Supporting Information

$Yb(OTf)_3$ Catalyzed [1,3]-Rearrangement of 3-Alkenyl Oxindoles

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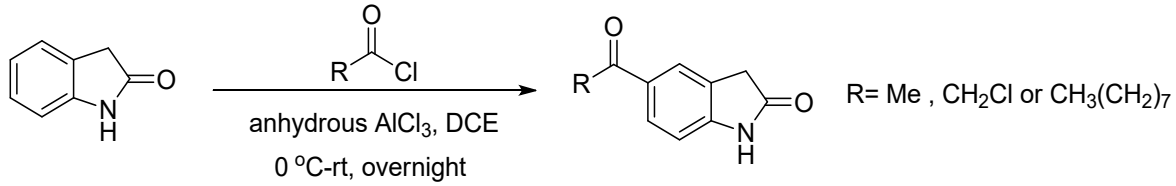
Contents

1. General Information

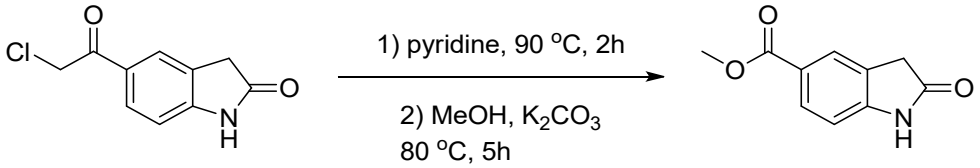
Chemicals were received from commercial sources without further purification or prepared by literature methods. Melting points are uncorrected and recorded on Digital Melting Point Apparatus WRS-1C. IR spectra were recorded on an NICOLETIS10 FI-Infrared Spectrophotometer. High-resolution mass spectrometry (HRMS) spectra were recorded on BRUKER micrOTOF-QII. X-ray crystallographic analysis was done at the X-ray crystallography facility. ^{1}H NMR and ^{13}C NMR spectra were measured on a 500 MHz Bruker spectrometer, using Actone-d_6 or $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts are given in δ (ppm) relative to TMS, the coupling constants J are given in Hz.

2. Preparation and Analytic Data of substrates 2a-n:

2.1. General Procedure for the synthesis of Oxindoles:

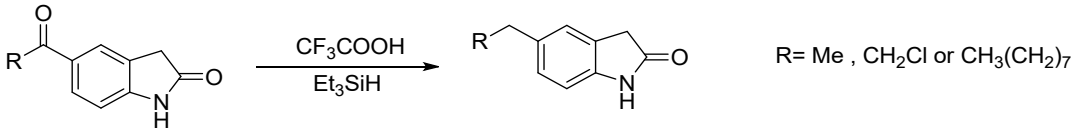


Anhydrous $AlCl_3$ (3.0 equiv.) was suspended in DCE and then acyl chloride (2.0 equiv.) was added dropwise under ice bath. Then the mixture was stirred for 1 hour and 2-oxindole (1.0 equiv.) was added in several portions. The solution was then allowed to warm to r.t and stir overnight. After the reaction was completed, it was stopped by pour into crushed ice. Then the mixture was stirred vigorously for 10 minutes. The resulting precipitate was collected by vacuum filtration, washed with water and dried under vacuum to afford the title compound.



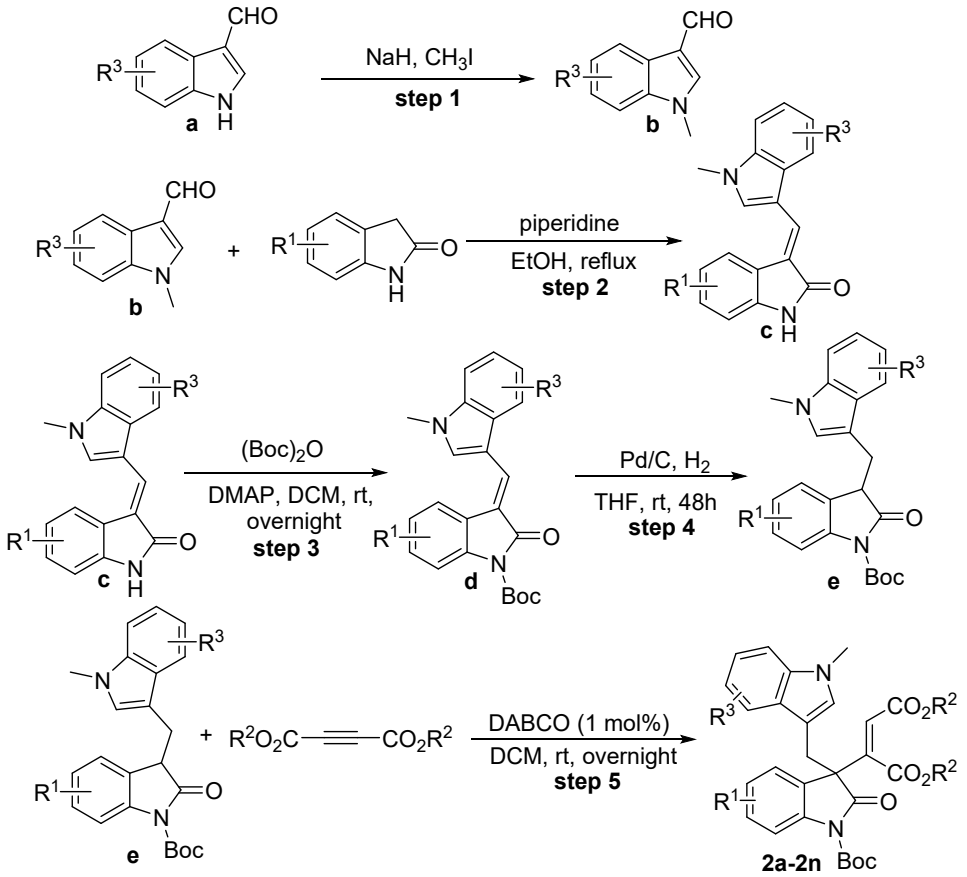
A solution of 5-(2-chloroacetyl) indolin-2-one (1.0 equiv) in pyridine was stirred at 90°C for 2h. After the reaction was completed, the mixture was cooled to room temperature and filtered precipitated solid. The solid was then washed with ethanol and dried under vacuo. The obtained compound was dissolved in MeOH, and K_2CO_3 (0.2 equiv.) was added. The

mixture was stirred at 80°C for 5h. After cooling to room temperature, 4M HCl/dioxane was added until PH = 3 and the solvent was concentrated in vacuo. The crude product was triturated in water, filtered, wshed with water and then dried under vacuo to get the product.



2-oxindole derivatives (10.0 mmol) was dissolved in 15 mL trifluoroacetic acid under ice bath then 2 mL triethylsilane was added dropwise to this solution. The mixture allowed to warm to r.t and stirred for 5h. Then 1 mL triethylsilane was added and the solution was stirred overnight. After the reaction was completed, the mixture was poured into ice water and the result precipitate was filtrated, washed with water, and dried under vacuum to get the product.

2.2. General Procedure for the synthesis of substrates 2a-n:



Step 1: 1H-indole-3-carbaldehyde **a** (3.0 g, 20.7 mmol) was treated with NaH (1.08 g, 26.9 mmol) in DMF (30 mL) at 0 °C for 15 min, and then iodomethane (1.7 mL, 26.9 mmol)

was added to the resulting mixture at room temperature. After being stirred at room temperature for 2 h, the reaction was quenched with H_2O and extracted with ethyl acetate. Combined organic layers were washed with H_2O and saturated brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by flash chromatography on silica gel to give **b** (2.51g, 83%) as a colorless solid.

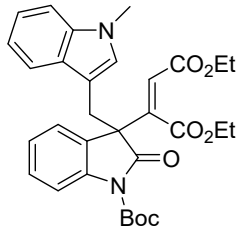
Step 2: A solution of aldehyde **b** (1 equiv.), 1,3-dihydro-indol-2-one (1 equiv.) and piperidine (1 equiv.) in EtOH is heated to reflux overnight. The crude mixture is allowed to come to room temperature, and then cooled in an ice bath. A precipitate is obtained which is filtered and washed with cold EtOH. If no precipitation occurs, the solvent is removed and the product is purified by flash chromatography. The title compound **c** was obtained as a yellow solid.

Step 3: Di-tert-butyldicarbonate (1.3 equiv.) was added in one portion to a solution of **c** (1 equiv.) and DMAP (1.3 equiv.) in DCM (20 mL). After completion of reaction (monitored by TLC), the reaction mixture was directly loaded onto by flash column chromatography (DCM) to afford the desired products **d**.

Step 4: Compound **d** (1 equiv.) was dissolved in THF and was allowed to react in the presence of Pd/C (0.8 mmol, 0.1 equiv.; 10 % loading in 50 % water) under a hydrogen atmosphere. After the starting material was consumed, the catalyst was removed via filtration through celite, followed by removal of the solvent by vacuum. The crude product was purified via flash chromatography on silica gel using hexanes/EtOAc. After the solvents were removed. Compound **e** was obtained as white solid.

Step 5: Compound **e** (1.0 equiv.) was dissolved in dichloromethane, then adding the corresponding alkyne ester (1.5 equiv.), DABCO (0.01 equiv.), stirring overnight at rt. After completion of reaction (monitored by TLC), the resulting crude product was purified through flash column chromatography (EtOAc : Petroleum ether= 1:5) to give the pure product **2a**.

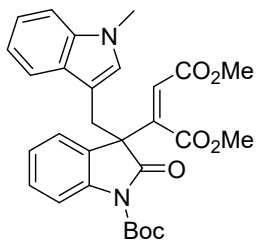
2.3. Analytic Data for the substrates:



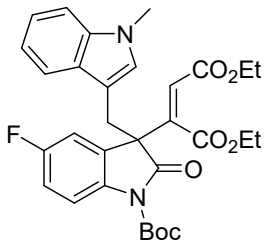
Diethyl-2-(1-(tert-butoxycarbonyl)-3-((1-methylindolin-3-yl)methyl)-2-oxoindolin-3-yl) maleate 2a: White solid , m.p. 133 - 134 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.01 (t, *J* = 7.0 Hz, 3H), 1.30 (t, *J* = 7.0 Hz, 3H), 1.43 (s, 9H), 3.42 (d, *J* = 13.5 Hz, 1H), 3.54 (s,

3H), 3.72 (d, J = 13.5 Hz, 1H), 3.99 - 4.02 (m, 2H), 4.22 (q, J = 7.0 Hz, 2H), 6.36 (s, 1H), 6.51 (m, 1H), 6.93 - 6.96 (m, 1H), 7.06 - 7.12 (m, 3H), 7.16-7.19 (m, 1H), 7.27 - 7.32 (m, 2H), 7.52 - 7.54 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.4, 14.0, 27.8, 32.4, 33.0, 57.2, 61.1, 61.4, 83.9, 106.1, 108.6, 114.7, 118.8, 119.0, 121.3, 124.0, 124.1, 125.5, 127.9, 128.2, 128.5, 128.9, 136.2, 140.4, 146.5, 148.6, 164.7, 165.8, 170.0. IR (KBr): 2987, 1726, 1479, 1346, 1150, 841, 739 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{31}H_{34}N_2O_7$ $[M+H]^+$: 547.2439, found 547.2454.

Dimethyl-2-(1-(tert-butoxycarbonyl)-3-((1-methyl-1H-indol-3-yl)methyl)-2-oxoindolin-3yl)maleate 2b: White solid, m.p. 131.8 - 133.2 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.44 (s, 9H), 3.45 (d, J = 13.5 Hz, 1H), 3.54 (s, 3H), 3.59 (s, 3H), 3.72 (d, J = 13.5 Hz, 1H), 3.77 (s, 3H), 6.37 (s, 1H), 6.49 (s, 1H), 6.93-6.96 (m, 1H), 7.06 - 7.12 (m, 3H), 7.17 - 7.20 (m, 1H), 7.26 - 7.27 (m, 1H), 7.30 - 7.32 (m, 1H), 7.54 - 7.56 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 27.8, 32.5, 33.2, 52.1, 52.3, 57.2, 84.0, 106.1, 108.7, 114.8, 118.8, 119.0, 121.3, 123.5, 124.0, 124.4, 127.9, 128.0, 128.5, 129.0, 136.1, 140.3, 147.3, 148.6, 165.1, 166.6, 173.9. IR (KBr): 2994, 1729, 1479, 1344, 1148, 846, 735 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{29}H_{30}N_2O_7$ $[M+H]^+$: 519.2126, found 519.2115.



Diethyl-2-(1-(tert-butoxycarbonyl)-5-fluoro-3-((1-methylindolin-3-yl)methyl)-2-oxoindolin-3-yl)maleate 2c: Yellow solid, m.p. 106 - 107 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.06 (t, J = 7.0 Hz, 3H), 1.31 (t, J = 7.0 Hz, 3H), 1.43 (s, 9H), 3.41 (d, J = 13.5 Hz, 1H), 3.57 (s, 3H), 3.72 (d, J = 13.5 Hz, 1H), 4.03 - 4.06 (m, 2H), 4.23 (q, J = 7.0 Hz, 2H), 6.42 (s, 1H), 6.52 (s, 1H), 6.84 - 6.88 (m, 1H), 6.96 - 6.99 (m, 1H), 7.02 - 7.04 (m, 1H), 7.07 - 7.14 (m, 2H), 7.32 - 7.34 (m, 1H), 7.50 - 7.53 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.5, 14.0, 27.8, 32.5, 33.1, 57.3, 61.3, 61.6, 84.1, 105.7, 108.8, 111.9 (d, J_{C-F} = 24.6 Hz), 115.38 (d, J_{C-F} = 22.5 Hz), 116.10 (d, J_{C-F} = 7.7 Hz), 118.8, 119.0, 121.4, 124.7, 127.7, 128.5, 130.1 (d, J_{C-F} = 8.1 Hz), 136.2, 136.4 (d, J_{C-F} = 2.3 Hz), 145.5, 148.5, 158.5 (d, J_{C-F} = 242.5 Hz), 164.6, 165.6, 173.7. IR (KBr): 2998, 1720, 1483, 1368, 1248, 1148, 829, 747 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{31}H_{33}FN_2O_7$ $[M+H]^+$: 565.2345, found 565.2354.



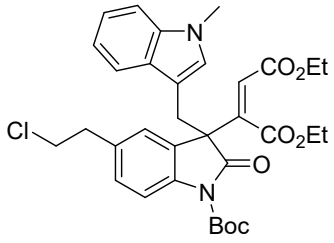
Diethyl-2-(1-(tert-butoxycarbonyl)-5-methyl-3-((1-methyl-1H-indol-3-yl)methyl)-2-oxoindolin-3-yl)maleate 2d: White solid, m.p. 89.8 - 95.2 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.03 (t, *J* = 7.0 Hz, 3H), 1.30 (t, *J* = 7.0 Hz, 3H), 1.44 (s, 9H), 2.28 (s, 3H), 3.42 (d, *J* = 13.5 Hz, 1H), 3.55 (s, 3H), 3.69 (d, *J* = 13.5 Hz, 1H), 3.98 - 4.07 (m, 2H), 4.22 (q, *J* = 7.0 Hz, 2H), 6.39 (s, 1H), 6.47 (s, 1H), 6.92 - 6.96 (m, 2H), 7.05 - 7.12 (m, 3H), 7.27 - 7.29 (m, 1H), 7.38 - 7.40 (m, 1H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 13.4, 14.0, 20.9, 27.8, 32.4, 32.9, 57.2, 61.1, 61.3, 83.7, 106.3, 108.6, 114.4, 118.6, 119.0, 121.2, 123.9, 125.1, 127.9, 128.0, 128.4, 129.3, 133.5, 136.2, 138.0, 146.7, 148.7, 164.7, 165.9, 174.1. IR (KBr): 3004, 1722, 1468, 1249, 1153, 824, 739 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{32}H_{36}N_2O_7$ $[M+H]^+$: 561.2596, found 561.2610.

Diethyl-2-(1-(tert-butoxycarbonyl)-5-ethyl-3-((1-methyl-1H-indol-3-yl)methyl)-2-oxoindolin-3-yl)maleate 2e: Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.5 Hz, 1H), 7.28 - 7.24 (m, 1H), 7.11 - 7.04 (m, 3H), 6.96 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.49 (s, 1H), 6.45 (s, 1H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.06 - 3.95 (m, 2H), 3.68 (d, *J* = 13.5 Hz, 1H), 3.55 (s, 3H), 3.45 (d, *J* = 13.5 Hz, 1H), 2.62 - 2.53 (m, 2H), 1.46 (s, 9H), 1.30 (t, *J* = 7.0 Hz, 3H), 1.17 (t, *J* = 7.5 Hz, 3H), 1.01 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.4, 14.0, 15.7, 27.8, 28.4, 32.4, 32.9, 57.3, 61.1, 61.3, 83.7, 106.4, 108.6, 114.5, 118.7, 119.0, 121.2, 123.8, 124.1, 127.9, 128.0, 128.2, 128.5, 136.1, 138.1, 140.1, 146.8, 148.7, 164.7, 165.9, 174.2. HRMS (BRUKER micrOTOF-QII) calcd for $C_{33}H_{38}N_2O_7$ $[M+H]^+$: 575.2752, found 575.2746.

Diethyl-2-(1-(tert-butoxycarbonyl)-3-((1-methyl-1H-indol-3-yl)methyl)-5-nonyl-2-oxoindolin-3-yl)maleate 2f: Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, J = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.13 - 7.09 (m, 1H), 7.08 - 7.04 (m, 2H), 6.96 - 6.90 (m, 2H), 6.49 (s, 1H), 6.42 (s, 1H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.04 - 3.95 (m, 2H), 3.69 (d, *J* = 13.5 Hz, 1H), 3.55 (s, 3H), 3.44 (d, *J* = 13.5 Hz, 1H), 2.58 - 2.47 (m, 2H), 1.45 (s, 9H), 1.33 - 1.23 (m, 17H), 1.01 (t, *J* = 7.0 Hz, 3H), 0.92 - 0.86 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.5, 14.0, 14.0, 22.6, 27.8, 29.3, 29.3, 29.5, 29.6, 31.6, 31.9, 32.4, 32.8, 35.5, 57.3, 61.1, 61.3, 83.7, 106.3, 108.6, 114.4, 118.8, 119.0,

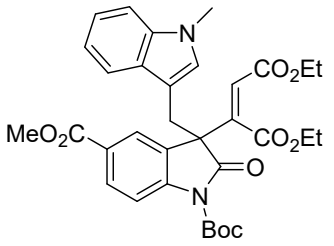
121.2, 123.9, 124.5, 127.9, 127.9, 128.5, 128.7, 136.1, 138.1, 138.8, 146.8, 148.7, 164.7, 165.9, 174.2. HRMS (BRUKER micrOTOF-QII) calcd for $C_{40}H_{52}N_2O_7$ $[M+H]^+$: 673.3848, found 673.3856.

Diethyl 2-(1-(tert-butoxycarbonyl)-5-(2-chloroethyl)-3-((1-methyl-1H-indol-3-yl)

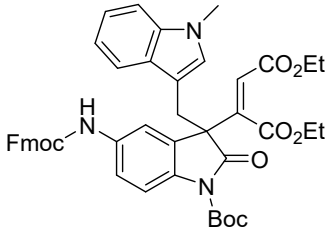


methyl)-2-oxoindolin-3-yl)maleate 2g: Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.5 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.13 - 7.10 (m, 1H), 7.09 - 7.04 (m, 2H), 7.02 - 6.98 (m, 1H), 6.97 - 6.90 (m, 1H), 6.50 (s, 1H), 6.46 (s, 1H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.06 - 3.94 (m, 2H), 3.68 (d, *J* = 13.5 Hz, 1H), 3.63 - 3.56 (m, 2H), 3.54 (s, 3H), 3.44 (d, *J* = 13.5 Hz, 1H), 2.97 (t, *J* = 7.0 Hz, 2H), 1.45 (s, 9H), 1.30 (t, *J* = 7.0 Hz, 3H), 1.01 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.5, 14.0, 27.8, 32.4, 32.9, 38.4, 45.0, 57.2, 61.1, 61.4, 83.9, 106.1, 108.7, 114.7, 118.8, 118.9, 121.3, 124.2, 125.0, 127.9, 128.4, 128.7, 129.4, 133.9, 136.1, 139.2, 146.4, 148.6, 164.7, 165.8, 174.0. HRMS (BRUKER micrOTOF-QII) calcd for $C_{33}H_{37}ClN_2O_7$ $[M+H]^+$: 609.2362, found 609.2359.

1-(tert-butyl) 5-methyl (Z)-3-(1,4-diethoxy-1,4-dioxobut-2-en-2-yl)-3-((1-methyl-1H-



indol-3-yl)methyl)-2-oxoindoline-1,5-dicarboxylate 2h: Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 1.9 Hz, 1H), 7.90 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.59 (d, *J* = 8.5 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.12 - 7.04 (m, 2H), 6.95 - 6.91 (m, 1H), 6.58 (s, 1H), 6.30 (s, 1H), 4.24 (q, *J* = 7.0 Hz, 2H), 4.06 - 3.97 (m, 2H), 3.93 (s, 3H), 3.76 (d, *J* = 13.5 Hz, 1H), 3.52 (s, 3H), 3.44 (d, *J* = 13.5 Hz, 1H), 1.42 (s, 9H), 1.31 (t, *J* = 7.0 Hz, 3H), 1.03 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 13.4, 14.0, 27.7, 32.4, 33.1, 52.1, 56.9, 61.2, 61.5, 84.4, 105.6, 108.7, 114.4, 118.9, 119.0, 121.4, 125.0, 125.5, 125.9, 127.6, 128.4, 128.7, 131.0, 136.2, 144.4, 145.1, 148.3, 164.7, 165.5, 166.3, 173.8. HRMS (BRUKER micrOTOF-QII) calcd for $C_{33}H_{36}N_2O_9$ $[M+H]^+$: 605.2494, found 605.2490.



Diethyl 2-(5-((((9H-fluoren-9-yl)methoxy)carbonyl)amino)-1-(tert-butoxycarbonyl)-3-((1-methyl-1H-indol-3-yl)methyl)-2-oxoindolin-3-yl)maleate 2i: Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ

7.80 (d, *J* = 7.5 Hz, 2H), 7.64 (d, *J* = 7.5 Hz, 2H), 7.48 - 7.40 (m, 4H), 7.38 - 7.32 (m, 3H), 7.13 - 7.02 (m, 3H), 6.96 - 6.90 (m, 1H), 6.66 (br, 1H), 6.49 (s, 1H), 6.43 (s, 1H), 4.56 (d, *J* = 6.5 Hz, 2H), 4.29 (t, *J* = 6.5 Hz, 1H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.08 - 3.97 (m, 2H), 3.71 (d, *J* = 13.5 Hz, 1H), 3.53 (s, 3H), 3.41 (d, *J* = 13.5 Hz, 1H), 1.42 (s, 9H), 1.29 (t, *J* = 7.0 Hz, 3H), 1.03 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.5, 14.0, 27.8, 32.4, 33.0, 47.1, 57.4, 61.1, 61.5, 66.9, 83.9, 105.9, 108.7, 115.2, 118.8, 119.1, 120.1, 121.3, 124.4, 124.9, 127.1, 127.8, 128.7, 129.1, 134.1, 136.2, 141.4, 143.7, 146.0, 148.6, 153.3, 164.7, 165.7, 173.9. HRMS (BRUKER micrOTOF-QII) calcd for $C_{46}H_{45}N_3O_9$ $[M+H]^+$: 784.3229, found 784.3215.

Diethyl-2-(1-(tert-butoxycarbonyl)-5-methoxy-3-((1-methyl-1H-indol-3-yl)methyl)-2-oxoindolin-3-yl)maleate 2j: White solid, m.p. 85.9 - 87.7 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.05 (t, *J* = 7.0 Hz, 3H), 1.30 (t, *J* = 7.0 Hz, 3H), 1.44 (s, 9H), 3.43 (d, *J* = 13.5 Hz, 1H), 3.55 (s, 3H), 3.67 - 3.69 (m, 4H), 4.02 - 4.06 (m, 2H), 4.22 (q, *J* = 7.0 Hz, 2H), 6.45 (s, 1H), 6.48 (s, 1H), 6.68 - 6.70 (m, 2H), 6.79 (d, *J* = 2.5 Hz, 1H), 6.93 - 6.96 (m, 1H), 7.06 - 7.12 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 1H),7.47 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.5, 14.0, 27.8, 32.4, 32.9, 55.6, 57.4, 61.1, 61.4, 83.7, 106.2, 108.7, 110.6, 114.3, 115.6, 118.8, 119.0, 121.3, 124.1, 128.0, 128.4, 129.2, 133.7, 136.2, 146.5, 148.7, 156.5, 164.7, 165.8, 174.0. IR (KBr): 2989, 1725, 1488, 1342,1247, 1155, 1011, 862, 742 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{32}H_{36}N_2O_8$ $[M+H]^+$: 577.2545, found 577.2538.

Diethyl-2-(1-(tert-butoxycarbonyl)-3-((4-methoxy-1-methylindolin-3-yl)methyl)-2-oxoindolin-3-yl)maleate 2k: White solid, m.p. 135.8 - 145.2 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.00 (t, *J* = 7.0 Hz, 3H), 1.29 (t, *J* = 7.0 Hz, 3H), 1.57 (s, 9H), 3.56 (s, 3H), 3.75 (s, 3H), 3.84 (d, *J* = 13.5 Hz, 1H), 3.91 - 4.00 (m, 3H), 4.19 - 4.23 (m, 2H), 6.28 (d, *J* = 7.5 Hz, 1H), 6.46 (s, 1H), 6.54(s, 1H) , 6.73(d, *J* = 8.0 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.5, 14.0, 28.0, 32.7, 32.9, 54.6, 57.8, 61.0, 61.2, 83.9, 99.0, 102.2, 106.8, 114.1, 117.9, 122.0, 123.2, 123.7, 125.6, 126.8, 127.6, 128.5, 137.7, 139.9, 147.2, 148.9, 154.4, 164.8, 166.0, 174.3. IR

(KBr): 3004, 1722, 1468, 1249, 1153, 824, 739 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{32}H_{36}N_2O_8$ $[M+H]^+$: 577.2545, found 577.2553.

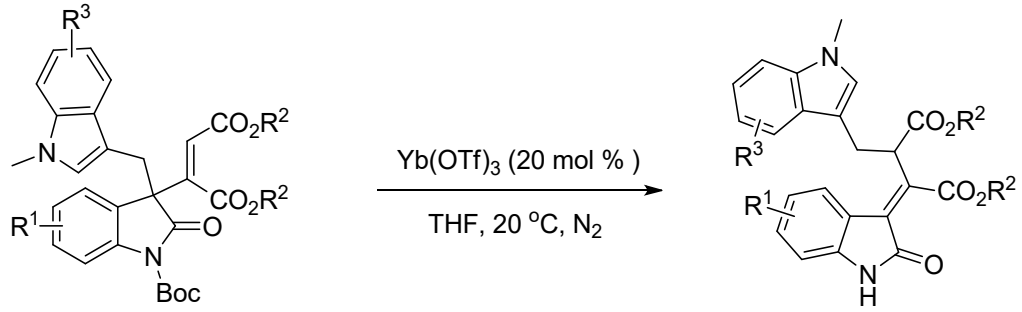
Diethyl-2-(1-(tert-butoxycarbonyl)-3-((1,6-dimethyl-1H-indol-3-yl)methyl)-2-oxoindolin-3-yl) maleate 2l: White solid, m.p. 104.4 - 107.0 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 1.01 (t, *J* = 7.0 Hz, 3H), 1.30 (t, *J* = 7.0 Hz, 3H), 1.46 (s, 9H), 2.62 (s, 3H), 3.40 (d, *J* = 14.0 Hz, 1H), 3.68 (d, *J* = 14.0 Hz, 1H), 3.79 (s, 3H), 3.98 - 4.02 (m, 2H), 4.22 (q, *J* = 7.0 Hz, 2H), 6.23 (s, 1H), 6.50 (s, 1H), 6.74 - 6.81 (m, 2H), 7.09 (t, *J* = 7.5 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.17 - 7.20 (m, 1H), 7.26 - 7.28 (m, 1H), 7.58 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.5, 14.0, 19.5, 26.9, 27.8, 32.8, 36.4, 51.1, 61.1, 61.4, 83.9, 105.9, 114.7, 117.1, 119.1, 120.5, 124.0, 124.1, 124.5, 128.2, 128.9, 129.1, 130.1, 134.9, 140.5, 146.7, 148.7, 164.7, 165.8, 174.0. IR (KBr): 2976, 1731, 1464, 1346, 1250, 1151, 1028, 876, 745 cm^{-1}. HRMS calcd for $C_{32}H_{36}N_2O_7$ $[M+H]^+$: 561.2596, found 561.2600.

Diethyl-2-(1-(tert-butoxycarbonyl)-3-((5-methoxy-1-methylindolin-3-yl)methyl)-2-oxoindolin-3-yl)maleate 2m: Yellow liquid.^1H NMR (500 MHz, $CDCl_3$) δ 1.19 (t, *J* = 7.0 Hz, 3H), 1.42 (t, *J* = 7.0 Hz, 3H), 3.25(dd, J_1 = 9.0 Hz, J_2 = 14.5 Hz, 1H), 3.59(dd, J_1 = 9.0 Hz, J_2 = 14.5 Hz, 1H), 3.65 (s, 3H), 3.81 (s, 3H), 4.11 - 4.23 (m, 2H), 4.23-4.50 (m, 2H), 4.54 (dd, J_1 = 5.0 Hz, J_2 = 9.0 Hz, 1H), 6.84 - 6.89 (m, 3H), 6.94 (s, 1H), 7.04 (d, *J* = 2.0 Hz, 1H), 7.14 (d, *J* = 10.5 Hz, 1H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 9.44 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 12.9, 12.9, 25.1, 31.7, 47.6, 54.8, 60.5, 60.7, 99.1, 108.9, 109.0, 109.3, 111.0, 120.0, 120.9, 123.3, 126.8, 127.3, 129.3, 131.1, 139.4, 141.2, 152.9, 166.0, 166.9, 169.4. IR (KBr): 3001, 1723, 1494, 1348, 1253, 1150, 1035, 879, 753 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{32}H_{36}N_2O_8$ $[M+H]^+$: 577.2545, found 577.2527.

Diethyl-2-(1-(tert-butoxycarbonyl)-3-((1,7-dimethyl-1H-indol-3-yl)methyl)-2-oxoindolin-3-yl)maleate 2n: White solid, m.p. 88.2 - 89.0 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 1.01 (t, *J* = 7.0 Hz, 3H), 1.30 (t, *J* = 7.0 Hz, 3H), 1.44 (s, 9H), 2.39 (s, 3H), 3.40 (d, *J* = 13.5 Hz, 1H), 3.49 (s, 3H), 3.70 (d, *J* = 13.5 Hz, 1H), 3.96 - 4.04 (m, 2H), 4.22 (q, *J* = 7.0

Hz, 2H), 6.27 (s, 1H), 6.50 (s, 1H), 6.77 (dd, J_1 = 1.0 Hz, J_2 = 7.5 Hz, 1H), 7.16 - 7.20 (m, 2H), 7.54 (d, J = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.5, 14.0, 21.7, 27.8, 32.3, 33.1, 57.2, 61.1, 61.4, 83.8, 106.0, 108.6, 114.7, 118.7, 120.7, 124.0, 124.1, 124.5, 125.8, 127.9, 128.2, 128.9, 131.0, 136.6, 140.5, 146.6, 148.7, 164.7, 165.8, 174.0. IR (KBr): 2991, 1711, 1467, 1346, 1289, 1152, 1035, 863, 754 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{32}H_{36}N_2O_7$ $[M+H]^+$: 561.2596, found 561.2614.

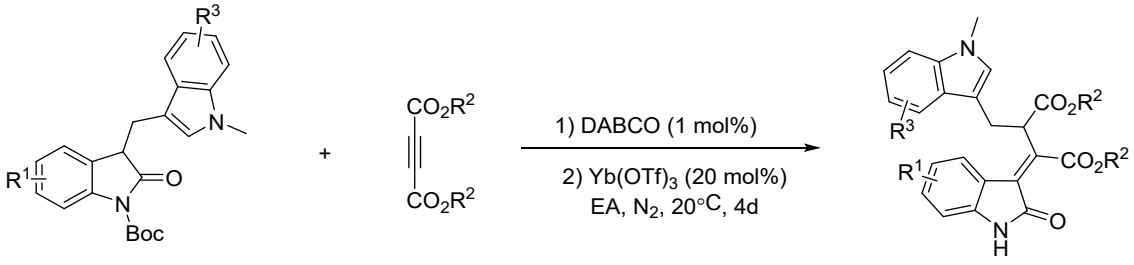
3. General Procedure for the rearrangement reaction



2a-2n **3a-3n**

2a-2n (0.1 mmol), catalyst (20 mol%) and THF (1 mL) was added to a sealed tube under N_2 atmosphere, then the reaction system was stirred at 20 °C. After completion of reaction (monitored by TLC), the reaction mixture was purified through flash column chromatography on a silica gel (eluent: petroleum ether: ethyl acetate= 4/1-2/1) to give the targeting products.

4. General Procedure for one-pot reaction

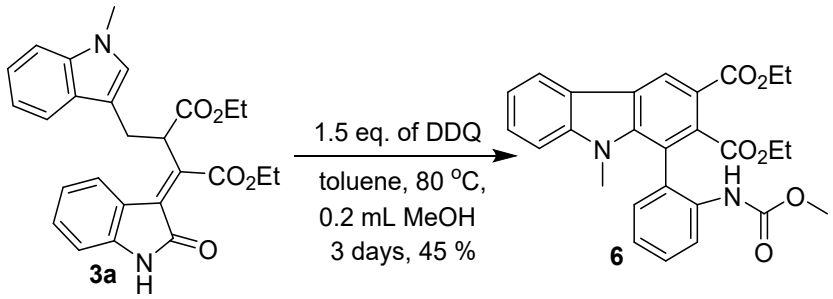


2a,2b,2c,2f,2g **3a,3b,3c,3f,3g**

Compound **2** (0.1 mmol), DABCO (1 mol%) were added to a tube. After the sealed tube was evacuated and refilled with N_2 three times, the corresponding alkyne ester (1.5 equiv.) and EtOAc (1 mL) was added and the reaction system was stirred at 20 °C. After completion of reaction (monitored by TLC), then the $Yb(OTf)_3$ (20 mol%) was added under N_2 atmosphere and the resulting mixture was stirred for 3 days at 20 °C (monitored

by TLC). The reaction mixture was purified through flash column chromatography on a silica gel (eluent: petroleum ether: ethyl acetate= 4/1-2/1) to yield the targeting products.

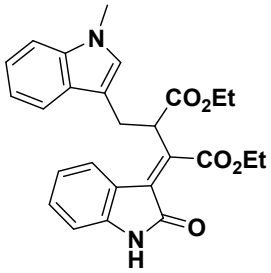
5. General Procedure for derivative 6



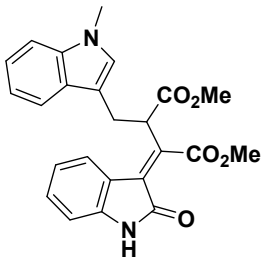
3a (0.1 mmol) and DDQ (0.15 mmol) was dissolved in solvent (Toluene：Methanol = 5:1，1.0 mL). The resulting mixture was stirred for 3 days at 80 °C. After completion of reaction, the reaction mixture was purified through flash column chromatography on a silica gel (petroleum ether: ethyl acetate = 8/1 - 4/1) to yield the targeting product **6** (white solid, 45% yield).

6. Analytical data for the products

Diethyl-(*Z*)-2-((1-methyl-1*H*-indol-3-yl)methyl)-3-(2-oxoindolin-3-ylidene)succinate



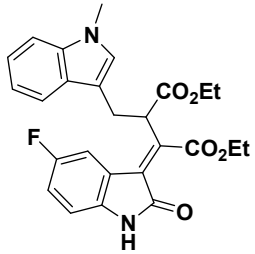
3a: Yellow solid (37.5 mg, 72% yield), m.p. 150 - 151 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.17 (t, J = 7.0 Hz, 3H), 1.40 (t, J = 7.0 Hz, 3H), 3.26 (dd, J_1 = 5.5 Hz, J_2 = 15.0 Hz, 1H), 3.60 (dd, J_1 = 9.0 Hz, J_2 = 15.0 Hz, 1H), 3.68 (s, 3H), 4.13 - 4.16 (m, 2H), 4.43 - 4.46 (m, 2H), 4.52 (dd, J_1 = 5.5 Hz, J_2 = 9.0 Hz, 1H), 6.96(s, 1H), 7.12 (t, J = 7.0 Hz, 1H), 7.18-7.25 (m, 2H), 7.46 (t, J = 8.0 Hz, 1H), 7.60 (t, J = 8.0 Hz, 1H), 8.66 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 14.0, 26.0, 32.6, 48.7, 61.5, 61.7, 109.2, 110.1, 110.4, 118.5, 119.0, 121.1, 121.6, 122.1, 124.6, 127.2, 127.7, 127.8, 130.3, 136.9, 140.5, 141.9, 167.0, 167.5, 170.3. IR (KBr): 3139, 2959, 1708, 1617, 1467, 1337, 1182, 1014, 856, 745 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{26}H_{26}N_2O_5$ $[M+H]^+$: 447.1915, found 447.1919.



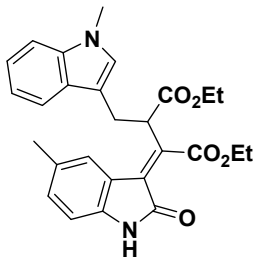
Dimethyl-(*Z*)-2-((1-methyl-1*H*-indol-3-yl)methyl)-3-(2-oxoindolin-3-ylidene) succinate 3b: Yellow solid (35.9 mg, 86% yield), m.p. 171-172 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.26 (dd, J_1 = 5.5 Hz, J_2 = 15.0 Hz, 1H), 3.60 (dd, J_1 = 9.0 Hz, J_2 = 15.0 Hz,

1H), 3.68 (s, 6H), 3.96 (s, 3H), 4.54 (dd, J_1 = 5.5 Hz, J_2 = 9.0 Hz, 1H), 6.80 - 6.83 (m, 2H), 6.95 (s, 1H), 7.12 (t, J = 7.0 Hz, 1H), 7.21 (dd, J_1 = 7.0 Hz, J_2 = 15.0 Hz, 2H), 7.25 (s, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 8.0 Hz, 1H), 8.54 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 26.0, 32.6, 48.6, 52.5, 52.7, 109.3, 110.2, 110.3, 118.4, 119.0, 120.9, 121.6, 122.2, 124.5, 127.5, 127.6, 127.8, 130.4, 136.9, 139.9, 141.9, 167.4, 167.6, 170.8. IR (KBr): 3381, 2948, 1719, 1615, 1435, 1324, 1253, 1175, 1097, 831 ,754, 673 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{24}H_{22}N_2O_5$ $[M+H]^+$: 419.1602, found 419.1602.

Diethyl-(*Z*)-2-(5-fluoro-2-oxoindolin-3-ylidene)-3-((1-methyl-1*H*-indol-3-yl)methyl) succinate 3c: Yellow solid (39.4 mg, 85% yield), m.p. 51.7 - 52.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.18 (t, J = 7.0 Hz, 3H), 1.40 (t, J = 7.0 Hz, 3H), 3.28 (dd, J_1 = 6.0 Hz, J_2 = 15.0 Hz, 1H), 3.59 (dd, J_1 = 8.5 Hz, J_2 = 15.0 Hz, 1H), 3.69 (s, 3H), 4.11 - 4.18 (m, 2H), 4.38 (dd, J_1 = 6.0 Hz, J_2 = 8.5 Hz, 1H), 4.40 - 4.47 (m, 2H), 6.73(dd, J_1 = 4.5 Hz, J_2 = 8.5 Hz, 1H), 6.91 (dt, J_1 = 2.5 Hz, J_2 = 8.5 Hz, 1H), 6.96 (s, 1H), 7.11 - 7.14 (m, 1H), 7.18 (dd, J_1 = 2.0 Hz, J_2 = 9.0 Hz, 1H), 7.20 - 7.25 (m, 2H), 7.61 (d, J = 8.0 Hz, 1H), 8.78 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 12.9, 12.9, 25.1, 31.5, 47.8, 60.6, 60.8, 108.2, 109.2, 109.4 (d, $J_{C\text{-}F}$ = 8.0 Hz), 111.1 (d, $J_{C\text{-}F}$ = 26.2 Hz), 115.6 (d, $J_{C\text{-}F}$ = 23.6 Hz), 117.3, 118.1, 120.7, 120.9 (d, $J_{C\text{-}F}$ = 8.6 Hz), 126.1 (d, $J_{C\text{-}F}$ = 2.7 Hz), 126.6, 126.8, 135.8, 136.8, 140.8, 157.4 (d, $J_{C\text{-}F}$ = 238.1 Hz), 165.6, 166.5, 169.0. IR (KBr): 3364, 2927, 1725, 1479, 1177, 1017, 859, 742 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{26}H_{25}FN_2O_5$ $[M+H]^+$: 465.1821, found 465.1821.



Diethyl-(*Z*)-2-((1-methyl-1*H*-indol-3-yl)methyl)-3-(5-methyl-2-oxoindolin-3-ylidene) succinate 3d: Yellow solid (35.4 mg, 77% yield), m.p. 163.0 - 164.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.20 (t, J = 7.0 Hz, 3H), 1.40 (t, J = 7.0 Hz, 3H), 2.08 (s, 3H), 3.25 (dd, J_1 = 6.0 Hz, J_2 = 14.5 Hz, 1H), 3.61 (dd, J_1 = 8.5 Hz, J_2 = 14.5 Hz, 1H), 3.66 (s, 3H), 4.11 - 4.20 (m, 2H), 4.41 - 4.45 (m, 2H), 4.49 (dd, J_1 = 6.0 Hz, J_2 = 8.5 Hz, 1H), 6.68 (d, J = 8.0 Hz, 1H), 6.95 (s, 1H), 6.98 (d, J = 8.0 Hz, 1H), 7.11 - 7.14 (m, 1H), 7.16 (s, 1H), 7.20 - 7.23 (m, 1H), 7.24 - 7.25 (m, 1H), 7.64 (d, J = 8.0 Hz, 1H), 8.62 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 14.0, 20.9, 23.1, 32.5, 48.8, 61.5, 61.7, 109.3, 109.8, 110.3, 118.3, 119.0, 121.1, 121.6, 125.1, 127.4, 127.7, 128.1, 130.7, 131.5, 136.8, 139.6,



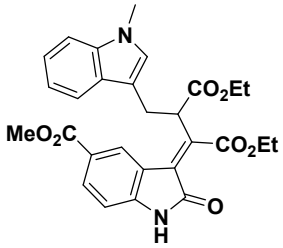
140.2, 167.1, 167.8, 170.5. IR (KBr): 3325, 2931, 1724, 1618, 1485, 1371, 1230, 1098, 1017, 809, 741 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calc d for $C_{27}H_{28}N_2O_5$ $[M+H]^+$: 461.2071, found 461.2090.

Diethyl-(*Z*)-2-(5-ethyl-2-oxoindolin-3-ylidene)-3-((1-methyl-1*H*-indol-3-yl)methyl) succinate 3e: Yellow oil (35.2 mg, 74% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 8.64 (s, 1H), 7.63 (d, J = 7.9 Hz, 1H), 7.27 - 7.19 (m, 3H), 7.14 - 7.08 (m, 1H), 7.05 - 7.01 (m, 1H), 6.96 (s, 1H), 6.72 (d, *J* = 7.9 Hz, 1H), 4.56 - 4.51 (m, 1H), 4.48 - 4.36 (m, 2H), 4.21 - 4.09 (m, 2H), 3.67 (s, 3H), 3.64 - 3.56 (m, 1H), 3.25 (dd, J_1 = 14.5 Hz, J_2 = 6.0 Hz, 1H), 2.39 (q, *J* = 7.5 Hz, 2H), 1.39 (t, *J* = 7.0 Hz, 3H), 1.18 (t, *J* = 7.0 Hz, 3H), 1.08 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 14.0, 15.9, 26.0, 28.4, 32.5, 48.7, 61.5, 61.7, 109.3, 109.9, 110.3, 118.3, 119.0, 121.2, 121.6, 124.1, 127.5, 127.7, 128.1, 129.6, 136.8, 138.2, 139.8, 140.2, 167.1, 167.7, 170.4. HRMS (BRUKER micrOTOF-QII) calcd for $C_{28}H_{30}N_2O_5$ $[M+H]^+$: 475.2228, found 475.2219.

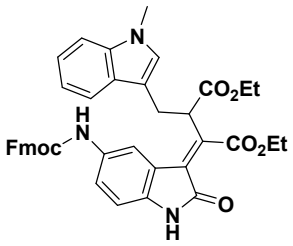
Diethyl-(*Z*)-2-((1-methyl-1*H*-indol-3-yl)methyl)-3-(5-nonyl-2-oxoindolin-3-ylidene) succinate 3f: Yellow oil (43.6 mg, 76% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.28 - 7.24 (m, 2H), 7.24 - 7.19 (m, 2H), 7.14 - 7.08 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 6.96 (s, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 4.54 - 4.50 (m, 1H), 4.48 - 4.37 (m, 2H), 4.19 - 4.08 (m, 2H), 3.67 (s, 3H), 3.60 (dd, J_1 = 14.5 Hz, J_2 = 9.0 Hz, 1H), 3.25 (dd, J_1 = 14.5 Hz, J_2 = 6.0 Hz, 1H), 2.38 - 2.30 (m, 2H), 1.39 (t, *J* = 7.0 Hz, 3H), 1.29 - 1.21 (m, 14H), 1.18 (t, *J* = 7.0 Hz, 3H), 0.88 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 14.0, 14.0, 22.6, 26.0, 29.3, 29.4, 29.5, 31.7, 31.8, 32.5, 35.5, 48.6, 61.4, 61.7, 109.2, 109.7, 110.4, 118.3, 119.0, 121.2, 121.6, 124.6, 127.4, 127.7, 128.0, 130.1, 136.8, 137.0, 139.6, 140.1, 167.1, 167.5, 170.4. HRMS (BRUKER micrOTOF-QII) calcd for $C_{35}H_{44}N_2O_5$ $[M+H]^+$: 573.3323, found 573.3335.

Diethyl-(*Z*)-2-(5-(2-chloroethyl)-2-oxoindolin-3-ylidene)-3-((1-methyl-1*H*-indol-3-yl)methyl)succinate 3g: Yellow oil (38.7 mg, 76% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.26 - 7.22 (m, 2H), 7.18 - 7.10 (m, 2H), 7.02 (d, *J* = 9.0 Hz, 1H), 6.96 (s, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 4.52 - 4.46 (m,

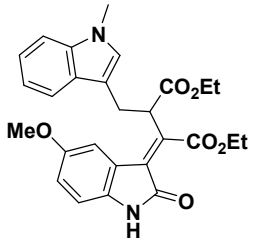
1H), 4.45 - 4.37 (m, 2H), 4.22 - 4.12 (m, 2H), 3.65 (s, 3H), 3.64 - 3.55 (m, 1H), 3.44 - 3.36 (m, 2H), 3.27 (dd, J = 14.5, 6.5 Hz, 1H), 2.79 - 2.65 (m, 2H), 1.39 (t, J = 7.0 Hz, 3H), 1.21 (t, J = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 14.0, 25.9, 32.5, 38.5, 44.9, 48.7, 61.6, 61.8, 109.4, 110.0, 110.2, 118.1, 119.1, 121.4, 121.7, 124.8, 127.2, 127.6, 128.1, 130.7, 132.0, 136.8, 140.6, 140.7, 166.9, 167.4, 170.3. HRMS (BRUKER micrOTOF-QII) calcd for $C_{28}H_{29}ClN_2O_5$ $[M+H]^+$: 509.1838, found 509.1829.

Diethyl-(*Z*)-2-(5-(methoxycarbonyl)-2-oxoindolin-3-ylidene)-3-((1-methyl-1*H*-indol-3-yl)methyl)succinate 3h: 

Yellow solid (41.4 mg, 82% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.13 (s, 1H), 7.95 - 7.91 (m, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.20 - 7.12 (m, 2H), 7.09 - 7.04 (m, 1H), 7.03 (s, 1H), 6.83 (d, J = 8.0 Hz, 1H), 4.60 - 4.54 (m, 1H), 4.51 - 4.36 (m, 2H), 4.20 - 4.06 (m, 2H), 3.82 (s, 3H), 3.67 - 3.59 (m, 1H), 3.65 (s, 3H), 3.31 (dd, J_1 = 14.5 Hz, J_2 =6.5 Hz, 1H), 1.40 (t, J = 7.0 Hz, 3H), 1.16 (t, J = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 26.6, 32.5, 49.3, 52.0, 61.6, 61.9, 109.0, 109.6, 110.2, 118.7, 119.0, 120.9, 121.5, 124.2, 125.6, 126.2, 127.7, 128.0, 132.3, 136.7, 142.4, 145.3, 166.3, 166.7, 167.4, 170.1. HRMS (BRUKER micrOTOF-QII) calcd for $C_{28}H_{28}N_2O_7$ $[M+H]^+$: 505.1970, found 505.1962.

Diethyl-(*Z*)-2-(5-((((9H-fluoren-9-yl)methoxy)carbonyl)amino)-2-oxoindolin-3-ylidene)-3-((1-methyl-1*H*-indol-3-yl)methyl)succinate 3i: 

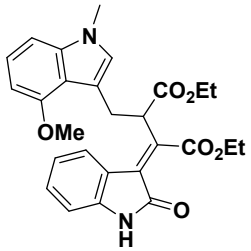
Yellow solid (58.2 mg, 85% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.83 (d, J = 7.5 Hz, 2H), 7.70 - 7.61 (m, 3H), 7.49 - 7.33 (m, 5H), 7.17 - 7.11 (m, 1H), 7.04 - 6.95 (m, 2H), 6.91 (s, 1H), 6.63 (d, J = 8.5 Hz, 1H), 6.45 (s, 1H), 4.58 - 4.48 (m, 2H), 4.47 - 4.36 (m, 2H), 4.33 - 4.23 (m, 2H), 4.23 - 4.14 (m, 2H), 3.59 (dd, J_1 = 14.5 Hz, J_2 = 6.0 Hz, 1H), 3.51 (s, 3H), 3.28 (dd, J_1 = 14.5 Hz, J_2 = 8.5 Hz, 1H), 1.39 (t, J = 7.0 Hz, 3H), 1.27 - 1.20 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 13.9, 14.0, 26.0, 32.4, 47.2, 48.8, 61.6, 61.8, 109.5, 109.8, 110.0, 118.2, 118.8, 120.0, 121.1, 121.7, 124.8, 124.9, 127.1, 127.8, 127.9, 128.5, 136.8, 141.4, 143.8, 166.9, 167.1, 170.4. HRMS (BRUKER micrOTOF-QII) calcd for $C_{41}H_{37}N_3O_7$ $[M+H]^+$: 684.2705, found 684.2720.

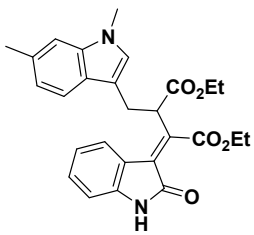
Diethyl-(*Z*)-2-(5-methoxy-2-oxoindolin-3-ylidene)-3-((1-methyl-1*H*-indol-3-yl)methyl) succinate 3j: 

Red solid (34.7 mg, 73% yield), m.p. 152.0 - 153.0 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 1.19 (t, J = 7.0 Hz, 3H), 1.41 (t, J = 7.0 Hz, 3H), 3.28 (dd, J_1 = 6.0 Hz, J_2 = 14.5 Hz, 1H), 3.51 (s, 3H), 3.60 (dd, J_1 = 9.0 Hz, J_2 = 14.5 Hz, 1H), 3.68 (s, 3H), 4.12 - 4.17 (m, 2H), 4.42 - 4.49 (m, 3H), 6.71 (d, J = 10.5 Hz, 1H),6.76 (dd, J_1 = 2.0 Hz, J_2 = 10.5 Hz, 1H), 6.97 (s, 1H), 7.01 (s, 1H), 7.11 (t, J = 7.0 Hz, 1H), 7.21 (t, J = 7.0 Hz, 3H), 7.25 (d, J = 10.5 Hz, 1H), 7.63 (d, J = 7.5 Hz, 1H), 8.96 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.0, 14.0, 26.0, 32.6, 48.6, 55.7, 61.6, 61.8, 109.2, 110.3, 110.5, 110.9, 115.9, 118.4, 119.0, 121.6, 121.8, 127.6, 127.9, 127.9, 135.8, 136.8, 140.6, 155.2, 167.1, 167.9, 170.3. IR (KBr): 3341, 2993, 1724, 1629, 1485, 1373, 1205, 1165, 1021, 858, 742 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{27}H_{28}N_2O_6$ $[M+H]^+$: 477.2020, found 477.2027.

Diethyl-(*Z*)-2-((4-methoxy-1-methyl-1*H*-indol-3-yl)methyl)-3-(2-oxoindolin-3-ylidene) succinate 3k: Yellow solid (42.4 mg, 89% yield), m.p. 97.6 - 99.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.16 (t, J = 7.0 Hz, 3H), 1.42 (t, J = 7.0 Hz, 3H), 3.45 (dd, J_1 = 6.0 Hz, J_2 = 14.0 Hz, 1H), 3.55 (dd, J_1 = 8.5 Hz, J_2 = 14.0 Hz, 1H), 3.63 (s, 3H), 3.69 (s, 3H), 4.09 - 4.17 (m, 2H), 4.42 - 4.49 (m, 2H), 4.87 (dd, J_1 = 6.0 Hz, J_2 = 8.5 Hz, 1H), 6.47 (d, J = 8.0 Hz, 1H), 6.78 (dd, J_1 = 6.0 Hz, J_2 = 7.5 Hz, 2H), 6.83 (s, 1H), 6.85 (d, J = 8.5 Hz, 1H), 7.10 (d, J = 8.0 Hz, 1H), 7.16 (d, J = 7.5 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 9.20 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.0, 14.0, 27.4, 32.7, 49.0, 54.9, 61.2, 61.6, 98.8, 102.7, 110.0, 110.7, 117.5, 121.3, 121.8, 122.2, 124.8, 127.3, 127.3, 130.0, 138.7, 140.7, 142.0, 154.3, 167.2, 168.1, 170.4. IR (KBr): 3673, 2988, 1723, 1466, 1254, 1153, 1057, 846, 737 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{27}H_{28}N_2O_6$ $[M+H]^+$: 477.2020, found 477.2020.

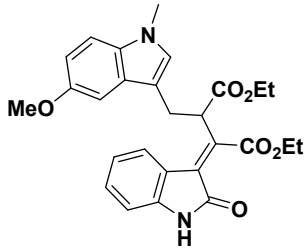




Diethyl-(*Z*)-2-((1,6-dimethyl-1*H*-indol-3-yl)methyl)-3-(2-oxoindolin-3-ylidene) succinate 3l: Yellow solid (36.3 mg, 79% yield), m.p. 80.0 - 81.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.18 (t, J = 7.0 Hz, 3H), 1.40 (t, J = 7.0 Hz, 3H), 2.72 (s, 3H), 3.21 (dd, J_1 = 5.5 Hz, J_2 = 14.5 Hz, 1H), 3.56 (dd, J_1 = 9.0 Hz, J_2 = 14.5 Hz, 1H), 3.94 (s, 3H), 4.11 - 4.18 (m, 2H), 4.40 - 4.47 (m, 2H), 4.50 (dd, J_1 = 5.5 Hz, J_2 = 9.0 Hz, 1H), 6.81-6.84 (m, 3H), 6.90 (d, J = 7.0 Hz, 1H), 6.97 (d, J = 8.0 Hz, 1H), 7.21 (t, J = 8.0 Hz, 1H), 7.41 (d, J = 7.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 8.66 (s, 1H); ^{13}C NMR (125

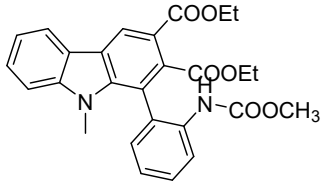
MHz, $CDCl_3$) δ 13.9, 14.0, 19.6, 25.9, 36.5, 48.6, 61.5, 61.7, 110.0, 110.1, 116.5, 119.3, 121.1, 121.3, 122.1, 124.2, 124.6, 127.1, 128.8, 129.5, 130.2, 135.6, 140.5, 141.8, 167.0, 167.5, 170.3. IR (KBr): 3354, 2961, 1725, 1609, 1466, 1367, 1218, 1142, 1016, 859, 743 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{27}H_{28}N_2O_5$ $[M+H]^+$: 461.2071, found 461.2085.

Diethyl-(*Z*)-2-((5-methoxy-1-methyl-1*H*-indol-3-yl)methyl)-3-(2-oxoindolin-3-ylidene) succinate 3m: Yellow solid (30.5 mg, 64% yield), m.p. 84.0 - 85.0 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 1.19 (t, J = 7.0 Hz, 3H), 1.42 (t, J = 7.0 Hz, 3H), 3.25 (dd, J_1 = 5.0 Hz, J_2 = 14.5 Hz, 1H), 3.59 (dd, J_1 = 9.0 Hz, J_2 = 14.5 Hz, 1H), 3.65(s, 3H), 3.81 (s, 3H), 4.11 - 4.23 (m, 2H), 4.23 - 4.50 (m, 2H), 4.54 (dd, J_1 = 5.0 Hz, J_2 = 9.0 Hz, 1H), 6.84 - 6.89 (m, 3H), 6.94 (s, 1H), 7.04 (d, J = 2.0 Hz, 1H), 7.14 (d, J = 10.5 Hz, 1H), 7.21 (t, J = 8.0 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 9.44 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 12.9, 12.9, 25.1, 31.7, 47.6, 54.8, 60.5, 60.7, 99.1, 108.9, 109.09, 109.3, 111.0, 120.0, 120.9, 123.3, 126.3, 126.8, 127.3, 131.1, 139.4, 141.2, 152.9, 166.0, 166.9, 169.4. IR (KBr): 3673, 2988, 1723, 1466, 1254, 1153, 1057, 846, 737 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{27}H_{28}N_2O_6$ $[M+H]^+$: 477.2020 , found 477.2023.



Diethyl-(*Z*)-2-((1,7-dimethyl-1*H*-indol-3-yl)methyl)-3-(2-oxoindolin-3-ylidene) succinate 3n: Yellow solid (37.3 mg, 81% yield), m.p. 190 - 191 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 1.18 (t, J = 7.0 Hz, 3H), 1.42 (t, J = 7.0 Hz, 3H), 2.51 (s, 3H), 3.24 (dd, J_1 = 5.0 Hz, J_2 = 14.5 Hz, 1H), 3.60 (dd, J_1 = 9.5 Hz, J_2 = 14.5 Hz, 1H), 3.66 (s, 3H), 4.10 - 4.20 (m, 2H), 4.42 - 4.49 (m, 2H), 4.53 (dd, J_1 = 5.0 Hz, J_2 = 9.5 Hz, 1H), 6.84 - 6.90 (m, 3H), 6.97 (d, J = 8.0 Hz, 1H), 7.07 (s, 1H), 7.23 (t, J = 8.0 Hz, 1H), 7.50 (dd, J_1 = 8.0 Hz, J_2 = 11.5 Hz, 1H), 9.20 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 14.0, 21.8, 26.1, 32.5, 48.8, 61.5, 61.7, 109.3, 110.3, 110.3, 118.2, 120.7, 121.1, 122.1, 124.6, 125.6, 127.2, 127.2, 130.3, 131.4, 137.3, 140.6, 142.1, 167.0, 167.8, 170.4. IR (KBr): 3189, 2981, 1745, 1706, 1615, 1466, 1345, 1289, 1176, 1096, 1014, 853, 793, 731 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{27}H_{28}N_2O_5$ $[M+H]^+$: 461.2071, found 461.2087.

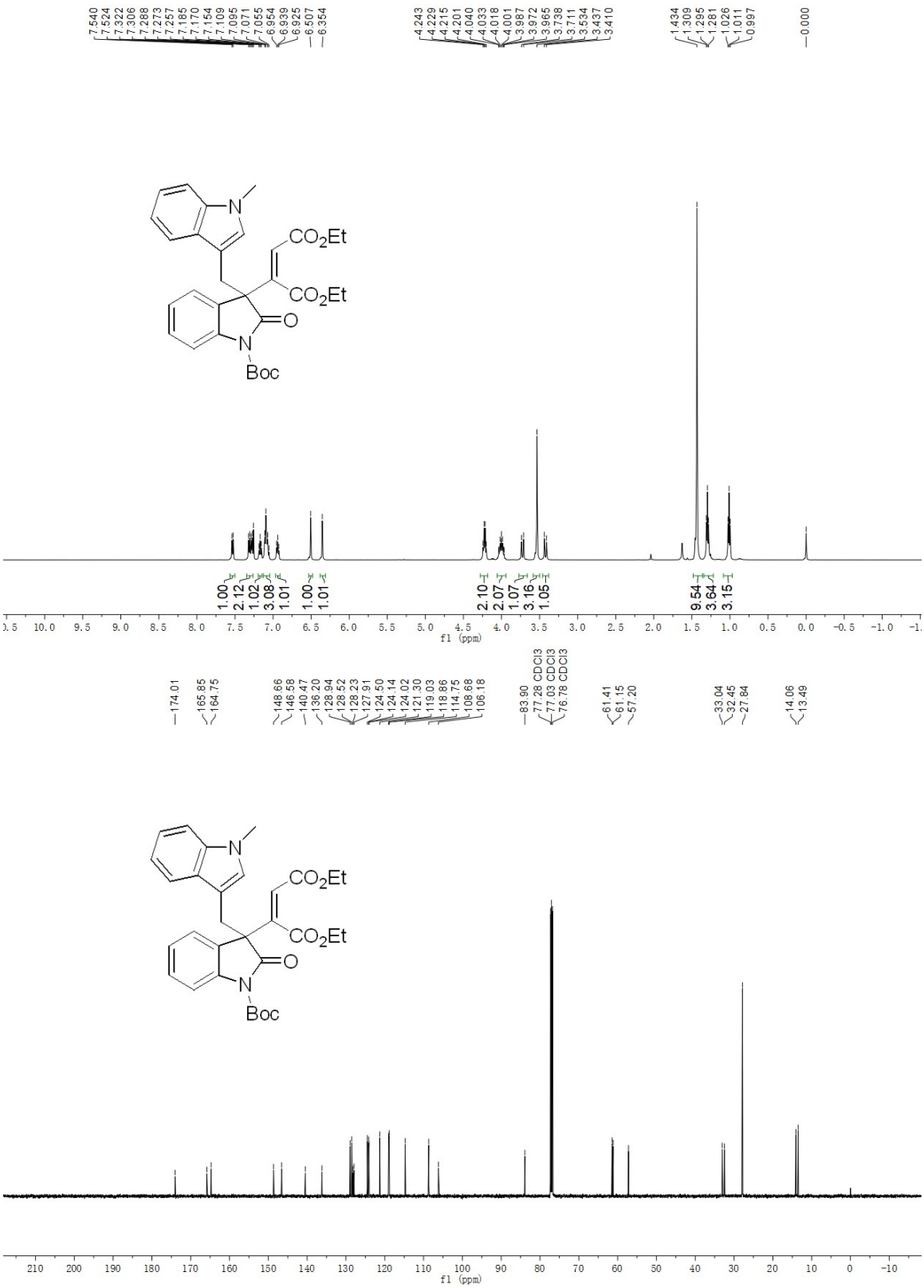
Diethyl-1-(2-((methoxycarbonyl)amino)phenyl)-9-methyl-9H-carbazole-2,3-dicarboxylate 6: White solid (45% yield), m.p. 155.6 - 156.7



°C. ^{1}H NMR (500 MHz, Actone-d_6) δ 0.99 (t, J = 7.5 Hz, 3H), 1.44 (t, J = 7.5 Hz, 3H), 3.22 (s, 3H), 3.59 (s, 3H), 4.04 - 4.08 (m, 2H), 4.41 - 4.45 (m, 2H), 6.58 (s, 1H), 7.17 (t, J = 7.5 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 7.33 - 7.37 (m, 2H), 7.49 (t, J = 7.5 Hz, 1H), 7.55 (t, J = 7.5 Hz, 1H), 8.04 (d, J = 7.5 Hz, 1H), 8.21 (d, J = 7.5 Hz, 1H), 8.88 (s, 1H); ^{13}C NMR (125 MHz, Actone-d_6) δ 13.6, 14.3, 30.9, 52.1, 61.3, 61.4, 109.4, 118.1, 118.2, 120.6, 120.6, 121.2, 122.2, 123.2, 123.3, 123.8, 126.2, 127.2, 130,0, 132.1, 134.9, 137.6, 139.9, 142.8, 154.1, 166.0, 169.0. IR (KBr): 3429, 3055, 2982, 2903, 1725, 1656, 1600, 1371, 1309, 1232, 1191, 1064, 950, 803, 735, 689 cm^{-1}. HRMS (BRUKER micrOTOF-QII) calcd for $C_{27}H_{25}F_3N_2O_5$ $[M+H]^+$: 475.1864, found 475.1860.

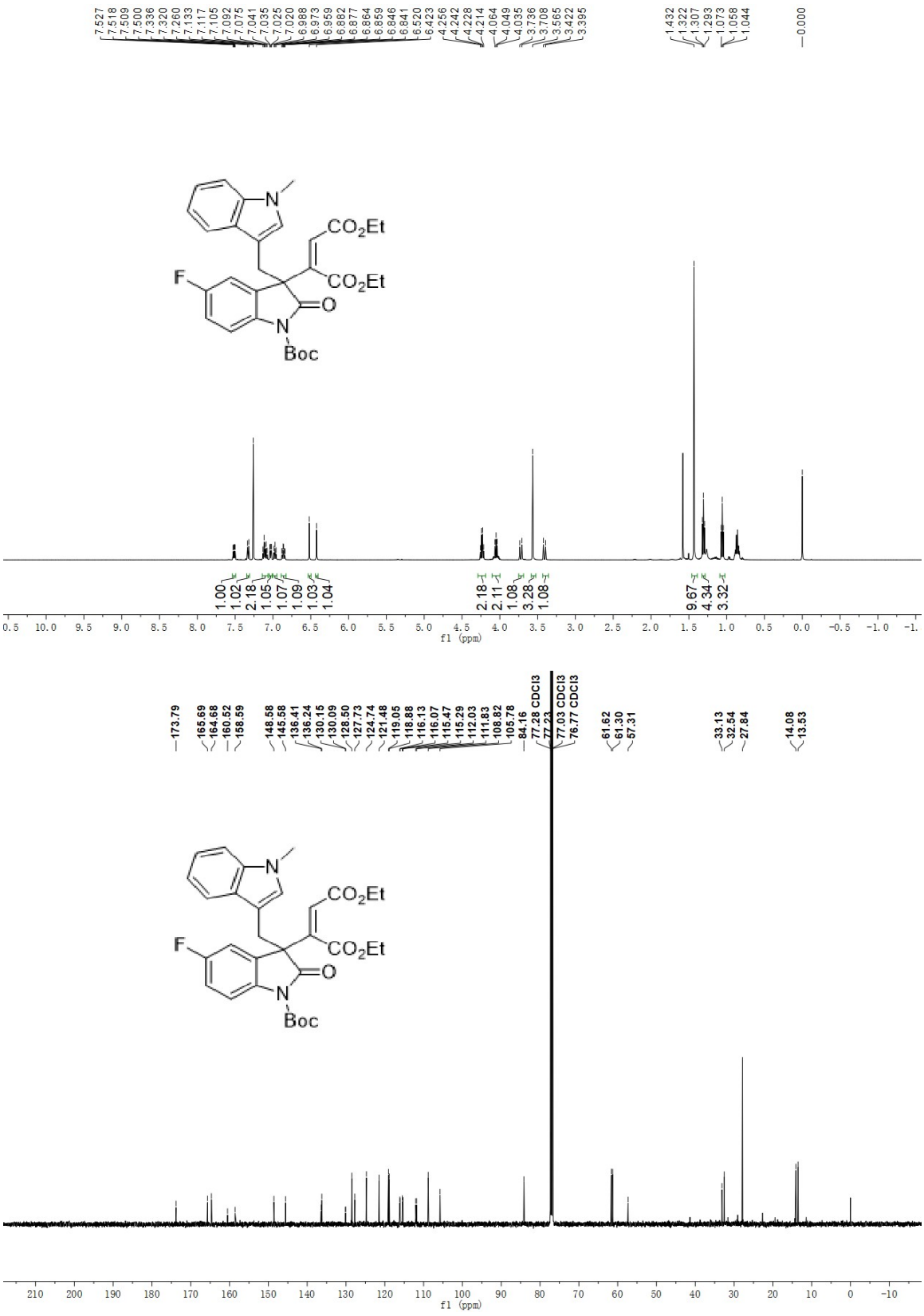
7. NMR spectra for substrates and products

2a ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

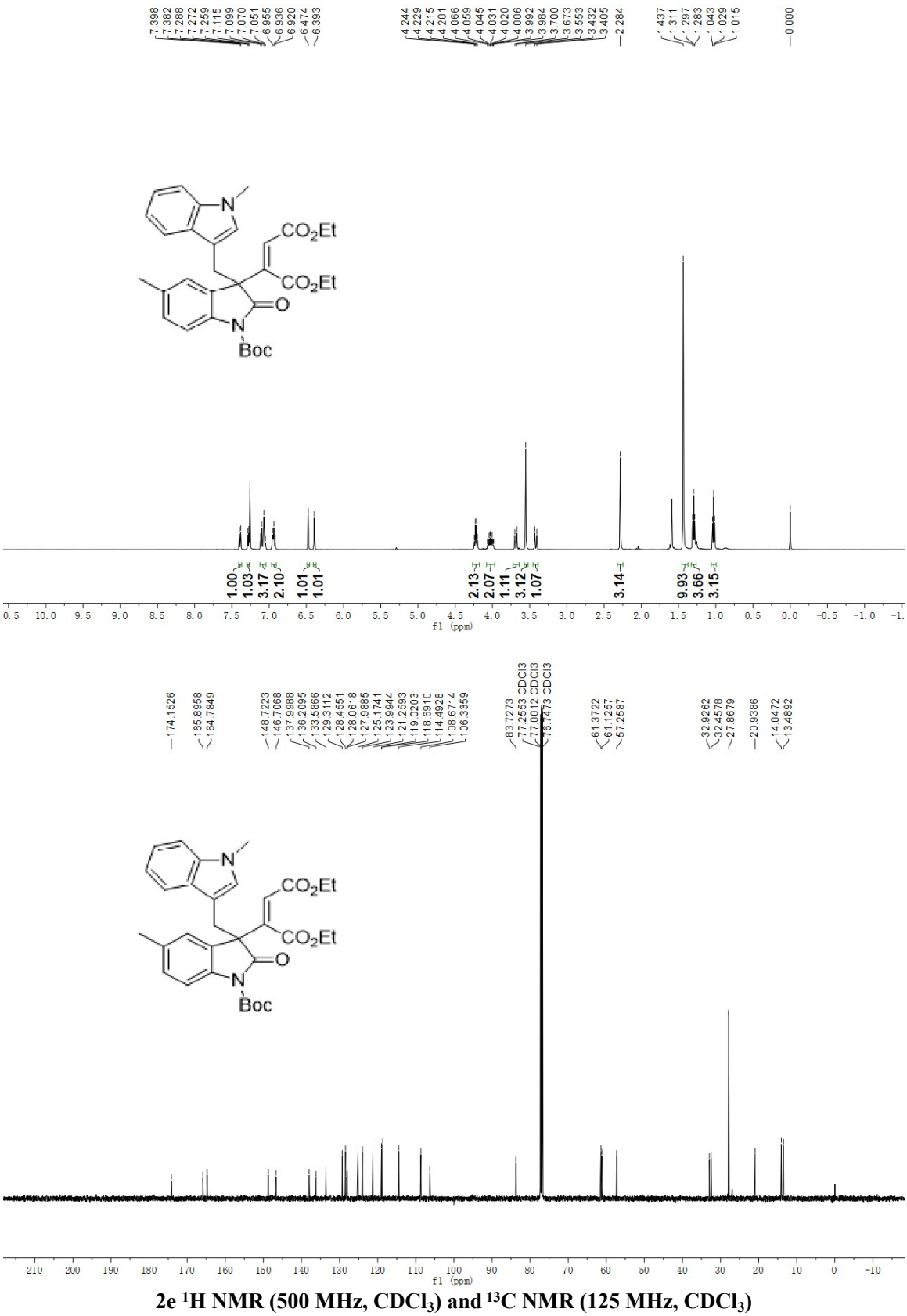


2b ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

2c ^{1}H NMR (500 MHz, $CDCl_3$), ^{13}C NMR (125 MHz, $CDCl_3$)

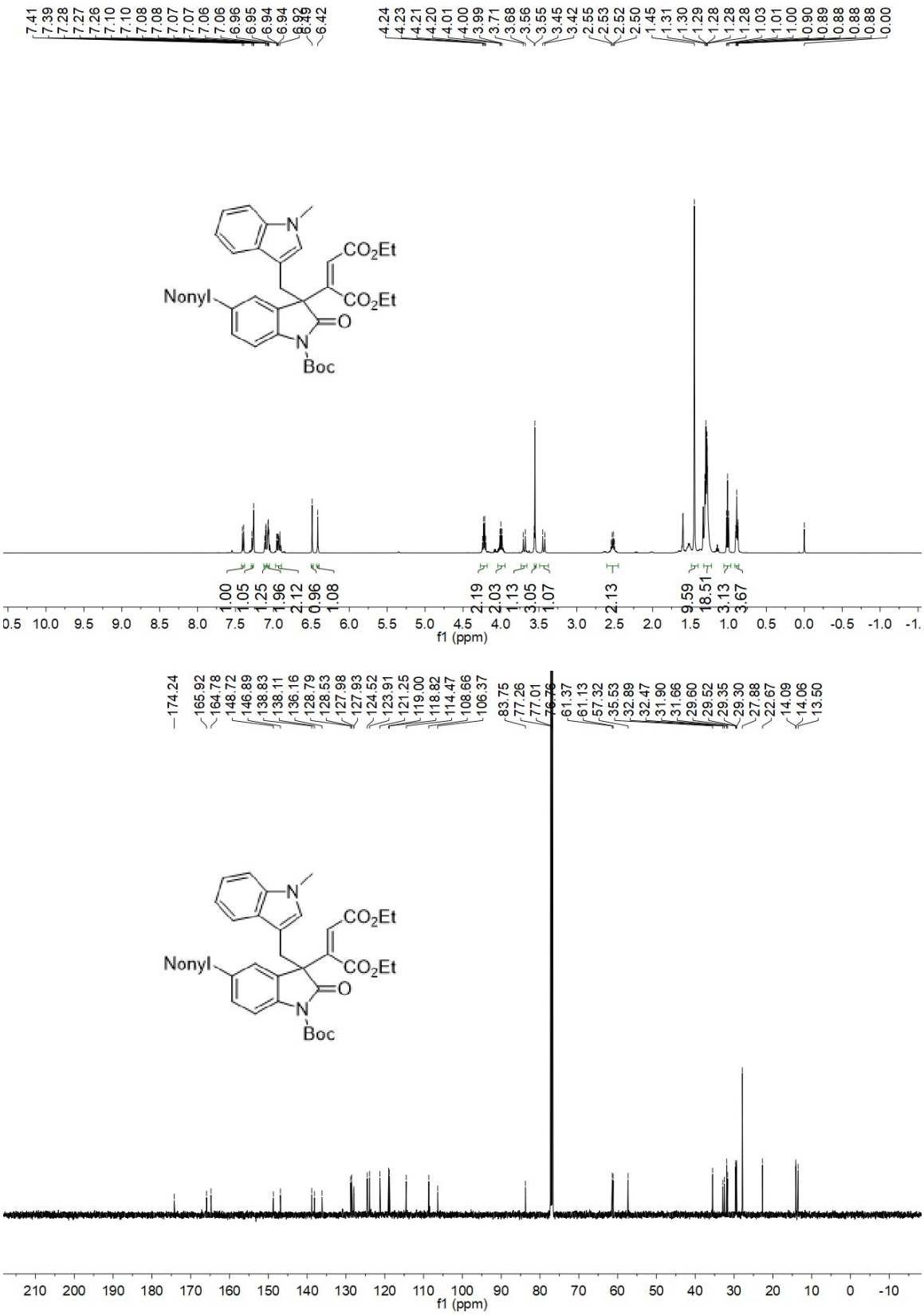


2d ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

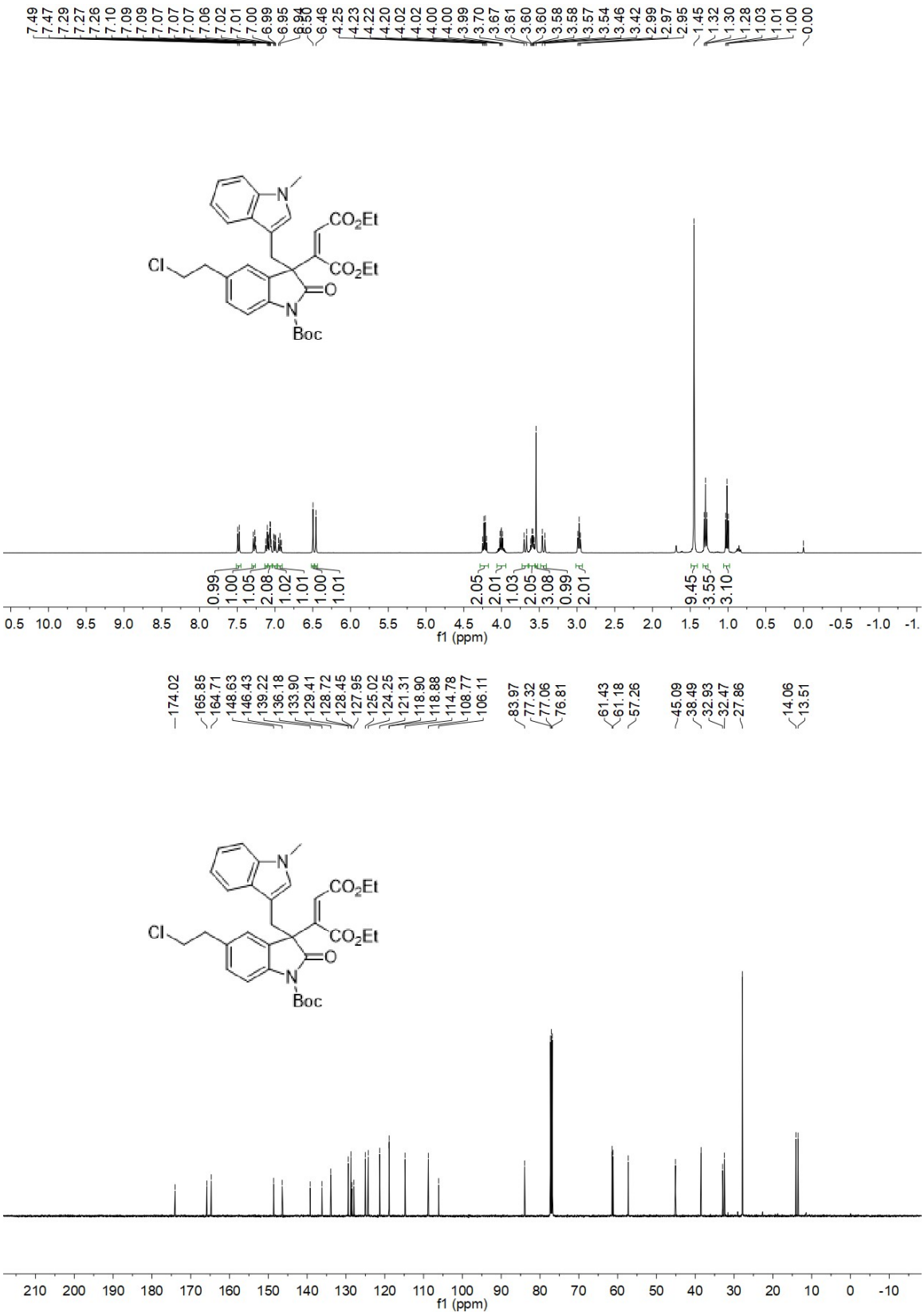


2e ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

2f ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

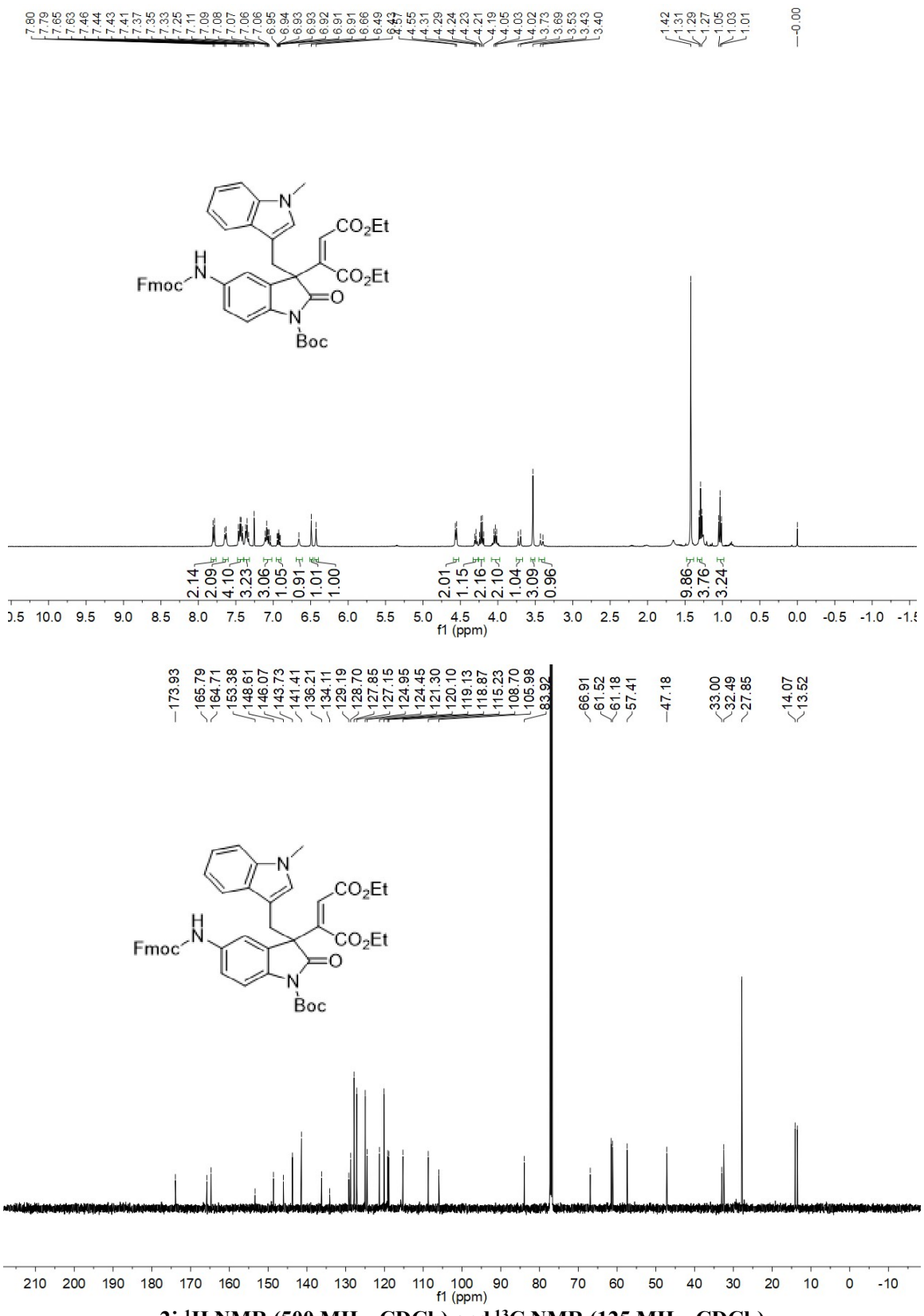


2g ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

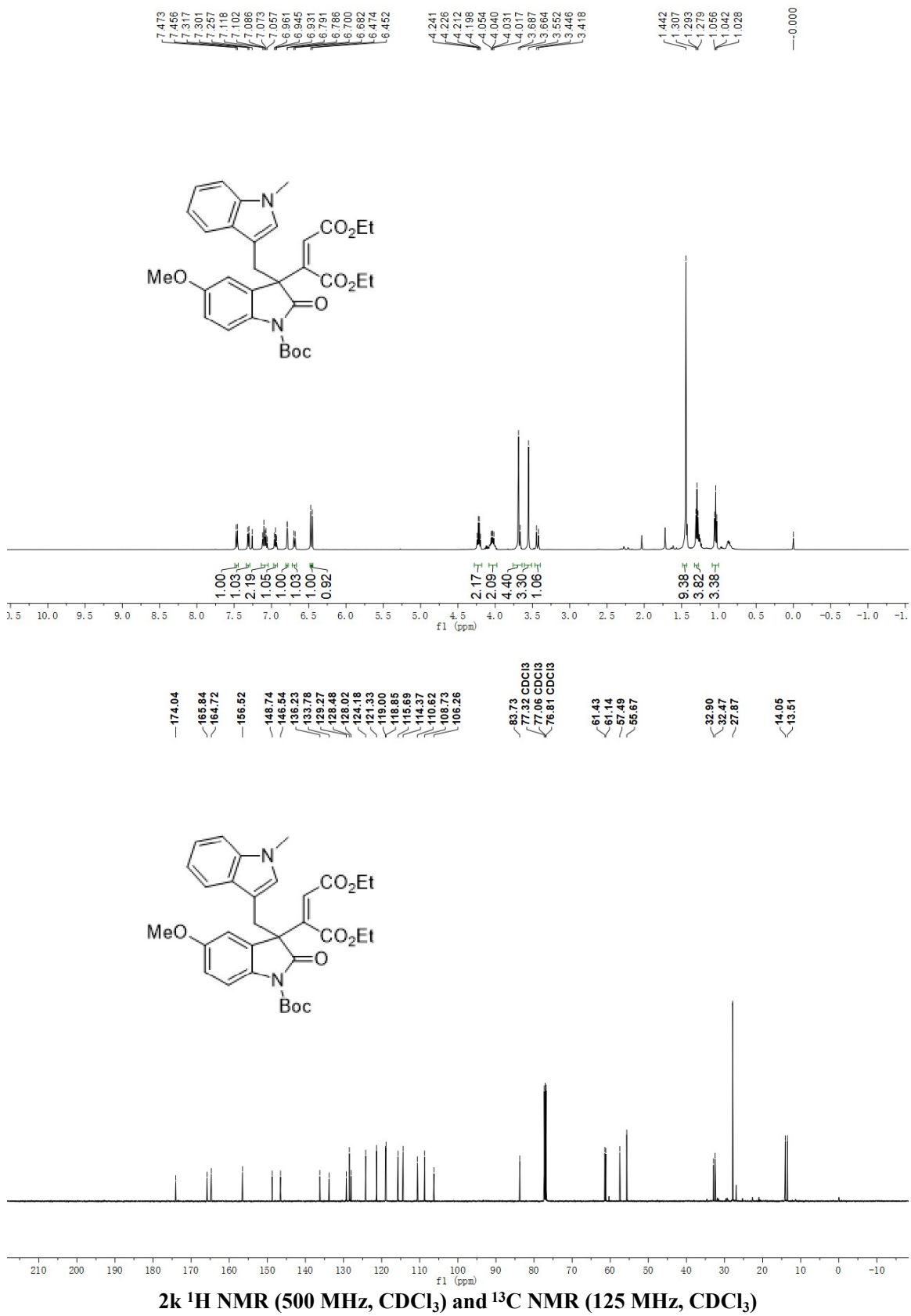


2h ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

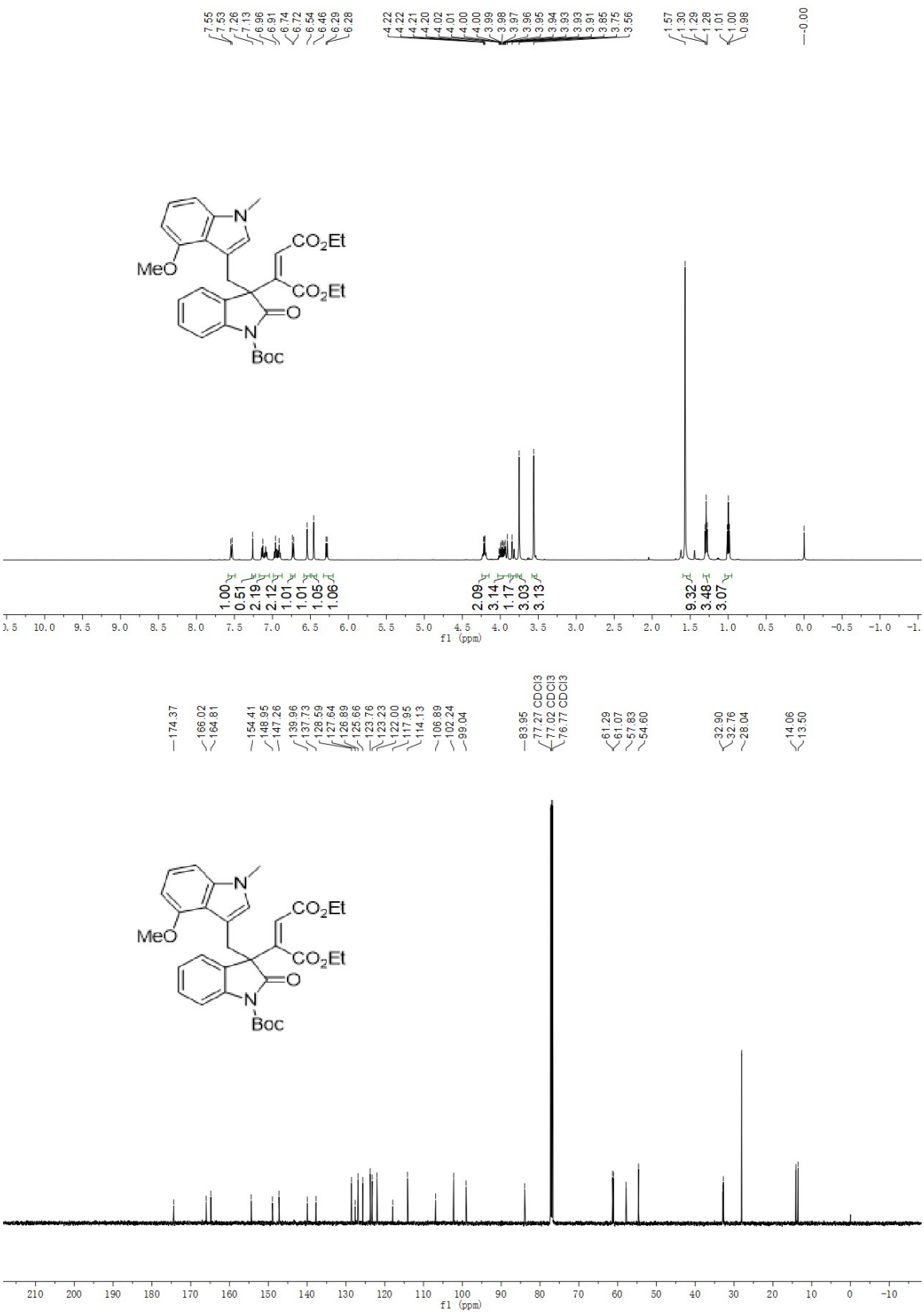
2i ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



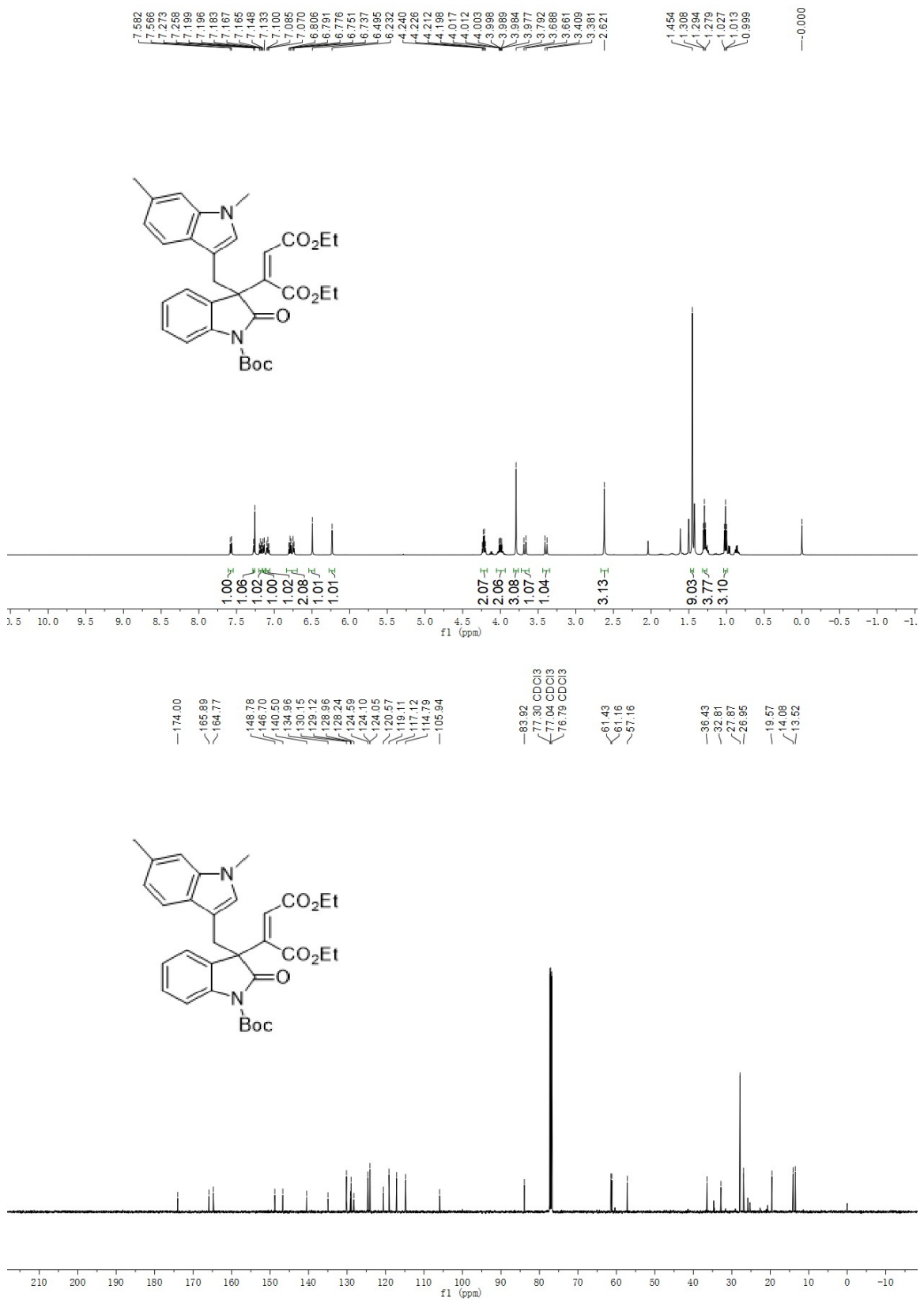
2j ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



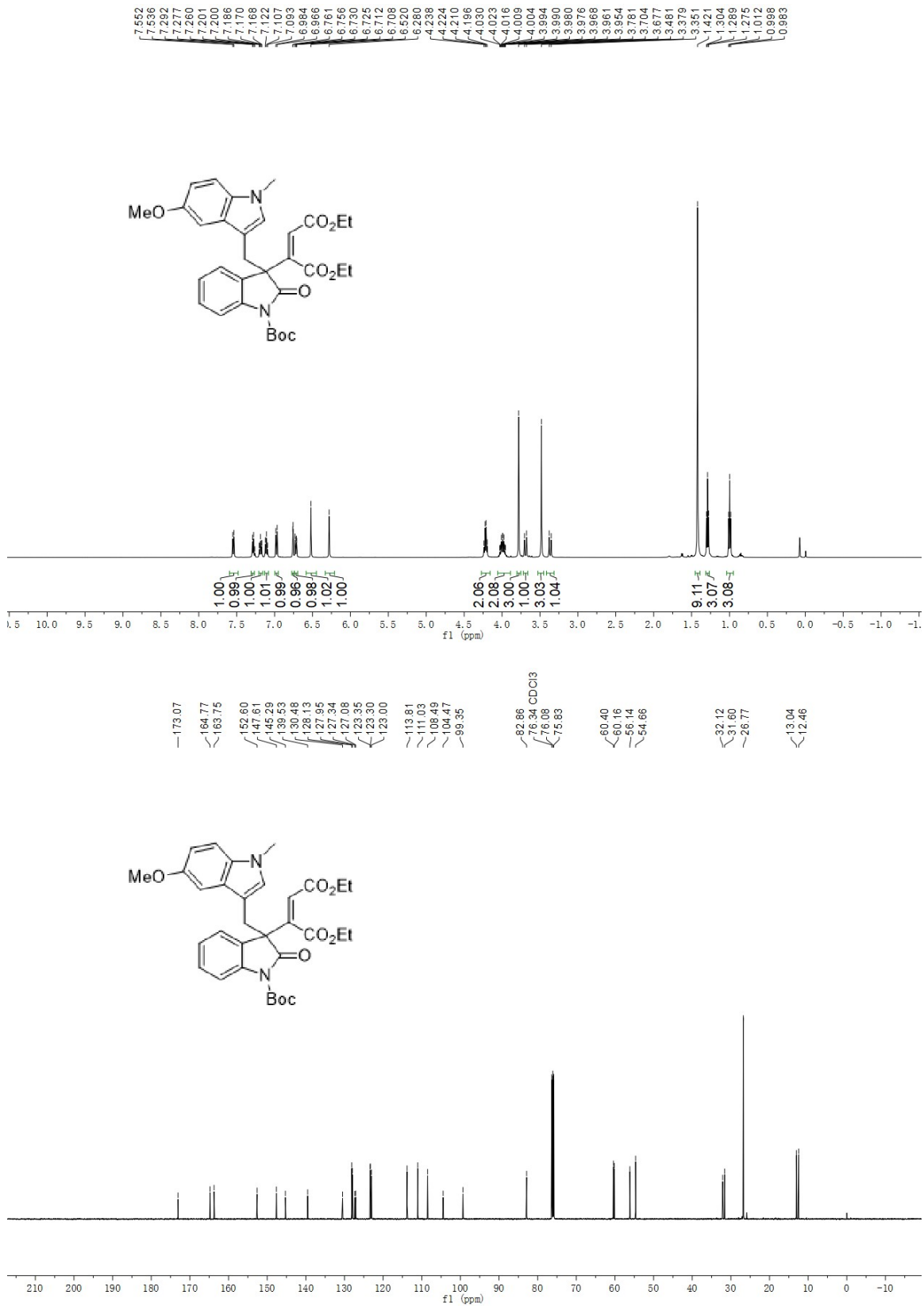
2k ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



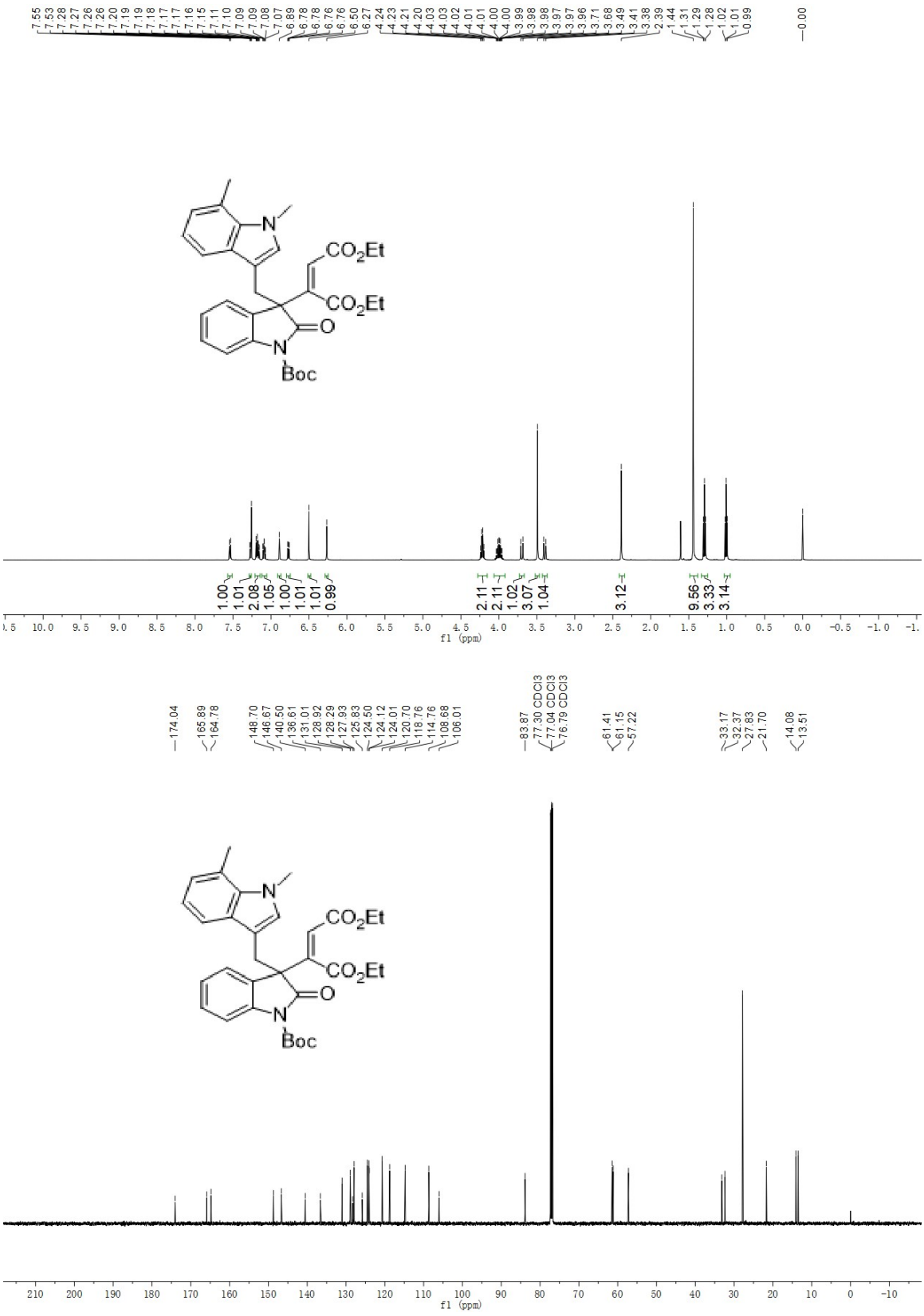
2l ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



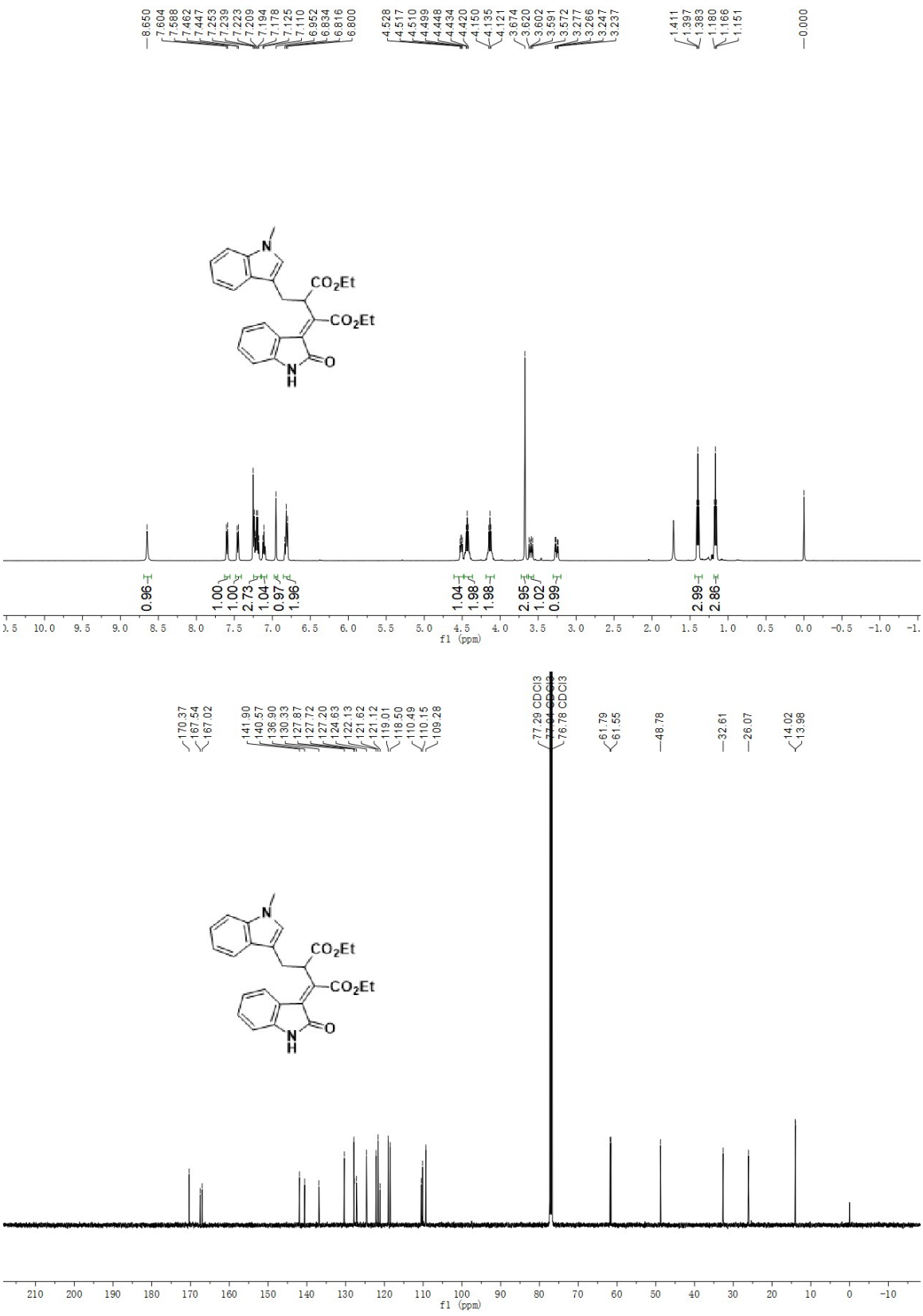
2m ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



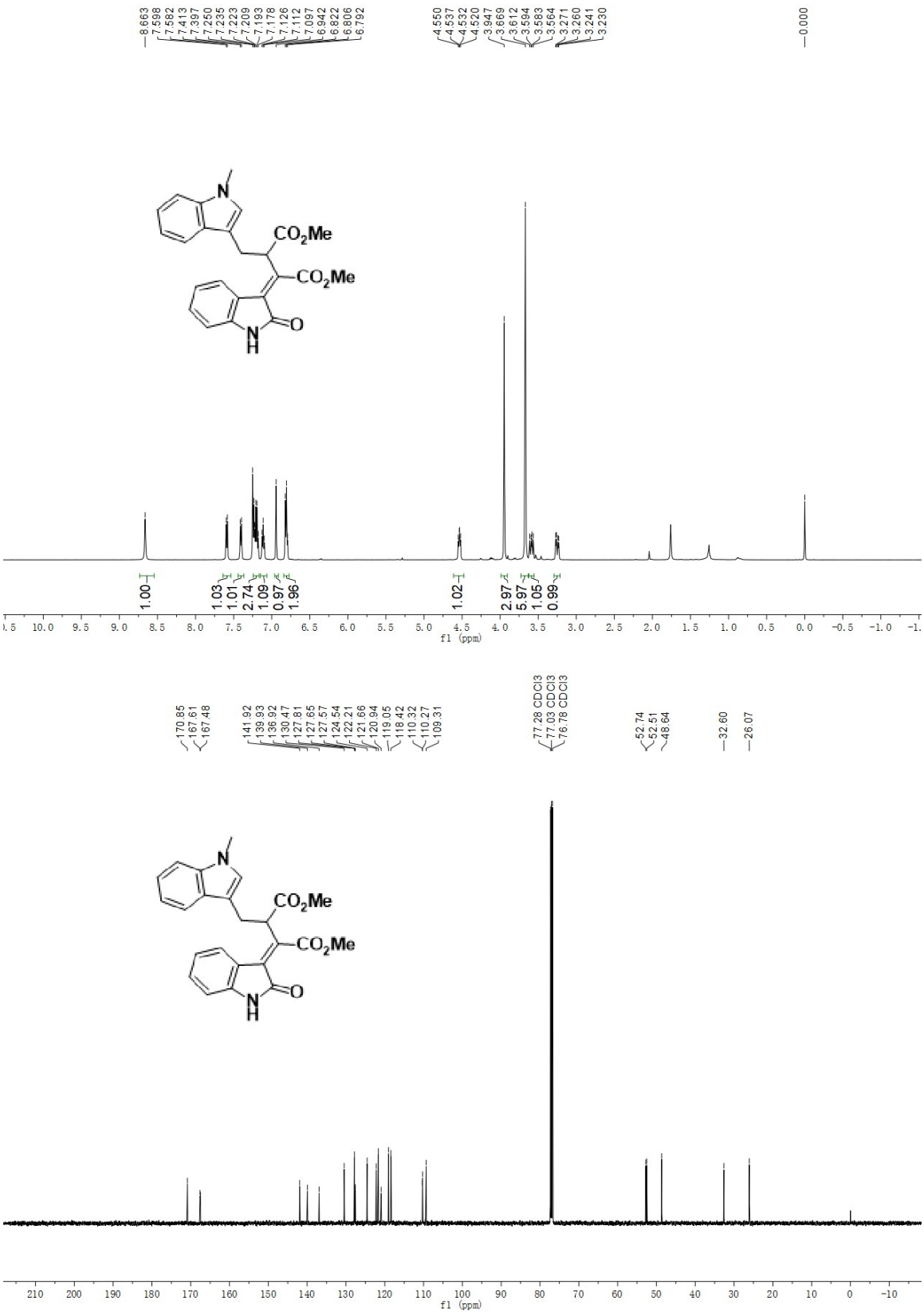
2n ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



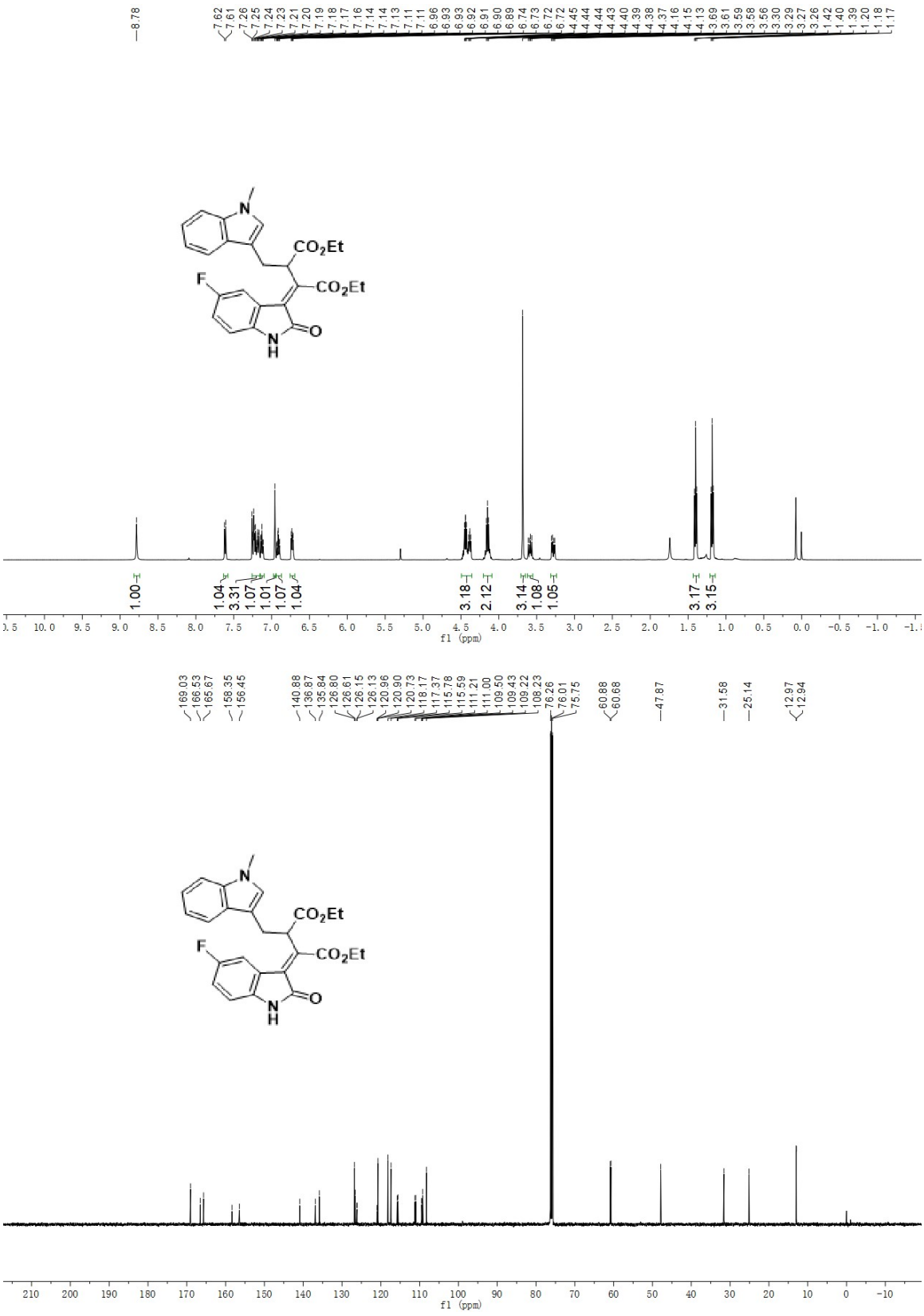
3a ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



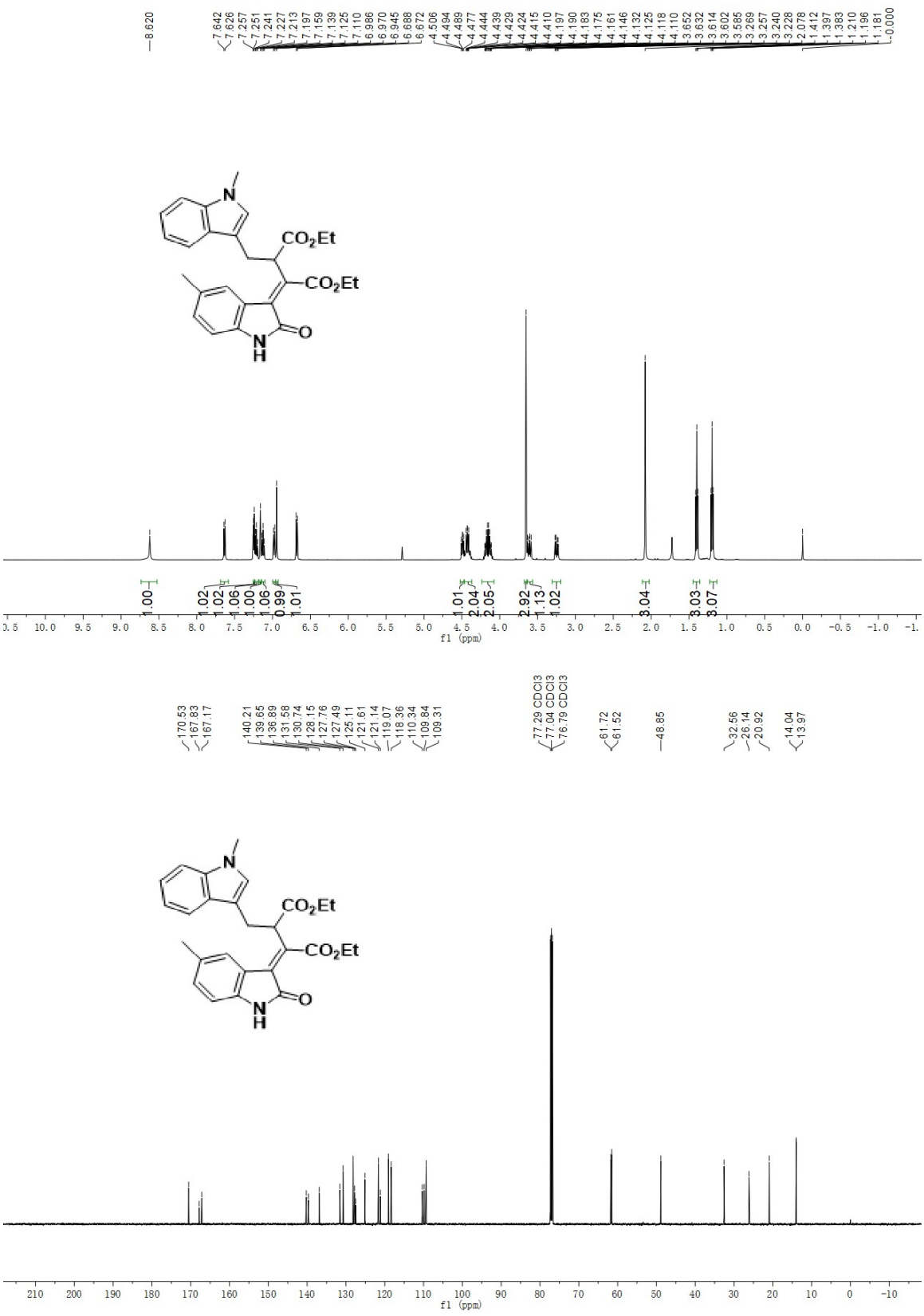
3b ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



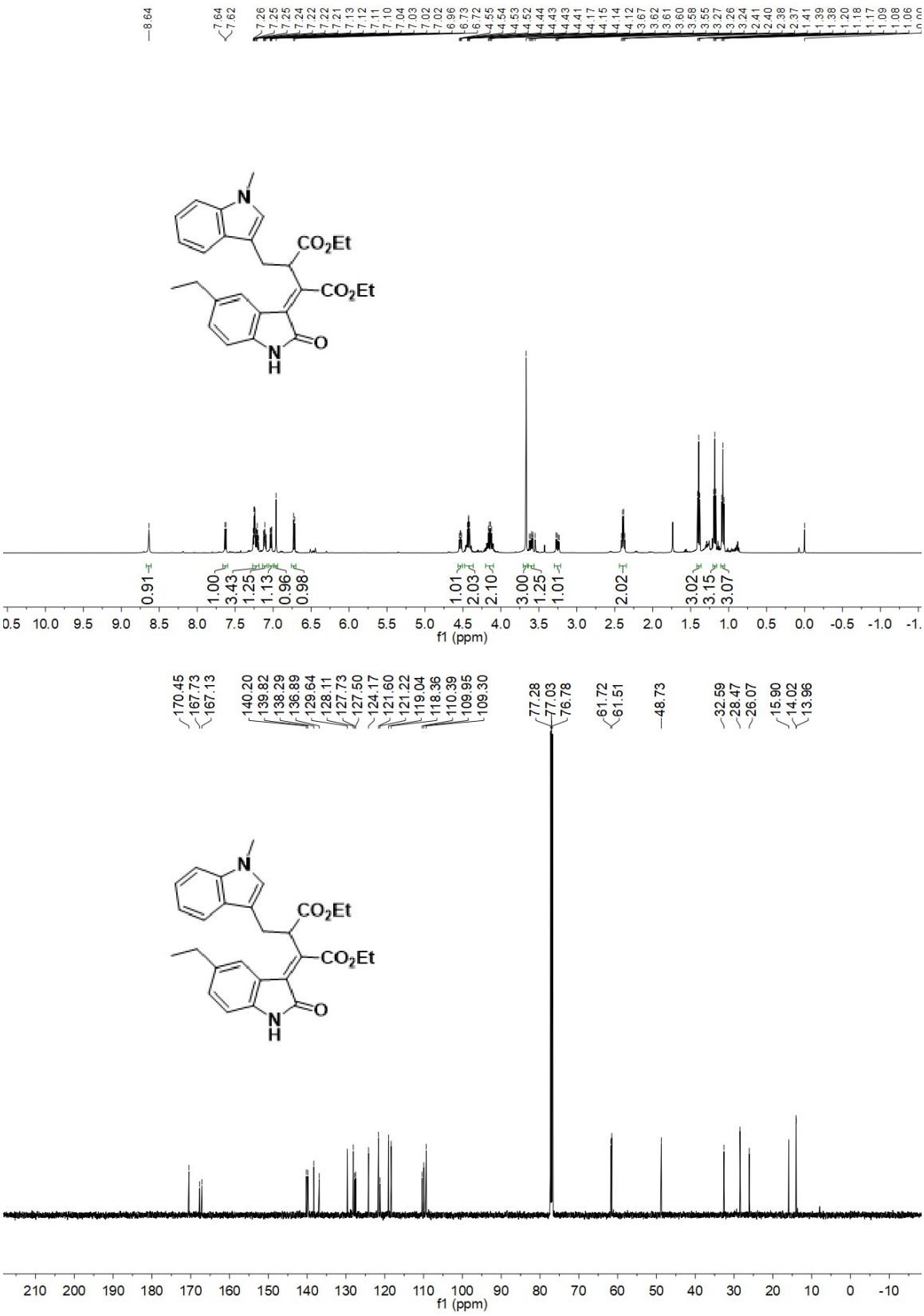
3c ^{1}H NMR (500 MHz, $CDCl_3$), ^{13}C NMR (125 MHz, $CDCl_3$)



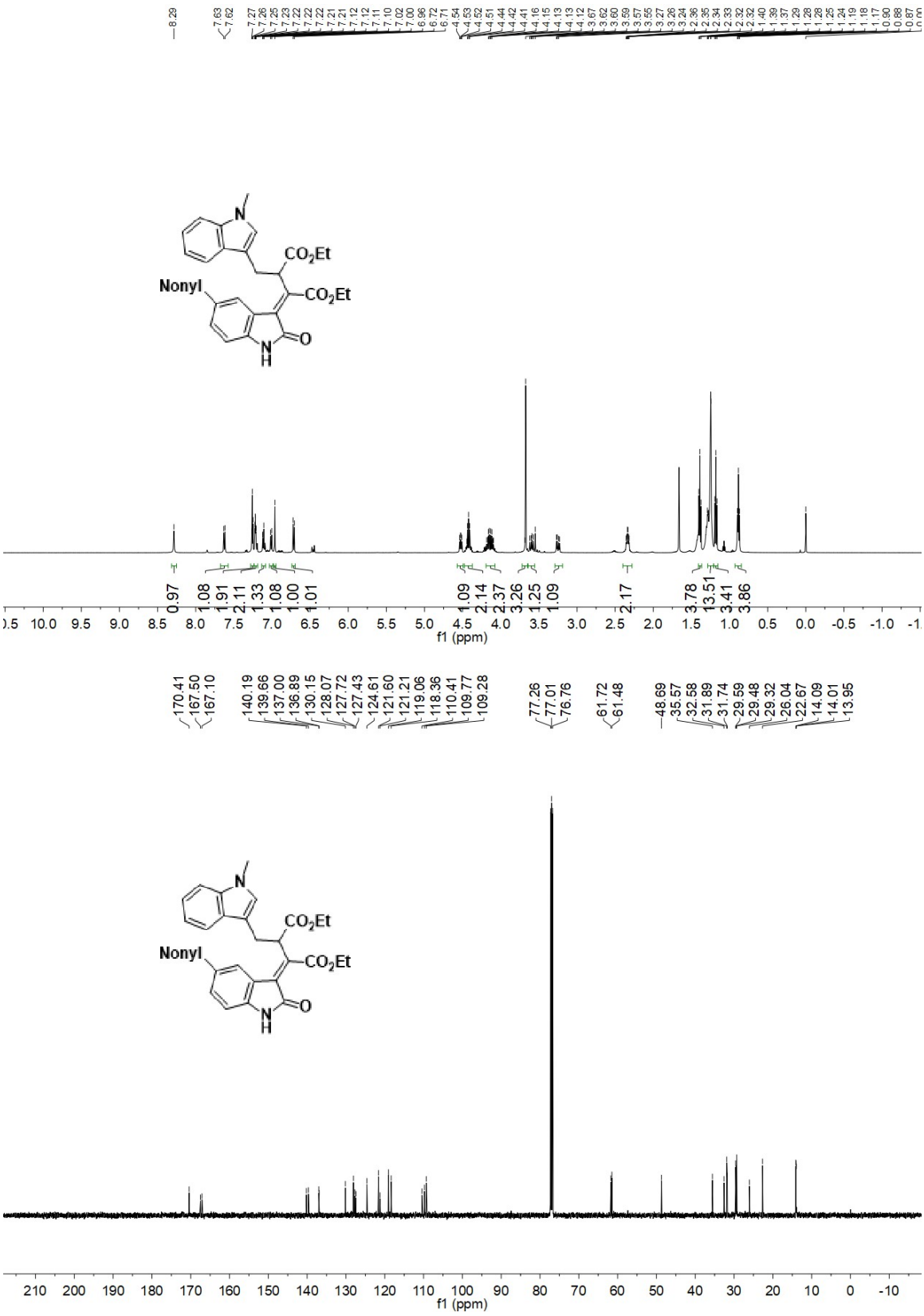
3d ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



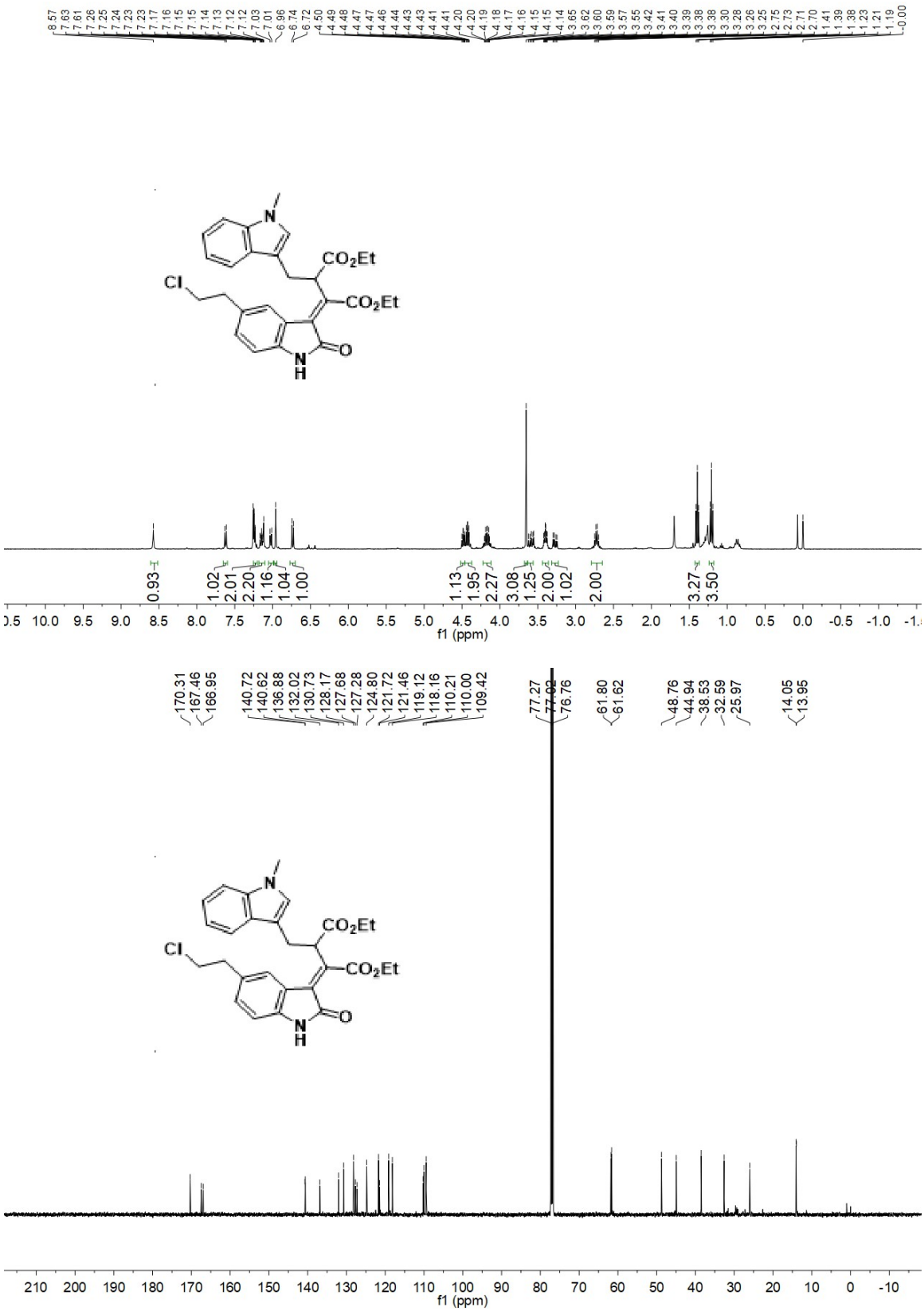
3e ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



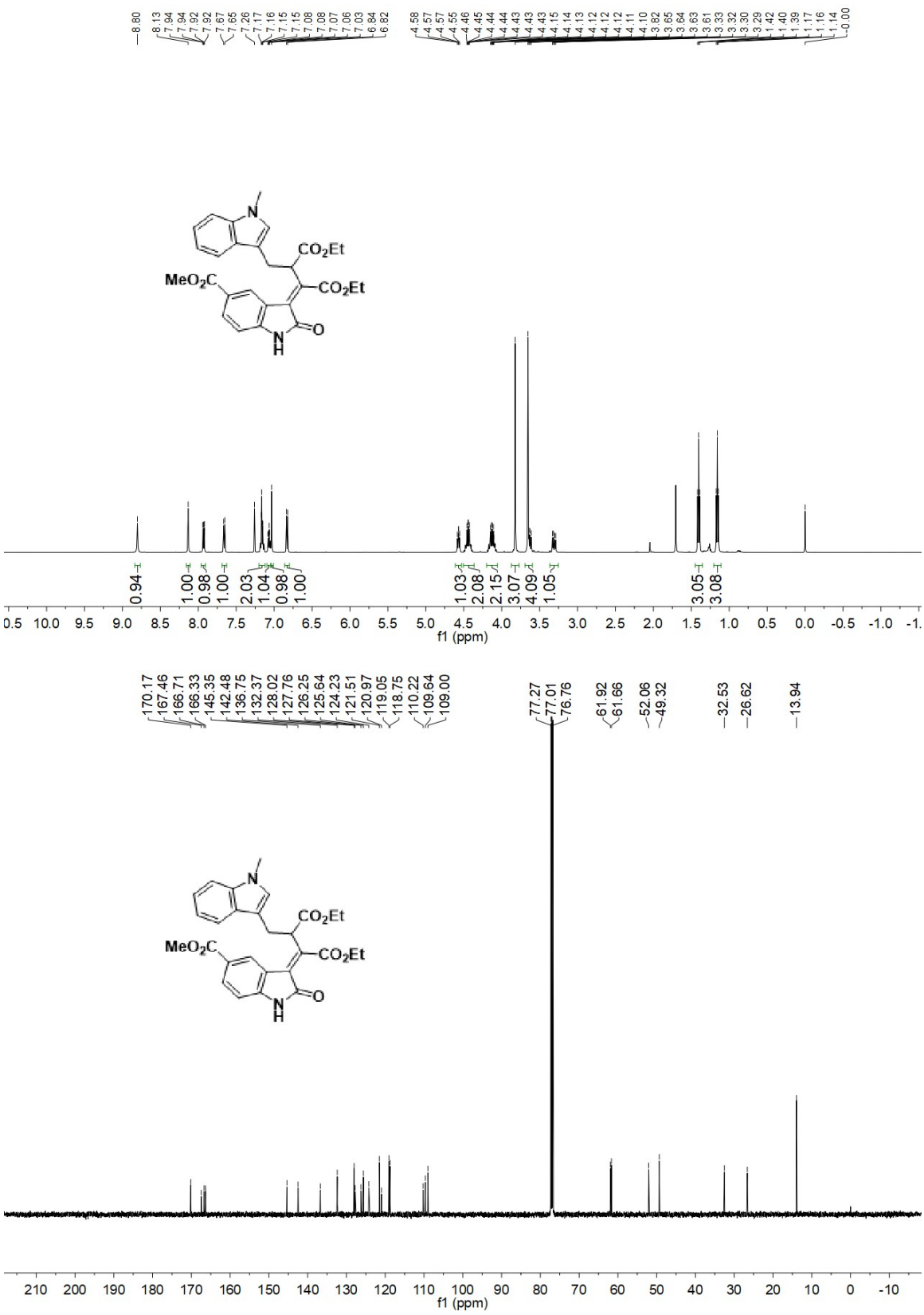
3f ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



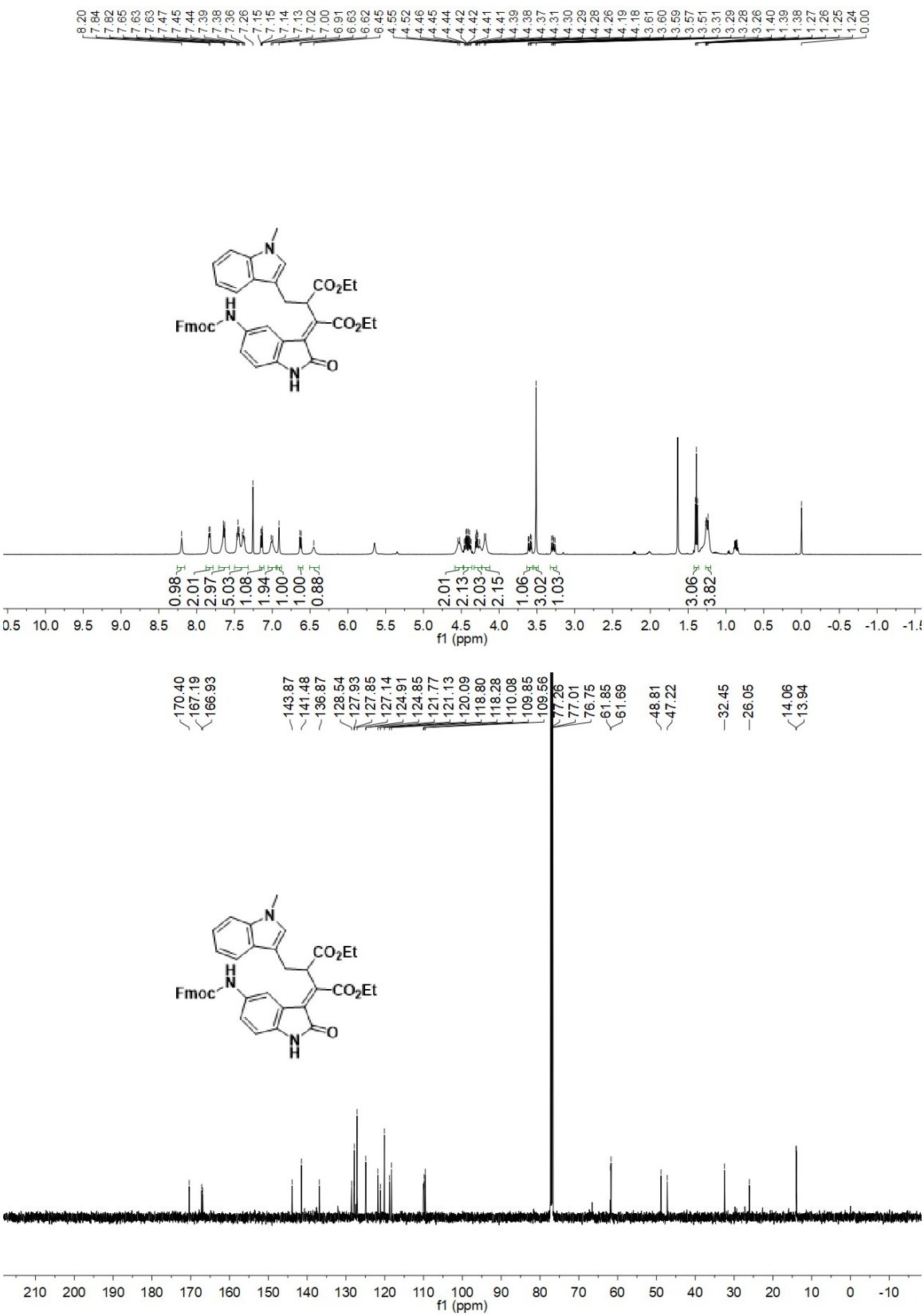
3g ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



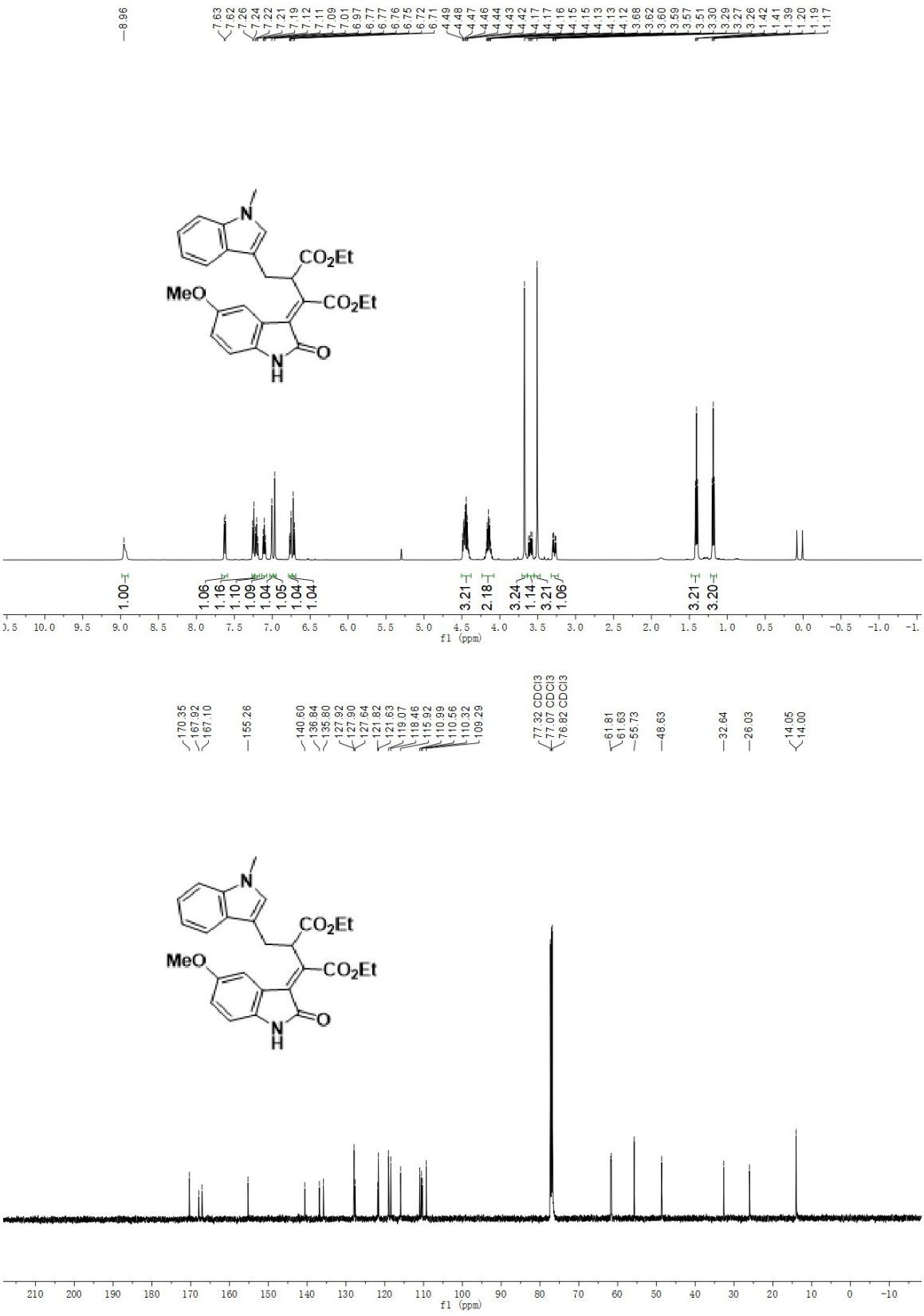
3h ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



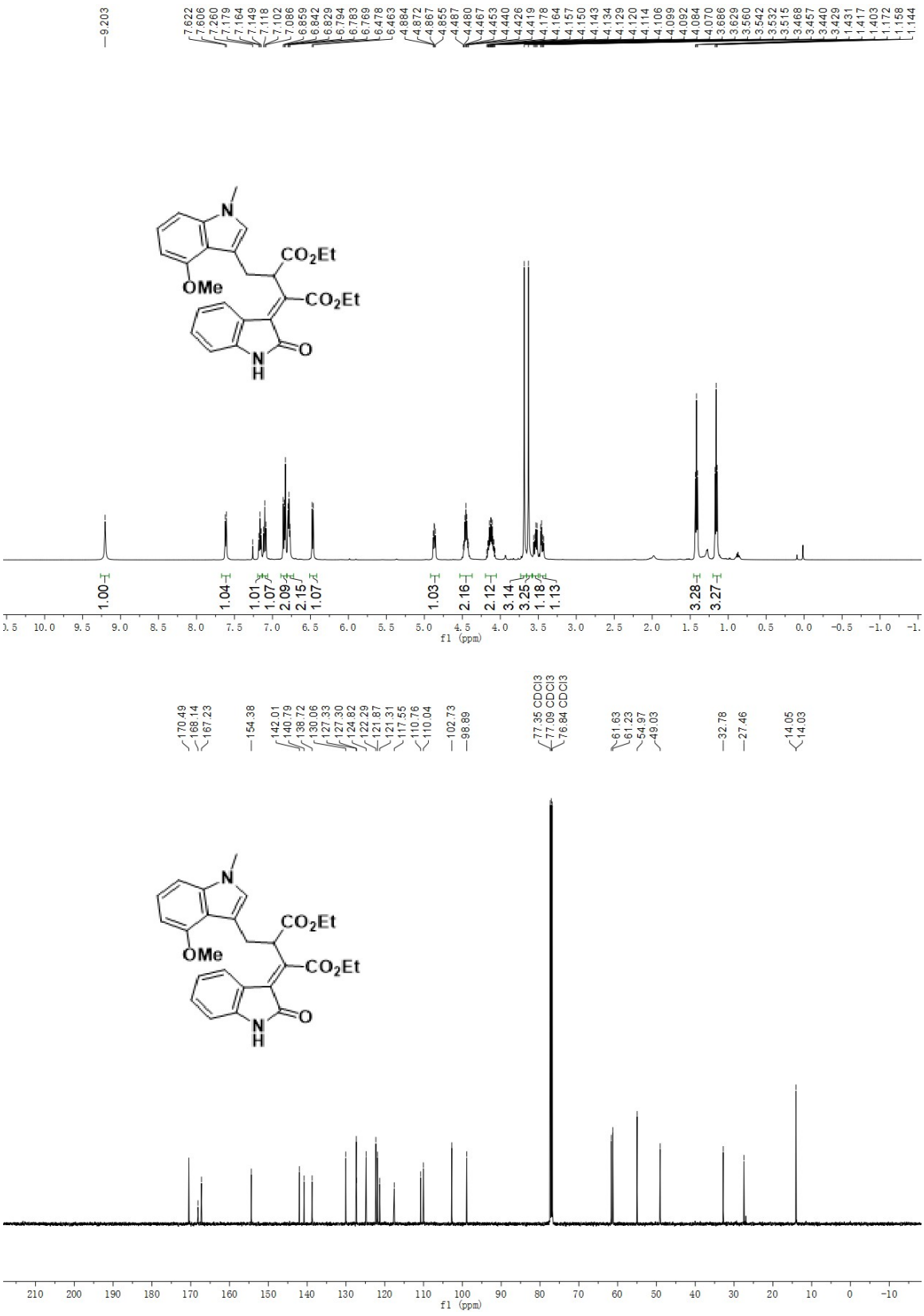
3i ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



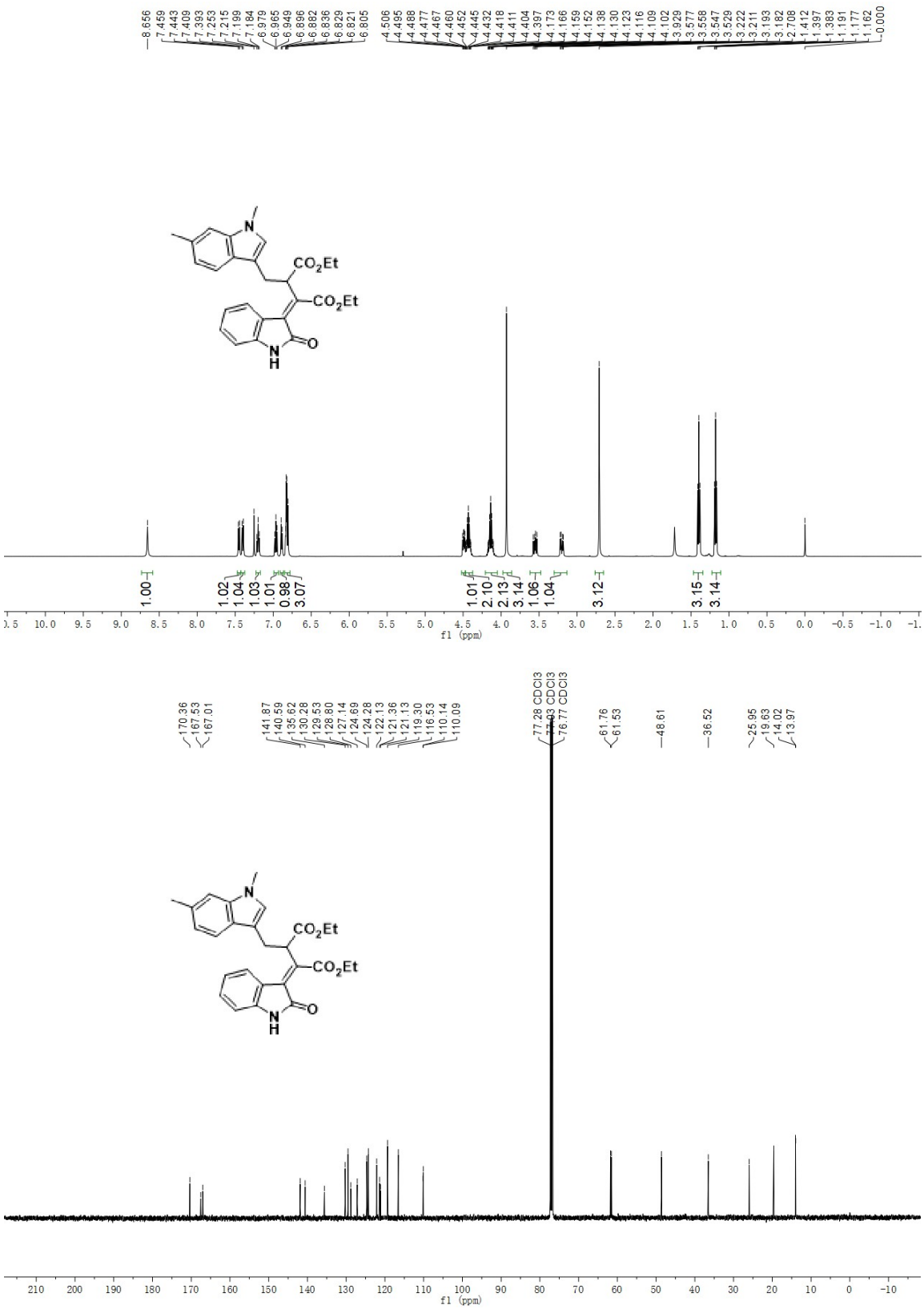
3j ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



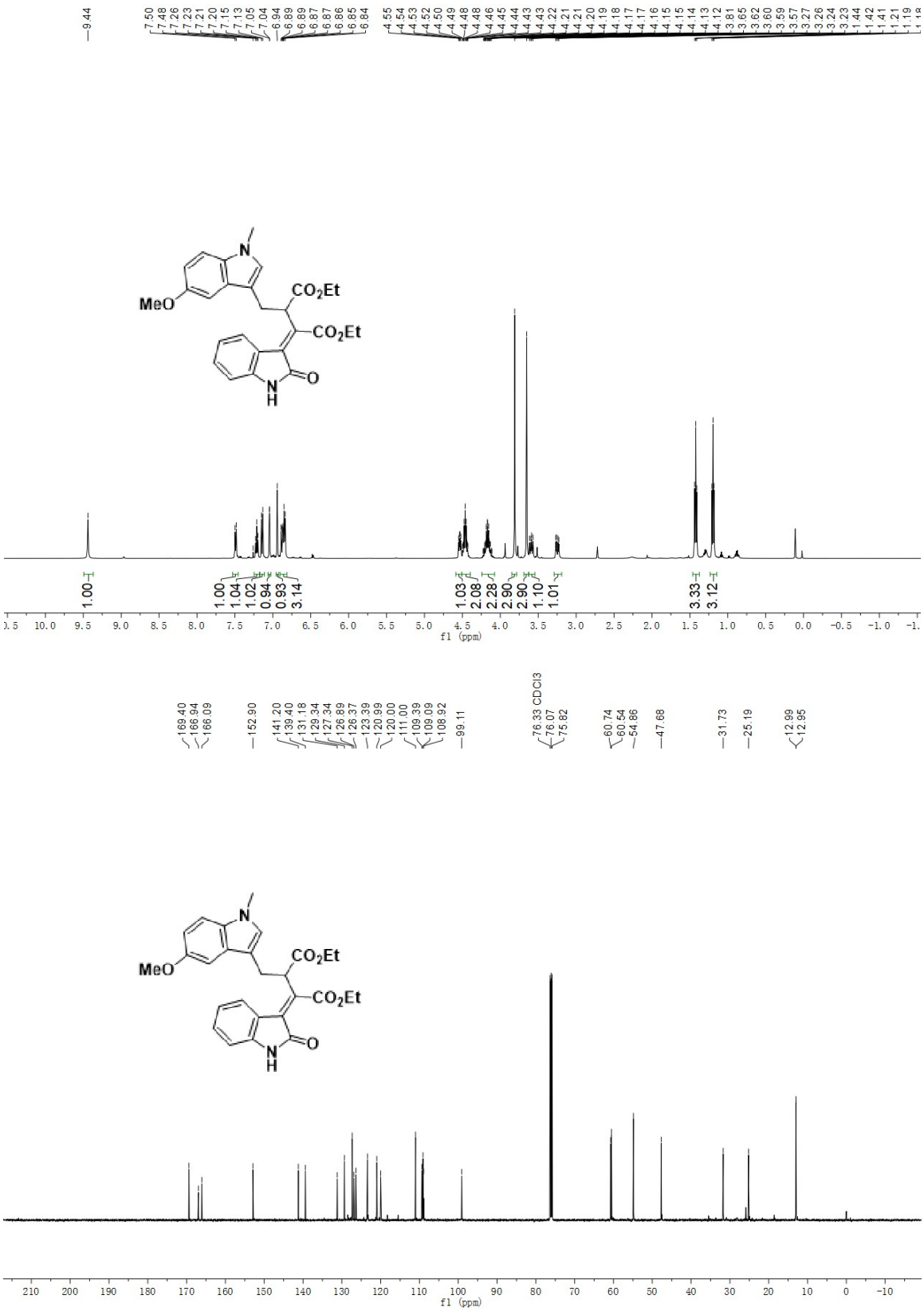
3k ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



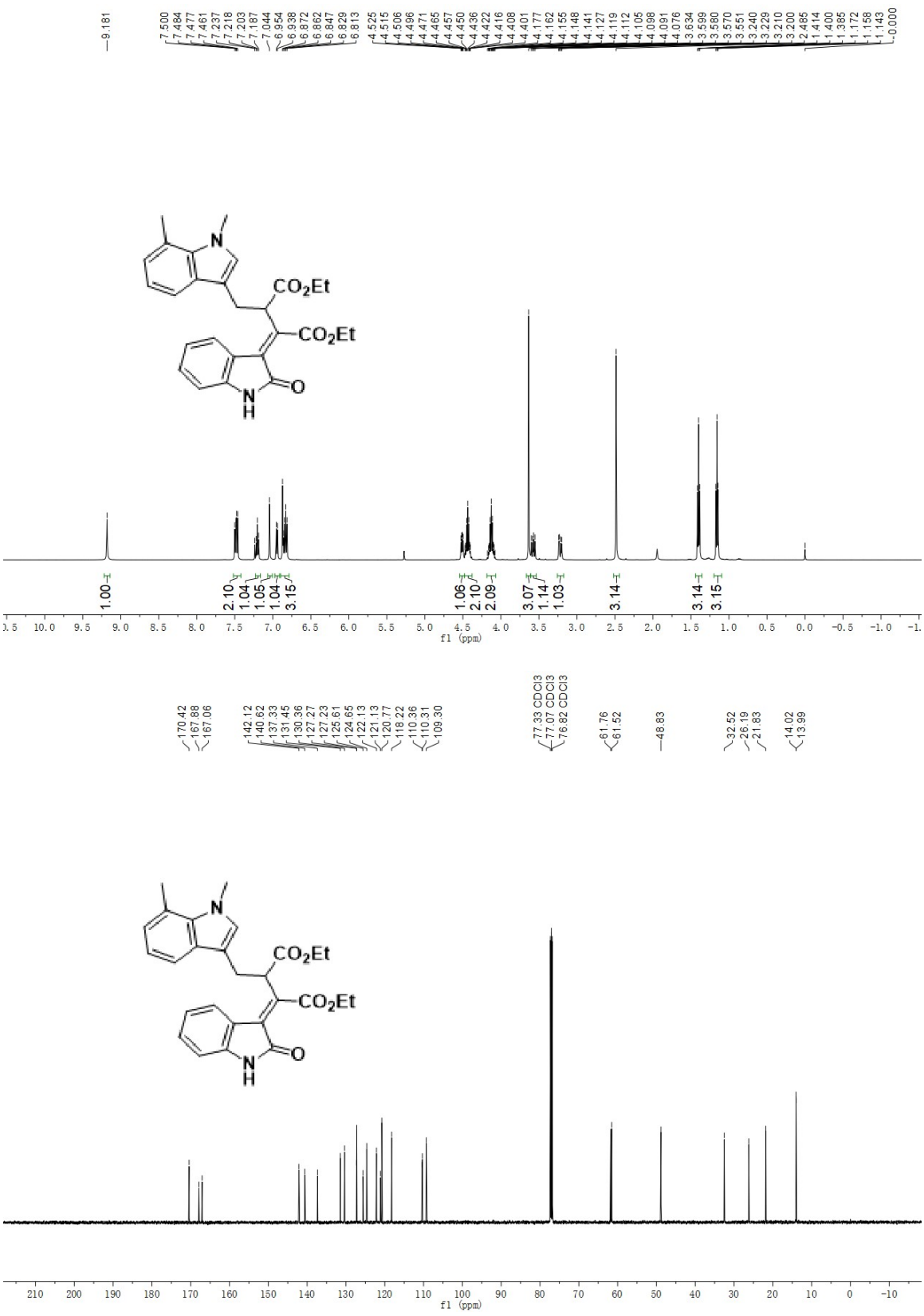
3l ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)



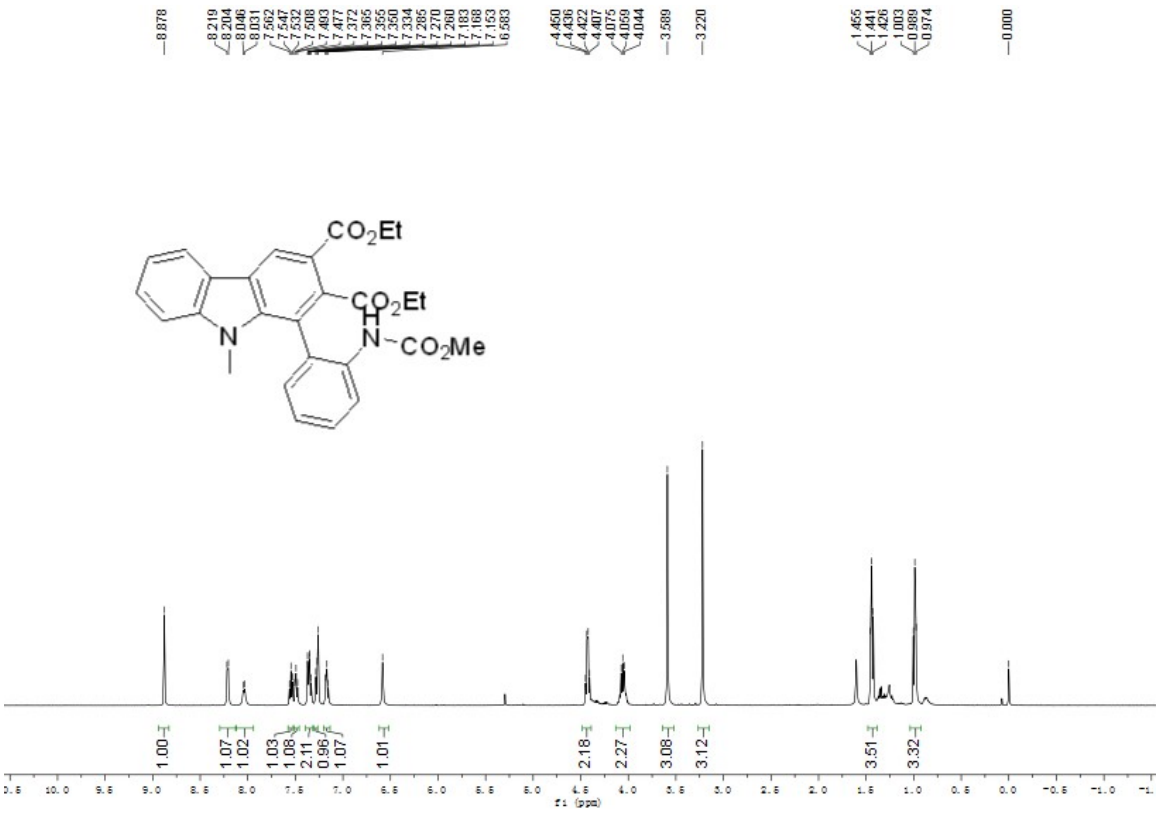
3m ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

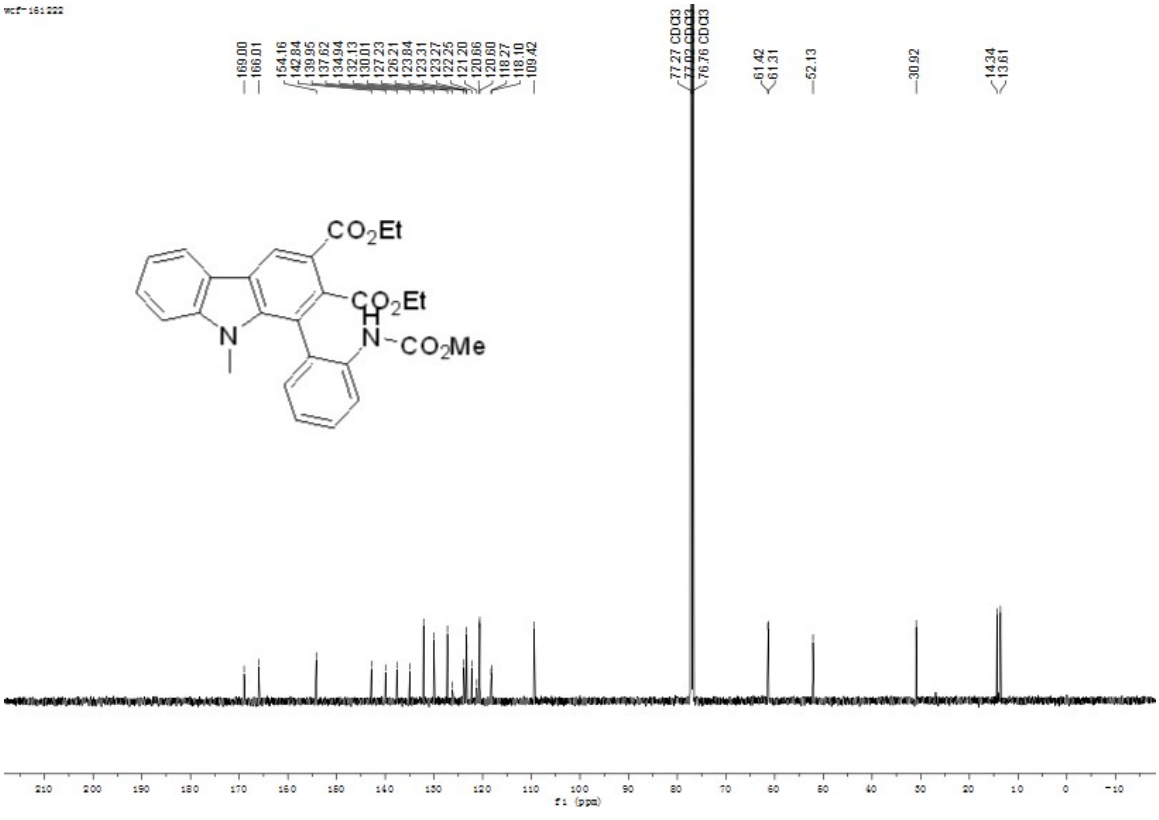


3n ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$)

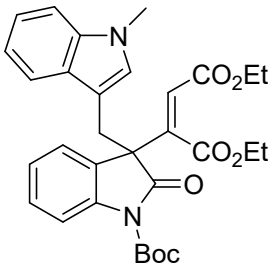


6 ^{1}H NMR (500 MHz, Actone-d_6) and ^{13}C NMR (125 MHz, Actone-d_6)

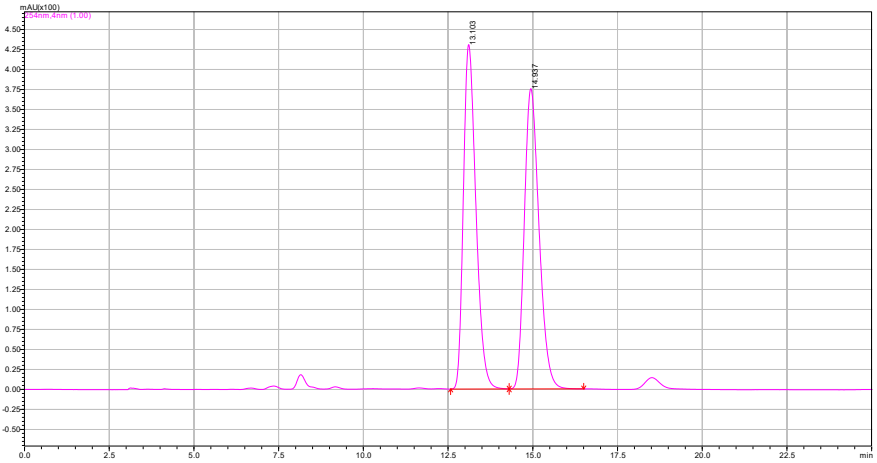




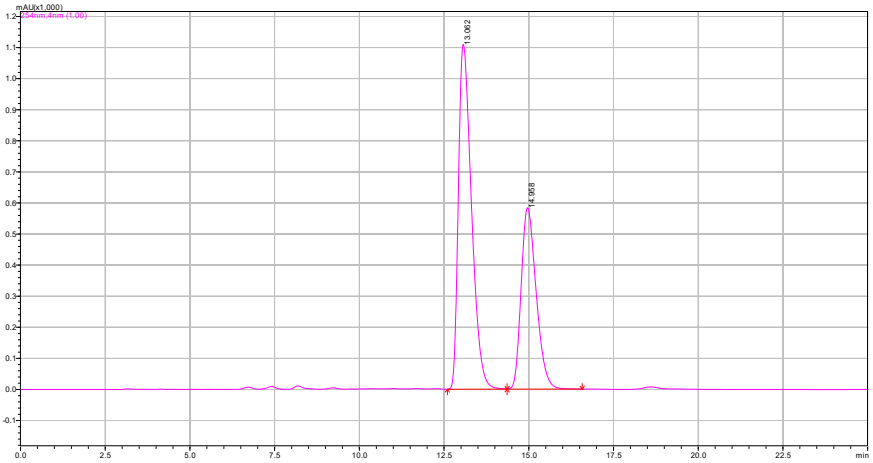
8. The HPLC of 2a and 3a



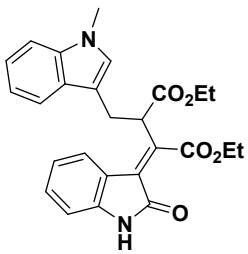
67% yield, 25% ee; Daicel Chiralpak IA-H, hexane/iso-propanol=90/10, flow rate 1.0 mL/min, t_1=13.06 min, t_2=14.96 min.



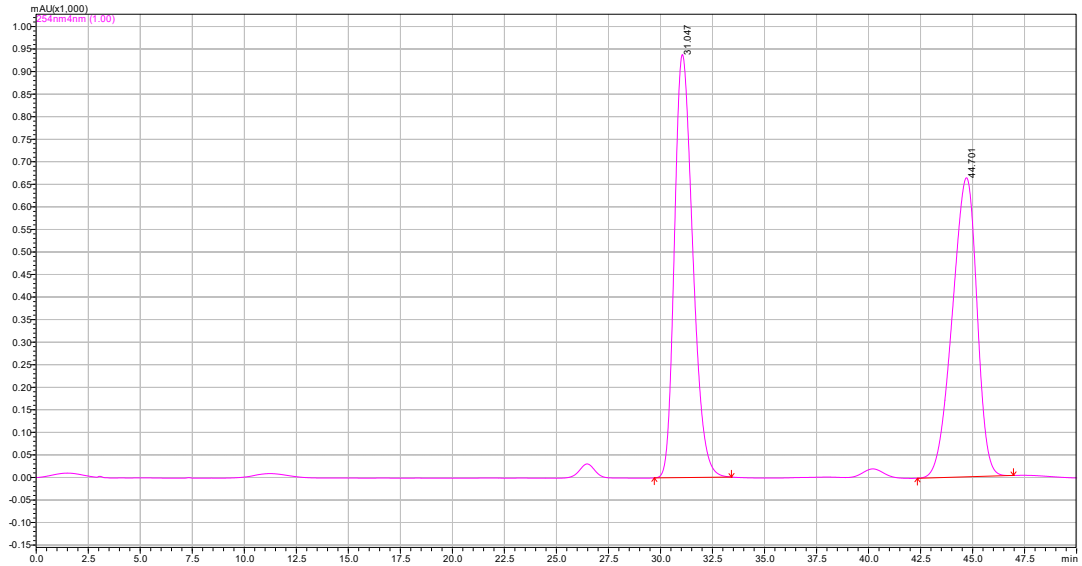
Peak	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	13.103	11072964	430581	12.576	14.304	49.3677
2	14.937	11356587	375524	14.304	16.501	50.6323



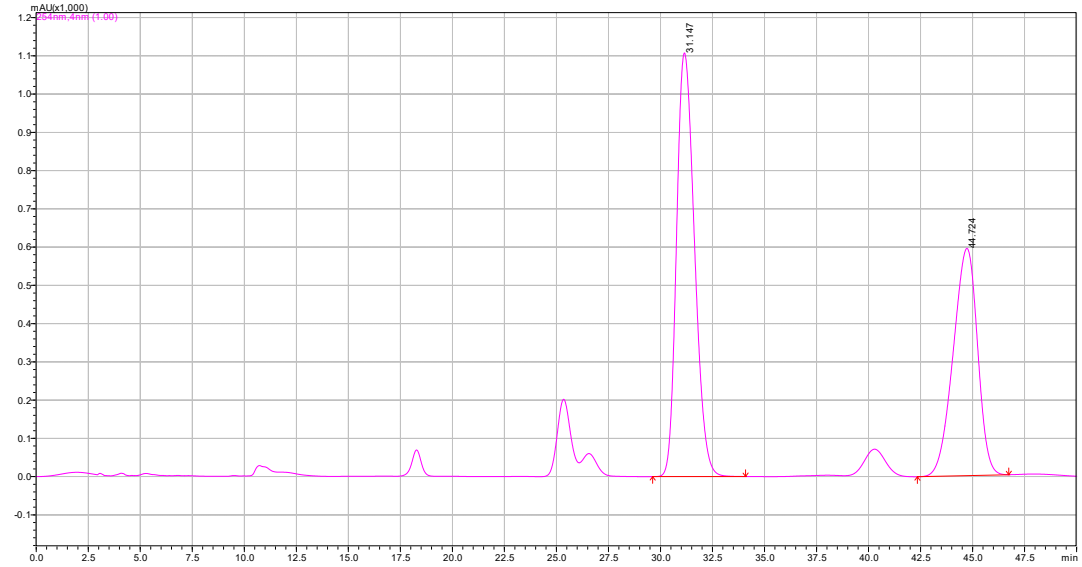
Peak	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	13.062	29825309	1109767	12.597	14.357	62.3568
2	14.958	18004750	583721	14.357	16.576	37.6432



Daicel Chiralpak AD-H, hexane/iso-propanol=90/10, flow rate 1.0 mL/min



Peak	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	31.047	57522716	938217	29.707	34.408	51.2725
2	44.701	54667421	663128	42.347	46.965	48.7275



Peak	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	31.147	66506773	1107586	29.621	34.091	57.9196
2	44.724	48319172	594027	42.347	46.741	42.0804

9. X-ray Crystallographic Data for Product 3a

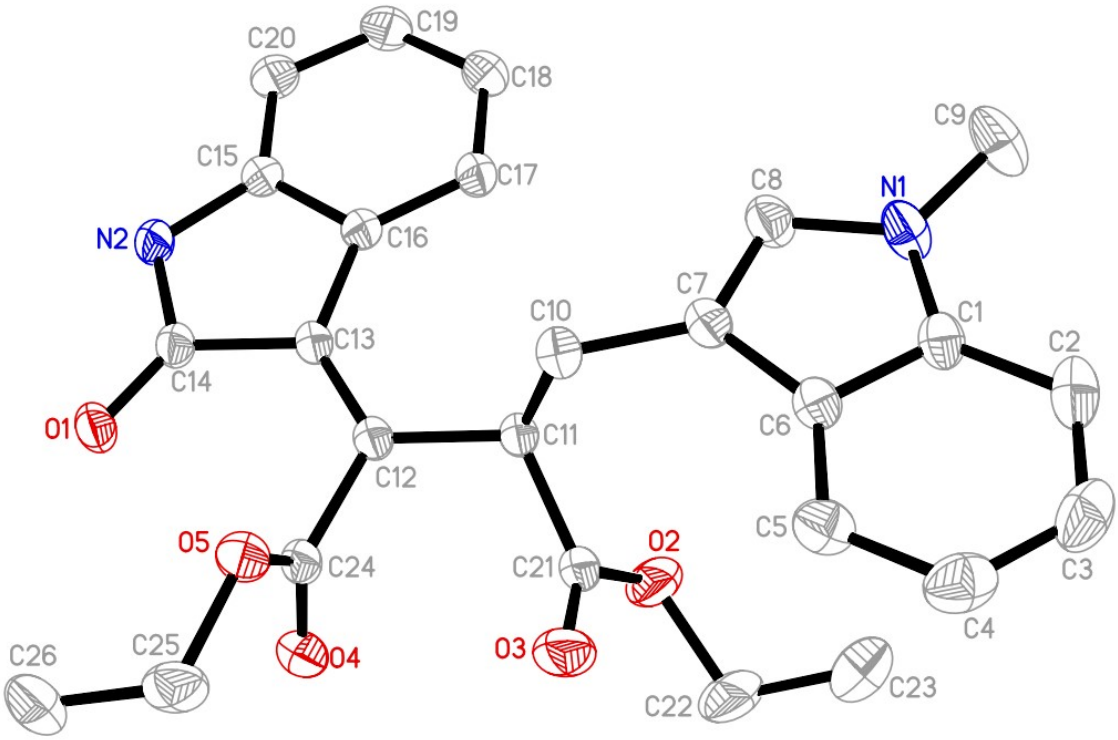


Figure 1. X-ray crystal structure of **3a**

Table 1. Crystal data and structure refinement for mo_20140522A_0m.

Identification code	mo_20140522a_0m
Empirical formula	C26 H26 N2 O5
Formula weight	446.49
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 9.084(4) A alpha = 90 deg. b = 17.370(7) A beta = 95.273(6) deg. c = 14.777(6) A gamma = 90 deg.
Volume	2321.8(16) A^3
Z, Calculated density	4, 1.277 Mg/m^3

Absorption coefficient	0.089 mm^-1
F(000)	944
Crystal size	0.36 x 0.25 x 0.20 mm
Theta range for data collection	2.54 to 25.50 deg.
Limiting indices	-9<=h<=11, -21<=k<=21, -17<=l<=17
Reflections collected / unique	13331 / 4279 [R(int) = 0.0196]
Completeness to theta = 25.50	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9824 and 0.9686
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4279 / 0 / 301
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0506, wR2 = 0.1629
R indices (all data)	R1 = 0.0661, wR2 = 0.1857
Largest diff. peak and hole	0.507 and -0.301 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for mo_20140522A_0m. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	8242(2)	10457(1)	4367(1)	49(1)
O(2)	3637(2)	9403(1)	1279(1)	76(1)
O(3)	2838(2)	10372(1)	2122(1)	66(1)
O(4)	5998(2)	10933(1)	2607(1)	51(1)
O(5)	5004(2)	10972(1)	3955(1)	48(1)
N(1)	750(2)	7458(1)	2594(1)	54(1)
N(2)	8923(2)	9189(1)	4674(1)	44(1)
C(1)	-179(2)	8062(1)	2304(1)	44(1)
C(2)	-1565(3)	8044(2)	1802(2)	61(1)
C(3)	-2263(3)	8746(2)	1623(2)	68(1)
C(4)	-1629(3)	9436(2)	1934(2)	66(1)
C(5)	-240(2)	9456(1)	2424(2)	53(1)
C(6)	514(2)	8757(1)	2616(1)	43(1)
C(7)	1908(2)	8553(1)	3103(1)	44(1)
C(8)	1983(2)	7758(1)	3077(2)	50(1)
C(9)	434(3)	6640(1)	2446(2)	72(1)
C(10)	3072(2)	9105(1)	3522(1)	47(1)
C(11)	4246(2)	9320(1)	2858(1)	38(1)
C(12)	5549(2)	9746(1)	3364(1)	37(1)
C(13)	6661(2)	9358(1)	3832(1)	37(1)
C(14)	8002(2)	9756(1)	4312(1)	39(1)
C(15)	8346(2)	8452(1)	4449(1)	40(1)
C(16)	6953(2)	8522(1)	3952(1)	37(1)
C(17)	6198(2)	7846(1)	3675(1)	44(1)
C(18)	6839(3)	7130(1)	3887(2)	53(1)
C(19)	8223(3)	7084(1)	4370(2)	55(1)
C(20)	9004(2)	7743(1)	4663(2)	51(1)
C(21)	3499(2)	9775(1)	2059(1)	47(1)
C(22)	2808(6)	9718(2)	456(2)	124(2)
C(23)	1672(6)	9209(3)	103(3)	135(2)
C(24)	5580(2)	10618(1)	3266(1)	39(1)
C(25)	4856(3)	11813(1)	3873(2)	60(1)
C(26)	6276(4)	12224(1)	4158(2)	80(1)

Table 3. Bond lengths [A] and angles [deg] for mo_20140522A_0m.

O(1)-C(14)	1.239(2)
O(2)-C(21)	1.338(3)
O(2)-C(22)	1.475(3)
O(3)-C(21)	1.206(3)
O(4)-C(24)	1.208(2)
O(5)-C(24)	1.337(2)
O(5)-C(25)	1.472(3)
N(1)-C(8)	1.375(3)
N(1)-C(1)	1.389(3)
N(1)-C(9)	1.462(3)
N(2)-C(14)	1.369(3)
N(2)-C(15)	1.411(2)
N(2)-H(2A)	0.8600
C(1)-C(2)	1.403(3)
C(1)-C(6)	1.419(3)
C(2)-C(3)	1.387(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.390(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.396(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.410(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.443(3)
C(7)-C(8)	1.383(3)
C(7)-C(10)	1.516(3)
C(8)-H(8)	0.9300
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-C(11)	1.559(3)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(21)	1.526(3)
C(11)-C(12)	1.531(2)
C(11)-H(11)	0.9800
C(12)-C(13)	1.351(3)
C(12)-C(24)	1.523(3)
C(13)-C(16)	1.483(3)
C(13)-C(14)	1.519(2)
C(15)-C(20)	1.393(3)
C(15)-C(16)	1.408(3)
C(16)-C(17)	1.402(3)
C(17)-C(18)	1.396(3)
C(17)-H(17)	0.9300
C(18)-C(19)	1.390(3)
C(18)-H(18)	0.9300
C(19)-C(20)	1.394(3)
C(19)-H(19)	0.9300

C(20)-H(20)	0.9300
C(22)-C(23)	1.421(5)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(25)-C(26)	1.500(4)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600

C(21)-O(2)-C(22)	116.7(3)
C(24)-O(5)-C(25)	115.61(16)
C(8)-N(1)-C(1)	108.39(17)
C(8)-N(1)-C(9)	125.9(2)
C(1)-N(1)-C(9)	125.6(2)
C(14)-N(2)-C(15)	111.15(15)
C(14)-N(2)-H(2A)	124.4
C(15)-N(2)-H(2A)	124.4
N(1)-C(1)-C(2)	129.6(2)
N(1)-C(1)-C(6)	107.75(17)
C(2)-C(1)-C(6)	122.7(2)
C(3)-C(2)-C(1)	117.0(2)
C(3)-C(2)-H(2)	121.5
C(1)-C(2)-H(2)	121.5
C(2)-C(3)-C(4)	121.8(2)
C(2)-C(3)-H(3)	119.1
C(4)-C(3)-H(3)	119.1
C(3)-C(4)-C(5)	121.4(2)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
C(4)-C(5)-C(6)	118.8(2)
C(4)-C(5)-H(5)	120.6
C(6)-C(5)-H(5)	120.6
C(5)-C(6)-C(1)	118.39(19)
C(5)-C(6)-C(7)	134.41(19)
C(1)-C(6)-C(7)	107.18(17)
C(8)-C(7)-C(6)	105.94(17)
C(8)-C(7)-C(10)	127.45(19)
C(6)-C(7)-C(10)	126.57(18)
N(1)-C(8)-C(7)	110.72(19)
N(1)-C(8)-H(8)	124.6
C(7)-C(8)-H(8)	124.6
N(1)-C(9)-H(9A)	109.5
N(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
N(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-C(11)	112.70(17)

C(7)-C(10)-H(10A)	109.1
C(11)-C(10)-H(10A)	109.1
C(7)-C(10)-H(10B)	109.1
C(11)-C(10)-H(10B)	109.1
H(10A)-C(10)-H(10B)	107.8
C(21)-C(11)-C(12)	113.40(15)
C(21)-C(11)-C(10)	109.25(16)
C(12)-C(11)-C(10)	110.54(15)
C(21)-C(11)-H(11)	107.8
C(12)-C(11)-H(11)	107.8
C(10)-C(11)-H(11)	107.8
C(13)-C(12)-C(24)	121.70(16)
C(13)-C(12)-C(11)	121.21(17)
C(24)-C(12)-C(11)	116.98(15)
C(12)-C(13)-C(16)	131.77(16)
C(12)-C(13)-C(14)	122.83(17)
C(16)-C(13)-C(14)	105.26(15)
O(1)-C(14)-N(2)	125.78(17)
O(1)-C(14)-C(13)	127.40(17)
N(2)-C(14)-C(13)	106.81(16)
C(20)-C(15)-C(16)	122.73(18)
C(20)-C(15)-N(2)	127.35(18)
C(16)-C(15)-N(2)	109.92(15)
C(17)-C(16)-C(15)	118.16(16)
C(17)-C(16)-C(13)	135.04(17)
C(15)-C(16)-C(13)	106.79(15)
C(18)-C(17)-C(16)	119.85(18)
C(18)-C(17)-H(17)	120.1
C(16)-C(17)-H(17)	120.1
C(19)-C(18)-C(17)	120.37(19)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(20)	121.50(19)
C(18)-C(19)-H(19)	119.2
C(20)-C(19)-H(19)	119.2
C(15)-C(20)-C(19)	117.39(19)
C(15)-C(20)-H(20)	121.3
C(19)-C(20)-H(20)	121.3
O(3)-C(21)-O(2)	124.6(2)
O(3)-C(21)-C(11)	125.1(2)
O(2)-C(21)-C(11)	110.29(18)
C(23)-C(22)-O(2)	111.8(3)
C(23)-C(22)-H(22A)	109.3
O(2)-C(22)-H(22A)	109.3
C(23)-C(22)-H(22B)	109.3
O(2)-C(22)-H(22B)	109.3
H(22A)-C(22)-H(22B)	107.9
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

O(4)-C(24)-O(5)	125.52(18)
O(4)-C(24)-C(12)	122.49(17)
O(5)-C(24)-C(12)	111.84(16)
O(5)-C(25)-C(26)	112.3(2)
O(5)-C(25)-H(25A)	109.1
C(26)-C(25)-H(25A)	109.1
O(5)-C(25)-H(25B)	109.1
C(26)-C(25)-H(25B)	109.1
H(25A)-C(25)-H(25B)	107.9
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for mo_20140522A_0m. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	43(1)	35(1)	66(1)	-3(1)	-12(1)	-5(1)
O(2)	113(2)	61(1)	47(1)	3(1)	-28(1)	2(1)
O(3)	58(1)	49(1)	89(1)	19(1)	-5(1)	8(1)
O(4)	55(1)	41(1)	56(1)	6(1)	5(1)	-5(1)
O(5)	51(1)	39(1)	53(1)	0(1)	2(1)	5(1)
N(1)	44(1)	39(1)	78(1)	-8(1)	8(1)	-7(1)
N(2)	38(1)	40(1)	51(1)	1(1)	-12(1)	-2(1)
C(1)	36(1)	50(1)	48(1)	-6(1)	7(1)	-6(1)
C(2)	44(1)	80(2)	59(1)	-16(1)	4(1)	-15(1)
C(3)	38(1)	102(2)	62(2)	4(1)	-2(1)	5(1)
C(4)	53(1)	74(2)	74(2)	18(1)	14(1)	18(1)
C(5)	51(1)	48(1)	63(1)	5(1)	13(1)	3(1)
C(6)	40(1)	43(1)	45(1)	-1(1)	6(1)	-4(1)
C(7)	42(1)	41(1)	50(1)	2(1)	3(1)	-6(1)
C(8)	39(1)	41(1)	70(1)	4(1)	2(1)	-3(1)
C(9)	66(2)	41(1)	111(2)	-16(1)	22(2)	-14(1)
C(10)	44(1)	46(1)	50(1)	1(1)	-2(1)	-9(1)
C(11)	36(1)	32(1)	45(1)	1(1)	-7(1)	-4(1)
C(12)	35(1)	33(1)	41(1)	-1(1)	-1(1)	-4(1)
C(13)	37(1)	33(1)	39(1)	-1(1)	-3(1)	-5(1)
C(14)	35(1)	38(1)	43(1)	-2(1)	-5(1)	-3(1)
C(15)	41(1)	38(1)	40(1)	2(1)	-2(1)	-1(1)
C(16)	38(1)	35(1)	37(1)	1(1)	0(1)	0(1)
C(17)	48(1)	37(1)	47(1)	-2(1)	-5(1)	-4(1)
C(18)	65(1)	34(1)	57(1)	-1(1)	-1(1)	-3(1)
C(19)	64(1)	37(1)	63(1)	5(1)	0(1)	10(1)
C(20)	48(1)	46(1)	56(1)	7(1)	-4(1)	7(1)
C(21)	39(1)	39(1)	59(1)	9(1)	-10(1)	-10(1)
C(22)	199(4)	86(2)	71(2)	23(2)	-75(2)	-17(3)
C(23)	147(4)	133(3)	110(3)	41(3)	-70(3)	-33(3)
C(24)	32(1)	35(1)	50(1)	1(1)	-6(1)	-2(1)
C(25)	77(2)	43(1)	61(1)	2(1)	4(1)	21(1)
C(26)	116(2)	41(1)	81(2)	-4(1)	-1(2)	-12(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for mo_20140522A_0m.

	x	y	z	U(eq)
H(2A)	9745	9271	4996	53
H(2)	-1997	7583	1597	73
H(3)	-3179	8754	1286	82
H(4)	-2141	9894	1814	80
H(5)	181	9923	2620	64
H(8)	2761	7467	3350	60
H(9A)	1231	6339	2732	108
H(9B)	329	6534	1805	108
H(9C)	-467	6509	2702	108
H(10A)	3568	8872	4063	57
H(10B)	2591	9571	3705	57
H(11)	4624	8840	2618	46
H(17)	5273	7874	3350	53
H(18)	6337	6682	3704	63
H(19)	8637	6603	4501	66
H(20)	9928	7710	4988	61
H(22A)	2373	10207	602	148
H(22B)	3484	9810	-3	148
H(23A)	2107	8748	-113	202
H(23B)	1089	9455	-390	202
H(23C)	1052	9080	573	202
H(25A)	4099	11988	4248	72
H(25B)	4540	11944	3247	72
H(26A)	6618	12078	4768	120
H(26B)	6114	12770	4131	120
H(26C)	7006	12086	3756	120

Table 6. Torsion angles [deg] for mo_20140522A_0m.

C(8)-N(1)-C(1)-C(2)	-179.2(2)
C(9)-N(1)-C(1)-C(2)	-1.8(4)
C(8)-N(1)-C(1)-C(6)	0.4(2)
C(9)-N(1)-C(1)-C(6)	177.7(2)
N(1)-C(1)-C(2)-C(3)	178.8(2)
C(6)-C(1)-C(2)-C(3)	-0.7(3)
C(1)-C(2)-C(3)-C(4)	-0.7(4)
C(2)-C(3)-C(4)-C(5)	1.6(4)
C(3)-C(4)-C(5)-C(6)	-1.1(3)
C(4)-C(5)-C(6)-C(1)	-0.2(3)
C(4)-C(5)-C(6)-C(7)	-178.6(2)
N(1)-C(1)-C(6)-C(5)	-178.42(17)
C(2)-C(1)-C(6)-C(5)	1.2(3)
N(1)-C(1)-C(6)-C(7)	0.3(2)
C(2)-C(1)-C(6)-C(7)	179.94(19)
C(5)-C(6)-C(7)-C(8)	177.5(2)
C(1)-C(6)-C(7)-C(8)	-0.9(2)
C(5)-C(6)-C(7)-C(10)	-4.7(4)
C(1)-C(6)-C(7)-C(10)	176.88(19)
C(1)-N(1)-C(8)-C(7)	-1.0(2)
C(9)-N(1)-C(8)-C(7)	-178.4(2)
C(6)-C(7)-C(8)-N(1)	1.2(2)
C(10)-C(7)-C(8)-N(1)	-176.57(19)
C(8)-C(7)-C(10)-C(11)	86.0(3)
C(6)-C(7)-C(10)-C(11)	-91.3(2)
C(7)-C(10)-C(11)-C(21)	65.6(2)
C(7)-C(10)-C(11)-C(12)	-168.95(16)
C(21)-C(11)-C(12)-C(13)	-154.18(19)
C(10)-C(11)-C(12)-C(13)	82.7(2)
C(21)-C(11)-C(12)-C(24)	22.1(2)
C(10)-C(11)-C(12)-C(24)	-101.01(19)
C(24)-C(12)-C(13)-C(16)	-173.50(18)
C(11)-C(12)-C(13)-C(16)	2.6(3)
C(24)-C(12)-C(13)-C(14)	1.5(3)
C(11)-C(12)-C(13)-C(14)	177.52(16)
C(15)-N(2)-C(14)-O(1)	-177.16(19)
C(15)-N(2)-C(14)-C(13)	2.3(2)
C(12)-C(13)-C(14)-O(1)	2.3(3)
C(16)-C(13)-C(14)-O(1)	178.39(19)
C(12)-C(13)-C(14)-N(2)	-177.17(18)
C(16)-C(13)-C(14)-N(2)	-1.06(19)
C(14)-N(2)-C(15)-C(20)	176.98(19)
C(14)-N(2)-C(15)-C(16)	-2.8(2)
C(20)-C(15)-C(16)-C(17)	0.9(3)
N(2)-C(15)-C(16)-C(17)	-179.39(16)
C(20)-C(15)-C(16)-C(13)	-177.82(18)
N(2)-C(15)-C(16)-C(13)	1.9(2)
C(12)-C(13)-C(16)-C(17)	-3.3(4)
C(14)-C(13)-C(16)-C(17)	-178.9(2)

C(12)-C(13)-C(16)-C(15)	175.1(2)
C(14)-C(13)-C(16)-C(15)	-0.53(19)
C(15)-C(16)-C(17)-C(18)	-0.6(3)
C(13)-C(16)-C(17)-C(18)	177.7(2)
C(16)-C(17)-C(18)-C(19)	-0.1(3)
C(17)-C(18)-C(19)-C(20)	0.5(4)
C(16)-C(15)-C(20)-C(19)	-0.5(3)
N(2)-C(15)-C(20)-C(19)	179.8(2)
C(18)-C(19)-C(20)-C(15)	-0.2(3)
C(22)-O(2)-C(21)-O(3)	-5.5(4)
C(22)-O(2)-C(21)-C(11)	172.3(3)
C(12)-C(11)-C(21)-O(3)	-65.4(3)
C(10)-C(11)-C(21)-O(3)	58.4(2)
C(12)-C(11)-C(21)-O(2)	116.74(19)
C(10)-C(11)-C(21)-O(2)	-119.48(19)
C(21)-O(2)-C(22)-C(23)	-113.3(4)
C(25)-O(5)-C(24)-O(4)	1.3(3)
C(25)-O(5)-C(24)-C(12)	-174.35(16)
C(13)-C(12)-C(24)-O(4)	96.4(2)
C(11)-C(12)-C(24)-O(4)	-79.8(2)
C(13)-C(12)-C(24)-O(5)	-87.8(2)
C(11)-C(12)-C(24)-O(5)	95.98(19)
C(24)-O(5)-C(25)-C(26)	-81.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_20140522A_0m [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(1)#1	0.86	2.03	2.889(2)	173.2

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+1

9. X-ray Crystallographic Data for Product 6

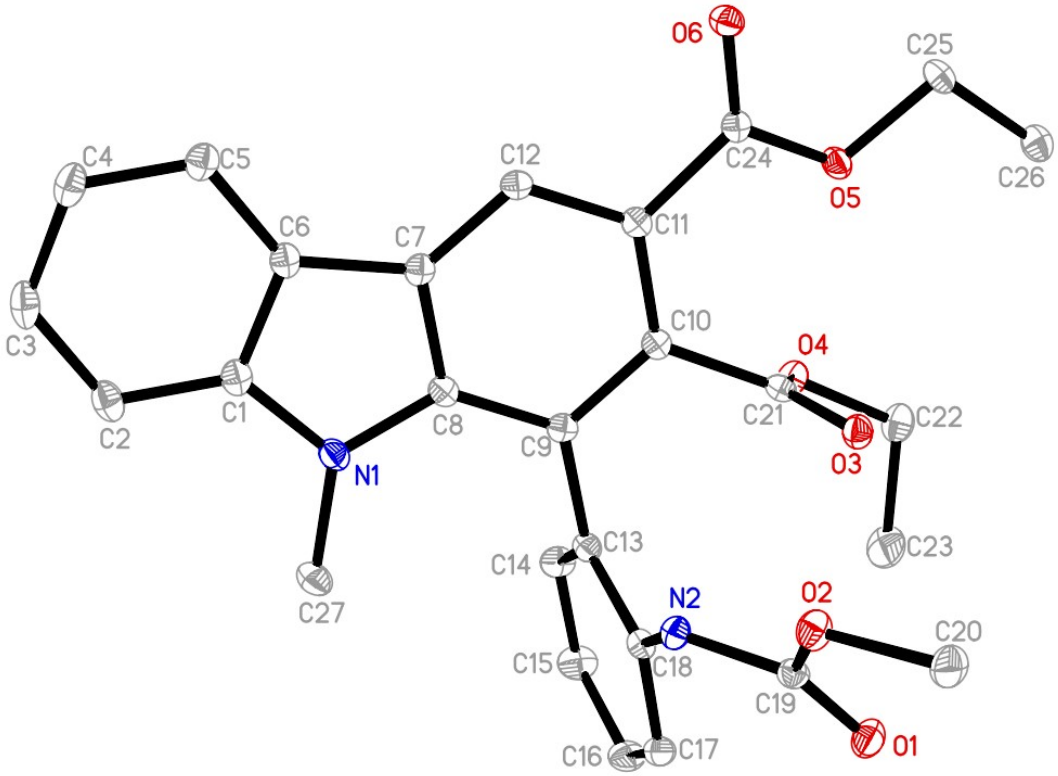


Figure 2. X-ray crystal structure of **6**

Table 2. Crystal data and structure refinement for mo_20170104a_0m.

Identification code	mo_20170104a_0m
Empirical formula	C27 H26 N2 O6
Formula weight	474.50
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 9.3272(8) A alpha = 90 deg. b = 13.2464(12) A beta = 95.3720(10) deg. c = 18.7695(16) A gamma = 90 deg.
Volume	2308.8(3) A^3

Z, Calculated density	4, 1.365 Mg/m^3
Absorption coefficient	0.097 mm^-1
F(000)	1000
Crystal size	0.34 x 0.25 x 0.21 mm
Theta range for data collection	1.88 to 26.00 deg.
Limiting indices	-11<=h<=11, -14<=k<=16, -23<=l<=21
Reflections collected / unique	16032 / 4528 [R(int) = 0.0223]
Completeness to theta = 26.00	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9799 and 0.9677
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4528 / 0 / 320
Goodness-of-fit on F^2	1.073
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.1019
R indices (all data)	R1 = 0.0423, wR2 = 0.1066
Largest diff. peak and hole	0.337 and -0.366 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for mo_20170104A_0m. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	1834(1)	5787(1)	10478(1)	27(1)
O(2)	-234(1)	6652(1)	10197(1)	23(1)
O(3)	2265(1)	8156(1)	11048(1)	21(1)
O(4)	4396(1)	8955(1)	11023(1)	22(1)
O(5)	2165(1)	10316(1)	11449(1)	21(1)
O(6)	604(1)	11450(1)	10941(1)	21(1)
N(1)	2531(1)	9372(1)	8153(1)	21(1)
N(2)	1670(1)	7051(1)	9638(1)	18(1)
C(1)	1858(1)	10148(1)	7745(1)	21(1)
C(2)	1741(2)	10281(1)	7006(1)	26(1)
C(3)	990(2)	11117(1)	6734(1)	28(1)
C(4)	361(2)	11802(1)	7180(1)	27(1)
C(5)	482(1)	11673(1)	7913(1)	23(1)
C(6)	1254(1)	10841(1)	8201(1)	19(1)
C(7)	1611(1)	10479(1)	8921(1)	18(1)
C(8)	2400(1)	9570(1)	8869(1)	18(1)
C(9)	2893(1)	9020(1)	9485(1)	18(1)
C(10)	2554(1)	9400(1)	10143(1)	17(1)
C(11)	1772(1)	10309(1)	10197(1)	17(1)
C(12)	1306(1)	10842(1)	9581(1)	17(1)
C(13)	3761(1)	8074(1)	9450(1)	19(1)
C(14)	5212(2)	8140(1)	9334(1)	25(1)
C(15)	6053(2)	7281(1)	9296(1)	29(1)
C(16)	5433(2)	6336(1)	9370(1)	27(1)
C(17)	3992(1)	6256(1)	9485(1)	22(1)
C(18)	3149(1)	7121(1)	9532(1)	18(1)
C(19)	1169(1)	6438(1)	10142(1)	19(1)
C(20)	-900(2)	6074(1)	10723(1)	27(1)
C(21)	3021(1)	8769(1)	10792(1)	18(1)
C(22)	4997(2)	8335(1)	11616(1)	28(1)
C(23)	5550(2)	7359(1)	11348(1)	42(1)
C(24)	1427(1)	10752(1)	10886(1)	17(1)
C(25)	1920(2)	10696(1)	12154(1)	23(1)
C(26)	2753(2)	10024(1)	12688(1)	28(1)
C(27)	3187(2)	8507(1)	7832(1)	29(1)

Table 3. Bond lengths [A] and angles [deg] for mo_20170104A_0m.

O(1)-C(19)	1.2055(16)
O(2)-C(19)	1.3516(16)
O(2)-C(20)	1.4366(17)
O(3)-C(21)	1.2050(16)
O(4)-C(21)	1.3374(15)
O(4)-C(22)	1.4529(16)
O(5)-C(24)	1.3371(15)
O(5)-C(25)	1.4538(16)
O(6)-C(24)	1.2121(16)
N(1)-C(8)	1.3840(17)
N(1)-C(1)	1.3953(17)
N(1)-C(27)	1.4566(18)
N(2)-C(19)	1.3629(17)
N(2)-C(18)	1.4149(16)
N(2)-H(2A)	0.8600
C(1)-C(2)	1.3925(19)
C(1)-C(6)	1.4088(19)
C(2)-C(3)	1.382(2)
C(2)-H(2)	0.9300
C(3)-C(4)	1.400(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.381(2)
C(4)-H(4)	0.9300
C(5)-C(6)	1.3970(19)
C(5)-H(5)	0.9300
C(6)-C(7)	1.4437(18)
C(7)-C(12)	1.3828(18)
C(7)-C(8)	1.4194(18)
C(8)-C(9)	1.4075(18)
C(9)-C(10)	1.3977(18)
C(9)-C(13)	1.4967(17)
C(10)-C(11)	1.4169(18)
C(10)-C(21)	1.5068(18)
C(11)-C(12)	1.3883(18)
C(11)-C(24)	1.4832(18)
C(12)-H(12)	0.9300
C(13)-C(14)	1.3936(19)
C(13)-C(18)	1.4001(18)
C(14)-C(15)	1.388(2)
C(14)-H(14)	0.9300
C(15)-C(16)	1.391(2)
C(15)-H(15)	0.9300
C(16)-C(17)	1.385(2)
C(16)-H(16)	0.9300
C(17)-C(18)	1.3968(18)
C(17)-H(17)	0.9300
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600

C(22)-C(23)	1.496(2)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(25)-C(26)	1.5012(19)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600

C(19)-O(2)-C(20)	115.12(10)
C(21)-O(4)-C(22)	115.71(10)
C(24)-O(5)-C(25)	117.16(10)
C(8)-N(1)-C(1)	108.51(11)
C(8)-N(1)-C(27)	128.97(11)
C(1)-N(1)-C(27)	122.47(11)
C(19)-N(2)-C(18)	122.58(11)
C(19)-N(2)-H(2A)	118.7
C(18)-N(2)-H(2A)	118.7
C(2)-C(1)-N(1)	129.04(13)
C(2)-C(1)-C(6)	121.63(13)
N(1)-C(1)-C(6)	109.33(11)
C(3)-C(2)-C(1)	117.29(14)
C(3)-C(2)-H(2)	121.4
C(1)-C(2)-H(2)	121.4
C(2)-C(3)-C(4)	121.69(13)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(5)-C(4)-C(3)	121.04(13)
C(5)-C(4)-H(4)	119.5
C(3)-C(4)-H(4)	119.5
C(4)-C(5)-C(6)	118.30(13)
C(4)-C(5)-H(5)	120.8
C(6)-C(5)-H(5)	120.8
C(5)-C(6)-C(1)	120.02(12)
C(5)-C(6)-C(7)	133.60(13)
C(1)-C(6)-C(7)	106.38(12)
C(12)-C(7)-C(8)	120.58(12)
C(12)-C(7)-C(6)	132.42(12)
C(8)-C(7)-C(6)	106.99(11)
N(1)-C(8)-C(9)	130.33(12)
N(1)-C(8)-C(7)	108.76(11)
C(9)-C(8)-C(7)	120.90(12)
C(10)-C(9)-C(8)	117.18(11)
C(10)-C(9)-C(13)	120.55(11)
C(8)-C(9)-C(13)	122.27(11)
C(9)-C(10)-C(11)	121.96(12)

C(9)-C(10)-C(21)	116.27(11)
C(11)-C(10)-C(21)	121.74(11)
C(12)-C(11)-C(10)	119.74(12)
C(12)-C(11)-C(24)	116.64(11)
C(10)-C(11)-C(24)	123.60(11)
C(7)-C(12)-C(11)	119.62(12)
C(7)-C(12)-H(12)	120.2
C(11)-C(12)-H(12)	120.2
C(14)-C(13)-C(18)	119.06(12)
C(14)-C(13)-C(9)	119.43(11)
C(18)-C(13)-C(9)	121.51(11)
C(15)-C(14)-C(13)	121.24(13)
C(15)-C(14)-H(14)	119.4
C(13)-C(14)-H(14)	119.4
C(14)-C(15)-C(16)	119.36(13)
C(14)-C(15)-H(15)	120.3
C(16)-C(15)-H(15)	120.3
C(17)-C(16)-C(15)	120.19(13)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.49(12)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-C(13)	119.66(12)
C(17)-C(18)-N(2)	121.20(12)
C(13)-C(18)-N(2)	119.11(11)
O(1)-C(19)-O(2)	124.39(12)
O(1)-C(19)-N(2)	126.61(12)
O(2)-C(19)-N(2)	108.97(11)
O(2)-C(20)-H(20A)	109.5
O(2)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
O(2)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(3)-C(21)-O(4)	125.01(12)
O(3)-C(21)-C(10)	124.05(11)
O(4)-C(21)-C(10)	110.89(10)
O(4)-C(22)-C(23)	110.55(12)
O(4)-C(22)-H(22A)	109.5
C(23)-C(22)-H(22A)	109.5
O(4)-C(22)-H(22B)	109.5
C(23)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	108.1
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
O(6)-C(24)-O(5)	123.09(12)
O(6)-C(24)-C(11)	124.48(12)
O(5)-C(24)-C(11)	112.40(11)

O(5)-C(25)-C(26)	106.61(11)
O(5)-C(25)-H(25A)	110.4
C(26)-C(25)-H(25A)	110.4
O(5)-C(25)-H(25B)	110.4
C(26)-C(25)-H(25B)	110.4
H(25A)-C(25)-H(25B)	108.6
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(1)-C(27)-H(27A)	109.5
N(1)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
N(1)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for mo_20170104A_0m. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	29(1)	25(1)	27(1)	7(1)	7(1)	5(1)
O(2)	18(1)	26(1)	26(1)	4(1)	6(1)	-2(1)
O(3)	23(1)	22(1)	19(1)	1(1)	2(1)	-4(1)
O(4)	17(1)	25(1)	24(1)	4(1)	-1(1)	0(1)
O(5)	23(1)	24(1)	15(1)	-2(1)	0(1)	4(1)
O(6)	21(1)	22(1)	21(1)	-3(1)	2(1)	3(1)
N(1)	23(1)	22(1)	18(1)	-2(1)	5(1)	-1(1)
N(2)	16(1)	19(1)	18(1)	2(1)	0(1)	-1(1)
C(1)	20(1)	24(1)	20(1)	1(1)	2(1)	-6(1)
C(2)	26(1)	33(1)	19(1)	-1(1)	4(1)	-8(1)
C(3)	27(1)	39(1)	18(1)	6(1)	0(1)	-9(1)
C(4)	26(1)	28(1)	25(1)	9(1)	-2(1)	-5(1)
C(5)	22(1)	22(1)	23(1)	2(1)	0(1)	-4(1)
C(6)	18(1)	21(1)	19(1)	1(1)	1(1)	-6(1)
C(7)	16(1)	19(1)	19(1)	1(1)	1(1)	-4(1)
C(8)	16(1)	19(1)	19(1)	-2(1)	4(1)	-5(1)
C(9)	15(1)	18(1)	21(1)	-1(1)	3(1)	-3(1)
C(10)	13(1)	18(1)	19(1)	-1(1)	2(1)	-4(1)
C(11)	14(1)	19(1)	18(1)	-1(1)	2(1)	-3(1)
C(12)	15(1)	16(1)	21(1)	-1(1)	2(1)	-2(1)
C(13)	19(1)	20(1)	17(1)	-1(1)	2(1)	1(1)
C(14)	21(1)	23(1)	30(1)	-2(1)	7(1)	-3(1)
C(15)	19(1)	30(1)	40(1)	-3(1)	10(1)	1(1)
C(16)	26(1)	24(1)	33(1)	-3(1)	6(1)	7(1)
C(17)	25(1)	19(1)	23(1)	-1(1)	4(1)	0(1)
C(18)	18(1)	21(1)	16(1)	-1(1)	2(1)	0(1)
C(19)	20(1)	18(1)	19(1)	-3(1)	2(1)	-2(1)
C(20)	28(1)	26(1)	30(1)	3(1)	12(1)	-4(1)
C(21)	17(1)	18(1)	18(1)	-4(1)	3(1)	1(1)
C(22)	22(1)	34(1)	26(1)	6(1)	-5(1)	2(1)
C(23)	46(1)	43(1)	38(1)	10(1)	2(1)	23(1)
C(24)	15(1)	18(1)	18(1)	0(1)	1(1)	-4(1)
C(25)	24(1)	27(1)	17(1)	-6(1)	2(1)	-1(1)
C(26)	35(1)	30(1)	19(1)	-2(1)	1(1)	-1(1)
C(27)	36(1)	28(1)	24(1)	-6(1)	9(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for mo_20170104A_0m.

	x	y	z	U(eq)
H(2A)	1064	7411	9374	22
H(2)	2151	9825	6707	31
H(3)	901	11228	6243	34
H(4)	-146	12353	6979	32
H(5)	60	12128	8208	27
H(12)	792	11439	9613	21
H(14)	5624	8772	9281	29
H(15)	7022	7337	9222	35
H(16)	5988	5757	9341	32
H(17)	3583	5622	9531	27
H(20A)	-802	5367	10625	41
H(20B)	-1904	6244	10705	41
H(20C)	-442	6223	11190	41
H(22A)	4260	8199	11936	33
H(22B)	5776	8696	11884	33
H(23A)	4756	6956	11148	63
H(23B)	6063	7001	11737	63
H(23C)	6187	7494	10986	63
H(25A)	902	10676	12222	27
H(25B)	2252	11388	12209	27
H(26A)	2428	9340	12620	42
H(26B)	2605	10240	13163	42
H(26C)	3760	10063	12621	42
H(27A)	4207	8612	7840	43
H(27B)	2780	8429	7346	43
H(27C)	3007	7909	8099	43

Table 6. Torsion angles [deg] for mo_20170104A_0m.

C(8)-N(1)-C(1)-C(2)	178.63(13)
C(27)-N(1)-C(1)-C(2)	-3.5(2)
C(8)-N(1)-C(1)-C(6)	-1.48(14)
C(27)-N(1)-C(1)-C(6)	176.39(12)
N(1)-C(1)-C(2)-C(3)	179.10(13)
C(6)-C(1)-C(2)-C(3)	-0.78(19)
C(1)-C(2)-C(3)-C(4)	-0.5(2)
C(2)-C(3)-C(4)-C(5)	0.8(2)
C(3)-C(4)-C(5)-C(6)	0.2(2)
C(4)-C(5)-C(6)-C(1)	-1.43(18)
C(4)-C(5)-C(6)-C(7)	179.12(13)
C(2)-C(1)-C(6)-C(5)	1.75(19)
N(1)-C(1)-C(6)-C(5)	-178.15(11)
C(2)-C(1)-C(6)-C(7)	-178.66(12)
N(1)-C(1)-C(6)-C(7)	1.44(14)
C(5)-C(6)-C(7)-C(12)	-0.2(2)
C(1)-C(6)-C(7)-C(12)	-179.69(13)
C(5)-C(6)-C(7)-C(8)	178.64(14)
C(1)-C(6)-C(7)-C(8)	-0.87(13)
C(1)-N(1)-C(8)-C(9)	179.91(12)
C(27)-N(1)-C(8)-C(9)	2.2(2)
C(1)-N(1)-C(8)-C(7)	0.91(14)
C(27)-N(1)-C(8)-C(7)	-176.78(12)
C(12)-C(7)-C(8)-N(1)	178.98(11)
C(6)-C(7)-C(8)-N(1)	-0.02(14)
C(12)-C(7)-C(8)-C(9)	-0.13(18)
C(6)-C(7)-C(8)-C(9)	-179.13(11)
N(1)-C(8)-C(9)-C(10)	-178.05(12)
C(7)-C(8)-C(9)-C(10)	0.85(17)
N(1)-C(8)-C(9)-C(13)	2.7(2)
C(7)-C(8)-C(9)-C(13)	-178.36(11)
C(8)-C(9)-C(10)-C(11)	-1.18(18)
C(13)-C(9)-C(10)-C(11)	178.04(11)
C(8)-C(9)-C(10)-C(21)	176.79(11)
C(13)-C(9)-C(10)-C(21)	-4.00(17)
C(9)-C(10)-C(11)-C(12)	0.79(18)
C(21)-C(10)-C(11)-C(12)	-177.06(11)
C(9)-C(10)-C(11)-C(24)	-178.18(11)
C(21)-C(10)-C(11)-C(24)	3.97(18)
C(8)-C(7)-C(12)-C(11)	-0.29(18)
C(6)-C(7)-C(12)-C(11)	178.40(12)
C(10)-C(11)-C(12)-C(7)	-0.02(18)
C(24)-C(11)-C(12)-C(7)	179.01(11)
C(10)-C(9)-C(13)-C(14)	-103.00(15)
C(8)-C(9)-C(13)-C(14)	76.17(16)
C(10)-C(9)-C(13)-C(18)	76.83(16)
C(8)-C(9)-C(13)-C(18)	-103.99(15)
C(18)-C(13)-C(14)-C(15)	0.3(2)
C(9)-C(13)-C(14)-C(15)	-179.83(13)

C(13)-C(14)-C(15)-C(16)	0.5(2)
C(14)-C(15)-C(16)-C(17)	-0.5(2)
C(15)-C(16)-C(17)-C(18)	-0.4(2)
C(16)-C(17)-C(18)-C(13)	1.2(2)
C(16)-C(17)-C(18)-N(2)	178.95(12)
C(14)-C(13)-C(18)-C(17)	-1.16(19)
C(9)-C(13)-C(18)-C(17)	179.00(12)
C(14)-C(13)-C(18)-N(2)	-178.96(12)
C(9)-C(13)-C(18)-N(2)	1.20(18)
C(19)-N(2)-C(18)-C(17)	47.00(18)
C(19)-N(2)-C(18)-C(13)	-135.24(13)
C(20)-O(2)-C(19)-O(1)	3.02(19)
C(20)-O(2)-C(19)-N(2)	-178.71(11)
C(18)-N(2)-C(19)-O(1)	-11.6(2)
C(18)-N(2)-C(19)-O(2)	170.14(11)
C(22)-O(4)-C(21)-O(3)	1.79(19)
C(22)-O(4)-C(21)-C(10)	-175.69(11)
C(9)-C(10)-C(21)-O(3)	-93.96(15)
C(11)-C(10)-C(21)-O(3)	84.00(16)
C(9)-C(10)-C(21)-O(4)	83.55(13)
C(11)-C(10)-C(21)-O(4)	-98.48(13)
C(21)-O(4)-C(22)-C(23)	85.27(15)
C(25)-O(5)-C(24)-O(6)	1.51(18)
C(25)-O(5)-C(24)-C(11)	179.56(10)
C(12)-C(11)-C(24)-O(6)	11.29(18)
C(10)-C(11)-C(24)-O(6)	-169.71(12)
C(12)-C(11)-C(24)-O(5)	-166.72(10)
C(10)-C(11)-C(24)-O(5)	12.27(17)
C(24)-O(5)-C(25)-C(26)	174.71(11)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_20170104A_0m [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(6)#1	0.86	2.21	3.0311(14)	160.3

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+2,-z+2