Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Iron-Catalyzed Stereoselective Haloamidation of Amide-tethered Alkynes

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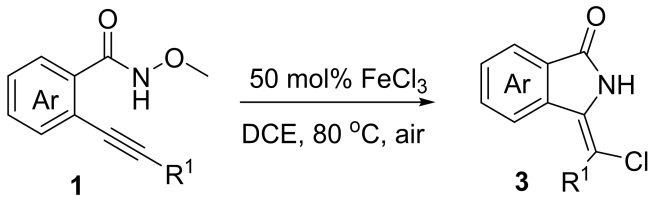
1. General information

The UV–Vis spectra were recorded on an Ultraviolet spectrophotometer (UV-2550). Emission spectra were performed on a Fluorescence spectrometer (F-4600). Error limits were estimated: λ (±1 nm); τ (±10%); φ (±10%). The solvents were distilled from standard drying agents. Unless otherwise stated, commercial reagents purchased from Alfa Aesar, Acros and Aldrich chemical companies were used without further purification. Purification of reaction products was carried out by flash chromatography using Qing Dao Sea Chemical Reagent silica gel (200–300 mesh). ^{1}H NMR spectra were recorded on a Bruker Avance III 400 (400 MHz) spectrometer and referenced internally to the residual proton resonance in $CDCl_3$ (δ = 7.26 ppm), or with tetramethylsilane (TMS, δ = 0.00 ppm) as the internal standard. Chemical shifts were reported as parts per million (ppm) in the δ scale downfield from TMS. Multiplicity is indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), m (multiplet), dd (doublet of doublet), bs (broad singlet). ^{13}C NMR spectra were recorded on Bruker spectrometer with complete proton decoupling, and chemical shifts were reported in ppm from TMS with the solvent as the internal reference ($CDCl_3$, δ = 77.0 ppm).

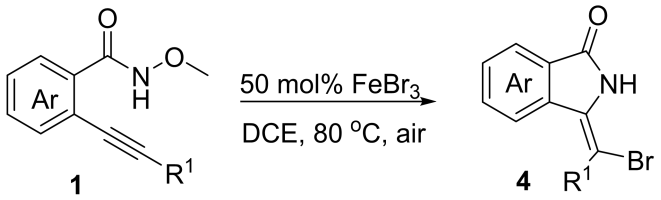
2. General procedure

(a) Synthesis of compounds 2:



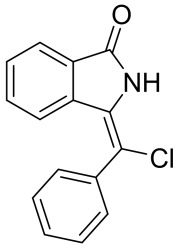
N-methoxy-2-(phenylethynyl)benzamide **1** (0.2 mmol), $FeCl_3$ (50 mol%) were added to a test tube, the solvent DCE was added. The mixture was stirred at 80 ºC for 6 h. After the disappearance of substrate as indicated by TLC, the mixture was filtrated, Evaporation of the solvent and purification by flash column chromatograph provided the desired products **3**.

(b) Synthesis of compounds 4:

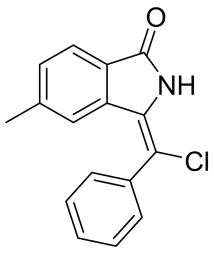


N-methoxy-2-(phenylethynyl)benzamide **1** (0.2 mmol), $FeBr_3$ (50 mol%) were added to a test tube, the solvent DCE was added. The mixture was stirred at 80 °C for 6 h. After the disappearance of substrate as indicated by TLC, the mixture was filtrated, Evaporation of the solvent and purification by flash column chromatograph provided the desired products **4**.

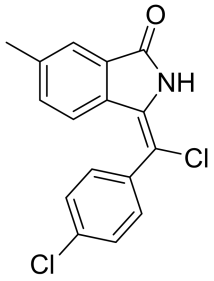
3. Characterization data



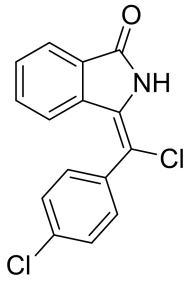
(*Z*)-3-(chloro(phenyl)methylene)isoindolin-1-one (3a): Following the general procedure, the reaction of *N*-methoxy-2-(phenylethynyl)benzamide (50.2 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3a** 50.0 mg (98% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.85 (d, *J* = 7.4 Hz, 1H), 7.53 – 7.50 (m, 5H), 7.43 – 7.39 (m, 1H), 7.30 – 7.26 (m, 1H), 6.75 (d, *J* = 7.7 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.3, 135.9, 135.1, 132.1, 131.7, 130.7, 130.1, 130.0, 129.2, 129.1, 123.8, 122.6, 113.5; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{11}ClNO^+$ 256.0524; Found: 256.0526.



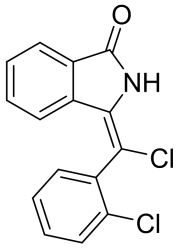
(*Z*)-3-(chloro(phenyl)methylene)-5-methylisoindolin-1-one (3b): Following the general procedure, the reaction of *N*-methoxy-4-methyl-2-(phenylethynyl)benzamide (53.0 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3b** 47.4 mg (88% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.52 (m, 2H), 7.49 – 7.48 (m, 3H), 7.20 (d, *J* = 7.8 Hz, 1H), 6.51 (m, 1H), 2.18 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.5, 142.8, 136.0, 135.5, 131.8, 130.3, 130.1, 129.9, 129.0, 128.2, 123.6, 123.0, 113.1, 22.1; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{13}ClNO^+$ 270.0680; Found: 270.0641.



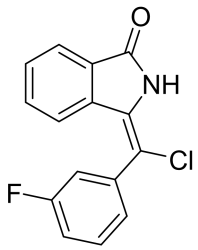
(*Z*)-3-(chloro(4-chlorophenyl)methylene)-6-methylisoindolin-1-one (3c): Following the general procedure, the reaction of (*Z*)-3-(chloro(4-chlorophenyl)methylene)-6-methylisoindolin-1-one (59.8 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3c** 55.1 mg (91% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 7.65 (m, 1H), 7.49 – 7.44 (m, 4H), 7.12 (d, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 8.1 Hz, 1H), 2.39 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.5, 140.0, 135.8, 134.6, 133.2, 132.4, 132.3, 131.5, 131.0, 129.3, 124.1, 122.2, 111.0, 21.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{12}Cl_2NO^+$ 304.0290; Found: 304.0318.



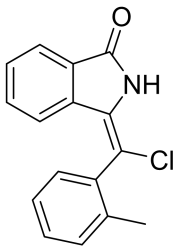
(*Z*)-3-(chloro(4-chlorophenyl)methylene)isoindolin-1-one(3d): Following the general procedure, the reaction of 2-((4-chlorophenyl)ethynyl)-*N*-methoxybenzamide (57.0 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3c** 52.0 mg (90% yield) as white solid;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.85 (d, *J* = 7.4 Hz, 1H), 7.48 – 7.42 (m, 5H), 7.35 – 7.31 (m, 1H), 6.81 (d, *J* = 7.9 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 167.0, 136.1, 134.8, 134.3, 132.3, 132.1, 131.5, 130.7, 130.6, 129.5, 124.0, 122.5, 105.0; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{10}Cl_2NO^+$ 290.0134; Found: 290.0152.



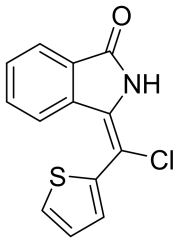
(Z)-3-(chloro(2-chlorophenyl)methylene)isoindolin-1-one (3e): Following the general procedure, the reaction of 2-((2-chlorophenyl)ethynyl)-*N*-methoxybenzamide (57.0 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3e** 50.9 mg (88% yield) as white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (s, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.43 – 7.41 (m, 1H), 7.40 – 7.38 (m, 1H), 7.30 – 7.26 (m, 1H), 6.35 (d, *J* = 7.9 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 167.7, 134.9, 133.5, 132.5, 131.4, 130.6, 129.4, 127.7, 123.9, 122.2, 109.6; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{10}Cl_2NO^+$ 290.0134; Found: 290.0173.



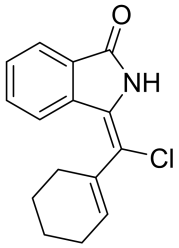
(*Z*)-3-(chloro(3-fluorophenyl)methylene)isoindolin-1-one (3f): Following the general procedure, the reaction of 2-((3-fluorophenyl)ethynyl)-*N*-methoxybenzamide (53.8 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3f** 44.8 mg (82% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.83 (s, 1H), 7.86 (d, J = 7.6 Hz, 1H), 7.49 – 7.41 (m, 2H), 7.34 – 7.29 (m, 2H), 7.27 – 7.23 (m, 1H), 7.22 – 7.18 (m, 1H), 6.78 (d, J = 7.9 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.6, 163.5 (J_{CF} = 247 Hz), 137.9 (J_{CF} = 9 Hz), 134.8, 132.4, 132.3, 130.8 (J_{CF} = 8 Hz), 129.5, 126.0, 124.0, 122.5, 117.2 (J_{CF} = 14 Hz), 117.1 (J_{CF} = 13 Hz), 111.7, 105.0; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{10}ClFNO^+$ 274.0429; Found: 274.0461.



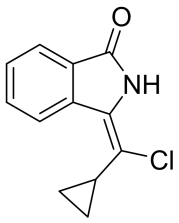
(Z)-3-(chloro(o-tolyl)methylene)isoindolin-1-one (3g): Following the general procedure, the reaction of *N*-methoxy-2-(*o*-tolylethynyl)benzamide (53.0 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3g** 45.7 mg (85% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.85 (d, J = 7.6 Hz, 1H), 7.44 – 7.29 (m, 6H), 7.27 – 7.23 (m, 1H), 2.31 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.4, 138.0, 135.1, 135.0, 132.4, 132.2, 130.9, 130.5, 130.2, 129.1, 126.8, 123.8, 122.2, 112.4, 105.0, 19.3; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{13}ClNO^+$ 270.0680; Found: 270.0662.



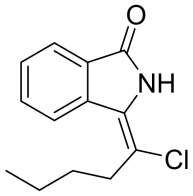
(*Z*)-3-(chloro(thiophen-2-yl)methylene)isoindolin-1-one (3h): Following the general procedure, the reaction of *N*-methoxy-2-(thiophen-2-ylethynyl)benzamide (51.4 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3h** 32.4 mg (62% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.26 (m, 1H), 7.70 – 7.67 (m, 1H), 7.59 (d, *J* = 3.6 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.39 (d, *J* = 5.0 Hz, 1H), 7.11 – 7.09 (m, 1H), 6.77 (m, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 161.7, 149.5, 137.4, 135.7, 134.9, 129.8, 128.1, 128.0, 127.4, 126.2, 125.7, 120.3, 100.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_9ClNOS^+$ 262.0088; Found: 262.0077.



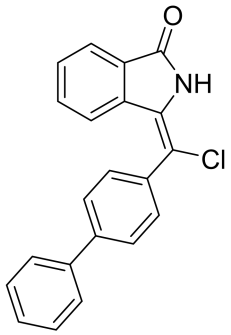
(*Z*)-3-(chloro(cyclohex-1-en-1-yl)methylene)isoindolin-1-one (3i): Following the general procedure, the reaction of 2-(cyclohex-2-en-1-ylethynyl)-*N*-methoxybenzamide (51.0 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3i** 36.3 mg (70% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.86 (d, *J* = 7.3 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.54 – 7.44 (m, 2H), 6.14 (m, 1H), 2.31 (s, 2H), 2.25 – 2.24 (m, 2H), 1.84 – 1.74 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 166.9, 135.6, 133.5, 133.5, 132.2, 130.7, 129.9, 128.9, 123.8, 122.6, 117.9, 26.7, 25.7, 22.4, 21.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{15}ClNO^+$ 260.0837; Found: 260.0847.



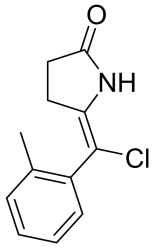
(*Z*)-3-(chloro(cyclopropyl)methylene)isoindolin-1-one (3j): Following the general procedure, the reaction of 2-(cyclopropylethynyl)-*N*-methoxybenzamide (43.0 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3j** 40.3 mg (92% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 7.5 Hz, 1H) 7.62 – 7.58 (m, 1H), 7.50 – 7.47 (m, 1H), 2.27 – 2.23 (m, 1H), 1.09 – 1.06 (m, 2H), 1.01 – 1.00 (m, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 166.8, 134.9, 132.3, 131.7, 130.8, 128.8, 124.1, 123.2, 119.4, 14.8, 8.9; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{12}H_{11}ClNO^+$ 220.0524; Found: 220.0481.



(*Z*)-3-(1-chloropentylidene)isoindolin-1-one (3k): Following the general procedure, the reaction of 2-(hex-1-yn-1-yl)-*N*-methoxybenzamide (46.2 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3k** 40.9 mg (87% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.62 – 7.58 (m, 1H), 7.50 – 7.46 (m, 1H), 2.91 – 2.87 (m, 2H), 1.76 – 1.68 (m, 2H), 1.50 – 1.41 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 166.7, 134.9, 132.4, 131.0, 130.5, 128.8, 124.2, 122.5, 119.0, 34.7, 30.0, 22.1, 13.9; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_{15}ClNO^+$ 236.0837; Found: 236.0861.

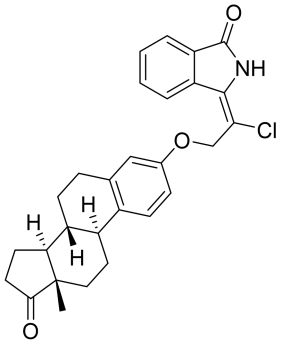


(*Z*)-3-([1,1'-biphenyl]-4-ylchloromethylene)isoindolin-1-one (3l): Following the general procedure, the reaction of 2-([1,1'-biphenyl]-4-ylethynyl)-*N*-methoxybenzamide (65.4 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 8/1) to give **3l** 60.9 mg (92% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 2H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.45 – 7.39 (m, 2H), 7.34 – 7.30 (m, 1H), 6.94 (d, *J* = 7.9 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.2, 142.7, 139.9, 135.1, 134.7, 132.2, 131.7, 130.7, 130.6, 129.3, 129.0, 128.0, 127.6, 127.1, 123,9, 122.7, 113.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{15}ClNO^+$ 332.00837; Found: 332.0864.

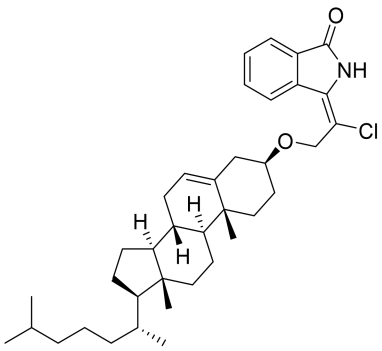


(*Z*)-5-(chloro(o-tolyl)methylene)pyrrolidin-2-one (3m): Following the general procedure, the reaction of *N*-methoxy-5-(*o*-tolyl)pent-4-ynamide (43.4 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **3m** 30.9 mg (70% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.22 – 7.17 (m, 2H), 2.57 (s, 3H), 2.29 – 2.27 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 176.5, 137.9, 137.6,

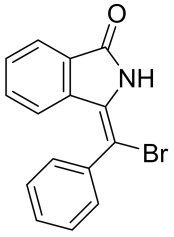
136.2, 130.5, 130.1, 129.1, 126.2, 91.4, 30.7, 24.4, 19.4; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{12}H_{13}ClNO^+$ 222.0680; Found: 222.0671.



(*Z*)-3-(1-chloro-2-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)ethylidene)isoindolin-1-one (3n): Following the general procedure, the reaction of *N*-methoxy-2-(3-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)prop-1-yn-1-yl)benzamide (91.4 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 ^oC for 6 h. The product was purified by flash chromatography (PE/EA = 5/1) to give **3n** 66.4 mg (72% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.84 (d, *J* = 7.4 Hz, 1H), 7.42 – 7.38 (m, 2H), 7.33 – 7.28 (m, 3H), 6.92 (d, *J* = 7.8 Hz, 1H), 2.95 (d, *J* = 4.7 Hz, 2H), 2.56 – 2.37 (m, 3H), 2.21 – 1.99 (m, 4H), 1.70 – 1.49 (m, 6H), 1.32 – 1.24 (m, 2H), 0.95 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 220.6, 167.2, 141.9, 137.4, 135.2, 133.3, 132.0, 131.4, 130.7, 130.4, 129.1, 127.3, 126.0, 123.8, 122.6, 114.0, 50.5, 48.0, 44.5, 37.9, 35.8, 31.5, 30.1, 29.2, 26.4, 25.6, 21.6, 13.9; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{28}H_{29}ClNO_3^+$ 462.1830; Found: 462.1862.

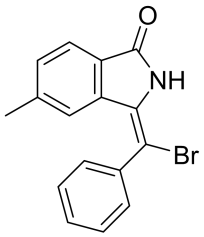


(Z)-**3-(1-chloro-2-(((3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methyl heptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a] phenanthren-3-yl)oxy)ethylidene)isoindolin-1-one (3o):** Following the general procedure, the reaction of *N*-methoxy-2-(3-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-dec ahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)prop-1-yn-1-yl)benzamide (91.4 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 5/1) to give **3o** 80.8 mg (70% yield) as white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.36 – 8.20 (m, 1H), 7.88 – 7.78 (m, 2H), 7.64 – 7.60 (m, 1H), 7.53 – 7.49 (m, 1H), 5.34 (s, 1H), 4.68 (s, 1H), 3.38 (s, 1H), 2.43 – 2.29 (m, 8.6 Hz, 2H), 2.00 – 1.94 (m, 2H), 1.88 – 1.80 (m, 2H), 1.58 – 1.41 (m, 6H), 1.32 – 1.24 (m, 6H), 1.10 – 1.05 (m, 6H), 1.15 – 1.03 (m, 6H), 0.99 (s, 6H), 0.90 – 0.89 (m, 4H), 0.86 – 0.84 (m, 6H), 0.66 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.1, 140.4, 140.0, 134.4, 132.7, 132.3, 129.5, 124.2, 123.4, 122.0, 113.2, 78.9, 67.9, 56.7, 56.1, 50.1, 42.3, 39.7, 39.5, 39.0, 37.2, 36.8, 36.2, 35.8, 31.9, 31.8, 28.2, 28.0, 24.3, 23.8, 22.8, 22.6, 21.1, 19.4, 18.7, 11.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{37}H_{53}ClNO_2^+$ 578.3759; Found: 578.3788.

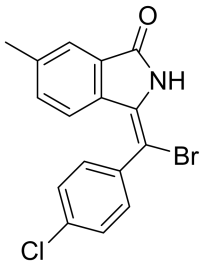


(*Z*)-3-(bromo(phenyl)methylene)isoindolin-1-one (4a): Following the general procedure, the reaction of *N*-methoxy-2-(phenylethynyl)benzamide (50.2 mg, 0.2

mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4a** 52.8 mg (88% yield) as white solid; ^1H NMR (400 MHz, DMSO-d_6) δ 10.59 (s, 1H), 7.70 (d, J = 7.5 Hz, 1H), 7.50 – 7.42 (m, 6H), 7.33 – 7.29 (m, 1H), 6.39 (d, J = 7.9 Hz, 1H); $^{13}C\{^1H\}$NMR (100 MHz, DMSO-d_6) δ 167.7, 138.5, 135.4, 134.8, 132.6, 131.2, 130.4, 130.2, 129.9, 129.7, 123.6, 122.7, 102.5; HRMS (ESI-TOF) m/z: [M + H]+ Calcd for C15H11BrNO 300.0019; Found: 300.0036.

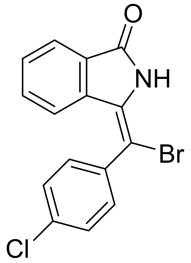


(*Z*)-3-(bromo(phenyl)methylene)-5-methylisoindolin-1-one (4b): Following the general procedure, the reaction of *N*-methoxy-4-methyl-2-(phenylethynyl)benzamide (53.1 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4b** 52.7 mg (84% yield) as white solid; ^1H NMR (400 MHz, DMSO-d_6) δ 10.48 (s, 1H), 7.58 (d, J = 7.8 Hz, 1H), 7.53 – 7.46 (m, 5H), 7.27 (d, J = 7.8 Hz, 1H), 6.14 (m, 1H), 2.06 (s, 3H); $^{13}C\{^1H\}$NMR (100 MHz, DMSO-d_6) δ 167.7, 142.6, 138.6, 135.9, 134.8, 130.7, 130.4, 130.2, 129.7, 128.9, 123.4, 123.1, 102.1, 22.0; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{12}NONaBr$ 336.0005; Found: 336.0000.

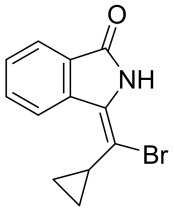


(*Z*)-3-(bromo(4-chlorophenyl)methylene)-6-methylisoindolin-1-one (4c): Following the general procedure, the reaction of 2-((4-chlorophenyl)ethynyl)-*N*-methoxy-5-methylbenzamide (60.0 mg, 0.2 mmol),

$FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4c** 53.7 mg (77% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.54 (s, 1H), 7.55 (d, J = 8.3 Hz, 2H), 7.50 – 7.48 (m, 3H), 7.17 (d, J = 8.1 Hz, 1H), 6.37 (d, J = 8.1 Hz, 1H), 2.29 (s, 3H); ^{13}C{^{1}H}NMR (100 MHz, DMSO-d_6) δ 167.8, 140.2, 137.5, 135.3, 134.8, 133.7, 132.9, 132.4, 131.5, 129.8, 123.7, 122.5, 99.8, 21.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{11}NONaClBr$ 369.9604; Found: 369.9610.

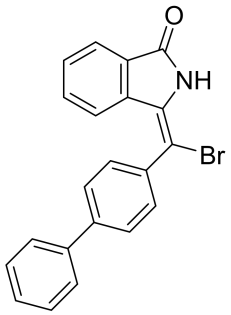


(*Z*)-3-(bromo(4-chlorophenyl)methylene)isoindolin-1-one (4d): Following the general procedure, the reaction of 2-((4-chlorophenyl)ethynyl)-*N*-methoxybenzamide (57.1 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4d** 50.8 mg (76% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.68 (s, 1H), 7.70 (d, J = 7.4 Hz, 1H), 7.58 – 7.51 (m, 4H), 7.50 – 7.45 (m, 1H), 7.40 – 7.37 (m, 1H), 6.48 (d, J = 7.8 Hz, 1H); ^{13}C{^{1}H}NMR (100 MHz, DMSO-d_6) δ 167.7, 137.4, 135.3, 135.2, 134.8, 132.9, 132.4, 131.2, 130.1, 129.9, 123.7, 122.7, 100.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_9NONaClBr$ 355.9453; Found: 355.9454.

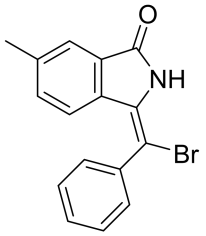


(*Z*)-3-(bromo(cyclopropyl)methylene)isoindolin-1-one (4e): Following the general procedure, the reaction of 2-(cyclopropylethynyl)-*N*-methoxybenzamide (43.1 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4e** 41.2 mg (78% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.25 (s, 1H), 8.11 (d, J = 7.9 Hz,

1H), 7.75 – 7.72 (m, 1H), 7.70 – 7.66 (m, 1H), 7.59 – 7.54 (m, 1H), 2.38 – 2.34 (m, 1H), 1.16 – 1.11 (m, 2H), 0.82 – 0.78 (m, 2H); $^{13}C\{^{1}H\}$NMR (100 MHz, DMSO-d_6) δ 167.2, 135.1, 135.0, 133.0, 131.3, 129.6, 124.4, 123.7, 112.1, 16.9, 11.5; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{12}H_{10}NONaBr$ 285.9843; Found: 285.9843.

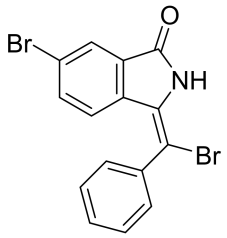


(*Z*)-3-([1,1'-biphenyl]-4-ylbromomethylene)isoindolin-1-one (4f): Following the general procedure, the reaction of 2-([1,1'-biphenyl]-4-ylethynyl)-*N*-methoxybenzamide (65.5 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4f** 57.1 mg (76% yield) as yellow solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.67 (s, 1H), 7.81 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 7.8 Hz, 2H), 7.71 (d, J = 7.5 Hz, 1H), 7.57 (d, J = 8.0 Hz, 2H), 7.50 – 7.44 (m, 3H), 7.40 – 7.33 (m, 2H), 6.60 (d, J = 7.9 Hz, 1H); $^{13}C\{^{1}H\}$NMR (100 MHz, DMSO-d_6) δ 167.7, 141.6, 139.4, 137.5, 135.4, 134.9, 132.8, 131.2, 131.1, 130.0, 129.5, 128.5, 127.8, 127.2, 123.6, 122.8, 102.3; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}NONaBr$ 398.0147; Found: 398.0156.

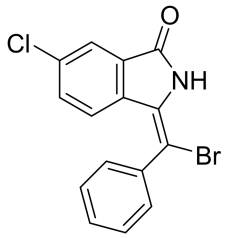


(*Z*)-3-(bromo(phenyl)methylene)-6-methylisoindolin-1-one (4g): Following the general procedure, the reaction of *N*-methoxy-5-methyl-2-(phenylethynyl)benzamide (53.1 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h.

The product was purified by flash chromatography (PE/EA = 10/1) to give **4g** 52.1 mg (83% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.57 (s, 1H), 7.50 – 7.47 (m, 6H), 7.14 (d, J = 8.2 Hz, 1H), 6.27 (d, J = 8.2 Hz, 1H), 2.29 (s, 3H); ^{13}C{^{1}H}NMR (100 MHz, DMSO-d_6) δ 167.8, 140.1, 138.6, 134.8, 133.5, 133.0, 131.5, 130.4, 130.2, 129.7, 123.7, 122.5, 101.5, 21.3; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{16}H_{12}NONaBr$ 335.9999; Found: 336.0000.

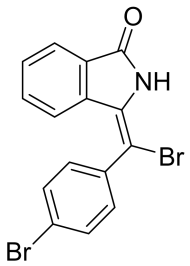


(*Z*)-6-bromo-3-(bromo(phenyl)methylene)isoindolin-1-one (4h): Following the general procedure, the reaction of 5-bromo-*N*-methoxy-2-(phenylethynyl)benzamide (66.0 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4h** 59.1 mg (78% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.68 (s, 1H), 7.75 – 7.69 (m, 3H), 7.51 – 7.46 (m, 3H), 7.43 – 7.39 (m, 1H), 6.51 (d, J = 7.8 Hz, 1H); ^{13}C{^{1}H}NMR (100 MHz, DMSO-d_6) δ 167.7, 137.8, 135.3, 135.2, 132.9, 132.8, 132.6, 131.2, 130.1, 123.7, 123.6, 122.7, 100.9;HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{15}H_9NONaBr_2$ 399.8940; Found: 399.8949.

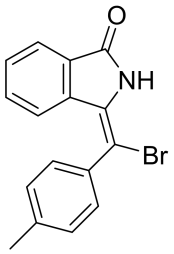


(*Z*)-3-(bromo(phenyl)methylene)-6-chloroisoindolin-1-one (4i): Following the general procedure, the reaction of 5-chloro-*N*-methoxy-2-(phenylethynyl)benzamide (57.1 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4i** 52.8 mg (79% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.85 (s, 1H), 7.73 (s,

1H), 7.52 (m, 6H), 7.45 (d, J = 8.6 Hz, 1H), 6.37 (d, J = 8.7 Hz, 1H); $^{13}C\{^{1}H\}$NMR (100 MHz, DMSO-d_6) δ 166.4, 138.2, 134.6, 134.0, 134.0, 133.1, 132.7, 130.4, 130.3, 129.8, 124.4, 123.4, 103.6;HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_9NONaClBr$ 355.9445; Found: 355.9454.

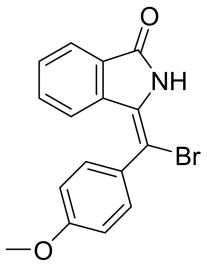


(*Z*)-3-(bromo(4-bromophenyl)methylene)isoindolin-1-one (4j): Following the general procedure, the reaction of 2-((4-bromophenyl)ethynyl)-*N*-methoxybenzamide (66.0 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4j** 57.6 mg (76% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.68 (s, 1H), 7.74 – 7.71 (m, 3H), 7.51 – 7.46 (m, 3H), 7.44 – 7.40 (m, 1H), 6.51 (d, J = 7.8 Hz, 1H); $^{13}C\{^{1}H\}$NMR (100 MHz, DMSO-d_6) δ 167.7, 137.7, 135.3, 135.2, 132.9, 132.8, 132.6, 131.2, 130.1, 123.7, 123.6, 122.7, 100.9; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_9NONaBr_2$ 399.8942; Found: 399.8949.

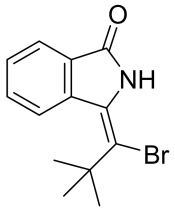


(*Z*)-3-(bromo(p-tolyl)methylene)isoindolin-1-one (4k): Following the general procedure, the reaction of *N*-methoxy-2-(p-tolylethynyl)benzamide (53.1 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4k** 52.7 mg (84% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.55 (s, 1H), 7.56 (d, J = 2.1 Hz,

1H), 7.55 – 7.54 (m, 1H), 7.51 – 7.48 (m, 4H), 7.17 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.37 (d, J = 8.1 Hz, 1H), 2.29 (s, 3H); $^{13}C\{^{1}H\}$NMR (100 MHz, DMSO-d_6) δ 167.7, 139.9, 135.6, 135.5, 134.6, 132.7, 131.2, 130.3, 130.3, 129.9, 123.6, 122.7, 103.0, 21.5;HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{12}NONaBr$ 336.0002; Found:336.0000.

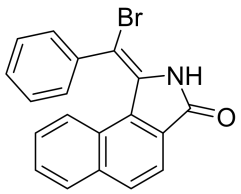


(*Z*)-3-(bromo(4-methoxyphenyl)methylene)isoindolin-1-one (4l): Following the general procedure, the reaction of *N*-methoxy-2-((4-methoxyphenyl)ethynyl)benzamide (56.2 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 ºC for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4l** 52.8 mg (80% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.59 (s, 1H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.47 – 7.35 (m, 4H), 7.06 – 7.04 (m, 2H), 6.51 (d, *J* = 7.9 Hz, 1H), 3.81 (s, 3H); $^{13}C\{^{1}H\}$NMR (100 MHz, DMSO-d_6) δ 167.7, 160.5, 135.6, 134.5, 132.7, 131.9, 131.2, 130.5, 129.8, 123.6, 122.7, 115.1, 103.2, 55.8;HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{12}NO_2NaBr$ 351.9945; Found: 351.9949.

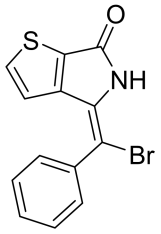


(*Z*)-3-(1-bromo-2,2-dimethylpropylidene)isoindolin-1-one (4m): Following the general procedure, the reaction of 2-(3,3-dimethylbut-1-yn-1-yl)-*N*-methoxybenzamide (46.2 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 ºC for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4m** 56.0 mg (82% yield) as white solid;

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.89 (s, 1H), 8.03 (d, J = 8.1 Hz, 1H), 7.75 – 7.70 (m, 2H), 7.59 – 7.56 (m, 1H), 1.49 (s, 9H); ^{13}C{^{1}H}NMR (100 MHz, DMSO-d_6) δ 166.6, 134.0, 133.6, 132.5, 132.4, 129.4, 127.3, 123.9, 123.2, 37.6, 31.8;HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_{14}NONaBr$ 302.0153; Found: 302.0156.

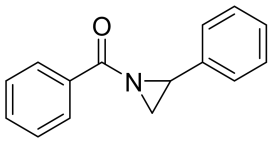


(*Z*)-1-(bromo(phenyl)methylene)-1,2-dihydro-3H-benzo[e]isoindol-3-one (4n): Following the general procedure, the reaction of *N*-methoxy-1-(phenylethynyl)-2-naphthamide (60.2 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4n** 39.2 mg (56% yield) as yellow solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.40 (s, 1H), 8.09 (d, J = 8.3 Hz, 1H), 7.94 (d, J = 8.3 Hz, 1H), 7.74 (d, J = 8.3 Hz, 1H), 7.44 – 7.33 (m, 6H), 6.87 – 6.83 (m, 1H), 6.74 (d, J = 8.7 Hz, 1H); ^{13}C{^{1}H}NMR (100 MHz, DMSO-d_6) δ 167.8, 140.2, 136.5, 136.4, 133.3, 132.7, 131.4, 131.3, 130.1, 129.7, 129.6, 127.5, 126.7, 126.1, 126.0, 119.5, 107.7;HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{12}NONaBr$ 371.9996; Found: 372.0000.

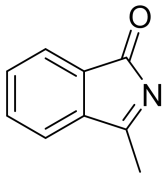


(*Z*)-4-(bromo(phenyl)methylene)-4,5-dihydro-6H-thieno[2,3-c]pyrrol-6-one (4o): Following the general procedure, the reaction of *N*-methoxy-3-(phenylethynyl)thiophene-2-carboxamide (51.4 mg, 0.2 mmol), $FeBr_3$ (29.6 mg, 50 mol %) in DCE was stirred at 80 °C for 6 h. The product was purified by flash chromatography (PE/EA = 10/1) to give **4o** 46.5 mg (76% yield) as white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.45 (s, 1H), 7.79 – 7.77 (m, 1H), 7.49 (m, 5H),

6.00 – 5.98 (m, 1H); $^{13}C\{^{1}H\}$NMR (100 MHz, DMSO-d_6) δ 163.2, 146.5, 138.1, 137.3, 135.2, 133.2, 130.4, 130.2, 129.3, 121.0, 103.4;HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_8NONaSBr$ 327.9404; Found: 327.9408.



phenyl(2-phenylaziridin-1-yl)methanone (6, Scheme 3): Following the general procedure, the reaction of *N*-methoxybenzamide (30.0 mg, 0.2 mmol), styrene (0.14 ml, 0.12 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 130 °C under nitrogen condition refluxed for 8 h. The product was purified by flash chromatography (PE/EA = 8/1) to give product **6** 32.1 mg (72% yield) as yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.50 (m, 1H), 7.45 (m, 3H), 7.37 (m, 4H), 5.66 (m, 1H), 4.49 (dd, *J* = 14.8, 10.2 Hz, 1H), 4.00 (dd, *J* = 14.8, 7.9 Hz, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 164.0, 141.1, 131.4, 128.8, 128.4, 128.3, 128.3, 127.6, 125.7, 81.0, 29.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{14}NO^+$ 224.1070; Found: 224.1098.



3-**methyl-1H-isoindol-1-one (8, Scheme 3):** Following the general procedure, the reaction of 2-ethyl-*N*-methoxybenzamide (36.0 mg, 0.2 mmol), $FeCl_3$ (16.2 mg, 50 mol%) in DCE was stirred at 130 °C under nitrogen condition refluxed for 8 h. The product was purified by flash chromatography (PE/EA = 10/1) to give product **8** 13.1 mg (45% yield) as white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.7 Hz, 1H), 7.83 – 7.80 (m, 1H), 7.73 – 7.68 (m, 1H), 7.67 – 7.63 (m, 1H), 2.69 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 196.1, 139.8, 135.3, 132.6, 132.5, 129.9, 118.1, 111.0, 27.8;HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_9H_8NO^+$ 146.0600; Found: 146.0626.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 20180425-1

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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/c P21/n Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
2 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

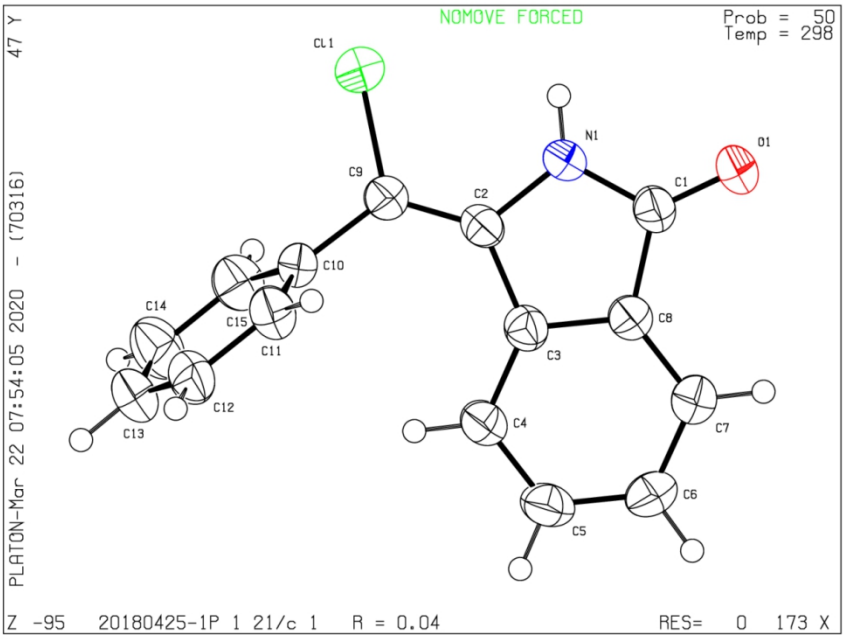
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

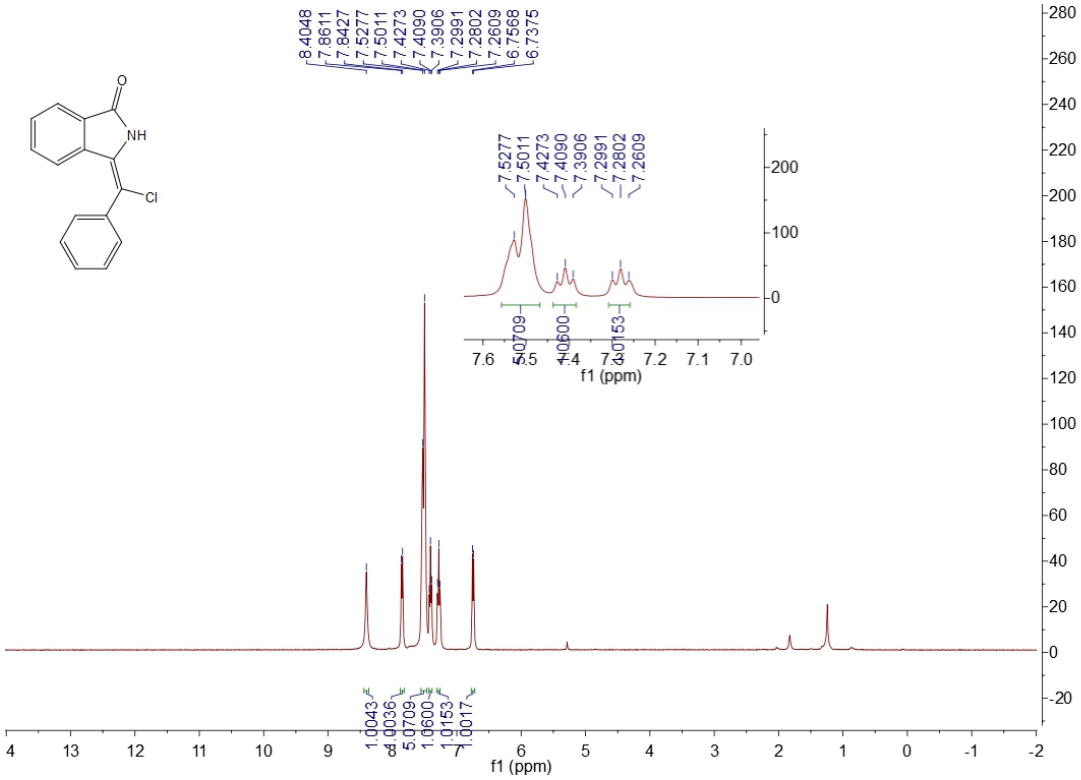
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock 20180425-1 - ellipsoid plot

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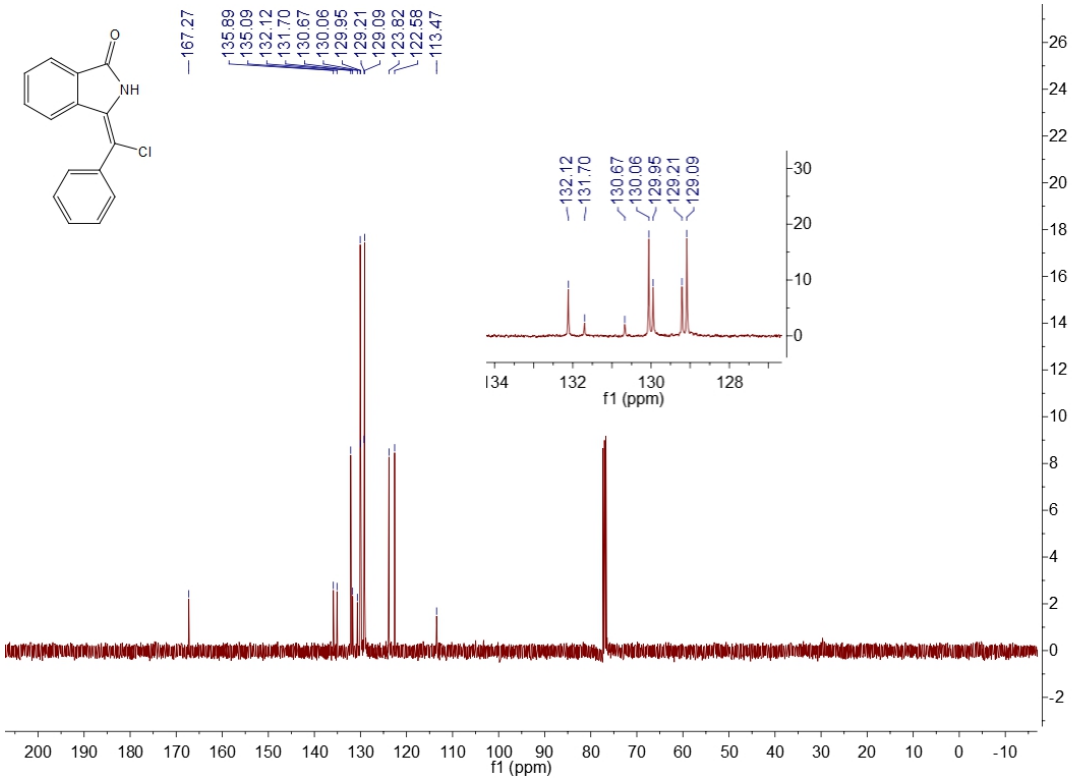
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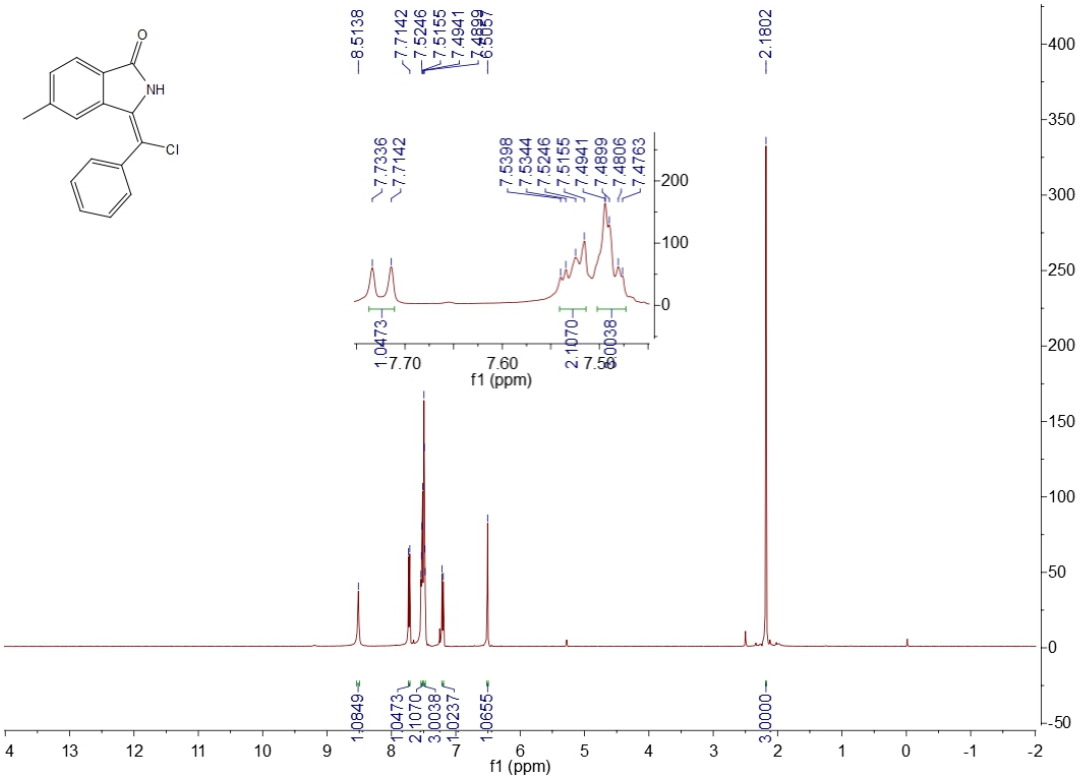
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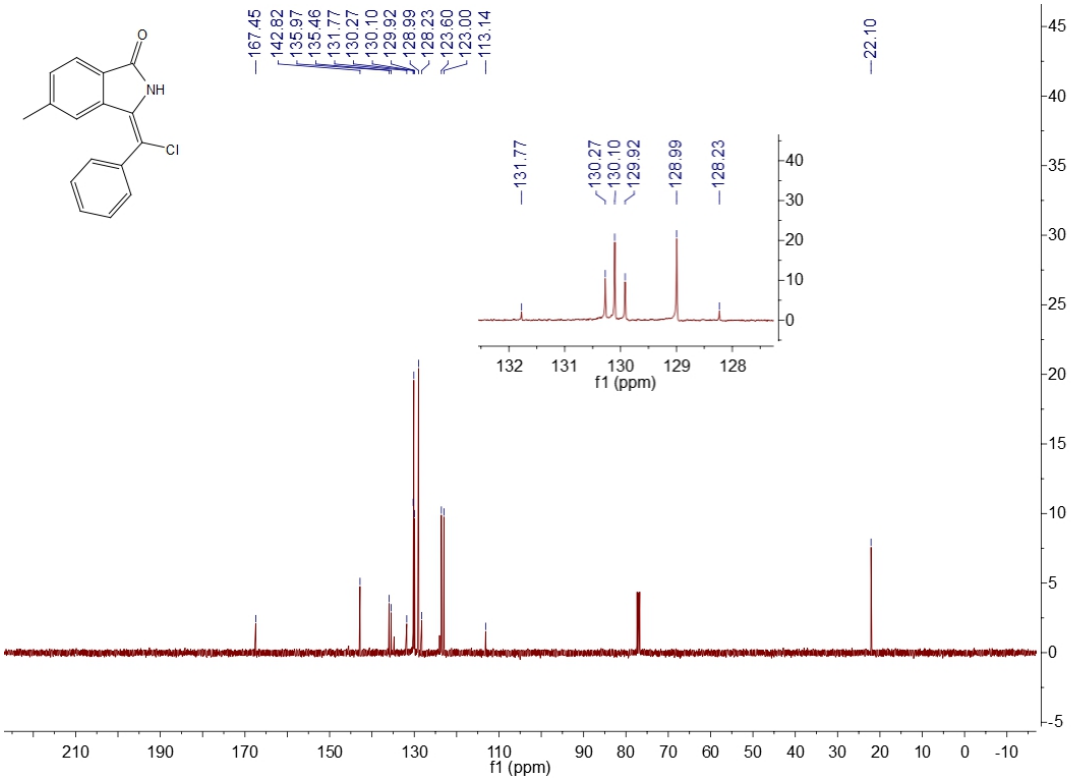
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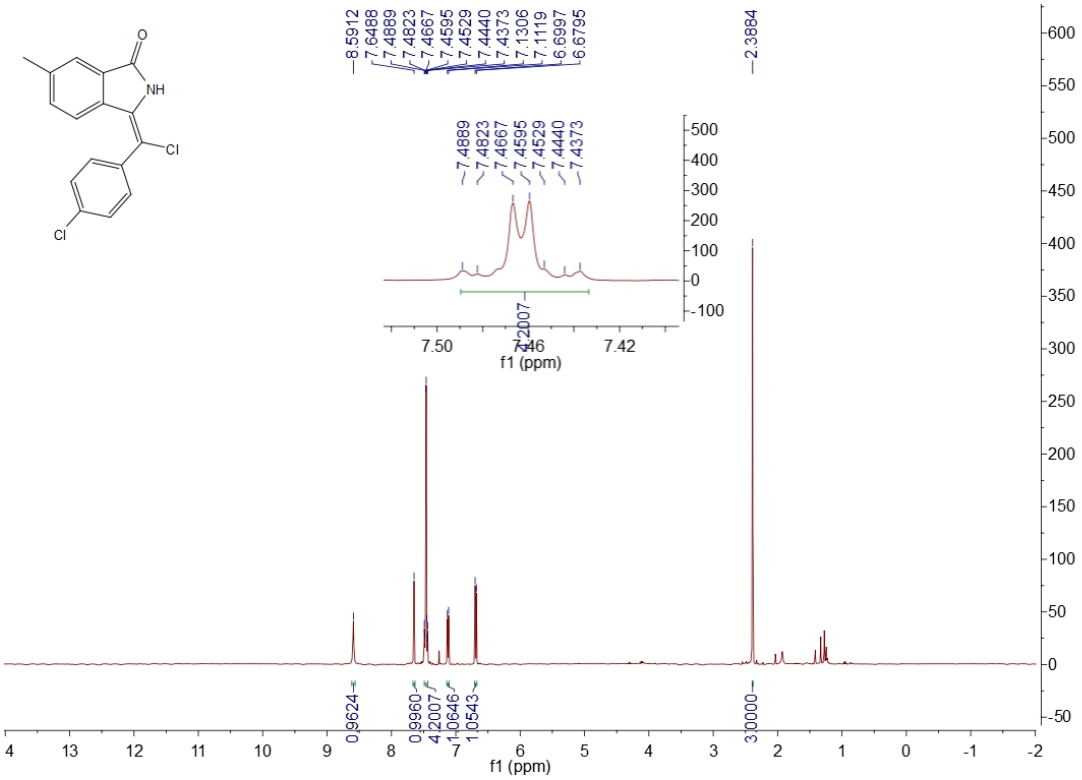
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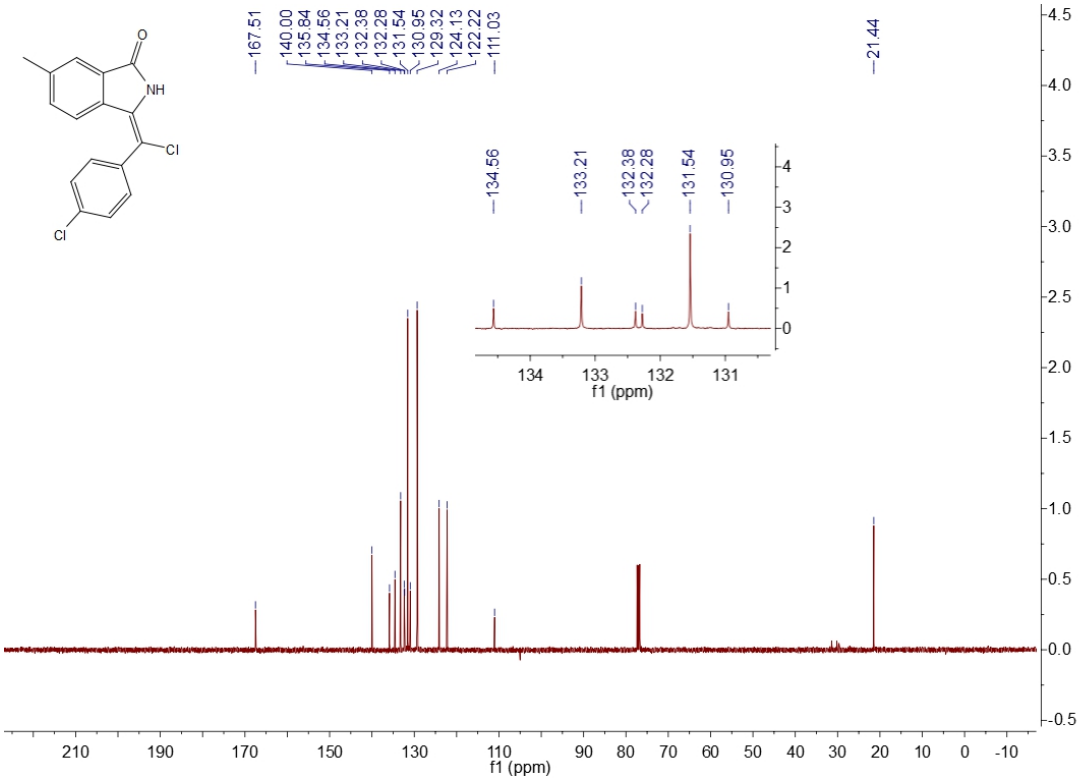
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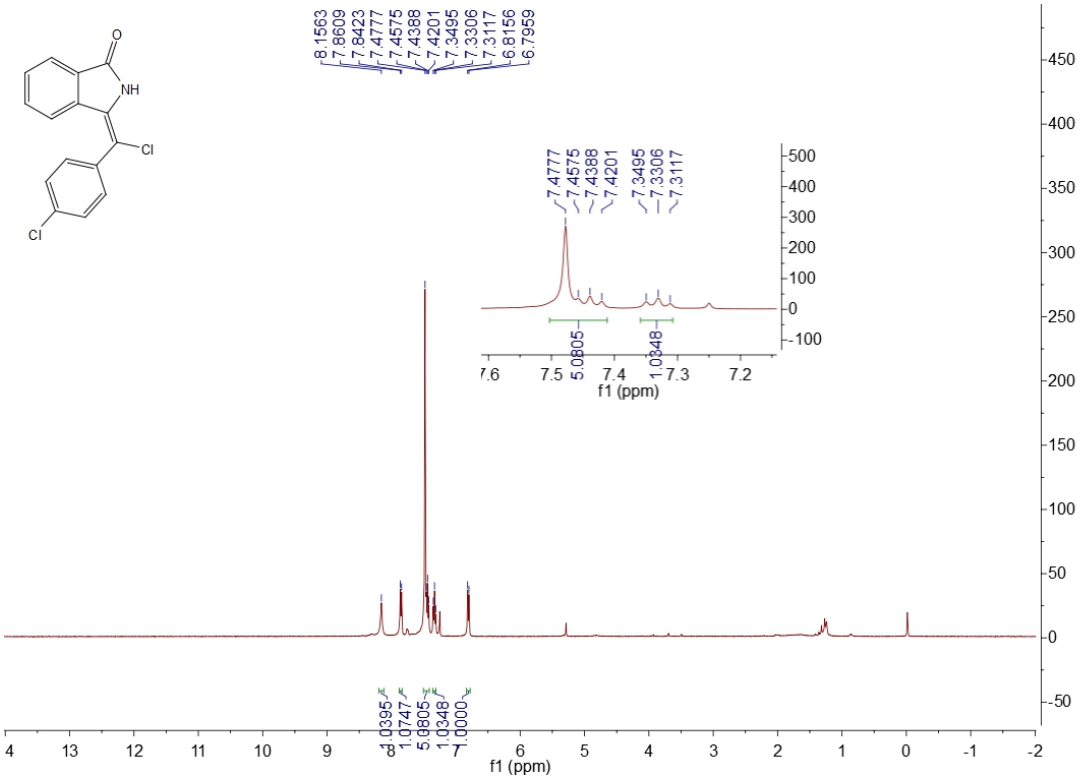
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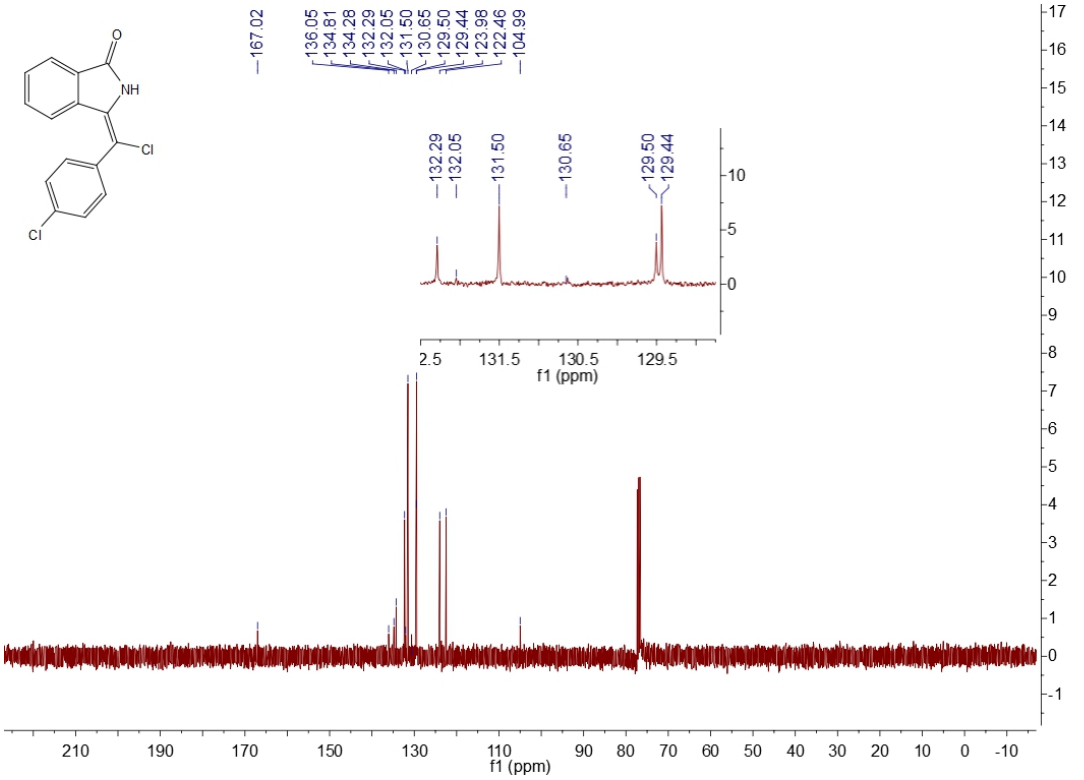
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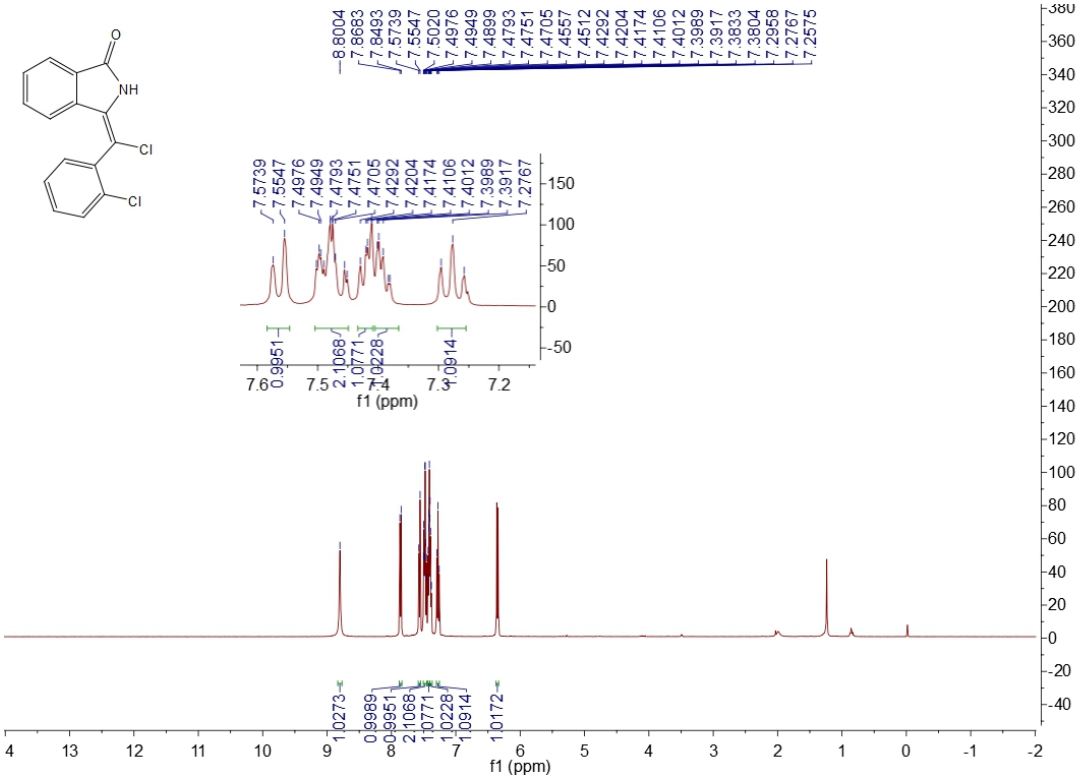
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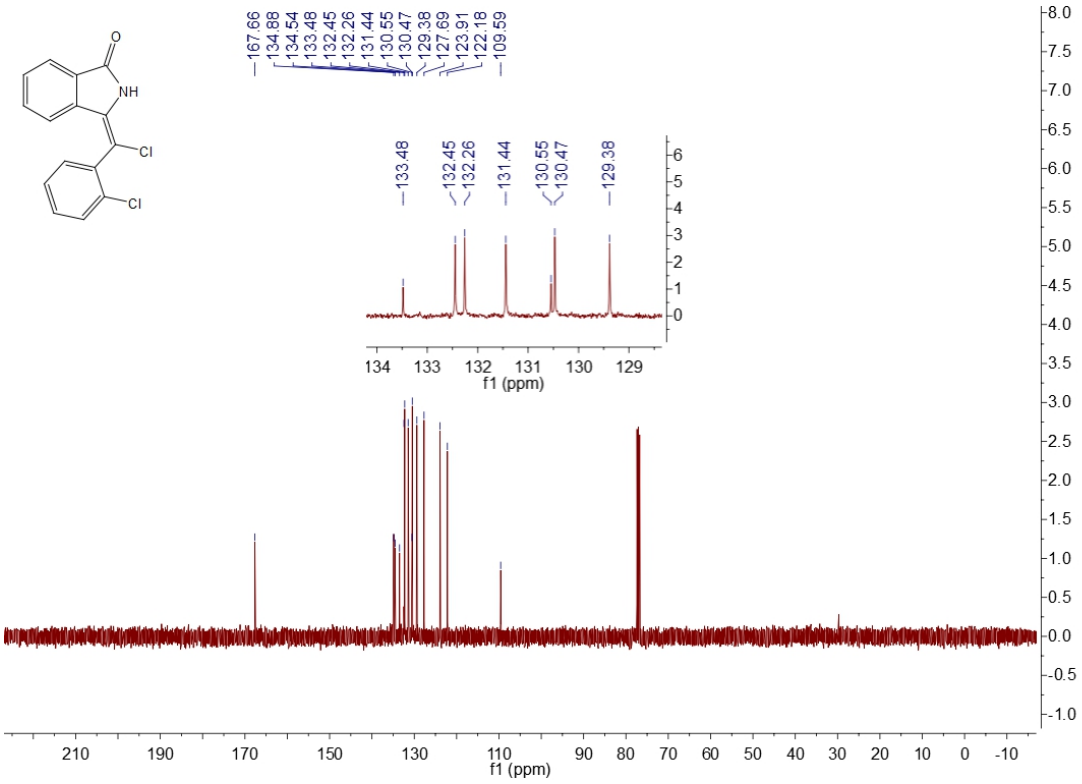
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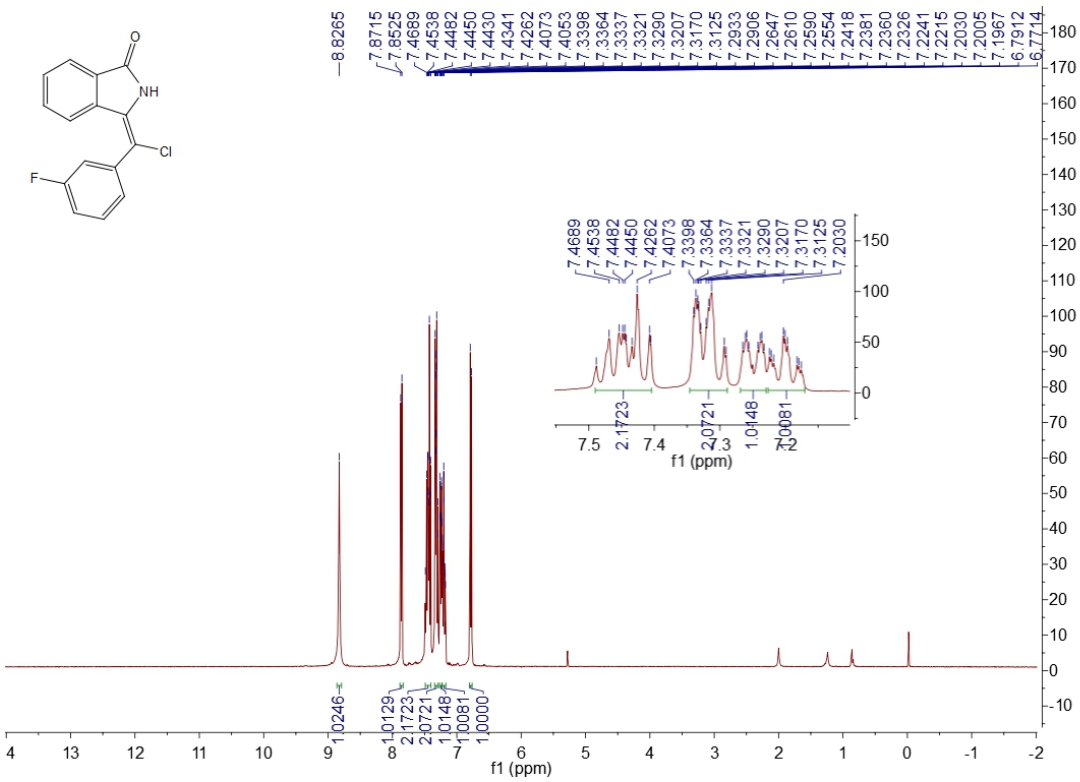
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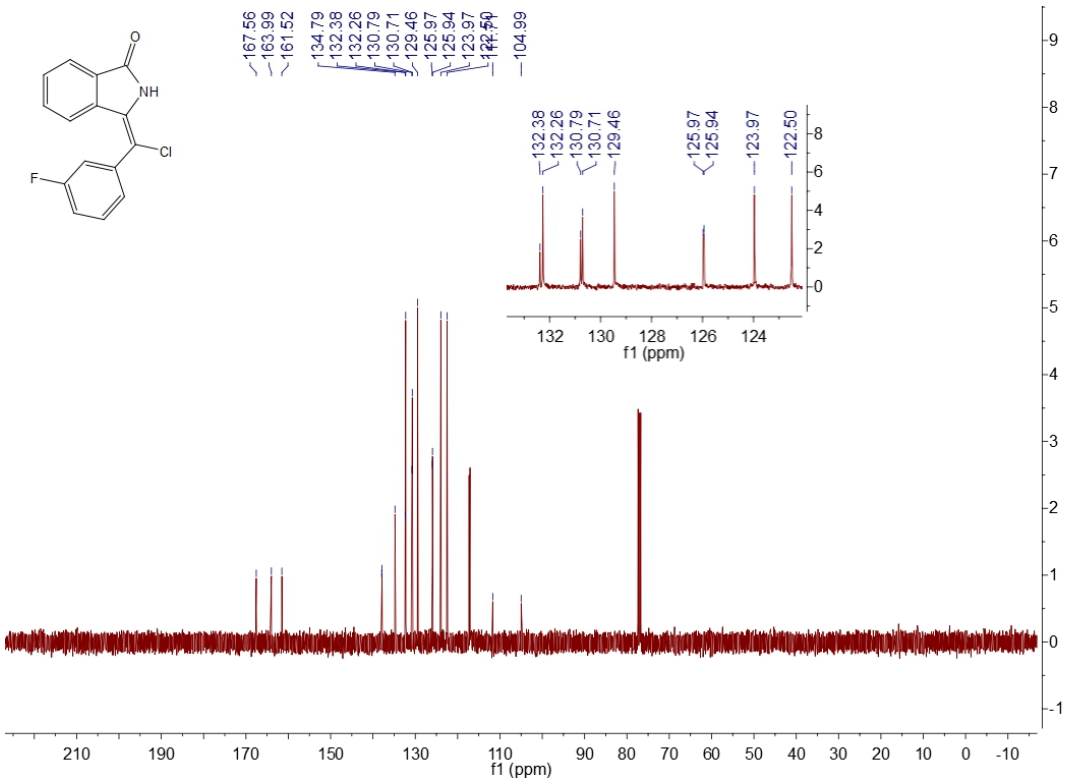
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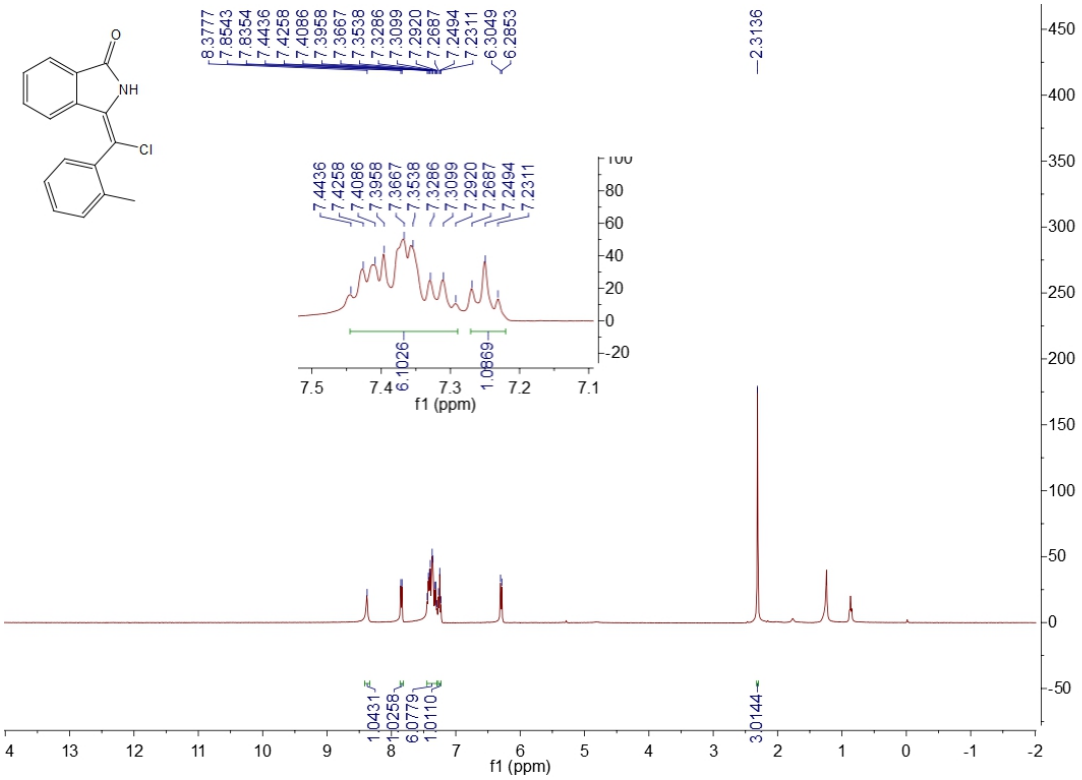
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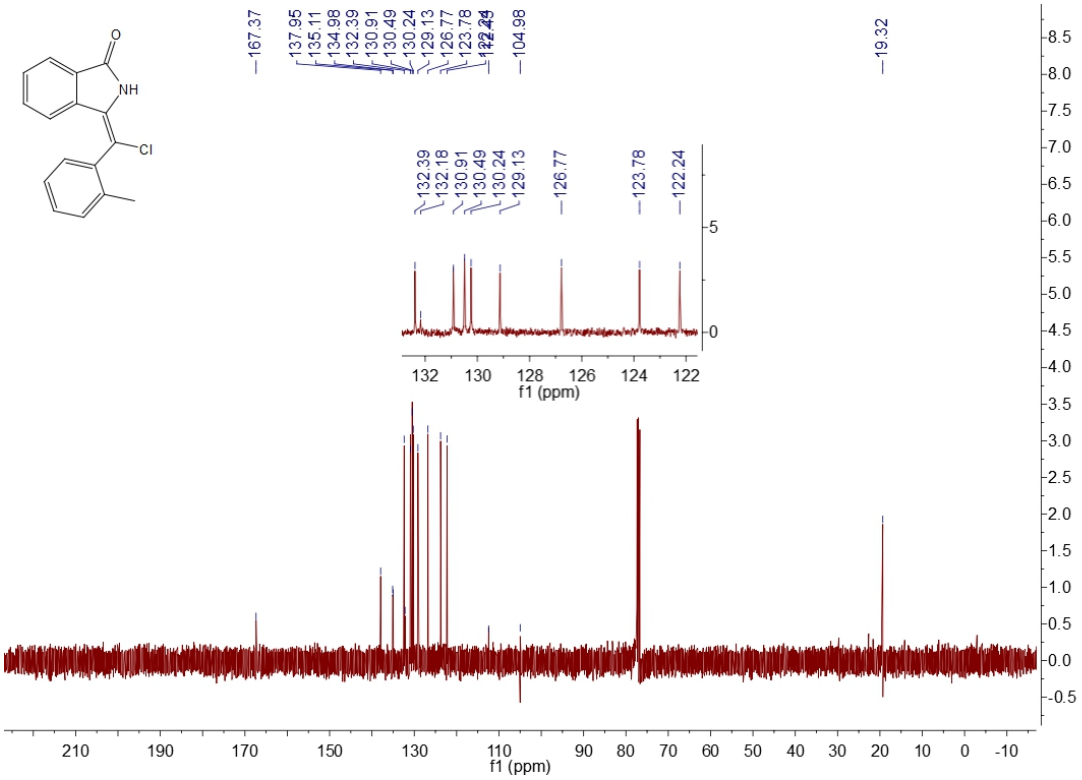
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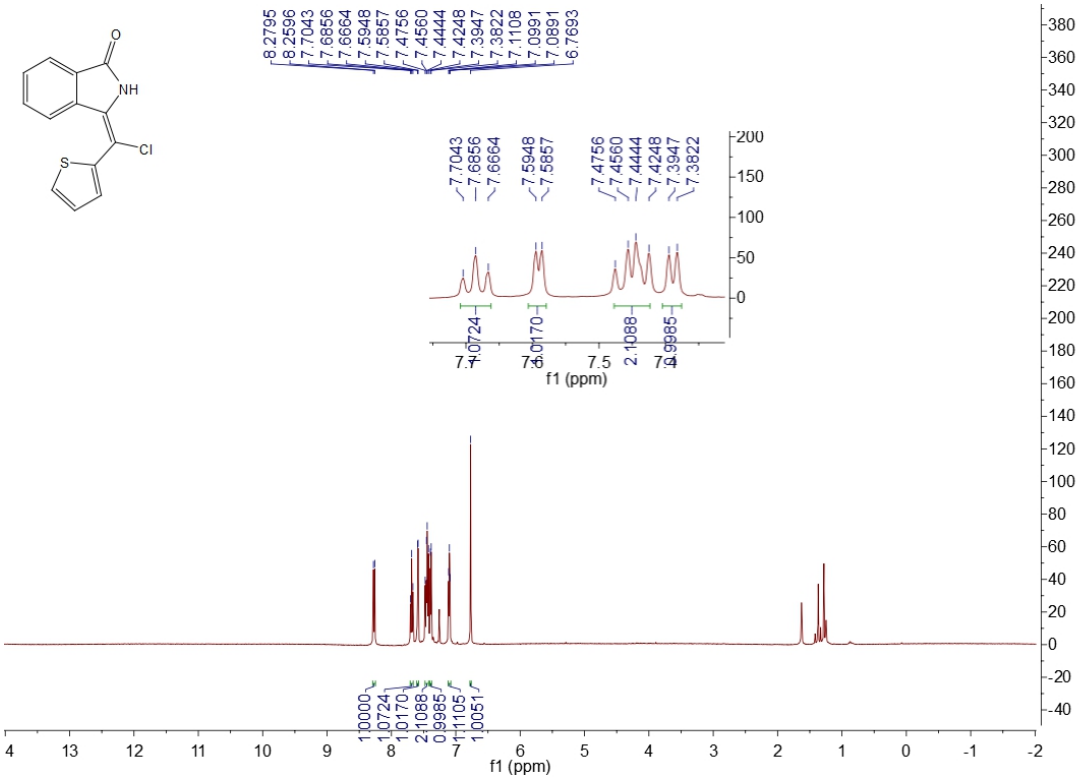
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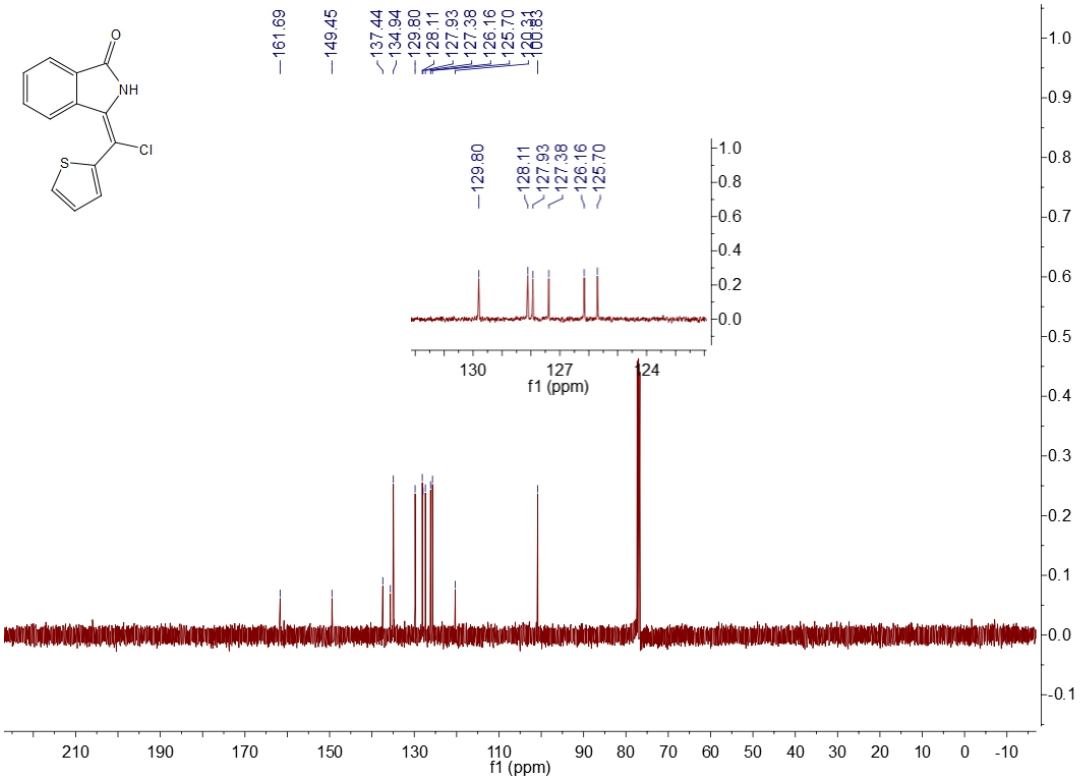
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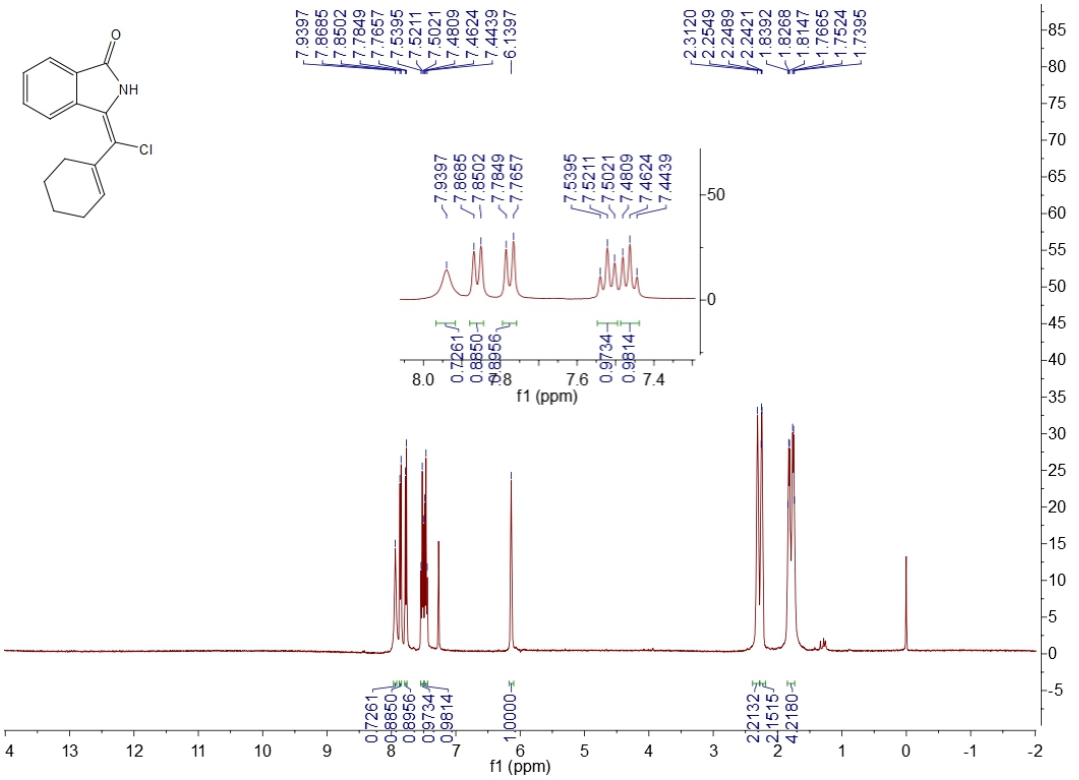
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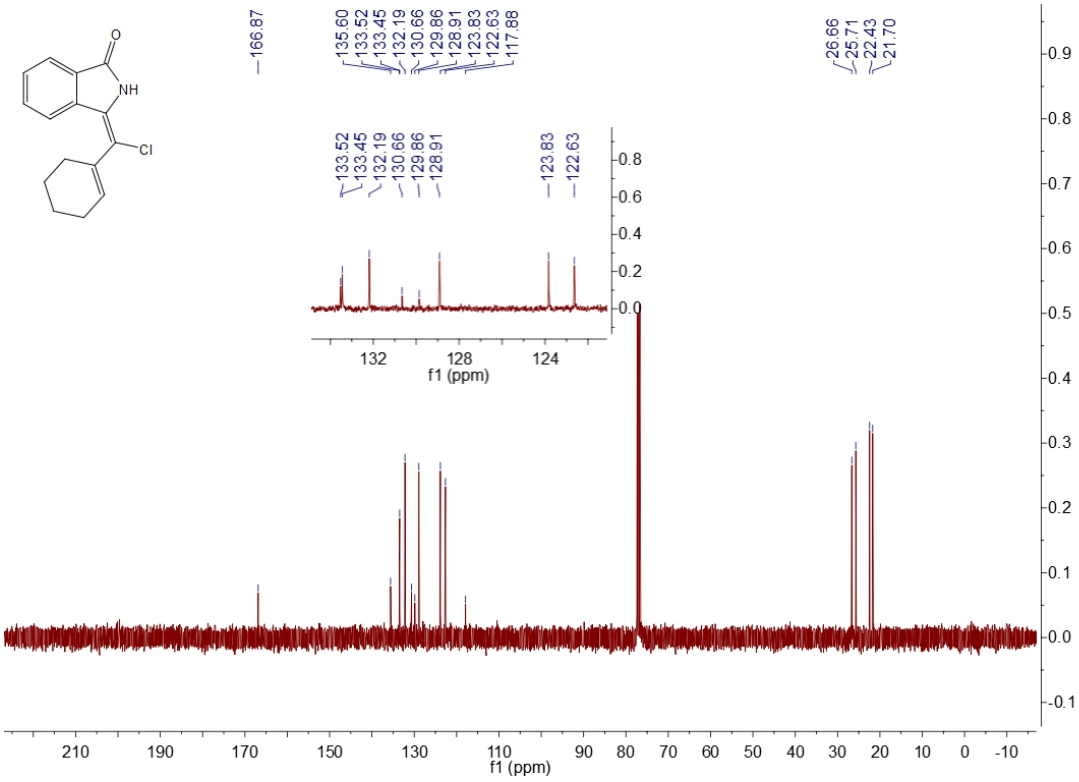
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NH
Cl
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133.52
133.45
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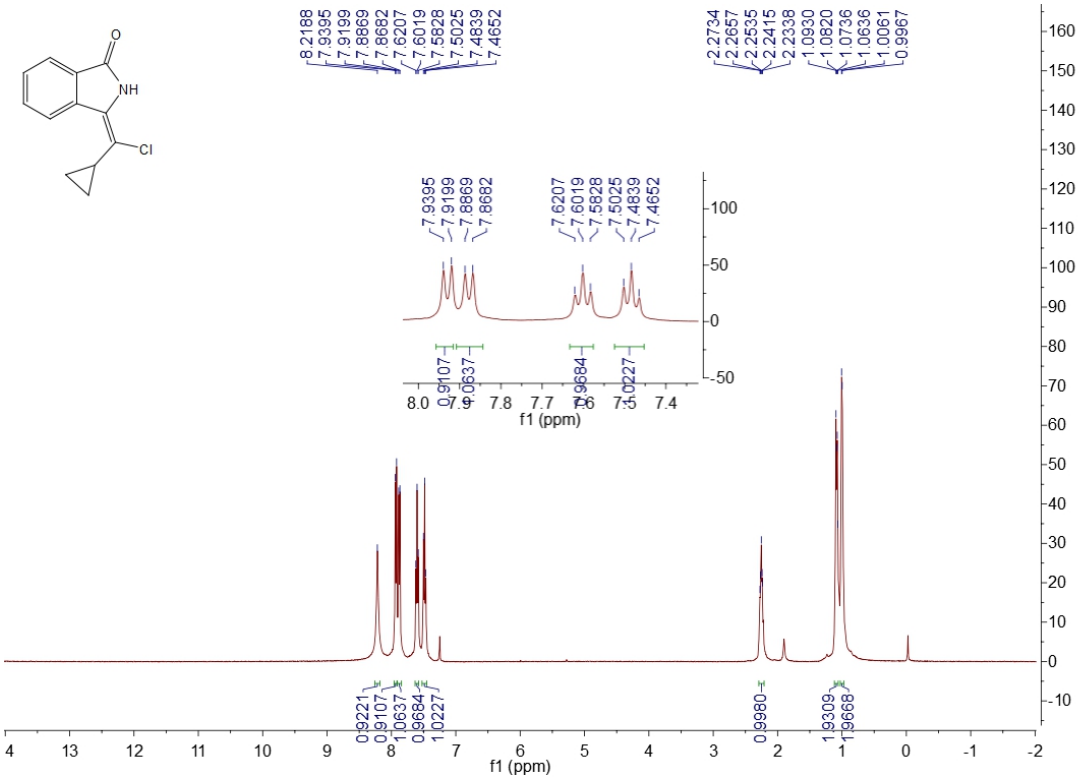
122.63
117.88
26.66
25.71
22.43
21.70
f1 (ppm)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Cl
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7.6019
7.5828
7.5025
7.4839
7.4652
2.2734
2.2657
2.2535
2.2415
2.2338
1.0930
1.0820
1.0736
1.0636
1.0061
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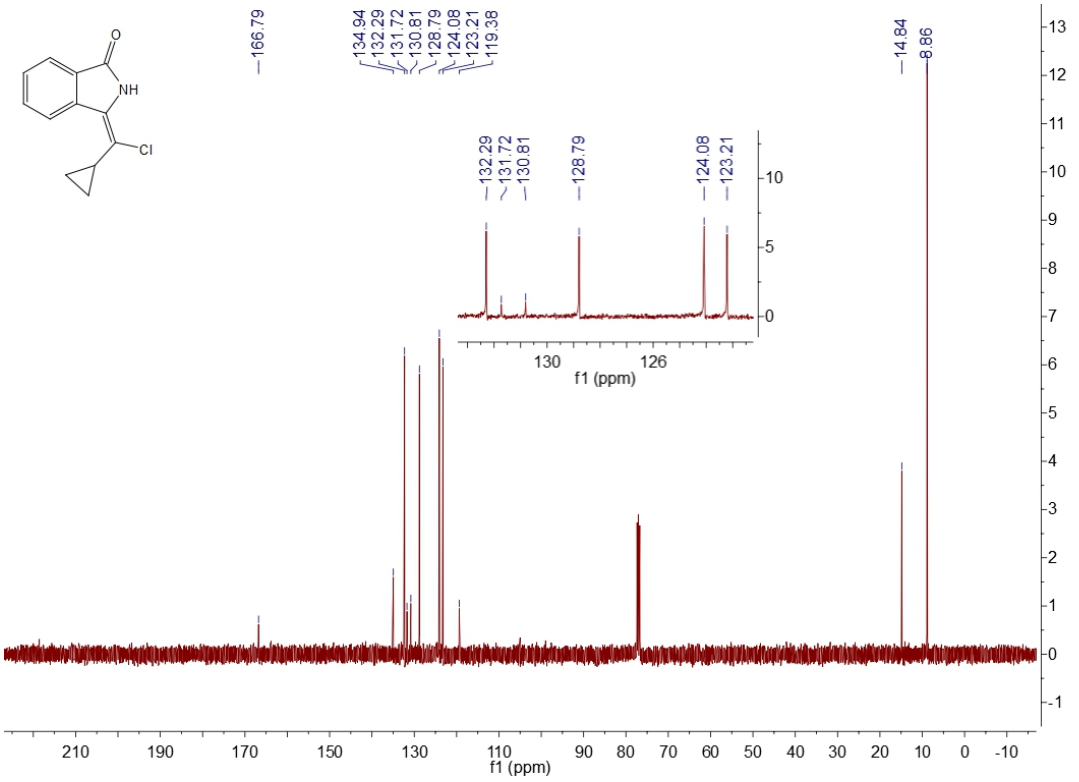
0.9684
1.0227
0.9980
1.9309
1.9668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NH
Cl
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128.79
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123.21
119.38
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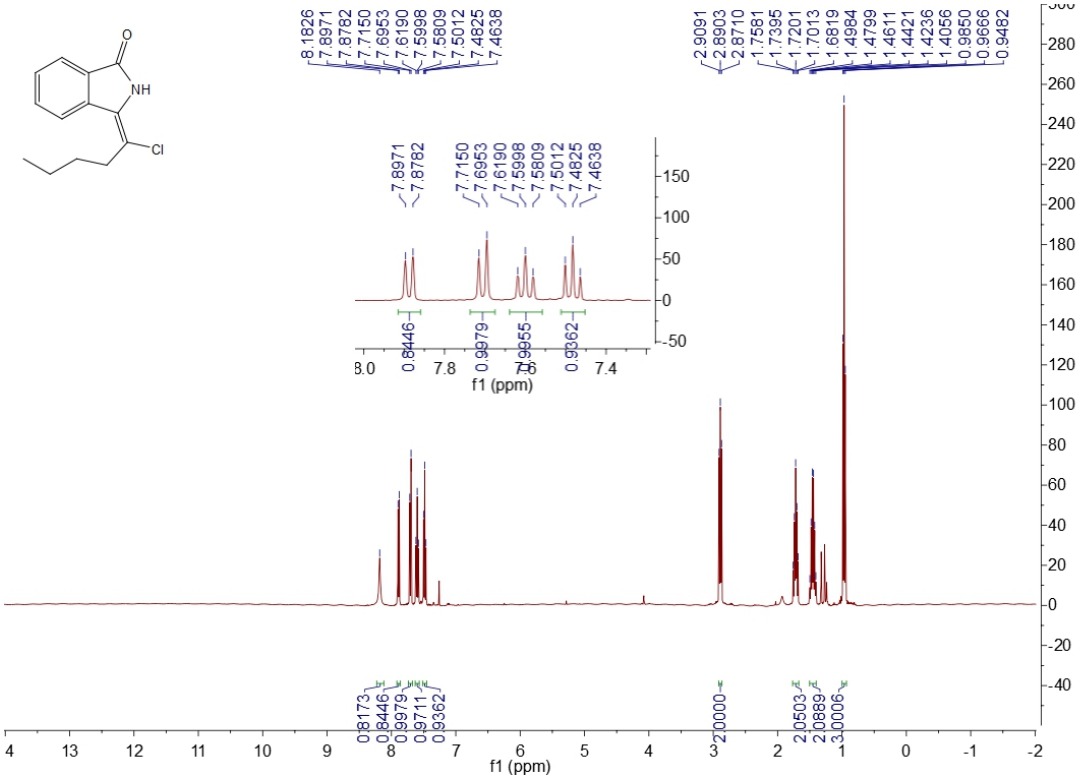
8.86
f1 (ppm)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2.9091
2.8903
2.8710
1.7581
1.7395
1.7201
1.7013
1.6819
1.4984
1.4799
1.4611
1.4421
1.4236
1.4056
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0.9666
0.9482
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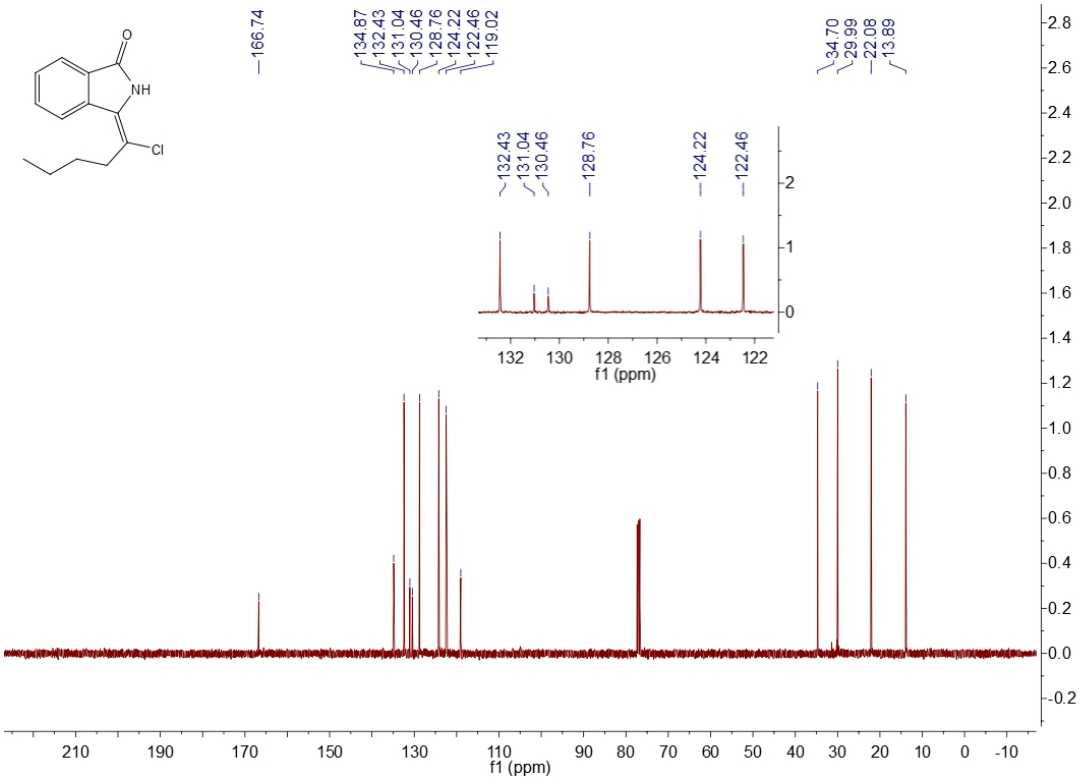
2.0000
2.0503
2.0889
3.0006
f1 (ppm)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122.46
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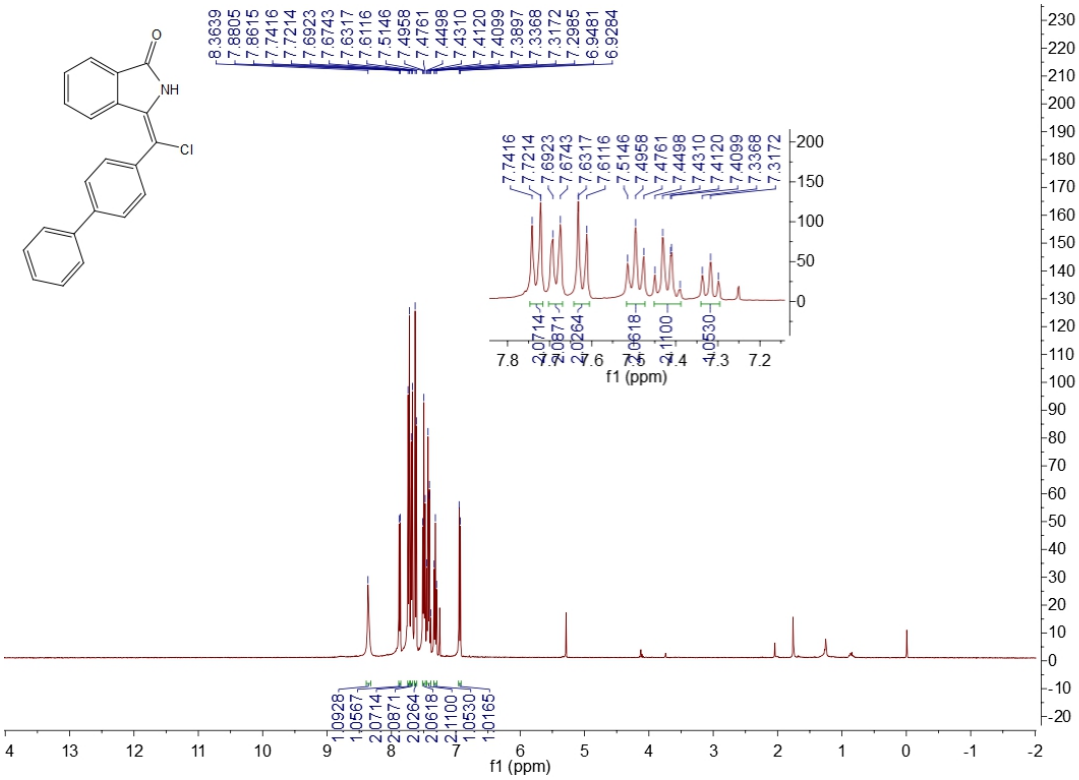
29.99
22.08
13.89
f1 (ppm)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7.8805
7.8615
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7.7214
7.6923
7.6743
7.6317
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7.4761
7.4498
7.4310
7.4120
7.4099
7.3897
7.3368
7.3172
7.2985
6.9481
6.9284
NH
O
Cl
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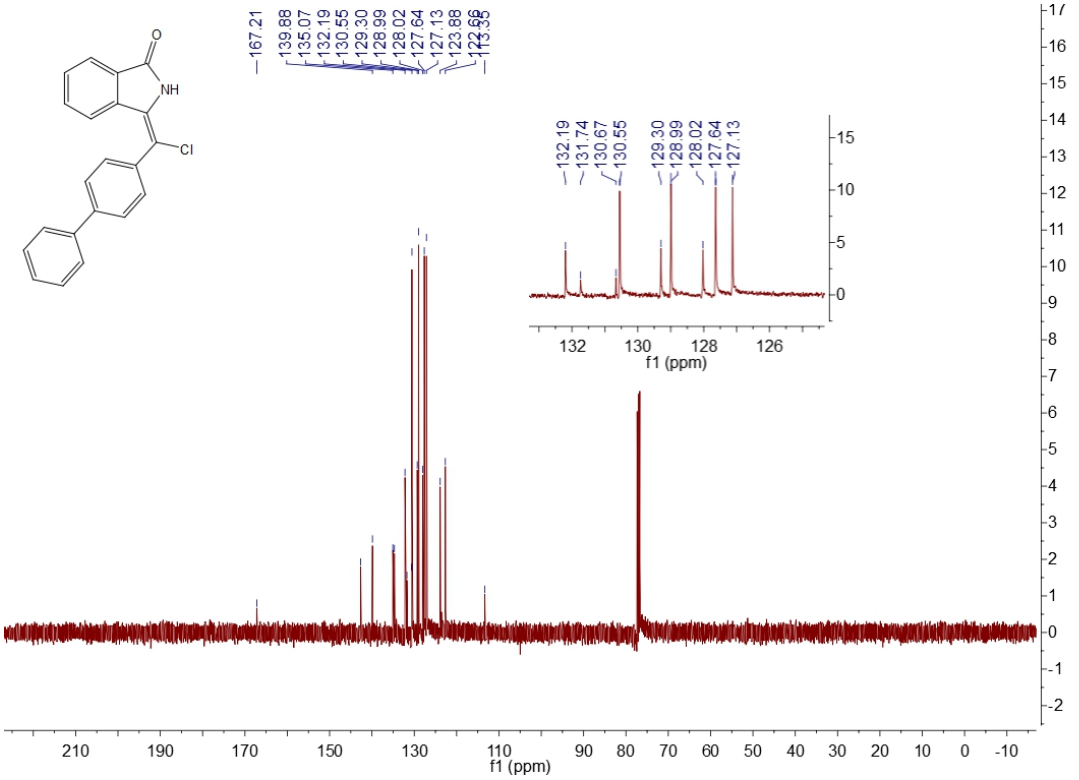
2.0714
2.0871
2.0264
2.0618
2.1100
1.0530
1.0165
f1 (ppm)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139.88
135.07
132.19
130.55
129.30
128.99
128.02
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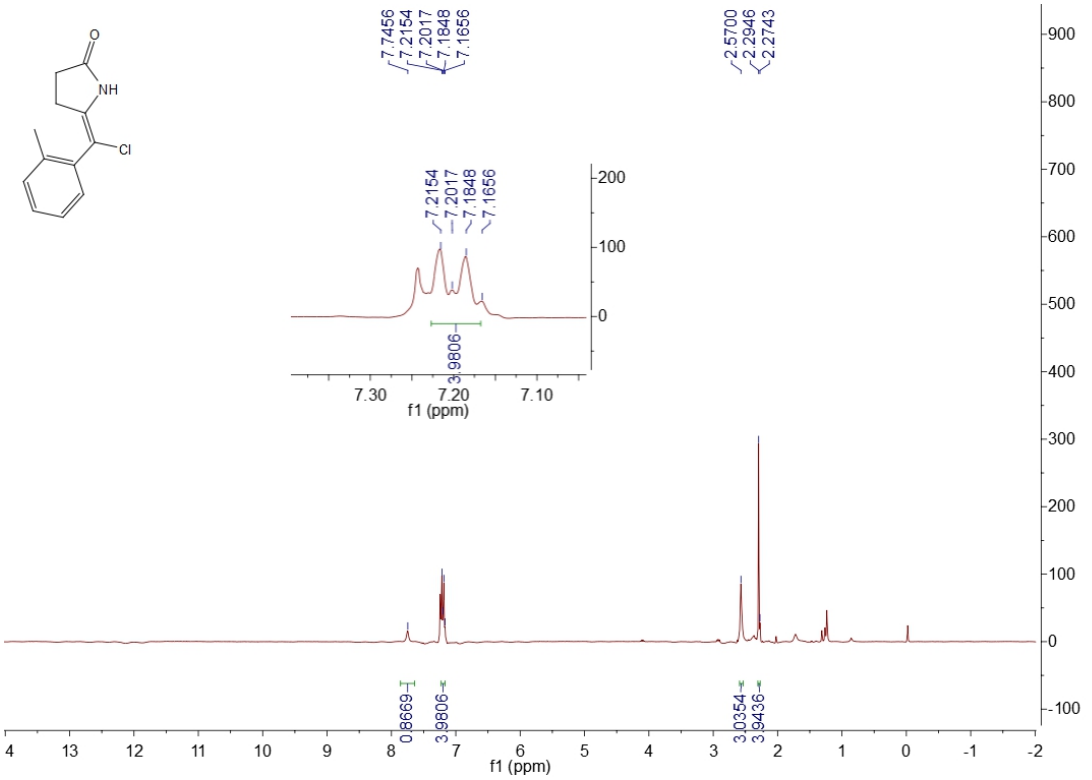
127.13
123.88
122.66
113.35
NH
O
Cl
f1 (ppm)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7.2154
7.2017
7.1848
7.1656
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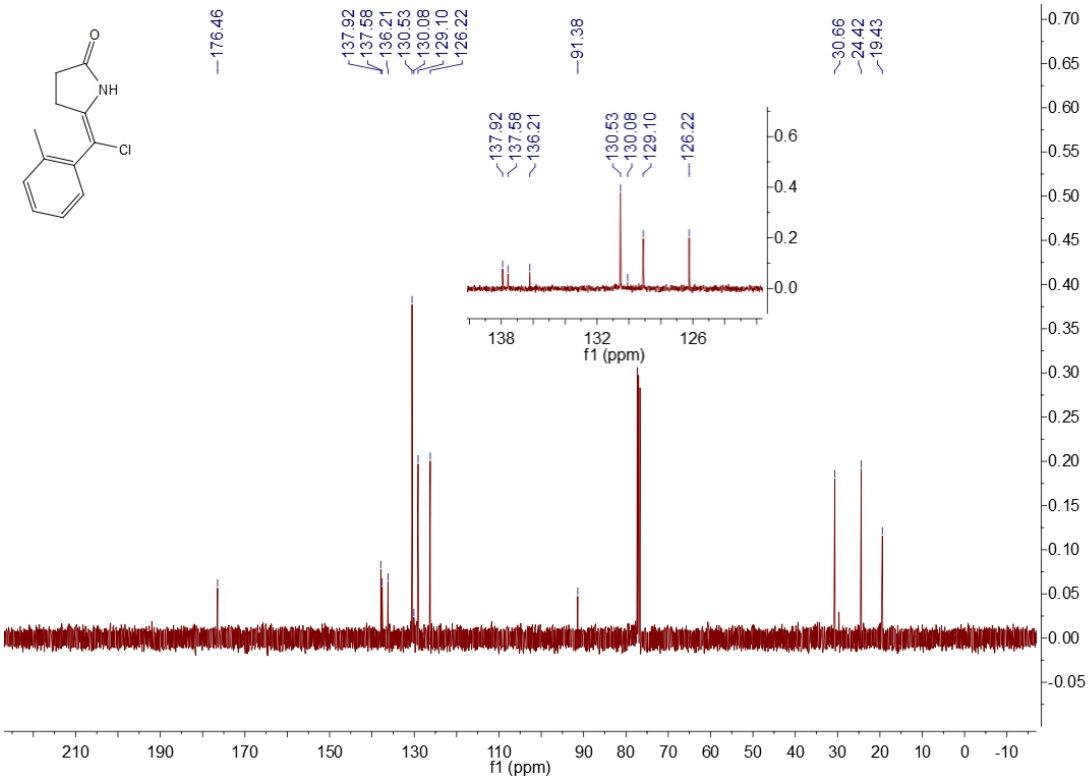
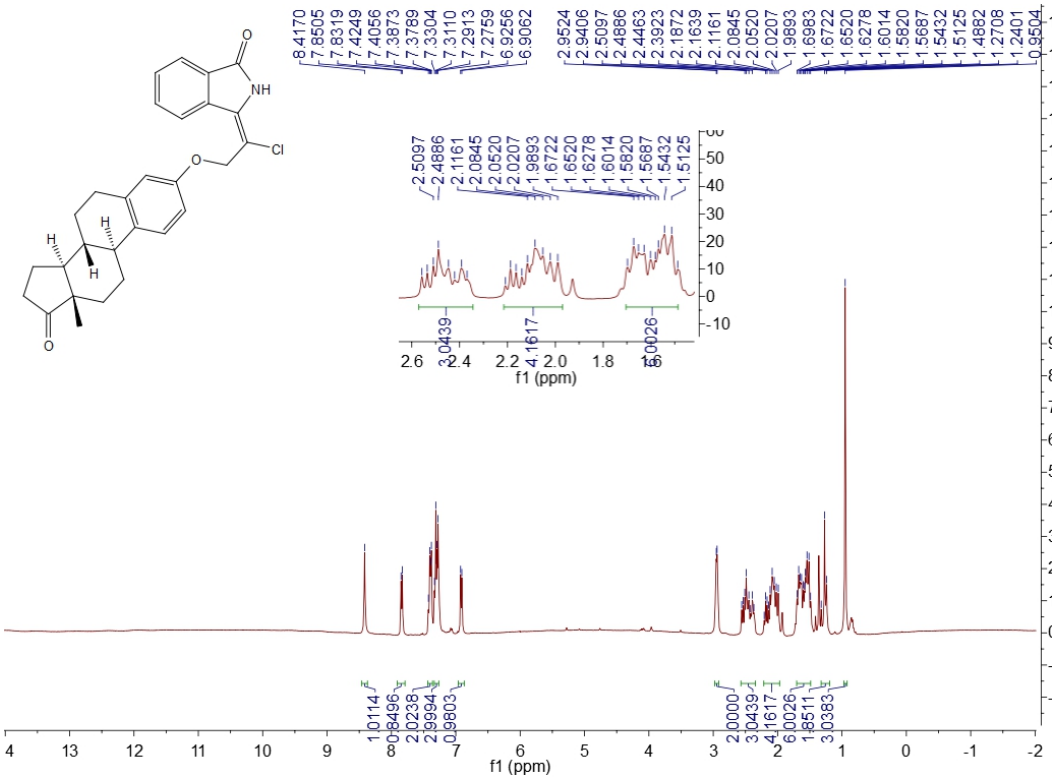
2.2946
2.2743
0.8669
3.9806
3.0354
3.9436
f1 (ppm)


176.46
137.92
137.58
136.21
130.53
130.08
129.10
126.22
91.38
30.66
24.42
19.43
f1 (ppm)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7.8505
7.8319
7.4249
7.4056
7.3873
7.3789
7.3304
7.3110
7.2913
7.2759
6.9256
6.9062
2.9524
2.9406
2.5097
2.4886
2.4463
2.3923
2.1672
2.1639
2.1161
2.0845
2.0520
2.0207
1.9893
1.6983
1.6722
1.6520
1.6278
1.6014
1.5820
1.5687
1.5432
1.5125
1.4882
1.2708
1.2401
0.9504
1.0114
0.8496
2.0238
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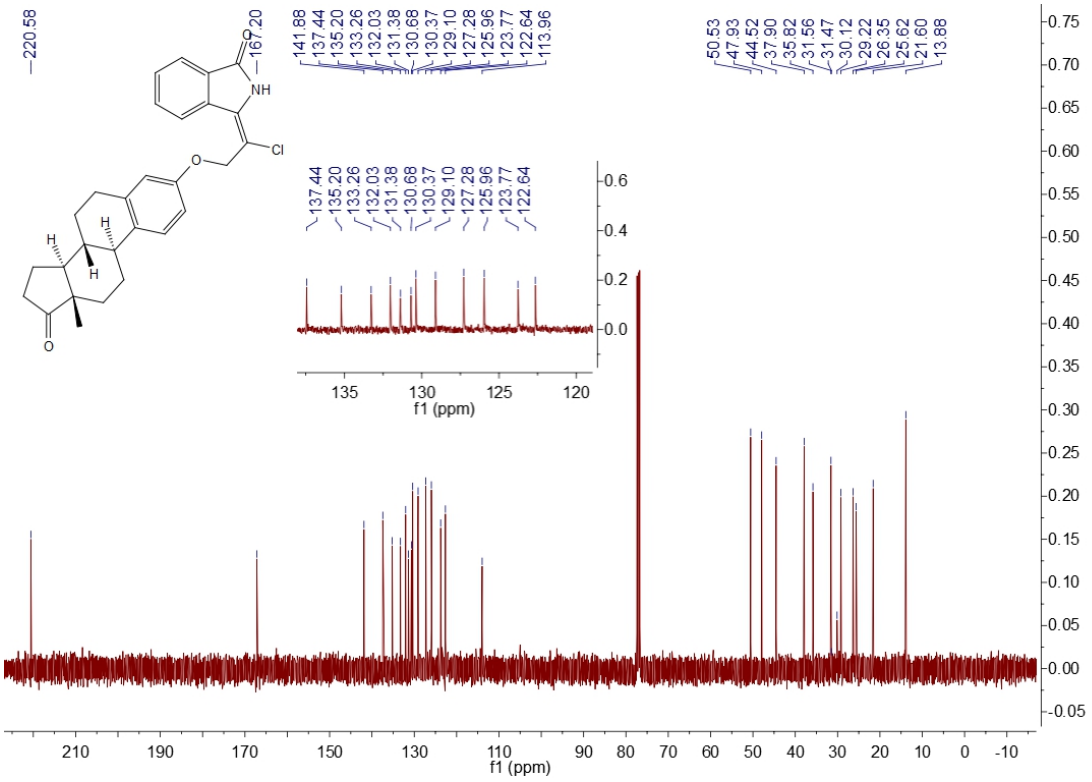
0.9803
2.0000
3.0439
4.1617
6.0026
1.8511
3.0383
f1 (ppm)


220.58
167.20
141.88
137.44
135.20
133.26
132.03
131.38
130.68
130.37
129.10
127.28
125.96
123.77
122.64
113.96
50.53
47.93
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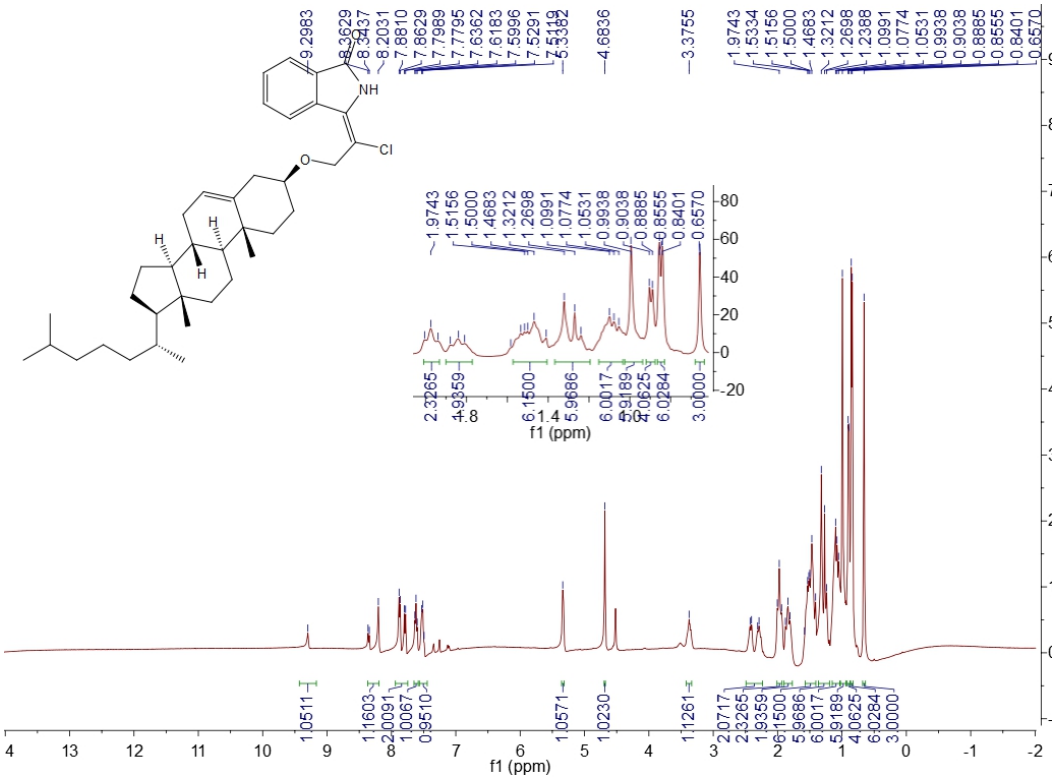
26.35
25.62
21.60
13.88
f1 (ppm)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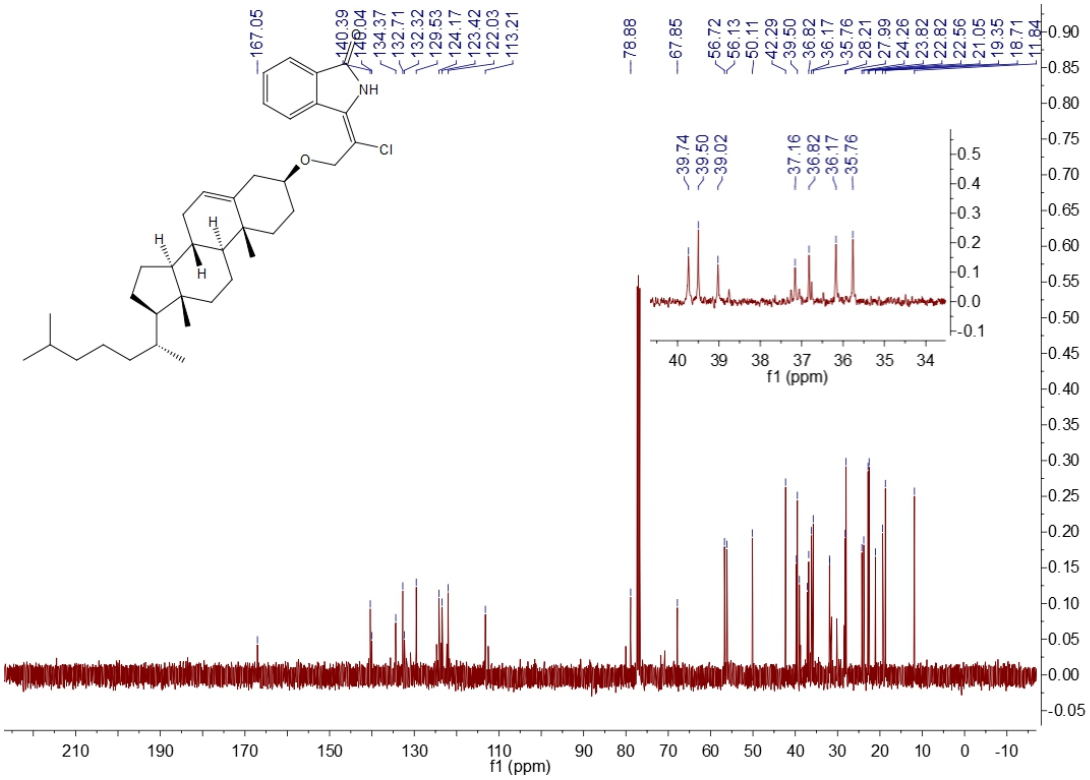
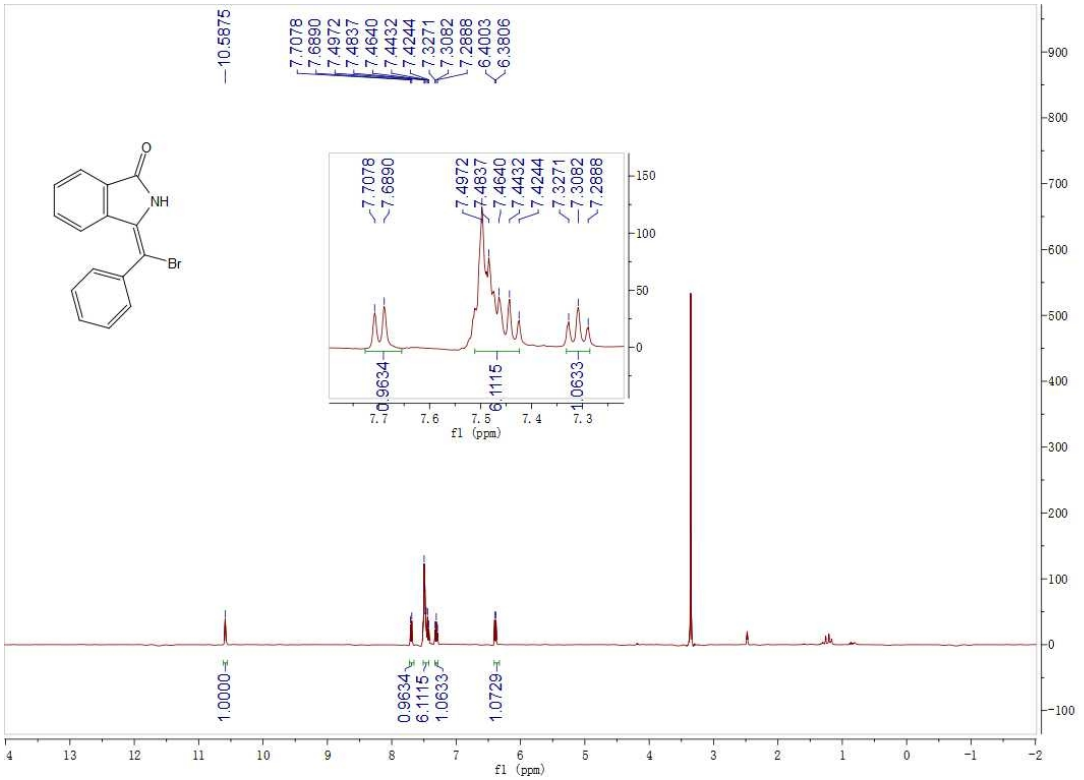

f1 (ppm)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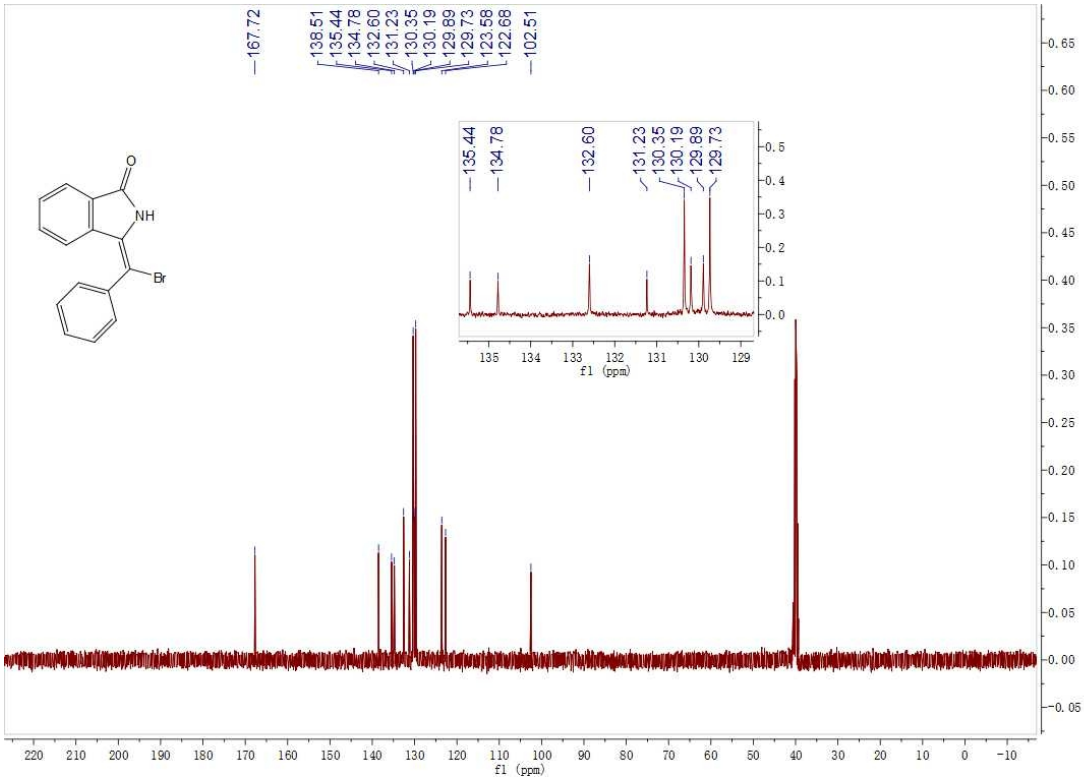
7.6890
7.4972
7.4837
7.4640
7.4432
7.4244
7.3271
7.3082
7.2888
6.4003
6.3806
O
NH
Br
1.0000
0.9634
6.1115
1.0633
1.0729
f1 (ppm)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138.51
135.44
134.78
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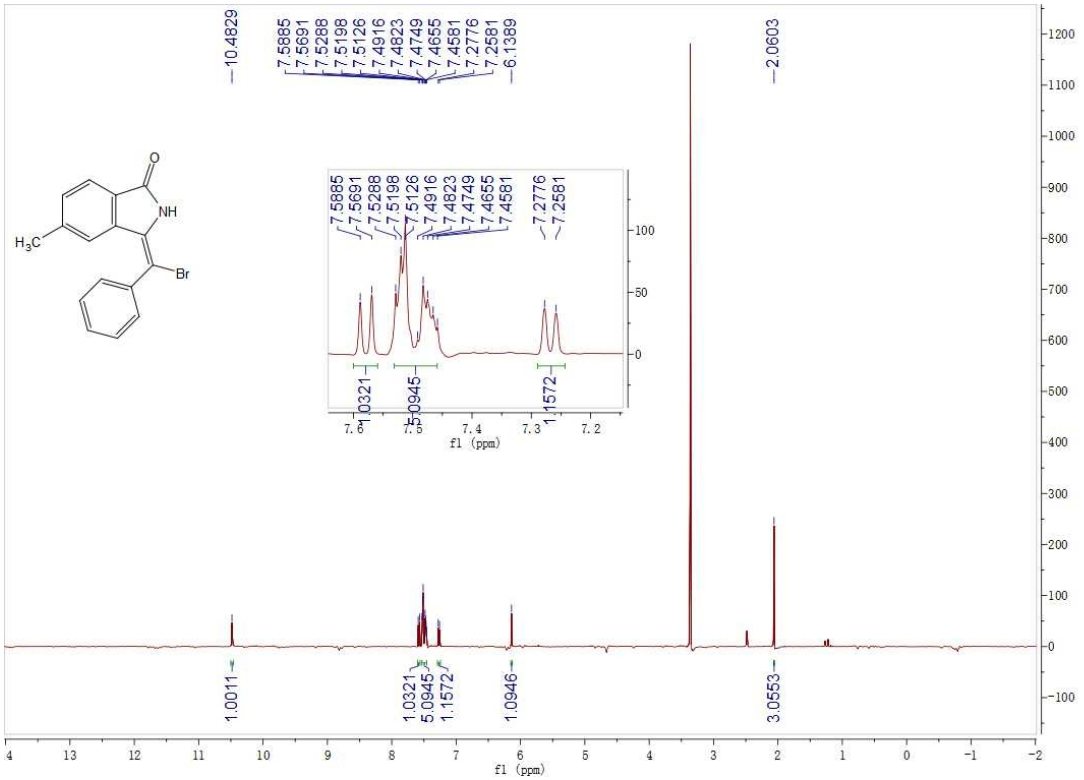
131.23
130.35
130.19
129.89
129.73
123.58
122.68
102.51
O
NH
Br
f1 (ppm)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7.5198
7.5126
7.4916
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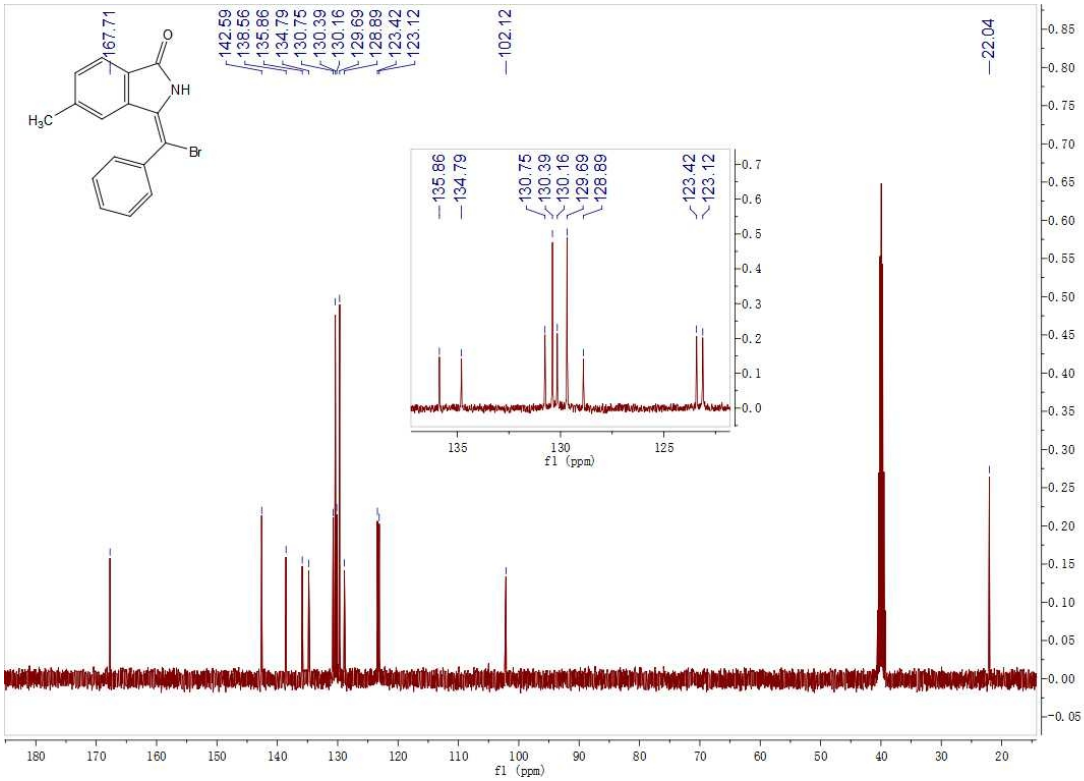
7.4749
7.4655
7.4581
7.2776
7.2581
6.1389
2.0603
NH
O
H3C
Br
1.0011
1.0321
5.0945
1.1572
1.0946
3.0553
f1 (ppm)


167.71
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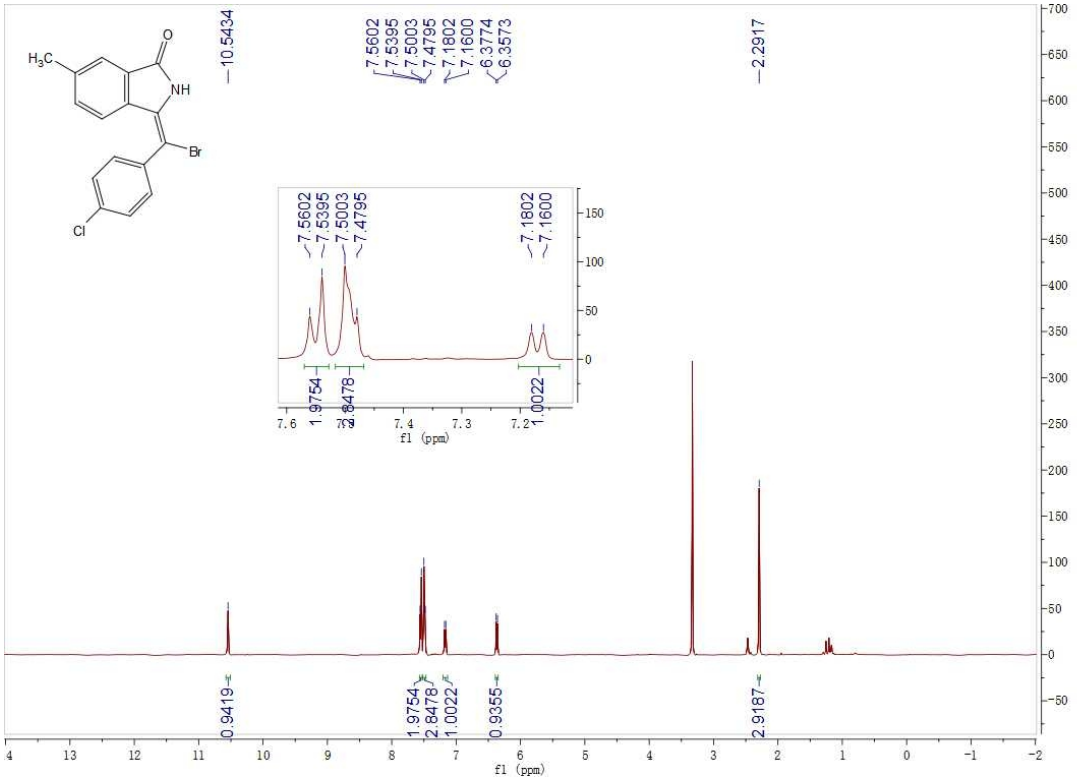
135.86
134.79
130.75
130.39
130.16
129.69
128.89
123.42
123.12
102.12
22.04
NH
O
H3C
Br
f1 (ppm)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7.5395
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7.4795
7.1802
7.1600
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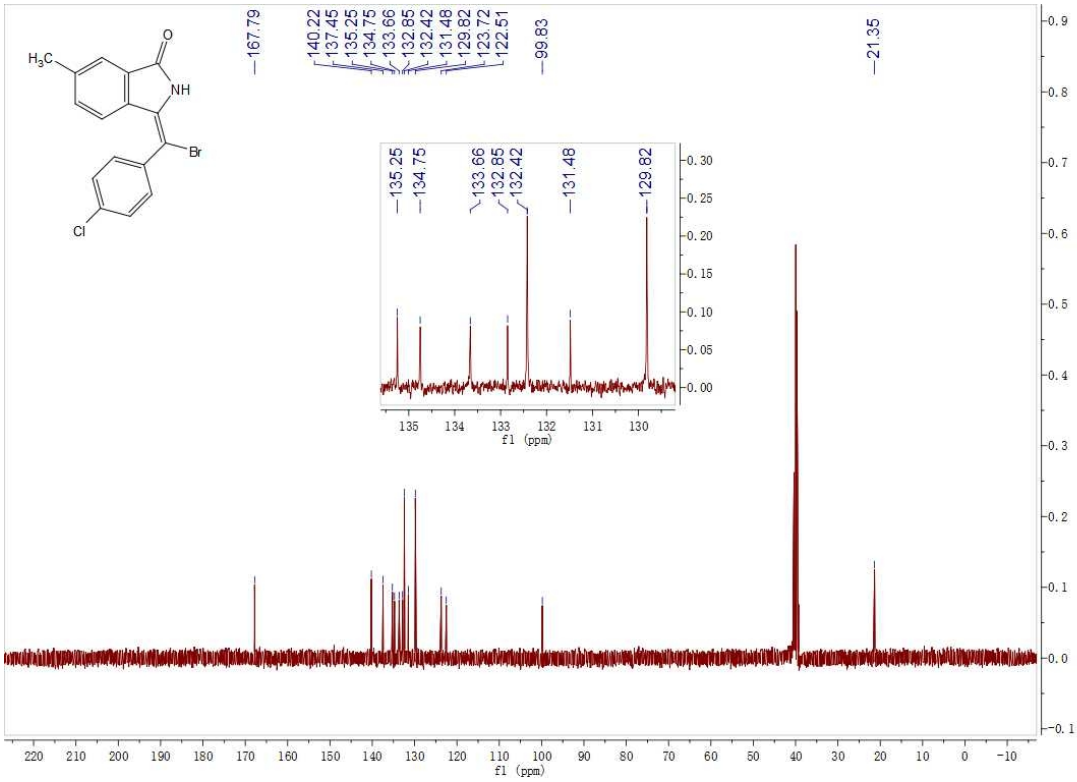
1.9754
2.8478
1.0022
0.9355
2.9187
f1 (ppm)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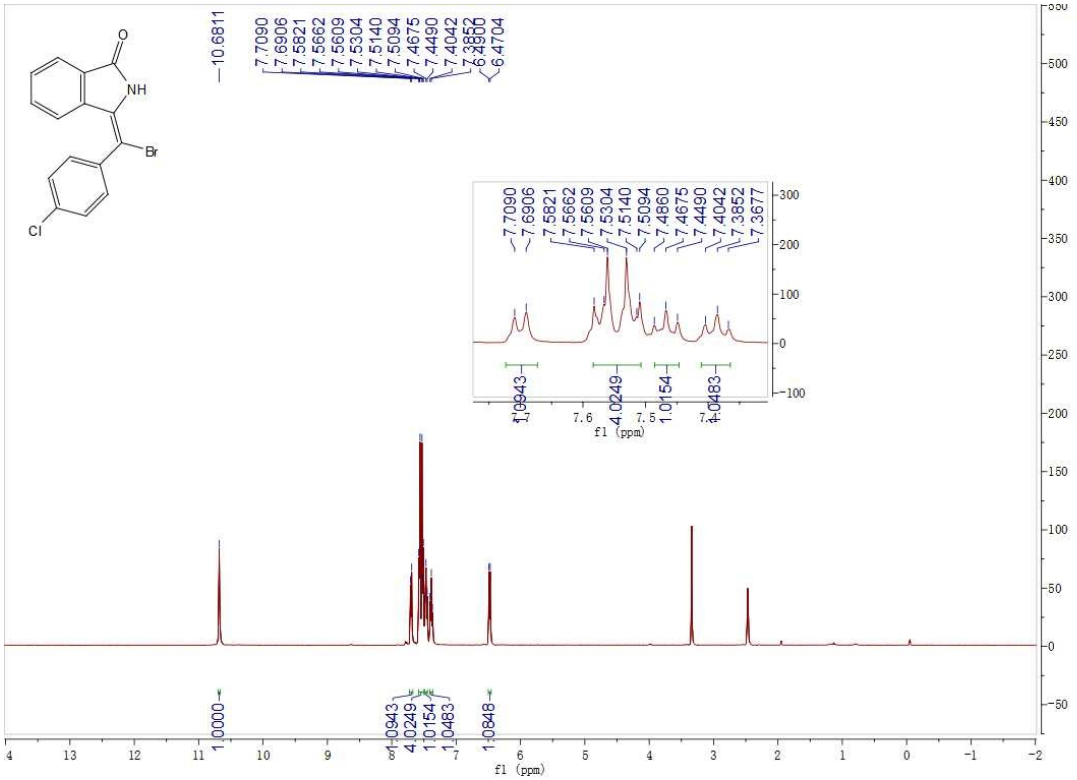
132.42
131.48
129.82
123.72
122.51
99.83
21.35
f1 (ppm)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7.6906
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7.5662
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7.5094
7.4675
7.4490
7.4042
7.3852
6.4900
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O
Br
Cl
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1.0943
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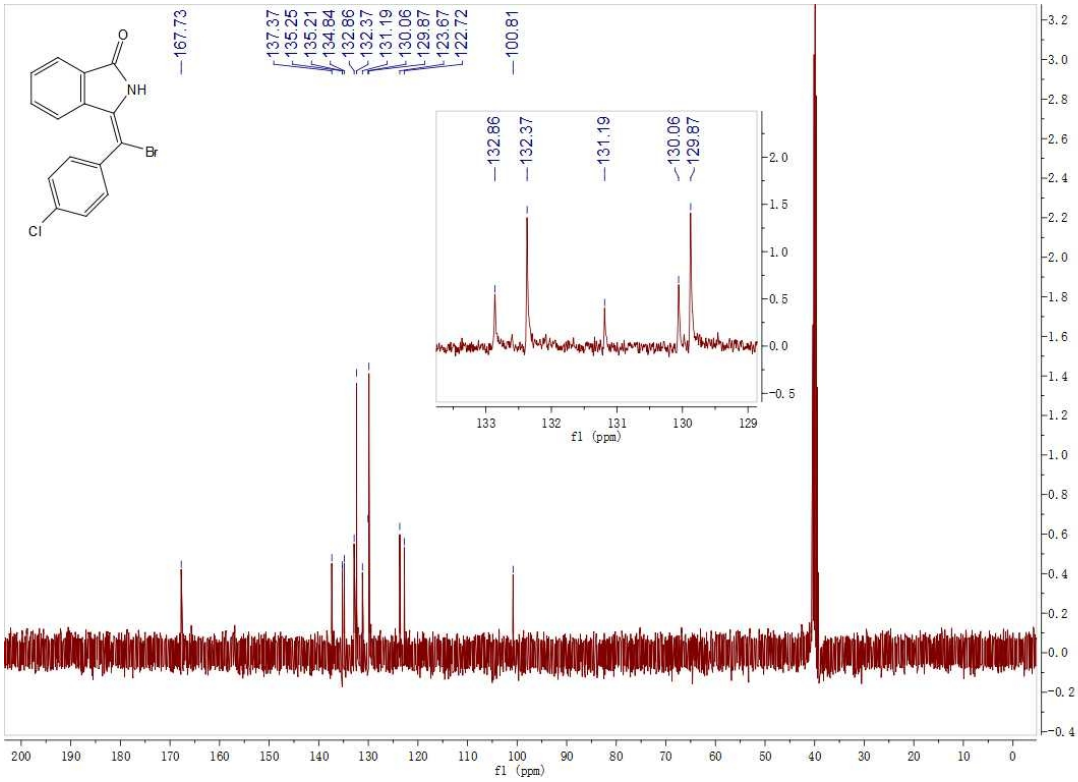
1.0154
1.0483
1.0848
f1 (ppm)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135.21
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130.06
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123.67
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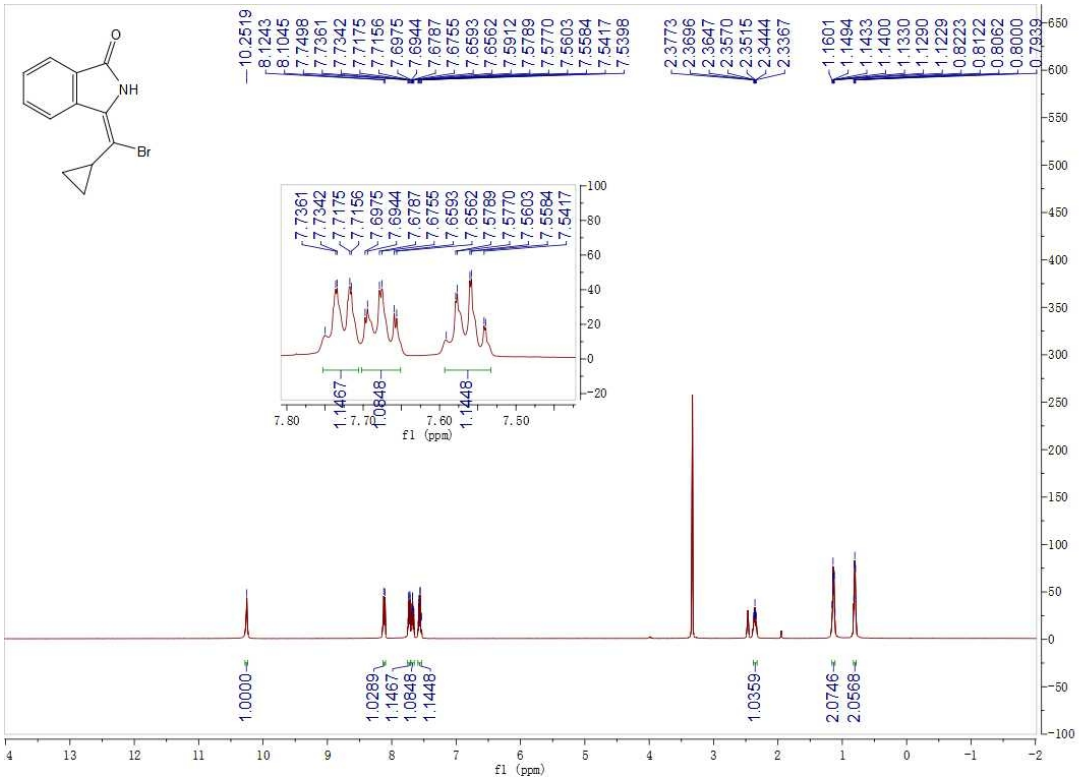
NH
O
Br
Cl
f1 (ppm)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Br
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7.7361
7.7342
7.7175
7.7156
7.6975
7.6944
7.6787
7.6755
7.6593
7.6562
7.5912
7.5789
7.5770
7.5603
7.5584
7.5417
7.5398
2.3773
2.3696
2.3647
2.3570
2.3515
2.3444
2.3367
1.1601
1.1494
1.1433
1.1400
1.1330
1.1290
1.1229
0.8223
0.8122
0.8062
0.8000
0.7939
1.1467
1.0848
1.1448
f1 (ppm)
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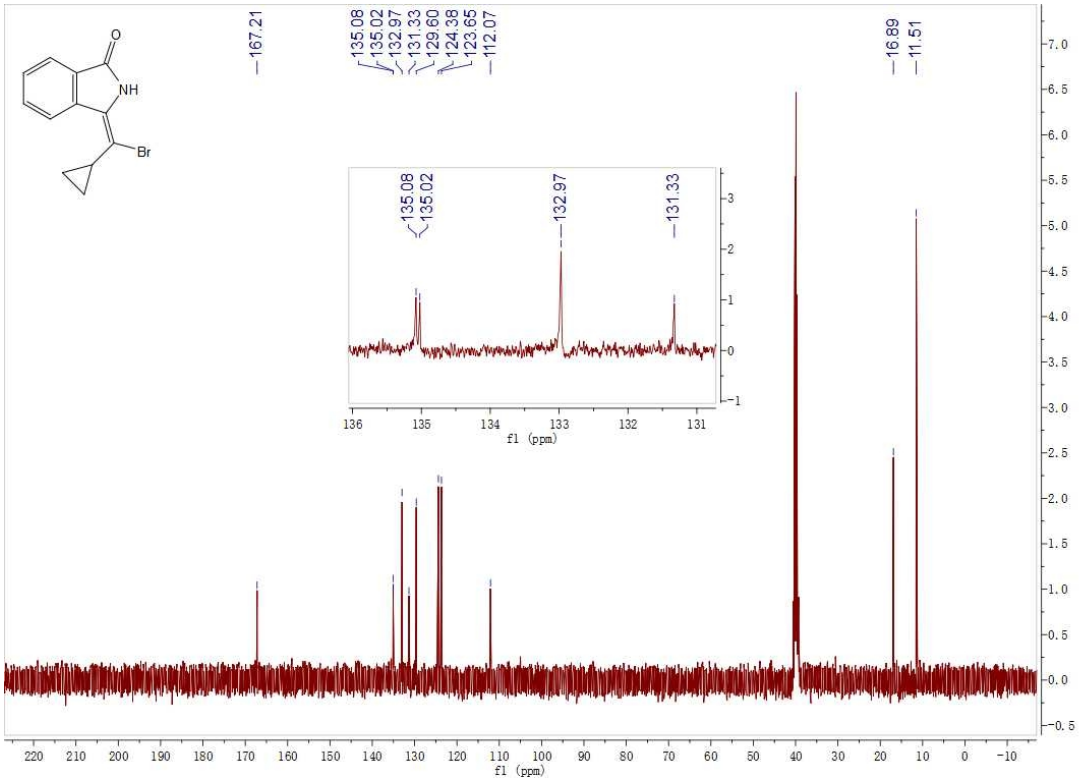
1.0289
1.1467
1.0848
1.1448
1.0359
2.0746
2.0568
f1 (ppm)


O
NH
Br
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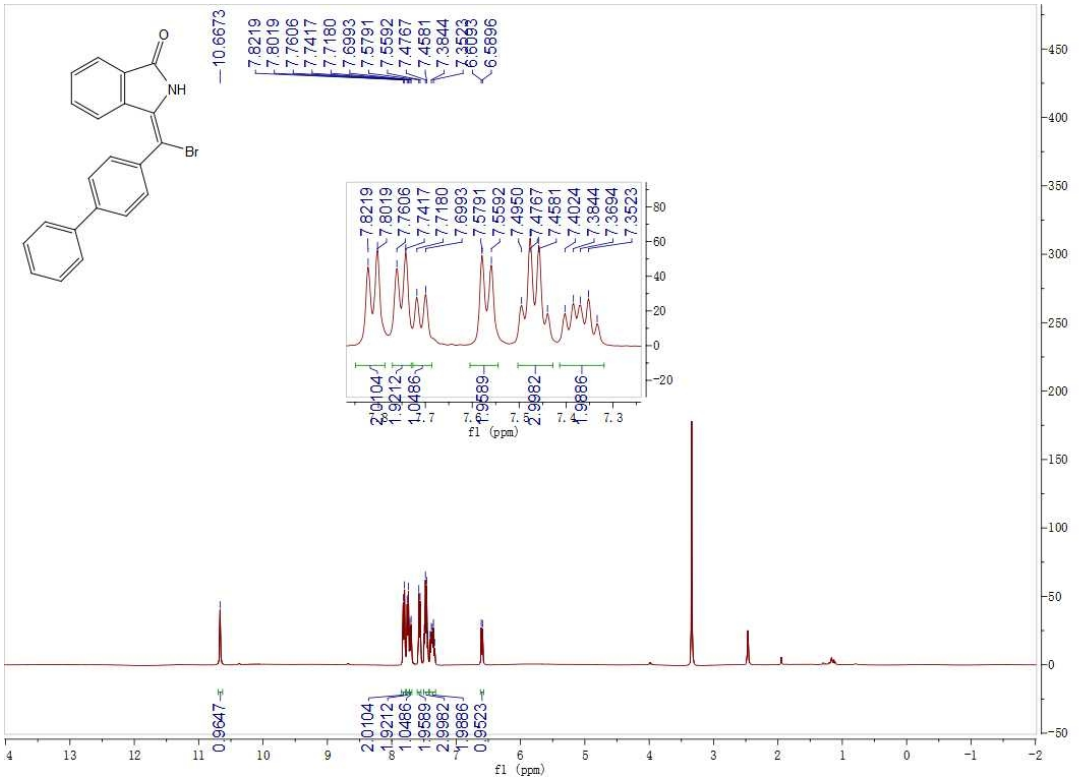
135.08
135.02
132.97
131.33
129.60
124.38
123.65
112.07
16.89
11.51
135.08
135.02
132.97
131.33
f1 (ppm)
f1 (ppm)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7.7606
7.7417
7.7180
7.6993
7.5791
7.5592
7.4767
7.4581
7.3844
7.3523
6.5896
NH
O
Br
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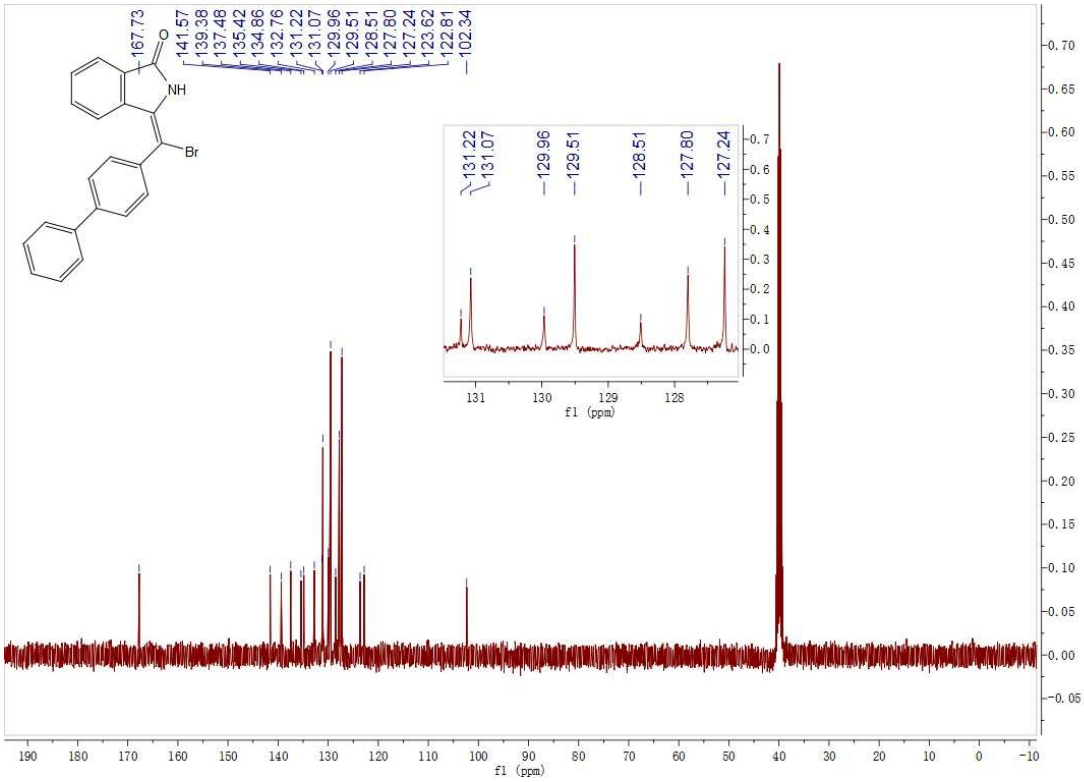
1.9212
1.0486
1.9589
2.9982
1.9886
0.9523
f1 (ppm)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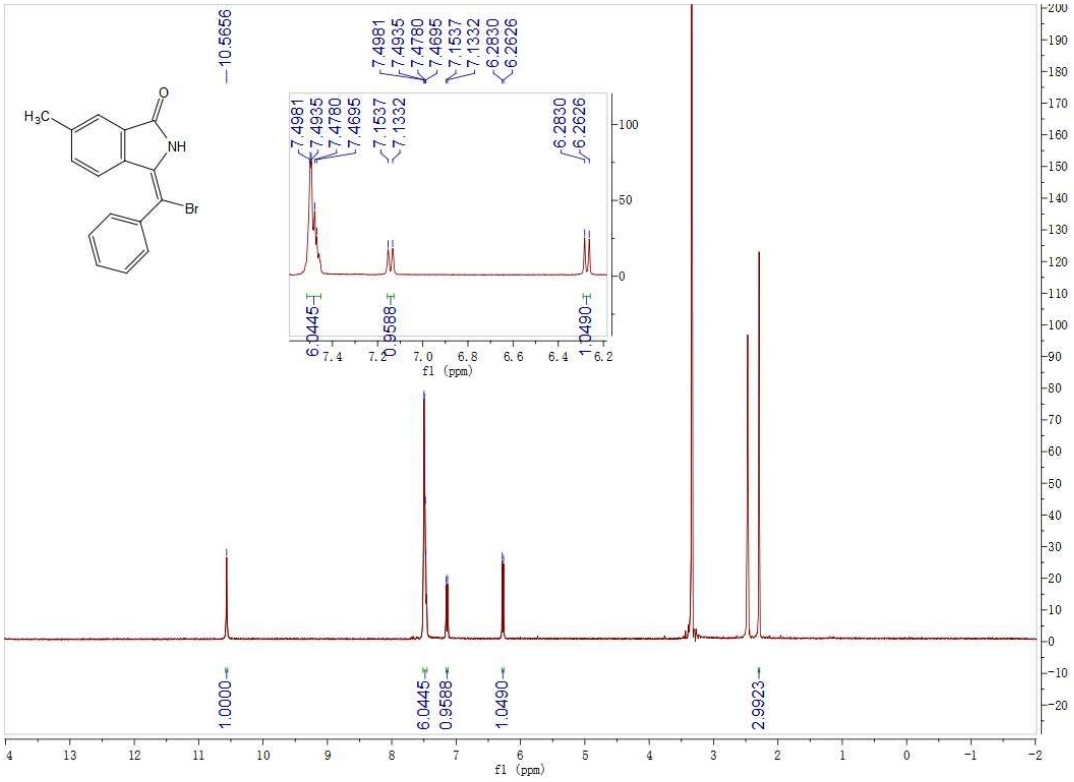
135.42
134.86
132.76
131.22
131.07
129.96
129.51
128.51
127.80
127.24
123.62
122.81
102.34
NH
O
Br
f1 (ppm)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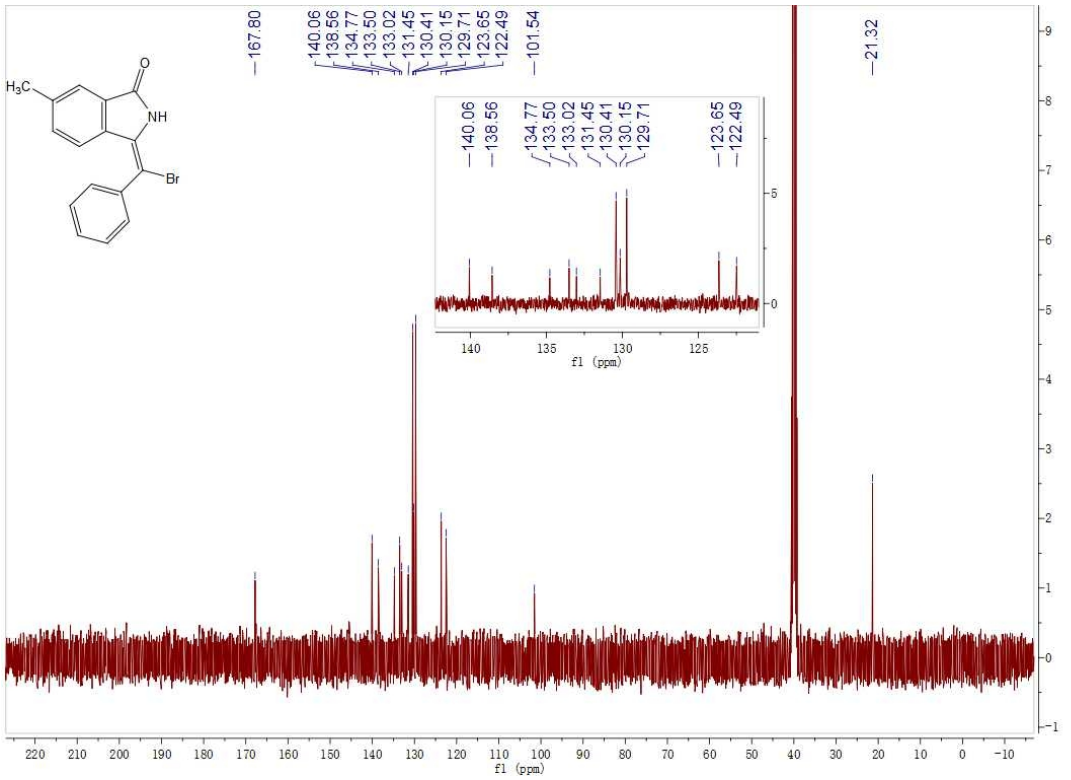
7.4935
7.4780
7.4695
7.1537
7.1332
6.2830
6.2626
1.0000
6.0445
0.9588
1.0490
2.9923
f1 (ppm)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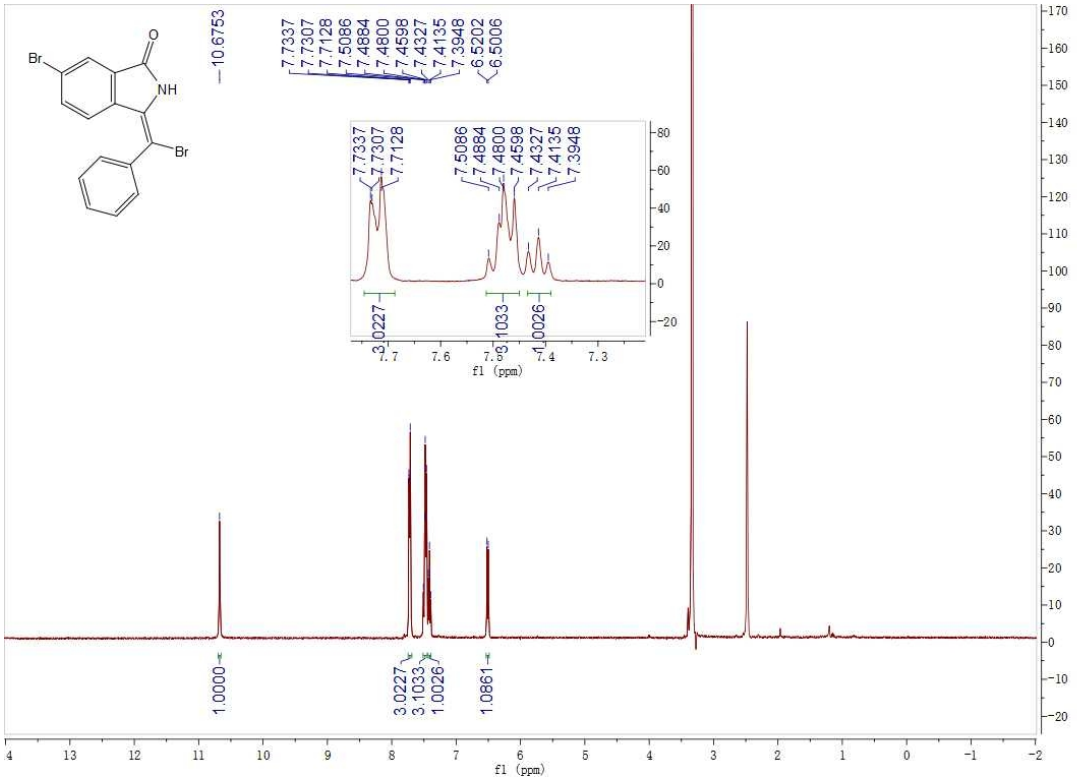
130.41
130.15
129.71
123.65
122.49
101.54
21.32
f1 (ppm)


Br
O
NH
Br
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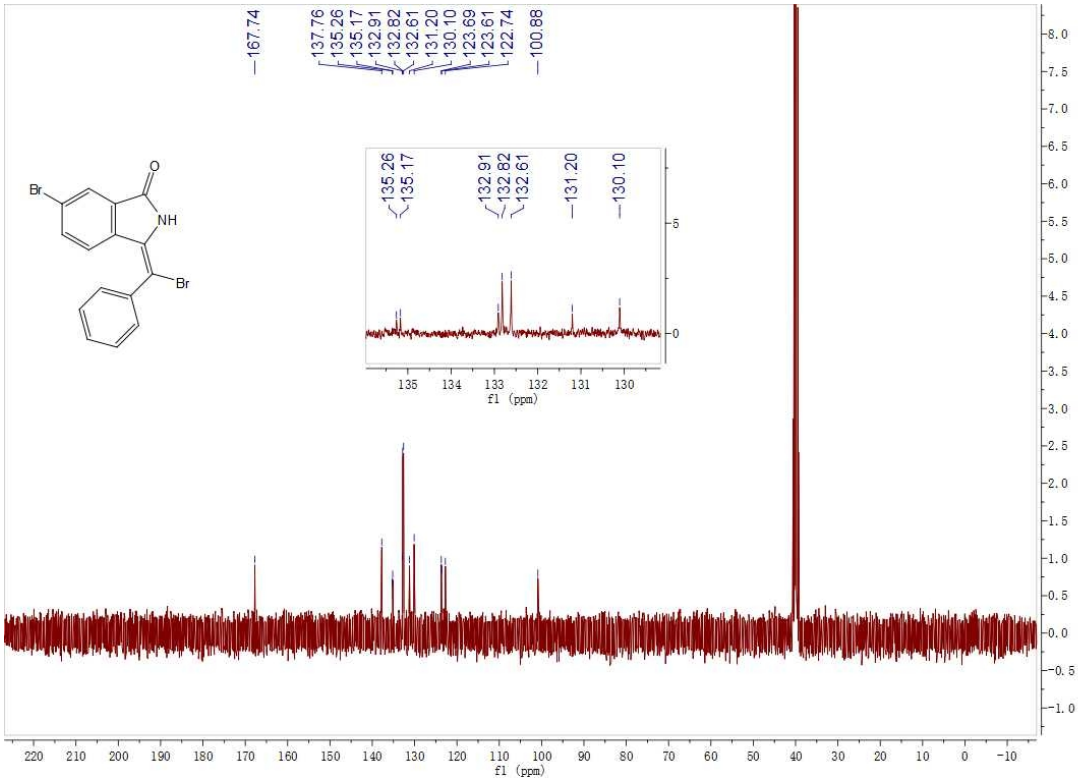
7.7337
7.7307
7.7128
7.5086
7.4884
7.4800
7.4598
7.4327
7.4135
7.3948
6.5202
6.5006
1.0000
3.0227
3.1033
1.0026
1.0861
f1 (ppm)


Br
O
NH
Br
167.74
137.76
135.26
135.17
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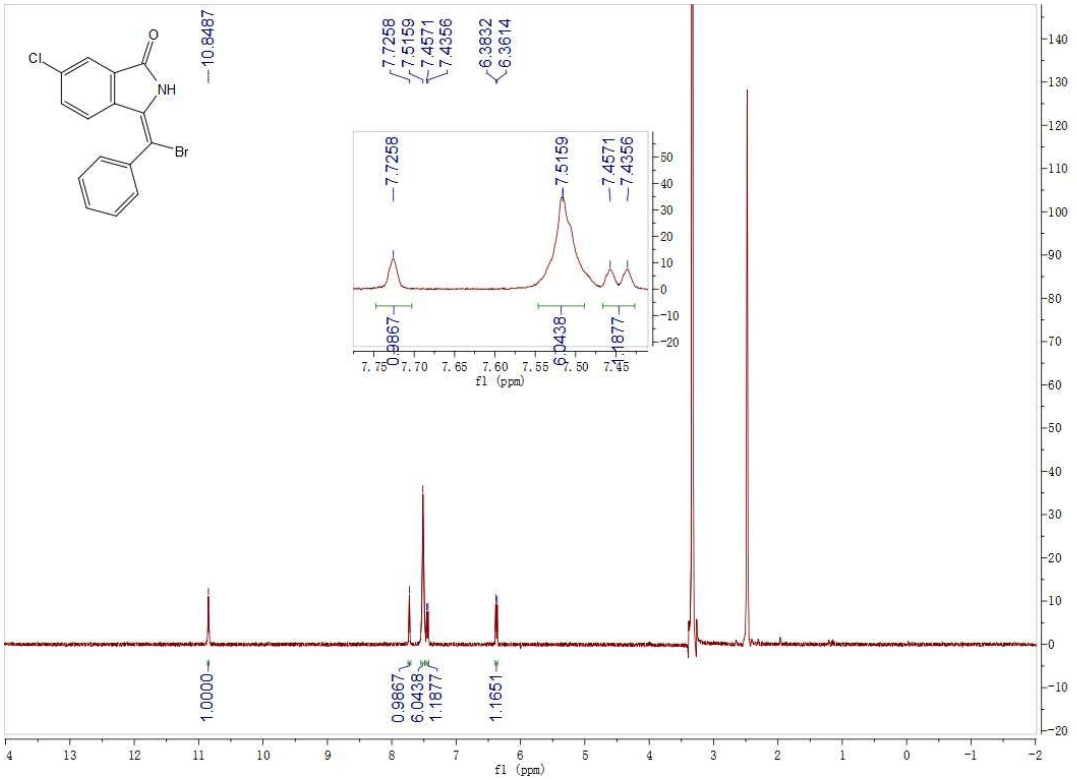
132.82
132.61
131.20
130.10
123.69
123.61
122.74
100.88
f1 (ppm)


Cl
O
NH
Br
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7.7258
7.5159
7.4571
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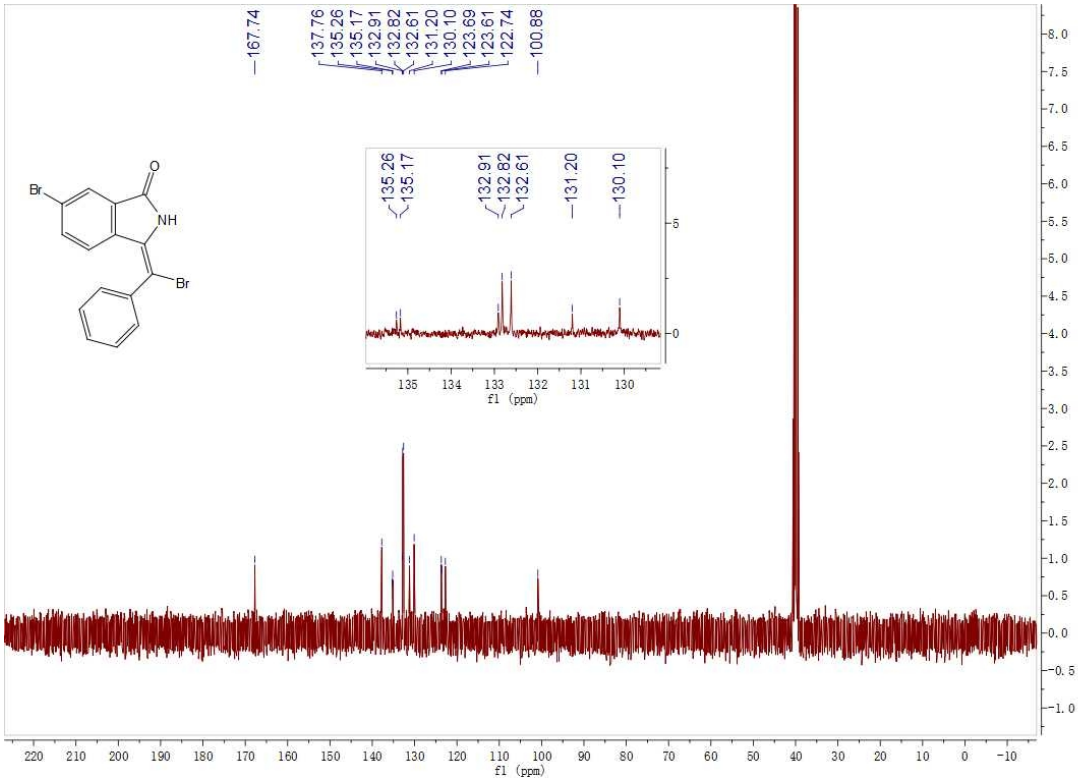
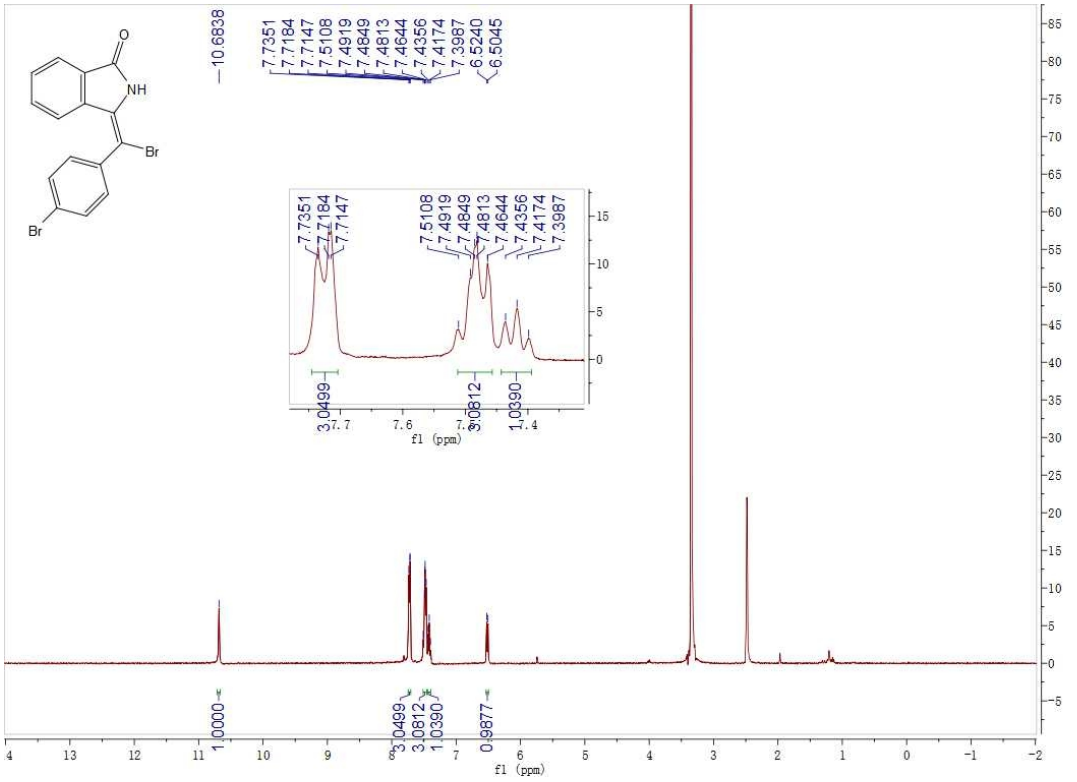
6.3614
1.0000
0.9867
6.0438
1.1877
1.1651
f1 (ppm)


Br
O
NH
Br
167.74
137.76
135.26
135.17
132.91
132.82
132.61
131.20
130.10
123.69
123.61
122.74
100.88
f1 (ppm)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7.7184
7.7147
7.5108
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7.4813
7.4644
7.4356
7.4174
7.3987
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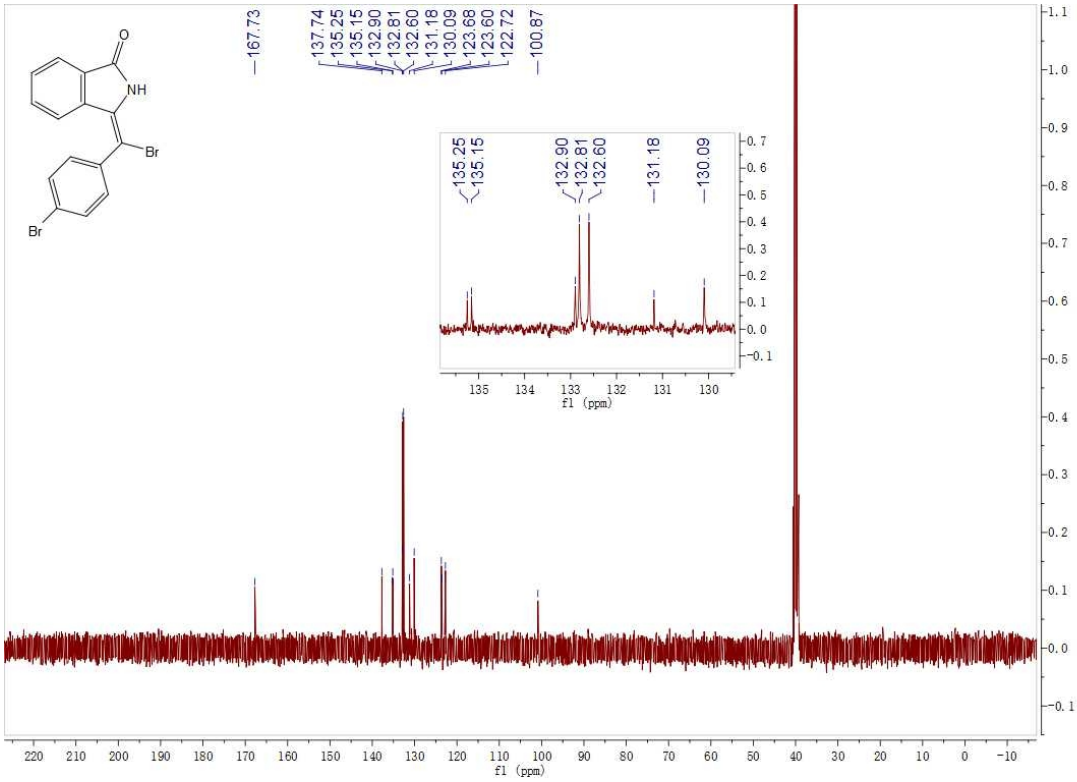
6.5045
NH
Br
Br
1.0000
3.0499
3.0812
1.0390
0.9877
f1 (ppm)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132.81
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131.18
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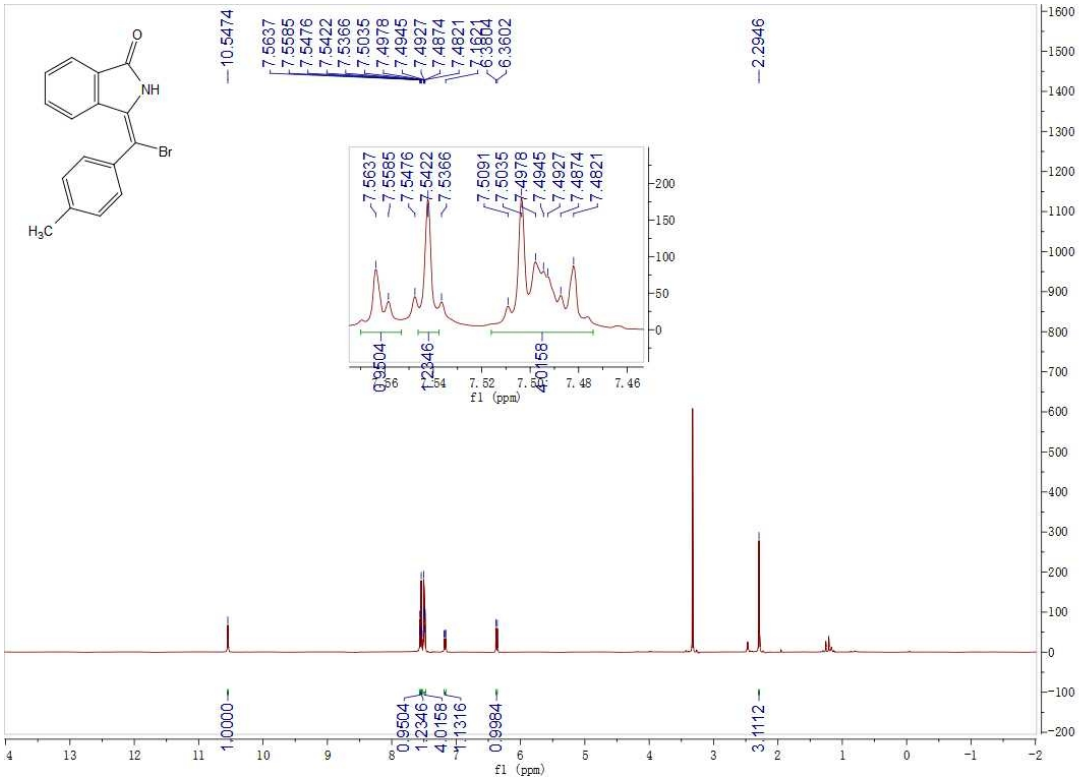
123.68
123.60
122.72
100.87
NH
Br
Br
f1 (ppm)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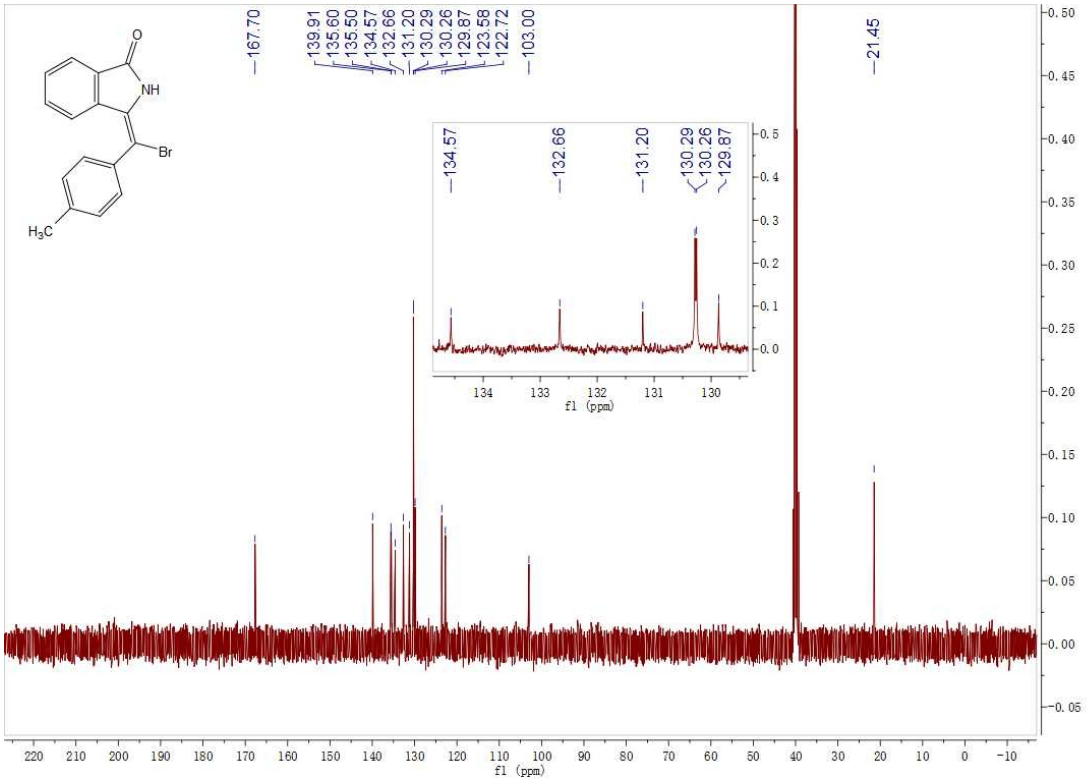
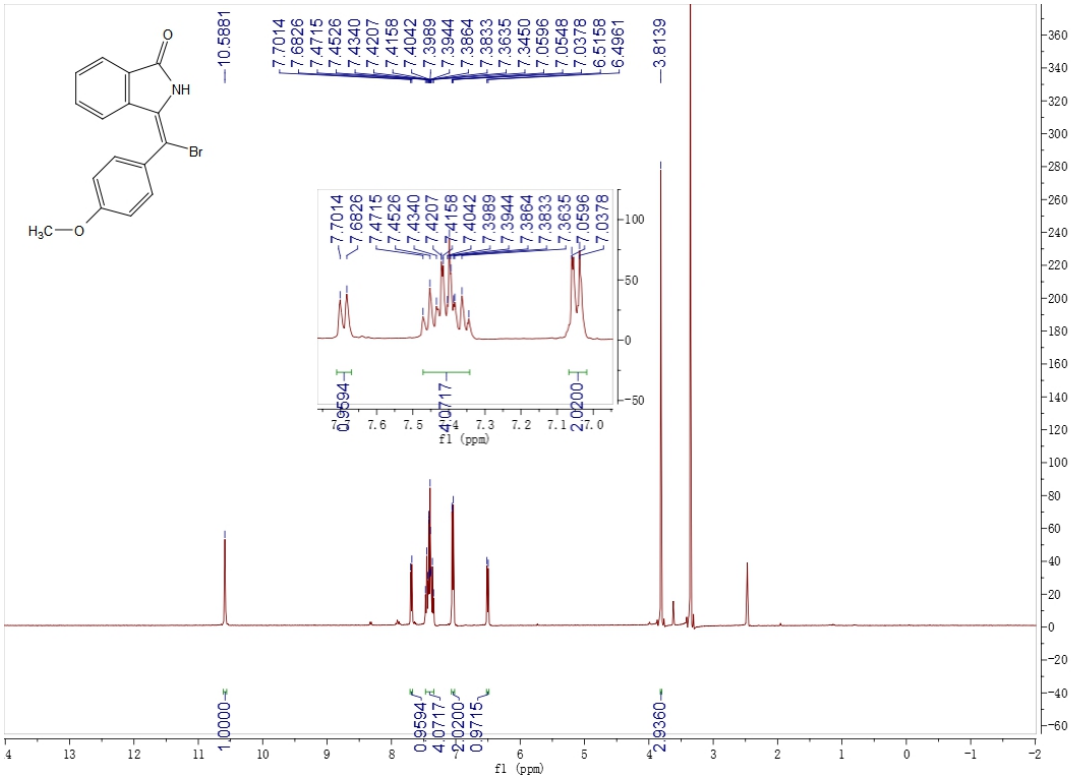
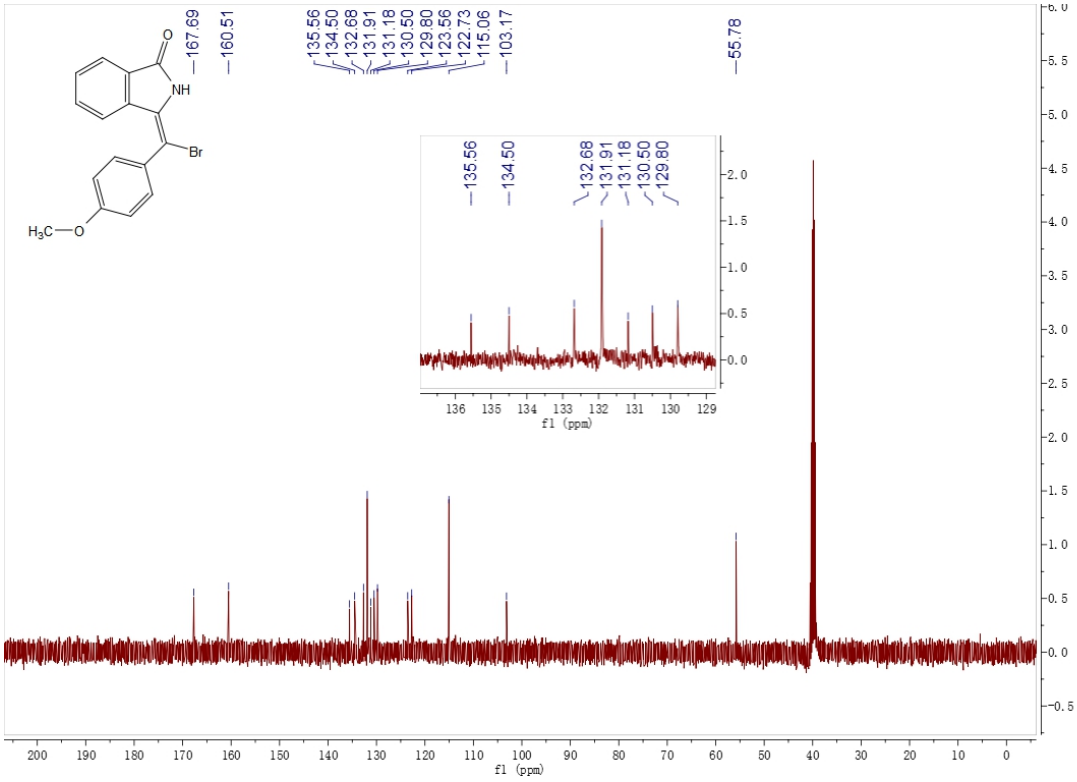
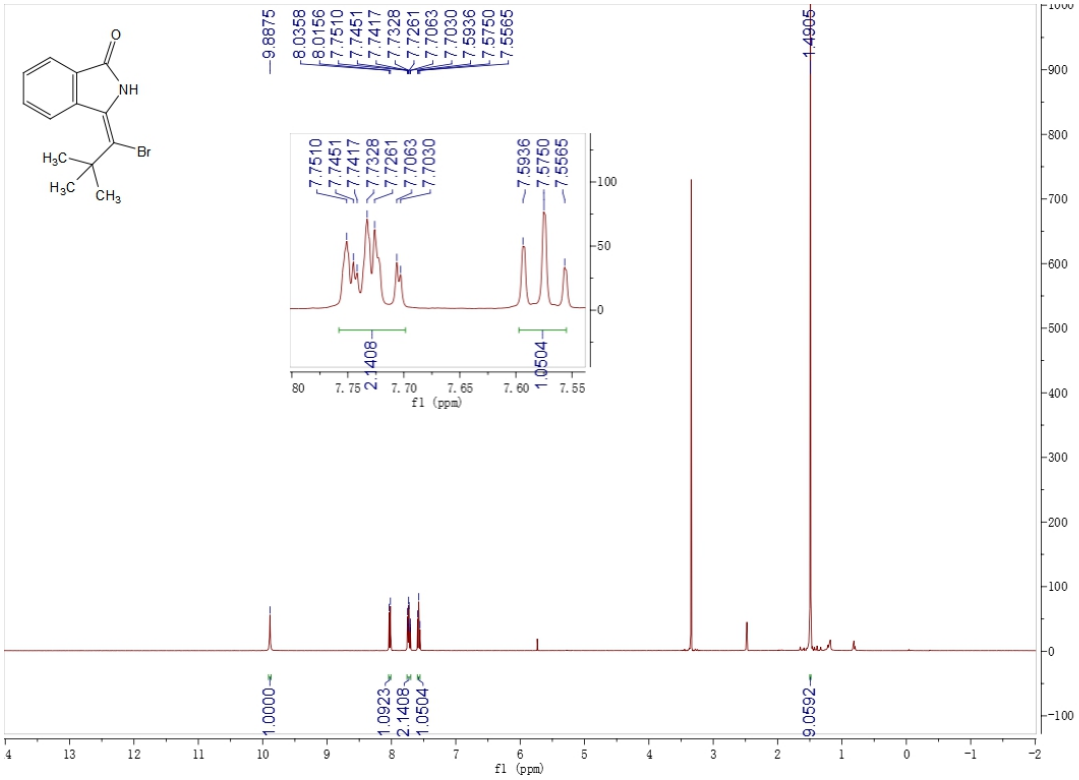
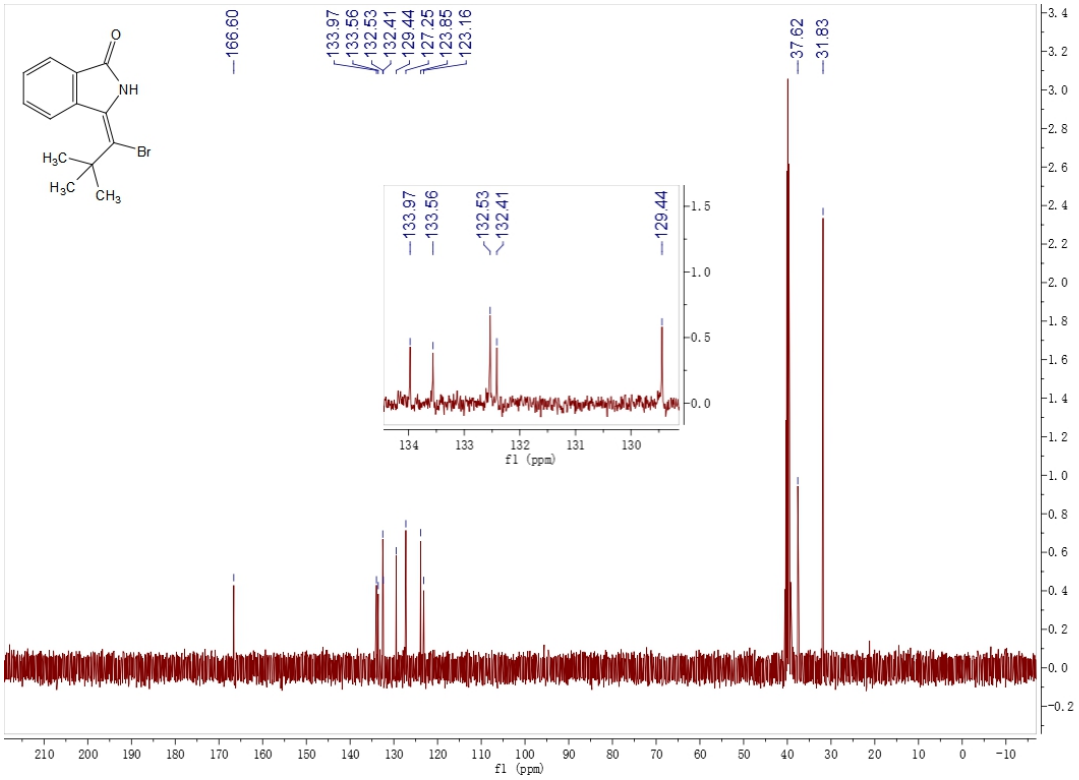
7.5637
7.5585
7.5476
7.5422
7.5366
7.5035
7.4978
7.4945
7.4927
7.4874
7.4821
7.1621
6.3864
6.3602
2.2946
NH
O
Br
H3C
f1 (ppm)

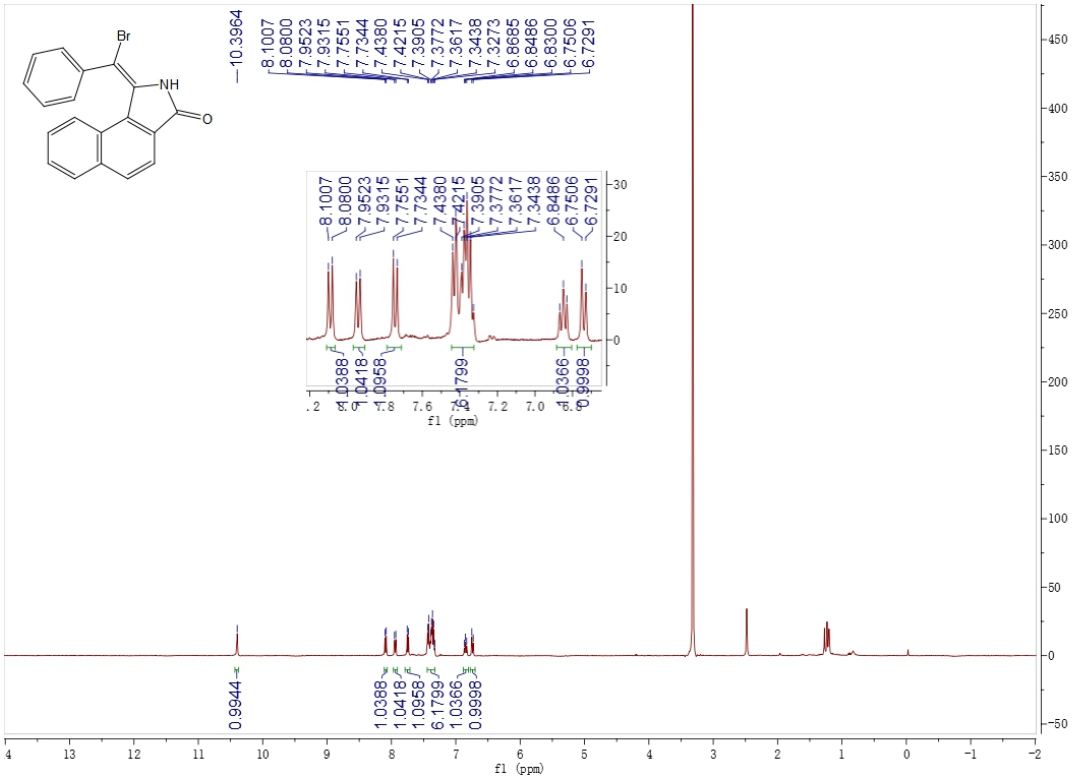

167.70
139.91
135.60
135.50
134.57
132.66
131.20
130.29
130.26
129.87
123.58
122.72
103.00
21.45
NH
O
Br
H3C
f1 (ppm)

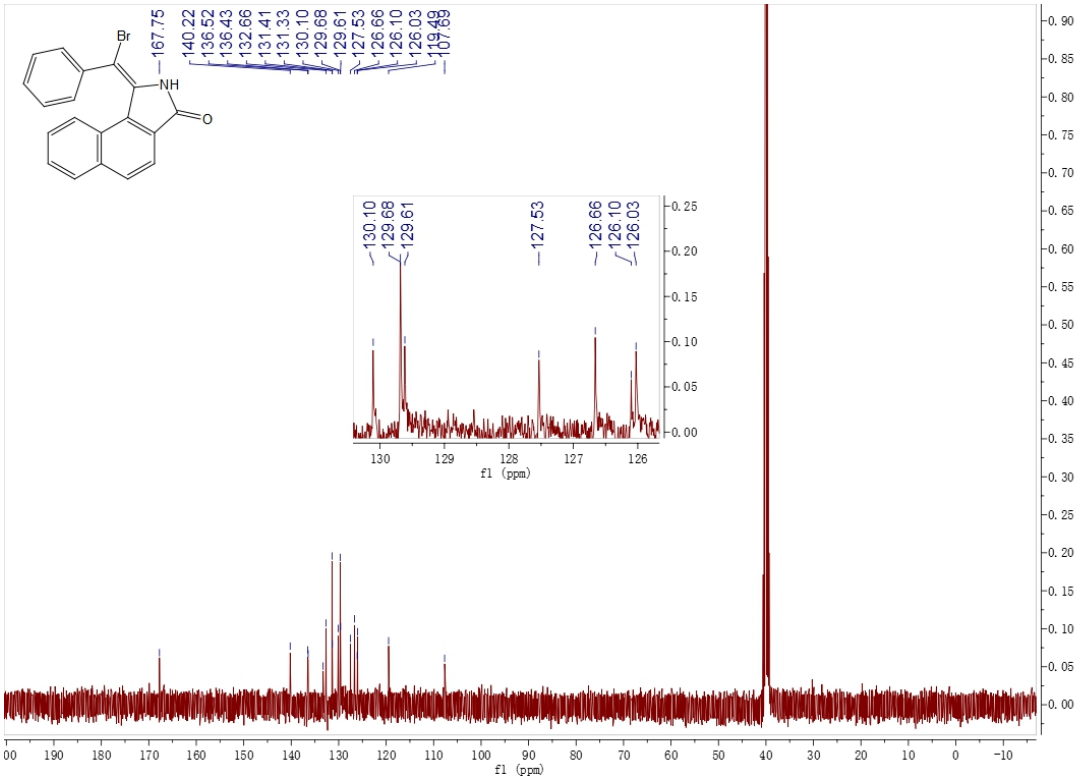

10.5881
7.7014
7.6826
7.4715
7.4526
7.4340
7.4207
7.4158
7.4042
7.3989
7.3944
7.3864
7.3833
7.3635
7.3450
7.0596
7.0548
7.0378
6.5158
6.4961
3.8139
NH
Br
H3C—O
1.0000
0.9594
4.0717
2.0200
0.9715
2.9360
f1 (ppm)

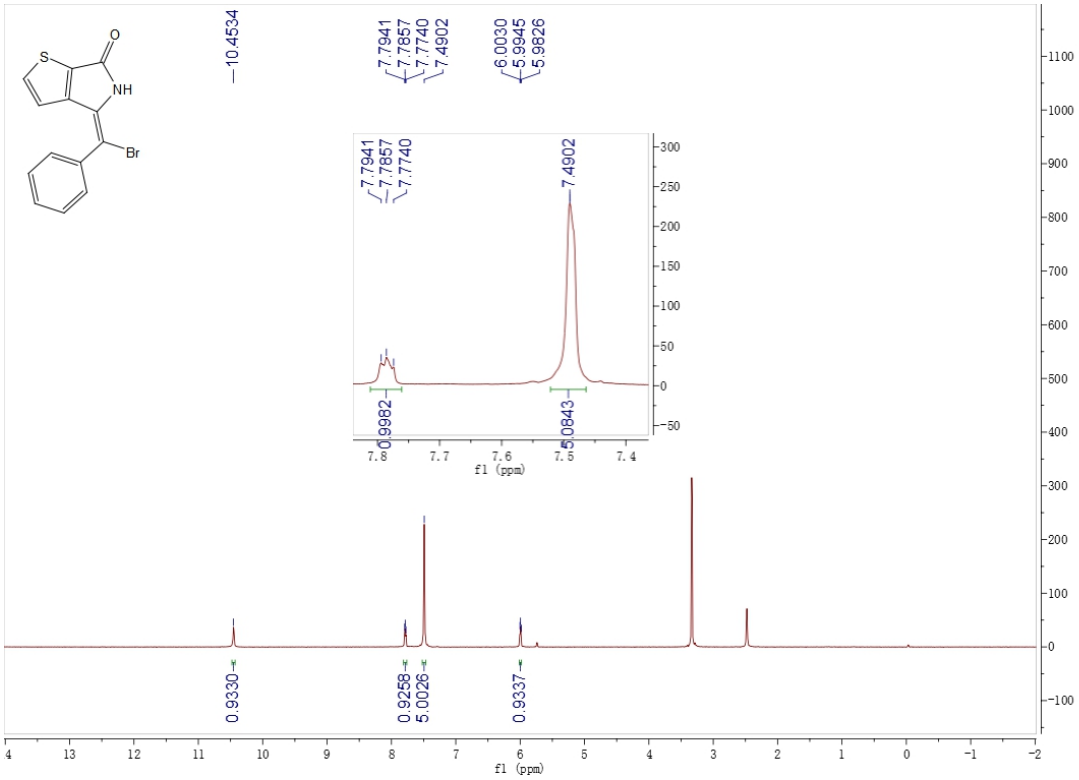

167.69
160.51
135.56
134.50
132.68
131.91
131.18
130.50
129.80
123.56
122.73
115.06
103.17
55.78
NH
Br
H3C—O
f1 (ppm)

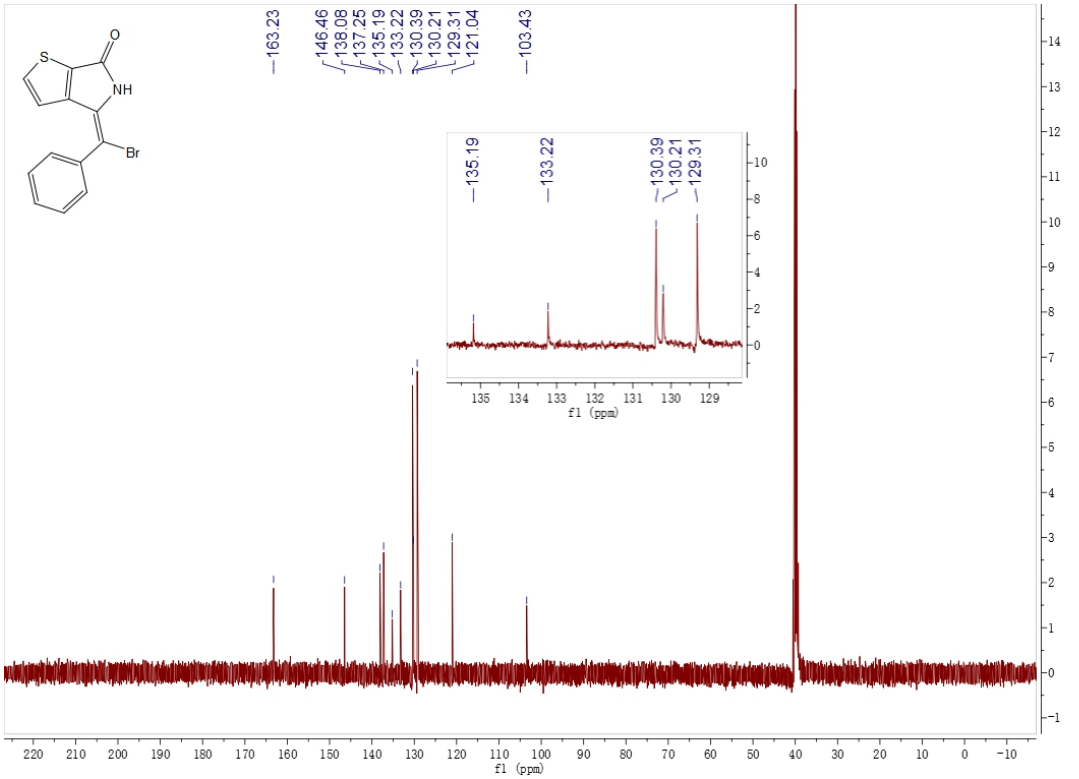

9.9875
8.0358
8.0156
7.7510
7.7451
7.7417
7.7328
7.7261
7.7063
7.7030
7.5936
7.5750
7.5565
1.4905
1.0000
1.0923
2.1408
1.0504
9.0592
f1 (ppm)

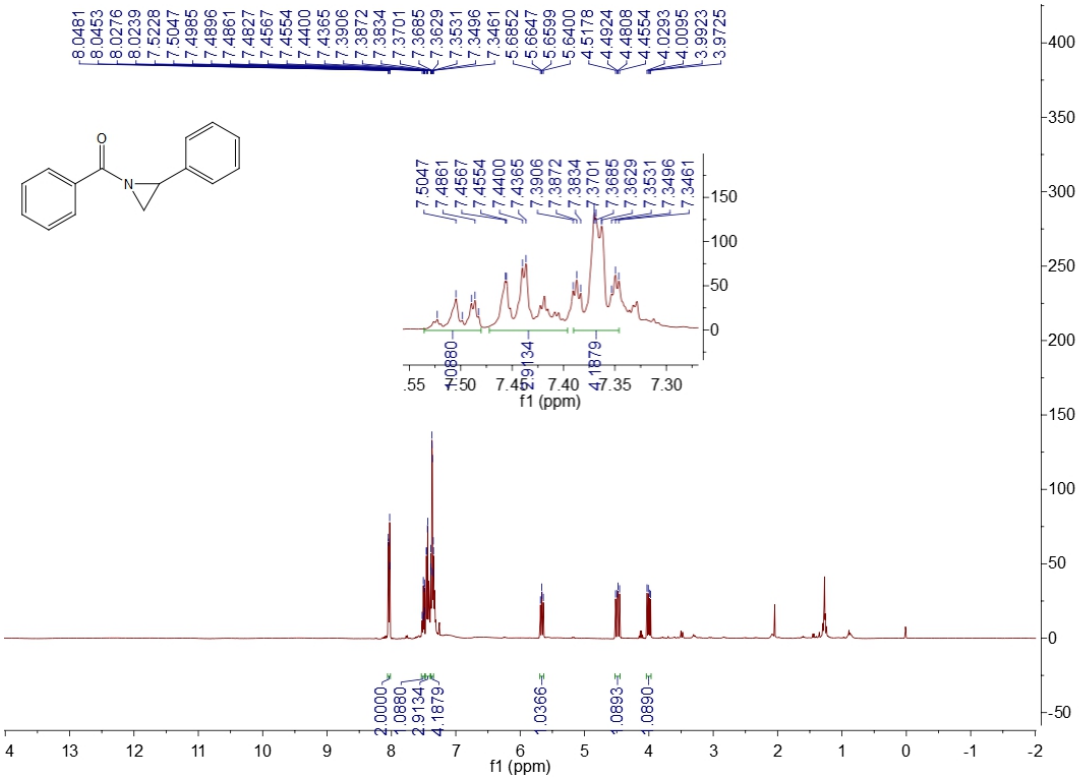

166.60
133.97
133.56
132.53
132.41
129.44
127.25
123.85
123.16
37.62
31.83
f1 (ppm)

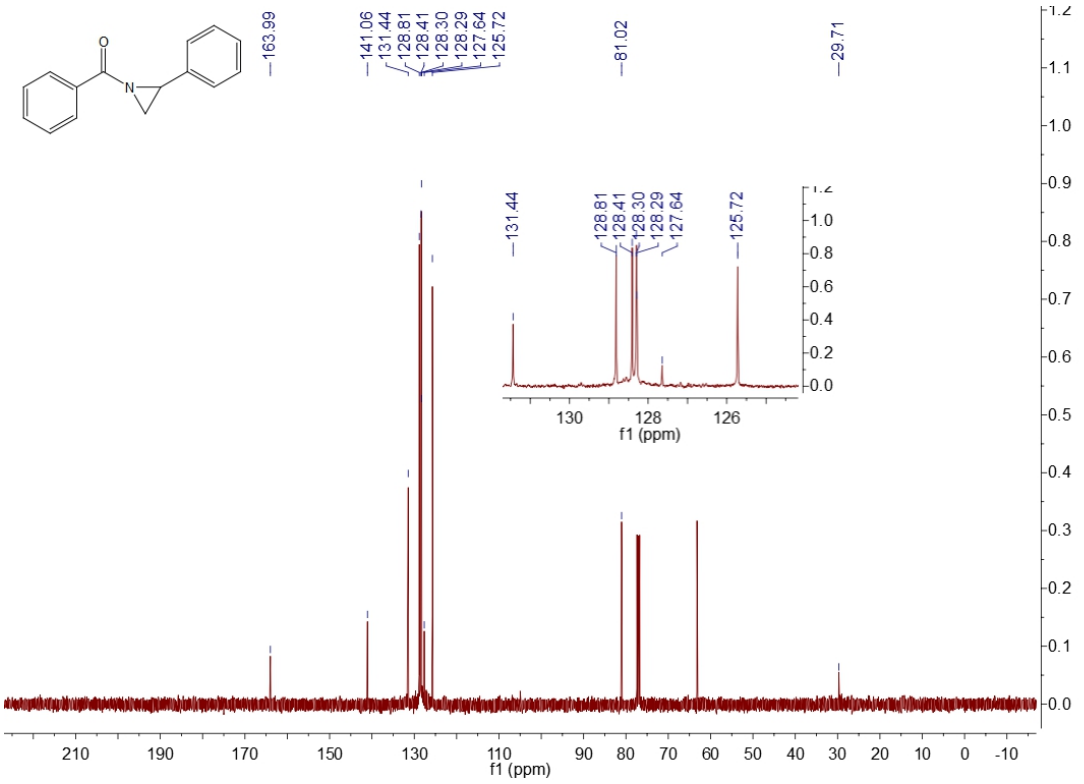

Br
NH
O
10.3964
8.1007
8.0800
7.9523
7.9315
7.7551
7.7344
7.4380
7.4215
7.3905
7.3772
7.3617
7.3438
7.3273
6.8685
6.8486
6.8300
6.7506
6.7291
0.9944
1.0388
1.0418
1.0958
6.1799
1.0366
0.9998
f1 (ppm)

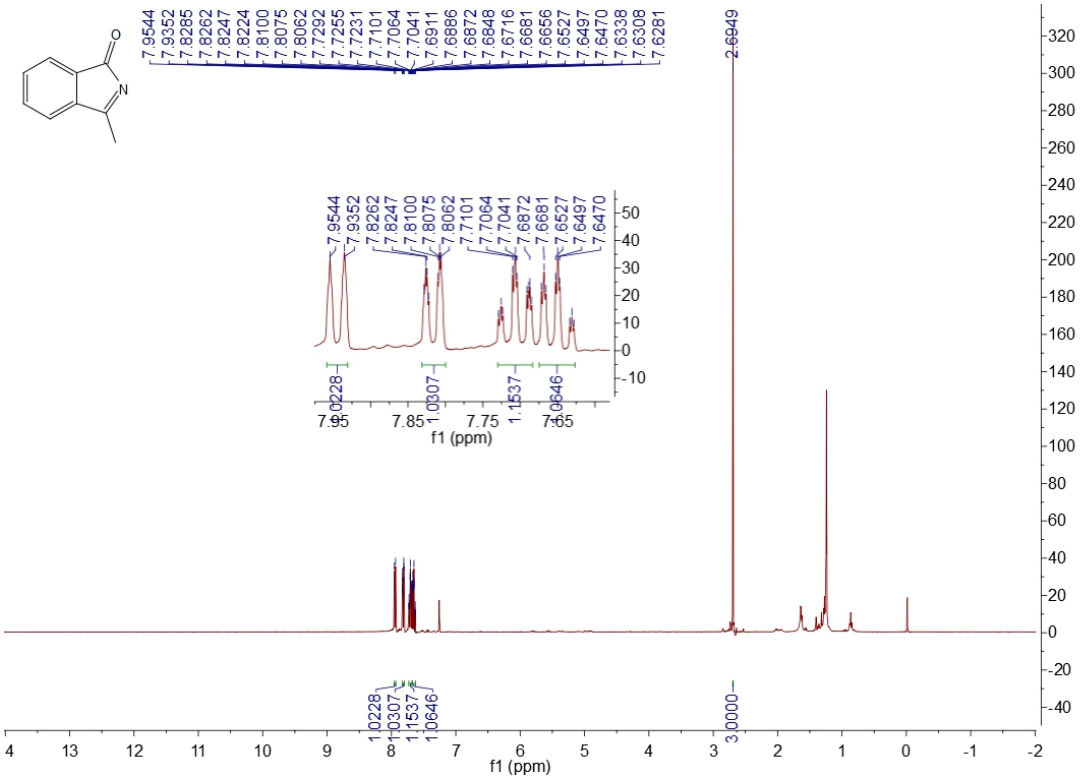

Br
NH
O
167.75
140.22
136.52
136.43
132.66
131.41
131.33
130.10
129.68
129.61
127.53
126.66
126.10
126.03
119.49
107.69
f1 (ppm)

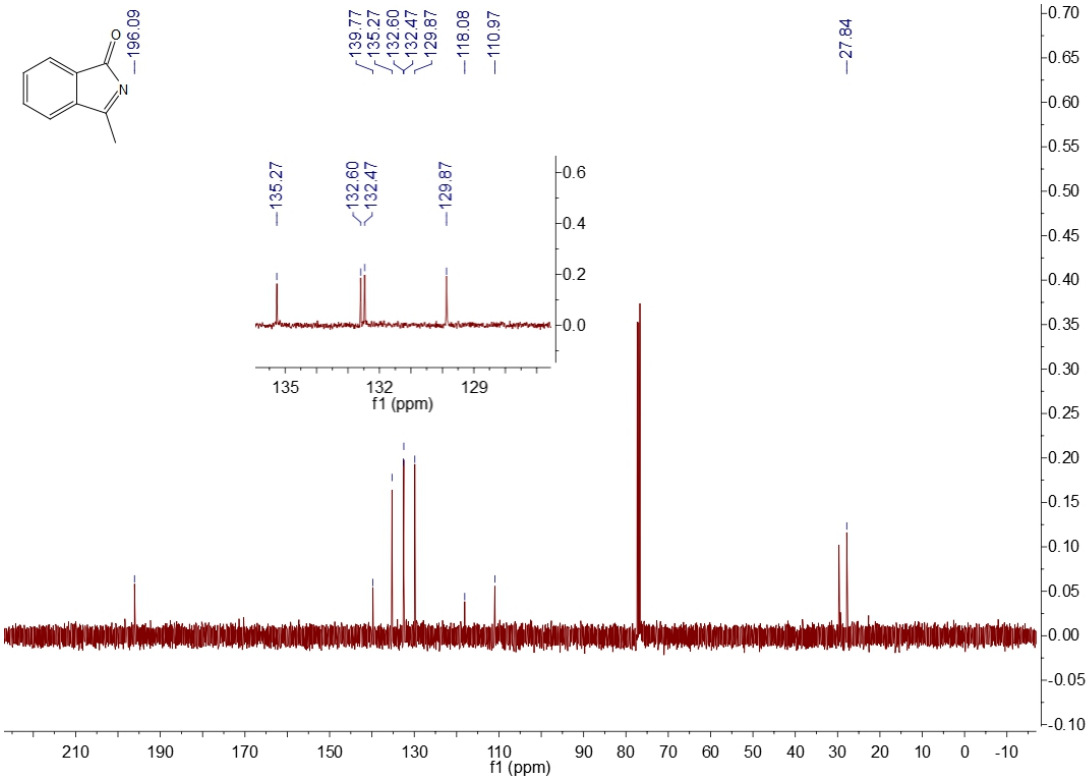

O
S
NH
Br
10.4534
7.7941
7.7857
7.7740
7.4902
6.0030
5.9945
5.9826
0.9982
5.0843
f1 (ppm)
0.9330
0.9258
5.0026
0.9337
f1 (ppm)


O
S
NH
Br
163.23
146.46
138.08
137.25
135.19
133.22
130.39
130.21
129.31
121.04
103.43
135.19
133.22
130.39
130.21
129.31
f1 (ppm)
f1 (ppm)


8.0481
8.0453
8.0276
8.0239
7.5228
7.5047
7.4985
7.4896
7.4861
7.4827
7.4567
7.4554
7.4400
7.4365
7.3906
7.3872
7.3834
7.3701
7.3685
7.3629
7.3531
7.3496
7.3461
5.6852
5.6647
5.6599
5.6400
4.5178
4.4924
4.4808
4.4554
4.0293
4.0095
3.9923
3.9725
O
N
2.0000
1.0880
2.9134
4.1879
1.0366
1.0893
1.0890
f1 (ppm)


O
N
163.99
141.06
131.44
128.81
128.41
128.30
128.29
127.64
125.72
81.02
29.71
f1 (ppm)


7.9544
7.9352
7.8285
7.8262
7.8247
7.8224
7.8100
7.8075
7.8062
7.7292
7.7255
7.7231
7.7101
7.7064
7.7041
7.6911
7.6886
7.6872
7.6848
7.6716
7.6681
7.6656
7.6527
7.6497
7.6470
7.6338
7.6308
7.6281
2.6949
1.0228
1.0307
1.1537
1.0646
3.0000
f1 (ppm)


196.09
139.77
135.27
132.60
132.47
129.87
118.08
110.97
27.84
f1 (ppm)