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SUPPORTING INFROMATION

Palladium-Catalyzed Dearomative Aryl/Cycloimidoylation of Indoles

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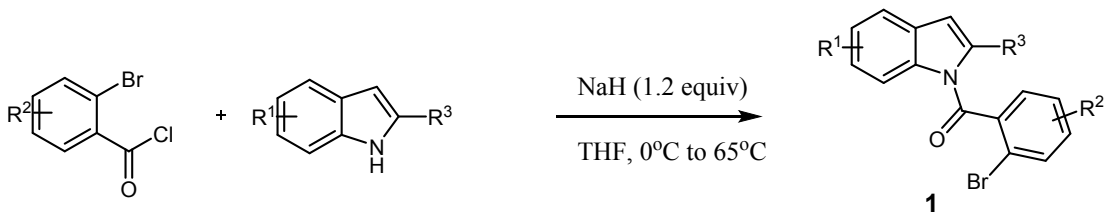
Contents

I. General Information

^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) were registered on 400 M spectrometers. Chemical shifts were reported in units (ppm) by assigning $CDCl_3$ resonance in the ^{1}H spectrum as 7.26 ppm, $CDCl_3$ resonance in the ^{13}C spectrum as 77.16 ppm, DMSO - D_6 resonance in the ^{1}H spectrum as 2.5 ppm, DMSO - D_6 resonance in the ^{13}C spectrum as 39.52 ppm. All coupling constants (J values) were reported in Hertz (Hz). NMR analysis was carried out at 298 K unless noted otherwise. HRMS was obtained on an ESI-LC-MS/MS spectrometer.

II. Preparation of Starting Materials

The staring materials N-(2-bromobenzoyl)indoles were synthesized following the procedure of jia[1] and Lautens[2], diethyl 2-allyl-2-isocyanomalonate were synthesized following the procedure of Dietrich[3], ethyl 2-isocyano-3,3-diphenylacrylate were synthesized following the procedure of Xu[4],and the data was in accordance with that of the reported literature.



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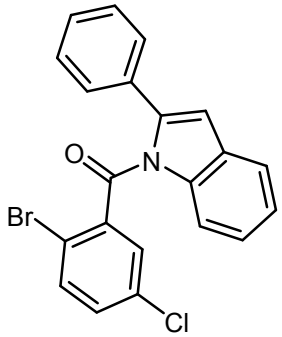
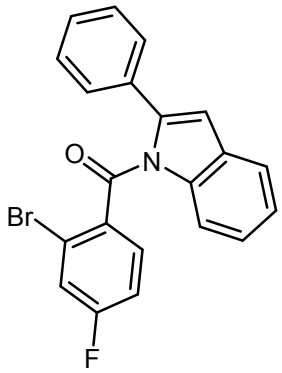
General procedure: A 60% dispersion of NaH in mineral oil (1.2 equiv) was added to a stirred solution of the appropriate indole derivative (1 equiv, ~0.5 M) in THF at 0 °C and the corresponding solution was stirred for 5 minutes before warming to room temperature where it was stirred for 30 minutes. The solution of the sodium indolate was re-cooled to 0 °C at which time a solution of appropriate 2-bromobenzoyl chloride derivative (2 equiv or 2.2 equiv, ~1 M) in THF was added dropwise. Once the addition was complete, the reaction was allowed to warm to room temperature and then was stirred at 65 °C for 30 minutes. At this time the extent of completion of the reaction was determined by conversion of the indole derivate by TLC analysis. The reaction was cooled to room temperature and quenched with a saturated solution of NH_4Cl. The reaction mixture was then diluted with water and EtOAc, and after separating the layers, the aqueous layer was extracted with EtOAc (3x). The combined organic layers were washed sequentially with water and brine, dried over sodium sulfate, filtered and concentrated under reduced pressure. The crude N-(2-bromobenzoyl)indole derivative was purified by flash column Si gel chromatography using the indicated solvent system.



(2-bromo-5-chlorophenyl)(2-phenyl-1*H*-indol-1-yl)methanone (1a)

white solid, MP = 156-157 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 6.8 Hz, 1H), 7.43 – 7.34 (m, 2H),, 7.25 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.21 – 7.12 (m, 4H), 7.10 (d, *J* = 2.4 Hz, 1H), 6.94 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.67 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.93, 140.22, 138.73, 137.92, 134.21, 133.12, 132.80, 131.53, 130.89, 129.59, 129.11, 128.15, 127.94, 125.49, 124.50, 120.78, 119.10, 115.73, 112.17.

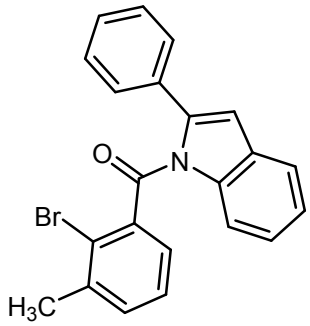
HRMS (ESI) Calc. for $C_{21}H_{13}BrClNO$ [M+H]: 409.9942; found: 409.9948.



(2-bromo-4-fluorophenyl)(2-phenyl-1*H*-indol-1-yl)methanone (1b)

white solid, MP = 128-129 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 7.2 Hz, 1H), 7.44 – 7.32 (m, 2H), 7.27 (dd, *J* = 7.6, 1.6 Hz, 2H), 7.22 – 7.11 (m, 4H), 7.03 (dd, *J* = 8.0, 2.4 Hz, 1H), 6.78 (td, *J* = 8.4, 2.4 Hz, 1H), 6.68 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 167.43, 163.1 (d, *J* = 255.1 Hz), 140.41, 137.93, 133.92, 133.88, 132.83, 132.66 (d, *J* = 9.2 Hz), 129.53, 128.89, 127.96, 127.94, 125.27, 124.23, 122.40 (d, *J* = 9.8 Hz), 120.75, 120.58 (d, *J* = 24.6 Hz), 115.33, 114.29 (d, *J* = 21.2 Hz), 111.68.

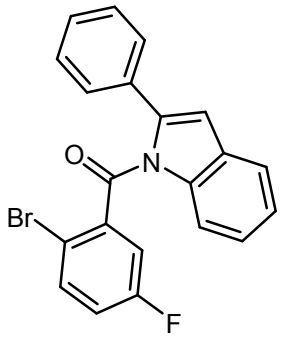
HRMS (ESI) Calc. for $C_{21}H_{13}BrFNO$ [M+H]: 395.0237; found: 394.0238.



(2-bromo-3-methylphenyl)(2-phenyl-1*H*-indol-1-yl)methanone (1c)

white solid, MP = 131-132 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.0 Hz, 1H), 7.62 (dd, *J* = 6.4, 1.2 Hz, 1H), 7.41 – 7.30 (m, 2H), 7.27 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.20 – 7.06 (m, 4H), 6.96 (d, *J* = 1.8 Hz, 1H), 6.82 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.67 (s, 1H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.40, 140.67, 137.97, 137.05, 136.94, 133.12, 132.98, 132.61, 131.65, 129.56, 128.94, 127.74, 127.70, 125.14, 124.08, 120.67, 117.96, 115.46, 111.57, 20.56.

HRMS (ESI) Calc. for $C_{22}H_{16}BrNO$ [M+H]: 390.0488; found: 390.0486.

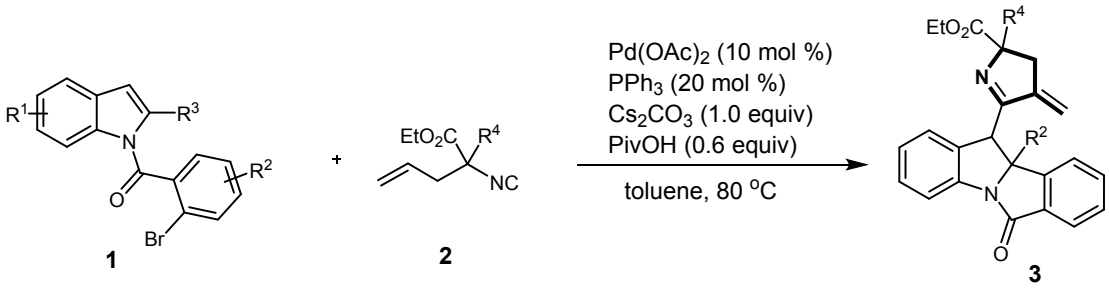


(3-bromo-5-fluorophenyl)(2-phenyl-1*H*-indol-1-yl)methanone (1d)

white solid, MP = 105-106 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.0 Hz, 1H), 7.66 – 7.59 (m, 1H), 7.44 – 7.39 (m, 1H), 7.37 (td, *J* = 7.2, 1.2 Hz, 1H), 7.29– 7.26 (m, 2H), 7.25 – 7.10 (m, 4H), 6.89 (dd, *J* = 8.0, 3.2 Hz, 1H), 6.76– 6.71 (m, 1H), 6.68 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.98 (d, *J* = 1.9 Hz), 160.97 (d, *J* = 247.9 Hz), 140.22, 138.87 (d, *J* = 7.0 Hz), 137.88, 134.64 (d, *J* = 7.9 Hz), 132.75, 129.59, 129.04, 128.10, 127.93, 125.43, 124.44, 120.78, 118.96 (d, *J* = 22.4 Hz), 118.12 (d, *J* = 24.4 Hz), 115.64, 115.60, 112.15.

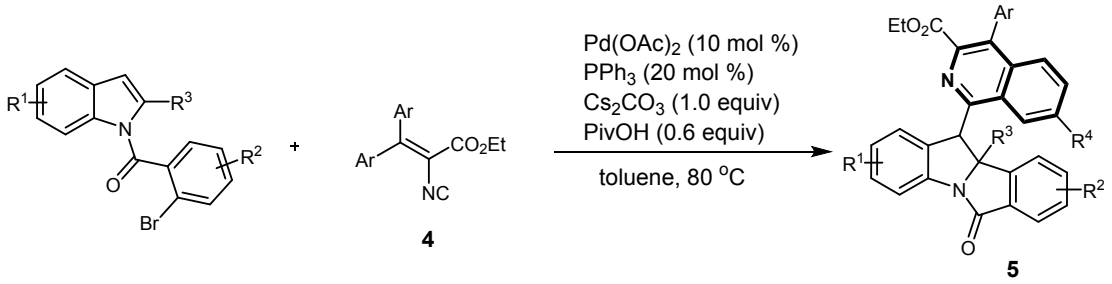
HRMS (ESI) Calc. for $C_{21}H_{13}BrFNO$ [M+H]: 395.0237; found: 394.0233.

III. General Procedures of Pd-Catalyzed Imidoylative Dearomatization of Indoles



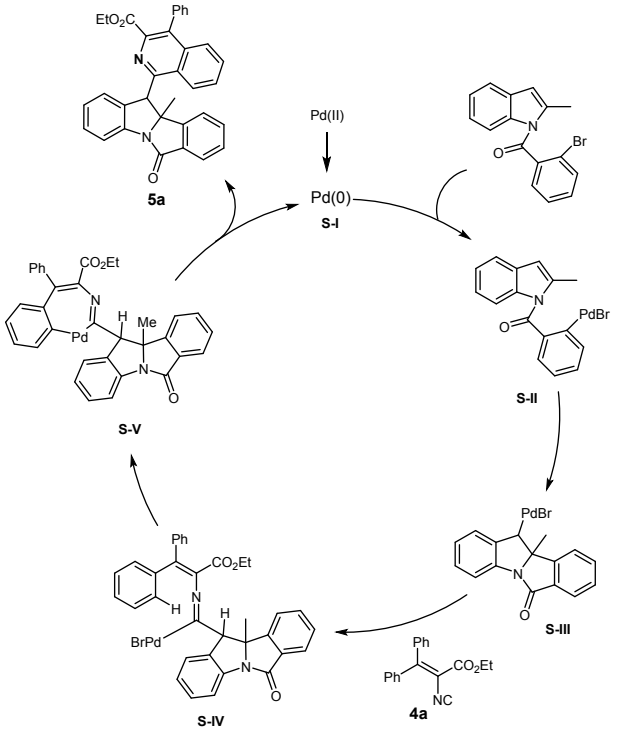
Procedure A: An oven-dried 25 mL schlenk tubecharged with $Pd(OAc)_2$ (0.02mmol, 4.48 mg, 10 mol%), PPh_3 (0.04mmol, 21.6mg, 20 mol%) and Cs_2CO_3 (0.2mmol, 65.2mg, 1.0 equiv) was refilled with Ar for 3 times. Then a solution of 1(0.2mmol, 1.5 equiv), PivOH (0.12 mmol, 12.2 mg, 0.6 equiv) in 1mL of dioxane was added by syringe and the tube was placed in an 80°C oil-bath. A solution of 2 (0.4mmol, 2 equiv) in 1.0 mL of dioxane was added dropwise with a syringe pump to

the reaction mixture. The addition was finished within 3 h. The crude reaction mixture was extracted with DCM (20 mL × 3) and washed with brine (20 mL). The organic phase was concentrated in vacuoand the residue was purified by silica gel flash column chromatography to afford the corresponding products.



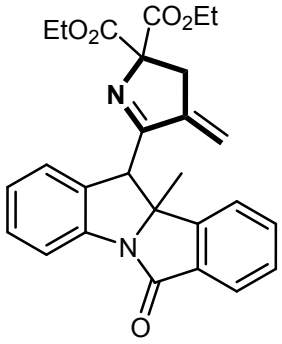
Procedure B: An oven-dried 25 mL schlenk tubecharged with $Pd(OAc)_2$ (0.02mmol, 4.48 mg, 10 mol%), PPh_3 (0.04mmol, 21.6mg, 20 mol%) and Cs_2CO_3 (0.2mmol, 65.2mg, 1.0 equiv) was refilled with Ar for 3 times. Then a solution of 1(0.2mmol, 1.5 equiv), PivOH (0.12 mmol, 12.2 mg, 0.6 equiv) in 1mL of dioxane was added by syringe and the tube was placed in an 80°C oil-bath. A solution of 4 (0.4mmol, 2 equiv) in 1.0 mL of dioxane was added dropwise with a syringe pump to the reaction mixture. The addition was finished within 3 h. The crude reaction mixture was extracted with DCM (20 mL × 3) and washed with brine (20 mL). The organic phase was concentrated in vacuoand the residue was purified by silica gel flash column chromatography to afford the corresponding products.

IV. Proposed mechanism of the formation of 5a.



Aryl-Pd^{II} intermediate **II** was generated *via* oxidative addition of Pd(0) to C(sp^2)-Br bond, followed by an intramolecular dearomative double bond insertion reaction, ffording benzylic Pd(II) species **III**. Then the imidoyl palladium intermediate **IV** was generated by coordination and insertion of isocyanide. Under the action of acid, **IV** removes a HBr to form a seven-membered ring intermediate **V,** followed by reductive elimination reaction to yield the desired product **5a**. Pd(0) was regenerated to complete the catalytic cycle.

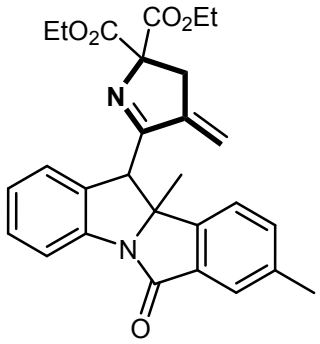
V. Characterization Data



diethyl 5-(10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3a)

59.6 mg, 65% yield, pale yellow solid, MP = 154-155 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.45 – 7.38 (m, 3H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.27 (d, *J* = 7.2 Hz, 1H), 7.12 (t, *J* = 7.6 Hz, 1H), 4.73 (d, *J* = 11.2 Hz, 2H), 4.28 (q, *J* = 7.2 Hz, 2H), 4.22 – 4.10 (m, 3H), 2.77 (d, *J* = 17.2 Hz, 1H), 2.42 (dt, *J* = 16.8, 2.8 Hz, 1H), 1.76 (s, 3H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.02, 168.84, 168.60, 168.42, 148.15, 145.28, 140.41, 134.14, 132.92, 132.47, 129.63, 128.82, 126.61, 125.17, 124.68, 123.68, 117.37, 113.62, 81.51, 74.27, 62.36, 62.21, 53.87, 37.75, 29.55, 14.16, 14.05.

HRMS (ESI) Calc. for $C_{27}H_{26}N_2O_5$ [M+H]: 459.1914; found: 459.1910.

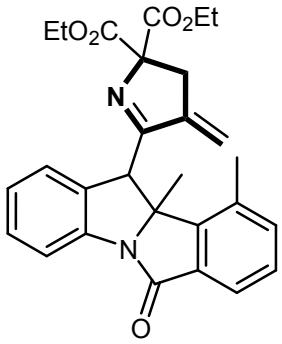


diethyl 5-(8,10b-dimethyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3b)

51.9 mg, 55% yield, pale yellow solid, MP = 101-102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8 Hz, 1H), 7.55 (s, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.27 – 7.25 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.12 (td, *J* = 7.6, 0.8 Hz, 1H), 4.76 (s, 1H), 4.70 (s, 1H), 4.33 – 4.27 (m, 2H), 4.25 – 4.10 (m, 3H), 2.78 (dt, *J* = 12.8, 2.0 Hz,

1H), 2.46 (dt, *J* = 12.8, 2.8 Hz, 1H), 2.40 (s, 3H), 1.74 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.16, 169.05, 168.70, 168.52, 145.55, 145.28, 140.51, 138.95, 134.21, 133.50, 133.07, 129.62, 126.63, 125.12, 124.92, 123.36, 117.35, 113.68, 81.56, 74.13, 62.38, 62.24, 53.90, 37.85, 29.76, 21.46, 14.20, 14.09.

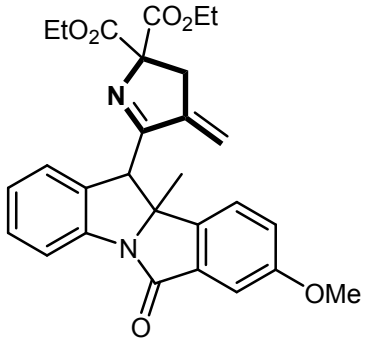
HRMS (ESI) Calc. for $C_{28}H_{28}N_2O_5$ [M+H]: 473.2071; found: 473.2072.



diethyl 5-(10,10b-dimethyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3c)

72.7 mg, 77% yield, yellow solid, MP = 112-113 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.27 – 7.25 (m, 1H), 7.14 – 7.10 (m, 1H), 4.78 (s, 1H), 4.77 (s, 1H), 4.29 – 4.20 (m, 1H), 4.18 – 4.12 (m, 2H), 2.65 (d, *J* = 16.8 Hz, 1H), 2.54 (dt, *J* = 16.8, 2.8 Hz, 1H), 2.36 (s, 3H), 1.78 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.22 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.95, 168.56, 168.45, 168.29, 145.60, 144.60, 139.69, 134.96, 134.74, 133.69, 133.20, 129.64, 129.27, 126.52, 125.18, 122.44, 117.39, 113.42, 81.21, 74.58, 62.30, 54.00, 38.26, 27.08, 19.11, 14.13, 14.06.

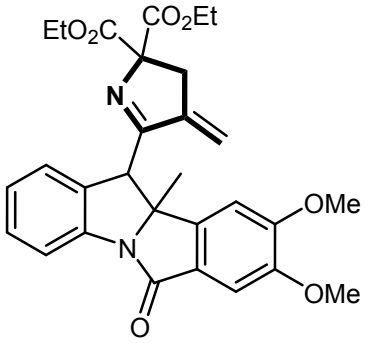
HRMS (ESI) Calc. for $C_{28}H_{28}N_2O_5$ [M+H]: 473.2071; found: 473.2067.



diethyl 5-(8-methoxy-10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3d)

74.2 mg, 76% yield, white solid, MP = 118-119 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.23 (m, 3H), 7.14 (td, *J* = 7.6, 0.8 Hz 1H), 7.01 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.78 (s, 1H), 4.71 (s, 1H), 4.32 – 4.15 (m, 4H), 4.10 (s, 1H), 3.84 (s, 3H), 2.83 (dt, *J* = 17.2, 1.6 Hz, 1H), 2.47 (dt, *J* = 17.2, 2.8 Hz, 1H), 1.75 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.11, 168.78, 168.62, 168.42, 160.40, 145.31, 140.50, 140.39, 134.31, 134.25, 129.57, 126.64, 125.13, 124.53, 120.58, 117.29, 113.58, 107.30, 81.50, 73.95, 62.33, 62.16, 55.72, 53.91, 37.84, 29.65, 14.15, 14.05.

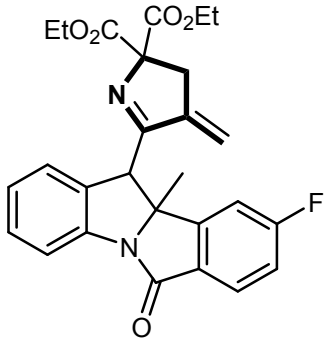
HRMS (ESI) Calc. for $C_{28}H_{28}N_2O_6$ [M+H]: 489.2020; found: 489.2012.



diethyl 5-(8,9-dimethoxy-10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3e)

74.6 mg, 72% yield, white solid, MP = 92-93 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.24 (d, *J* = 7.6 Hz, 1H), 7.19 (s, 1H), 7.10 (td, *J* = 7.6, 0.8 Hz, 1H), 6.86 (s, 1H), 4.75 (s, 1H), 4.71 (s, 1H), 4.24 – 4.15 (m, 4H), 4.04 (s, 1H), 3.98 (s, 3H), 3.90 (s, 3H), 2.92 (dt, *J* = 16.8, 1.6 Hz, 1H), 2.40 (dt, *J* = 16.8, 2.8 Hz, 1H), 1.74 (s, 3H), 1.26 (t, *J* = 6.8 Hz, 3H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.26, 169.33, 168.84, 168.27, 153.63, 150.06, 144.82, 142.62, 140.62, 134.04, 129.63, 126.59, 124.93, 124.69, 117.12, 114.14, 105.80, 105.69, 81.25, 73.74, 62.44, 62.10, 58.56, 56.43, 56.26, 54.30, 38.07, 30.09, 14.11.

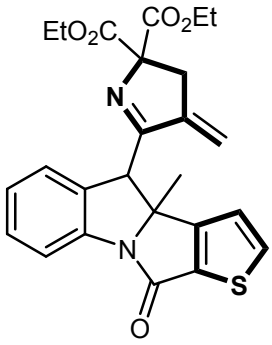
HRMS (ESI) Calc. for $C_{29}H_{30}N_2O_7$ [M+H]: 519.2126; found: 519.2122.



Diethyl 5-(9-fluoro-10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3f)

52.4 mg, 55% yield, pale yellow solid, MP = 199-200 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (dd, *J* = 8.4, 5.2 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.14 – 7.09 (m, 2H), 7.02 (dd, *J* = 8, 2 Hz, 1H), 4.75 (d, *J* = 22.4 Hz, 2H), 4.36 – 4.26 (m, 2H), 4.26 – 4.16 (m, 2H), 4.10 (s, 1H), 2.84 (dt, *J* = 17.2, 2.0 Hz, 1H), 2.55 (dt, *J* = 17.2, 2.1 Hz, 1H), 1.77 (s, 3H), 1.32 (t, *J* = 6.8 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.66, 168.51, 167.77, 165.57 (d, *J* = 252.6 Hz), 150.79 (d, *J* = 9.7 Hz), 145.32, 140.34, 133.79, 129.79, 128.95, 126.89 (d, *J* = 10.0 Hz), 126.70, 125.35, 117.36, 116.71 (d, *J* = 23.4 Hz), 113.91, 111.31 (d, *J* = 24.1 Hz), 81.72, 73.83, 62.50, 62.46, 53.89, 37.76, 29.52, 14.14, 14.10.

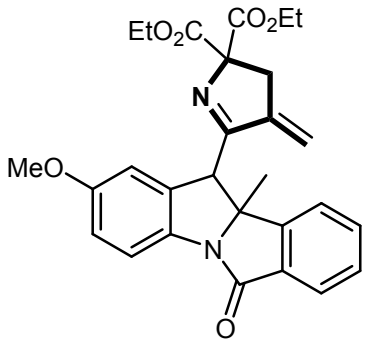
HRMS (ESI) Calc. for $C_{27}H_{25}FN_2O_5$ [M+H]: 477.1820; found: 477.1818.



diethyl 5-(3b-methyl-10-oxo-3b,10-dihydro-4*H*-thieno[3',2':3,4]pyrrolo[1,2-*a*]indol-4-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3g)

37.1 mg, 40% yield, yellow solid, MP = 139-140 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 4.8 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.28 (s, 1H), 7.14 (td, *J* = 7.6, 1.2 Hz, 1H), 6.92 (d, *J* = 4.8 Hz, 1H), 4.93 (s, 1H), 4.67 (s, 1H), 4.28 – 4.17 (m, 5H), 2.91 (dt, *J* = 17.2, 2.0 Hz, 1H), 2.62 (dt, *J* = 17.2, 2.8 Hz, 1H), 1.79 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 1.28 (t, *J* = 7.2 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.08, 168.75, 168.49, 164.96, 159.31, 145.50, 140.95, 137.05, 135.77, 133.87, 129.68, 126.68, 125.04, 121.74, 117.17, 113.78, 81.66, 73.58, 62.48, 62.27, 53.44, 37.85, 28.52, 14.20, 14.12.

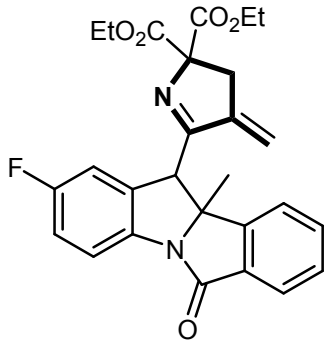
HRMS (ESI) Calc. for $C_{25}H_{24}N_2O_5S$ [M+H]: 465.1473; found: 465.1470.



diethyl 5-(2-methoxy-10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3h)

75.2 mg, 77% yield, white solid, MP = 113-114 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.2 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.43 – 7.35 (m, 2H), 7.27 (d, *J* = 7.6 Hz, 1H), 6.89 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.80 (d, *J* = 2.4 Hz, 1H), 4.74 (s, 1H), 4.64 (s, 1H), 7.28 – 7.10 (m, 5H), 3.74 (s, 3H), 2.74 (d, *J* = 17.2 Hz, 1H), 2.39 (dt, *J* = 17.2, 2.4 Hz, 1H), 1.72 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.21 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.85, 168.72, 168.46, 168.32, 157.50, 147.89, 145.05, 135.54, 133.90, 133.02, 132.19, 128.71, 124.45, 123.56, 117.82, 114.22, 113.70, 112.78, 81.43, 74.57, 62.26, 62.12, 55.71, 54.10, 37.63, 29.31, 14.07, 13.97.

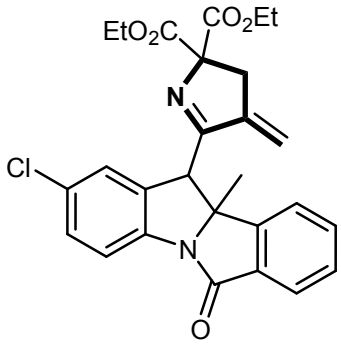
HRMS (ESI) Calc. for $C_{28}H_{28}N_2O_6$ [M+H489.2020; found: 489.2019.



diethyl 5-(2-fluoro-10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3i)

71.4 mg, 75% yield, pale yellow solid, MP = 164-165 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.6 Hz, 1H), 7.68 (dd, *J* = 8.8, 4.8 Hz, 1H), 7.47 – 7.38 (m, *2*H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.09 (td, *J* = 8.8, 2.4 Hz, 1H), 6.97 (dd, *J* = 8.0, 2.4 Hz, 1H), 4.83 (s, 1H), 4.66 (s, 1H), 4.27 – 4.09 (m, 5H), 2.79 (d, *J* = 17.2 Hz, 1H), 2.45 (dt, *J* = 17.2, 2.4 Hz, 1H), 1.76 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.23 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.49, 168.88, 168.51, 168.25, 160.39 (d, *J* = 243.3 Hz), 147.87, 145.53, 136.62 (d, *J* = 2.0 Hz), 136.12 (d, *J* = 8.5 Hz), 132.73, 132.56, 128.95, 124.71, 123.58, 118.19 (d, *J* = 8.2 Hz), 116.23 (d, *J* = 23.5 Hz), 113.96 (d, *J* = 24.1 Hz), 113.36, 81.67, 74.81, 62.41, 62.24, 53.54, 37.60, 29.35, 14.11, 14.03.

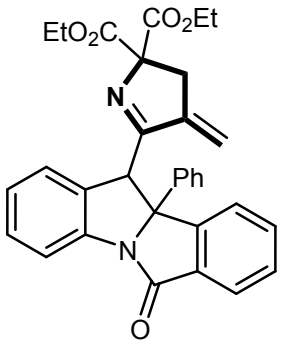
HRMS (ESI) Calc. for $C_{27}H_{25}FN_2O_5$ [M+H]: 477.1820; found: 477.1825.



diethyl 5-(2-chloro-10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3j)

65.9 mg, 67% yield, pale yellow solid, MP = 148-149 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.2 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.48 – 7.35 (m, 3H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.23 (d, *J* = 1.2 Hz, 1H), 4.85 (s, 1H), 4.65 (s, 1H), 4.25 – 4.07 (m, 5H), 2.80 (d, *J* = 17.2 Hz, 1H), 2.47 (d, *J* = 17.2 Hz, 1H), 1.75 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 174.46, 168.74, 168.52, 168.23, 147.82, 145.62, 139.06, 136.14, 132.68, 132.63, 130.39, 129.70, 128.99, 126.68, 124.77, 123.60, 118.23, 113.35, 81.73, 74.65, 62.43, 62.26, 53.24, 37.55, 29.42, 14.11, 14.03.

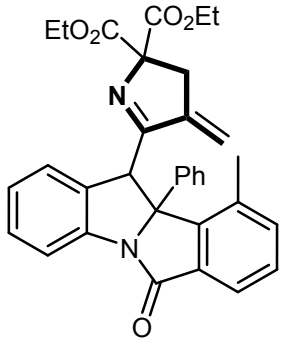
HRMS (ESI) Calc. for $C_{27}H_{25}ClN_2O_5$ [M+H]: 493.1525; found: 493.1524.



diethyl 4-methylene-5-(6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3k)

84.2 mg, 81% yield, yellow solid, MP = 83-84 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 7.2 Hz, 2H), 7.73 (d, *J* = 7.2 Hz, 1H), 7.45 (d, *J* = 7.2 Hz, 1H), 7.42 – 7.28 (m, 5H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 5.36 (s, 1H), 4.88 (s, 1H), 4.36 – 4.29 (m, 3H), 4.23 – 4.14 (m, 2H), 2.84 (d, *J* = 16.8 Hz, 1H), 2.56 – 2.51(m, 1H), 1.33 (t, *J* = 7.2 Hz, 3H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.97, 169.17, 168.44, 168.20, 147.34, 145.64, 143.70, 140.79, 133.95, 132.49, 132.18, 129.40, 128.81, 128.59, 127.97, 126.03, 125.27, 124.86, 124.47, 124.40, 117.01, 113.24, 81.47, 79.05, 62.16, 62.03, 55.44, 37.81, 14.00, 13.86.

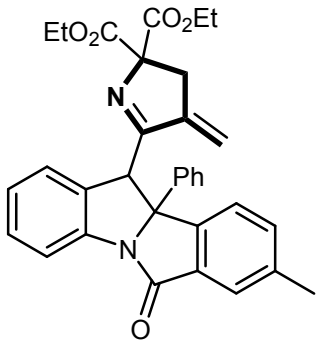
HRMS (ESI) Calc. for $C_{32}H_{28}N_2O_5$ [M+H]: 521.2071; found: 521.2064.



diethyl 5-(10-methyl-6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3l)

87.6 mg, 82% yield, pale yellow solid, MP = 107-108 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.2 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.40 – 7.33 (m, 5H), 7.26 – 7.20 (m, 4H), 7.12 (t, *J* = 7.6 Hz, 1H), 5.73 (s, 1H), 4.85 (s, 1H), 4.26 – 4.14 (m, 5H), 2.64 (d, *J* = 16.8 Hz, 1H), 2.48 (dt, *J* = 16.8, 2.8 Hz, 1H), 2.02 (s, 3H), 1.27 (t, *J* = 7.2 Hz, 3H), 1.24 (t, *J* = 6.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.68, 169.20, 168.50, 168.33, 145.37, 144.98, 140.14, 139.82, 135.48, 135.25, 134.38, 134.01, 129.77, 129.72, 128.68, 128.47, 126.27, 125.78, 125.43, 122.36, 117.79, 113.56, 80.93, 79.21, 62.33, 62.31, 51.04, 38.50, 19.30, 14.12, 14.07.

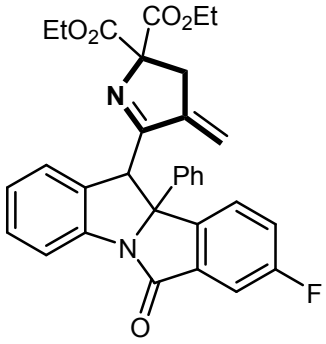
HRMS (ESI) Calc. for $C_{33}H_{30}N_2O_5$ [M+H]: 535.2227; found: 535.2222.



diethyl 5-(8-methyl-6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3m)

91.9 mg, 86% yield, yellow solid, MP = 119-120 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.6 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.52 (s, 1H), 7.40 (t, *J* = 7.2 Hz, 1H), 7.32 – 7.29 (m, 3H), 7.24 – 7.16 (m, 3H), 7.09 (td, *J* = 7.6, 0.8 Hz, 1H), 5.32 (s, 1H), 4.86 (s, 1H), 4.41 – 4.09 (m, 5H), 2.82 (d, *J* = 17.2 Hz, 1H), 2.54 (dt, *J* = 17.2, 2.8 Hz, 1H), 2.35 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.33, 169.64, 168.76, 168.53, 145.75, 144.99, 144.26, 141.09, 138.97, 134.15, 133.72, 132.50, 129.61, 129.00, 128.07, 126.28, 125.43, 125.04, 124.93, 124.25, 117.20, 113.60, 81.68, 79.07, 62.40, 62.29, 55.77, 38.13, 21.34, 14.24, 14.09.

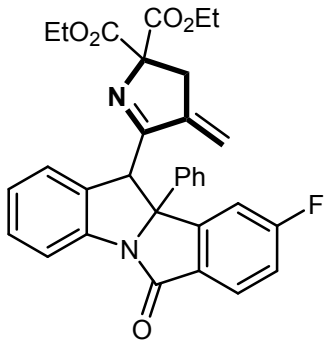
HRMS (ESI) Calc. for $C_{33}H_{30}N_2O_5$ [M+H]: 535.2227; found: 535.2226.



diethyl 5-(8-fluoro-6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3n)

62.4 mg, 58% yield, white solid, MP = 115-116 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 2H), 7.45 – 7.39 (m, 3H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.28 – 7.20 (m, 2H), 7.15 – 7.09 (m, 2H), 5.33 (s, 1H), 4.94 (s, 1H), 4.39 (s, 1H), 4.31 (q, *J* = 7.2 Hz, 2H), 4.25 – 4.14 (m, 2H), 2.92 (d, *J* = 16.8 Hz, 1H), 2.56 (d, *J* = 16.8 Hz, 1H), 1.33 (t, *J* = 7.2 Hz, 3H), 1.30 – 1.26 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.13, 168.71, 168.36, 168.14, 163.05 (d, *J* = 248.5 Hz), 145.94, 143.57, 143.13, 140.70, 134.64 (d, *J* = 8.2 Hz), 134.12, 129.72, 129.14, 128.32, 126.33, 126.23, 125.74, 125.00, 120.15 (d, *J* = 24.4 Hz), 117.28, 113.60, 111.32 (d, *J* = 24.4 Hz), 81.71, 78.99, 62.46, 62.30, 55.45, 38.00, 14.18, 14.09.

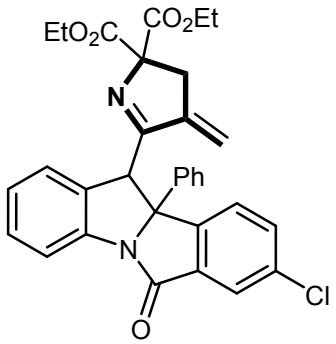
HRMS (ESI) Calc. for $C_{32}H_{27}FN_2O_5$ [M+H]: 539.1977; found: 539.1972.



diethyl 5-(9-fluoro-6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3o)

75.3 mg, 70% yield, pale yellow solid, MP = 145-146 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.6 Hz, 1H), 7.76 – 7.70 (m, 3H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.10 – 7.02 (m, 3H), 5.34 (s, 1H), 4.89 (s, 1H), 4.38 – 4.29 (m, 3H), 4.26 – 4.17 (m, 2H), 2.88 (dt, *J* = 17.2, 2 Hz, 1H), 2.62 (dt, *J* = 17.2, 2.4 Hz, 1H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.83, 168.56, 168.49, 168.36, 165.54 (d, *J* = 252.6 Hz), 150.18 (d, *J* = 9.8 Hz), 145.74, 143.33, 140.85, 133.75, 129.74, 129.18, 128.44, 128.30 (d, *J* = 2.0 Hz), 126.83 (d, *J* = 9.9 Hz), 126.32, 125.62, 125.06, 117.20, 116.66 (d, *J* = 23.4 Hz), 113.79, 112.25 (d, *J* = 24.6 Hz), 81.79, 78.72, 62.48, 62.45, 55.75, 38.03, 14.15, 14.08.

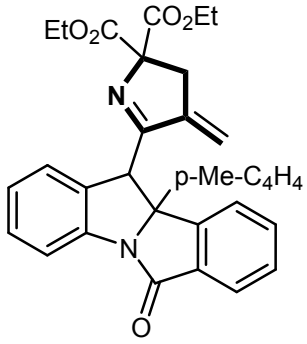
HRMS (ESI) Calc. for $C_{32}H_{27}FN_2O_5$ [M+H]: 539.1977; found: 539.1973.



diethyl 5-(8-chloro-6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3p)

62.1 mg, 56% yield, pale yellow solid, MP = 133-134 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.6 Hz, 1H), 7.75 – 7.71 (m, 3H), 7.44 – 7.32 (m, 5H), 7.29 – 7.20 (m, 2H), 7.13 (t, *J* = 7.6 Hz, 1H), 5.32 (s, 1H), 4.97 (s, 1H), 4.43 (s, 1H), 4.33 – 4.12 (m, 4H), 2.94 (d, *J* = 16.8 Hz, 1H), 2.58 (dt, *J* = 16.8, 2.4 Hz, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 1.29 – 1.26 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.06, 168.71, 168.35, 167.92, 146.02, 145.79, 143.39, 140.62, 135.16, 134.23, 134.09, 132.78, 129.72, 129.17, 128.39, 126.28, 125.79, 125.75, 124.98, 124.71, 117.27, 113.57, 81.78, 79.06, 62.48, 62.30, 55.24, 37.96, 29.82, 14.18, 14.09.

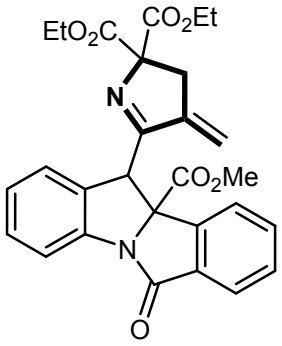
HRMS (ESI) Calc. for $C_{32}H_{27}ClN_2O_5$ [M+H]: 555.1681; found: 555.1674.



diethyl4-methylene-5-(6-oxo-10b-(p-tolyl)-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3q)

86.5 mg, 81% yield, yellow solid, MP = 103-104 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.8 Hz, 1H), 7.73 – 7.71 (m, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.41 – 7.32 (m, 4H), 7.19 (d, *J* = 7.6 Hz, 1H), 7.13 – 7.07 (m, 3H), 5.33 (s, 1H), 4.85 (s, 1H), 4.34 – 4.29 (m, 3H), 4.26 – 4.10 (m, 2H), 2.80 (dt, *J* = 16.8, 1.6 Hz, 1H), 2.49 (dt, *J* = 16.8, 2.4 Hz, 1H), 2.26 (s, 3H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.26 (t, *J* = 6.8 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 175.23, 169.38, 168.64, 168.43, 147.73, 145.71, 140.95, 140.87, 137.99, 134.17, 132.65, 132.34, 129.64, 129.57, 128.66, 126.27, 125.42, 124.99, 124.65, 124.51, 117.21, 113.51, 81.57, 79.16, 62.37, 62.23, 55.69, 38.05, 21.00, 14.18, 14.04.

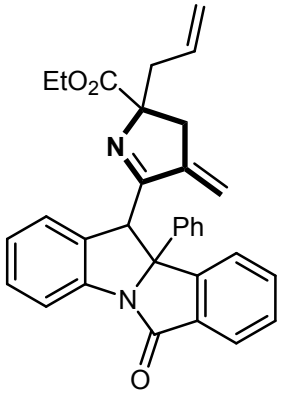
HRMS (ESI) Calc. for $C_{33}H_{30}N_2O_5$ [M+H]: 535.2227; found: 535.2223.



diethyl 5-(10b-(methoxycarbonyl)-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-methylene-3,4-dihydro-2*H*-pyrrole-2,2-dicarboxylate (3r)

60.3 mg, 60% yield, white solid, MP = 127-128 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.74 (m, 2H), 7.47 – 7.37 (m, 4H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.11 (td, *J* = 7.6, 1.2 Hz, 1H), 5.42 (s, 1H), 5.06 (s, 1H), 4.80 (s, 1H), 4.15 – 3.98 (m, 4H), 3.70 (s, 3H), 2.83 (dt, *J* = 17.2, 2.0 Hz, 1H), 2.58 (dt, *J* = 17.2, 2.4 Hz, 1H), 1.22 (t, *J* = 7.2 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.08, 171.27, 168.66, 168.63, 168.15, 146.72, 141.25, 140.70, 133.86, 133.82, 132.66, 129.92, 129.58, 125.85, 125.34, 124.69, 124.48, 117.00, 112.92, 82.07, 79.08, 62.24, 62.16, 53.91, 48.73, 37.34, 14.06, 13.99.

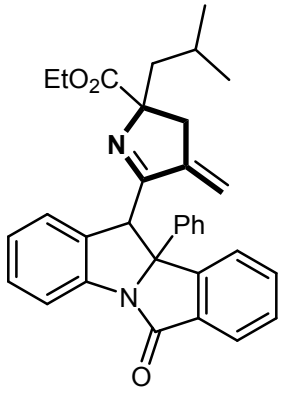
HRMS (ESI) Calc. for $C_{28}H_{26}N_2O_7$ [M+H]: 503.1813; found: 503.1814.



ethyl 2-allyl-4-methylene-5-(6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-3,4-dihydro-2*H*-pyrrole-2-carboxylate (3s)

73.2 mg, 75% yield, white solid, MP = 142-143 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.6 Hz, 1H), 7.75 (d, *J* = 7.2 Hz, 3H), 7.45 – 7.30 (m, 6H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.14 (t, *J* = 6.8 Hz, 1H), 7.08 (tdd, *J* = 7.2, 2.8, 0.8 Hz, 1H), 5.65 – 5.32 (m, 1H), 5.21 (d, *J* = 4.8 Hz, 1H), 5.09 – 5.03 (m, 1H), 5.03 – 4.87 (m, 2H), 4.57 (s, 1H), 4.23 – 3.97 (m, 2H), 2.73 – 2.02 (m, 4H), 1.24 (dt, *J* = 21.2, 7.2 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 172.64 (d, *J* = 23.1 Hz), 172.28 (d, *J* = 6.2Hz), 169.26 (d, *J* = 16.0 Hz), 147.58 (d, *J* = 22.4 Hz), 143.88 (d, *J* = 10.3 Hz), 140.81 (d, *J* = 12.0 Hz), 135.23 (d, *J* = 23.2 Hz), 132.82 (d, *J* = 7.5 Hz), 132.71, 132.41 (d, *J* = 9.1 Hz), 132.28, 129.37 (d, *J* = 3.0 Hz), 129.03 (d, *J* = 2.0 Hz), 128.73, 128.14 (d, *J* = 2.0 Hz), 125.94 (d, *J* = 11.4 Hz), 125.31, 125.10 (d, *J* = 2.2 Hz), 124.76 (d, *J* = 10.5 Hz), 124.42, 119.16 (d, *J* = 14.4 Hz), 117.28 (d, *J* = 8.1 Hz), 111.60, 79.45 (d, *J* = 5.2 Hz), 78.20 (d, *J* = 55.4 Hz), 61.41 (d, *J* = 8.2 Hz), 54.46, 42.71 (d, *J* = 55.1 Hz), 38.77 (d, *J* = 55.1 Hz), 14.30 (d, *J* = 11.0 Hz).

HRMS (ESI) Calc. for $C_{32}H_{28}N_2O_3$ [M+H]: 489.2173; found: 489.2180.

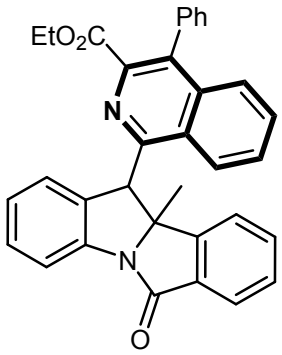


ethyl 2-isobutyl-4-methylene-5-(6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-3,4-dihydro-2*H*-pyrrole-2-carboxylate (3t)

70.6 mg, 70% yield, yellow solid, MP = 137-138 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 7.6, 2.8 Hz, 1H), 7.79 – 7.70 (m, 3H), 7.48 – 7.28 (m, 6H), 7.26 – 7.19 (m, 1H), 7.18 – 7.02 (m, 2H), 5.21 (d, *J* = 5.6 Hz, 1H), 4.88 (d, *J* = 8.4 Hz, 1H), 4.49 (s, 1H), 4.29 – 3.94 (m, 2H), 2.76 – 2.46 (m, 1H), 2.07 (dd, *J* = 80.8, 16.8 Hz, 1H), 1.72 – 1.61 (m, 1H), 1.59 – 1.41 (m, 2H), 1.26 (dt, *J* = 22.4, 7.2 Hz, 3H), 0.94 – 0.79 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.46 (d, *J* = 40.4 Hz), 171.39 (d, *J* = 22.8 Hz), 169.29 (d, *J* = 21.7 Hz), 147.65 (d, *J* = 24.3 Hz), 147.41, 143.93 (d, *J* = 10.6 Hz), 140.85 (d, *J* = 16.3 Hz), 135.16 (d, *J* = 22.8 Hz), 132.82 (d, *J* = 12.7 Hz), 132.33 (d, *J* = 11.8 Hz), 129.34 (d, *J* = 1.0 Hz), 129.02 (d, *J* = 1.4 Hz), 128.68 (d, *J* = 1.8 Hz), 128.12 (d, *J* = 1.2 Hz), 125.96 (d, *J* = 13.8 Hz), 125.31, 125.13, 124.75 (d, *J* = 6.9 Hz), 124.47,

117.24 (d, *J* = 6.4 Hz), 111.17, 79.46 (d, *J* = 11.7 Hz), 78.61 (d, *J* = 49.6 Hz), 61.24 (d, *J* = 6.6 Hz), 54.63 (d, *J* = 5.2 Hz), 47.79 (d, *J* = 81.8 Hz), 40.72 (d, *J* = 56.4 Hz), 25.07 (d, *J* = 34.2 Hz), 24.09, 23.84 (d, *J* = 5.7 Hz), 14.26 (d, *J* = 13.5 Hz).

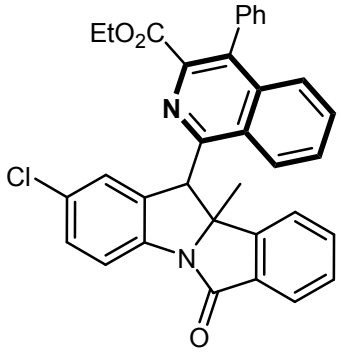
HRMS (ESI) Calc. for $C_{33}H_{32}N_2O_3$ [M+H]: 505.2486; found: 505.2490.



ethyl 1-(10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylate (5a)

89.8 mg, 88% yield, white solid, MP = 190-191 °C. ^{1}H NMR (400 MHz, DMSO) δ 9.01 (d, *J* = 8.0 Hz, 1H), 7.93 (t, *J* = 7.2 Hz, 1H), 7.79 (t, *J* = 7.6 Hz, 1H), 7.62 (dd, *J* = 13.6, 8.0 Hz, 2H), 7.49 – 7.32 (m, 5H), 7.28 (t, *J* = 6.0 Hz, 2H), 7.19 – 7.04 (m, 3H), 6.88 (d, *J* = 7.2 Hz, 2H), 5.78 (s, 1H), 3.74 (dd, *J* = 13.6, 6.4 Hz, 2H), 1.82 (s, 3H), 0.86 (t, *J* = 7.2 Hz, 4H). ^{13}C NMR (100 MHz, DMSO) δ 168.07, 165.64, 159.04, 148.63, 141.30, 140.01, 139.11, 134.94, 134.66, 133.18, 131.69, 131.10, 129.58, 128.88, 128.21, 128.10, 127.90, 127.78, 126.04, 125.85, 125.56, 124.17, 123.51, 121.83, 116.80, 75.44, 60.13, 50.75, 27.88, 13.43.

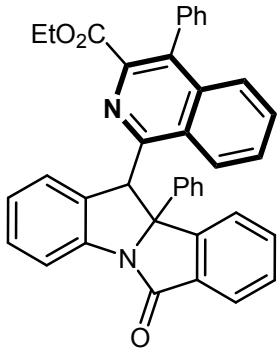
HRMS (ESI) Calc. for $C_{32}H_{22}N_2O_3$ [M+H]: 483.1703; found: 483.1705.



ethyl 1-(2-chloro-10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylate (5b)

90.3 mg, 83% yield, white solid, MP = 103-104 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.98 (d, *J* = 8.4 Hz, 1H), 7.93 (t, *J* = 7.6 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.61 (dd, *J* = 16.4, 7.6 Hz, 2H), 7.49 – 7.33 (m, 6H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.18 – 7.07 (m, 2H), 6.86 (d, *J* = 7.6 Hz, 2H), 5.80 (s, 1H), 3.76 (q, *J* = 6.8 Hz, 2H), 1.84 (s, 3H), 0.87 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 168.07, 165.55, 158.48, 148.15, 141.32, 141.18, 139.30, 134.89, 134.69, 132.74, 131.80, 131.17, 129.75, 129.52, 128.94, 128.19, 128.07, 127.97, 127.90, 126.12, 126.06, 125.83, 125.60, 123.58, 121.91, 117.91, 75.97, 60.14, 50.80, 27.53, 13.42.

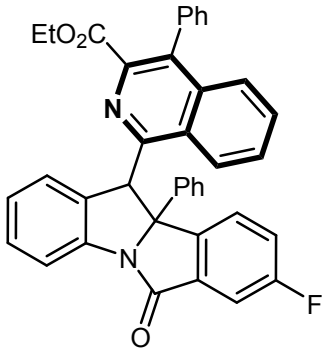
HRMS (ESI) Calc. for $C_{34}H_{25}ClN_2O_3$ [M+H]: 545.1626; found: 545.1634.



ethyl 1-(6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylate (5c)

97.3 mg, 83% yield, yellow solid, MP = 119-120 °C. ^{1}H NMR (400 MHz, DMSO) δ 9.15 (d, *J* = 7.8 Hz, 1H), 8.00 (d, *J* = 6.4 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 2H), 7.84 – 7.78 (m, 2H), 7.62 (d, *J* = 7.2 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.45 – 7.20 (m, 10H), 7.15 (d, *J* = 3.6 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 7.03 (t, *J* = 7.2 Hz, 1H), 6.98 – 6.87 (m, 2H), 6.26 (s, 1H), 3.80 (d, *J* = 6.4 Hz, 2H), 0.92 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 168.68, 166.07, 158.98, 148.09, 144.10, 141.83, 141.01, 139.10, 135.40, 135.31, 133.29, 132.34, 131.68, 130.31, 130.04, 129.75, 129.48, 128.92, 128.71, 128.58, 128.42, 128.36, 128.30, 126.60, 126.53, 126.22, 125.69, 124.92, 124.15, 123.08, 117.23, 81.10, 60.67, 53.04, 13.95.

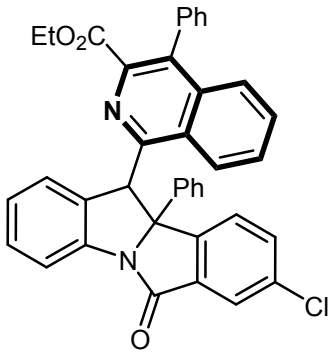
HRMS (ESI) Calc. for $C_{39}H_{28}N_2O_3$ [M+H]: 573.2173; found: 573.2170.



ethyl 1-(8-fluoro-6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylate (5d)

85.1 mg, 72% yield, yellow solid, MP = 108-109 °C. ^{1}H NMR (400 MHz, DMSO) δ 9.13 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 3H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.44 – 7.30 (m, 8H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.16 (, *J* = 2.7 Hz, 1H), 7.08 – 6.97 (m, 4H), 6.24 (s, 1H), 3.80 (dd, *J* = 6.8, 4.4 Hz, 2H), 0.89 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (100 MHz, DMSO) δ 167.04, 164.40 (d, *J* = 256.9 Hz), 160.68, 158.52, 143.81, 143.79, 143.26, 141.43, 140.04, 138.53, 134.81, 131.36, 129.81, 129.60, 129.33, 129.06, 128.57, 128.30, 128.18, 128.04, 127.99, 126.05, 126.02, 125.82, 125.39, 125.19, 124.73, 119.29, 119.05, 116.85, 110.15 (d, *J* = 23.3 Hz), 80.23, 60.27, 52.49, 13.44.

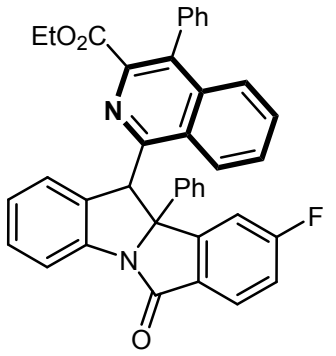
HRMS (ESI) Calc. for $C_{39}H_{27}FN_2O_3$ [M+H]: 591.2078; found: 591.2071.



ethyl 1-(8-chloro-6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylate (5e)

93.4 mg, 77% yield, yellow solid, MP = 252-253 °C. ^{1}H NMR (400 MHz, DMSO) δ 9.13 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 7.2 Hz, 1H), 7.79 – 7.76 (m, 4H), 7.62 (d, *J* = 1.6 Hz, 1H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.44 – 7.17 (m, 10H), 7.07 – 6.98 (m, 3H), 6.25 (s, 1H), 3.86 – 3.77 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 166.76, 165.63, 158.44, 146.63, 143.00, 141.35, 139.88, 138.34, 134.86, 134.80, 132.78, 131.77, 131.39, 129.93, 129.60, 129.33, 129.08, 128.61, 128.30, 128.16, 128.05, 126.06, 125.99, 125.81, 125.44, 125.20, 124.78, 124.54, 123.37, 116.86, 80.31, 60.29, 52.59, 13.47.

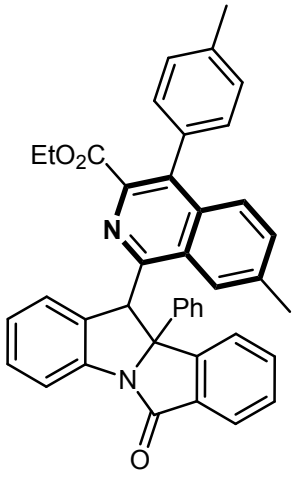
HRMS (ESI) Calc. for $C_{39}H_{27}ClN_2O_3$ [M+H]: 607.1783; found: 607.1776.



ethyl 1-(9-fluoro-6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylate (5f)

95.6 mg, 81% yield, yellow solid, MP = 111-112 °C. ^{1}H NMR (400 MHz, DMSO) δ 9.14 (d, *J* = 7.2 Hz, 1H), 7.99 (s, 1H), 7.92 (d, *J* = 7.6 Hz, 2H), 7.83 (d, *J* = 7.6 Hz, 2H), 7.72 (dd, *J* = 8.0, 5.2 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.48 – 7.22 (m, 8H), 7.21 – 7.08 (m, 2H), 7.05 – 6.98 (m, 3H), 6.27 (s, 1H), 3.81 (d, *J* = 6.0 Hz, 2H), 0.92 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 167.11, 164.48 (d, *J* = 232.2 Hz), 163.32, 158.44, 150.90 (d, *J* = 9.9 Hz), 143.30, 141.31, 139.99, 138.06, 134.95, 134.87, 131.30, 130.02, 129.60, 129.29, 129.07, 128.59, 128.30, 128.15, 128.04, 126.16, 126.07, 125.73, 125.56, 125.30, 124.53, 116.67, 115.32 (d, *J* = 23.4 Hz), 110.29 (d, *J* = 24.7 Hz), 79.94, 60.32, 53.00, 13.47.

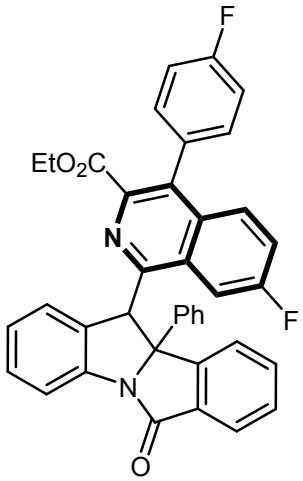
HRMS (ESI) Calc. for $C_{39}H_{27}FN_2O_3$ [M+H]: 591.2078; found: 591.2081.



ethyl 7-methyl-1-(6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-(p-tolyl)isoquinoline-3-carboxylate (5g)

102.1 mg, 85% yield, pale yellow solid, MP = 209-210 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.91 (s, 1H), 7.86 (d, *J* = 7.6 Hz, 2H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 3H), 7.37 – 7.18 (m, 6H), 7.12 (t, *J* = 7.2 Hz, 1H), 7.00 (t, *J* = 11.2 Hz, 3H), 6.82 (d, *J* = 6.0 Hz, 1H), 6.22 (s, 1H), 3.81 (dd, *J* = 12.0, 6.8 Hz, 2H), 2.72 (s, 3H), 2.32 (s, 3H), 0.95 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (100 MHz, DMSO) δ 168.12, 165.71, 157.56, 147.90, 143.83, 140.60, 140.30, 139.20, 138.69, 137.11, 133.25, 133.13, 132.97, 132.09, 131.92, 129.81, 129.48, 129.40, 128.97, 128.77, 128.63, 128.38, 127.80, 127.69, 126.27, 125.98, 125.66, 125.21, 124.35, 123.90, 123.60, 122.66, 116.66, 80.46, 60.11, 52.43, 21.60, 20.78, 13.53.

HRMS (ESI) Calc. for $C_{41}H_{32}N_2O_3$ [M+H]: 601.2486; found: 601.2492.

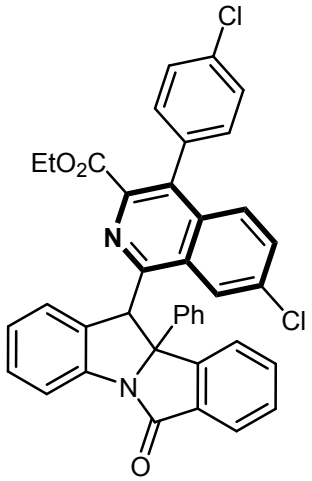


ethyl 7-fluoro-4-(4-fluorophenyl)-1-(6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)isoquinoline-3-carboxylate (5h)

99.8 mg, 82% yield, yellow solid, MP = 102-103 °C. ^{1}H NMR (400 MHz, DMSO) δ 9.01 (d, *J* = 9.6 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.78 (d, *J* = 7.6 Hz, 2H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.53 (dd, *J* = 9.2, 5.6 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.19 (m, 7H), 7.16 – 7.09 (m, 1H), 7.02 (dd, *J* = 17.6, 7.6 Hz, 2H), 6.93 (s, 1H), 6.21 (s, 1H), 3.82 (d, *J* = 6.8 Hz, 2H), 0.96 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (100 MHz, DMSO) δ 168.13, 165.27, 161.85 (d, *J* = 243.4 Hz), 159.33 (d, *J* = 238.8 Hz), 158.50 (d, *J* = 4.4 Hz), 147.70, 143.42, 140.88 (d, *J* = 2.3 Hz), 140.42, 138.57, 132.86, 132.24, 131.96, 131.65 (d, *J* = 8.1 Hz), 130.98 (d, *J* = 3.4 Hz),

129.44 (d, *J* = 9.7 Hz), 129.15, 128.92, 128.46, 127.83 (d, *J* = 4.4 Hz), 127.25 (d, *J* = 9.4 Hz), 125.86, 125.32, 124.39, 123.63, 122.63, 121.72, 121.47, 116.70, 115.34 (d, *J* = 9.8 Hz), 115.13 (d, *J* = 9.4 Hz), 109.51 (d, *J* = 18.7 Hz), 80.63, 60.35, 52.45, 13.51.

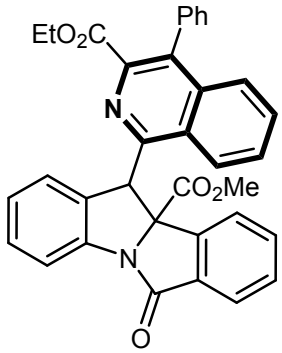
HRMS (ESI) Calc. for $C_{39}H_{26}F_2N_2O_3$ [M+H]: 609.1984; found: 609.1980.



ethyl 7-chloro-4-(4-chlorophenyl)-1-(6-oxo-10b-phenyl-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)isoquinoline-3-carboxylate (5i)

94.7 mg, 74% yield, pale yellow solid, MP = 131-132 °C.^{1}H NMR (400 MHz, DMSO) δ 9.31 (s, 1H), 7.92 – 7.75 (m, 4H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.54 – 7.17 (m, 10H), 7.13 (td, *J* = 7.6, 0.8 Hz, 1H), 7.02 (d, *J* = 7.6 Hz, 2H), 6.92 (d, *J* = 7.2 Hz, 1H), 6.28 (s, 1H), 3.83 (d, *J* = 6.8 Hz, 2H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 168.09, 165.08, 158.52, 151.42, 147.75, 143.44, 141.19, 140.35, 138.52, 134.48, 133.47, 133.39, 133.09, 132.95, 132.03, 131.52, 131.41, 129.06, 128.93, 128.50, 128.44, 128.37, 128.31, 127.89, 126.85, 125.93, 125.35, 124.43, 123.66, 122.71, 116.70, 80.59, 60.53, 52.29, 13.51.

HRMS (ESI) Calc. for $C_{39}H_{26}Cl_2N_2O_3$ [M+H]: 641.1393; found: 641.1386.



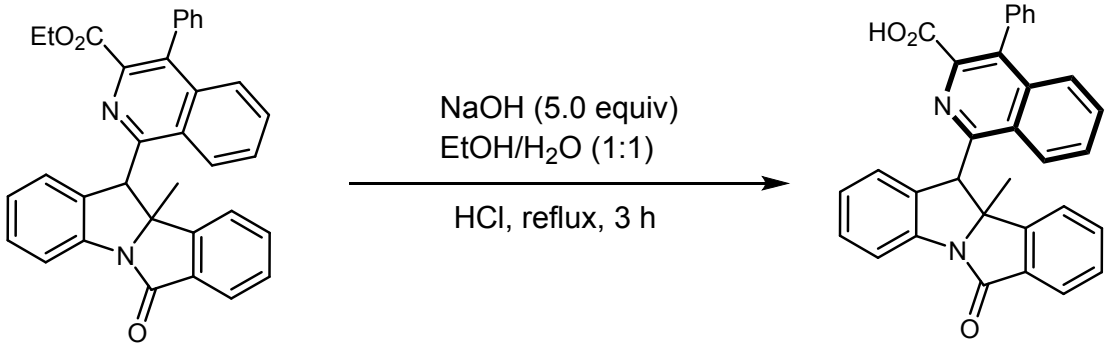
methyl 11-(3-(ethoxycarbonyl)-4-phenylisoquinolin-1-yl)-6-oxo-6*H*-isoindolo[2,1-*a*]indole-10b(11*H*)-carboxylate (5j)

78.7 mg, 72% yield, white solid, MP = 212-213 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (s, 1H), 7.95 – 7.49 (m, 5H), 7.42 – 7.32 (m, 4H), 7.31 – 7.24 (m, 1H), 7.20 – 7.12 (m, 2H), 7.06 (td, *J* = 7.6, 0.8 Hz, 2H), 6.95 (s, 1H), 6.85 (d, *J* = 7.6 Hz, 1H), 6.33 (s, 1H), 3.92 (d, *J* = 6.8 Hz, 2H), 3.75 (s, 3H), 1.01 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (100 MHz, DMSO) δ 171.26, 168.17, 165.48, 157.50, 141.44, 141.30, 140.52, 137.44, 134.83, 134.78, 133.47, 132.24, 131.39, 130.19, 129.57, 129.49, 129.33, 129.23, 128.54, 128.21,

128.15, 127.98, 126.30, 126.07, 125.75, 125.09, 124.60, 123.88, 122.69, 116.25, 80.31, 60.20, 53.82, 48.28, 13.39.

HRMS (ESI) Calc. for $C_{35}H_{26}N_2O_5$ [M+H]: 555.1914; found: 555.1918.

VI. Diversifications



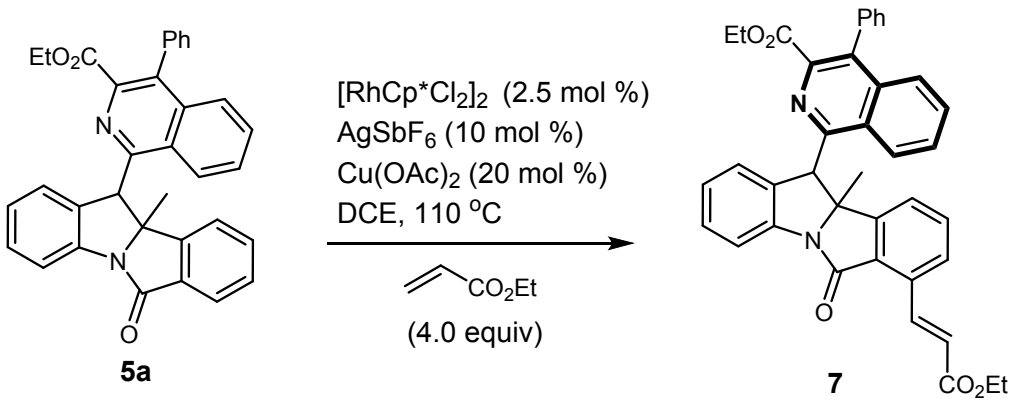
5a **6**

NaOH (5 equiv) was added to solution of the **5a** (0.1 mmol) in H_2O and EtOH (1:1) and was stirred at reflux for 3h. The solution acidified using 2N HCl, filtered and concentrated. The desired product was obtained by column chromatography using appropriate eluent.

1-(10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylic acid (6)

84% yield, brown solid, MP = 258-259 °C. ^{1}H NMR (400 MHz, DMSO) δ 11.99 (s, 1H), 9.01 (d, *J* = 8.4 Hz, 1H), 7.92 (t, *J* = 7.6 Hz, 1H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.38 (d, *J* = 4.8 Hz, 5H), 7.33 – 7.21 (m, 2H), 7.18 – 7.06 (m, 3H), 6.88 (d, *J* = 7.6 Hz, 2H), 5.80 (s, 1H), 1.85 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 168.15, 166.63, 158.64, 148.21, 141.46, 140.11, 139.17, 135.12, 134.97, 132.89, 131.68, 131.06, 129.64, 129.57, 129.10, 128.76, 128.24, 128.11, 128.03, 127.75, 126.16, 125.87, 125.64, 124.33, 123.63, 121.98, 116.80, 75.59, 50.92, 27.72.

HRMS (ESI) Calc. for $C_{32}H_{22}N_2O_3$ [M+H]: 483.1703; found:483.1705.



5a **7**

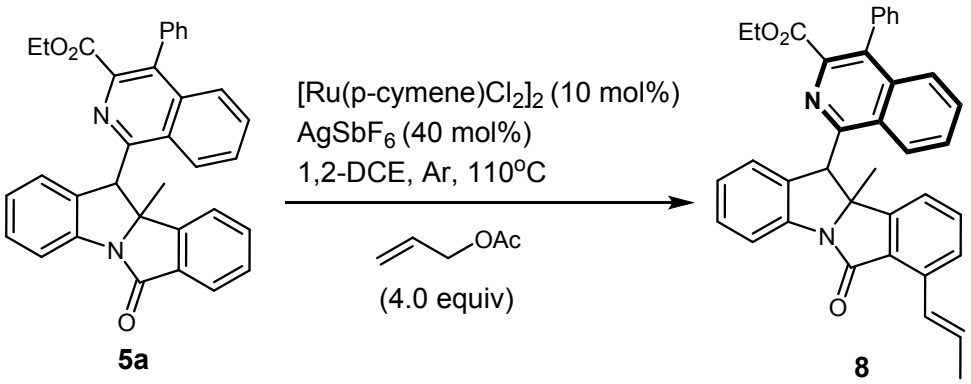
To a 1 mL screw-capped vial equipped with a 10 x 5 mm spinvane-shaped Teflon stirrer bar were charged with **5a** (0.1 mmol), ethyl acrylate (0.4 mmol, 4 equiv), $[Cp^*RhCl_2]_2$ (0.0025 mmol, 2.5 mol %), $AgSbF_6$ (0.01 mmol, 10 mol %), and $Cu(OAc)_2$ (0.02 mmol, 20 mol %) with 1,2-dichloroethane (1 mL) in air condition. The resulting mixture was sealed with Teflon-lined cap

and stirred at 110 °C for 12 h in an oil bath. The reaction was cooled to room temperature, filtered through a plug of celite and washed with dichloromethane (15 mL). The desired product was obtained by column chromatography using appropriate eluent.

ethyl (E)-1-(7-(3-ethoxy-3-oxoprop-1-en-1-yl)-10b-methyl-6-oxo-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylate (7)

79% yield, yellow solid, MP = 264-265 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.98 (d, *J* = 8.4 Hz, 1H), 8.30 (d, *J* = 16.0 Hz, 1H), 7.92 (t, *J* = 7.6 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.79 (t, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.38 (dd, *J* = 21.2, 7.2 Hz, 5H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.22 – 7.07 (m, 3H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.82 (s, 1H), 6.68 (d, *J* = 16.1 Hz, 1H), 5.75 (s, 1H), 4.28 – 4.14 (m, 2H), 3.76 (q, *J* = 6.9 Hz, 2H), 1.87 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H), 0.83 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (100 MHz, DMSO) δ 168.98, 166.98, 166.16, 159.16, 148.05, 143.33, 142.09, 141.98, 141.07, 135.30, 135.03, 133.04, 132.30, 131.64, 130.03, 129.80, 129.33, 128.68, 128.60, 128.42, 126.64, 126.21, 216.13, 126.02, 125.03, 124.07, 122.34, 117.71, 77.12, 60.60, 60.43, 51.14, 27.24, 14.77, 13.89.

HRMS (ESI) Calc. for $C_{39}H_{32}N_2O_5$ [M+H]: 609.2384; found:609.2386.



5a **8**

An oven-dried, screw-cap vial was charged with $[RuCl_2(pcymene)]_2$ (0.01 mmol, 10 mol%), AgSbF6 (0.02 mmol, 20 mol%) and DCE (1 mL). Then, **5a** (1.0 equiv., 0.1 mmol) and allyl acetate (4 equiv., 0.4 mmol) were added into the solution in sequence. The vial was sealed under argon and heated to 110 °C with stirring for 18 hours. After cooling down, the mixture was diluted with DCM, filtered and washed with water and brine. The organic layer was dried, filtered and concentrated to give the crude product which was directly applied to a flash column chromatography (EtOAc/hexanes mixtures).

ethyl (E)-1-(10b-methyl-6-oxo-7-(prop-1-en-1-yl)-10b,11-dihydro-6*H*-isoindolo[2,1-*a*]indol-11-yl)-4-phenylisoquinoline-3-carboxylate (8)

61% yield, yellow solid, MP = 264-265 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.96 (d, *J* = 8.4 Hz, 1H), 7.91 (t, *J* = 7.6 Hz, 1H), 7.82 – 7.71 (m, 1H), 7.62 – 7.49 (m, 2H), 7.45 – 7.36 (m, 4H), 7.28 – 7.06 (m, 6H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.85 (s, 1H), 6.39– 6.30 (m, 1H), 5.66 (s, 1H), 3.78 (q, *J* = 7.2 Hz, 2H), 1.93 (dd, *J* = 6.4, 1.2 Hz, 3H), 1.82 (s, 3H), 0.87 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 168.44, 165.81, 158.87, 147.60, 141.66, 141.20, 138.07, 134.87, 134.55, 133.31, 131.48, 131.09, 129.59, 129.06, 128.79, 128.32, 128.23, 128.14, 127.95, 126.15, 125.73, 125.65, 125.23, 124.39, 124.23, 123.38, 121.73, 76.39, 60.16, 50.64, 26.88, 18.77, 13.46.

HRMS (ESI) Calc. for $C_{37}H_{30}N_2O_3$ [M+H]: 551.2329; found: 551.2321.

VII. References

[1] C. Shen, R.-R. Liu, R.-J. Fan, Y.-L. Li, T.-F. Xu, J.-R. Gao, Y.-X. Jia, *J. Am. Chem. Soc*. 2015, **137**, 4936.

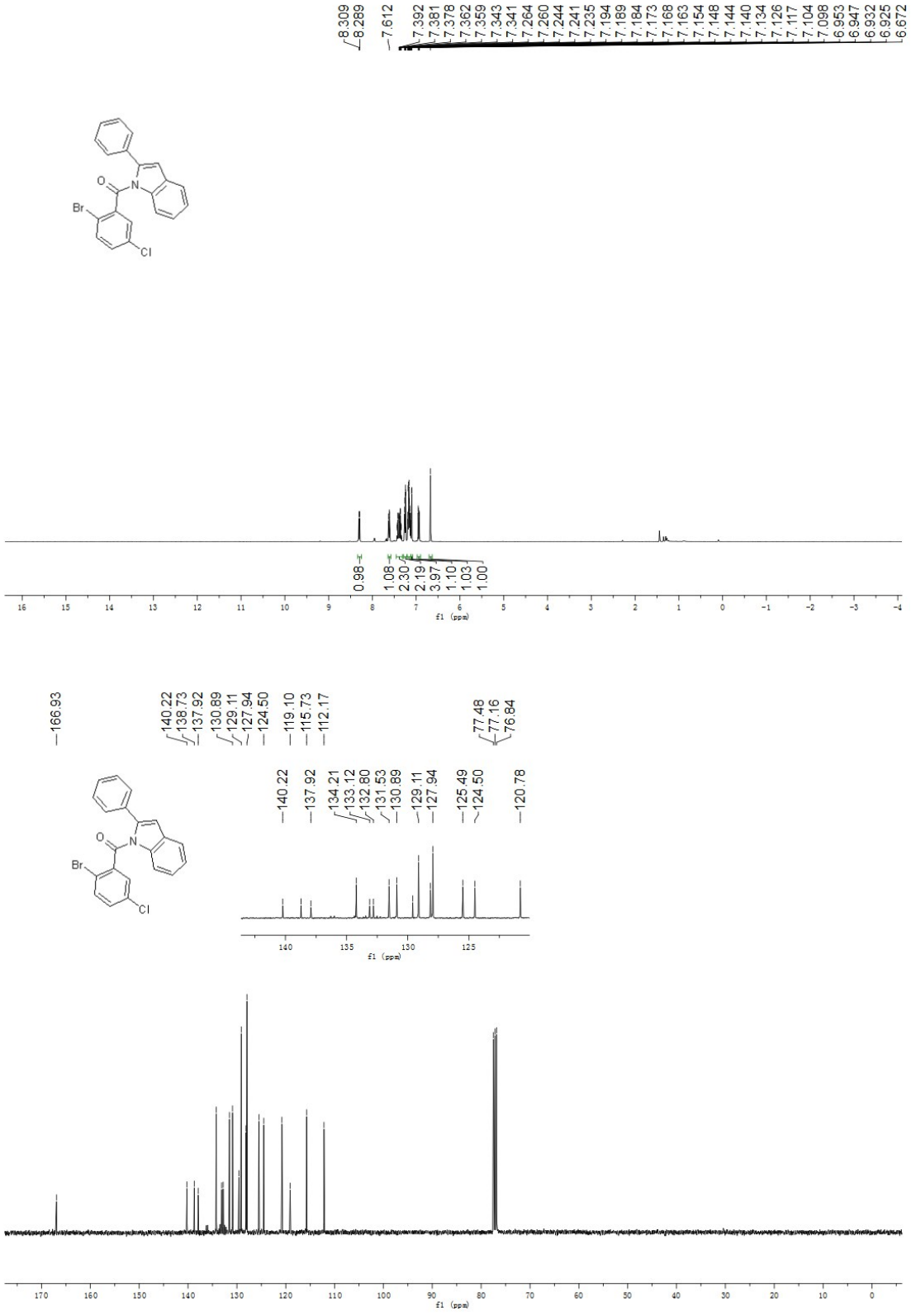
[2] D. A. Petrone, A. Yen, N. Zeidan, M. Lautens, *Org. Lett.* 2015, **17**, 4838.

[3] A. D. Silvia, B. Luca, B. Andrea, D. Gianluca, G. Giuseppe, R. Renata, *Org. Biomol. Chem.* 2005, **3**, 97.

[4] W.-Q. Shi, S. Liu, C. -Z. Wang, Y. Huang, F. -L. Qing, X. -H. Xu, *J. Org. Chem*. 2018, **83**, 15236.

VIII. Copies of ^{1}H and ^{13}C NMR Spectra

1a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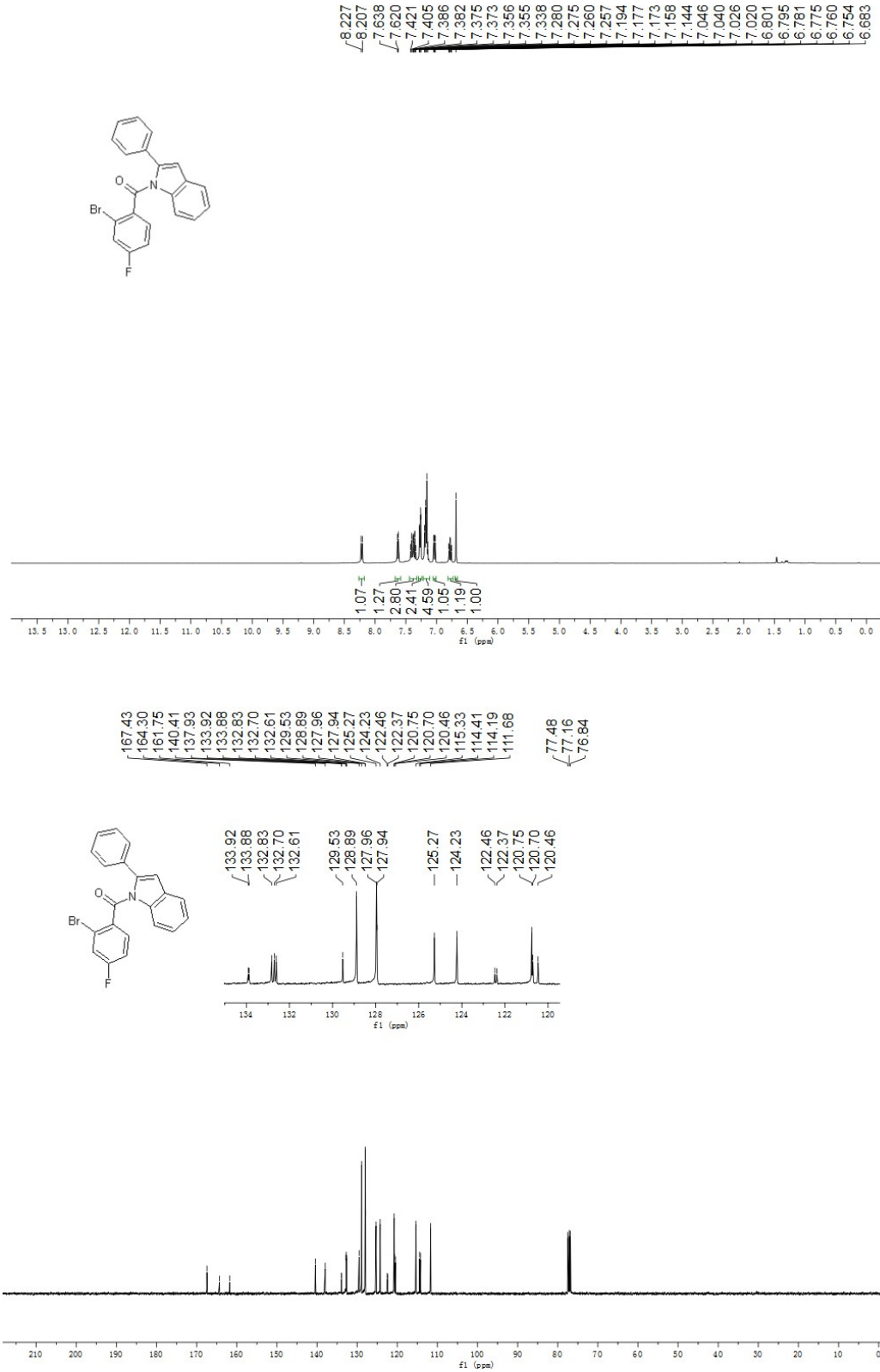
f1 (ppm)

1b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O
N
F
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1.00
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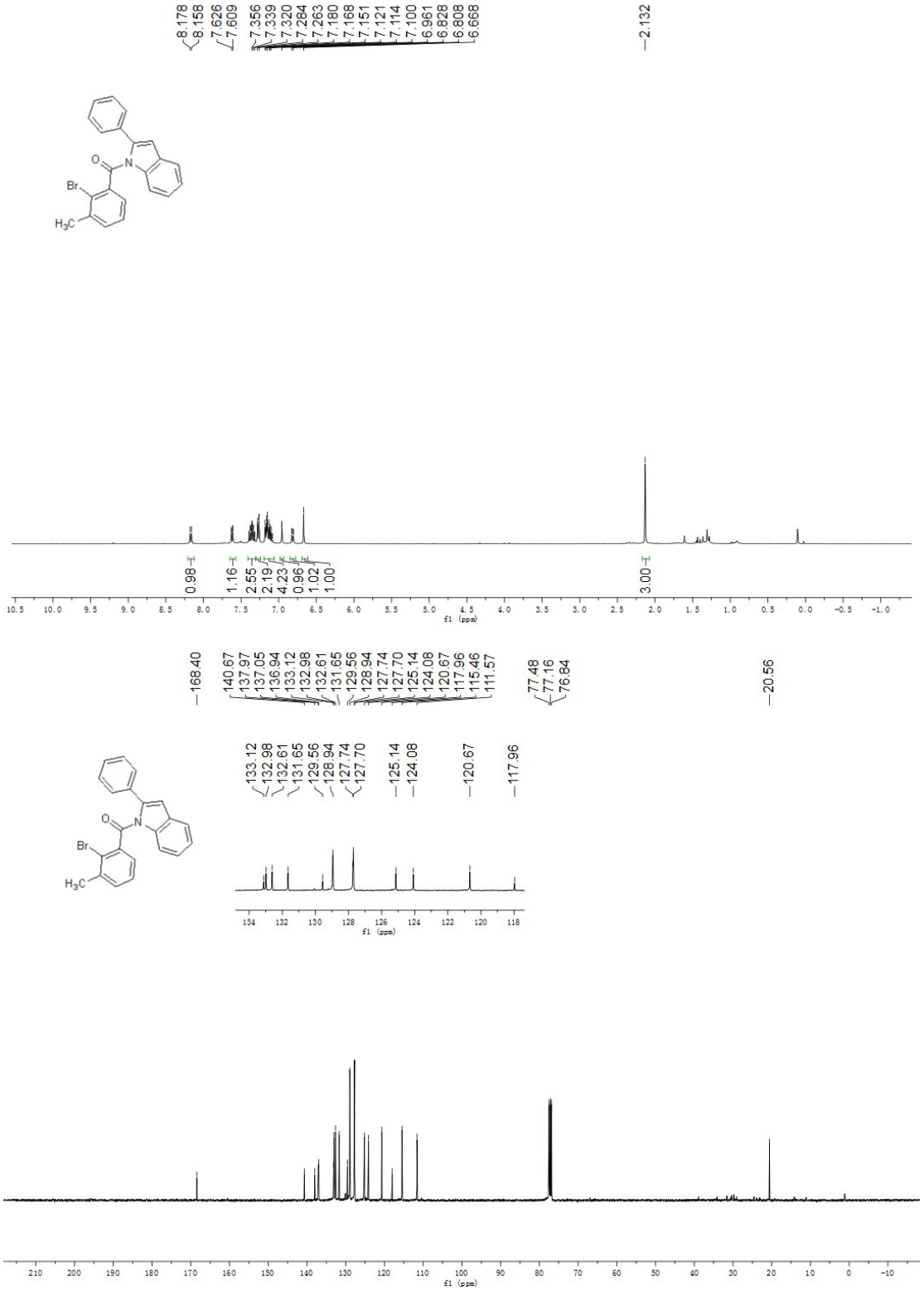
f1 (ppm)

1c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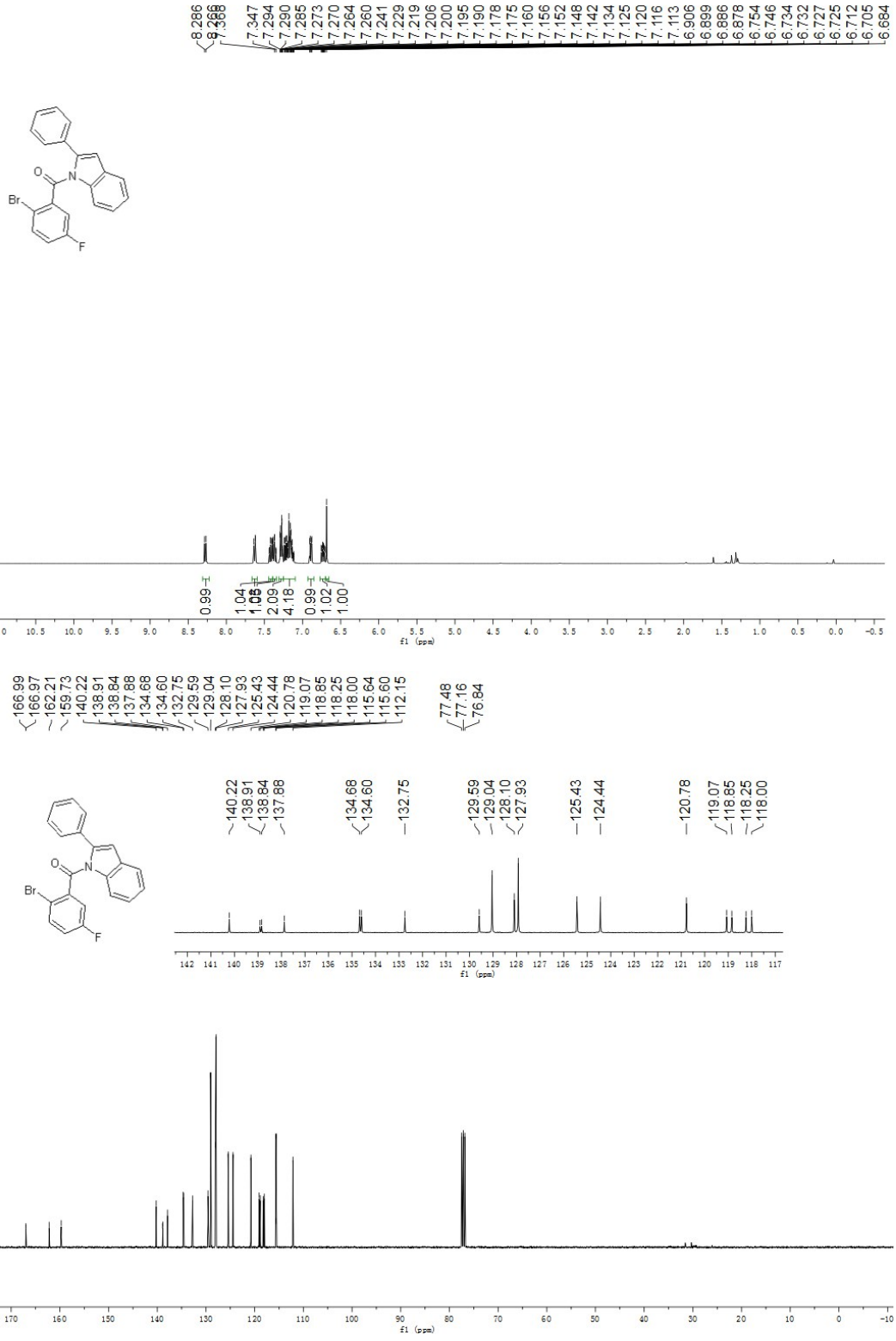
1d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Br
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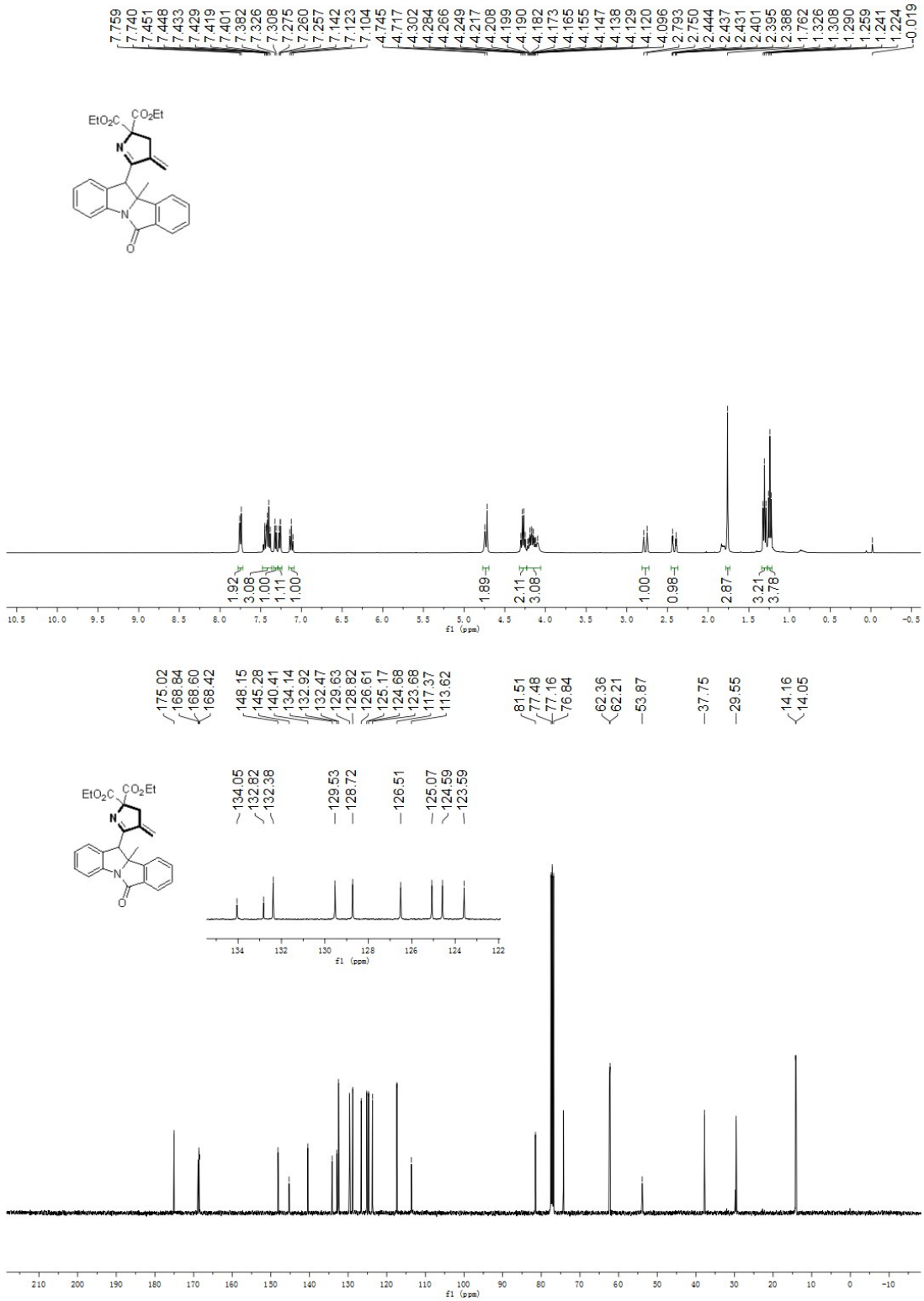
f1 (ppm)
f1 (ppm)

3a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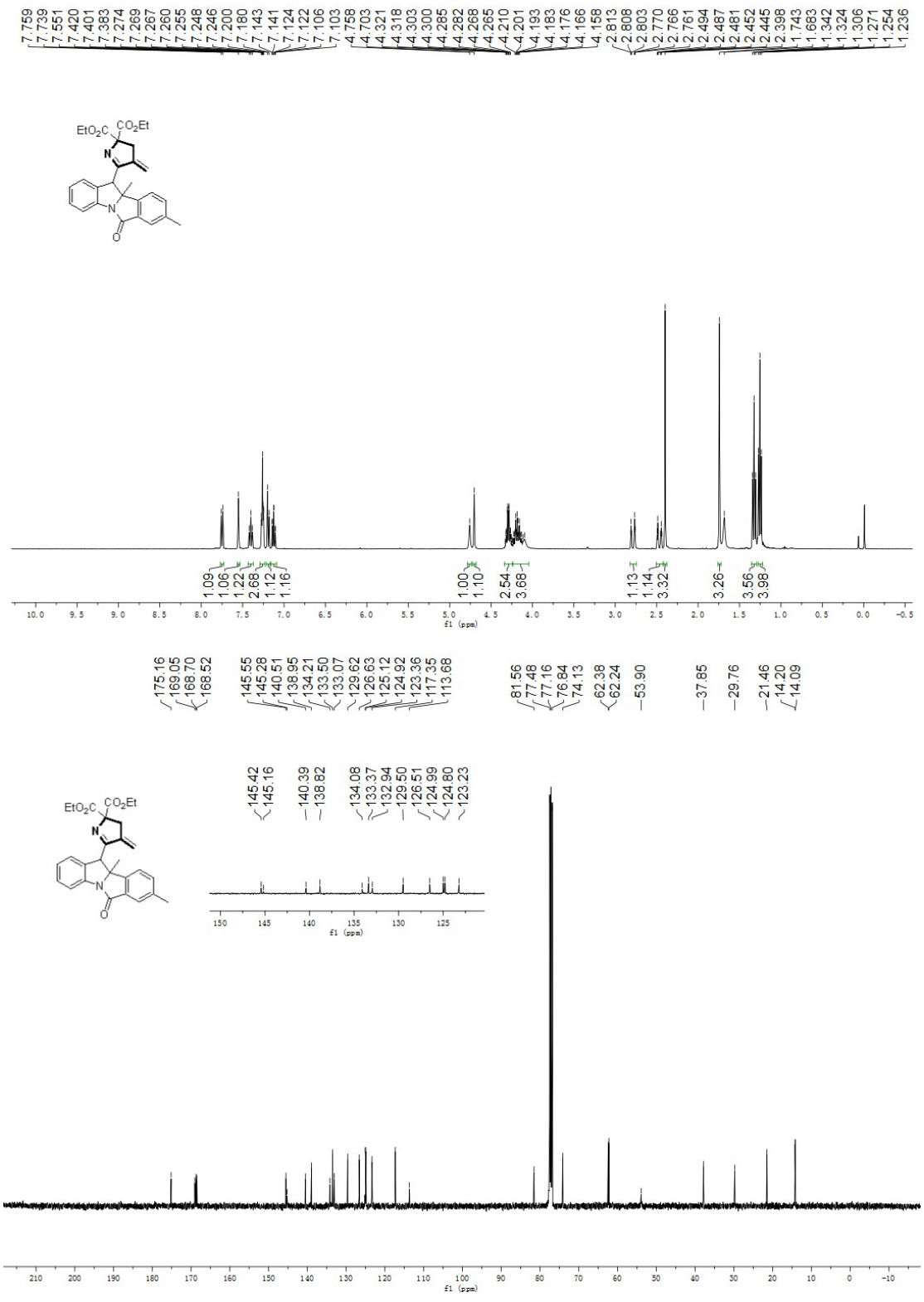
3b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f1 (ppm)

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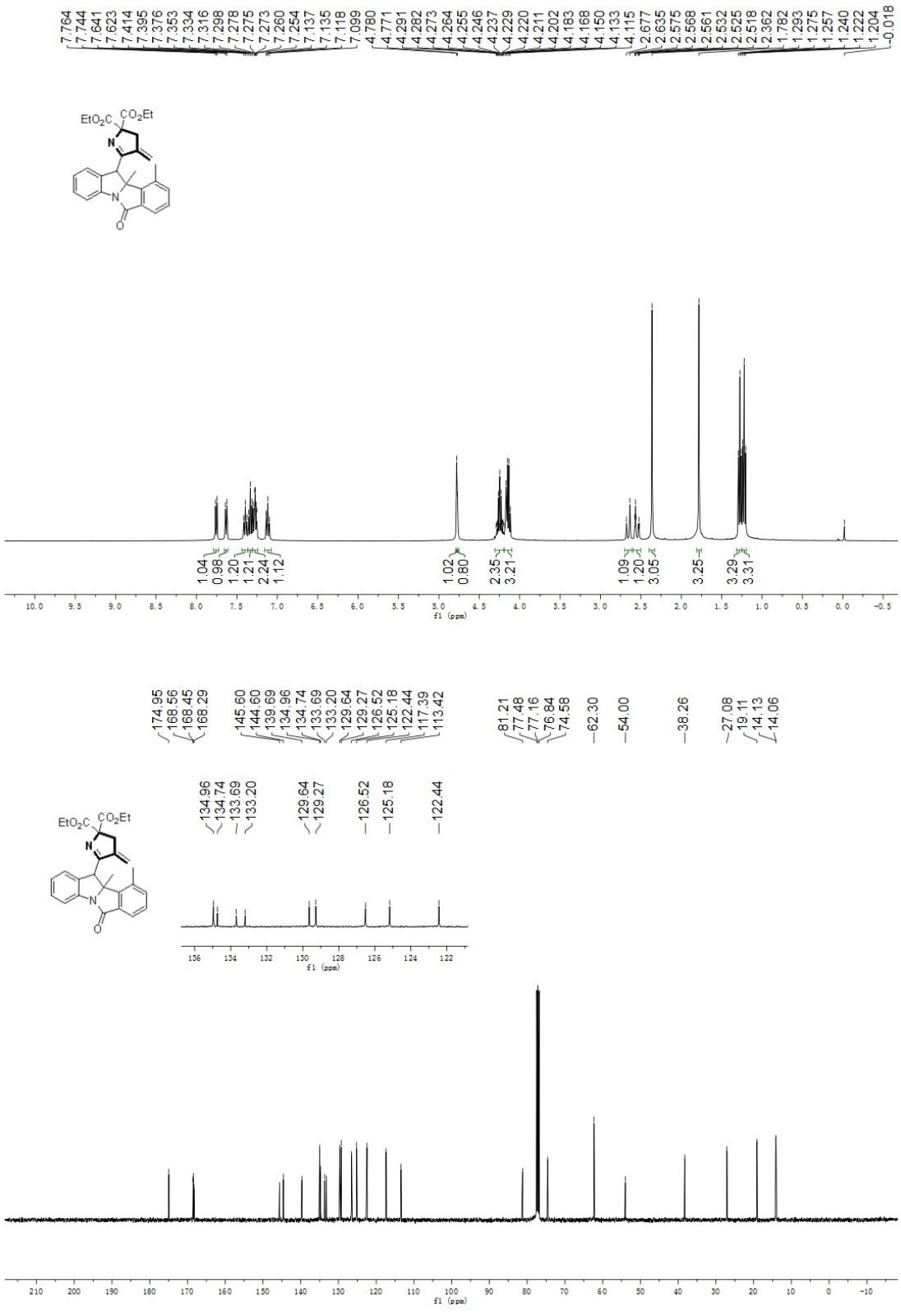
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3d


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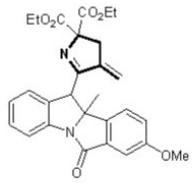
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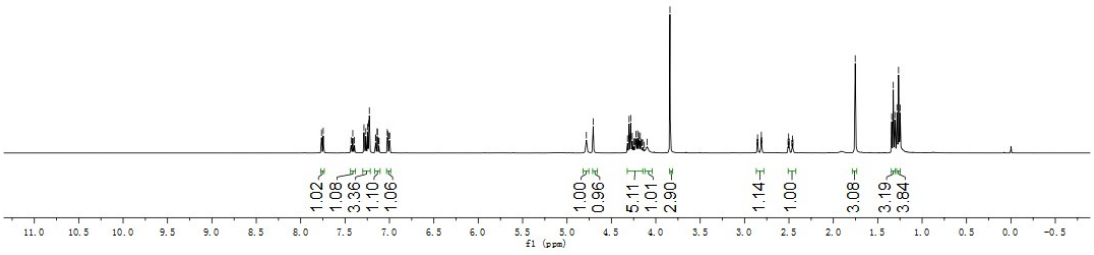
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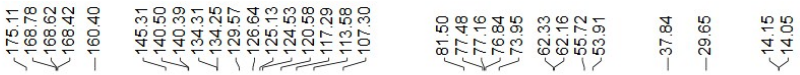
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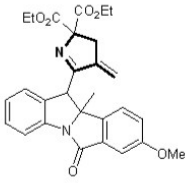
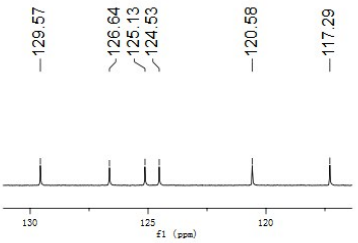
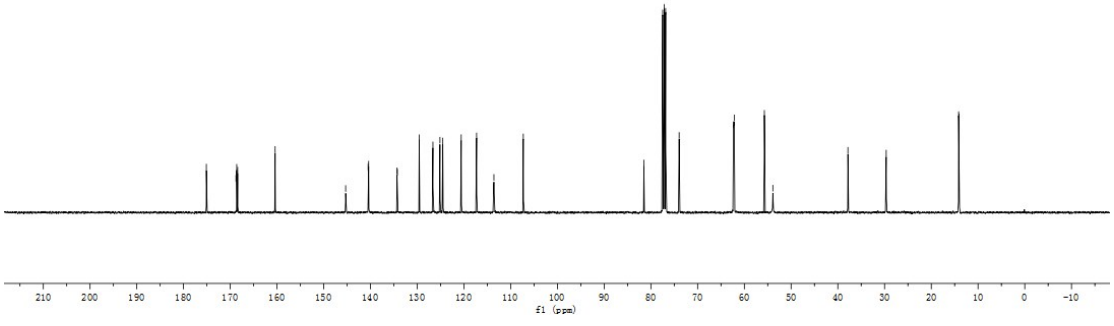
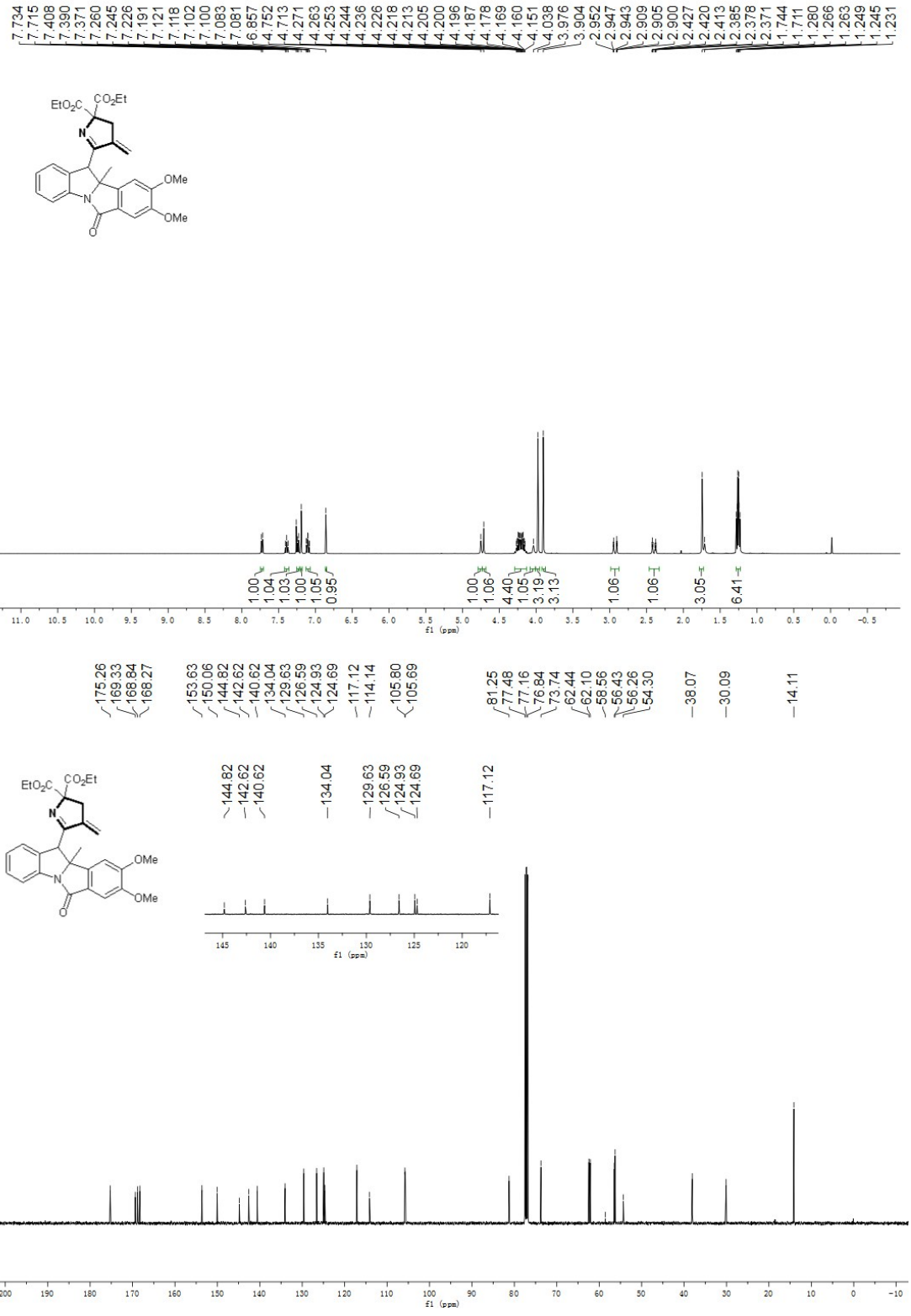
14.15
14.05


EtO2C
CO2Et
N
OMe
O


129.57
126.64
125.13
124.53
120.58
117.29
130
125
120
f1 (ppm)


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3e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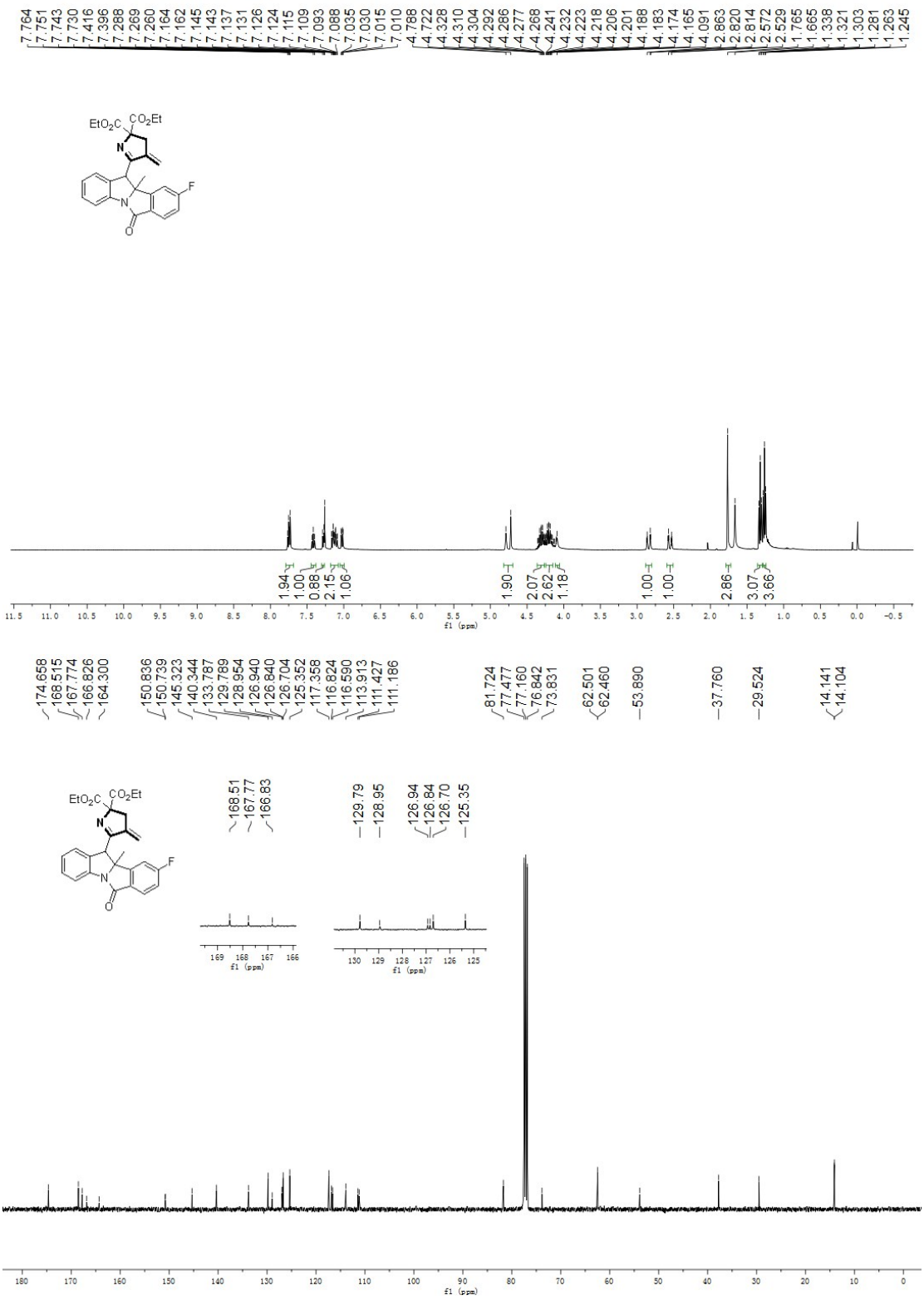
7.715
7.408
7.390
7.371
7.260
7.245
7.226
7.191
7.121
7.118
7.102
7.100
7.083
7.081
6.857
4.752
4.713
4.271
4.263
4.253
4.244
4.236
4.226
4.218
4.213
4.205
4.200
4.196
4.187
4.178
4.169
4.160
4.151
4.038
3.976
3.904
2.952
2.947
2.943
2.909
2.905
2.900
2.427
2.420
2.413
2.385
2.378
2.371
1.744
1.711
1.280
1.266
1.263
1.249
1.245
1.231
EtO2C
CO2Et
N
OMe
OMe
O
1.00
1.04
1.03
1.00
1.05
0.95
1.00
1.06
4.40
1.05
3.19
3.13
1.06
1.06
3.05
6.41
f1 (ppm)
175.26
169.33
168.84
168.27
153.63
150.06
144.82
142.62
140.62
134.04
129.63
126.59
124.93
124.69
117.12
114.14
105.80
105.69
81.25
77.48
77.16
76.84
73.74
62.44
62.10
58.56
56.43
56.26
54.30
38.07
30.09
14.11
144.82
142.62
140.62
134.04
129.63
126.59
124.93
124.69
117.12
f1 (ppm)

3f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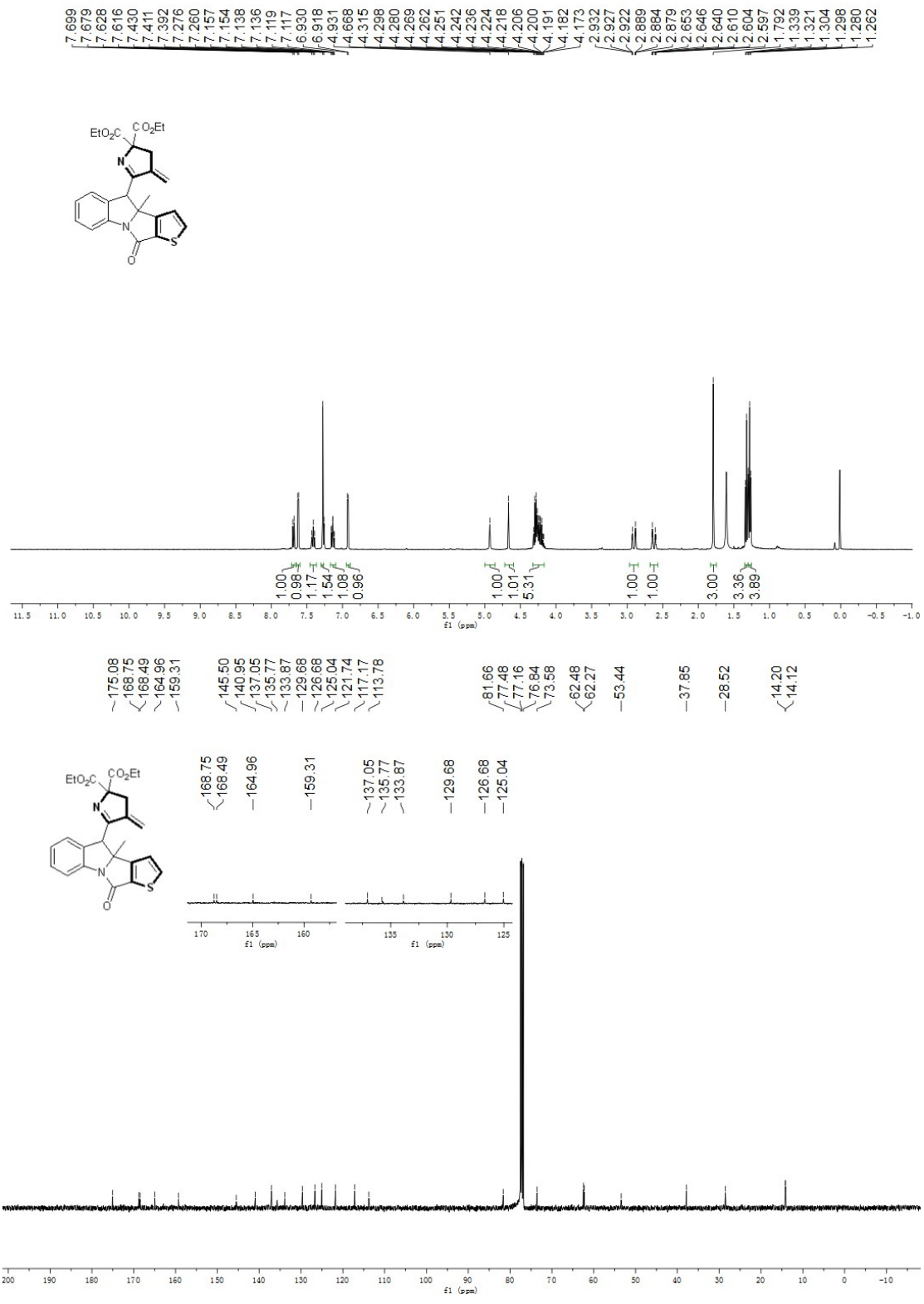
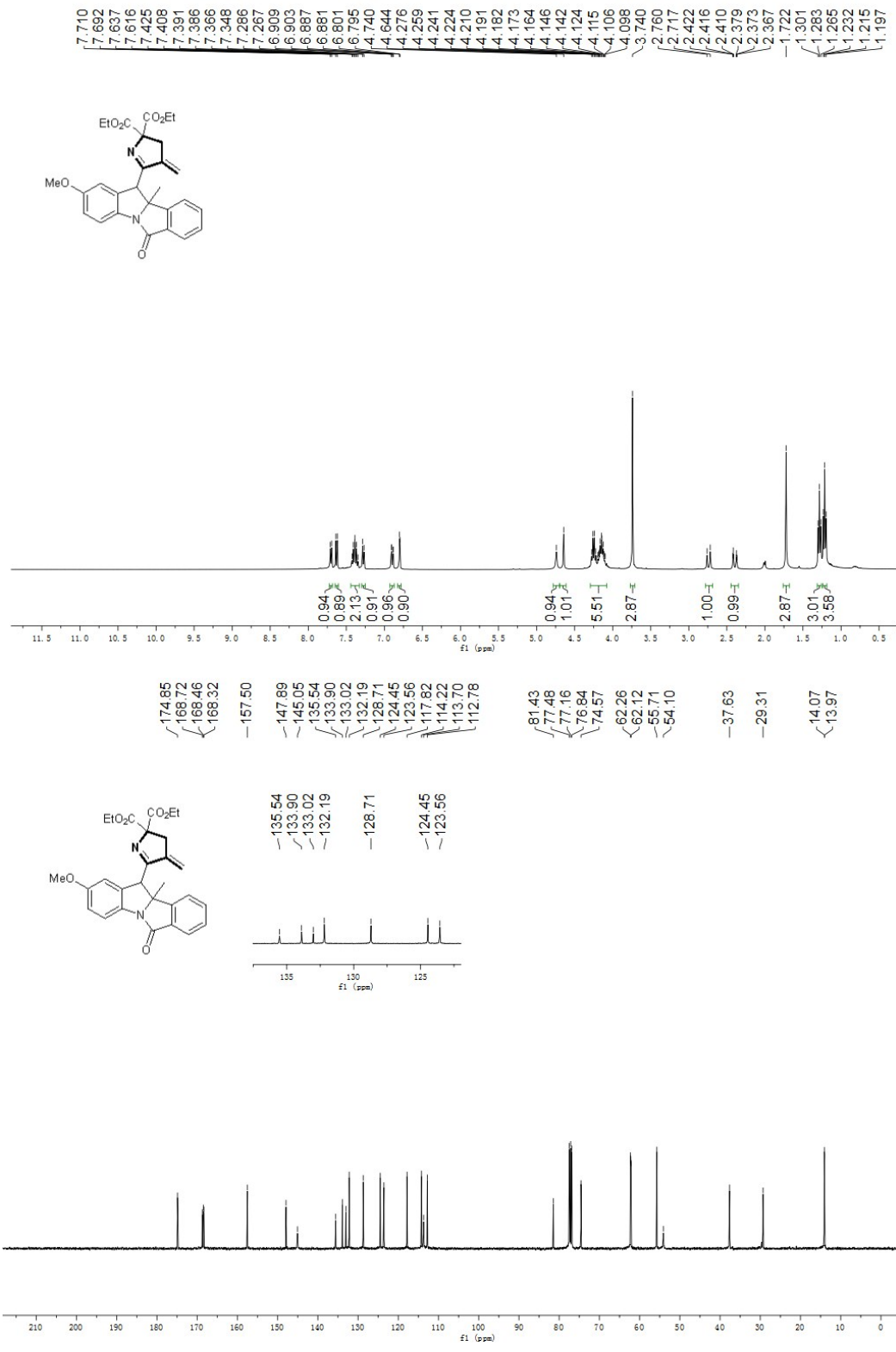
7.751
7.743
7.730
7.416
7.396
7.288
7.269
7.260
7.164
7.162
7.145
7.143
7.137
7.131
7.126
7.124
7.115
7.109
7.093
7.088
7.035
7.030
7.015
7.010
4.788
4.722
4.328
4.310
4.304
4.292
4.286
4.277
4.268
4.241
4.232
4.223
4.218
4.206
4.201
4.188
4.183
4.174
4.165
4.091
2.863
2.820
2.814
2.572
2.529
1.765
1.665
1.338
1.321
1.303
1.281
1.263
1.245
EtO2C
CO2Et
N
F
O
1.94
1.00
0.88
2.15
1.06
1.90
2.07
2.62
1.18
1.00
1.00
2.86
3.07
3.66
f1 (ppm)
174.658
168.515
167.774
166.826
164.300
150.836
150.739
145.323
140.344
133.787
129.789
128.954
126.940
126.840
126.704
125.352
117.358
116.824
116.590
113.913
111.427
111.186
81.724
77.477
77.160
76.842
73.831
62.501
62.460
53.890
37.760
29.524
14.141
14.104
168.51
167.77
166.83
129.79
128.95
126.94
126.84
126.70
125.35

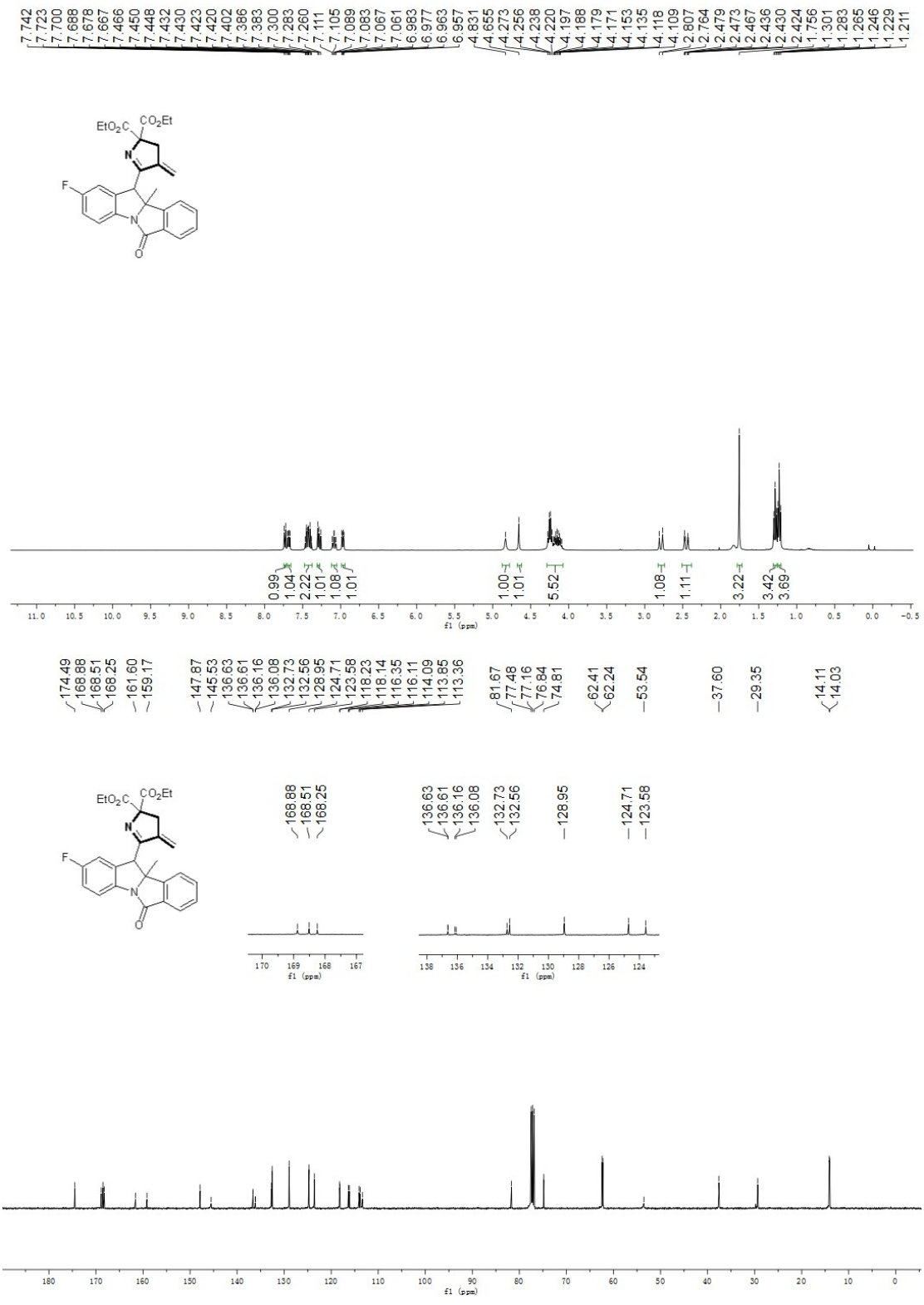
3g


7.699
7.679
7.628
7.616
7.430
7.411
7.392
7.276
7.260
7.157
7.154
7.138
7.136
7.119
7.117
6.930
6.918
4.931
4.668
4.315
4.298
4.280
4.269
4.262
4.251
4.242
4.236
4.224
4.218
4.206
4.200
4.191
4.182
4.173
2.932
2.927
2.922
2.889
2.884
2.879
2.653
2.646
2.640
2.610
2.604
2.597
1.792
1.339
1.321
1.304
1.298
1.280
1.262
EtO2C
CO2Et
N
N
S
O
1.00
0.98
1.17
1.54
1.08
0.96
1.00
1.01
5.31
1.00
1.00
3.00
3.36
3.89
f1 (ppm)
175.08
168.75
168.49
164.96
159.31
145.50
140.95
137.05
135.77
133.87
129.68
126.68
125.04
121.74
117.17
113.78
81.66
77.48
77.16
76.84
73.58
62.48
62.27
53.44
37.85
28.52
14.20
14.12
f1 (ppm)

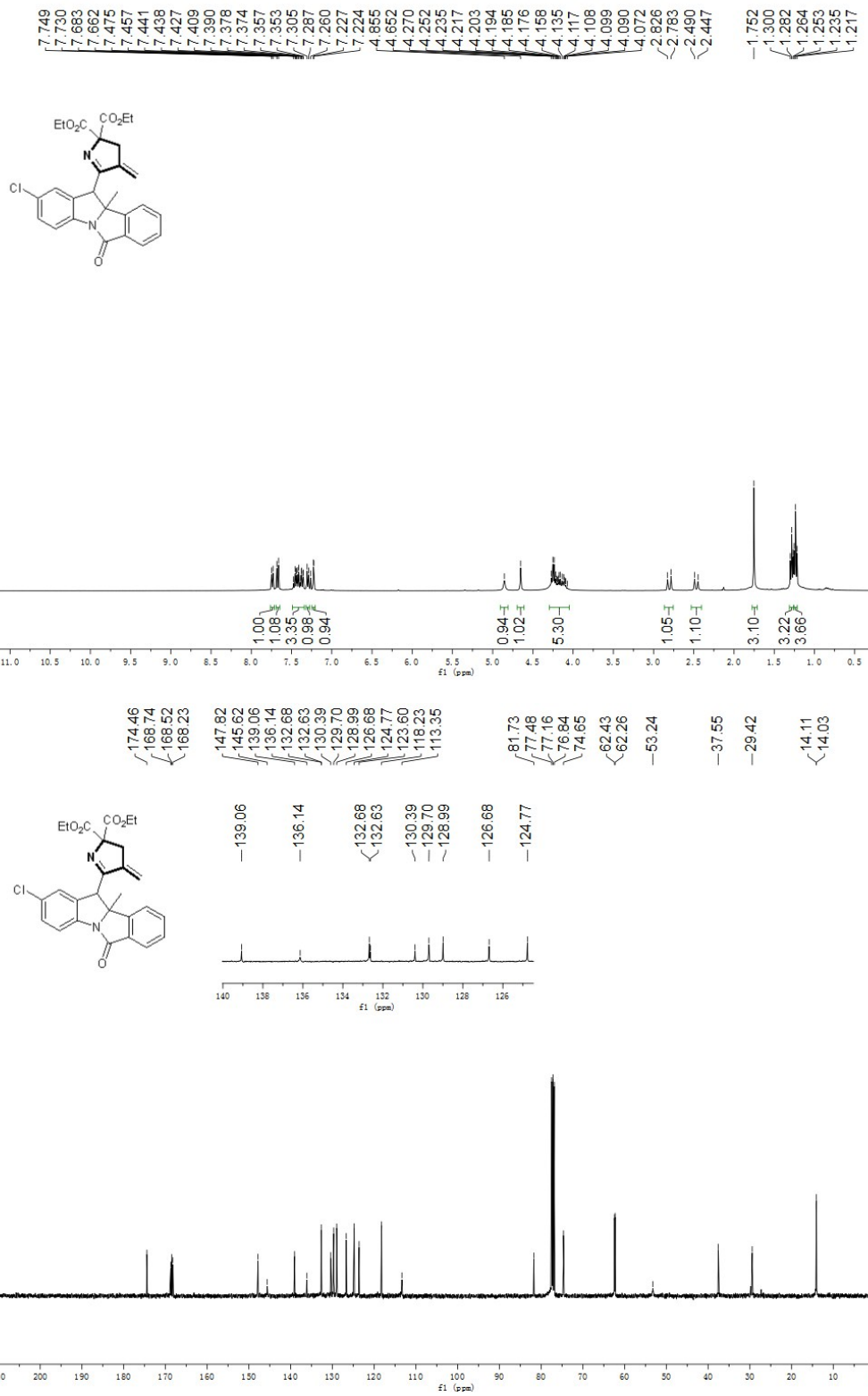
3h


7.710
7.692
7.637
7.616
7.425
7.408
7.391
7.386
7.366
7.348
7.286
7.267
6.909
6.903
6.887
6.881
6.801
6.795
4.740
4.644
4.276
4.259
4.241
4.224
4.210
4.191
4.182
4.173
4.164
4.146
4.142
4.124
4.115
4.106
4.098
3.740
2.760
2.717
2.422
2.416
2.410
2.379
2.373
2.367
1.722
1.301
1.283
1.265
1.232
1.215
1.197
EtO2C
CO2Et
MeO
0.94
0.89
2.13
0.91
0.96
0.90
0.94
1.01
5.51
2.87
1.00
0.99
2.87
3.01
3.58
f1 (ppm)
174.85
168.72
168.46
168.32
157.50
147.89
145.05
135.54
133.90
133.02
132.19
128.71
124.45
123.56
117.82
114.22
113.70
112.78
81.43
77.48
77.16
76.84
74.57
62.26
62.12
55.71
54.10
37.63
29.31
14.07
13.97

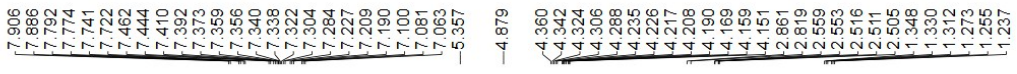
3i

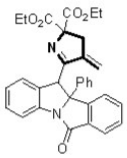

7.742
7.723
7.700
7.688
7.678
7.667
7.466
7.450
7.448
7.432
7.430
7.423
7.420
7.402
7.386
7.383
7.300
7.283
7.260
7.111
7.105
7.089
7.083
7.067
7.061
6.983
6.977
6.963
6.957
4.831
4.655
4.273
4.256
4.238
4.220
4.197
4.188
4.179
4.171
4.153
4.135
4.118
4.109
2.807
2.764
2.479
2.473
2.467
2.436
2.430
2.424
1.756
1.301
1.283
1.265
1.246
1.229
1.211
EtO2C
CO2Et
N
F
N
O
0.99
1.04
2.22
1.01
1.08
1.01
1.00
1.01
5.52
1.08
1.11
3.22
3.42
3.69
f1 (ppm)
174.49
168.88
168.51
168.25
161.60
159.17
147.87
145.53
136.63
136.61
136.16
136.08
132.73
132.56
128.95
124.71
123.58
118.23
118.14
116.35
116.11
114.09
113.85
113.36
81.67
77.48
77.16
76.84
74.81
62.41
62.24
53.54
37.60
29.35
14.11
14.03
f1 (ppm)
f1 (ppm)
f1 (ppm)

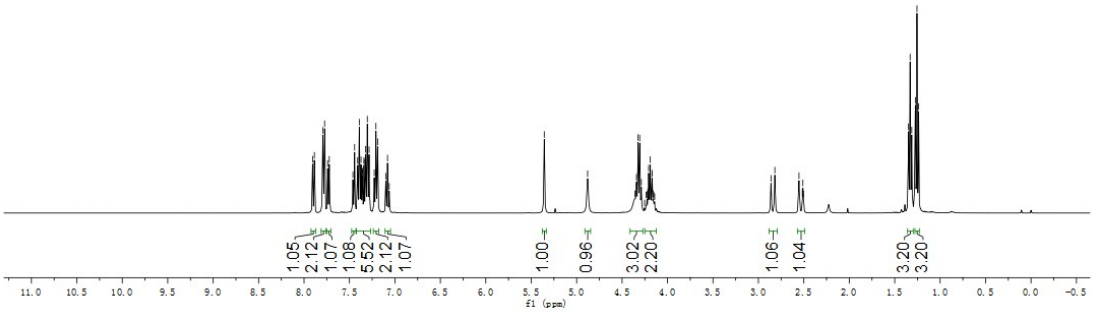
3j

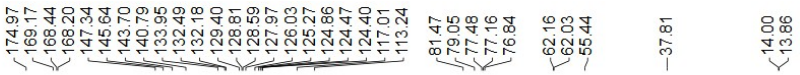

7.749
7.730
7.683
7.662
7.475
7.457
7.441
7.438
7.427
7.409
7.390
7.378
7.374
7.357
7.353
7.305
7.287
7.260
7.227
7.224
4.855
4.652
4.270
4.252
4.235
4.217
4.203
4.194
4.185
4.176
4.158
4.135
4.117
4.108
4.099
4.090
4.072
2.826
2.783
2.490
2.447
1.752
1.300
1.282
1.264
1.253
1.235
1.217
EtO2C
CO2Et
Cl
N
O
1.00
1.08
3.35
0.98
0.94
0.94
1.02
5.30
1.05
1.10
3.10
3.22
3.66
f1 (ppm)
174.46
168.74
168.52
168.23
147.82
145.62
139.06
136.14
132.68
132.63
130.39
129.70
128.99
126.68
124.77
123.60
118.23
113.35
81.73
77.48
77.16
76.84
74.65
62.43
62.26
53.24
37.55
29.42
14.11
14.03

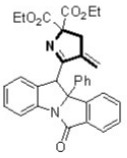
3k

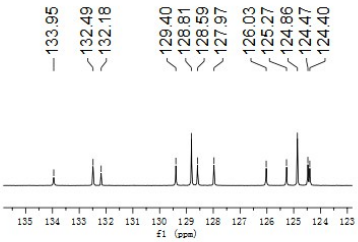

7.906
7.886
7.792
7.774
7.741
7.722
7.462
7.444
7.410
7.392
7.373
7.359
7.356
7.340
7.338
7.322
7.304
7.284
7.227
7.209
7.190
7.100
7.081
7.063
5.357
4.879
4.360
4.342
4.324
4.306
4.288
4.235
4.226
4.217
4.208
4.190
4.169
4.159
4.151
2.861
2.819
2.559
2.553
2.516
2.511
2.505
1.348
1.330
1.312
1.273
1.255
1.237

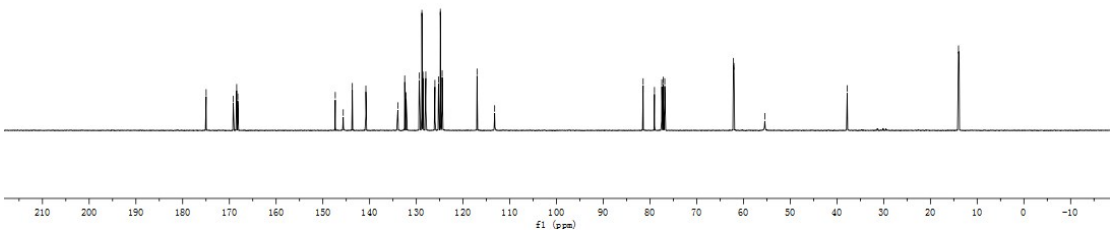

EtO2C
CO2Et
N
Ph
N
O


1.05
2.12
1.07
1.08
5.52
2.12
1.07
1.00
0.96
3.02
2.20
1.06
1.04
3.20
3.20
f1 (ppm)

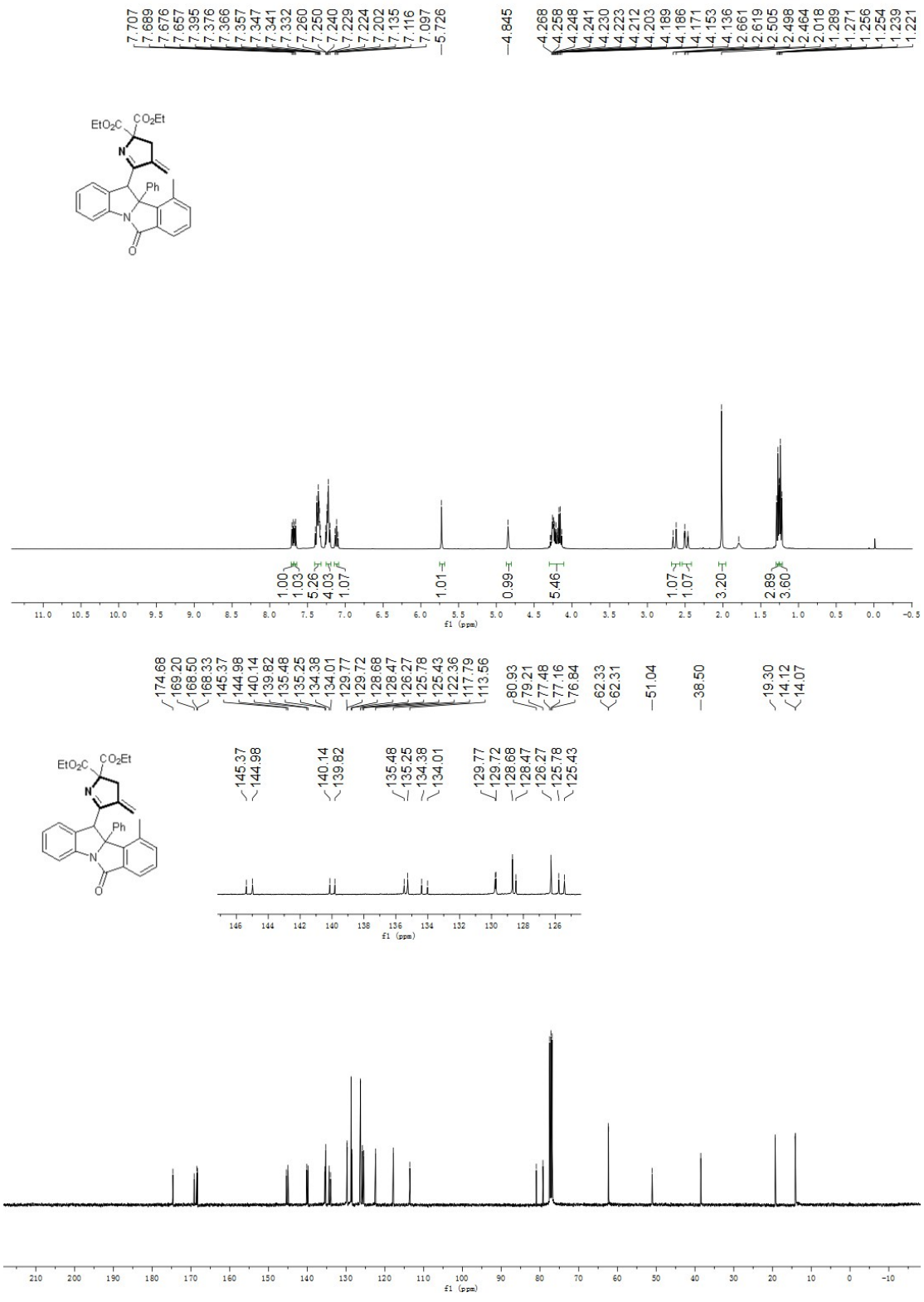

174.97
169.17
168.44
168.20
147.34
145.64
143.70
140.79
133.95
132.49
132.18
129.40
128.81
128.59
127.97
126.03
125.27
124.86
124.47
124.40
117.01
113.24
81.47
79.05
77.48
77.16
76.84
62.16
62.03
55.44
37.81
14.00
13.86


EtO2C
CO2Et
N
Ph
N
O


133.95
132.49
132.18
129.40
128.81
128.59
127.97
126.03
125.27
124.86
124.47
124.40
f1 (ppm)


f1 (ppm)

3l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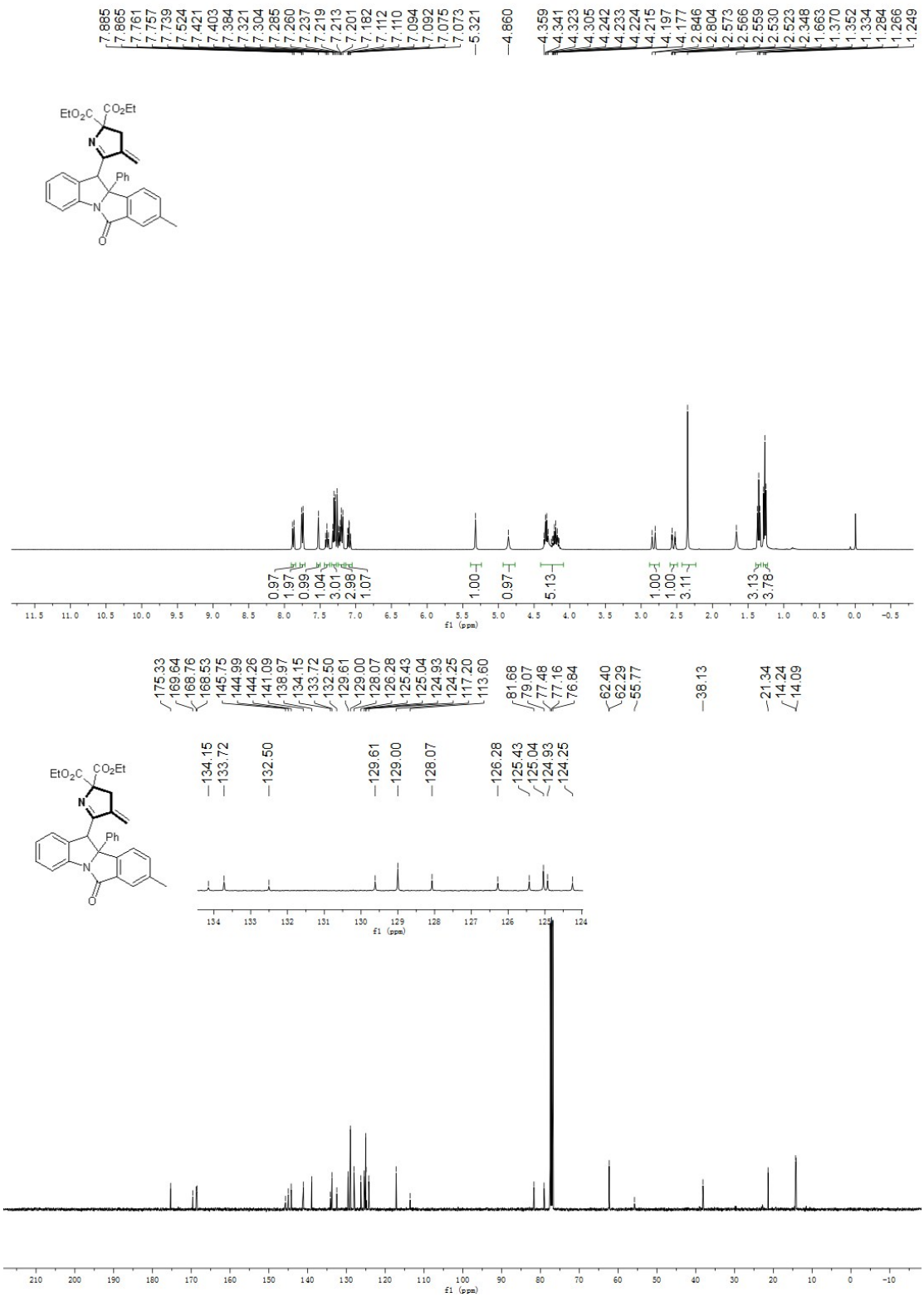
7.395
7.376
7.366
7.357
7.347
7.341
7.332
7.260
7.250
7.240
7.229
7.224
7.202
7.135
7.116
7.097
5.726
4.845
4.268
4.258
4.248
4.241
4.230
4.223
4.212
4.203
4.189
4.186
4.171
4.153
4.136
2.661
2.619
2.505
2.498
2.464
2.018
1.289
1.271
1.256
1.254
1.239
1.221
EtO2C
CO2Et
Ph
1.00
1.03
5.26
4.03
1.07
1.01
0.99
5.46
1.07
1.07
3.20
2.89
3.60
f1 (ppm)
174.68
169.20
168.50
168.33
145.37
144.98
140.14
139.82
135.48
135.25
134.38
134.01
129.77
129.72
128.68
128.47
126.27
125.78
125.43
122.36
117.79
113.56
80.93
79.21
77.48
77.16
76.84
62.33
62.31
51.04
38.50
19.30
14.12
14.07

3m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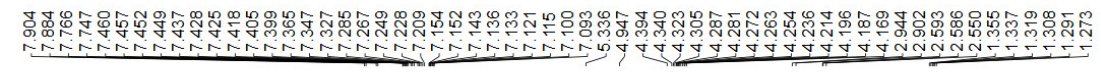
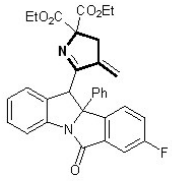
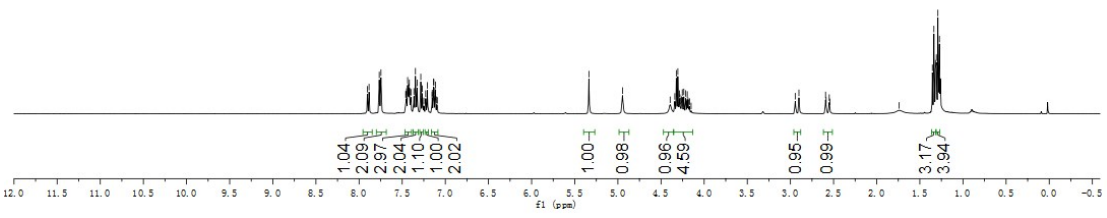
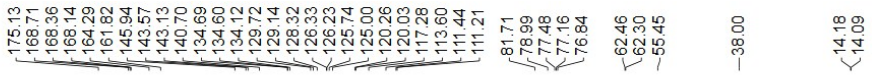
7.761
7.757
7.739
7.524
7.421
7.403
7.384
7.321
7.304
7.285
7.260
7.237
7.219
7.213
7.201
7.182
7.112
7.110
7.094
7.092
7.075
7.073
5.321
4.860
4.359
4.341
4.323
4.305
4.242
4.233
4.224
4.215
4.197
4.177
2.846
2.804
2.573
2.566
2.559
2.530
2.523
2.348
1.663
1.370
1.352
1.334
1.284
1.266
1.249
EtO2C
CO2Et
N
Ph
O
0.97
1.97
0.99
1.04
3.01
2.98
1.07
1.00
0.97
5.13
1.00
1.00
3.11
3.13
3.78
f1 (ppm)
175.33
169.64
168.76
168.53
145.75
144.99
144.26
141.09
138.97
134.15
133.72
132.50
129.61
129.00
128.07
126.28
125.43
125.04
124.93
124.25
117.20
113.60
81.68
79.07
77.48
77.16
76.84
62.40
62.29
55.77
38.13
21.34
14.24
14.09

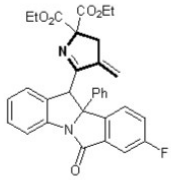
3n

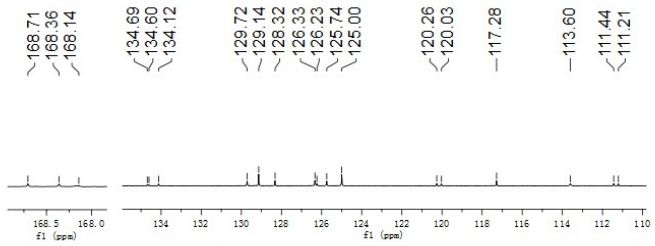


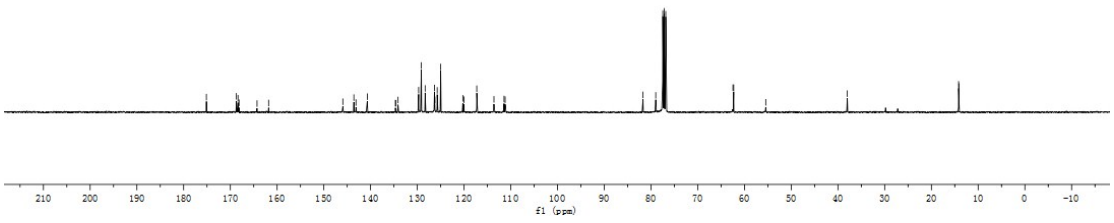




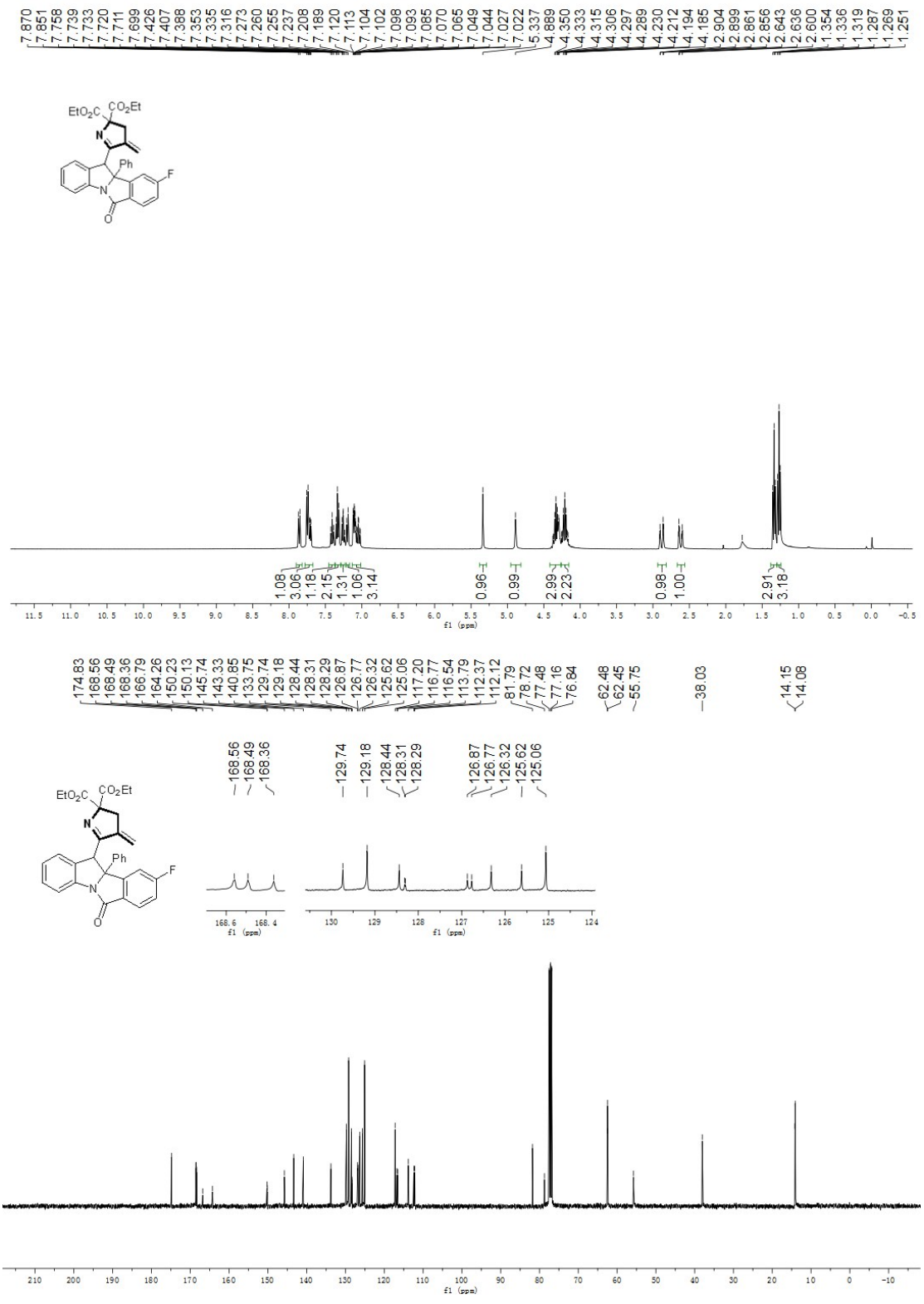








3o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7.699
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7.407
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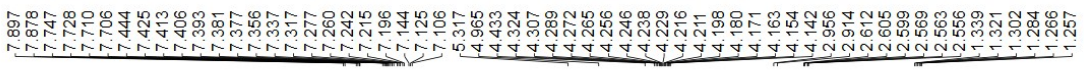
7.353
7.335
7.316
7.273
7.260
7.255
7.237
7.208
7.189
7.120
7.113
7.104
7.102
7.098
7.093
7.085
7.070
7.065
7.049
7.044
7.027
7.022
5.337
4.889
4.350
4.333
4.315
4.306
4.297
4.289
4.230
4.212
4.194
4.185
2.904
2.899
2.861
2.856
2.643
2.636
2.600
1.354
1.336
1.319
1.287
1.269
1.251
EtO2C
CO2Et
Ph
F
O
1.08
3.06
1.18
2.15
1.31
1.06
3.14
0.96
0.99
2.99
2.23
0.98
1.00
2.91
3.18
f1 (ppm)
174.83
168.56
168.49
168.36
166.79
164.26
150.23
150.13
145.74
143.33
140.85
133.75
129.74
129.18
128.44
128.31
128.29
126.87
126.77
126.32
125.62
125.06
117.20
116.77
116.54
113.79
112.37
112.12
81.79
78.72
77.48
77.16
76.84
62.48
62.45
55.75
38.03
14.15
14.08

3p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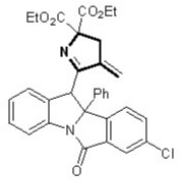
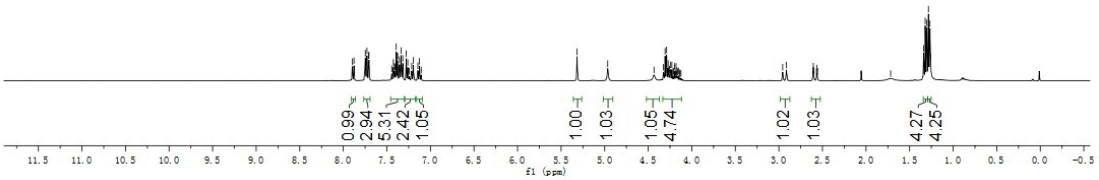
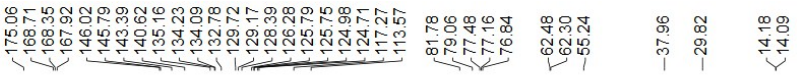
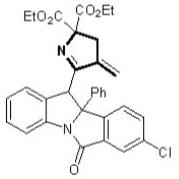
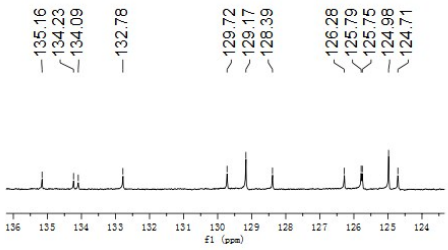
7.878
7.747
7.728
7.710
7.706
7.444
7.425
7.413
7.406
7.393
7.381
7.377
7.356
7.337
7.317
7.277
7.260
7.242
7.215
7.196
7.144
7.125
7.106
5.317
4.965
4.433
4.324
4.307
4.289
4.272
4.265
4.256
4.246
4.238
4.229
4.216
4.211
4.198
4.180
4.171
4.163
4.154
4.142
2.956
2.914
2.612
2.605
2.599
2.569
2.563
2.556
1.339
1.321
1.302
1.284
1.266
1.257

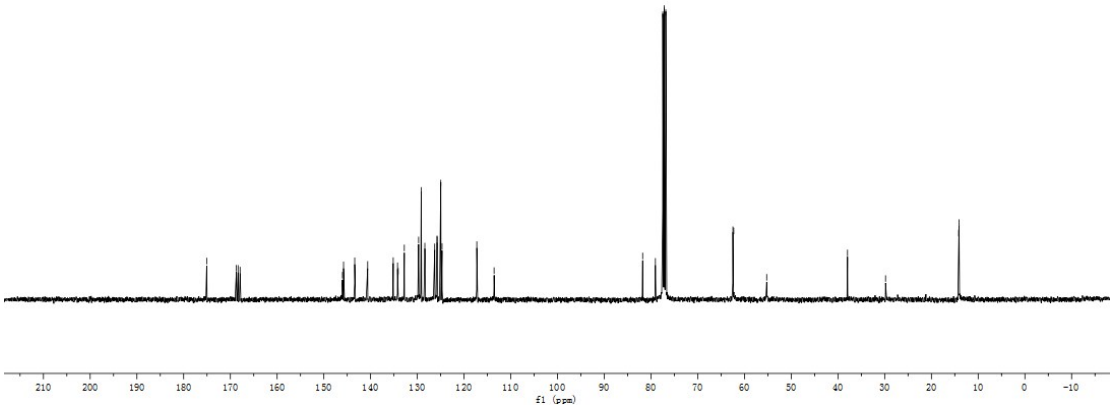

EtO2C
CO2Et
N
Ph
N
O
Cl


0.99
2.94
5.31
2.42
1.05
1.00
1.03
1.05
4.74
1.02
1.03
4.27
4.25
f1 (ppm)

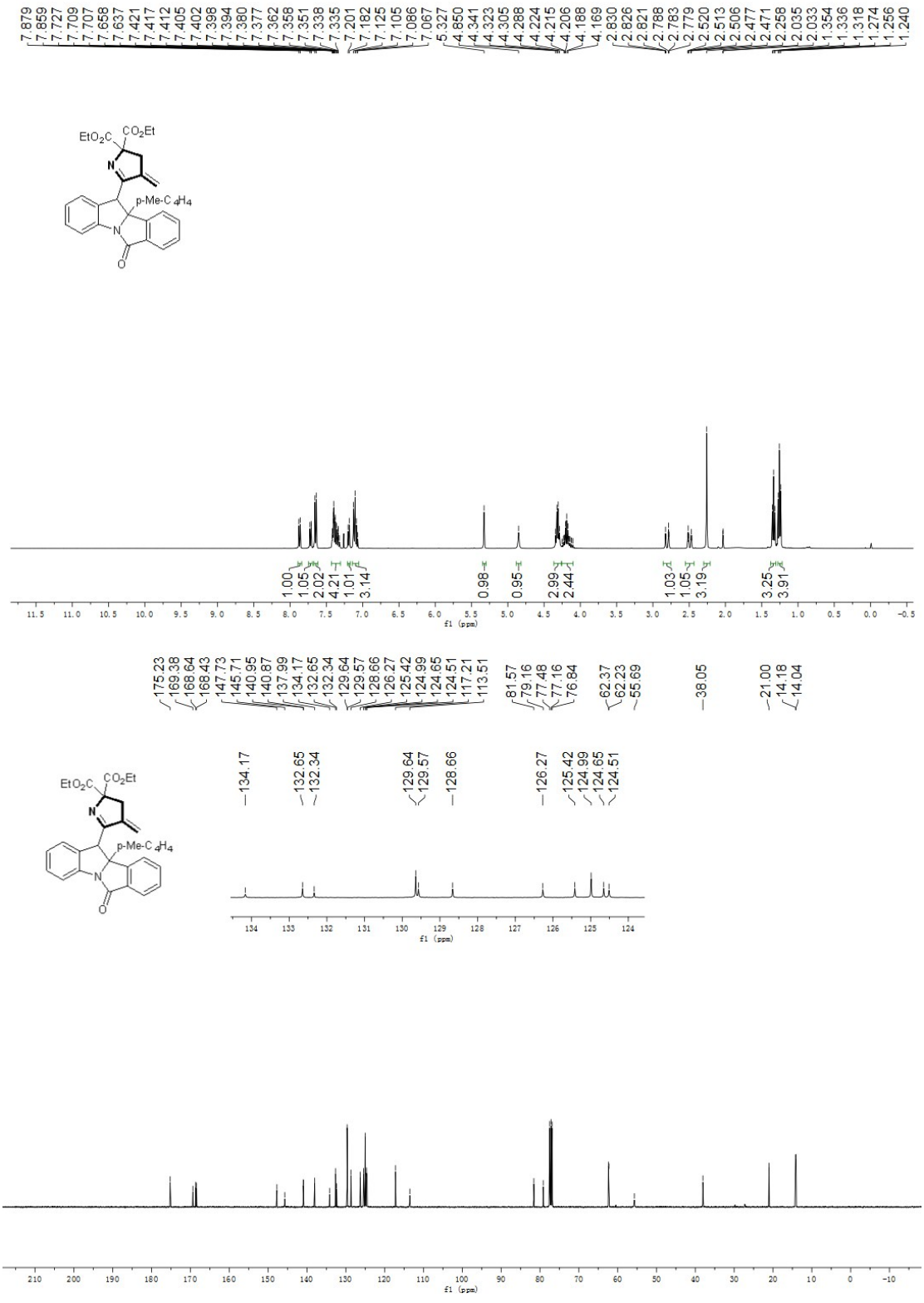

175.06
168.71
168.35
167.92
146.02
145.79
143.39
140.62
135.16
134.23
134.09
132.78
129.72
129.17
128.39
126.28
125.79
125.75
124.98
124.71
117.27
113.57
81.78
79.06
77.48
77.16
76.84
62.48
62.30
55.24
37.96
29.82
14.18
14.09


EtO2C
CO2Et
N
Ph
N
O
Cl


135.16
134.23
134.09
132.78
129.72
129.17
128.39
126.28
125.79
125.75
124.98
124.71
f1 (ppm)


f1 (ppm)

3q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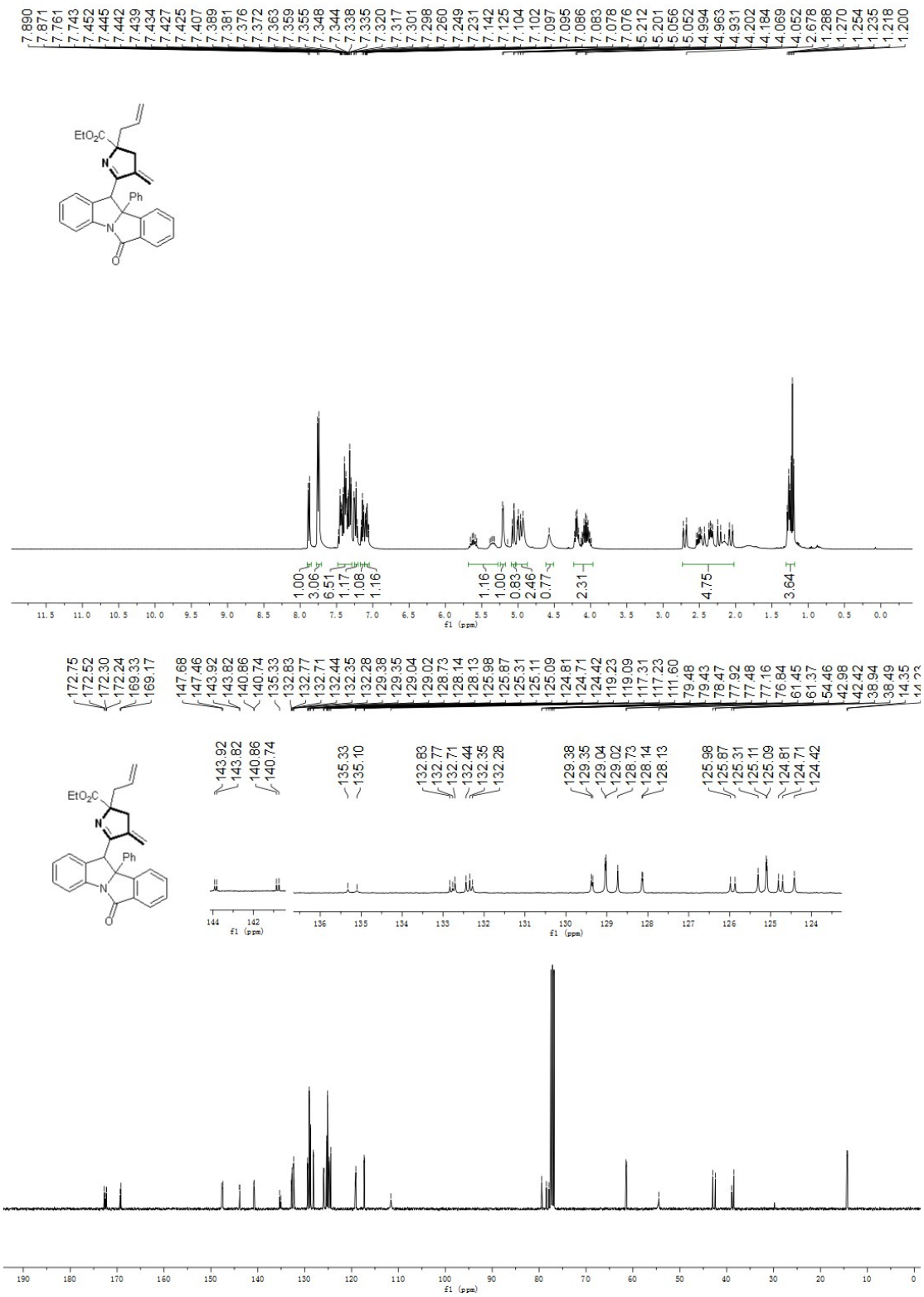
7.859
7.727
7.709
7.707
7.658
7.637
7.421
7.417
7.412
7.405
7.402
7.398
7.394
7.380
7.377
7.362
7.358
7.351
7.338
7.335
7.201
7.182
7.125
7.105
7.086
7.067
5.327
4.850
4.341
4.323
4.305
4.288
4.224
4.215
4.206
4.188
4.169
2.830
2.826
2.821
2.788
2.783
2.779
2.520
2.513
2.506
2.477
2.471
2.258
2.035
2.033
1.354
1.336
1.318
1.274
1.256
1.240
EtO2C
CO2Et
p-Me-C6H4
1.00
1.05
2.02
4.21
1.01
3.14
0.98
0.95
2.99
2.44
1.03
1.05
3.19
3.25
3.91
f1 (ppm)
175.23
169.38
168.64
168.43
147.73
145.71
140.95
140.87
137.99
134.17
132.65
132.34
129.64
129.57
128.66
126.27
125.42
124.99
124.65
124.51
117.21
113.51
81.57
79.16
77.48
77.16
76.84
62.37
62.23
55.69
38.05
21.00
14.18
14.04
f1 (ppm)

3r


7.795
7.776
7.769
7.767
7.762
7.754
7.478
7.470
7.463
7.456
7.445
7.442
7.432
7.424
7.417
7.407
7.404
7.385
7.367
7.365
7.260
7.225
7.206
7.134
7.131
7.115
7.112
7.096
7.094
5.421
5.060
4.203
4.186
4.168
4.150
4.109
4.091
4.082
4.064
4.022
4.004
3.996
3.704
2.858
2.853
2.815
2.810
2.804
2.610
2.604
2.597
2.561
1.237
1.219
1.201
1.198
1.180
1.162
EtO2C
CO2Et
CO2Me
1.91
4.04
0.93
1.00
1.02
0.94
0.83
3.83
2.95
1.01
1.03
3.19
3.03
f1 (ppm)
174.08
171.27
168.66
168.63
168.15
146.72
141.25
140.70
133.86
133.82
132.66
129.92
129.58
125.85
125.34
124.69
124.48
117.00
112.92
82.07
79.08
77.48
77.16
76.84
62.24
62.16
53.91
48.73
37.34
14.06
13.99

3s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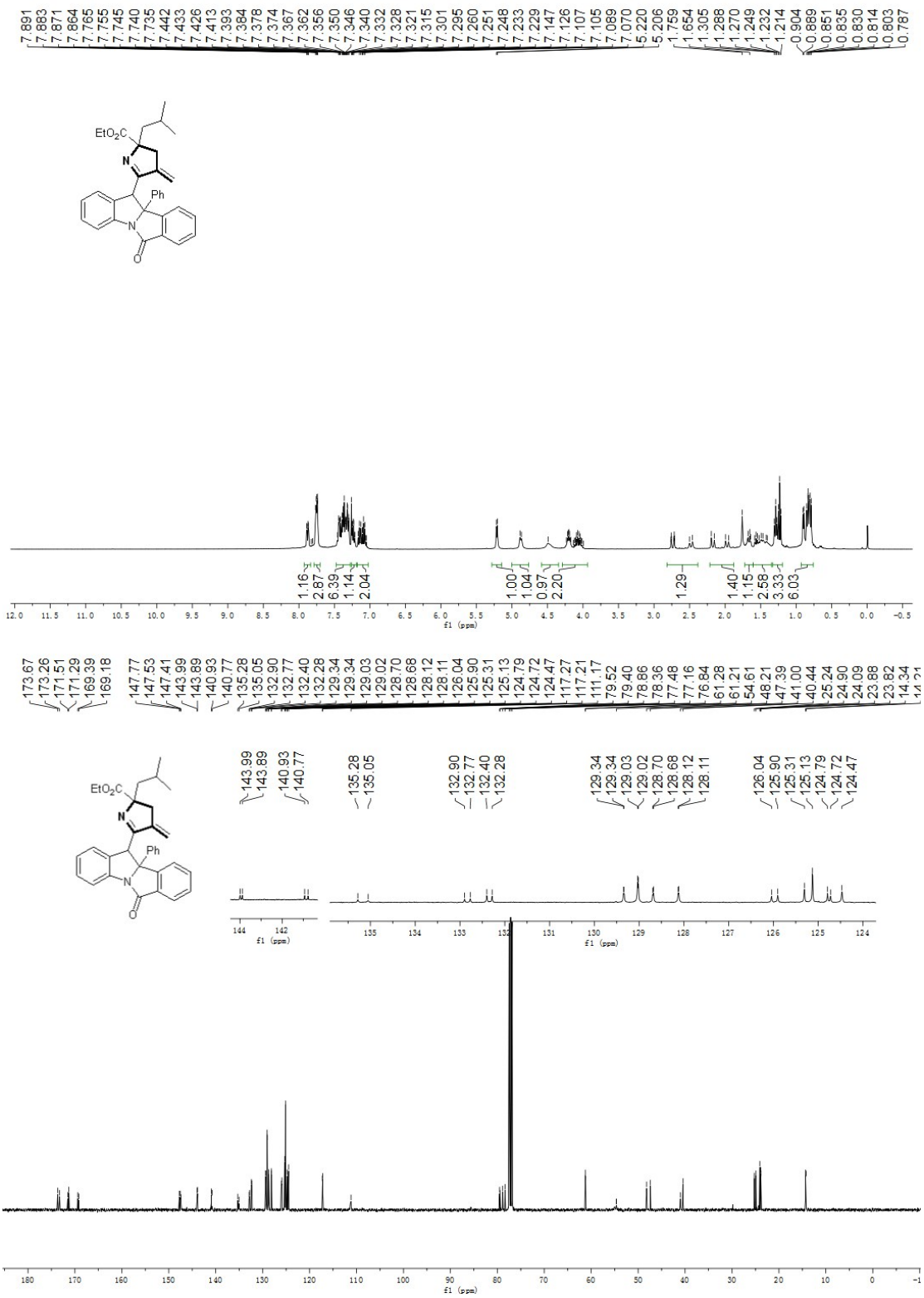
7.442
7.439
7.434
7.427
7.425
7.407
7.389
7.381
7.376
7.372
7.363
7.359
7.355
7.348
7.344
7.338
7.335
7.320
7.317
7.301
7.298
7.260
7.249
7.231
7.142
7.125
7.104
7.102
7.097
7.095
7.086
7.083
7.078
7.076
5.212
5.201
5.056
5.052
4.994
4.963
4.931
4.202
4.184
4.069
4.052
2.678
1.288
1.270
1.254
1.235
1.218
1.200
EtO2C
N
Ph
O
1.00
3.06
6.51
1.17
1.08
1.16
1.16
1.00
0.83
2.46
0.77
2.31
4.75
3.64
f1 (ppm)
172.75
172.52
172.30
172.24
169.33
169.17
147.68
147.46
143.92
143.82
140.86
140.74
135.33
135.10
132.83
132.77
132.71
132.44
132.35
132.28
129.38
129.35
129.04
129.02
128.73
128.14
128.13
125.98
125.87
125.31
125.11
125.09
124.81
124.71
124.42
119.23
119.09
117.31
117.23
111.60
79.48
79.43
78.47
77.92
77.48
77.16
76.84
61.45
61.37
54.46
42.98
42.42
38.94
38.49
14.35
f1 (ppm)

3t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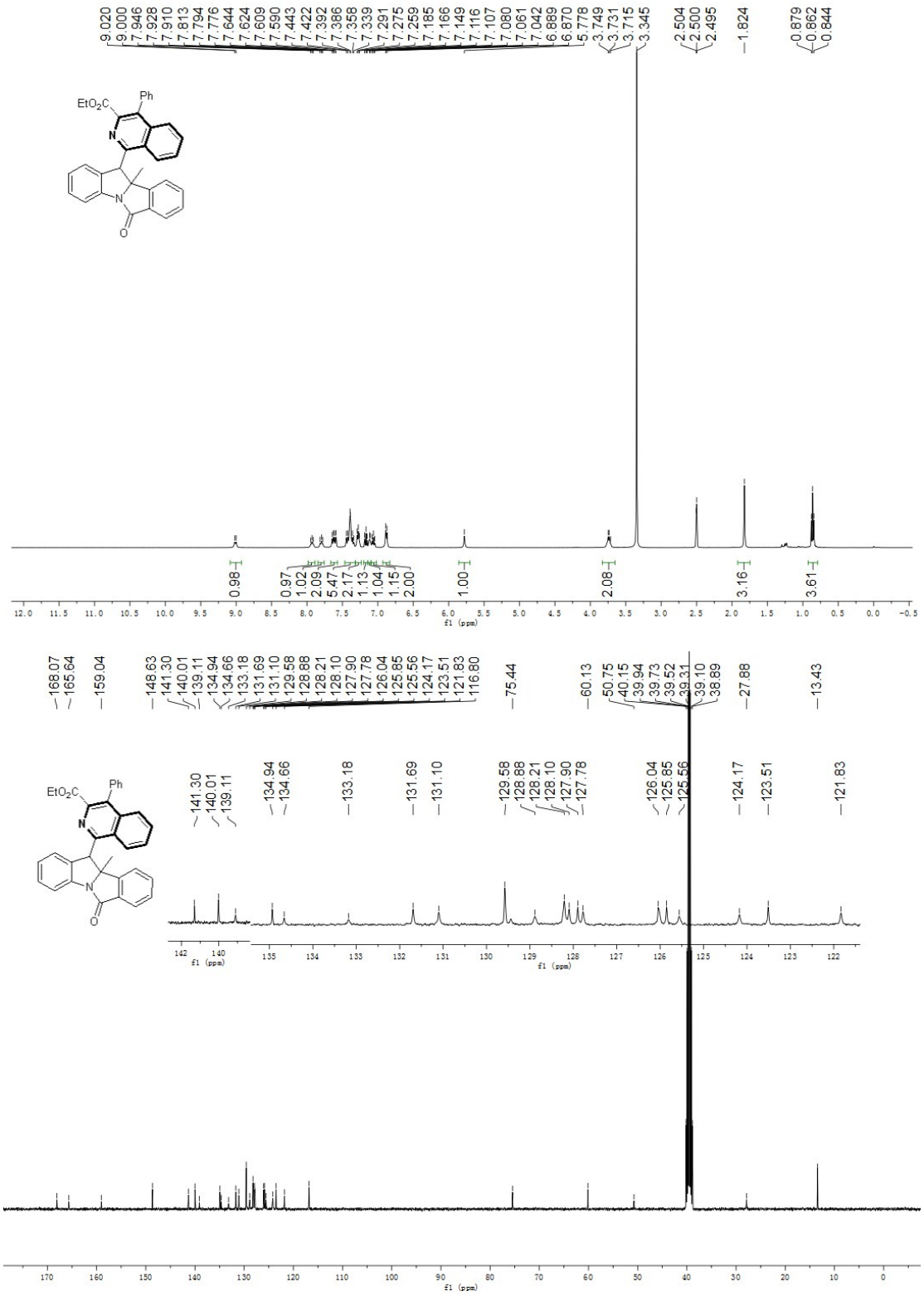
7.426
7.413
7.393
7.384
7.378
7.374
7.367
7.362
7.356
7.350
7.346
7.340
7.332
7.328
7.321
7.315
7.301
7.295
7.260
7.251
7.248
7.233
7.229
7.147
7.126
7.107
7.105
7.089
7.070
5.220
5.206
1.759
1.654
1.305
1.288
1.270
1.249
1.232
1.214
0.904
0.889
0.851
0.835
0.830
0.814
0.803
0.787
EtO2C
N
Ph
O
1.16
2.87
6.39
1.14
2.04
1.00
1.04
0.97
2.20
1.29
1.40
1.15
2.58
3.33
6.03
f1 (ppm)
173.67
173.26
171.51
171.29
169.39
169.18
147.77
147.53
147.41
143.99
143.89
140.93
140.77
135.28
135.05
132.90
132.77
132.40
132.28
129.34
129.34
129.03
129.02
128.70
128.68
128.12
128.11
126.04
125.90
125.31
125.13
124.79
124.72
124.47
79.52
79.40
78.86
78.36
77.48
77.16
76.84
61.28
61.21
54.61
48.21
47.39
41.00
40.44
25.24
24.90
24.09
23.88
23.82
14.34
f1 (ppm)

5a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9.000
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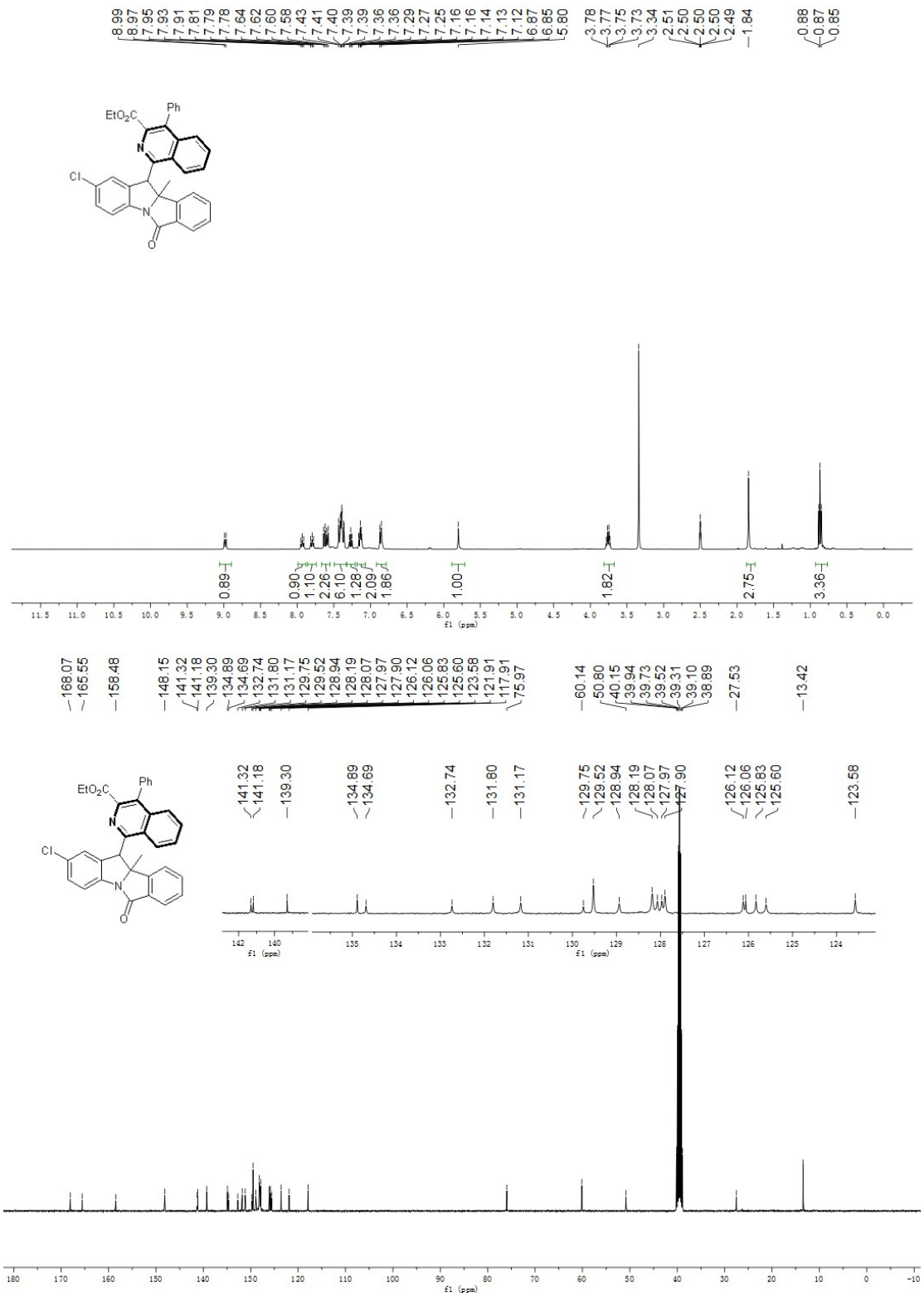
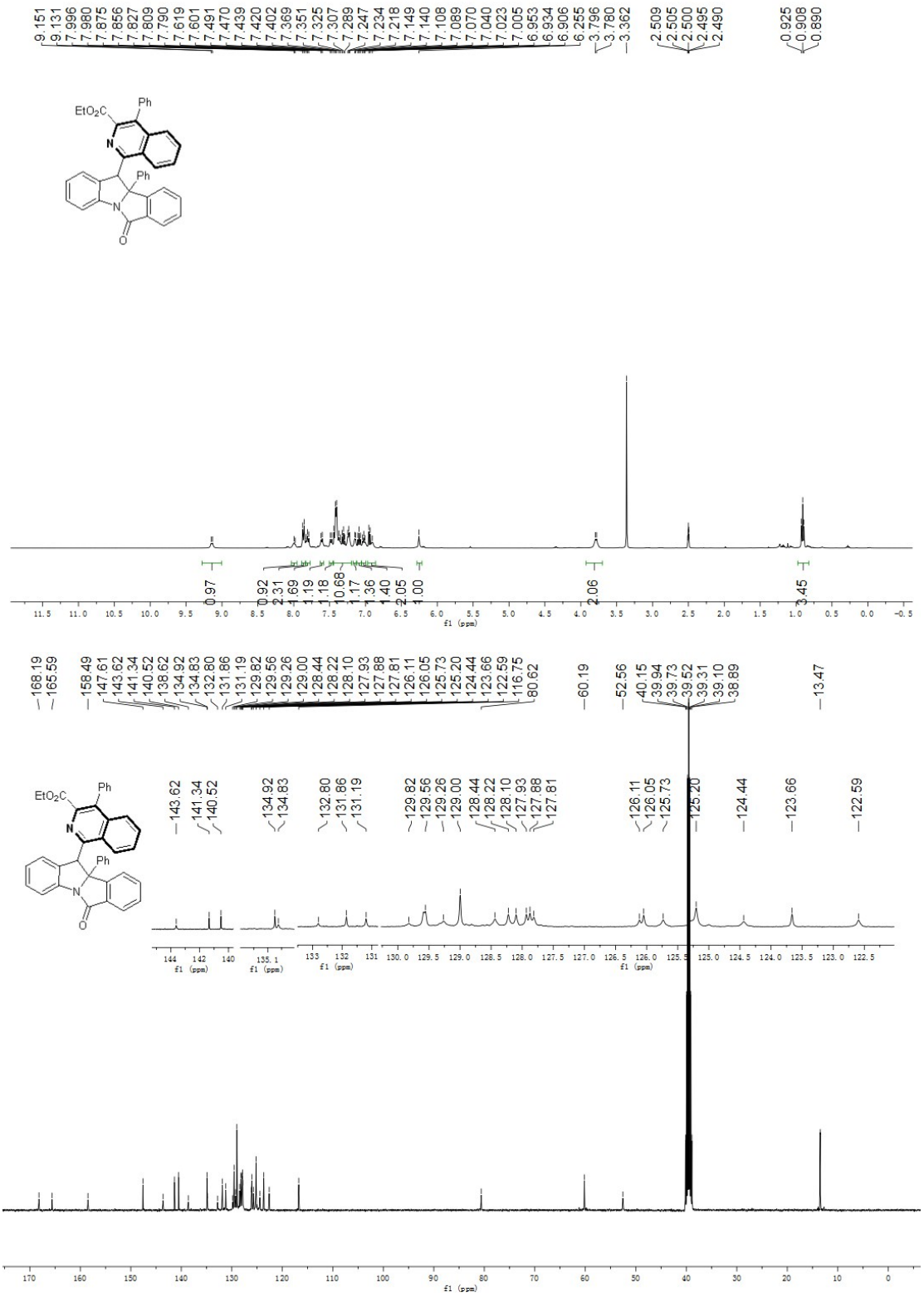
7.910
7.813
7.794
7.776
7.644
7.624
7.609
7.590
7.443
7.422
7.392
7.386
7.358
7.339
7.291
7.275
7.259
7.185
7.166
7.149
7.116
7.107
7.080
7.061
7.042
6.889
6.870
5.778
3.749
3.731
3.715
3.345
2.504
2.500
2.495
1.824
0.879
0.862
0.844
EtO2C
Ph
N
O
0.98
0.97
1.02
2.09
5.47
2.17
1.13
1.04
1.15
2.00
1.00
2.08
3.16
3.61
f1 (ppm)
168.07
165.64
159.04
148.63
141.30
140.01
139.11
134.94
134.66
133.18
131.69
131.10
129.58
128.88
128.21
128.10
127.90
127.78
126.04
125.85
125.56
124.17
123.51
121.83
116.80
75.44
60.13
50.75
40.15
39.94
39.73
39.52
39.31
39.10
38.89
27.88
13.43

5b


8.99
8.97
7.95
7.93
7.91
7.81
7.79
7.78
7.64
7.62
7.60
7.58
7.43
7.41
7.40
7.39
7.39
7.36
7.36
7.29
7.27
7.25
7.16
7.16
7.14
7.13
7.12
6.87
6.85
5.80
3.78
3.77
3.75
3.73
3.34
2.51
2.50
2.50
2.50
2.49
1.84
0.88
0.87
0.85
EtO2C
Ph
Cl
N
O
0.89
0.90
1.10
2.26
6.10
1.28
2.09
1.86
1.00
1.82
2.75
3.36
f1 (ppm)
168.07
165.55
158.48
148.15
141.32
141.18
139.30
134.89
134.69
132.74
131.80
131.17
129.75
129.52
128.94
128.19
128.07
127.97
127.90
126.12
126.06
125.83
125.60
123.58
121.91
117.91
75.97
60.14
50.80
40.15
39.94
39.73
39.52
39.31
39.10
38.89
27.53
13.42
f1 (ppm)

5c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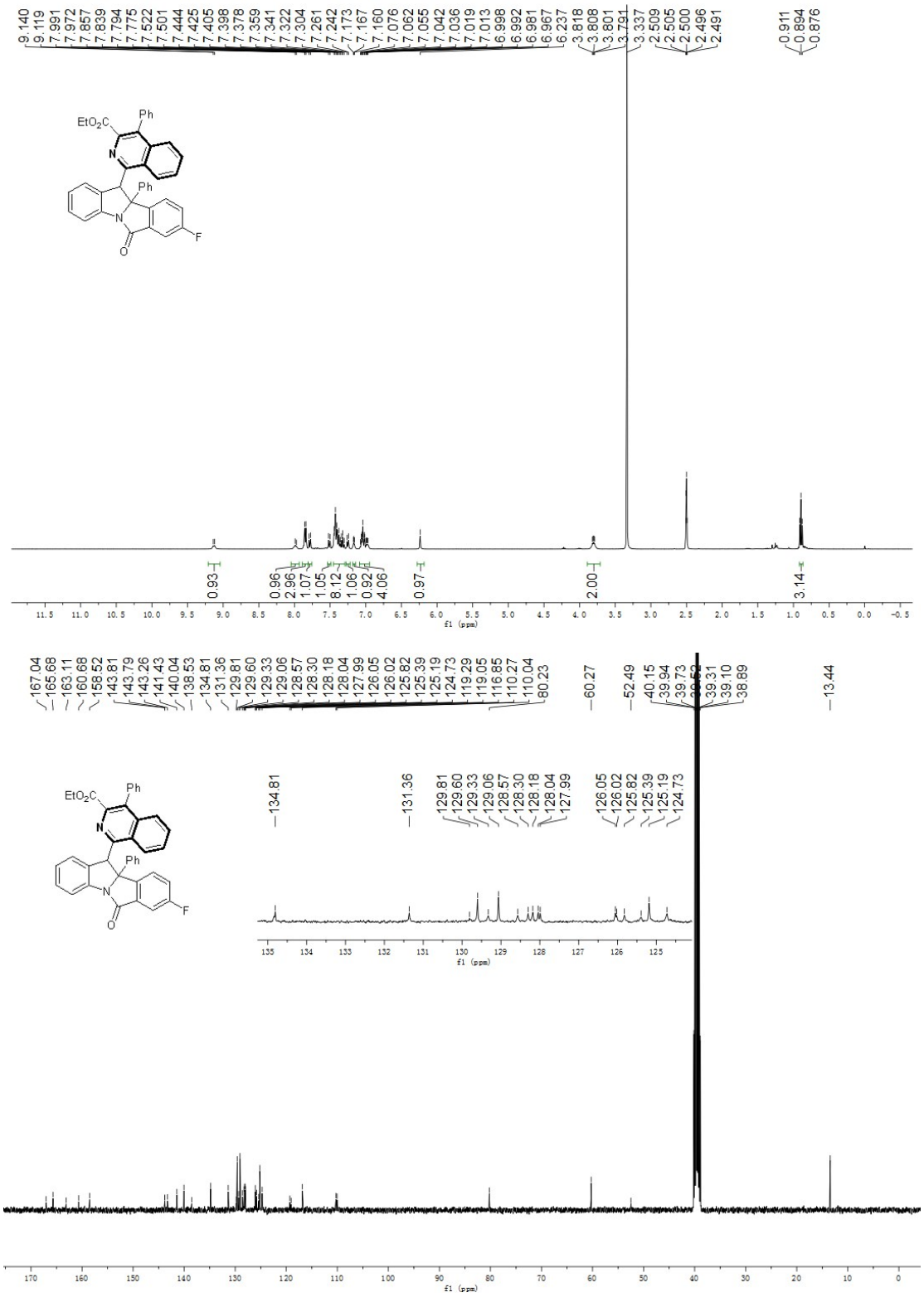
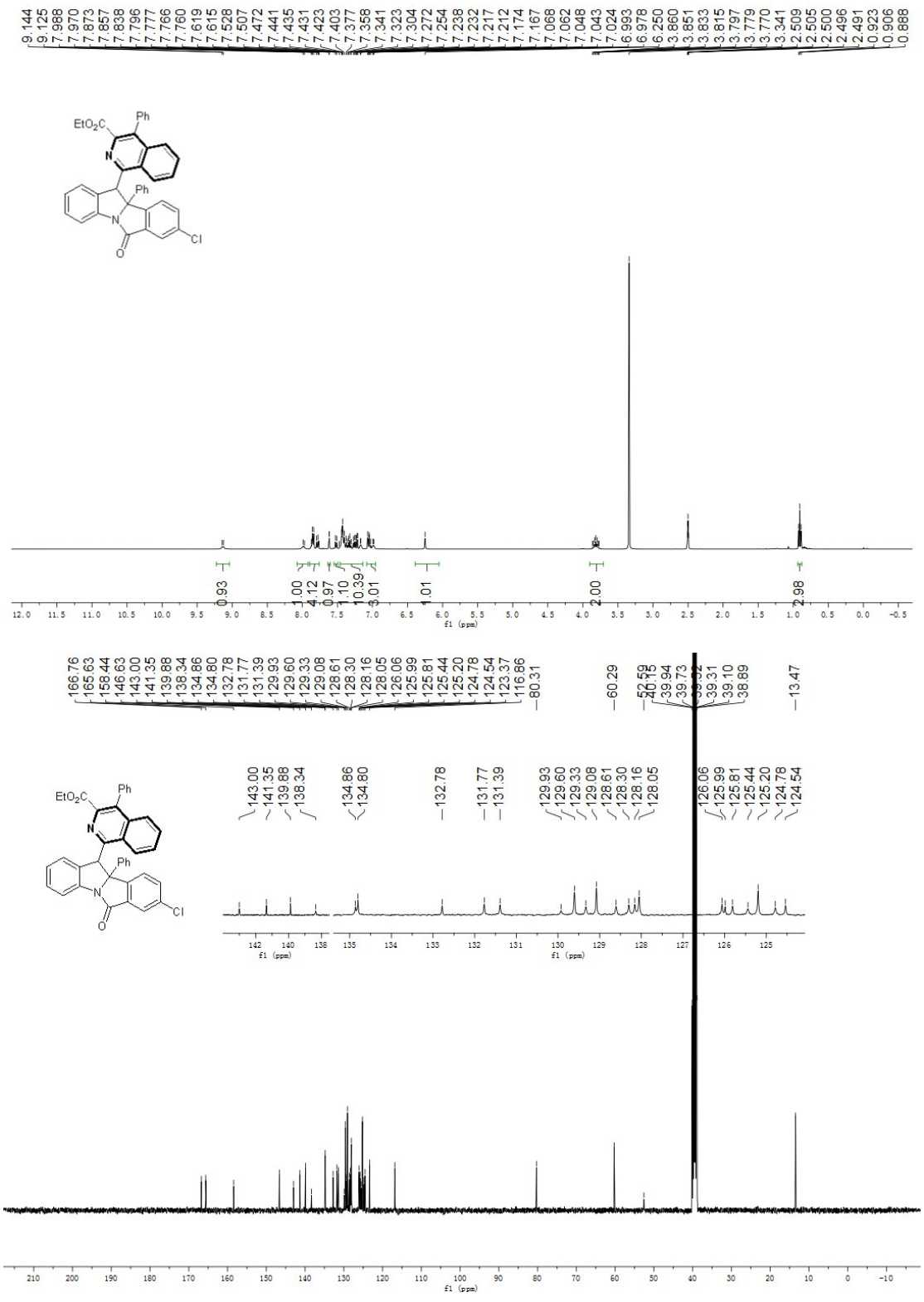
7.996
7.980
7.875
7.856
7.827
7.809
7.790
7.619
7.601
7.491
7.470
7.439
7.420
7.402
7.369
7.351
7.325
7.307
7.289
7.247
7.234
7.218
7.149
7.140
7.108
7.089
7.070
7.040
7.023
7.005
6.953
6.934
6.906
6.255
3.796
3.780
3.362
2.509
2.505
2.500
2.495
2.490
0.925
0.908
0.890
EtO2C
Ph
N
Ph
N
O
0.97
0.92
2.31
1.69
1.19
1.18
10.68
1.17
1.36
1.40
2.05
1.00
2.06
3.45
f1 (ppm)
168.19
165.59
158.49
147.61
143.62
141.34
140.52
138.62
134.92
134.83
132.80
131.86
131.19
129.82
129.56
129.26
129.00
128.44
128.22
128.10
127.93
127.88
127.81
126.11
126.05
125.73
125.20
124.44
123.66
122.59
116.75
80.62
60.19
52.56
40.15
39.94
39.73
39.52
39.31
39.10
38.89
13.47
f1 (ppm)

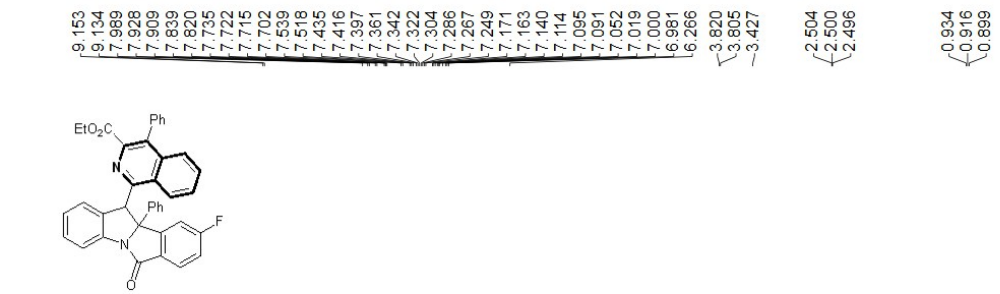
5d

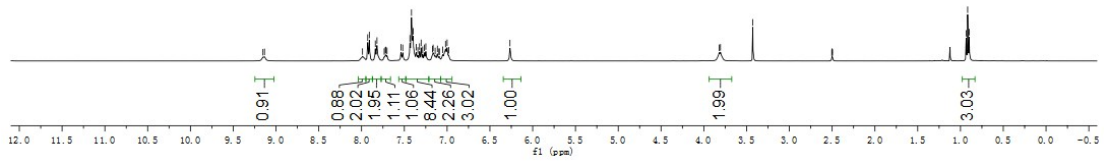

9.140
9.119
7.991
7.972
7.857
7.839
7.794
7.775
7.522
7.501
7.444
7.425
7.405
7.398
7.378
7.359
7.341
7.322
7.304
7.261
7.242
7.173
7.167
7.160
7.076
7.062
7.055
7.042
7.036
7.019
7.013
6.998
6.992
6.981
6.967
6.237
3.818
3.808
3.801
3.791
3.337
2.509
2.505
2.500
2.496
2.491
0.911
0.894
0.876
EtO2C
Ph
Ph
F
O
0.93
0.96
2.96
1.07
1.05
8.12
1.06
0.92
4.06
0.97
2.00
3.14
f1 (ppm)
167.04
165.68
163.11
160.68
158.52
143.81
143.79
143.26
141.43
140.04
138.53
134.81
131.36
129.81
129.60
129.33
129.06
128.57
128.30
128.18
128.04
127.99
126.05
126.02
125.82
125.39
125.19
124.73
119.29
119.05
116.85
110.27
110.04
80.23
60.27
52.49
40.15
39.94
39.73
39.52
39.31
39.10
38.89
13.44
f1 (ppm)
f1 (ppm)

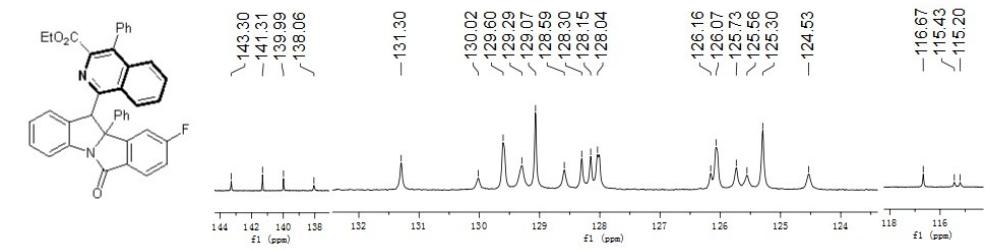
5e

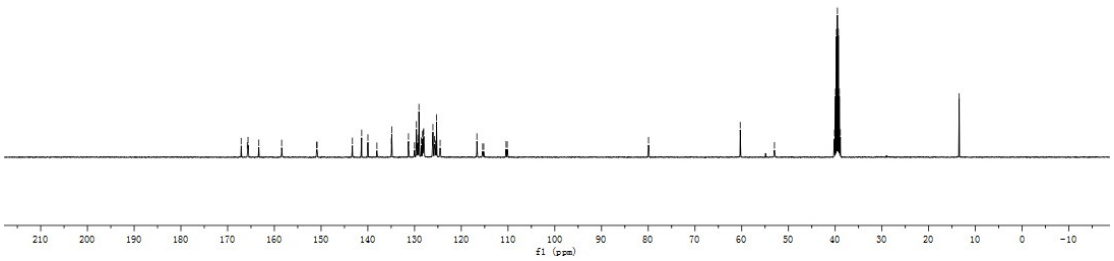

9.144
9.125
7.988
7.970
7.873
7.857
7.838
7.796
7.777
7.766
7.760
7.619
7.615
7.528
7.507
7.472
7.441
7.435
7.431
7.423
7.403
7.377
7.358
7.341
7.323
7.304
7.272
7.254
7.238
7.232
7.217
7.212
7.174
7.167
7.068
7.062
7.048
7.043
7.024
6.993
6.978
6.250
3.860
3.851
3.833
3.815
3.797
3.779
3.770
3.341
2.509
2.505
2.500
2.496
2.491
0.923
0.906
0.888
EtO2C
Ph
Ph
Cl
O
N
0.93
1.00
4.12
0.97
1.10
10.39
3.01
1.01
2.00
2.98
f1 (ppm)
166.76
165.63
158.44
146.63
143.00
141.35
139.88
138.34
134.86
134.80
132.78
131.77
131.39
129.93
129.60
129.33
129.08
128.61
128.30
128.16
128.05
126.06
125.99
125.81
125.44
125.20
124.78
124.54
123.37
116.86
80.31
60.29
52.59
40.15
39.94
39.73
39.52
39.31
39.10
38.89
13.47

5f

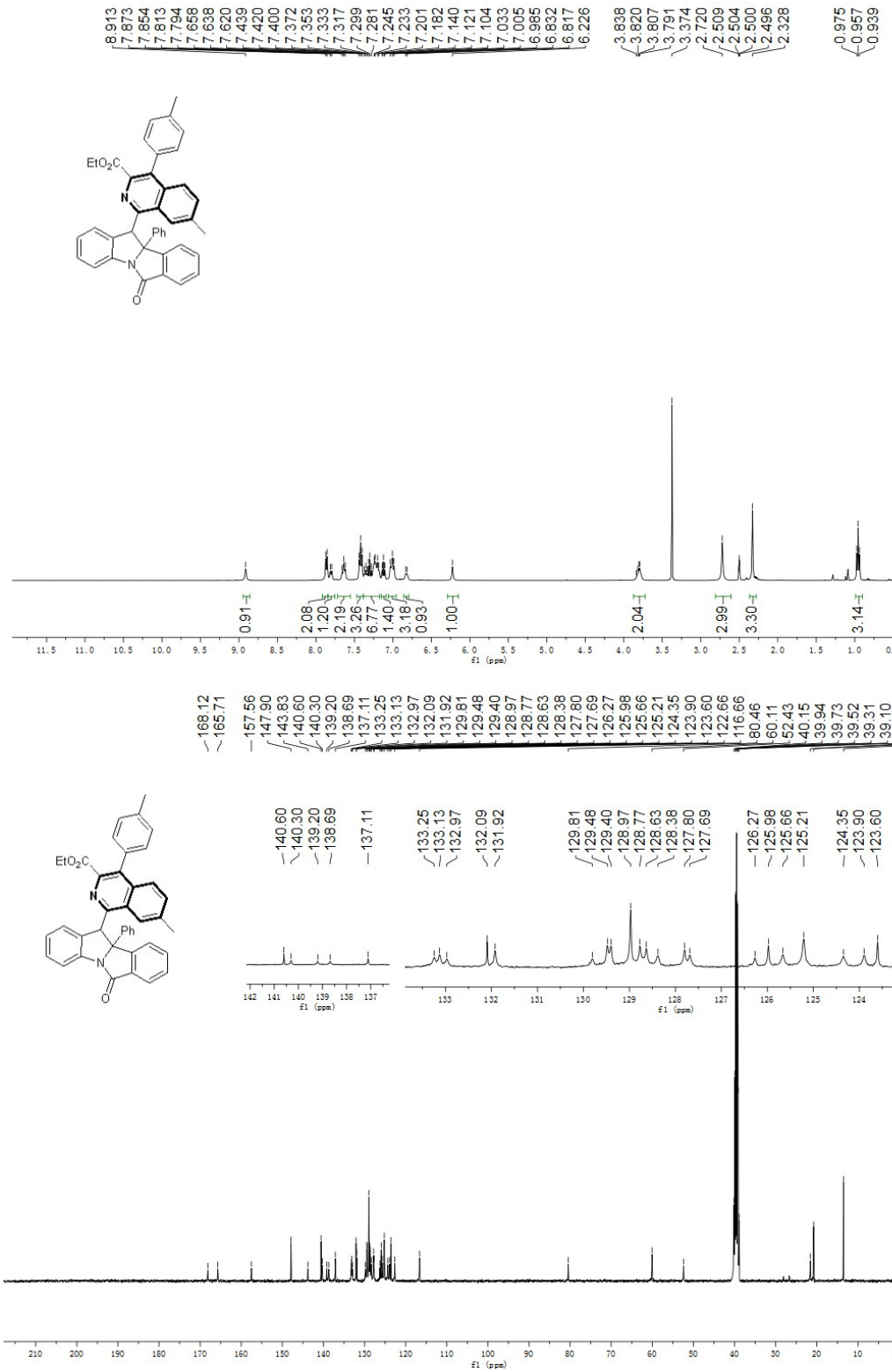




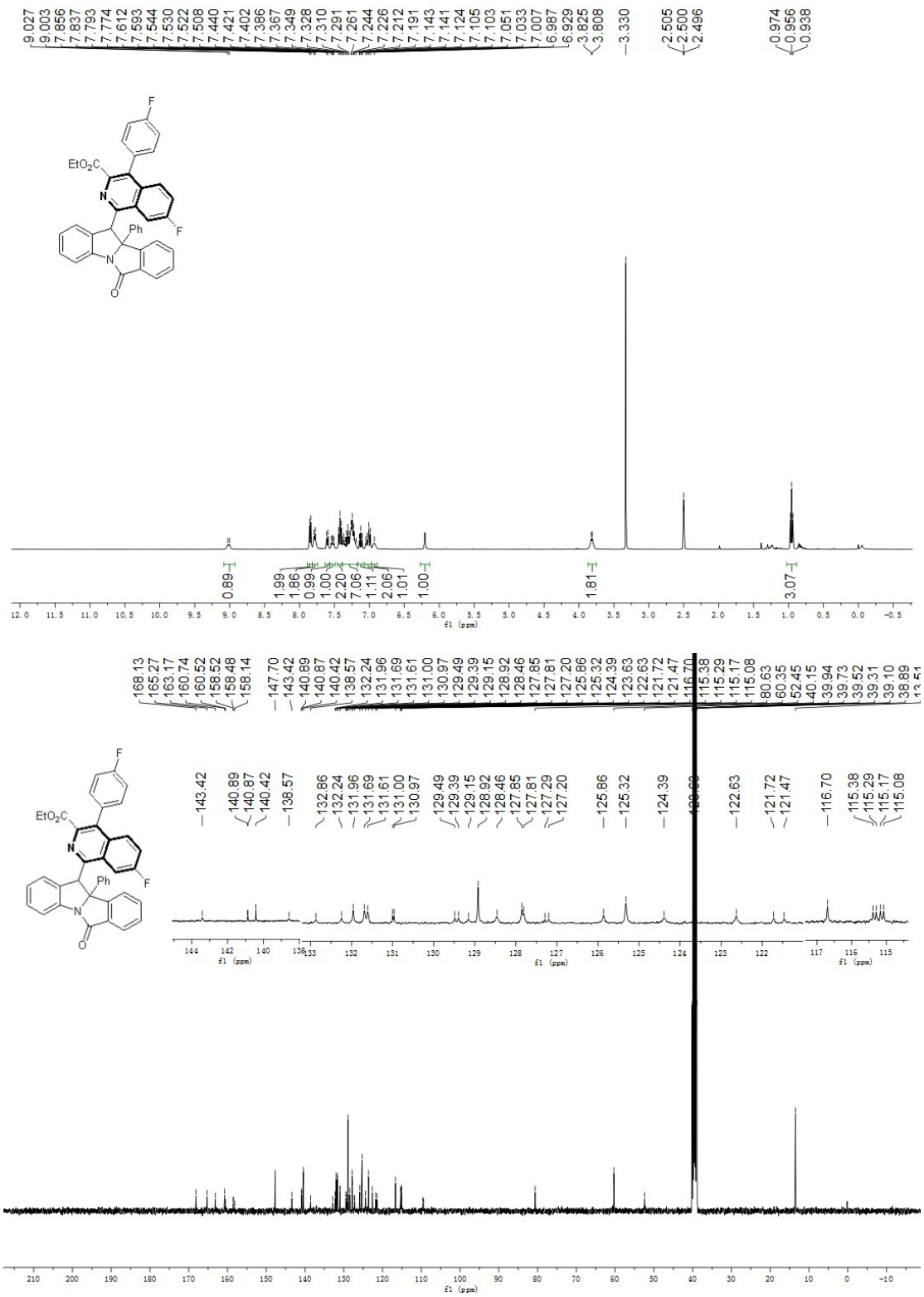




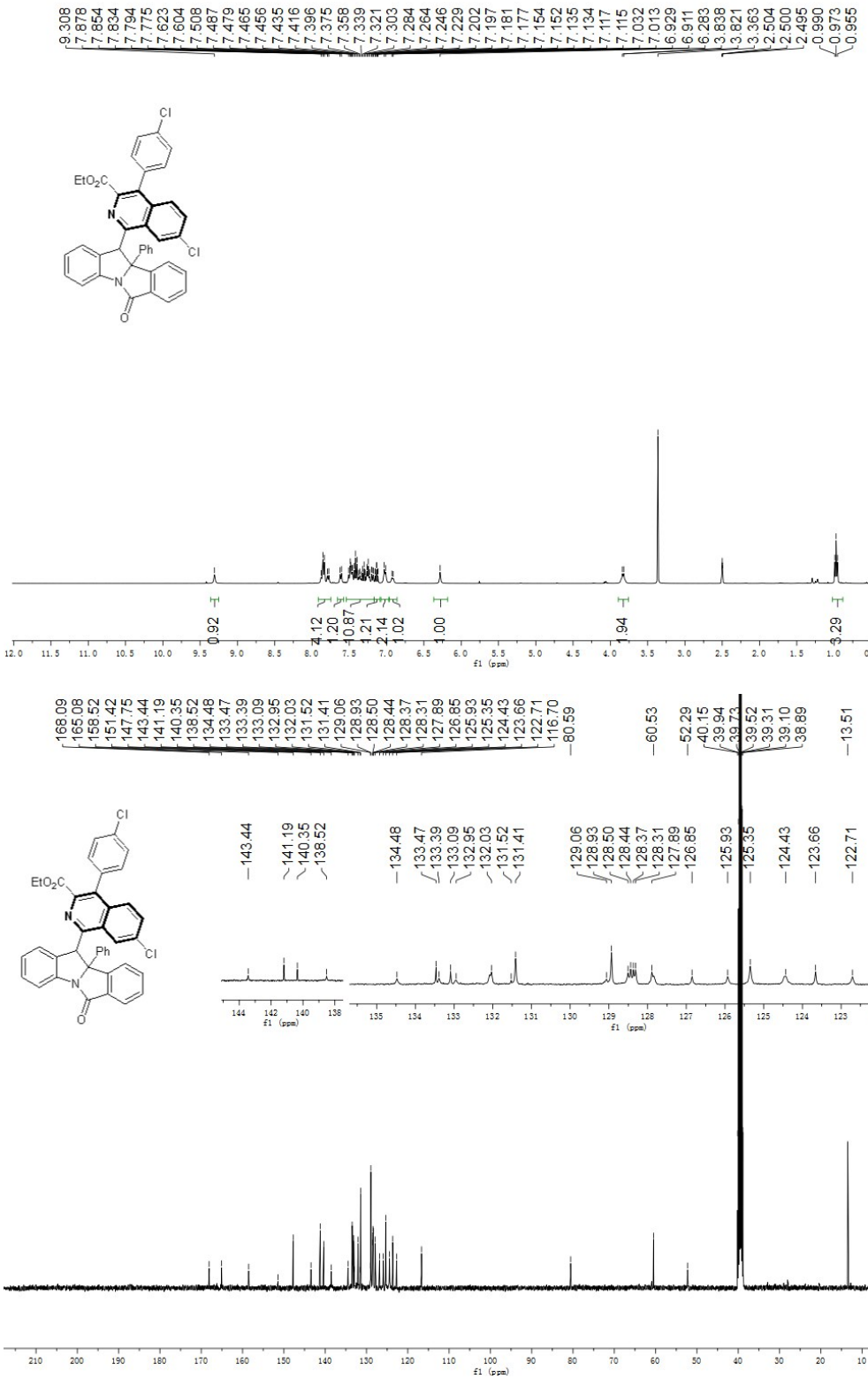
5g


8.913
7.873
7.854
7.813
7.794
7.658
7.638
7.620
7.439
7.420
7.400
7.372
7.353
7.333
7.317
7.299
7.281
7.245
7.233
7.201
7.182
7.140
7.121
7.104
7.033
7.005
6.985
6.832
6.817
6.226
3.838
3.820
3.807
3.791
3.374
2.720
2.509
2.504
2.500
2.496
2.328
0.975
0.957
0.939
EtO2C
N
Ph
O
0.91
2.08
1.20
2.19
3.26
6.77
1.40
3.18
0.93
1.00
2.04
2.99
3.30
3.14
f1 (ppm)
168.12
165.71
157.56
147.90
143.83
140.60
140.30
139.20
138.69
137.11
133.25
133.13
132.97
132.09
131.92
129.81
129.48
129.40
128.97
128.77
128.63
128.38
127.80
127.69
126.27
125.98
125.66
125.21
124.35
123.90
123.60
122.66
116.66
80.46
60.11
52.43
40.15
39.94
39.73
39.52
39.31
39.10
38.89
21.60
20.78
13.53

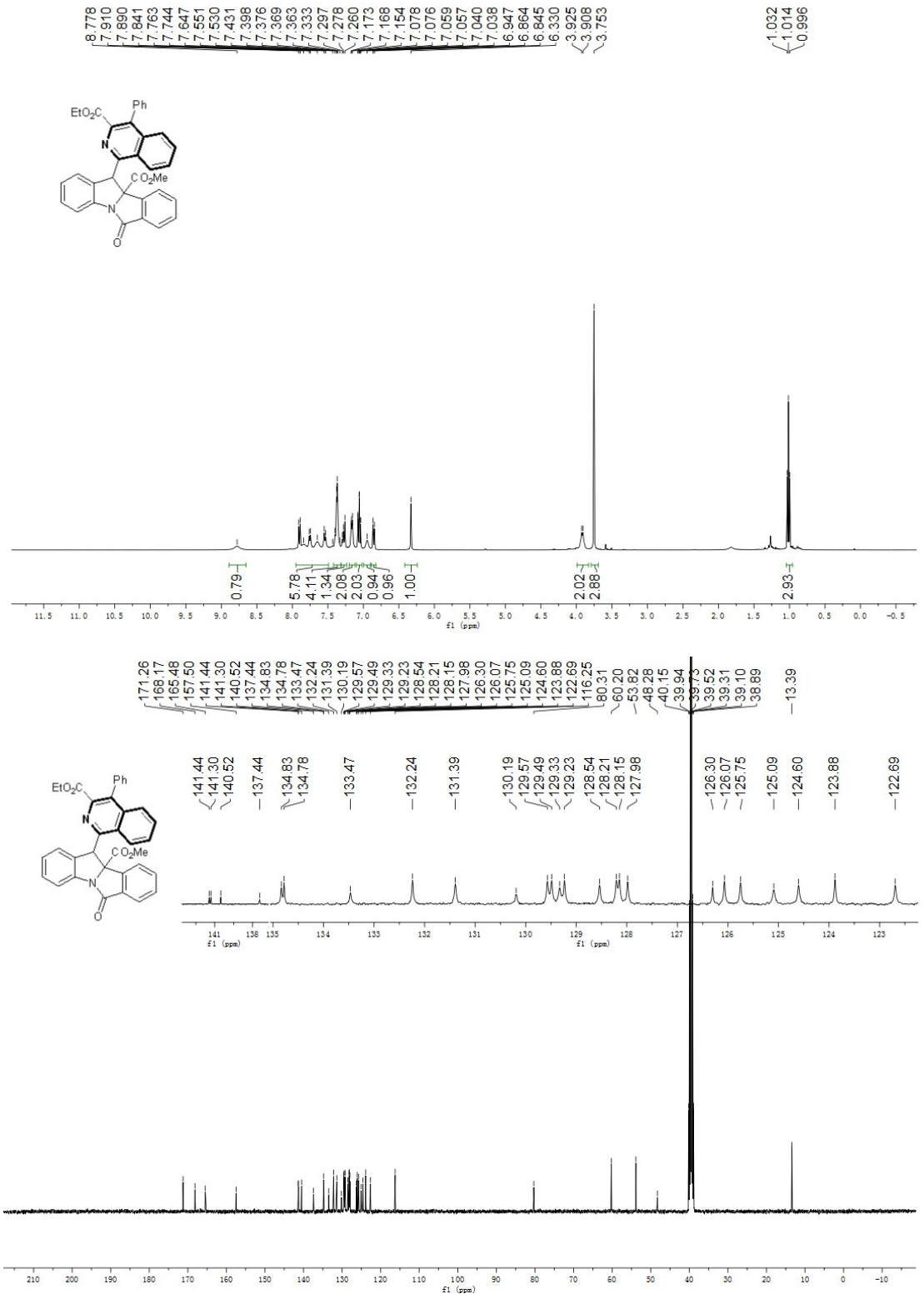
5h



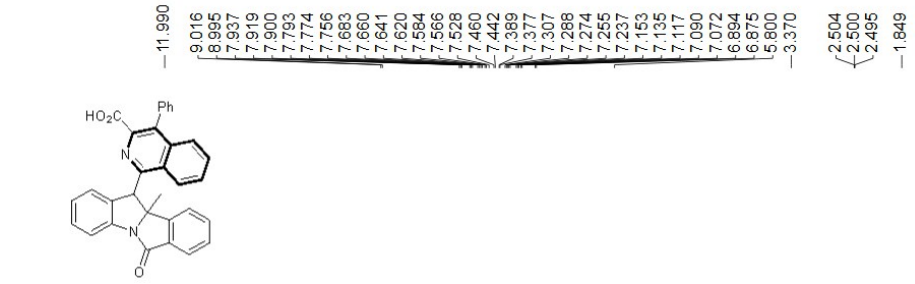
5i

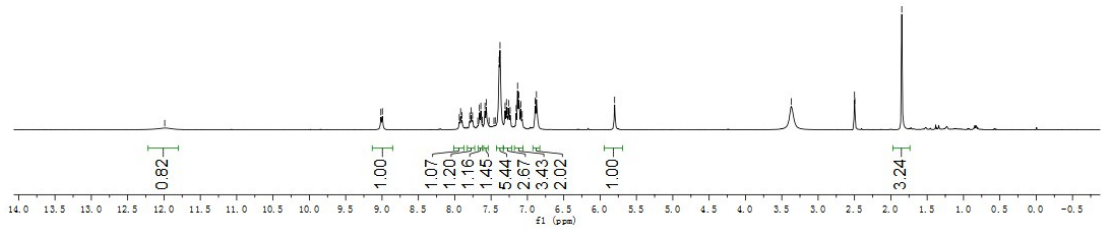

9.308
7.878
7.854
7.834
7.794
7.775
7.623
7.604
7.508
7.487
7.479
7.465
7.456
7.435
7.416
7.396
7.375
7.358
7.339
7.321
7.303
7.284
7.264
7.246
7.229
7.202
7.197
7.181
7.177
7.154
7.152
7.135
7.134
7.117
7.115
7.032
7.013
6.929
6.911
6.283
3.838
3.821
3.363
2.504
2.500
2.495
0.990
0.973
0.955
Cl
EtO2C
N
Ph
Cl
N
O
0.92
4.12
1.20
0.87
1.21
2.14
1.02
1.00
1.94
3.29
f1 (ppm)
168.09
165.08
158.52
151.42
147.75
143.44
141.19
140.35
138.52
134.48
133.47
133.39
133.09
132.95
132.03
131.52
131.41
129.06
128.93
128.50
128.44
128.37
128.31
127.89
126.85
125.93
125.35
124.43
123.66
122.71
116.70
80.59
60.53
52.29
40.15
39.94
39.73
39.52
39.31
39.10
38.89
13.51
f1 (ppm)
f1 (ppm)

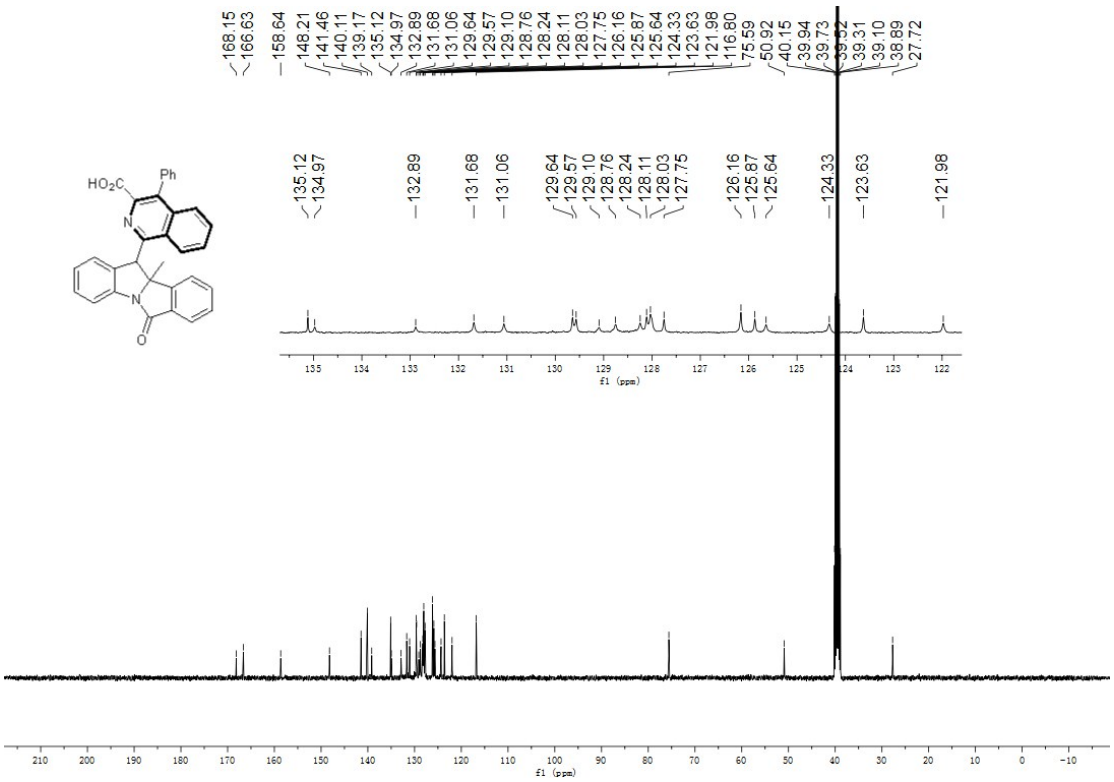
5j


8.778
7.910
7.890
7.841
7.763
7.744
7.647
7.551
7.530
7.431
7.398
7.376
7.369
7.363
7.333
7.297
7.278
7.260
7.173
7.168
7.154
7.078
7.076
7.059
7.057
7.040
7.038
6.947
6.864
6.845
6.330
3.925
3.908
3.753
1.032
1.014
0.996
EtO2C
Ph
N
CO2Me
N
O
0.79
5.78
4.11
1.34
2.08
2.03
0.94
0.96
1.00
2.02
2.88
2.93
f1 (ppm)
171.26
168.17
165.48
157.50
141.44
141.30
140.52
137.44
134.83
134.78
133.47
132.24
131.39
130.19
129.57
129.49
129.33
129.23
128.54
128.21
128.15
127.98
126.30
126.07
125.75
125.09
124.60
123.88
122.69
116.25
80.31
60.20
53.82
48.28
40.15
39.94
39.73
39.52
39.31
39.10
38.89
13.39
f1 (ppm)
f1 (ppm)

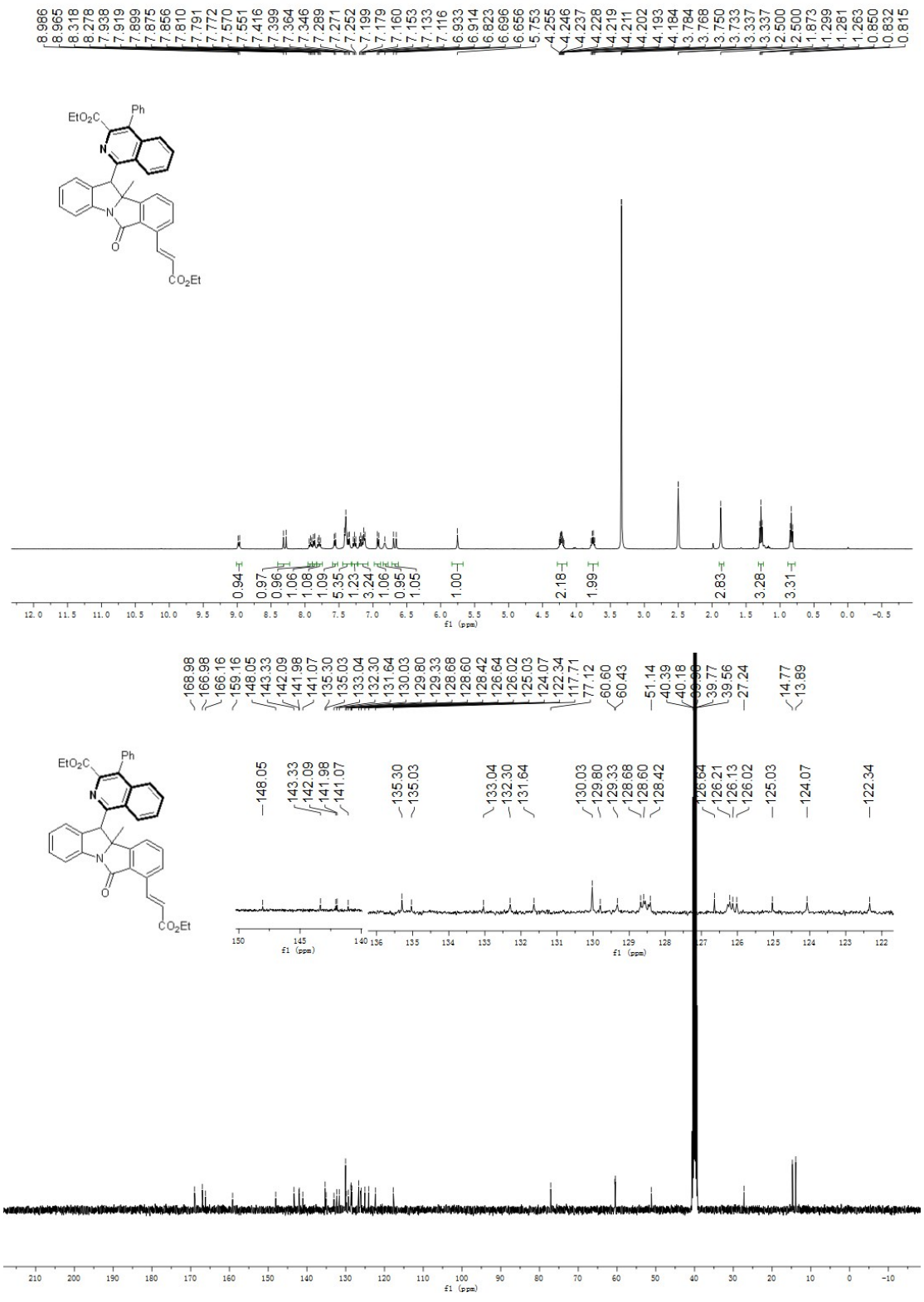
6


11.990
9.016
8.995
7.937
7.919
7.900
7.793
7.774
7.756
7.683
7.660
7.641
7.620
7.584
7.566
7.528
7.460
7.442
7.389
7.377
7.307
7.288
7.274
7.255
7.237
7.153
7.135
7.117
7.090
7.072
6.894
6.875
5.800
3.370
2.504
2.500
2.495
1.849
HO2C
Ph
N
N
O

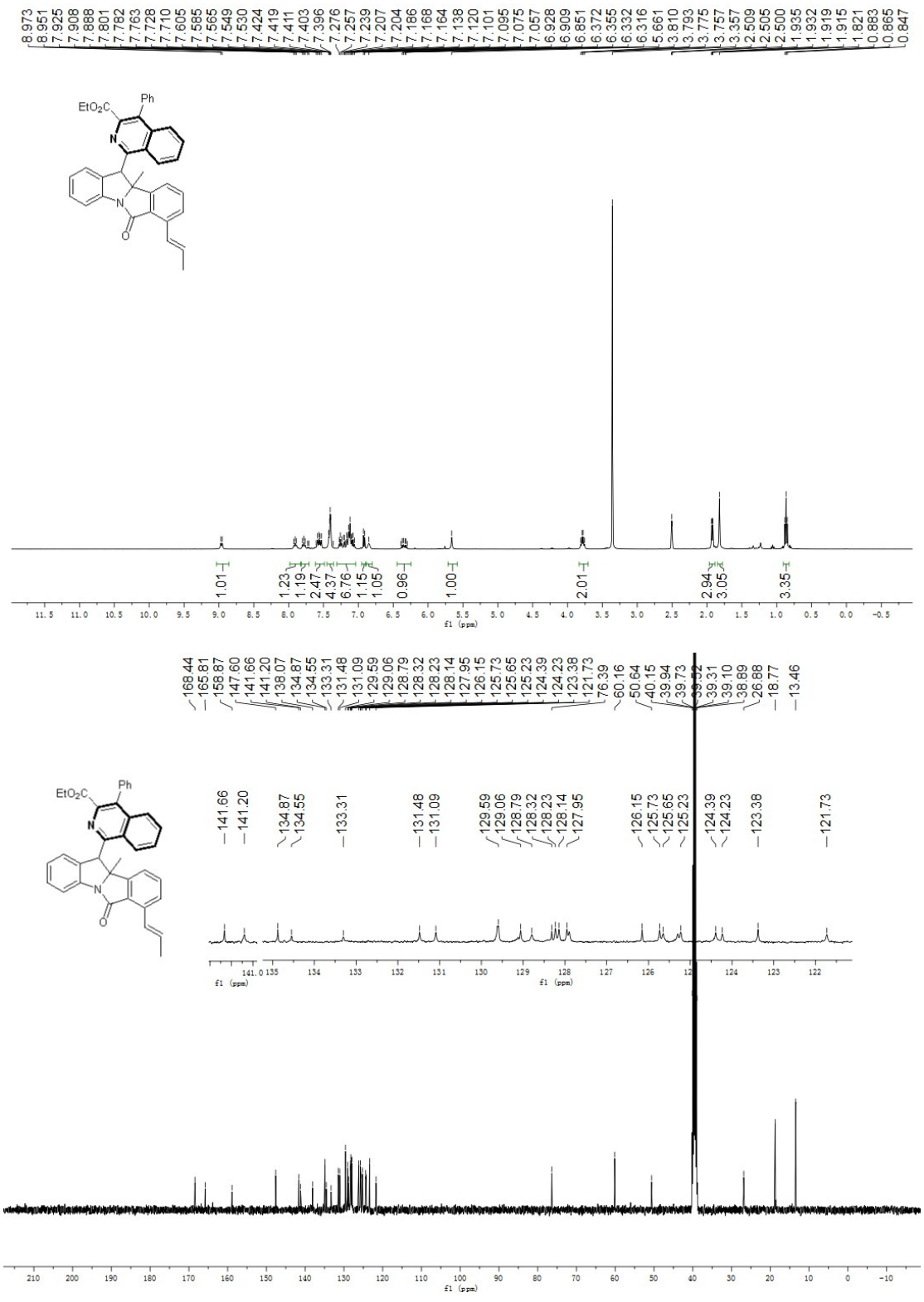

0.82
1.00
1.07
1.20
1.16
1.45
5.44
2.67
3.43
2.02
1.00
3.24
f1 (ppm)


168.15
166.63
158.64
148.21
141.46
140.11
139.17
135.12
134.97
132.89
131.68
131.06
129.64
129.57
129.10
128.76
128.24
128.11
128.03
127.75
126.16
125.87
125.64
124.33
123.63
121.98
116.80
75.59
50.92
40.15
39.94
39.73
39.52
39.31
39.10
38.89
27.72
HO2C
Ph
N
N
O
f1 (ppm)

7



8


8.973
8.951
7.925
7.908
7.888
7.801
7.782
7.763
7.728
7.710
7.605
7.585
7.565
7.549
7.530
7.424
7.419
7.411
7.403
7.396
7.276
7.257
7.239
7.207
7.204
7.186
7.168
7.164
7.138
7.120
7.101
7.095
7.075
7.057
6.928
6.909
6.851
6.372
6.355
6.332
6.316
5.661
3.810
3.793
3.775
3.757
3.357
2.509
2.505
2.500
1.935
1.932
1.919
1.915
1.821
0.883
0.865
0.847
EtO2C
Ph
N
O
1.01
1.23
1.19
2.47
4.37
6.76
1.15
1.05
0.96
1.00
2.01
2.94
3.05
3.35
f1 (ppm)
168.44
165.81
158.87
147.60
141.66
141.20
138.07
134.87
134.55
133.31
131.48
131.09
129.59
129.06
128.79
128.32
128.23
128.14
127.95
126.15
125.73
125.65
125.23
124.39
124.23
123.38
121.73
76.39
60.16
50.64
40.15
39.94
39.73
39.52
39.31
39.10
38.89
26.88
18.77
13.46
f1 (ppm)