Supporting Information

Access to Distal Biaxial Atropisomers by Iridium Catalyzed Asymmetric C−H Alkylation

Xueqing Hu,[†,a] Yunxu Zhao,[†,a] Tong He,[b] Caoyue Niu,[a] Feipeng Liu,[a] Wei Jia,[a] Yi Mu,[a] Xingwei Li*[b] and Zi-Qiang Rong*[a]

[a] Frontiers Science Center for Flexible Electronics (FSCFE), Shaanxi Institute of Flexible Electronics (SIFE), Northwestern Polytechnical University (NPU), Xi'an 710072, China

[b] School of Chemistry and Chemical Engineering, Shaanxi Normal University (SNNU), Xi'an 710119, China

*Corresponding author. Email: lixw@snnu.edu.cn; iamzqrong@nwpu.edu.cn

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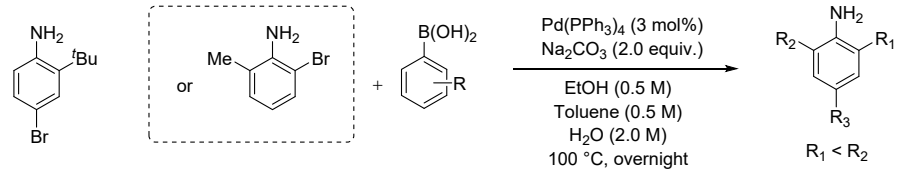
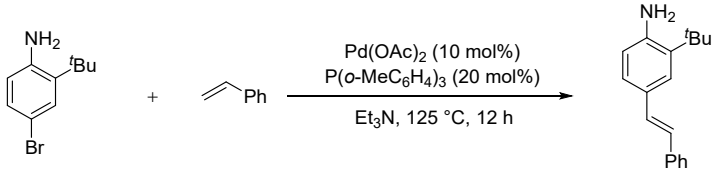
I. General Information

Unless noted otherwise, all solvents were dried by filtration through a Pure–Solv MD–5 Solvent Purification System (Innovative Technology). Sensitive reagents and solvents were transferred under nitrogen into a nitrogen–filled glovebox with standard techniques. Analytical thin–layer chromatography (TLC) was carried out using 0.2 mm commercial silica gel plates (silica gel 60, F254, Leyan chemical). Nuclear magnetic resonance spectra (^{1}H NMR, ^{2}H NMR, ^{13}C NMR and ^{19}F NMR) were recorded with a Bruker Model DMX 500 (500 MHz, ^{1}H at 500 MHz, ^{13}C at 126 MHz,). Chemical shifts were reported in parts per million (ppm, δ), downfield from tetramethylsilane (TMS, δ=0.00 ppm) and were referenced to residual solvent ($CDCl_3$, δ=7.26 ppm (^{1}H) and 77.00 ppm (^{13}C). All the ^{19}F chemical shifts were not referenced. Coupling constants were reported in Hertz (Hz). Data for ^{1}H NMR spectra were reported as follows: chemical shift (ppm, referenced to protium, s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, coupling constant (Hz), and integration). Commercially available materials were obtained from Rhawn Corporation, Leyan, Aladdin Bio–Chem Technology or Energy chemical and were used as received. High-resolution mass spectra (HRMS) were performed on a Waters Xevo G2-XS Tof Mass Spectrometry by electrospray ionization (ESI). IR spectra were collected on a Bruker Tensor II. and reported in unit of cm^{-1}. Melting Point were measured with Hanon MP430 Fully Automatic Video Melting Point Instrument. Absorption spectra were measured with a UV-Vis spectrophotometer (MAPADA, P7). Emission spectra were measured with an Edinburgh FLS 1000 spectrometer. Circular polarized luminescence (CPL) spectra were measured on a JASCO CPL-300 spectrometer. Circular dichroism (CD) spectra were measured on a JASCO J-815 CD Spectrometer. Chiral HPLC chromatograms were obtained from a Dionex UltiMate 3000 system. Optical rotation was measured on Anton Paar MCP 150 Automatic Polarimeter at concentrations of 0.1 g/10 mL in $CHCl_3$.

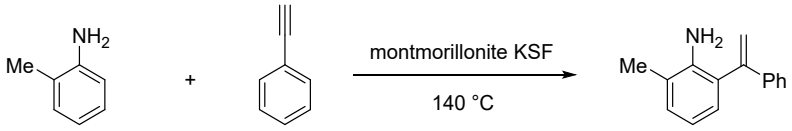
II. Synthesis of substrates 1



General procedure A[1]: To an oven-dried round bottom flask with reflux condenser equipped with a stir bar were added $Pd(PPh_3)_4$ (3 mol%), Na_2CO_3 (2.0 equiv.), substituted aniline (3 mmol, 1.0 equiv.), aryl boronic acid (1.5 equiv.), ethyl alcohol (0.5 M), toluene (0.5 M) and H_2O (2.0 M). The reaction mixture was heated to 100 °C overnight. The reaction mixture was then allowed to stand at room temperature and the residue was concentrated. The crude mixture was purified by silica gel flash column chromatography to provide the desired compound for the next step.



The synthesis of (*E*)-2-(*tert*-Butyl)-4-styrylaniline was carried out according to published procedures.[2] To a flask charged with 4-bromo-2-(*tert*-butyl)aniline (456.2 mg, 2.0 mmol, 1.0 equiv.), styrene (312.5 mg, 3.0 mmol, 1.5 equiv.), $Pd(OAc)_2$ (45 mg, 0.2 mmol, 0.1 equiv.) and P(*o*-$MeC_6H_4)_3$ (138.2 mg, 0.4 mmol, 0.2 equiv.), then Et_3N (10 mL) was added. The mixture was stirred at 125 °C for 12 h under Ar. After the mixture was cooled to room temperature, filtered and concentrated in vacuo. The residue was purified by silica gel flash column chromatography to provide the desired compound for the next step.



The synthesis of 2-methyl-6-(1-phenylvinyl)aniline was carried out according to published procedures.[3] Aniline (2 mmol), phenylacetylene (0.21 g, 2 mmol) and montmorillonite KSF (0.20 g) are introduced in a round bottomed flask equipped with magnetic stirrer and reflux condenser. The reaction mixture is heated at 140 °C (heating mantle) for 5 hours and then cooled to room temperature. The mixture was dissolved with dichloromethane and filtered. Then the solvent was concentrated in vacuo and the crude was purified by silica gel flash column chromatography to provide the desired compound for the next step.

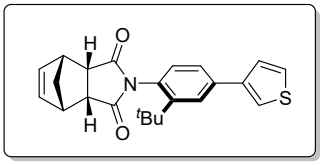
The substrates **1** were prepared according to the general procedure B.[4]

$R_1 < R_2$

General procedure B: To a solution of the cis-5-norbornene-endo-2,3-dicarboxylic anhydride (4.5 mmol) in acetic acid (2.0 M) was added slowly primary amine (3 mmol) and the mixture was stirred at room temperature

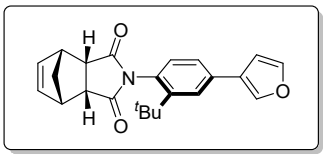
until anhydride dissolved completely. Then the reaction mixture was refluxed for 3-5 h at 110 °C in preheated oil bath. After completion of the reaction, the reaction mixture was then allowed to cool down to room temperature and the whole reaction mixture was transferred to a 250 mL beaker. Saturated Na_2CO_3 aqueous solution was added to the beaker containing reaction mixture until effervescence stop. The resulting mixture was extracted with DCM (60 mL × 3) and the combined organic layers were washed with brine (30 mL), dried over Na_2SO_4 and filtered. Then organic solvent was concentrated under reduced pressure, the residue was purified by column chromatography (ethyl acetate/petroleum ether/dichloromethane = 1/3/1, v/v/v) to give the products **1**.

(3a*R*,4*S*,7*R*,7a*S*)-2-(2-(*tert*-butyl)-4-(thiophen-3-yl)phenyl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (1c)



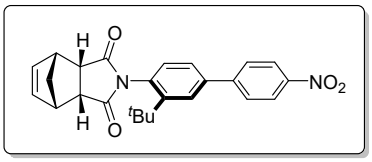
White solid, **m.p.** = 148–150 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 2.1 Hz, 1H), 7.42 - 7.40 (m, 2H), 7.38 - 7.37 (m, 1H), 7.33 (dd, *J* = 5.0, 1.4 Hz, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 6.35 - 6.34 (m, 2H), 3.53 - 3.51 (m, 2H), 3.46 - 3.45 (m, 2H), 1.81 - 1.79 (m, 1H), 1.63 - 1.61 (m, 1H), 1.32 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.3, 148.3, 142.0, 137.3, 135.1, 131.1, 129.8, 126.9, 126.6, 126.3, 125.5, 121.1, 52.4, 46.1, 45.2, 35.7, 31.6. **HRMS (ESI)**: Calculated for $[C_{23}H_{23}NNaO_2S, M+Na]^+$: 400.1342; Found: 400.1348.

(3a*R*,4*S*,7*R*,7a*S*)-2-(2-(*tert*-butyl)-4-(furan-3-yl)phenyl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (1d)



White solid, **m.p.** = 129–131 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.70 - 7.69 (m, 1H), 7.61 (d, *J* = 2.0 Hz, 1H), 7.47 - 7.46 (m, 1H), 7.31 (dd, *J* = 8.1, 2.0 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 6.66 - 6.65 (m, 1H), 6.34 - 6.33 (m, 2H), 3.53 - 3.51 (m, 2H), 3.46 - 3.45 (m, 2H), 1.81 - 1.79 (m, 1H), 1.62 - 1.61 (m, 1H), 1.31 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.3, 148.4, 143.7, 138.9, 135.1, 133.9, 131.1, 129.6, 126.25, 126.17, 125.0, 109.0, 52.4, 46.0, 45.2, 35.6, 31.6. **HRMS (ESI)**: Calculated for $[C_{23}H_{23}NNaO_3, M+Na]^+$: 384.1570; Found: 384.1575.

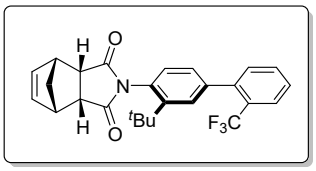
(3a*R*,4*S*,7*R*,7a*S*)-2-(3-(*tert*-butyl)-4'-nitro-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (1g)



Yellow solid, **m.p.** = 217–219 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.31 - 8.28 (m, 2H), 7.73 (d, *J* = 2.0 Hz, 1H), 7.70 - 7.67 (m, 2H), 7.45 - 7.44 (m, 1H), 6.82 (d, *J* = 8.1 Hz, 1H), 6.37 - 6.36 (m, 2H), 3.56 - 3.53 (m,

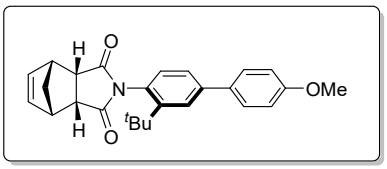
2H), 3.50 - 3.49 (m, 2H), 1.84 - 1.82 (m, 1H), 1.66 - 1.64 (m, 1H), 1.35 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.2, 149.0, 147.3, 147.2, 140.1, 135.1, 131.62, 131.58, 128.1, 127.9, 126.3, 124.1, 52.5, 46.1, 45.3, 35.9, 31.6. **HRMS (ESI)**: Calculated for $[C_{25}H_{24}N_2NaO_4, M+Na]^+$: 439.1628; Found: 439.1630.

(3a*R*,4*S*,7*R*,7a*S*)-2-(3-(*tert*-butyl)-2'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (1h)



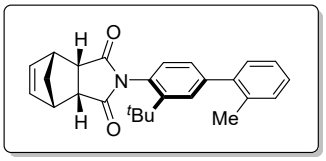
White solid, **m.p.** = 157–159 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.9 Hz, 1H), 7.57 - 7.54 (m, 1H), 7.49 - 7.45 (m, 2H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.19 - 7.17 (m, 1H), 6.72 (d, *J* = 7.9 Hz, 1H), 6.36 - 6.35 (m, 2H), 3.54 - 3.52 (m, 2H), 3.47 - 3.46 (m, 2H), 1.82 - 1.79 (m, 1H), 1.64 - 1.62 (m, 1H), 1.29 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 147.4, 140.7, 135.1, 132.0, 131.4, 130.3, 130.1, 129.6, 128.5 (q, $J_{C\text{-}F}$= 30.3 Hz), 127.64, 127.56, 126.2 (q, $J_{C\text{-}F}$= 5.4 Hz), 125.1, 123.0, 52.4, 46.0, 45.3, 35.7, 31.6. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -56.6. **HRMS (ESI)**: Calculated for $[C_{26}H_{24}F_3NNaO_2, M+Na]^+$: 462.1651; Found: 462.1660.

(3a*R*,4*S*,7*R*,7a*S*)-2-(3-(*tert*-butyl)-4'-methoxy-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (1i)



White solid, **m.p.** = 147–149 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 2.1 Hz, 1H), 7.49 - 7.46 (m, 2H), 7.37 - 7.35 (m, 1H), 6.98 - 6.95 (m, 2H), 6.72 (d, *J* = 8.1 Hz, 1H), 6.35 - 6.34 (m, 2H), 3.84 (s, 3H), 3.53 -3.51 (m, 2H), 3.47 -3.46 (m, 2H), 1.81 - 1.79 (m, 1H), 1.63 - 1.61 (m, 1H), 1.32 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.3, 159.4, 148.1, 142.2, 135.1, 133.4, 130.9, 129.4, 128.4, 127.3, 125.8, 114.2, 55.4, 52.4, 46.0, 45.3, 35.7, 31.7. **HRMS (ESI)**: Calculated for $[C_{26}H_{27}NNaO_3, M+Na]^+$: 424.1883; Found: 424.1889.

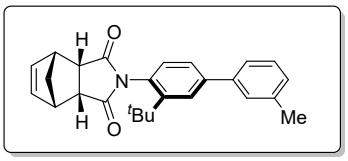
(3a*R*,4*S*,7*R*,7a*S*)-2-(3-(*tert*-butyl)-2'-methyl-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (1j)



White solid, **m.p.** = 171–173 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 2.0 Hz, 1H), 7.27 - 7.26 (m, 2H), 7.24 - 7.23 (m, 2H), 7.19 - 7.17 (m, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 6.36 - 6.35 (m, 2H), 3.54 - 3.51 (m, 2H), 3.47 - 3.46 (m, 2H), 2.29 (s, 3H), 1.82 - 1.79 (m, 1H), 1.64 - 1.61 (m, 1H), 1.30 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.3, 147.5, 142.9, 141.3, 135.4, 135.1, 130.5, 130.3, 129.9, 129.8, 129.4, 128.0, 127.5, 125.9, 52.4, 46.0, 45.3, 35.7, 31.7, 20.6. **HRMS (ESI)**: Calculated for $[C_{26}H_{27}NNaO_2, M+Na]^+$: 408.1934; Found:

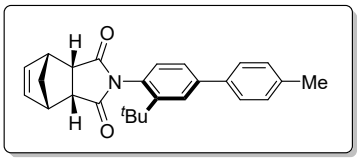
408.1941.

(3a*R*,4*S*,7*R*,7a*S*)-2-(3-(*tert*-butyl)-3'-methyl-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (1k)



White solid, **m.p.** = 163–165 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 2.0 Hz, 1H), 7.39 (dd, *J* = 8.0, 2.1 Hz, 1H), 7.34 - 7.31 (m, 3H), 7.18 - 7.16 (m, 1H), 6.74 (d, *J* = 8.1 Hz, 1H), 6.36 - 6.35 (m, 2H), 3.54 - 3.51 (m, 2H), 3.47 - 3.46 (m, 2H), 2.41 (s, 3H), 1.81 - 1.79 (m, 1H), 1.63 - 1.61 (m, 1H), 1.33 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.3, 148.1, 142.7, 140.9, 138.4, 135.1, 130.9, 129.9, 128.7, 128.3, 128.2, 127.8, 126.2, 124.6, 52.4, 46.1, 45.3, 35.8, 31.7, 21.6. **HRMS (ESI)**: Calculated for $[C_{26}H_{27}NNaO_2, M+Na]^+$: 408.1934; Found: 408.1938.

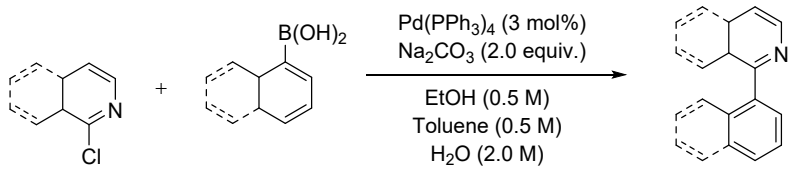
(3a*R*,4*S*,7*R*,7a*S*)-2-(3-(*tert*-butyl)-4'-methyl-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (1l)



White solid, **m.p.** = 185–187 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 2.0 Hz, 1H), 7.44 - 7.42 (m, 2H), 7.39 (dd, *J* = 8.0, 2.1 Hz, 1H), 7.25 - 7.23 (m, 2H), 6.73 (d, *J* = 8.1 Hz, 1H), 6.36 - 6.35 (m, 2H), 3.54 - 3.52 (m, 2H), 3.47 - 3.46 (m, 2H), 2.39 (s, 3H), 1.82 - 1.79 (m, 1H), 1.64 - 1.61 (m, 1H), 1.32 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.3, 148.1, 142.5, 138.0, 137.4, 135.1, 130.9, 129.7, 129.5, 127.6, 127.2, 126.0, 52.4, 46.1, 45.3, 35.7, 31.7, 21.1. **HRMS (ESI)**: Calculated for $[C_{26}H_{27}NNaO_2, M+Na]^+$: 408.1934; Found: 408.1939.

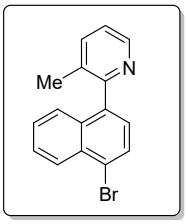
III. Synthesis of substrates 2

The substrates **2** were prepared according to the general procedure C.[5]



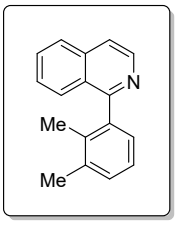
General procedure C: To an oven-dried round bottom flask with reflux condenser equipped with a stir bar were added $Pd(PPh_3)_4$ (3 mol%), Na_2CO_3 (2.0 equiv.), substituted quinoline (5 mmol, 1.0 equiv.), aryl boronic acid (1.5 equiv.), ethyl alcohol (0.5 M), toluene (0.5 M) and H_2O (2.0 M). The reaction mixture was heated to 100 °C overnight. The reaction mixture was then allowed to stand at room temperature and the residue was concentrated. The crude mixture was purified by column chromatography (ethyl acetate/petroleum ether = 1/5, v/v) to afford the resulting product **2**.

2-(4-bromonaphthalen-1-yl)-3-methylpyridine (2f)



Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 - 8.58 (m, 1H), 8.32 (d, *J* = 8.5 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.64 - 7.62 (m, 1H), 7.59 - 7.56 (m, 1H), 7.44 - 7.38 (m, 2H), 7.28 - 7.25 (m, 2H), 2.04 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.7, 147.1, 138.4, 138.0, 132.7, 132.6, 132.2, 129.5, 127.6, 127.3, 127.2, 126.8, 126.0, 123.1, 122.8, 19.3. **HRMS (ESI)**: Calculated for $[C_{16}H_{12}BrNNa, M+Na]^+$: 320.0045; Found: 320.0050.

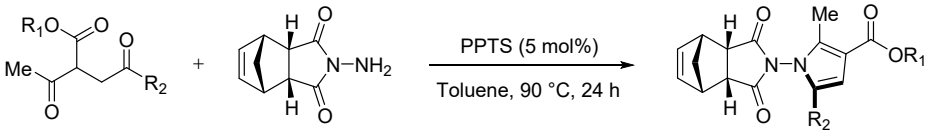
1-(2,3-dimethylphenyl)isoquinoline (2i)



White solid, **m.p.** = 74–76 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 5.8 Hz, 1H), 7.88 - 7.86 (m, 1H), 7.68 - 7.64 (m, 3H), 7.48 - 7.45 (m, 1H), 7.28 - 7.26 (m, 1H), 7.23 - 7.20 (m, 1H), 7.17 - 7.15 (m, 1H), 2.37 (s, 3H), 1.94 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.1, 142.2, 139.2, 137.2, 136.3, 134.9, 130.1, 129.9, 127.7, 127.4, 127.1, 126.8, 125.3, 119.8, 20.4, 16.7. **HRMS (ESI)**: Calculated for $[C_{17}H_{15}NNa, M+Na]^+$: 256.1097; Found: 256.1105.

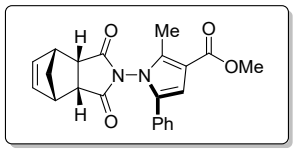
IV. Synthesis of substrates 4

The substrates **4** were prepared according to the general procedure D.[6]



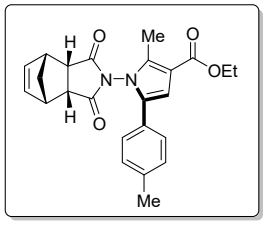
General procedure D: To a seal tube with oven-dried stir bar was added hydrazine (6 mmol, 1.2 equiv.) and PPTS (5 mol%) in toluene (25 mL). 1,4-dione (5 mmol, 1.0 equiv.) were then added. The mixture was allowed to stir at 90 ℃ for 24 h and cooled to room temperature. The residue was purified by column chromatography (ethyl acetate/petroleum ether = 1/5, v/v) as eluent to give N-aminopyrrole **4**.

methyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (4a)



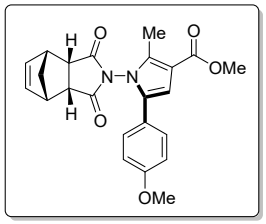
White solid, **m.p.** =171–173 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 - 7.30 (m, 3H), 7.21 - 7.19 (m, 2H), 6.66 (s, 1H), 6.31 - 6.30 (m, 2H), 3.81 (s, 3H), 3.48 - 3.46 (m, 2H), 3.244 - 3.235 (m, 2H), 2.30 (s, 3H), 1.82 - 1.79 (m, 1H), 1.55 - 1.53 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.8, 164.9, 137.1, 135.7, 130.5, 127.4, 126.2, 125.7, 125.5, 112.0, 109.5, 52.3, 51.1, 45.0, 44.7, 11.1. **HRMS (ESI)**: Calculated for $[C_{22}H_{21}N_2O_4, M+H]^+$: 377.1496; Found: 377.1506.

ethyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-(p-tolyl)-1*H*-pyrrole-3-carboxylate (4b)



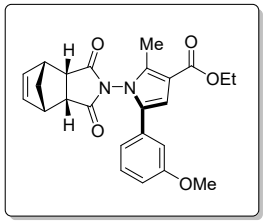
White solid, **m.p.** = 172–174 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.15 - 7.10 (m, 4H), 6.66 (s, 1H), 6.334 - 6.326 (m, 2H), 4.32 - 4.28 (m, 2H), 3.50 - 3.49 (m, 2H), 3.28 - 3.27 (m, 2H), 2.36 (s, 3H), 2.31 (s, 3H), 1.84 - 1.82 (m, 1H), 1.57 - 1.55 (m, 1H), 1.37 - 1.34 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.0, 164.8, 138.1, 136.3, 135.6, 133.0, 129.3, 128.2, 127.3, 112.1, 108.4, 59.7, 52.2, 44.9, 44.4, 21.2, 14.5, 11.1. **HRMS (ESI)**: Calculated for $[C_{24}H_{24}N_2NaO_4, M+Na]^+$: 427.1628; Found: 427.1637.

methyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-5-(4-methoxyphenyl)-2-methyl-1*H*-pyrrole-3-carboxylate (4c)



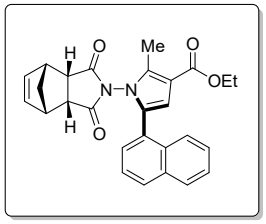
White solid, **m.p.** = 152–154 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.13 - 7.11 (m, 2H), 6.85 - 6.83 (m, 2H), 6.58 (s, 1H), 6.31 - 6.30 (m, 2H), 3.804 - 3.798 (m, 6H), 3.47 - 3.46 (m, 2H), 3.24 - 3.23 (m, 2H), 2.28 (s, 3H), 1.81 - 1.79 (m, 1H), 1.54 - 1.52 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.0, 165.2, 159.6, 136.2, 135.5, 132.8, 129.9, 122.5, 114.0, 111.7, 108.1, 55.3, 52.2, 51.0, 44.9, 44.4, 11.1. **HRMS (ESI)**: Calculated for $[C_{23}H_{22}N_2NaO_5, M+Na]^+$: 429.1421; Found: 429.1429.

ethyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-5-(3-methoxyphenyl)-2-methyl-1*H*-pyrrole-3-carboxylate (4d)



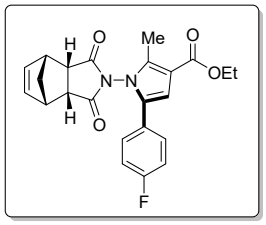
White solid, **m.p.** = 118–120 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.24 - 7.20 (m, 1H), 6.85 - 6.83 (m, 1H), 6.78 - 6.76 (m, 2H), 6.68 (s, 1H), 6.32 - 6.31 (m, 2H), 4.31 - 4.26 (m, 2H), 3.77 (s, 3H), 3.48 - 3.47 (m, 2H), 3.27 - 3.26 (m, 2H), 2.30 (s, 3H), 1.83 - 1.80 (m, 1H), 1.56 - 1.54 (m, 1H), 1.35 - 1.32 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.0, 164.7, 159.6, 136.7, 135.6, 132.9, 131.4, 129.6, 120.3, 114.3, 113.4, 112.2, 108.9, 59.8, 55.3, 52.2, 44.9, 44.4, 14.5, 11.1. **HRMS (ESI)**: Calculated for $[C_{24}H_{24}N_2NaO_5, M+Na]^+$: 443.1577; Found: 443.1584.

ethyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-(naphthalen-1-yl)-1*H*-pyrrole-3-carboxylate (4e)



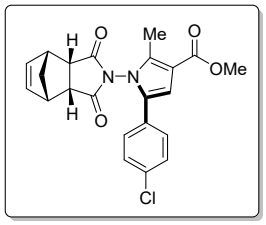
White solid, **m.p.** = 158–160 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.82 - 7.78 (m , 3H), 7.68 - 7.67 (m, 1H), 7.50 - 7.46 (m, 2H), 7.33 - 7.31 (m, 1H), 6.78 (s, 1H), 6.313 - 6.306 (m, 2H), 4.32 - 4.28 (m, 2H), 3.45 - 3.44 (m, 2H), 3.19 - 3.18 (m, 2H), 2.33 (s, 3H), 1.79 - 1.77 (m, 1H), 1.50 - 1.48 (m, 1H), 1.36 - 1.33 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.0, 164.7, 136.9, 135.6, 133.2, 133.0, 132.8, 128.3, 128.1, 127.7, 127.6, 127.3, 126.54, 126.47, 125.9, 112.4, 109.2, 59.8, 52.2, 44.9, 44.4, 14.5, 11.2. **HRMS (ESI)**: Calculated for $[C_{27}H_{24}N_2NaO_4, M+Na]^+$: 463.1628; Found: 463.1635.

ethyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-5-(4-fluorophenyl)-2-methyl-1*H*-pyrrole-3-carboxylate (4f)



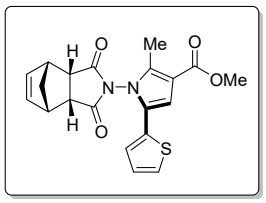
White solid, **m.p.** = 192–194 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.19 - 7.16 (m, 2H), 7.03 - 7.00 (m, 2H), 6.64 (s, 1H), 6.31 - 6.30 (m, 2H), 4.30 - 4.26 (m, 2H), 3.48 - 3.47 (m, 2H), 3.24 (dd, J = 2.9, 1.6 Hz, 2H), 2.29 (s, 3H), 1.83 - 1.80 (m, 1H), 1.56 - 1.53 (m, 1H), 1.35 - 1.32 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.0, 164.6, 162.7 (d, $J_{C\text{-}F}$ = 248.9 Hz), 136.5, 135.6, 131.9, 130.3 (d, $J_{C\text{-}F}$ = 8.2 Hz), 126.3 (d, $J_{C\text{-}F}$ = 3.4 Hz), 115.6 (d, $J_{C\text{-}F}$ = 21.7 Hz), 112.2, 108.9, 59.8, 52.3, 45.0, 44.3, 14.5, 11.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -112.90 – -112.96 (m). **HRMS (ESI)**: Calculated for [$C_{23}H_{21}FN_2NaO_4$, M+Na]$^+$: 431.1378; Found: 431.1389.

methyl 5-(4-chlorophenyl)-1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-1*H*-pyrrole-3-carboxylate (4g)



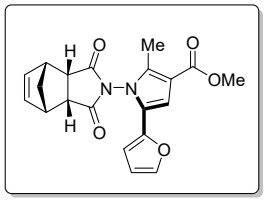
White solid, **m.p.** = 210–212 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.31 - 7.29 (m, 2H), 7.14 - 7.12 (m, 2H), 6.65 (s, 1H), 6.315 - 6.307 (m, 2H), 3.81 (s, 3H), 3.49 - 3.48 (m, 2H), 3.274 - 3.265 (m, 2H), 2.29 (s, 3H), 1.83 - 1.81 (m, 1H), 1.57 - 1.54 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.9, 165.0, 137.1, 135.6, 134.3, 131.8, 129.6, 128.9, 128.6, 112.1, 109.1, 52.3, 51.1, 45.0, 44.4, 11.1. **HRMS (ESI)**: Calculated for [$C_{22}H_{19}ClN_2NaO_4$, M+Na]$^+$: 433.0926; Found: 433.0931.

methyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-(thiophen-2-yl)-1*H*-pyrrole-3-carboxylate (4h)



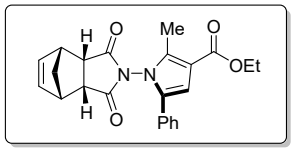
White solid, **m.p.** = 179–181 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.24 - 7.23 (m, 1H), 6.99 - 6.97 (m, 2H), 6.79 (s, 1H), 6.34 - 6.33 (m, 2H), 3.81 (s, 3H), 3.53 - 3.51 (m , 2H), 3.434 - 3.425 (m, 2H), 2.29 (s, 3H), 1.86 - 1.83 (m, 1H), 1.62 - 1.60 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.8, 164.9, 137.1, 135.7, 130.5, 127.4, 126.2, 125.7, 125.5, 112.0, 109.5, 52.3, 51.1, 45.0, 44.7, 11.1. **HRMS (ESI)**: Calculated for [$C_{20}H_{18}N_2NaO_4S$, M+Na]$^+$: 405.0879; Found: 405.0887.

methyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-5-(furan-2-yl)-2-methyl-1*H*-pyrrole-3-carboxylate (4i)



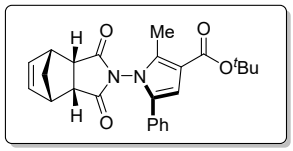
White solid, **m.p.** = 154–156 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.312 - 7.307 (m, 1H), 6.82 (s, 1H), 6.38 - 6.37 (m, 1H), 6.345 - 6.337 (m, 2H), 6.31 - 6.30 (m, 1H), 3.81 (s, 3H), 3.55 - 3.53 (m, 2H), 3.49 - 3.48 (m, 2H), 2.28 (s, 3H), 1.87 - 1.85 (m, 1H), 1.65 - 1.62 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.8, 164.8, 144.8, 141.8, 137.1, 135.6, 122.8, 112.0, 111.3, 108.4, 106.8, 52.3, 51.2, 45.1, 44.7, 10.8. **HRMS (ESI)**: Calculated for $[C_{20}H_{19}N_2O_5, M+H]^+$: 367.1288; Found: 367.1294.

ethyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (4j)



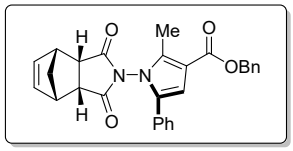
White solid, **m.p.** = 147–149 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36 - 7.32 (m, 3H), 7.23 - 7.21 (m, 2H), 6.70 (s, 1H), 6.34 - 6.33 (m, 2H), 4.33 - 4.29 (m, 2H), 3.50 - 3.49 (m, 2H), 3.27 - 3.26 (m, 2H), 2.32 (s, 3H), 1.84 - 1.82 (m, 1H), 1.57 - 1.55(m, 1H), 1.37 - 1.34 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.0, 164.7, 136.6, 135.6, 133.0, 130.2, 128.6, 128.3, 128.2, 112.2, 108.8, 59.8, 52.2, 44.9, 44.4, 14.5, 11.1. **HRMS (ESI)**: Calculated for $[C_{23}H_{22}N_2NaO_4, M+Na]^+$: 413.1472; Found: 413.1479.

***tert*-butyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (4k)**



White solid, **m.p.** = 189–191 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 - 7.29 (m, 3H), 7.20 - 7.18 (m, 2H), 6.63 (s, 1H), 6.31 - 6.30 (m, 2H), 3.47 - 3.46 (m, 2H), 3.24 - 3.23 (m, 2H), 2.27 (s, 3H), 1.81 - 1.79 (m, 1H), 1.608 - 1.606 (m, 1H), 1.55 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.1, 164.1, 135.8, 135.6, 132.6, 130.3, 128.5, 128.3, 128.1, 113.7, 109.1, 52.2, 44.9, 44.4, 28.4, 11.1. **HRMS (ESI)**: Calculated for $[C_{25}H_{26}N_2NaO_4, M+Na]^+$: 441.1785; Found: 441.1792.

benzyl 1-((3a*R*,4*S*,7*R*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (4l)

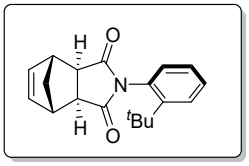


White solid, **m.p.** = 193–195 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.42 - 7.40 (m, 2H), 7.38 - 7.35 (m, 2H), 7.33 - 7.29 (m, 4H), 7.20 - 7.18 (m, 2H), 6.70 (s, 1H), 6.30 - 6.29 (m, 2H), 5.28 (s, 2H), 3.46 - 3.45 (m, 2H), 3.23 - 3.22 (m, 2H), 2.30 (s, 3H), 1.81 - 1.78 (m, 1H), 1.53 - 1.51 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.0, 164.4, 136.9, 136.6, 135.6, 133.1, 130.1, 128.6, 128.5, 128.3, 128.2, 128.02, 127.98, 111.9, 108.9, 65.6, 52.2, 44.9, 44.4, 11.2. **HRMS (ESI)**: Calculated for $[C_{28}H_{25}N_2O_4, M+H]^+$: 453.1809; Found: 453.1820.

V. Synthesis of substrates 6

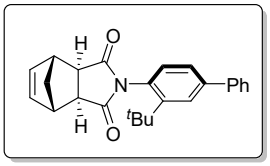
The substrates **6a-6g** were prepared according to the general procedure B with cis-5-norbornene-exo-2,3-dicarboxylic anhydride. The substrates **6h-6i** were prepared according to the general procedure D with corresponding exo-hydrazine.

(3a*R*,4*R*,7*S*,7a*S*)-2-(2-(*tert*-butyl)phenyl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (6a)



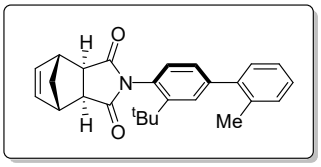
White solid, **m.p.** = 162–164 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.58 (d, *J* = 9.7 Hz, 1H), 7.40 - 7.38 (m, 1H), 7.29 - 7.27 (m, 1H), 6.81 - 6.79 (m, 1H), 6.353 - 6.345 (m, 2H), 3.46 - 3.45 (m, 2H), 2.882 - 2.879 (m, 2H), 1.69 - 1.66 (m, 1H), 1.57 - 1.55 (m, 1H), 1.30 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.4, 148.0, 138.1, 130.5, 130.0, 129.8, 128.8, 127.4, 48.1, 45.8, 43.6, 35.6, 31.6. **HRMS (ESI)**: Calculated for $[C_{19}H_{21}NNaO_2, M+Na]^+$: 318.1465; Found: 318.1476.

(3a*R*,4*R*,7*S*,7a*S*)-2-(3-(*tert*-butyl)-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (6b)



White solid, **m.p.** = 190–192 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.75 (d, *J* = 2.0 Hz, 1H), 7.57 - 7.55 (m, 2H), 7.47 - 7.43 (m, 3H), 7.38 - 7.35 (m, 1H), 6.88 - 6.87 (m, 1H), 6.36 - 6.35 (m, 2H), 3.475 - 3.467 (m, 2H), 2.903 - 2.900 (m, 2H), 1.70 - 1.68 (m, 1H), 1.59 - 1.57 (m, 1H), 1.35 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.5, 148.2, 142.8, 140.8, 138.1, 130.4, 129.6, 128.8, 128.0, 127.7, 127.4, 126.3, 48.2, 45.82, 45.79, 43.6, 35.8, 31.7. **HRMS (ESI)**: Calculated for $[C_{25}H_{26}NO_2, M+H]^+$: 372.1958; Found: 372.1964.

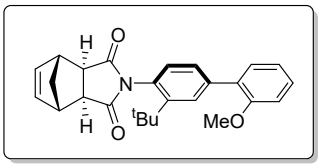
(3a*R*,4*R*,7*S*,7a*S*)-2-(3-(*tert*-butyl)-2'-methyl-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (6c)



White solid, **m.p.** = 168–170 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.53 - 7.52 (m, 1H), 7.29 - 7.27 (m, 3H), 7.25 - 7.23 (m, 2H), 6.86 - 6.84 (m, 1H), 6.37 - 6.36 (m, 2H), 3.48 - 3.47 (m, 2H), 2.91 - 2.90 (m, 2H), 2.31 (s, 3H), 1.70 - 1.68 (m, 1H), 1.58 - 1.56 (m, 1H), 1.33 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.5, 147.6, 143.1, 141.2, 138.1, 135.4, 130.5, 130.0, 129.9, 129.7, 129.1, 128.1, 127.6, 125.9, 48.1, 45.9, 43.6,

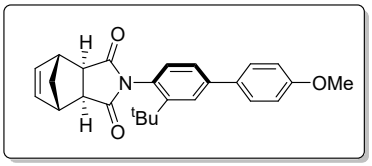
35.8, 31.7, 20.6. **HRMS (ESI)**: Calculated for $[C_{26}H_{27}NNaO_2$, M+Na$]^+$: 408.1934; Found: 408.1937.

(3a*R*,4*R*,7*S*,7a*S*)-2-(3-(*tert*-butyl)-2'-methoxy-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (6d)



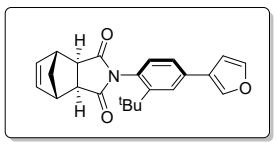
White solid, **m.p.** = 157–159 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.72 (d, *J* = 2.0 Hz, 1H), 7.44 - 7.42 (m, 1H), 7.34 - 7.31 (m, 2H), 7.05 - 7.02 (m, 1H), 6.99 - 6.98 (m, 1H), 6.83 - 6.81 (m, 1H), 6.36 - 6.35 (m, 2H), 3.80 (s, 3H), 3.47 - 3.46 (m, 2H), 2.90 - 2.89 (m, 2H), 1.69 - 1.67 (m, 1H), 1.58 - 1.56 (m, 1H), 1.33 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.6, 156.5, 147.2, 139.8, 138.1, 130.9, 130.4, 130.0, 129.4, 129.0, 128.9, 128.6, 120.9, 111.3, 55.5, 48.1, 45.8, 43.6, 35.7, 31.7. **HRMS (ESI)**: Calculated for $[C_{26}H_{27}NNaO_3$, M+Na$]^+$: 424.1883; Found: 424.1883.

(3a*R*,4*R*,7*S*,7a*S*)-2-(3-(*tert*-butyl)-4'-methoxy-[1,1'-biphenyl]-4-yl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (6e)



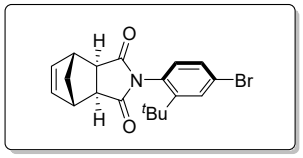
White solid, **m.p.** = 171–173 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.71 (d, *J* = 2.1 Hz, 1H), 7.50 - 7.48 (m, 2H), 7.43 - 7.41 (m, 1H), 6.99 - 6.97 (m, 2H), 6.85 - 6.84 (m, 1H), 6.36 - 6.35 (m, 2H), 3.86 (s, 3H), 3.48 - 3.47 (m, 2H), 2.902 - 2.899 (m, 2H), 1.70 - 1.68 (m, 1H), 1.57 - 1.56 (m, 1H), 1.35 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.5, 159.4, 148.1, 142.4, 138.1, 133.3, 130.3, 129.2, 128.5, 127.6, 125.8, 114.3, 55.4, 48.1, 45.8, 43.6, 35.7, 31.6. **HRMS (ESI)**: Calculated for $[C_{26}H_{27}NNaO_3$, M+Na$]^+$: 424.1883; Found: 424.1891.

(3a*R*,4*R*,7*S*,7a*S*)-2-(2-(*tert*-butyl)-4-(tetrahydrofuran-3-yl)phenyl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (6f)



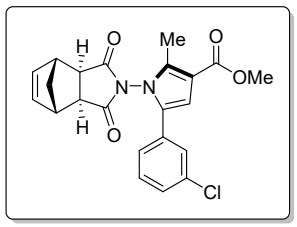
White solid, **m.p.** = 202–204 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.88 (d, *J* = 2.0 Hz, 1H), 7.55 - 7.53 (m, 1H), 7.481 - 7.476 (m, 1H), 6.82 - 6.80 (m, 1H), 6.68 - 6.67 (m, 1H), 6.48 - 6.47 (m, 1H), 6.36 - 6.35 (m, 2H), 3.47 - 3.45 (m, 2H), 2.89 - 2.88 (m, 2H), 1.69 - 1.68 (m, 1H), 1.55 - 1.52 (m, 1H), 1.34 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.4, 153.3, 148.4, 142.5, 138.1, 132.1, 130.5, 129.5, 124.2, 122.8, 111.8, 106.0, 48.1, 45.8, 43.6, 35.7, 31.6. **HRMS (ESI)**: Calculated for $[C_{23}H_{24}NO_3$, M+H$]^+$: 362.1751; Found: 362.1757.

(3a*R*,4*R*,7*S*,7a*S*)-2-(4-bromo-2-(*tert*-butyl)phenyl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (6g)



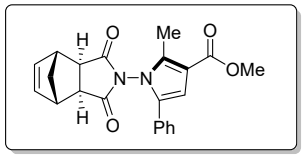
White solid, **m.p.** = 185–187 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.69 (d, *J* = 2.3 Hz, 1H), 7.41 - 7.39 (m, 1H), 6.68 - 6.66 (m, 1H), 6.35 - 6.34 (m, 2H), 3.45 - 3.44 (m, 2H), 2.879 - 2.876 (m, 2H), 1.69 - 1.66 (m, 1H), 1.49 - 1.47 (m, 1H), 1.29 (s, 9H). **^{13}C NMR** (126 MHz, CDCl3) δ 178.5, 150.4, 138.0, 132.2, 131.7, 130.5, 129.7, 124.1, 48.1, 45.8, 43.6, 35.8, 31.4. **HRMS (ESI)**: Calculated for $[C_{19}H_{20}BrNNaO_2, M+Na]^+$: 396.0570; Found: 396.0576.

methyl 5-(3-chlorophenyl)-1-((3a*R*,4*R*,7*S*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-1*H*-pyrrole-3-carboxylate (6h)



White solid, **m.p.** = 192–194 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.28 - 7.26 (m, 2H), 7.223 - 7.215 (m, 1H), 7.11 - 7.09 (m, 1H), 6.73 (s, 1H), 6.31 - 6.30 (m, 2H), 3.83 (s, 3H), 3.42 - 3.41 (m, 2H), 2.69 - 2.68 (m,, 2H), 2.40 (s, 3H), 1.71 - 1.68 (m, 1H), 1.55 - 1.53 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.5, 164.9, 137.5, 137.1, 134.6, 131.8, 131.6, 129.9, 128.3, 128.0, 126.1, 112.3, 109.5, 51.2, 45.7, 45.0, 43.4, 10.7. **HRMS (ESI)**: Calculated for $[C_{22}H_{19}ClN_2NaO_4, M+Na]^+$: 433.0926; Found: 433.0936.

methyl 1-((3a*R*,4*R*,7*S*,7a*S*)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (6i)

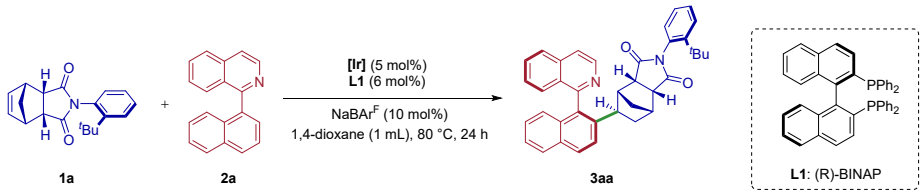


White solid, **m.p.** = 143–145 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.33 - 7.29 (m, 3H), 7.23 - 7.21 (m, 2H), 6.70 (s, 1H), 6.29 - 6.28 (m, 2H), 3.83 (s, 3H), 3.40 - 3.39 (m, 2H), 2.630 - 2.627 (m, 2H), 2.40 (s, 3H), 1.69 - 1.67 (m, 1H), 1.56 - 1.53 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.6, 165.1, 137.5, 136.5, 133.2, 130.1, 128.6, 128.29, 128.26, 112.1, 108.8, 51.1, 45.7, 44.9, 43.4, 10.7. **HRMS (ESI)**: Calculated for $[C_{22}H_{20}N_2NaO_4, M+Na]^+$: 399.1315; Found: 399.1323.

VI. Optimization of the reaction conditions

1. Construction of C−C and C−N atropisomers:

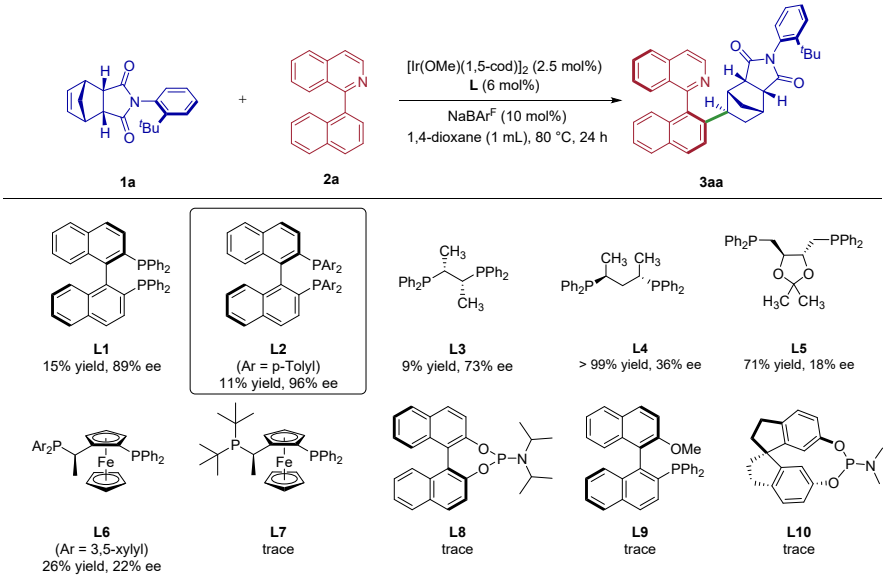
Table S1. Screening of catalyst.[a][b][c]



entry	cat.	yield (%)	ee (%)
1	$[Ir(coe)_2Cl]_2$	-	-
2	$[Ir(1,5\text{-}cod)_2]BF_4$	-	-
3	$[IrCl(1,5\text{-}cod)]_2$	-	-
4	**$[Ir(OMe)(1,5\text{-}cod)]_2$**	**15**	**89**

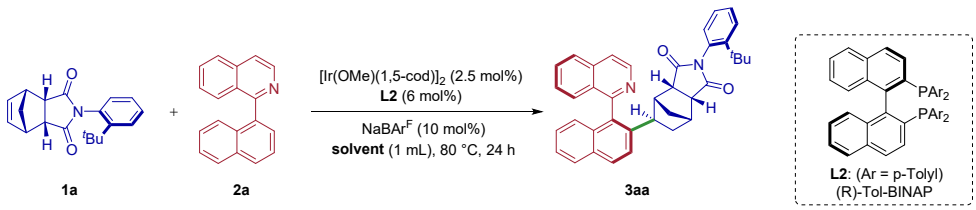
[a] Conditions: **1a** (0.05 mmol), **2a** (0.06 mmol), cat. (5 mol%), **L1** (6 mol %), $NaBAr^F$ (10 mol%) in 1,4-dioxane (1.0 mL) at 80 °C under N_2 for 24 h. [b] Yield was detected by ^1H NMR using 1,1,2,2-tetrachloroethane as the internal standard. [c] The enantiomeric ratio were determined by HPLC analysis with a chiral column.

Table S2. Screening of ligand.[a][b][c]



[a] Conditions: **1a** (0.05 mmol), **2a** (0.06 mmol), $[Ir(OMe)(1,5\text{-}cod)]_2$ (2.5 mol%), **L** (6 mol %), $NaBAr^F$ (10 mol%) in 1,4-dioxane (1.0 mL) at 80 °C under N_2 for 24 h. [b] Yield was detected by ^1H NMR using 1,1,2,2-tetrachloroethane as the internal standard. [c] The enantiomeric ratio were determined by HPLC analysis with a chiral column.

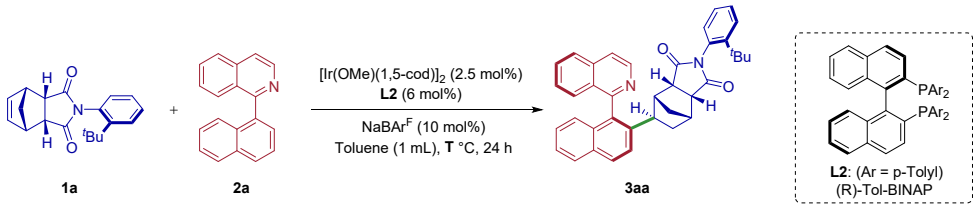
Table S3. Screening of amount of the solvent[a][b][c]



entry	cat.	yield (%)	ee (%)
1	Xylene	98	97
2	DCE	76	96
3	MTBE	>99	96
4	DCM	72	95
5	**Toluene**	**>99**	**97**
6	THF	37	95
7	Ph-F	>99	96

[a] Conditions: **1a** (0.05 mmol), **2a** (0.06 mmol), $[Ir(OMe)(1,5\text{-cod})]_2$ (2.5 mol%), **L2** (6 mol %), $NaBAr^F$ (10 mol%) in solvent (1.0 mL) at 80 °C under N_2 for 24 h. [b] Yield was detected by ^1H NMR using 1,1,2,2-tetrachloroethane as the internal standard. [c] The enantiomeric ratio were determined by HPLC analysis with a chiral column. Abbreviations: DCE, dichloroethane. MTBE, methyl tert-butyl ether. DCM, dichloromethane. THF, tetrahydrofuran. Ph-F, fluorobenzene.

Table S4. Screening of temperature[a][b][c]

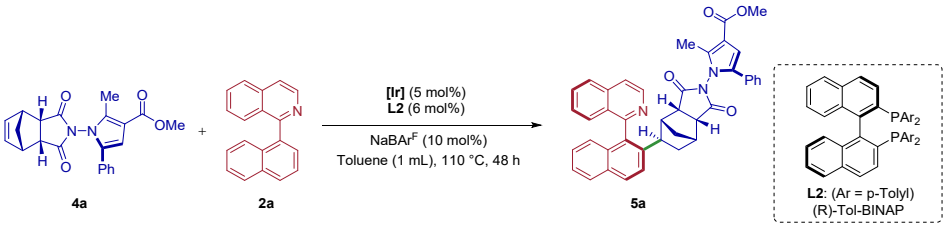


entry	T (°C)	yield (%)	ee (%)
1	60	42	95
2	**80**	**>99**	**97**
3	110	>99	96

[a] Conditions: **1a** (0.05 mmol), **2a** (0.06 mmol), $[Ir(OMe)(1,5\text{-cod})]_2$ (2.5 mol%), **L2** (6 mol %), $NaBAr^F$ (10 mol%) in toluene (1.0 mL) at T °C under N_2 for 24 h. [b] Yield was detected by ^1H NMR using 1,1,2,2-tetrachloroethane as the internal standard. [c] The enantiomeric ratio were determined by HPLC analysis with a chiral column.

2. Construction of C−C and N−N atropisomers:

Table S5. Screening of catalyst[a][b][c]

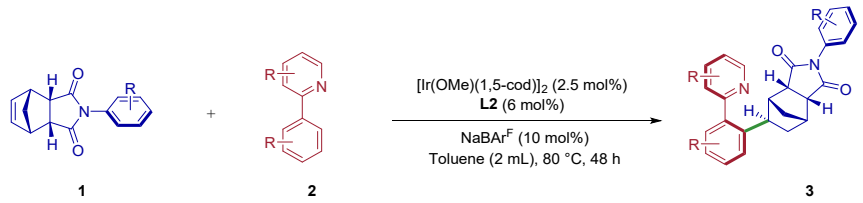


entry	cat.	yield (%)	ee (%)
1	$[Ir(OMe)(1,5\text{-cod})]_2$	47	96
2	**$[IrCl(1,5\text{-cod})]_2$**	**95**	**96**
3	$[Ir(coe)_2Cl]_2$	79	96
4	$Ir(cod)_2BARF$	-	-
5	$[Ir(1,5\text{-cod})_2]BF_4$	trace	-

[a] Conditions: **4a** (0.05 mmol), **2a** (0.06 mmol), cat. (5 mol%), **L2** (6 mol %), NaBAr^F (10 mol%) in toluene (1.0 mL) at 110 ℃ under N_2 for 48 h. [b] Yield was detected by ^{1}H NMR using 1,1,2,2-tetrachloroethane as the internal standard. [c] The enantiomeric ratio were determined by HPLC analysis with a chiral column.

VII. General synthetic procedure and analytical data for distal biaxial chiral compounds 3, 5 and 7

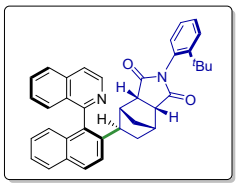
1. Construction of C−C and C−N atropisomers 3:



1 2 3

General procedure E: To an oven-dried 10 mL Schlenk tube containing a stirring bar was charged with $[Ir(OMe)(1,5\text{-cod})]_2$ (0.0025 mmol, 1.7 mg), **L2** (0.006 mmol, 4.1 mg) and 1.0 mL dry toluene in a nitrogen-filled glove-box, the mixture was stirred for 10 min at room temperature. Then corresponding substrate **1** (0.1 mmol, 1.0 equiv.), corresponding substrate **2** (0.12 mmol, 1.2 equiv.), $NaBAr^F$ (0.01 mmol, 8.9 mg) and another 1.0 mL dry toluene were added sequentially. The mixture was stirred at 80 °C for 48 hours, concentrated to dryness and the crude mixture was purified by flash column chromatography on silica gel using a mixture of Hexane/EtOAc (3/1, v/v) as eluent to obtain the desired product.

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3aa)



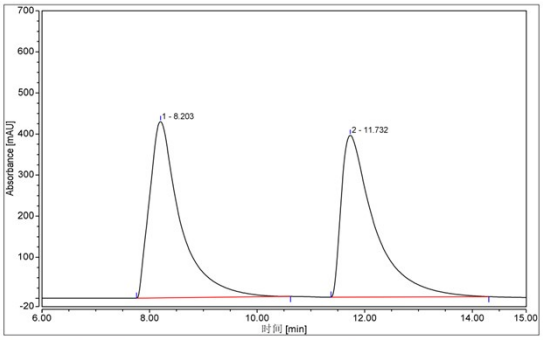
99% yield, white solid, **m.p.** = 159–161 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.7 Hz, 1H), 7.99 - 7.97 (m, 2H), 7.87 - 7.86 (m, 1H), 7.79 - 7.77 (m, 1H), 7.69 - 7.67 (m, 1H), 7.66 - 7.63 (m, 1H), 7.46 - 7.44 (m, 1H), 7.39 - 7.30 (m, 4H), 7.18 - 7.14 (m, 1H), 7.11 - 7.08 (m, 1H), 6.73 - 6.71 (m, 1H), 5.38 - 5.36 (m, 1H), 3.15 - 3.11 (m, 3H), 3.01 - 2.98 (m, 1H), 2.88 - 2.86 (m, 1H), 2.28 - 2.26 (m, 1H), 2.05 - 2.00 (m, 1H), 1.75 - 1.73 (m, 1H), 1.69 - 1.64 (m, 1H), 1.15 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 176.9, 159.9, 147.6, 142.8, 140.7, 136.4, 135.5, 133.2, 132.1, 130.8, 130.4, 130.0, 129.3, 128.9, 128.7, 128.4, 127.9, 127.8, 127.2, 127.0, 126.8, 126.5, 125.8, 125.5, 123.1, 120.4, 49.0, 48.7, 44.3, 41.3, 39.5, 39.4, 36.2, 35.6, 31.6.

HRMS (ESI): Calculated for $[C_{38}H_{34}N_2NaO_2, M+Na]^+$: 573.2512; Found: 573.2516.

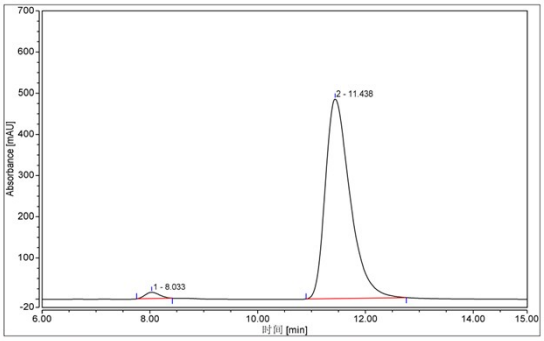
Optical Rotation: $[\alpha]^{25}_D$ = –107.1° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2343, 1708, 1367, 1172, 815, 749, 606.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 11.438 min (major) and 8.033 min (minor). 96% ee.

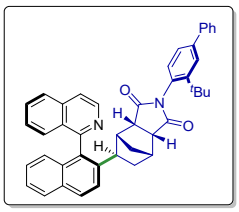


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.203	284.765	429.298	50.21	52.15
2	11.732	282.373	393.885	49.79	47.85



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.033	4.746	15.264	1.81	3.05
2	11.438	257.786	484.653	98.19	96.95

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(3-(*tert*-butyl)-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ab)



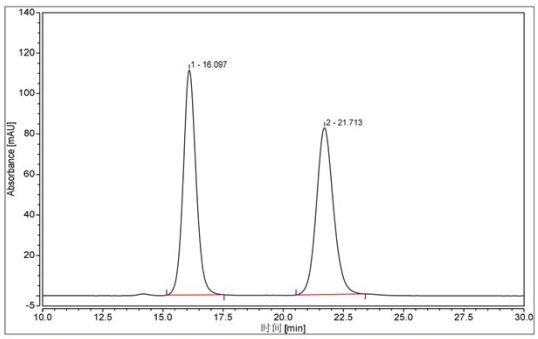
99% yield, white solid, **m.p.** = 288–290 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 5.8 Hz, 1H), 8.01 - 7.99 (m, 2H), 7.88 - 7.87 (m, 1H), 7.82 - 7.81 (m, 1H), 7.71 - 7.66 (m, 2H), 7.631 - 7.627 (m, 1H), 7.59 - 7.57 (m, 2H), 7.53 - 7.50 (m, 2H), 7.44 - 7.36 (m, 4H), 7.27 - 7.26 (m, 1H), 7.19 - 7.15 (m, 1H), 6.73 - 6.71 (m, 1H), 5.41 - 5.40 (m, 1H), 3.18 - 3.16 (m, 3H), 3.04 - 3.01 (m, 1H), 2.90 - 2.89 (m, 1H), 2.30 - 2.28 (m, 1H), 2.07 - 2.02 (m, 1H), 1.78 - 1.76 (m, 1H), 1.71 - 1.65 (m, 1H), 1.21 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 177.0, 159.9, 147.9, 142.8, 142.2, 141.0, 140.7, 136.4, 135.5, 133.3, 132.1, 130.8, 130.7, 129.2, 128.91, 128.89, 128.4, 128.0, 127.9, 127.8, 127.7, 127.4, 127.0, 126.8, 126.5, 126.1, 125.8, 125.5, 123.1, 120.4, 49.0, 48.7, 44.3, 41.4, 39.6, 39.4, 36.3, 35.8, 31.6.

HRMS (ESI): Calculated for $[C_{44}H_{39}N_2O_2, M+H]^+$: 627.3006; Found: 627.3008.

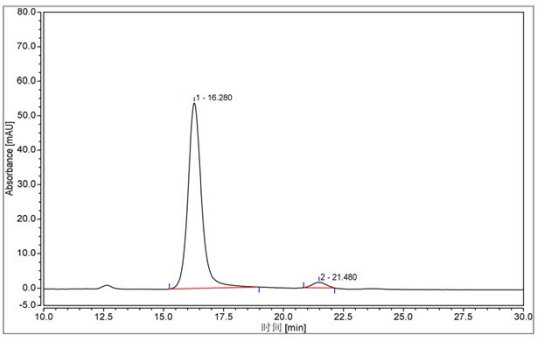
Optical Rotation: $[\alpha]^{25}_D$ = –169.5° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2359, 2340, 1749, 1698, 1684, 1653, 1558, 1541, 1507, 1457, 669.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 16.280 min (major) and 21.480 min (minor). 94% ee.

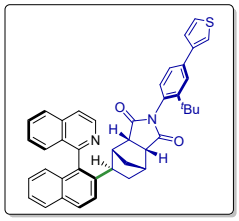


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	16.097	68.988	111.281	50.53	57.43
2	21.713	67.552	82.500	49.47	42.57

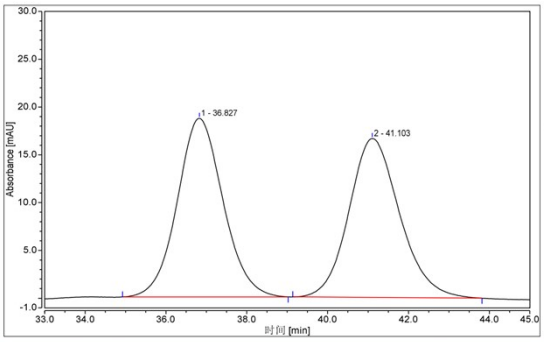


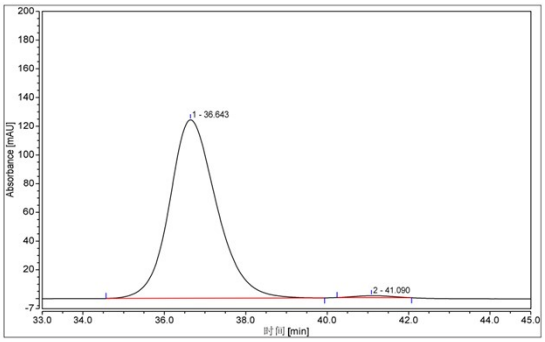
peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	16.280	35.333	53.856	97.11	97.17
2	21.480	1.053	1.566	2.89	2.83

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)-4-(thiophen-3-yl)phenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ac)



54% yield, white solid, **m.p.** = 282–284 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.70 (d, *J* = 5.7 Hz, 1H), 8.01 - 7.98 (m, 2H), 7.88 - 7.86 (m, 1H), 7.81 - 7.80 (m, 1H), 7.70 - 7.64 (m, 3H), 7.47 - 7.44 (m, 2H), 7.40 - 7.35 (m, 4H), 7.28 - 7.26 (m, 1H), 7.18 - 7.15 (m, 1H), 6.72 - 6.70 (m, 1H), 5.43 - 5.42 (m, 1H), 3.17 - 3.11 (m, 3H), 3.04 - 3.01 (m, 1H), 2.90 - 2.88 (m, 1H), 2.30 - 2.27 (m, 1H), 2.07 - 2.02 (m, 1H), 1.76 - 1.74 (m, 1H), 1.71 - 1.66 (m, 1H), 1.19 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 176.9, 159.9, 148.0, 142.8, 142.1, 140.7, 136.9, 136.4, 135.5, 133.2, 132.1, 130.8, 129.0, 128.9, 128.4, 127.9, 127.8, 127.1, 127.0, 126.9, 126.6, 126.52, 126.47, 125.8, 125.6, 125.4, 123.1, 121.0, 120.4, 49.0, 48.7, 44.4, 41.3, 39.6, 39.4, 36.1, 35.7, 31.6.
HRMS (ESI): Calculated for $[C_{42}H_{37}N_2O_2S, M+H]^+$: 633.2570; Found: 633.2573.
Optical Rotation: $[\alpha]^{25}_D$ = –179.0° (c = 1.0, $CHCl_3$).
IR (neat, cm^{-1}) = 2361, 2341, 1772, 1748, 1699, 1652, 1522, 1473, 1419, 669.
HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 80 : 20, 1.0 mL/min), 30 °C, 254 nm, R*t* = 36.643 min (major) and 41.090 min (minor). 98% ee.

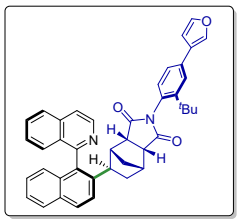




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	36.827	24.536	18.678	50.37	52.92
2	41.103	24.172	16.619	49.63	47.08

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	36.643	166.857	124.211	99.16	98.91
2	41.090	1.418	1.371	0.84	1.09

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)-4-(furan-3-yl)phenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ad)



60% yield, white solid, **m.p.** = 257–259 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.70 (d, *J* = 5.8 Hz, 1H), 8.00 - 7.98 (m, 2H), 7.88 - 7.86 (m, 1H), 7.81 - 7.80 (m, 1H), 7.76 - 7.75 (m, 1H), 7.70 - 7.65 (m, 2H), 7.54 - 7.53

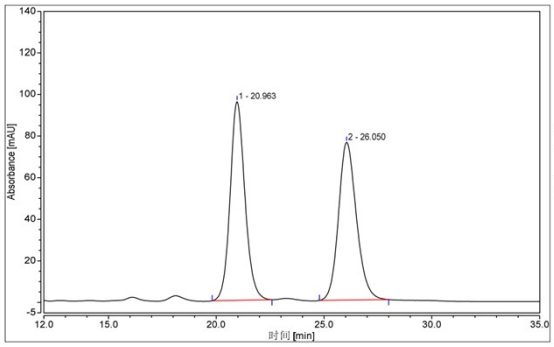
(m, 2H), 7.40 - 7.34 (m, 3H), 7.18 - 7.15 (m, 2H), 6.72 - 6.70 (m, 2H), 5.43 - 5.42 (m, 1H), 3.16 - 3.09 (m, 3H), 3.03 - 3.00 (m, 1H), 2.90 - 2.88 (m, 1H), 2.29 - 2.27 (m, 1H), 2.08 - 2.02 (m, 1H), 1.75 - 1.67 (m, 2H), 1.18 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 176.9, 159.9, 148.1, 143.9, 142.8, 140.7, 138.8, 136.4, 135.5, 133.5, 133.2, 132.1, 130.9, 130.8, 128.91, 128.87, 128.4, 127.9, 127.8, 127.0, 126.9, 126.5, 126.4, 126.3, 125.8, 125.6, 124.9, 123.2, 120.4, 109.1, 49.0, 48.7, 44.5, 41.2, 39.6, 39.4, 36.0, 35.6, 31.6.

HRMS (ESI): Calculated for $[C_{42}H_{37}N_2O_3, M+H]^+$: 617.2799; Found: 617.2805.

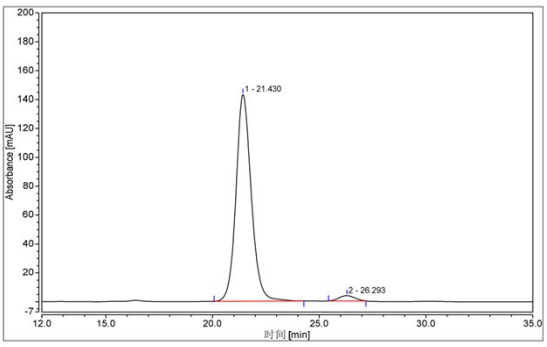
Optical Rotation: $[\alpha]^{25}_D$ = –174.9° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2346, 1705, 1369, 1161, 1062, 873, 812, 758.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 21.430 min (major) and 26.293 min (minor). 95% ee.

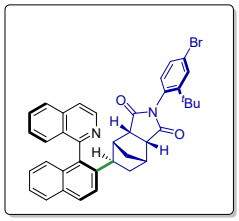


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	20.963	76.013	95.620	50.96	55.73
2	26.050	73.162	75.958	49.04	44.27



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	21.430	118.876	143.138	97.42	97.48
2	26.293	3.146	3.700	2.58	2.52

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(4-bromo-2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ae)



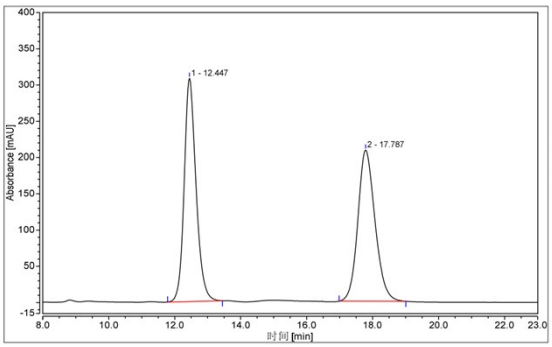
61% yield, white solid, **m.p.** = 275–277 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.8 Hz, 1H), 8.01 - 7.98 (m, 1H), 7.88 - 7.86 (m, 1H), 7.81 - 7.80 (m, 2H), 7.71 - 7.67 (m, 2H), 7.573 - 7.569 (m, 1H), 7.40 - 7.32 (m, 3H), 7.23 - 7.21 (m, 1H), 7.19 - 7.16 (m, 1H), 6.72 - 6.70 (m, 1H), 5.26 - 5.24 (m, 1H), 3.17 - 3.09 (m, 3H), 2.97 - 2.94 (m, 1H), 2.89 - 2.87 (m, 1H), 2.30 - 2.27 (m, 1H), 2.06 - 2.00 (m, 1H), 1.76 - 1.73 (m, 1H), 1.64 - 1.59 (m, 1H), 1.14 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.7, 176.6, 159.9, 150.1, 142.8, 140.5, 136.4, 135.5, 133.2, 132.1, 132.0, 131.9, 130.9, 130.3, 129.2, 128.9, 128.4, 128.0, 127.8, 127.0, 126.8, 126.5, 125.8, 125.6, 123.6, 123.0, 120.4, 49.0, 48.7, 44.4, 41.3, 39.5, 39.4, 36.0, 35.8, 31.4.

HRMS (ESI): Calculated for $[C_{38}H_{34}BrN_2O_2, M+H]^+$: 629.1798; Found: 629.1806.

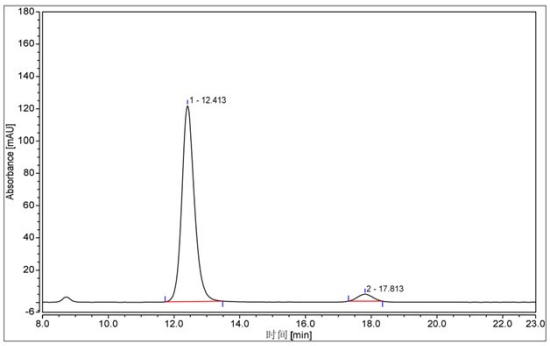
Optical Rotation: $[\alpha]^{25}_D$ = –156.0° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2967, 2347, 1706, 1389, 1362, 1260, 1161, 1085, 1016, 873, 792, 751, 696, 592.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 12.413 min (major) and 17.813 min (minor). 92% ee.

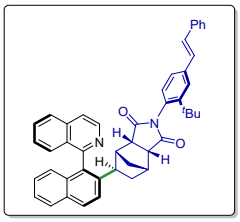


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.447	128.107	307.848	50.46	59.61
2	17.787	125.756	208.615	49.54	40.39



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.413	54.008	121.389	95.99	96.57
2	17.813	2.256	4.312	4.01	3.43

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)-4-((*E*)-styryl)phenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3af)



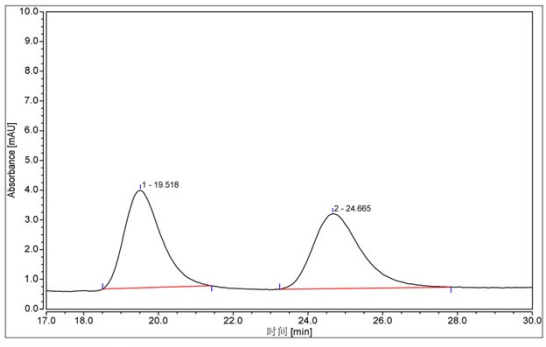
40% yield, white solid, **m.p.** = 116–118 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 5.7 Hz, 1H), 8.03 - 7.99 (m, 2H), 7.88 - 7.87 (m, 1H), 7.84 - 7.82 (m, 1H), 7.70 - 7.67 (m, 2H), 7.61 - 7.59 (m, 2H), 7.555 - 7.551 (m, 1H), 7.43 - 7.29 (m, 7H), 7.19 - 7.16 (m, 1H), 7.13 - 7.12 (m, 2H), 6.74 - 6.72 (m, 1H), 5.44 - 5.42 (m, 1H), 3.18 - 3.13 (m, 2H), 3.09 - 3.08 (m, 1H), 3.03 - 3.00 (m, 1H), 2.90 - 2.88 (m, 1H), 2.30 - 2.27 (m, 1H), 2.08 - 2.02 (m, 1H), 1.75 - 1.73 (m, 1H), 1.71 - 1.66 (m, 1H), 1.19 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 176.9, 159.9, 147.9, 142.8, 140.7, 138.2, 137.1, 136.5, 135.6, 133.2, 132.1, 130.8, 129.9, 129.3, 128.9, 128.8, 128.5, 128.3, 128.0, 127.9, 127.8, 127.2, 127.0, 126.9, 126.7, 126.5, 125.8, 125.6, 124.8, 123.2, 120.5, 49.0, 48.7, 44.5, 41.2, 39.6, 39.4, 36.0, 35.7, 31.6.

HRMS (ESI): Calculated for $[C_{46}H_{41}N_2O_2, M+H]^+$: 653.3163; Found: 653.3165.

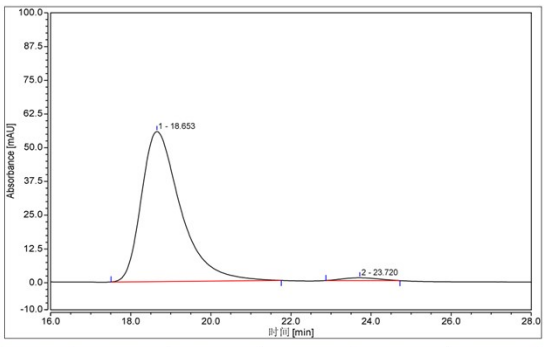
Optical Rotation: $[\alpha]^{25}_D$ = –164.9° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2960, 2921, 2350, 1707, 1495, 1452, 1402, 1366, 1260, 1169, 1083, 1017, 797, 691, 630.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 80 : 20, 1.0 mL/min), 30 °C, 254 nm, R*t* = 18.653 min (major) and 23.720 min (minor). 96% ee.

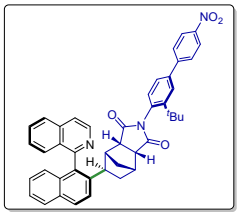


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	19.518	3.742	3.281	49.74	56.55
2	24.665	3.781	2.521	50.26	43.45



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	18.653	63.077	55.594	98.35	98.19
2	23.720	1.056	1.025	1.65	1.81

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(3-(*tert*-butyl)-4'-nitro-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ag)



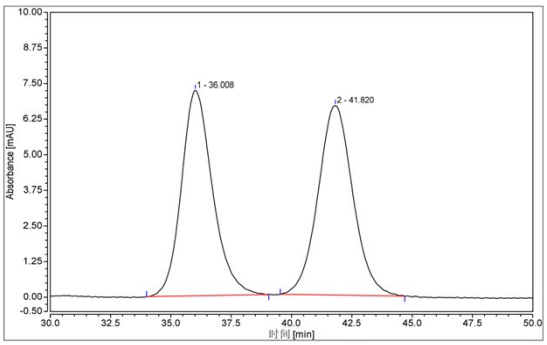
52% yield, white solid, **m.p.** = 150–152 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 5.8 Hz, 1H), 8.38 - 8.36 (m, 2H), 8.02 - 7.99 (m, 2H), 7.89 - 7.87 (m, 1H), 7.82 - 7.81 (m, 1H), 7.74 - 7.66 (m, 5H), 7.40 - 7.36 (m, 3H), 7.31 - 7.29 (m, 1H), 7.19 - 7.16 (m, 1H), 6.71 - 6.69 (m, 1H), 5.55 - 5.54 (m, 1H), 3.21 - 3.16 (m, 2H), 3.13 - 3.12 (m, 1H), 3.05 - 3.02 (m, 1H), 2.92 - 2.90 (m, 1H), 2.32 - 2.30 (m, 1H), 2.09 - 2.05 (m, 1H), 1.78 - 1.76 (m, 1H), 1.72 - 1.67 (m, 1H), 1.22 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.9, 176.8, 160.0, 148.7, 147.4, 147.3, 142.8, 140.5, 139.8, 136.4, 135.4, 133.2, 132.1, 131.3, 130.8, 129.0, 128.5, 128.1, 128.0, 127.8, 126.95, 126.89, 126.5, 126.2, 125.8, 125.6, 124.3, 123.1, 120.3, 49.1, 48.8, 44.5, 41.3, 39.6, 39.5, 36.1, 35.9, 31.6.

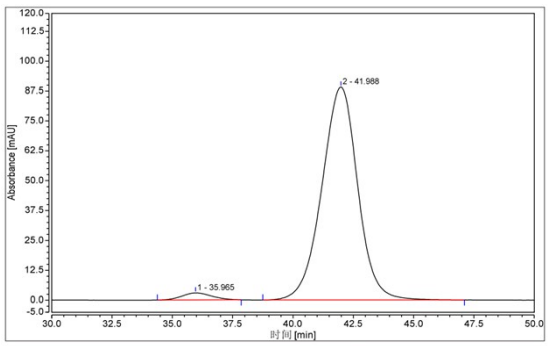
HRMS (ESI): Calculated for $[C_{44}H_{38}N_3O_4, M+H]^+$: 672.2857; Found: 672.2857.

Optical Rotation: $[\alpha]^{25}_D$ = –145.1° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2960, 2923, 1709, 1596, 1513, 1343, 1260, 1169, 1084, 1015, 812, 797, 750, 694, 629.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 41.988 min (major) and 35.965 min (minor). 95% ee.

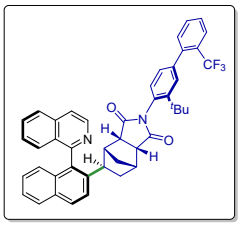




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	36.008	10.801	7.212	49.25	52.01
2	41.820	11.130	6.655	50.75	47.99

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	35.965	4.180	2.955	2.64	3.21
2	41.988	153.873	89.107	97.36	96.79

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(3-(*tert*-butyl)-2'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ah)



99% yield, white solid, **m.p.** = 140–142 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.65 (d, *J* = 5.7 Hz, 1H), 8.00 -

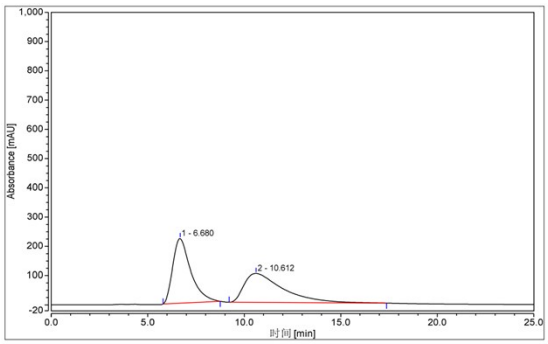
7.98 (m, 1H), 7.93 - 7.91 (m, 1H), 7.87 - 7.86 (m, 1H), 7.83 - 7.81 (m, 1H), 7.72 - 7.69 (m, 2H), 7.66 - 7.60 (m, 2H), 7.54 - 7.51 (m, 1H), 7.42 - 7.41 (m, 1H), 7.39 - 7.32 (m, 4H), 7.18 - 7.13 (m, 2H), 6.75 - 6.73 (m, 1H), 5.59 - 5.57 (m, 1H), 3.17 - 3.14 (m, 1H), 3.11 - 3.08 (m, 1H), 3.05 - 3.02 (m, 2H), 2.92 - 2.90 (m, 1H), 2.32 - 2.30 (m, 1H), 2.07 - 2.03 (m, 1H), 1.77 - 1.72 (m, 2H), 1.16 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 176.6, 159.7, 147.2, 142.8, 140.9, 140.7, 140.4, 136.6, 135.6, 133.2, 132.1, 131.6, 130.7, 130.0, 129.7, 129.5, 128.9, 128.6, 128.45, 128.37, 127.8, 127.74, 127.67, 127.1, 126.7, 126.5, 126.3 (q, $J_{C\text{-}F}$= 5.2 Hz), 125.9, 125.6, 124.2 (q, $J_{C\text{-}F}$= 274.3 Hz), 123.3, 120.5, 49.1, 48.6, 44.9, 41.1, 39.6, 39.4, 35.7, 31.6. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -56.41.

HRMS (ESI): Calculated for $[C_{45}H_{38}F_3N_2O_2, M+H]^+$: 695.2880; Found: 695.2883.

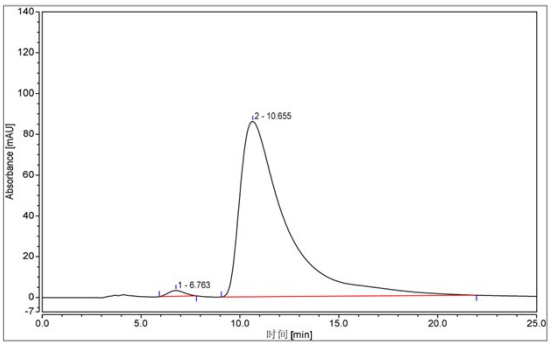
Optical Rotation: $[\alpha]^{25}_D$ = –168.7° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2964, 2350, 1709, 1484, 1394, 1366, 1312, 1168, 1107, 814, 747, 688, 596.

HPLC: Daicel Chiralcel OJ-H Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 10.655 min (major) and 6.763 min (minor). 98% ee.

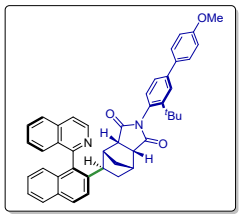


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	6.680	237.717	220.863	50.69	69.07
2	10.612	231.228	98.915	49.31	30.93



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	6.763	2.714	2.866	1.17	3.23
2	10.655	228.817	85.966	98.83	96.77

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(3-(*tert*-butyl)-4'-methoxy-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ai)



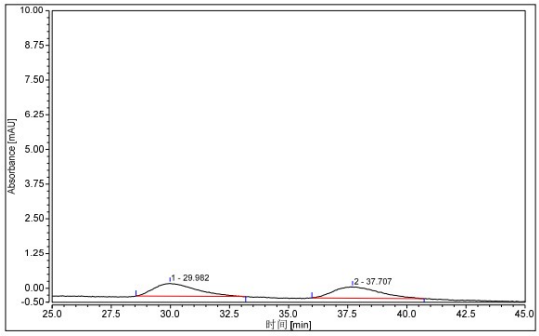
95% yield, white solid, **m.p.** = 258–260 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 5.8 Hz, 1H), 8.01 - 7.98 (m, 2H), 7.88 - 7.86 (m, 1H), 7.82 - 7.80 (m, 1H), 7.70 - 7.65 (m, 2H), 7.59 - 7.58 (m, 1H), 7.53 - 7.51 (m, 2H), 7.39 - 7.35 (m, 3H), 7.23 - 7.21 (m, 1H), 7.18 - 7.15 (m, 1H), 7.05 - 7.04 (m, 2H), 6.72 - 6.71 (m, 1H), 5.39 - 5.38 (m, 1H), 3.88 (s, 3H), 3.17 - 3.14 (m, 3H), 3.03 - 3.00 (m, 1H), 2.89 - 2.88 (m, 1H), 2.29 - 2.27 (m, 1H), 2.06 - 2.01 (m, 1H), 1.76 - 1.74 (m, 1H), 1.70 - 1.65 (m, 1H), 1.20 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 177.0, 159.9, 159.5, 147.8, 142.8, 141.8, 140.7, 136.4, 135.5, 133.5, 133.3, 132.1, 130.8, 130.6, 128.9, 128.6, 128.44, 128.41, 128.0, 127.8, 127.4, 127.0, 126.9, 126.5, 125.8, 125.7, 125.6, 123.1, 120.4, 114.4, 55.4, 49.0, 48.7, 44.3, 41.4, 39.6, 39.5, 36.2, 35.7, 31.7.

HRMS (ESI): Calculated for $[C_{45}H_{41}N_2O_3, M+H]^+$: 657.3112; Found: 657.3120.

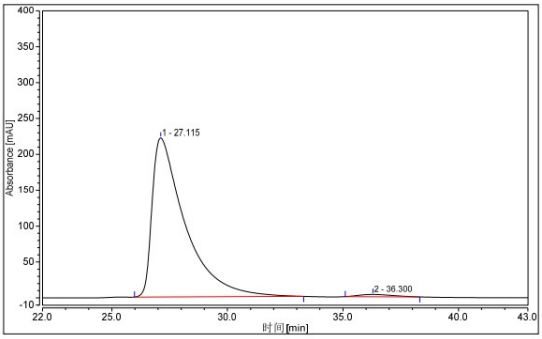
Optical Rotation: $[\alpha]^{25}_D$ = –164.2° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2920, 1708, 1607, 1488, 1364, 1247, 1176, 1028, 812, 748, 692.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 35.395 min (major) and 28.953 min (minor). 97% ee.

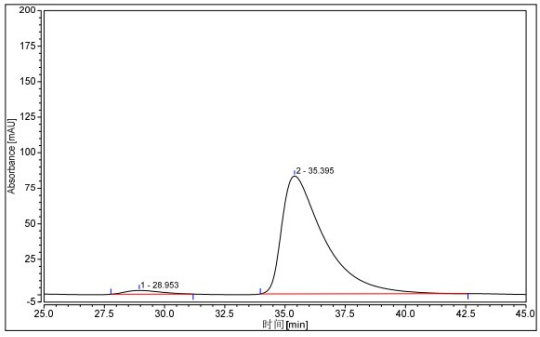


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	29.982	0.949	0.472	50.66	53.15
2	37.707	0.925	0.417	49.34	46.85



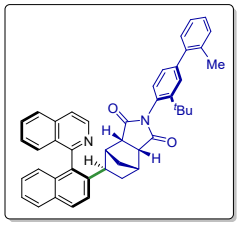
peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	27.115	367.069	221.624	98.56	98.57
2	36.300	5.363	3.210	1.44	1.43

(*ent*)-**3ai**: 95% ee



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	28.953	4.452	2.654	2.57	3.10
2	35.395	168.571	82.899	97.43	96.90

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(3-(*tert*-butyl)-2'-methyl-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3aj)



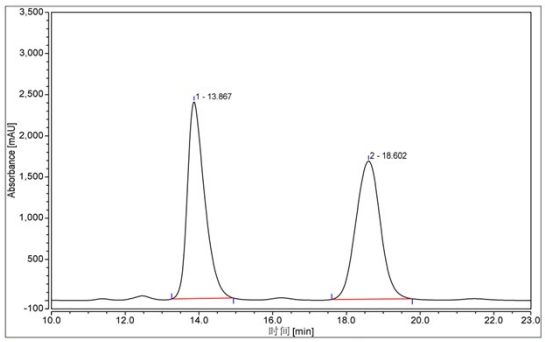
89% yield, white solid, **m.p.** = 220–222 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 7.8 Hz, 1H), 7.99 - 7.98 (m, 1H), 7.95 - 7.93 (m, 1H), 7.87 - 7.85 (m, 1H), 7.76 - 7.75 (m, 1H), 7.70 - 7.68 (m, 1H), 7.65 - 7.62 (m, 1H), 7.40 - 7.26 (m, 8H), 7.17 - 7.13 (m, 1H), 7.07 - 7.05 (m, 1H), 6.72 - 6.70 (m, 1H), 5.39 - 5.38 (m, 1H), 3.16 - 3.14 (m, 3H), 3.03 - 3.00 (m, 1H), 2.89 - 2.87 (m, 1H), 2.36 (s, 3H), 2.29 - 2.27 (m, 1H), 2.05 - 2.01 (m, 1H), 1.76 - 1.74 (m, 1H), 1.71 - 1.66 (m, 1H), 1.17 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 177.0, 159.9, 147.2, 142.8, 142.5, 141.4, 140.8, 136.4, 135.5, 135.4, 133.3, 132.1, 130.8, 130.6, 130.0, 129.9, 128.9, 128.7, 128.4, 128.0, 127.9, 127.8, 127.6, 127.0, 126.8, 126.5, 126.0, 125.8, 125.6, 123.1, 120.4, 49.0, 48.7, 44.4, 41.4, 39.6, 39.5, 36.3, 35.8, 31.7, 20.7.

HRMS (ESI): Calculated for $[C_{45}H_{41}N_2O_2, M+H]^+$: 641.3163; Found: 641.3163.

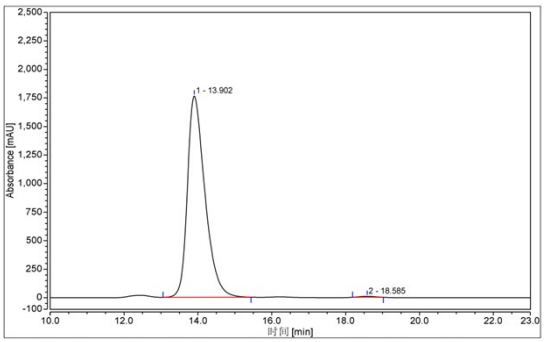
Optical Rotation: $[\alpha]^{25}_{D}$ = –164.5° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2962, 2338, 1706, 1480, 1392, 1365, 1260, 1163, 1017, 758, 693, 629, 588.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 13.902 min (major) and 18.585 min (minor). 99% ee.

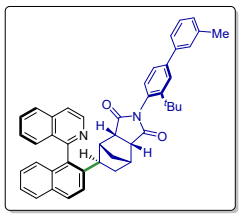


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	13.867	1293.265	2389.226	50.10	58.76
2	18.602	1288.203	1676.517	49.90	41.24



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	13.902	972.180	1763.997	99.59	99.53
2	18.585	3.996	8.293	0.41	0.47

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(3-(*tert*-butyl)-3'-methyl-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ak)



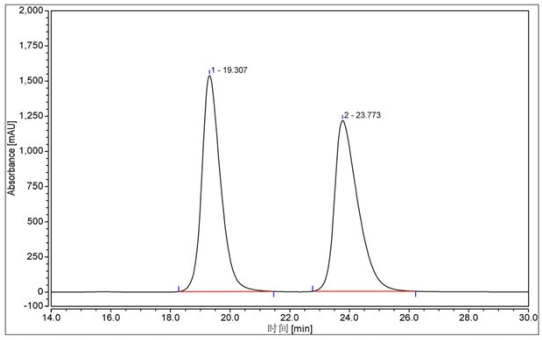
89% yield, white solid, **m.p.** = 289–291 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 5.7 Hz, 1H), 8.00 - 7.98 (m, 2H), 7.87 - 7.86 (m, 1H), 7.81 - 7.80 (m, 1H), 7.70 - 7.61 (m, 3H), 7.40 - 7.35 (m, 6H), 7.26 - 7.24 (m, 2H), 7.18 - 7.15 (m, 1H), 6.73 - 6.71 (m, 1H), 5.43 - 5.41 (m, 1H), 3.17 - 3.12 (m, 3H), 3.03 - 3.00 (m, 1H), 2.89 - 2.88 (m, 1H), 2.48 (s, 3H), 2.29 - 2.27 (m, 1H), 2.07 - 2.02 (m, 1H), 1.76 - 1.74 (m, 1H), 1.71 - 1.66 (m, 1H), 1.20 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 177.0, 159.9, 147.8, 142.8, 142.4, 141.1, 140.7, 138.5, 136.5, 135.5, 133.3, 132.1, 130.8, 130.6, 129.1, 128.9, 128.8, 128.4, 128.2, 128.0, 127.9, 127.8, 127.0, 126.8, 126.5, 126.1, 125.8, 125.6, 124.6, 123.1, 120.4, 49.1, 48.7, 44.3, 41.4, 39.6, 39.5, 36.2, 35.8, 31.7, 21.7.

HRMS (ESI): Calculated for $[C_{45}H_{41}N_2O_2, M+H]^+$: 641.3163; Found: 641.3199.

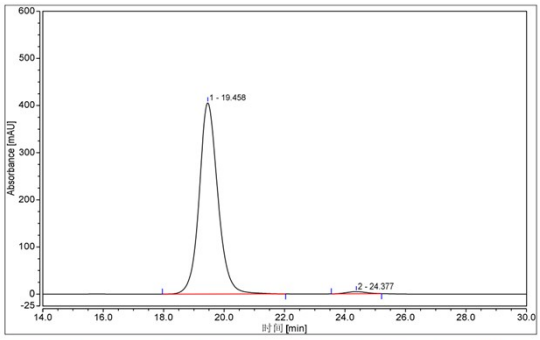
Optical Rotation: $[\alpha]^{25}_{D}$ = –167.7° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2920, 2350, 1705, 1485, 1365, 1160, 1079, 813, 758, 604, 589.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 80 : 20, 1.0 mL/min), 30 °C, 254 nm, R*t* = 19.458 min (major) and 24.377 min (minor). 98% ee.

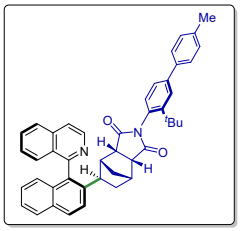


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	19.307	1118.392	1536.151	50.29	55.85
2	23.773	1105.437	1214.515	49.71	44.15



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	19.458	290.457	405.712	98.87	98.93
2	24.377	3.315	4.371	1.13	1.07

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(3-(tert-butyl)-4'-methyl-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3al)



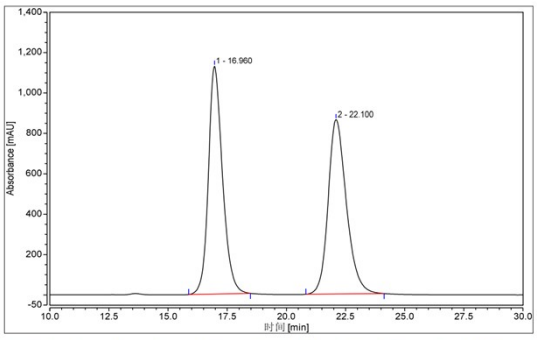
75% yield, white solid, **m.p.** = 302–304 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 5.7 Hz, 1H), 8.01 - 7.98 (m, 2H), 7.88 - 7.86 (m, 1H), 7.81 - 7.80 (m, 1H), 7.70 - 7.65 (m, 2H), 7.612 - 7.608 (m, 1H), 7.49 - 7.47 (m, 2H), 7.40 - 7.31 (m, 5H), 7.25 - 7.23 (m, 1H), 7.18 - 7.15 (m, 1H), 6.72 - 6.71 (m, 1H), 5.39 - 5.37 (m, 1H), 3.18 - 3.15 (m, 3H), 3.03 - 3.00 (m, 1H), 2.89 - 2.88 (m, 1H), 2.44 (s, 3H), 2.30 - 2.27 (m, 1H), 2.06 - 2.01 (m, 1H), 1.77 - 1.75 (m, 1H), 1.70 - 1.65 (m, 1H), 1.20 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 177.0, 159.9, 147.8, 142.8, 142.2, 140.7, 138.2, 137.5, 136.4, 135.5, 133.3, 132.1, 130.8, 130.6, 129.6, 128.9, 128.4, 128.0, 127.8, 127.7, 127.3, 127.0, 126.8, 126.5, 125.9, 125.8, 125.5, 123.1, 120.4, 49.0, 48.7, 44.3, 41.4, 39.6, 39.4, 36.3, 35.7, 31.7, 21.2.

HRMS (ESI): Calculated for $[C_{45}H_{41}N_2O_2, M+H]^+$: 641.3163; Found: 641.3168.

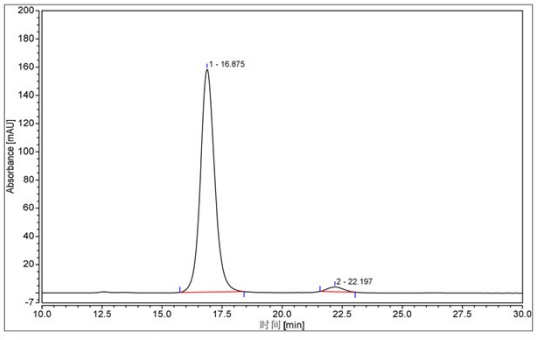
Optical Rotation: $[\alpha]^{25}_D$ = –163.1° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2922, 2357, 1705, 1486, 1364, 1084, 690, 837, 809, 758, 693.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 16.875 min (major) and 22.197 min (minor). 95% ee.

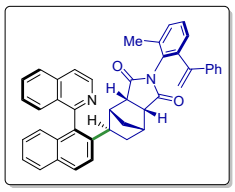


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	16.960	780.333	1128.896	50.19	56.65
2	22.100	774.336	863.747	49.81	43.35



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	16.875	108.529	157.908	97.72	97.89
2	22.197	2.536	3.410	2.28	2.11

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-2-(2-methyl-6-(1-phenylvinyl)phenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3am)



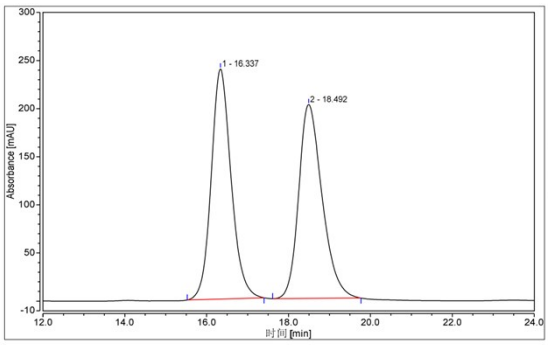
91% yield, white solid, **m.p.** = 94–96 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 5.7 Hz, 1H), 7.95 - 7.90 (m, 2H), 7.83 - 7.82 (m, 1H), 7.70 - 7.69 (m, 1H), 7.65 - 7.61 (m, 2H), 7.35 - 7.26 (m, 4H), 7.20 - 7.06 (m, 8H), 6.60 - 6.58 (m, 1H), 5.42 (s, 1H), 5.11 (s, 1H), 2.98 - 2.96 (m, 1H), 2.80 - 2.79 (m, 1H), 2.72 - 2.70 (m, 1H), 2.44 - 2.37 (m, 2H), 2.15 - 2.07 (m, 2H), 1.64 - 1.59 (m, 1H), 1.49 - 1.47 (m, 1H), 1.41 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 176.1, 174.8, 159.7, 147.2, 142.5, 140.6, 140.4, 140.1, 136.75, 136.70, 135.7, 133.3, 132.0, 130.4, 130.3, 129.7, 129.2, 128.9, 128.74, 128.65, 128.3, 128.0, 127.69, 127.66, 127.2, 126.9, 126.8, 126.4, 125.9, 125.5, 123.6, 120.6, 117.3, 48.8, 48.7, 44.4, 40.7, 39.3, 39.1, 35.0, 18.0.

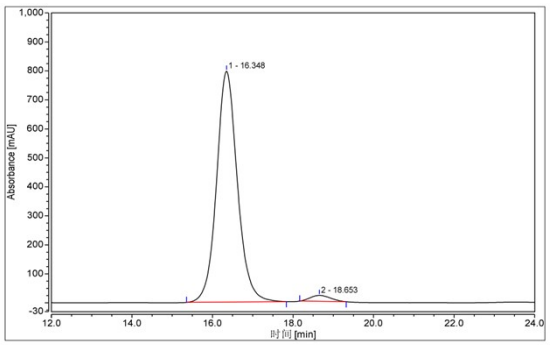
HRMS (ESI): Calculated for $[C_{43}H_{35}N_2O_2, M+H]^+$: 611.2693; Found: 611.2703.

Optical Rotation: $[\alpha]^{25}_D$ = –63.0° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2964, 2360, 1708, 1358, 1259, 1174, 1046, 795, 747, 698, 629.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 80 : 20, 1.0 mL/min), 30 °C, 254 nm, R*t* = 16.348 min (major) and 18.653 min (minor). 95% ee.

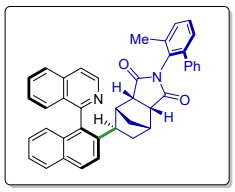




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	16.337	134.509	239.147	50.15	54.27
2	18.492	133.693	201.526	49.85	45.73

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	16.348	477.219	796.572	97.57	97.50
2	18.653	11.872	20.458	2.43	2.50

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-2-(3-methyl-[1,1'-biphenyl]-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3an)



99% yield, white solid, **m.p.** = 133–135 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.66 (d, *J* = 5.8 Hz, 1H), 7.96 - 7.94 (m, 2H), 7.84 - 7.83 (m, 1H), 7.77 - 7.76 (m, 1H), 7.67 - 7.63 (m, 2H), 7.36 - 7.28 (m, 4H), 7.22 - 7.19 (m, 4H), 7.14 - 7.11 (m, 2H), 7.04 - 7.02 (m, 2H), 6.64 - 6.62 (m, 1H), 3.18 - 3.15 (m, 1H), 2.80 - 2.78 (m, 1H), 2.72 - 2.70 (m, 1H), 2.62 - 2.54 (m, 2H), 2.24 - 2.15 (m, 2H), 1.74 - 1.71 (m, 1H), 1.68 (s, 3H), 1.46 -

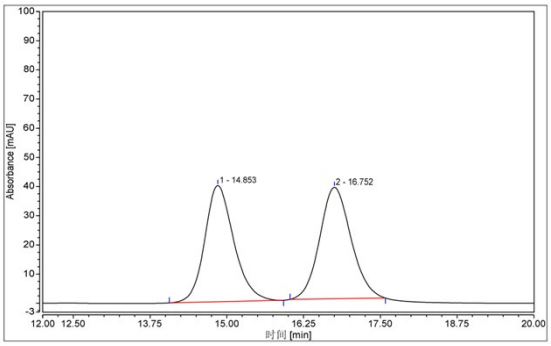
1.44 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.0, 175.7, 159.7, 142.7, 141.1, 140.3, 139.1, 136.8, 136.5, 135.8, 133.3, 132.0, 130.4, 130.0, 129.7, 129.3, 128.8, 128.7, 128.3, 128.1, 128.0, 127.7, 127.6, 127.4, 127.3, 127.0, 126.4, 125.9, 125.6, 123.9, 120.7, 49.0, 48.8, 45.1, 40.1, 39.6, 39.2, 34.0, 18.1.

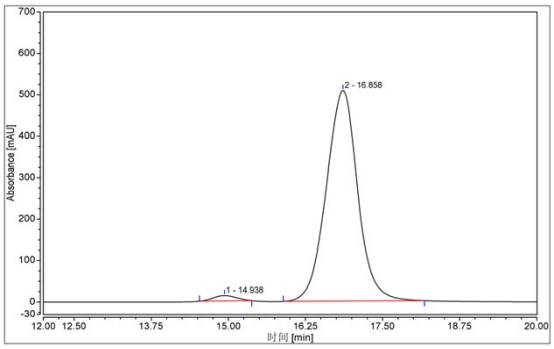
HRMS (ESI): Calculated for $[C_{41}H_{33}N_2O_2, M+H]^+$: 585.2537; Found: 585.2549.

Optical Rotation: $[\alpha]^{25}_D$ = –57.4° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2922, 2852, 1706, 1465, 1359, 1175, 815, 749, 701.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 80 : 20, 1.0 mL/min), 30 °C, 254 nm, R*t* = 16.858 min (major) and 14.938 min (minor). 96% ee.

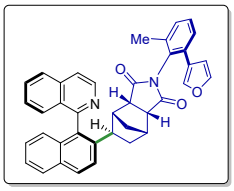




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	14.853	21.880	39.859	49.20	51.07
2	16.752	22.596	38.190	50.80	48.93

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	14.938	5.639	12.936	1.84	2.48
2	16.858	300.273	508.284	98.16	97.52

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(furan-3-yl)-6-methylphenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ao)



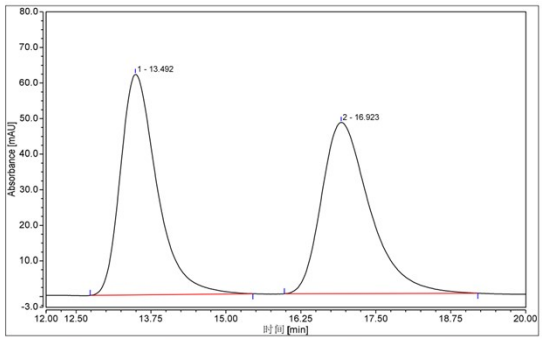
87% yield, white solid, **m.p.** = 101–103 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.8 Hz, 1H), 7.99 - 7.97 (m, 1H), 7.94 - 7.92 (m, 1H), 7.86 - 7.84 (m, 1H), 7.75 - 7.73 (m, 1H), 7.68 - 7.63 (m, 2H), 7.38 - 7.32 (m, 2H), 7.30 - 7.26 (m, 3H), 7.21 - 7.19 (m, 2H), 7.15 - 7.12 (m, 2H), 6.66 - 6.65 (m, 1H), 6.16 - 6.15 (m, 1H), 3.23 - 3.20 (m, 1H), 2.95 - 2.89 (m, 2H), 2.80 - 2.77 (m, 1H), 2.71 - 2.70 (m, 1H), 2.30 - 2.26 (m, 1H), 2.24 - 2.22 (m, 1H), 1.83 - 1.79 (m, 1H), 1.76 (s, 3H), 1.54 - 1.51 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.1, 175.6, 159.7, 142.8, 142.6, 140.3, 139.6, 136.8, 135.8, 133.2, 132.0, 130.4, 130.1, 129.9, 129.4, 128.9, 128.7, 128.3, 127.7, 127.5, 127.3, 127.0, 126.5, 126.0, 125.6, 124.0, 123.1, 120.8, 110.5, 49.2, 49.1, 45.6, 40.1, 39.6, 39.3, 33.7, 18.2.

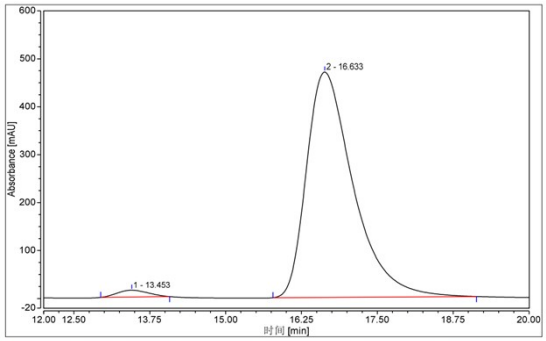
HRMS (ESI): Calculated for $[C_{39}H_{31}N_2O_3, M+H]^+$: 575.2329; Found: 575.2335.

Optical Rotation: $[\alpha]^{25}_D$ = –80.4° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2921, 2349, 1705, 1462, 1364, 1175, 1259, 1175, 1086, 1019, 798, 747, 673, 629, 600.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 16.633 min (major) and 13.453 min (minor). 96% ee.

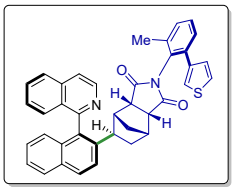




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	13.492	43.835	61.990	49.40	56.29
2	16.923	44.908	48.128	50.60	43.71

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	13.453	8.331	14.224	1.95	2.94
2	16.633	419.193	470.160	98.05	97.06

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-2-(2-methyl-6-(thiophen-3-yl)phenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ap)



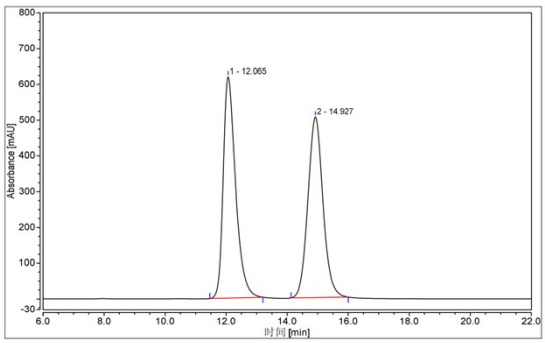
60% yield, white solid, **m.p.** = 117–119 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.65 (d, *J* = 5.8 Hz, 1H), 7.98 - 7.93 (m, 2H), 7.85 - 7.84 (m, 1H), 7.76 - 7.75 (m, 1H), 7.67 - 7.64 (m, 2H), 7.37 - 7.32 (m, 2H), 7.30 - 7.27 (m, 2H), 7.21 - 7.20 (m, 1H), 7.17 - 7.12 (m, 3H), 6.954 - 6.946 (m, 1H), 6.80 - 6.79 (m, 1H), 6.65 - 6.63 (m, 1H), 3.21 - 3.18 (m, 1H), 2.86 - 2.84 (m, 1H), 2.77 - 2.71 (m, 2H), 2.68 - 2.65 (m, 1H), 2.27 - 2.18 (m, 2H), 1.78 - 1.74 (m, 1H), 1.71 (s, 3H), 1.51 - 1.48 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.1, 175.7, 159.7, 142.6, 140.3, 139.1, 136.8, 136.6, 136.1, 135.8, 133.2, 132.0, 130.4, 130.1, 129.9, 129.2, 128.8, 128.7, 128.2, 128.0, 127.7, 127.5, 127.3, 127.0, 126.4, 125.9, 125.5, 125.3, 124.0, 122.6, 120.7, 49.1, 49.0, 45.3, 40.1, 39.6, 39.2, 33.8, 18.1.

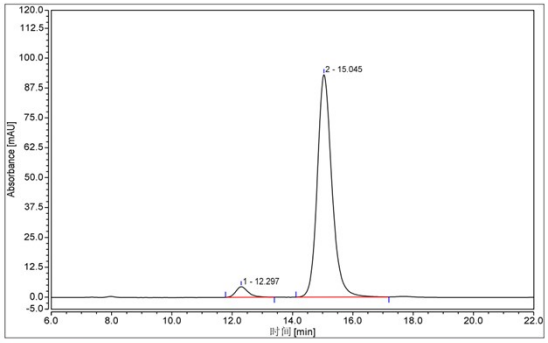
HRMS (ESI): Calculated for $[C_{39}H_{31}N_2O_2S, M+H]^+$: 591.2101; Found: 591.2104.

Optical Rotation: $[\alpha]^{25}_D$ = –52.1° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2362, 2921, 2349, 1706, 1463, 1365, 1259, 1178, 1083, 1015, 780, 748, 673, 659, 630, 604.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 15.045 min (major) and 12.297 min (minor). 92% ee.

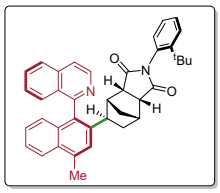




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.065	290.134	619.504	50.14	55.08
2	14.927	288.468	505.196	49.86	44.92

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.297	2.104	4.423	3.87	4.54
2	15.045	52.206	93.110	96.13	95.46

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)-4-methylnaphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ba)



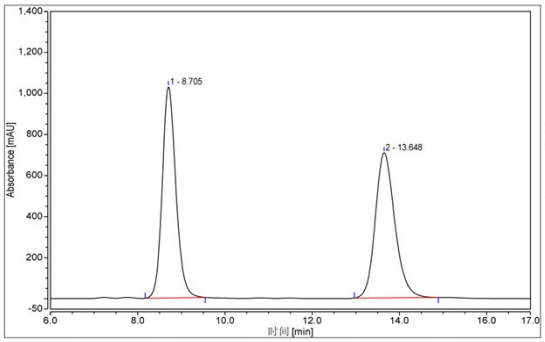
75% yield, white solid, **m.p.** = 262–264 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.7 Hz, 1H), 8.03 - 8.01 (m, 1H), 7.98 - 7.96 (m, 1H), 7.77 - 7.76 (m, 1H), 7.66 - 7.62 (m, 1H), 7.51 (s, 1H), 7.46 - 7.40 (m, 2H), 7.34 - 7.28 (m, 3H), 7.18 - 7.15 (m, 1H), 7.11 - 7.08 (m, 1H), 6.74 - 6.72 (m, 1H), 5.38 - 5.36 (m, 1H), 3.15 - 3.11 (m, 3H), 2.97 - 2.94 (m, 1H), 2.88 - 2.86 (m, 1H), 2.82 (s, 3H), 2.31 - 2.28 (m, 1H), 2.05 - 2.00 (m, 1H), 1.76 - 1.74 (m, 1H), 1.68 - 1.65 (m, 1H), 1.15 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 176.9, 160.2, 147.6, 142.8, 140.2, 136.4, 135.1, 133.8, 133.4, 131.2, 130.7, 130.4, 130.0, 129.3, 128.63, 128.57, 127.8, 127.2, 127.0, 126.9, 126.4, 126.1, 125.3, 124.0, 123.9, 120.3, 49.0, 48.7, 44.3, 41.4, 39.5, 39.3, 36.1, 35.6, 31.6, 20.1.

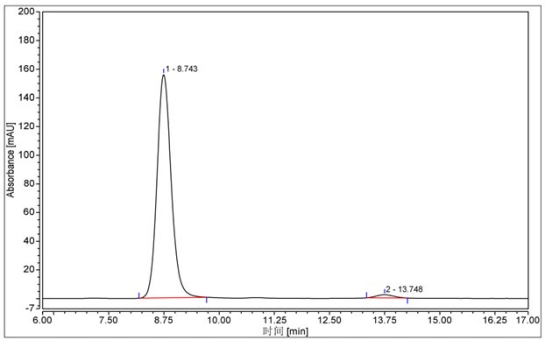
HRMS (ESI): Calculated for $[C_{39}H_{37}N_2O_2, M+H]^+$: 565.2850; Found: 565.2855.

Optical Rotation: $[\alpha]^{25}_D$ = –132.0° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2962, 2365, 2155, 2012, 1706, 1443, 1369, 1259, 1166, 1085, 1017, 798, 754, 691, 603.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 8.743 min (major) and 13.748 min (minor). 97% ee.

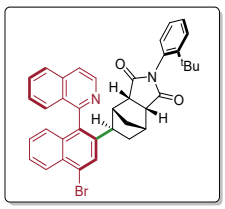




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.705	373.011	1029.182	50.44	59.27
2	13.648	366.536	707.205	49.56	40.73

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.743	57.926	155.837	98.28	98.58
2	13.748	1.011	2.243	1.72	1.42

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(4-bromo-1-(isoquinolin-1-yl)naphthalen-2-yl)-2-(2-(*tert*-butyl)phenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ca)



95% yield, white solid, **m.p.** = 275–277 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.8 Hz, 1H), 8.28 - 8.26 (m, 1H), 7.99 - 7.97 (m, 2H), 7.80 - 7.79 (m, 1H), 7.67 - 7.63 (m, 1H), 7.50 - 7.44 (m, 2H), 7.36 - 7.29 (m, 3H), 7.22 - 7.19 (m, 1H), 7.10 - 7.07 (m, 1H), 6.73 - 6.72 (m, 1H), 5.33 - 5.32 (m, 1H), 3.17 - 3.14 (m, 2H), 3.09 - 3.08 (m, 1H), 2.97 - 2.94 (m, 1H), 2.88 - 2.87 (m, 1H), 2.25 - 2.23 (m, 1H), 2.02 - 1.97 (m, 1H),

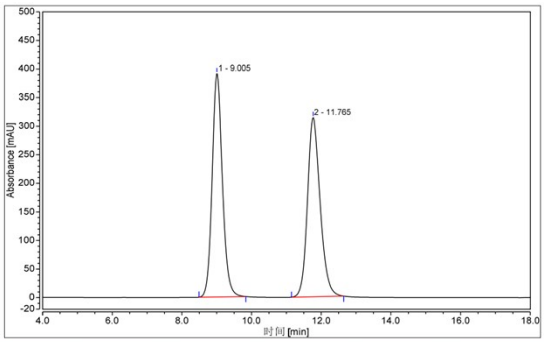
1.77 - 1.74 (m, 1H), 1.67 - 1.63 (m, 1H), 1.15 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.8, 176.7, 158.9, 147.7, 142.8, 141.6, 136.4, 135.6, 134.4, 130.9, 130.7, 130.3, 130.0, 129.3, 128.7, 128.3, 128.1, 127.4, 127.3, 127.15, 127.13, 127.0, 126.5, 126.3, 124.0, 120.7, 48.9, 48.6, 44.2, 41.3, 39.5, 39.3, 36.2, 35.6, 31.6.

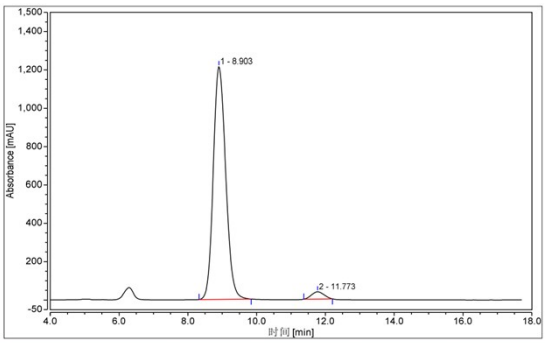
HRMS (ESI): Calculated for $[C_{38}H_{34}BrN_2O_2, M+H]^+$: 629.1798; Found: 629.1803.

Optical Rotation: $[\alpha]^{25}_D$ = –114.3° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 3871, 3750, 3689, 3675, 2361, 1749, 1699, 1684, 1558, 1541, 1489.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 8.903 min (major) and 11.773 min (minor). 94% ee.

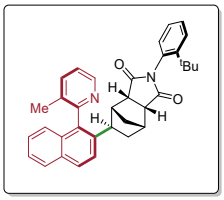




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.005	133.204	390.933	50.19	55.47
2	11.765	132.195	313.770	49.81	44.53

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.903	507.245	1213.297	96.99	96.98
2	11.773	15.744	37.723	3.01	3.02

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(3-methylpyridin-2-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3da)



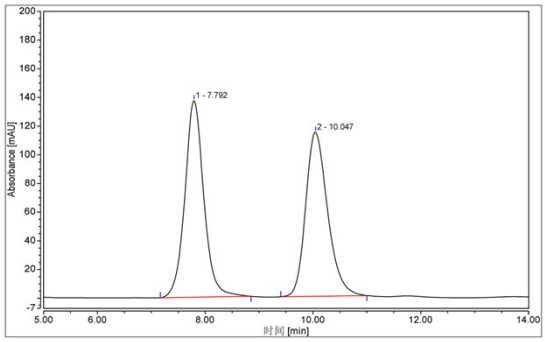
99% yield, white solid, **m.p.** = 285–287 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 6.5 Hz, 1H), 7.90 - 7.89 (m, 1H), 7.84 - 7.82 (m, 1H), 7.72 - 7.70 (m, 1H), 7.61 - 7.60 (m, 1H), 7.55 - 7.53 (m, 1H), 7.41 - 7.38 (m, 2H), 7.35 - 7.33 (m, 1H), 7.30 - 7.26 (m, 2H), 6.89 - 6.87 (m, 1H), 5.91 - 5.89 (m, 1H), 3.33 - 3.30 (m, 1H), 3.26 - 3.22 (m, 1H), 3.14 - 3.13 (m, 1H), 2.98 - 2.95 (m, 1H), 2.92 - 2.90 (m, 1H), 2.34 - 2.32 (m, 1H), 1.93 (s, 3H), 1.90 - 1.89 (m, 1H), 1.82 - 1.77 (m, 2H), 1.25 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 177.7, 157.8, 147.9, 147.6, 139.7, 138.1, 136.5, 133.4, 132.22, 132.21, 131.0, 130.3, 129.6, 128.8, 128.6, 127.9, 127.2, 126.5, 125.5, 125.1, 123.1, 122.7, 49.4, 48.7, 44.5, 41.7, 39.6, 39.2, 36.2, 35.6, 31.7, 18.5.

HRMS (ESI): Calculated for $[C_{35}H_{35}N_2O_2, M+H]^+$: 515.2693; Found: 515.2704.

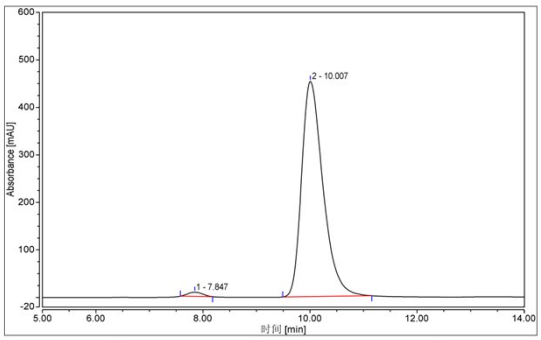
Optical Rotation: $[\alpha]^{25}_D$ = –58.5° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2922, 1710, 1442, 1361, 1259, 1160, 1018, 808, 749, 621, 590.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 10.007 min (major) and 7.847 min (minor). 97% ee.

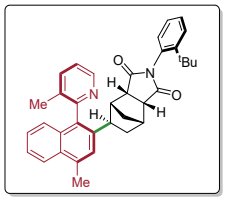


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.792	55.866	137.038	50.87	54.48
2	10.047	53.965	114.490	49.13	45.52



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.847	2.801	8.734	1.32	1.89
2	10.007	209.185	453.258	98.68	98.11

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(4-methyl-1-(3-methylpyridin-2-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ea)



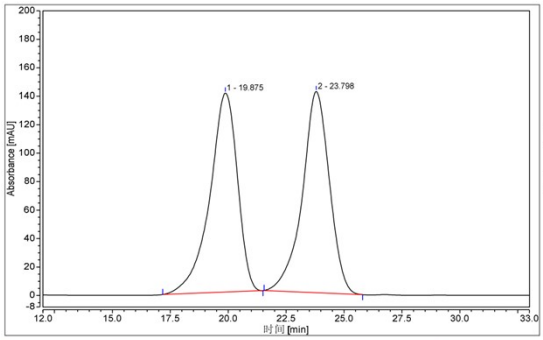
85% yield, white solid, **m.p.** = 256–258 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.62 (d, *J* = 6.7 Hz, 1H), 8.00 - 7.98 (m, 1H), 7.71 - 7.69 (m, 1H), 7.55 - 7.53 (m, 1H), 7.45 - 7.42 (m, 2H), 7.40 - 7.37 (m, 1H), 7.34 - 7.32 (m, 1H), 7.28 - 7.23 (m, 2H), 6.89 - 6.87 (m, 1H), 5.91 - 5.89 (m, 1H), 3.33 - 3.30 (m, 1H), 3.26 - 3.22 (m, 1H), 3.15 - 3.13 (m, 1H), 2.95 - 2.90 (m, 2H), 2.76 (s, 3H), 2.37 - 2.35 (m, 1H), 1.92 (s, 3H), 1.91 - 1.88 (m, 1H), 1.84 - 1.74 (m, 2H), 1.24 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 177.7, 158.1, 147.9, 147.5, 139.2, 138.0, 134.9, 134.7, 133.6, 132.3, 131.4, 131.0, 130.3, 129.6, 128.8, 127.2, 126.2, 125.7, 125.3, 124.1, 123.9, 122.5, 49.4, 48.7, 44.5, 41.8, 39.6, 39.1, 36.2, 35.6, 31.7, 20.0, 18.6.

HRMS (ESI): Calculated for $[C_{36}H_{37}N_2O_2, M+H]^+$: 529.2850; Found: 529.2854.

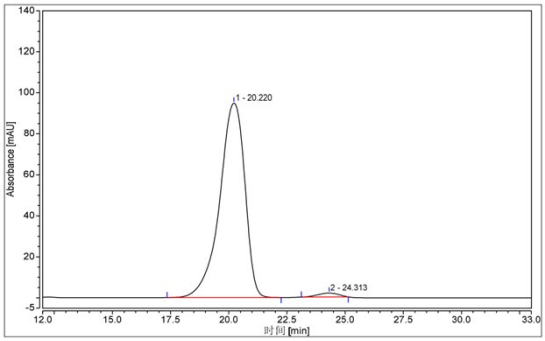
Optical Rotation: $[\alpha]^{25}_D$ = –75.5° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1709, 1443, 1369, 1260, 1167, 1084, 801, 757, 728, 619, 597.

HPLC: Daicel Chiralpak AD-H Column (*n*-Hexane/*i*-PrOH = 90 : 10, 1.0 mL/min), 30 °C, 254 nm, R*t* = 20.220 min (major) and 24.313 min (minor). 97% ee.

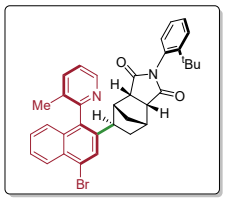


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	19.875	193.472	139.850	50.19	49.73
2	23.798	192.034	141.362	49.81	50.27



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	20.220	119.107	94.885	98.34	97.99
2	24.313	2.005	1.948	1.66	2.01

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(4-bromo-1-(3-methylpyridin-2-yl)naphthalen-2-yl)-2-(2-(*tert*-butyl)phenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3fa)



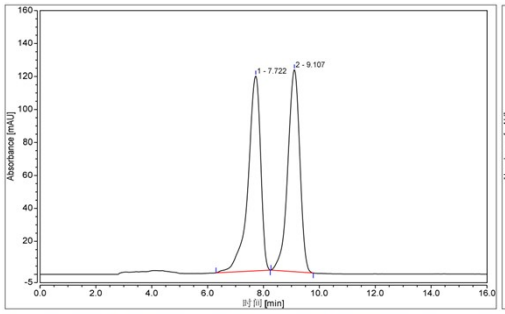
99% yield, white solid, **m.p.** = 242–244 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 6.5 Hz, 1H), 8.25 - 8.23 (m, 1H), 7.91 (s, 1H), 7.72 - 7.70 (m, 1H), 7.55 - 7.49 (m, 2H), 7.39 - 7.31 (m, 3H), 7.24 - 7.22 (m, 1H), 6.89 - 6.87 (m, 1H), 5.87 - 5.85 (m, 1H), 3.34 - 3.31 (m, 1H), 3.26 - 3.23 (m, 1H), 3.12 - 3.11 (m, 1H), 2.94 - 2.91 (m, 2H), 2.31 - 2.29 (m, 1H), 1.92 (s, 3H), 1.90 - 1.86 (m, 1H), 1.84 - 1.82 (m, 1H), 1.79 - 1.74 (m, 1H), 1.24 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.8, 177.6, 157.0, 147.9, 147.7, 140.7, 138.3, 136.6, 133.42, 133.40, 130.9, 130.8, 130.3, 129.6, 128.8, 127.41, 127.39, 127.24, 127.16, 127.0, 125.6, 123.5, 122.9, 49.3, 48.6, 44.4, 41.7, 39.6, 39.1, 36.2, 35.6, 31.7, 18.5.

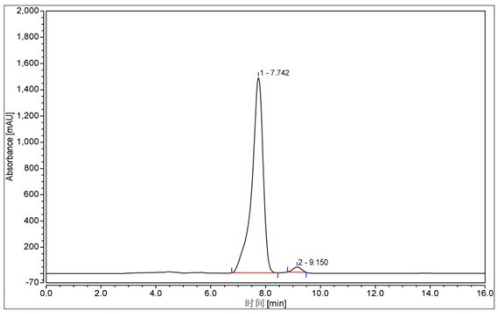
HRMS (ESI): Calculated for $[C_{35}H_{34}BrN_2O_2, M+H]^+$: 593.1798; Found: 593.1804.

Optical Rotation: $[\alpha]^{25}_D$ = –53.4° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2960, 1711, 1442, 1370, 1260, 1168, 1018, 798, 756, 698, 595.

HPLC: Daicel Chiralpak AD-H Column (*n*-Hexane/*i*-PrOH = 80 : 20, 1.0 mL/min), 30 °C, 254 nm, R*t* = 7.742 min (major) and 9.150 min (minor). 96% ee.

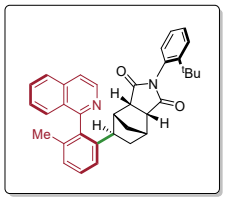




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.722	61.537	118.293	50.22	49.11
2	9.107	60.990	122.575	49.78	50.89

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.742	709.289	1487.987	98.09	97.49
2	9.150	13.798	38.347	1.91	2.51

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(2-(isoquinolin-1-yl)-3-methylphenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ga)



60% yield, white solid, **m.p.** = 104–106 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 5.8 Hz, 1H), 7.96 - 7.95 (m, 1H), 7.71 - 7.70 (m, 1H), 7.68 - 7.65 (m, 1H), 7.46 - 7.43 (m, 3H), 7.37 - 7.28 (m, 3H), 7.19 - 7.18 (m, 1H), 7.06 - 7.03 (m, 1H), 5.24 - 5.22 (m, 1H), 3.11 - 3.10 (m, 2H), 3.04 - 3.03 (m, 1H), 2.83 - 2.76 (m, 2H), 2.19 - 2.16 (m, 1H), 1.93 - 1.88 (m, 1H), 1.73 (s, 3H), 1.69 - 1.66 (m, 1H), 1.50 - 1.46 (m, 1H), 1.14 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 177.0, 160.7, 147.6, 143.2, 142.7, 138.6, 137.5, 136.4, 130.7, 130.2, 130.0, 129.2, 128.6, 128.32, 128.26, 127.9, 127.5, 127.1, 127.0, 126.3, 122.6, 120.0, 48.9, 48.6, 44.0,

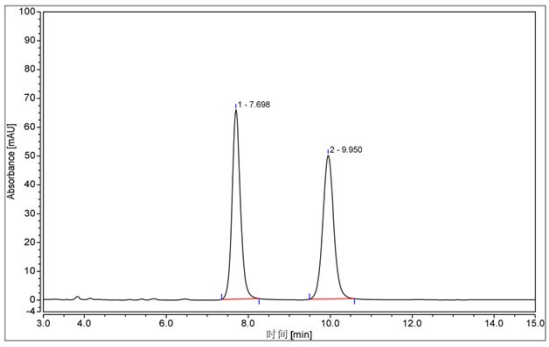
41.0, 39.6, 39.2, 36.0, 35.6, 31.6, 19.9.

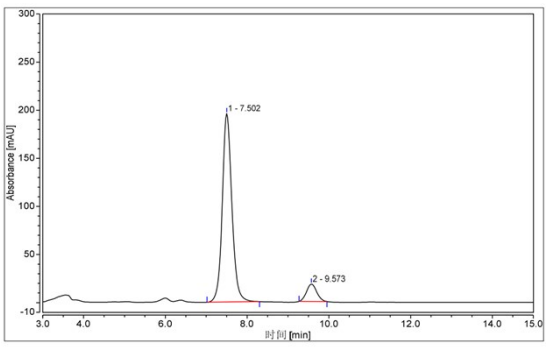
HRMS (ESI): Calculated for $[C_{35}H_{35}N_2O_2, M+H]^+$: 515.2693; Found: 515.2699.

Optical Rotation: $[\alpha]^{25}_D = -103.2^o$ (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2959, 1708, 1582, 1488, 1441, 1175, 973, 875, 826, 783, 753, 726, 687, 618.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 7.502 min (major) and 9.573 min (minor). 82% ee.

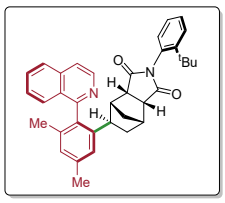




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.698	15.566	65.699	50.19	56.84
2	9.950	15.446	49.894	49.81	43.16

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.502	53.288	195.810	91.12	91.58
2	9.573	5.196	18.009	8.88	8.42

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(2-(isoquinolin-1-yl)-3,5-dimethylphenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ha)



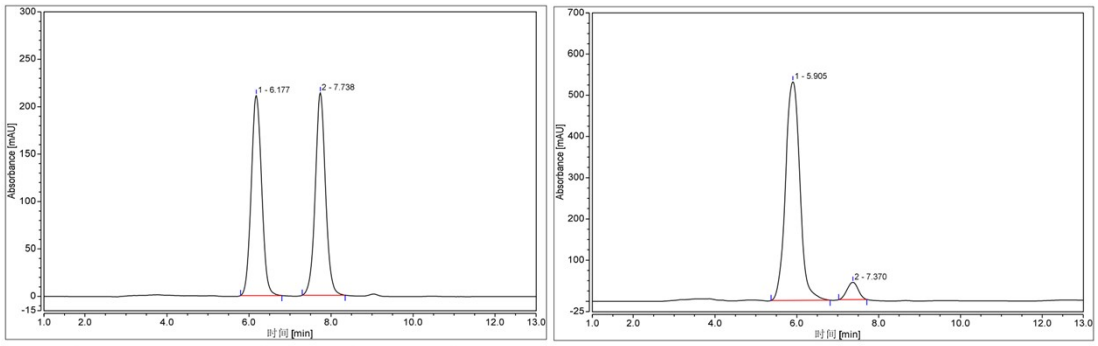
60% yield, white solid, **m.p.** = 118–120 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.7 Hz, 1H), 7.95 - 7.93 (m, 1H), 7.69 - 7.68 (m, 1H), 7.67 - 7.64 (m, 1H), 7.49 - 7.47 (m, 1H), 7.45 - 7.42 (m, 2H), 7.29 - 7.28 (m, 1H), 7.11 (s, 1H), 7.05 - 7.01 (m, 2H), 5.24 - 5.22 (m, 1H), 3.11 - 3.10 (m, 2H), 3.03 - 3.02 (m, 1H), 2.82 - 2.81 (m, 1H), 2.77 - 2.74 (m, 1H), 2.42 (s, 3H), 2.19 - 2.17 (m, 1H), 1.92 - 1.88 (m, 1H), 1.70 (s, 3H), 1.68 - 1.66 (m, 1H), 1.50 - 1.45 (m, 1H), 1.14 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 177.0, 160.9, 147.6, 143.1, 142.7, 137.7, 137.3, 136.4, 130.6, 130.3, 130.0, 129.2, 128.9, 128.6, 127.8, 127.7, 127.1, 127.0, 126.4, 123.3, 119.9, 48.9, 48.7, 44.0, 41.1, 39.6, 39.1, 36.0, 35.6, 31.6, 21.7, 19.9.

HRMS (ESI): Calculated for $[C_{36}H_{37}N_2O_2, M+H]^+$: 529.2850; Found: 529.2854.

Optical Rotation: $[\alpha]^{25}_D = -102.7^o$ (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2920, 2850, 1708, 1441, 1367, 1173, 826, 753, 727, 691, 617.

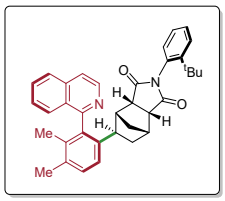
HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 5.905 min (major) and 7.370 min (minor). 88% ee.



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	6.177	62.224	211.158	50.17	49.71
2	7.738	61.795	213.610	49.83	50.29

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	5.905	215.462	530.984	94.17	92.66
2	7.370	13.331	42.056	5.83	7.34

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(2-(isoquinolin-1-yl)-3,4-dimethylphenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ia)



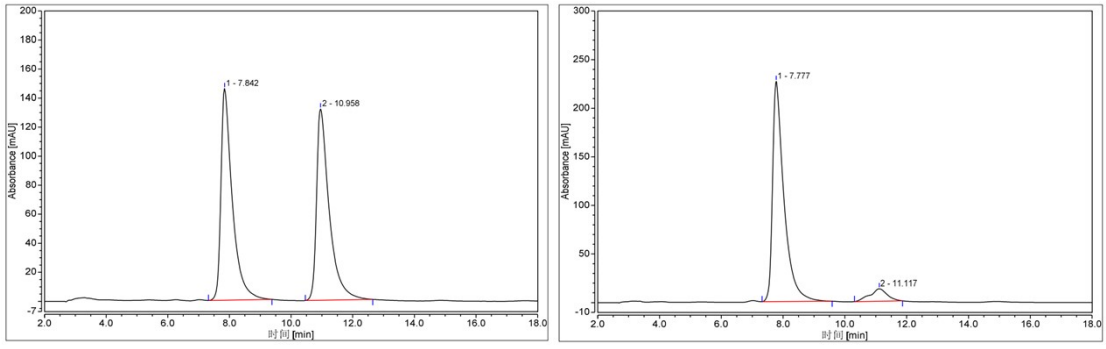
57% yield, white solid, **m.p.** = 133–135 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.8 Hz, 1H), 7.96 - 7.94 (m, 1H), 7.71 - 7.65 (m, 2H), 7.48 - 7.42 (m, 3H), 7.30 - 7.21 (m, 4H), 7.08 - 7.05 (m, 1H), 5.26 - 5.24 (m, 1H), 3.10 - 3.09 (m, 2H), 3.004 - 2.996 (m, 1H), 2.81 - 2.80 (m, 1H), 2.72 - 2.69 (m, 1H), 2.29 (s, 3H), 2.17 - 2.15 (m, 1H), 1.91 - 1.86 (m, 1H), 1.66 - 1.64 (m, 1H), 1.61 (s, 3H), 1.46 - 1.41 (m, 1H), 1.14 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 177.0, 161.3, 147.6, 142.5, 140.8, 138.4, 136.4, 135.8, 135.0, 130.7, 130.3, 130.0, 129.8, 129.2, 128.6, 127.85, 127.78, 127.1, 127.0, 126.5, 122.3, 120.0, 48.9, 48.7, 44.0, 41.0, 39.6, 39.1, 36.0, 35.6, 31.6, 20.1, 16.6.

HRMS (ESI): Calculated for $[C_{36}H_{37}N_2O_2, M+H]^+$: 529.2850; Found: 529.2852.

Optical Rotation: $[\alpha]^{25}_D$ = –117.2° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2967, 2332, 1708, 1440, 1367, 1175, 825, 753, 688, 618.

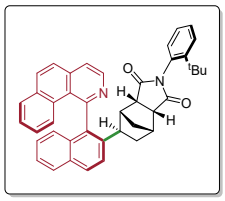
HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 7.777 min (major) and 11.117 min (minor). 84% ee.



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.842	62.528	145.796	49.86	52.52
2	10.958	62.866	131.827	50.14	47.48

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.777	97.135	226.548	92.21	94.64
2	11.117	8.211	12.834	7.79	5.36

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(benzo[h]isoquinolin-1-yl)naphthalen-2-yl)-2-(2-(*tert*-butyl)phenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ja)



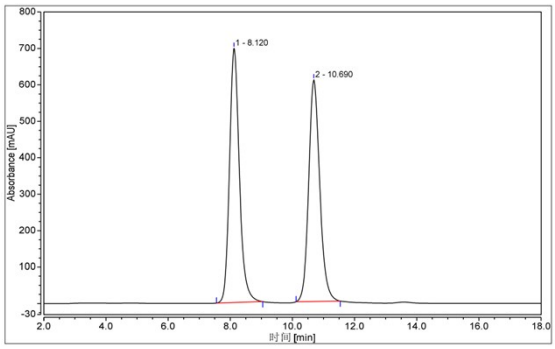
69% yield, white solid, **m.p.** = 108–110 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.82 (d, *J* = 5.2 Hz, 1H), 8.07 - 8.05 (m, 1H), 7.97 - 7.95 (m, 1H), 7.88 - 7.76 (m, 6H), 7.45 - 7.43 (m, 1H), 7.36 - 7.29 (m, 4H), 7.12 - 7.08 (m, 1H), 7.07 - 7.03 (m, 1H), 7.00 - 6.97 (m, 1H), 6.71 - 6.69 (m, 1H), 5.66 - 5.64 (m, 1H), 3.15 - 3.09 (m, 2H), 2.95 - 2.89 (m, 3H), 2.33 - 2.30 (m, 1H), 2.18 - 2.15 (m, 1H), 1.81 - 1.76 (m, 1H), 1.68 - 1.66 (m, 1H), 1.11 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 176.5, 156.7, 147.6, 144.3, 140.3, 138.9, 138.4, 133.3, 132.68, 132.66, 131.9, 130.6, 130.1, 129.3, 129.2, 128.8, 128.6, 127.8, 127.3, 127.1, 126.9, 126.6, 126.0, 125.9, 125.8, 125.6, 125.3, 124.2, 121.8, 49.0, 48.6, 44.5, 41.1, 39.5, 39.3, 35.6, 35.2, 31.6.

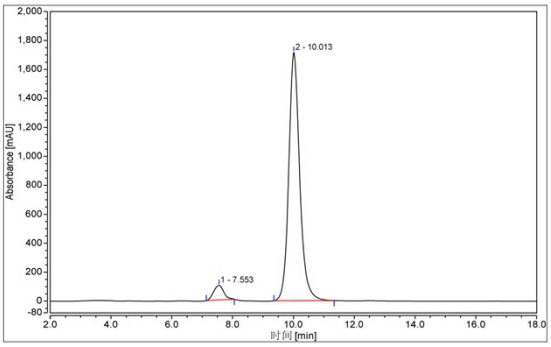
HRMS (ESI): Calculated for $[C_{42}H_{37}N_2O_2, M+H]^+$: 601.2850; Found: 601.2858.

Optical Rotation: $[\alpha]^{25}_D$ = –52.8° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2954, 2922, 2853, 1708, 1461, 1375, 1260, 1169, 1084, 1021, 789, 749.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 10.013 min (major) and 7.553 min (minor). 90% ee.

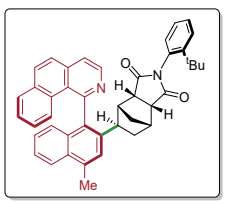




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.120	256.445	697.657	50.62	53.42
2	10.690	250.133	608.441	49.38	46.58

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.553	39.257	101.831	5.21	5.61
2	10.013	714.825	1714.884	94.79	94.39

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(benzo[h]isoquinolin-1-yl)-4-methylnaphthalen-2-yl)-2-(2-(*tert*-butyl)phenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ka)



98% yield, white solid, **m.p.** = 248–250 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 5.2 Hz, 1H), 7.95 - 7.94 (m, 1H), 7.88 - 7.86 (m, 1H), 7.75 - 7.74 (m, 1H), 7.71 - 7.69 (m, 2H), 7.51 (s, 1H), 7.37 - 7.27 (m, 4H), 7.24 - 7.21 (m, 1H), 7.04 - 6.91 (m, 3H), 6.65 - 6.64 (m, 1H), 5.58 - 5.56 (m, 1H), 3.04 - 3.01 (m, 2H), 2.87 - 2.82 (m, 3H), 2.80 (s, 3H), 2.27 - 2.24 (m, 1H), 2.11 - 2.07 (m, 1H), 1.72 - 1.67 (m, 1H), 1.60 - 1.58 (m, 1H), 1.04 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.1, 176.4, 157.0, 147.6, 144.3, 138.7, 138.4, 135.1, 133.2,

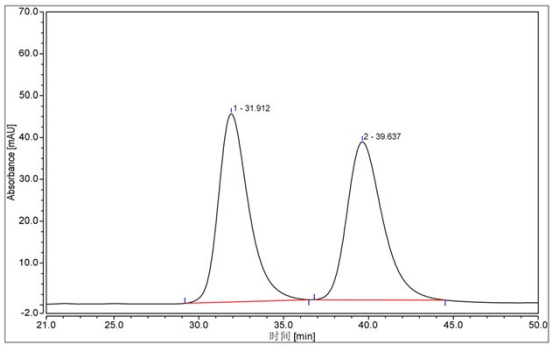
132.6, 132.0, 131.9, 130.6, 130.1, 129.3, 129.23, 129.15, 128.6, 127.3, 127.1, 126.8, 126.3, 126.2, 125.92, 125.90, 125.7, 125.6, 125.0, 124.0, 121.7, 49.1, 48.6, 44.5, 41.2, 39.4, 39.3, 35.6, 35.1, 31.6, 20.2.

HRMS (ESI): Calculated for $[C_{43}H_{39}N_2O_2, M+H]^+$: 615.3006; Found: 615.3011.

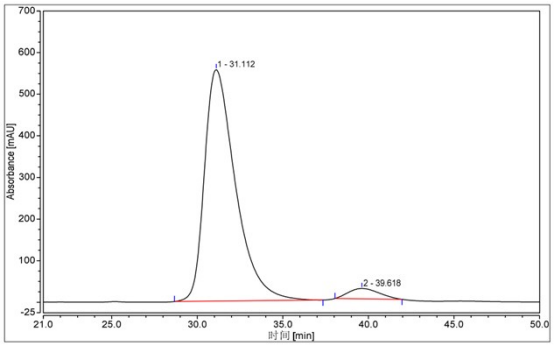
Optical Rotation: $[\alpha]^{25}_D$ = –64.2° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2922, 1710, 1442, 1364, 1259, 1169, 1017, 858, 795, 748, 604.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 90 : 10, 1.0 mL/min), 30 °C, 254 nm, R*t* = 31.112 min (major) and 39.618 min (minor). 92% ee.

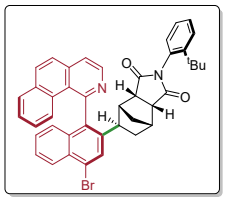


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	31.912	93.423	44.965	50.42	54.37
2	39.637	91.879	37.734	49.58	45.63



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	31.112	1169.281	556.260	95.79	95.73
2	39.618	51.388	24.794	4.21	4.27

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(benzo[h]isoquinolin-1-yl)-4-bromonaphthalen-2-yl)-2-(2-(*tert*-butyl)phenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3la)



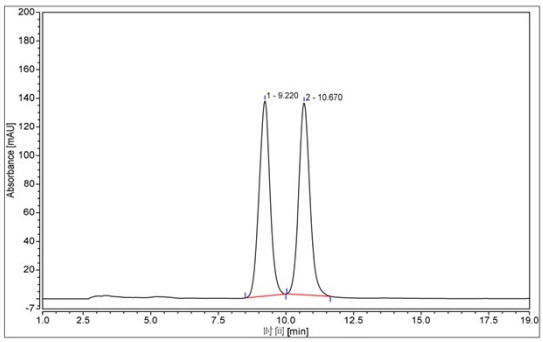
73% yield, white solid, **m.p.** = 271–273 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.80 (d, *J* = 5.2 Hz, 1H), 8.28 - 8.26 (m, 1H), 8.070 - 8.067 (m, 1H), 7.95 - 7.93 (m, 1H), 7.82 - 7.77 (m, 3H), 7.45 - 7.42 (m, 2H), 7.38 - 7.35 (m, 2H), 7.31 - 7.28 (m, 1H), 7.10 - 7.03 (m, 3H), 6.72 - 6.71 (m, 1H), 5.61 - 5.59 (m, 1H), 3.12 - 3.08 (m, 2H), 2.96 - 2.88 (m, 3H), 2.28 - 2.26 (m, 1H), 2.14 - 2.10 (m, 1H), 1.79 - 1.74 (m, 1H), 1.69 - 1.66 (m, 1H), 1.10 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.9, 176.3, 155.7, 147.7, 144.4, 140.5, 139.9, 138.4, 133.3, 133.0, 132.8, 131.3, 130.5, 130.0, 129.4, 129.3, 129.0, 128.7, 128.6, 127.6, 127.5, 127.3, 127.2, 127.1, 126.0, 125.9, 125.8, 125.5, 123.7, 122.0, 49.0, 48.5, 44.4, 41.1, 39.4, 39.3, 35.6, 35.2, 31.6.

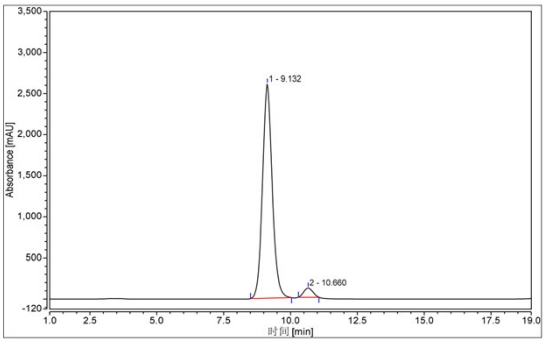
HRMS (ESI): Calculated for $[C_{42}H_{36}BrN_2O_2, M+H]^+$: 679.1955; Found: 679.1965.

Optical Rotation: $[\alpha]^{25}_D$ = –79.3° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2919, 2849, 1710, 1645, 1364, 1260, 1017, 856, 801, 747, 605.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 80 : 20, 1.0 mL/min), 30 °C, 254 nm, R*t* = 9.132 min (major) and 10.660 min (minor). 92% ee.

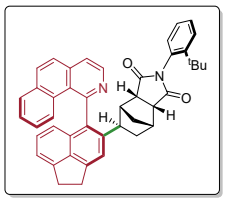




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.220	63.939	136.253	50.05	50.39
2	10.670	63.812	134.157	49.95	49.61

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.132	1098.436	2604.438	96.19	95.91
2	10.660	43.475	110.957	3.81	4.09

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(5-(benzo[h]isoquinolin-1-yl)-1,2-dihydroacenaphthylen-4-yl)-2-(2-(*tert*-butyl)phenyl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (3ma)



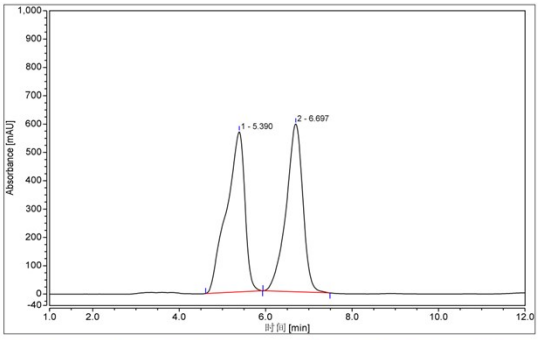
99% yield, white solid, **m.p.** = 136–138 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 5.2 Hz, 1H), 7.88 - 7.86 (m, 1H), 7.76 - 7.74 (m, 1H), 7.71 - 7.69 (m, 2H), 7.51 - 7.48 (m, 2H), 7.36 - 7.34 (m, 1H), 7.30 - 7.27 (m, 1H), 7.22 - 7.19 (m, 1H), 7.07 - 7.05 (m, 1H), 6.99 - 6.92 (m, 3H), 6.30 - 6.28 (m, 1H), 5.55 - 5.54 (m, 1H), 3.52 - 3.36 (m, 4H), 3.21 - 3.18 (m, 1H), 3.06 - 3.03 (m, 1H), 2.92 - 2.89 (m, 2H), 2.85 - 2.83 (m, 1H), 2.30 - 2.28 (m, 1H), 2.14 - 2.09 (m, 1H), 1.79 - 1.74 (m, 1H), 1.62 - 1.60 (m, 1H), 1.04 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.1, 175.5, 155.7, 146.5, 145.6, 144.6, 143.3, 139.8, 137.3, 137.2, 135.2, 132.2, 131.5, 129.5, 129.0, 128.9, 128.2, 128.0, 127.5, 127.4, 126.2, 126.1, 125.7, 125.0, 124.8, 124.7, 120.4, 119.3, 118.2, 116.6, 48.1, 47.6, 43.7, 40.2, 38.9, 38.3, 34.6, 34.5, 30.5, 29.6, 29.5.

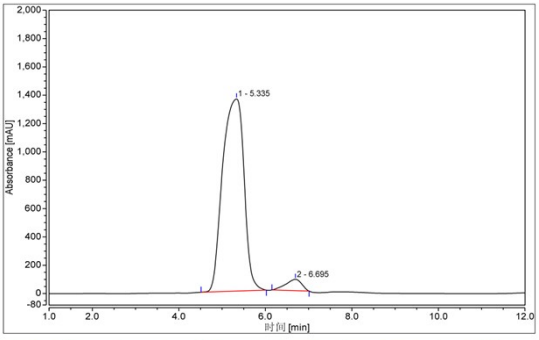
HRMS (ESI): Calculated for $[C_{44}H_{39}N_2O_2, M+H]^+$: 627.3006; Found: 627.3019.

Optical Rotation: $[\alpha]^{25}_D$ = –64.5° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2923, 2342, 2173, 1978, 1453, 1259, 1066, 796.

HPLC: Daicel Chiralpak AD-H Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 5.335 min (major) and 6.695 min (minor). 92% ee.

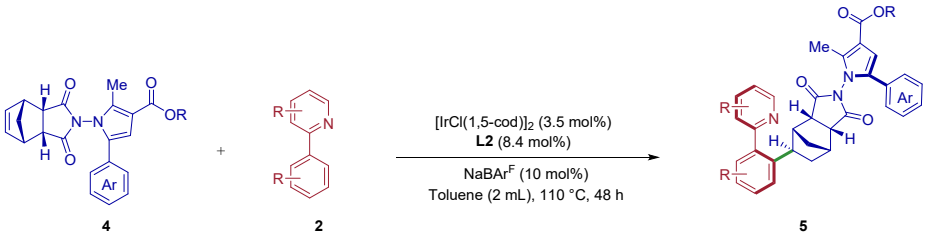




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	5.390	276.278	565.407	50.94	48.81
2	6.697	266.037	592.892	49.06	51.19

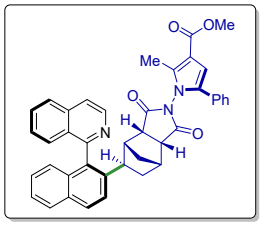
peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	5.335	779.289	1356.559	95.82	94.45
2	6.695	33.964	79.710	4.18	5.55

2. Construction of C−C and N−N atropisomers 5:



General procedure F: To an oven-dried 10 mL Schlenk tube containing a stirring bar was charged with $[IrCl(1,5\text{-cod})]_2$ (0.0035 mmol, 2.4 mg), **L2** (0.0084 mmol, 5.7 mg) and 1.0 mL dry toluene in a nitrogen-filled glove-box, the mixture was stirred for 10 min at room temperature. Then corresponding substrate **4** (0.1 mmol, 1.0 equiv.), corresponding substrate **2** (0.12 mmol, 1.2 equiv.), $NaBAr^F$ (0.01 mmol, 8.9 mg) and another 1.0 mL dry toluene were added sequentially. The mixture was stirred at 110 °C for 48 hours, concentrated to dryness and the crude mixture was purified by flash column chromatography on silica gel using a mixture of Hexane/EtOAc (3/1, v/v) as eluent to obtain the desired product.

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5a)



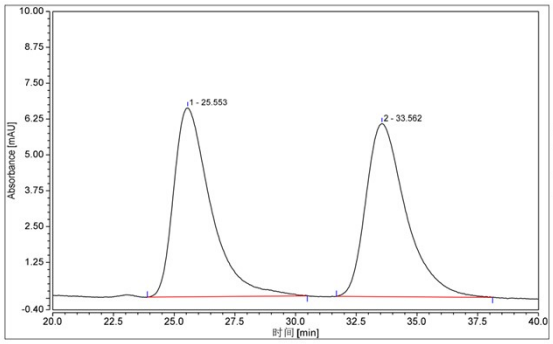
99% yield, white solid, **m.p.** = 121–123 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.8 Hz, 1H), 8.02 - 7.98 (m, 2H), 7.87 - 7.82 (m, 2H), 7.72 - 7.69 (m, 1H), 7.64 - 7.62 (m, 1H), 7.40 - 7.35 (m, 2H), 7.29 - 7.27 (m, 1H), 7.21 - 7.15 (m, 4H), 7.06 - 7.03 (m, 2H), 6.69 - 6.67 (m, 1H), 6.62 (s, 1H), 3.87 (s, 3H), 3.14 - 3.11 (m, 1H), 2.93 - 2.91 (m, 1H), 2.88 - 2.84 (m, 1H), 2.73 - 2.69 (m, 2H), 2.32 - 2.24 (m, 2H), 1.97 (s, 3H), 1.75 - 1.70 (m, 1H), 1.49 - 1.47 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3, 171.9, 165.2, 159.4, 139.5, 136.9, 136.8, 133.1, 132.9, 132.1, 130.5, 130.1, 128.9, 128.8, 128.5, 128.1, 127.7, 127.6, 127.5, 126.8, 126.6, 126.0, 125.8, 123.7, 121.1, 111.7, 108.7, 51.2, 46.60, 46.57, 45.5, 39.5, 39.4, 39.2, 33.5, 10.1.

HRMS (ESI): Calculated for $[C_{41}H_{34}N_3O_4, M+H]^+$: 632.2544; Found: 632.2552.

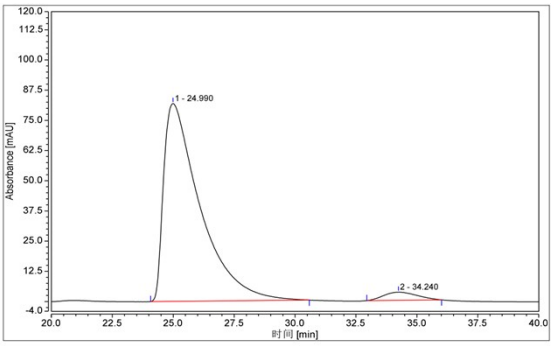
Optical Rotation: $[\alpha]^{25}_D$ = –85.7° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1737, 1706, 1438, 1398, 1241, 1199, 1166, 1072, 815, 749, 699, 630, 502.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 24. 990 min (major) and 34. 240 min (minor). 93% ee.

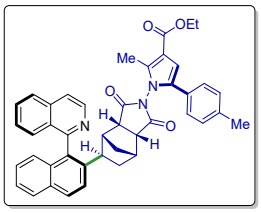


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	25.553	11.638	6.592	50.27	52.20
2	33.562	11.514	6.037	49.73	47.80



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	24.990	142.227	81.883	96.40	96.05
2	34.240	5.306	3.368	3.60	3.95

ethyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-(p-tolyl)-1*H*-pyrrole-3-carboxylate (5b)



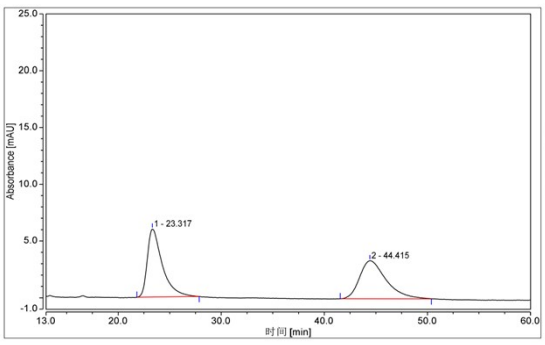
95% yield, white solid, **m.p.** = 147–149 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.7 Hz, 1H), 8.00 - 7.97 (m, 2H), 7.86 - 7.84 (m, 1H), 7.81 - 7.80 (m, 1H), 7.70 - 7.66 (m, 1H), 7.64 - 7.62 (m, 1H), 7.39 - 7.33 (m, 2H), 7.28 - 7.26 (m, 1H), 7.17 - 7.13 (m, 1H), 7.00 - 6.99 (m, 2H), 6.94 - 6.92 (m, 2H), 6.69 - 6.67 (m, 1H), 6.60 (s, 1H), 4.37 - 4.30 (m, 2H), 3.15 - 3.12 (m, 1H), 2.92 - 2.85 (m, 2H), 2.73 - 2.67 (m, 2H), 2.32 - 2.27 (m, 1H), 2.25 - 2.23 (m, 4H), 1.99 (s, 3H), 1.76 - 1.70 (m, 1H), 1.48 - 1.46 (m, 1H), 1.40 - 1.37 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 171.9, 164.8, 159.4, 142.7, 139.6, 137.9, 136.9, 136.3, 136.0, 133.2, 132.9, 132.1, 130.5, 129.2, 128.9, 128.8, 128.0, 127.7, 127.54, 127.53, 127.2, 126.8, 126.6, 126.0, 125.7, 123.8, 121.1, 111.9, 108.4, 59.8, 46.61, 46.58, 45.5, 39.5, 39.4, 39.2, 33.5, 21.2, 14.6, 10.2.

HRMS (ESI): Calculated for $[C_{43}H_{37}N_3NaO_4, M+Na]^+$: 682.2676; Found: 682.2687.

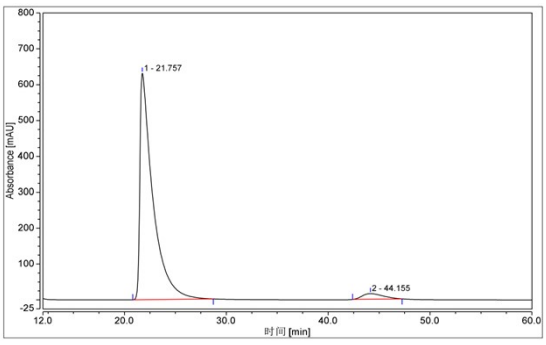
Optical Rotation: $[\alpha]^{25}_D$ = –85.9° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1737, 1701, 1403, 1240, 1195, 1166, 1069, 814, 772, 747, 593, 508.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 21.757 min (major) and 44. 155 min (minor). 92% ee.

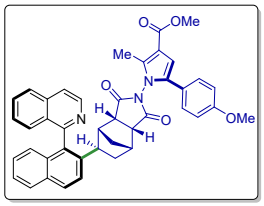


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	23.317	10.152	6.000	50.31	64.13
2	44.415	10.025	3.356	49.69	35.87



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	21.757	927.597	631.681	96.16	97.57
2	44.155	37.090	15.753	3.84	2.43

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-5-(4-methoxyphenyl)-2-methyl-1*H*-pyrrole-3-carboxylate (5c)



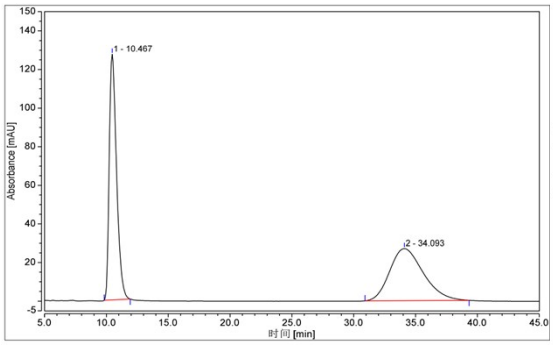
87% yield, white solid, **m.p.** = 150–152 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.8 Hz, 1H), 7.92 - 7.89 (m, 2H), 7.78 - 7.76 (m, 1H), 7.73 - 7.72 (m, 1H), 7.62 - 7.58 (m, 1H), 7.55 - 7.54 (m, 1H), 7.30 - 7.25 (m, 2H), 7.20 - 7.17 (m, 1H), 7.09 - 7.05 (m, 1H), 6.89 - 6.87 (m, 2H), 6.64 - 6.59 (m, 3H), 6.46 (s, 1H), 3.77 (s, 3H), 3.63 (s, 3H), 3.07 - 3.04 (m, 1H), 2.83 - 2.81 (m, 1H), 2.78 - 2.75 (m, 1H), 2.63 - 2.59 (m, 2H), 2.23 - 2.14 (m, 2H), 1.89 (s, 3H), 1.66 - 1.61 (m, 1H), 1.39 - 1.37 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 171.9, 165.2, 159.5, 159.4, 142.7, 139.5, 136.9, 136.3, 136.0, 133.2, 132.7, 132.1, 130.5, 129.7, 128.84, 128.79, 127.7, 127.6, 127.5, 126.8, 126.6, 126.0, 125.7, 123.8, 122.4, 121.1, 113.9, 111.4, 108.1, 55.2, 51.1, 46.60, 46.57, 45.5, 39.5, 39.4, 39.2, 33.5, 10.1.

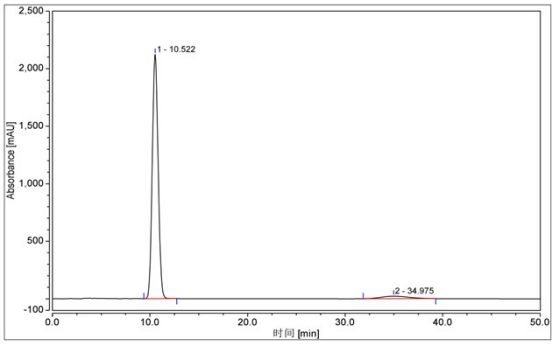
HRMS (ESI): Calculated for $[C_{42}H_{36}N_3O_5, M+H]^+$: 662.2649; Found: 662.2671.

Optical Rotation: $[\alpha]^{25}_D$ = –84.2° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1737, 1705, 1587, 1496, 1439, 1395, 1245, 1199, 1167, 1074, 1027, 814, 773, 747, 595.

HPLC: Daicel Chiralpak AD-H Column (*n*-Hexane/*i*-PrOH = 50 : 50, 1.0 mL/min), 30 °C, 254 nm, R*t* = 10.522 min (major) and 34.975 min (minor). 90% ee.

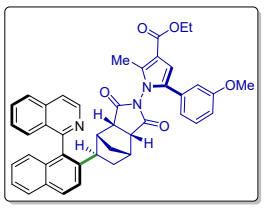




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	10.467	87.137	127.268	50.64	82.51
2	34.093	84.951	26.975	49.36	17.49

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	10.522	1471.942	2122.237	95.36	98.99
2	34.975	71.699	21.626	4.64	1.01

ethyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-5-(3-methoxyphenyl)-2-methyl-1*H*-pyrrole-3-carboxylate (5d)



78% yield, white solid, **m.p.** = 116–118 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.7 Hz, 1H), 8.00 - 7.97 (m, 2H), 7.86 - 7.85 (m, 1H), 7.81 - 7.80 (m, 1H), 7.69 - 7.66 (m, 1H), 7.64 - 7.62 (m, 1H), 7.39 - 7.33 (m, 2H), 7.28 - 7.26 (m, 1H), 7.17 - 7.14 (m, 1H), 7.10 - 7.07 (m, 1H), 6.74 - 6.72 (m, 1H), 6.69 - 6.67 (m,

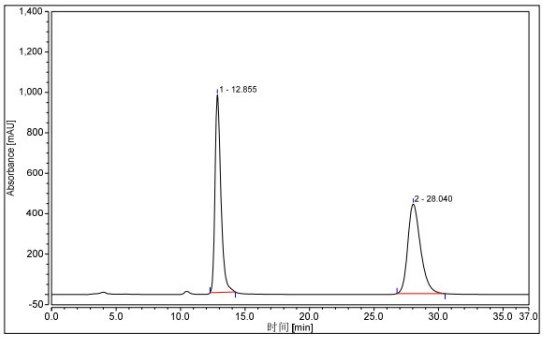
1H), 6.65 - 6.63 (m, 2H), 6.60 - 6.58 (m, 1H), 4.37 - 4.30 (m, 2H), 3.68 (s, 3H), 3.15 - 3.12 (m, 1H), 2.93 - 2.87 (m, 2H), 2.74 - 2.68 (m, 2H), 2.32 - 2.24 (m, 2H), 1.99 (s, 3H), 1.77 - 1.71 (m, 1H), 1.49-1.47 (m, 1H), 1.41 - 1.38 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 171.9, 164.7, 159.6, 159.4, 142.7, 139.5, 136.9, 136.7, 136.0, 133.1, 132.7, 132.1, 131.4, 130.5, 129.5, 128.9, 128.8, 127.7, 127.6, 127.5, 126.8, 126.6, 126.0, 125.7, 123.8, 121.1, 120.0, 114.0, 113.5, 112.0, 108.9, 59.8, 55.2, 46.7, 46.6, 45.5, 39.6, 39.4, 39.2, 33.5, 14.6, 10.2.

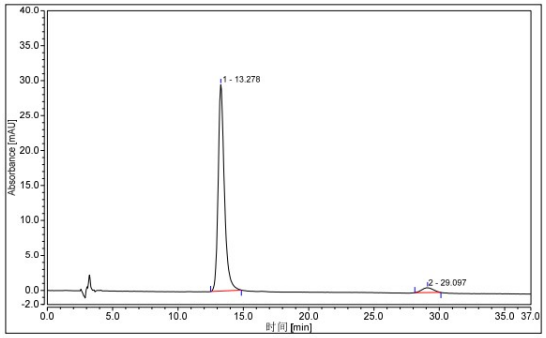
HRMS (ESI): Calculated for $[C_{43}H_{38}N_3O_5, M+H]^+$: 676.2806; Found: 676.2843.

Optical Rotation: $[\alpha]^{25}_D$ = –92.5° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 3853, 3839, 3802, 3750, 3675, 3649, 2359,1698, 1653, 1558, 1507, 1457.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 13.278 min (major) and 29.097 min (minor). 92% ee.

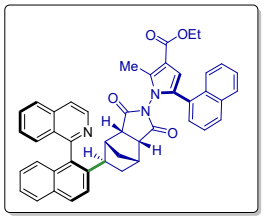




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.855	520.740	977.960	50.58	68.82
2	28.040	508.836	443.140	49.42	31.18

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	13.278	16.312	29.552	95.97	97.74
2	29.097	0.684	0.684	4.03	2.26

ethyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-(naphthalen-1-yl)-1*H*-pyrrole-3-carboxylate (5e)



53% yield, white solid, **m.p.** = 115–117 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.7 Hz, 1H), 8.02 - 7.97 (m, 2H), 7.86 - 7.82 (m, 2H), 7.73 - 7.65 (m, 5H), 7.62 - 7.61 (m, 1H), 7.52 - 7.51 (m, 1H), 7.42 - 7.33 (m, 5H), 7.27 - 7.26 (m, 1H), 7.17 - 7.14 (m, 2H), 6.75 (s, 1H), 6.69 - 6.68 (m, 1H), 4.38 - 4.34 (m, 2H), 3.16 - 3.13 (m, 1H), 2.90 - 2.88 (m, 1H), 2.82 - 2.79 (m, 1H), 2.66 - 2.64 (m, 2H), 2.32 - 2.27 (m, 1H), 2.23 - 2.21 (m, 1H), 2.03 (s, 3H), 1.76 - 1.71 (m, 1H), 1.42 - 1.39 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 171.9, 164.8, 159.4, 142.6, 139.5, 136.92, 136.85, 135.9, 133.1, 132.9, 132.7, 132.1, 130.5, 128.9, 128.8, 128.2, 128.0, 127.7, 127.62, 127.59, 127.55, 127.50, 127.0, 126.8, 126.6, 126.5, 126.4, 126.0, 125.8, 125.7, 123.8, 121.1, 112.2, 109.3, 59.9, 46.62, 46.60, 45.5, 39.6, 39.3, 39.2, 33.5, 14.6, 10.2.

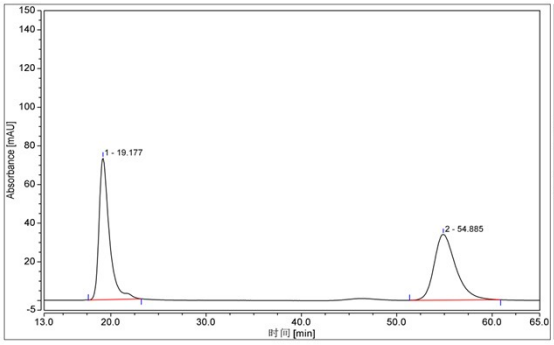
HRMS (ESI): Calculated for $[C_{46}H_{38}N_3O_4, M+H]^+$: 696.2857; Found: 696.2868.

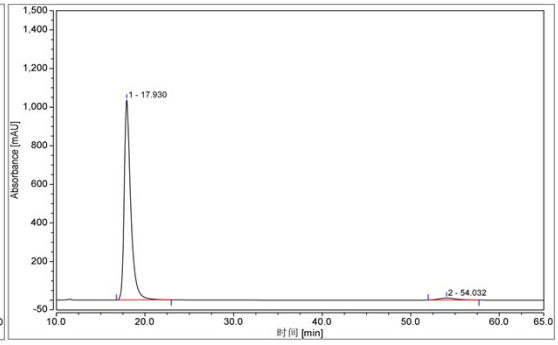
Optical Rotation: $[\alpha]^{25}_D$ = –65.7° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1738, 1704, 1227, 1166, 1069, 815, 773, 747.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 17.930

min (major) and 54.032 min (minor). 95% ee.

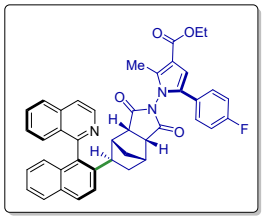




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	19.177	91.704	73.260	50.53	68.28
2	54.885	89.772	34.039	49.47	31.72

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	17.930	891.801	1036.596	97.40	99.02
2	54.032	23.782	10.269	2.60	0.98

ethyl 5-(4-fluorophenyl)-1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-1*H*-pyrrole-3-carboxylate (5f)



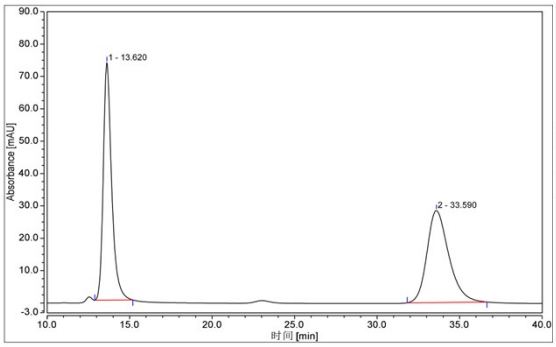
94% yield, white solid, **m.p.** = 141–143 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.7 Hz, 1H), 8.00 - 7.98 (m, 2H), 7.87 - 7.85 (m, 1H), 7.81 - 7.80 (m, 1H), 7.70 - 7.67 (m, 1H), 7.64 - 7.62 (m, 1H), 7.39 - 7.34 (m, 2H), 7.28 - 7.27 (m, 1H), 7.17 - 7.14 (m, 1H), 7.03 - 7.00 (m, 2H), 6.90 - 6.87 (m, 2H), 6.69 - 6.68 (m, 1H), 6.60 (s, 1H), 4.38 - 4.30 (m, 2H), 3.15 - 3.13 (m, 1H), 2.93 - 2.91 (m, 1H), 2.87 - 2.84 (m, 1H), 2.70 - 2.66 (m, 2H), 2.33 - 2.30 (m, 1H), 2.26 - 2.24 (m, 1H), 2.02 (s, 3H), 1.76 - 1.71 (m, 1H), 1.48 - 1.45 (m, 1H), 1.41 - 1.38 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ173.3, 171.9, 164.7, 162.5 (d, $J_{C\text{-}F}$ = 249.0 Hz), 159.4, 142.7, 139.4, 136.9, 136.5, 136.0, 133.1, 132.1, 131.8, 130.5, 130.2 (d, $J_{C\text{-}F}$ = 8.2 Hz), 128.9, 128.8, 127.6 (d, $J_{C\text{-}F}$ = 21.5 Hz), 127.5 (d, $J_{C\text{-}F}$ = 5.2 Hz), 126.8, 126.6, 126.2 (d, $J_{C\text{-}F}$ = 3.2 Hz), 126.0, 125.8, 123.8, 121.1, 115.6, 115.4, 112.0, 108.9, 59.9, 46.6, 45.6, 39.6, 39.3, 39.2, 33.4, 14.6, 10.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -112.98 – -113.04 (m).

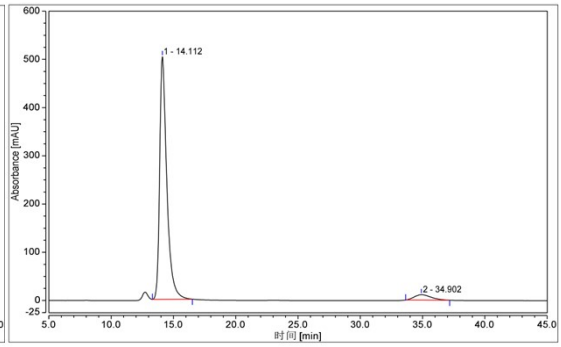
HRMS (ESI): Calculated for $[C_{42}H_{35}FN_3O_4, M+H]^+$: 664.2606; Found: 664.2639.

Optical Rotation: $[\alpha]^{25}_D$ = –97.3° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1737, 1703, 1583, 1494, 1243, 1196, 1166, 1070, 813, 773, 748, 591, 519, 472.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 14.112 min (major) and 34.902 min (minor). 90% ee.

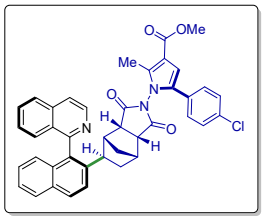




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	13.620	43.250	73.385	49.85	72.08
2	33.590	43.514	28.422	50.15	27.92

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	14.112	334.926	503.172	95.04	97.84
2	34.902	17.475	11.114	4.96	2.16

methyl 5-(4-chlorophenyl)-1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-1*H*-pyrrole-3-carboxylate (5g)



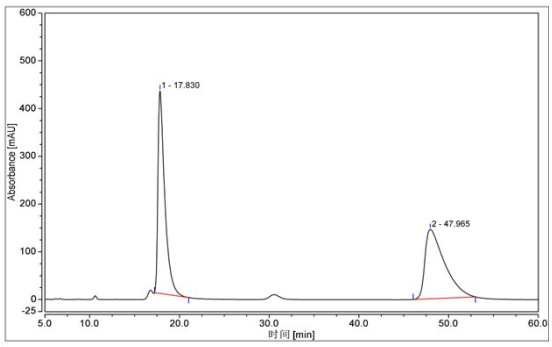
63% yield, white solid, **m.p.** = 146–148 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.66 (d, *J* = 5.7 Hz, 1H), 8.01 - 7.99 (m, 2H), 7.87 - 7.86 (m, 1H), 7.82 - 7.80 (m, 1H), 7.72 - 7.68 (m, 1H), 7.64 - 7.63 (m, 1H), 7.70 - 7.35 (m, 2H), 7.28 - 7.26 (m, 1H), 7.19 - 7.15 (m, 3H), 6.99 - 6.96 (m, 2H), 6.69 - 6.67 (m, 1H), 6.61 (s, 1H), 3.87 (s, 3H), 3.15 - 3.12 (m, 1H), 2.95 - 2.93 (m, 1H), 2.91 - 2.88 (m, 1H), 2.74 - 2.71 (m, 1H), 2.69 - 2.68 (m, 1H), 2.34 - 2.30 (m, 1H), 2.28 - 2.25 (m, 1H), 2.00 (s, 3H), 1.76 - 1.70 (m, 1H), 1.50 - 1.48 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3, 171.8, 165.0, 159.4, 142.7, 139.4, 137.1, 136.9, 136.0, 134.2, 133.1, 132.1, 131.7, 130.5, 129.4, 128.9, 128.8, 128.6, 127.7, 127.6, 127.5, 126.8, 126.6, 126.0, 125.8, 123.7, 121.0, 111.8, 109.1, 51.2, 46.6, 45.6, 39.5, 39.4, 39.3, 33.4, 29.7, 10.1.

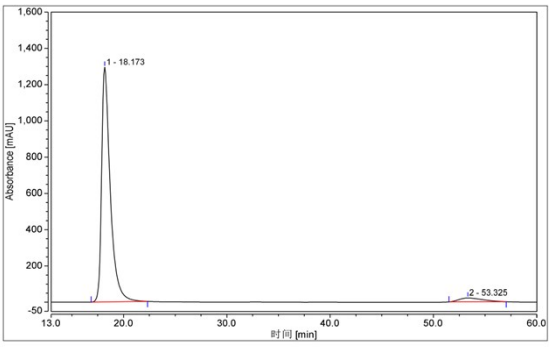
HRMS (ESI): Calculated for $[C_{41}H_{33}ClN_3O_4, M+H]^+$: 666.2154; Found: 666.2184.

Optical Rotation: $[\alpha]^{25}_D$ = –68.9° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2920, 1738,. 1707, 1583, 1438, 1399, 1259, 1199, 1163, 1074, 1014, 813, 773, 746, 687.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 18.173 min (major) and 53.325 min (minor). 91% ee.

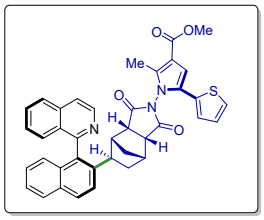




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	17.830	374.538	424.518	50.58	74.48
2	47.965	365.876	145.421	49.42	25.52

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	18.173	1257.733	1294.362	95.66	98.38
2	53.325	57.044	21.364	4.34	1.62

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-((*R*)-isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-(thiophen-2-yl)-1*H*-pyrrole-3-carboxylate (5h)



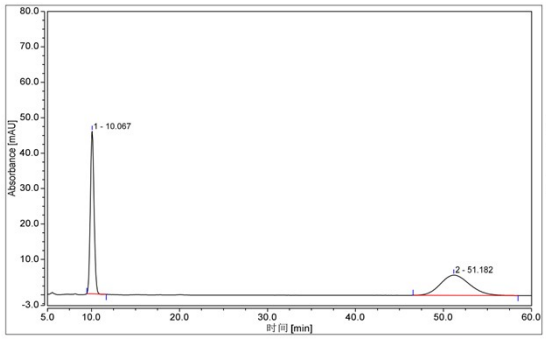
68% yield, white solid, **m.p.** = 149–151 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.66 (d, *J* = 5.8 Hz, 1H), 8.01 - 7.98 (m, 2H), 7.87 - 7.86 (m, 1H), 7.81 - 7.79 (m, 1H), 7.69 - 7.64 (m, 2H), 7.40 - 7.34 (m, 2H), 7.29 - 7.27 (m, 1H), 7.18 - 7.15 (m, 1H), 7.11 - 7.09 (m, 1H), 6.88 - 6.86 (m, 1H), 6.84 - 6.83 (m, 1H), 6.75 (s, 1H), 6.70 - 6.68 (m, 1H), 3.86 (s, 3H), 3.18 - 3.15 (m, 1H), 3.10 - 3.07 (m, 1H), 2.99 - 2.97 (m, 1H), 2.91 - 2.88 (m, 1H), 2.72 - 2.71 (m, 1H), 2.36 - 2.27 (m, 2H), 2.00 (s, 3H), 1.78 - 1.73 (m, 1H), 1.55 - 1.53 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3 171.7, 165.0, 159.4, 142.7, 139.5, 137.1, 136.9, 136.0, 133.1, 132.1, 130.49, 130.47, 128.9, 128.8, 127.7, 127.6, 127.5, 127.4, 126.8, 126.6, 126.04, 125.95, 125.8, 125.6, 125.3, 123.8, 121.1, 111.8, 109.5, 51.2, 47.0, 46.9, 45.6, 39.6, 39.4, 39.3, 33.5, 10.0.

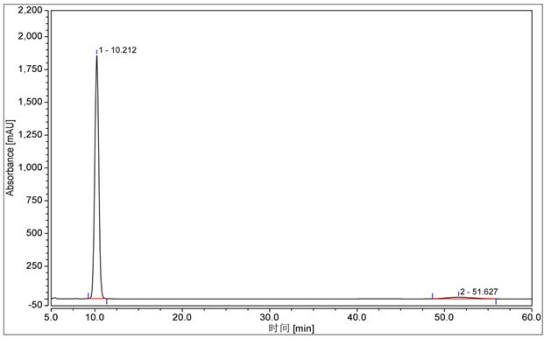
HRMS (ESI): Calculated for $[C_{39}H_{32}N_3O_4S, M+H]^+$: 638.2108; Found: 638.2122.

Optical Rotation: $[\alpha]^{25}_D$ = –99.1° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1739, 1705, 1439, 1217, 1242, 1192, 1160, 1075, 815, 772, 747, 690, 629.

HPLC: Daicel Chiralpak AD-H Column (*n*-Hexane/*i*-PrOH = 50 : 50, 1.0 mL/min), 30 °C, 254 nm, R*t* = 10.212 min (major) and 51.627 min (minor). 90% ee.

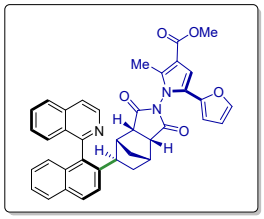




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	10.067	22.302	45.880	50.14	88.89
2	51.182	22.181	5.737	49.86	11.11

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	10.212	979.257	1853.343	95.69	99.34
2	51.627	44.062	12.374	4.31	0.66

methyl 5-(furan-2-yl)-1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-1*H*-pyrrole-3-carboxylate (5i)



90% yield, white solid, **m.p.** = 156–158 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.65 (d, *J* = 5.7 Hz, 1H), 8.01 -

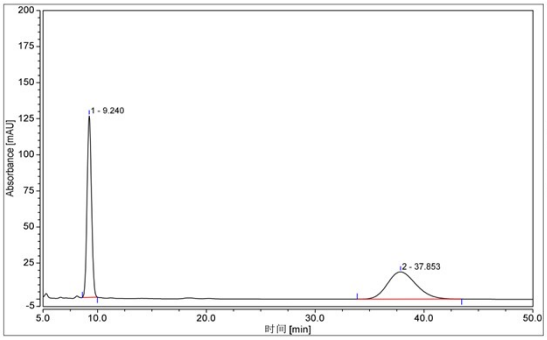
7.96 (m, 2H), 7.88 - 7.86 (m, 1H), 7.79 - 7.78 (m, 1H), 7.69 - 7.65 (m, 2H), 7.40 - 7.34 (m, 2H), 7.29 - 7.28 (m, 1H), 7.18 - 7.15 (m, 1H), 7.114 - 7.110 (m, 1H), 6.77 (s, 1H), 6.71 - 6.69 (m, 1H), 6.25 - 6.24 (m, 1H), 6.18 - 6.17 (m, 1H), 3.85 (s, 3H), 3.21 - 3.12 (m, 2H), 3.01 - 2.99 (m, 1H), 2.95 - 2.92 (m, 1H), 2.71 - 2.70 (m, 1H), 2.37 - 2.28 (m, 2H), 2.04 (s, 3H), 1.82 - 1.76 (m, 1H), 1.57 - 1.55 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3, 171.8, 164.9, 159.4, 144.8, 142.6, 141.5, 139.5, 137.1, 136.9, 136.0, 133.1, 132.1, 130.5, 128.9, 128.8, 127.7, 127.6, 127.5, 126.8, 126.6, 126.1, 125.8, 123.8, 122.5, 121.1, 111.8, 111.3, 108.3, 106.5, 51.2, 47.0, 45.8, 39.7, 39.4, 39.3, 33.4, 9.8.

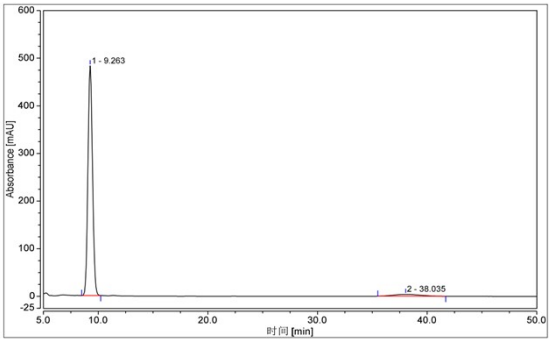
HRMS (ESI): Calculated for $[C_{39}H_{32}N_3O_5, M+H]^+$: 622.2336; Found: 622.2349.

Optical Rotation: $[\alpha]^{25}_D$ = –26.4° (c = 0.5, $CHCl_3$).

IR (neat, cm^{-1}) = 2961, 1741, 1708, 1439, 1258, 1161, 1076, 1014, 798, 746, 592.

HPLC: Daicel Chiralpak AD-H Column (*n*-Hexane/*i*-PrOH = 50 : 50, 1.0 mL/min), 30 °C, 254 nm, R*t* = 9.263 min (major) and 38.035 min (minor). 90% ee.

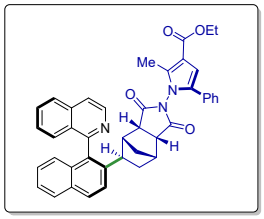




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.240	59.039	125.722	50.57	86.93
2	37.853	57.710	18.895	49.43	13.07

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.263	232.920	482.224	95.49	99.21
2	38.035	11.011	3.821	4.51	0.79

ethyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5j)



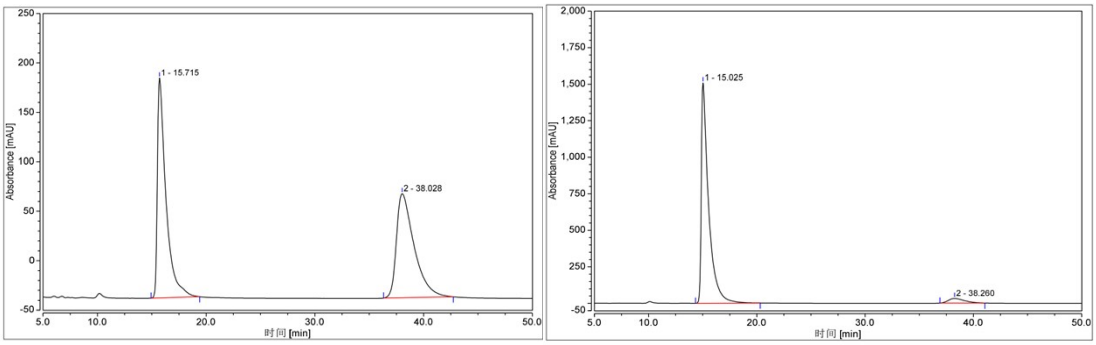
32% yield, white solid, **m.p.** = 140–142 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.8 Hz, 1H), 8.01 - 7.98 (m, 2H), 7.87 - 7.85 (m, 1H), 7.82 - 7.81 (m, 1H), 7.70 - 7.67 (m, 1H), 7.64 - 7.62 (m, 1H), 7.39 - 7.34 (m, 2H), 7.28 - 7.26 (m, 1H), 7.20 - 7.14 (m, 4H), 7.05 - 7.04 (m, 2H), 6.69 - 6.67 (m, 1H), 6.64 (s, 1H), 4.38 - 4.30 (m, 2H), 3.16 - 3.13 (m, 1H), 2.93 - 2.91 (m, 1H), 2.87 - 2.84 (m, 1H), 2.72 - 2.67 (m, 2H), 2.32 - 2.24 (m, 2H), 2.00 (s, 3H), 1.76 - 1.71 (m, 1H), 1.48 - 1.46 (m, 1H), 1.41 - 1.38 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 171.9, 164.7, 159.4, 142.7, 139.5, 136.9, 136.5, 136.0, 133.1, 132.8, 132.1, 130.5, 130.1, 128.9, 128.8, 128.5, 128.1, 128.0, 127.7, 127.54, 127.52, 126.8, 126.6, 126.0, 125.7, 123.8, 121.1, 112.0, 108.8, 59.8, 46.6, 45.5, 39.5, 39.4, 39.2, 33.5, 14.6, 10.2.

HRMS (ESI): Calculated for $[C_{42}H_{36}N_3O_4, M+H]^+$: 646.2700; Found: 646.2715.

Optical Rotation: $[\alpha]^{25}_D$ = –97.9° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2355, 1738, 1701, 1404, 1240, 1196, 1167, 1069, 815, 749, 699, 630, 501.

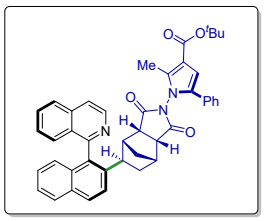
HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 15.025 min (major) and 38.260 min (minor). 91% ee.



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	15.715	203.810	222.472	50.73	67.86
2	38.028	197.981	105.374	49.27	32.14

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	15.025	1170.652	1508.367	95.52	97.93
2	38.260	54.959	31.913	4.48	2.07

***tert*-butyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5k)**



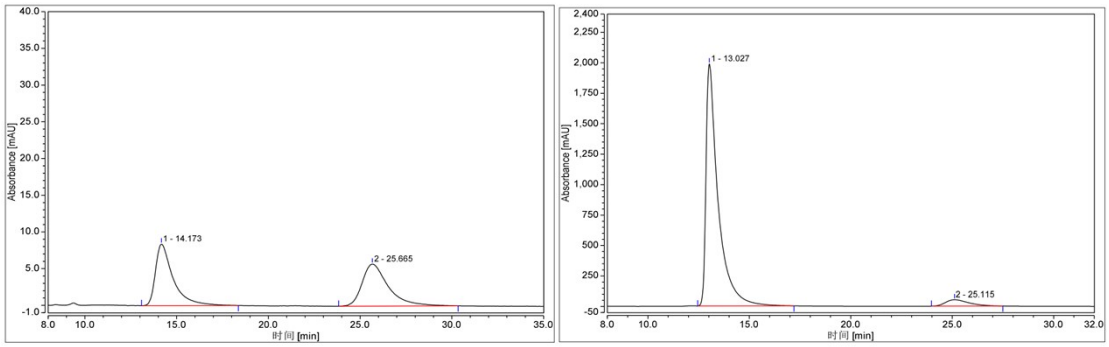
46% yield, white solid, **m.p.** = 158–160 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.8 Hz, 1H), 8.00 - 7.98 (m, 2H), 7.87 - 7.81 (m, 2H), 7.70 - 7.62 (m, 2H), 7.39 - 7.34 (m, 2H), 7.28 - 7.27 (m, 1H), 7.19 - 7.15 (m, 4H), 7.04 - 7.03 (m, 2H), 6.70 - 6.69 (m, 1H), 6.61 (s, 1H), 3.16 - 3.14 (m, 1H), 2.93 - 2.91 (m, 1H), 2.85 - 2.82 (m, 1H), 2.68 - 2.62 (m, 2H), 2.32 - 2.24 (m, 2H), 2.03 (s, 3H), 1.77 - 1.72 (m, 1H), 1.62 (s, 9H), 1.46 - 1.44 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.5, 171.9, 164.1, 159.4, 142.7, 139.5, 136.9, 136.0, 135.6, 133.1, 132.6, 132.1, 130.4, 130.3, 128.9, 128.8, 128.5, 128.1, 128.0, 127.7, 127.53, 127.50, 126.8, 126.6, 126.1, 125.7, 123.9, 121.1, 113.6, 109.1, 46.6, 45.7, 39.6, 39.3, 39.2, 33.2, 28.6, 10.4.

HRMS (ESI): Calculated for $[C_{44}H_{40}N_3O_4, M+H]^+$: 674.3013; Found: 674.3022.

Optical Rotation: $[\alpha]^{25}_D$ = –102.9° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2349, 1739, 1695, 1402, 1250, 1155, 1068, 815, 748, 699, 630, 467.

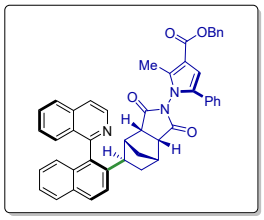
HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 13.027 min (major) and 25.115 min (minor). 90% ee.



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	14.173	9.304	8.382	49.58	59.39
2	25.665	9.464	5.731	50.42	40.61

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	13.027	1371.771	1986.473	95.09	97.43
2	25.115	70.885	52.447	4.91	2.57

benzyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5l)



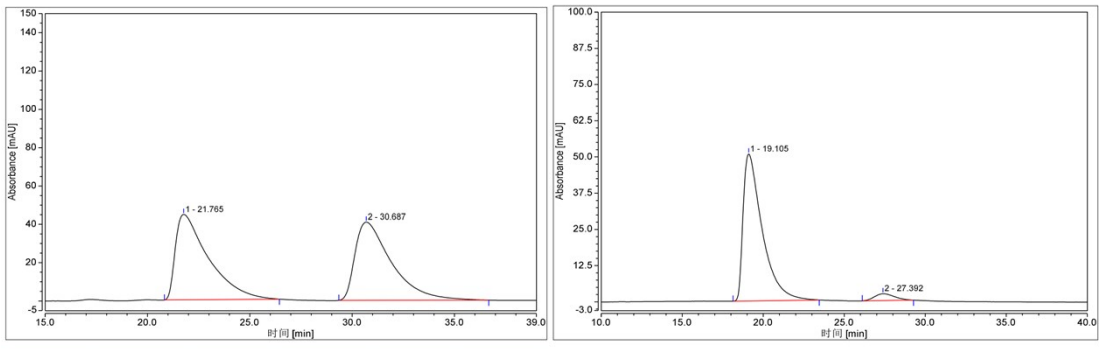
33% yield, white solid, **m.p.** = 118–120 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.61 (d, *J* = 5.8 Hz, 1H), 7.99 - 7.97 (m, 1H), 7.87 - 7.85 (m, 2H), 7.72 - 7.71 (m, 1H), 7.66 - 7.62 (m, 2H), 7.50 - 7.48 (m, 2H), 7.45 - 7.42 (m, 2H), 7.40 - 7.33 (m, 3H), 7.27 (s, 1H), 7.22 - 7.19 (m, 3H), 7.18 - 7.14 (m, 1H), 7.06 - 7.03 (m, 2H), 6.67 - 6.65 (m, 2H), 5.38 - 5.30 (m, 2H), 3.11 - 3.08 (m, 1H), 2.92 - 2.90 (m, 1H), 2.87 - 2.84 (m, 1H), 2.75 - 2.72 (m, 2H), 2.30 - 2.24 (m, 2H), 1.91 (s, 3H), 1.72 - 1.67 (m, 1H), 1.51 - 1.48 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3, 171.9, 164.5, 159.4, 142.6, 139.5, 136.8, 136.7, 136.6, 135.9, 133.2, 132.9, 132.1, 130.5, 130.0, 128.8, 128.7, 128.6, 128.5, 128.22, 128.15, 128.1, 127.7, 127.6, 127.5, 126.7, 126.6, 126.0, 125.7, 123.6, 121.0, 111.7, 108.9, 65.7, 46.61, 46.57, 45.4, 39.53, 39.49, 39.2, 33.7, 29.7, 29.3, 14.1, 10.2.

HRMS (ESI): Calculated for $[C_{47}H_{38}N_3O_4, M+H]^+$: 708.2857; Found: 708.2869.

Optical Rotation: $[\alpha]^{25}_D$ = –77.7° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1736, 1701, 1406, 1237, 1176, 1066, 765, 754, 747, 720, 702, 598.

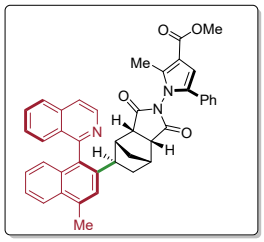
HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 19.105 min (major) and 27.392 min (minor). 91% ee.



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	21.765	83.458	44.607	49.76	52.23
2	30.687	84.279	40.799	50.24	47.77

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	19.105	69.284	50.747	95.41	95.59
2	27.392	3.337	2.340	4.59	4.41

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(isoquinolin-1-yl)-4-methylnaphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5m)



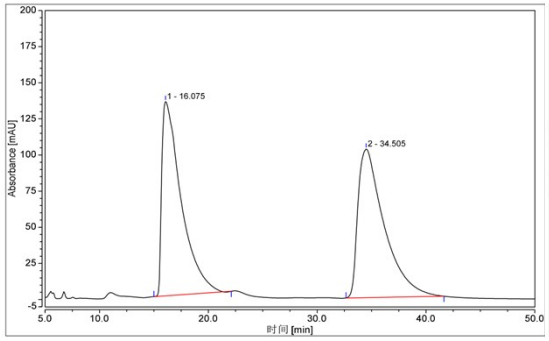
99% yield, white solid, **m.p.** = 254–256 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.8 Hz, 1H), 8.04 - 8.01 (m, 2H), 7.87 (s, 1H), 7.74 (s, 1H), 7.46 - 7.38 (m, 3H), 7.34 - 7.32 (m, 1H), 7.21 - 7.16 (m, 4H), 7.05 - 7.03 (m, 2H), 6.67 - 6.66 (m, 1H), 6.61 (s, 1H), 3.87 (s, 3H), 3.04 (s, 1H), 2.95 - 2.93 (m, 1H), 2.88 - 2.85 (m, 1H), 2.82 (s, 3H), 2.73 - 2.67 (m, 2H), 2.35 - 2.32 (m, 1H), 2.29 - 2.27 (m, 1H), 1.96 (s, 3H), 1.75 - 1.70 (m, 1H), 1.50 - 1.48 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 171.9, 165.2, 159.7, 142.6, 139.0, 136.90, 136.87, 135.2, 134.3, 133.3, 132.9, 131.3, 130.4, 130.1, 129.0, 128.5, 128.10, 128.06, 127.5, 127.0, 126.7, 126.3, 125.6, 124.6, 124.0, 121.0, 111.7, 108.7, 51.2, 46.6, 45.6, 39.5, 39.4, 39.2, 33.4, 20.2, 10.1.

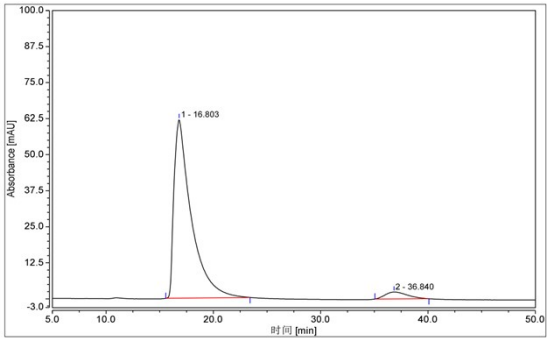
HRMS (ESI): Calculated for $[C_{42}H_{36}N_3O_4, M+H]^+$: 646.2700; Found: 646.2710.

Optical Rotation: $[\alpha]^{25}_D$ = –91.3° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2353, 1738, 1715, 1443, 1297, 1243, 1189, 1164, 1070, 826, 759, 697, 581, 500.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 16.803 min (major) and 36.840 min (minor). 91% ee.

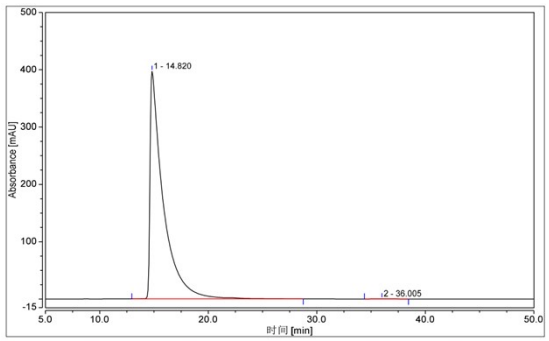




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	16.075	276.628	134.532	49.05	56.69
2	34.505	287.375	102.790	50.95	43.31

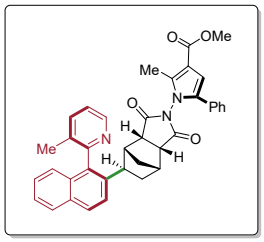
peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	16.803	115.379	61.972	95.29	96.27
2	36.840	5.701	2.402	4.71	3.73

Recrystallized **5m** for X-Ray analysis : >99% ee



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	14.820	556.109	397.065	99.92	99.95
2	36.005	0.427	0.216	0.08	0.05

methyl 2-methyl-1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(3-methylpyridin-2-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (5n)



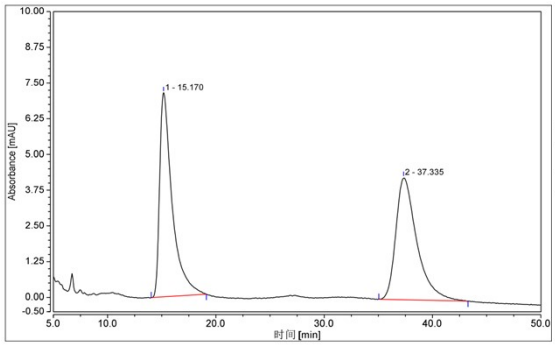
69% yield, white solid, **m.p.** = 114–116 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.57 (d, *J* = 5.6 Hz, 1H), 7.90 - 7.88 (m, 1H), 7.83 - 7.82 (m, 1H), 7.72 - 7.71 (m, 1H), 7.56 - 7.54 (m, 1H), 7.42 - 7.39 (m, 1H), 7.33 - 7.26 (m, 5H), 7.15 - 7.13 (m, 2H), 6.89 - 6.87 (m, 1H), 6.66 (s, 1H), 3.86 (s, 3H), 3.12 - 3.09 (m, 1H), 2.99 - 2.91 (m, 3H), 2.78 - 2.77 (m, 1H), 2.30 - 2.28 (m, 1H), 2.24 - 2.21 (m, 1H), 2.19 (s, 3H), 1.96 (s, 3H), 1.81 - 1.76 (m, 1H), 1.57 - 1.54 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 172.4, 165.2, 156.9, 147.6, 138.62, 138.57, 136.9, 136.8, 133.3, 133.0, 132.2, 132.1, 130.2, 129.1, 128.6, 128.5, 128.23, 128.20, 127.9, 126.7, 125.7, 125.2, 123.7, 123.2, 111.7, 108.7, 51.2, 46.9, 46.7, 45.4, 39.7, 39.4, 39.2, 33.8, 18.8, 10.6.

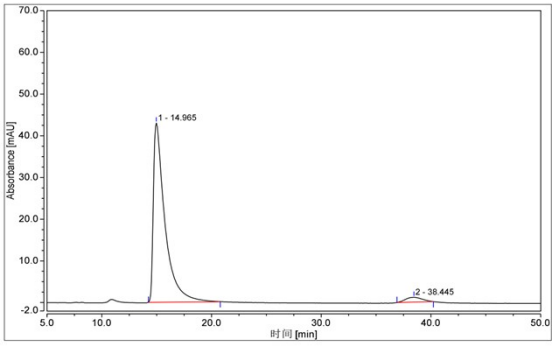
HRMS (ESI): Calculated for $[C_{38}H_{34}N_3O_4, M+H]^+$: 596.2544; Found: 596.2563.

Optical Rotation: $[\alpha]^{25}_D$ = –69.0° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2919, 1738, 1706, 1438, 1243, 1200, 1075, 814, 763, 700, 627, 472.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 14.965 min (major) and 38.445 min (minor). 93% ee.

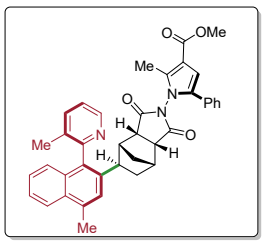




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	15.170	9.582	7.149	49.95	62.53
2	37.335	9.600	4.284	50.05	37.47

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	14.965	52.543	42.981	96.27	97.38
2	38.445	2.037	1.155	3.73	2.62

methyl 2-methyl-1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(4-methyl-1-(3-methylpyridin-2-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (5o)



47% yield, white solid, **m.p.** = 130–132 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.56 (d, *J* = 6.7 Hz, 1H), 7.99 - 7.97 (m, 1H), 7.71 - 7.69 (m, 1H), 7.46 - 7.43 (m, 1H), 7.37 (s, 1H), 7.31 - 7.26 (m, 6H), 7.15 - 7.13 (m, 2H),

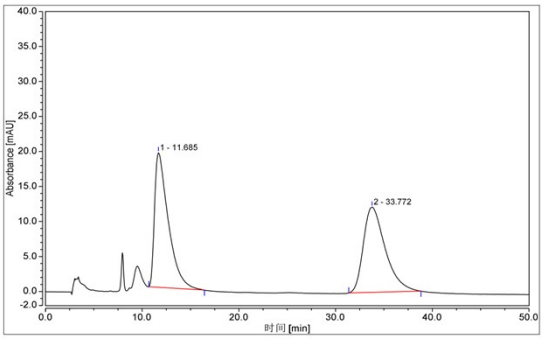
6.90 - 6.88 (m, 1H), 6.66 (s, 1H), 3.87 (s, 3H), 3.09 - 3.06 (m, 1H), 3.00 - 2.97 (m, 2H), 2.94 - 2.91 (m, 1H), 2.78 - 2.77 (m, 1H), 2.75 (s, 3H), 2.33 - 2.31 (m, 1H), 2.25 - 2.21 (m, 1H), 2.18 (s, 3H), 1.95 (s, 3H), 1.80 - 1.75 (m, 1H), 1.58 - 1.56 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 172.4, 165.2, 157.3, 147.7, 138.4, 138.0, 136.8, 135.4, 134.7, 133.4, 133.0, 132.2, 131.4, 130.2, 128.6, 128.2, 126.3, 125.8, 125.5, 124.5, 124.1, 123.0, 111.7, 108.6, 51.2, 46.9, 46.8, 45.4, 39.8, 39.3, 39.2, 33.7, 20.1, 18.9, 10.6.

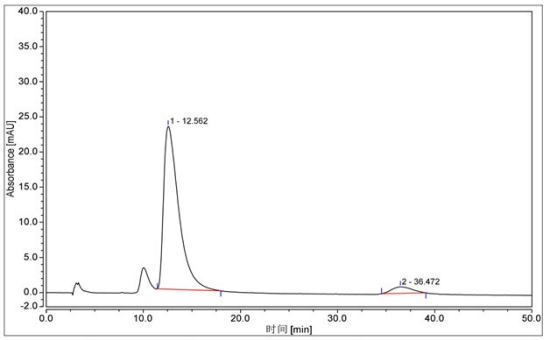
HRMS (ESI): Calculated for $[C_{39}H_{36}N_3O_4, M+H]^+$: 610.2700; Found: 610.2708.

Optical Rotation: $[\alpha]^{25}_D$ = –61.5° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2917, 1737, 1705, 1438, 1397, 1242, 1199, 1167, 1074, 796, 755, 700, 663.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 12.562 min (major) and 36.472 min (minor). 90% ee.

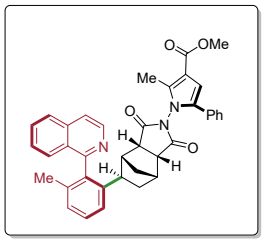




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	11.685	31.573	19.241	49.69	61.22
2	33.772	31.972	12.190	50.31	38.78

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.562	41.722	23.190	94.98	96.14
2	36.472	2.205	0.930	5.02	3.86

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(2-(isoquinolin-1-yl)-3-methylphenyl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5p)



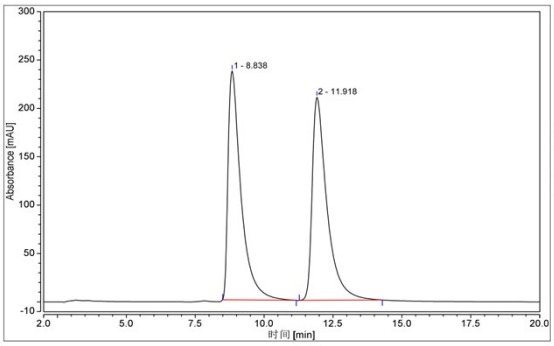
56% yield, white solid, **m.p.** = 92–94 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.8 Hz, 1H), 7.98 - 7.96 (m, 1H), 7.74 - 7.70 (m, 2H), 7.49 - 7.43 (m, 2H), 7.38 - 7.35 (m, 1H), 7.29 - 7.27 (m, 1H), 7.20 - 7.19 (m, 4H), 7.04 - 7.02 (m, 2H), 6.60 (s, 1H), 3.86 (s, 3H), 2.95 - 2.92 (m, 1H), 2.86 - 2.80 (m, 2H), 2.70 - 2.67 (m, 1H), 2.60 - 2.59 (m, 1H), 2.19 - 2.12 (m, 2H), 1.89 (s, 3H), 1.71 (s, 3H), 1.61 - 1.56 (m, 1H), 1.42 - 1.40 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3, 171.9, 165.1, 160.2, 142.5, 142.1, 138.8, 137.6, 136.9, 136.8, 132.8, 130.4, 130.1, 128.53, 128.48, 128.3, 128.1, 127.9, 127.61, 127.57, 126.2, 123.6, 120.7, 111.6, 108.6, 51.1, 46.6, 46.4, 45.2, 39.2, 39.11, 39.07, 33.4, 20.0, 9.9.

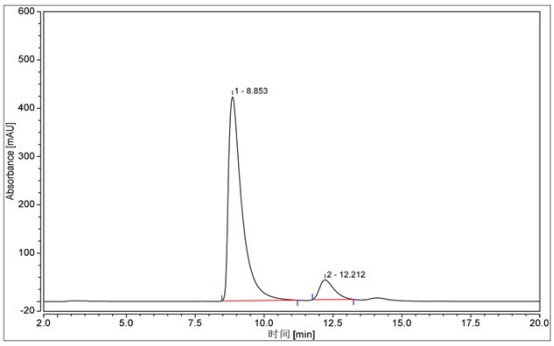
HRMS (ESI): Calculated for $[C_{38}H_{34}N_3O_4, M+H]^+$: 596.2544; Found: 596.2551.

Optical Rotation: $[\alpha]^{25}_D$ = –123.3° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1738, 1706, 1438, 1397, 1242, 1199, 1166, 1073, 825, 759, 700, 647, 593.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 8.853 min (major) and 12.212 min (minor). 81% ee.

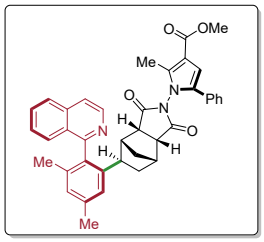




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.838	129.041	236.657	49.74	52.98
2	11.918	130.414	210.023	50.26	47.02

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.853	238.914	423.271	90.52	91.21
2	12.212	25.014	40.776	9.48	8.79

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(2-(isoquinolin-1-yl)-3,5-dimethylphenyl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5q)



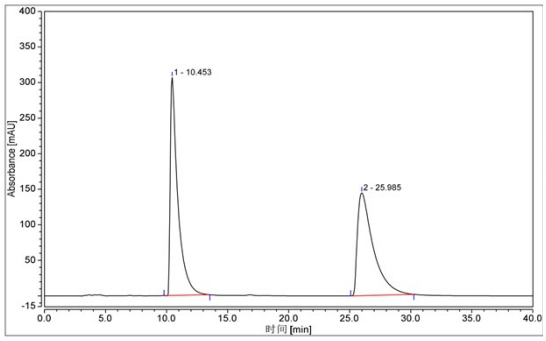
84% yield, white solid, **m.p.** = 136–138 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.57 (d, *J* = 5.8 Hz, 1H), 7.96 - 7.94 (m, 1H), 7.71 - 7.68 (m, 2H), 7.46 - 7.45 (m, 2H), 7.19 - 7.18 (m, 3H), 7.07 - 7.01 (m, 4H), 6.60 (s, 1H), 3.86 (s, 3H), 2.93 - 2.90 (m, 1H), 2.85 - 2.79 (m, 2H), 2.69 - 2.65 (m, 1H), 2.59 - 2.58 (m, 1H), 2.41 (s, 3H), 2.18 - 2.12 (m, 2H), 1.90 (s, 3H), 1.67 (s, 3H), 1.60 - 1.55 (m, 1H), 1.41 - 1.39 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 171.9, 165.1, 160.4, 142.5, 142.0, 137.7, 137.4, 136.9, 136.8, 136.0, 132.8, 130.3, 130.1, 129.2, 128.5, 128.11, 128.05, 127.52, 127.49, 126.3, 124.3, 120.6, 111.6, 108.6, 51.1, 46.6, 46.4, 45.2, 39.1, 33.3, 21.7, 19.9, 9.9.

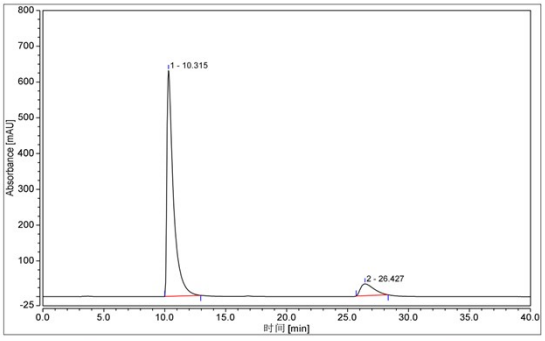
HRMS (ESI): Calculated for $[C_{39}H_{36}N_3O_4, M+H]^+$: 610.2700; Found: 610.2714.

Optical Rotation: $[\alpha]^{25}_D$ = –96.4° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1738, 1706, 1438, 1396, 1242, 1199, 1166, 1073, 824, 760, 699.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 10.315 min (major) and 26.427 min (minor). 80% ee.

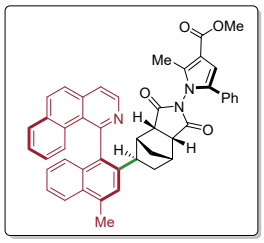




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	10.453	219.468	306.395	50.43	67.95
2	25.985	215.688	144.532	49.57	32.05

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	10.315	392.033	631.237	90.24	95.01
2	26.427	42.407	33.140	9.76	4.99

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(benzo[h]isoquinolin-1-yl)-4-methylnaphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5r)



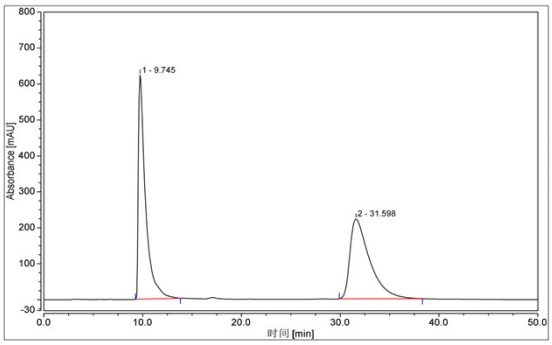
99% yield, white solid, **m.p.** = 138–140 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.82 (d, *J* = 5.3 Hz, 1H), 8.02 - 8.00 (m, 1H), 7.95 - 7.93 (m, 1H), 7.84 - 7.79 (m, 3H), 7.51 (s, 1H), 7.38 - 7.30 (m, 3H), 7.13 - 7.12 (m, 3H), 7.06 - 7.03 (m, 1H), 6.99 - 6.95 (m, 3H), 6.78 - 6.76 (m, 1H), 6.60 (s, 1H), 3.85 (s, 3H), 3.19 - 3.16 (m, 1H), 2.91 - 2.89 (m, 1H), 2.85 (s, 3H), 2.78 - 2.75 (m, 1H), 2.49 - 2.46 (m, 2H), 2.38 - 2.35 (m, 1H), 2.25 - 2.22 (m, 1H), 2.09 (s, 3H), 1.76 - 1.71 (m, 1H), 1.33 - 1.31 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 171.7, 165.2, 156.7, 144.4, 139.0, 138.8, 136.8, 135.1, 133.4, 133.0, 132.5, 132.1, 132.0, 130.1, 129.3, 129.2, 128.5, 128.04, 128.00, 127.1, 126.8, 126.52, 126.45, 126.4, 126.1, 125.9, 125.6, 124.1, 122.2, 111.7, 108.6, 51.2, 46.61, 46.58, 44.6, 39.7, 39.2, 39.1, 32.7, 20.3, 10.3.

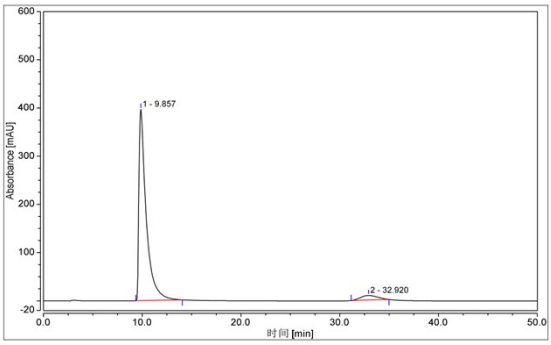
HRMS (ESI): Calculated for $[C_{46}H_{38}N_3O_4, M+H]^+$: 696.2857; Found: 696.2872.

Optical Rotation: $[\alpha]^{25}_D$ = –93.3° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2349, 1738, 1705, 1438, 1241, 1198, 1166, 1073, 855, 750, 699, 497.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 9.857 min (major) and 32.920 min (minor). 89% ee.

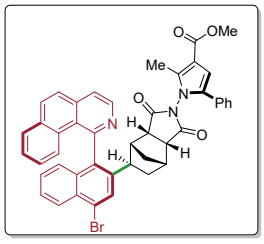




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.745	524.434	622.339	50.60	73.74
2	31.598	512.069	221.622	49.40	26.26

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.857	339.929	396.844	94.70	97.66
2	32.920	19.041	9.498	5.30	2.34

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(1-(benzo[h]isoquinolin-1-yl)-4-bromonaphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5s)



99% yield, white solid, **m.p.** = 149–151 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.82 (d, *J* = 5.2 Hz, 1H), 8.28 - 8.26 (m, 1H), 8.00 - 7.97 (m, 2H), 7.87 - 7.82 (m, 3H), 7.46 - 7.43 (m, 1H), 7.40 - 7.37 (m, 1H), 7.29 - 7.28

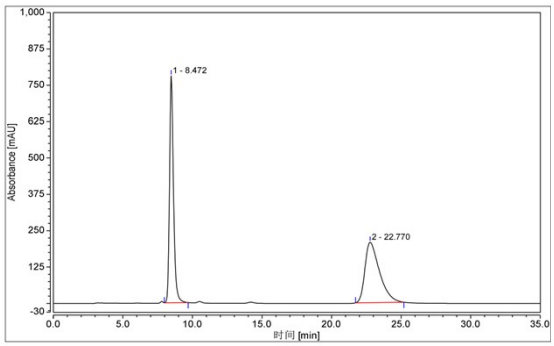
(m, 1H), 7.15 - 7.09 (m, 4H), 7.04 - 7.01 (m, 1H), 7.00 - 6.97 (m, 2H), 6.77 - 6.75 (m, 1H), 6.60 - 6.59 (m, 1H), 3.86 (s, 3H), 3.18 - 3.15 (m, 1H), 2.93 - 2.91 (m, 1H), 2.80 - 2.77 (m, 1H), 2.52 - 2.50 (m, 2H), 2.33 - 2.28 (m, 1H), 2.19 - 2.17 (m, 1H), 2.051 - 2.047 (m, 3H), 1.77 - 1.73 (m, 1H), 1.38 - 1.36 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.2, 171.5, 165.2, 155.4, 144.5, 140.8, 138.9, 138.4, 136.7, 133.5, 133.1, 133.0, 132.7, 131.3, 130.0, 129.5, 129.0, 128.9, 128.5, 128.1, 128.0, 127.8, 127.5, 127.4, 127.2, 127.0, 126.4, 126.2, 126.0, 125.6, 123.8, 122.5, 111.7, 108.6, 51.2, 46.5, 44.5, 39.6, 39.2, 39.0, 32.9, 10.2.

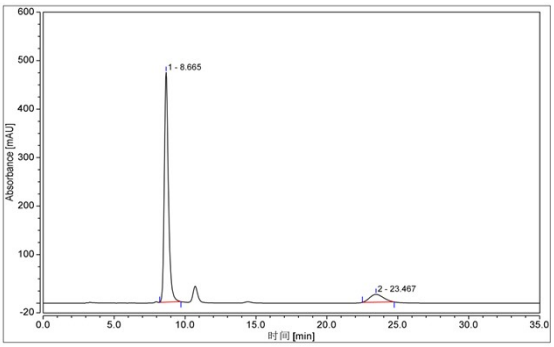
HRMS (ESI): Calculated for $[C_{45}H_{35}BrN_3O_4, M+H]^+$: 760.1805; Found: 760.1810.

Optical Rotation: $[\alpha]^{25}_D$ = –85.9° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 3853, 3735, 3649, 3629, 2361, 2341, 1698, 1653, 1558, 1507, 1541, 1457.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 8.665 min (major) and 23.467 min (minor). 80% ee.

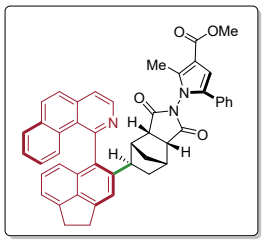




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.472	257.079	779.929	50.55	78.95
2	22.770	251.520	207.899	49.45	21.05

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.665	157.865	473.611	89.81	96.73
2	23.467	17.902	16.026	10.19	3.27

methyl 1-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-5-(5-(benzo[h]isoquinolin-1-yl)-1,2-dihydroacenaphthylen-4-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5t)



99% yield, white solid, **m.p.** = 143–145 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.80 (d, *J* = 5.3 Hz, 1H), 7.95 - 7.93 (m, 1H), 7.83 - 7.79 (m, 3H), 7.51 (s, 1H), 7.47 - 7.45 (m, 1H), 7.36 - 7.33 (m, 1H), 7.14 - 7.12 (m, 4H), 7.03 - 6.97 (m, 4H), 6.60 (s, 1H), 6.43 - 6.41 (m, 1H), 3.85 (s, 3H), 3.55 - 3.35 (m, 5H), 2.91 - 2.89 (m, 1H), 2.80 - 2.76 (m, 1H), 2.57 - 2.50 (m, 2H), 2.41 - 2.37 (m, 1H), 2.26 - 2.24 (m, 1H), 2.10 (s, 3H), 1.79 - 1.74 (m, 1H), 1.35 - 1.33 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.5, 171.8, 165.2, 156.4, 146.7, 145.7, 144.5, 139.3, 138.7, 138.5, 136.9, 133.4, 133.0, 132.4, 130.1, 129.4, 129.3, 128.7, 128.5, 128.03, 128.01, 127.1, 126.7, 126.4, 126.2, 125.9, 122.0, 120.5, 119.6, 118.2, 111.7, 108.6, 51.2, 46.7, 46.6, 44.8, 40.1, 39.2, 39.1, 32.9, 30.7, 30.6, 10.2.

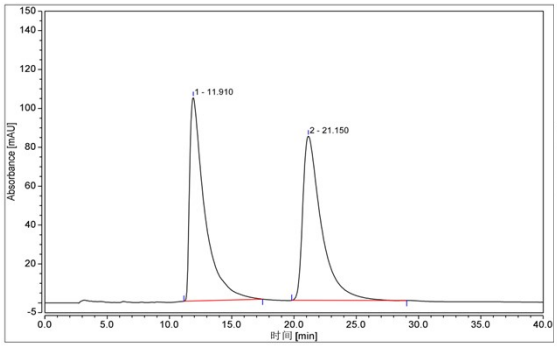
HRMS (ESI): Calculated for $[C_{47}H_{38}N_3O_4, M+H]^+$: 708.2857; Found: 708.2887.

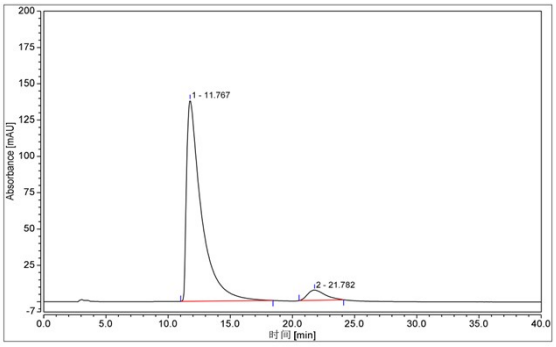
Optical Rotation: $[\alpha]^{25}_D$ = –89.6° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 3853, 3735, 3649, 2361, 2341,1699, 1558, 1541, 1508, 1457, 750, 699.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 11.767

min (major) and 21.782 min (minor). 89% ee.

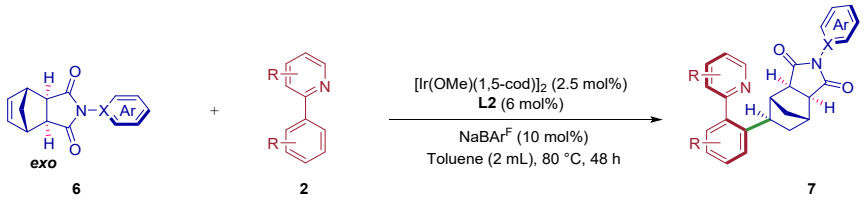




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	11.910	147.160	104.713	50.29	55.34
2	21.150	145.443	84.520	49.71	44.66

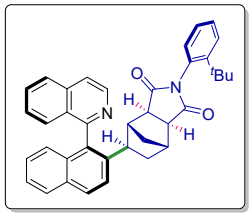
peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	11.767	191.591	138.301	94.33	95.15
2	21.782	11.525	7.048	5.67	4.85

3. Construction of exo-atropisomers 7:



General procedure G: To an oven-dried 10 mL Schlenk tube containing a stirring bar was charged with $[Ir(OMe)(1,5\text{-cod})]_2$ (0.0025 mmol, 1.7 mg), **L2** (0.006 mmol, 4.1 mg) and 1.0 mL dry toluene in a nitrogen-filled glove-box, the mixture was stirred for 10 min at room temperature. Then corresponding substrate **6** (0.1 mmol, 1.0 equiv.), corresponding substrate **2** (0.12 mmol, 1.2 equiv.), $NaBAr^F$ (0.01 mmol, 8.9 mg) and another 1.0 mL dry toluene were added sequentially. The mixture was stirred at 80 °C for 48 hours, concentrated to dryness and the crude mixture was purified by flash column chromatography on silica gel using a mixture of Hexane/EtOAc (3/1, v/v) as eluent to obtain the desired product.

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (7a)



95% yield, white solid, **m.p.** = 157–159 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 5.8 Hz, 1H), 8.01 - 7.99 (m, 1H), 7.98 - 7.96 (m, 1H), 7.91 - 7.89 (m, 1H), 7.81 - 7.80 (m, 1H), 7.74 - 7.71 (m, 1H), 7.63 - 7.61 (m, 1H), 7.53 - 7.52 (m, 1H), 7.47 - 7.35 (m, 4H), 7.28 - 7.26 (m, 1H), 7.24 - 7.21 (m, 1H), 6.91 - 6.89 (m, 1H), 6.78 - 6.76 (m, 1H), 3.13 (s, 1H), 2.88 - 2.87 (m, 1H), 2.61 - 2.59 (m, 1H), 2.50 - 2.47 (m, 1H), 2.30 - 2.28 (m, 1H), 1.99 - 1.96 (m, 1H), 1.89 - 1.84 (m, 1H), 1.51 - 1.46 (m, 2H), 1.18 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.8, 178.5, 160.2, 147.8, 142.5, 140.8, 136.3, 135.0, 133.0, 132.1, 130.74, 130.68, 130.4, 129.8, 129.2, 128.7, 128.4, 128.1, 127.9, 127.4, 127.1, 126.9, 126.6, 125.8, 125.6, 122.8, 120.5, 49.8, 48.3, 44.9,

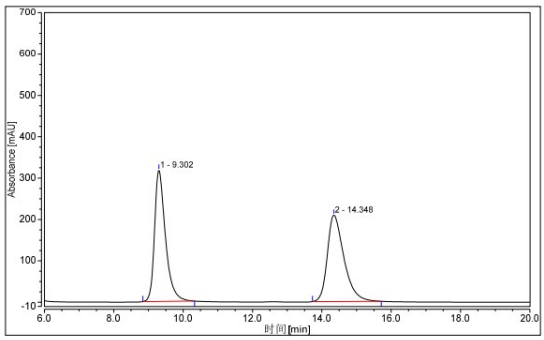
43.5, 40.8, 39.6, 35.5, 33.4, 31.5.

HRMS (ESI): Calculated for $[C_{38}H_{34}N_2NaO_2, M+Na]^+$: 573.2512; Found: 573.2521.

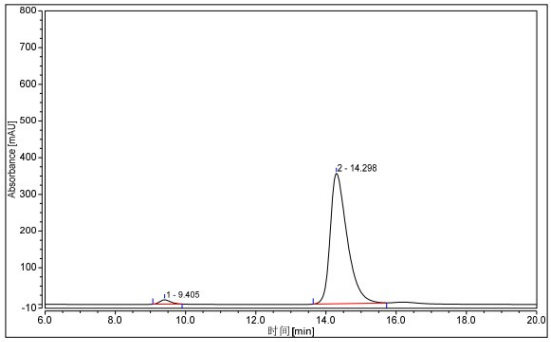
Optical Rotation: $[\alpha]^{25}_D$ = –12.3 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2963, 1710, 1492, 1442, 1371, 1182, 810, 751, 691, 624, 463.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 14.298 min (major) and 9.405 min (minor). 96% ee.

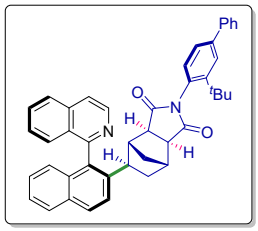


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.302	115.621	317.310	49.96	60.31
2	14.348	115.786	208.821	50.04	39.69



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.405	4.148	11.554	2.05	3.15
2	14.298	198.629	355.131	97.95	96.85

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(3-(*tert*-butyl)-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1H-4,7-methanoisoindole-1,3(2*H*)-dione (7b)



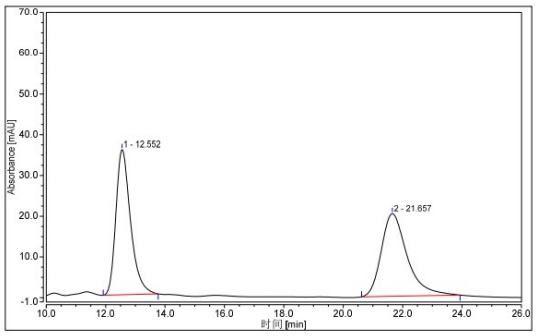
90% yield, white solid, **m.p.** = 146–148 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.74 (d, *J* = 5.8 Hz, 1H), 8.00 - 7.99 (m, 1H), 7.96 - 7.94 (m, 1H), 7.89 - 7.88 (m, 1H), 7.80 - 7.79 (m, 1H), 7.72 - 7.69 (m, 2H), 7.64 - 7.62 (m, 1H), 7.54 - 7.52 (m, 2H), 7.46 - 7.38 (m, 6H), 7.36 - 7.33 (m, 1H), 7.22 - 7.20 (m, 1H), 6.92 - 6.90 (m, 1H), 6.86 - 6.84 (m, 1H), 3.14 (s, 1H), 2.90 - 2.89 (m, 1H), 2.62 - 2.60 (m, 1H), 2.52 - 2.49 (m, 1H), 2.30 - 2.28 (m, 1H), 2.00 - 1.98 (m, 1H), 1.91 - 1.86 (m, 1H), 1.53 - 1.48 (m, 2H), 1.23 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.9, 178.6, 160.2, 148.0, 142.8, 142.5, 140.80, 140.76, 136.3, 135.1, 133.0, 132.1, 130.8, 130.7, 129.8, 129.2, 128.8, 128.4, 128.1, 127.95, 127.89, 127.7, 127.4, 127.1, 126.9, 126.6, 126.3, 125.9, 125.6, 122.8, 120.5, 49.8, 48.4, 44.9, 43.5, 40.8, 39.6, 35.7, 33.5, 31.6.

HRMS (ESI): Calculated for $[C_{44}H_{39}N_2O_2, M+H]^+$: 627.3006; Found: 627.3012.

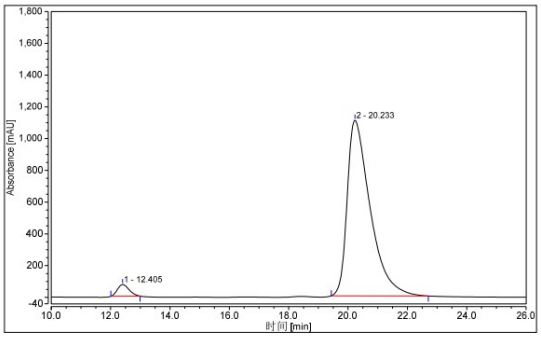
Optical Rotation: $[\alpha]^{25}_D$ = 12.2 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1710, 1483, 1367, 1179, 807, 749, 696, 621.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 20.233 min (major) and 12.405 min (minor). 93% ee.

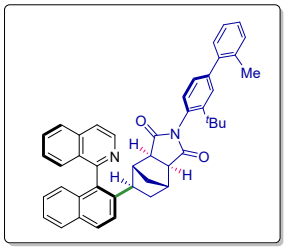


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.552	20.405	35.654	49.93	63.73
2	21.657	20.466	20.290	50.07	36.27



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.405	33.464	73.514	3.27	6.23
2	20.233	990.717	1106.253	96.73	93.77

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(3-(*tert*-butyl)-2'-methyl-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (7c)



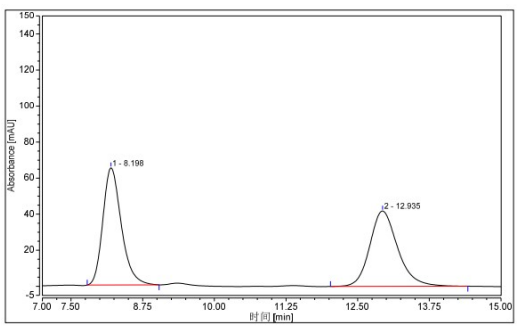
95% yield, white solid, **m.p.** = 135–137 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.75 (d, *J* = 5.8 Hz, 1H), 8.01 - 7.99 (m, 1H), 7.97 - 7.95 (m, 1H), 7.90 - 7.88 (m, 1H), 7.80 - 7.79 (m, 1H), 7.73 - 7.70 (m, 1H), 7.64 - 7.62 (m, 1H), 7.471 - 7.467 (m, 1H), 7.45 - 7.42 (m, 1H), 7.41 - 7.39 (m, 2H), 7.26 - 7.25 (m, 2H), 7.24 - 7.20 (m, 4H), 6.93 - 6.91 (m, 1H), 6.82 - 6.81 (m, 1H), 3.12 (s, 1H), 2.90 - 2.89 (m, 1H), 2.62 - 2.61 (m, 1H), 2.53 - 2.50 (m, 1H), 2.28 - 2.27 (m, 4H), 1.99 - 1.97 (m, 1H), 1.92 - 1.87 (m, 1H), 1.54 - 1.48 (m, 2H), 1.20 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 179.0, 178.6, 160.2, 147.4, 143.1, 142.6, 141.2, 140.7, 136.3, 135.4, 135.1, 133.0, 132.1, 130.7, 130.5, 130.1, 129.94, 129.85, 129.3, 129.2, 128.4, 128.14, 128.06, 127.9, 127.6, 127.1, 126.9, 126.6, 125.90, 125.86, 125.6, 122.8, 120.4, 49.8, 48.3, 45.0, 43.5, 40.8, 39.6, 35.7, 33.4, 31.6, 20.6.

HRMS (ESI): Calculated for $[C_{45}H_{40}N_2NaO_2, M+Na]^+$: 663.2982; Found: 663.2987.

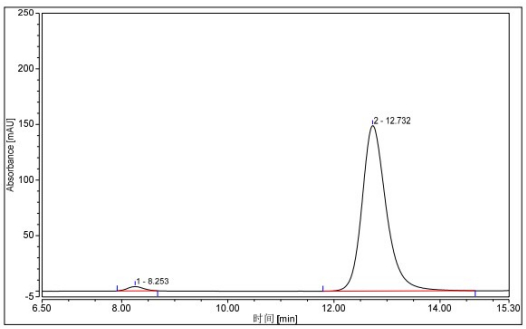
Optical Rotation: $[\alpha]^{25}_D$ = 7.9 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1710, 1481, 1392, 1367, 955, 807, 748, 694, 623, 442.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 12.732 min (major) and 8.253 min (minor). 97% ee.

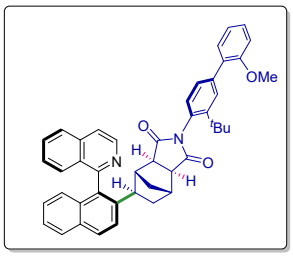


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.198	24.306	65.012	50.64	60.85
2	12.935	23.694	41.829	49.36	39.15



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.253	1.337	3.847	1.67	2.52
2	12.732	78.857	148.749	98.33	97.48

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(3-(*tert*-butyl)-2'-methoxy-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (7d)



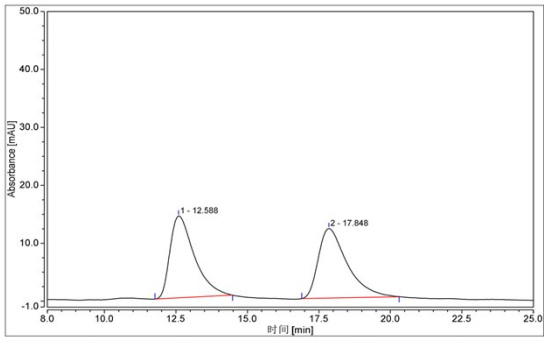
93% yield, white solid, **m.p.** = 126–128 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.75 (d, *J* = 5.7 Hz, 1H), 8.01 - 7.99 (m, 1H), 7.98 - 7.96 (m, 1H), 7.91 - 7.89 (m, 1H), 7.81 - 7.80 (m, 1H), 7.74 - 7.71 (m, 1H), 7.67 - 7.66 (m, 1H), 7.64 - 7.62 (m, 1H), 7.47 - 7.44 (m, 1H), 7.43 - 7.38 (m, 3H), 7.34 - 7.28 (m, 2H), 7.24 - 7.21 (m, 1H), 7.03 - 7.00 (m, 1H), 6.98 - 6.96 (m, 1H), 6.92 - 6.90 (m, 1H), 6.79 - 6.78 (m, 1H), 3.78 (s, 3H), 3.12 (s, 1H), 2.89 - 2.88 (m, 1H), 2.61 - 2.60 (m, 1H), 2.52 - 2.48 (m, 1H), 2.29 - 2.27 (m, 1H), 1.99 - 1.96 (m, 1H), 1.90 - 1.86 (m, 1H), 1.53 - 1.48 (m, 2H), 1.21 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.9, 178.6, 160.2, 148.0, 142.8, 142.5, 140.80, 140.76, 136.3, 135.1, 133.0, 132.1, 130.8, 130.7, 129.8, 129.2, 128.8, 128.4, 128.1, 127.95, 127.89, 127.7, 127.4, 127.1, 126.9, 126.6, 126.3, 125.9, 125.6, 122.8, 120.5, 49.8, 48.4, 44.9, 43.5, 40.8, 39.6, 35.7, 33.5, 31.6.

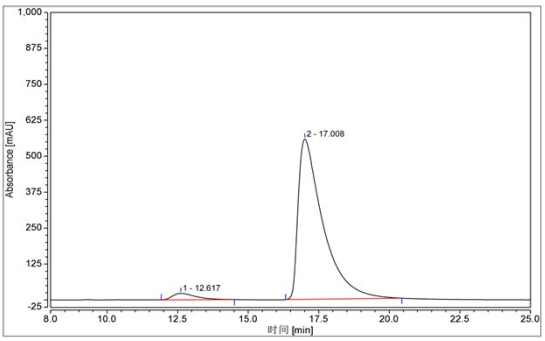
HRMS (ESI): Calculated for $[C_{45}H_{40}N_2NaO_3, M+Na]^+$: 679.2931; Found: 679.2937.

Optical Rotation: $[\alpha]^{25}_D$ = 11.5 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2921, 1709, 1483, 1393, 1367, 1259, 1181, 1019, 805, 749, 694, 442.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 17.008 min (major) and 12.617 min (minor). 93% ee.

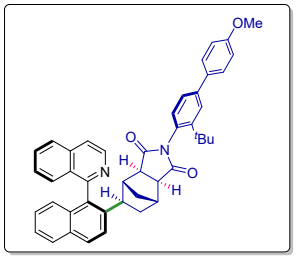




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.588	13.980	14.131	49.89	54.08
2	17.848	14.043	12.000	50.11	45.92

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.617	21.323	22.374	3.62	3.86
2	17.008	567.829	557.255	96.38	96.14

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(3-(tert-butyl)-4'-methoxy-[1,1'-biphenyl]-4-yl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (7e)



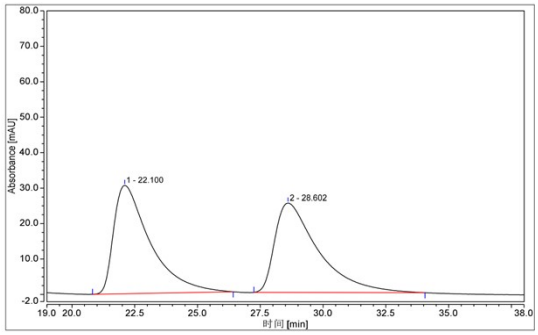
93% yield, white solid, **m.p.** = 139–141 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.74 (d, *J* = 5.7 Hz, 1H), 8.00 - 7.99 (m, 1H), 7.96 - 7.94 (m, 1H), 7.89 - 7.88 (m, 1H), 7.80 - 7.79 (m, 1H), 7.72 - 7.69 (m, 1H), 7.66 - 7.62 (m, 2H), 7.47 - 7.39 (m, 6H), 7.23 - 7.20 (m, 1H), 6.97 - 6.95 (m, 2H), 6.92 - 6.90 (m, 1H), 6.83 - 6.81 (m, 1H), 3.82 (s, 3H), 3.14 (s, 1H), 2.89 - 2.88 (m, 1H), 2.62 - 2.60 (m, 1H), 2.52 - 2.49 (m, 1H), 2.30 - 2.28 (m, 1H), 2.00 - 1.97 (m, 1H), 1.90 - 1.86 (m, 1H), 1.53 - 1.48 (m, 2H), 1.22 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.9, 178.6, 160.2, 159.5, 147.9, 142.6, 142.4, 140.8, 136.3, 135.1, 133.3, 133.0, 132.1, 130.7, 129.23, 129.20, 128.45, 128.41, 128.1, 127.9, 127.5, 127.1, 126.9, 126.6, 125.94, 125.85, 125.6, 122.8, 120.4, 114.3, 55.4, 49.8, 48.3, 44.9, 43.5, 40.8, 39.7, 35.6, 33.5, 31.6.

HRMS (ESI): Calculated for $[C_{45}H_{40}N_2NaO_3, M+Na]^+$: 679.2931; Found: 679.2939.

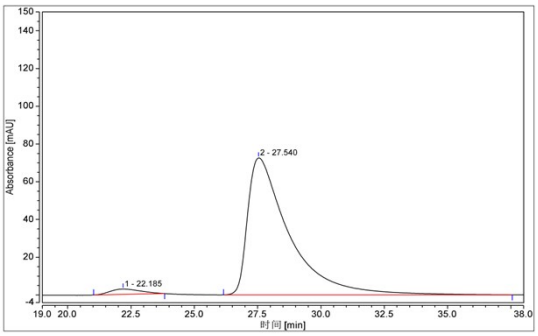
Optical Rotation: $[\alpha]^{25}_D$ = 16.3 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2921, 1709, 1491, 1368, 1247, 1178, 1027, 806, 748, 623, 441.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 27.250 min (major) and 22.185 min (minor). 94% ee.

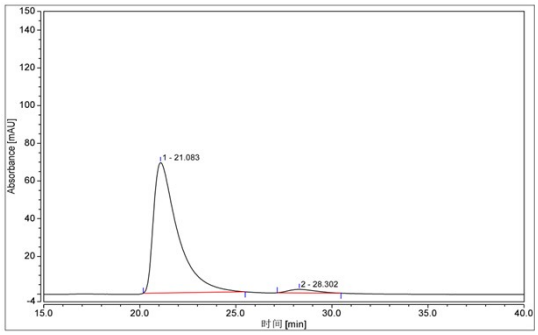


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	22.100	51.392	30.576	50.45	54.81
2	28.602	50.479	25.209	49.55	45.19



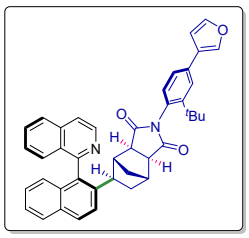
peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	22.185	3.971	2.829	2.80	3.75
2	27.540	137.790	72.560	97.20	96.25

(*ent*)-**7e**: 94% ee



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	21.083	100.640	69.170	97.07	97.38
2	28.302	3.034	1.858	2.93	2.62

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(2-(*tert*-butyl)-4-(furan-3-yl)phenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (7f)



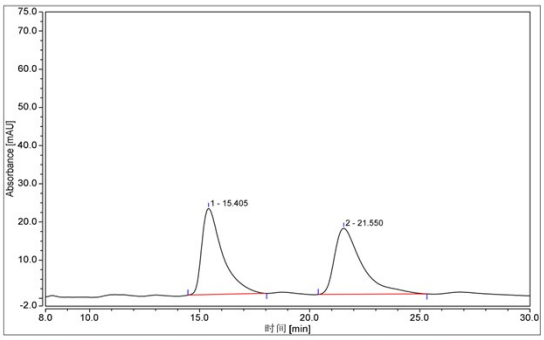
99% yield, white solid, **m.p.** = 153–155 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.74 (d, *J* = 5.7 Hz, 1H), 8.01 - 7.99 (m, 1H), 7.97 - 7.95 (m, 1H), 7.90 - 7.88 (m, 1H), 7.832 - 7.828 (m, 1H), 7.80 - 7.79 (m, 1H), 7.73 - 7.70 (m, 1H), 7.63 - 7.61 (m, 1H), 7.54 - 7.52 (m, 1H), 7.46 - 7.38 (m, 4H), 7.24 - 7.21 (m, 1H), 6.92 - 6.90 (m, 1H), 6.79 - 6.77 (m, 1H), 6.654 - 6.648 (m, 1H), 6.46 - 6.45 (m, 1H), 3.12 (s, 1H), 2.88 - 2.87 (m, 1H), 2.60 - 2.59 (m, 1H), 2.51 - 2.48 (m, 1H), 2.28 - 2.27 (m, 1H), 1.99 - 1.97 (m, 1H), 1.90 - 1.85 (m, 1H), 1.52 - 1.46 (m, 2H), 1.22 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.8, 178.4, 160.2, 153.3, 148.2, 142.5, 140.7, 136.3, 135.0, 133.0, 132.1, 130.8, 130.7, 129.6, 129.2, 128.4, 128.1, 127.9, 127.1, 126.9, 126.5, 125.8, 125.5, 124.1, 122.9, 122.8, 120.4, 111.8, 106.0, 49.8, 48.3, 44.9, 43.4, 40.7, 39.6, 35.6, 33.4, 31.5.

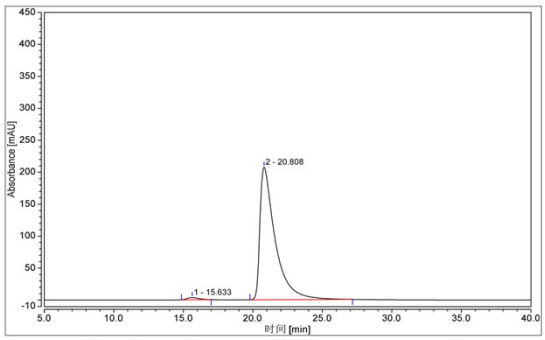
HRMS (ESI): Calculated for $[C_{42}H_{36}N_2NaO_3, M+Na]^+$: 639.2618; Found: 639.2624.

Optical Rotation: $[\alpha]^{25}_D$ = 23.4 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1711, 1376, 1180, 1013, 806, 747, 695, 623, 591, 490, 444.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 20.808 min (major) and 15.633 min (minor). 97% ee.

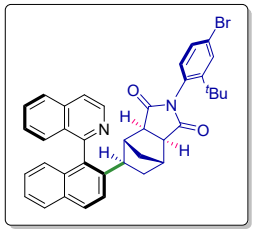




peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	15.405	24.631	22.556	49.75	56.60
2	21.550	24.876	17.297	50.25	43.40

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	15.633	3.362	3.408	1.26	1.62
2	20.808	264.092	207.494	98.74	98.38

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(4-bromo-2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (7g)



43% yield, white solid, **m.p.** = 143–145 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.74 (d, *J* = 5.8 Hz, 1H), 8.01 - 7.99 (m, 1H), 7.97 - 7.96 (m, 1H), 7.90 - 7.88 (m, 1H), 7.81 - 7.80 (m, 1H), 7.74 - 7.70 (m, 1H), 7.64 -

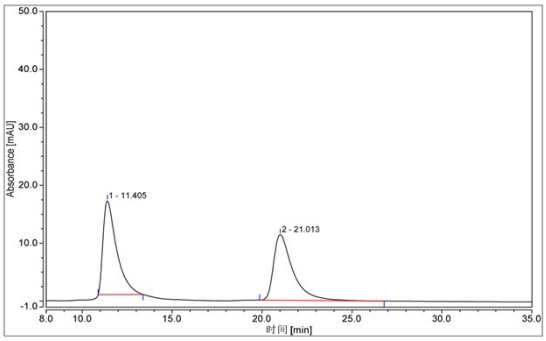
7.63 (m, 1H), 7.62 - 7.60 (m, 1H), 7.46 - 7.37 (m, 4H), 7.24 - 7.21 (m, 1H), 6.91 - 6.89 (m, 1H), 6.64 - 6.63 (m, 1H), 3.09 (s, 1H), 2.87 - 2.86 (m, 1H), 2.60 - 2.58 (m, 1H), 2.49 - 2.46 (m, 1H), 2.26 - 2.25 (m, 1H), 1.99 - 1.96 (m, 1H), 1.90 - 1.85 (m, 1H), 1.51 - 1.47 (m, 1H), 1.42 - 1.40 (m, 1H), 1.16 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.5, 178.2, 160.1, 150.1, 142.4, 140.6, 136.3, 134.9, 133.0, 132.1, 132.0, 130.8, 130.6, 129.9, 129.2, 128.4, 128.1, 127.9, 127.1, 126.9, 126.6, 125.8, 125.6, 124.1, 122.7, 120.5, 49.8, 48.3, 44.9, 43.4, 40.7, 39.5, 35.7, 33.4, 31.3.

HRMS (ESI): Calculated for $[C_{38}H_{33}BrN_2NaO_2, M+Na]^+$: 651.1618; Found: 651.1627.

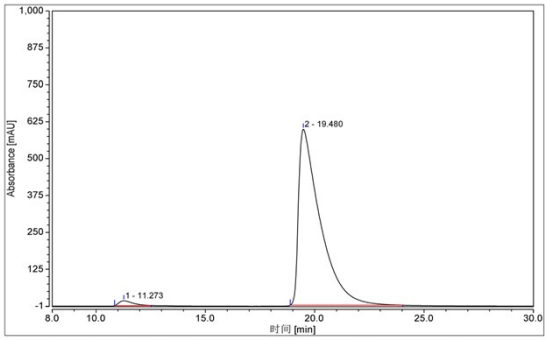
Optical Rotation: $[\alpha]^{25}_D$ = 5.8 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1711, 1484, 1390, 1365, 1178, 804, 747, 694, 622, 589, 492.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 19.480 min (major) and 11.273 min (minor). 96% ee.

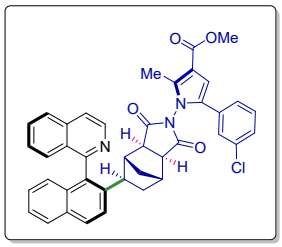


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	11.405	14.204	16.207	50.39	58.87
2	21.013	13.982	11.324	49.61	41.13



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	11.273	11.729	16.338	1.69	2.67
2	19.480	681.946	596.504	98.31	97.33

methyl 5-(3-chlorophenyl)-1-((3a*R*,4*R*,5*R*,7*S*,7a*S*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-1*H*-pyrrole-3-carboxylate (7h)



83% yield, white solid, **m.p.** = 165–167 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.72 (d, *J* = 5.8 Hz, 1H), 7.99 - 7.94 (m, 2H), 7.89 - 7.87 (m, 1H), 7.79 - 7.78 (m, 1H), 7.72 - 7.69 (m, 1H), 7.58 - 7.56 (m, 1H), 7.44 - 7.39 (m, 2H), 7.36 - 7.34 (m, 1H), 7.23 - 7.19 (m, 2H), 7.17 - 7.12 (m, 2H), 6.98 - 6.97 (m, 1H), 6.91 - 6.89 (m, 1H), 6.67 (s, 1H), 3.80 (s, 3H), 2.99 (s, 1H), 2.83 - 2.82 (m, 1H), 2.47 - 2.43 (m, 2H), 2.38 (s, 3H), 2.05 - 2.00 (m, 2H), 1.94 - 1.89 (m, 1H), 1.51 - 1.46 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.7, 173.3, 164.8, 160.0, 142.6, 140.0, 137.1, 136.3, 135.2, 134.5, 133.0, 132.2, 131.7, 131.6, 130.7, 129.9, 129.2, 128.4, 128.2, 128.09, 128.06, 127.9, 127.2, 126.8, 126.7, 126.0, 125.9, 125.7, 122.6, 120.5, 112.5, 109.7, 51.2, 47.7, 46.3, 44.3, 43.2, 40.1, 39.2, 33.3, 10.8.

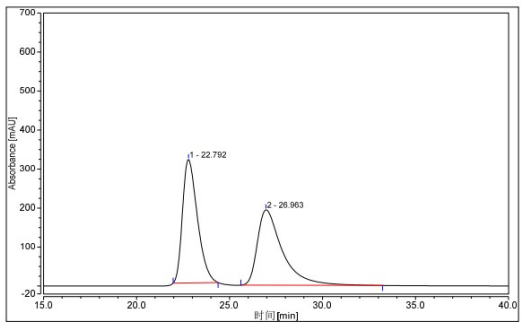
HRMS (ESI): Calculated for $[C_{41}H_{32}ClN_3NaO_4, M+Na]^+$: 688.1974; Found: 688.1984.

Optical Rotation: $[\alpha]^{25}_D$ = –18.9 ° (c = 1.0, $CHCl_3$).

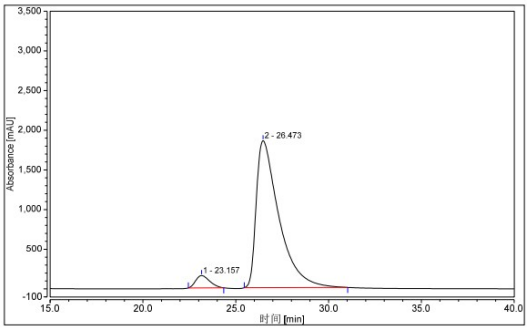
IR (neat, cm^{-1}) = 1738, 1707, 1583, 1438, 1397, 1243, 1200, 1074, 822, 802, 774, 748, 694, 632, 442.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 26.473

min (major) and 23.157 min (minor). 90% ee.

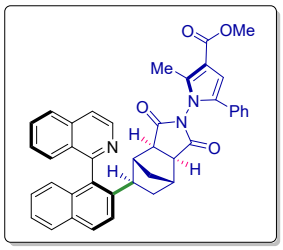


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	22.792	293.893	316.319	49.36	62.08
2	26.963	301.456	193.235	50.64	37.92



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	23.157	134.817	155.066	4.88	7.72
2	26.473	2625.958	1852.535	95.12	92.28

methyl 1-((3a*R*,4*R*,5*R*,7*S*,7a*S*)-5-(1-(isoquinolin-1-yl)naphthalen-2-yl)-1,3-dioxooctahydro-2*H*-4,7-methanoisoindol-2-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (7i)



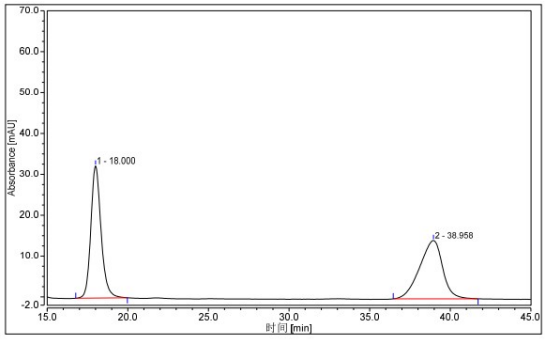
54% yield, white solid, **m.p.** = 157–158 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.71 - 8.70 (m, 1H), 7.98 - 7.92 (m, 2H), 7.88 - 7.86 (m, 1H), 7.77 - 7.76 (m, 1H), 7.70 - 7.67 (m, 1H), 7.58 - 7.56 (m, 1H), 7.42 - 7.37 (m, 2H), 7.34 - 7.32 (m, 1H), 7.22 - 7.18 (m, 4H), 7.12 - 7.10 (m, 2H), 6.88 - 6.87 (m, 1H), 6.65 (s, 1H), 3.79 (s, 3H), 3.01 (s, 1H), 2.81 - 2.80 (m, 1H), 2.46 - 2.41 (m, 2H), 2.39 (s, 3H), 2.05 - 1.99 (m, 2H), 1.91 - 1.87 (m, 1H), 1.53 - 1.50 (m, 1H), 1.47 - 1.43 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.8, 173.4, 165.0, 160.0, 142.6, 140.1, 136.5, 136.3, 135.2, 133.1, 133.0, 132.2, 130.7, 130.0, 129.2, 128.6, 128.4, 128.2, 128.12, 128.06, 127.9, 127.2, 126.8, 126.6, 125.9, 125.7, 122.6, 120.5, 112.3, 108.9, 51.2, 47.7, 46.4, 44.2, 43.3, 40.0, 39.4, 33.3, 10.8.

HRMS (ESI): Calculated for $[C_{41}H_{34}N_3O_4, M+H]^+$: 632.2544; Found: 632.2552.

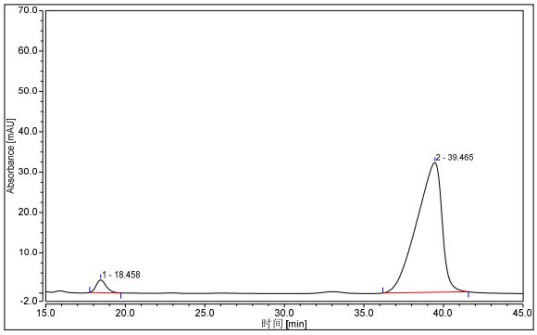
Optical Rotation: $[\alpha]^{25}_D$ = 9.000 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1738, 1704, 1439, 1398, 1241, 1199, 1072, 802, 749, 696, 632, 443.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 39.465 min (major) and 18.458 min (minor). 93% ee.

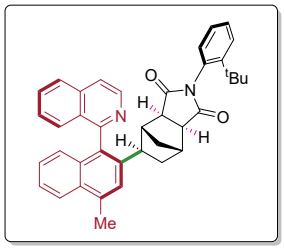


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	18.000	23.819	32.308	50.30	69.38
2	38.958	23.537	14.261	49.70	30.62



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	18.458	2.284	3.151	3.72	8.93
2	39.465	59.184	32.116	96.28	91.07

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)-4-methylnaphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (7j)



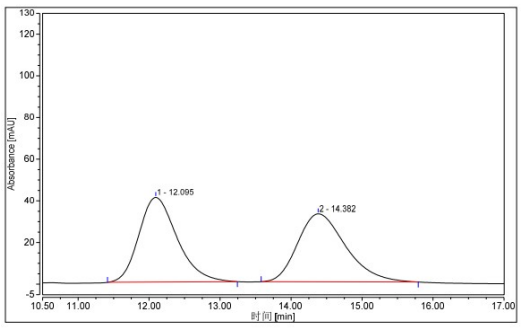
82% yield, white solid, **m.p.** = 133–135 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.73 (d, *J* = 5.8 Hz, 1H), 8.05 - 8.03 (m, 1H), 7.94 - 7.93 (m, 1H), 7.78 - 7.76 (m, 1H), 7.70 - 7.67 (m, 1H), 7.52 - 7.51 (m, 1H), 7.45 - 7.40 (m, 4H), 7.36 - 7.33 (m, 1H), 7.27 - 7.25 (m, 1H), 7.23 - 7.20 (m, 1H), 6.93 - 6.91 (m, 1H), 6.78 - 6.77 (m, 1H), 3.12 (s, 1H), 2.87 - 2.86 (m, 1H), 2.81 (s, 3H), 2.59 - 2.58 (m, 1H), 2.47 - 2.43 (m, 1H), 2.27 - 2.26 (m, 1H), 2.00 - 1.98 (m, 1H), 1.88 - 1.85 (m, 1H), 1.50 - 1.46 (m, 2H), 1.18 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.9, 178.5, 160.5, 147.8, 142.6, 140.3, 136.3, 135.5, 133.4, 133.1, 131.3, 130.7, 130.6, 130.4, 129.8, 128.7, 128.6, 128.0, 127.4, 127.1, 127.0, 126.5, 126.2, 125.4, 124.1, 123.6, 120.3, 49.8, 48.3, 44.8, 43.4, 40.7, 39.7, 35.5, 33.5, 31.5, 20.1.

HRMS (ESI): Calculated for $[C_{39}H_{36}N_2NaO_2, M+Na]^+$: 587.2669; Found: 587.2678.

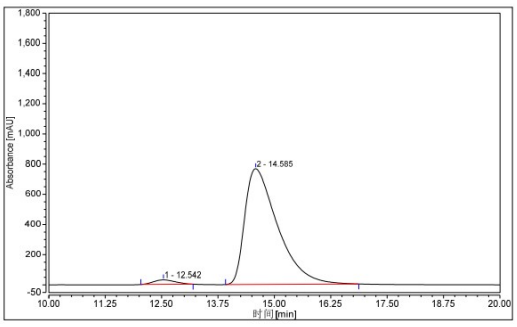
Optical Rotation: $[\alpha]^{25}_D$ = –25.5 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2963, 1709, 1442, 1369, 1181, 812, 753, 692, 621, 463.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 14.585 min (major) and 12.542 min (minor). 95% ee.

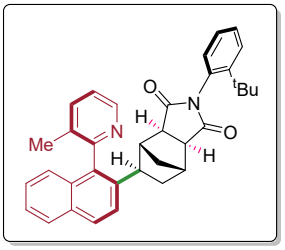


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.095	25.408	40.602	49.79	55.44
2	14.382	25.619	32.635	50.21	44.56



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	12.542	16.670	29.549	2.51	3.71
2	14.585	648.695	766.654	97.49	96.29

(3a*R*,4*R*,5*R*,7*S*,7a*S*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(3-methylpyridin-2-yl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (7k)



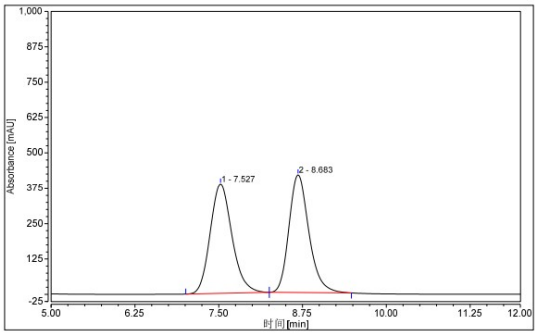
74% yield, white solid, **m.p.** = 196–198 °C. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.64 (d, *J* = 4.8 Hz, 1H), 7.91 - 7.89 (m, 1H), 7.86 - 7.84 (m, 1H), 7.72 - 7.70 (m, 1H), 7.56 - 7.54 (m, 2H), 7.43 - 7.31 (m, 4H), 7.30 - 7.26 (m, 1H), 7.03 - 7.01 (m, 1H), 6.81 - 6.79 (m, 1H), 3.06 (s, 1H), 2.93 - 2.92 (m, 1H), 2.76 - 2.74 (m, 1H), 2.64 - 2.61 (m, 1H), 2.59 - 2.57 (m, 1H), 1.99 - 1.96 (m, 4H), 1.90 - 1.87 (m, 1H), 1.66 - 1.61 (m, 1H), 1.50 - 1.47 (m, 1H), 1.25 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.9, 178.5, 158.0, 147.8, 147.4, 139.6, 138.1, 136.3, 133.0, 132.2, 132.0, 130.7, 130.4, 129.8, 128.8, 128.7, 128.0, 127.5, 126.6, 125.5, 125.2, 123.1, 122.7, 50.2, 48.4, 45.3, 43.3, 40.7, 39.0, 35.6, 33.2, 31.6, 18.8.

HRMS (ESI): Calculated for $[C_{35}H_{34}N_2NaO_2, M+Na]^+$: 537.2512; Found: 537.2521.

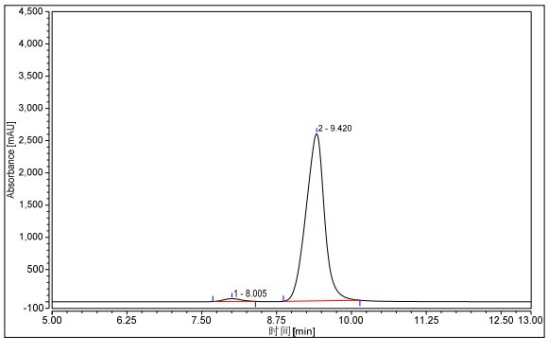
Optical Rotation: $[\alpha]^{25}_D$ = 50.8 ° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2921, 1709, 1444, 1371, 1171, 807, 756, 584.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 ℃, 254 nm, R*t* = 9.420 min (major) and 8.005 min (minor). 97% ee.

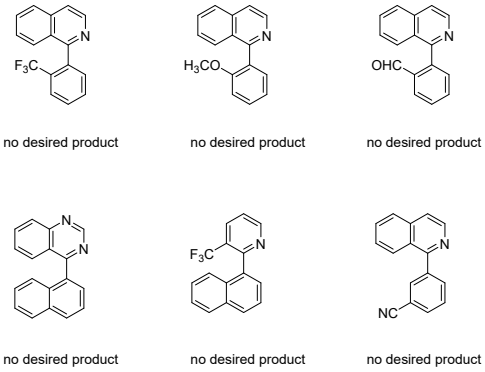


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.527	145.725	386.033	50.35	48.15
2	8.683	143.695	415.636	49.65	51.85



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.005	14.950	43.691	1.59	1.66
2	9.420	927.999	2591.891	98.41	98.34

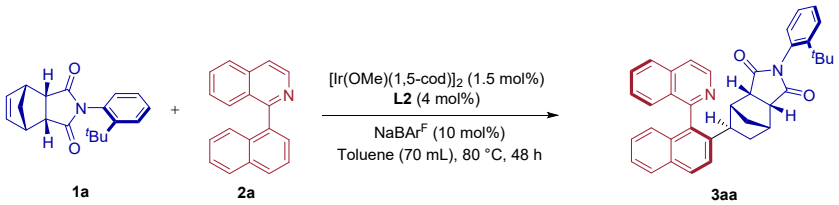
Scheme S1. Unsuccessful substrates



Several substrates (Scheme S1) were tested in this reaction without success. Studies are ongoing to find solutions for these problematic substrates.

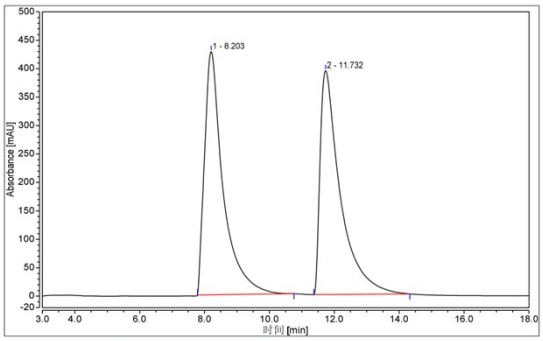
VIII. Gram-scale reaction and synthetic transformations

1. Gram-Scale Preparation:

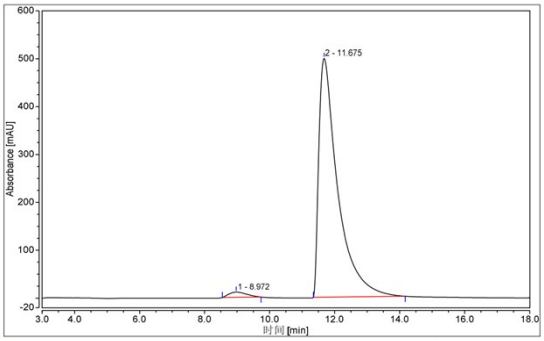


To an flame–dried 250 mL Schlenk tube containing a stirring bar was charged with $[Ir(OMe)(1,5\text{-cod})]_2$ (0.05 mmol, 35 mg), **L2** (0.14 mmol, 95 mg) and 35 mL dry toluene in a nitrogen-filled glove-box, the mixture was stirred for 20 min at room temperature. Then **1a** (3.5 mmol, 1.03 g, 1.0 equiv.), **2a** (4.2 mmol, 1.07 g, 1.2 equiv.), $NaBAr^F$ (0.35 mmol, 310 mg) and another 35 mL dry toluene were added sequentially. The mixture was stirred at 80 °C for 48 hours, concentrated to dryness and the crude mixture was purified by flash column chromatography on silica gel using a mixture of Hexane/EtOAc (3/1, v/v) as eluent to obtain the desired product **3aa** in 99% isolated yield (1.91 g) with 96% ee.

HPLC: Daicel Chiralpak IC Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 11.675 min (major) and 8.972 min (minor).

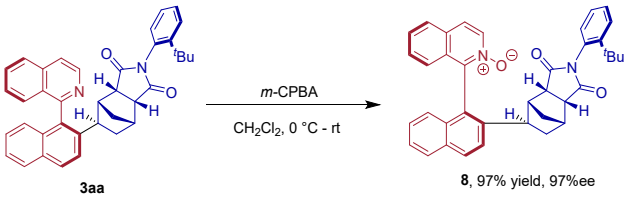


peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.203	282.444	427.736	49.97	52.05
2	11.732	282.750	394.019	50.03	47.95



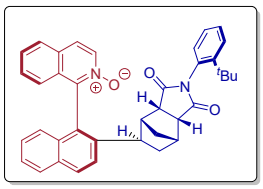
peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.972	6.904	10.906	2.01	2.14
2	11.675	336.032	499.090	97.99	97.86

2. Synthetic transformations



The following reaction was carried out by the published procedures[7]. To a solution of the substituted isoquinoline **3aa** (96% ee, 110.1 mg,0.2 mmol) in CH_2Cl_2 (2 mL) was added m-chloroperoxybenzoic acid (69 mg, 0.4 mmol) at 0 °C. The reaction mixture was stirred at room temperature for 4 hours. Then the reaction mixture was quenched with saturated Na_2CO_3 aqueous solution and extracted with CH_2Cl_2 (3 × 20 mL). The combined organic layers were washed with brine, dried over Na_2SO_4 and filtrated. The solvent was removed under reduced pressure and the residue was purified by silica gel column chromatography(CH_2Cl_2/EtOAc 1:1, v/v) to afford product **8** as a white solid (110.0 mg, 97% yield).

1-(2-((3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-1,3-dioxooctahydro-1*H*-4,7-methanoisoindol-5-yl)naphthalen-1-yl)isoquinoline 2-oxide (8)



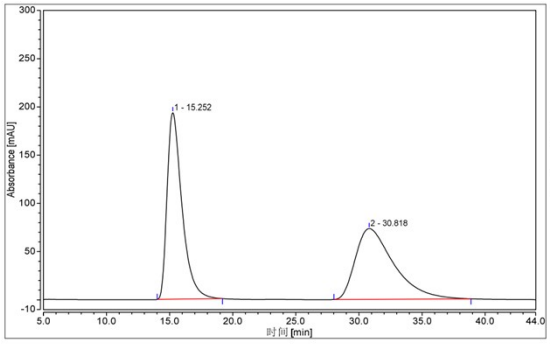
97% yield, white solid, **m.p.** = 186–188 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.28 - 8.27 (m, 1H), 8.09 - 8.07 (m, 1H), 7.98 - 7.93 (m, 2H), 7.81 - 7.79 (m, 1H), 7.76 - 7.74 (m, 1H), 7.58 - 7.52 (m, 2H), 7.47 - 7.44 (m, 1H), 7.41 - 7.35 (m, 2H), 7.32 - 7.30 (m, 1H), 7.20 - 7.17 (m, 1H), 7.05 - 7.04 (m, 1H), 6.94 - 6.93 (m, 1H), 5.78 - 5.76 (m, 1H), 3.21 - 3.18 (m, 2H), 3.14 - 3.13 (m, 1H), 3.04 - 3.01 (m, 1H), 2.96 - 2.94 (m, 1H), 2.36 - 2.31 (m, 1H), 2.21 - 2.19 (m, 1H), 1.74 - 1.69 (m, 2H), 1.22 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.9, 177.2, 147.8, 145.1, 142.2, 137.7, 132.4, 131.9, 130.4, 130.2, 130.1, 129.9, 129.7, 129.4, 129.2, 129.0, 128.8, 128.3, 127.6, 127.4, 127.3, 127.1, 126.0, 124.9, 124.5, 124.2, 123.5, 48.8, 48.7, 44.0, 40.7, 39.8, 39.7, 35.6, 33.1, 31.6.

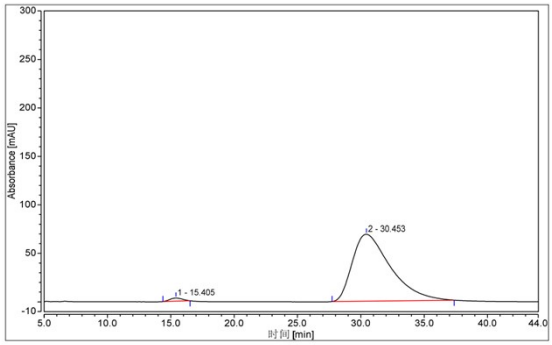
HRMS (ESI): Calculated for $[C_{38}H_{35}N_2O_3, M+H]^+$: 567.2642; Found: 567.2653.

Optical Rotation: $[\alpha]^{25}_D$ = –187.6° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1705, 1441, 1366, 1318, 1224, 1170, 814, 744, 608, 511, 442.

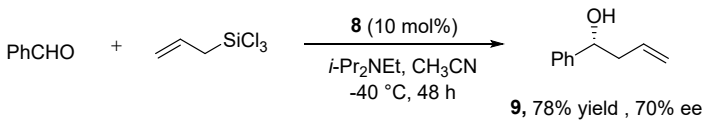
HPLC: Daicel Chiralcel OD-H Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 30.453 min (major) and 15.405 min (minor). 97% ee.





peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	15.252	265.255	193.501	50.65	72.51
2	30.818	258.407	73.356	49.35	27.49

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	15.405	3.649	3.245	1.49	4.49
2	30.453	241.110	69.055	98.51	95.51



9, 78% yield , 70% ee

The following reaction was carried out by the published procedures[7]. The catalyst was recovered in 83% yield without racemization. Allyltrichlorosilane (69.5 μL,0.48 mmol) was added dropwise to a solution of catalyst **8** (97% ee, 23 mg, 0.04 mmol), *i*-Pr_2NEt (82.6 μL,0.5 mmol), and benzaldehyde (41 μL, 0.4 mmol) in MeCN (2 mL) under argon at -40 °C. The reaction mixture was stirred at -40 °C for 48 h. The reaction was quenched with saturated aqueous $NaHCO_3$ (5 mL) and diluted with water. The aqueous layer was extracted with DCM (3 × 5 mL). The combined organic extracts were washed with brine (5 mL) and dried over Na_2SO_4. The solvent was removed in vacuo. The residue was purified by column chromatography on silica gel with a petroleum

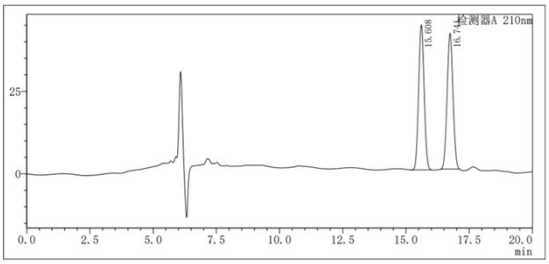
ether/ethyl acetate mixture (20:1) to afford **9** as a colorless oil (46.5 mg, 78% yield, 70% ee).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 - 7.32 (m, 4H), 7.27 - 7.23 (m, 1H), 5.82 - 5.74 (m, 1H), 5.15 - 5.10 (m, 2H), 4.70 - 4.67 (m, 1H), 2.53 - 2.47 (m, 2H), 2.45 - 2.34 (m, 1H).

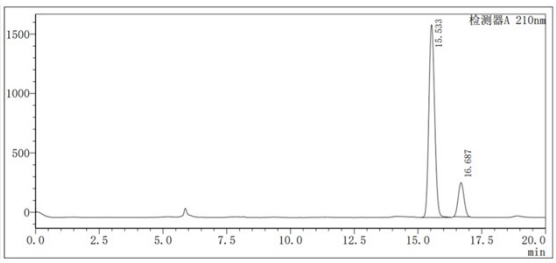
Optical Rotation: $[\alpha]^{25}_D$ = 36.8° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 3353, 2924, 1641, 1493, 1453, 1045, 986, 913, 870, 756, 698, 608, 537.

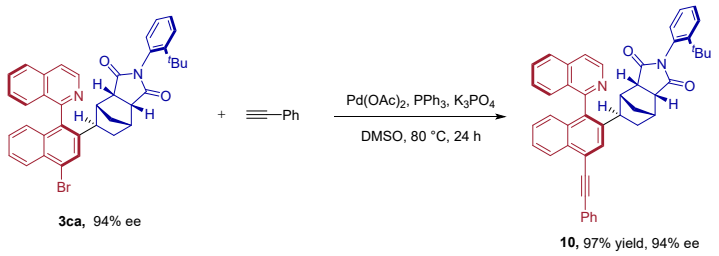
HPLC: Daicel Chiralcel OD-H Column (*n*-Hexane/*i*-PrOH = 95 : 5, 1.0 mL/min), 30 °C, 210 nm, R*t* = 15.533 min (major) and 16.687 min (minor). 70% ee.



peak	RT / min	Area	Height	Area / %
1	15.608	666045	43895	50.005
2	16.741	665902	41104	49.995



peak	RT / min	Area	Height	Area / %
1	15.533	25809102	1622348	84.937
2	16.687	4577188	287853	15.063

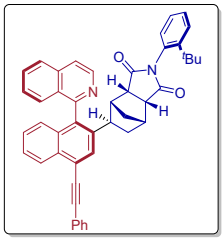


3ca, 94% ee

10, 97% yield, 94% ee

The following reaction was carried out by the published procedures.[8] To a reaction tube equipped with a stir bar were charged with **3ca** (63.0 mg, 0.1 mmol), DMSO (1 mL), $Pd(OAc)_2$ (1.1 mg, 0.005 mmol), PPh_3 (5.2 mg, 0.02 mmol), K_3PO_4 (25.5 mg, 0.12 mmol) and ethynylbenzene (16.5 μL, 0.15 mmol). The tube was then sealed, and the resulting mixture was stirred at 80 °C for 24 h under argon atmosphere. Upon completion, it was diluted with ethyl acetate (20 mL) and washed with water and brine. The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (5:1) as the eluent to give **10** as a white solid (62.9 mg, 97% yield).

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)-4-(phenylethynyl)naphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (10)



97% yield, white solid, **m.p.** = 163–165 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.74 (d, *J* = 5.8 Hz, 1H), 8.56 -

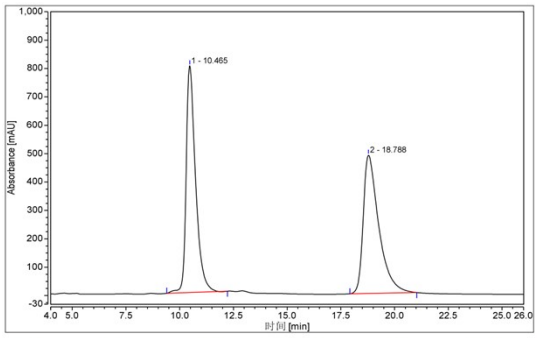
8.54 (m, 1H), 8.03 - 8.02 (m, 2H), 7.84 - 7.83 (m, 1H), 7.78 - 7.76 (m, 2H), 7.71 - 7.68 (m, 1H), 7.53 - 7.36 (m, 8H), 7.27 - 7.25 (m, 1H), 7.18 - 7.14 (m, 1H), 6.82 - 6.80 (m, 1H), 5.45 - 5.43 (m, 1H), 3.20 - 3.17 (m, 3H), 3.06 - 3.03 (m, 1H), 2.95 - 2.93 (m, 1H), 2.37 - 2.35 (m, 1H), 2.11 - 2.07 (m, 1H), 1.81 - 1.79 (m, 1H), 1.76 - 1.71 (m, 1H), 1.21 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 176.8, 159.3, 147.7, 142.8, 140.5, 136.5, 136.4, 133.2, 132.0, 131.8, 130.9, 130.4, 130.1, 129.3, 128.70, 128.68, 128.6, 128.3, 128.1, 127.7, 127.2, 127.12, 127.06, 126.6, 126.5, 126.3, 126.2, 123.3, 121.9, 120.6, 94.7, 87.9, 49.0, 48.6, 44.3, 41.4, 39.6, 39.3, 36.1, 35.6, 31.6.

HRMS (ESI): Calculated for $[C_{46}H_{39}N_2O_2, M+H]^+$: 651.3006; Found: 651.3015.

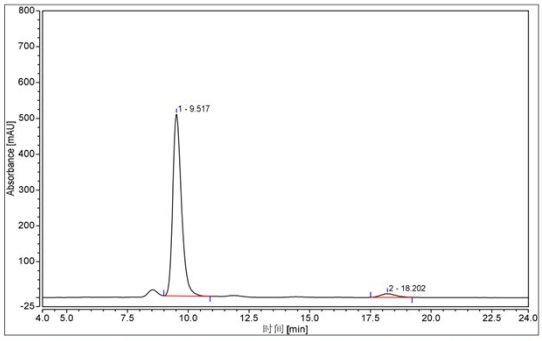
Optical Rotation: $[\alpha]^{25}_D = -112.9^o$ (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2961, 1709, 1488, 1440, 1366, 1172, 827, 753, 690, 618.

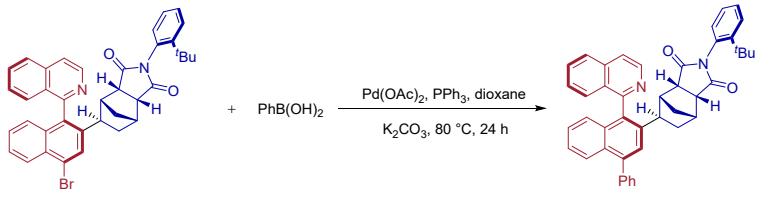
HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 9.517 min (major) and 18.202 min (minor). 93% ee.



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	10.465	405.557	798.265	49.85	62.10
2	18.788	408.053	487.118	50.15	37.90



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	9.517	210.894	507.005	96.61	98.06
2	18.202	7.397	10.049	3.39	1.94

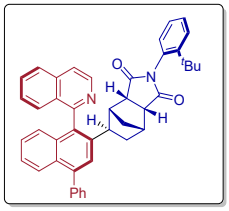


3ca, 94% ee

11, 99% yield, 94% ee

The following reaction was carried out by the published procedures.[8] To a reaction tube equipped with a stir bar were charged with **3ca** (63.0 mg, 0.1 mmol), dioxane (1 mL), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol), PPh_3 (15.7 mg, 0.06 mmol), K_2CO_3 (55.3 mg, 0.4 mmol) and phenylboronic acid (13.4 mg, 0.11 mmol). The tube was then sealed, and the resulting mixture was stirred at 80 °C for 24 h under argon atmosphere. Upon completion, it was diluted with ethyl acetate (20 mL) and washed with water and brine. The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (5:1) as the eluent to give **11** as a white solid (62.5 mg, 99% yield).

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)-4-phenylnaphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (11)



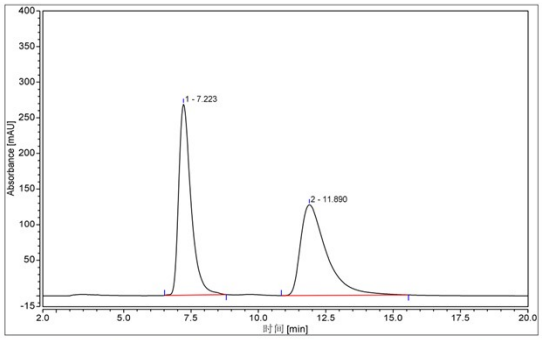
99% yield, white solid, **m.p.** = 257–259 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 5.8 Hz, 1H), 8.06 - 8.05 (m, 1H), 7.95 - 7.93 (m, 1H), 7.86 - 7.85 (m, 1H), 7.74 - 7.71 (m, 1H), 7.67 - 7.59 (m, 5H), 7.55 - 7.50 (m, 3H), 7.46 - 7.43 (m, 1H), 7.38 - 7.35 (m, 2H), 7.23 - 7.20 (m, 1H), 7.17 - 7.14 (m, 1H), 6.85 - 6.83 (m, 1H), 5.43 - 5.41 (m, 1H), 3.19 - 3.18 (m, 3H), 3.10 - 3.07 (m, 1H), 2.91 - 2.90 (m, 1H), 2.32 - 2.30 (m, 1H), 2.16 - 2.11 (m, 1H), 1.76 - 1.69 (m, 2H), 1.21 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.0, 176.9, 160.0, 147.7, 142.9, 141.2, 141.1, 140.2, 136.5, 135.1, 133.6, 130.9, 130.45, 130.39, 130.2, 130.1, 129.3, 128.7, 128.49, 128.46, 128.0, 127.6, 127.2, 127.1, 126.9, 126.4, 126.2, 126.0, 125.6, 124.3, 120.5, 49.0, 48.7, 44.3, 41.5, 39.54, 39.46, 36.1, 35.6, 31.7.

HRMS (ESI): Calculated for $[C_{44}H_{39}N_2O_2, M+H]^+$: 627.3006; Found: 627.3019.

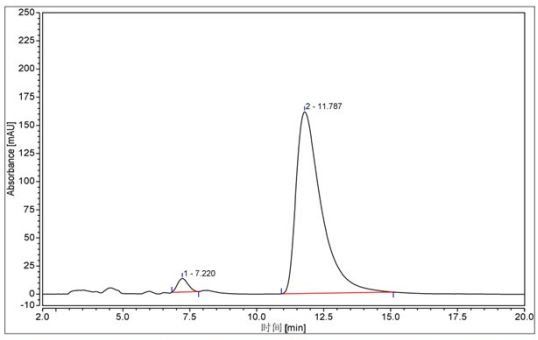
Optical Rotation: $[\alpha]^{25}_D$ = –106.6° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 2921, 1708, 1441, 1368, 1178, 754, 707, 614.

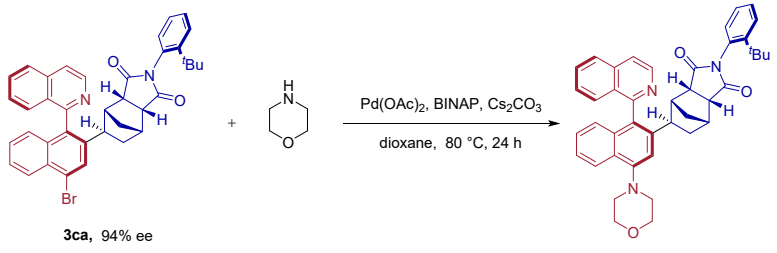
HPLC: Daicel Chiralcel OX-H Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 11.787 min (major) and 7.220 min (minor). 94% ee.



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.223	141.467	268.086	50.03	67.79
2	11.890	141.318	127.374	49.97	32.21



peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	7.220	5.476	12.039	3.02	6.94
2	11.787	175.872	161.399	96.98	93.06



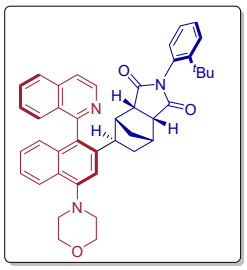
3ca, 94% ee

12, 60% yield, 96% ee

The following reaction was carried out by the published procedures.[8] To a reaction tube equipped with a stir bar were charged with **3ca** (63.0 mg, 0.1 mmol), dioxane (1 mL), $Pd(OAc)_2$ (5.6 mg, 0.025 mmol), BINAP (18.7 mg, 0.03 mmol), Cs_2CO_3 (91.2 mg, 0.28 mmol) and morpholine (70 μL, 0.8 mmol). The tube was then sealed, and the resulting mixture was stirred at 80 °C for 24 h under argon atmosphere. Upon completion, it was quenched with water , extracted with CH_2Cl_2, and washed with brine. The organic layer was dried over

anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (5:1) as the eluent to give **12** as a white solid (38.1 mg, 60% yield).

(3a*S*,4*R*,5*R*,7*S*,7a*R*)-2-(2-(*tert*-butyl)phenyl)-5-(1-(isoquinolin-1-yl)-4-morpholinonaphthalen-2-yl)hexahydro-1*H*-4,7-methanoisoindole-1,3(2*H*)-dione (12)



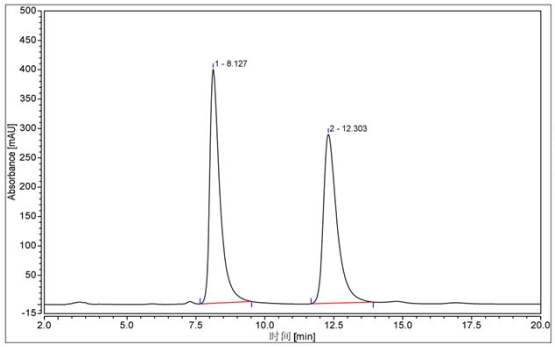
60% yield, white solid, **m.p.** = 158–160 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.70 (d, *J* = 5.7 Hz, 1H), 8.29 - 8.27 (m, 1H), 8.02 - 8.00 (m, 1H), 7.81 - 7.80 (m, 1H), 7.70 - 7.67 (m, 1H), 7.49 - 7.47 (m, 1H), 7.43 - 7.38 (m, 3H), 7.35 - 7.31 (m, 2H), 7.20 - 7.17 (m, 1H), 7.13 - 7.10 (m, 1H), 6.74 - 6.72 (m, 1H), 5.35 - 5.33 (m, 1H), 4.09 - 4.07 (m, 4H), 3.28 - 3.16 (m, 7H), 3.01 - 2.98 (m, 1H), 2.92 - 2.90 (m, 1H), 2.29 - 2.27 (m, 1H), 2.07 - 2.02 (m, 1H), 1.82 - 1.80 (m, 1H), 1.70 - 1.64 (m, 1H), 1.18 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.9, 176.9, 160.0, 150.1, 147.6, 142.7, 140.7, 136.4, 134.6, 130.8, 130.3, 130.0, 129.3, 128.7, 128.6, 127.9, 127.4, 127.2, 127.0, 126.9, 126.5, 126.4, 125.1, 123.2, 120.4, 112.0, 67.5, 53.7, 49.0, 48.6, 44.2, 41.5, 39.6, 39.5, 36.2, 35.6, 31.6.

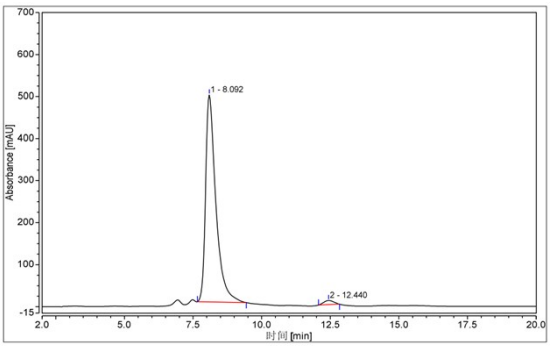
HRMS (ESI): Calculated for $[C_{42}H_{42}N_3O_3, M+H]^+$: 636.3221; Found: 636.3233.

Optical Rotation: $[\alpha]^{25}_D$ = –109.9° (c = 1.0, $CHCl_3$).

IR (neat, cm^{-1}) = 1709, 1370, 1172, 1113, 1017, 752, 668, 619, 484, 439.

HPLC: Daicel Chiralpak IA Column (*n*-Hexane/*i*-PrOH = 70 : 30, 1.0 mL/min), 30 °C, 254 nm, R*t* = 8.092 min (major) and 12.440 min (minor). 96% ee.





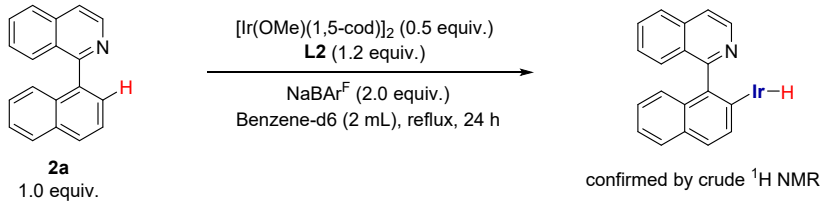
peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.127	169.572	398.600	50.86	58.06
2	12.303	163.868	287.947	49.14	41.94

peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.092	214.133	492.396	98.12	98.08
2	12.440	4.109	9.625	1.88	1.92

IX. Mechanistic studies

Mechanistic Studies. To explore the mechanism of this C−H alkylation reaction, an equivalent reaction of substrate **2a** with the iridium metal catalyst was carried out. The presence of [Ir]−H intermediates was successfully observed by crude NMR, albeit not in significant amounts. This experimental result indicate that the reaction involves a C−H activation process and substrate **2a** is the source of the H atoms going through the asymmetric activation process.

Iridium intermediate detection experiment:

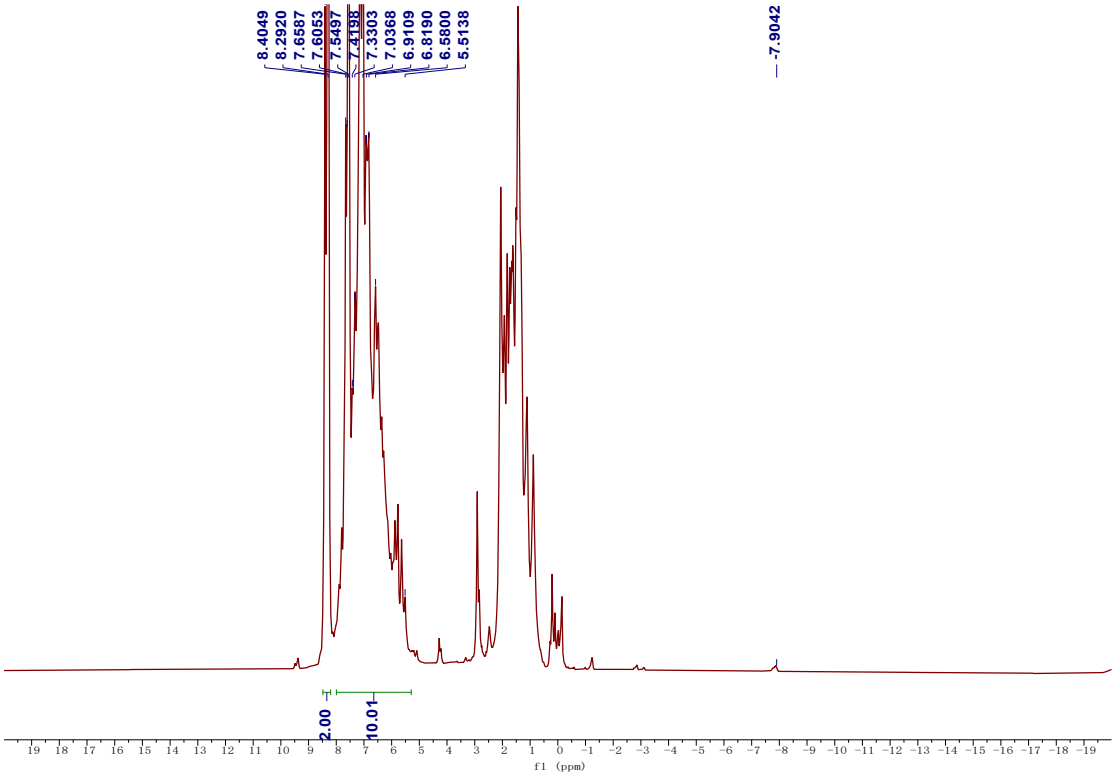


2a
1.0 equiv.

confirmed by crude ^{1}H NMR

To an oven-dried 10 mL Schlenk tube containing a stirring bar was charged with $[Ir(OMe)(1,5\text{-cod})]_2$ (0.015 mmol, 10.0 mg), **L2** (0.035 mmol, 24.4 mg) and 0.3 mL dry C_6D_6 in a nitrogen-filled glove-box, the mixture was stirred for 10 min at room temperature. Then corresponding substrate **2a** (0.03 mmol, 1.0 equiv.), $NaBAr^F$ (0.06 mmol, 53.2 mg) and another 0.3 mL dry C_6D_6 were added sequentially. The mixture was stirred at 110 °C for 24 hours. The presence of Ir−H intermediates was observed through crude ^{1}H NMR.

^{1}H-NMR for [Ir]−H:



X. Photophysical properties of selected compounds

Table S6. Absorption maxima and emission maxima of selected compounds

compound	λ_{abs} (nm)[a]	λ_{em} (nm)[b]
3ai	322	380
3ak	322	382
3ga	308	346
3ha	310	350
3ia	310	344
3la	317	366
7e	327	388

[a] Absorption maximum in CH_2Cl_2 at 10^{-3} mol/L. [b] Emission maximum in CH_2Cl_2 at 10^{-3} mol/L.

XI. References

[1] K. Kim, J. Hyun, J. Kim, H. Kim, *Asian J. Org. Chem.* **2016**, *5*, 1107-1110.

[2] Z.-S. Liu, P.-P. Xie, Y. Hua, C. Wu, Y. Ma, J. Chen, H.-G. Cheng, X. Hong, Q. Zhou, *Chem* **2021**, *7*, 1917-1932.

[3] L. Liu, J. Lin, M. Pang, H. Jin, X. Yu, S. Wang, *Org. Lett.* **2022**, *24*, 1146-1151.

[4] a) X.-W. Gu, Y.-L. Sun, J.-L. Xie, X.-B. Wang, Z. Xu, G.-W. Yin, L. Li, K.-F. Yang, L.-W. Xu, *Nat. Commun.* **2020**, *11*, 2904; b) F. Sun, T. Wang, G.-J. Cheng, X. Fang, *ACS Catal.* **2021**, *11*, 7578-7583.

[5] J. Zheng, S.-L. You, *Angew. Chem. Int. Ed.* **2014**, *53*, 13244-13247.

[6] X.-M. Wang, P. Zhang, Q. Xu, C.-Q. Guo, D.-B. Zhang, C.-J. Lu, R.-R. Liu, *J. Am. Chem. Soc.* **2021**, *143*, 15005-15010.

[7] a) A. V. Malkov, P. Ramírez-López, L. Biedermannová, L. Rulíšek, L. Dufková, M. Kotora, F. Zhu, P. Kočovský, *J. Am. Chem. Soc.* **2008**, *130*, 5341-5348; b) Q. Wang, Z.-J. Cai, C.-X. Liu, Q. Gu, S.-L. You, *J. Am. Chem. Soc.* **2019**, *141*, 9504-9510.

[8] a) X. Song, X. Cai, X. Zhang, X. Fan, *Org. Chem. Front.* **2021**, *8*, 6265-6272; b) X. Song, Q. Zhou, J. Zhao, Y. Jiang, X. Zhang, X. Zhang, X. Fan, *Org. Lett.* **2020**, *22*, 9506-9512.

[9] A. Romero-Arenas, V. Hornillos, J. Iglesias-Sigüenza, R. Fernández, J. López-Serrano, A. Ros, J. M. Lassaletta, *J. Am. Chem. Soc.* **2020**, *142*, 2628-2639.

XII. X-ray Crystallographic data for 3ca, 5m, 7i and 7k

Single crystals for X-ray studies were grown by slow evaporation of a solution of compound **3ca** in a mixture of EtOAc and $CHCl_3$ at room temperature. X-Ray structural analysis of single crystal **3ca** was obtained to confirm the absolute configuration. The X-ray data of **3ca** is deposited in the Cambridge Crystallographic Data Centre with a number CCDC 2278431.

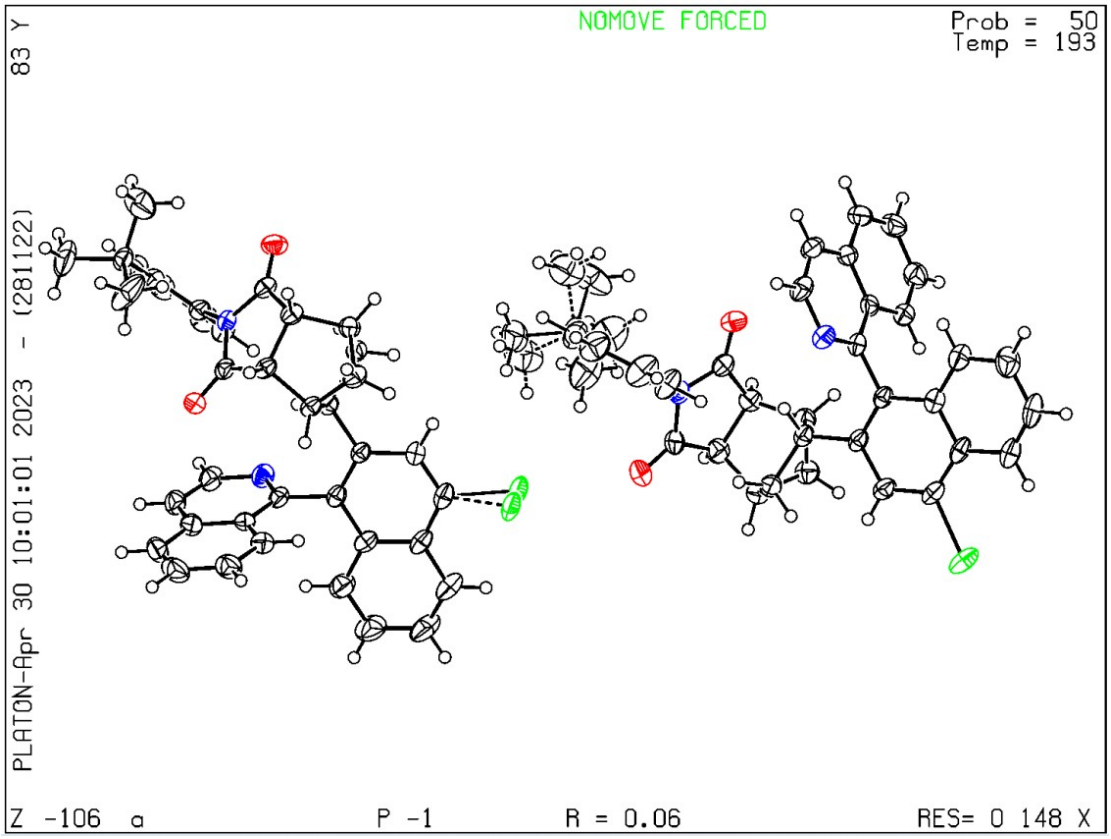


Figure S1. X-ray structure of **3ca**

Table S7. Crystal data and structure refinement for 3ca

Identification code	A	
Empirical formula	$C_{38}H_{33}BrN_2O_2$	
Formula weight	629.57	
Temperature	193.00 K	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.7215(5) Å	α = 99.0400(10)°.
	b = 15.7043(6) Å	β = 90.0390(10)°.
	c = 16.4829(6) Å	γ = 111.104(2)°.
Volume	3028.1(2) $Å^3$	
Z	4	
Density (calculated)	1.381 Mg/m^3	

Absorption coefficient	1.395 mm^{-1}
F(000)	1304.0
Crystal size	0.13 × 0.12 × 0.1 mm^3
Radiation	MoKα (λ = 0.71073)
Theta range for data collection	3.564 to 55.072°.
Index ranges	-14≤h≤16, -20≤k≤20, -20≤l≤21
Reflections collected	28882
Independent reflections	13858 [R_{int} = 0.0591, R_{sigma} = 0.0918]
Data / restraints / parameters	13858 / 88 / 816
Goodness-of-fit on F^2	0.995
Final R indices [I>2sigma(I)]	R_1 = 0.0574, wR_2 = 0.1179
R indices (all data)	R_1 = 0.1090, wR_2 = 0.1440
Largest diff. peak and hole	0.59 and -0.73 e.$Å^{-3}$

Single crystals for X-ray studies were grown by slow evaporation of a solution of recrystallized compound **5m** in a mixture of hexane and DCM at room temperature. X-Ray structural analysis of single crystal **5m** was obtained to confirm the absolute configuration. The X-ray data of **5m** is deposited in the Cambridge Crystallographic Data Centre with a number CCDC 2283545.

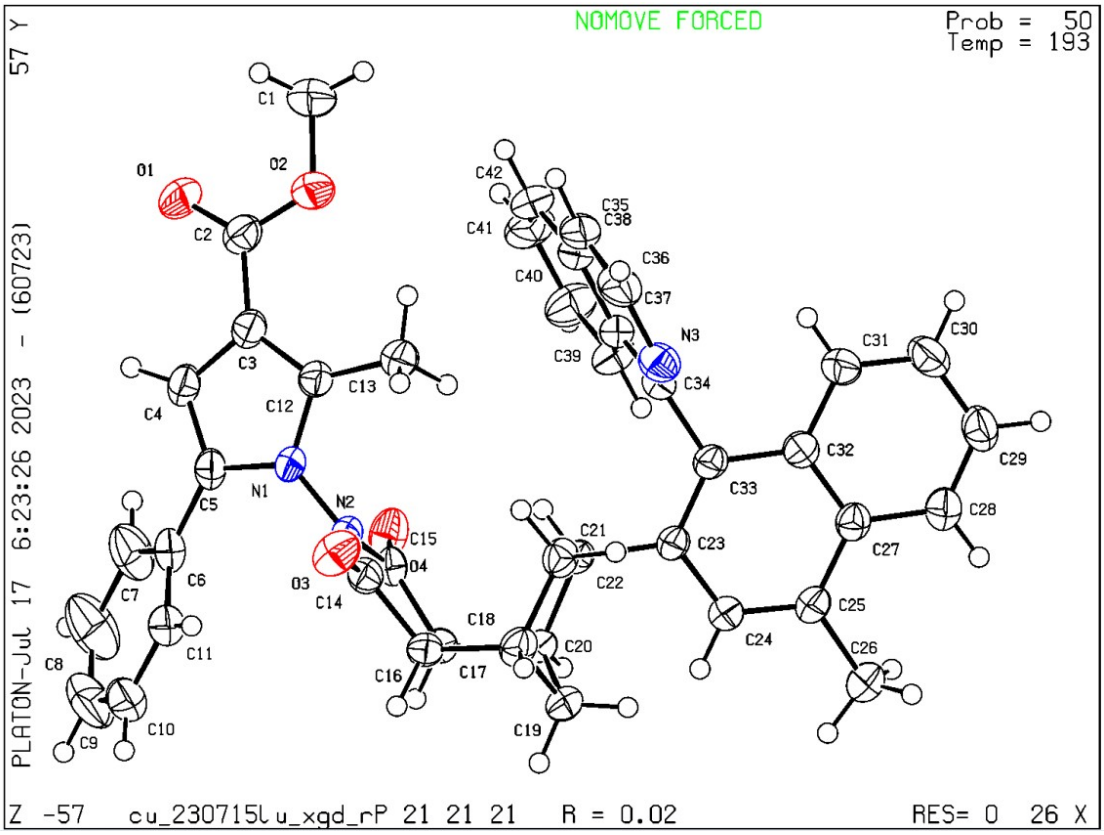


Figure S2. X-ray structure of **5m**

Table S8. Crystal data and structure refinement for 5m

Identification code	cu_230715LU_XGD_RZQ_HXQ_0m	
Empirical formula	$C_{42}H_{35}N_3O_4$	
Formula weight	645.73	
Temperature	193.00 K	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 11.4007(3) Å	α = 90°.
	b = 12.6971(3) Å	β = 90°.
	c = 23.0034(6) Å	γ = 90°.
Volume	3329.88(15) $Å^3$	
Z	4	
Density (calculated)	1.288 Mg/m^3	
Absorption coefficient	0.665 mm^{-1}	
F(000)	1360.0	

Crystal size	0.13 × 0.12 × 0.1 mm^3
Radiation	CuKα (λ = 1.54178)
Theta range for data collection	7.686 to 136.604°.
Index ranges	-13≤h≤13, -15≤k≤15, -27≤l≤27
Reflections collected	77740
Independent reflections	6111 [R_{int} = 0.0374, R_{sigma} = 0.0166]
Data / restraints / parameters	6111 / 0 / 446
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R_1 = 0.0245, wR_2 = 0.0645
R indices (all data)	R_1 = 0.0249, wR_2 = 0.0648
Largest diff. peak and hole	0.17 and -0.09 e.$Å^{-3}$
Flack parameter	0.01(3)

Single crystals for X-ray studies were grown by slow evaporation of a solution of compound **7i** in a mixture of EtOAc and $CHCl_3$ at room temperature. X-Ray structural analysis of single crystal **7i** was obtained to confirm the absolute configuration. The X-ray data of **7i** is deposited in the Cambridge Crystallographic Data Centre with a number CCDC 2309607.

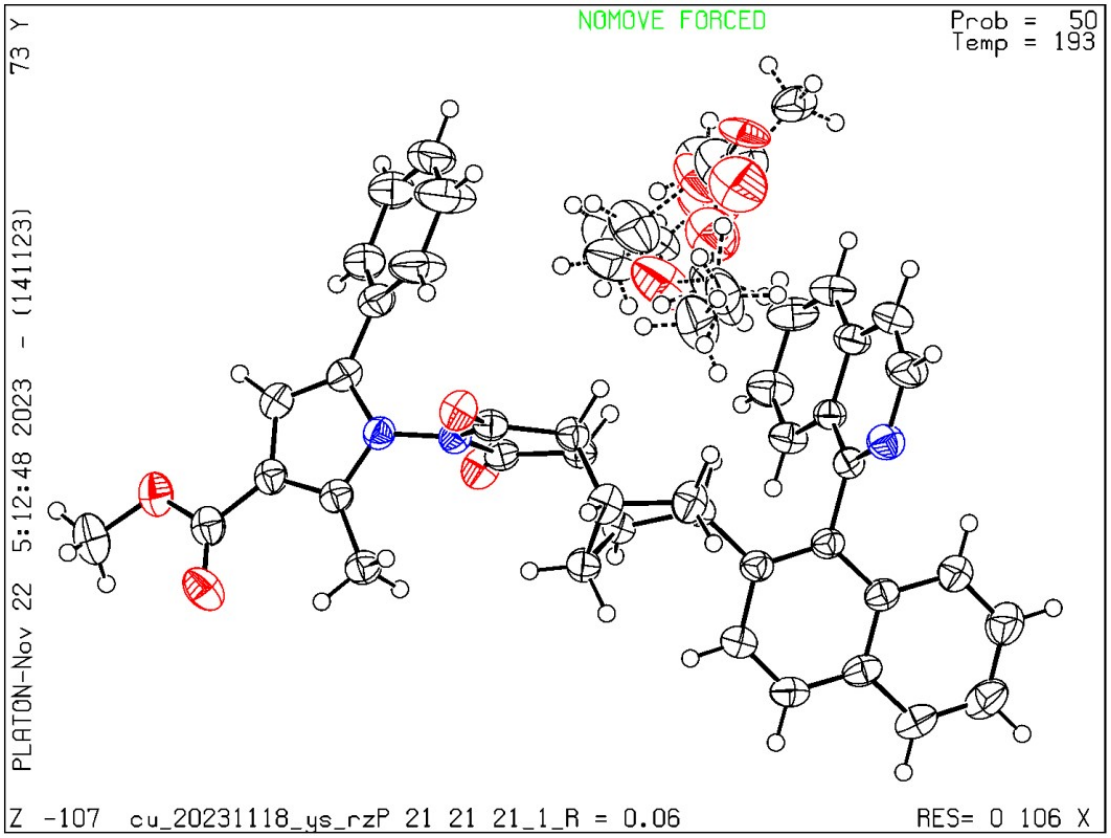


Figure S3. X-ray structure of **7i**

Table S9. Crystal data and structure refinement for 7i

Identification code	cu_20231118_YS_RZQ_ZYX1_138_1_	
Empirical formula	$C_{45}H_{41}N_3O_6$	
Formula weight	719.81	
Temperature	193.00 K	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.0009(5) Å	α =90°.
	b = 11.0174(6) Å	β = 90°.
	c = 34.0362(18) Å	γ =90°.
Volume	3750.2(3) $Å^3$	
Z	4	
Density (calculated)	1.275 Mg/m^3	
Absorption coefficient	0.684 mm^{-1}	

F(000)	1520.0
Crystal size	0.13 × 0.12 × 0.1 mm^3
Radiation	CuKα (λ = 1.54178)
Theta range for data collection	8.436 to 136.858°.
Index ranges	-12≤h≤11, -13≤k≤13, -40≤l≤41
Reflections collected	59003
Independent reflections	6840 [R_{int} = 0.0454, R_{sigma} = 0.0275]
Data / restraints / parameters	6840 / 285 / 602
Goodness-of-fit on F^2	1.086
Final R indices [I>2sigma(I)]	R_1 = 0.0557, wR_2 = 0.1536
R indices (all data)	R_1 = 0.0575, wR_2 = 0.1570
Largest diff. peak and hole	0.73 and -0.43 e.$Å^{-3}$
Flack parameter	0.00(7)

Single crystals for X-ray studies were grown by slow evaporation of a solution of compound **7k** in a mixture of EtOH and $CHCl_3$ at room temperature. X-Ray structural analysis of single crystal **7k** was obtained to confirm the absolute configuration. The X-ray data of **7k** is deposited in the Cambridge Crystallographic Data Centre with a number CCDC 2309606.

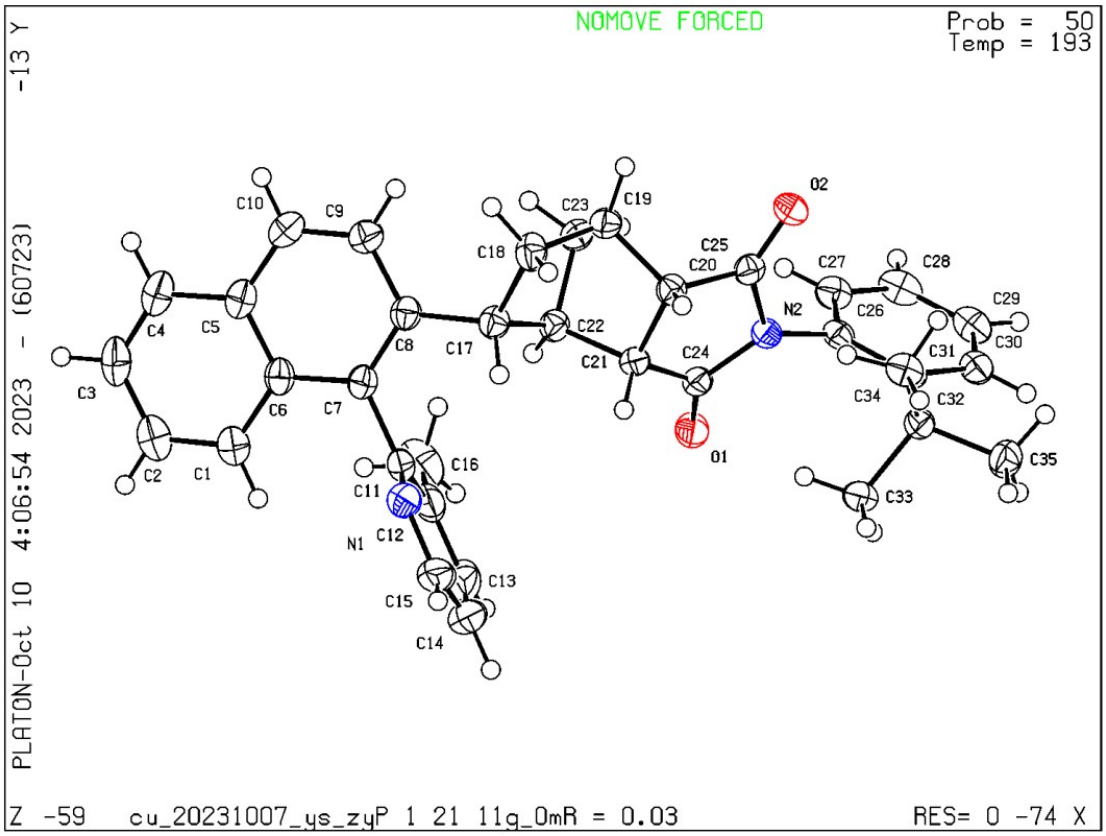


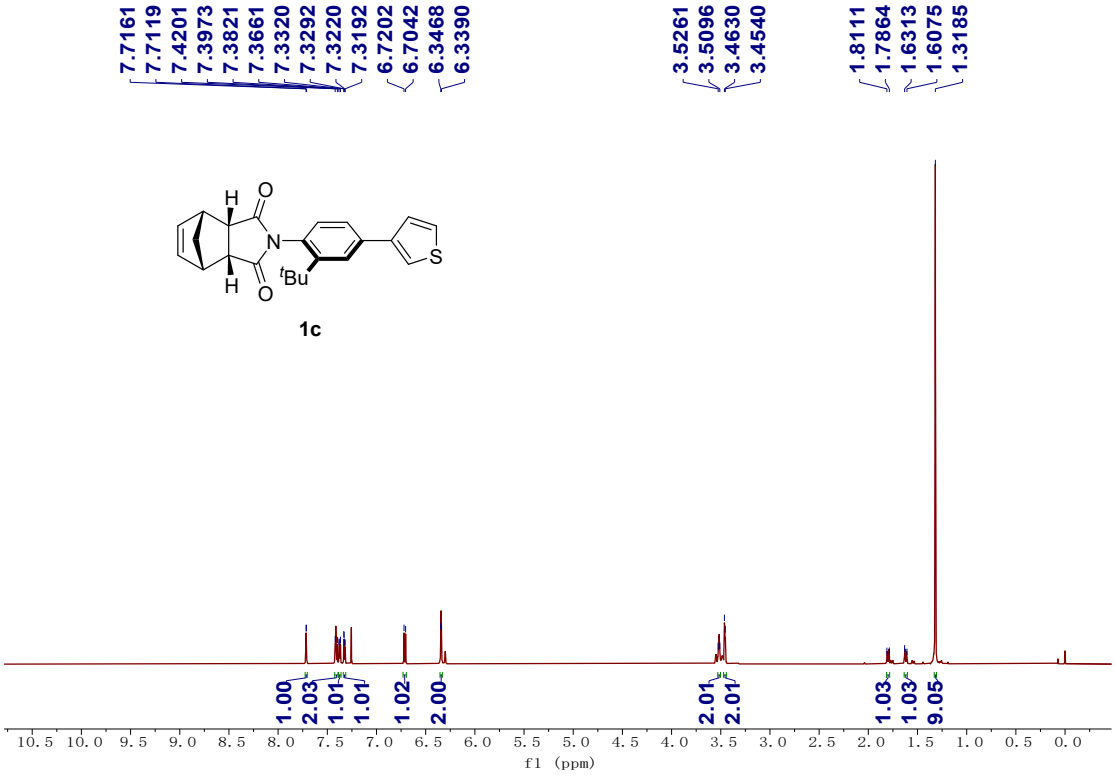
Figure S4. X-ray structure of **7k**

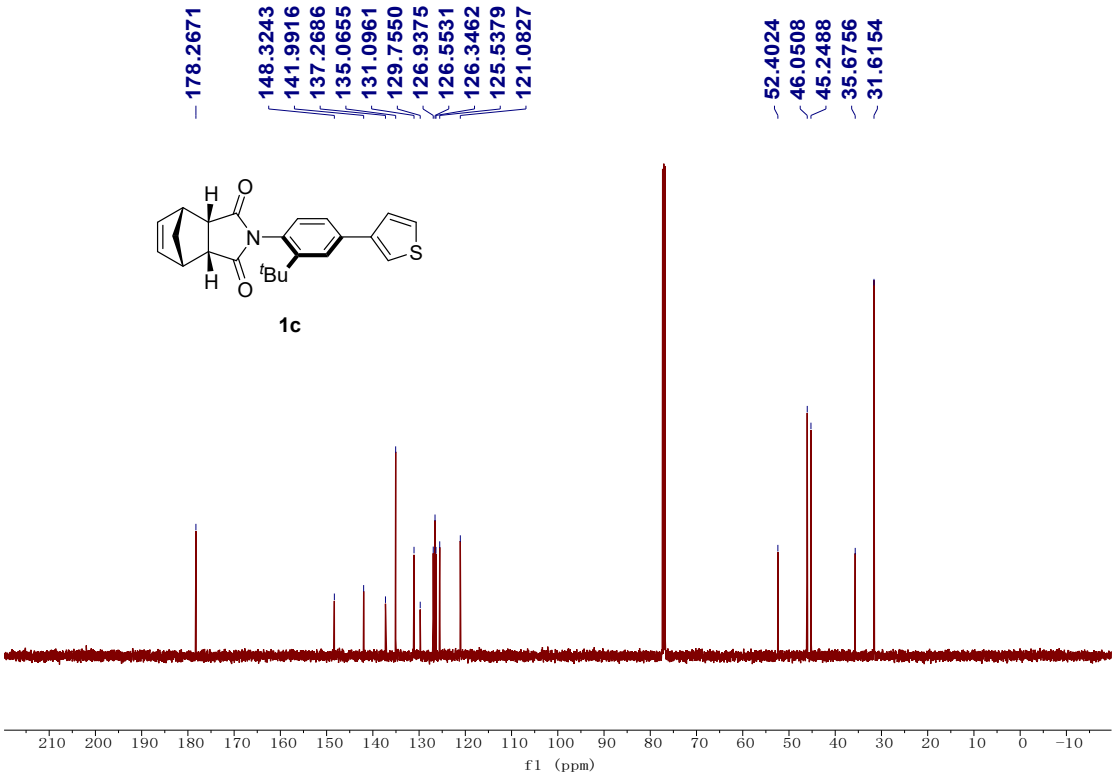
Table S10. Crystal data and structure refinement for 7k

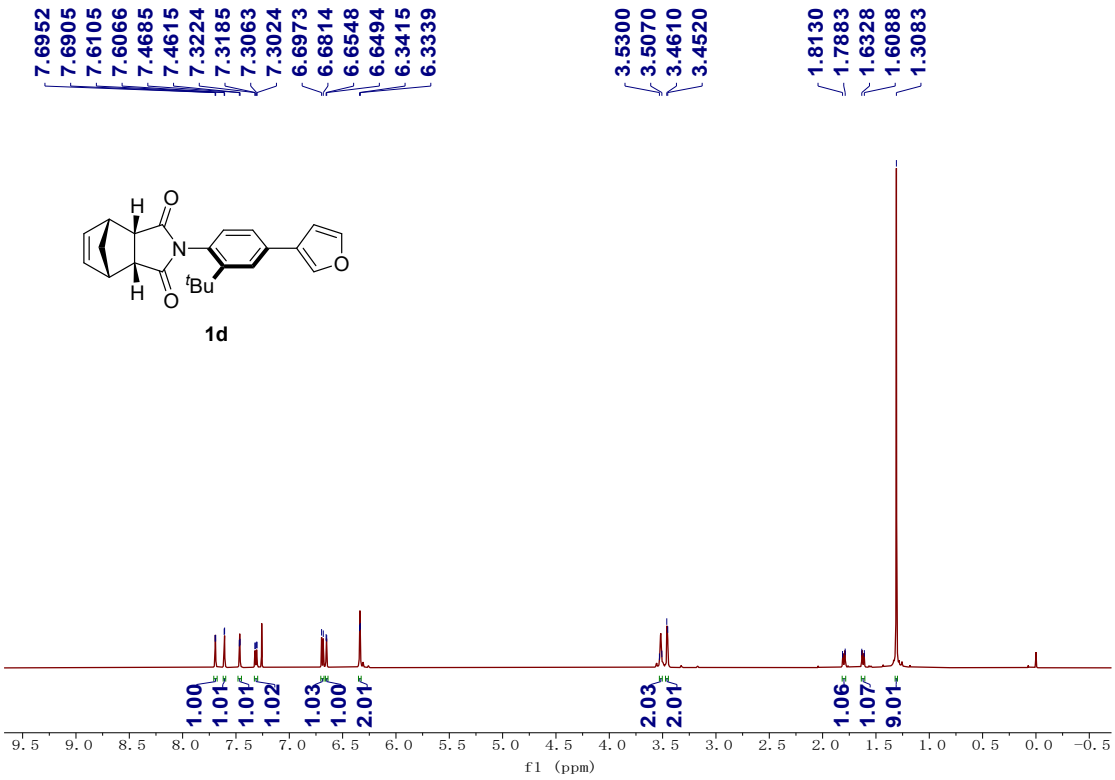
Identification code	cu_20231007_YS_ZYX_1_121_1G_0m	
Empirical formula	$C_{35}H_{34}N_2O_2$	
Formula weight	514.64	
Temperature	193.00 K	
Crystal system	monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 10.8233(6) Å	α =90°.
	b = 7.0541(4) Å	β = 94.633(2)°.
	c = 18.1771(10) Å	γ =90°.
Volume	1383.26(13) $Å^3$	
Z	2	
Density (calculated)	1.236 Mg/m^3	
Absorption coefficient	0.596 mm^{-1}	
F(000)	548.0	

Crystal size	0.13 × 0.12 × 0.1 mm^3
Radiation	CuKα (λ = 1.54178)
Theta range for data collection	4.878 to 136.546°.
Index ranges	-13≤h≤13, -8≤k≤8, -21≤l≤20
Reflections collected	25438
Independent reflections	5006 [R_{int} = 0.0372, R_{sigma} = 0.0332]
Data / restraints / parameters	5006 / 1 / 356
Goodness-of-fit on F^2	1.088
Final R indices [I>2sigma(I)]	R_1 = 0.0319, wR_2 = 0.0804
R indices (all data)	R_1 = 0.0321, wR_2 = 0.0806
Largest diff. peak and hole	0.17 and -0.23 e.$Å^{-3}$
Flack parameter	0.06(4)

XIII. ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra



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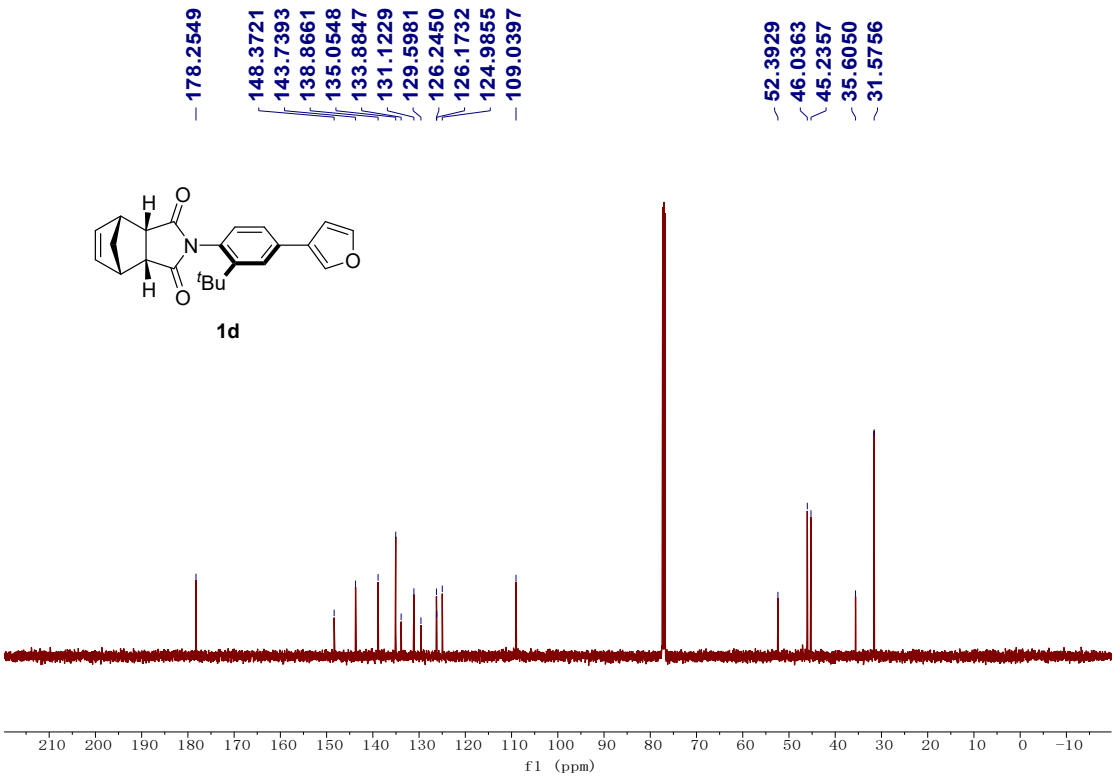
1.07
9.01
f1 (ppm)

1d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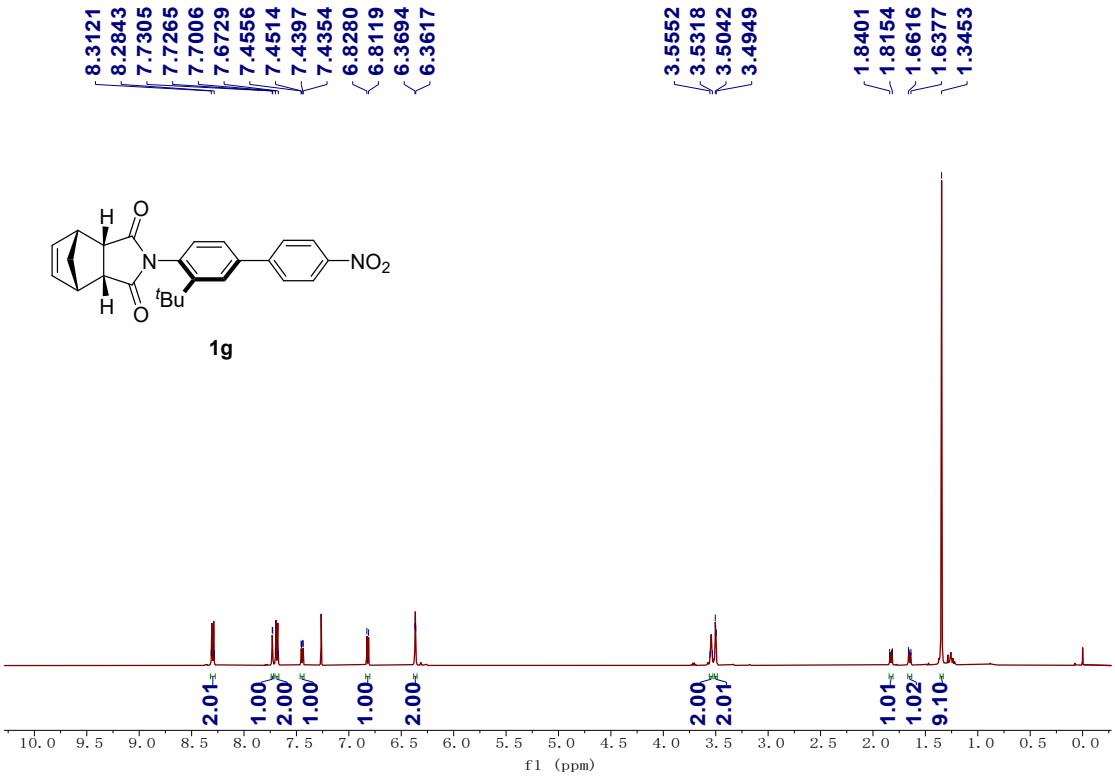
1d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NO2
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H
O
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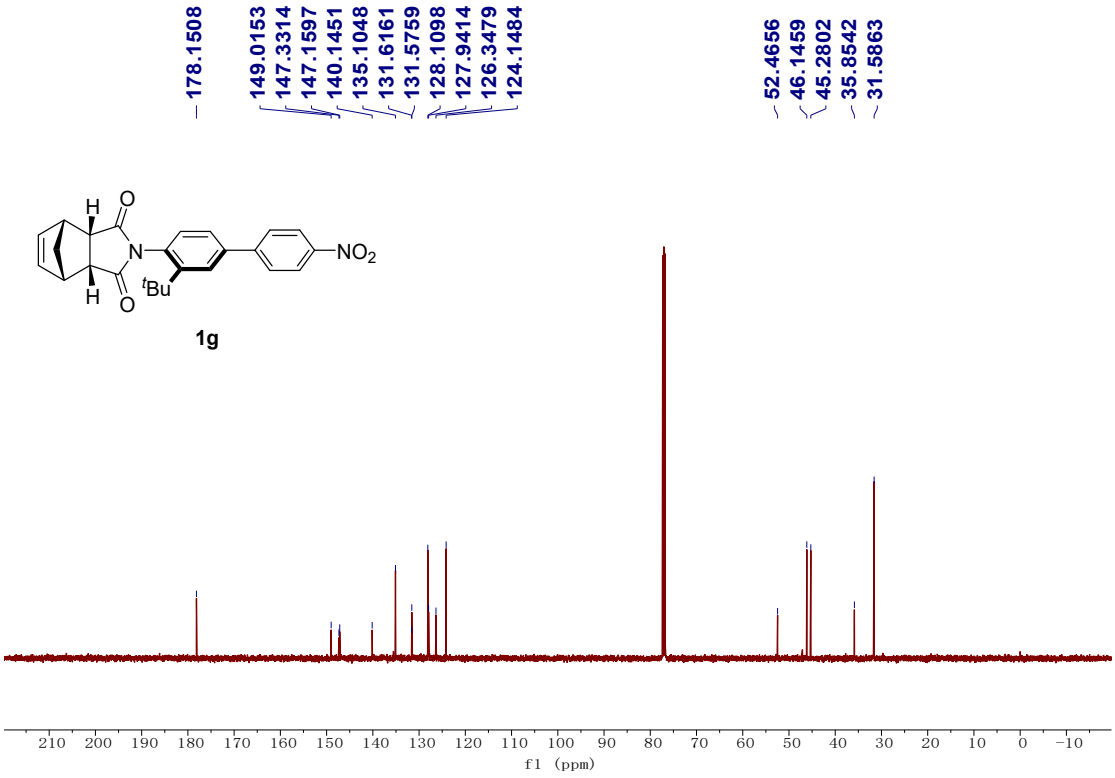
f1 (ppm)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H
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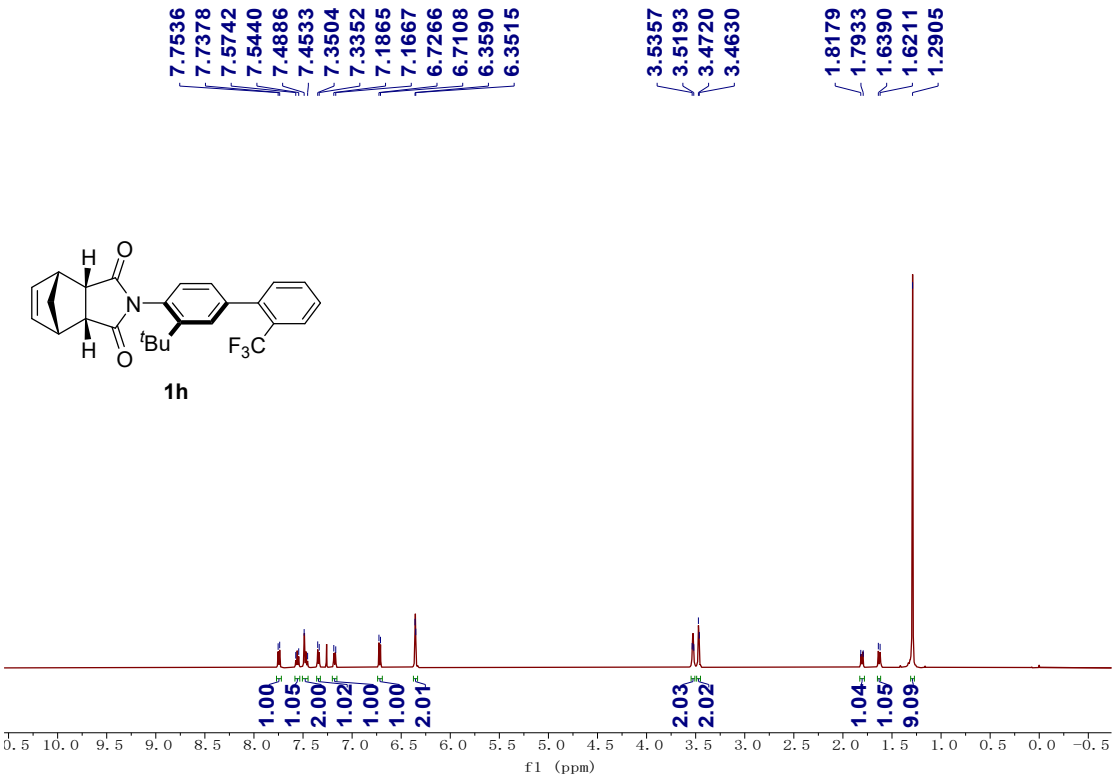
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N
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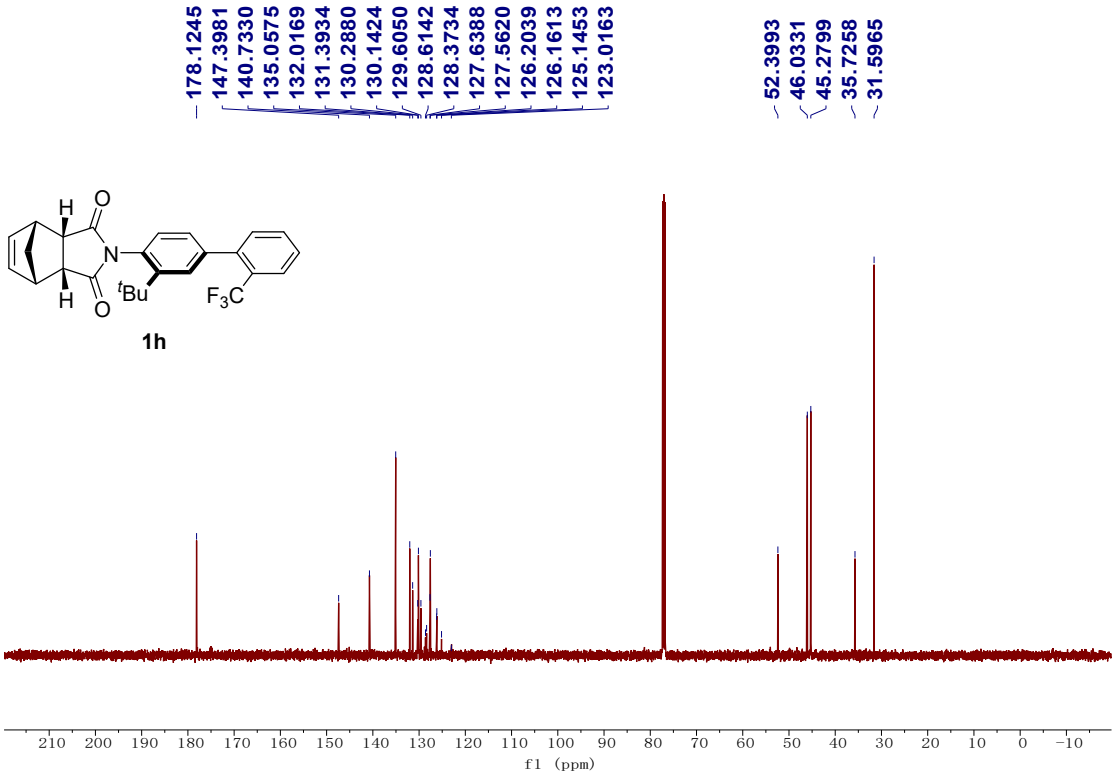
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127.5620
126.2039
126.1613
125.1453
123.0163
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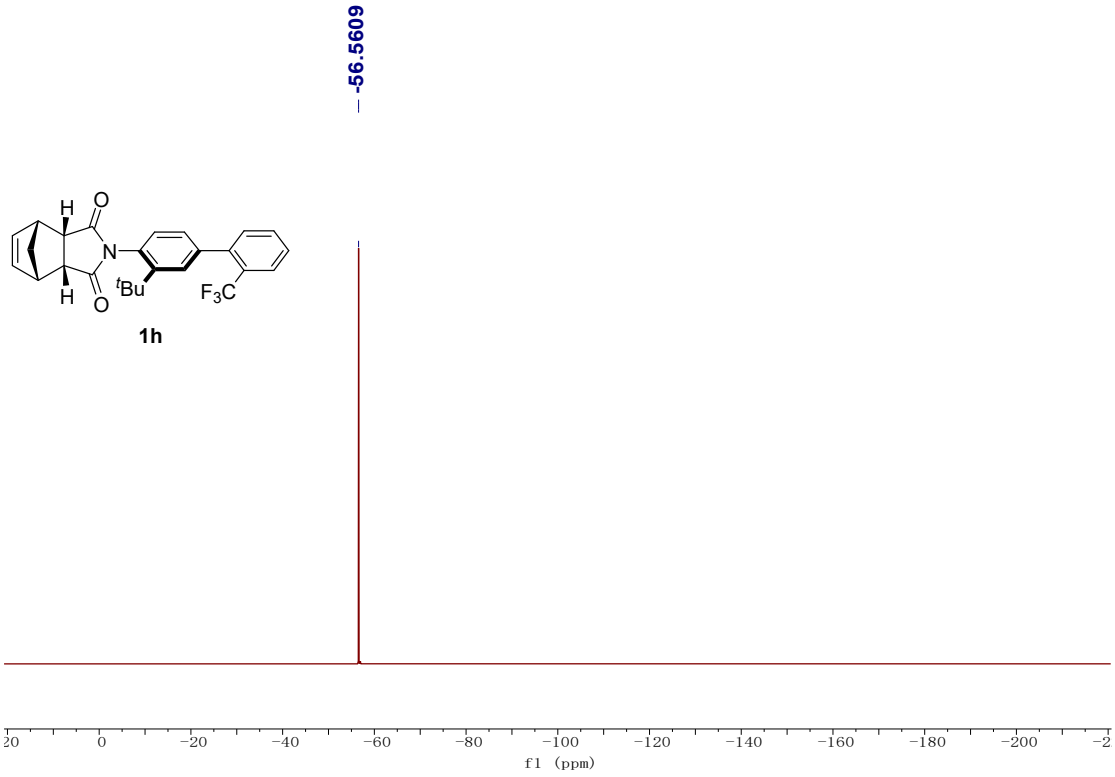
N
tBu
F3C
1h
f1 (ppm)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O
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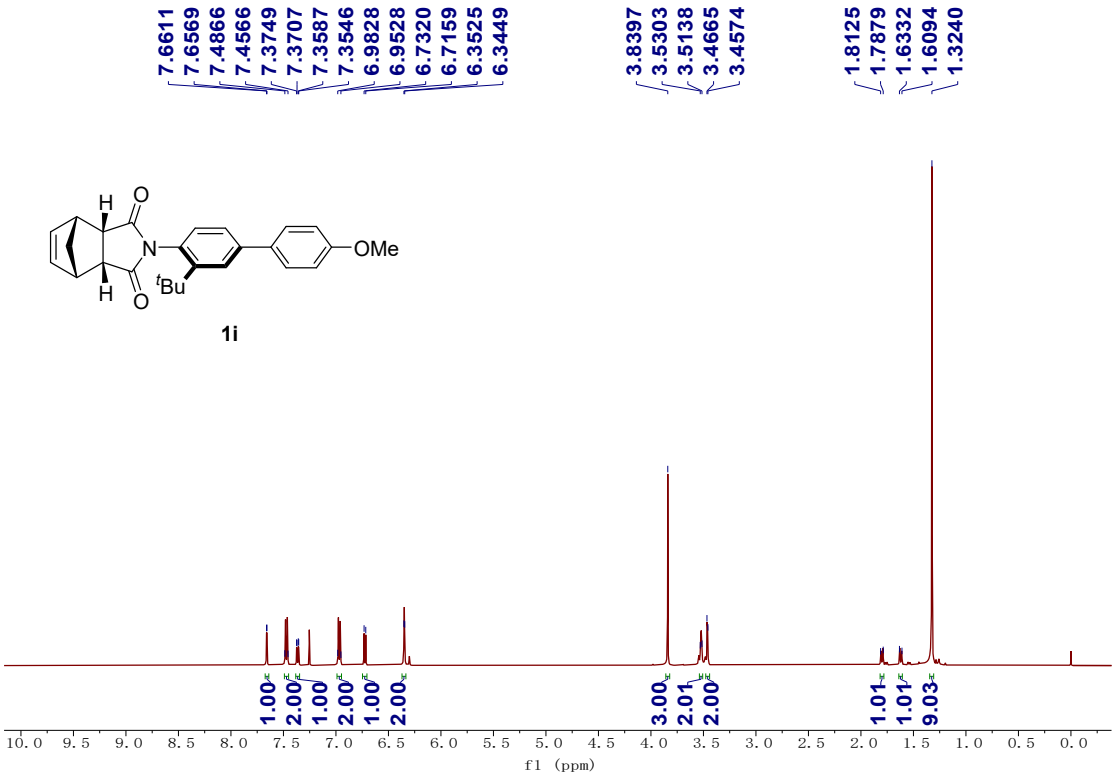
f1 (ppm)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OMe
tBu
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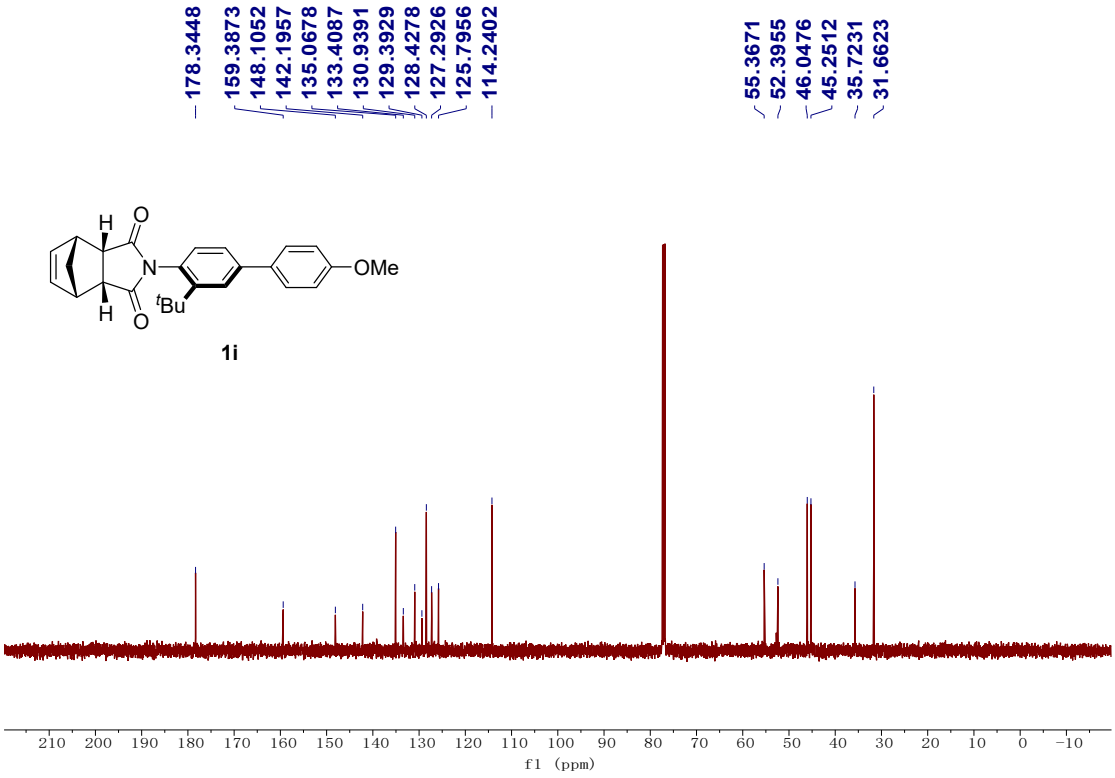
f1 (ppm)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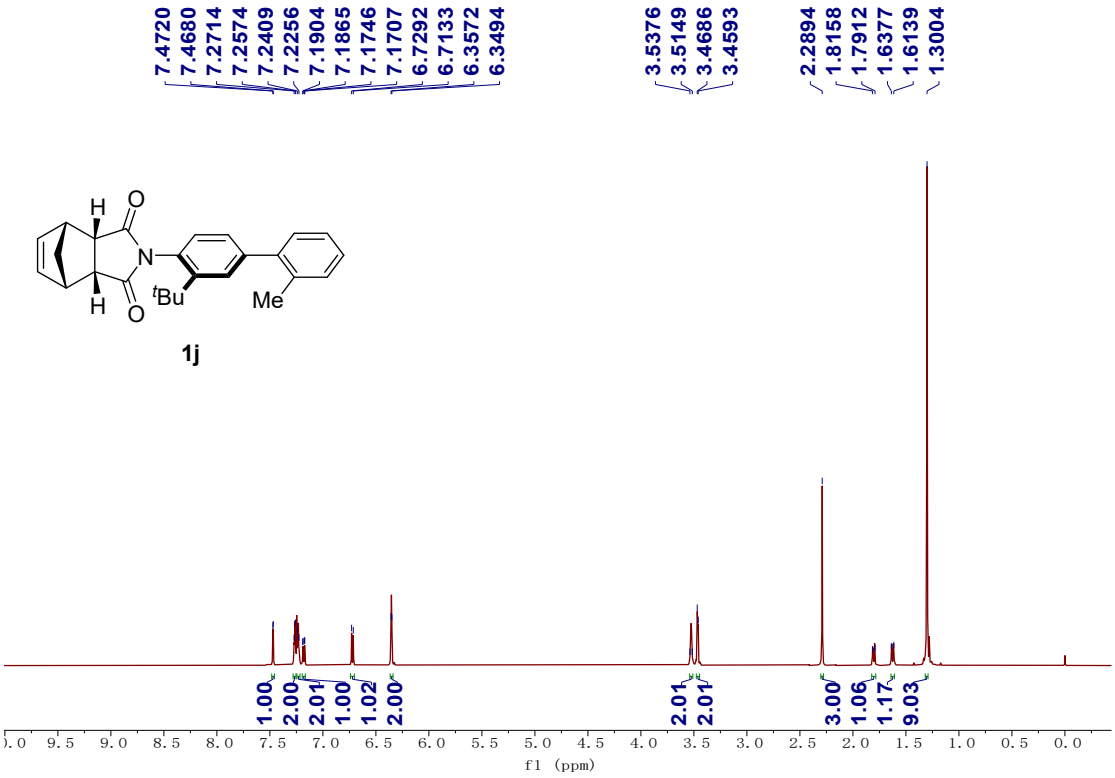
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H
O

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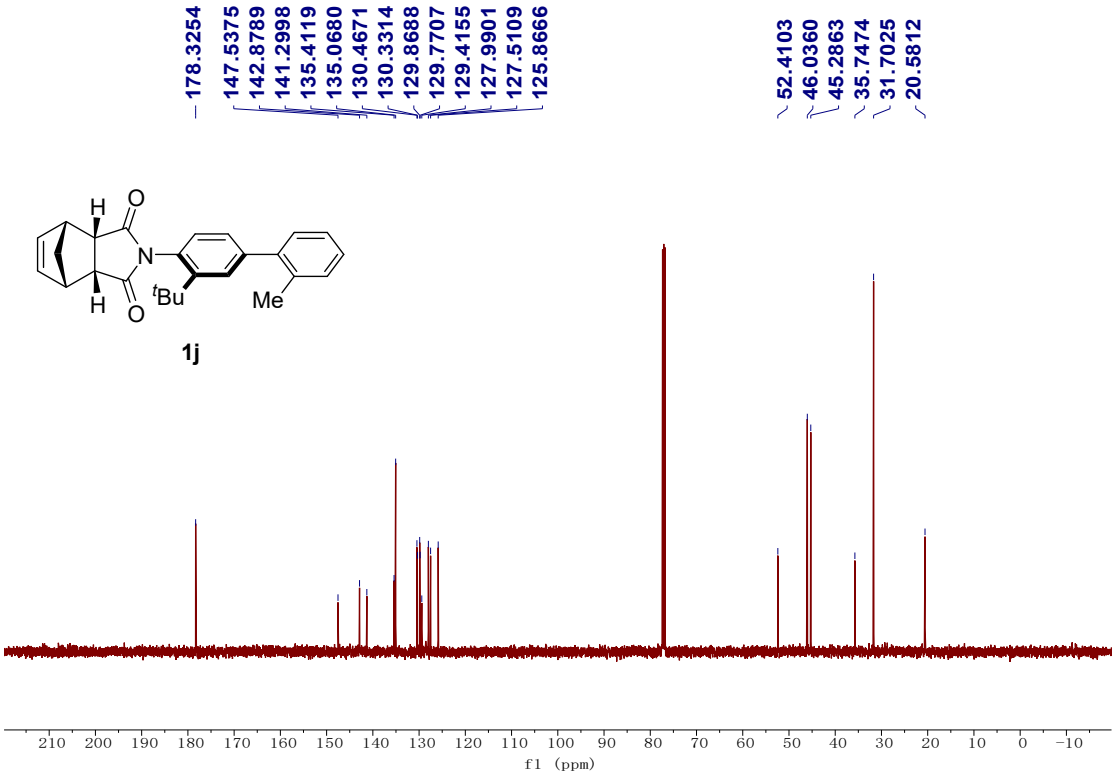
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f1 (ppm)

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O
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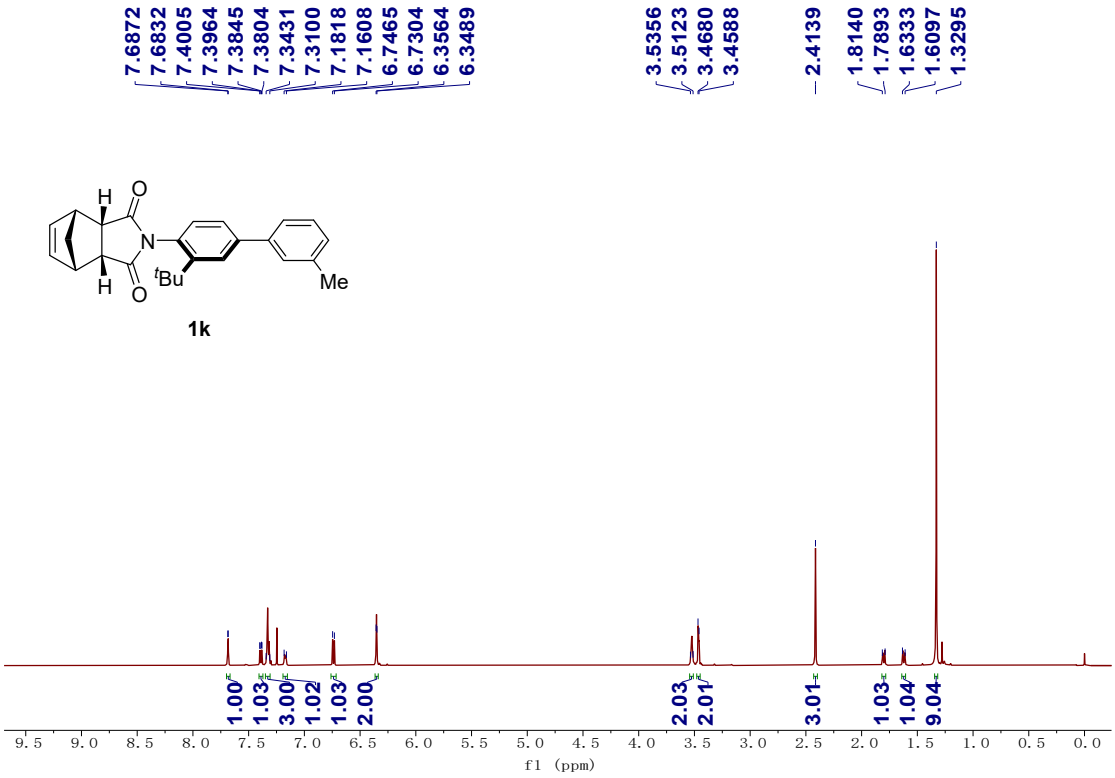
Me
H
O

1j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O
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Me
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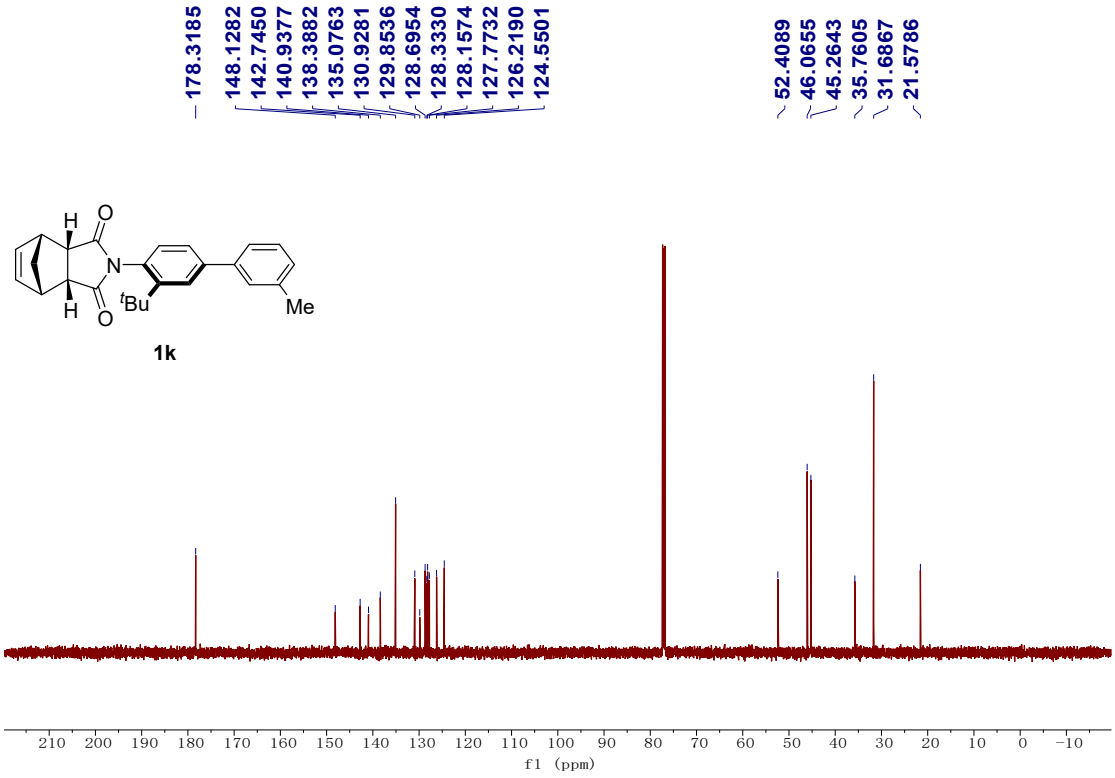
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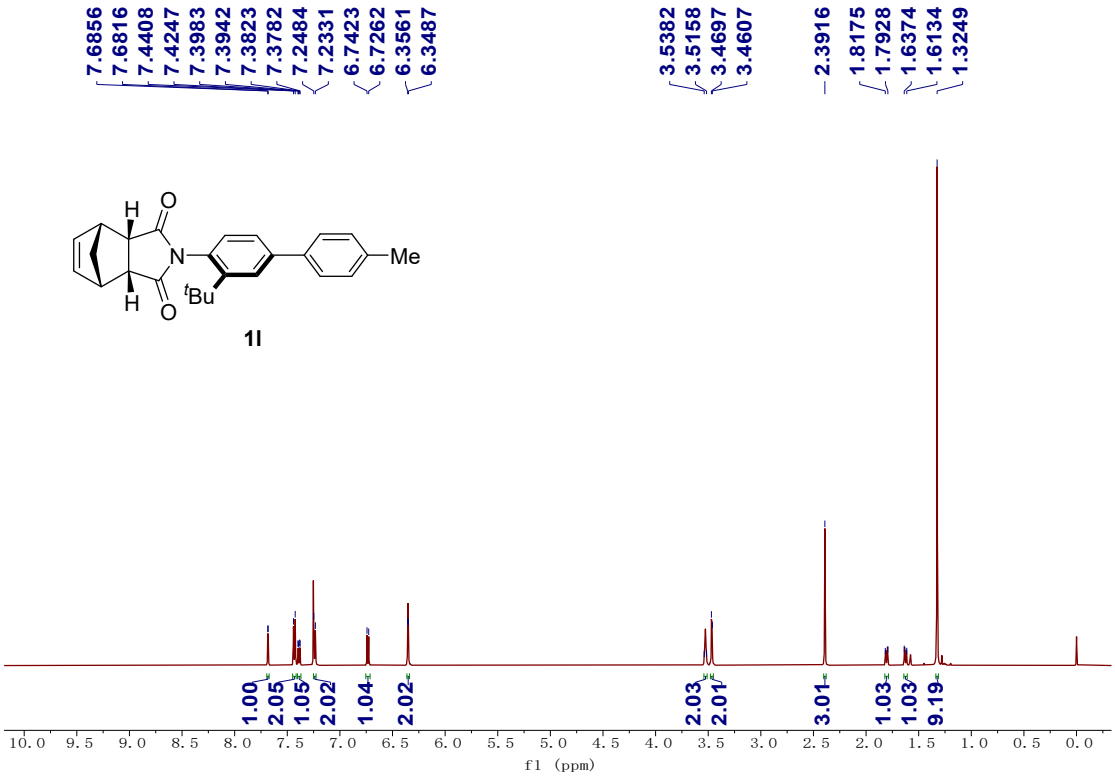
O
1k
f1 (ppm)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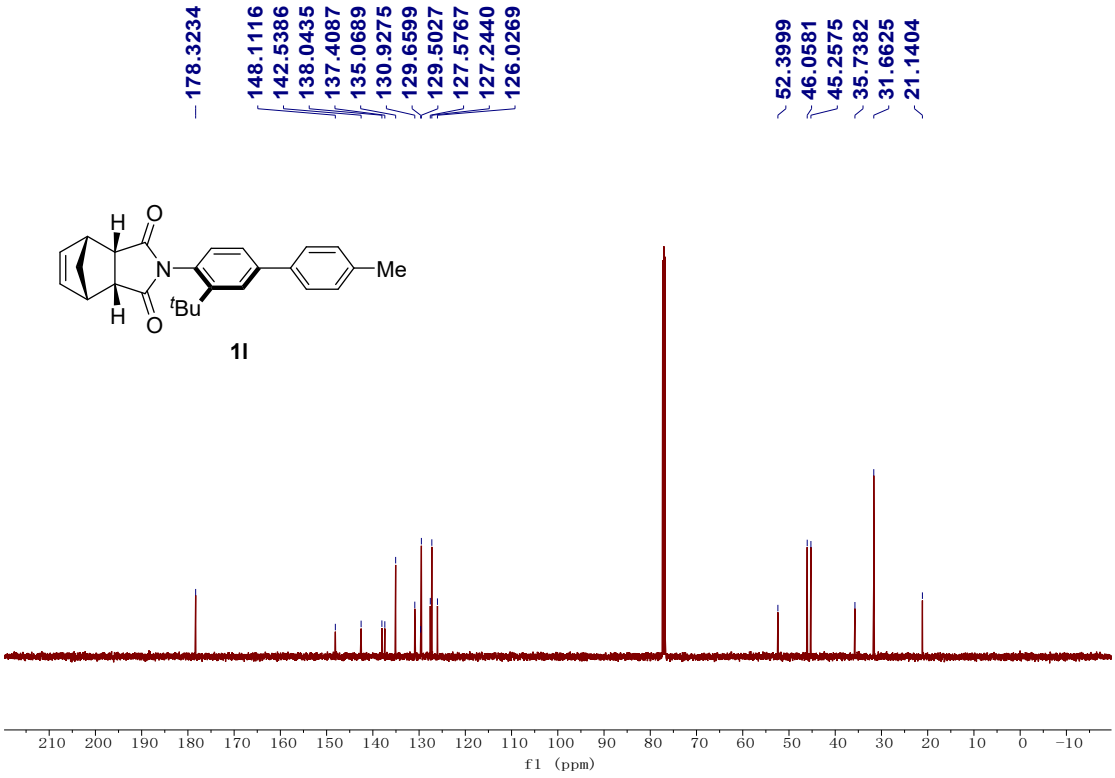
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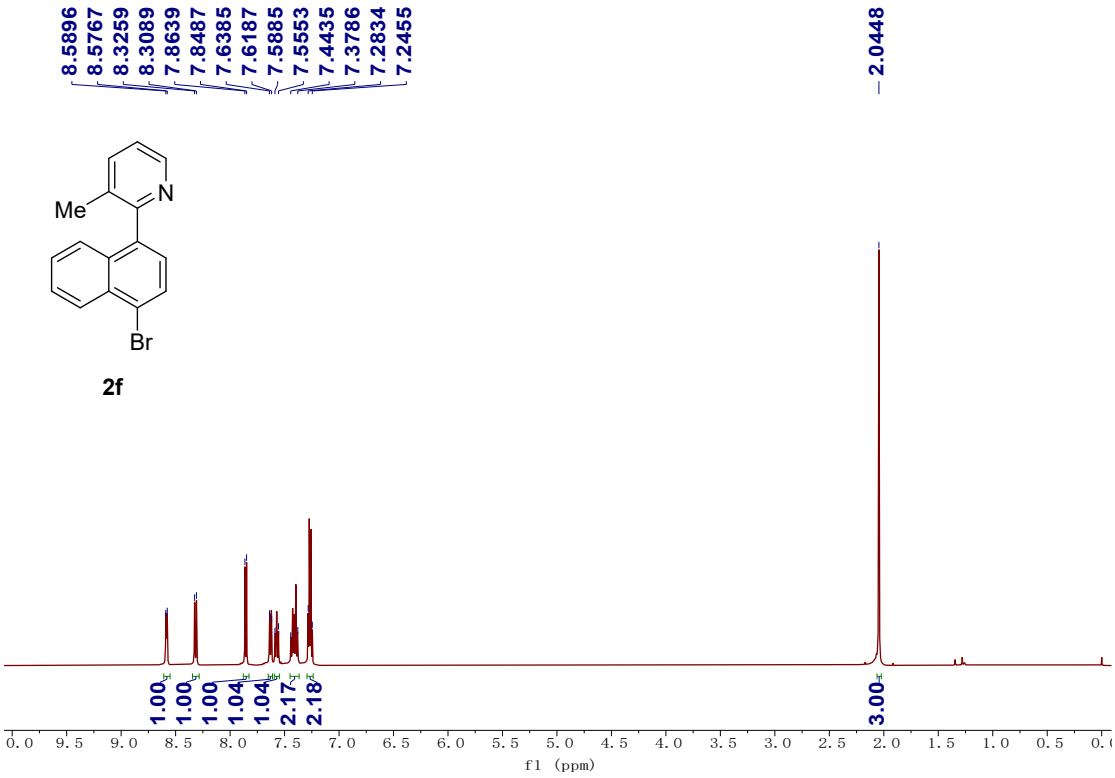
O
1l
f1 (ppm)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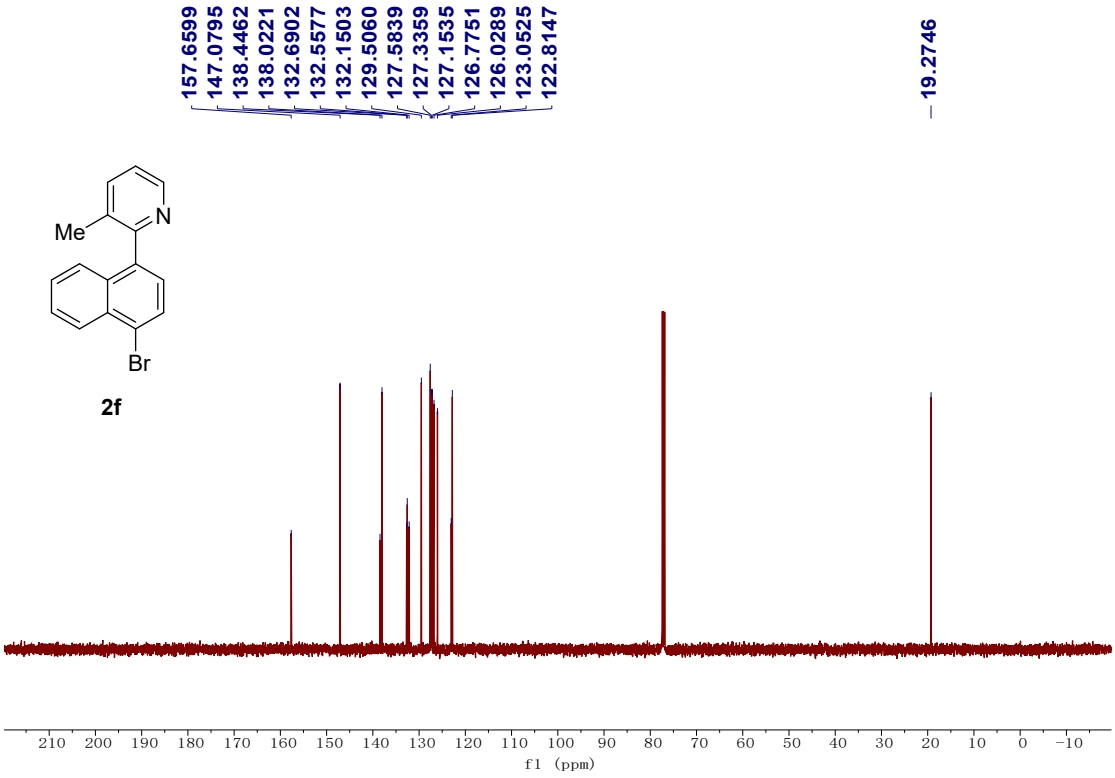
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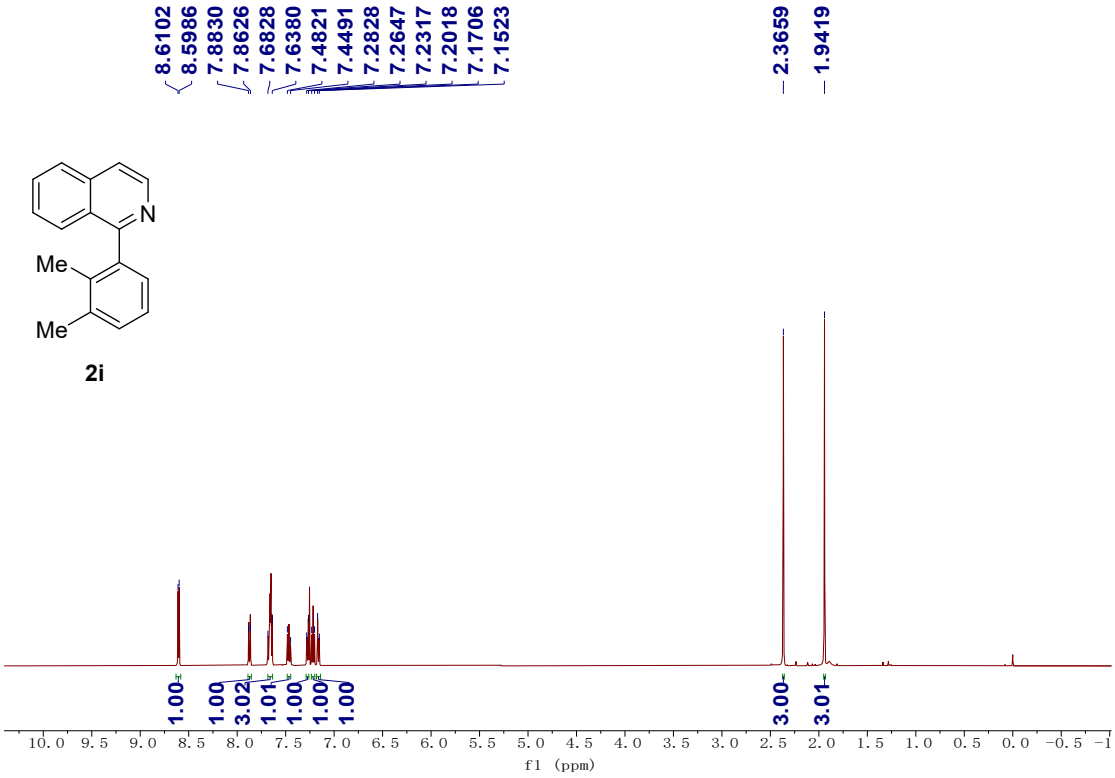
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7.1706
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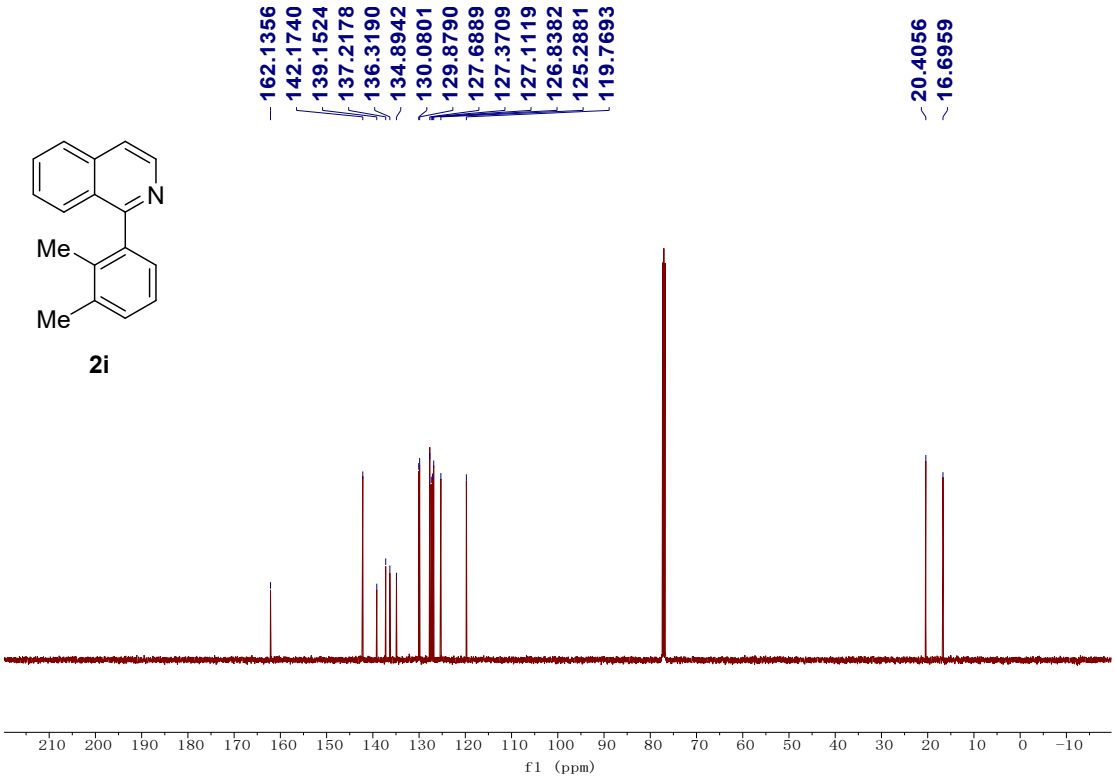
2i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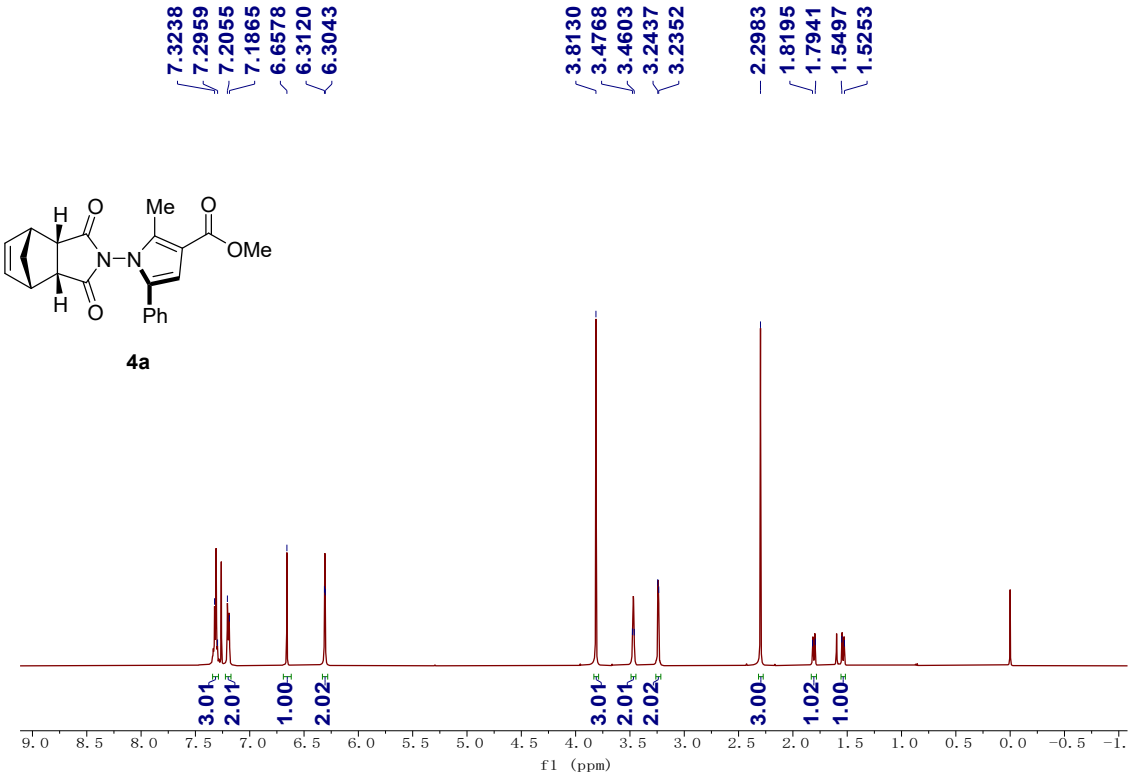
2i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3.2352
2.2983
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OMe
N–N
Ph
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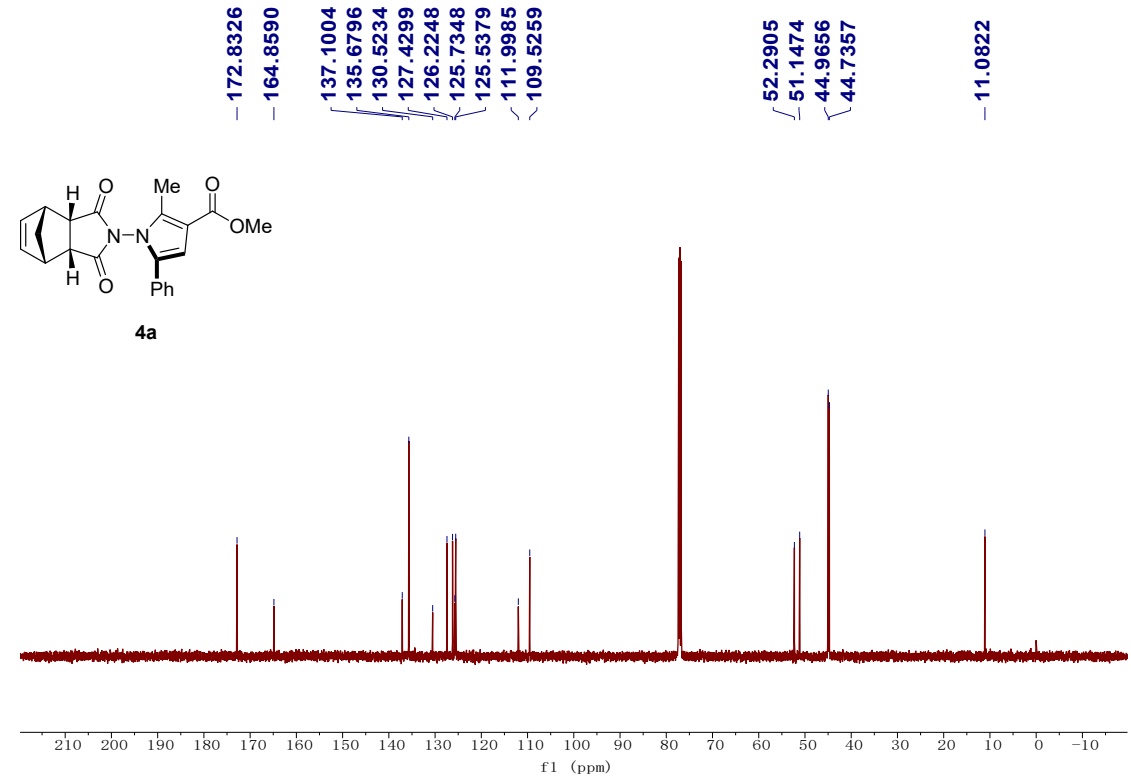
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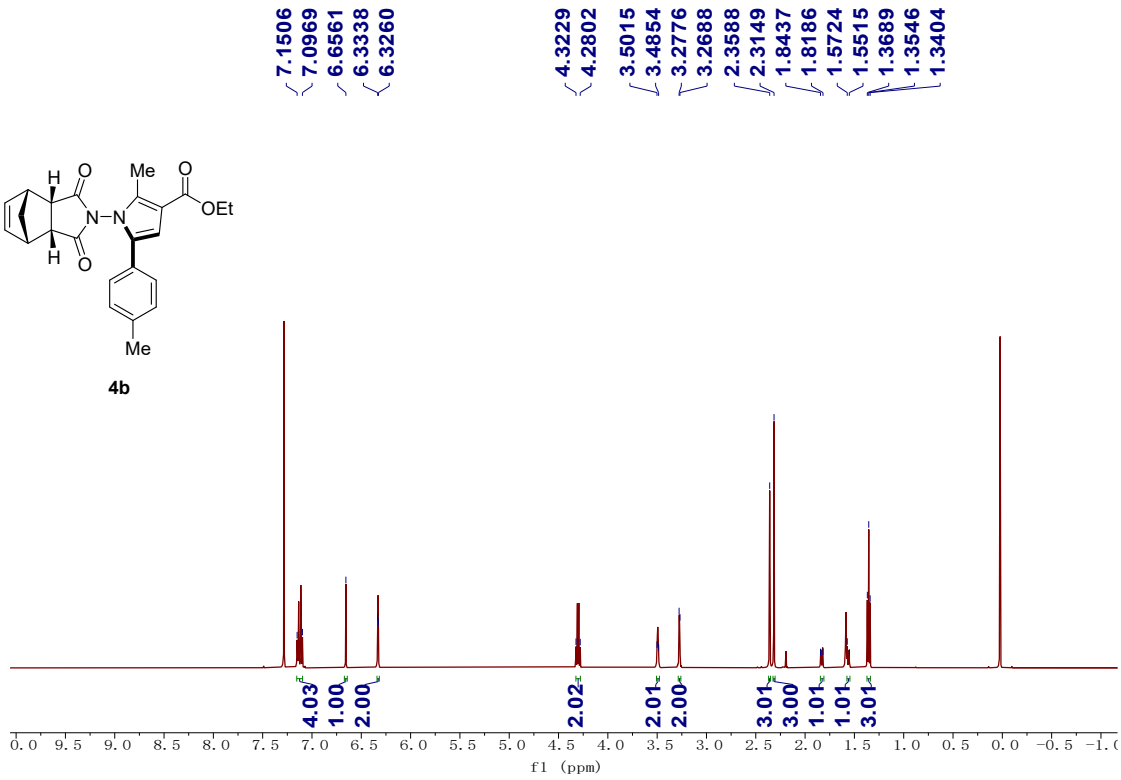
O
OMe
N–N
Ph
4a
f1 (ppm)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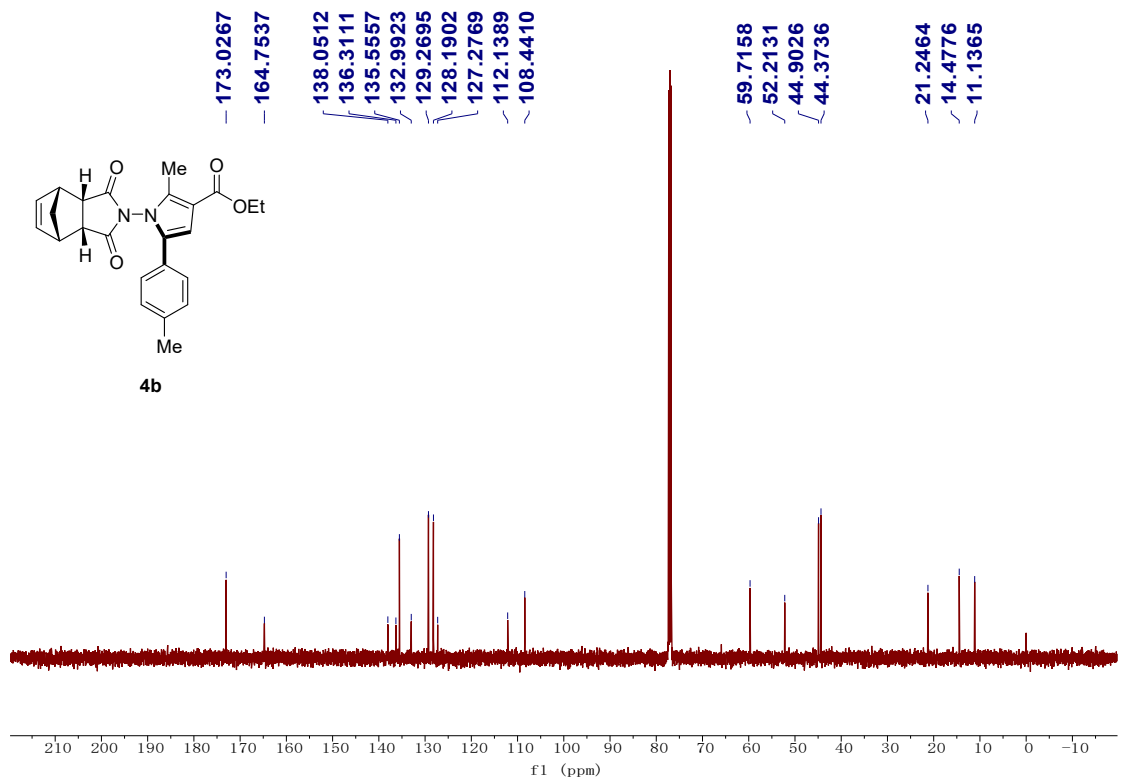
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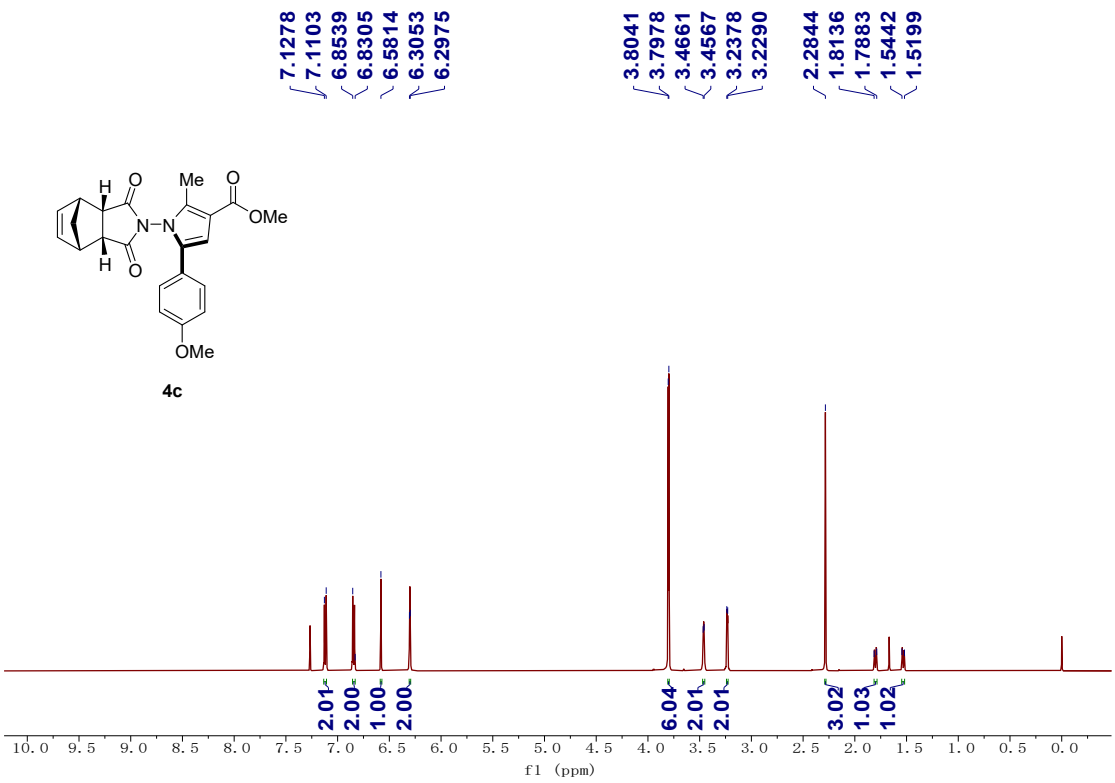
Me
O
OEt
H
O
N–N
H
O
Me
4b
f1 (ppm)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7.1103
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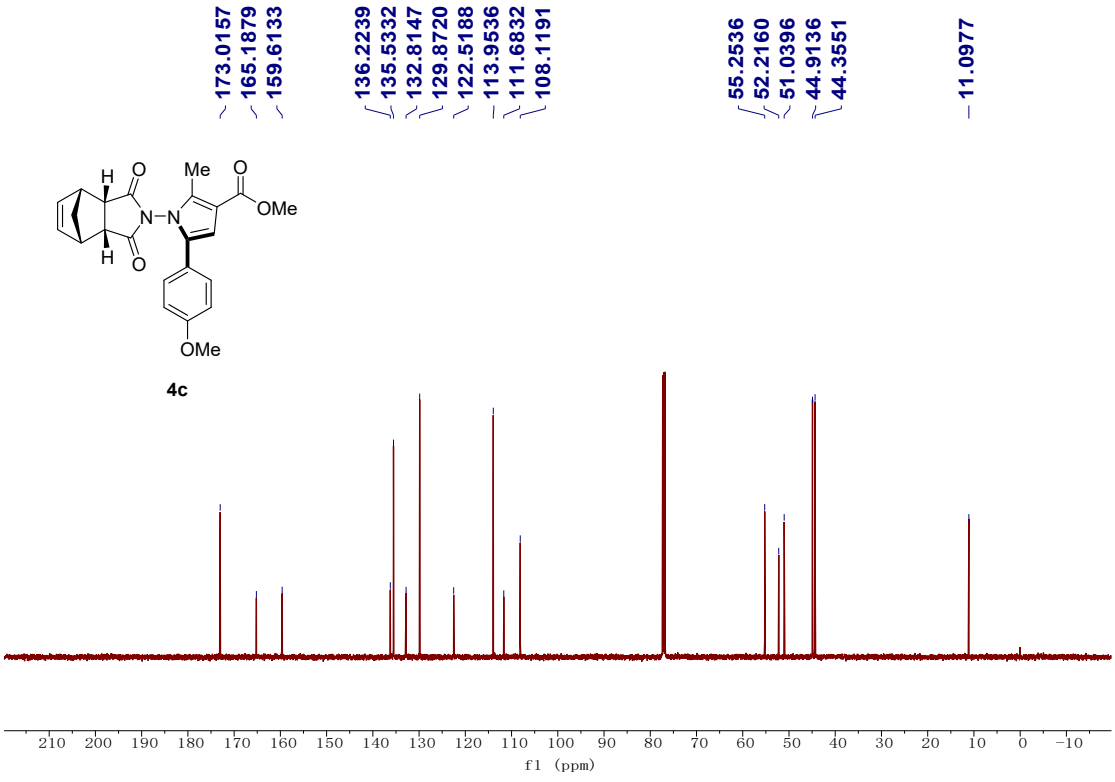
6.8305
6.5814
6.3053
6.2975
3.8041
3.7978
3.4661
3.4567
3.3378
3.2290
2.2844
1.8136
1.7883
1.5442
1.5199
Me
O
OMe
H
O
N–N
H
O
OMe
2.01
2.00
1.00
2.00
6.04
2.01
2.01
3.02
1.03
1.02
f1 (ppm)

4c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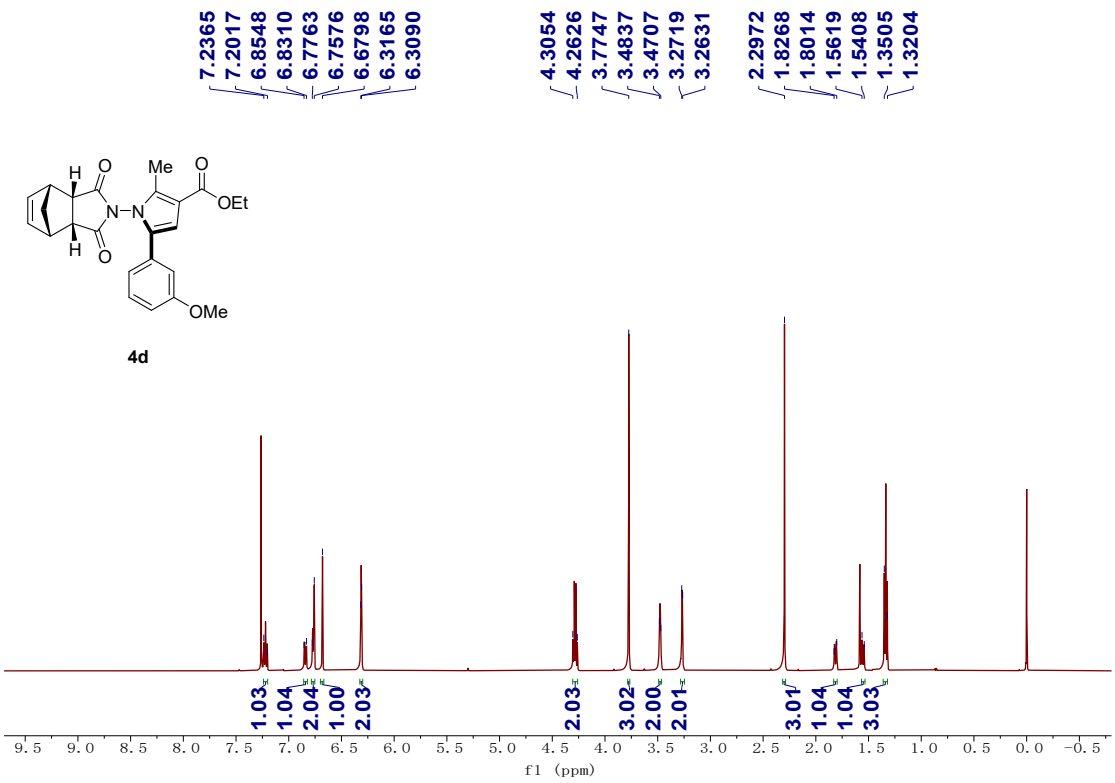
135.5332
132.8147
129.8720
122.5188
113.9536
111.6832
108.1191
55.2536
52.2160
51.0396
44.9136
44.3551
11.0977
Me
O
OMe
H
O
N–N
H
O
OMe
f1 (ppm)

4c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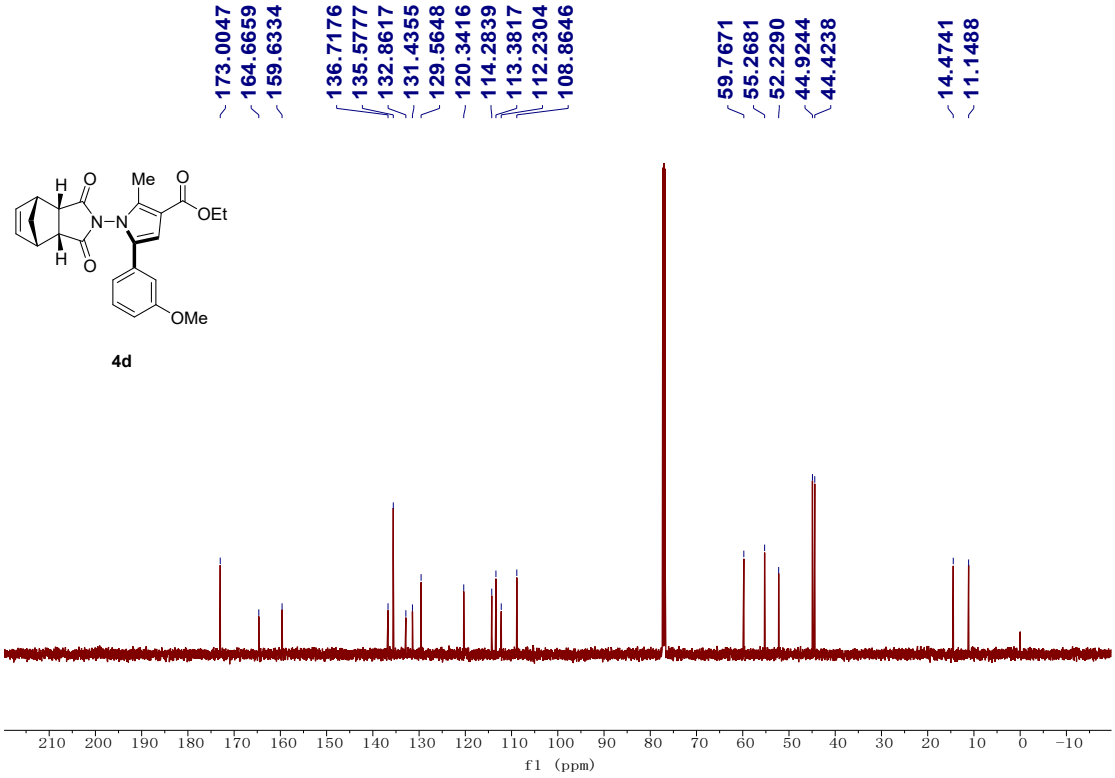
7.2017
6.8548
6.8310
6.7763
6.7576
6.6798
6.3165
6.3090
4.3054
4.2626
3.7747
3.4837
3.4707
3.2719
3.2631
2.2972
1.8268
1.8014
1.5619
1.5408
1.3505
1.3204
H
O
Me
O
N–N
OEt
H
O
OMe
4d
1.03
1.04
2.04
1.00
2.03
2.03
3.02
2.00
2.01
3.01
1.04
1.04
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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131.4355
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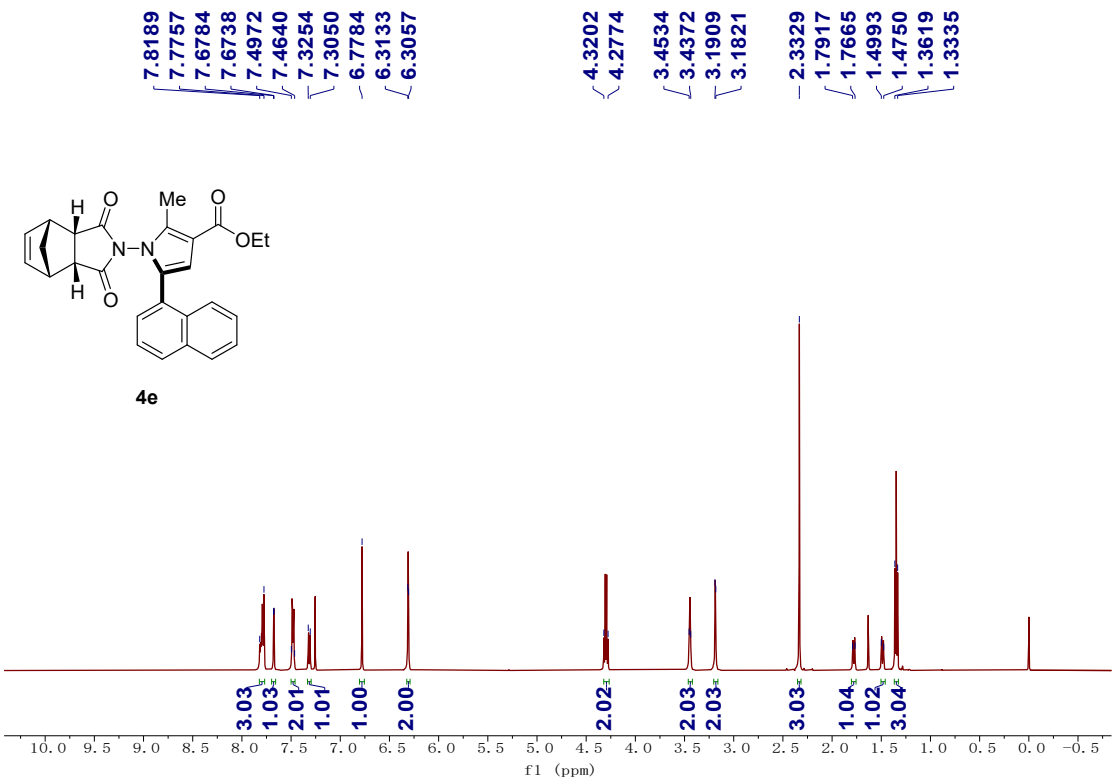
114.2839
113.3817
112.2304
108.8646
59.7671
55.2681
52.2290
44.9244
44.4238
14.4741
11.1488
H
O
Me
O
N–N
OEt
H
O
OMe
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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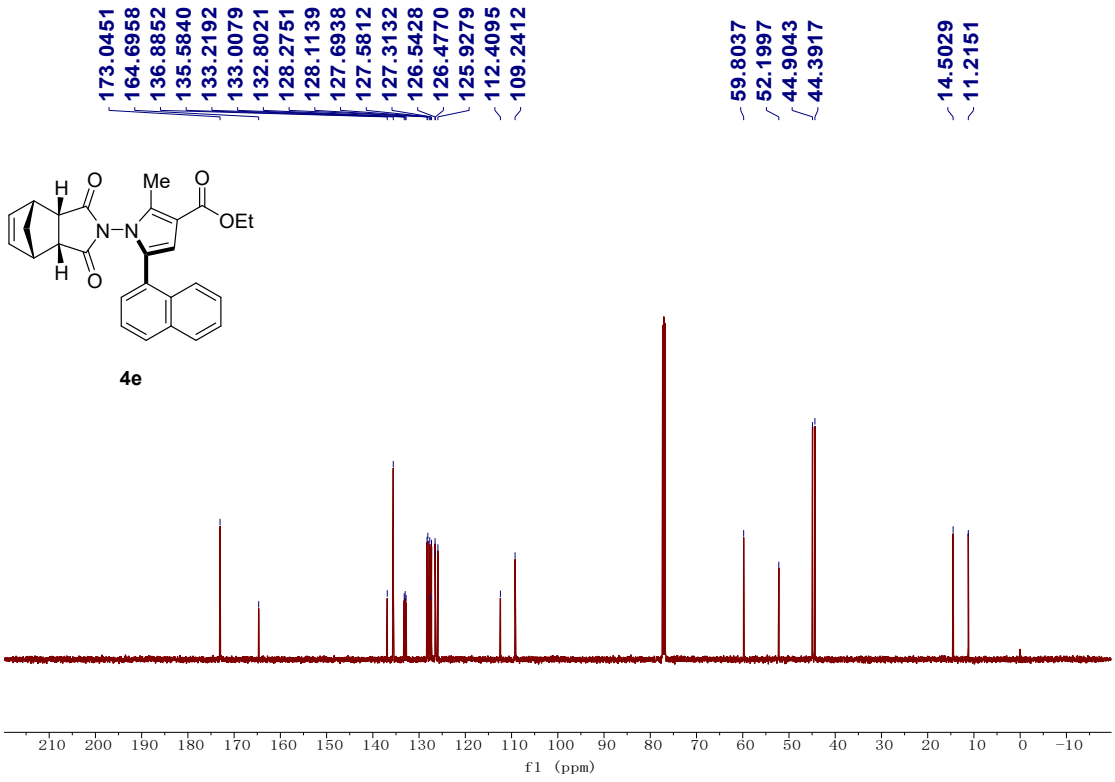
7.7757
7.6784
7.6738
7.4972
7.4640
7.3254
7.3050
6.7784
6.3133
6.3057
4.3202
4.2774
3.4534
3.4372
3.1909
3.1821
2.3329
1.7917
1.7665
1.4993
1.4750
1.3619
1.3335
Me
O
OEt
N–N
H
O
4e
3.03
1.03
2.01
1.01
1.00
2.00
2.02
2.03
2.03
3.03
1.04
1.02
3.04
f1 (ppm)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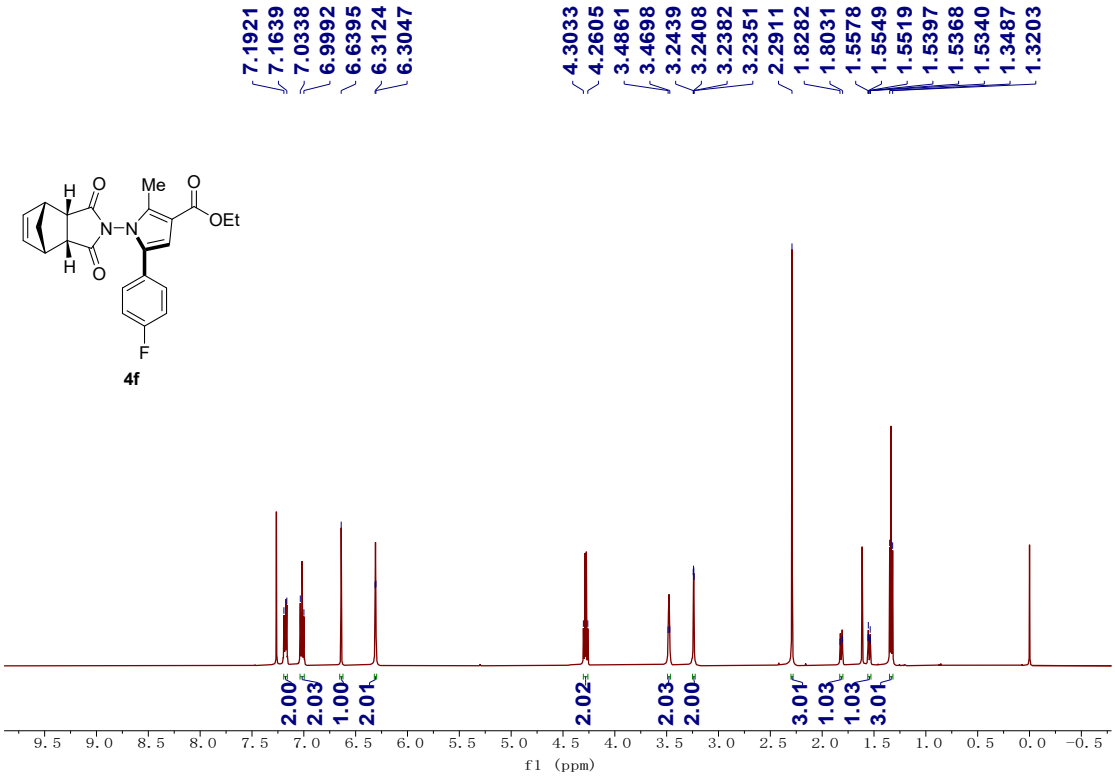
133.2192
133.0079
132.8021
128.2751
128.1139
127.6938
127.5812
127.3132
126.5428
126.4770
125.9279
112.4095
109.2412
59.8037
52.1997
44.9043
44.3917
14.5029
11.2151
Me
O
OEt
N–N
H
O
4e
f1 (ppm)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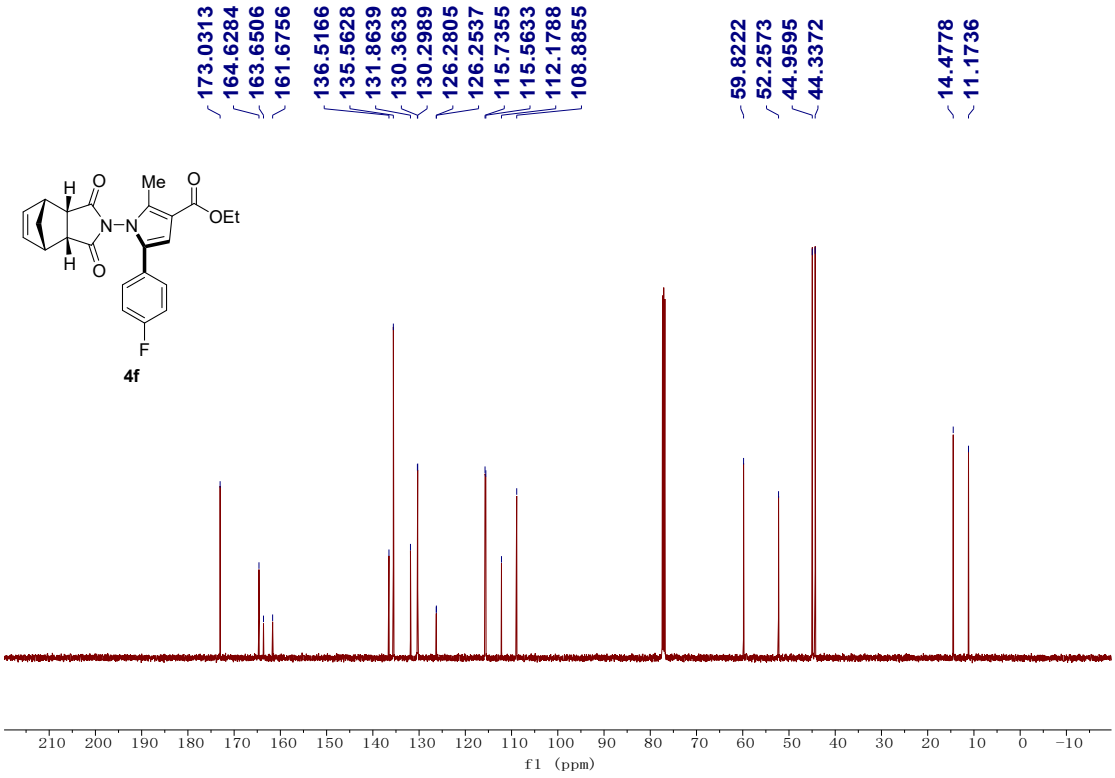
7.0338
6.9992
6.6395
6.3124
6.3047
4.3033
4.2605
3.4861
3.4698
3.2439
3.2408
3.2382
3.2351
2.2911
1.8282
1.8031
1.5578
1.5549
1.5519
1.5397
1.5368
1.5340
1.3487
1.3203
Me
O
OEt
N
H
O
F
4f
2.00
2.03
1.00
2.01
2.02
2.03
2.00
3.01
1.03
1.03
3.01
f1 (ppm)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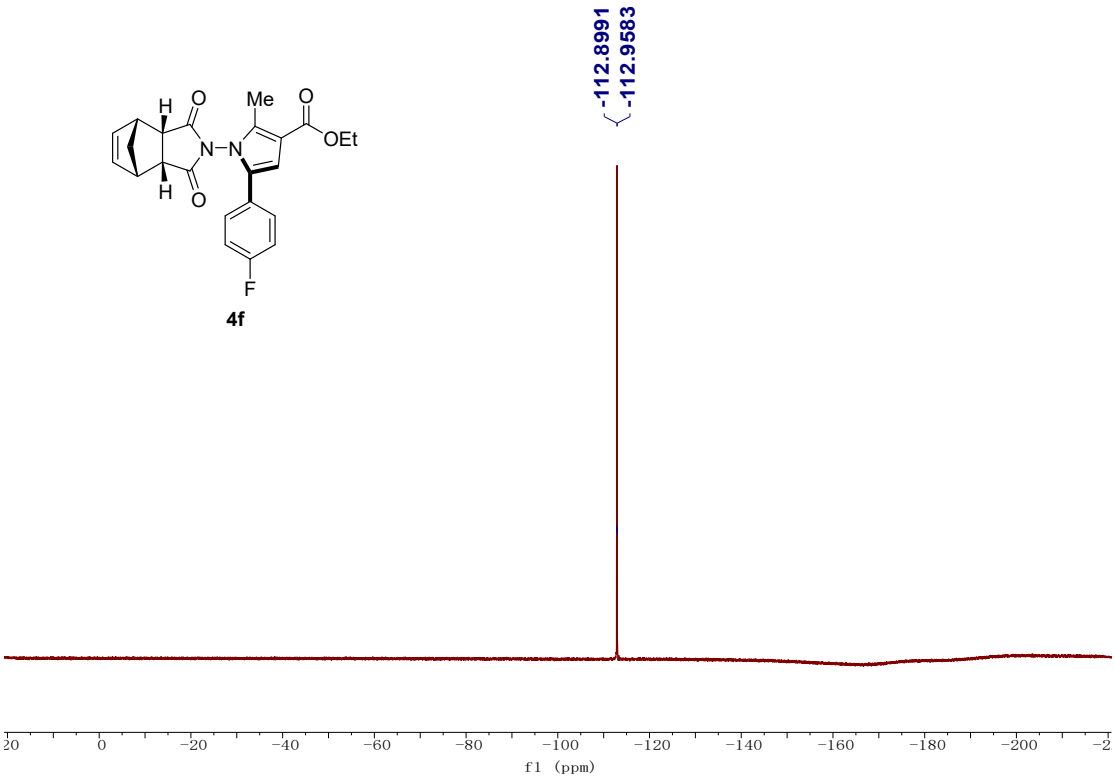
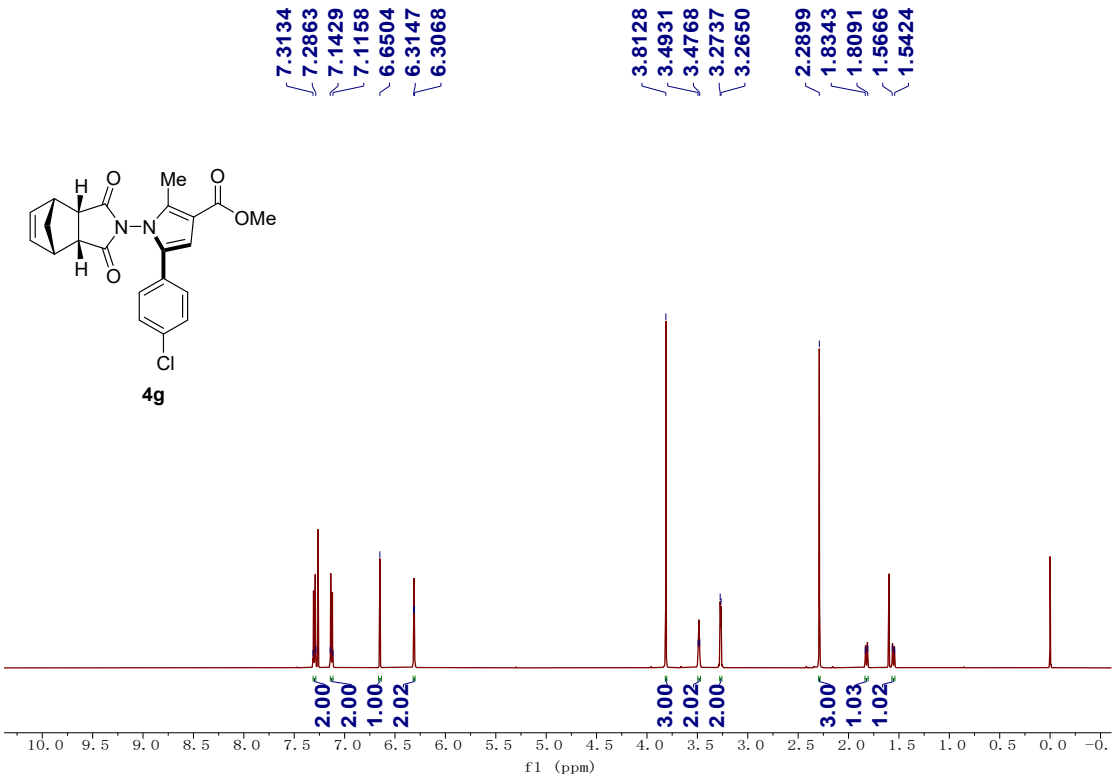
163.6506
161.6756
136.5166
135.5628
131.8639
130.3638
130.2989
126.2805
126.2537
115.7355
115.5633
112.1788
108.8855
59.8222
52.2573
44.9595
44.3372
14.4778
11.1736
Me
O
OEt
N
H
O
F
4f
f1 (ppm)


-112.8991
-112.9583
H
O
Me
O
N
N
OEt
H
O
F
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

4f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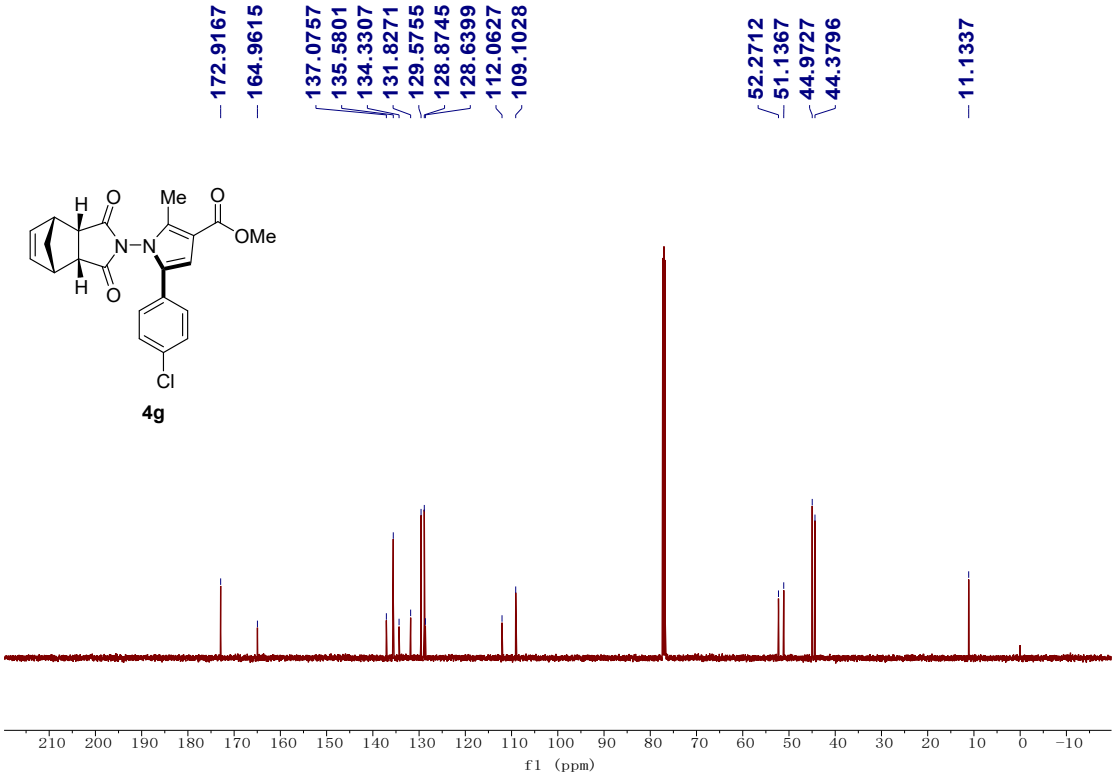
7.2863
7.1429
7.1158
6.6504
6.3147
6.3068
3.8128
3.4931
3.4768
3.2737
3.2650
2.2899
1.8343
1.8091
1.5666
1.5424
2.00
2.00
1.00
2.02
3.00
2.02
2.00
3.00
1.03
1.02
f1 (ppm)

H
O
Me
O
N
N
OMe
H
O
Cl

4g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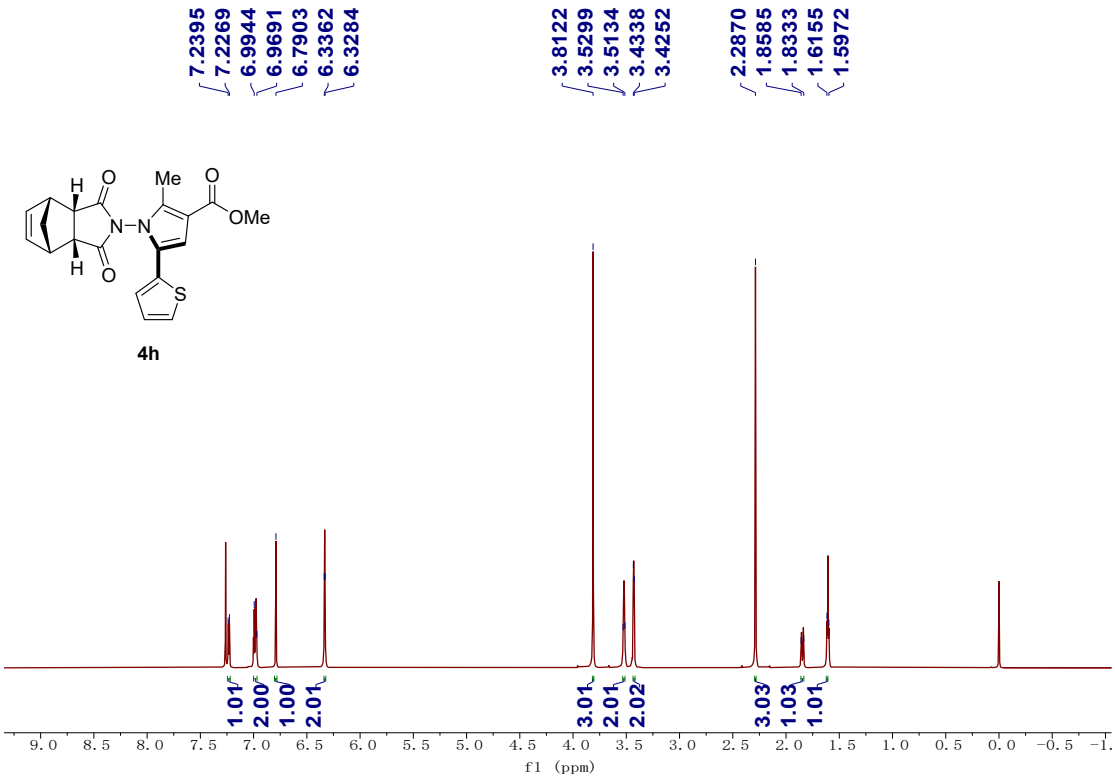
135.5801
134.3307
131.8271
129.5755
128.8745
128.6399
112.0627
109.1028
52.2712
51.1367
44.9727
44.3796
11.1337
f1 (ppm)

H
O
Me
O
N
N
OMe
H
O
Cl

4g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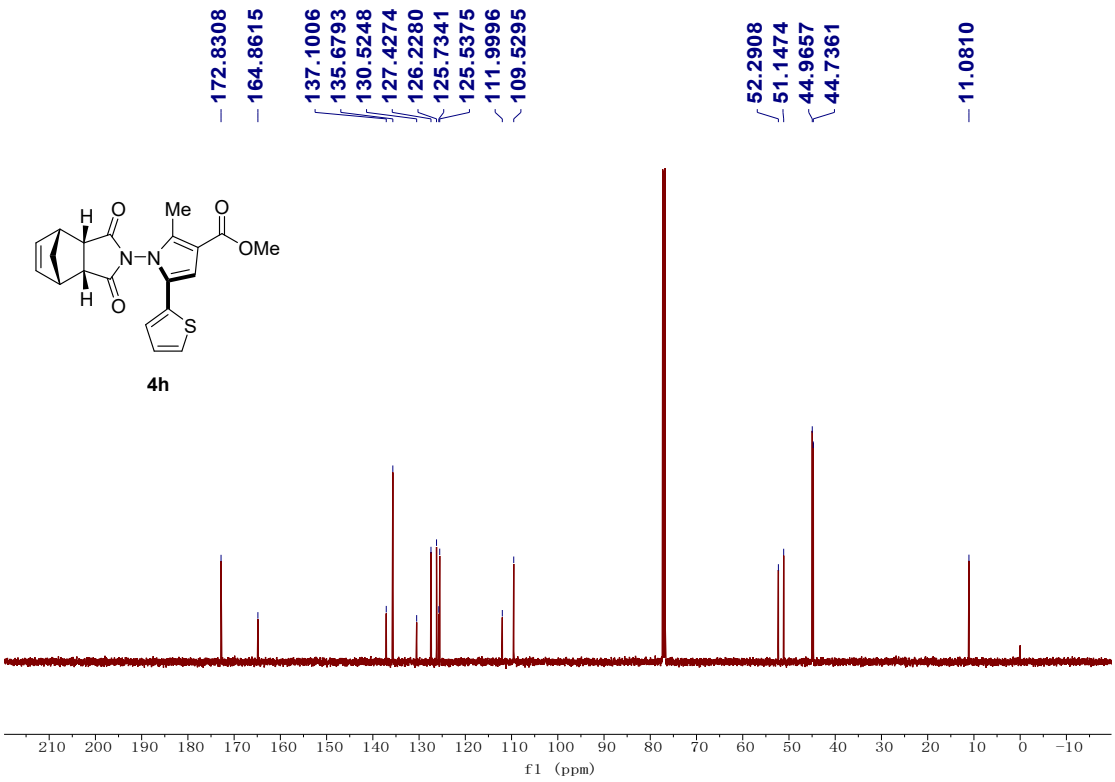
7.2269
6.9944
6.9691
6.7903
6.3362
6.3284
3.8122
3.5299
3.5134
3.4338
3.4252
2.2870
1.8585
1.8333
1.6155
1.5972
H
O
Me
O
N–N
OMe
H
O
S
4h
1.01
2.00
1.00
2.01
3.01
2.01
2.02
3.03
1.03
1.01
f1 (ppm)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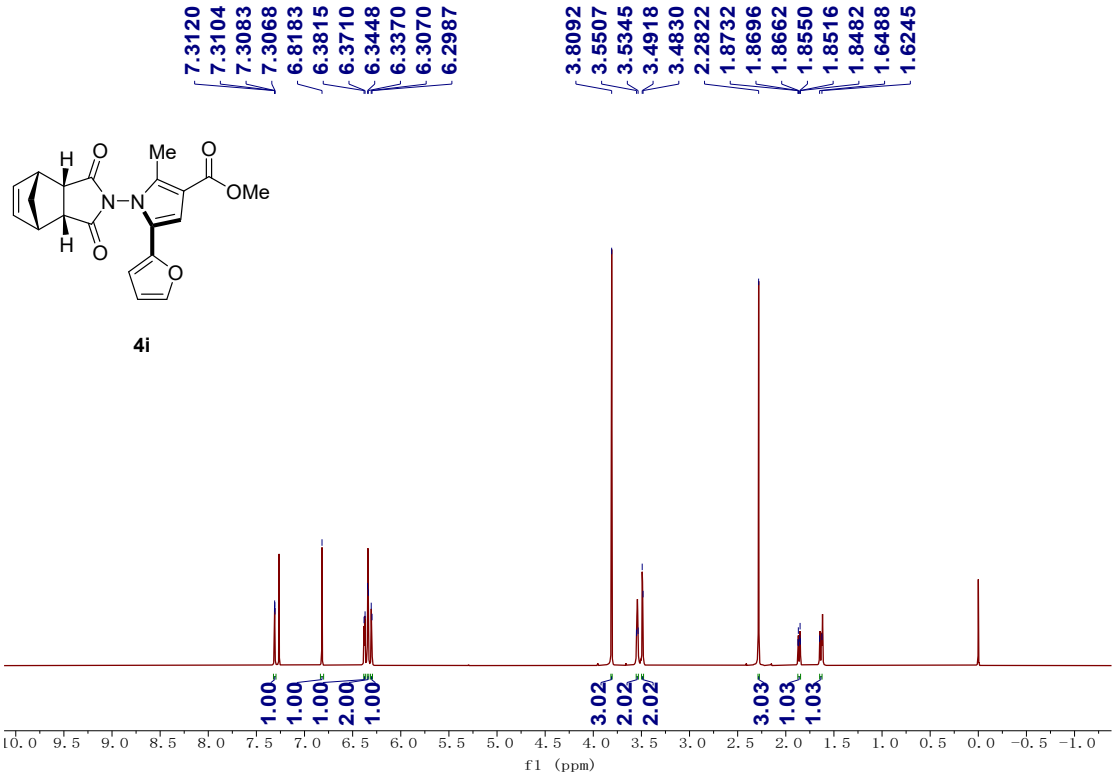
127.4274
126.2280
125.7341
125.5375
111.9996
109.5295
52.2908
51.1474
44.9657
44.7361
11.0810
H
O
Me
O
N–N
OMe
H
O
S
4h
f1 (ppm)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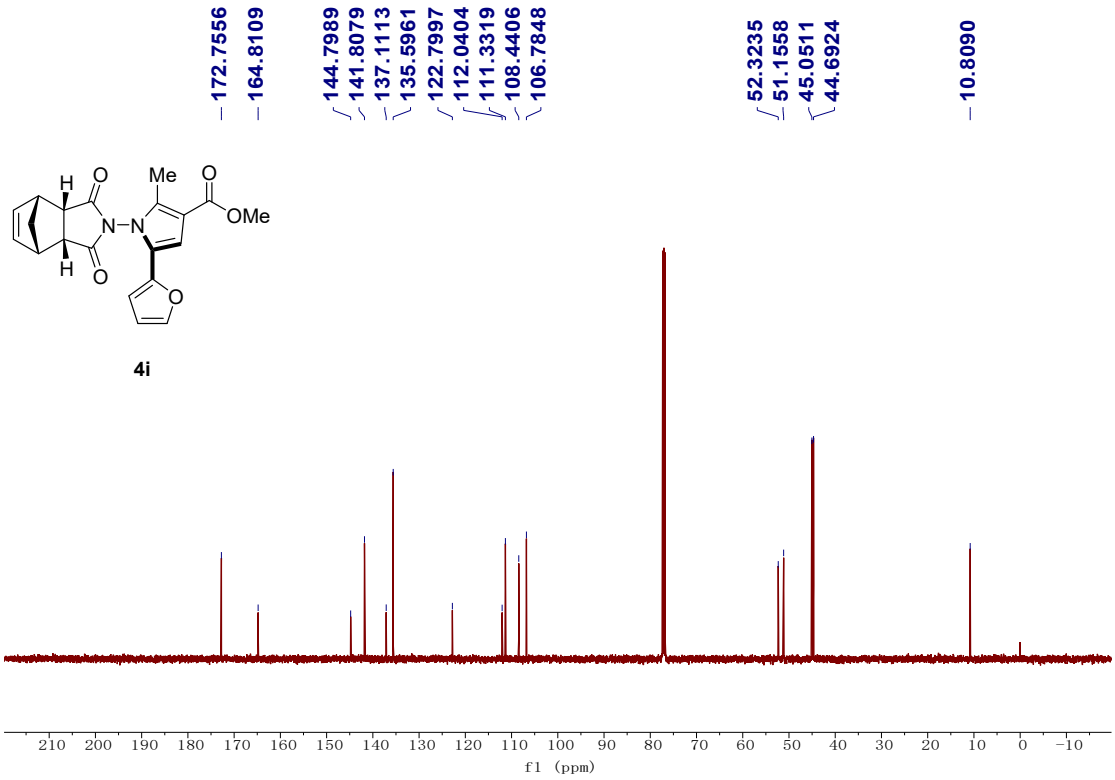
7.3104
7.3083
7.3068
6.8183
6.3815
6.3710
6.3448
6.3370
6.3070
6.2987
3.8092
3.5507
3.5345
3.4918
3.4830
2.2822
1.8732
1.8696
1.8662
1.8550
1.8516
1.8482
1.6488
1.6245
Me
O
OMe
H
N–N
1.00
1.00
1.00
2.00
1.00
3.02
2.02
2.02
3.03
1.03
1.03
f1 (ppm)

4i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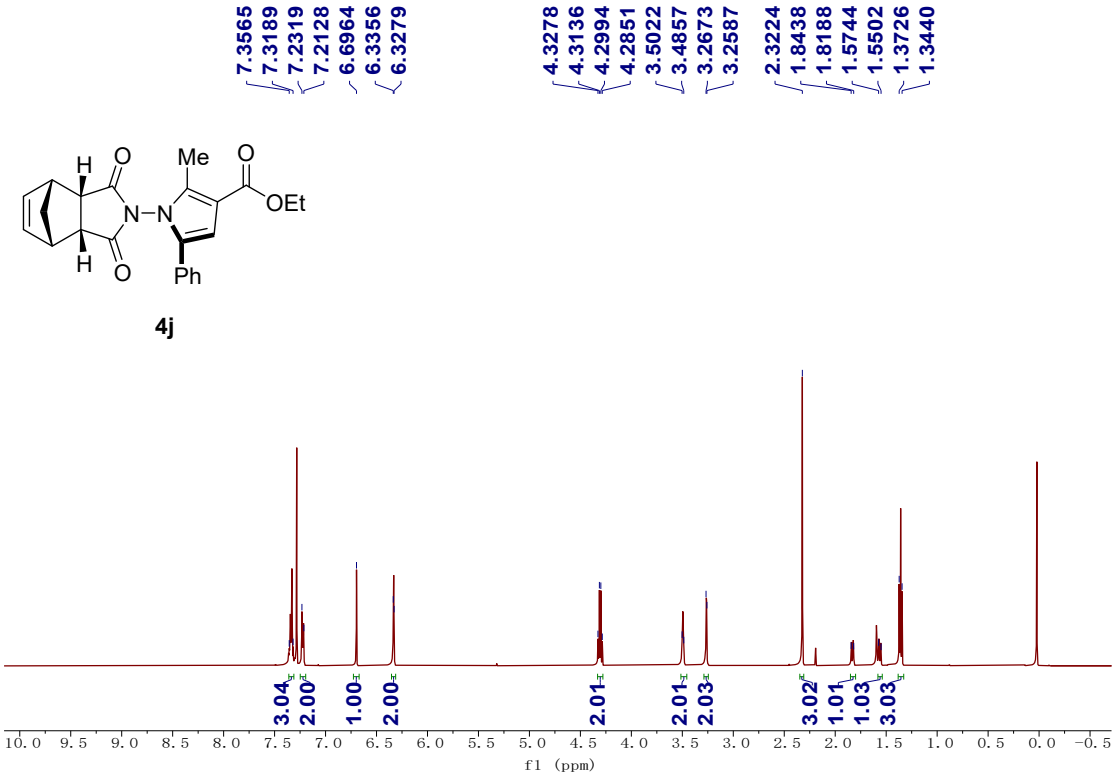
141.8079
137.1113
135.5961
122.7997
112.0404
111.3319
108.4406
106.7848
52.3235
51.1558
45.0511
44.6924
10.8090
Me
O
OMe
H
N–N
f1 (ppm)

4i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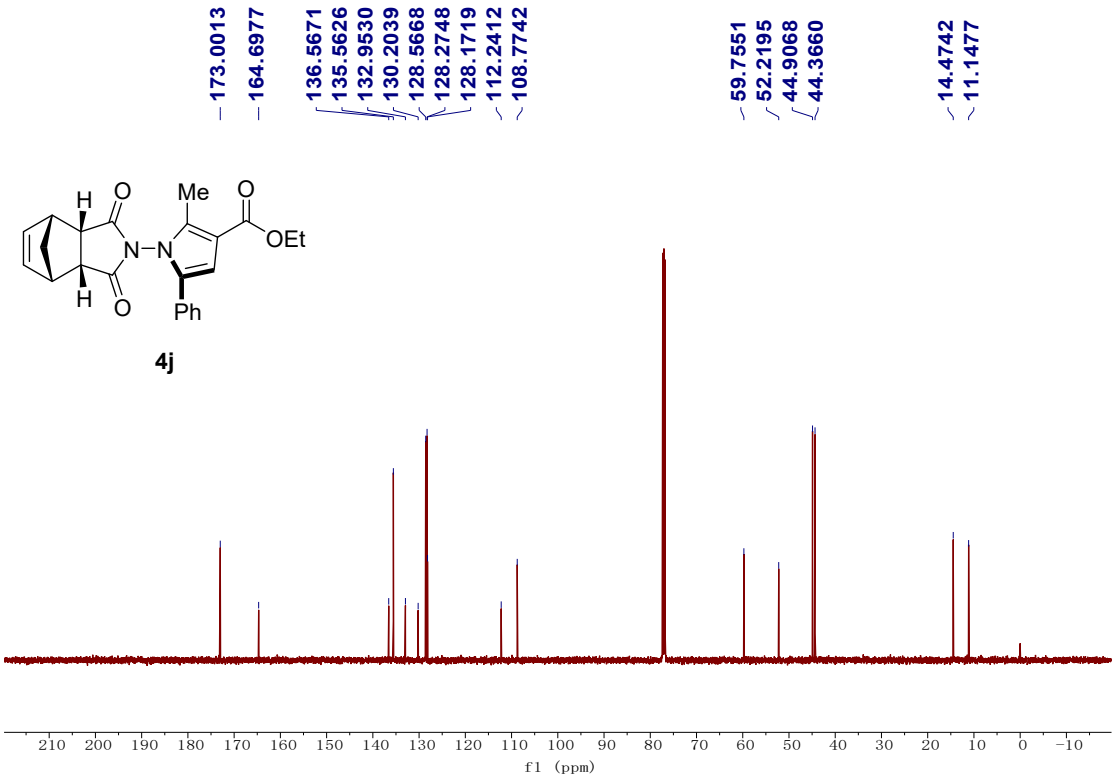
7.2319
7.2128
6.6964
6.3356
6.3279
4.3278
4.3136
4.2994
4.2851
3.5022
3.4857
3.2673
3.2587
2.3224
1.8438
1.8188
1.5744
1.5502
1.3726
1.3440
H
O
Me
O
N–N
OEt
H
O
Ph
3.04
2.00
1.00
2.00
2.01
2.01
2.03
3.02
1.01
1.03
3.03
f1 (ppm)

4j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128.5668
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128.1719
112.2412
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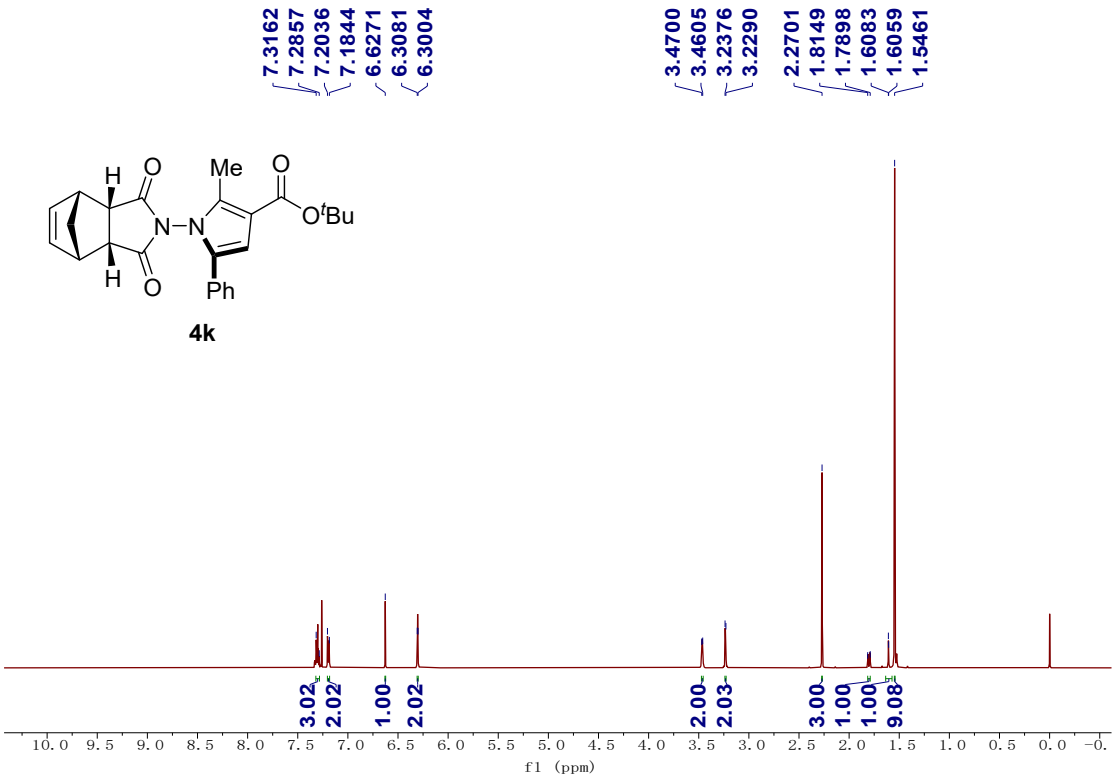
59.7551
52.2195
44.9068
44.3660
14.4742
11.1477
H
O
Me
O
N–N
OEt
H
O
Ph
f1 (ppm)

4j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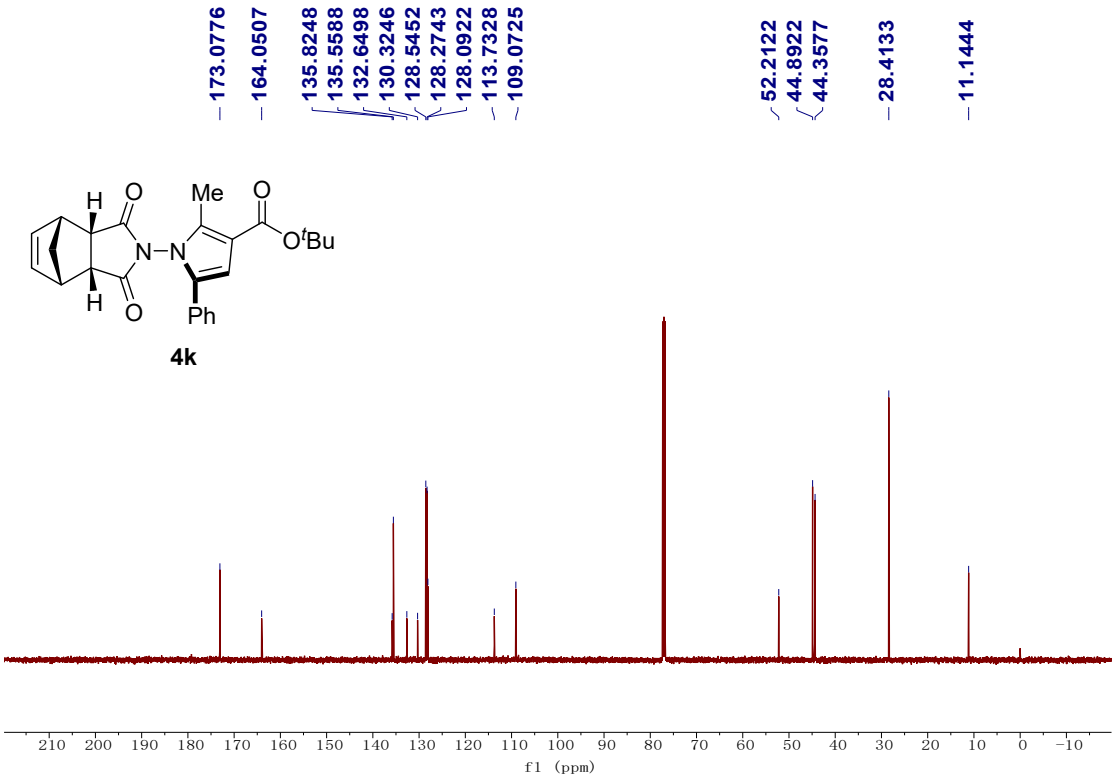
7.2036
7.1844
6.6271
6.3081
6.3004
3.4700
3.4605
3.2376
3.2290
2.2701
1.8149
1.7898
1.6083
1.6059
1.5461
H
O
Me
O
N–N
O
O^{t}Bu
H
O
Ph
4k
3.02
2.02
1.00
2.02
2.00
2.03
3.00
1.00
1.00
9.08
f1 (ppm)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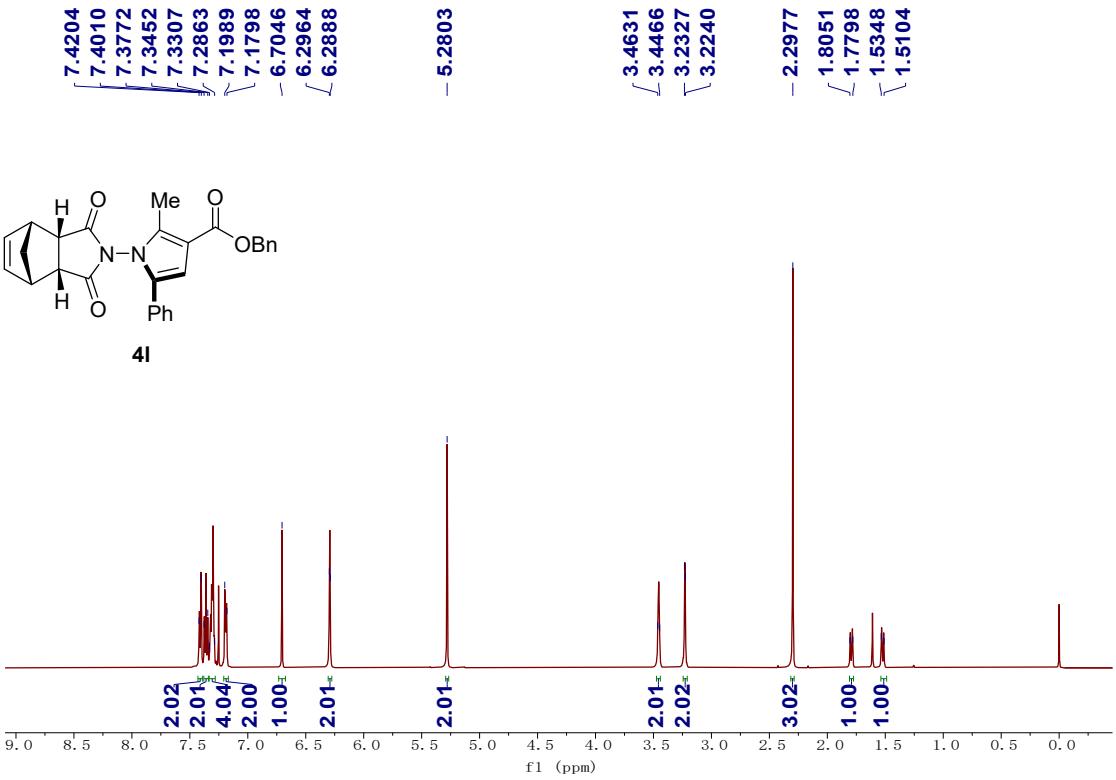
130.3246
128.5452
128.2743
128.0922
113.7328
109.0725
52.2122
44.8922
44.3577
28.4133
11.1444
H
O
Me
O
N–N
O
O^{t}Bu
H
O
Ph
4k
f1 (ppm)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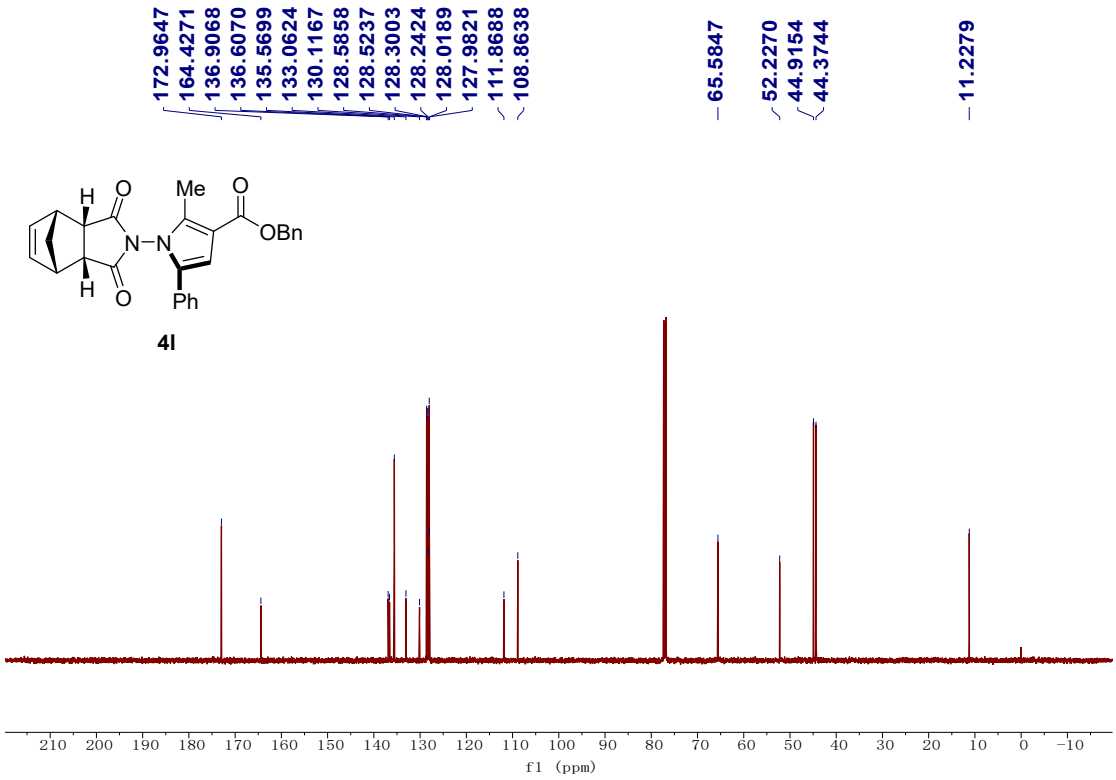
7.3307
7.2863
7.1989
7.1798
6.7046
6.2964
6.2888
5.2803
3.4631
3.4466
3.2327
3.2240
2.2977
1.8051
1.7798
1.5348
1.5104
H
O
Me
O
N–N
OBn
H
O
Ph
2.02
2.01
4.04
2.00
1.00
2.01
2.01
2.01
2.02
3.02
1.00
1.00
f1 (ppm)

4l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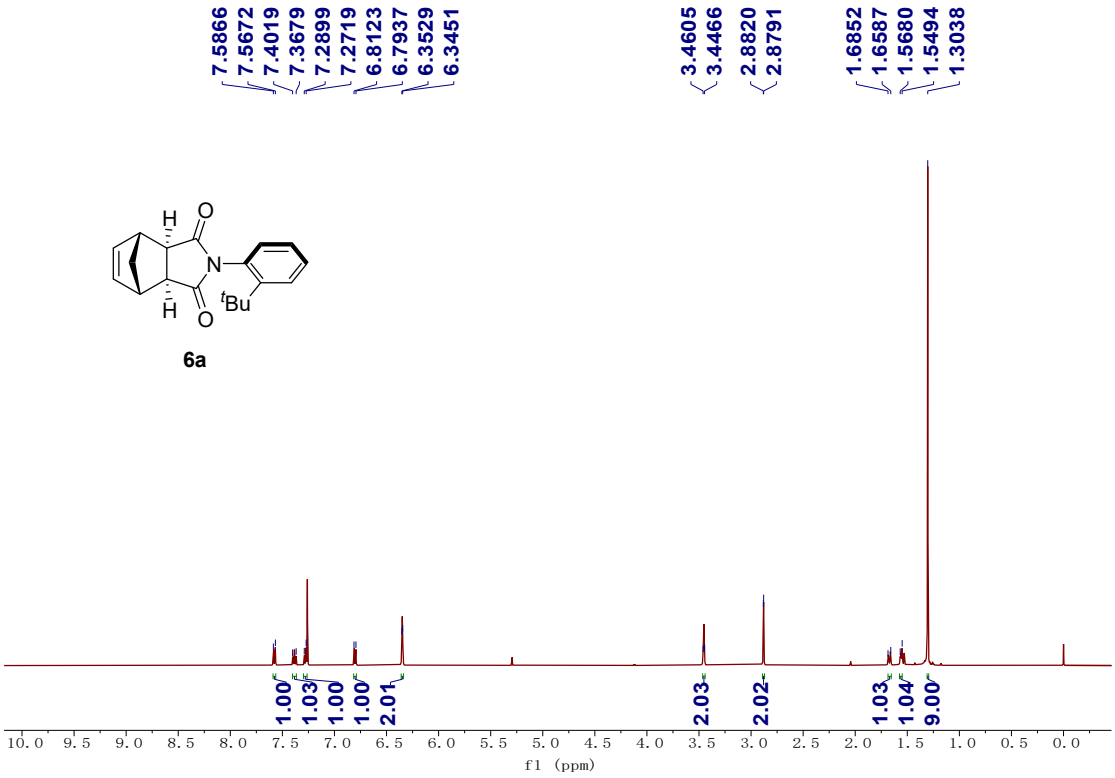
128.3003
128.2424
128.0189
127.9821
111.8688
108.8638
65.5847
52.2270
44.9154
44.3744
11.2279
H
O
Me
O
N–N
OBn
H
O
Ph
f1 (ppm)

4l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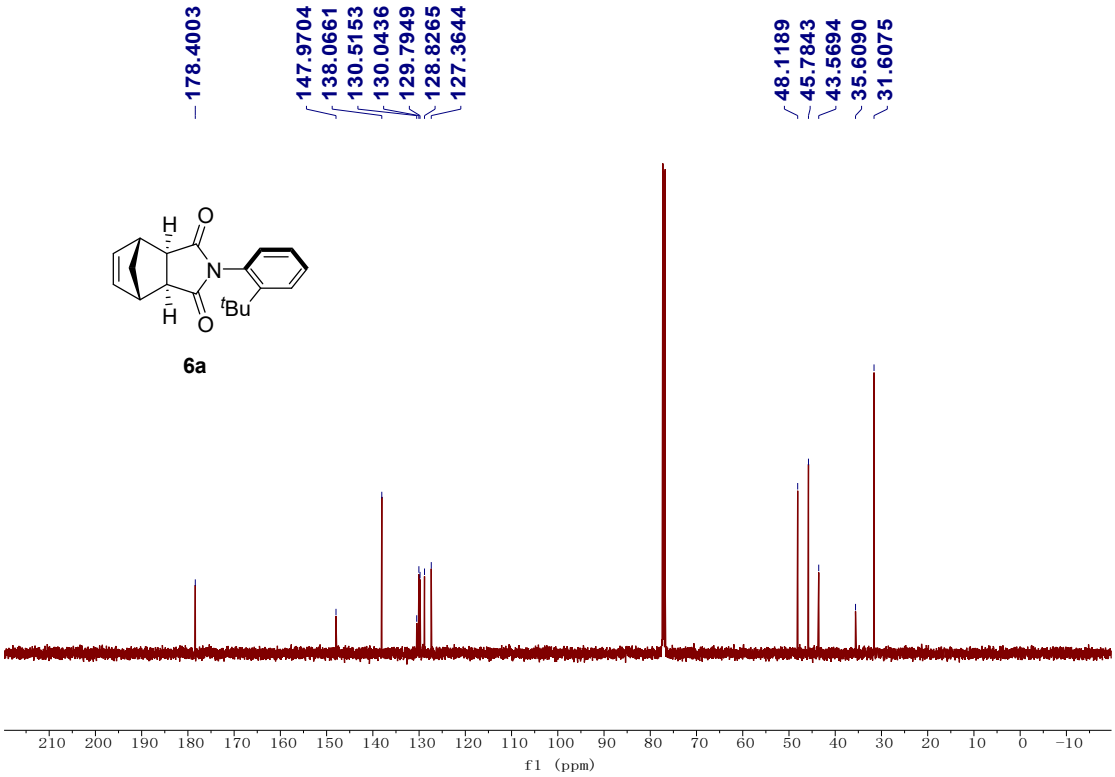
7.3679
7.2899
7.2719
6.8123
6.7937
6.3529
6.3451
3.4605
3.4466
2.8820
2.8791
1.6852
1.6587
1.5680
1.5494
1.3038
1.00
1.03
1.00
1.00
2.01
2.03
2.02
1.03
1.04
9.00
f1 (ppm)

H
O
N
tBu
H
O

6a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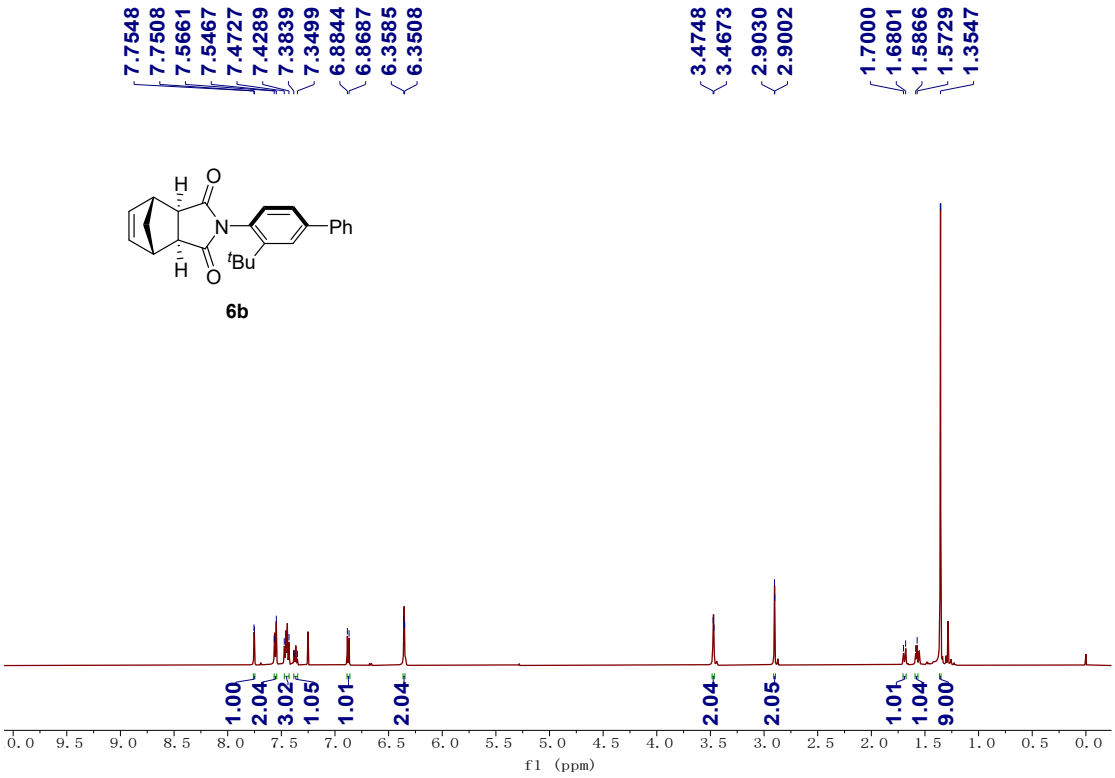
138.0661
130.5153
130.0436
129.7949
128.8265
127.3644
48.1189
45.7843
43.5694
35.6090
31.6075
f1 (ppm)

H
O
N
tBu
H
O

6a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7.4289
7.3839
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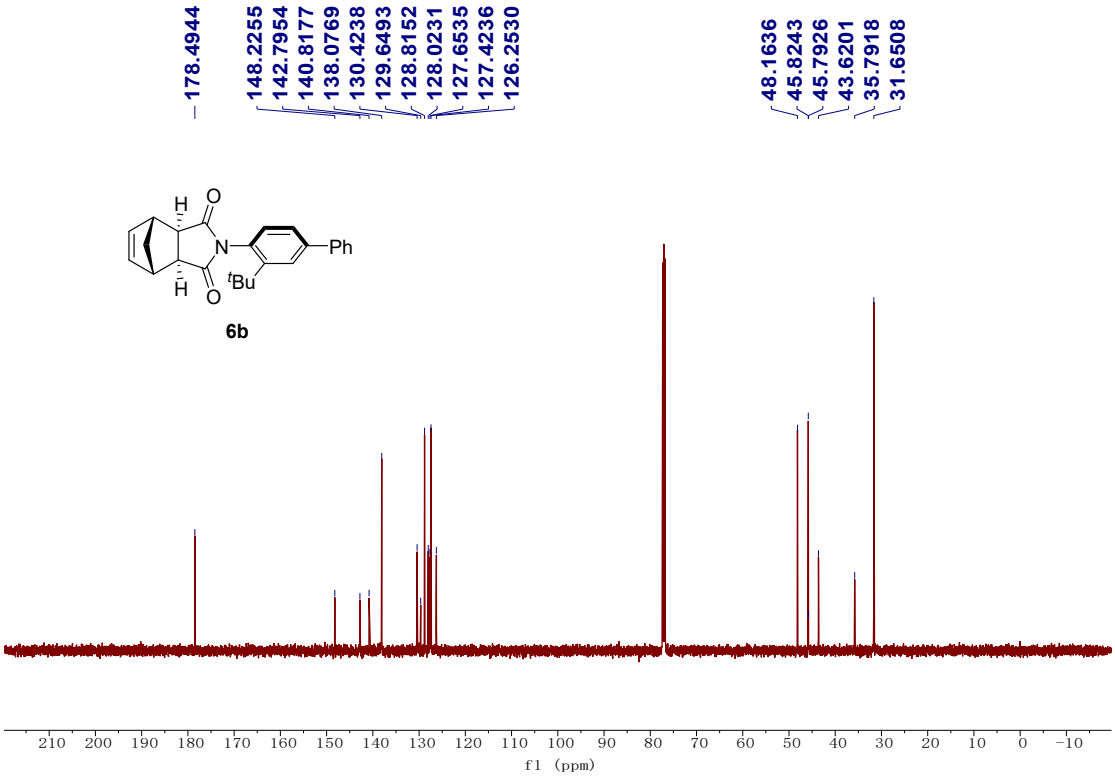
6.8844
6.8687
6.3585
6.3508
3.4748
3.4673
2.9030
2.9002
1.7000
1.6801
1.5866
1.5729
1.3547
H
O
N
Ph
tBu
H
O
6b
1.00
2.04
3.02
1.05
1.01
2.04
2.04
2.05
1.01
1.04
9.00
f1 (ppm)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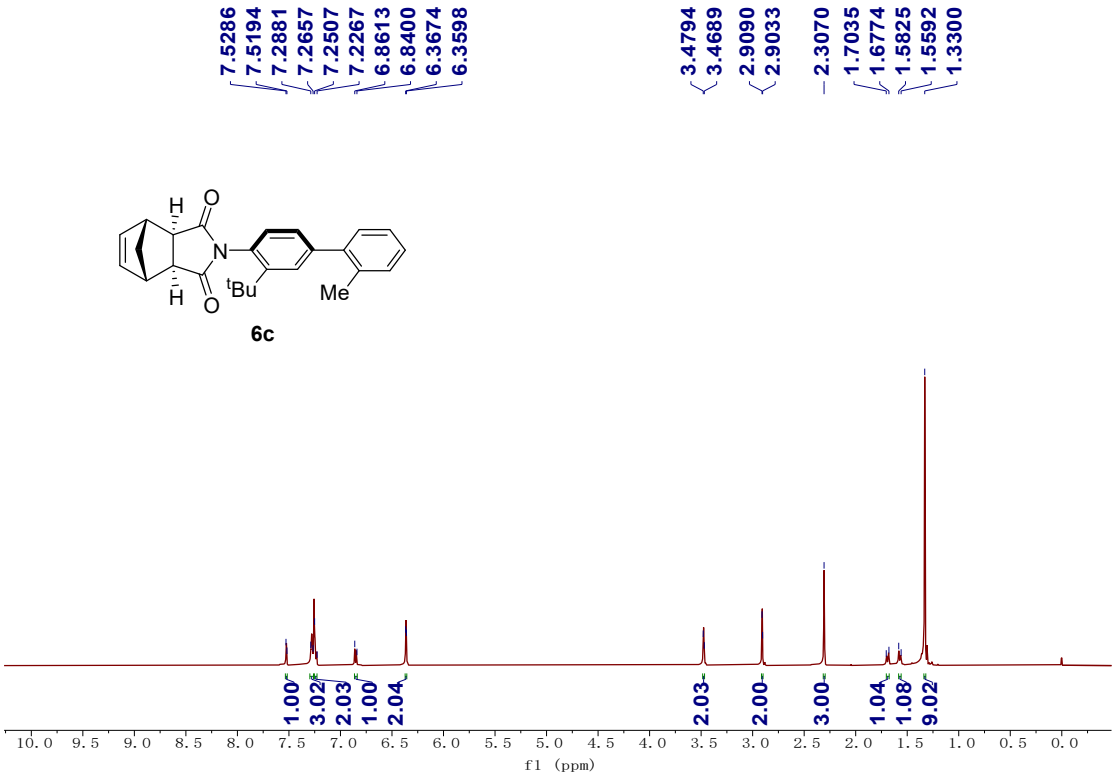
142.7954
140.8177
138.0769
130.4238
129.6493
128.8152
128.0231
127.6535
127.4236
126.2530
48.1636
45.8243
45.7926
43.6201
35.7918
31.6508
H
O
N
Ph
tBu
H
O
6b
f1 (ppm)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7.5194
7.2881
7.2657
7.2507
7.2267
6.8613
6.8400
6.3674
6.3598
3.4794
3.4689
2.9090
2.9033
2.3070
1.7035
1.6774
1.5825
1.5592
1.3300
H
O
N
tBu
Me
H
O
6c
1.00
3.02
2.03
1.00
2.04
2.03
2.00
3.00
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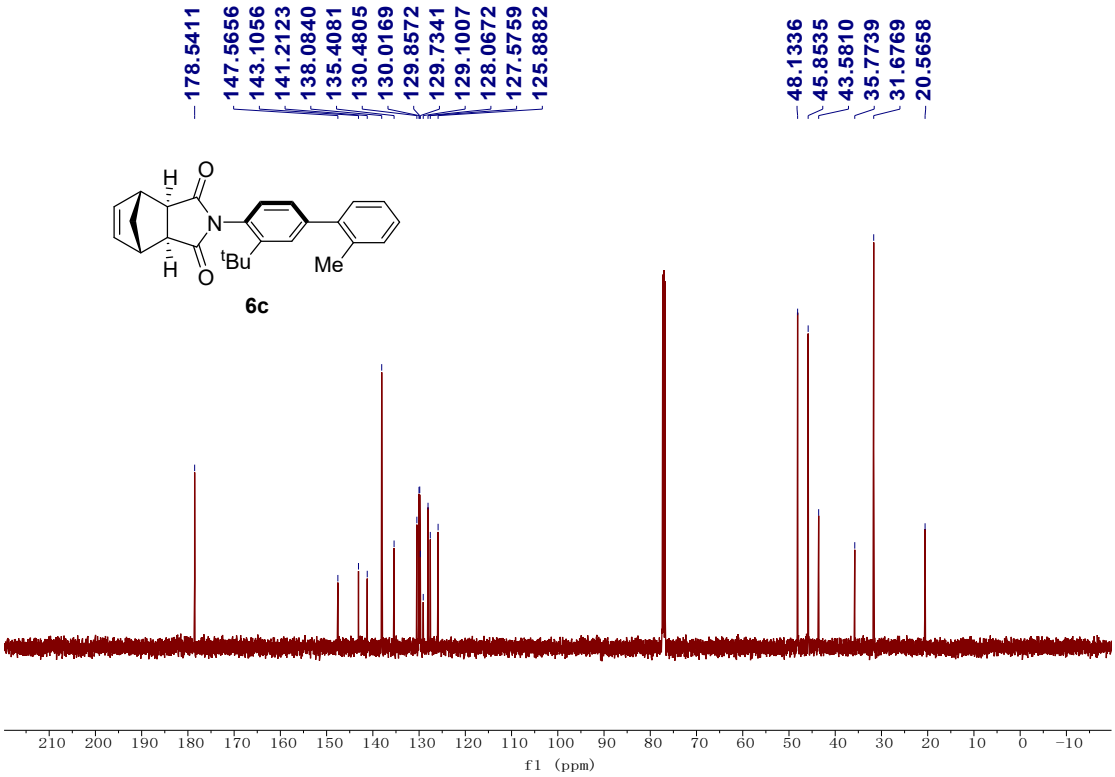
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O
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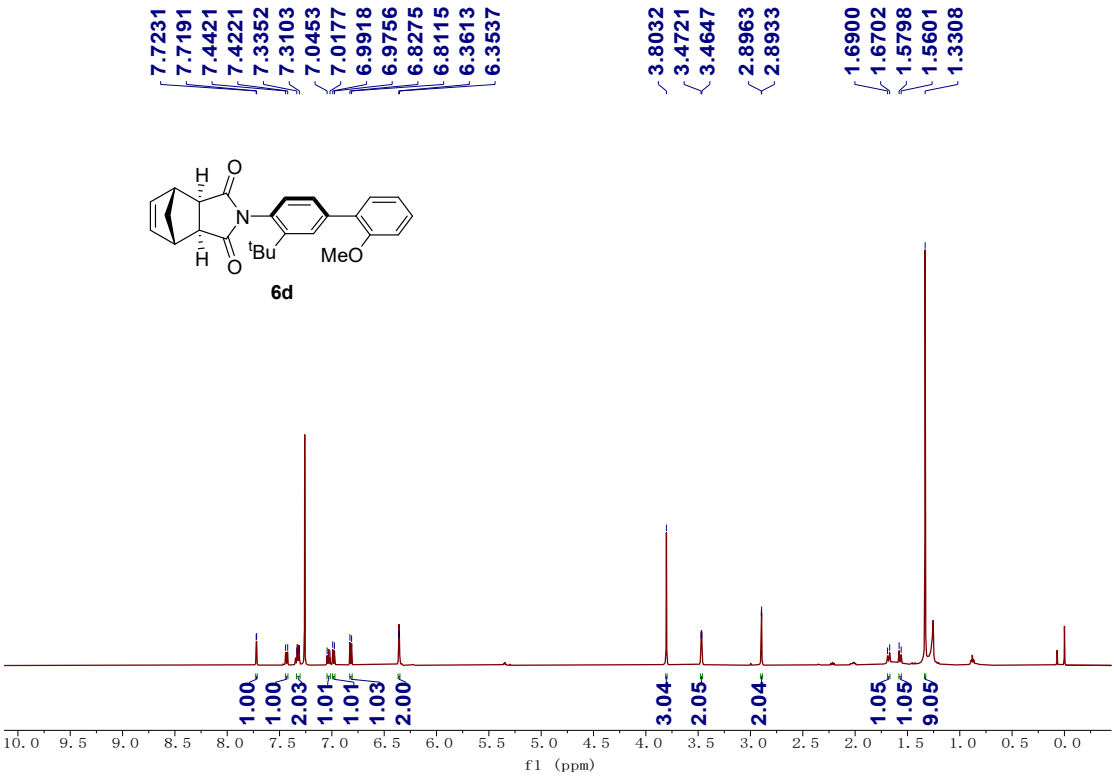
f1 (ppm)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1.6702
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1.3308
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O
N
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MeO
H
O
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1.00
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1.03
2.00
3.04
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2.04
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1.05
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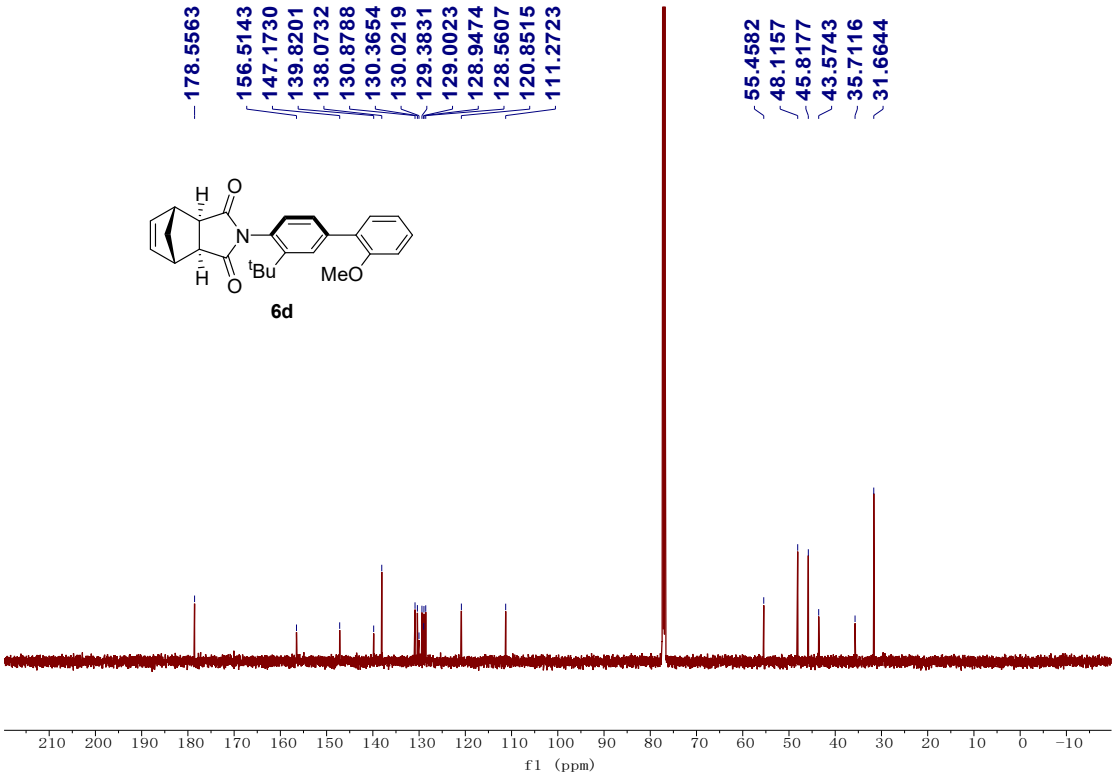
f1 (ppm)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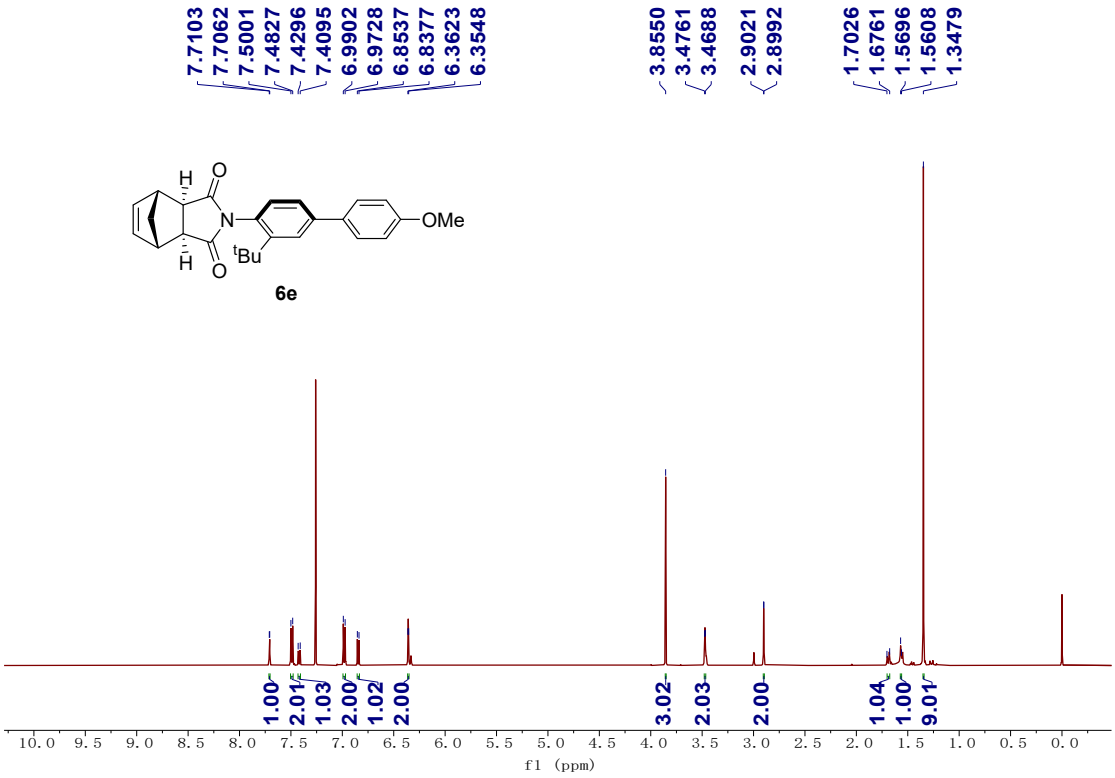
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3.4761
3.4688
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1.6761
1.5696
1.5608
1.3479
OMe
tBu
6e
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2.00
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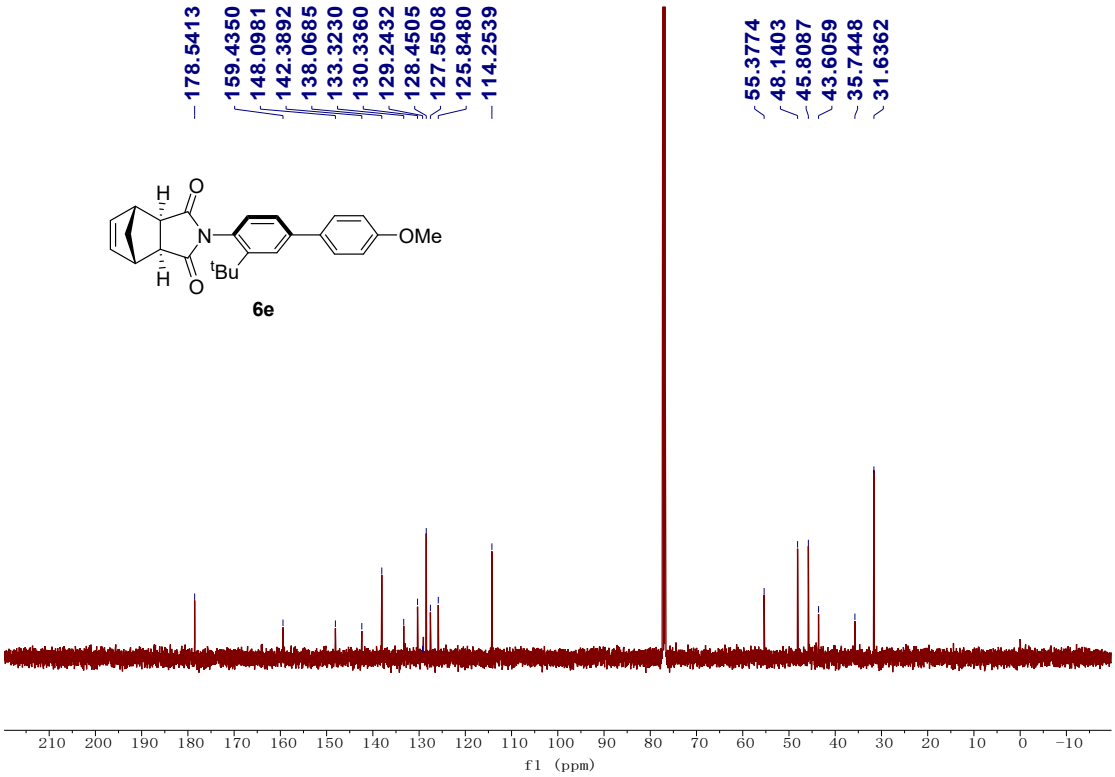
f1 (ppm)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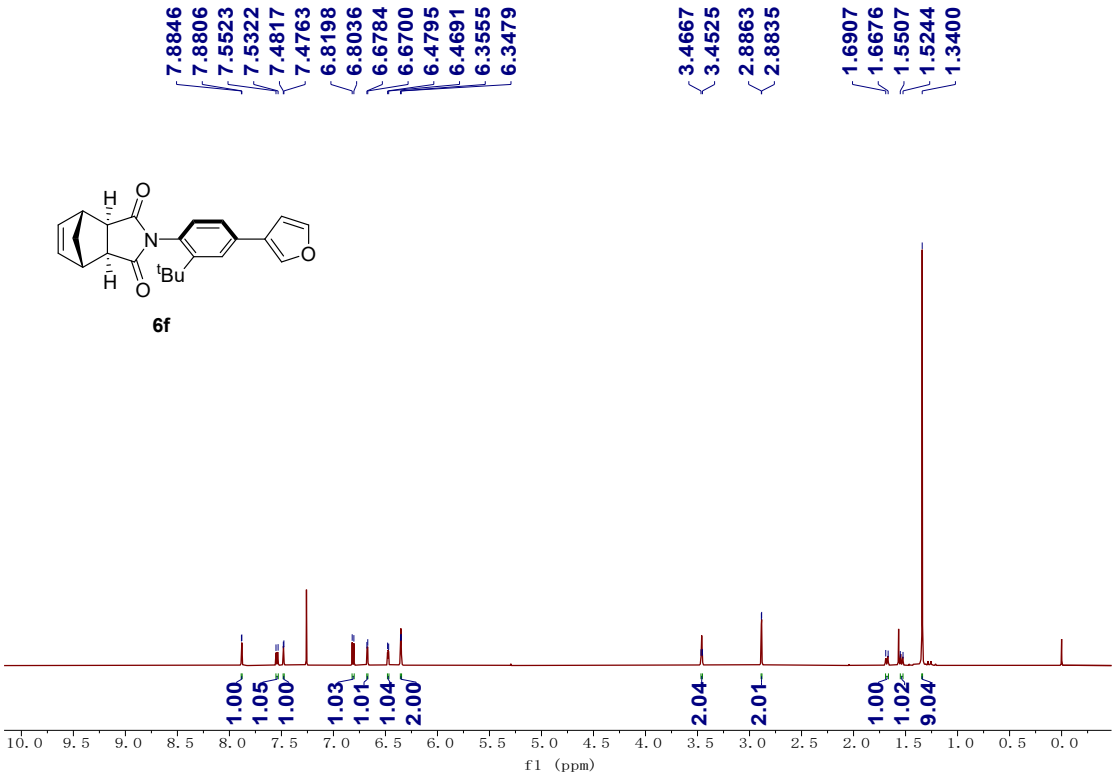
f1 (ppm)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1.3400
1.00
1.05
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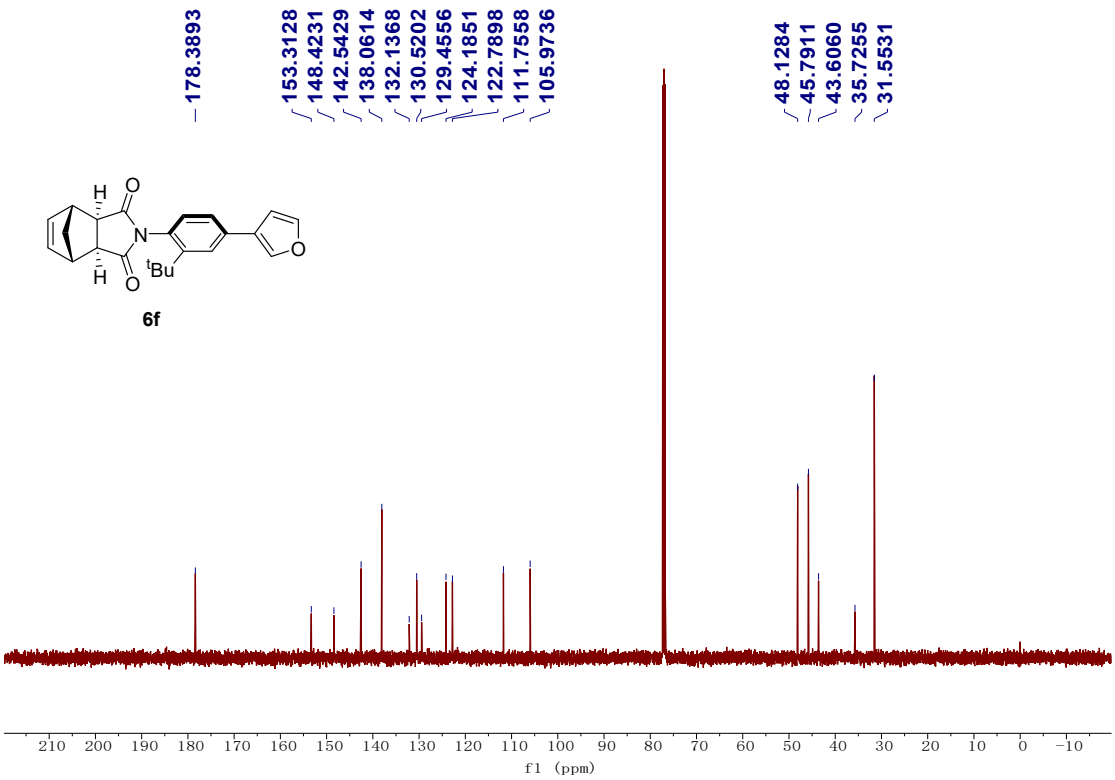
1.00
1.02
9.04
f1 (ppm)

6f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45.7911
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35.7255
31.5531
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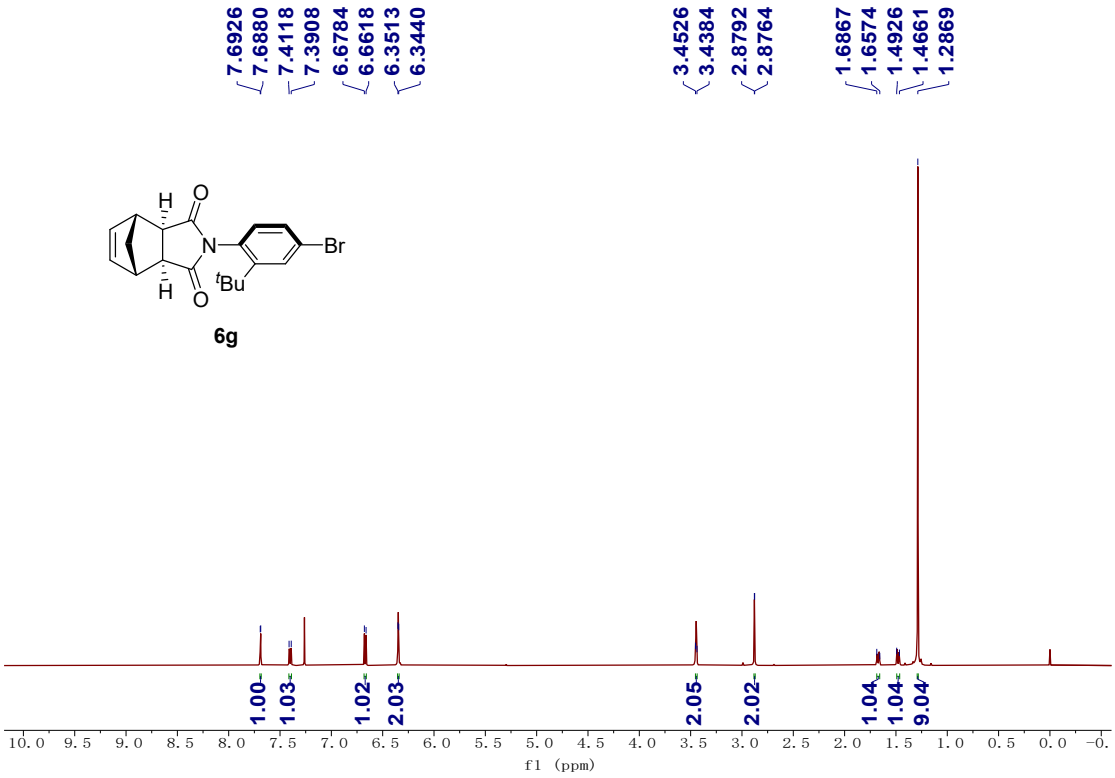
6f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2.8792
2.8764
1.6867
1.6574
1.4926
1.4661
1.2869
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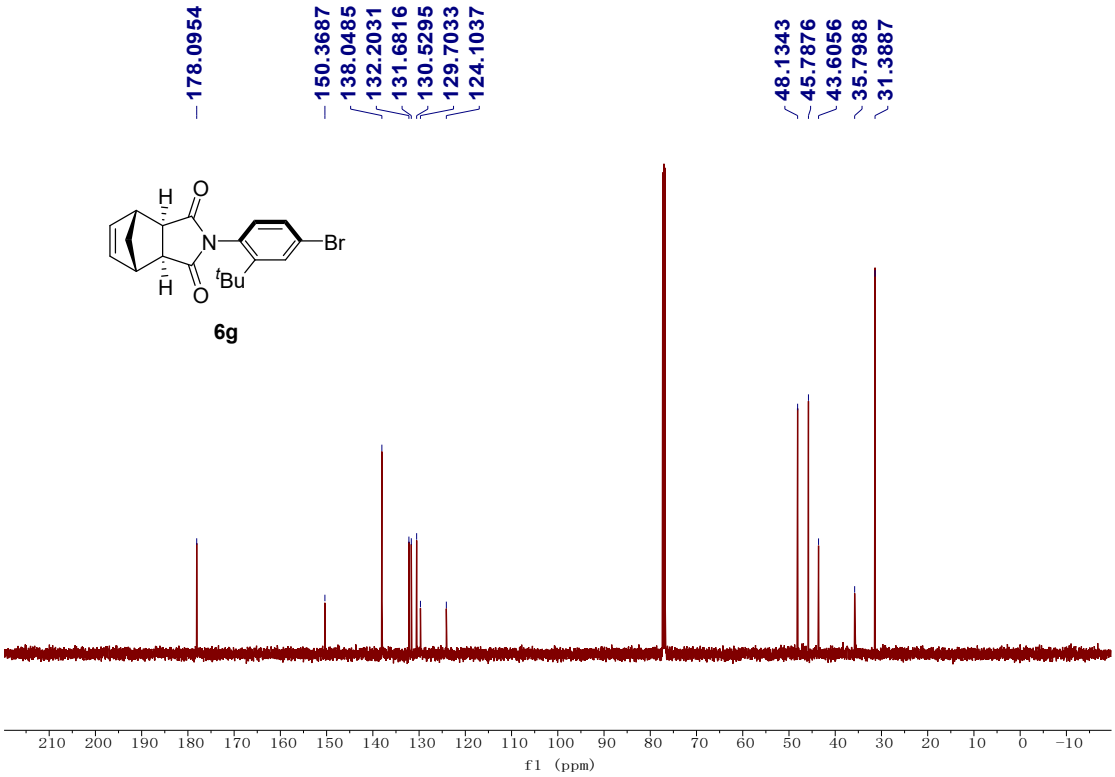
1.03
1.02
2.03
2.05
2.02
1.04
1.04
9.04
f1 (ppm)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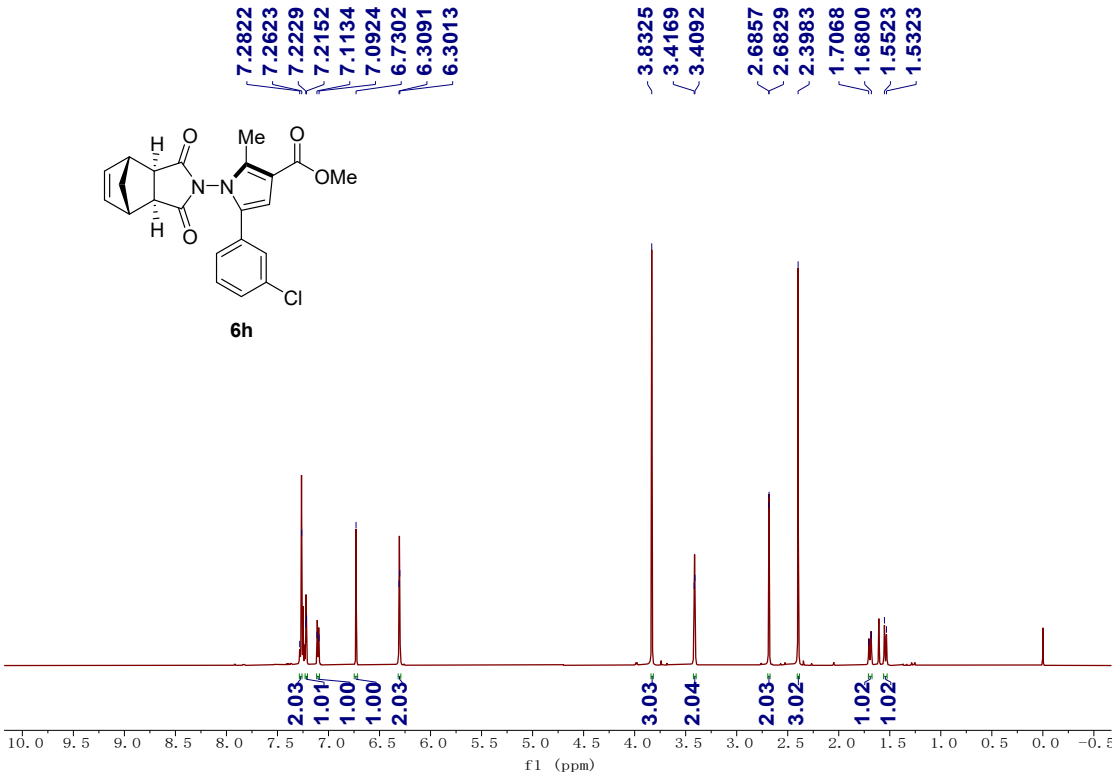
31.3887
Br
tBu
6g
f1 (ppm)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3.4092
2.6857
2.6829
2.3983
1.7068
1.6800
1.5523
1.5323
H
O
N–N
Me
O
OMe
H
O
Cl
6h
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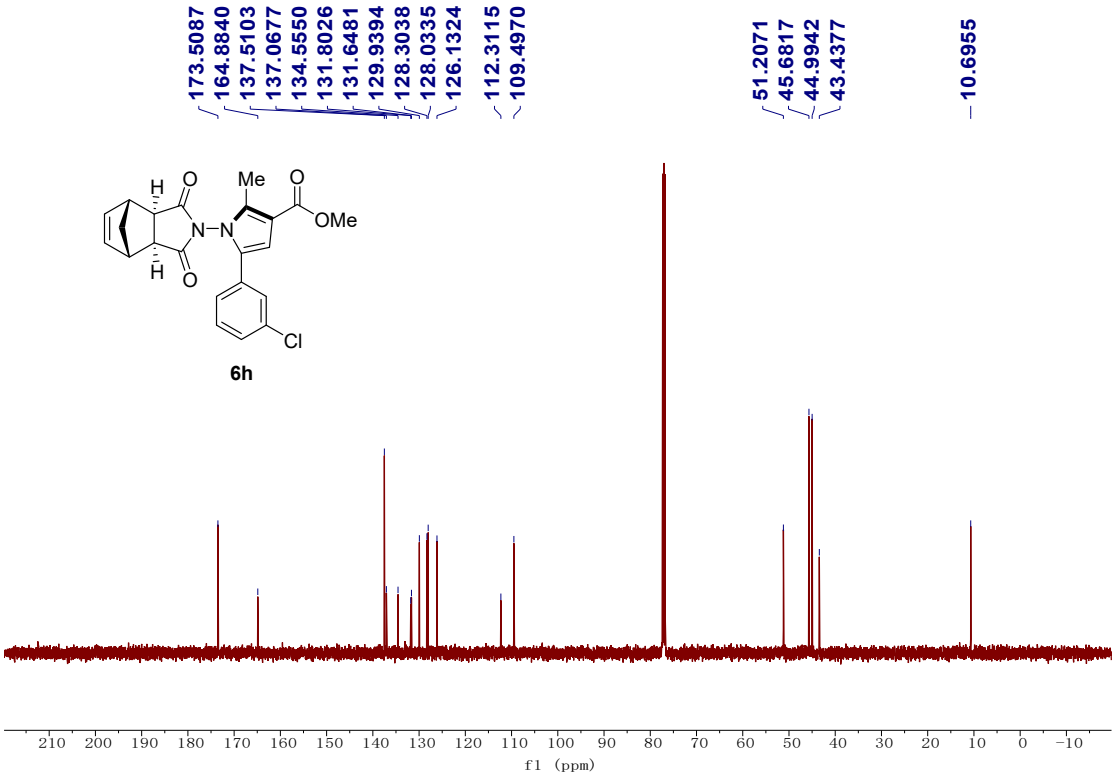
1.00
2.03
3.03
2.04
2.03
3.02
1.02
1.02
f1 (ppm)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45.6817
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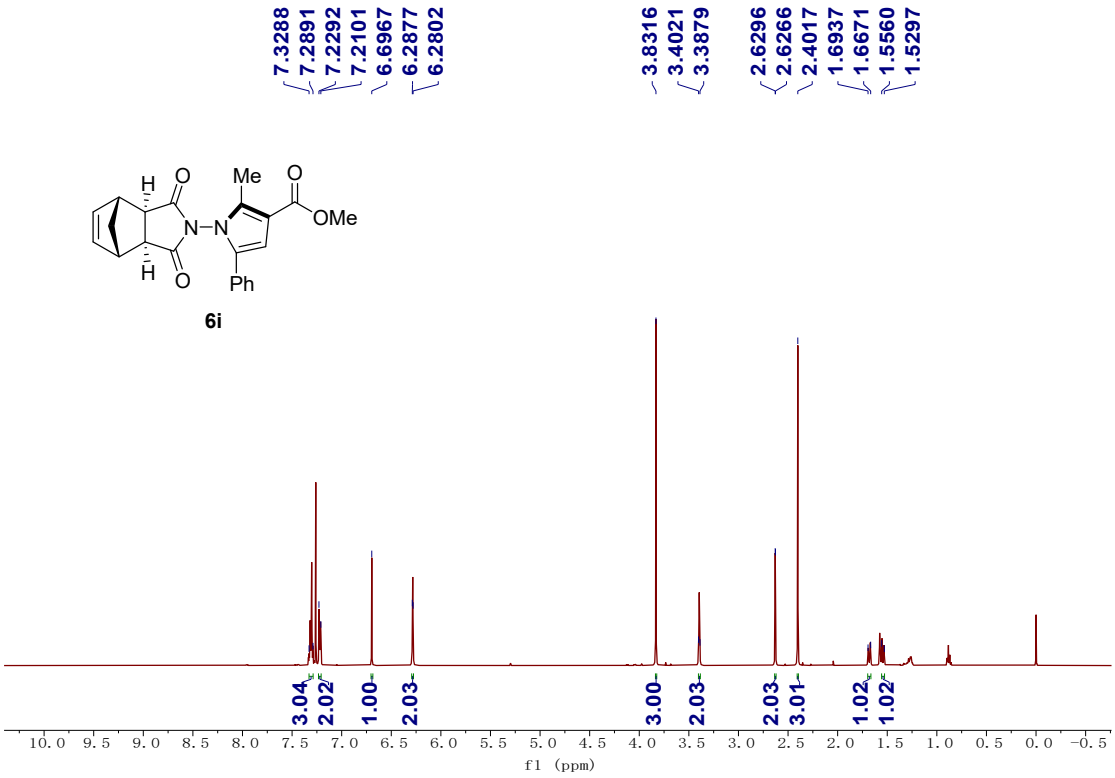
Me
O
OMe
H
O
Cl
6h
f1 (ppm)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2.6266
2.4017
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1.6671
1.5560
1.5297
Me
O
OMe
H
O
N–N
H
O
Ph
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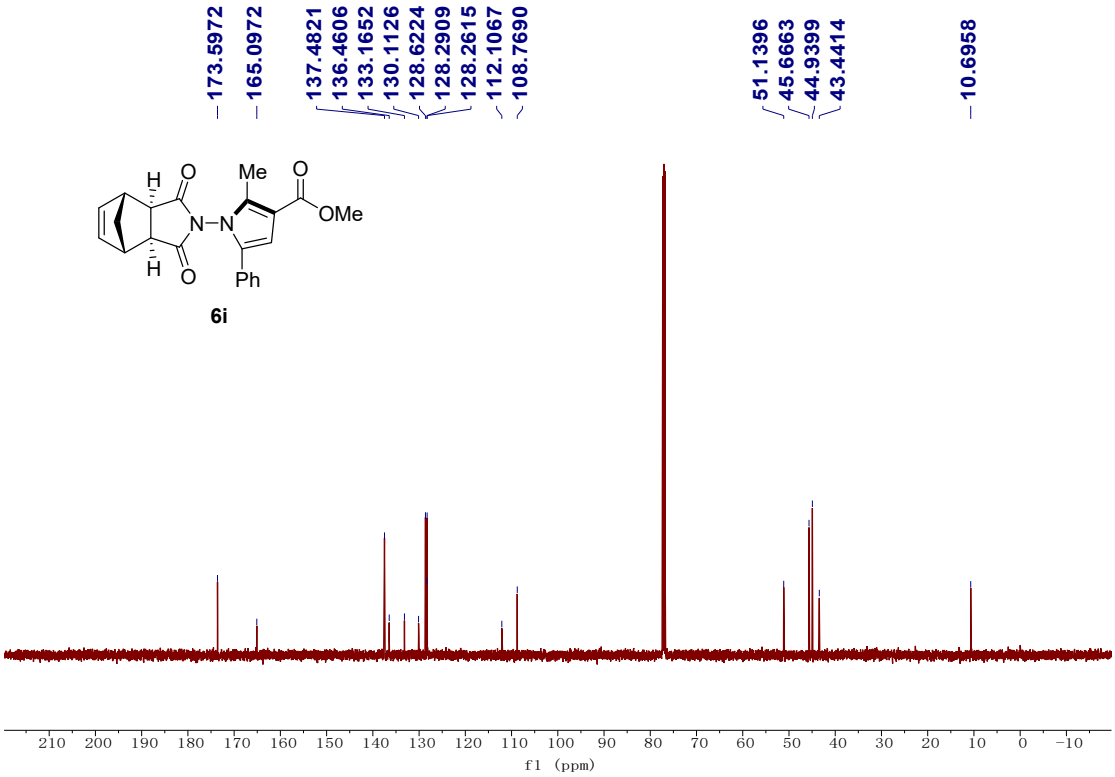
2.03
3.00
2.03
2.03
3.01
1.02
1.02
f1 (ppm)

6i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108.7690
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45.6663
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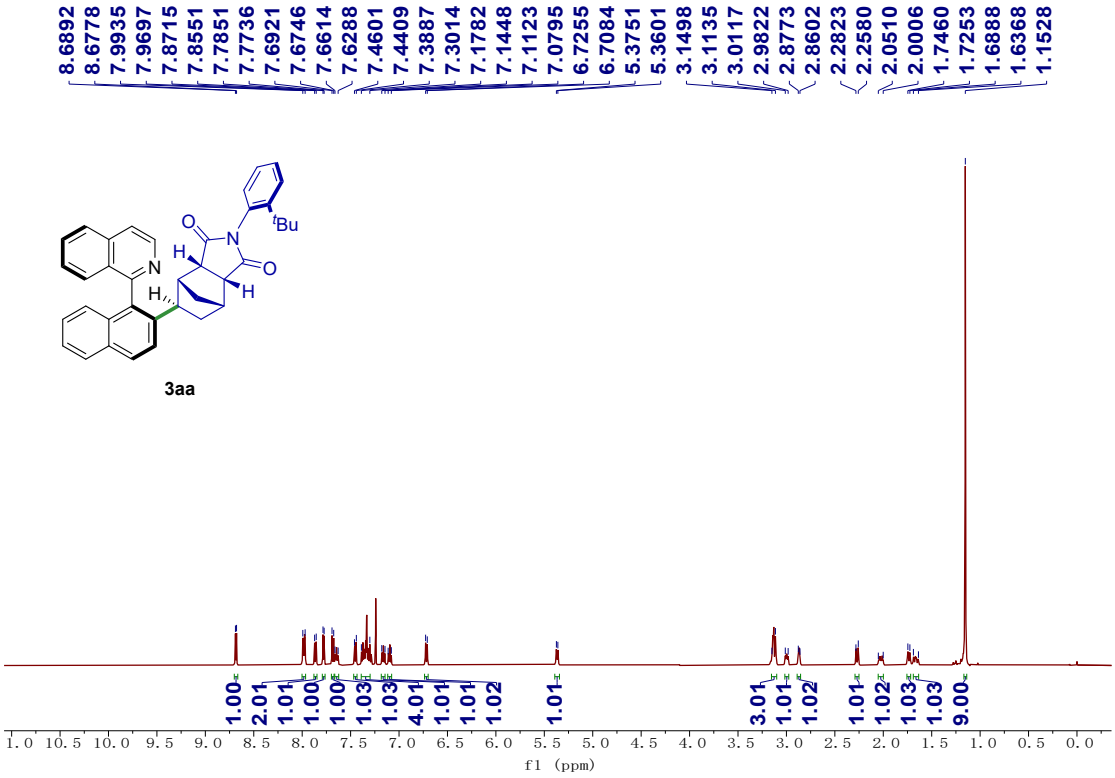
10.6958
Me
O
OMe
H
O
N–N
H
O
Ph
f1 (ppm)

6i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7.1123
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1.1528
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N
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H
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1.01
1.00
1.00
1.03
1.03
4.01
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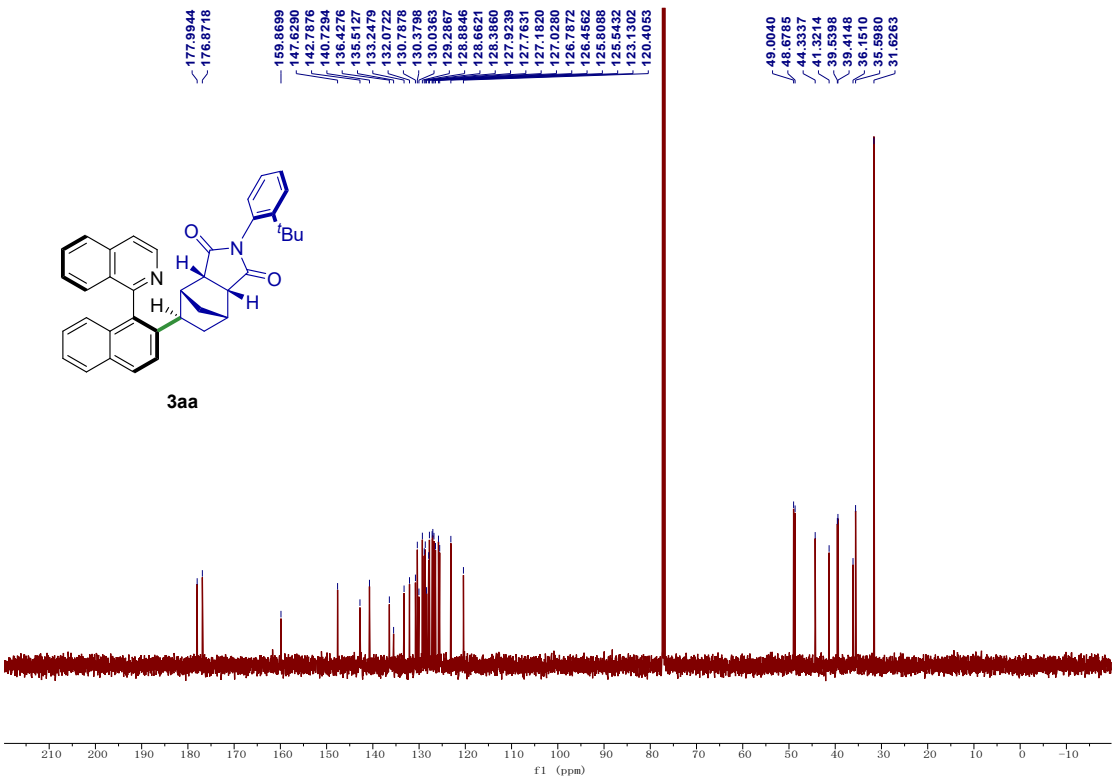
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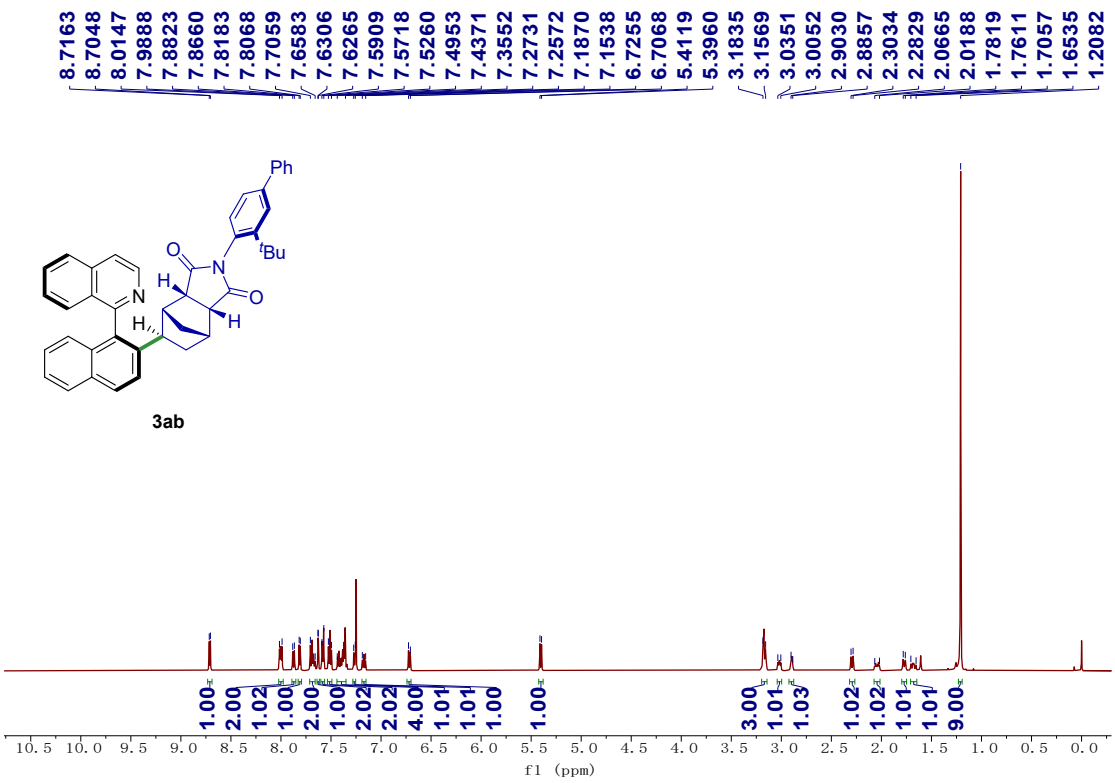
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Ph
tBu
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N
O
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N
H
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1.02
1.00
2.00
1.00
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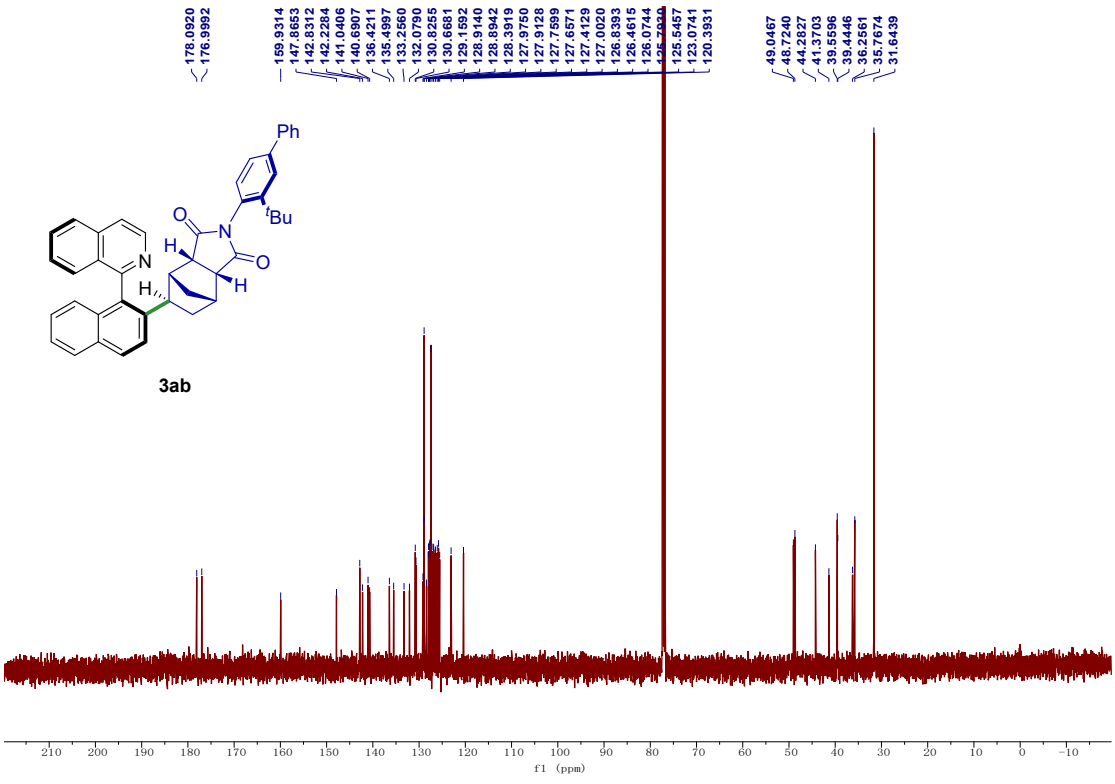
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tBu
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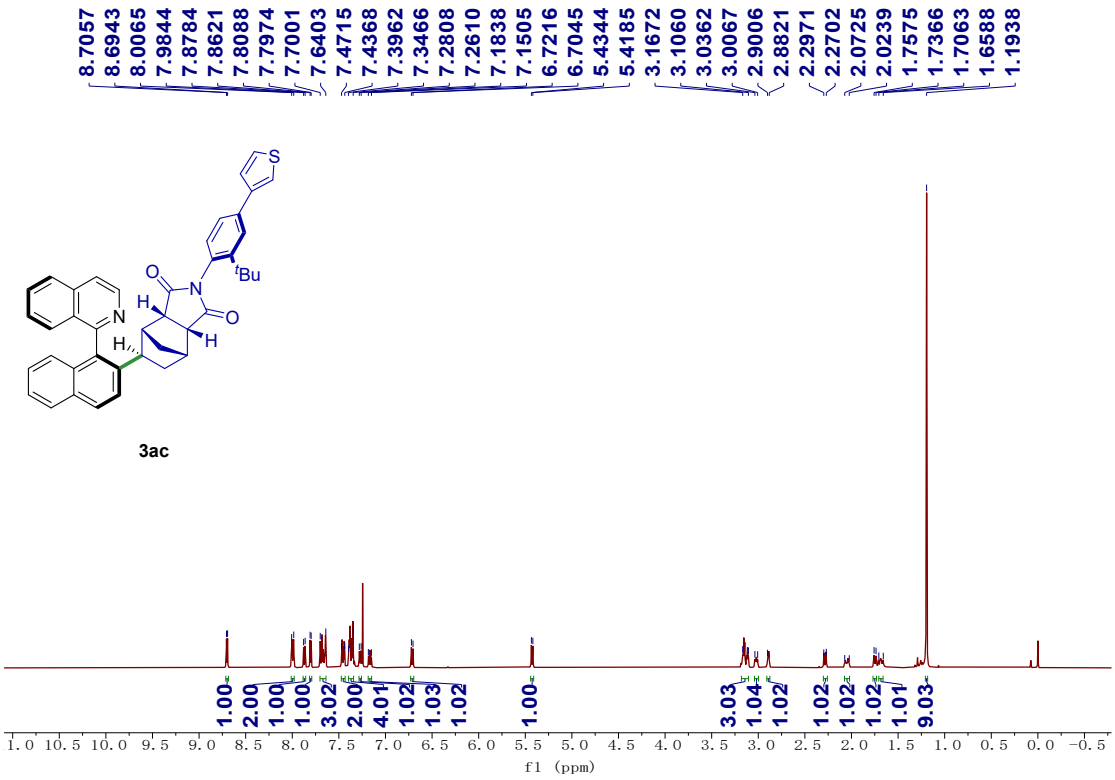
H
3ab
f1 (ppm)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S
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1.00
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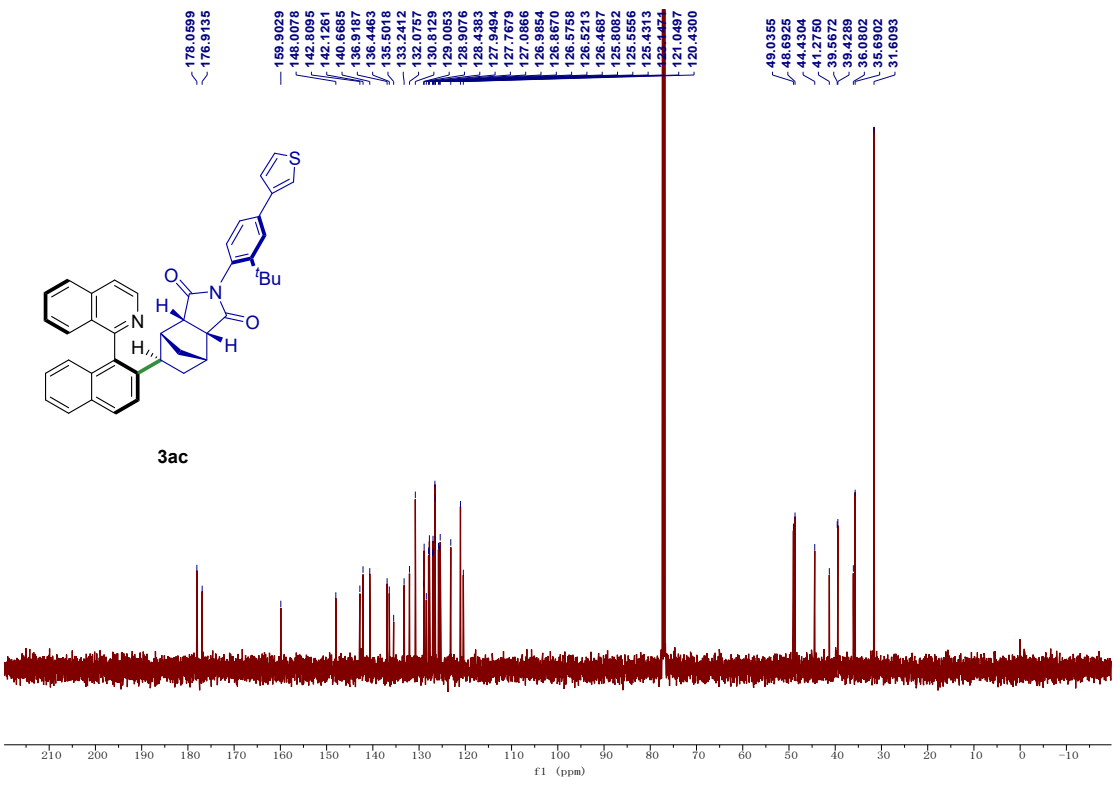
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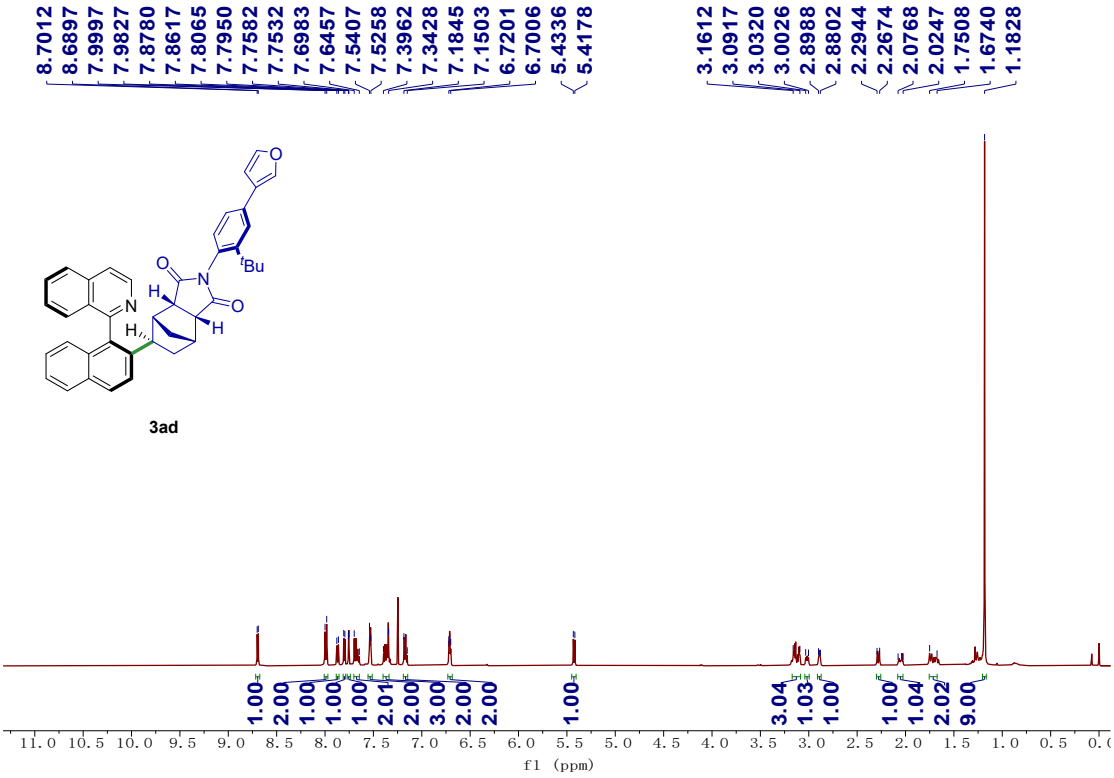
3ac
f1 (ppm)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1.1828
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1.00
1.00
1.00
2.01
2.00
3.00
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1.00
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f1 (ppm)

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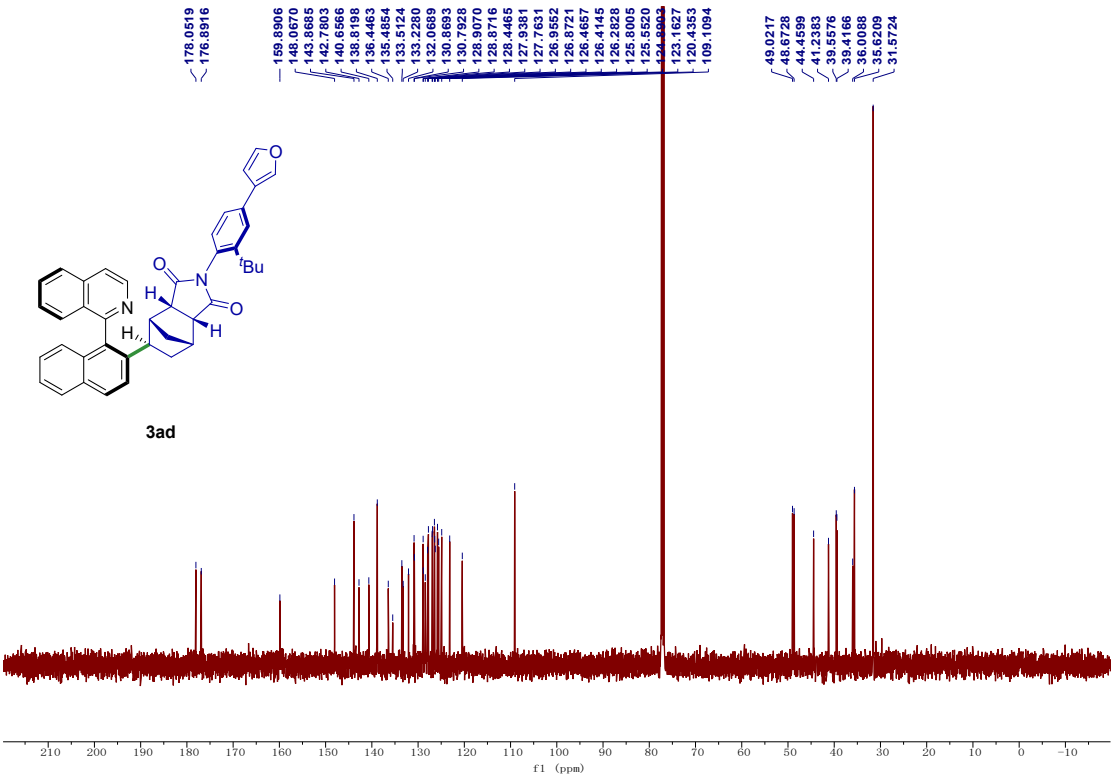
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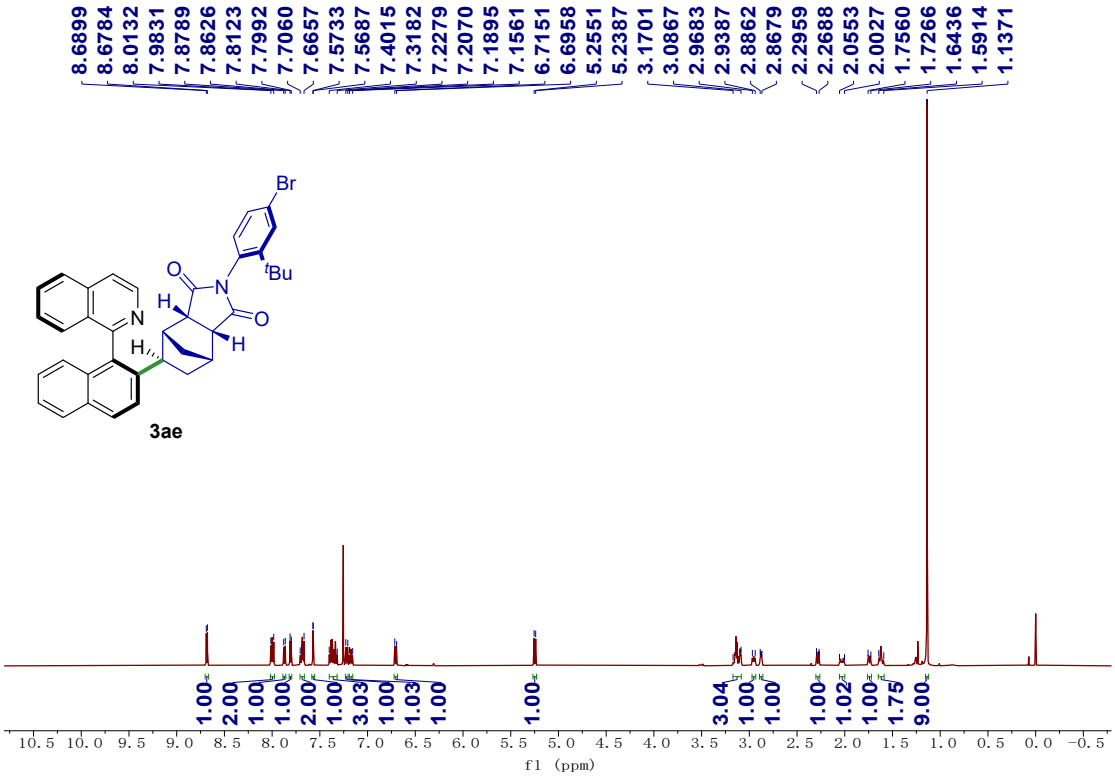
3ad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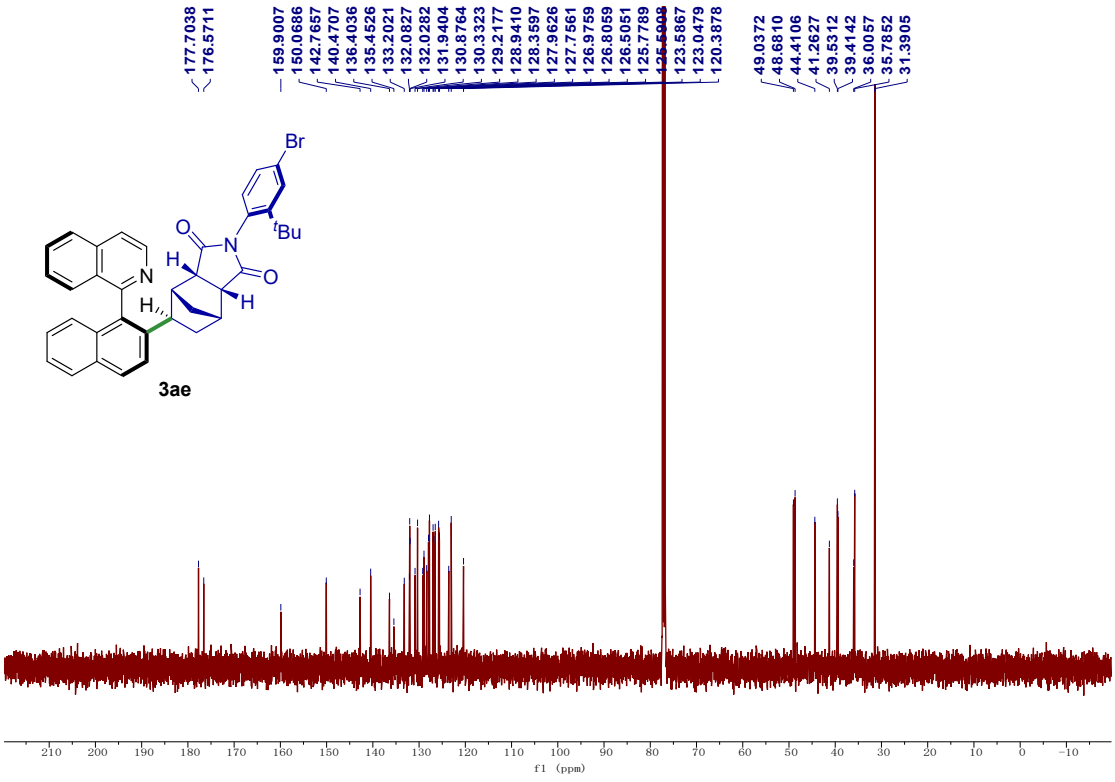
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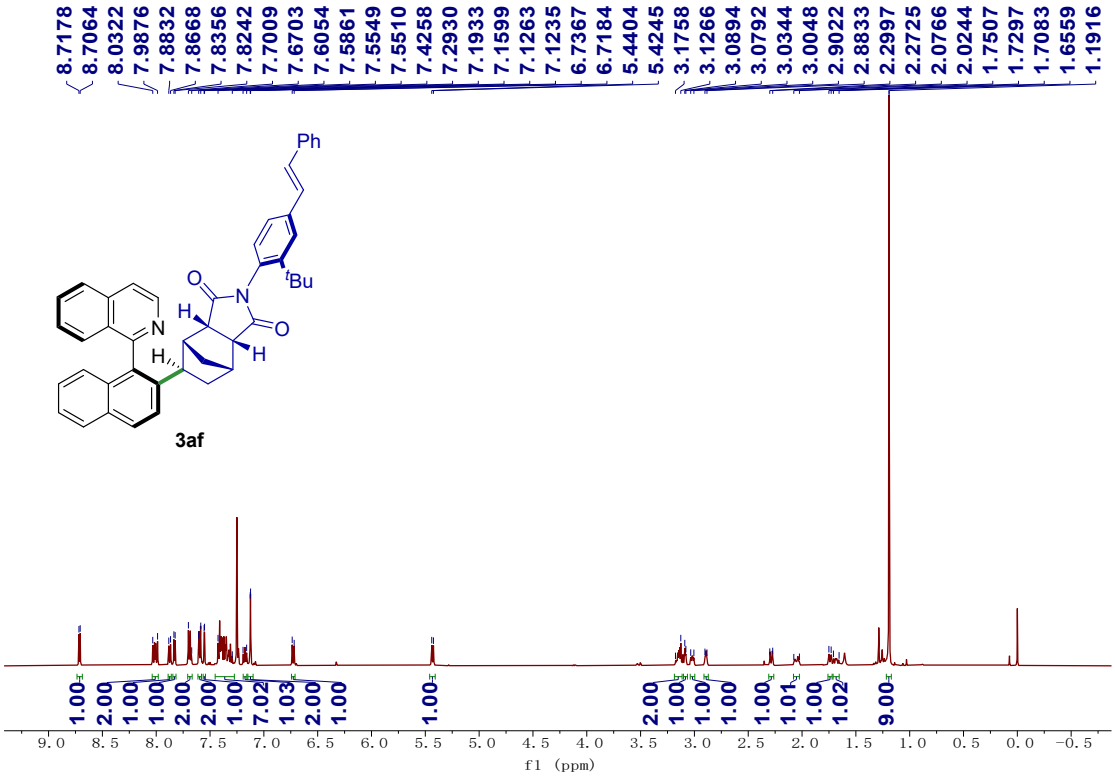
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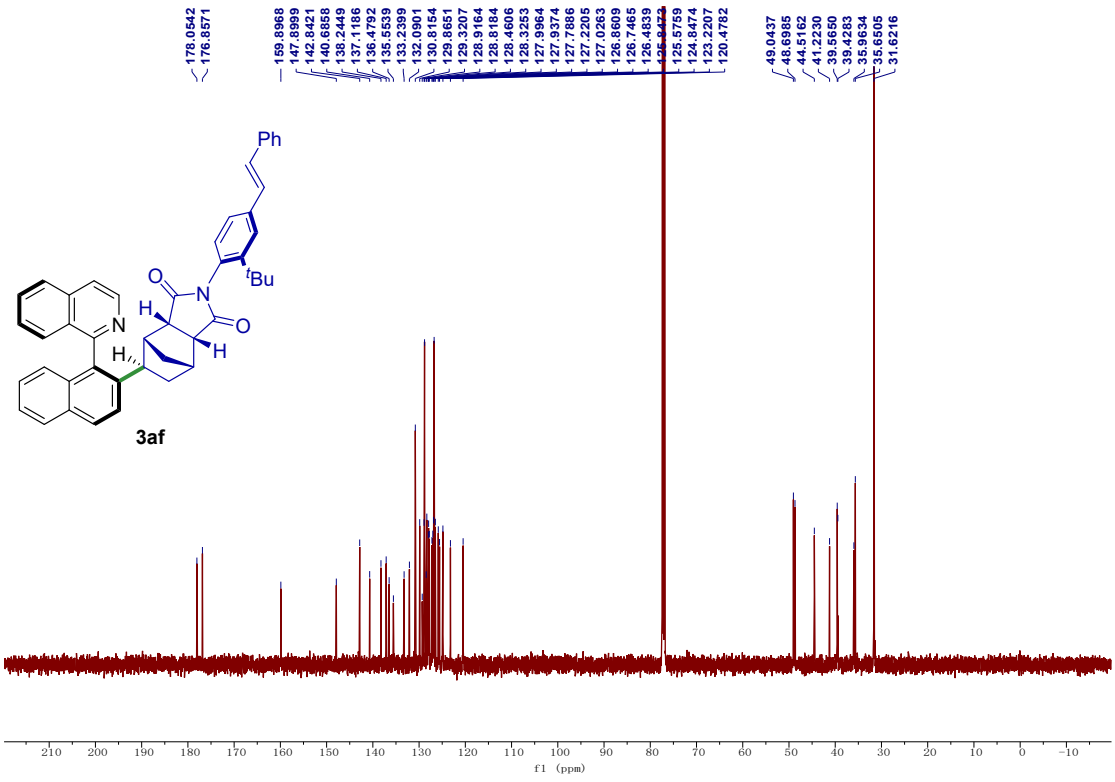
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H
O
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H
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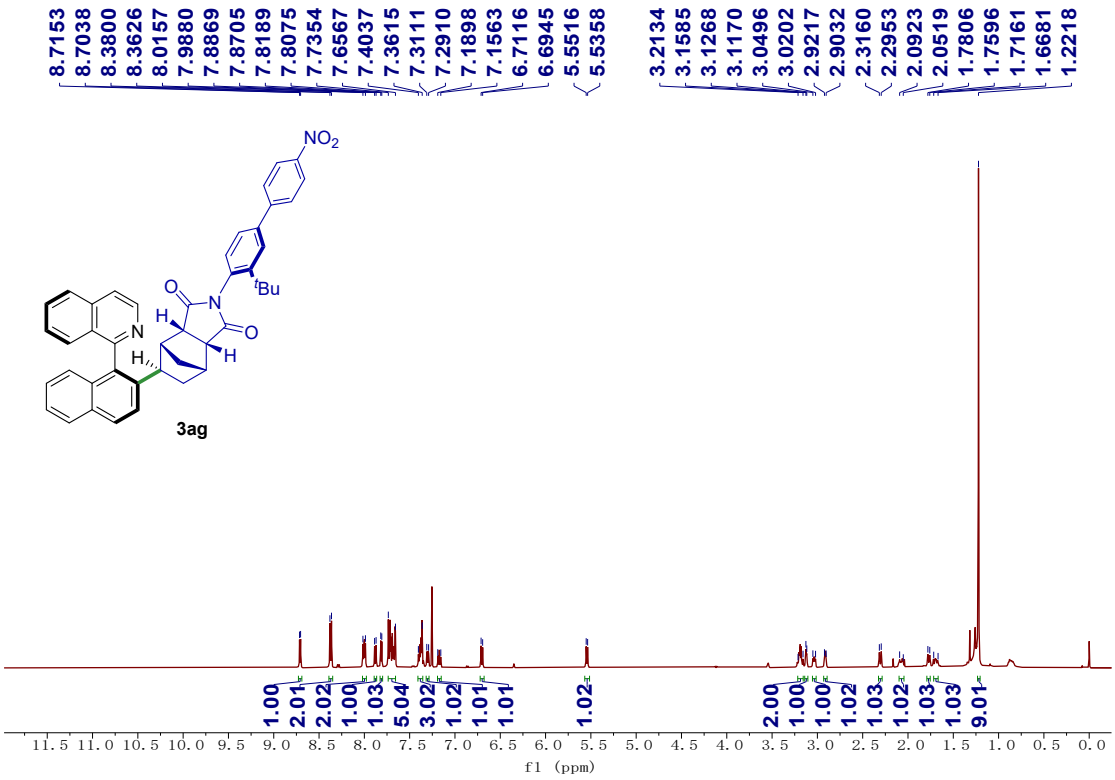
f1 (ppm)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1.7161
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1.2218
NO2
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O
N
H
O
H
N
H
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3.02
1.02
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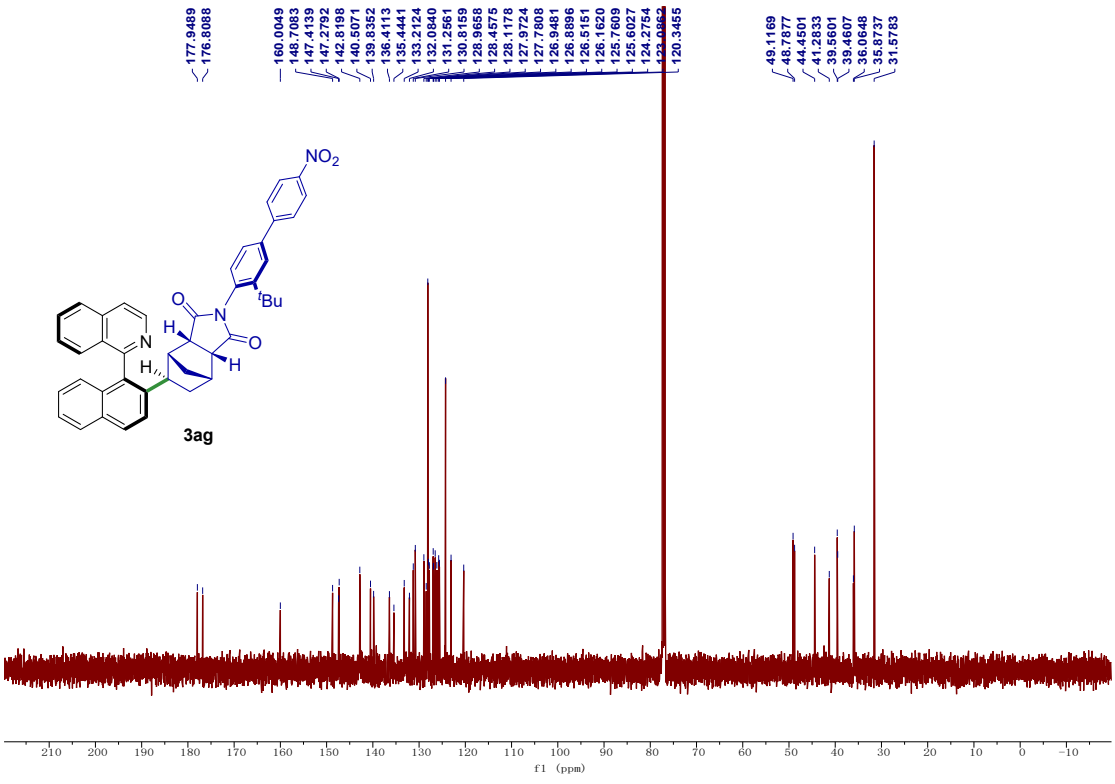
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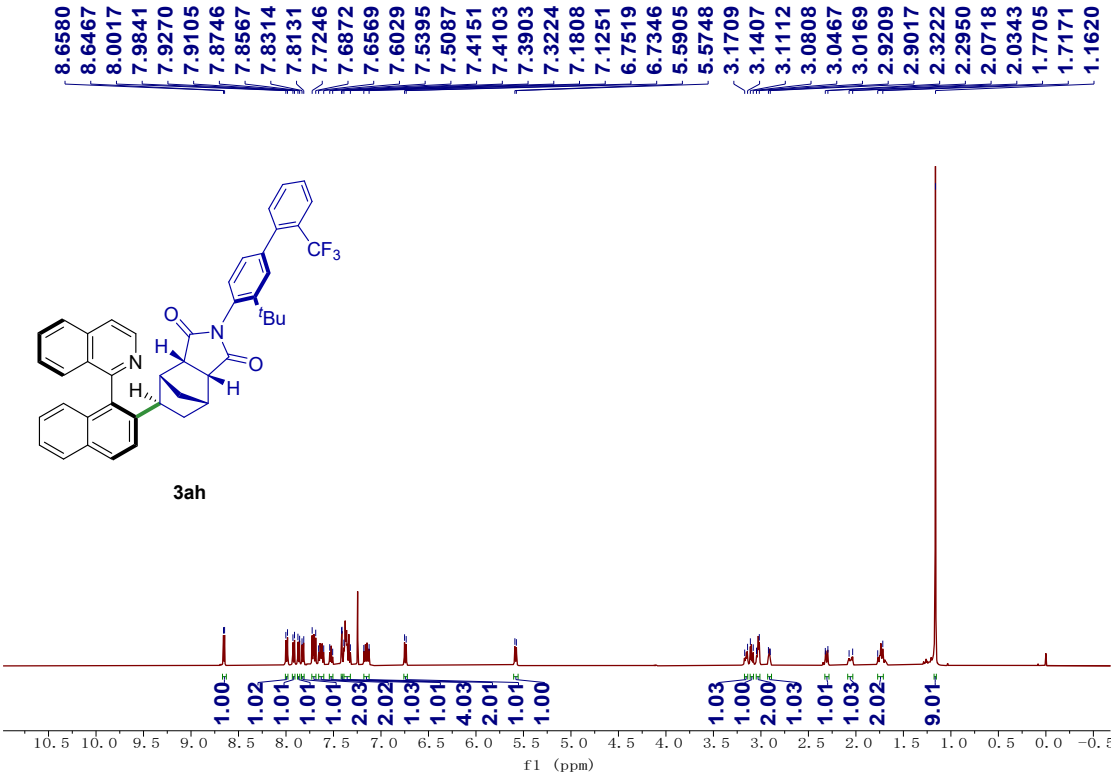
3ag
f1 (ppm)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2.0718
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1.7171
1.1620
CF3
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O
N
H
O
H
N
H
3ah
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1.02
1.01
1.01
1.01
2.03
2.02
1.03
1.01
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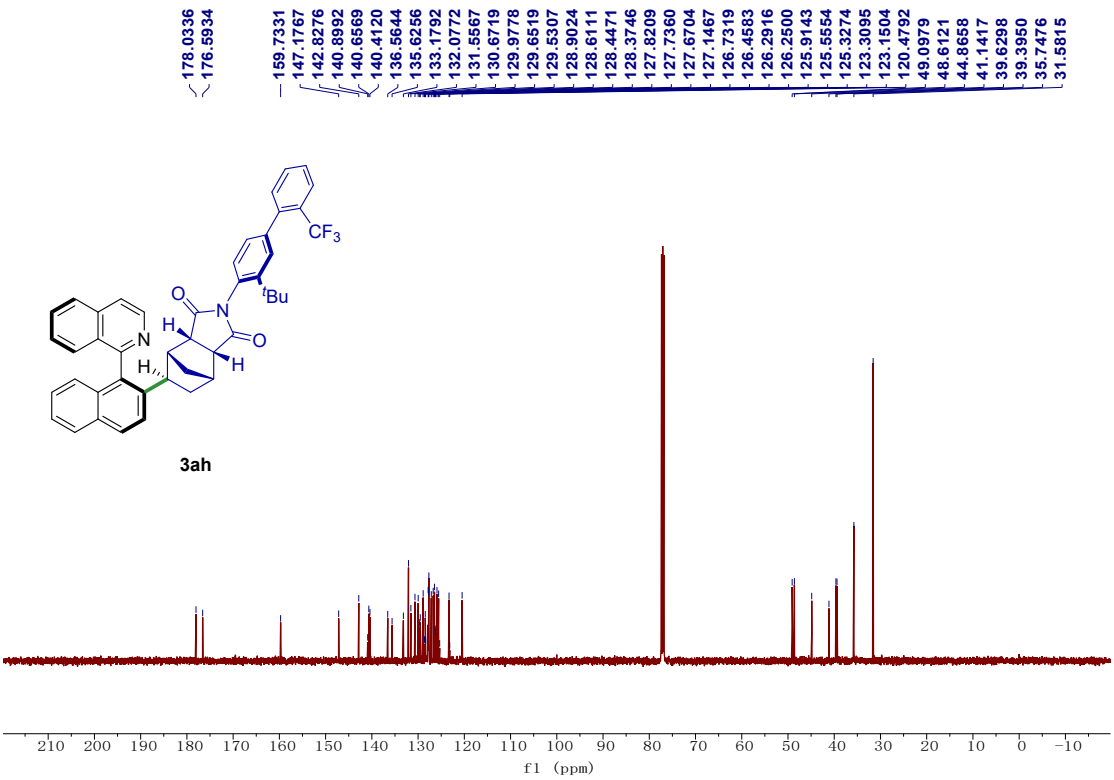
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44.8658
41.1417
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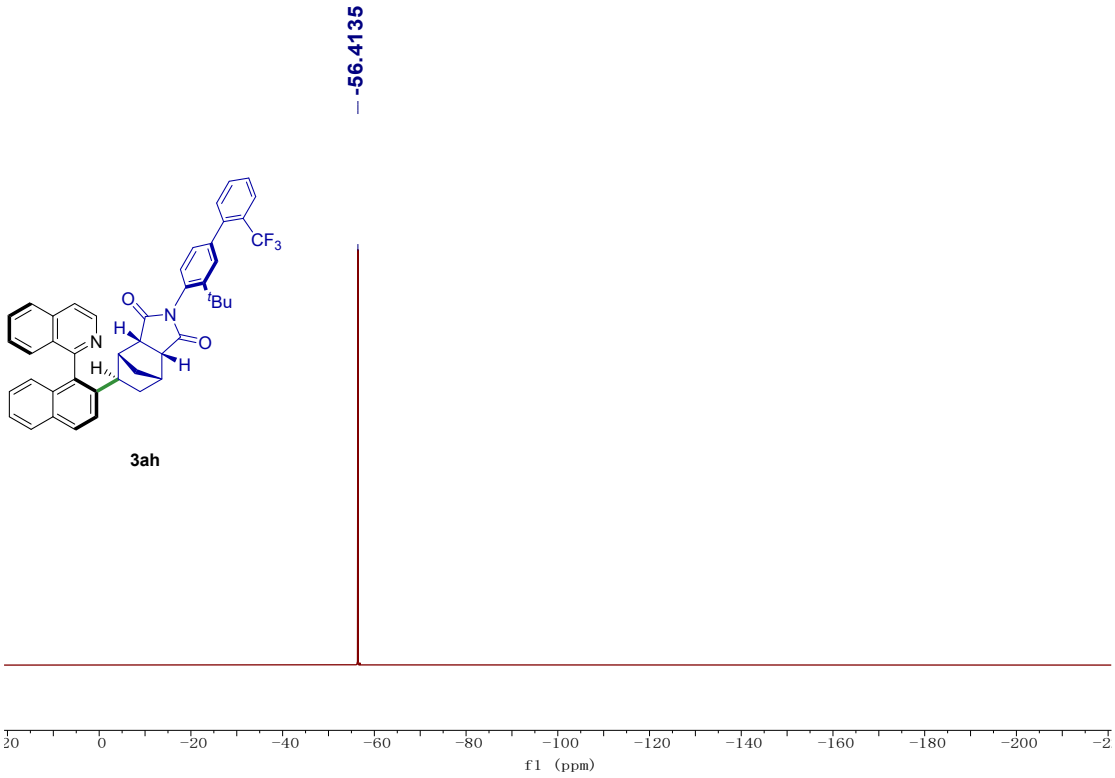
N
H
3ah
f1 (ppm)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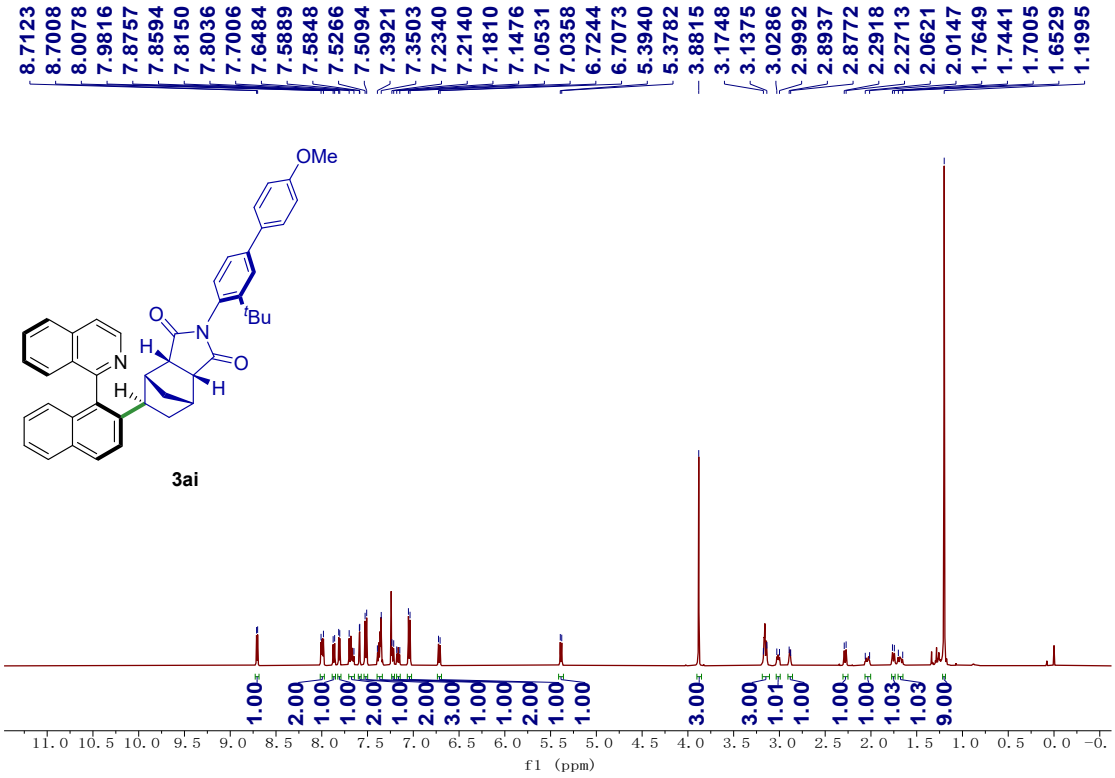
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OMe
tBu
O
N
H
O
H
N
H
3ai
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2.00
1.00
1.00
2.00
1.00
2.00
3.00
1.00
1.00
2.00
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9.00
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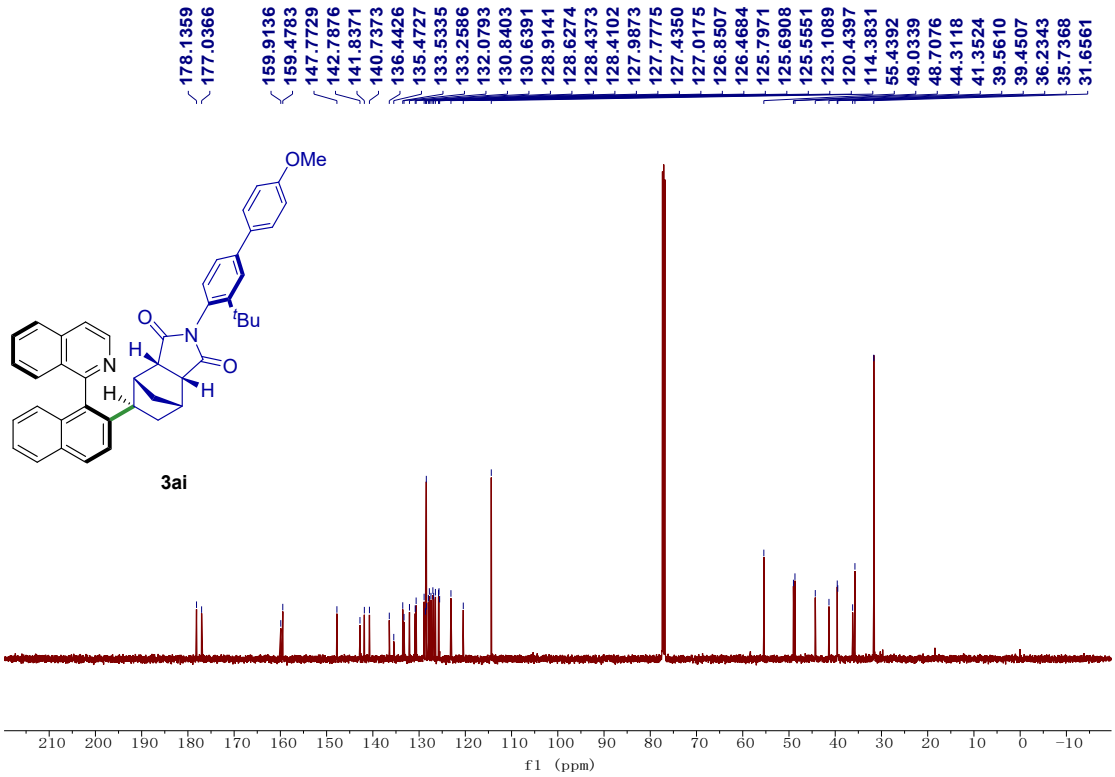
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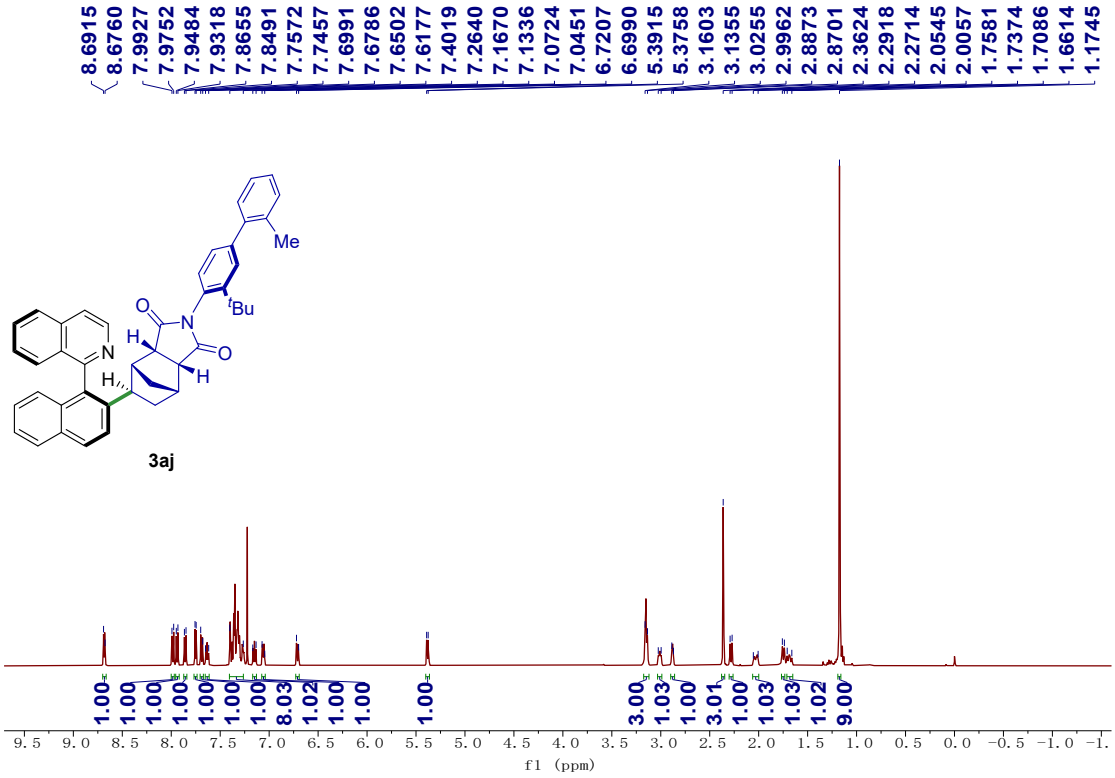
3ai
f1 (ppm)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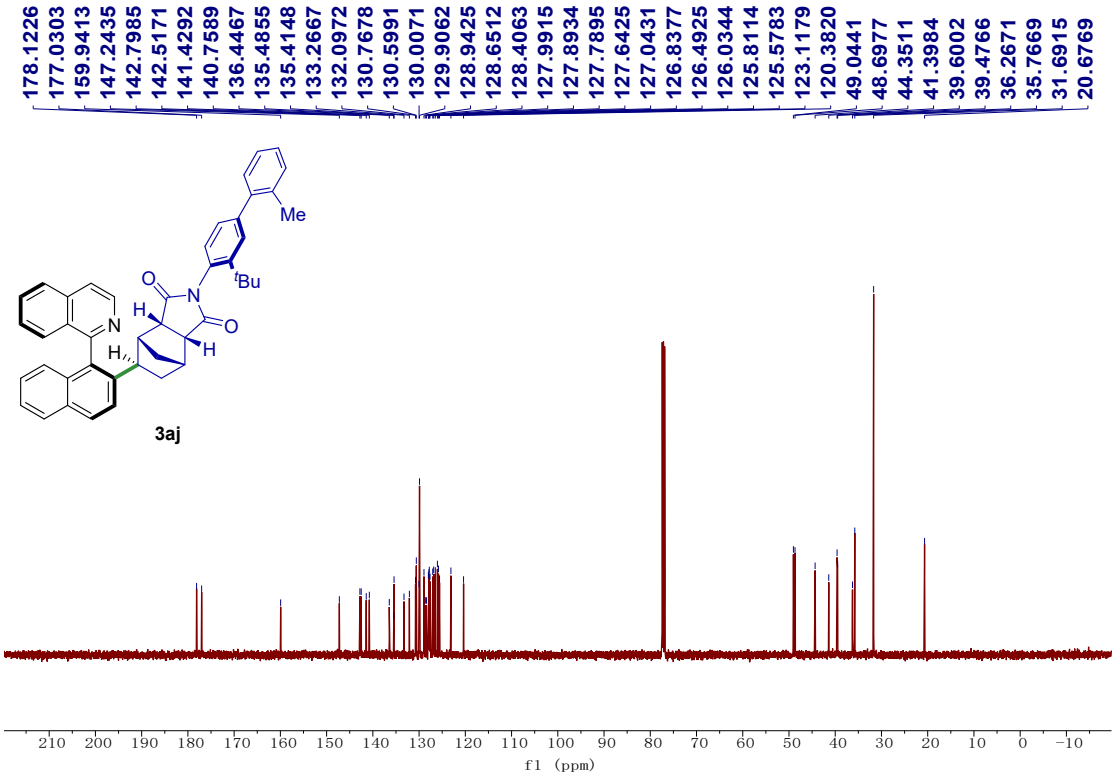
Me
tBu
O
N
H
O
H
N
H
3aj
1.00 1.00 1.00 1.00 1.00 1.00 1.00 8.03 1.02 1.00 1.00 1.00 3.00 1.03 1.00 3.01 1.00 1.03 1.03 1.02 9.00
f1 (ppm)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H
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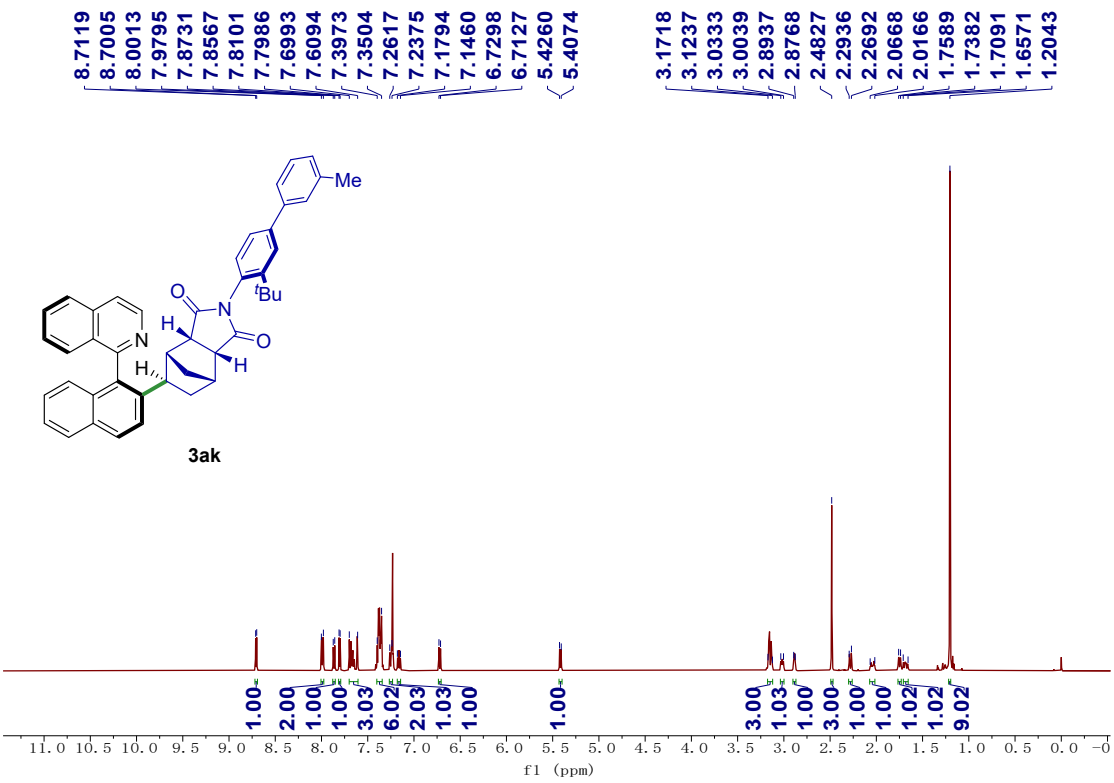
f1 (ppm)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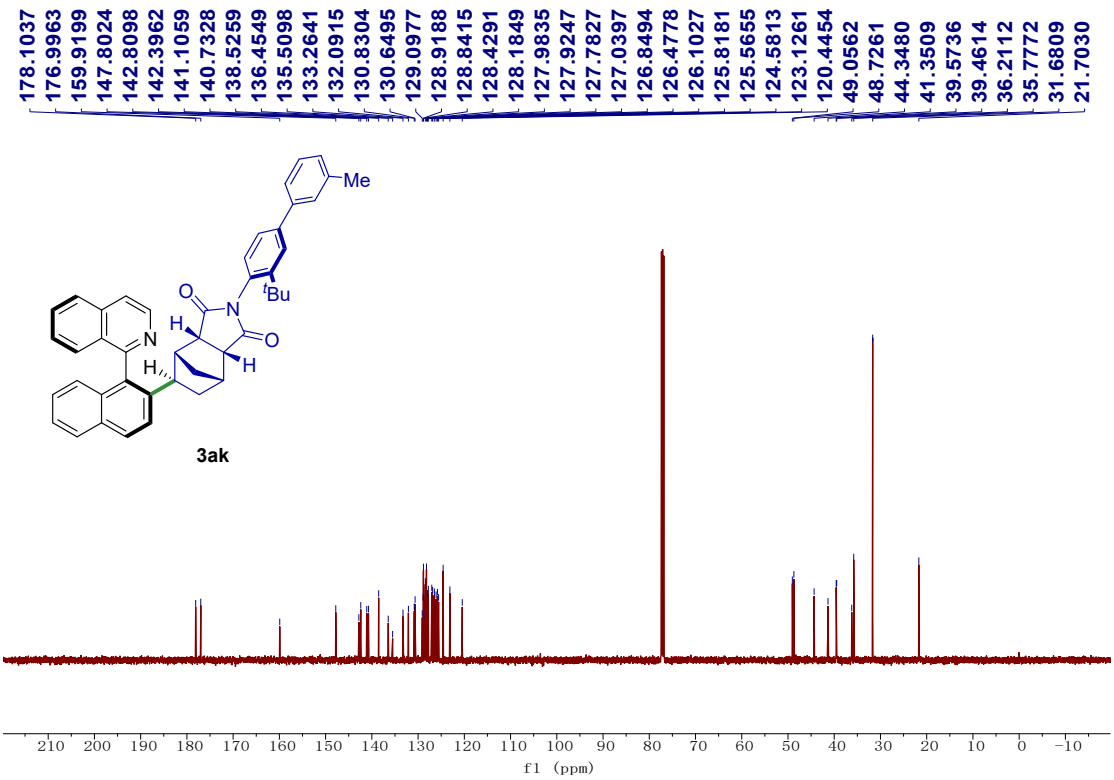
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O
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N
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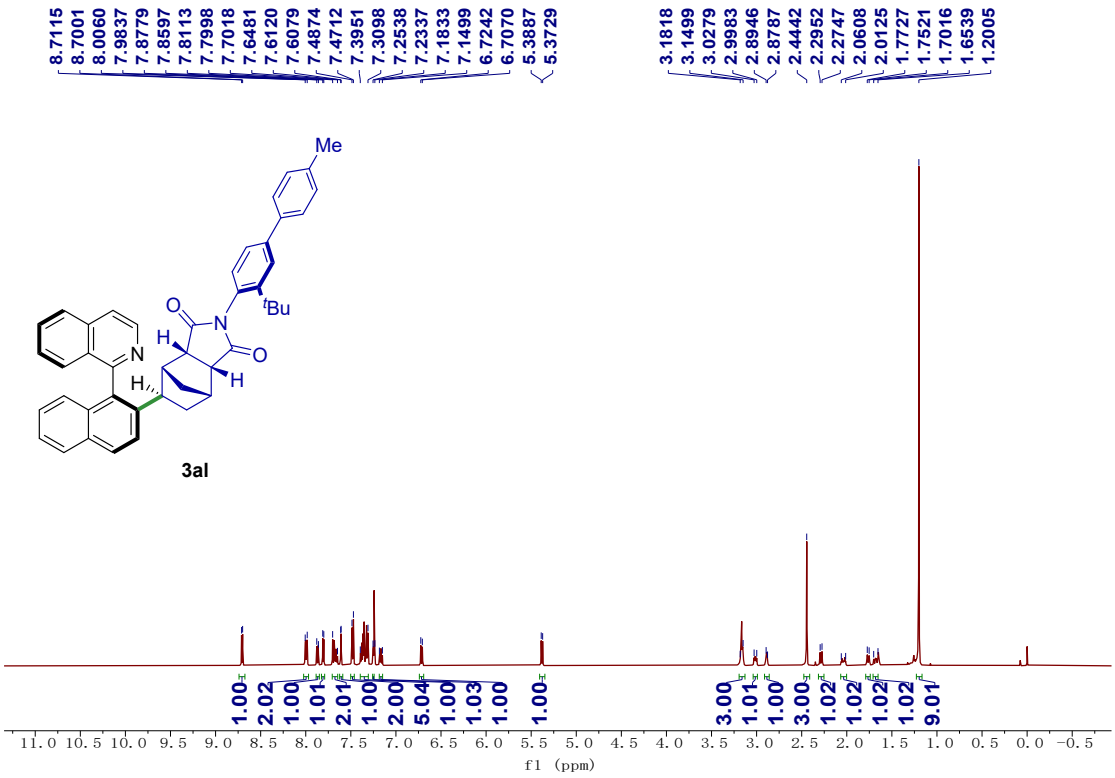
f1 (ppm)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1.00
1.00
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1.01
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1.02
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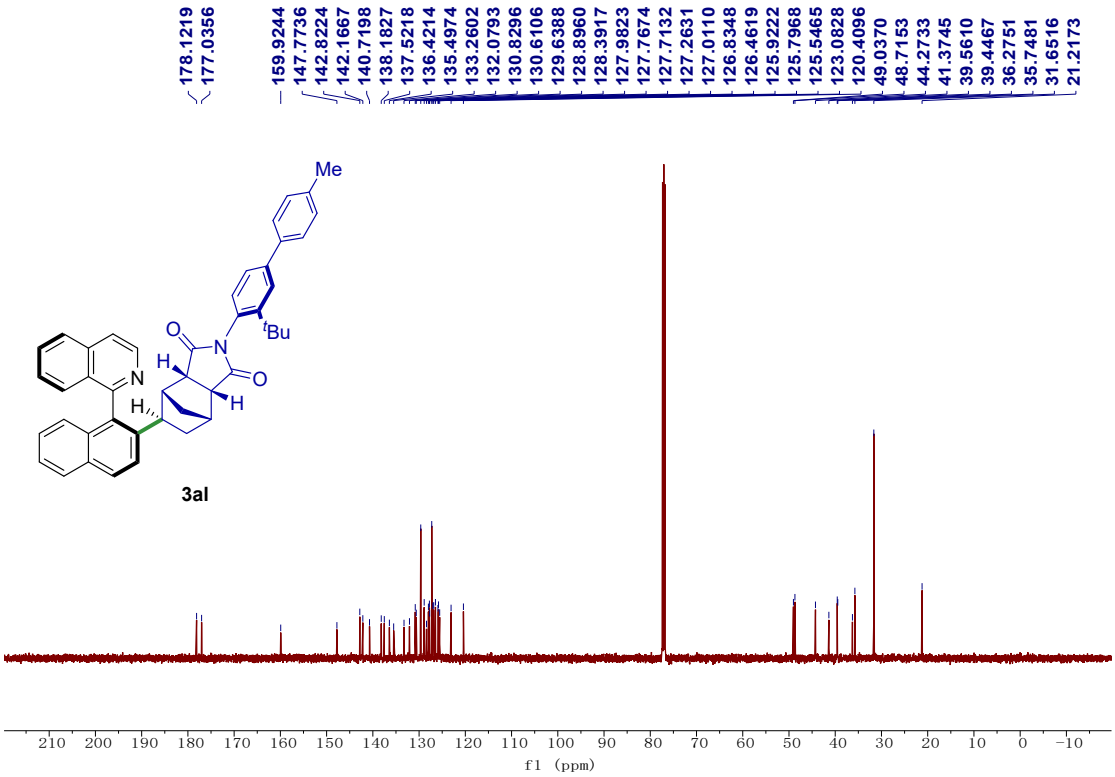
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36.2751
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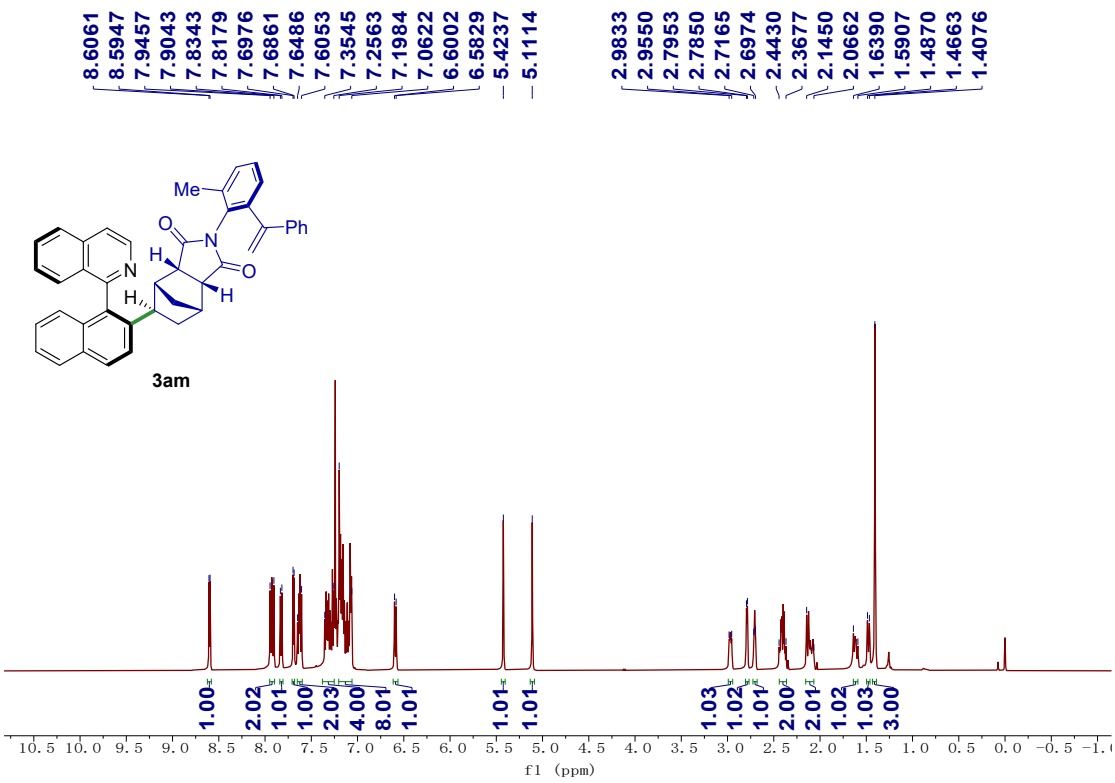
f1 (ppm)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4.00
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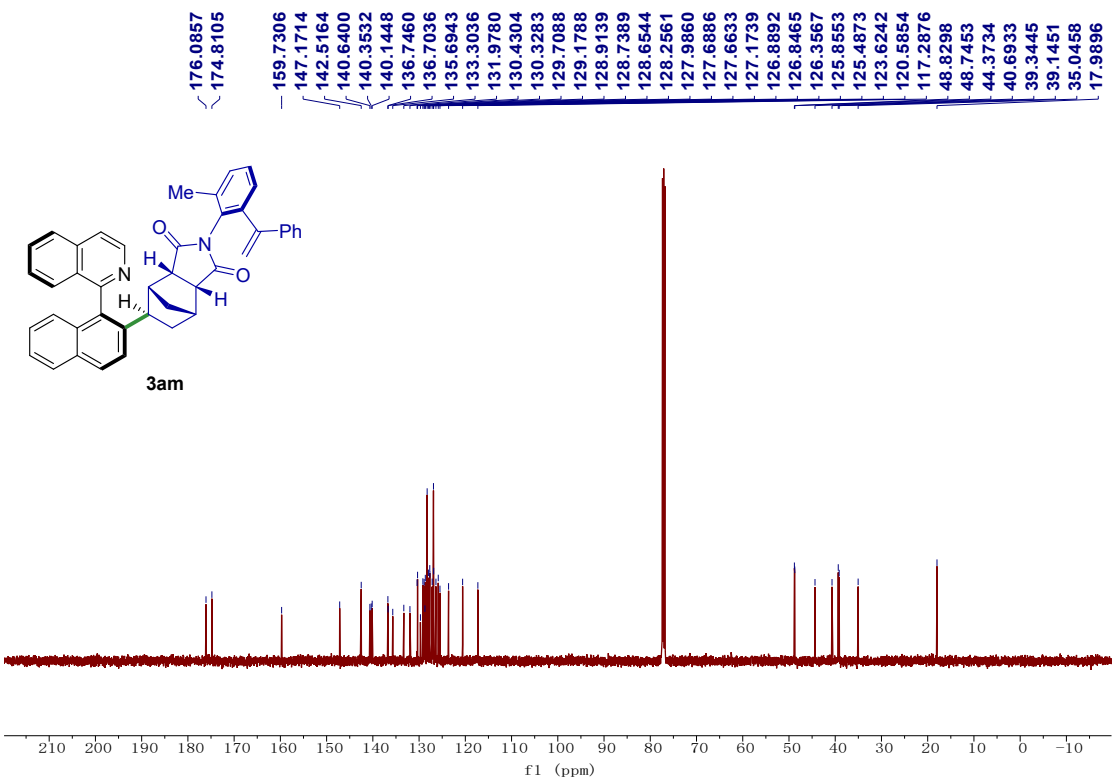
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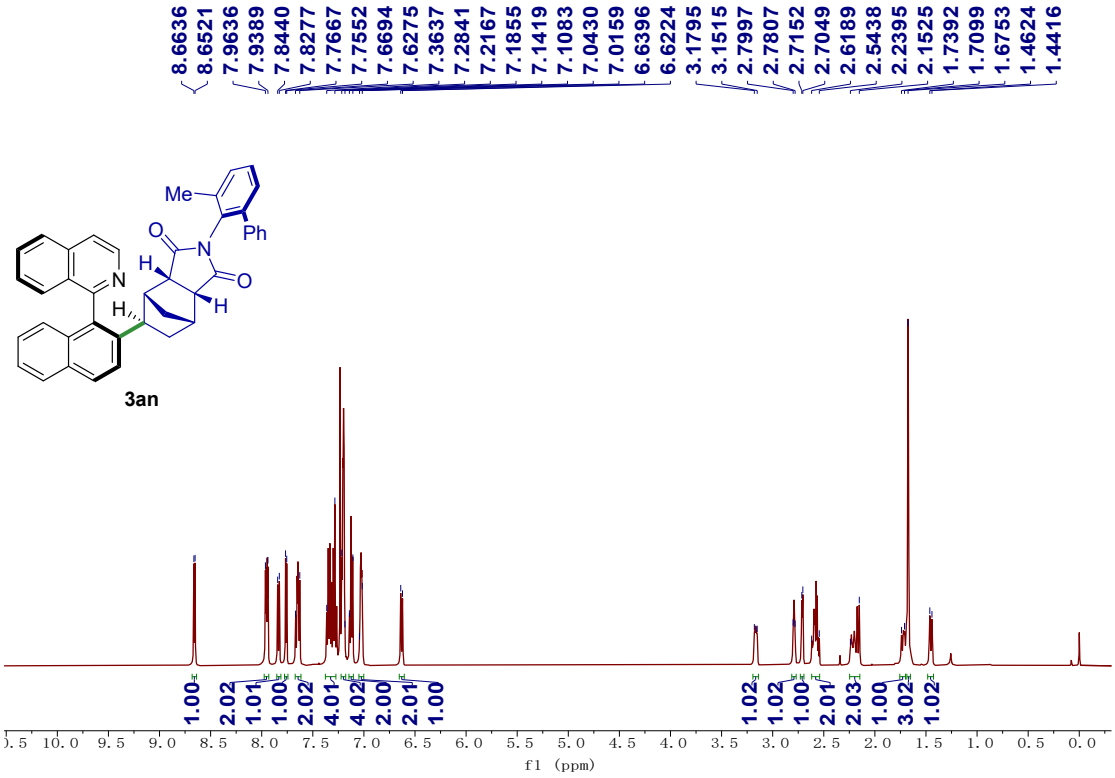
3am
f1 (ppm)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Ph
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H
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H
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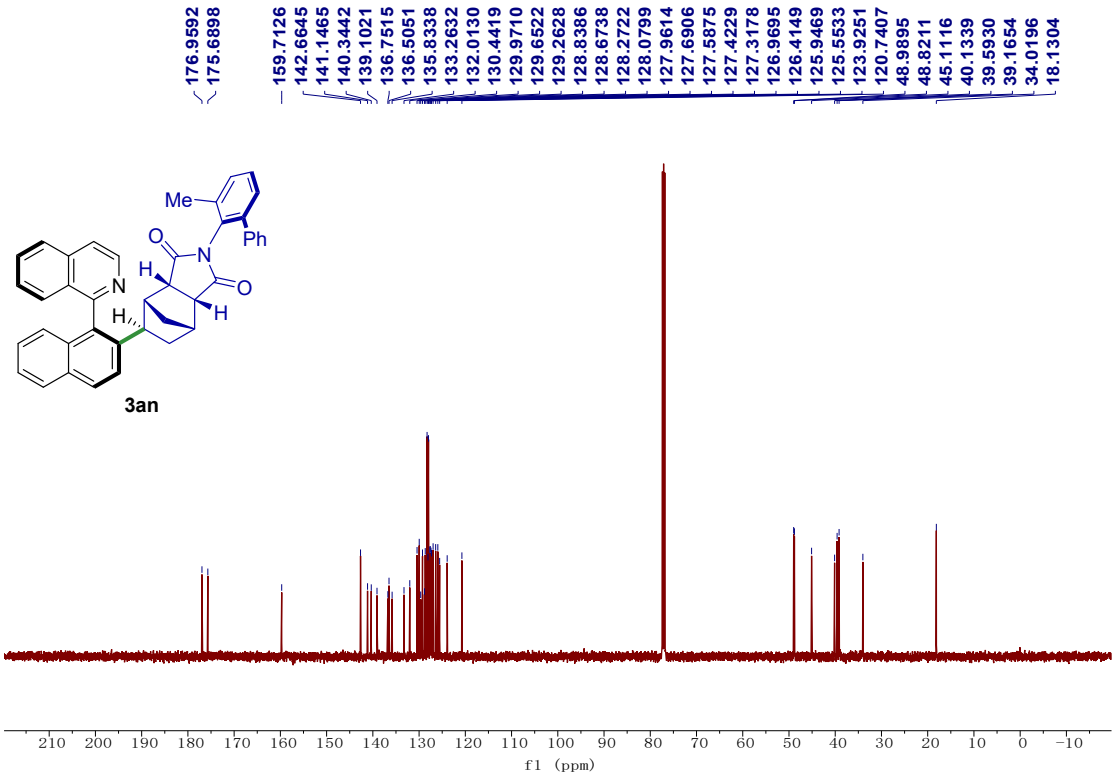
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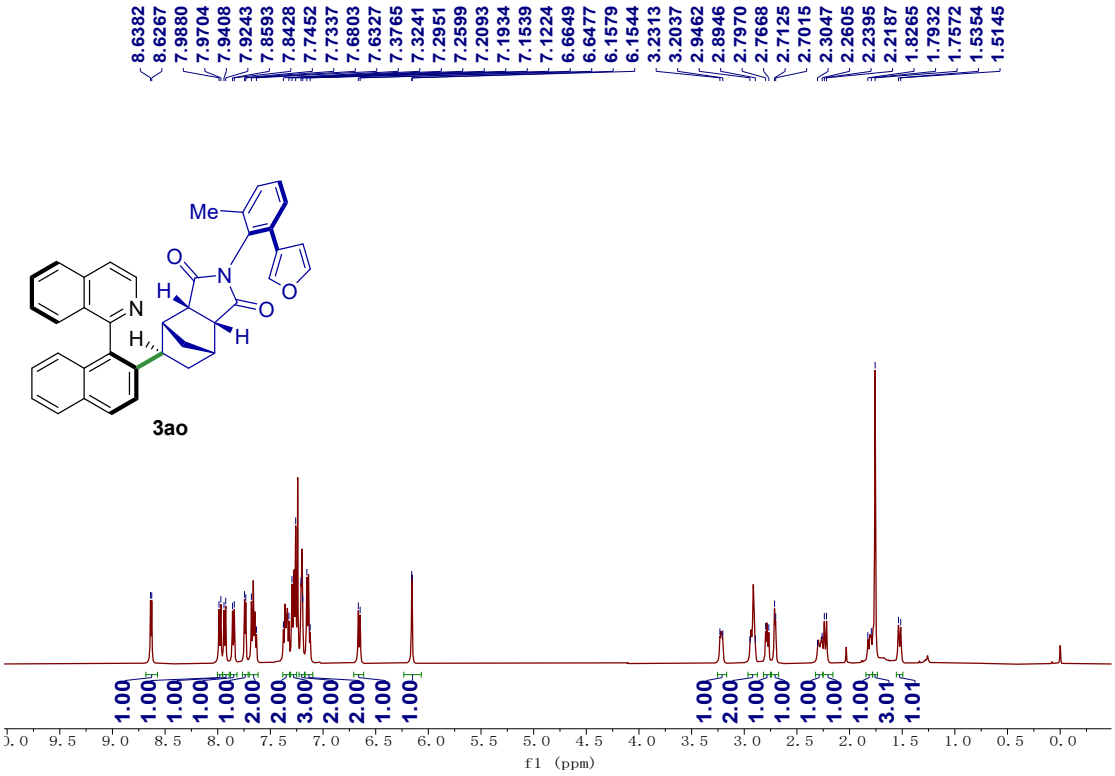
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H
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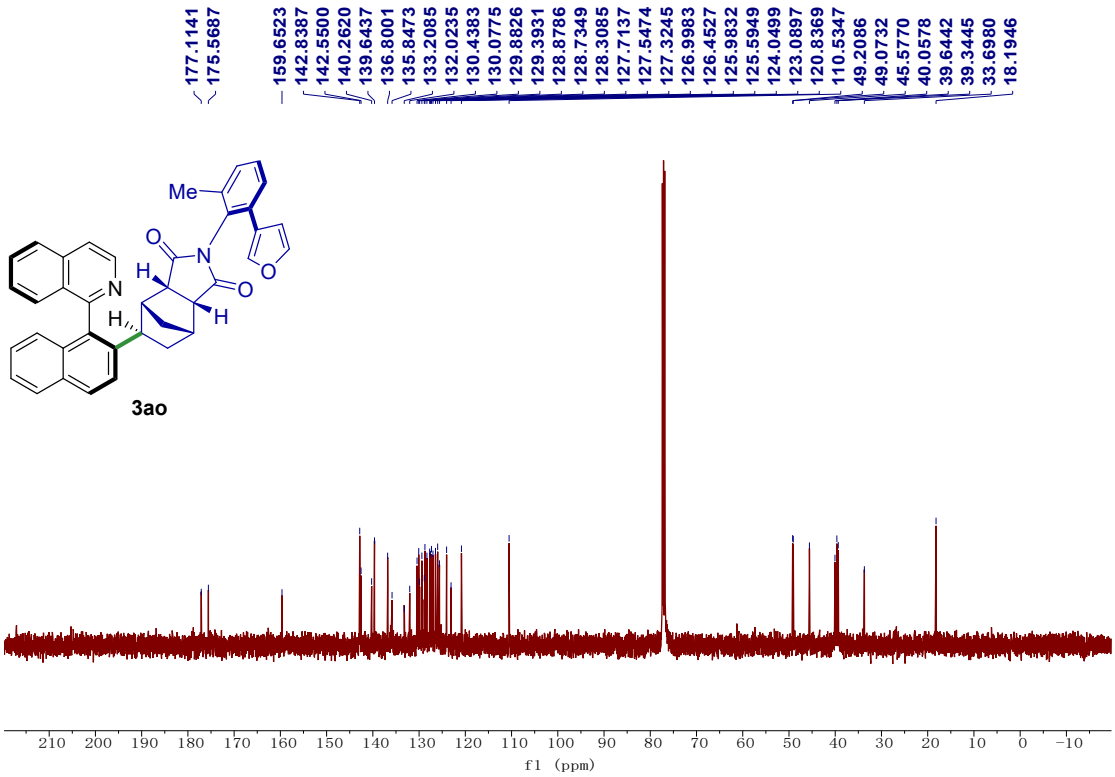
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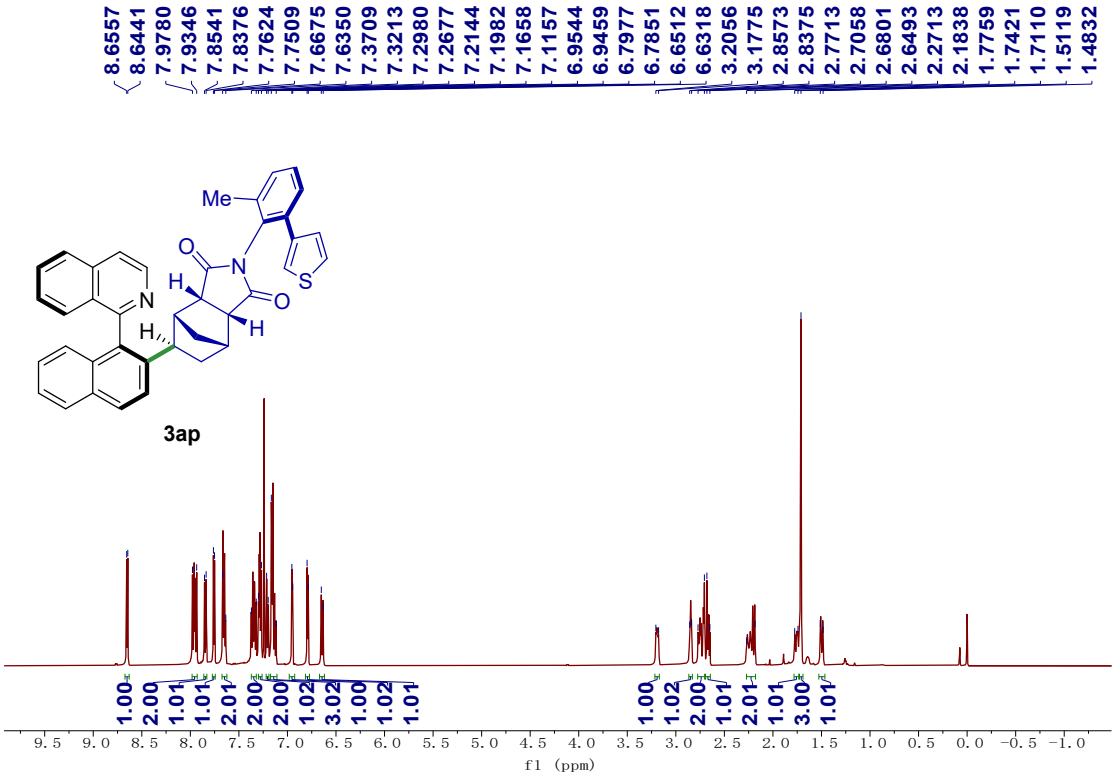
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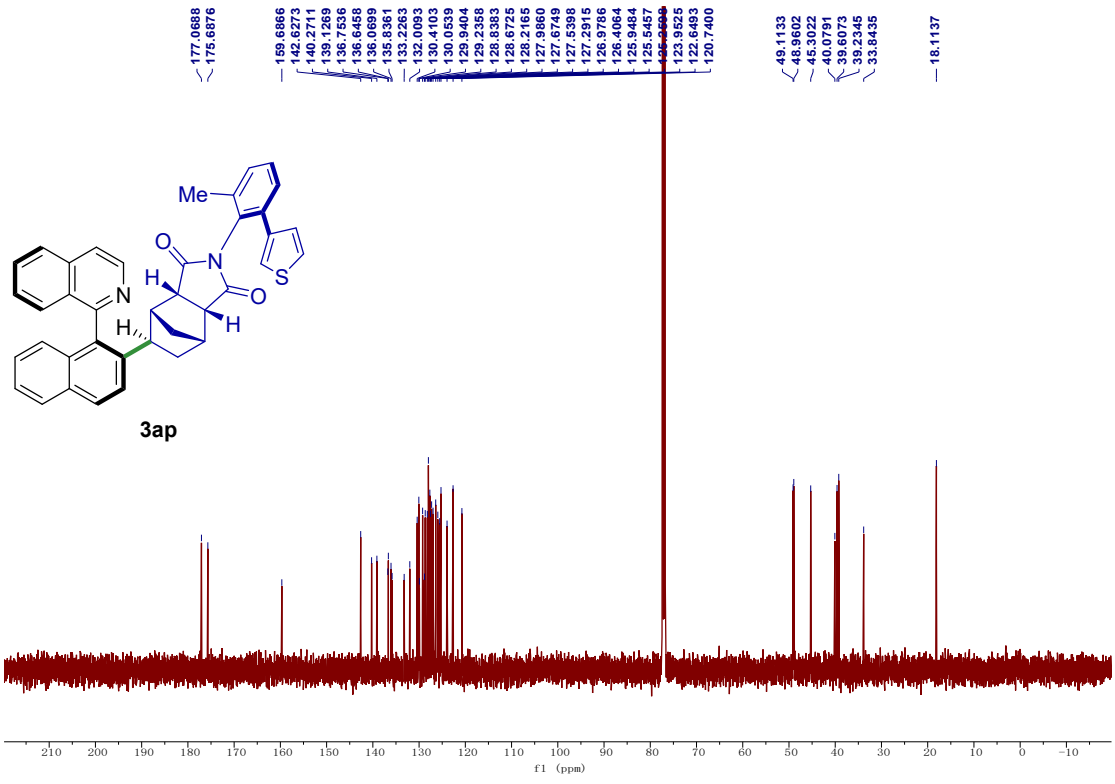
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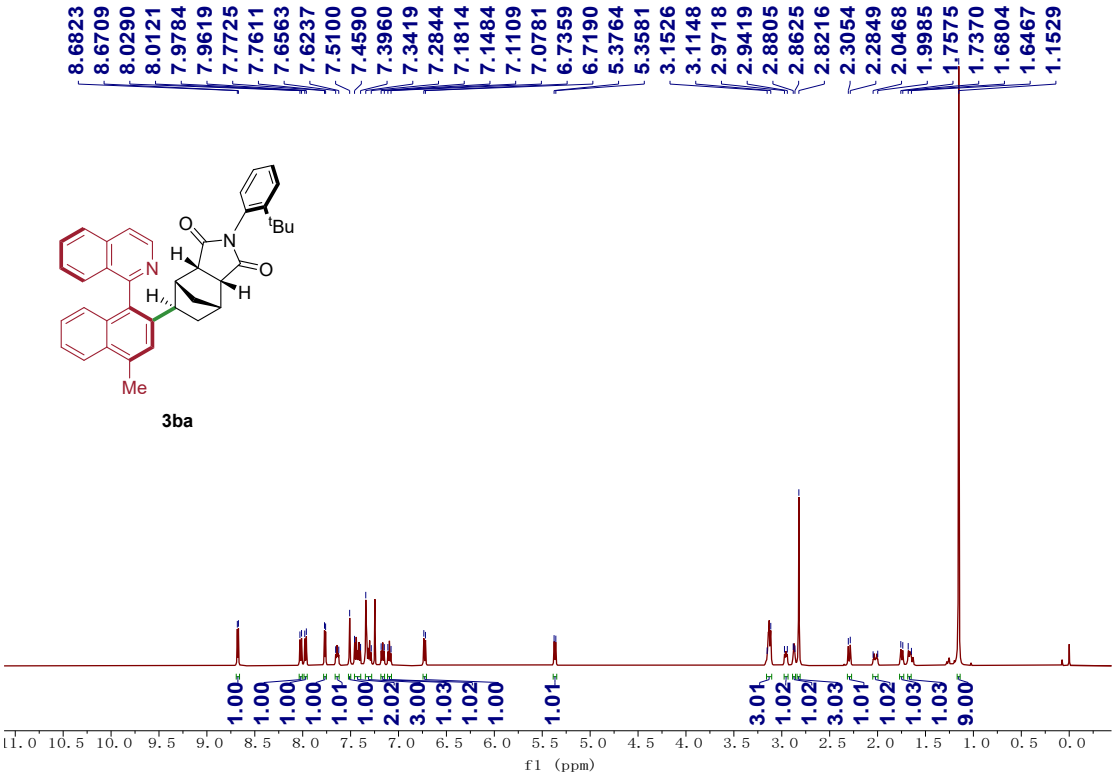
H
H
3ap
f1 (ppm)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H
N
Me
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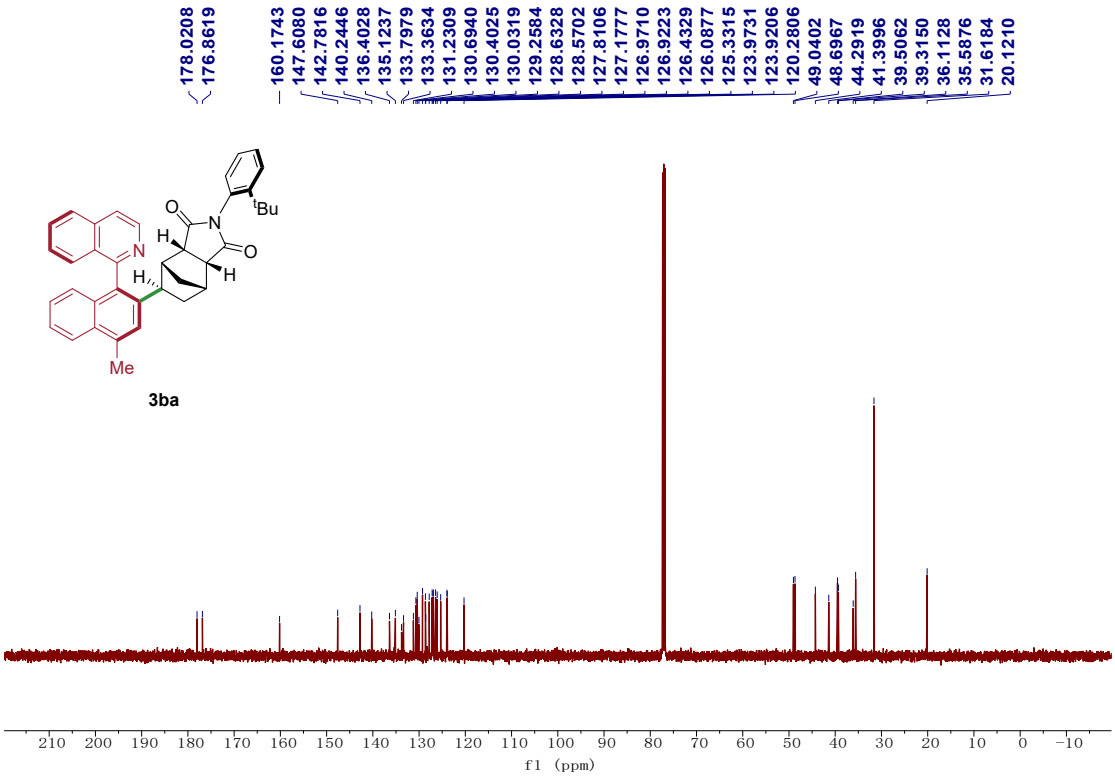
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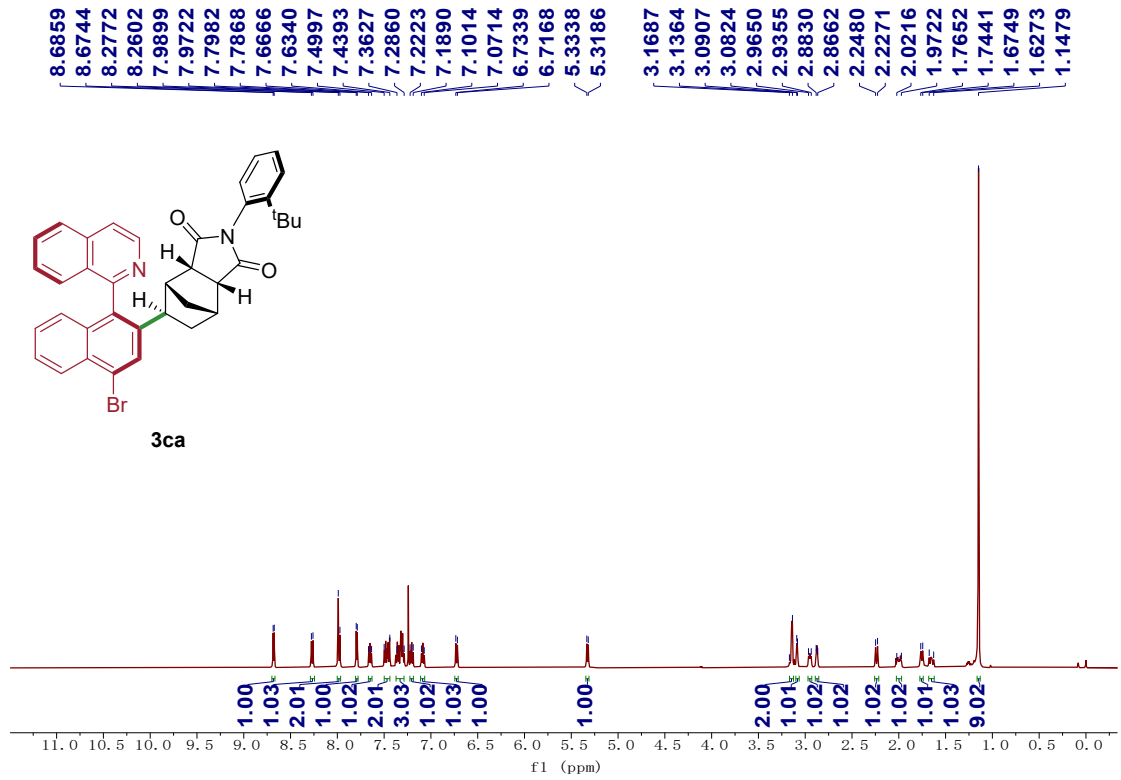
Me
3ba
f1 (ppm)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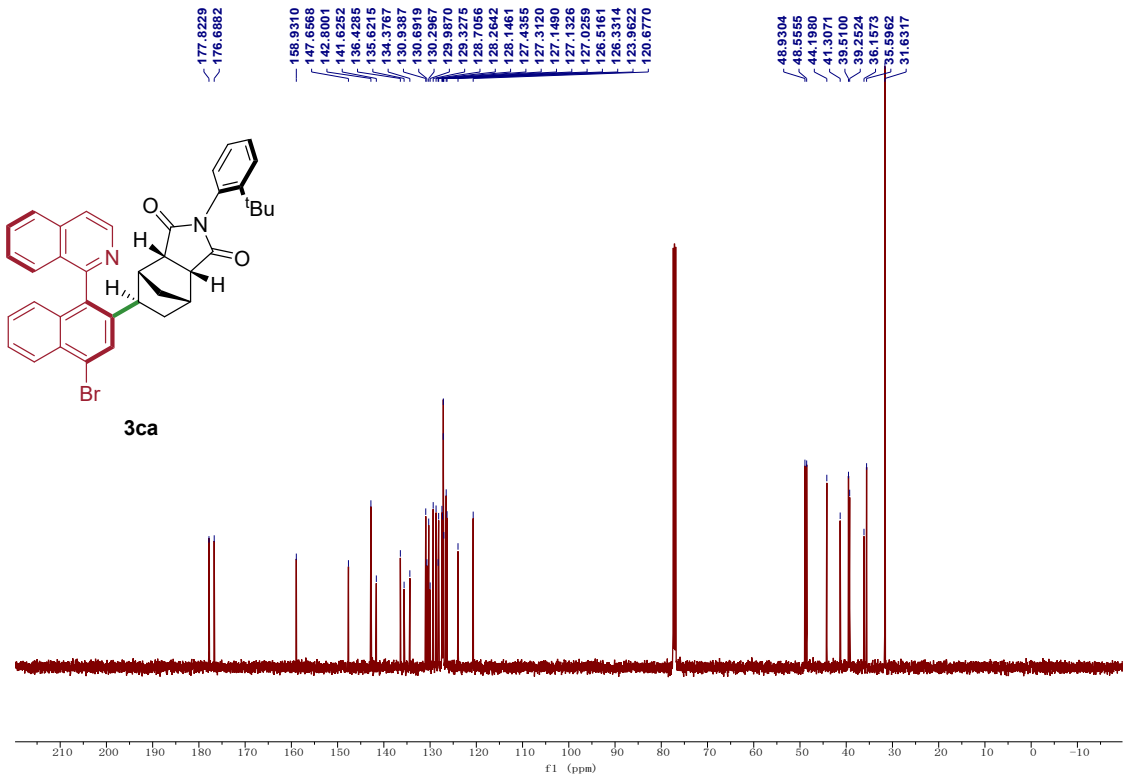
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Br
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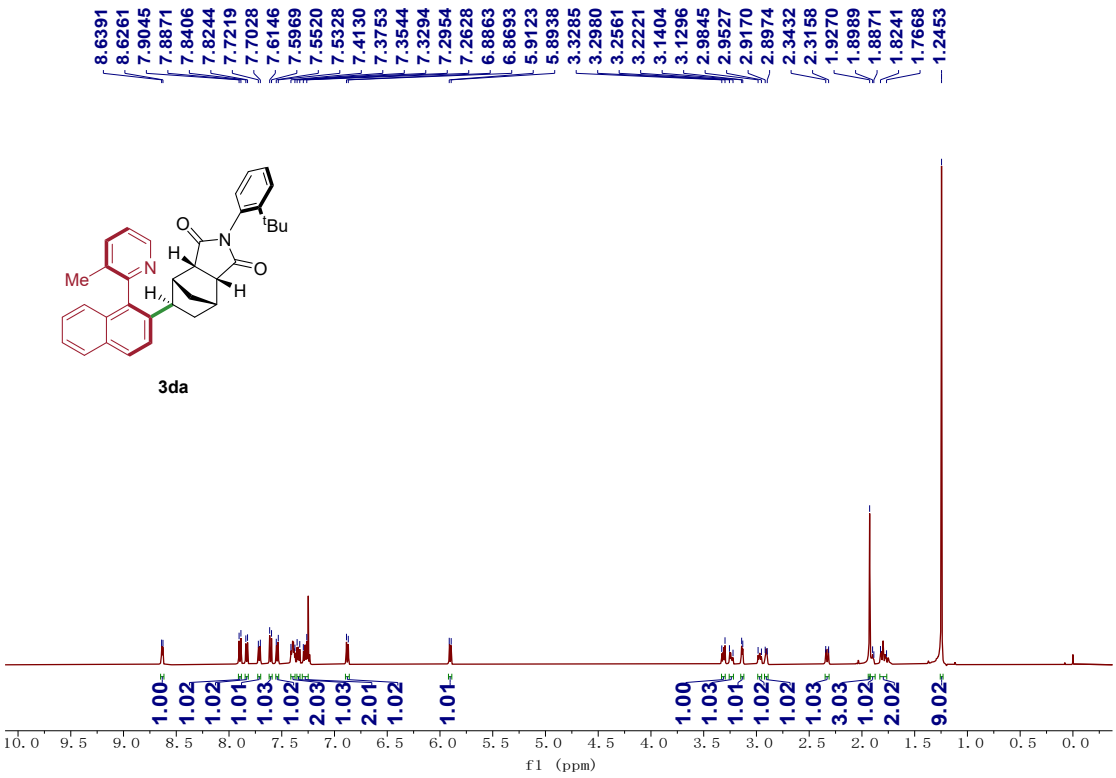
f1 (ppm)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10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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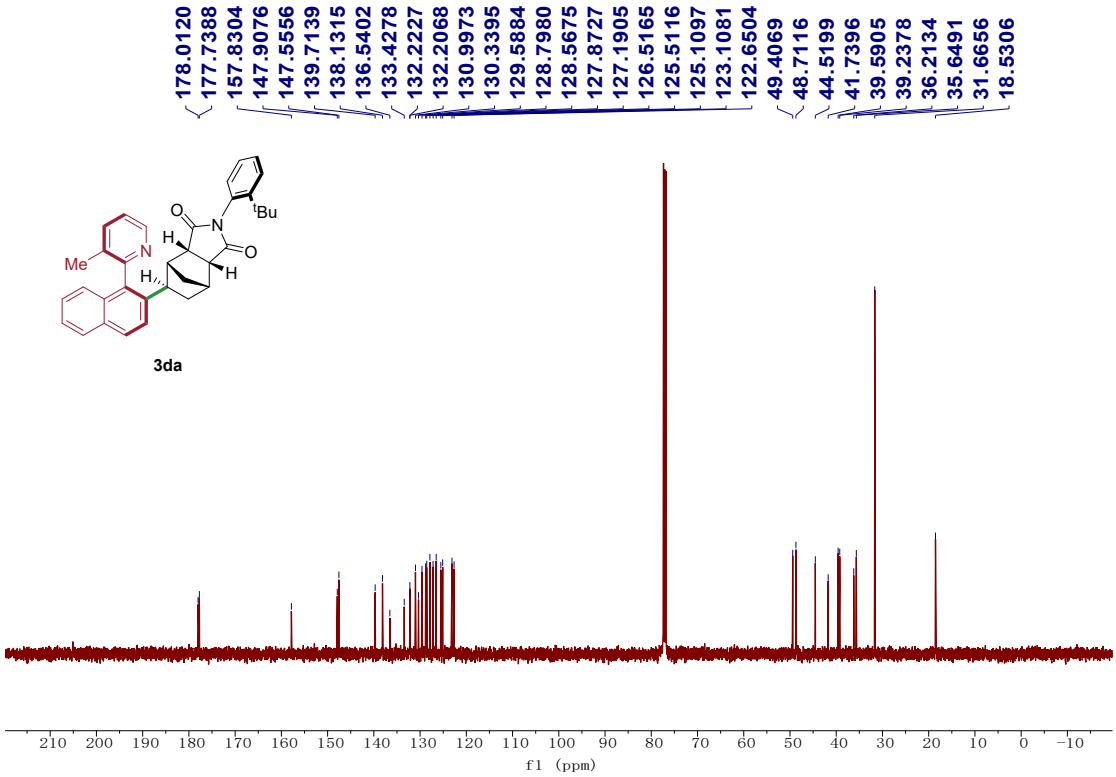
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35.6491
31.6656
18.5306
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H
Me
N
H
3da
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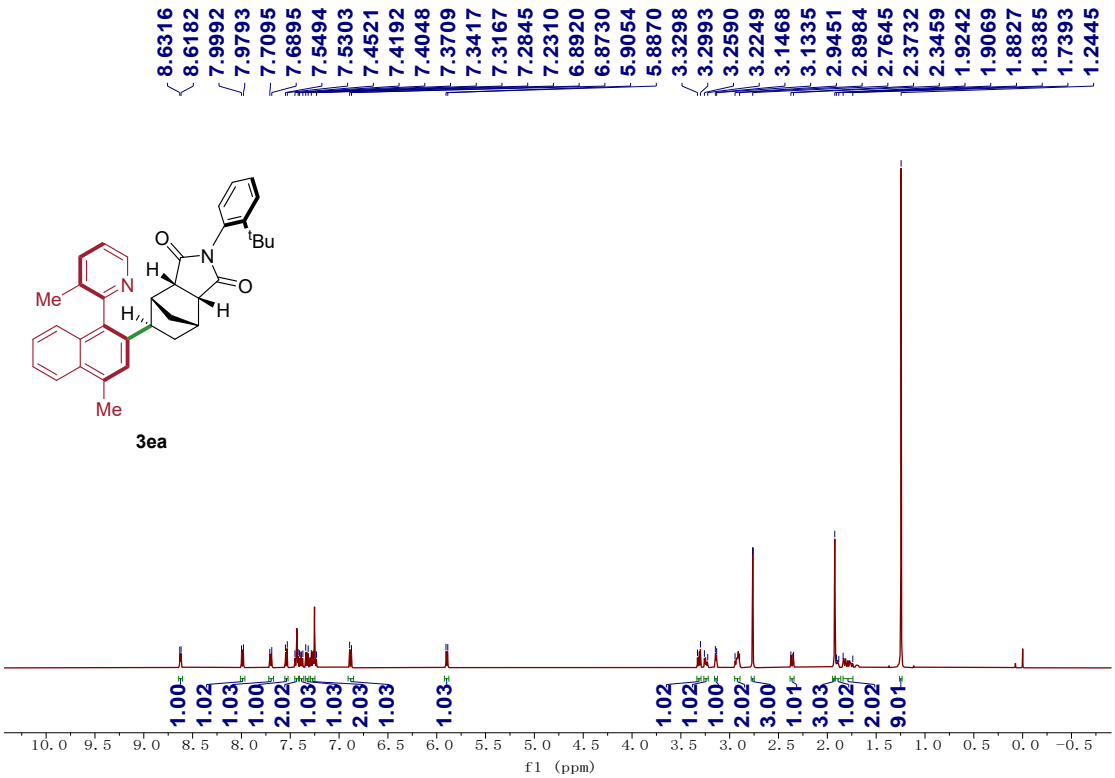
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1.7393
1.2445
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N
tBu
H
O
H
H
Me
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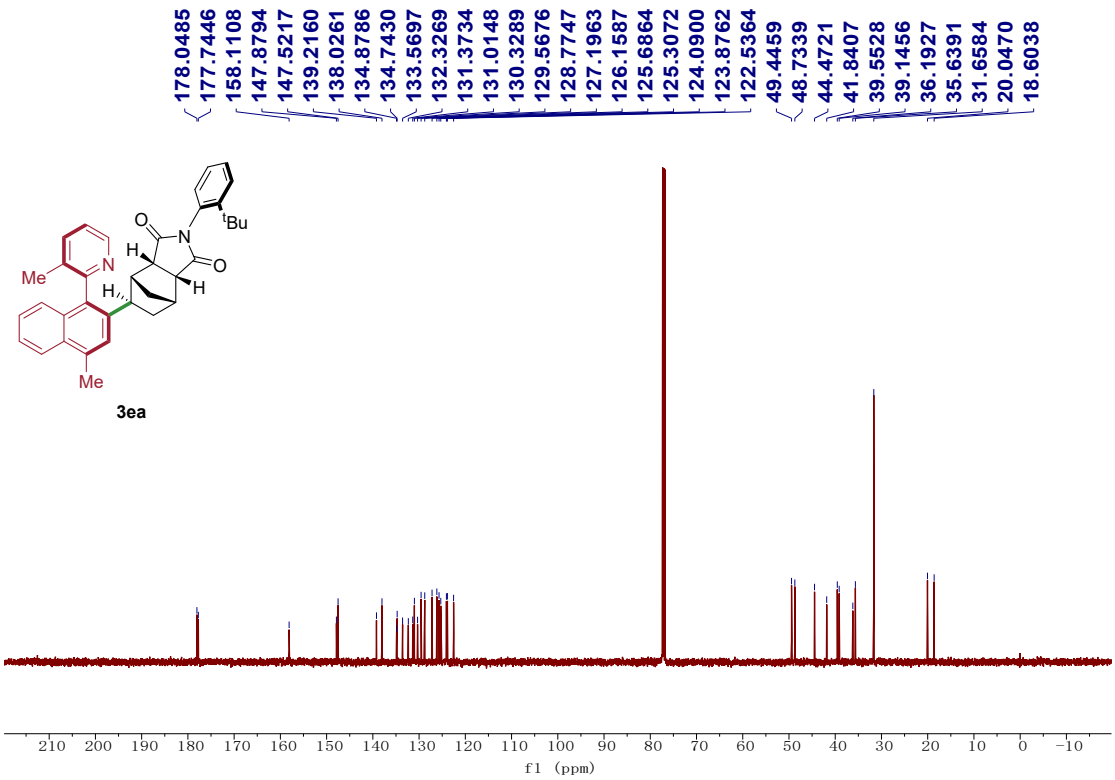
9.01
f1 (ppm)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Me
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tBu
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O
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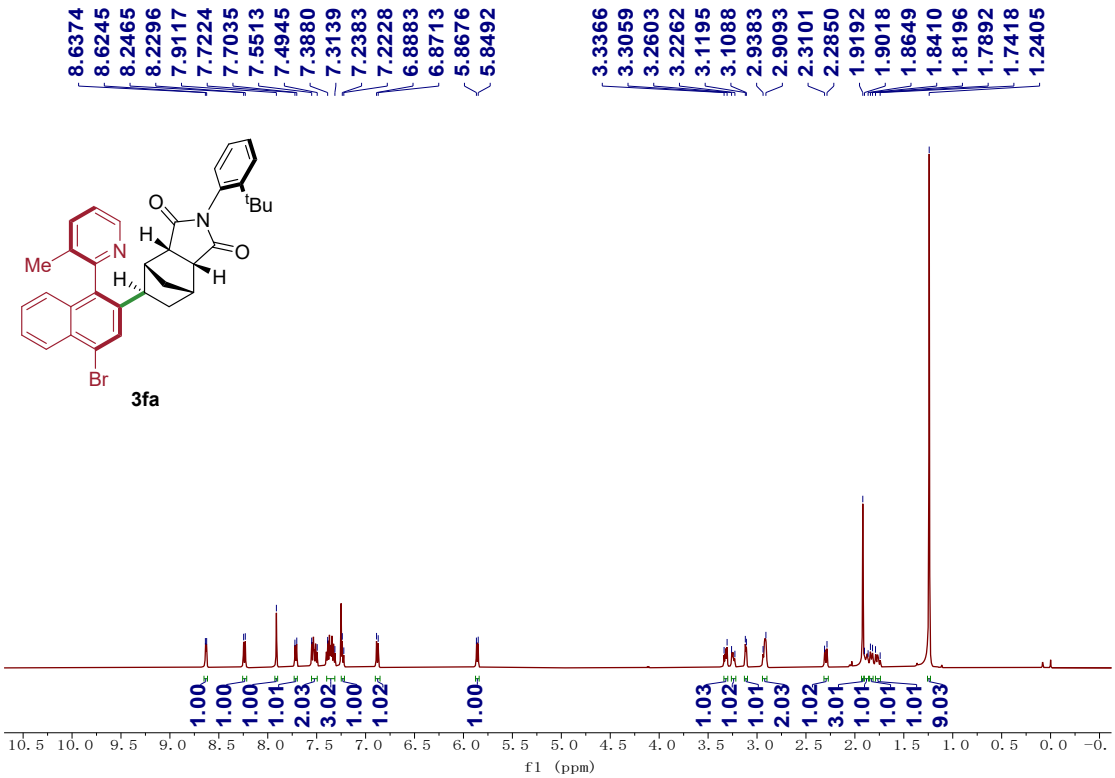
Me
3ea
f1 (ppm)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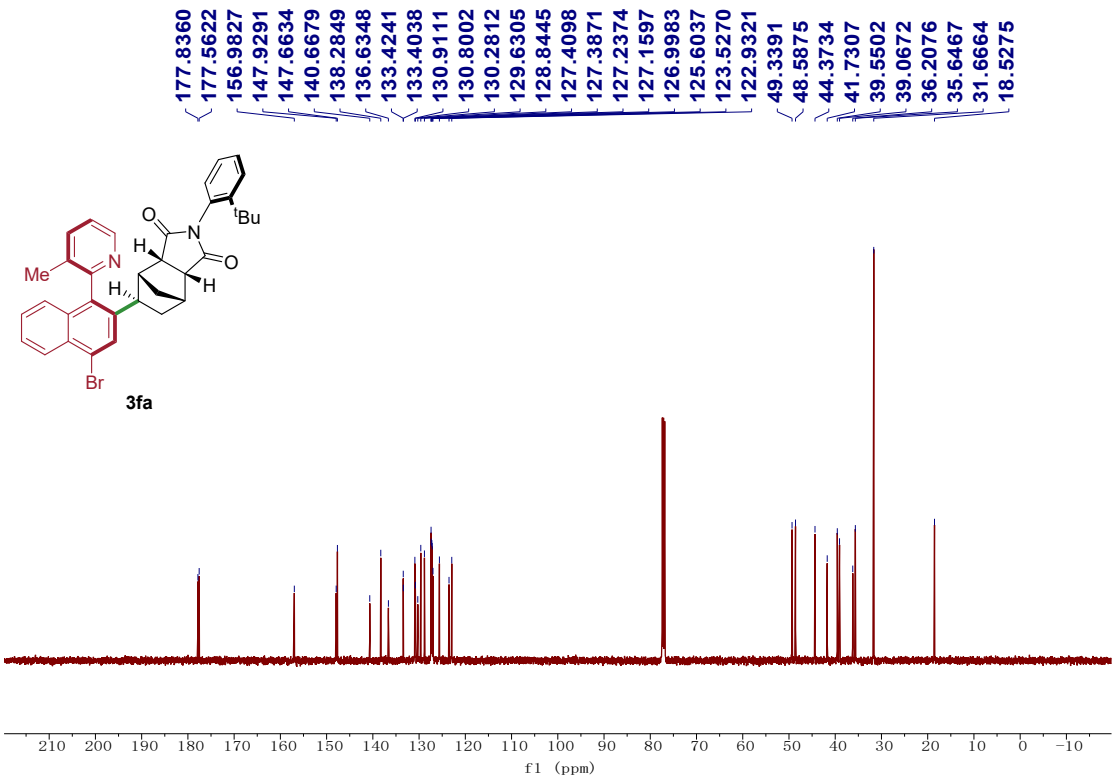
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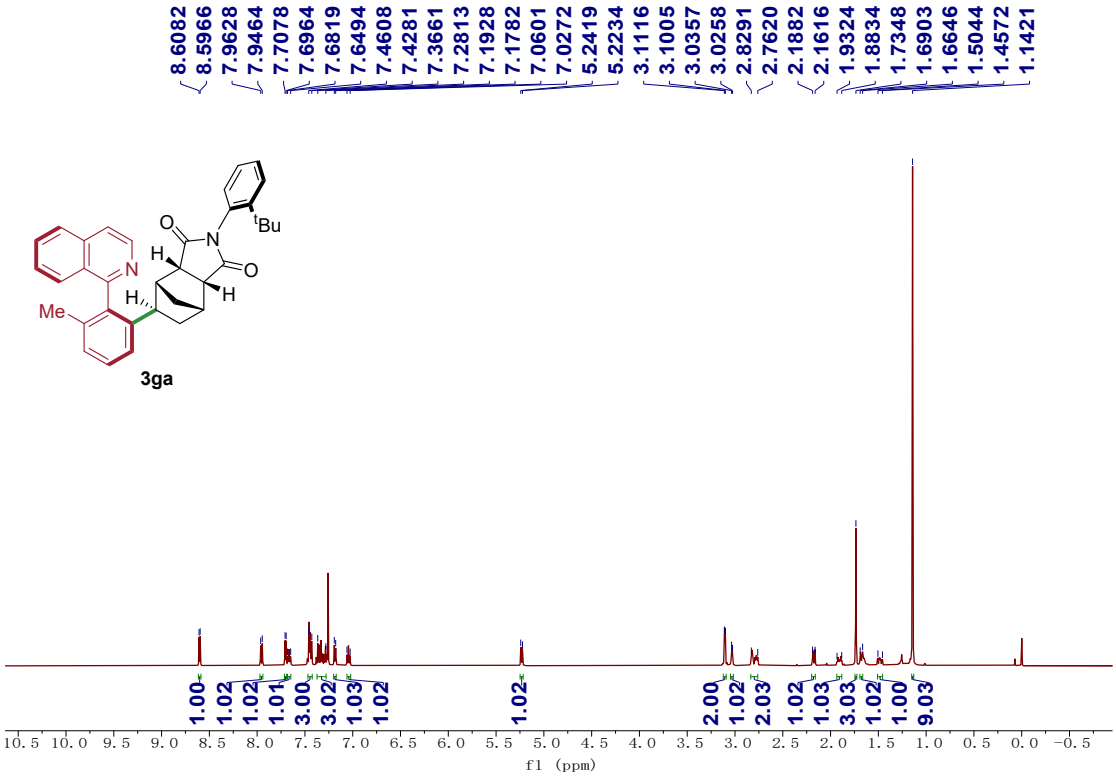
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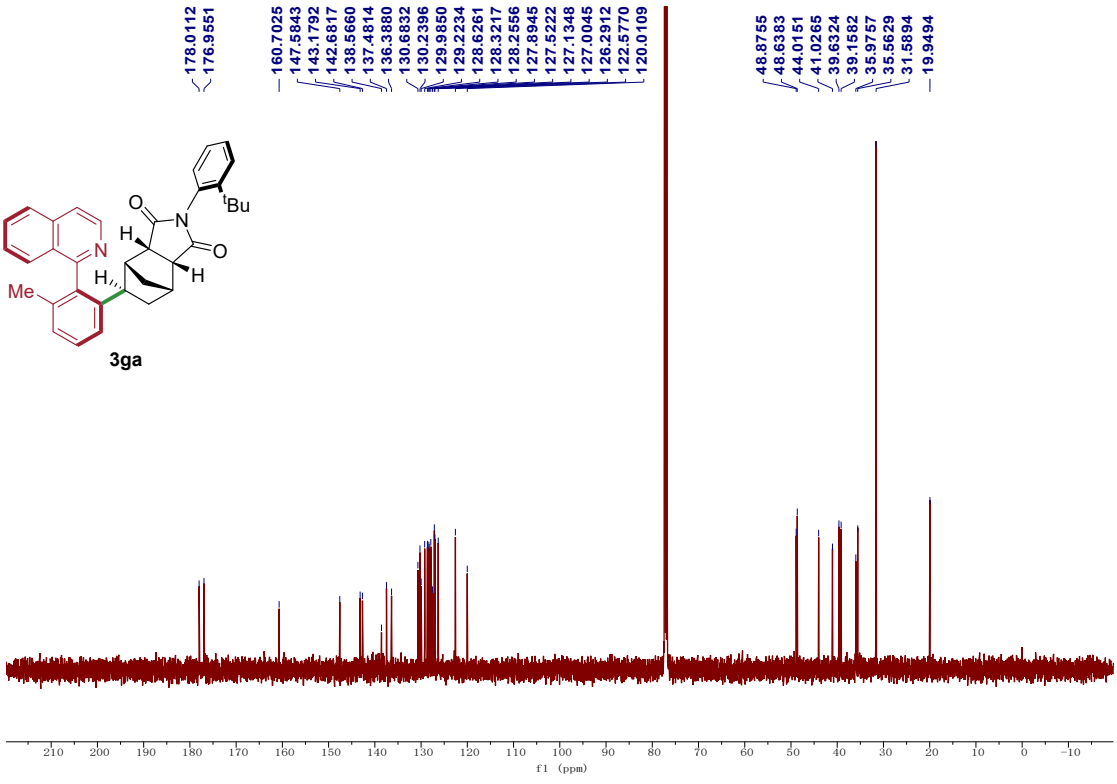
f1 (ppm)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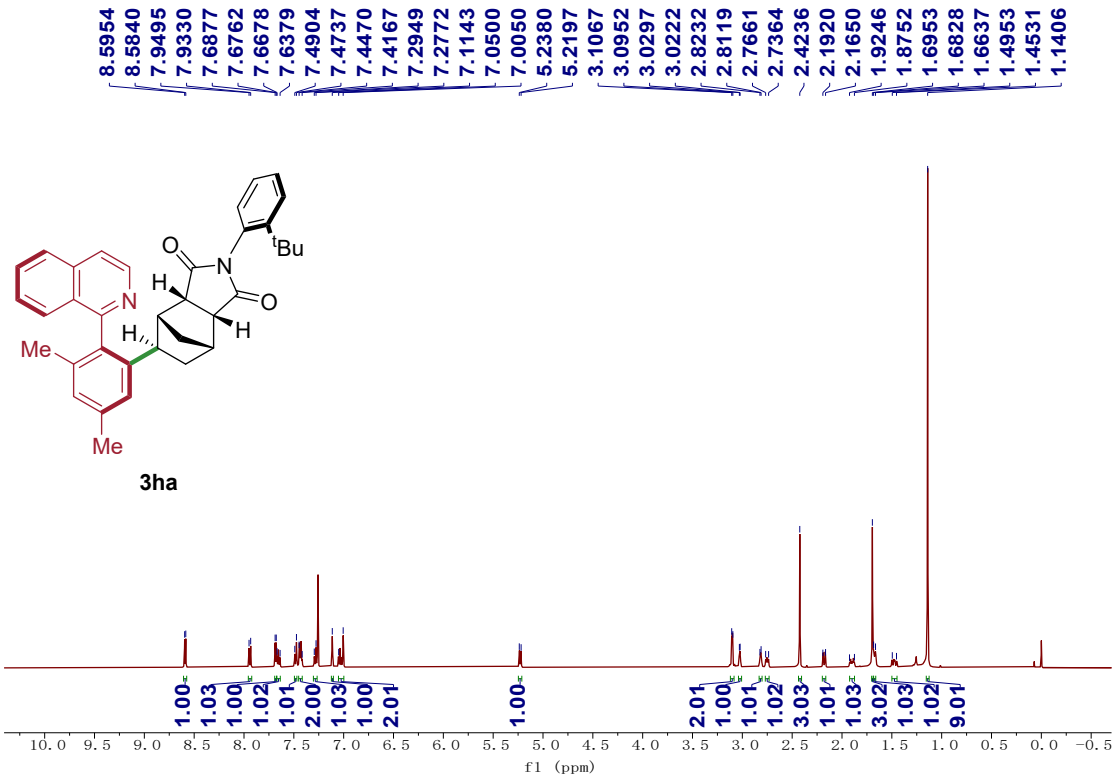
f1 (ppm)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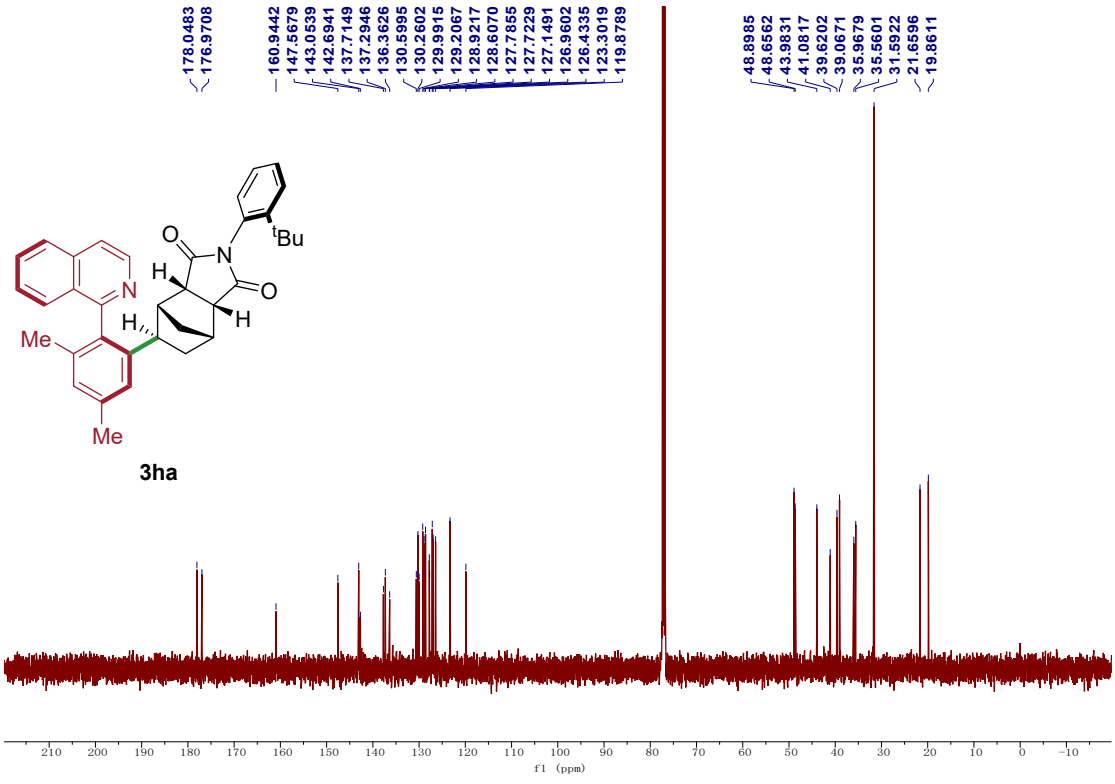
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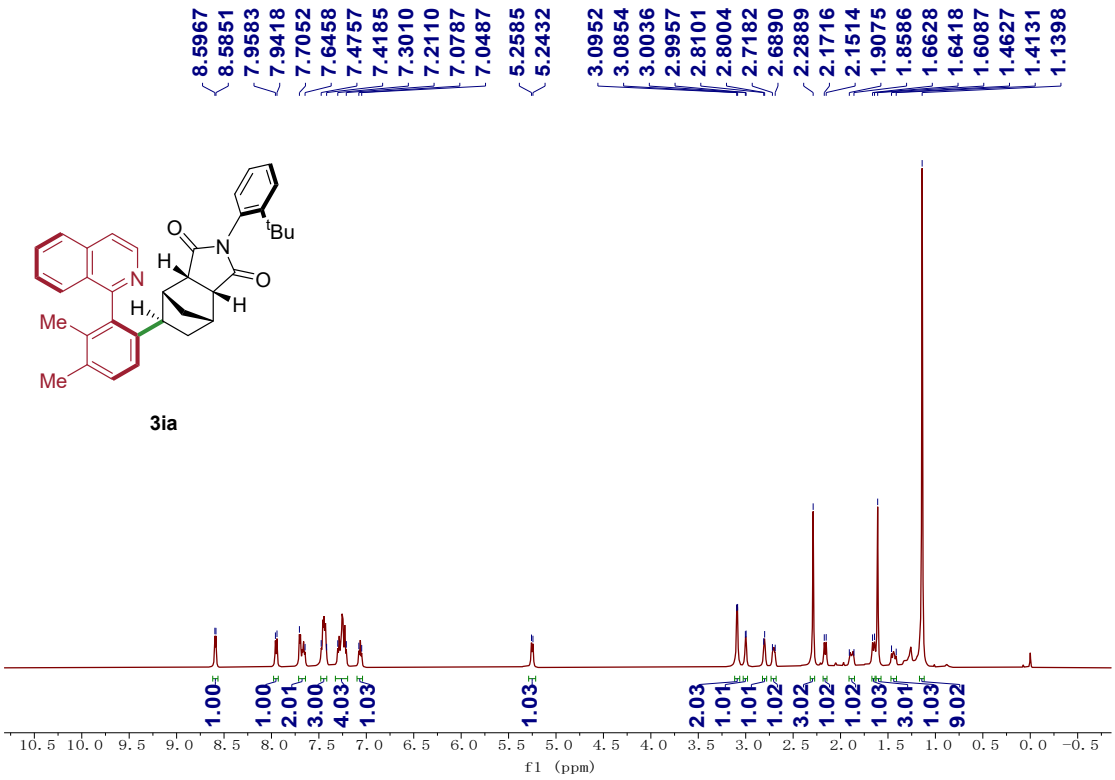
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H
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Me
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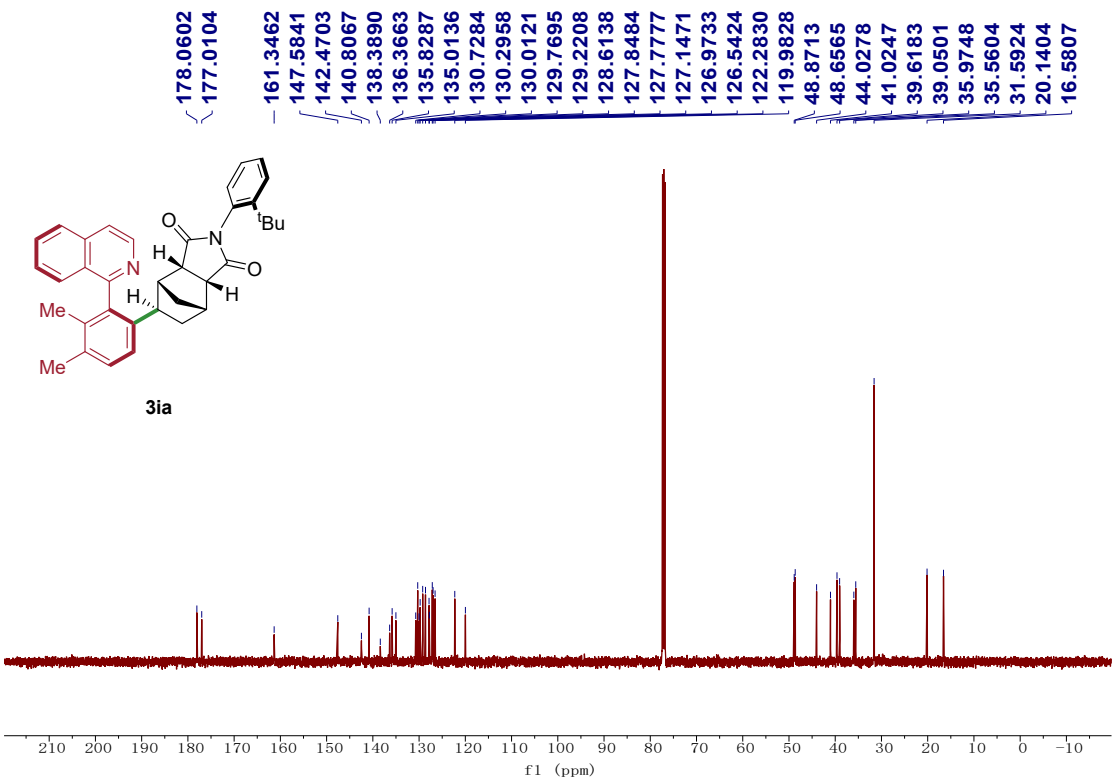
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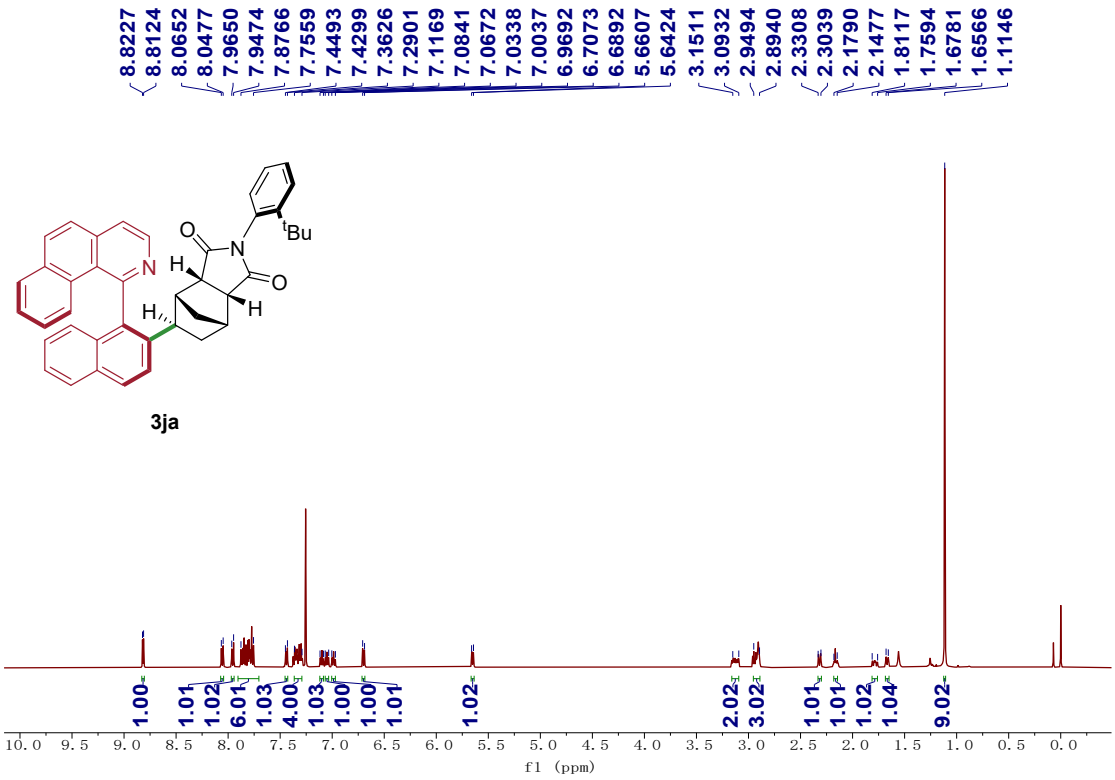
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H
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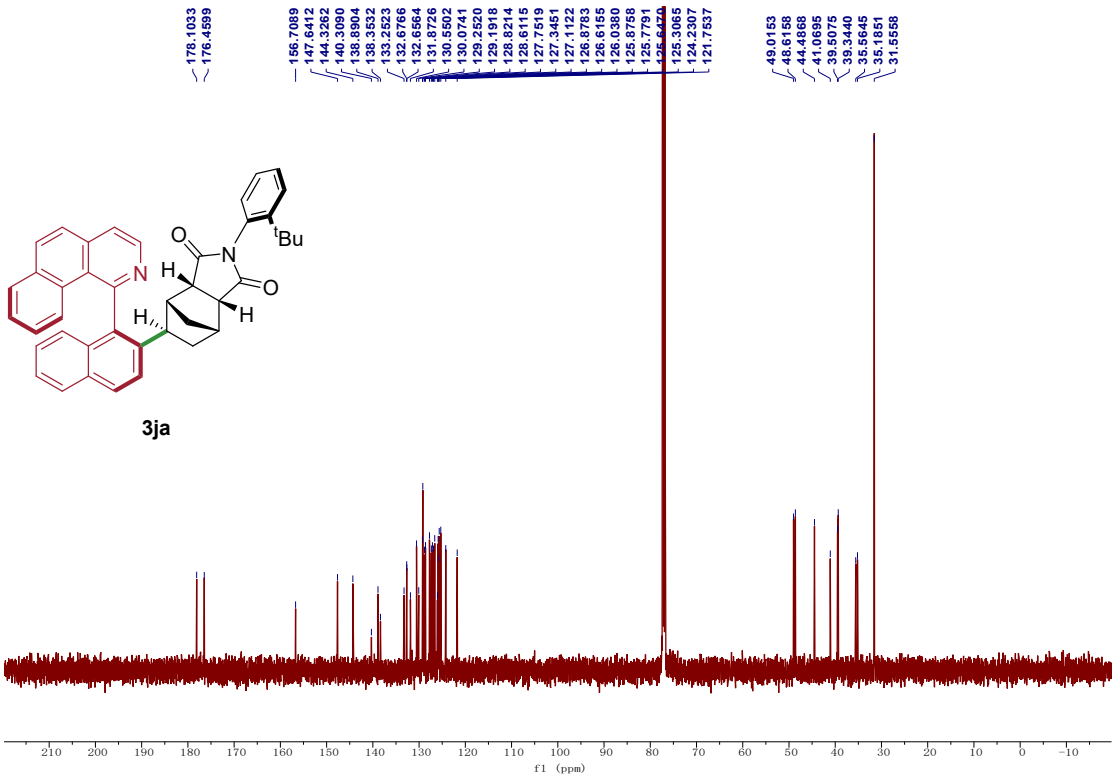
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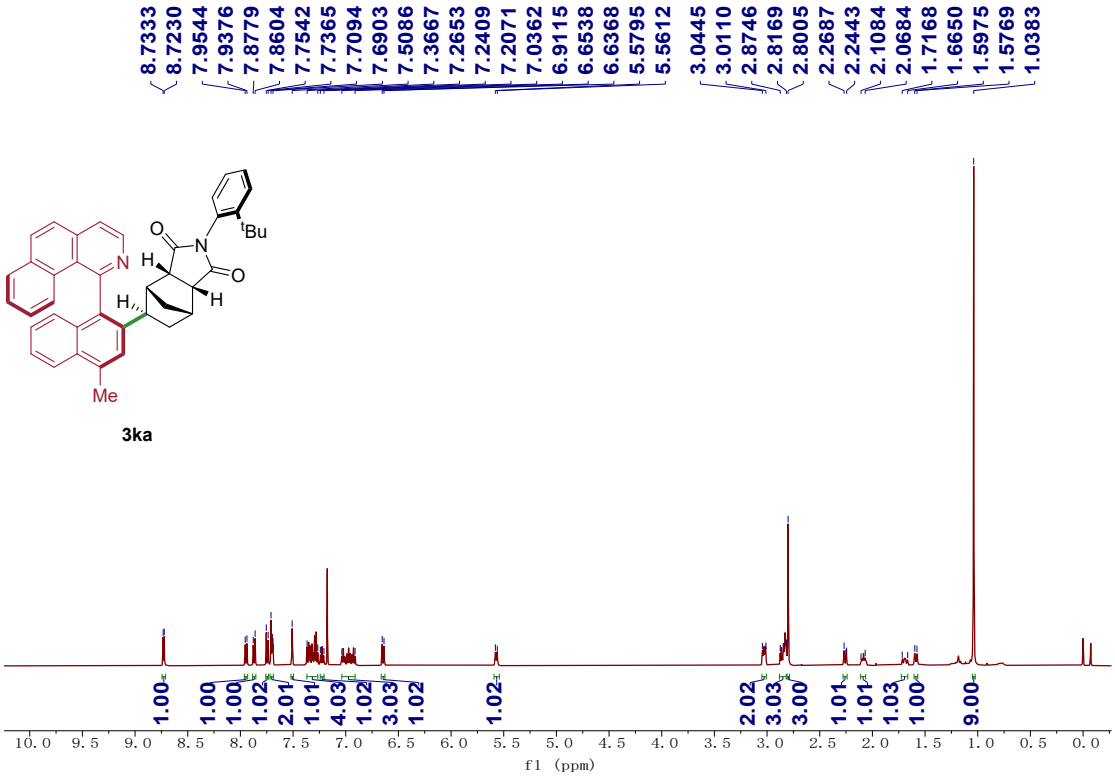
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H
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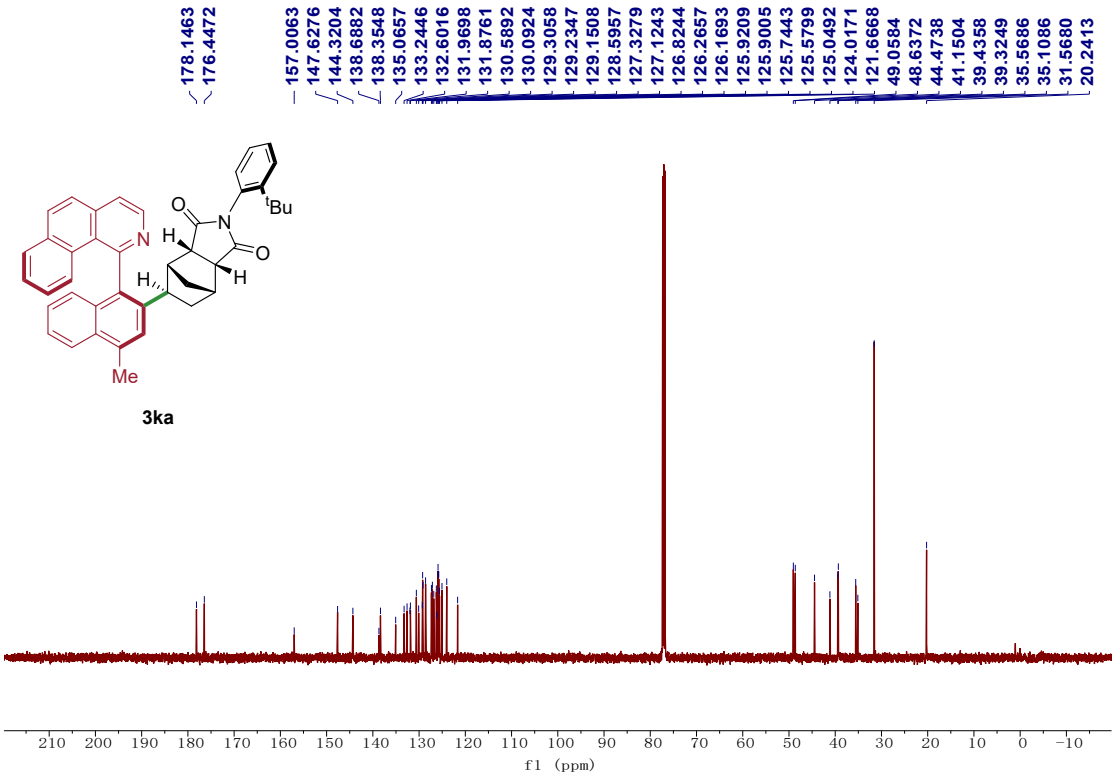
9.00
f1 (ppm)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H
H
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Me
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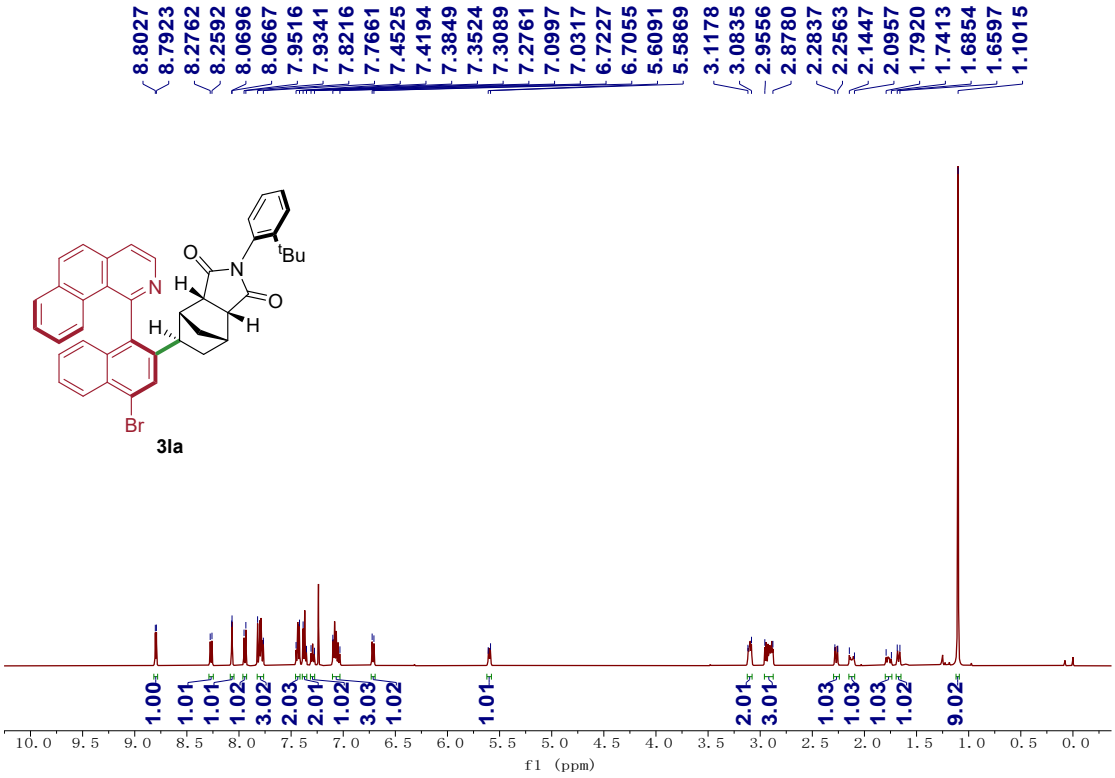
f1 (ppm)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H
N
Br
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1.01
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9.02
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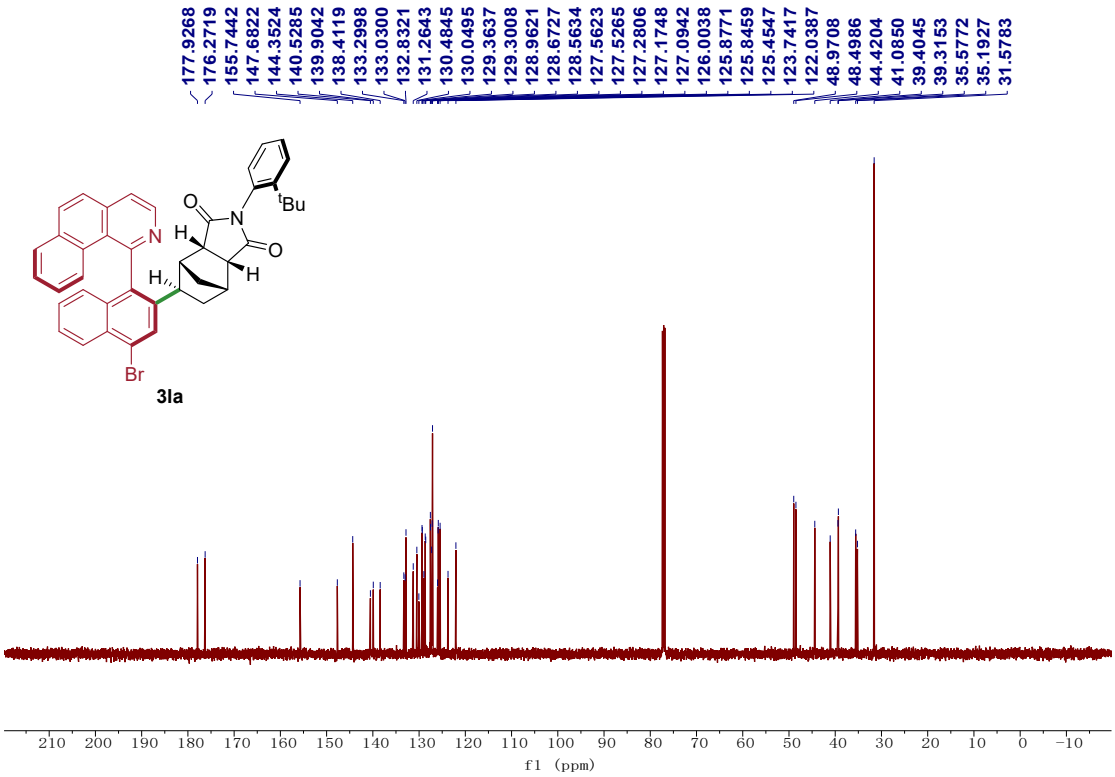
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Br
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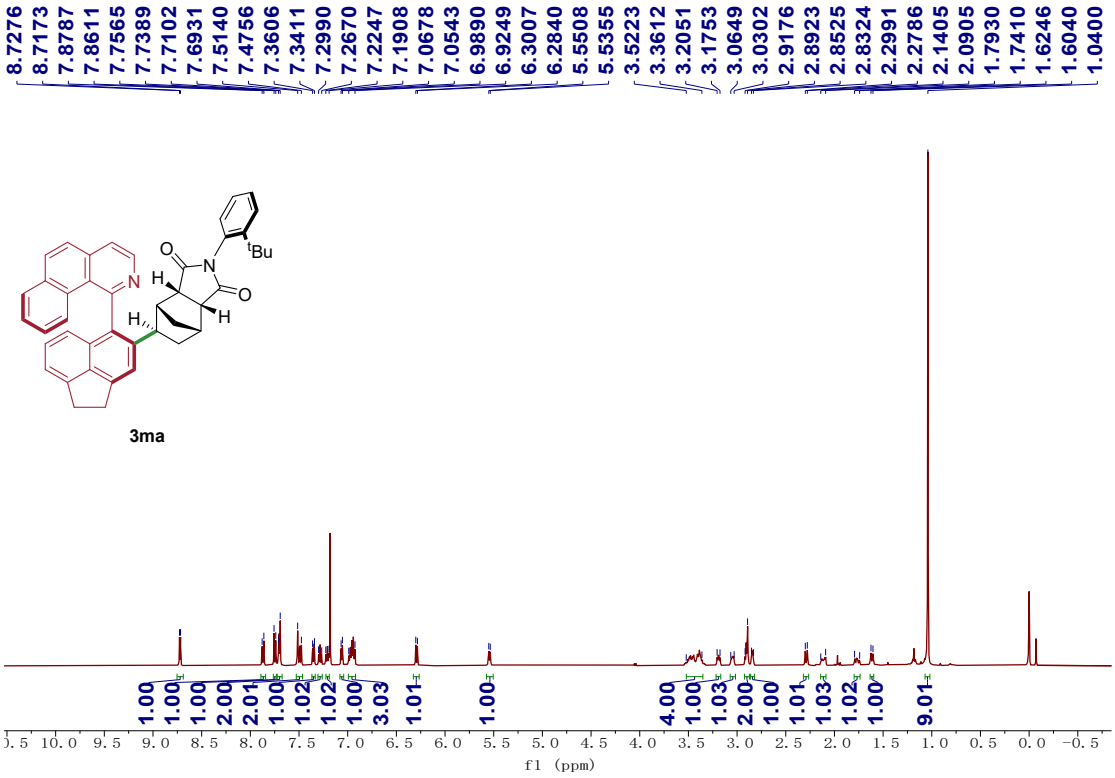
f1 (ppm)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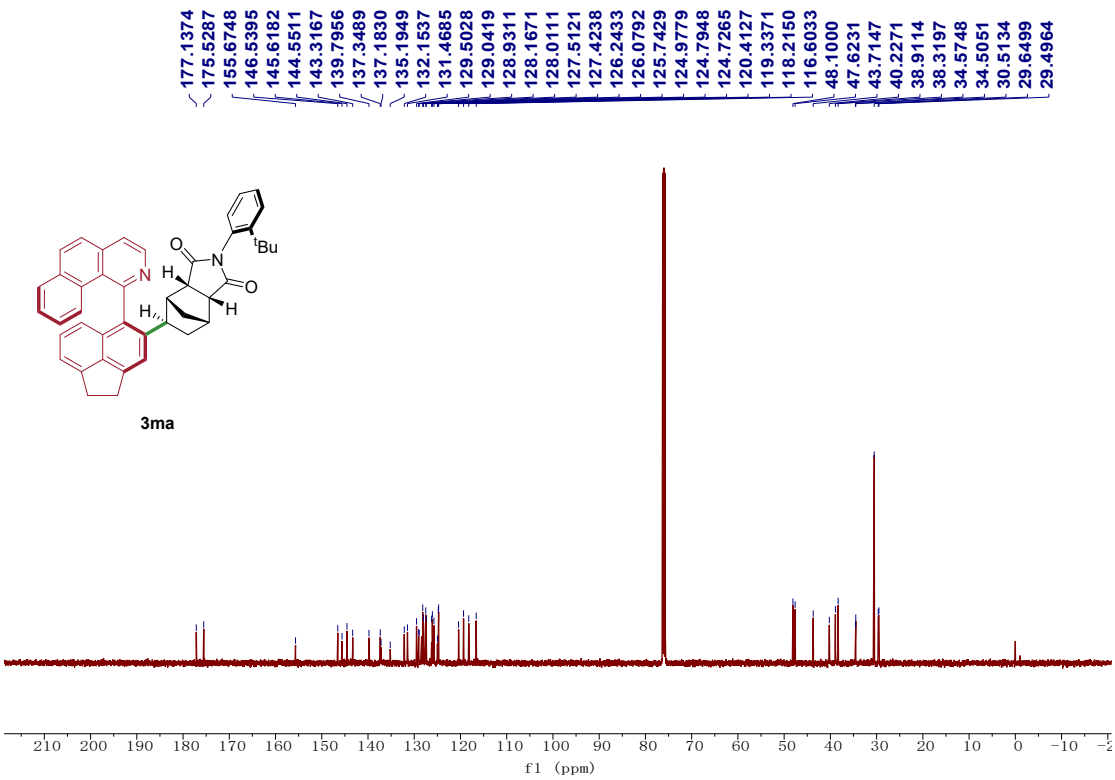
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H
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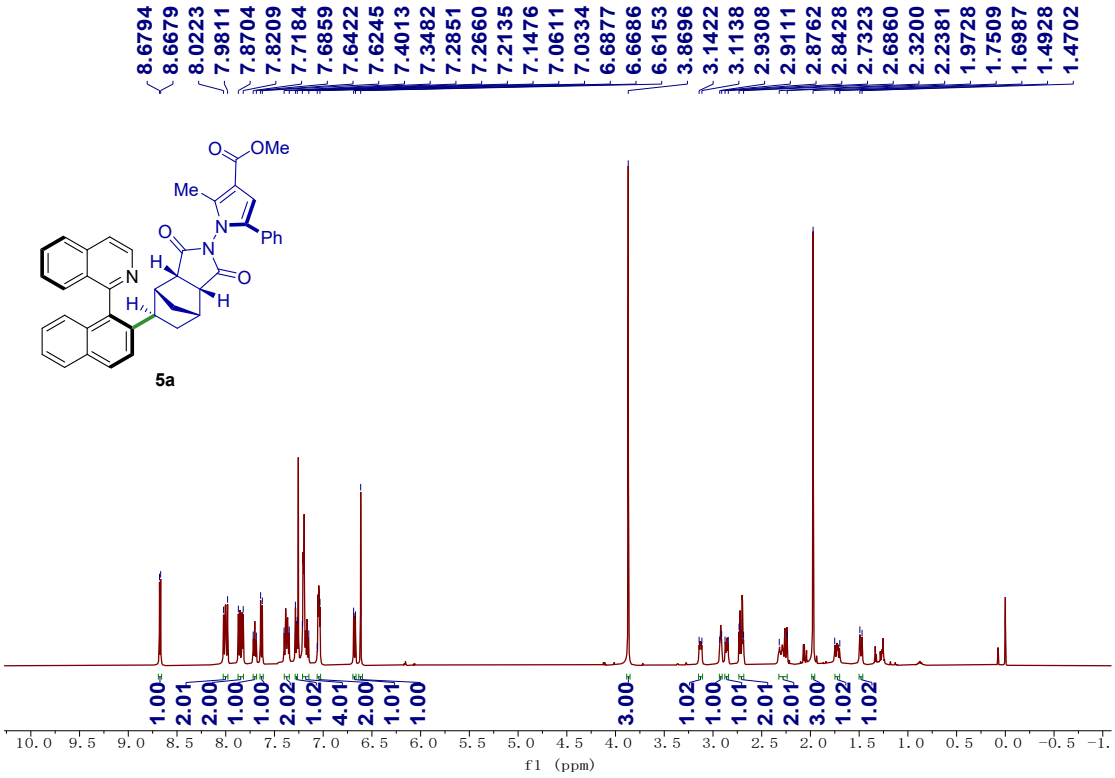
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Me
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Ph
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H
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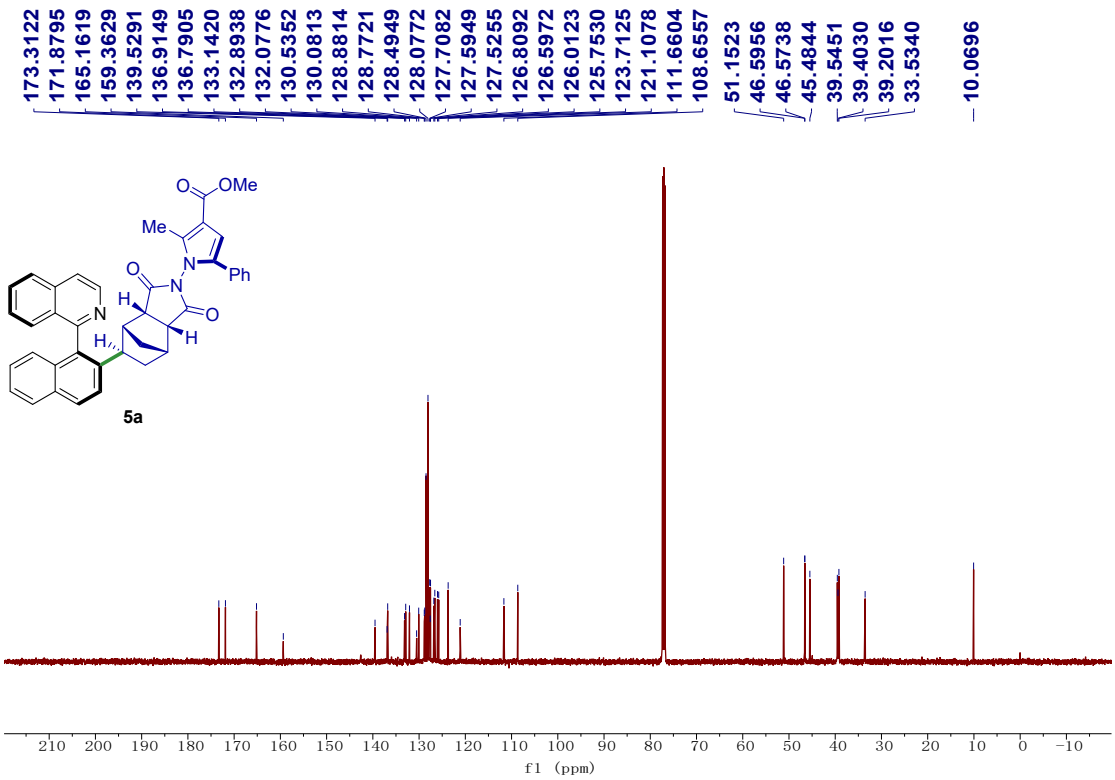
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33.5340
10.0696
O
OMe
Me
N
Ph
O
N
H
O
N
H
H
5a
210
200
190
180
170
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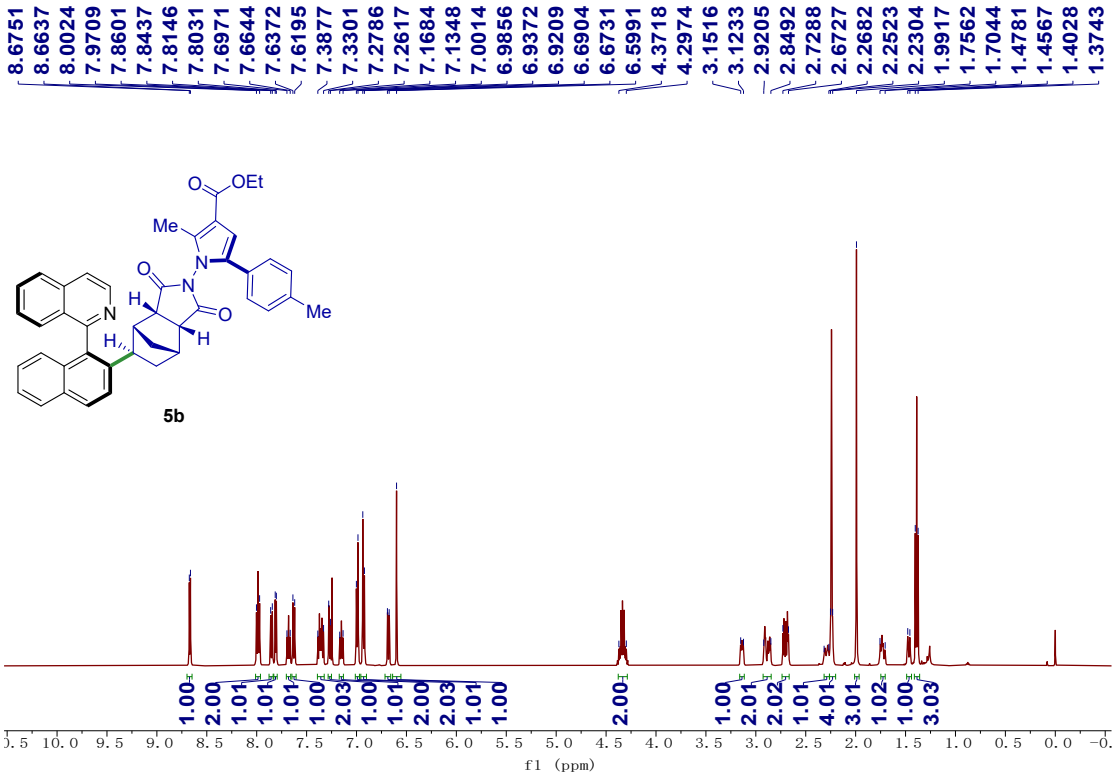
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3.03
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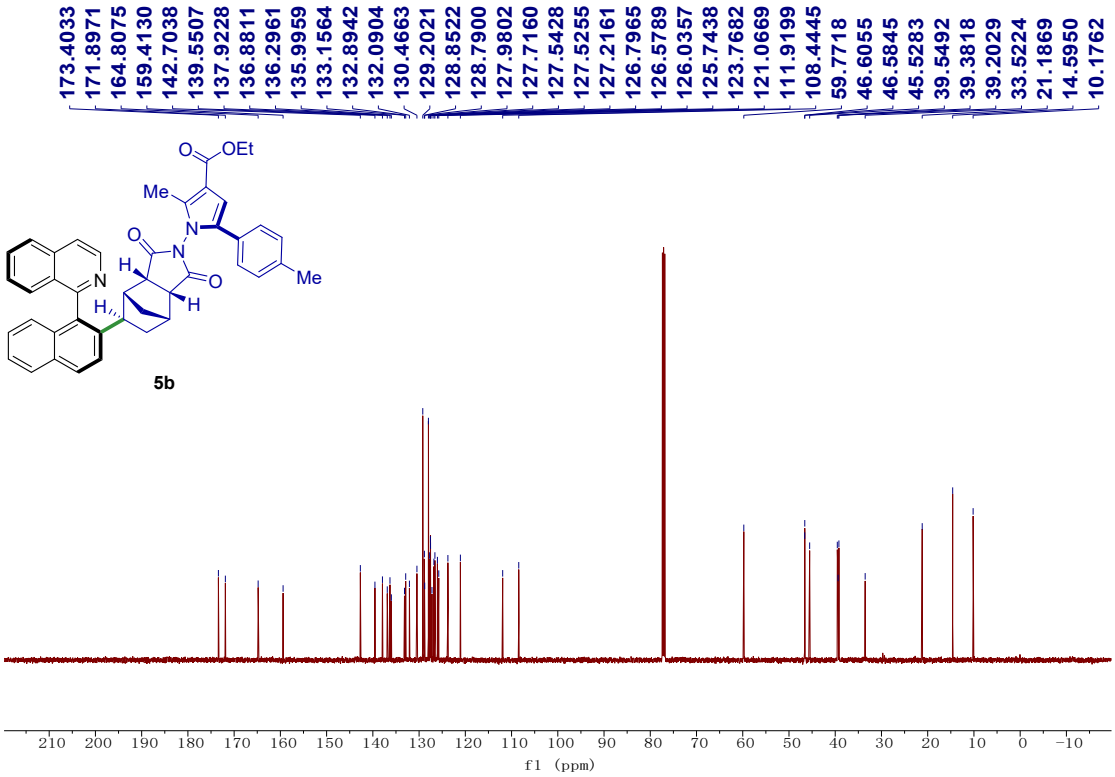
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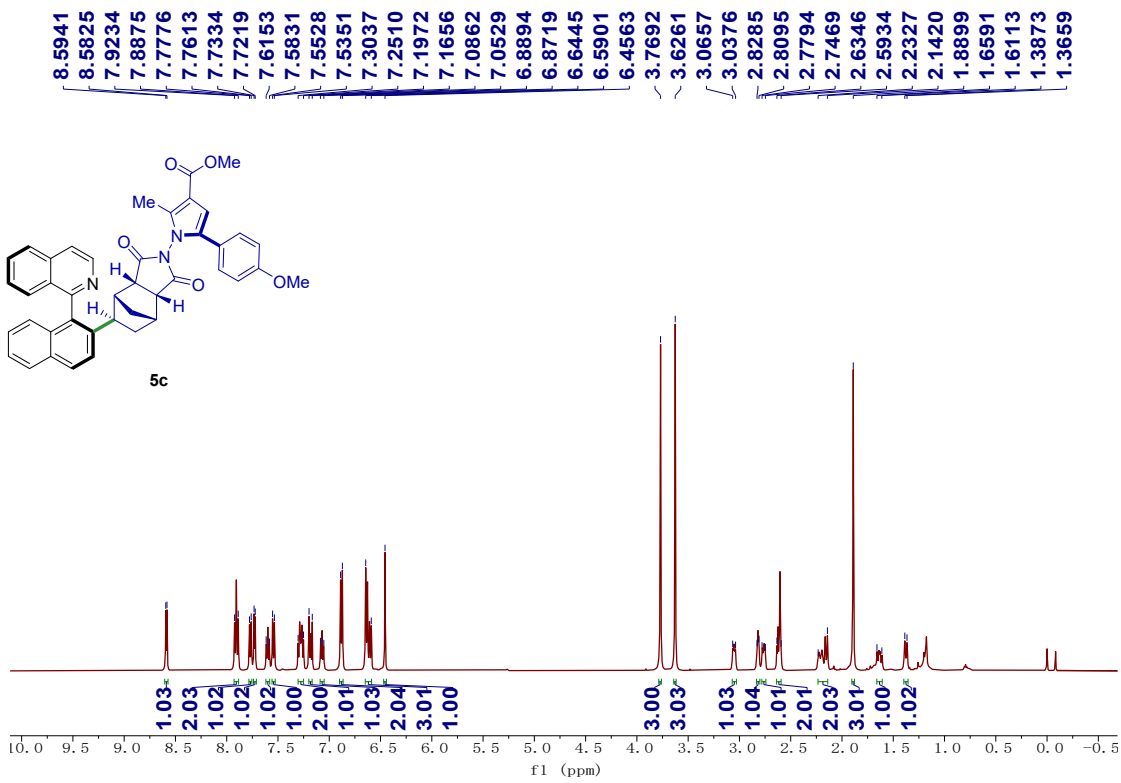
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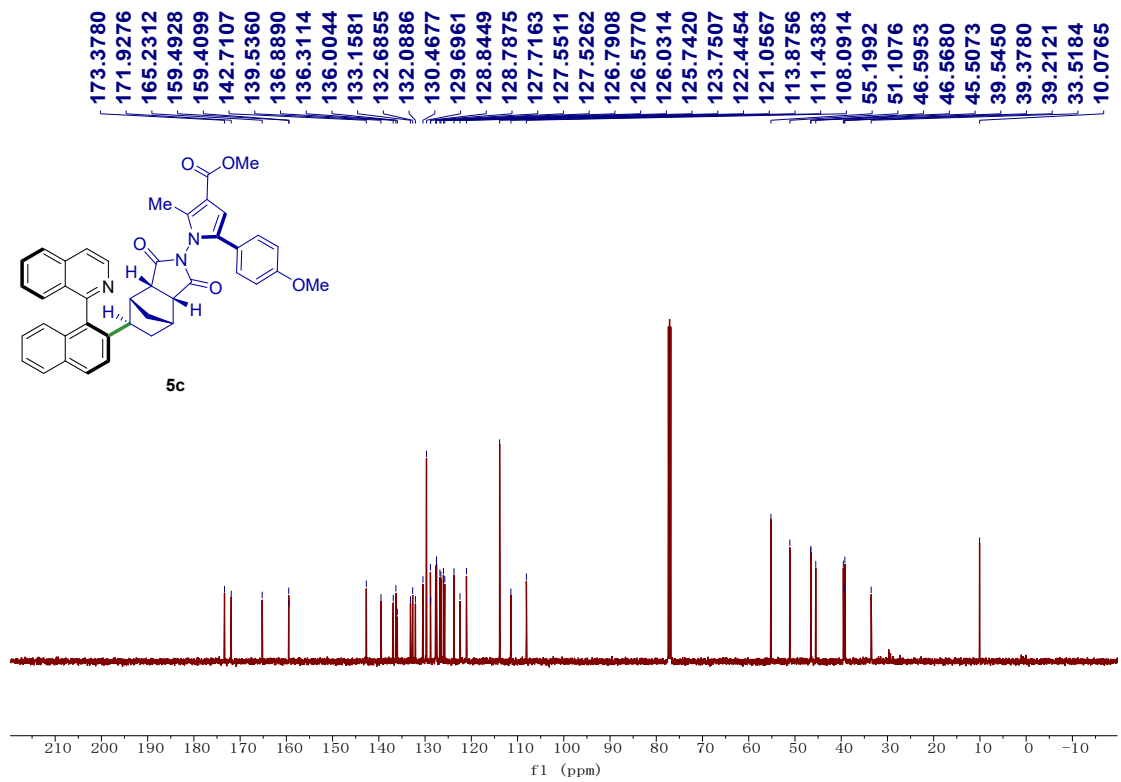
f1 (ppm)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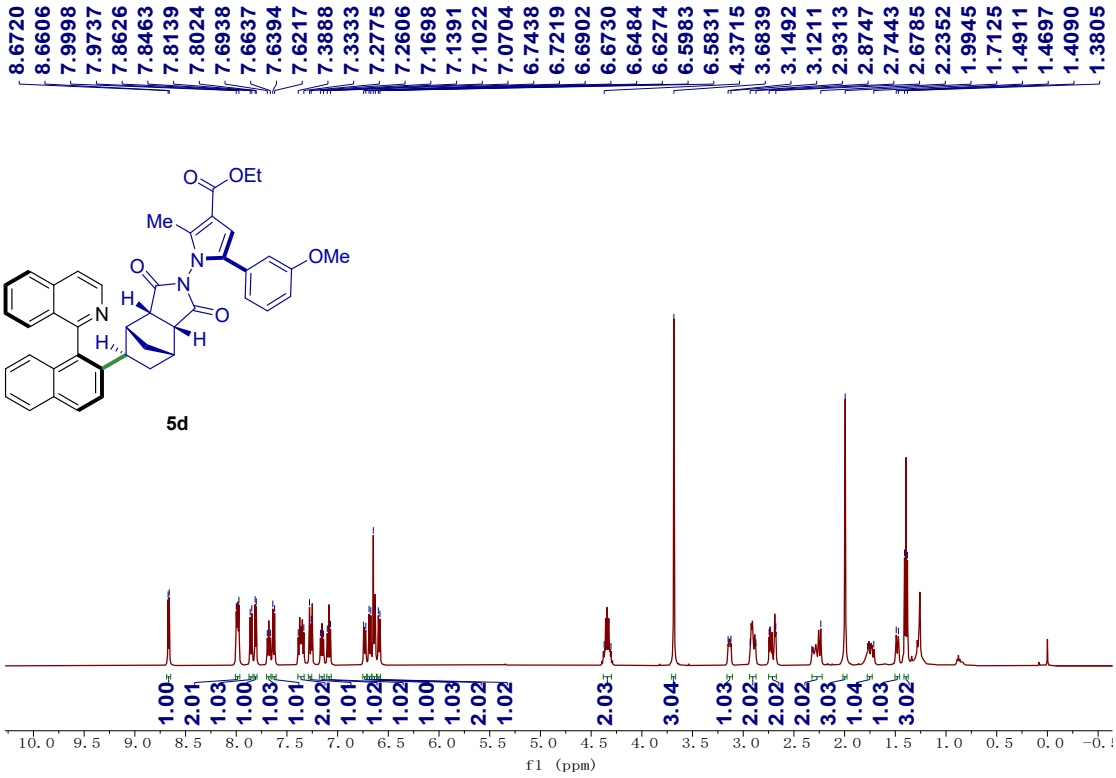
5c
f1 (ppm)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OEt
Me
OMe
N
O
H
5d
1.00 2.01 1.03 1.00 1.03 1.01 2.02 1.01 1.02 1.02 1.00 1.03 2.02 1.02 2.03 3.04 1.03 2.02 2.02 2.02 3.03 1.04 1.03 3.02
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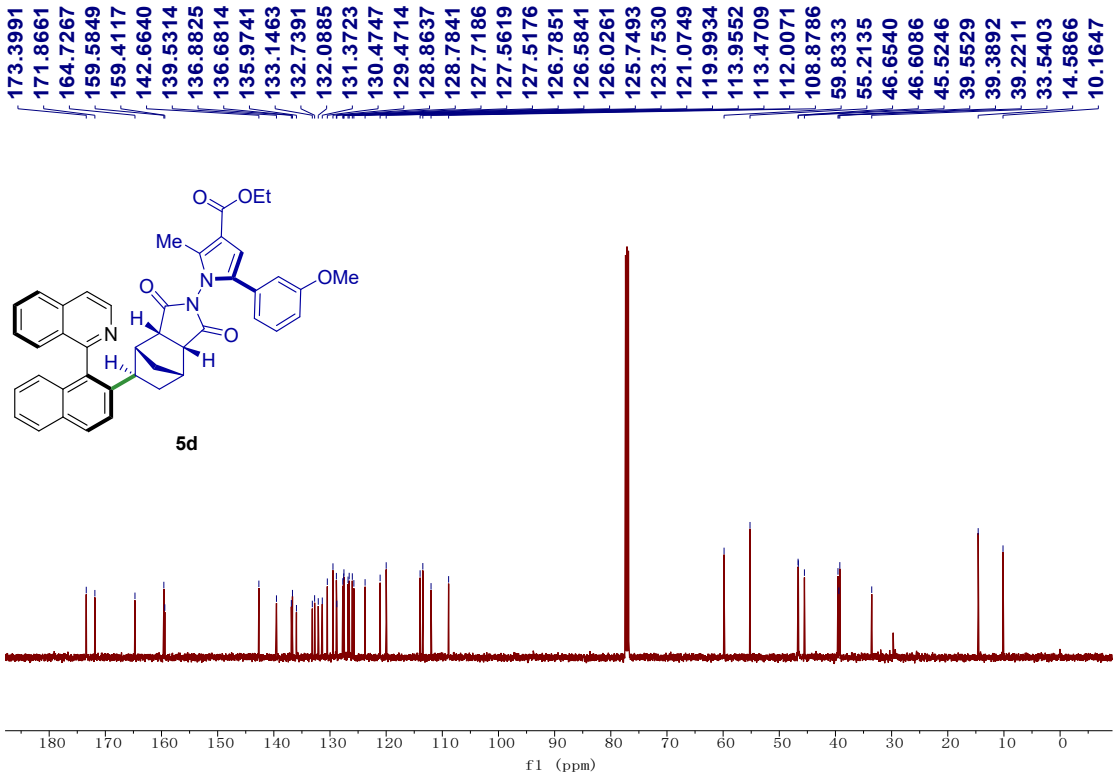
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OEt
Me
OMe
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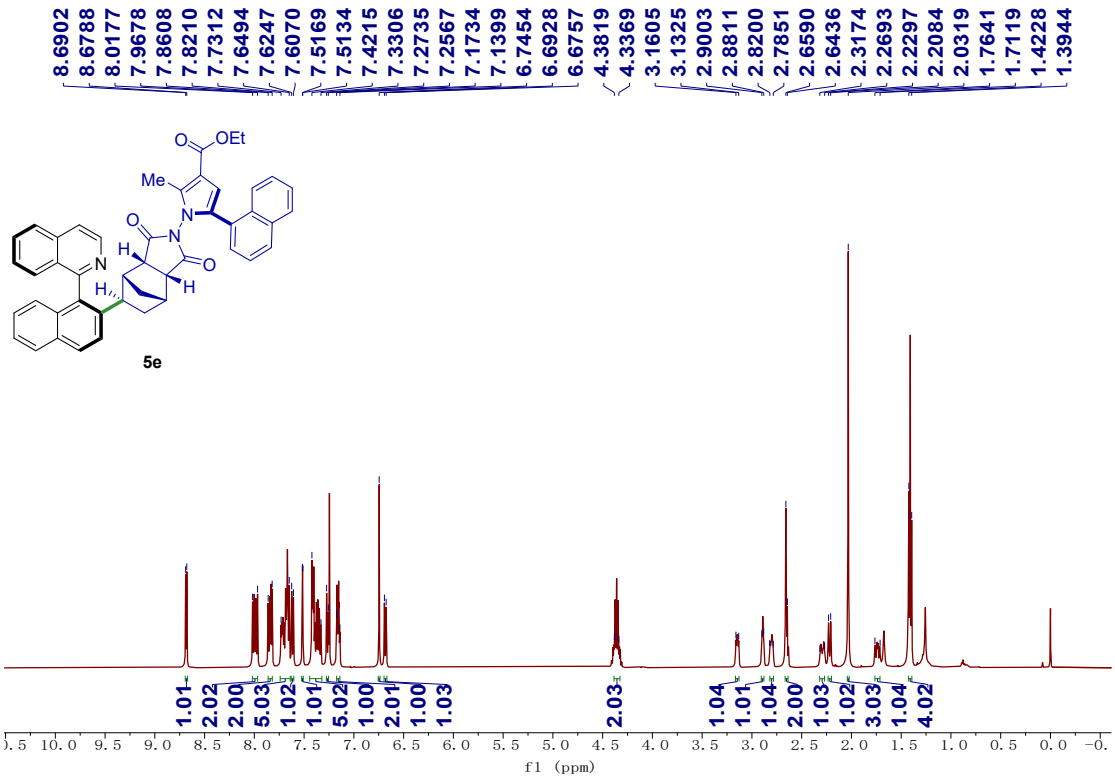
O
H
5d
f1 (ppm)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6.6928
6.6757
4.3819
4.3369
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2.3174
2.2693
2.2297
2.2084
2.0319
1.7641
1.7119
1.4228
1.3944
OEt
Me
N
O
H
5e
1.01
2.02
2.00
5.03
1.02
1.01
5.02
1.00
2.01
1.00
1.03
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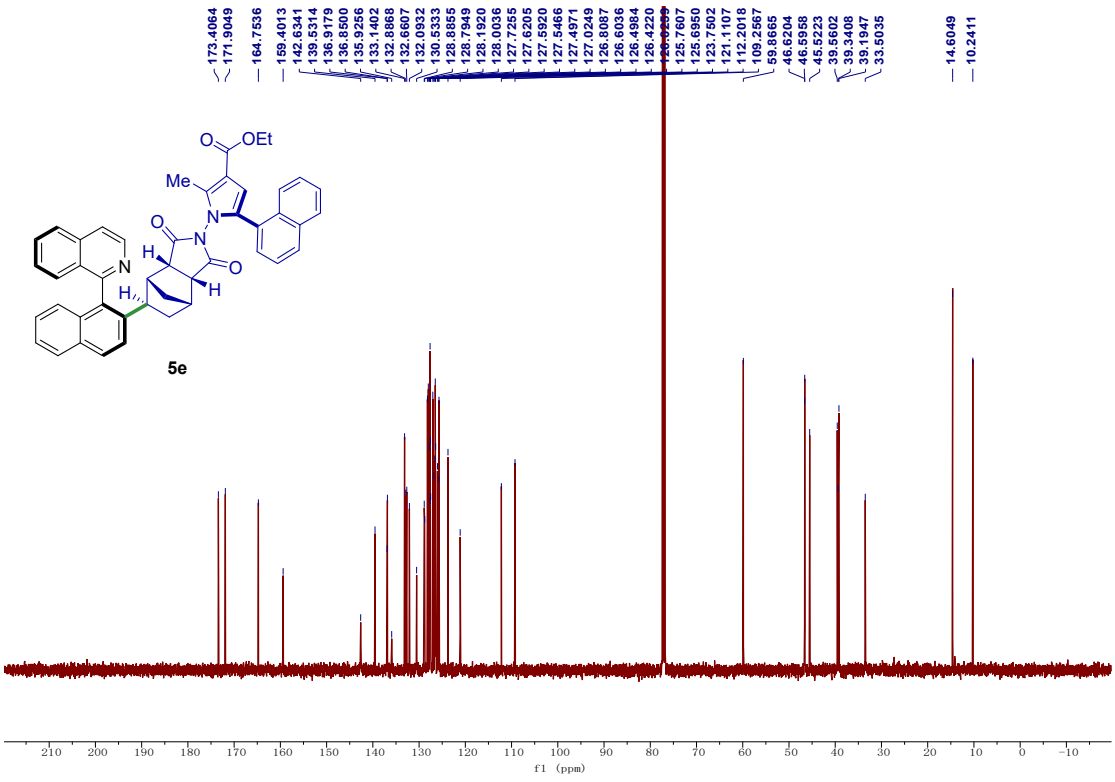
1.02
3.03
1.04
4.02
f1 (ppm)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46.6204
46.5958
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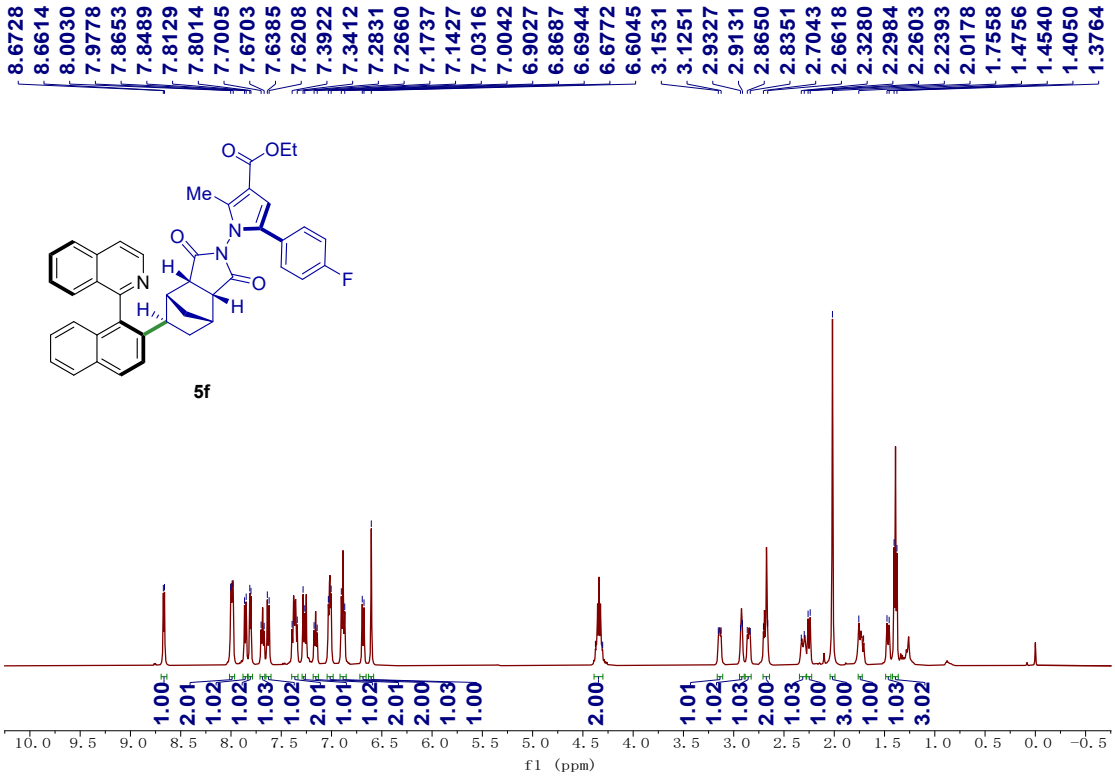
OEt
Me
N
O
H
5e
f1 (ppm)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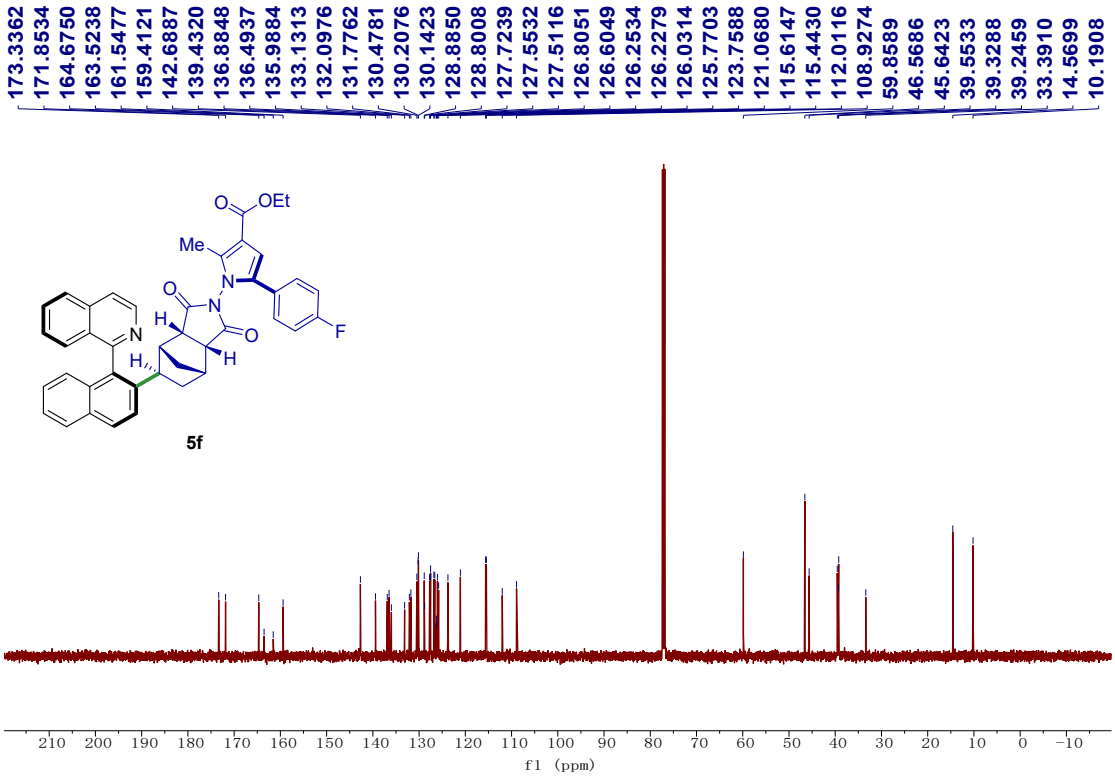
O
OEt
Me
N
O
H
N
O
H
N
H
F
5f
1.00 2.01 1.02 1.02 1.03 1.02 2.01 1.01 1.02 2.01 2.00 1.03 1.00 2.00 1.01 1.02 1.03 2.00 1.03 1.00 3.00 1.00 1.03 3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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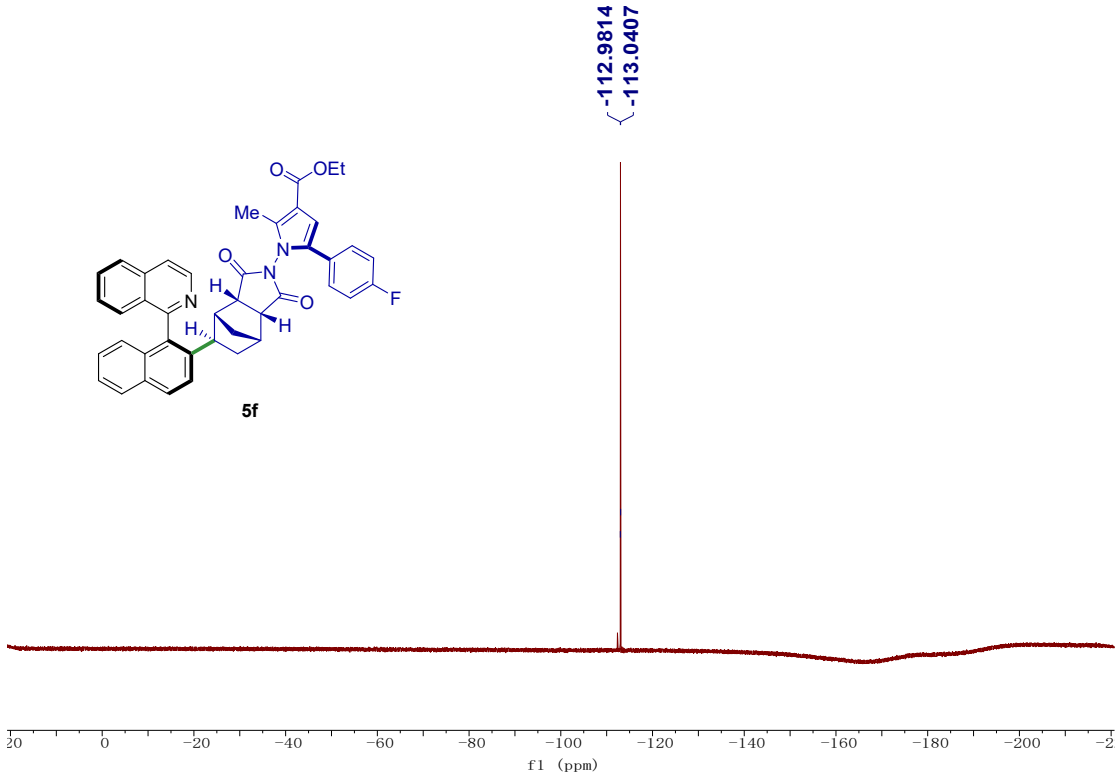
O
OEt
Me
N
O
H
N
O
H
N
H
F
5f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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-113.0407
O
OEt
Me
N
O
N
O
H
H
H
N
F
5f
20
0
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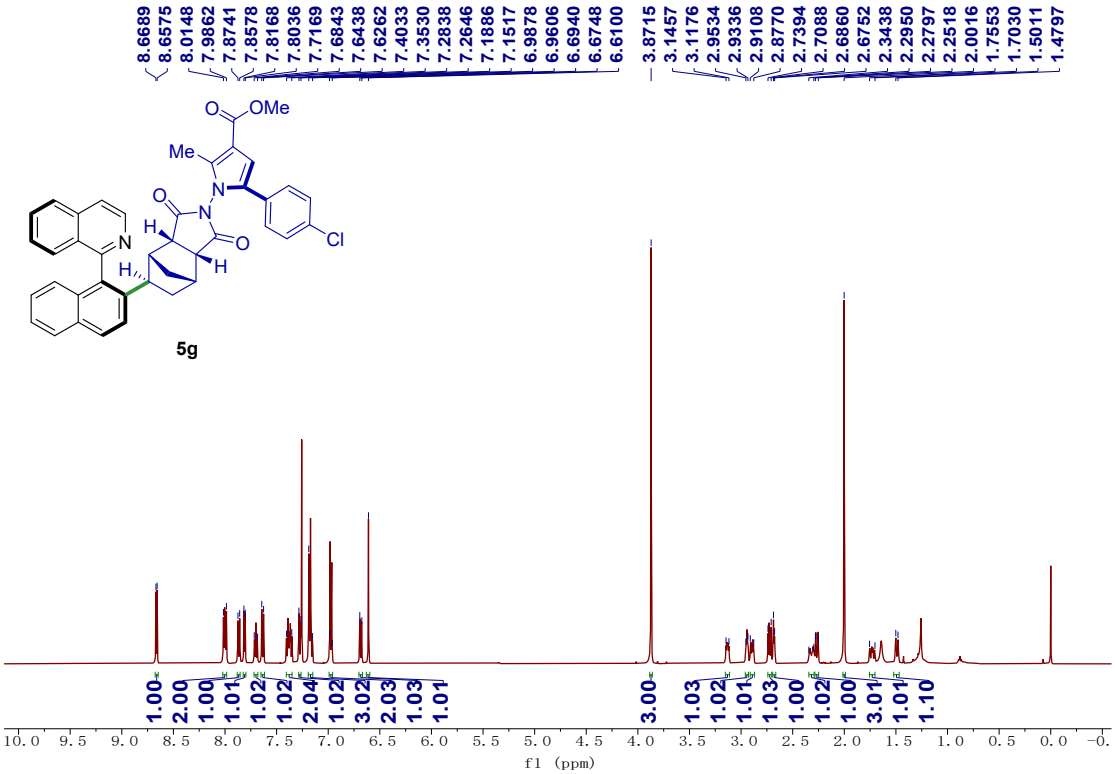
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)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7.4033
7.3530
7.2838
7.2646
7.1886
7.1517
6.9878
6.9606
6.6940
6.6748
6.6100
3.8715
3.1457
3.1176
2.9534
2.9336
2.9108
2.8770
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2.3438
2.2950
2.2797
2.2518
2.0016
1.7553
1.7030
1.5011
1.4797
OMe
Me
N
O
H
Cl
5g
1.00
2.00
1.00
1.01
1.02
1.02
2.04
1.02
3.02
2.03
1.03
1.01
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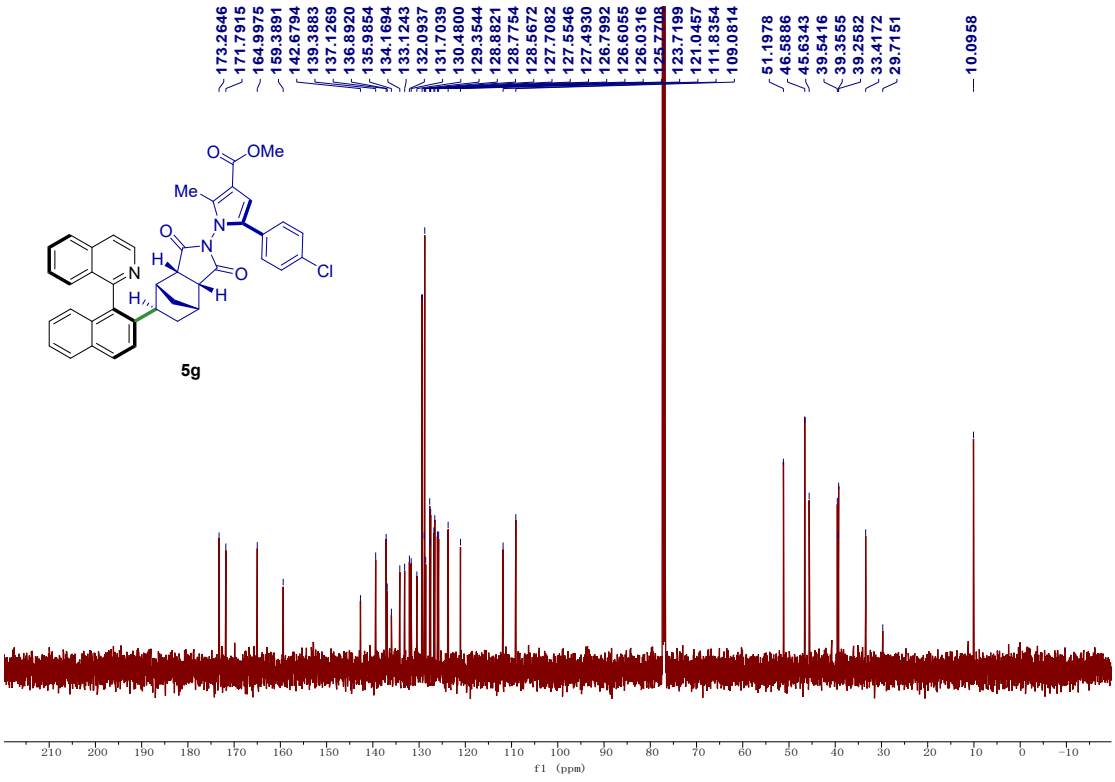
3.01
1.01
1.10
f1 (ppm)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132.0937
131.7039
130.4800
129.3544
128.8821
128.7754
128.5672
127.7082
127.5546
127.4930
126.7992
126.6055
126.0316
125.7708
123.7199
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46.5886
45.6343
39.5416
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Me
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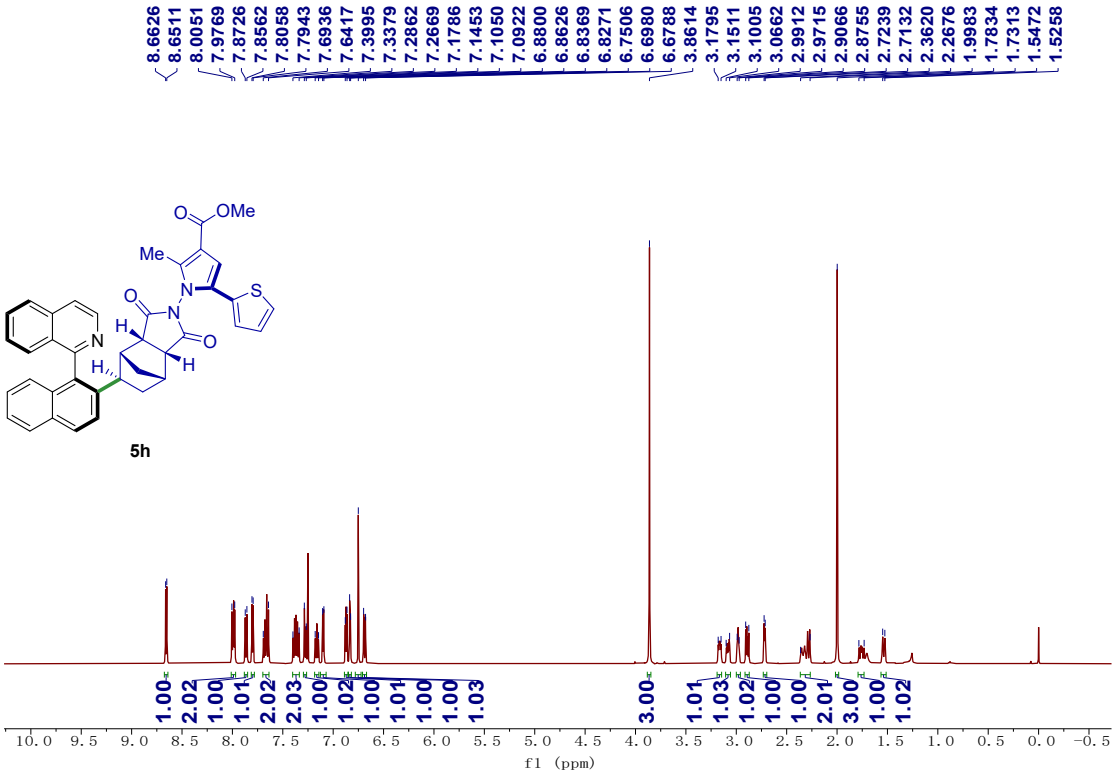
H
Cl
5g
f1 (ppm)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7.3379
7.2862
7.2669
7.1786
7.1453
7.1050
7.0922
6.8800
6.8626
6.8369
6.8271
6.7506
6.6980
6.6788
3.8614
3.1795
3.1511
3.1005
3.0662
2.9912
2.9715
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2.8755
2.7239
2.7132
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2.2676
1.9983
1.7834
1.7313
1.5472
1.5258
OMe
Me
N
S
O
H
5h
1.00
2.02
1.00
1.01
2.02
2.03
1.00
1.02
1.00
1.01
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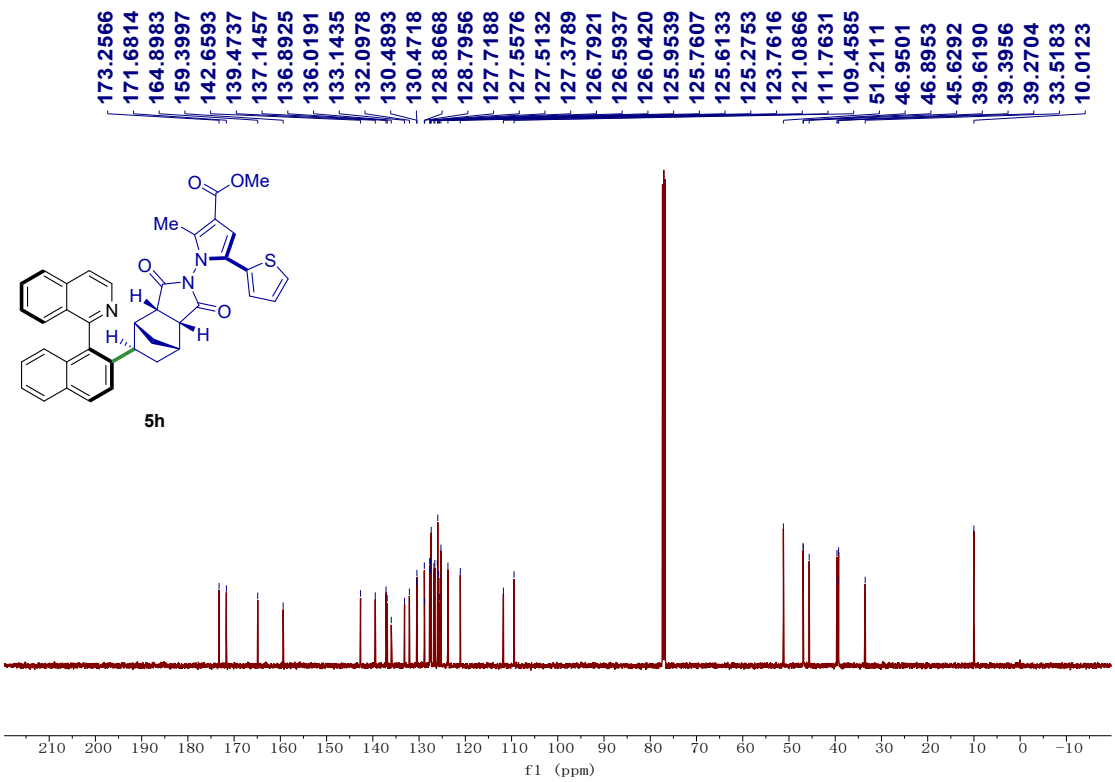
1.02
f1 (ppm)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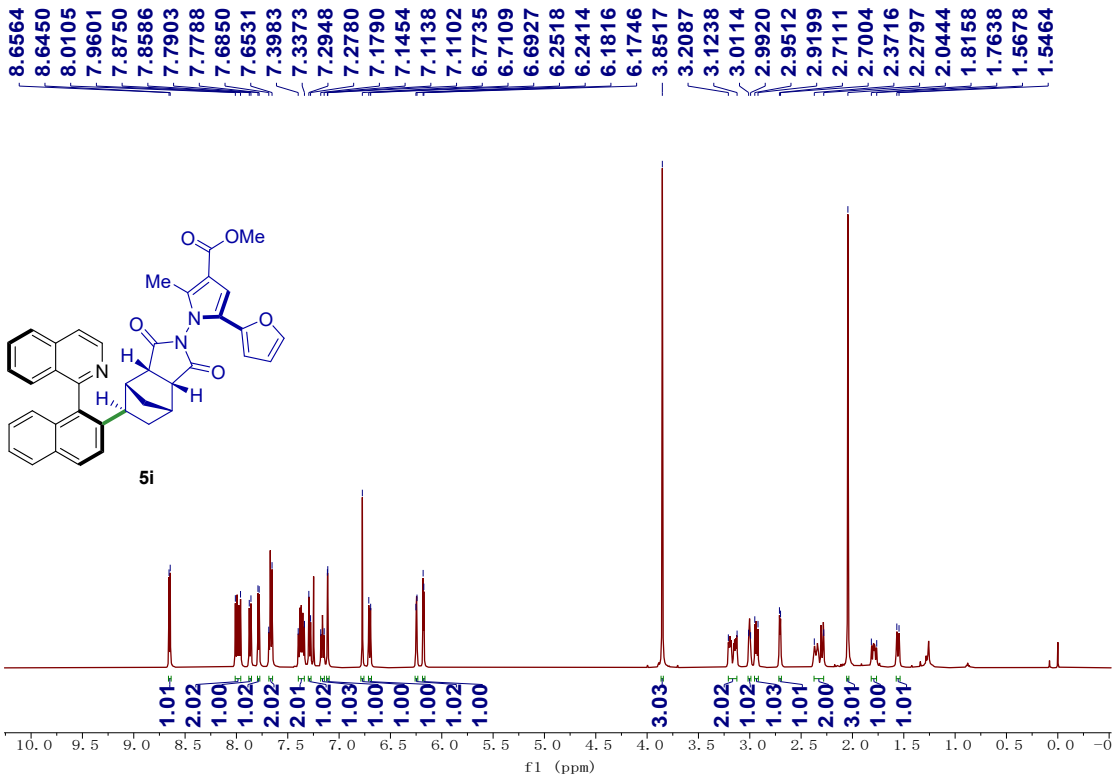
S
O
H
5h
f1 (ppm)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7.1790
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7.1138
7.1102
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6.7109
6.6927
6.2518
6.2414
6.1816
6.1746
3.8517
3.2087
3.1238
3.0114
2.9920
2.9512
2.9199
2.7111
2.7004
2.3716
2.2797
2.0444
1.8158
1.7638
1.5678
1.5464
OMe
Me
N
O
H
5i
1.01
2.02
1.00
1.02
2.02
2.01
1.02
1.03
1.00
1.00
1.00
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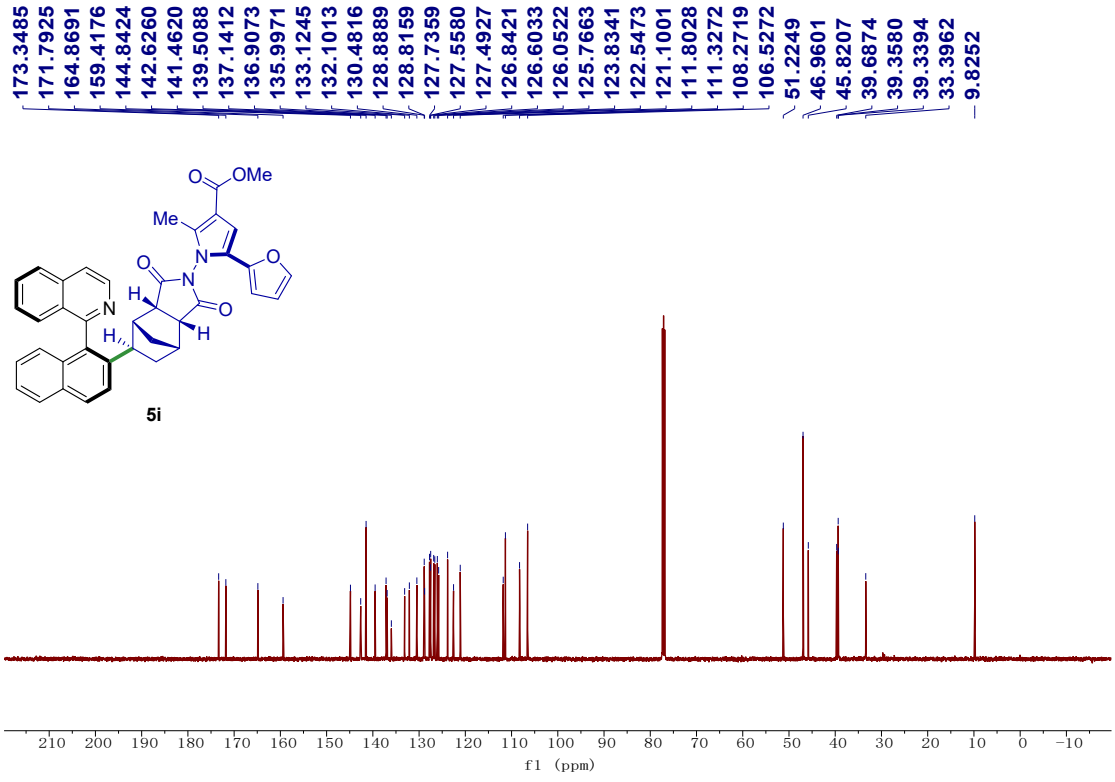
3.01
1.00
1.01
f1 (ppm)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127.4927
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126.0522
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46.9601
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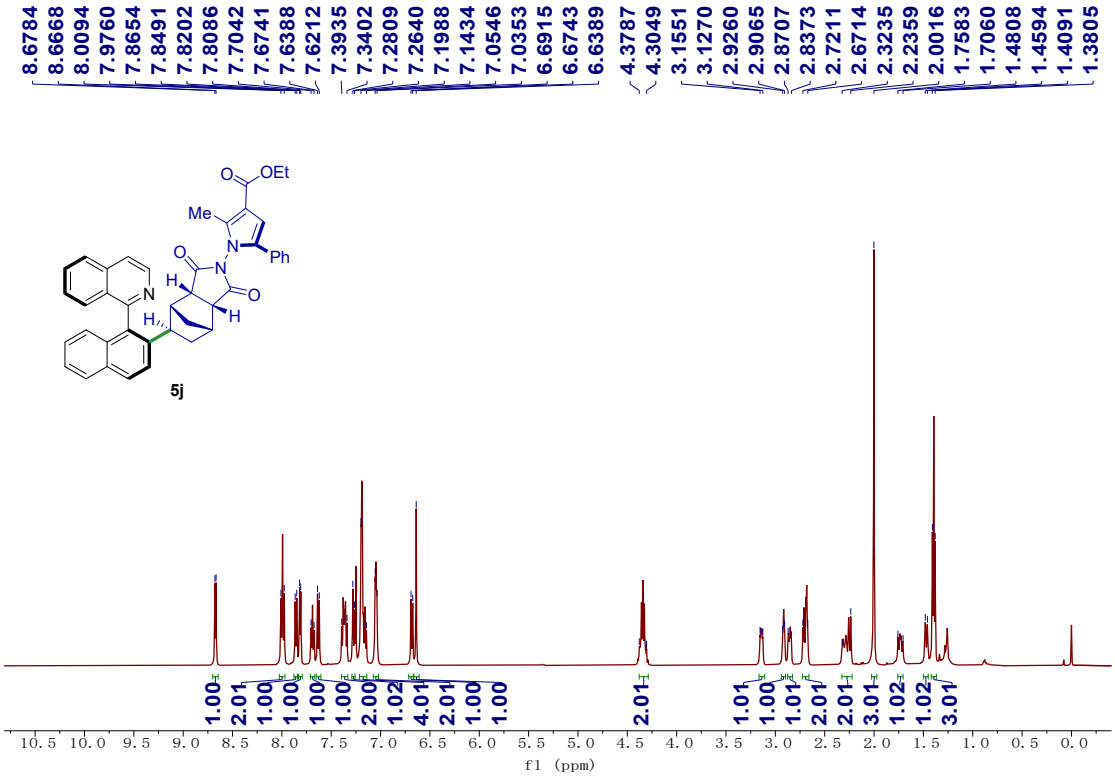
Me
N
O
H
5i
f1 (ppm)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Me
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Ph
O
H
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1.00
1.00
1.00
1.00
2.00
1.02
4.01
2.01
1.00
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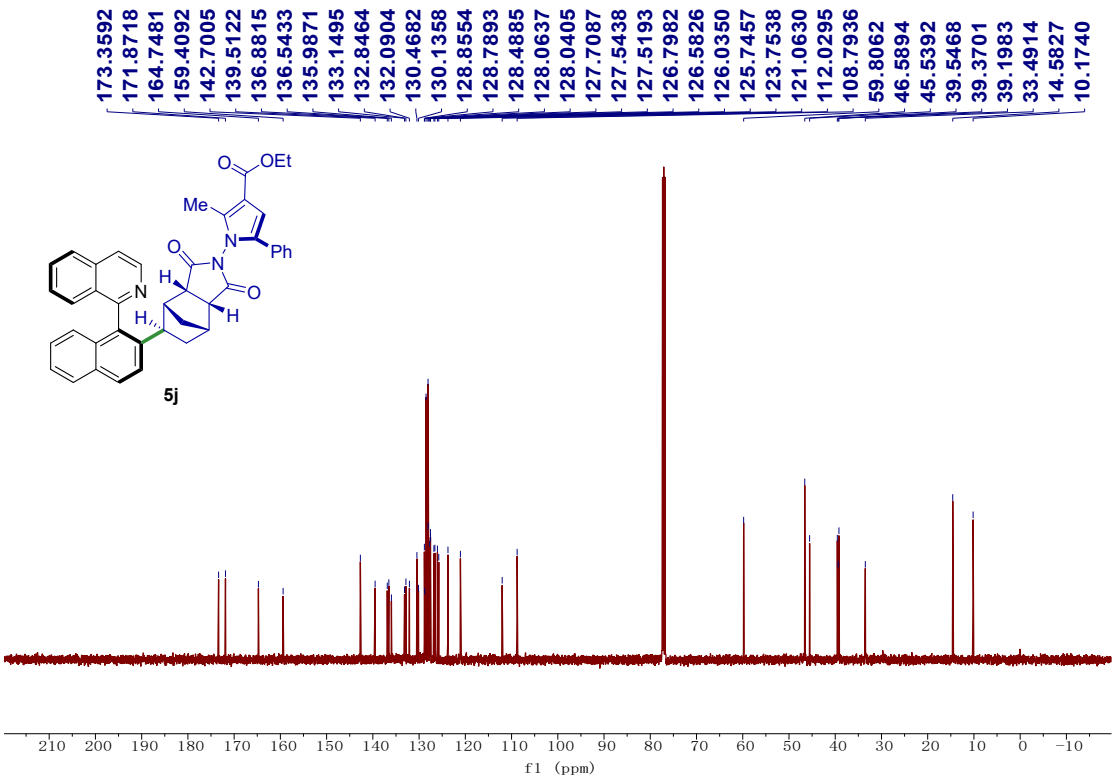
1.02
3.01
f1 (ppm)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127.5438
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126.5826
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125.7457
123.7538
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45.5392
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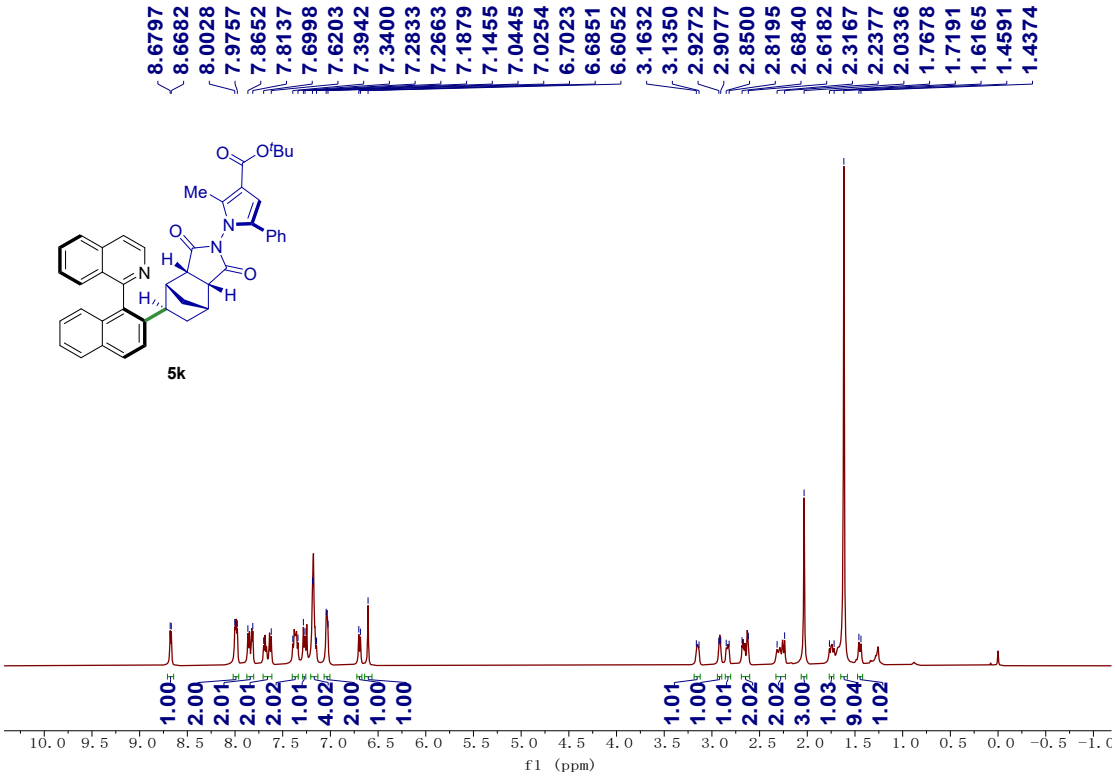
14.5827
10.1740
OEt
Me
N
Ph
O
H
5j
f1 (ppm)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7.0254
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6.6052
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3.1350
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1.7191
1.6165
1.4591
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O
O^{t}Bu
Me
N
Ph
O
N
O
H
H
H
5k
1.00
2.00
2.01
2.04
2.02
1.01
4.02
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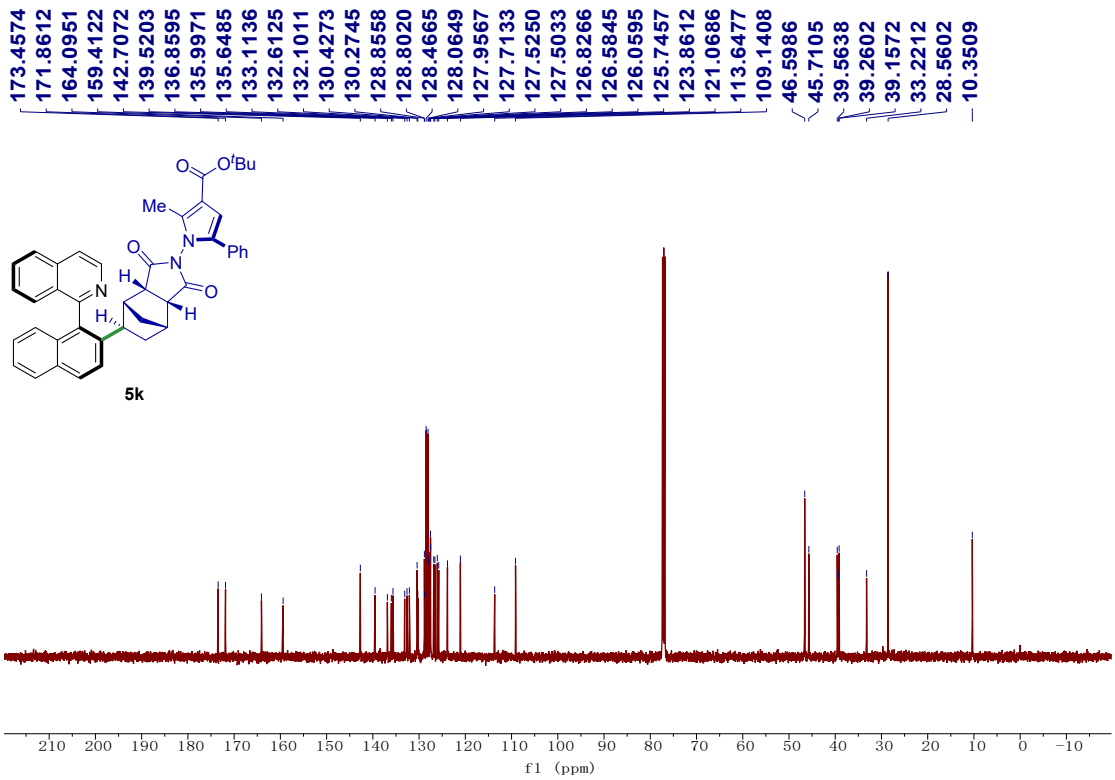
3.00
1.03
9.04
1.02
f1 (ppm)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132.1011
130.4273
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128.8020
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127.7133
127.5250
127.5033
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126.5845
126.0595
125.7457
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121.0686
113.6477
109.1408
46.5986
45.7105
39.5638
39.2602
39.1572
33.2212
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O
O^{t}Bu
Me
N
Ph
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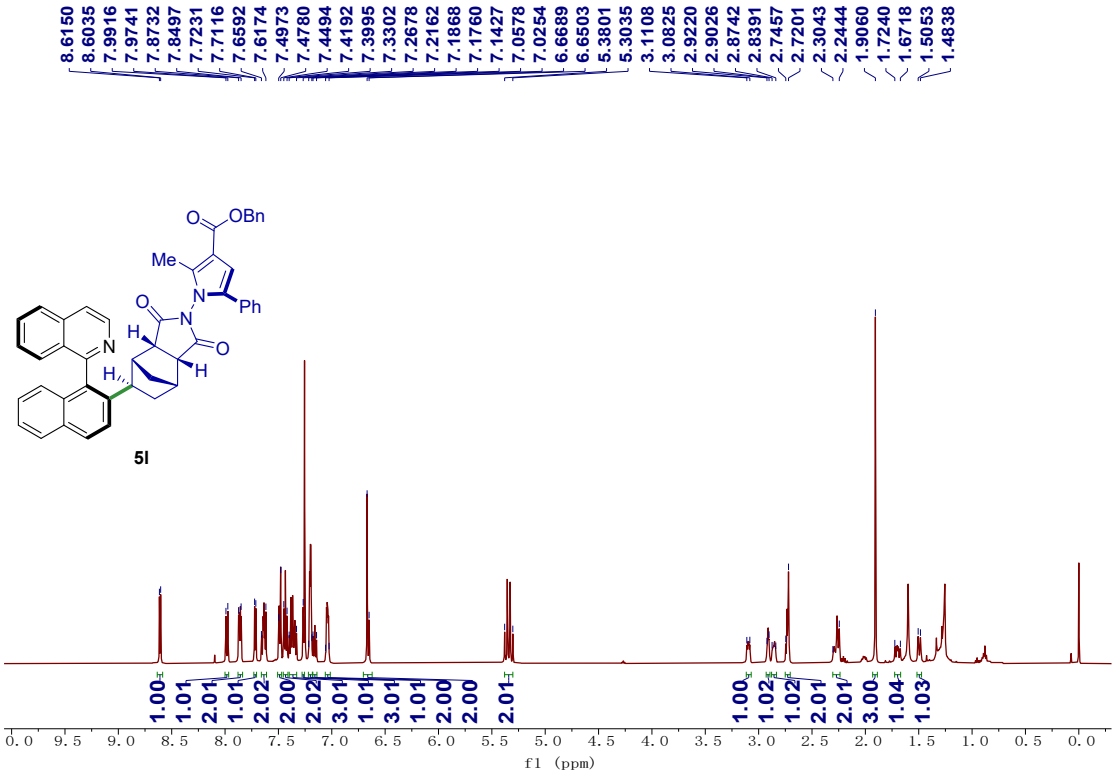
N
O
H
H
H
5k
f1 (ppm)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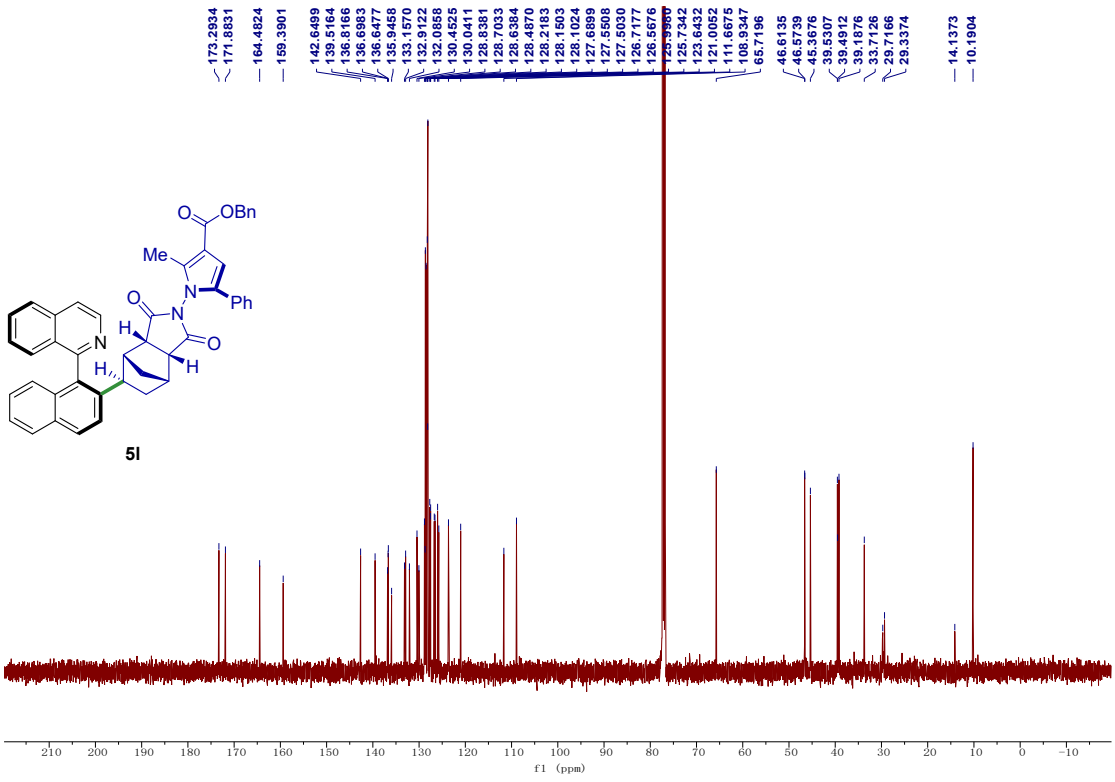
OBn
Me
Ph
5l
1.00 1.01 2.01 1.01 2.02 2.00 2.02 3.01 1.01 3.01 1.01 2.00 2.00 2.01 1.00 1.02 1.02 2.01 2.01 3.00 1.04 1.03
f1 (ppm)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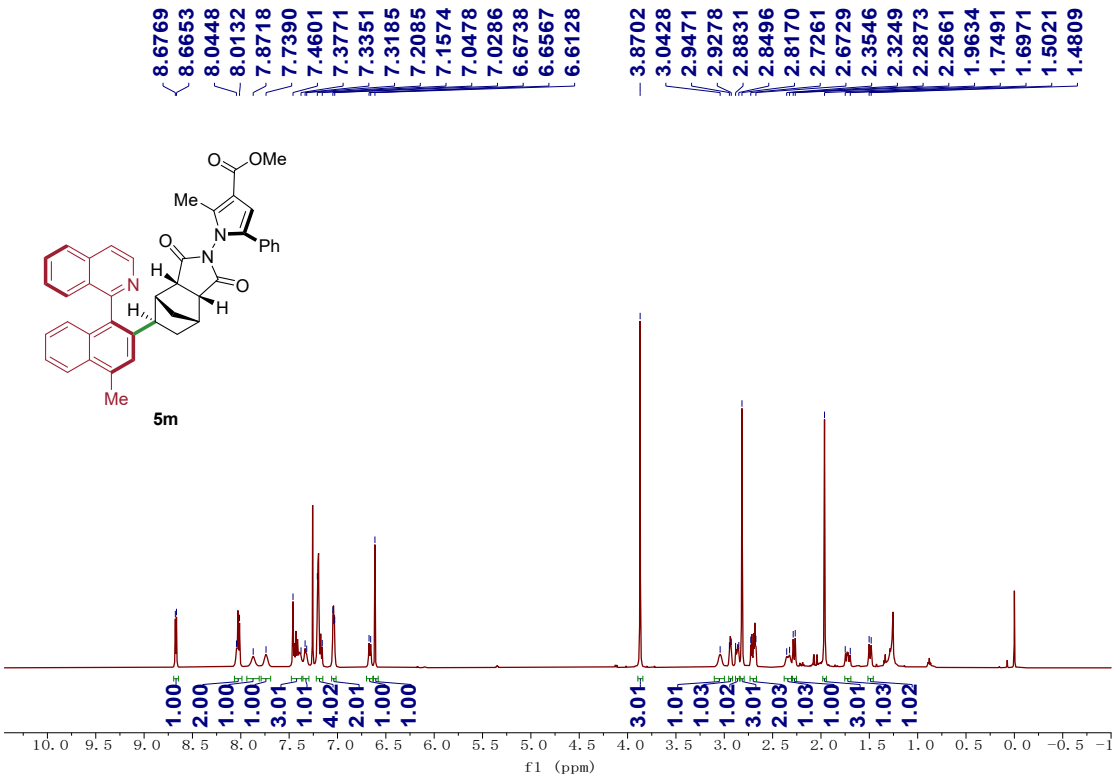
OBn
Me
Ph
5l
f1 (ppm)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2.2661
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Me
Ph
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O
H
Me
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2.00
1.00
1.00
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1.01
4.02
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1.00
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1.03
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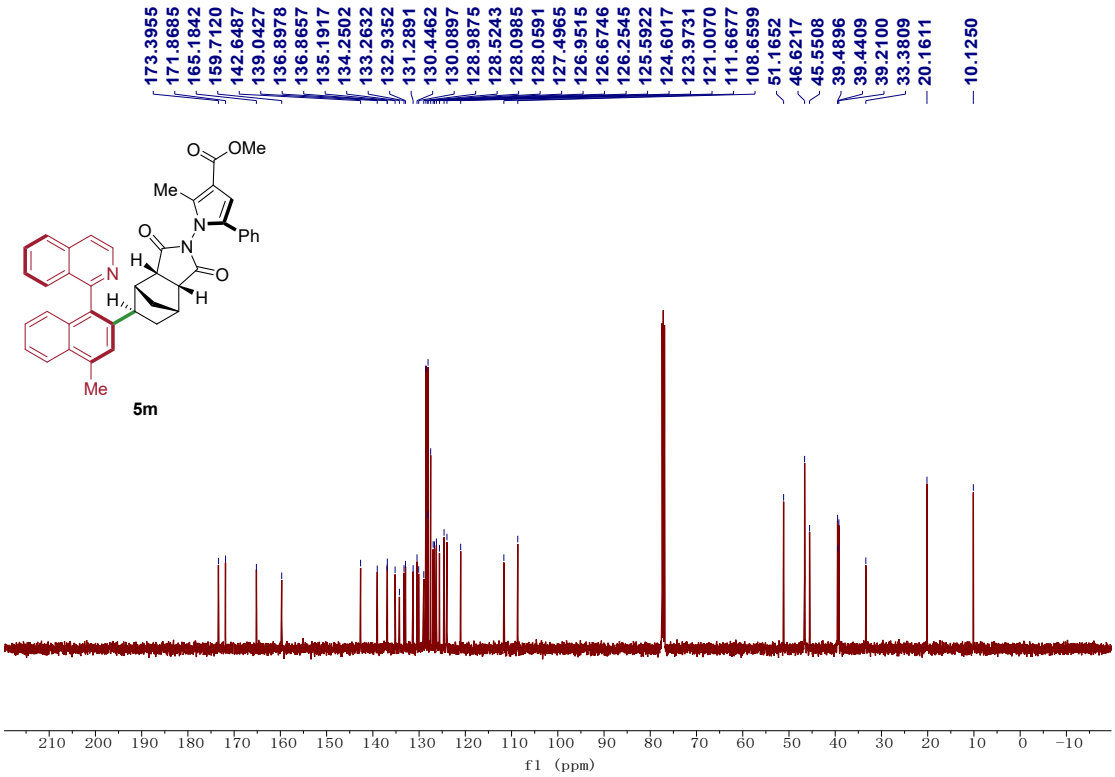
1.03
1.02
f1 (ppm)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Ph
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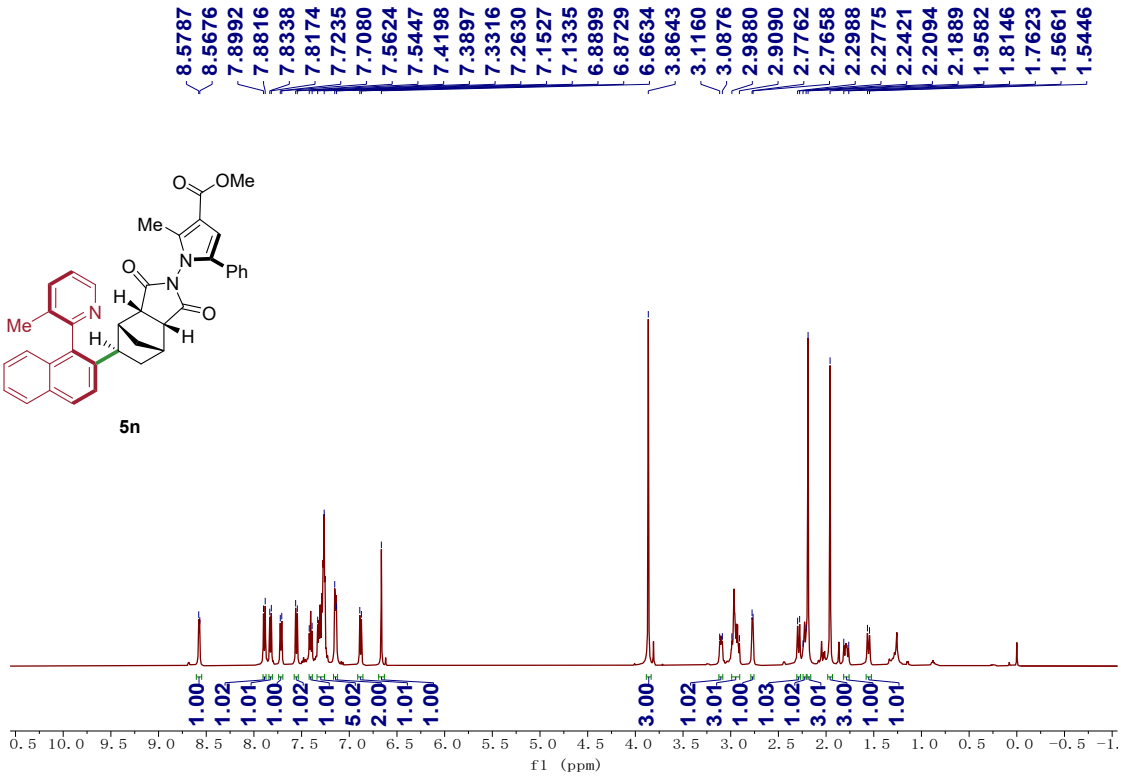
O
H
Me
5m
f1 (ppm)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1.5661
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OMe
Me
Ph
N
O
H
Me
5n
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5.02
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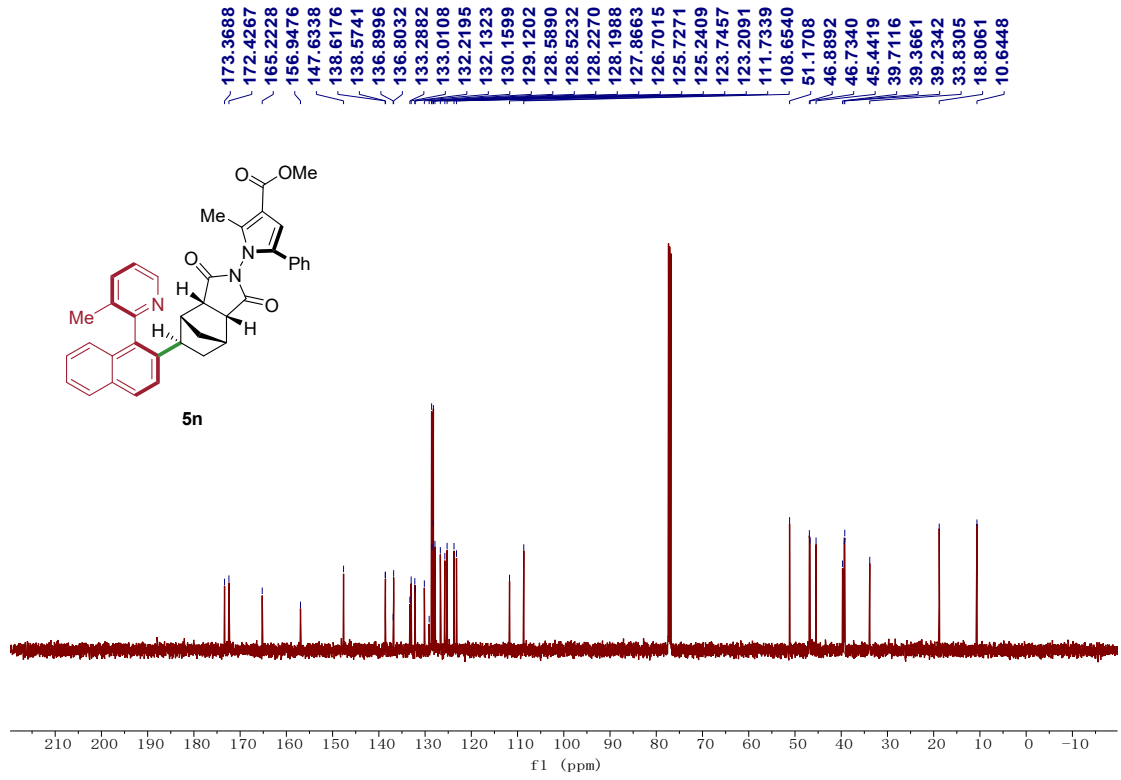
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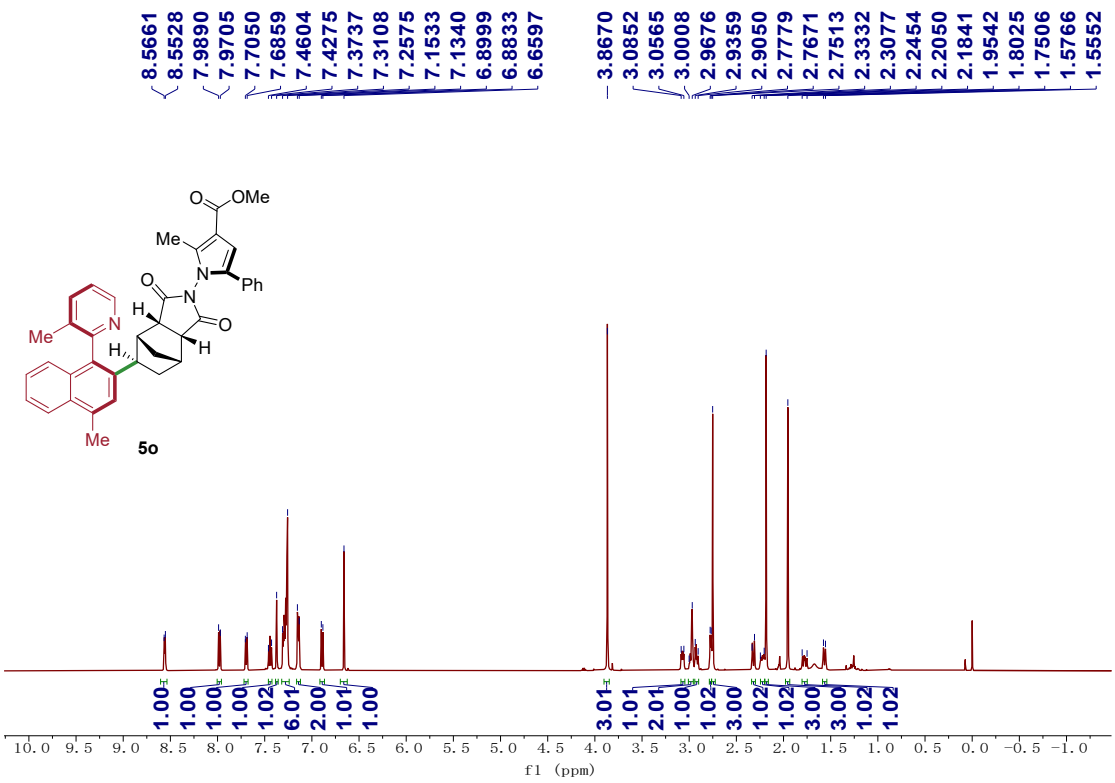
Ph
N
O
H
Me
5n
f1 (ppm)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Me
N
Ph
O
H
Me
5o
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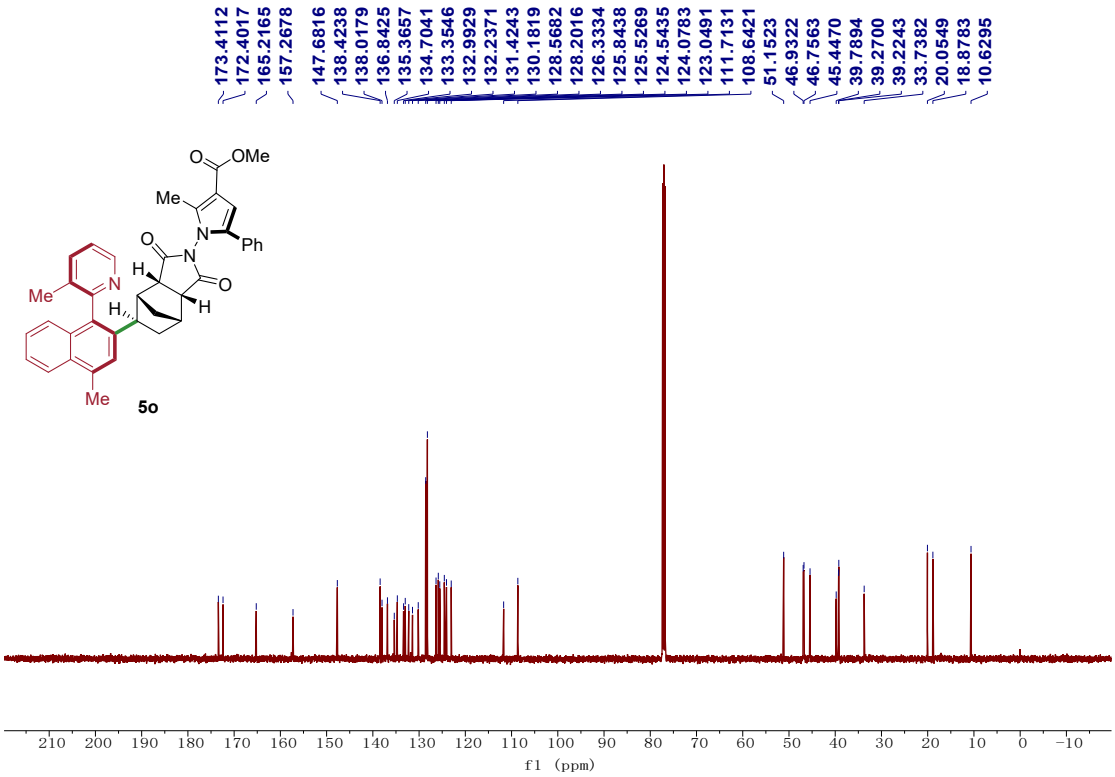
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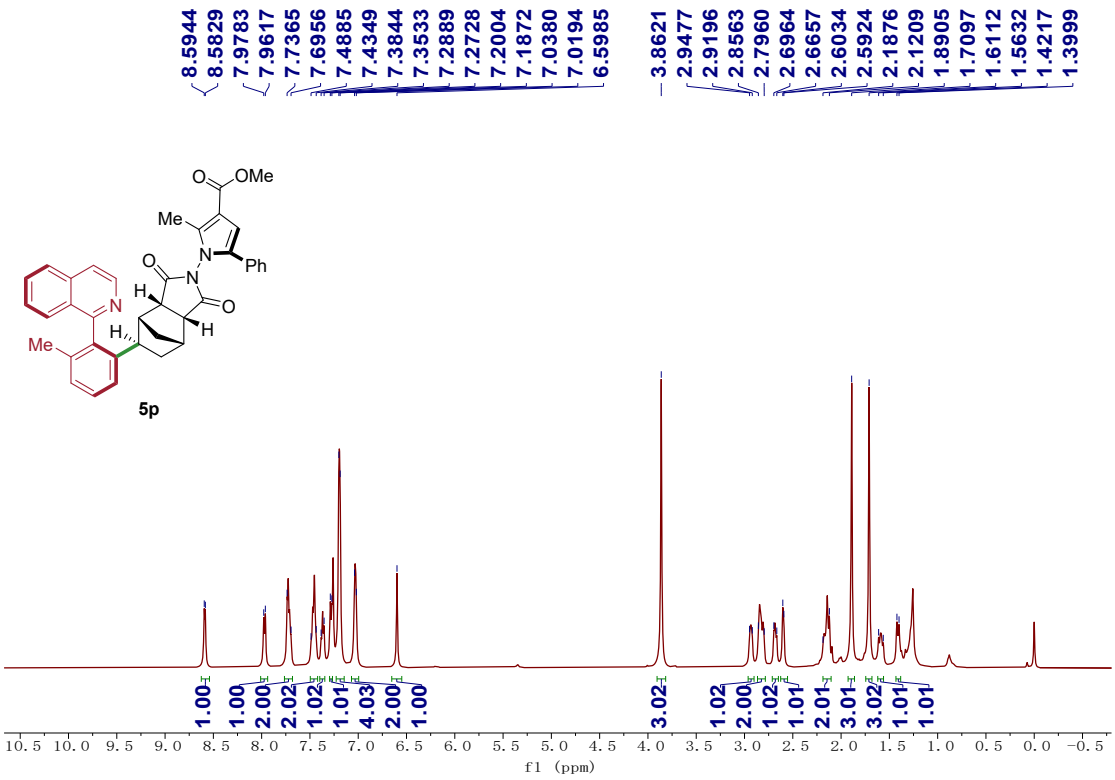
Ph
O
H
Me
5o
f1 (ppm)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7.1872
7.0380
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1.3999
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OMe
Me
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Ph
O
N
O
H
H
N
H
Me
5p
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1.00
2.00
2.02
1.02
1.01
4.03
2.00
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3.02
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1.01
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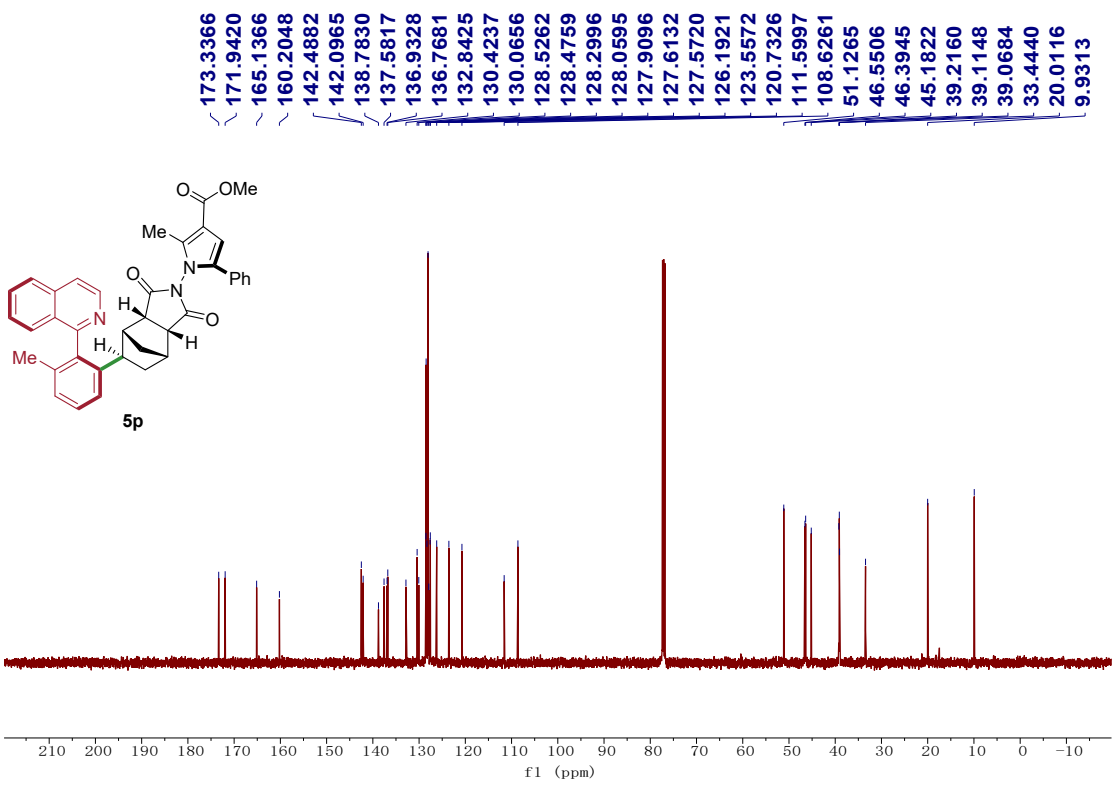
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Me
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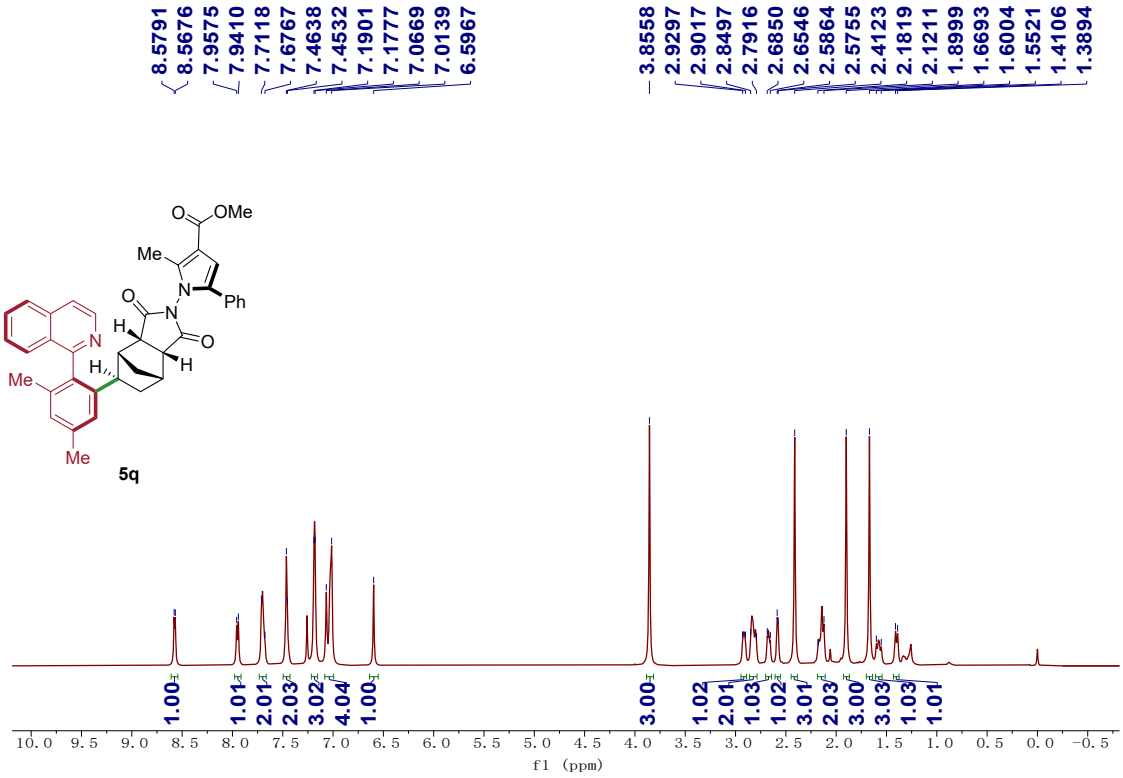
H
N
H
Me
5p
f1 (ppm)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Ph
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O
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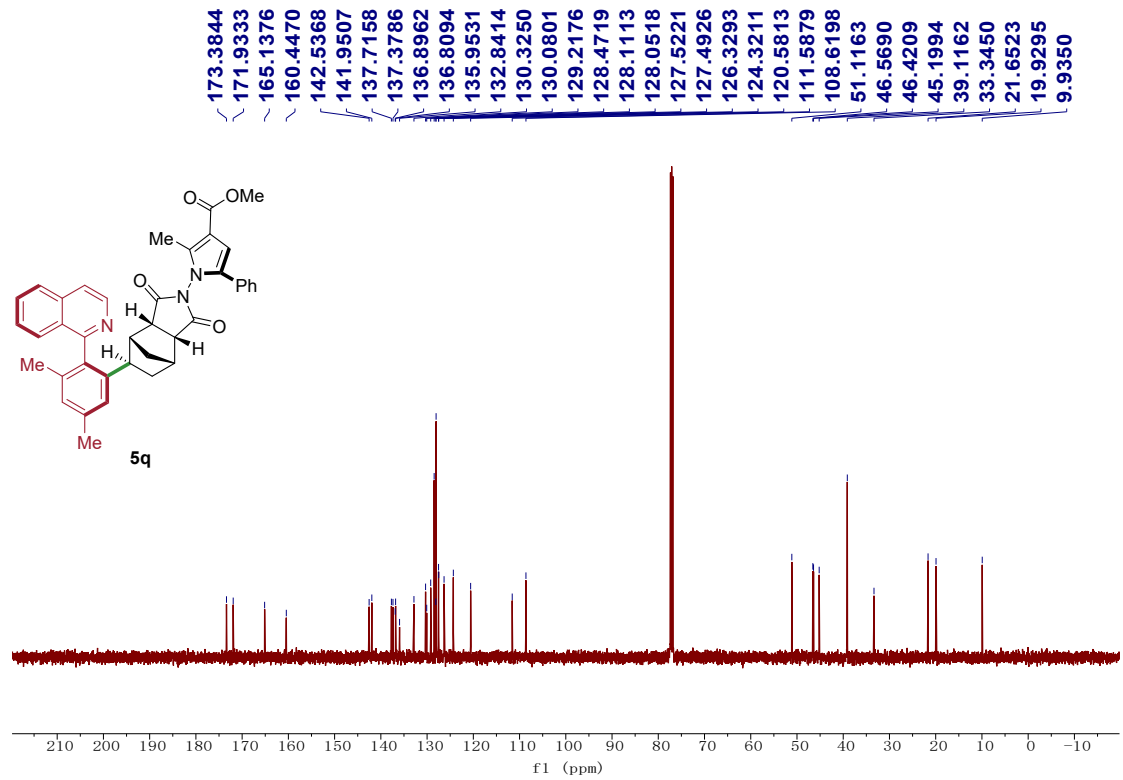
1.01
f1 (ppm)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Me
Ph
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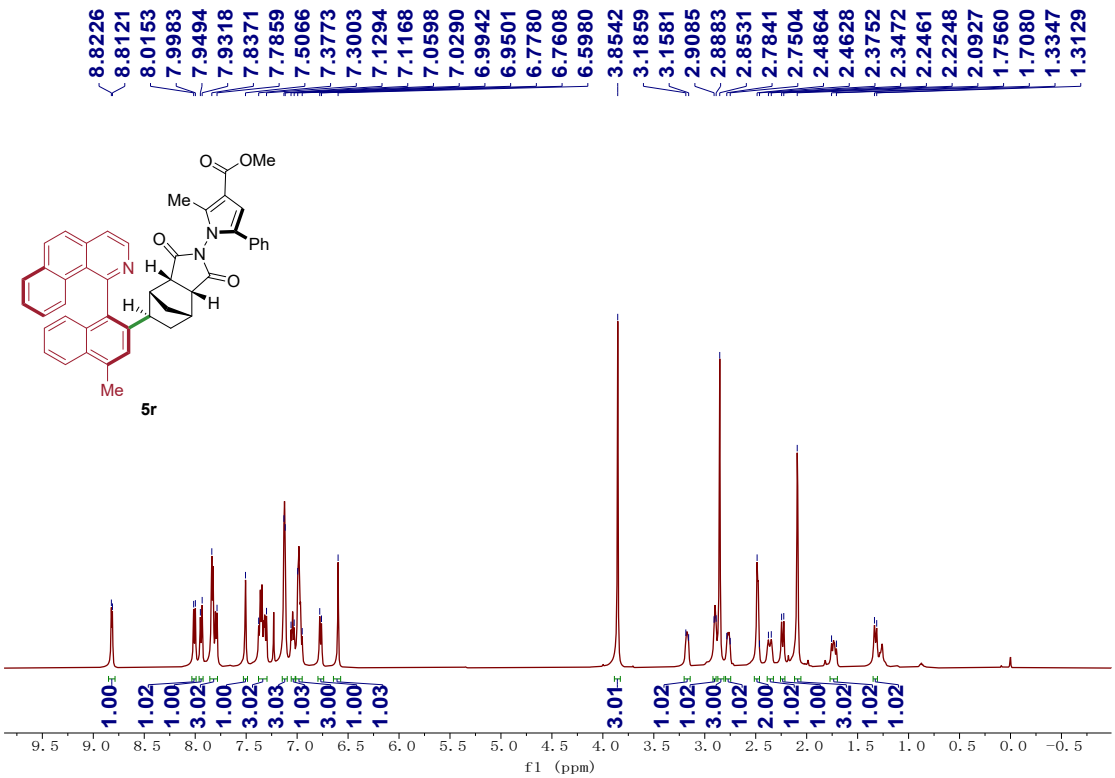
O
H
Me
Me
5q
f1 (ppm)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Ph
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O
H
Me
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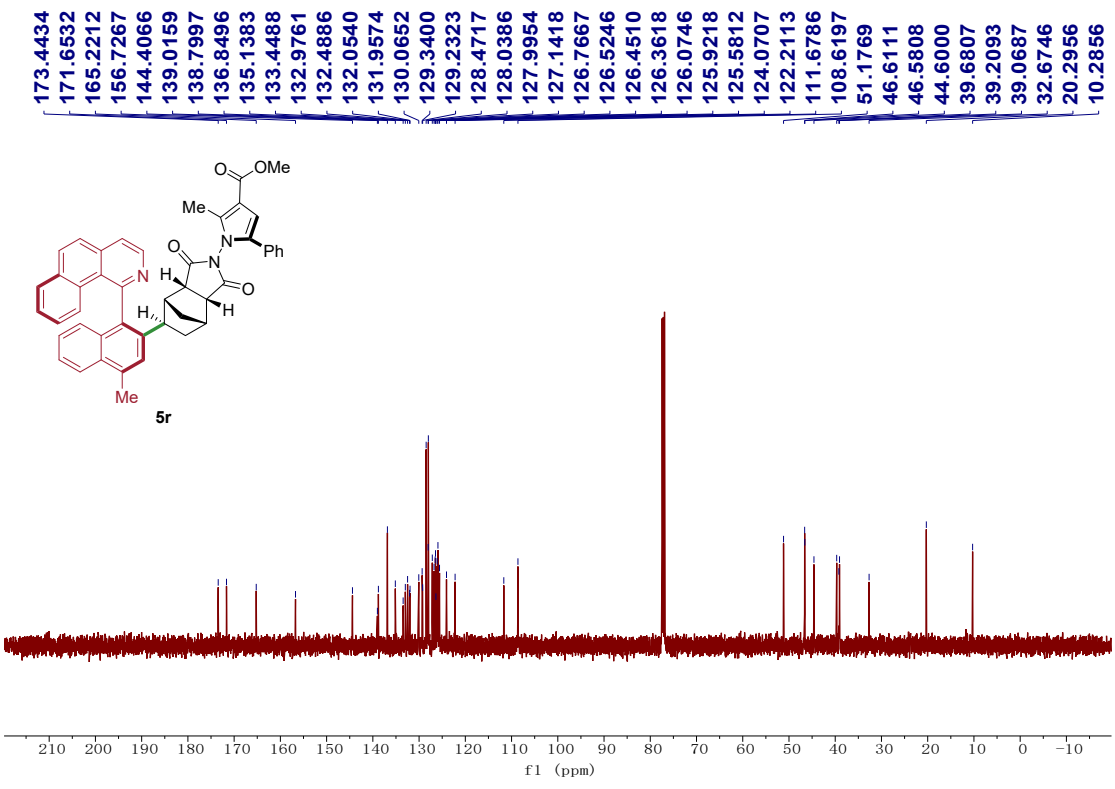
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Ph
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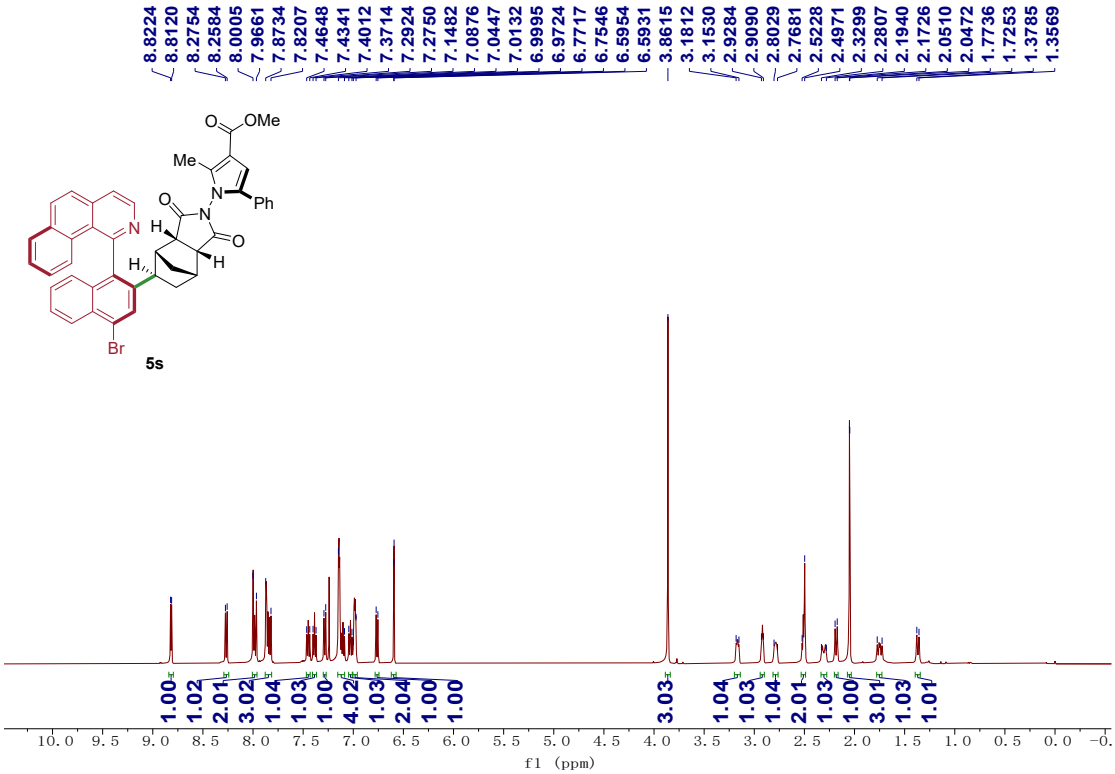
Me
5r
f1 (ppm)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Ph
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Br
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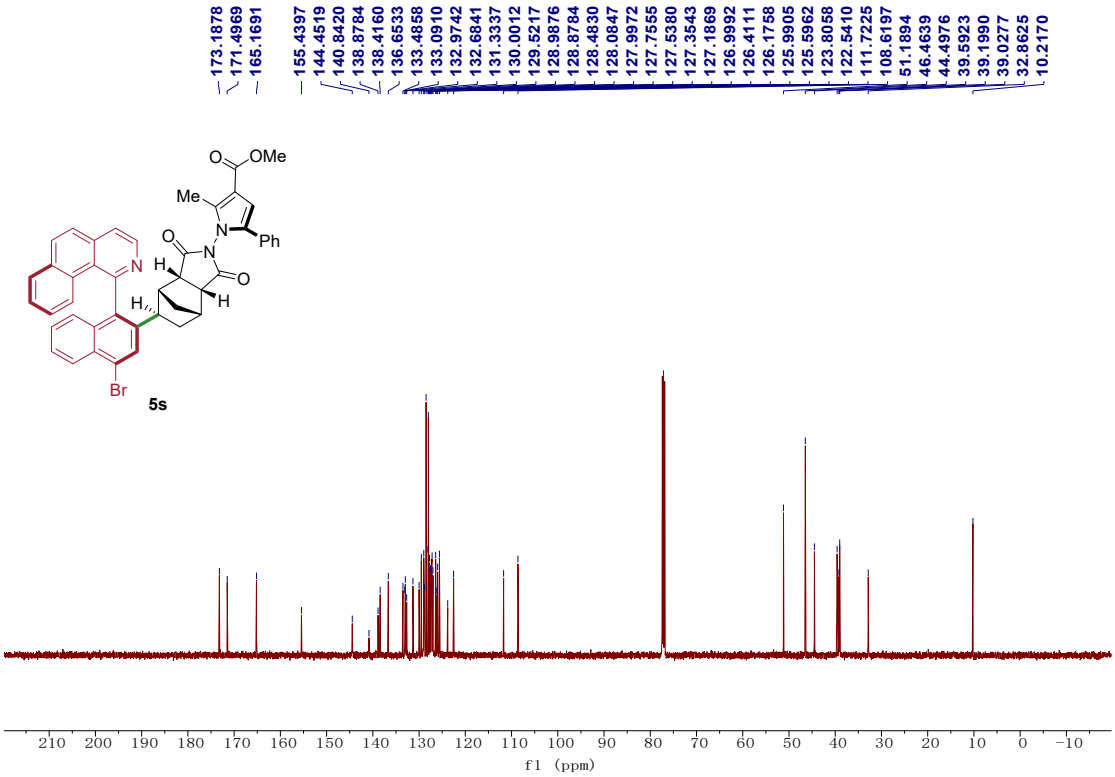
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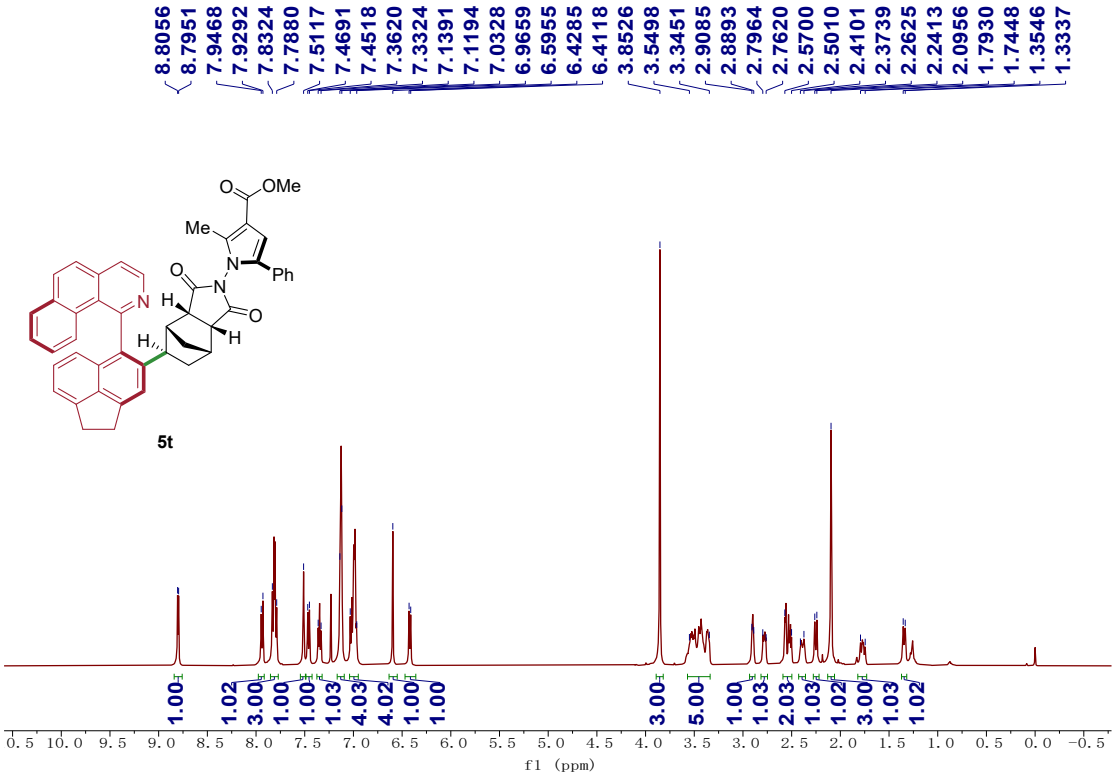
Br
5s
f1 (ppm)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H
H
5t
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1.02
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1.00
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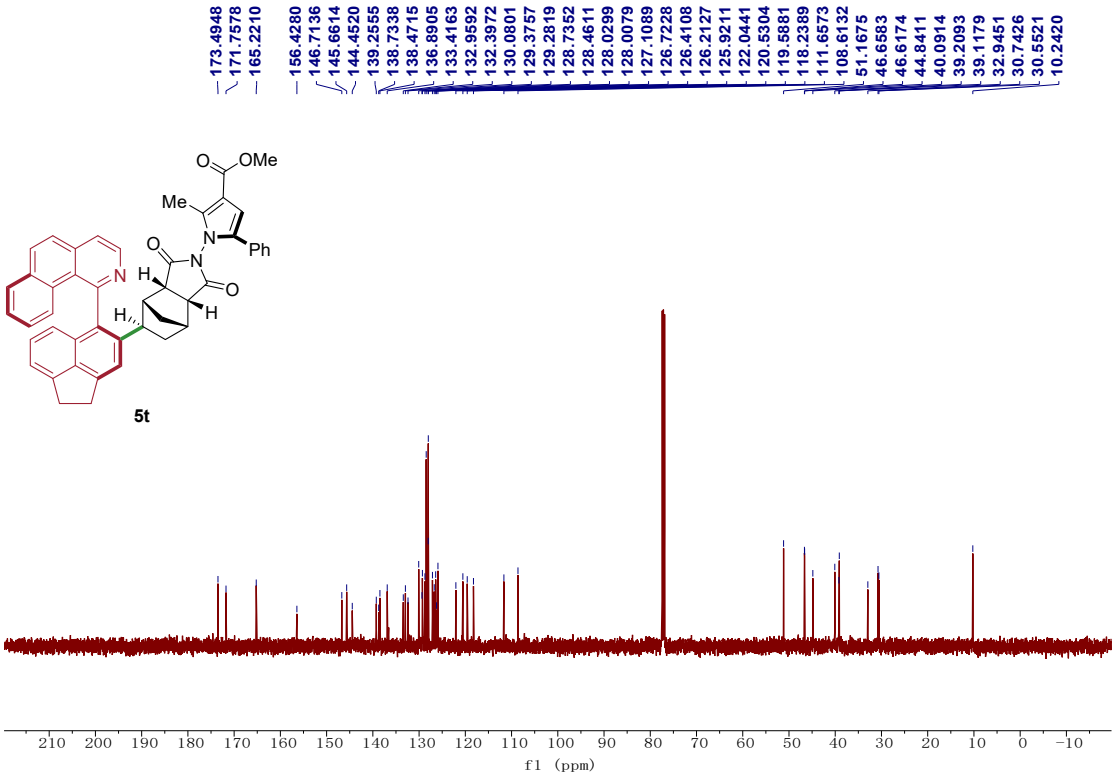
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Me
Ph
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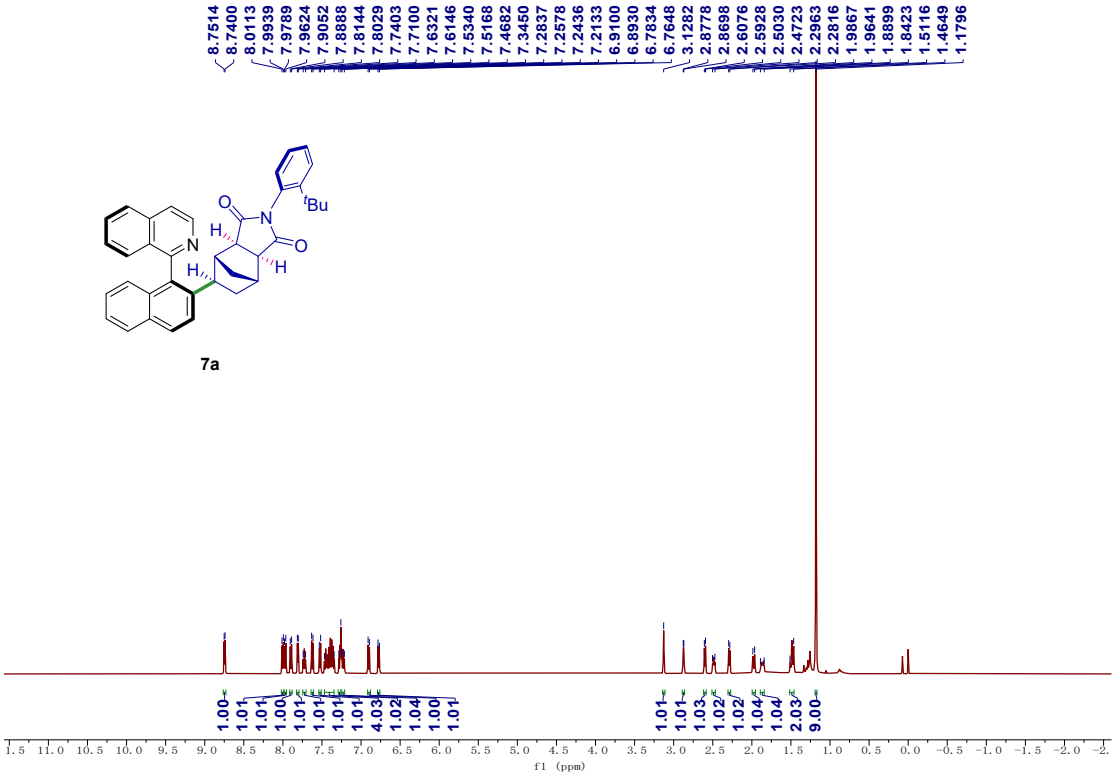
H
5t
f1 (ppm)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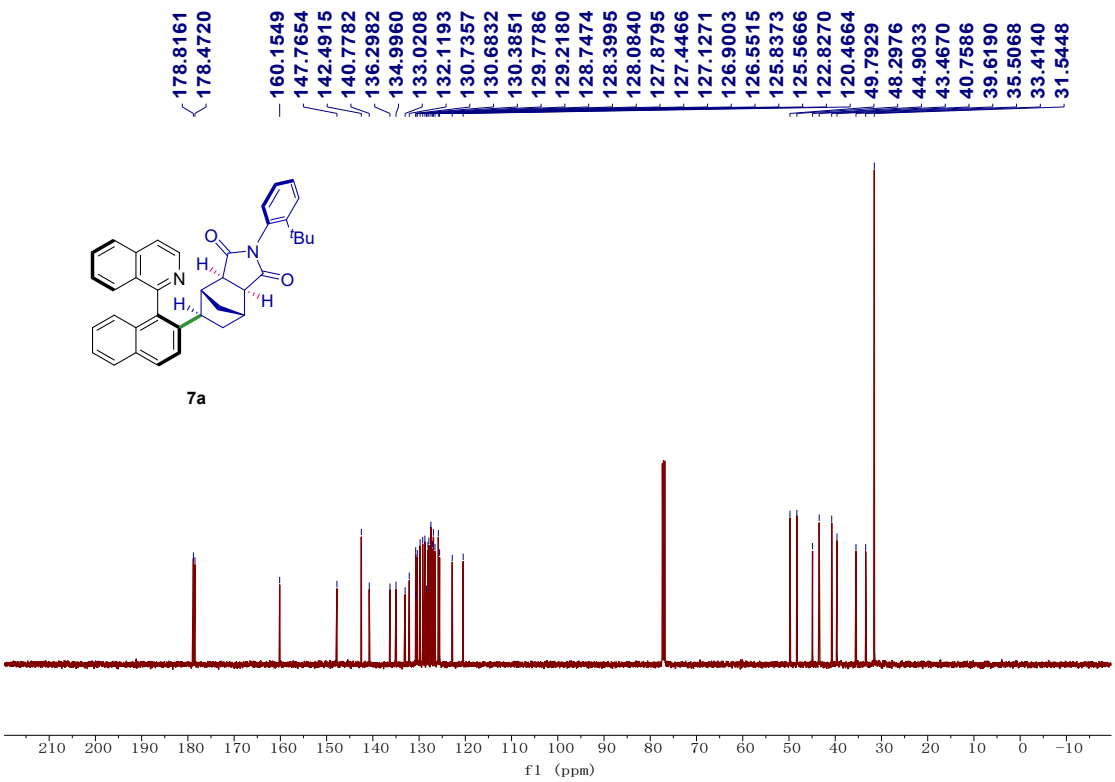
1.04
2.03
9.00
f1 (ppm)

7a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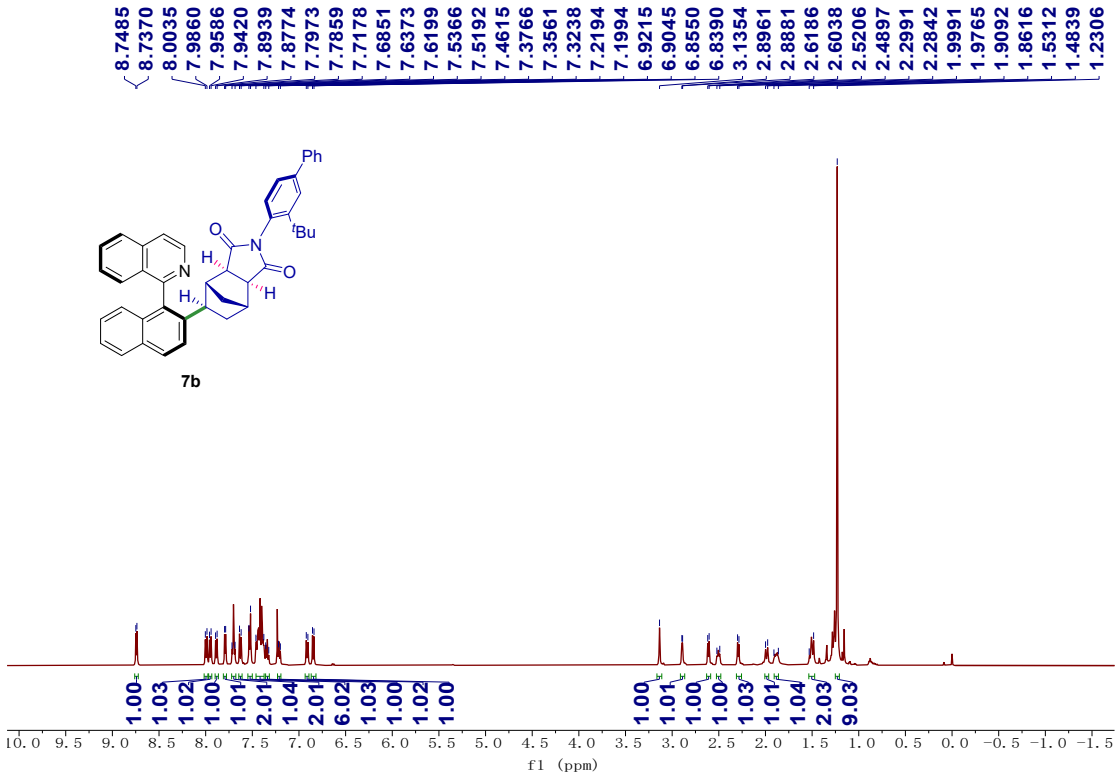
tBu
f1 (ppm)

7a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Ph
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O
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H
N
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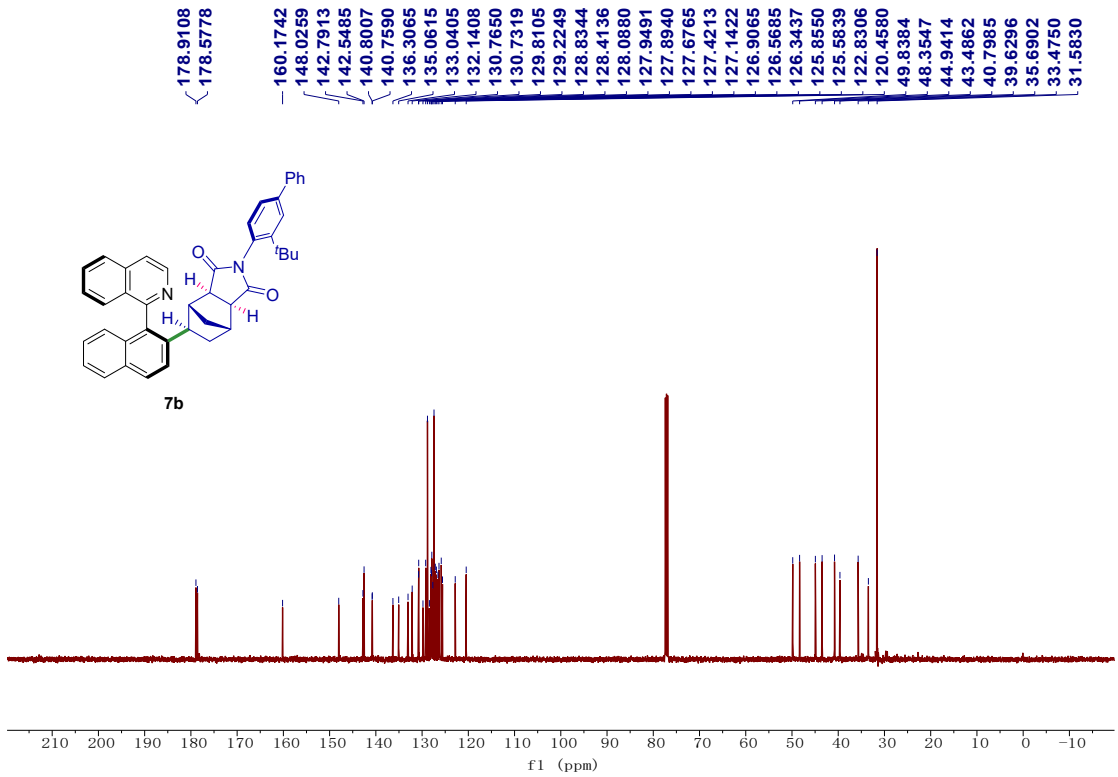
f1 (ppm)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Ph
tBu
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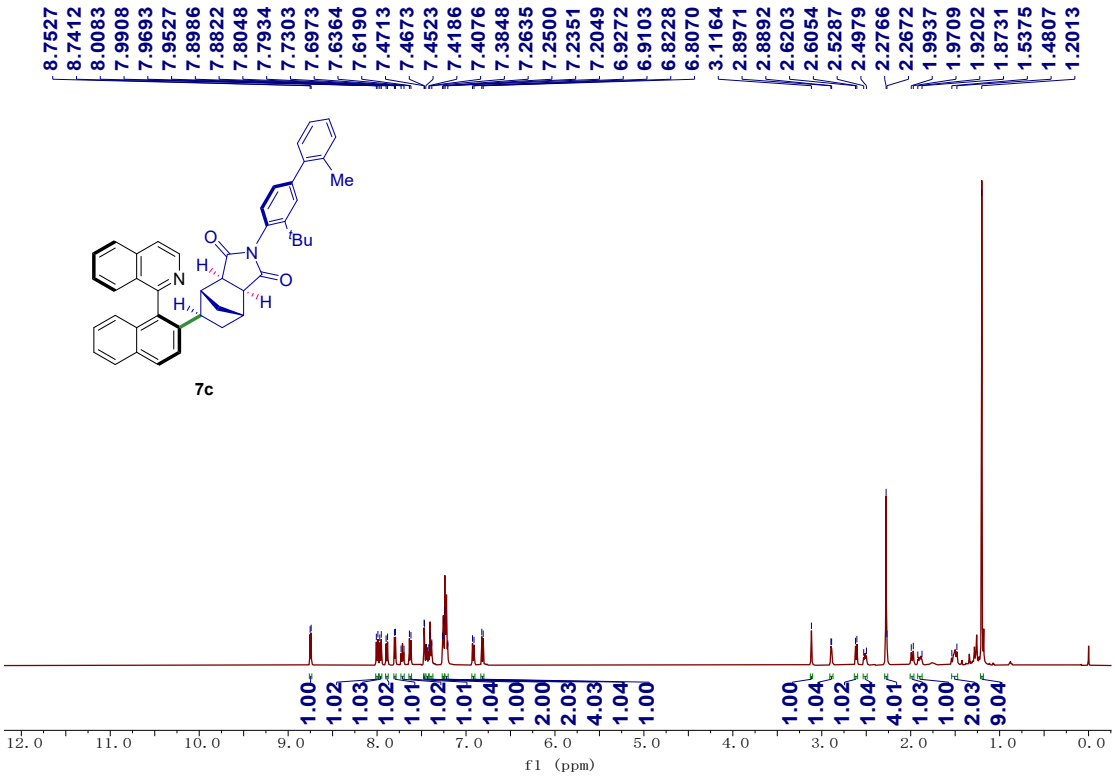
O
H
H
N
7b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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7.6190
7.4713
7.4673
7.4523
7.4186
7.4076
7.3848
7.2635
7.2500
7.2351
7.2049
6.9272
6.9103
6.8228
6.8070
3.1164
2.8971
2.8892
2.6203
2.6054
2.5287
2.4979
2.2766
2.2672
1.9937
1.9709
1.9202
1.8731
1.5375
1.4807
1.2013
Me
tBu
O
N
H
O
H
N
H
7c
1.00
1.02
1.03
1.02
1.01
1.02
1.01
1.04
1.00
2.00
2.03
4.03
1.04
1.00
1.00
1.04
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9.04
12.0
11.0
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5.0
4.0
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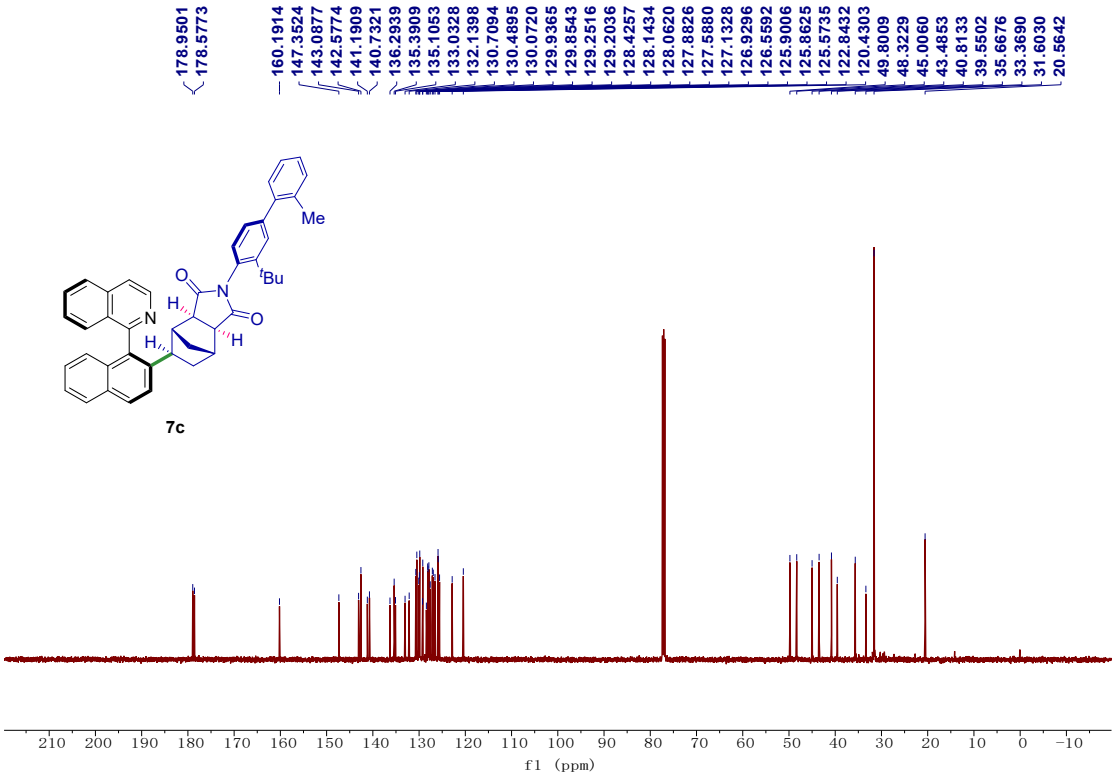
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135.1053
133.0328
132.1398
130.7094
130.4895
130.0720
129.9365
129.8543
129.2516
129.2036
128.4257
128.1434
128.0620
127.8826
127.5880
127.1328
126.9296
126.5592
125.9006
125.8625
125.5735
122.8432
120.4303
49.8009
48.3229
45.0060
43.4853
40.8133
39.5502
35.6676
33.3690
31.6030
20.5642
Me
tBu
O
N
H
O
H
N
H
7c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
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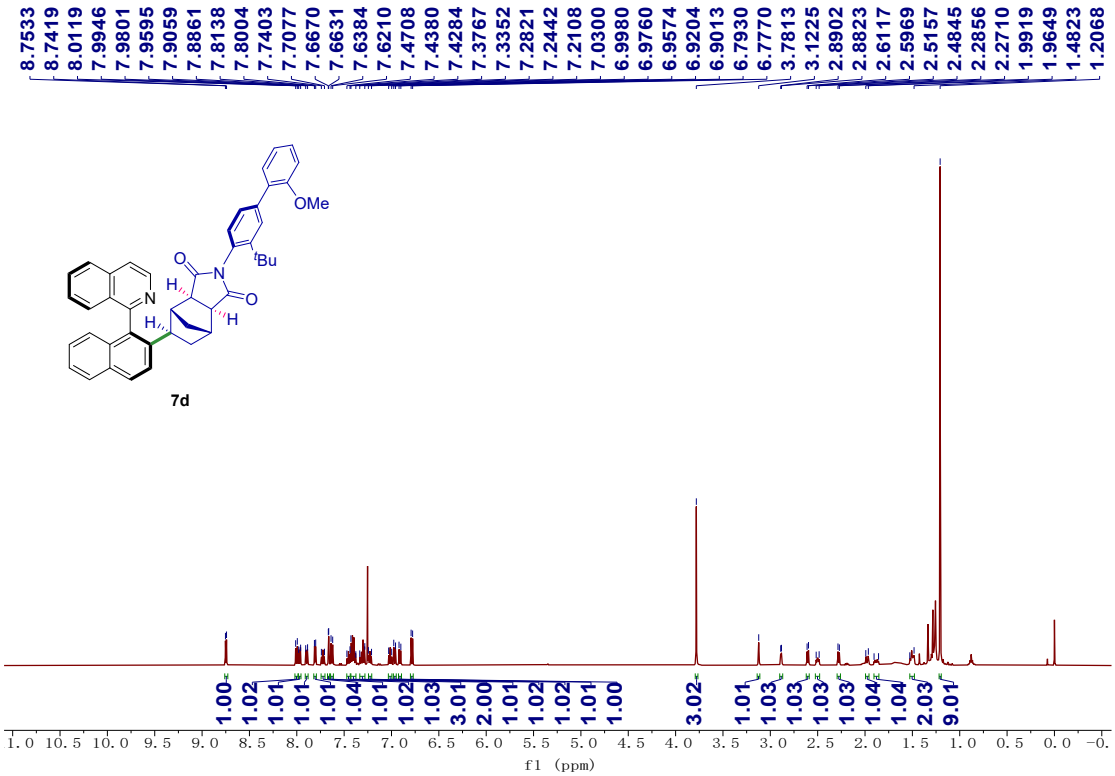
40
30
20
10
0
−10
f1 (ppm)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7.7403
7.7077
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7.6631
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7.6210
7.4708
7.4380
7.4284
7.3767
7.3352
7.2821
7.2442
7.2108
7.0300
6.9980
6.9760
6.9574
6.9204
6.9013
6.7930
6.7770
3.7813
3.1225
2.8902
2.8823
2.6117
2.5969
2.5157
2.4845
2.2856
2.2710
1.9919
1.9649
1.4823
1.2068
OMe
tBu
O
N
O
H
H
H
N
7d
1.00
1.02
1.01
1.01
1.01
1.04
1.01
1.02
1.03
3.01
2.00
1.01
1.02
1.02
1.01
1.00
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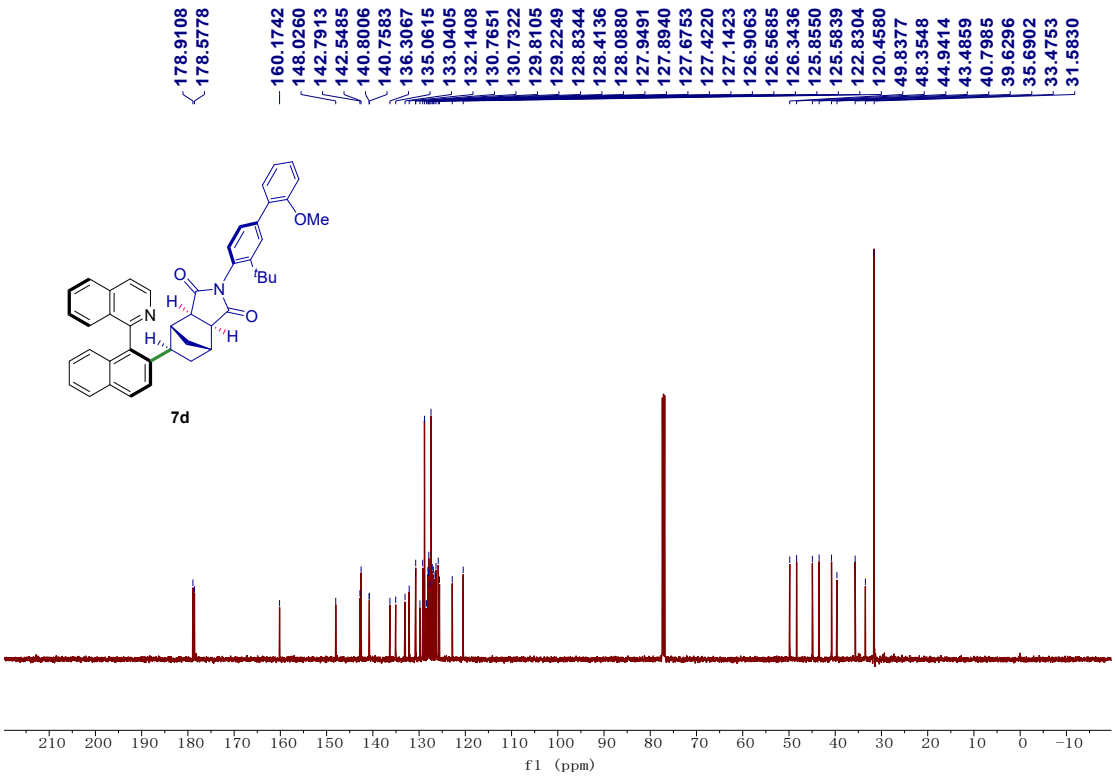
1.03
1.03
1.03
1.03
1.04
1.04
2.03
9.01
f1 (ppm)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132.1408
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130.7322
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129.2249
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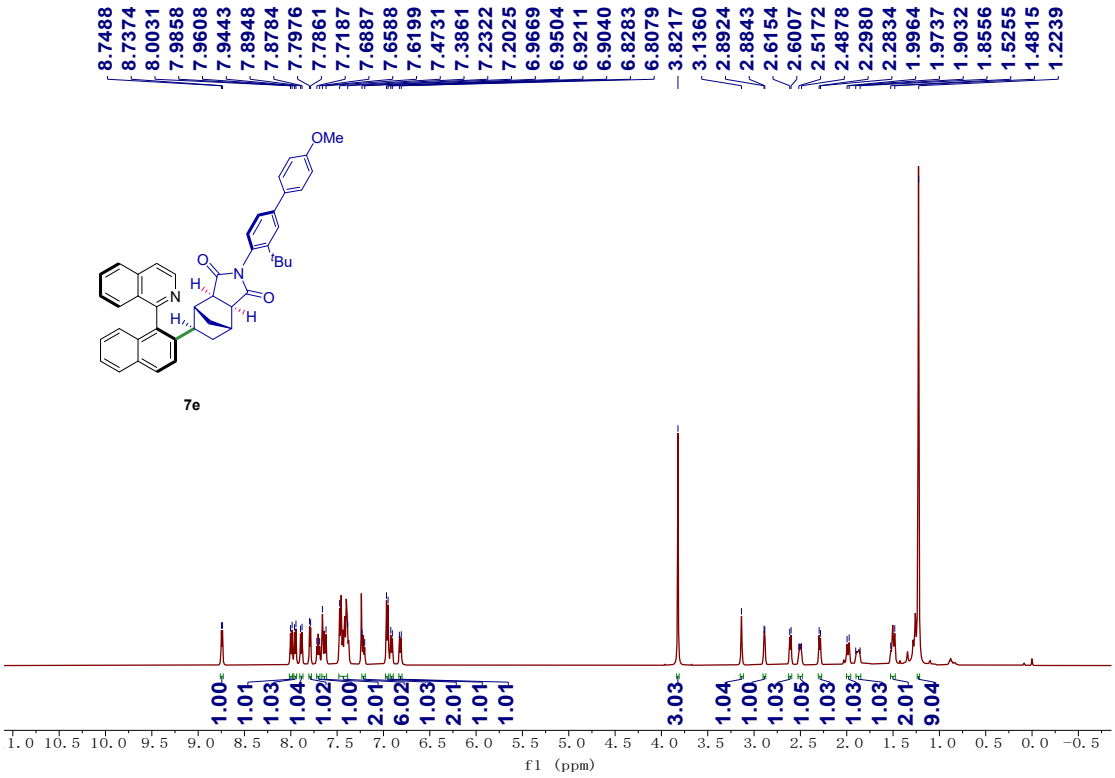
128.4136
128.0880
127.9491
127.8940
127.6753
127.4220
127.1423
126.9063
126.5685
126.3436
125.8550
125.5839
122.8304
120.4580
49.8377
48.3548
44.9414
43.4859
40.7985
39.6296
35.6902
33.4753
31.5830
OMe
tBu
O
N
O
H
H
H
N
7d
f1 (ppm)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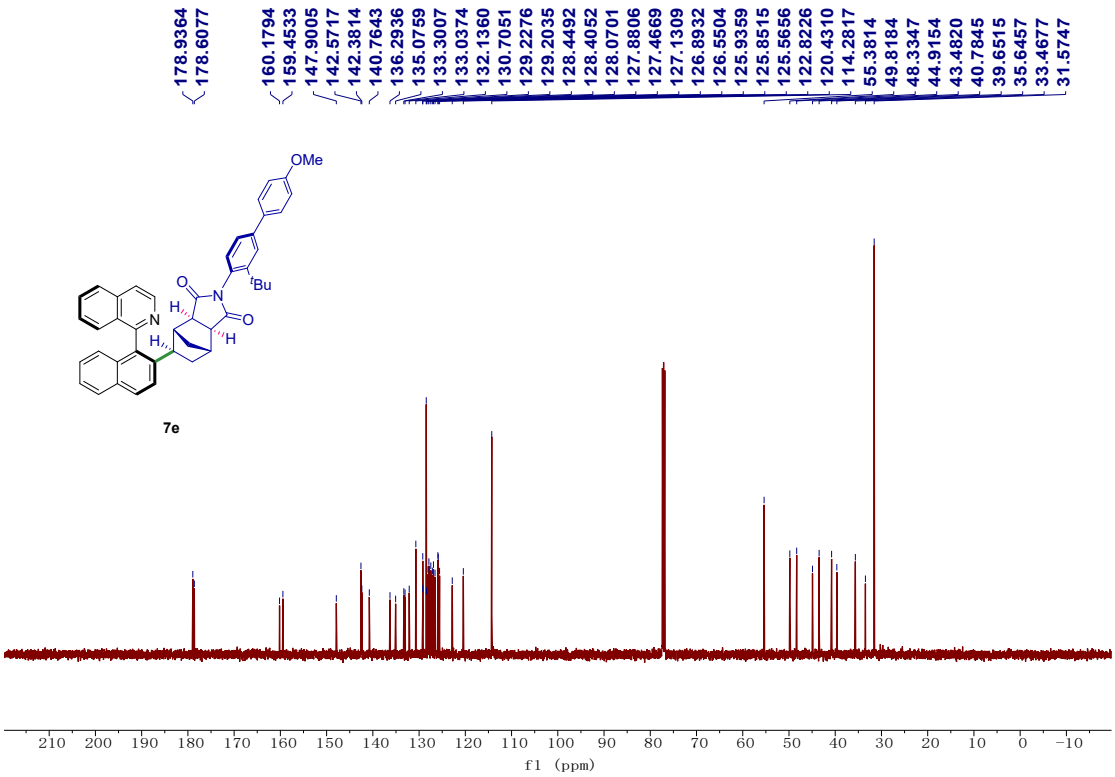
7.7187
7.6887
7.6588
7.6199
7.4731
7.3861
7.2322
7.2025
6.9669
6.9504
6.9211
6.9040
6.8283
6.8079
3.8217
3.1360
2.8924
2.8843
2.6154
2.6007
2.5172
2.4878
2.2980
2.2834
1.9964
1.9737
1.9032
1.8556
1.5255
1.4815
1.2239
OMe
tBu
O
N
H
O
H
N
H
7e
1.00
1.01
1.03
1.04
1.02
1.00
2.01
6.02
1.03
2.01
1.01
1.01
3.03
1.04
1.00
1.03
1.05
1.03
1.03
1.03
2.01
9.04
f1 (ppm)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142.3814
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133.0374
132.1360
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129.2035
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128.4052
128.0701
127.8806
127.4669
127.1309
126.8932
126.5504
125.9359
125.8515
125.5656
122.8226
120.4310
114.2817
55.3814
49.8184
48.3347
44.9154
43.4820
40.7845
39.6515
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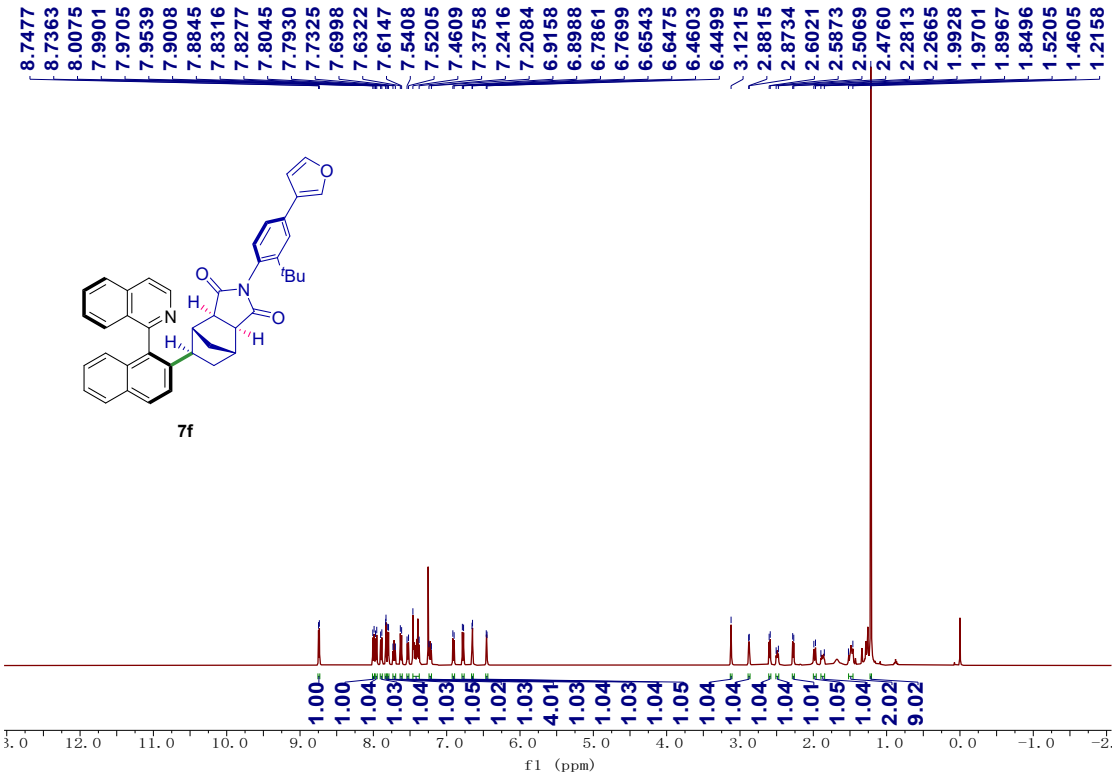
33.4677
31.5747
OMe
tBu
O
N
H
O
H
N
H
7e
f1 (ppm)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7.7930
7.7325
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7.6322
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7.5205
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7.3758
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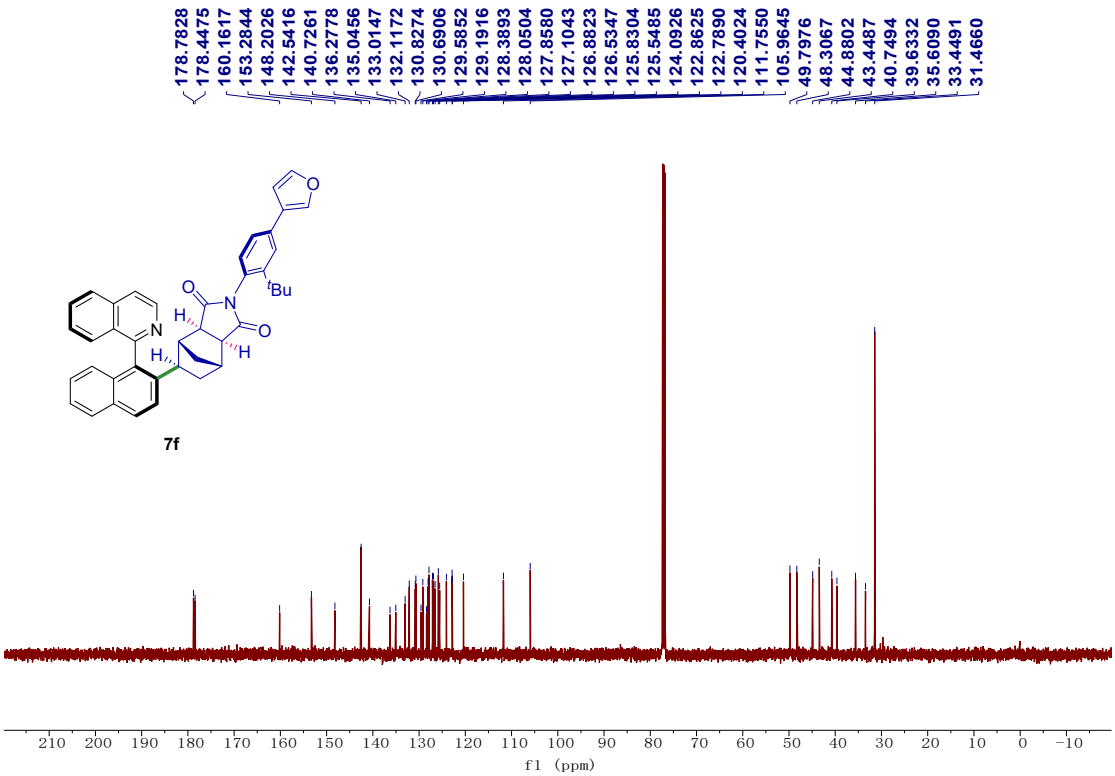
6.4603
6.4499
3.1215
2.8815
2.8734
2.6021
2.5873
2.5069
2.4760
2.2813
2.2665
1.9928
1.9701
1.8967
1.8496
1.5205
1.4605
1.2158
tBu
7f
1.00 1.00 1.04 1.03 1.04 1.03 1.05 1.02 1.03 4.01 1.03 1.04 1.03 1.04 1.05 1.04 1.04 1.04 1.04 1.01 1.05 1.04 2.02 9.02
f1 (ppm)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130.6906
129.5852
129.1916
128.3893
128.0504
127.8580
127.1043
126.8823
126.5347
125.8304
125.5485
124.0926
122.8625
122.7890
120.4024
111.7550
105.9645
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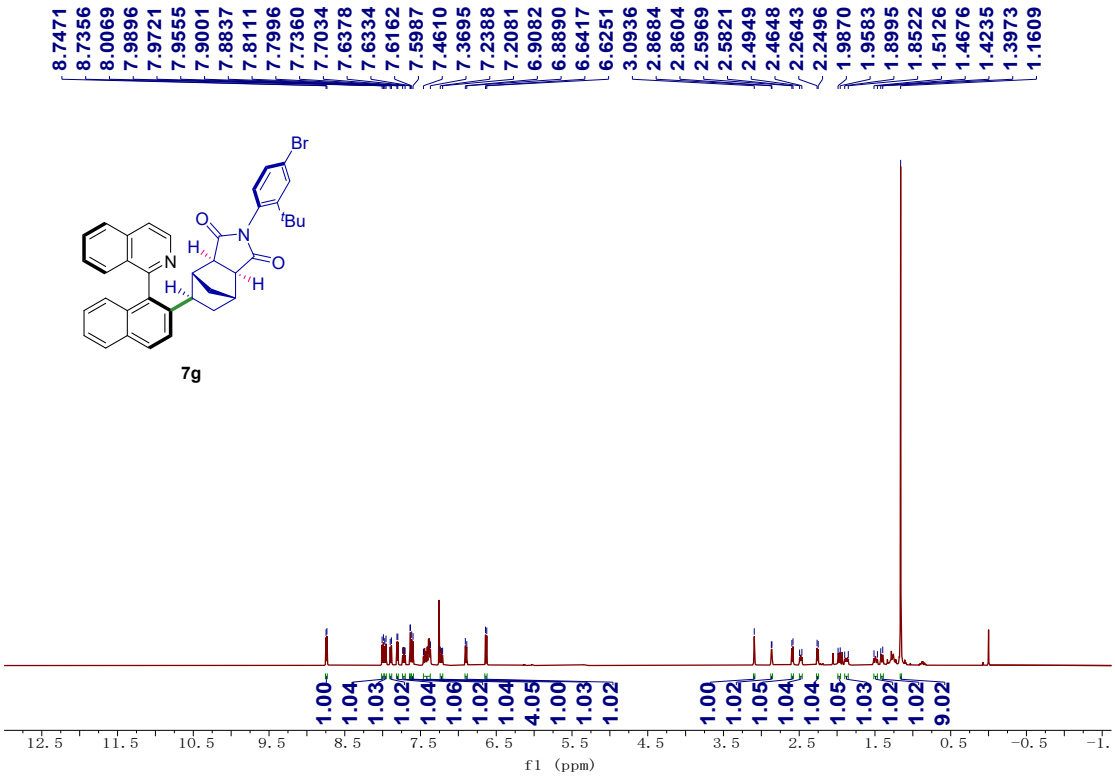
31.4660
tBu
7f
f1 (ppm)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7.7360
7.7034
7.6378
7.6334
7.6162
7.5987
7.4610
7.3695
7.2388
7.2081
6.9082
6.8890
6.6417
6.6251
3.0936
2.8684
2.8604
2.5969
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2.4648
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1.8995
1.8522
1.5126
1.4676
1.4235
1.3973
1.1609
Br
tBu
O
N
O
H
H
H
N
7g
1.00
1.04
1.03
1.02
1.04
1.06
1.02
1.04
4.05
1.00
1.03
1.02
1.00
1.02
1.05
1.04
1.04
1.05
1.03
1.02
1.02
9.02
12.5
11.5
10.5
9.5
8.5
7.5
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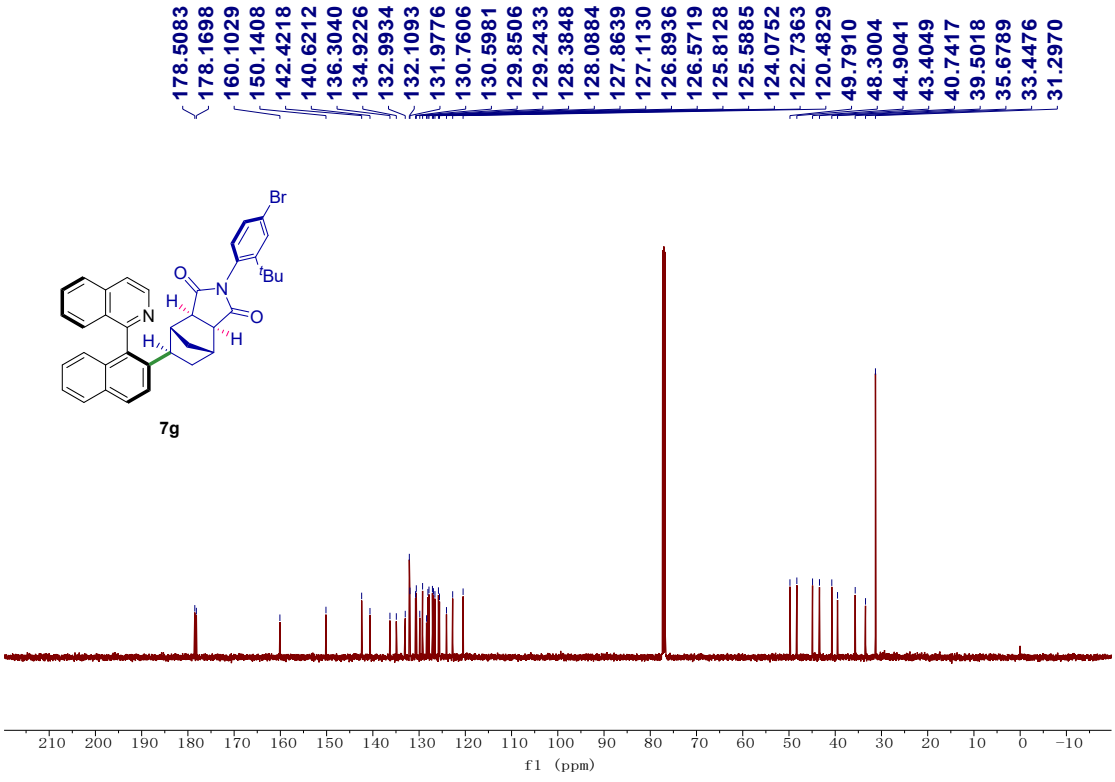
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
−1.
f1 (ppm)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130.5981
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127.1130
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126.5719
125.8128
125.5885
124.0752
122.7363
120.4829
49.7910
48.3004
44.9041
43.4049
40.7417
39.5018
35.6789
33.4476
31.2970
Br
tBu
O
N
O
H
H
H
N
7g
210
200
190
180
170
160
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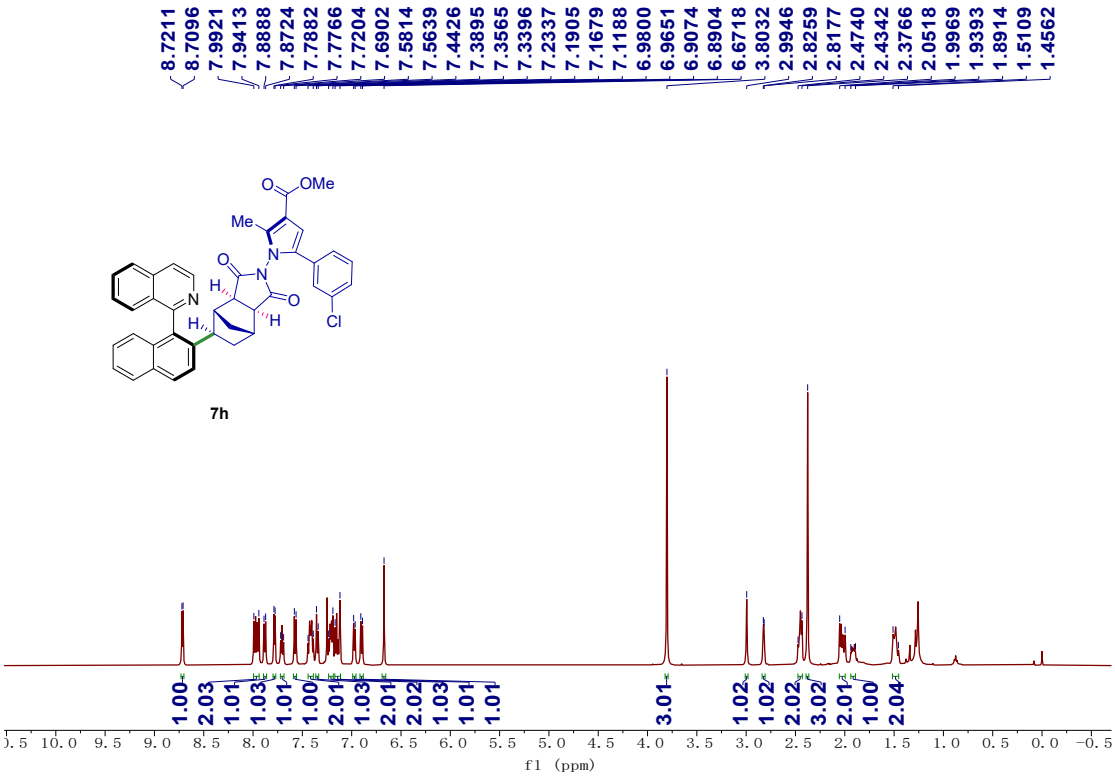
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.5639
7.4426
7.3895
7.3565
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7.2337
7.1905
7.1679
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6.9800
6.9651
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6.8904
6.6718
3.8032
2.9946
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2.4740
2.4342
2.3766
2.0518
1.9969
1.9393
1.8914
1.5109
1.4562
OMe
Me
N
O
H
Cl
7h
1.00
2.03
1.01
1.03
1.01
1.00
2.01
1.03
2.01
2.02
1.03
1.01
1.01
3.01
1.02
1.02
2.02
3.02
2.01
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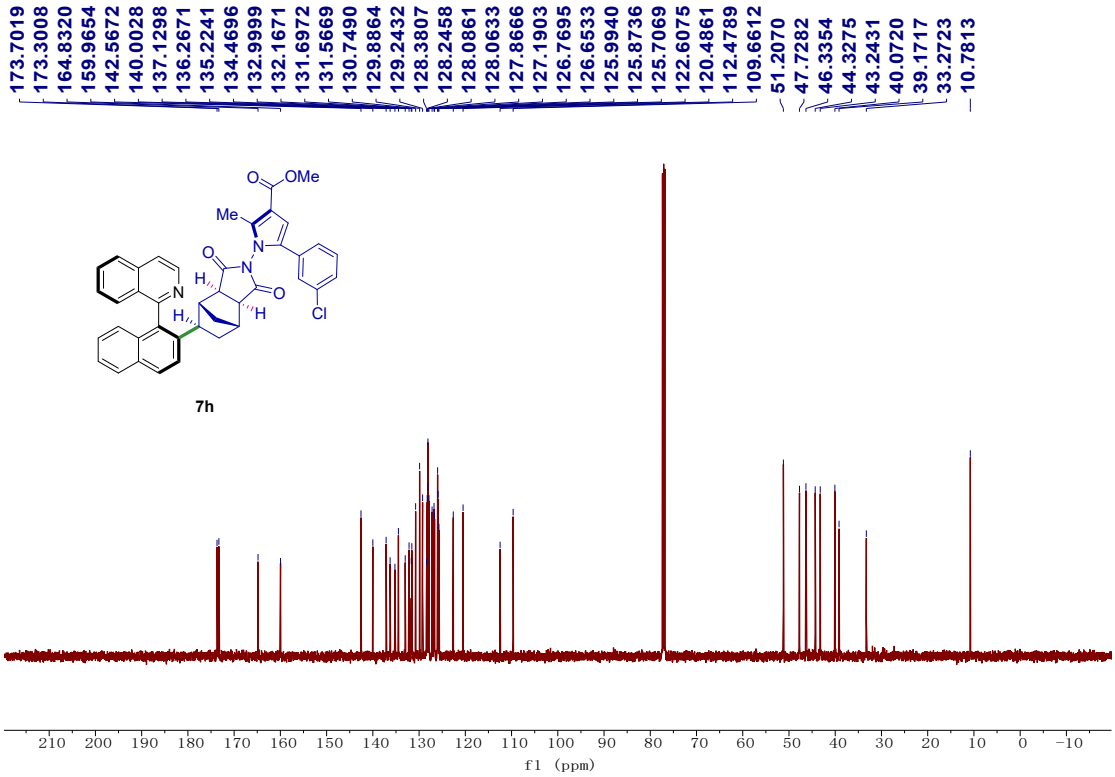
2.04
f1 (ppm)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47.7282
46.3354
44.3275
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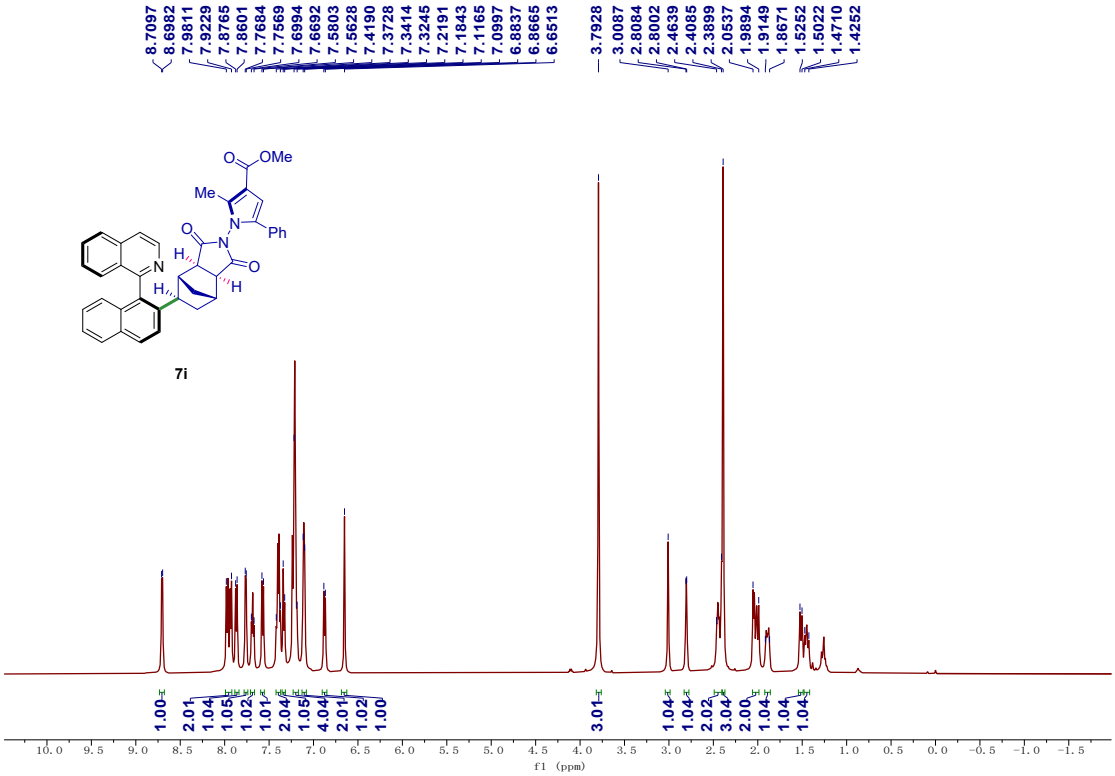
OMe
Me
N
O
H
Cl
7h
f1 (ppm)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7.4190
7.3728
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7.3245
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7.1843
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7.0997
6.8837
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3.7928
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1.5252
1.5022
1.4710
1.4252
OMe
Me
Ph
N
O
H
7i
1.00
2.01
1.04
1.05
1.02
1.01
2.04
1.05
4.04
2.01
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1.04
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2.02
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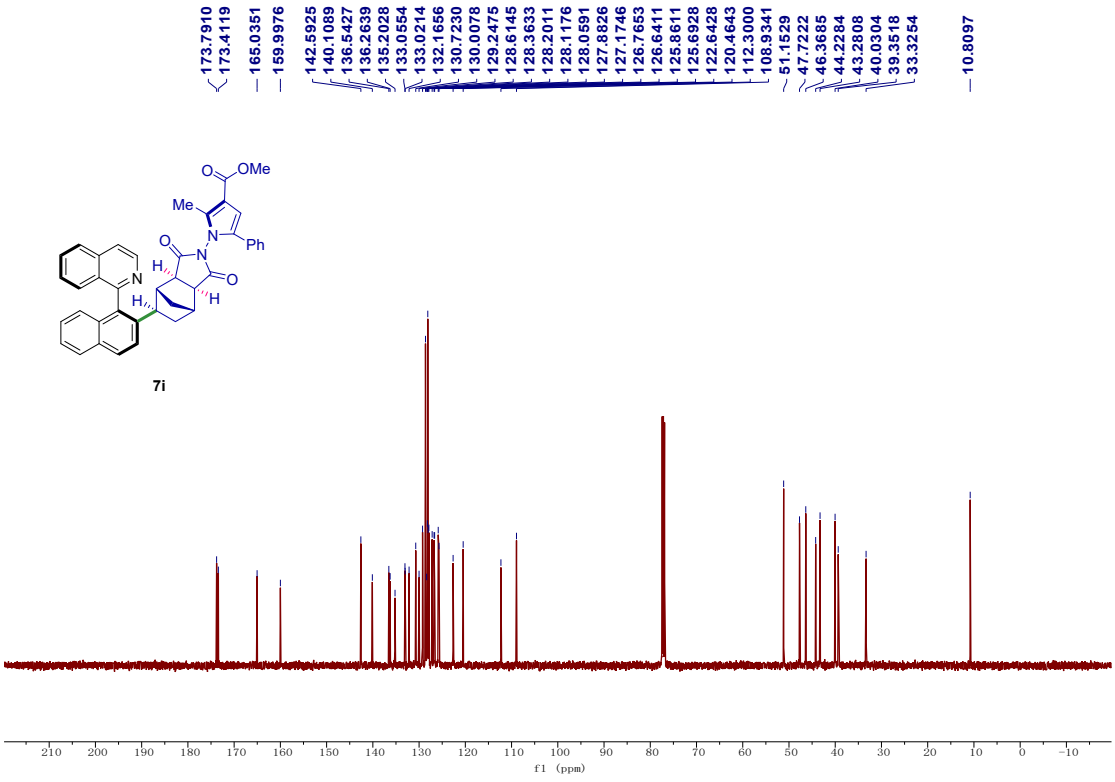
1.04
f1 (ppm)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130.7230
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128.2011
128.1176
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127.8826
127.1746
126.7653
126.6411
125.8611
125.6928
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120.4643
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47.7222
46.3685
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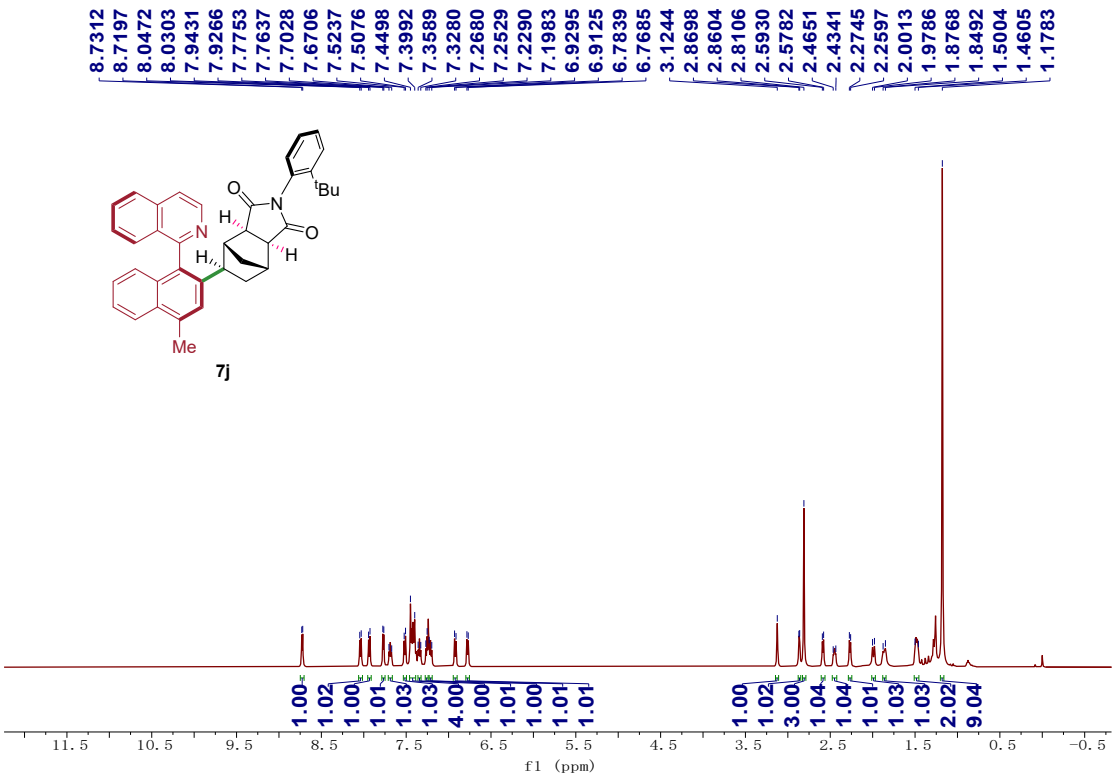
Me
Ph
N
O
H
7i
f1 (ppm)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7.3589
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7.2680
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6.7839
6.7685
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1.5004
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1.1783
tBu
Me
7j
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1.02
1.00
1.01
1.03
1.03
4.00
1.00
1.01
1.00
1.01
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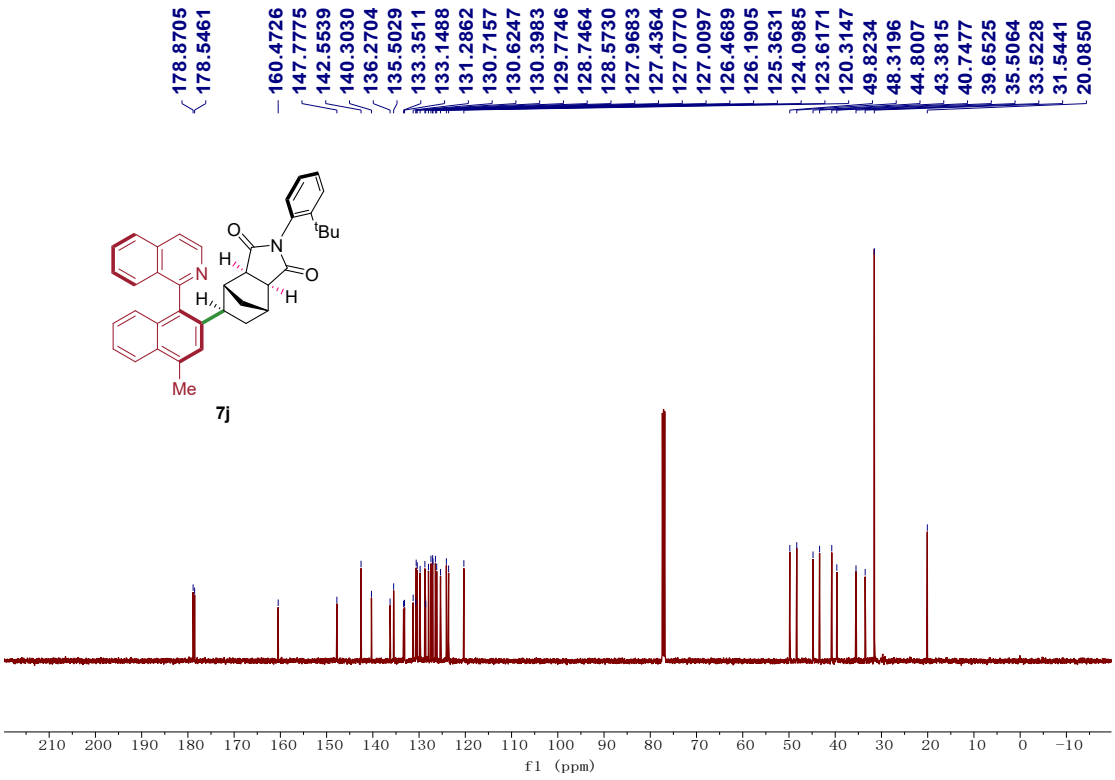
1.03
1.03
2.02
9.04
f1 (ppm)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128.7464
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124.0985
123.6171
120.3147
49.8234
48.3196
44.8007
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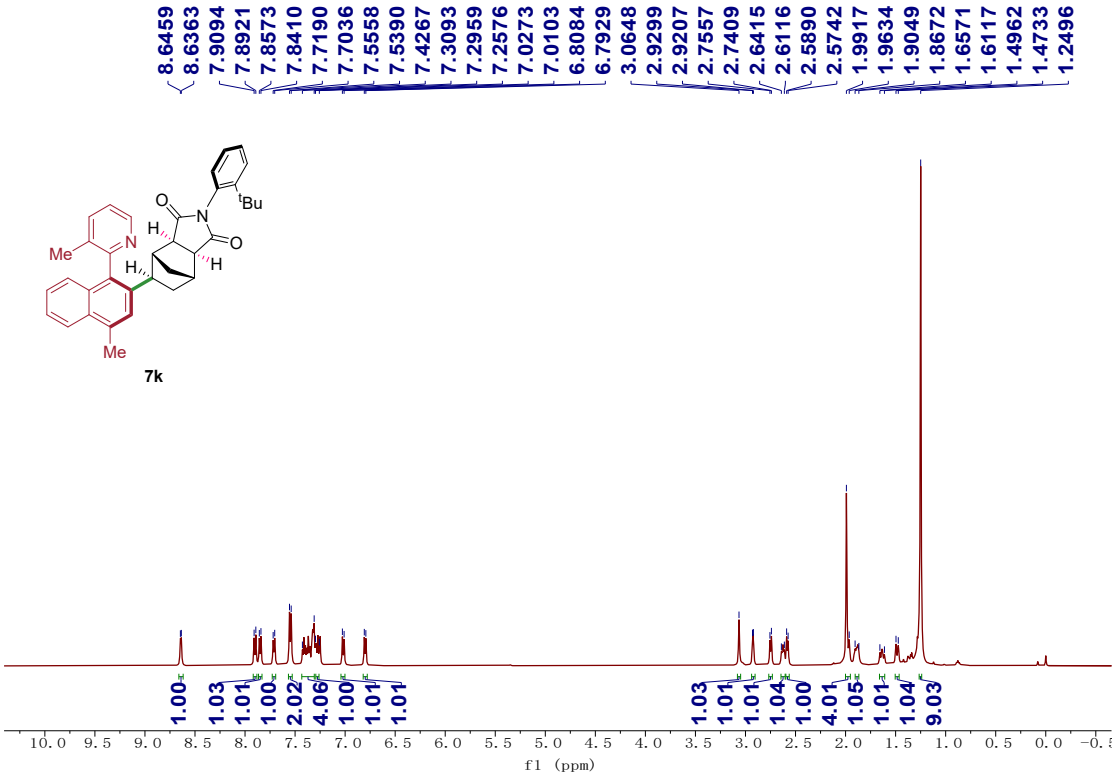
39.6525
35.5064
33.5228
31.5441
20.0850
tBu
Me
7j
f1 (ppm)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7.2576
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6.7929
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2.9207
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2.7409
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2.5890
2.5742
1.9917
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1.9049
1.8672
1.6571
1.6117
1.4962
1.4733
1.2496
tBu
O
N
O
H
H
H
Me
N
Me
1.00
1.03
1.01
1.00
2.02
4.06
1.00
1.01
1.01
1.03
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1.04
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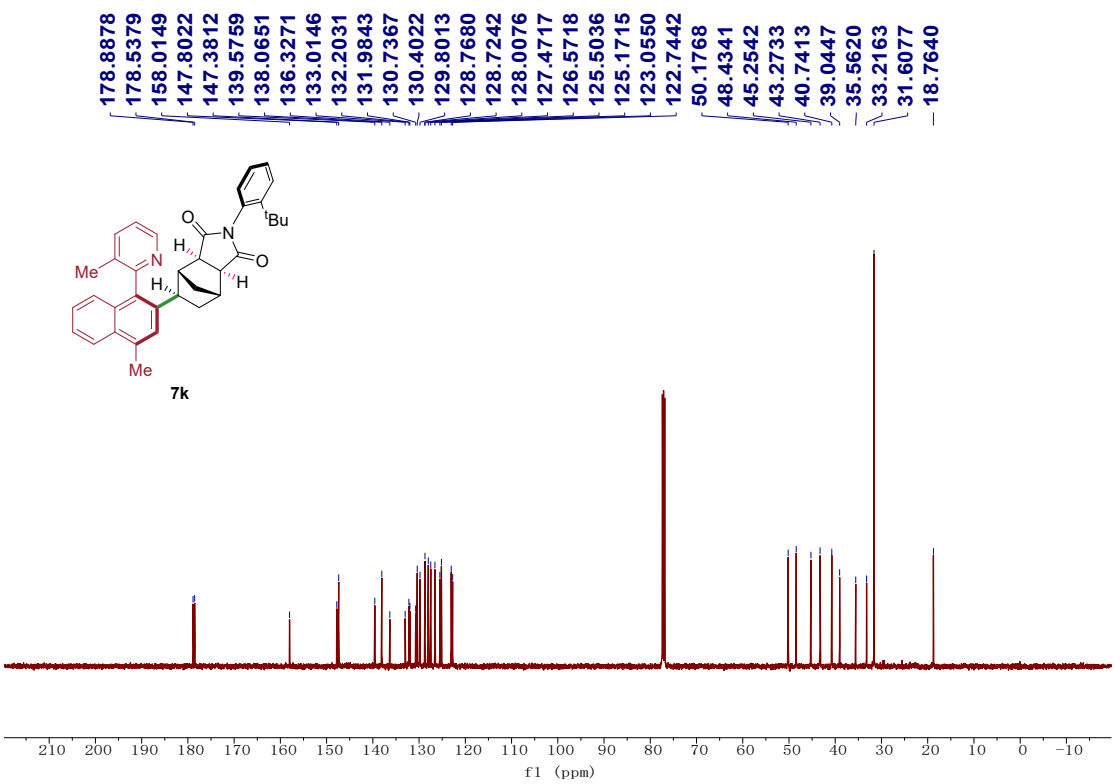
7k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128.7242
128.0076
127.4717
126.5718
125.5036
125.1715
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122.7442
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45.2542
43.2733
40.7413
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35.5620
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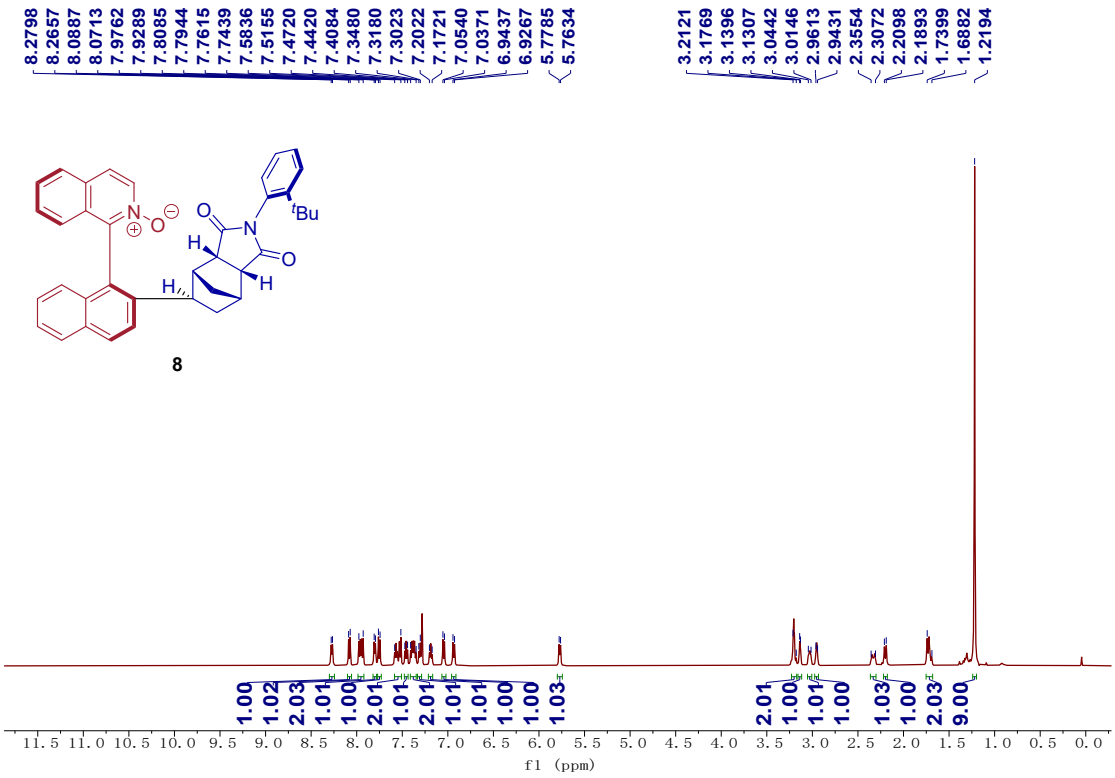
tBu
O
N
O
H
H
H
Me
N
Me
f1 (ppm)

7k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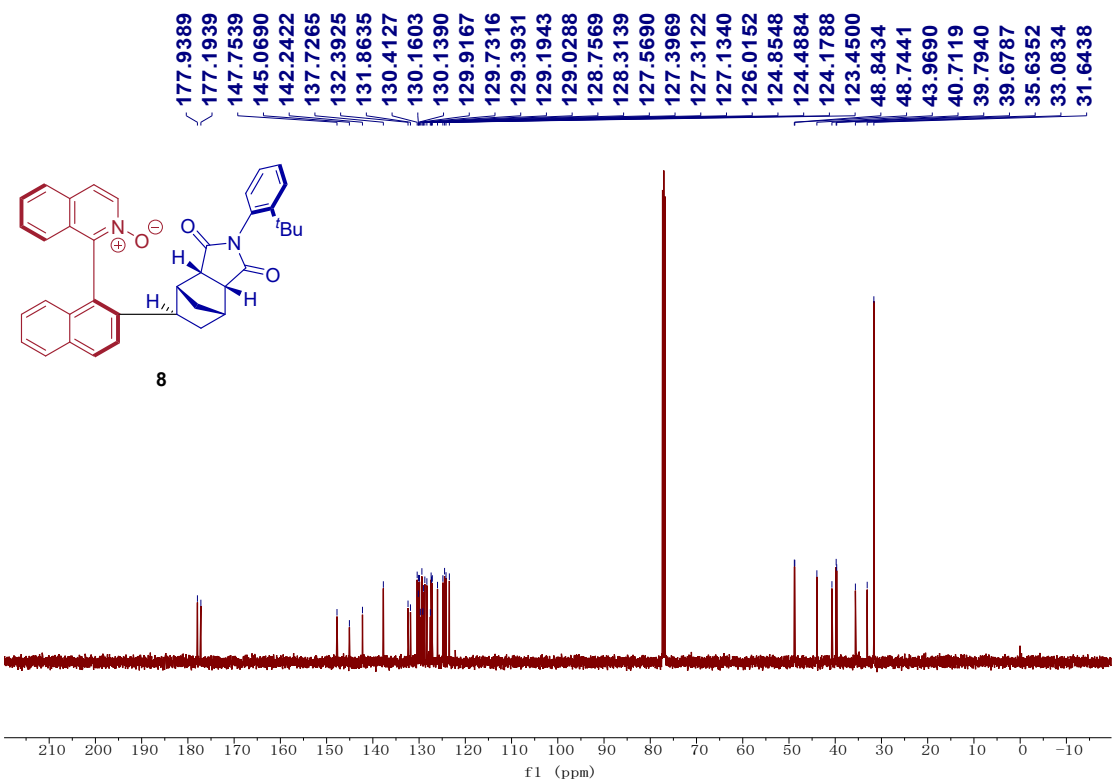
7.5155
7.4720
7.4420
7.4084
7.3480
7.3180
7.3023
7.2022
7.1721
7.0540
7.0371
6.9437
6.9267
5.7785
5.7634
3.2121
3.1769
3.1396
3.1307
3.0442
3.0146
2.9613
2.9431
2.3554
2.3072
2.2098
2.1893
1.7399
1.6882
1.2194
tBu
8
1.00 1.02 2.03 1.01 1.00 2.01 1.01 2.01 1.01 1.01 1.00 1.00 1.03
2.01 1.00 1.01 1.00 1.03 1.00 2.03 9.00
f1 (ppm)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129.3931
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127.3969
127.3122
127.1340
126.0152
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124.4884
124.1788
123.4500
48.8434
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39.6787
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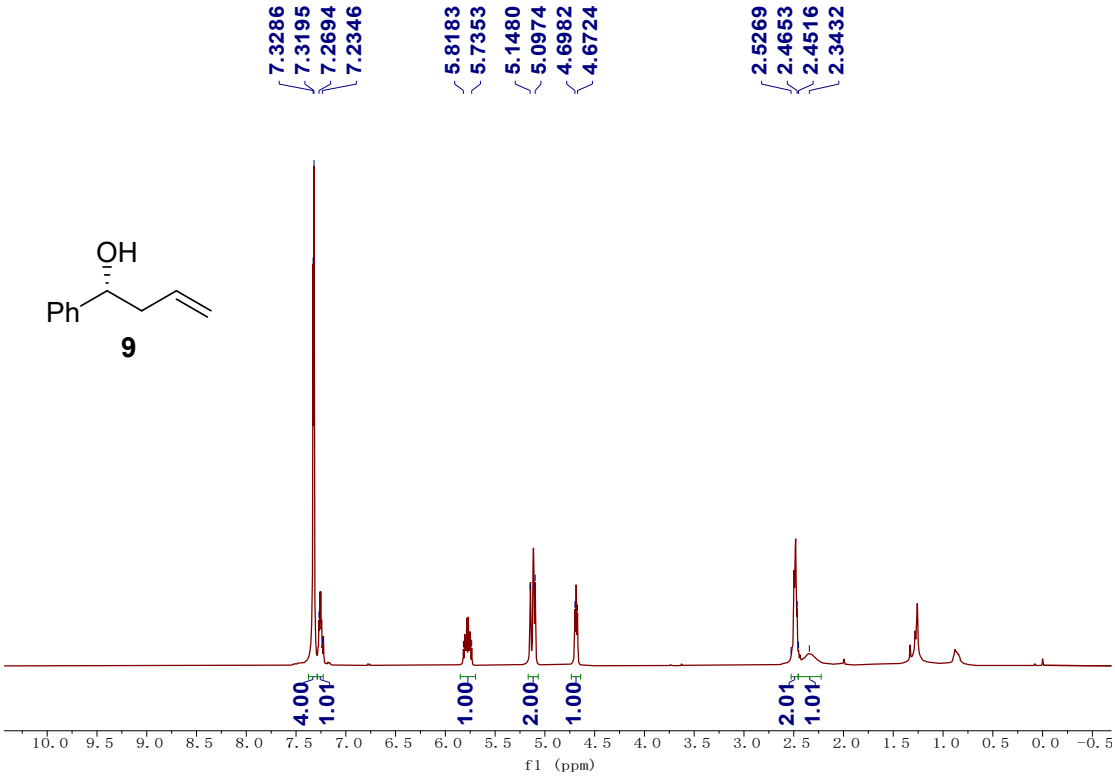
tBu
8
f1 (ppm)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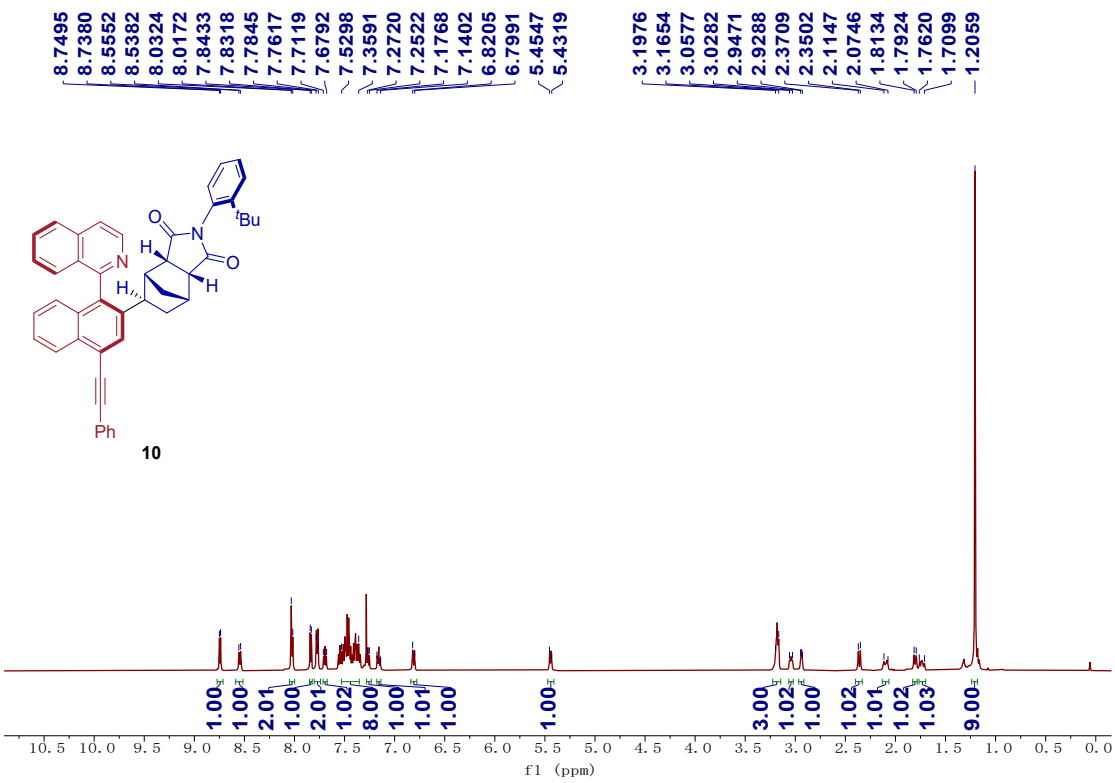
4.6982
4.6724
2.5269
2.4653
2.4516
2.3432
OH
Ph
9
4.00
1.01
1.00
2.00
1.00
2.01
1.01
f1 (ppm)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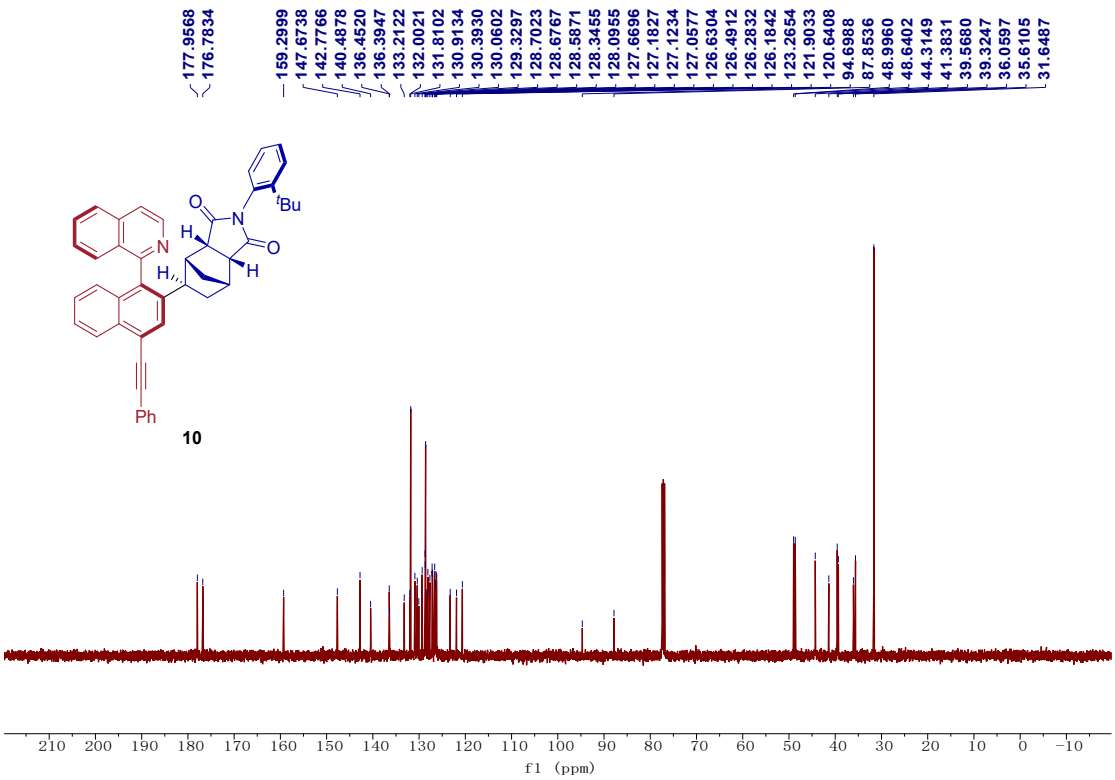
7.6792
7.5298
7.3591
7.2720
7.2522
7.1768
7.1402
6.8205
6.7991
5.4547
5.4319
3.1976
3.1654
3.0577
3.0282
2.9471
2.9288
2.3709
2.3502
2.1147
2.0746
1.8134
1.7924
1.7620
1.7099
1.2059
tBu
Ph
10
1.00
1.00
2.01
1.00
2.01
1.02
8.00
1.00
1.01
1.00
1.00
3.00
1.02
1.00
1.02
1.01
1.02
1.03
9.00
f1 (ppm)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130.9134
130.3930
130.0602
129.3297
128.7023
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128.3455
128.0955
127.6696
127.1827
127.1234
127.0577
126.6304
126.4912
126.2832
126.1842
123.2654
121.9033
120.6408
94.6988
87.8536
48.9960
48.6402
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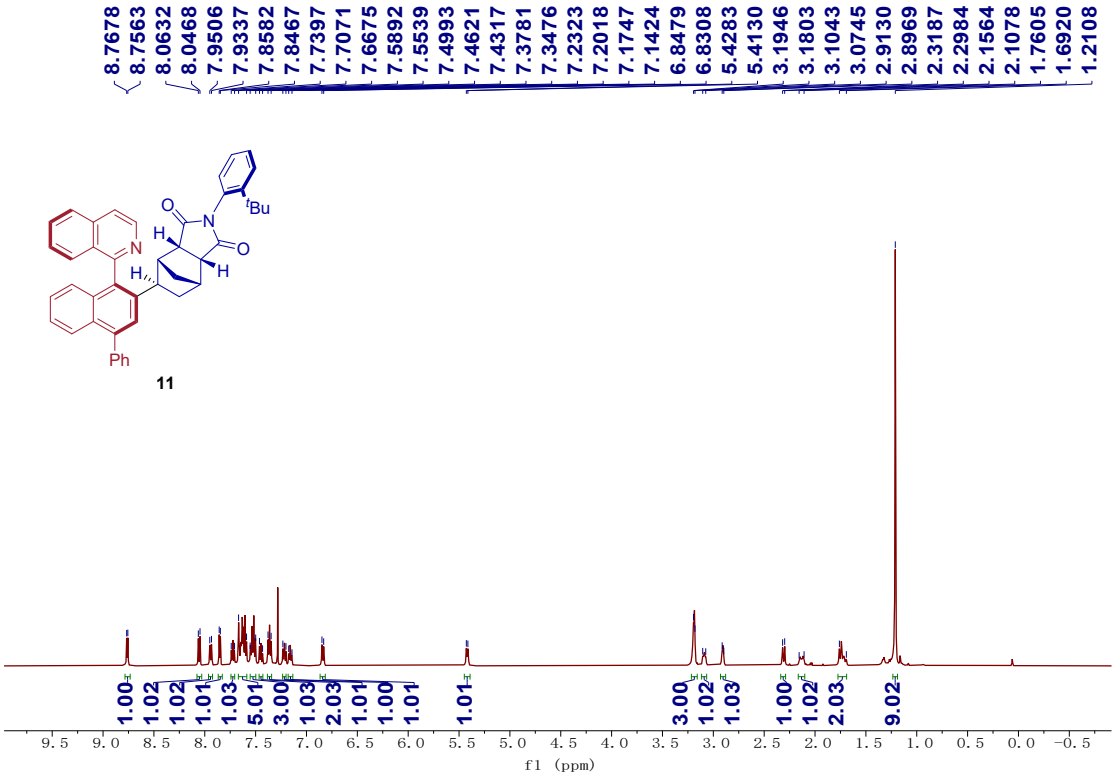
39.5680
39.3247
36.0597
35.6105
31.6487
tBu
Ph
10
f1 (ppm)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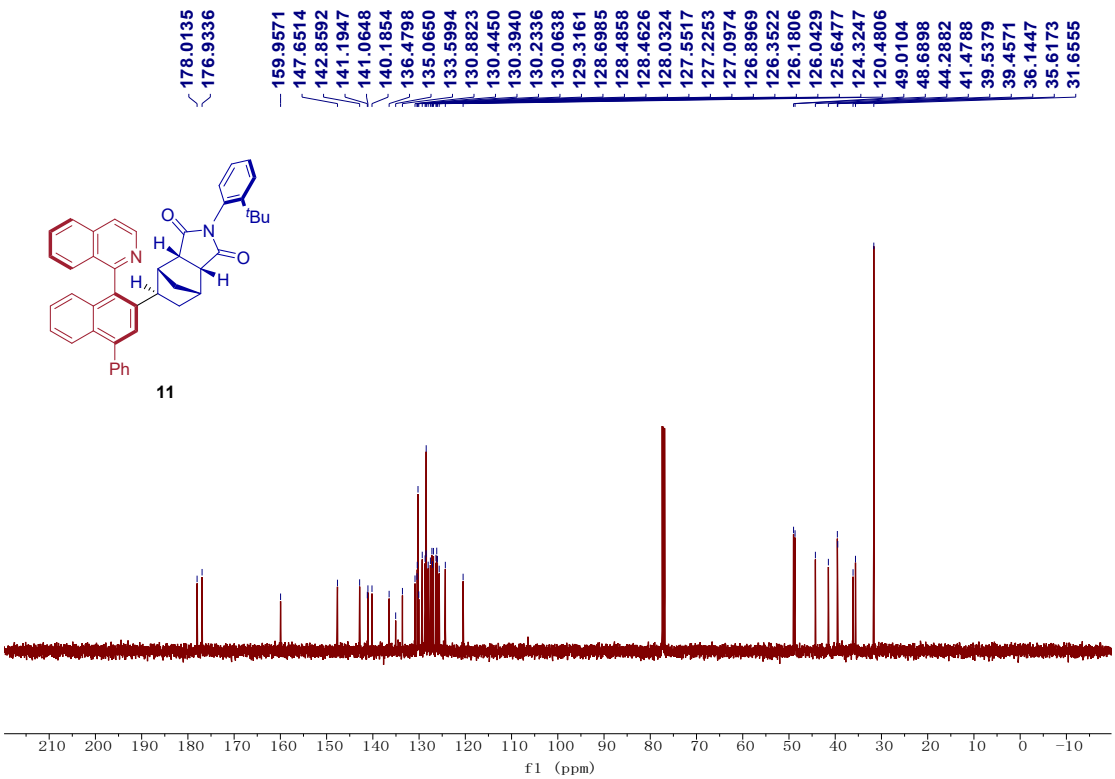
tBu
N
O
H
O
H
H
Ph
11
1.00 1.02 1.02 1.01 1.03 5.01 3.00 1.03 2.03 1.01 1.00 1.01 1.01 3.00 1.02 1.03 1.00 1.02 2.03 9.02
f1 (ppm)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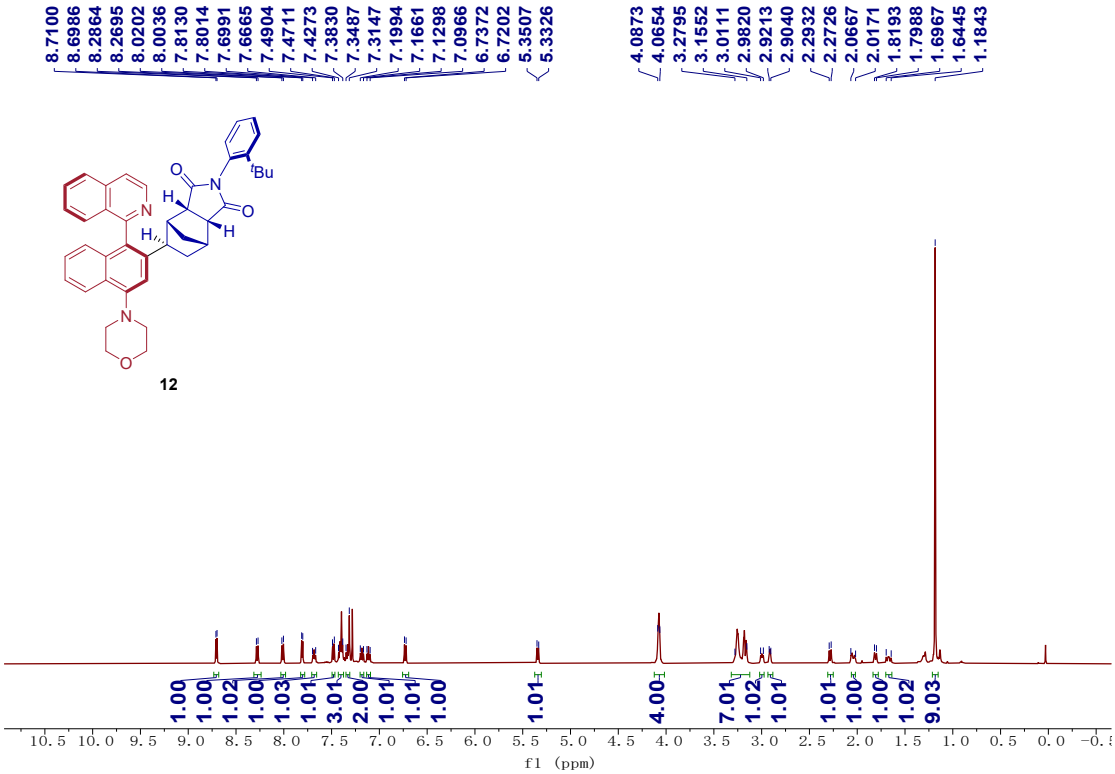
tBu
N
O
H
O
H
H
Ph
11
f1 (ppm)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7.4711
7.4273
7.3830
7.3487
7.3147
7.1994
7.1661
7.1298
7.0966
6.7372
6.7202
5.3507
5.3326
4.0873
4.0654
3.2795
3.1552
3.0111
2.9820
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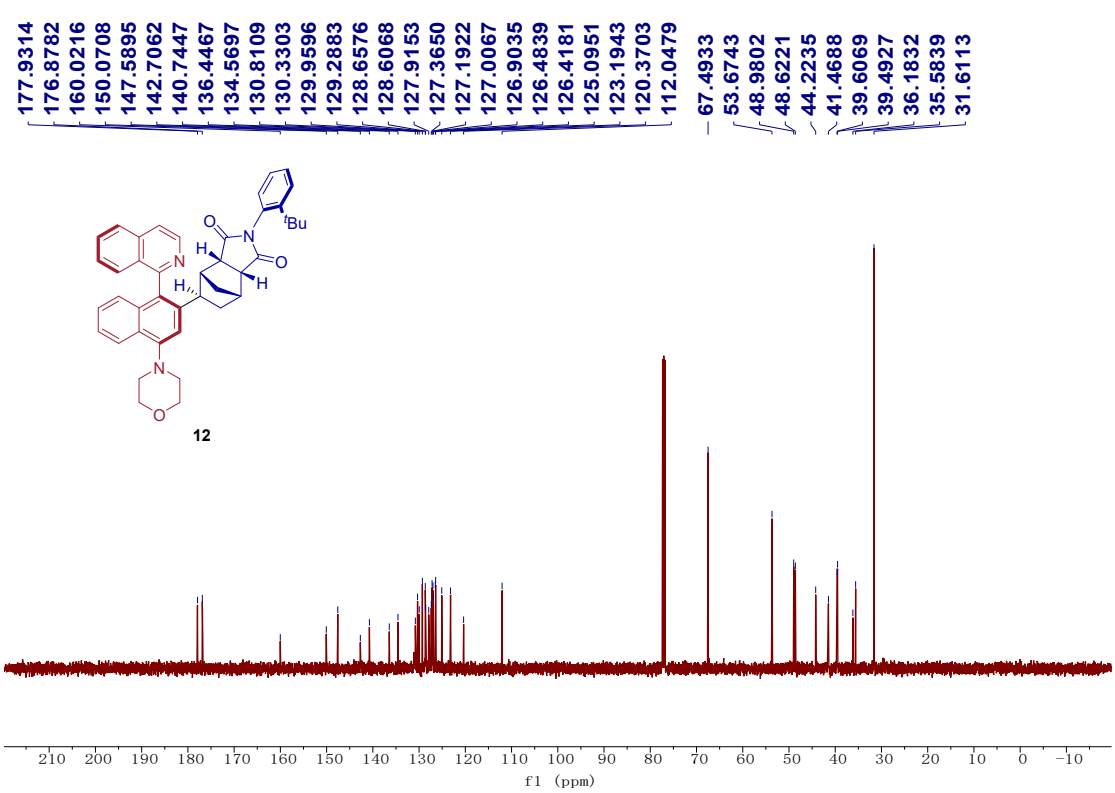
2.2932
2.2726
2.0667
2.0171
1.8193
1.7988
1.6967
1.6445
1.1843
tBu
12
1.00
1.00
1.02
1.00
1.03
1.01
3.01
2.00
1.01
1.01
1.00
1.01
4.00
7.01
1.02
1.01
1.01
1.00
1.00
1.02
9.03
f1 (ppm)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128.6576
128.6068
127.9153
127.3650
127.1922
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126.4839
126.4181
125.0951
123.1943
120.3703
112.0479
67.4933
53.6743
48.9802
48.6221
44.2235
41.4688
39.6069
39.4927
36.1832
35.5839
31.6113
tBu
12
f1 (ppm)