Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Synthesis of 2-substituted 3-chlorobenzofurans *via* TMSCl-mediated nucleophilic annulation of isatin-derived propargylic alcohol

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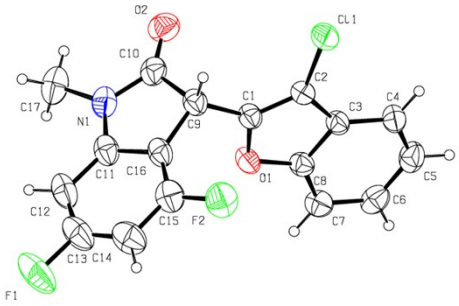
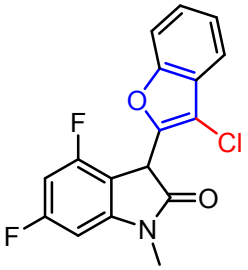
X-Ray Single Crystal Diffraction Data of 3-(3-chlorobenzofuran-2-yl)-4,6-difluoro-1-methylindolin-2-one (2r).

The CCDC deposition number: CCDC (**2r**): 1832855





Bond precision: C-C = 0.0064 A Wavelength=1.54184

Cell: a=8.1375(4) b=8.1375(4) c=22.6700(15)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1501.18(18)	1501.17(18)
Space group	P 41	P 41
Hall group	P 4w	P 4w
Moiety formula	C17 H10 Cl F2 N O2	C17 H10 Cl F2 N O2
Sum formula	C17 H10 Cl F2 N O2	C17 H10 Cl F2 N O2
Mr	333.71	333.71
Dx,g cm-3	1.477	1.477
Z	4	4
Mu (mm-1)	2.545	2.545
F000	680.0	680.0
F000'	683.71	
h,k,lmax	9,9,26	9,9,26
Nref	2657[1365]	1878
Tmin,Tmax	0.625,0.683	0.480,1.000
Tmin'	0.558	

Correction method= # Reported T Limits: Tmin=0.480 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.38/0.71 Theta(max)= 66.583

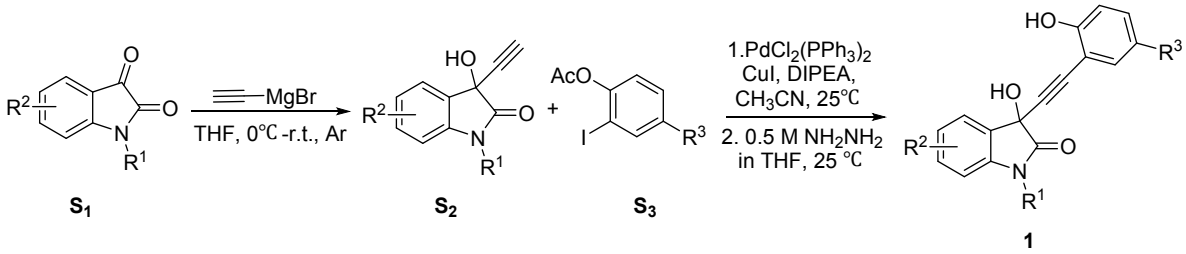
R(reflections)= 0.0368(1739) wR2(reflections)= 0.0986(1878)

S = 1.050 Npar= 209

General Procedure for the Preparation of Isatin Derived Propargylic Alcohols [1].

Step 1: Synthesis of 3-alkynyloxindoles ***S₂***. To a solution of $\mathbf{S_1}$ (2 mmol, 1.0 equiv) in dry THF (5 mL) was added ethynylmagnesium bromide (0.5 M in THF, 6 mL, 1.5 equiv) at 0˚C under argon for 6 hours. After the reaction was completed as determined by TLC, the reaction mixture was quenched with saturated aqueous NH_4Cl, extracted with ethyl acetate, washed with brine and dried over anhydrous Na_2SO_4. The solvent was evaporated under the reduced pressure and the residue was purified by column chromatography on silica gel to afford the desired product $\mathbf{S_2}$.

Step 2: Synthesis of Isatin derived propargylic alcohols ***1***. A mixture of phenyl iodide $\mathbf{S_3}$ (0.5 mmol, 1.0 equiv), $\mathbf{S_2}$ (1.0 mmol, 2.0 equiv), CuI (0.025 mmol) and $Pd(PPh_3)_2Cl_2$ (0.025 mmol) in dry CH_3CN (10 mL) was degassed with argon for 10 minutes, and the reaction mixture was treated with DIPEA (0.45 mL, 2.5 mmol), then stirred at 25˚C for 24 hours. The reaction mixture was concentrated and the residue was purified by flash column chromatography to afford the corresponding *o*-propynolphenol acetate. This acetate was treated with 0.5 M NH_2NH_2 in THF (3 mL) at 25˚C for 30 min., and then purified by flash column chromatography to afford corresponding Isatin derived propargylic alcohols.



Scheme 1 Preparation of 2-propynolphenols

3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methylindolin-2-one(1a).

Light grey solid **1a** (51% yield over two steps), mp 157-158°C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.92 (s, 1H), 7.49 (d, *J* = 3.6 Hz, 1H), 7.38 (t, *J* = 7.6, 1H), 7.24-7.17 (m, 2H), 7.12 (t, *J* = 8.0Hz, 1H), 7.08 (s, 1H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.86 (d, *J* = 8.0Hz, 1H), 6.76 (t, *J* = 7.6 Hz, 1H), 3.16 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.1, 158.5, 142.6, 133.2, 130.6, 130.4, 129.9, 124.1, 123.0, 119.0, 115.5, 109.1, 108.7, 90.4, 81.8, 68.8, 26.2; HRMS-ESI (m/z): calcd for $C_{17}H_{13}NO_3$ $[M+Na]^+$: 302.0793; found 302.0796.

1-ethyl-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)indolin-2-one(1b).

Light grey solid **1b** (53% yield over two steps), mp 158-159˚C. ^{1}H NMR (DMSO-d_6,400 MHz): *δ* 10.01 (s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.17–7.08 (m, 3H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.77 (t, *J* = 7.6 Hz, 1H), 3.81–3.60 (m, 2H), 1.17 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): *δ* 172.9, 158.6, 141.6, 133.3, 130.8, 130.5, 130.0, 124.5, 122.9, 119.1, 115.6, 109.2, 108.7, 90.5, 81.9, 69.0, 34.4, 12.4; HRMS-ESI (m/z): calcd for $C_{18}H_{15}NO_3$ $[M+Na]^+$: 316.0950; found: 316.0955.

3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-isopropylindolin-2-one(1c).

Light grey solid **1c** (52% yield over two steps), mp 160-161˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): *δ* 9.96 (s, 1H), 7.54 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.37 (td, *J* = 8.0, 1.2 Hz, 1H), 7.28–7.20 (m, 3H), 7.13 (t, *J* = 7.2 Hz, 1H),7.07 (s, 1H), 6.90 (d, *J* = 7.6 Hz, 1H), 6.81-6.77 (m, 1H), 4.48 (septet, J = 6.8 Hz 1H), 1.42

(d, J = 6.8, 3H), 1.41 (d, J = 6.8, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.9, 158.5, 141.2, 133.2, 131.0, 130.4, 129.8, 124.5, 122.5, 119.0, 115.5, 110.2, 108.7, 90.6, 81.7, 68.8, 43.7, 19.0, 18.8; HRMS-ESI (m/z): calcd for $C_{19}H_{17}NO_3$ $[M+Na]^+$: 330.1106; found: 330.1110.

1-benzyl-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)indolin-2-one(1d).

Light yellow solid **1d** (49% yield over two steps), mp 175-176˚C. ^{1}H NMR (Acetone-d_6, 400 MHz): δ 8.59 (s, 1H), 7.60 (dd, J = 7.6, 0.8 Hz, 1H), 7.41-7.39 (m, 2H), 7.35–7.21 (m, 6H), 7.11 (td, J = 7.6, 0.8 Hz, 1H), 6.93-6.89 (m, 2H), 6.83 (td, J = 7.6, 0.8 Hz, 1H), 6.32 (s, 1H), 4.97 (d, J = 1.2 Hz, 2H); ^{13}C NMR (Acetone-d_6, 100 MHz): δ 174.4, 159.2, 143.0, 137.0, 133.8, 131.4, 131.1, 130.7, 129.5, 128.3, 128.0, 125.4, 124.0, 120.4, 116.4, 110.5, 109.9, 91.9, 82.4, 70.3, 43.9; HRMS-ESI (m/z): calcd for $C_{23}H_{17}NO_3$ $[M+Na]^+$: 378.1106; found: 378.1112.

3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1,5-dimethylindolin-2-one(1e).

Light grey solid **1e** (58% yield over two steps) as, mp 159-160˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.92 (s, 1H), 7.31 (s, 1H), 7.24 (dd, J = 7.6, 1.6 Hz, 1H), 7.22–7.15 (m, 2H), 7.04 (s, 1H), 6.93 (d, J = 8.0 Hz, 1H), 6.87 (d, J = 7.6 Hz, 1H), 6.77 (td, J = 7.6, 0.8 Hz, 1H), 3.13 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz)**:** δ 173.1, 158.5, 140.2, 133.2, 132.0, 130.5, 130.3, 130.0, 124.7, 119.0, 115.5, 108.8, 108.7, 90.5, 81.7, 69.0, 26.2, 20.6; HRMS-ESI (m/z): calcd for $C_{18}H_{15}NO_3$[M+Na]$^+$: 316.0950; found: 316.0955.

3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1,7-dimethylindolin-2-one(1f).

Light yellow solid **1f** (55% over two steps), mp 157-158˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.89 (s, 1H), 7.32 (d, J = 6.8 Hz, 1H), 7.25–7.15 (m, 2H), 7.11 (d, J = 7.6 Hz, 1H), 7.01–6.97 (m, 2H), 6.85 (d, J = 7.6 Hz, 1H), 6.76 (td, J = 7.2, 0.8 Hz, 1H), 3.42 (s, 3H), 3,33 (H_2O), 2.55 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.7, 158.5, 140.1, 133.3, 133.2, 131.2, 130.3, 122.9, 122.2, 120.3, 119.0, 115.5, 108.7, 90.6, 81.7, 68.3, 29.2, 18.4; HRMS-ESI (m/z): calcd for $C_{18}H_{15}NO_3$[M+Na]$^+$: 316.0950; found: 316.0955.

3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-5-methoxy-1-meth-ylindolin-2-one(1g).

White solid **1g** (54% over two steps), mp 164-166˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.92 (s, 1H), 7.24 (dd, J = 7.6, 1.6 Hz, 1H), 7.22–7.16 (m, 1H), 7.10 (d, J = 2.0 Hz, 1H), 7.07 (s, 1H), 6.97–6.93 (m, 2H), 6.86 (d, J = 7.6 Hz, 1H), 6.76 (td, J = 7.6, 1.2 Hz, 1H), 3.76 (s, 3H), 3.13 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.3, 159.0, 156.3, 136.3, 133.7, 132.2, 130.9, 119.5, 116.0, 114.7, 111.7, 110.1, 109.1, 90.9, 82.4, 69.7, 56.1, 26.8; **HRMS-ESI** (m/z): calcd for $C_{18}H_{15}NO_4$[M+Na]$^+$: 332.0899; found: 332.0904.

5-fluoro-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methyl-indolin-2-one(1h).

White solid **1h** (49% over two steps), mp 159-160˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.97 (s, 1H), 7.37 (dd, J = 7.6, 2.4 Hz, 1H), 7.31–7.17 (m, 4H), 7.07-6.89 (m, 1H), 6.88 (d, J = 7.6 Hz, 1H), 6.78 (t, J = 7.6 Hz, 1H), 3.17 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.0, 158.8 (d, $J_{C\text{-}F}$ = 237.7), 186.6, 138.8 (d, $J_{C\text{-}F}$ = 1.7Hz), 133.3, 132.2 (d, $J_{C\text{-}F}$ = 7.8Hz), 130.6, 119.1, 116.3, 116.0, 115.6, 111.9 (d, $J_{C\text{-}F}$ = 2.5Hz), 108.5, 89.8, 82.3. 69.0, 26.4; HRMS-ESI (m/z): calcd for $C_{17}H_{12}FNO_3$[M+Na]$^+$: 320.0699; found: 320.0703.

6-fluoro-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methyl-indolin-2-one(1i).

White solid **1i** (50% over two steps), mp 158˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.93 (s, 1H), 7.51–7.48 (m, 1H), 7.26–7.16 (m, 2H), 7.13 (s, 1H), 7.04 (dd, J = 9.6, 2.0 Hz, 1H), 6.94–6.83 (m, 2H), 6.76 (t, J = 7.6 Hz, 1H), 3.33 (H_2O); 3.16 (s, 3H); ^{13}C NMR (DMSO-d_6,100 MHz): δ 173.4, 163.3 (d, $J_{C\text{-}F}$ = 242.6 Hz) 158.5, 144.5 (d, $J_{C\text{-}F}$ = 12.4 Hz), 133.2, 130.5, 126.4, 125.6 (d, $J_{C\text{-}F}$ = 10.0 Hz), 119.0, 115.5, 108.8 (d, $J_{C\text{-}F}$ = 22.4 Hz), 108.5, 98.0 (d, $J_{C\text{-}F}$ = 28.1 Hz), 90.0, 81.9, 68.4, 26.5; **HRMS-ESI** (m/z): calcd for $C_{17}H_{12}FNO_3$[M+Na]$^+$: 320.0699; found: 320.0703.

4-bromo-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methyl-indolin-2-one(1j).

Light yellow solid **1j** (45% over two steps), mp 173-175˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.99 (s, 1H), 7.45 (d, J = 7.8 Hz, 1H), 7.40–7.29 (m, 2H), 7.29–7.17 (m, 3H), 6.88 (d, J = 8.0 Hz, 1H), 6.77 (t, J = 7.6 Hz, 1H), 3.18 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.0, 158.6, 144.2, 133.3, 130.6, 129.8, 125.8, 125.6, 122.8, 119.1, 115.5, 112.4, 108.5, 89.7, 82.2, 68.5, 26.5; HRMS-ESI (m/z): calcd for $C_{17}H_{12}BrNO_3$[M+Na]$^+$: 379.9898, found: 379.9903.

5-bromo-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methyl-indolin-2-one(1k).

Light yellow solid **1k** (50% yield over two steps) as, mp 176-177˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.98 (s, 1H), 7.64–7.55 (m, 2H), 7.29–7.17 (m, 3H), 7.05 (d, J = 7.6 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 6.78 (td, J = 7.6, 0.8 Hz, 1H), 3.16 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.2, 158.4, 138.0, 133.3, 133.0, 131.7, 130.4, 124.3, 123.2, 118.8, 115.3, 114.4, 108.2, 89.5, 82.2, 68.2, 29.3; HRMS-ESI (m/z): calcd for $C_{17}H_{12}BrNO_3$[M+Na]$^+$: 379.9898; found: 379.9903.

3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methyl-5-(trifleoromethoxy)indolin-2-one(1l).

Light yellow solid **1l** (44% yield over two steps), mp 178-179˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.02 (s, 1H), 7.51 (d, J = 1.2 Hz, 1H), 7.43 (dd, J = 8.4, 1.6 Hz, 1H), 7.35 (s, 1H), 7.27 (dd, J = 7.6, 1.6 Hz, 1H), 7.25–7.15 (m, 2H), 6.89 (d, J = 8.0 Hz, 1H), 6.83–6.75 (m, 1H), 3.20 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.0, 158.7, 144.5 (q, $J_{C\text{-}F}$ = 2.0Hz), 141.7, 133.3, 132.2, 130.7, 123.2, 120.6 (d, $J_{C\text{-}F}$ = 25.4Hz), 119.1, 117.8, 115.6, 110.4, 108.4, 89.5, 82.5, 68.8, 26.5; HRMS-ESI (m/z): calcd for $C_{18}H_{12}F_3NO_4$[M+Na]$^+$: 386.0616; found: 386.0622.

3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methyl-7-(trifleoromethyl)indolin-2-one(1m).

Light yellow solid **1m** (45% over two steps), mp 173-175˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.06 (s, 1H), 7.89 (d, J = 6.8 Hz, 1H), 7.78–7.72 (m, 1H), 7.59–7.34 (m, 2H), 7.30 (dd, J = 7.6, 1.5 Hz, 1H), 7.27–7.21 (m, 1H), 6.93 (d, J = 8.0 Hz, 1H), 6.81 (t, J = 7.6 Hz, 1H), 3.36 (s, 3H)； ^{13}C NMR (DMSO-d_6 100 MHz): δ 174.1, 158.8, 140.3, 133.4, 132.0 (d, $J_{C\text{-}F}$ = 261.7Hz), 128.7, 127.6 (q, $J_{C\text{-}F}$ = 25.4Hz), 124.8, 123.3, 122.1, 119.1, 115.6, 111.5 (q, $J_{C\text{-}F}$ = 5.9Hz), 108.4, 89.4, 82.6, 67.2, 28.9 (d, $J_{C\text{-}F}$ = 6.0Hz); HRMS-ESI (m/z): calcd for $C_{18}H_{12}F_3NO_3$[M+Na]$^+$: 370.0667; found: 370.0674.

4-chloro-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methyl-indolin-2-one(1n).

Light yellow solid **1n** (46% over two steps), mp 169-171˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.93 (s, 1H), 7.39 (t, J = 8.0 Hz, 1H), 7.26 (dd, J = 7.6, 1.6 Hz, 1H), 7.23–7.17 (m, 1H), 7.12 (m, 2H), 7.03 (d, J = 7.7 Hz, 1H), 6.88 (d, J = 7.9 Hz, 1H), 6.78 (t, J = 7.5 Hz, 1H), 3.17 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.1, 159.0, 144.9, 133.9, 131.9, 130.9, 130.8, 127.0, 124.1, 119.5, 116.0, 109.1, 108.5, 88.6, 82.3, 69.5, 27.0; HRMS-ESI (m/z): calcd for $C_{17}H_{12}ClNO_3$[M+Na]$^+$: 336.0403; found: 336.0409.

5-chloro-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methylin-dolin-2-one(1o).

Light gray solid **1o** (51% over two steps), mp 174-176˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.97 (s, 1H), 7.50 (d, J = 1.8 Hz, 1H), 7.46 (dd, J = 7.6, 2.0 Hz, 1H), 7.27-7.25 (m, 2H), 7.20 (t, J = 7.8 Hz, 1H), 7.10 (d, J = 8.3 Hz, 1H), 6.86 (d, J = 8.4 Hz, 1H), 6.77 (t, J = 7.6 Hz, 1H), 3.35 (H_2O), 3.16 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.7, 158.6, 141.4, 133.3, 132.4, 130.6, 129.7, 126.9, 124.1, 119.0, 115.5, 110.8, 108.4, 89.6, 82.3, 68.7, 26.4; HRMS-ESI (m/z): calcd for $C_{17}H_{12}ClNO_3$[M+Na]$^+$: 336.0403; found: 336.0409.

6-chloro-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methylin-dolin-2-one(1p).

Light yellow solid **1p** (51%), mp 169-170°C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.97 (s, 1H), 7.50 (dd, J = 7.2, 1.0 Hz, 1H), 7.38 (dd, J = 8.0, 1.2 Hz, 1H), 7.30–7.18 (m, 3H), 7.16–7.10 (m, 1H), 6.88 (d, J = 8.0 Hz, 1H), 6.78 (t, J = 8.0 Hz, 1H), 3.49 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.4, 158.6, 138.2, 133.5, 133.2, 131.9, 130.6, 124.5, 123.3, 119.0, 115.5, 114.6, 108.4, 89.7, 82.4, 68.4, 29.5; HRMS-ESI (m/z): calcd for $C_{17}H_{12}ClNO_3[M+Na]^+$**:** 336.0403; found: 336.0409.

7-chloro-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-methylin-dolin-2-one(1q)

light yellow solid **1q** (45% over two steps) as, mp 176-177°C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.97 (s, 1H), 7.50 (dd, J = 7.2, 1.2 Hz, 1H), 7.38 (dd, J = 8.0, 1.2 Hz, 1H), 7.26 (m, 2H), 7.23–7.18 (m, 1H), 7.14 (d, J = 8.0, 1H), 6.88 (d, J = 8.0 Hz, 1H), 6.77 (td, J = 7.6, 0.8 Hz, 1H), 3.49 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.5, 158.6, 138.2, 133.6, 133.2, 131.9, 130.6, 124.5, 123.4, 119.0, 115.5, 1147, 108.4, 89.7, 82.4, 68.4, 29.5; HRMS-ESI (m/z): calcd for $C_{17}H_{12}ClNO_3[M+Na]^+$: 336.0403; found: 336.0409.

4,6-difluoro-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-meth-ylindolin-2-one(1r).

Light yellow solid **1r** (40% over two steps), mp 179-180°C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.01 (s, 1H), 7.32 (s, 1H), 7.30–7.18 (m, 2H), 7.03–6.92 (m, 2H), 6.88 (d, J = 8.4 Hz, 1H), 6.79 (t, J = 7.6 Hz, 1H), 3.18 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.0, 164.0 (dd, J_{C-F} = 244.8, 13.1 Hz), 158.0 (dd, J_{C-F} = 250.6, 15.3 Hz), 145.8 (d, J_{C-F} = 25.3 Hz), 133.4, 130.7, 119.1, 115.6, 112.1 (dd, J_{C-F} = 19.3, 3.0 Hz), 108.4, 98.37, 98.36 (d, J_{C-F} = 51.2Hz), 95.0 (dd, J_{C-F} = 27.9, 3.3Hz), 88.3, 81.9, 67.4, 27.0; HRMS-ESI (m/z): calcd for $C_{17}H_{11}F_2NO_3[M+Na]^+$: 338.0605; found: 338.0612.

3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1,5,7-trimethylin-dolin-2-one(1s).

Light yellow solid **1s** (42% over two steps), mp 179-180°C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.97 (s, 1H), 7.26–7.13 (m, 3H), 7.01 (s, 1H), 6.92 (s, 1H), 6.87 (d, J = 8.0 Hz, 1H), 6.77 (d, J = 7.6 Hz, 1H), 3.39 (s, 3H), 2.49 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.8, 158.5, 137.8, 133.7, 133.3, 132.0, 131.2, 130.4, 122.8, 120.1, 119.1, 115.5, 108.8, 90.8, 81.7, 68.5, 29.3, 20.4, 18.3; HRMS-ESI (m/z): calcd for $C_{19}H_{17}NO_3[M+Na]^+$: 330.1106; found: 330.1110.

4,7-dichloro-3-hydroxy-3-((2-hydroxyphenyl)ethynyl)-1-meth-ylindolin-2-one(1t).

Light gray solid **1t** (44% yield over two steps), mp 185-187°C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.99 (s, 1H), 7.47 (d, J = 8.8 Hz, 1H), 7.30 (dd, J = 7.6, 1.6 Hz, 1H), 7.28–7.22 (m, 2H), 7.20 (d, J = 8.8 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 6.85–6.79 (m, 1H), 3.54 (s, 3H), 3.39(H_2O); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.0, 158.6, 139.9, 133.4, 133.2, 130.6, 129.6, 128.9, 124.9, 119.0, 115.5, 113.6, 108.4, 87.3, 82.2, 68.6, 29.6; HRMS-ESI (m/z): calcd for $C_{17}H_{11}Cl_2NO_3[M+Na]^+$: 370.0014; found: 370.0021.

3-hydroxy-3-((2-hydroxy-5-methylphenyl)ethynyl)-1-methyl-indolin-2-one(1u).

Light yellow solid **1u** (55% over two steps), mp 161-163°C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.66 (s, 1H), 7.49 (d, J = 7.3 Hz, 1H), 7.37 (td, J = 7.7, 1.1 Hz, 1H), 7.12 (dd, J = 11.0, 4.0 Hz, 1H), 7.08–7.02 (m, 3H), 6.99 (dd, J = 8.3, 1.8 Hz, 1H), 6.75 (d, J = 8.3 Hz, 1H), 3.33 (H_2O), 3.16 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.2, 156.3, 142.6, 133.2, 131.0, 130.6, 123.0, 127.6, 124.1, 123.0, 115.4, 109.0, 108.3, 90.1, 82.0, 68.9, 26.2, 19.7; HRMS-ESI (m/z): calcd for $C_{18}H_{15}NO_3[M+Na]^+$: 316.0950; found: 316.0955.

3-((5-fluoro-2-hydroxyphenyl)ethynyl)-3-hydroxy-1-methylin-dolin-2-one(1v)

Light yellow solid **1v** (43% over two steps), mp 174-176°C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.97 (s, 1H), 7.49 (dd, J = 7.2, 0.8 Hz, 1H), 7.38 (td, J = 7.6, 1.2 Hz, 1H), 7.15–7.10 (m, 2H), 7.09–7.02 (m, 3H), 6.85 (dd, J = 9.7, 4.8 Hz, 1H), 3.16 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.9, 155.7, 155.2 (d,

J_{C-F} = 1.7Hz), 153.4, 142.6, 130.3, 130.0, 124.2, 123.0, 118.6 (d, J_{C-F} = 23.9Hz), 117.3 (d, J_{C-F} = 22.8), 116.5 (d, J_{C-F} = 10.3Hz), 109.1, 91.2, 80.6, 68.8, 26.3; HRMS-ESI (m/z): calcd for $C_{17}H_{12}FNO_3$[M+Na]$^+$: 320.0699; found: 320.0703.

3-((5-chloro-2-hydroxyphenyl)ethynyl)-3-hydroxy-1-methyl-indolin-2-one(1w).

Light yellow solid **1w** (44% yield over two steps), mp 163-164˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.30 (s, 1H), 7.49 (d, J = 6.8 Hz, 1H), 7.38 (td, J = 7.6, 1.2 Hz, 1H), 7.28–7.21 (m, 2H), 7.12 (t, J = 7.2 Hz, 2H), 7.05 (d, J = 7.8 Hz, 1H), 6.87 (dd, J = 8.8, 2.0 Hz, 1H), 3.33(H_2O), 3.16 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.0, 158.6, 144.2, 133.3, 130.6, 129.8, 125.8, 125.6, 122.8, 119.1, 115.5, 112.4, 108.5, 89.7, 82.2, 68.5, 26.5; HRMS-ESI (m/z): calcd for $C_{17}H_{12}ClNO_3$[M+Na]$^+$: 336.0403; found: 336.0409.

3-((5-(tert-butyl)-2-hydroxyphenyl)ethynyl)-3-hydroxy-1-methylindolin-2-one(1x).

Light yellow solid **1x** (52% over two steps), mp 182-184˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 7.70 (d, J = 7.2 Hz, 1H), 7.43 (dd, J = 7.8, 1.2 Hz, 1H), 7.27–7.20 (m, 3H), 7.00–6.89 (m, 2H), 6.83 (d, J = 8.4 Hz, 1H), 6.13 (s, 1H), 3.30 (s, 3H), 1.23 (s, 9H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 175.4, 155.6, 142.8, 142.6, 130.5, 129.0, 128.8, 128.4, 125.0, 124.3, 115.2, 109.1, 107.2, 90.7, 82.5, 34.0, 31.3, 26.9; HRMS-ESI (m/z): calcd for $C_{21}H_{21}NO_3$[M+Na]$^+$: 358.1419; found: 358.1426.

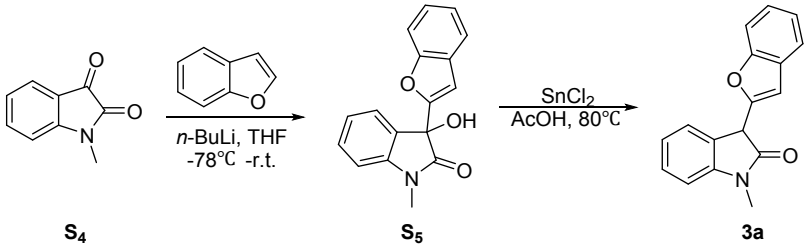
3-hydroxy-3-((4-hydroxy-[1,1'-biphenyl]-3-yl)ethynyl)-1-methylindolin-2-one(1y).

Light yellow solid **1y** (46% over two steps), mp 188-189˚C. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.16 (s, 1H), 7.60–7.50 (m, 5H), 7.42-7.37 (m, 3H), 7.3-7.27 (m, 1H), 7.18–7.10 (m, 2H), 7.06 (d, J = 7.6 Hz, 1H), 6.98 (dd, J = 7.6, 1.2 Hz, 1H), 3.39 (H_2O), 3.17 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 173.1, 158.2, 142.6, 139.1, 131.1, 131.0, 130.5, 129.9, 128.9, 126.8, 126.0, 124.2, 123.0, 116.1, 109.2, 109.1, 90.6, 81.7, 68.9, 26.3; HRMS-ESI (m/z): calcd for $C_{23}H_{17}NO_3$[M+Na]$^+$: 378.1106, found: 378.1112.

Procedure for Synthesis of compound 3a[2].

Step 1: To a solution of benzofuran (1.2 mmol, 1.2 equiv) in anhydrous THF (20 mL) at -78 °C was added *n*-BuLi (1.1 mmol, 1.1 equiv). After the resulting light yellow coloured solution stirring for 2 h, the N-methylisatin **S_4** (1.0 mmol, 1.0 equiv) in anhydrous THF (20 mL) was added to the mixture dropwise and the stirring was continued for 1 h at the same temperature. The reaction was allowed to warm to room temperature for 1 h and then quenched by saturated aqueous NH_4Cl. Then the mixture was extracted with EtOAc, and the organic layer was separated and washed with water and brine respectively. Then the organic layer was dried over Na_2SO_4, filtered and concentrated in vacuo. The crude product was purified by flash chromatography on silica gel (Petroleum Ether/EtOAc = 4:1) to afford the alcohol **S_5** (76% yield).

Step 2: The alcohol **S_5** (0.5 mmol, 1.0 equiv) was dissolved in 10 ml of glacial acetic acid and $SnCl_2$ (10.0 mmol, 2.0 equiv) was added. The reaction mixture was stirred at 80 ℃ for 2 h. Next, the solution was cooled to room temperature, concentrated in vacuo, and then diluted with EtOAc (50 ml). The solution was washed with water, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried with anhydrous $MgSO_4$, filtered, and concentrated in vacuo. The residue was purified by flash column chromatography (Petroleum Ether/EtOAc = 8:1) to afford **3a** (82% yield) as light yellow solid.



S4 **S5** **3a**

Scheme 2 Preparation of **3a**

3-(benzofuran-2-yl)-1-methylindolin-2-one(3a).

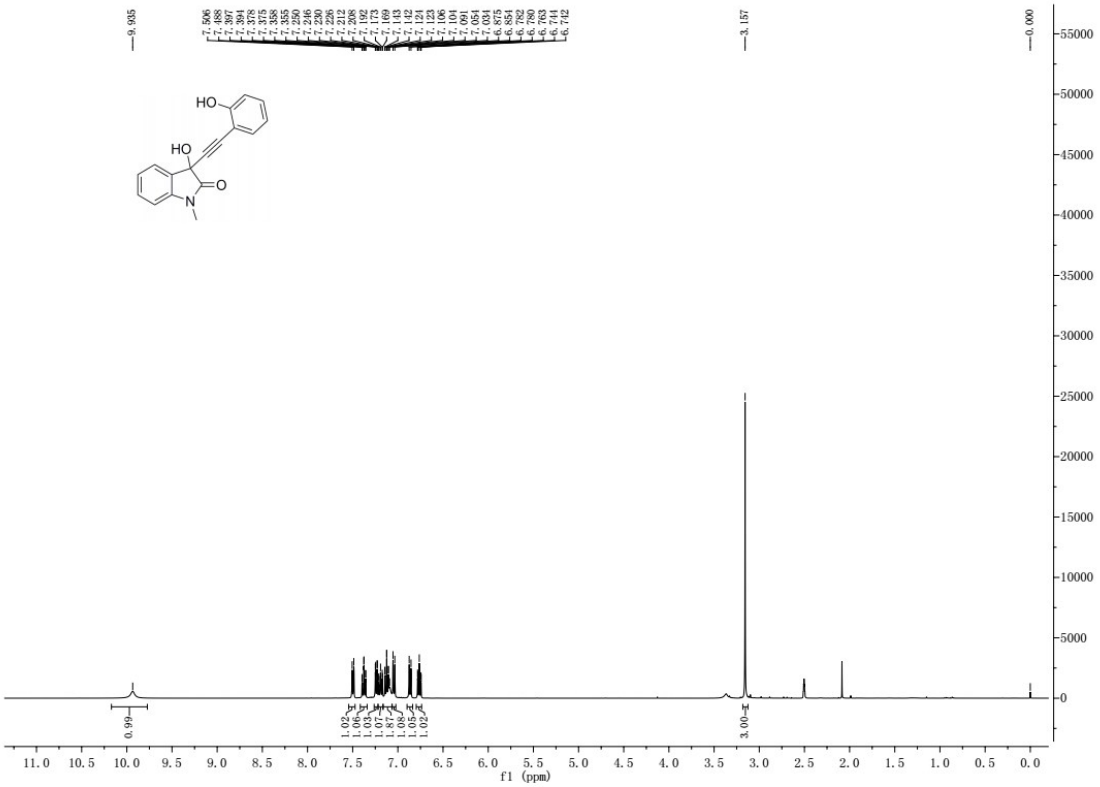
Light yellow solid **3a** (62% yield over two steps), mp 183-184˚C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.50 (dd, J = 7.6, 1.0 Hz, 1H), 7.42 (d, J = 8.4 Hz, 1H), 7.36-7.34 (m, 2H), 7.24-7.08 (m, 3H), 6.89 (d, J = 7.8 Hz, 1H), 6.67 (s, 1H), 4.87 (s, 1H), 3.27 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 172.9, 155.3, 151.8, 144.2, 128.9, 128.2, 125.9, 125.0, 124.1, 122.9, 122.8, 120.8, 111.2, 108.4, 105.1, 46.3, 26.6; HRMS-ESI (m/z): calcd for $C_{17}H_{13}NO_2$ $[M+Na]^+$: 286.0844; found 286.0849.

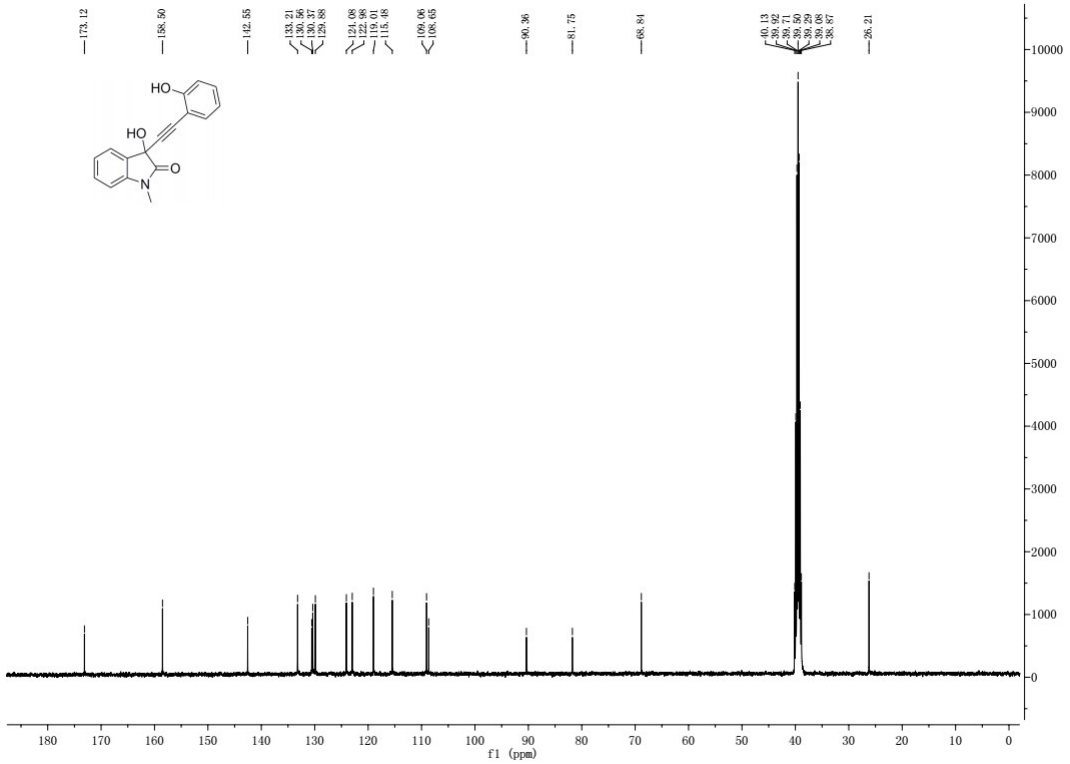
References

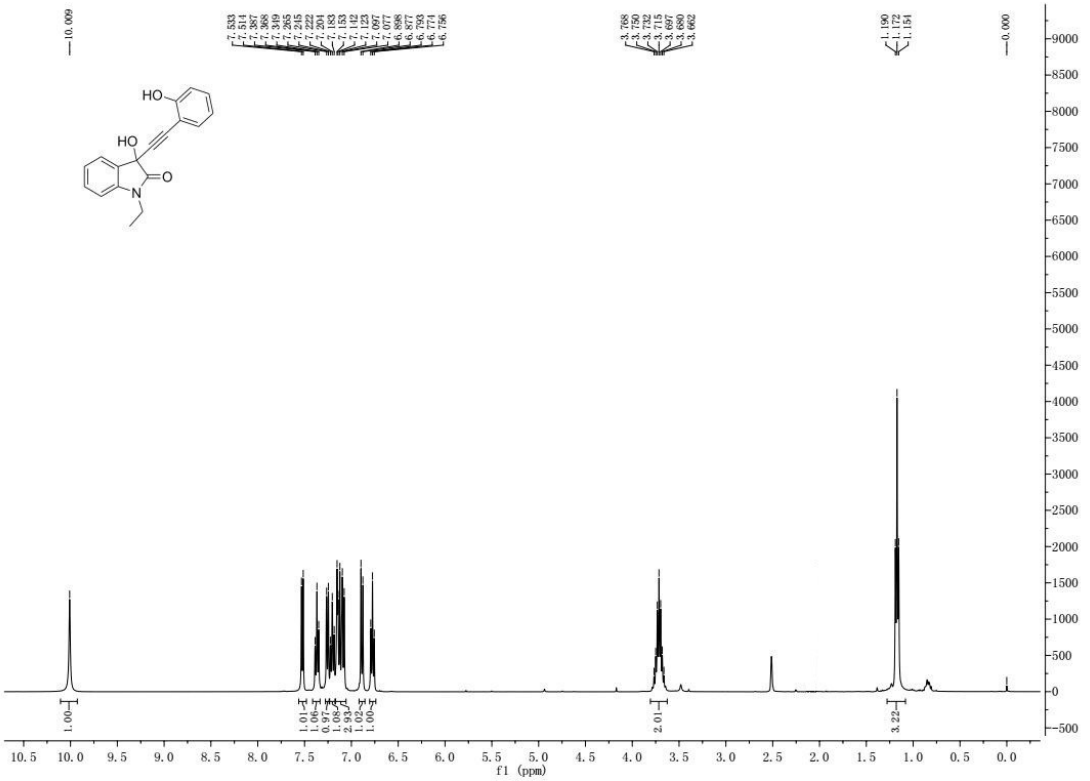
1. Y.-H. Hu, Z. Yang, *Org. Lett.,* 2001, **3**, 1387.

2. B. M. Trost, J. Xie, J. D. Sieber, *J. Am. Chem. Soc.,* 2011, **133**, 20611.

NMR Spectra of Compounds



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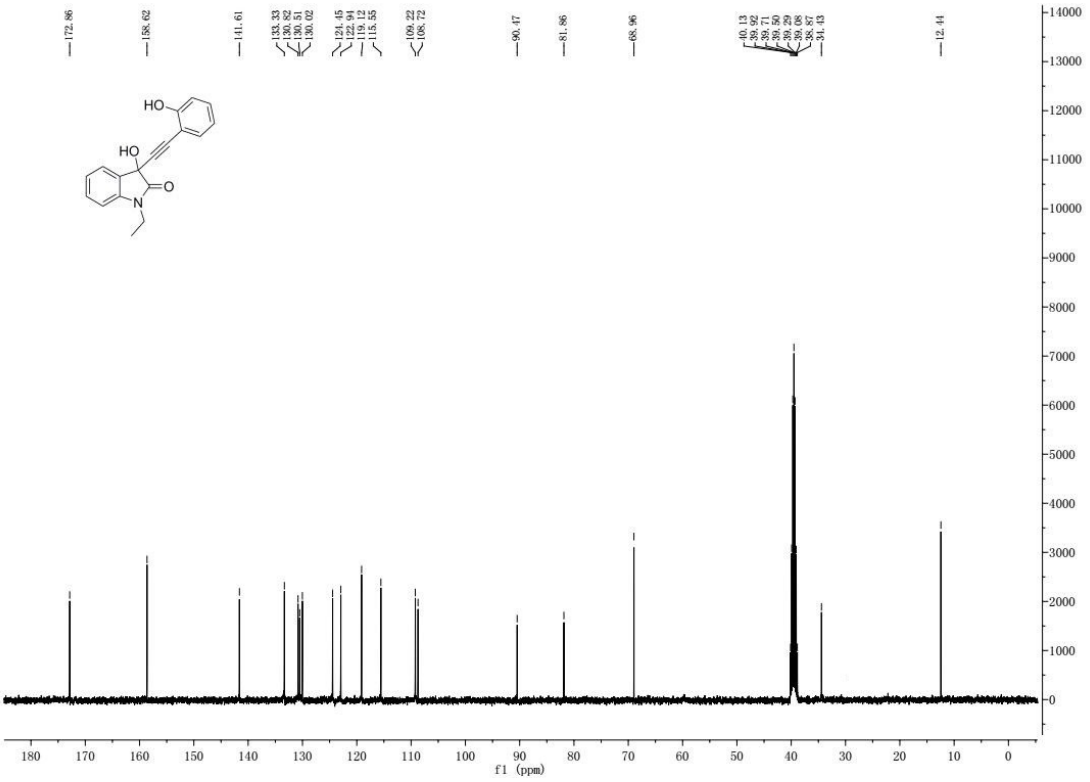
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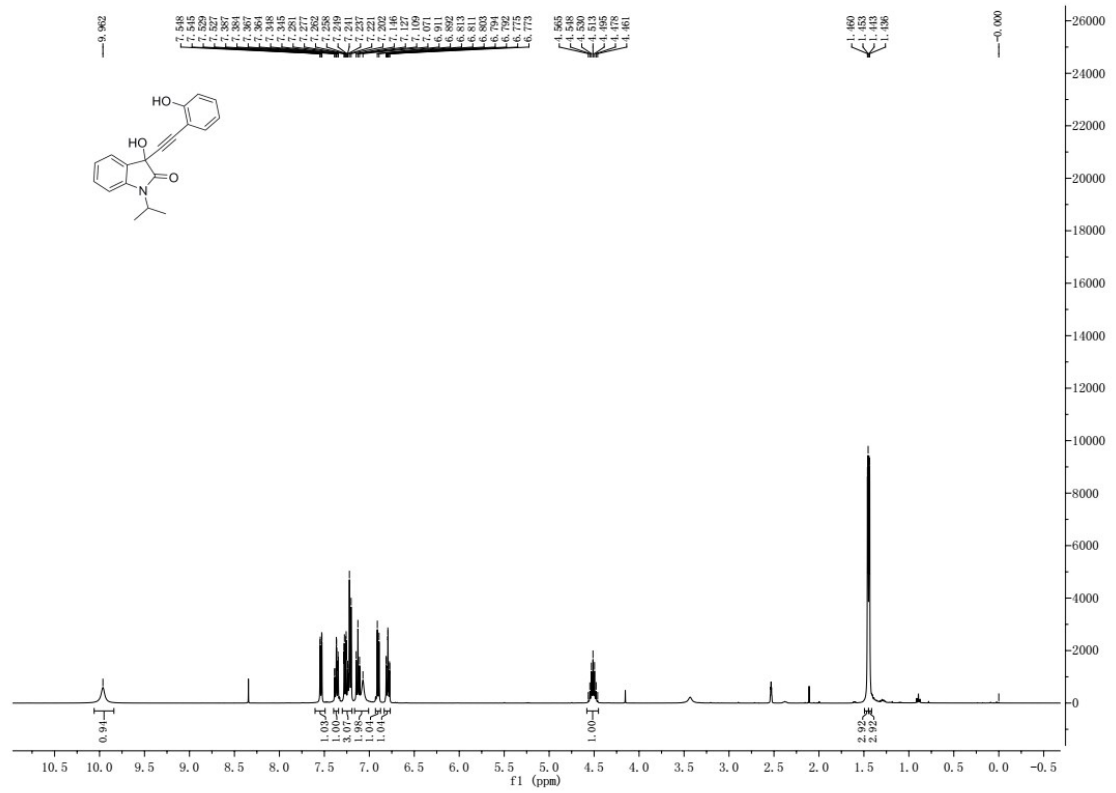
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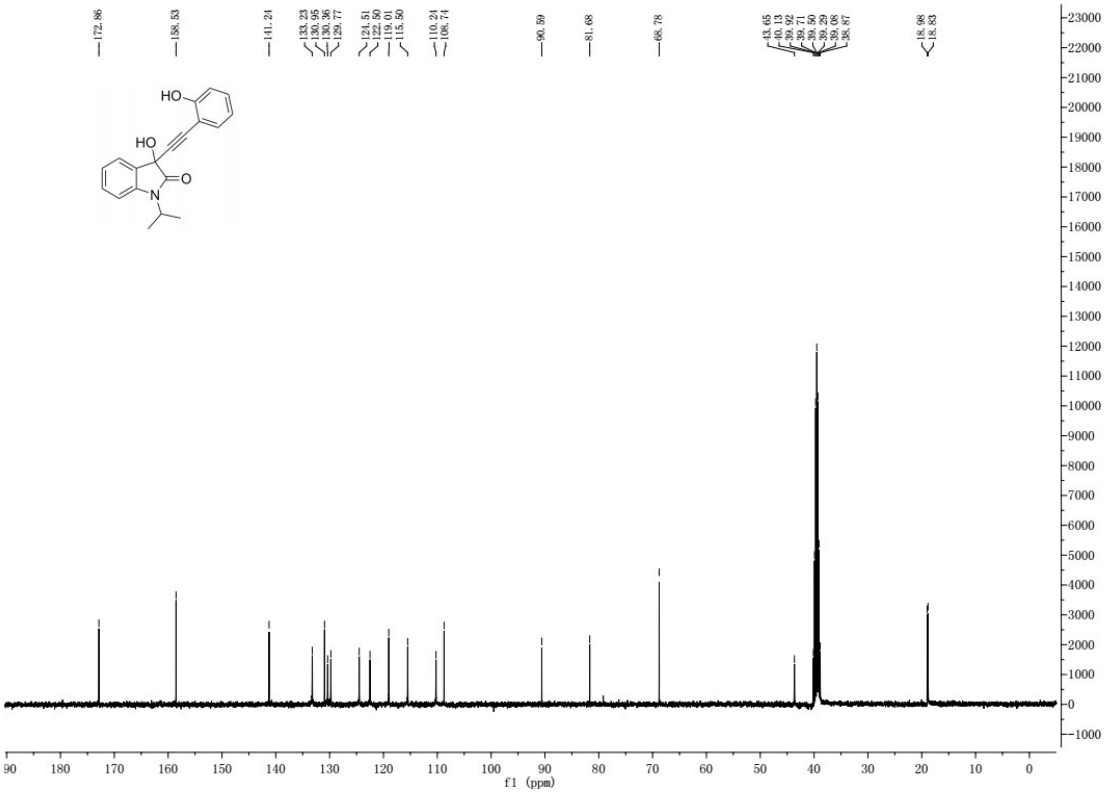
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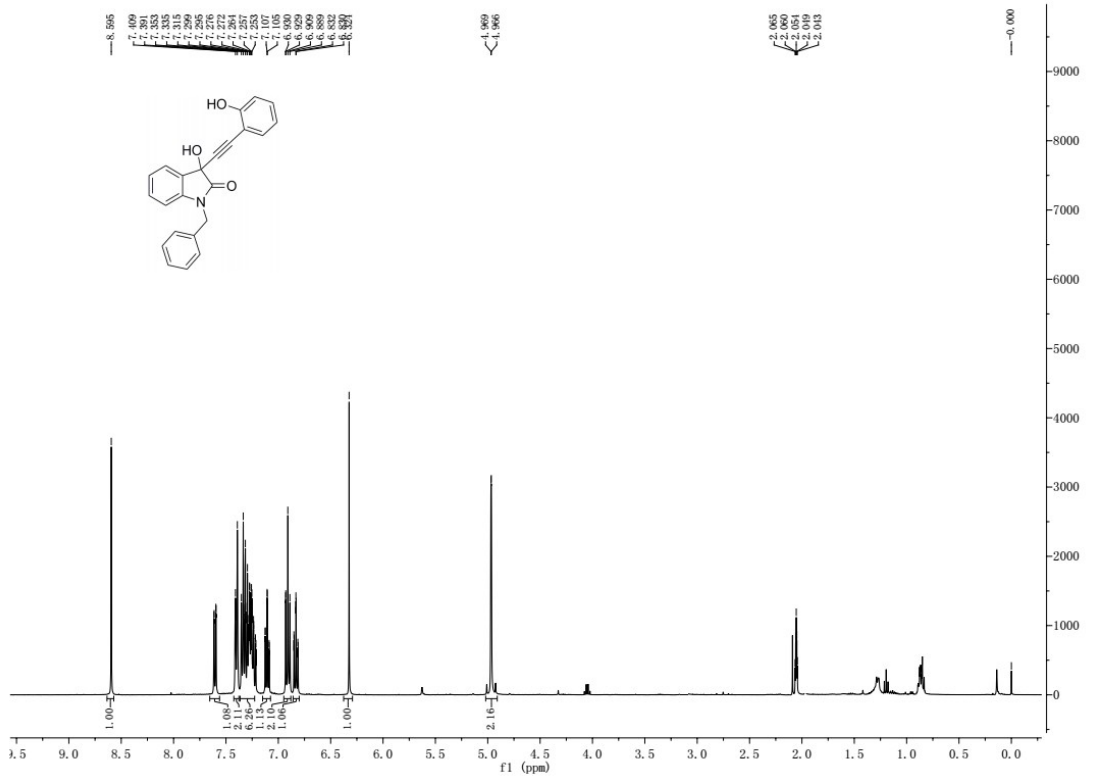
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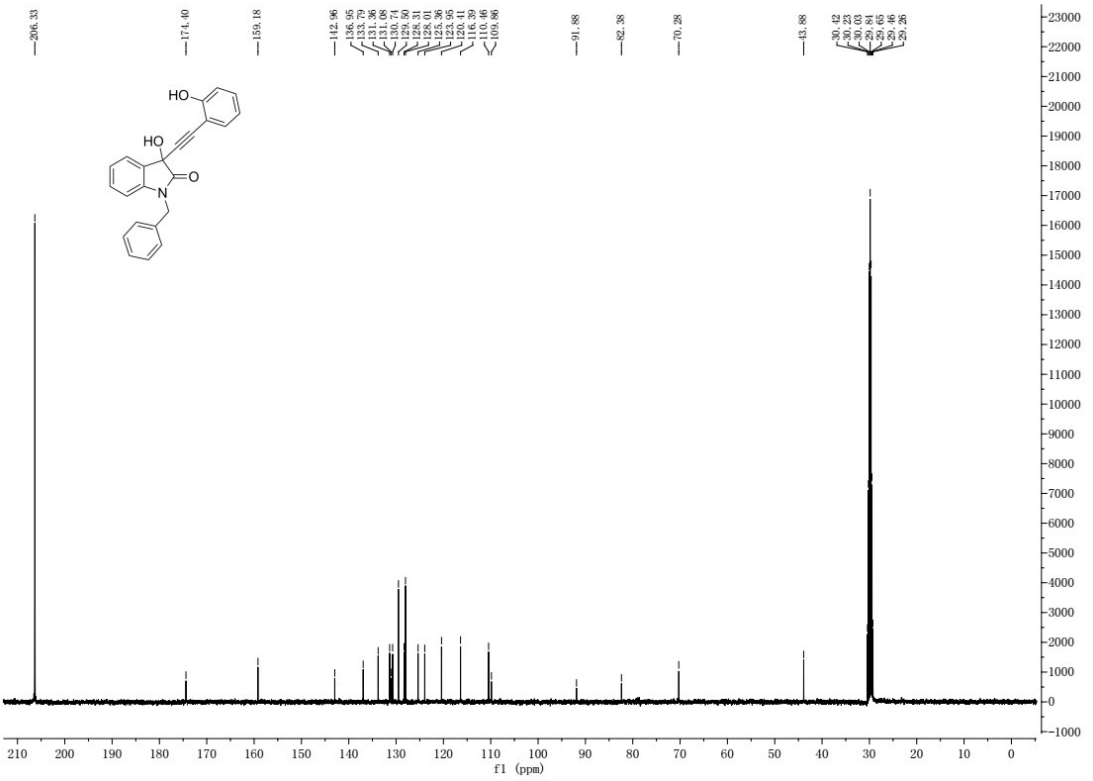
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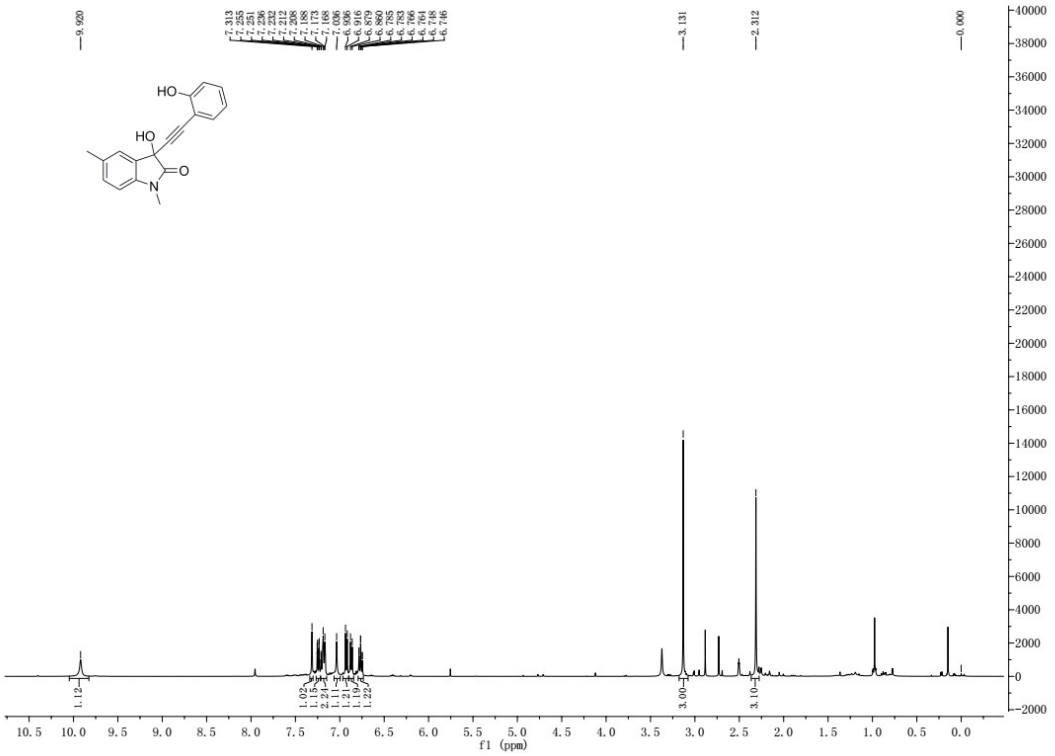
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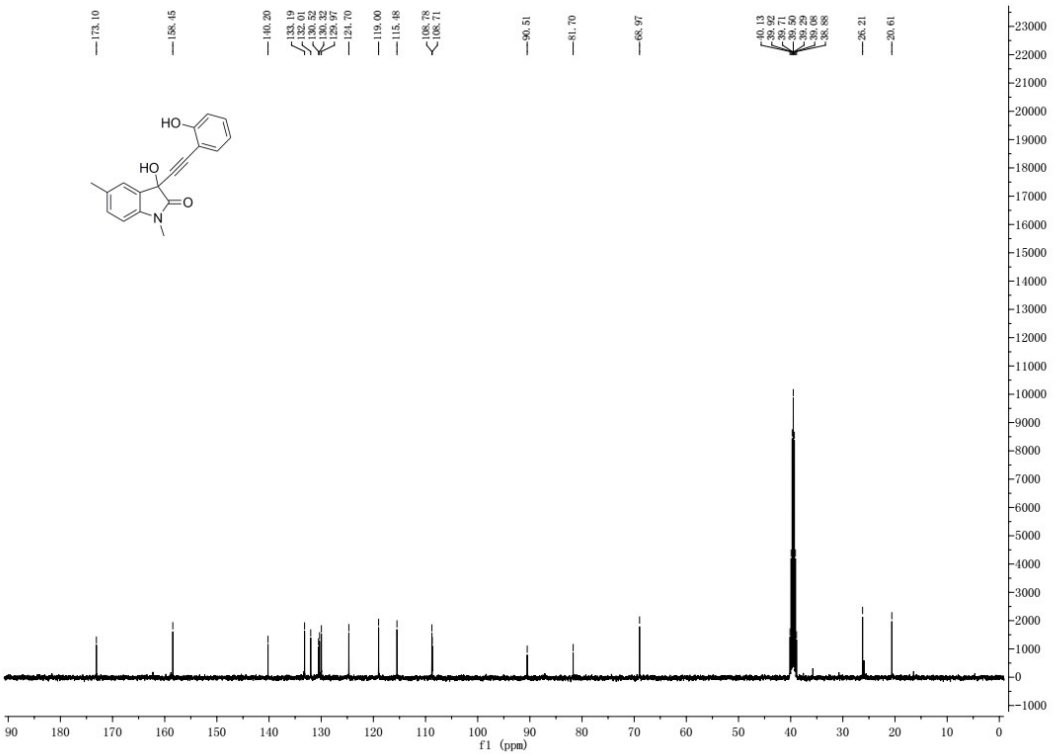
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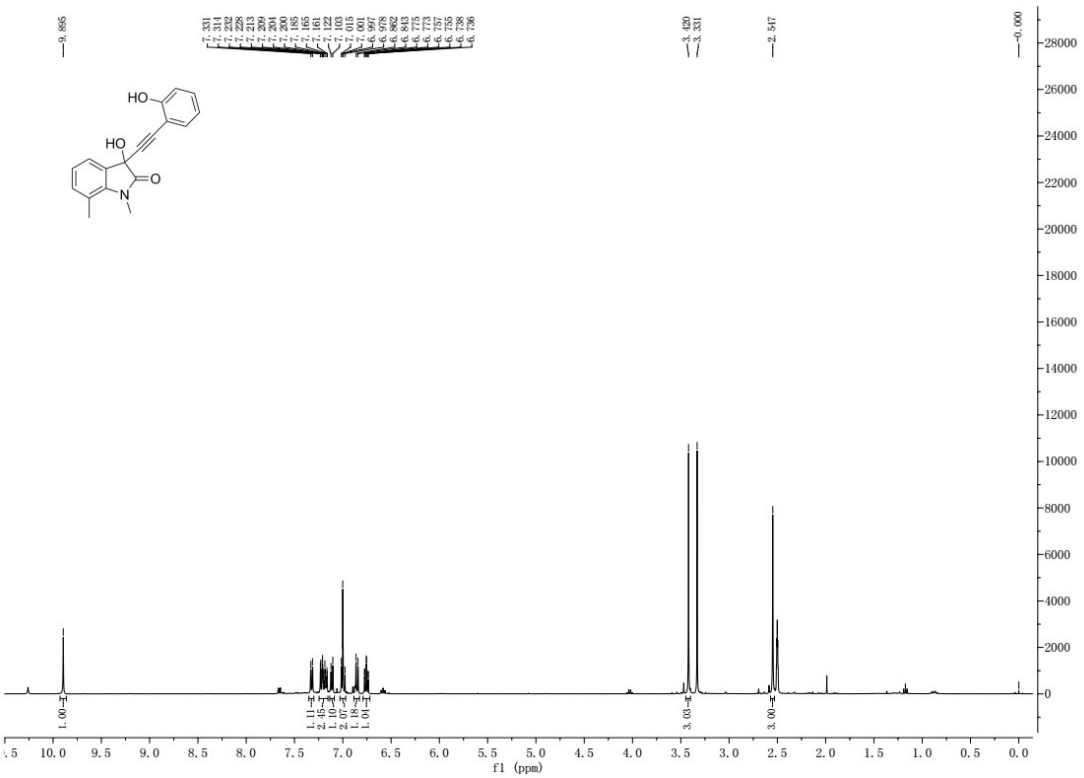
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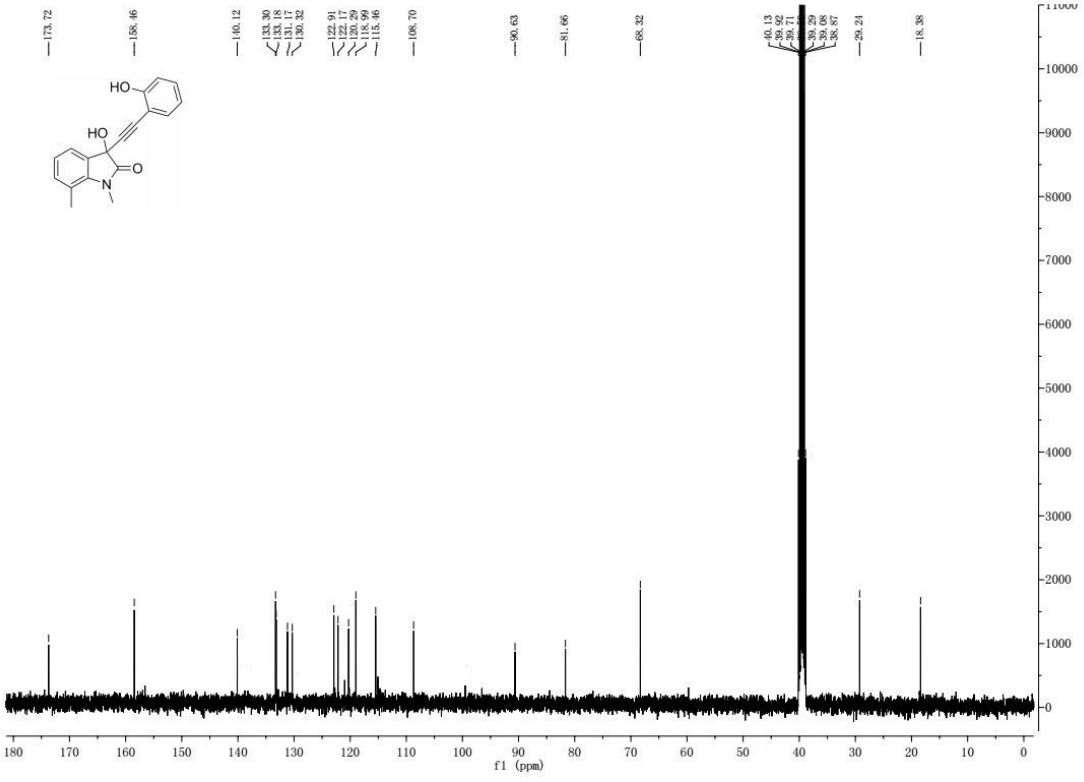
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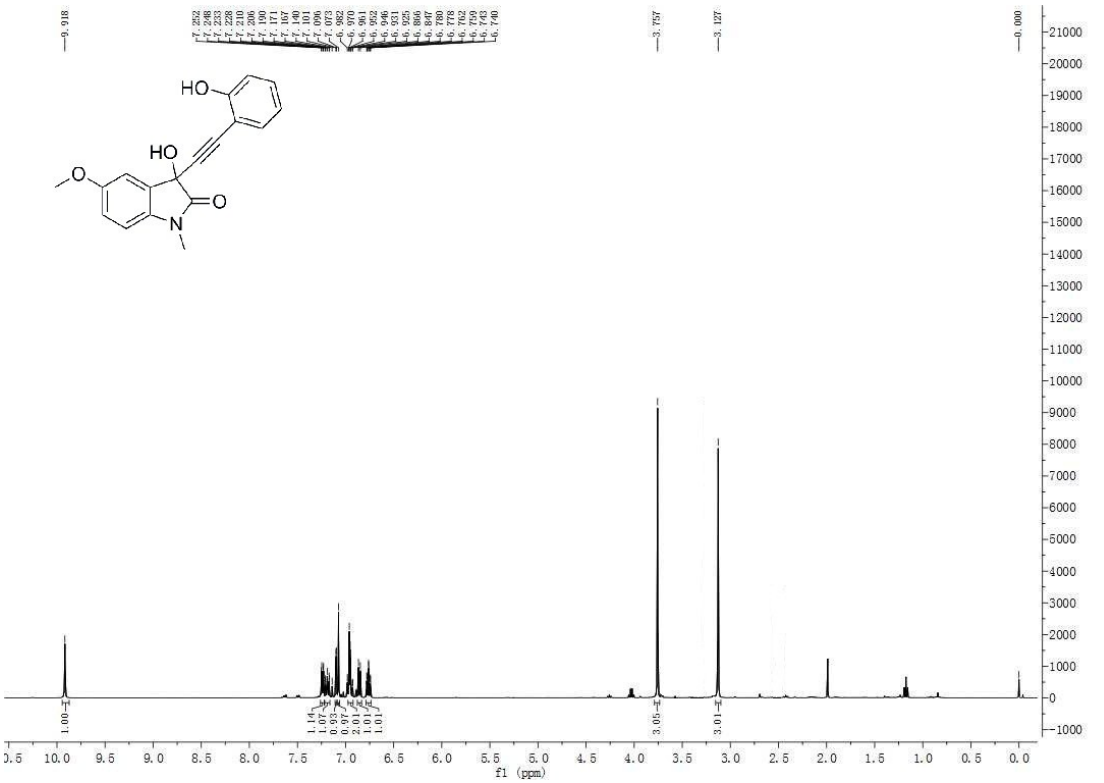
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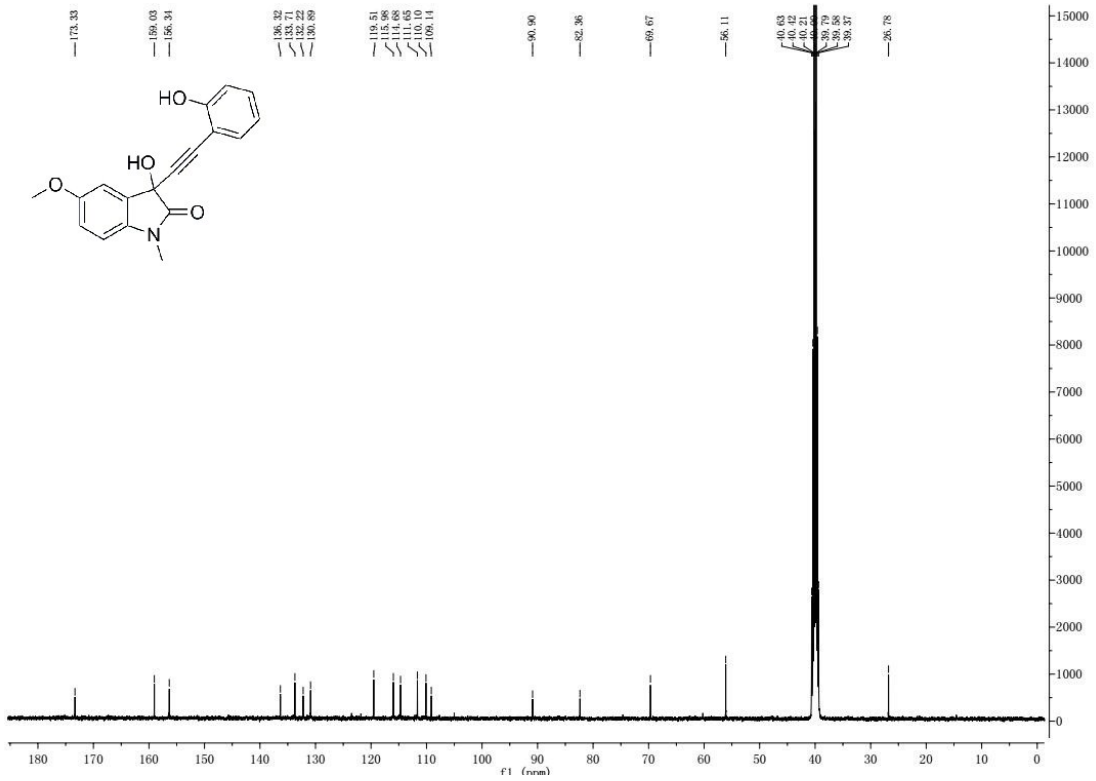
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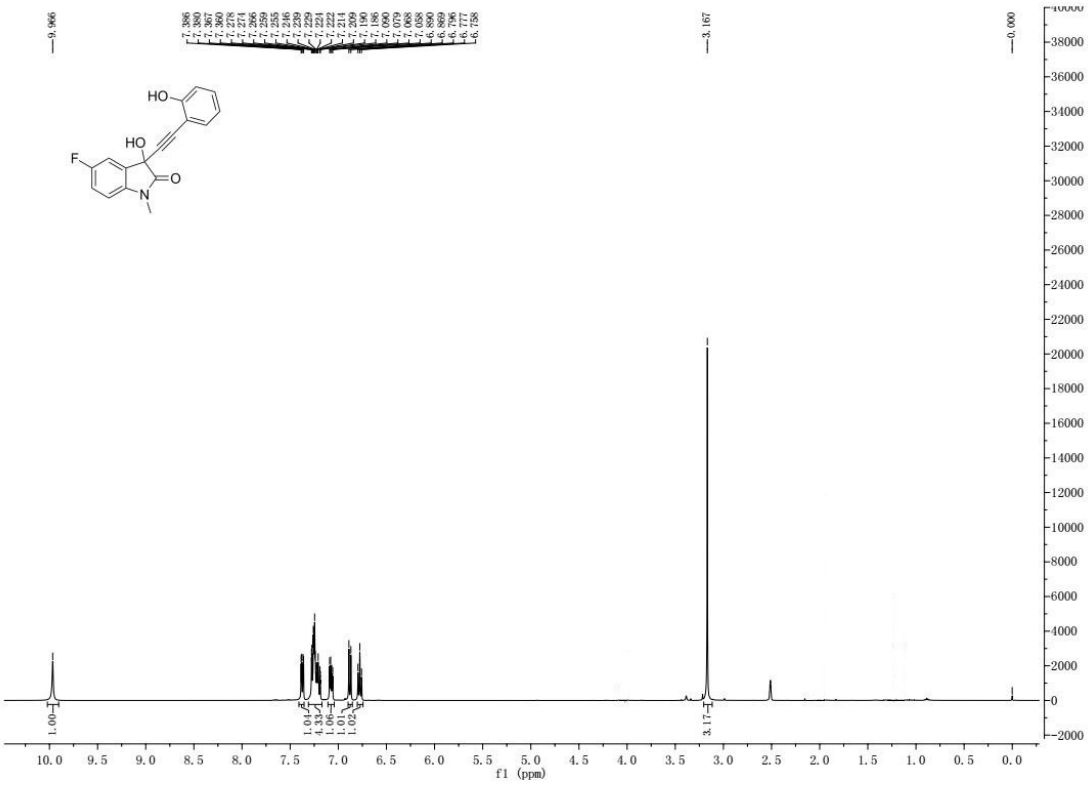
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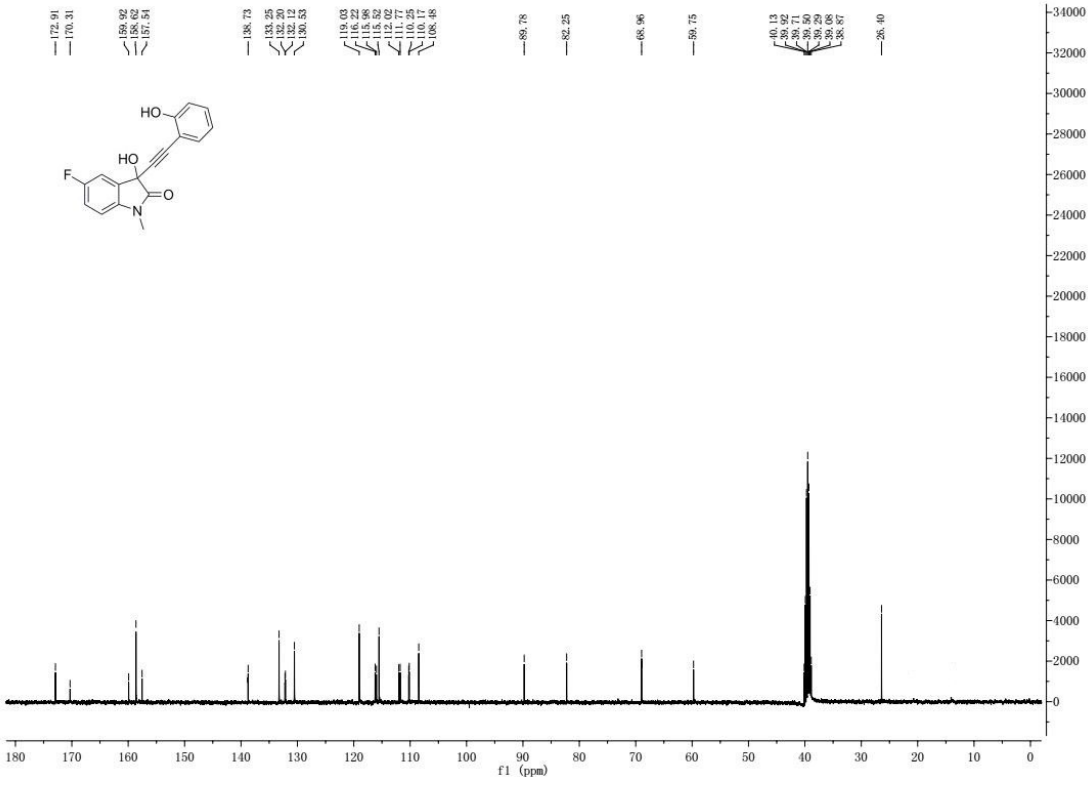
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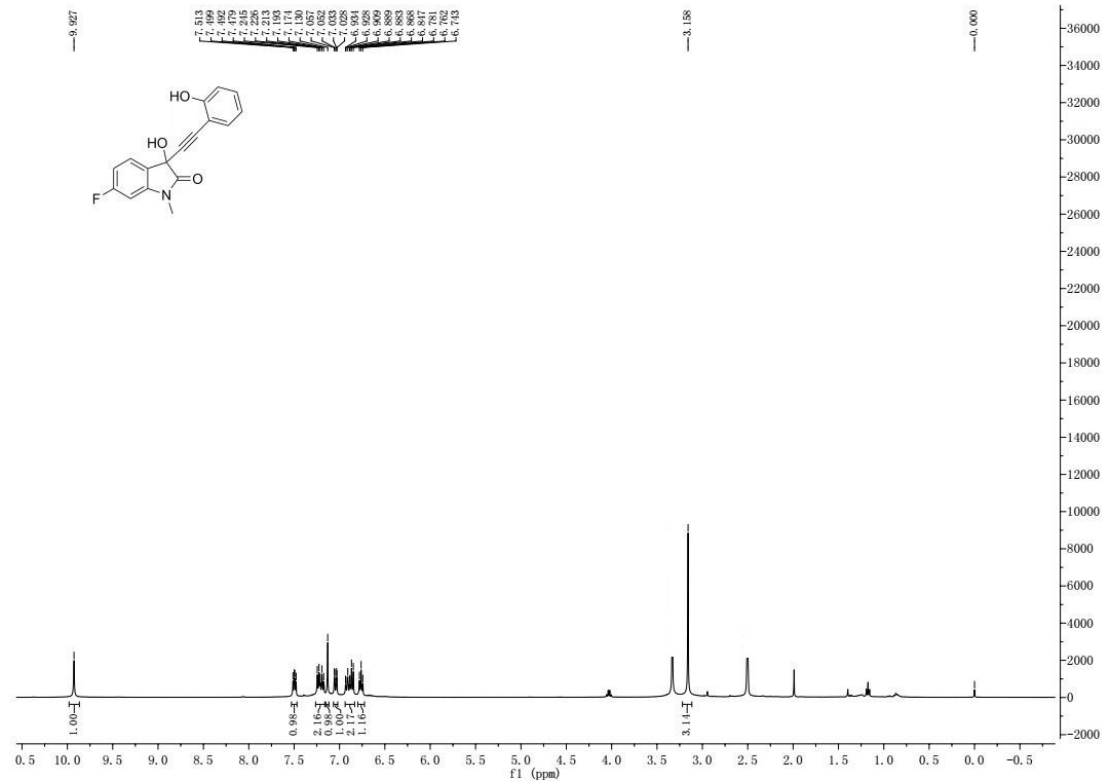
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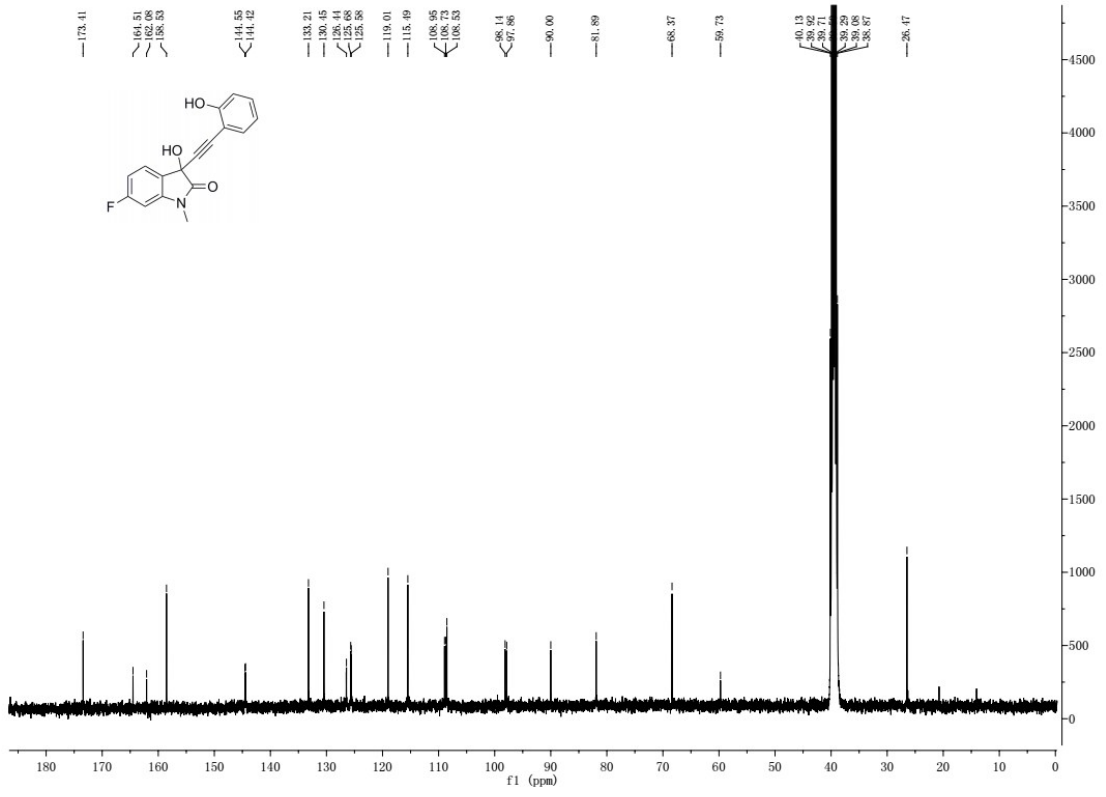
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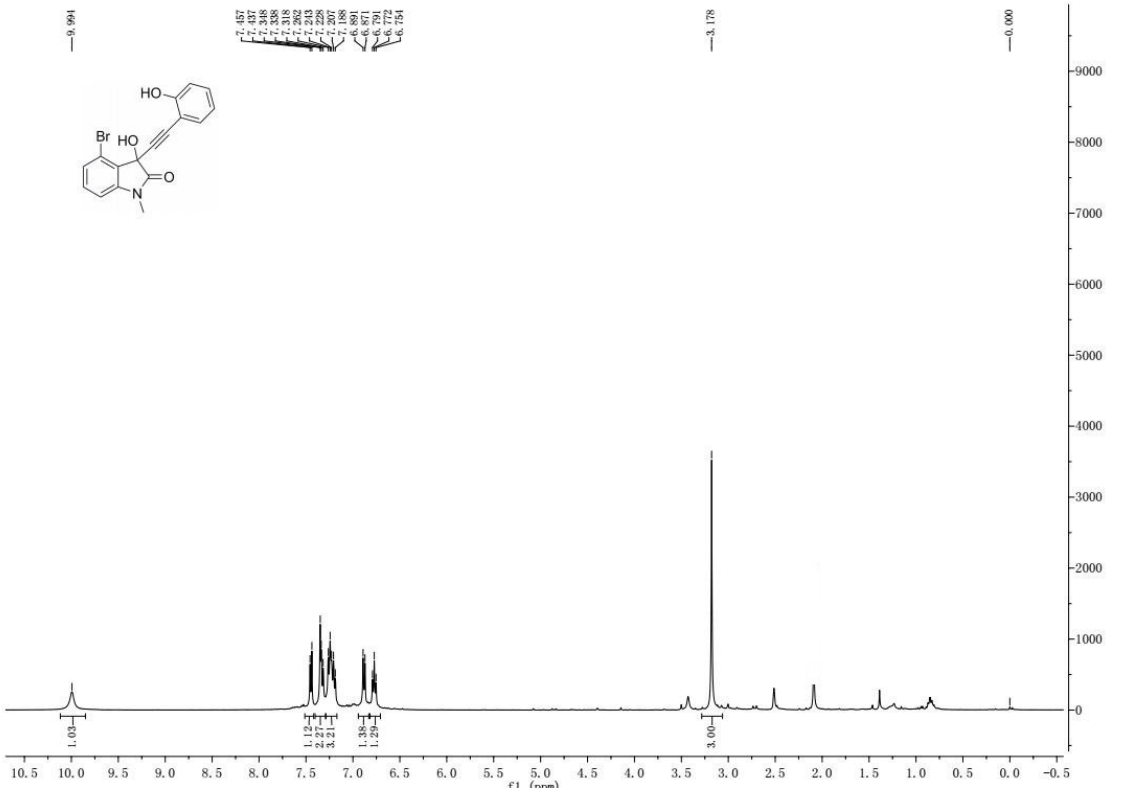
f1 (ppm)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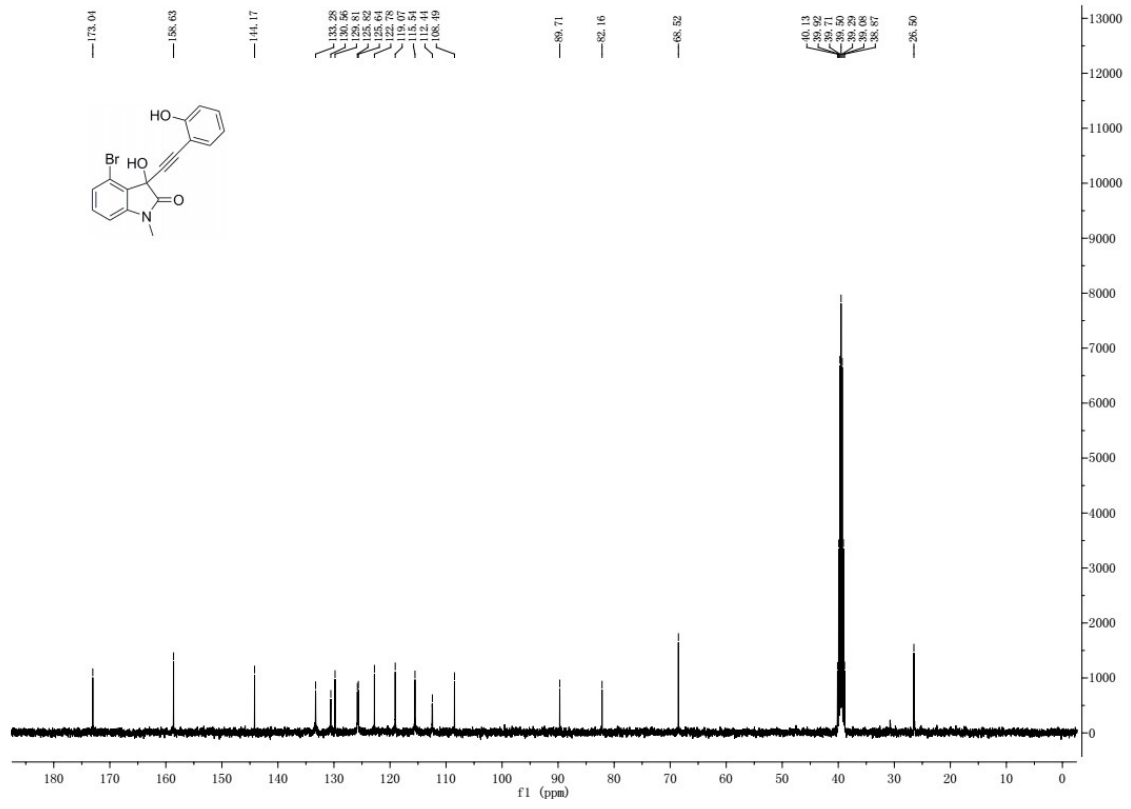
7.437
7.348
7.338
7.318
7.302
7.243
7.228
7.207
7.188
6.894
6.871
6.791
6.772
6.754
3.178
0.000
HO
Br
HO
O
N
1.03
1.12
2.27
3.21
1.38
1.29
3.00
f1 (ppm)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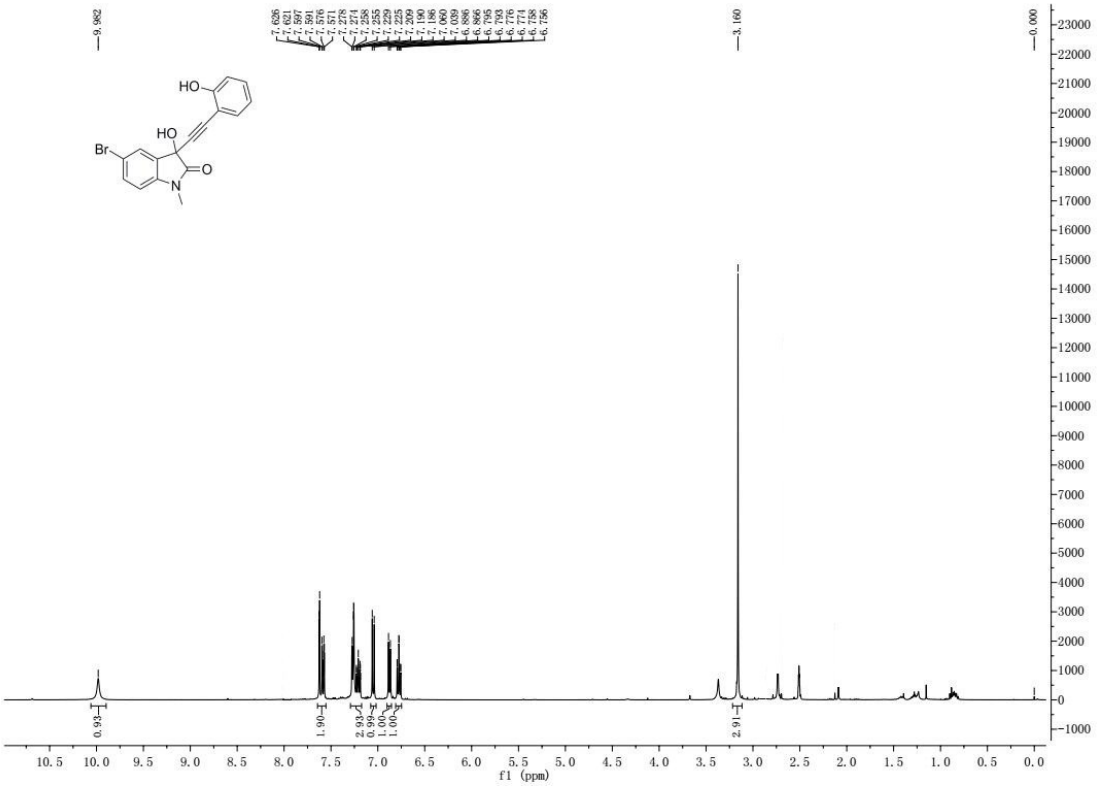
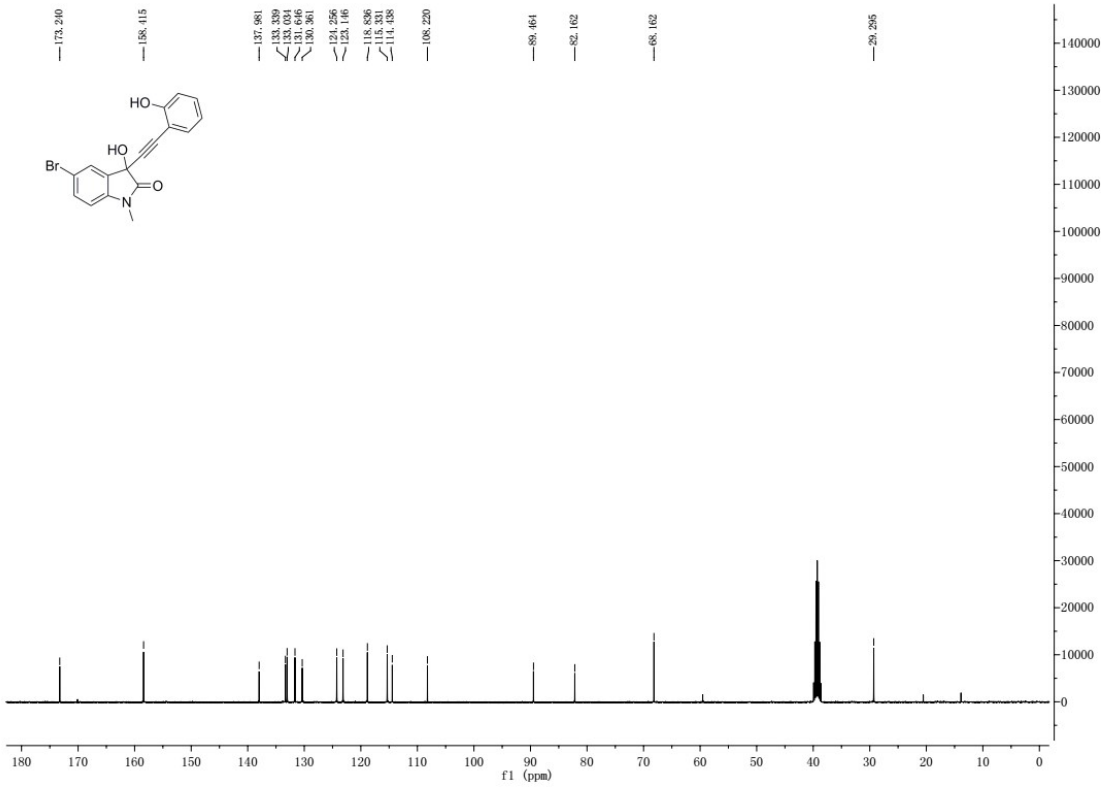
158.63
144.17
133.28
130.96
129.81
128.82
125.64
122.78
119.07
115.54
112.44
108.49
89.71
82.16
68.52
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.50
HO
Br
HO
O
N
f1 (ppm)


9.982
7.636
7.621
7.597
7.591
7.576
7.571
7.278
7.274
7.258
7.255
7.229
7.225
7.209
7.190
7.186
7.060
7.039
6.886
6.865
6.795
6.793
6.776
6.774
6.738
6.736
3.160
0.000
HO
HO
Br
O
N
0.93
1.90
2.93
0.89
1.00
1.00
2.91
f1 (ppm)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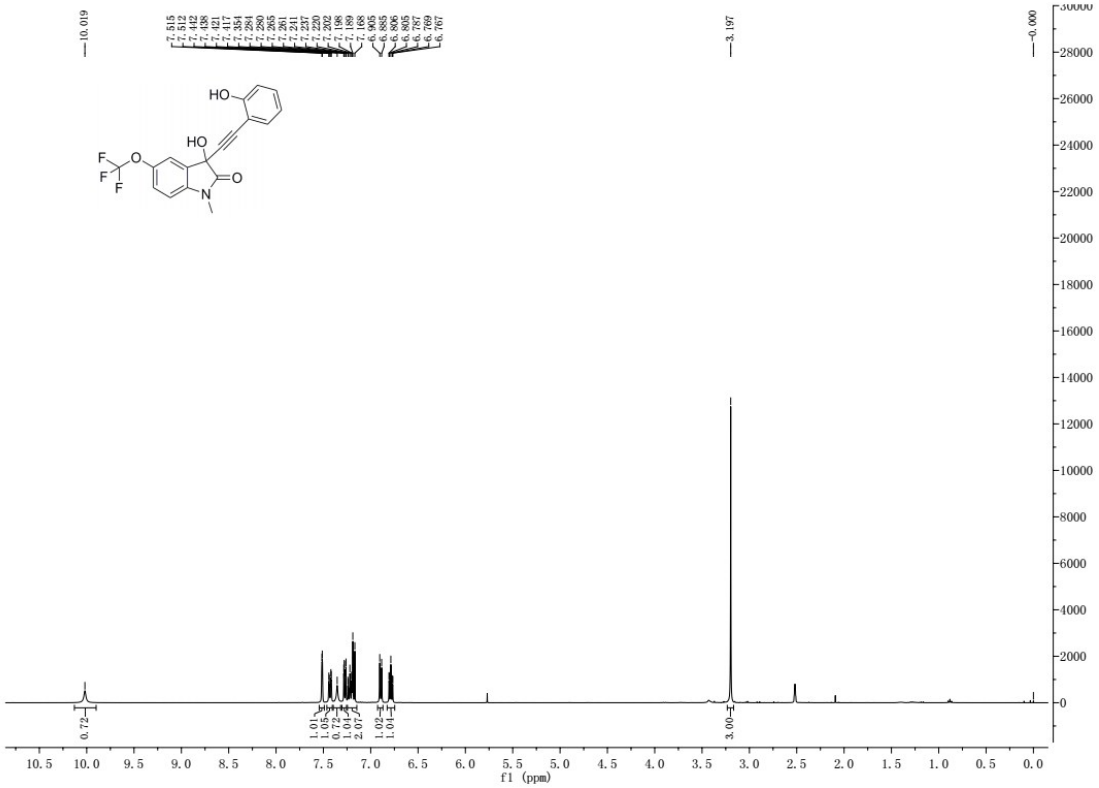
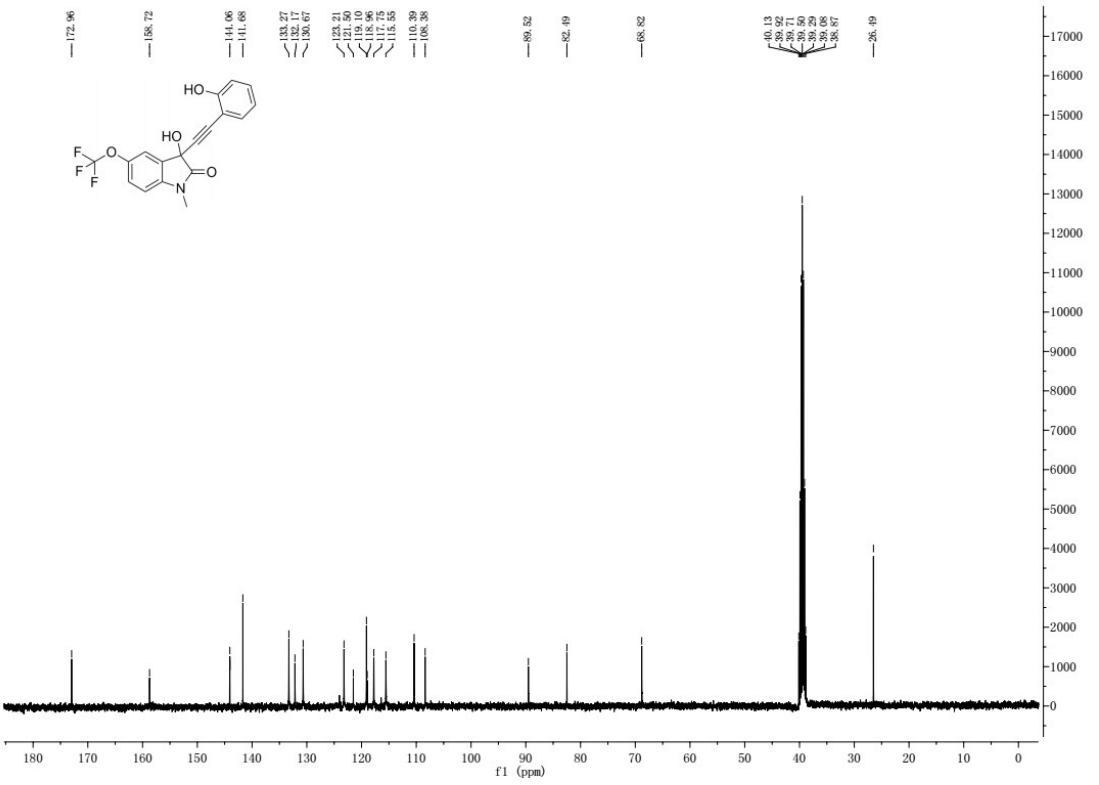
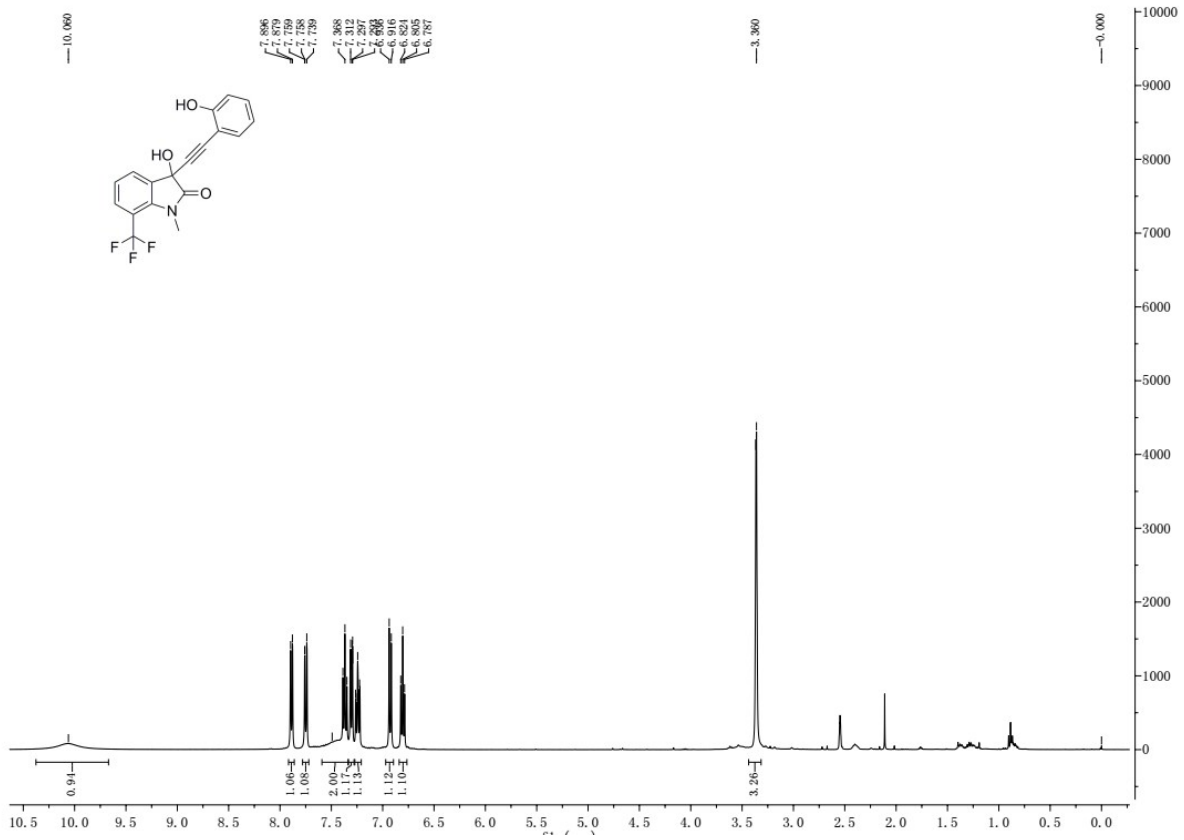
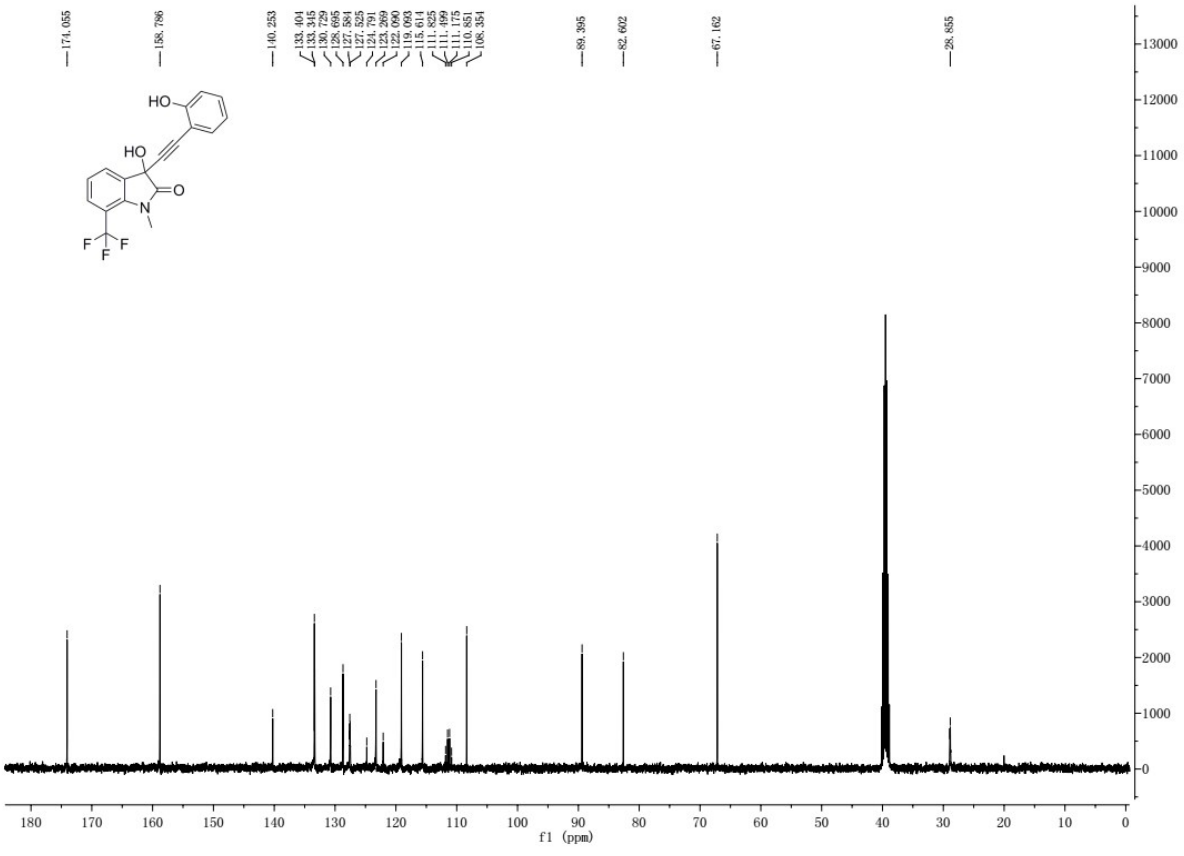
158.415
137.981
133.339
133.034
131.645
130.361
124.256
123.146
118.836
115.331
114.438
108.220
89.464
82.162
68.162
29.295
HO
HO
Br
O
N
f1 (ppm)


10.019
7.515
7.512
7.442
7.438
7.421
7.417
7.354
7.284
7.280
7.265
7.261
7.231
7.237
7.220
7.202
7.199
7.196
7.189
7.168
6.905
6.885
6.805
6.787
6.769
6.767
3.197
0.000
HO
HO
F
F
F
O
O
N
0.73
1.01
1.05
0.72
1.04
2.07
1.02
1.04
3.00
f1 (ppm)


172.96
158.72
144.06
141.68
133.27
132.17
130.67
123.21
121.50
119.10
118.96
117.75
115.55
110.39
108.38
89.52
82.49
68.82
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.49
HO
HO
F
F
F
O
O
N
f1 (ppm)


10.060
7.896
7.879
7.799
7.758
7.739
7.368
7.312
7.297
6.916
6.824
6.805
6.787
3.360
0.000
HO
HO
O
N
F
F
F
0.94
1.06
1.08
2.00
1.17
1.13
1.12
1.10
3.26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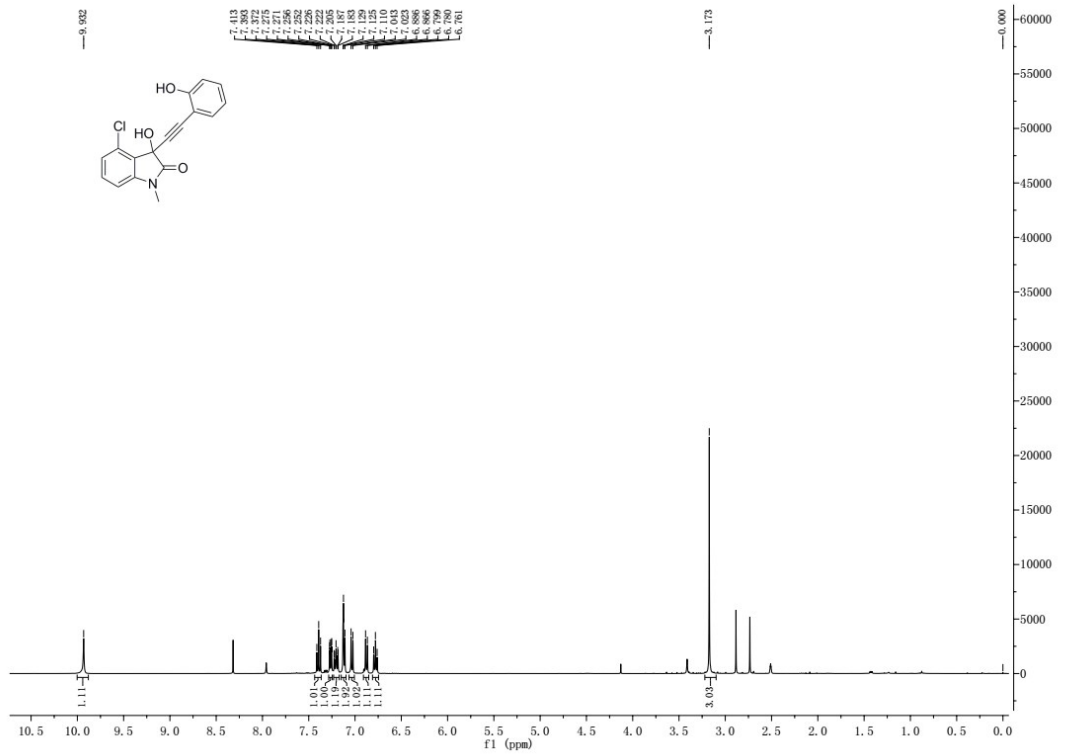
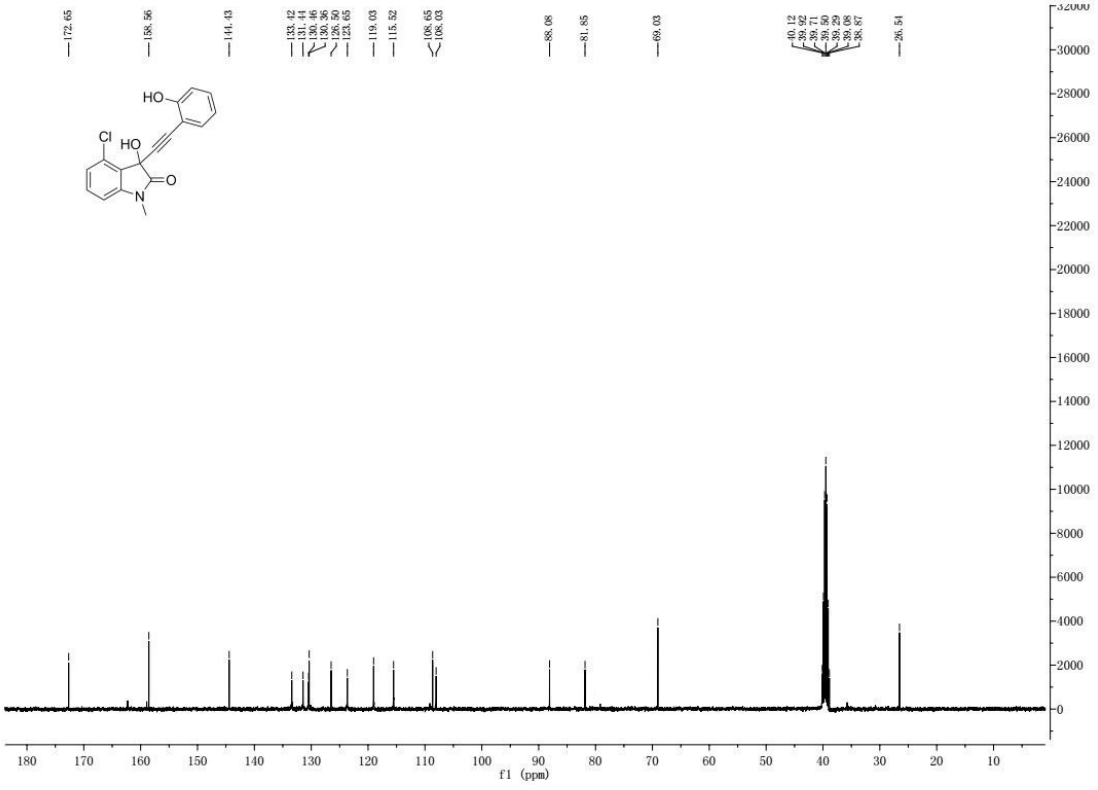
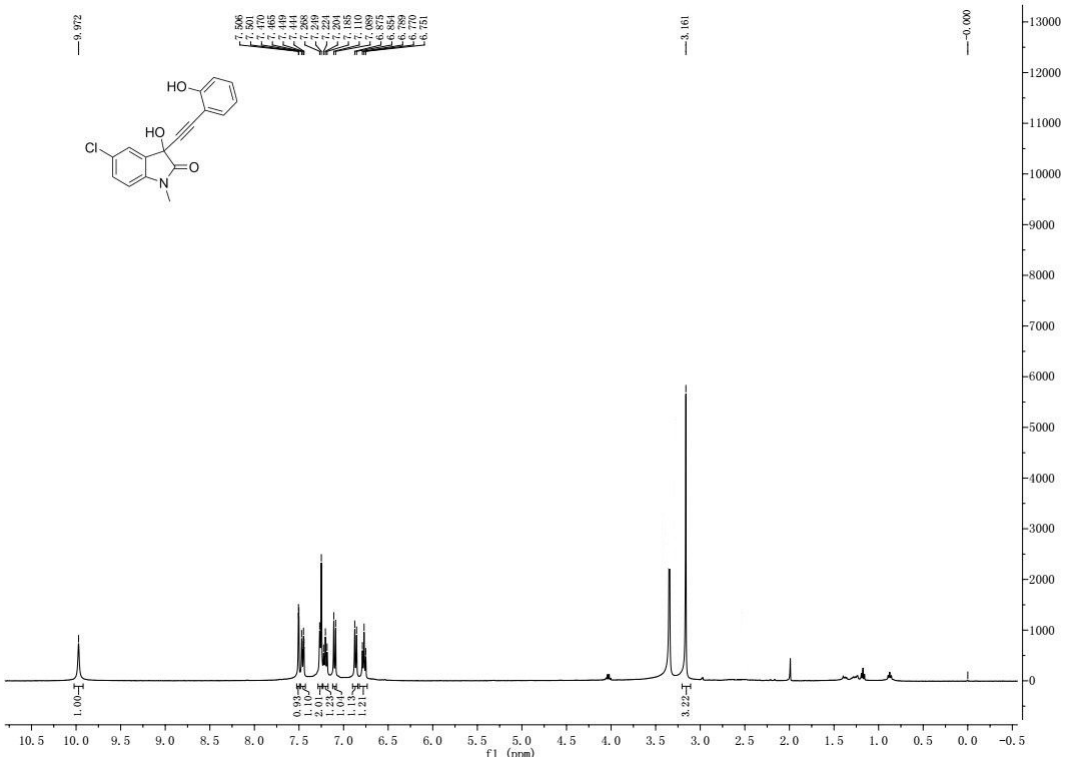
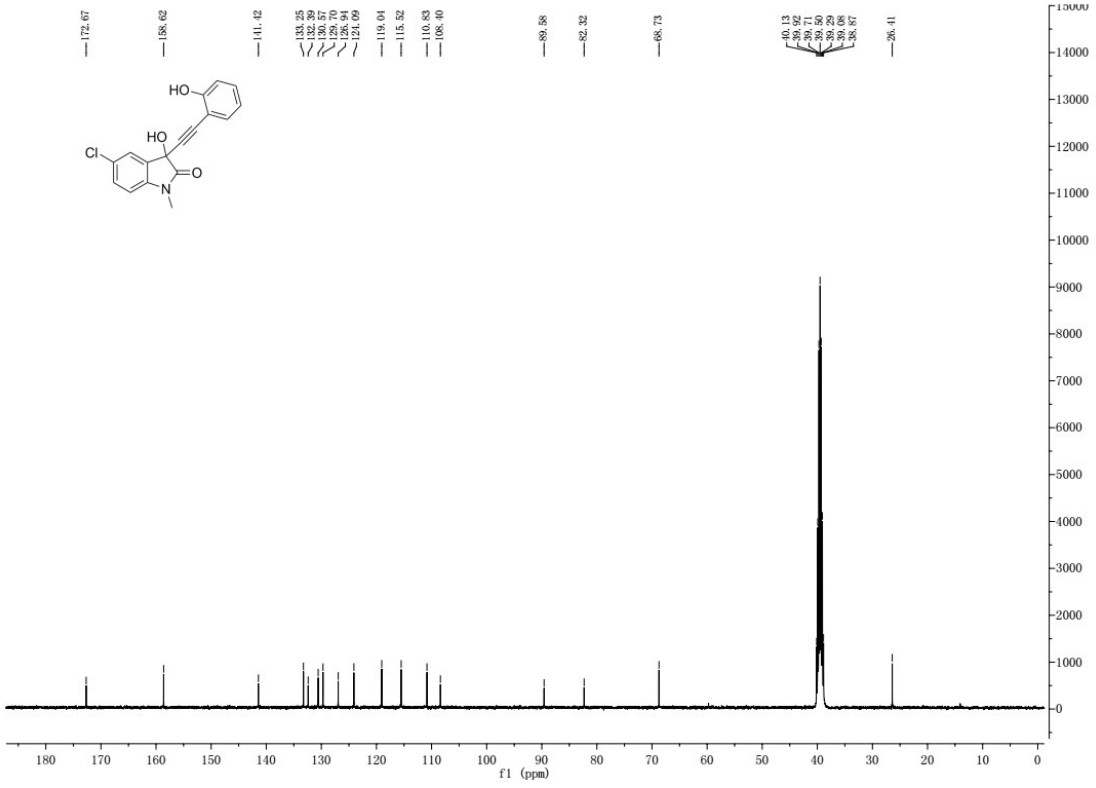
158.786
140.253
133.404
133.345
130.729
128.695
127.584
127.525
124.791
123.899
122.606
119.060
115.614
111.825
111.499
111.175
110.851
108.384
89.395
82.602
67.162
28.855
HO
HO
O
N
F
F
F
f1 (ppm)


9.932
7.413
7.393
7.372
7.275
7.271
7.256
7.252
7.222
7.205
7.187
7.165
7.129
7.125
7.110
7.045
7.023
6.896
6.896
6.789
6.789
6.761
3.173
0.000
HO
Cl
HO
O
N
1.11
1.01
1.00
1.19
1.92
1.02
1.11
1.11
3.03
f1 (ppm)


172.65
158.56
144.43
133.42
131.44
130.46
130.36
126.50
123.65
119.03
115.52
108.65
108.03
88.08
81.85
69.03
40.12
39.97
39.71
39.50
39.29
39.08
38.87
26.54
HO
Cl
HO
O
N
f1 (ppm)


9.972
7.506
7.501
7.470
7.465
7.449
7.444
7.268
7.239
7.221
7.204
7.185
7.110
7.089
6.875
6.854
6.789
6.770
6.751
3.161
0.000
HO
HO
Cl
O
N
1.00
0.93
1.01
2.01
1.23
1.04
1.13
1.21
3.22
f1 (ppm)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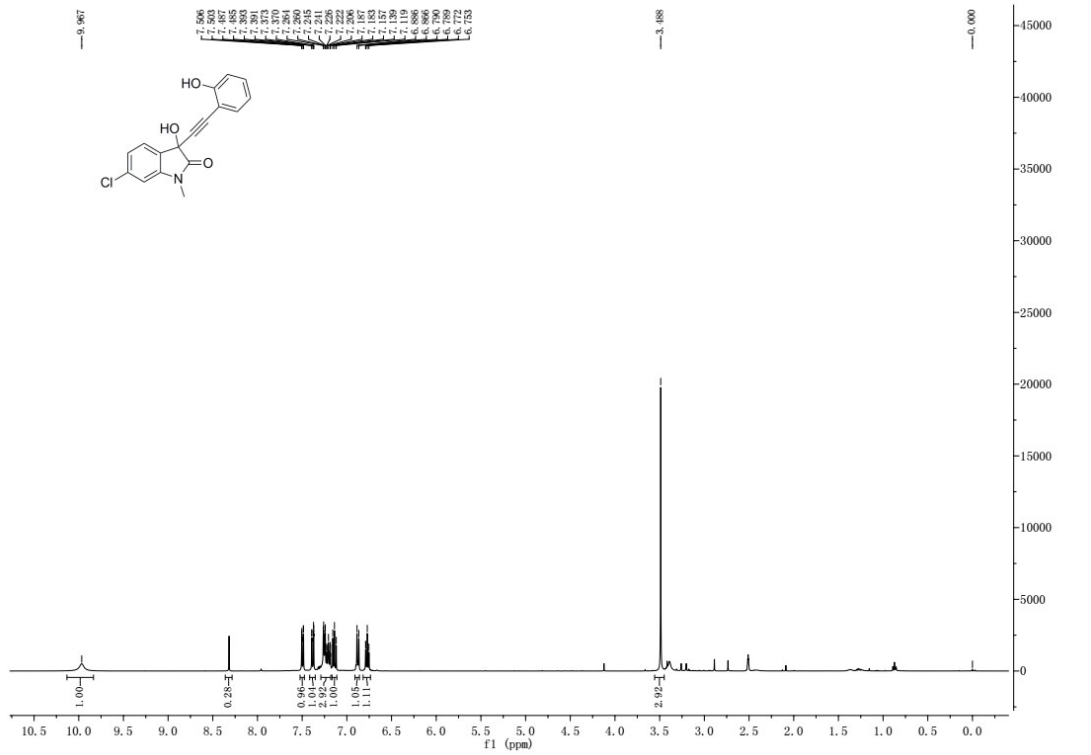
158.62
141.42
133.25
132.39
130.57
129.70
126.94
124.09
119.04
115.52
110.83
108.40
89.58
82.32
68.73
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.41
HO
HO
Cl
O
N
f1 (ppm)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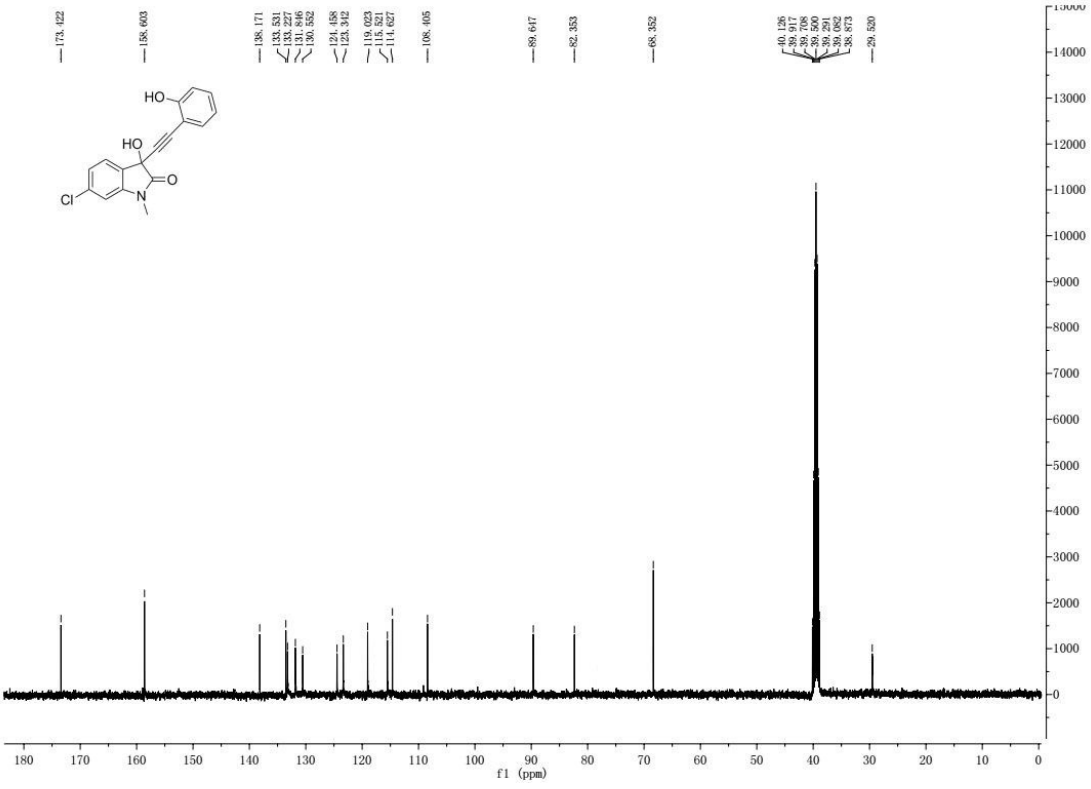
7.505
7.487
7.485
7.393
7.391
7.371
7.370
7.264
7.260
7.245
7.241
7.226
7.222
7.205
7.187
7.183
7.157
7.139
7.119
6.896
6.896
6.790
6.789
6.772
6.753
3.488
0.000
HO
HO
O
N
Cl
1.00
0.28
0.96
1.01
2.02
1.00
1.05
1.11
2.92
f1 (ppm)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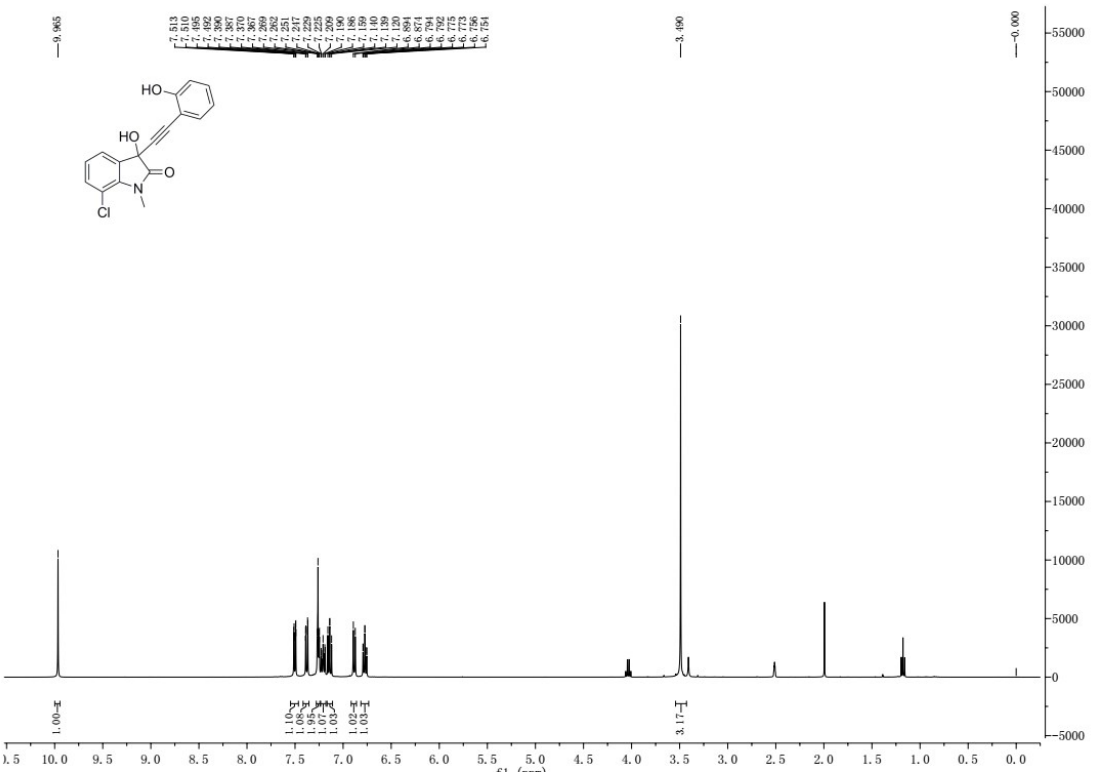
138.171
133.531
133.227
131.646
130.552
124.458
123.342
119.023
115.521
114.627
108.405
89.647
82.353
68.352
40.126
39.917
39.708
39.500
39.291
39.082
38.873
29.520
HO
HO
O
N
Cl
f1 (ppm)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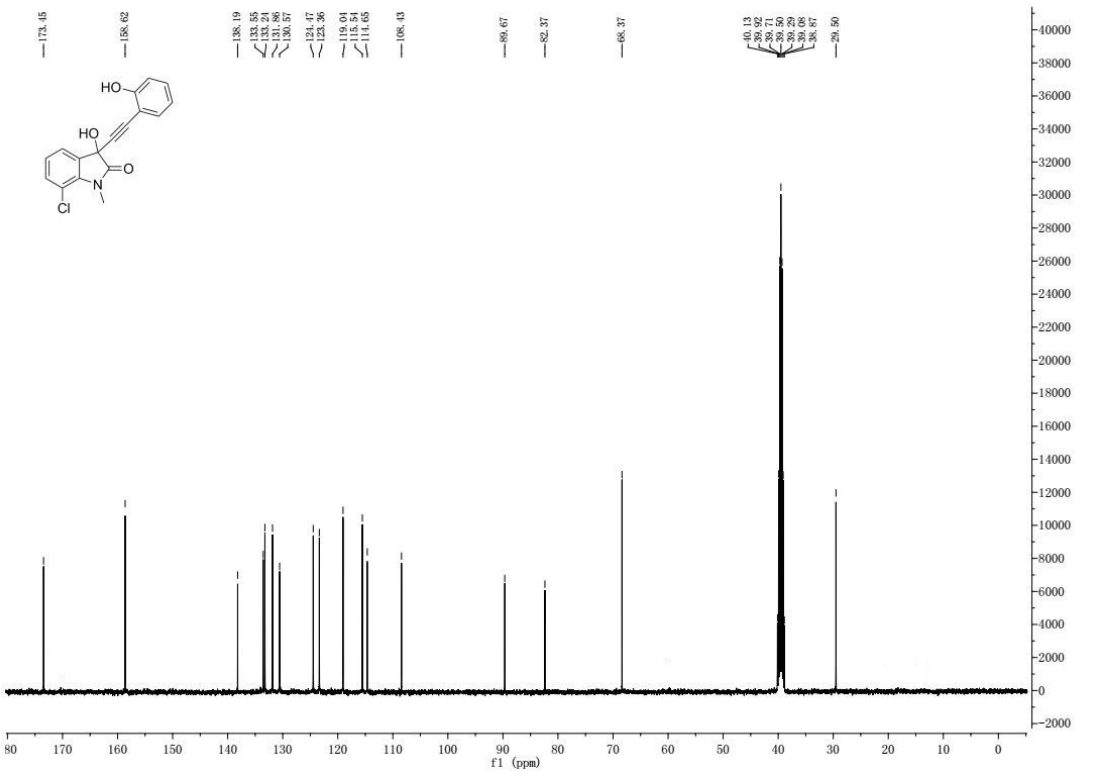
7.510
7.495
7.492
7.390
7.387
7.370
7.367
7.269
7.262
7.251
7.241
7.229
7.225
7.209
7.198
7.186
7.159
7.140
7.139
7.110
6.894
6.874
6.794
6.792
6.775
6.773
6.756
6.754
3.490
0.000
HO
HO
O
N
Cl
1.00
1.10
1.08
1.05
1.07
1.03
1.02
1.03
3.17
f1 (ppm)


173.45
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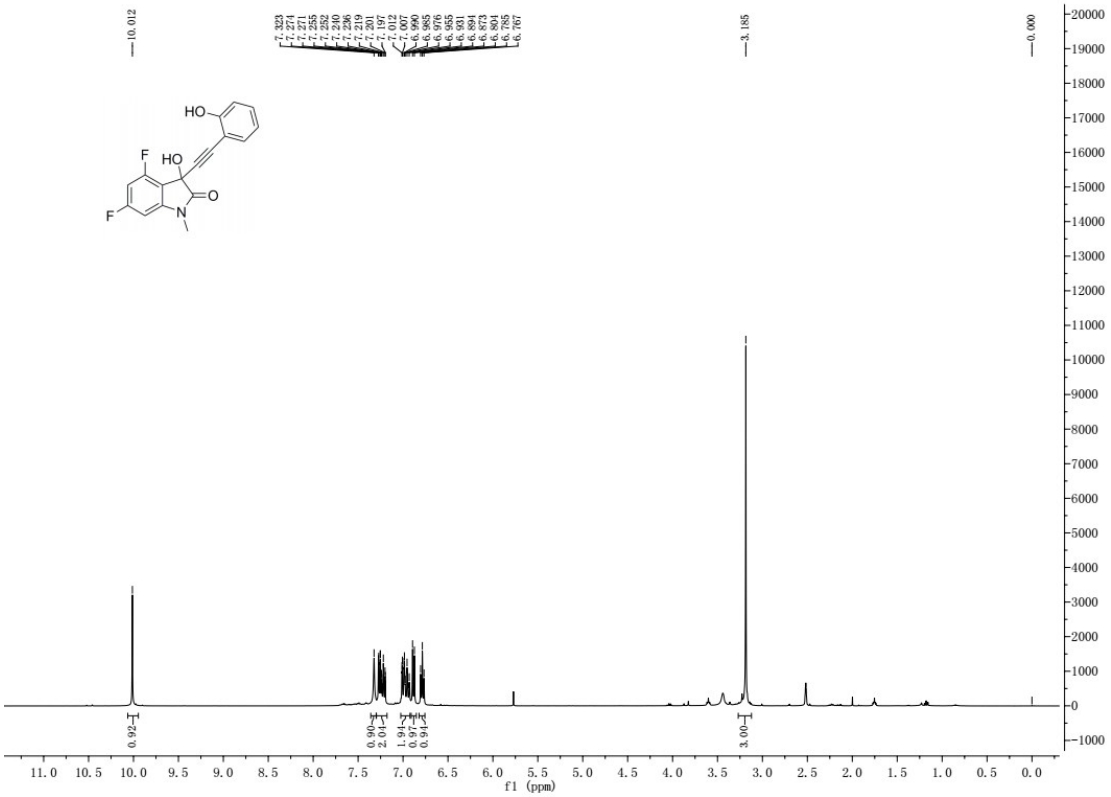
138.19
133.55
133.24
131.86
130.57
124.47
123.36
119.01
115.54
114.65
108.43
89.67
82.37
68.37
40.13
39.92
39.71
39.50
39.29
39.08
38.87
29.50
HO
HO
O
N
Cl
f1 (ppm)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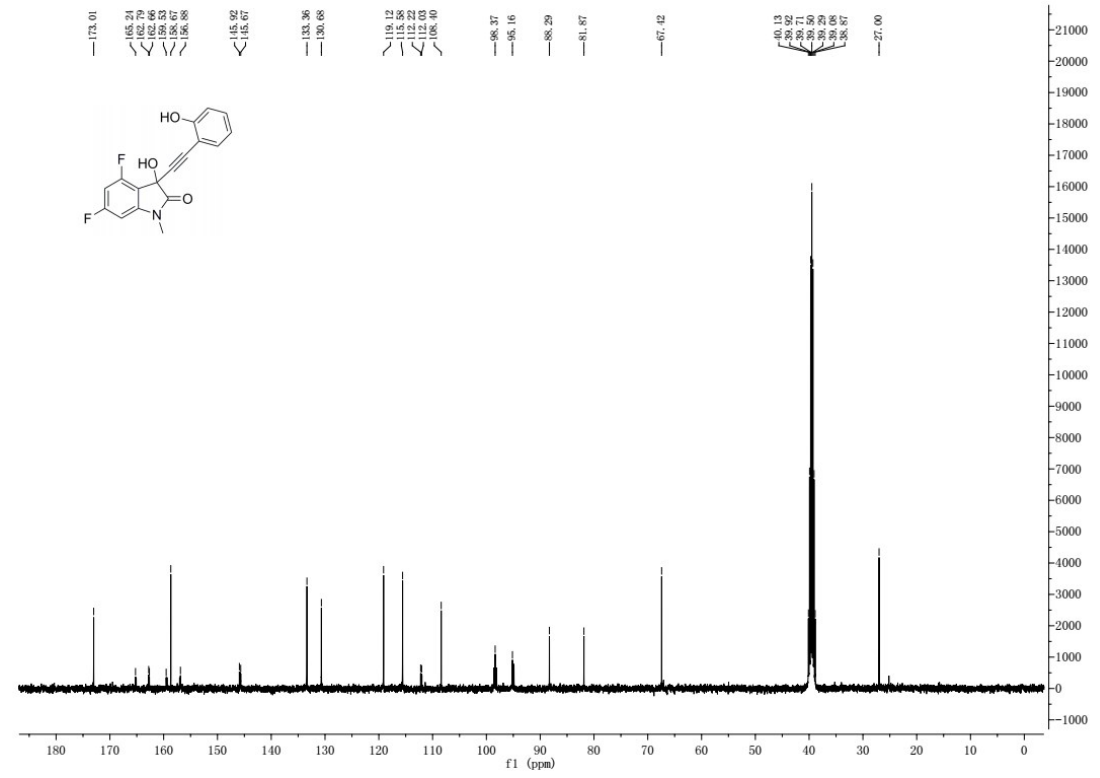
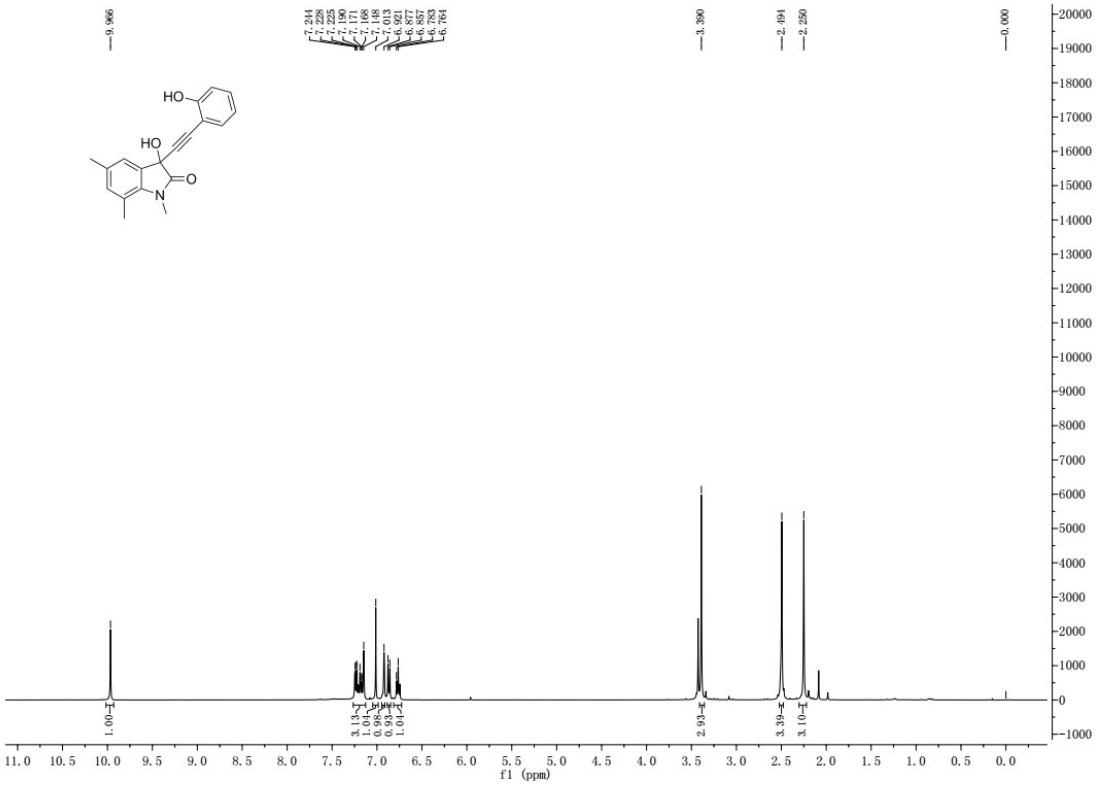
7.274
7.271
7.255
7.252
7.240
7.236
7.219
7.201
7.197
7.012
7.007
6.990
6.985
6.976
6.955
6.931
6.894
6.873
6.804
6.785
6.767
3.185
0.000
HO
F
HO
O
F
N
0.92
0.90
2.04
1.94
0.97
0.94
3.00
f1 (ppm)


173.01
165.24
163.79
162.66
159.53
156.67
156.88
145.92
145.67
133.36
130.68
119.12
115.58
112.22
112.03
108.40
98.37
95.16
88.29
81.87
67.42
40.13
39.92
39.71
39.50
39.29
39.08
38.87
27.00
HO
F
HO
O
F
N
f1 (ppm)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7.171
7.169
7.148
7.013
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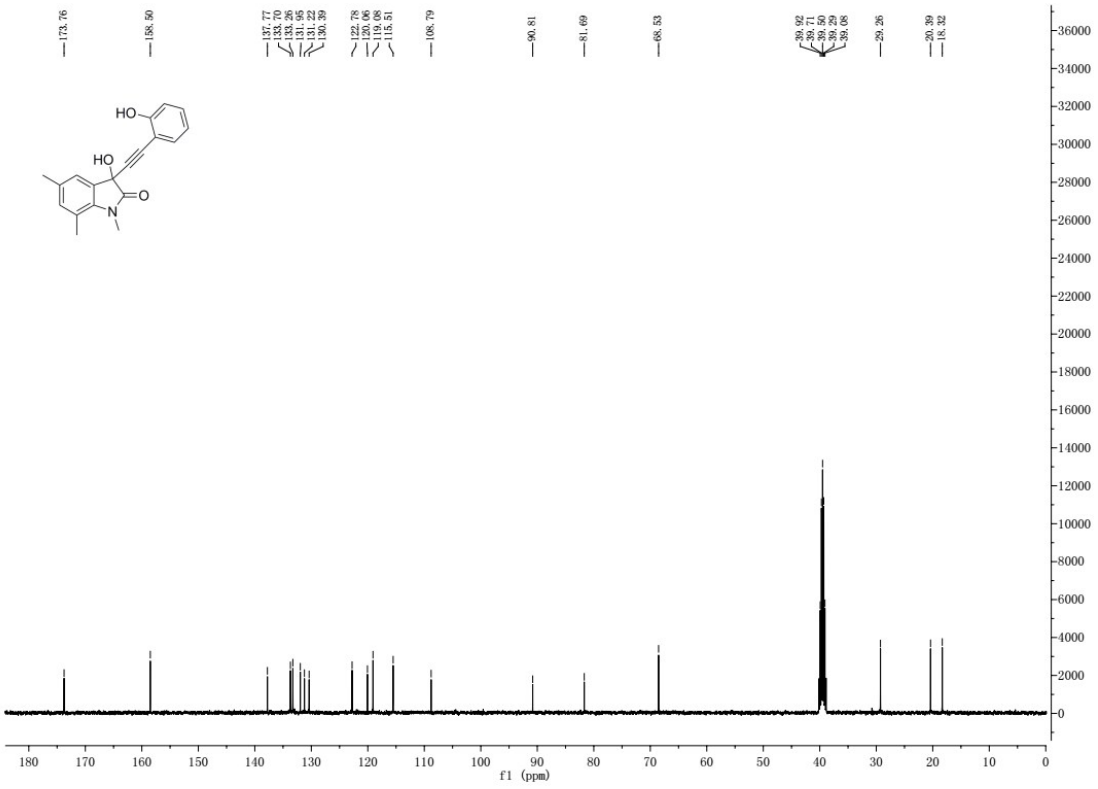
6.857
6.783
6.764
3.390
2.494
2.250
0.000
HO
HO
O
N
1.00
3.13
1.00
0.98
0.93
1.04
2.93
3.39
3.10
f1 (ppm)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131.95
131.71
130.39
122.78
120.06
119.08
115.51
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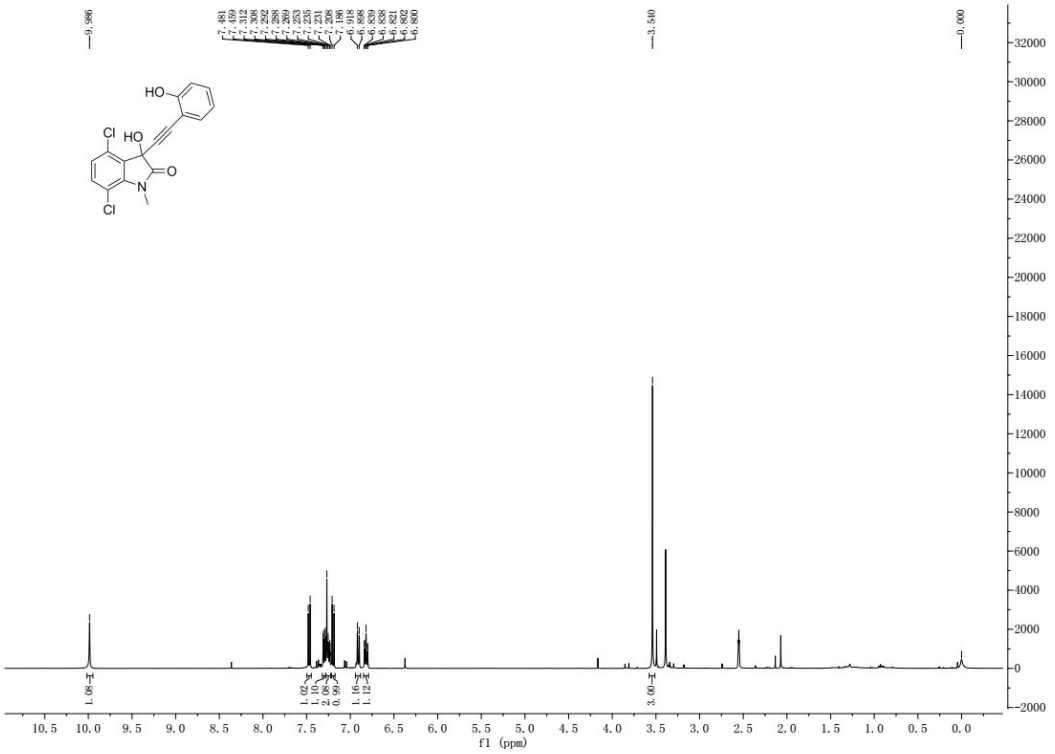
90.81
81.69
68.53
39.92
39.71
39.50
39.29
39.08
29.26
20.39
16.32
HO
HO
O
N
f1 (ppm)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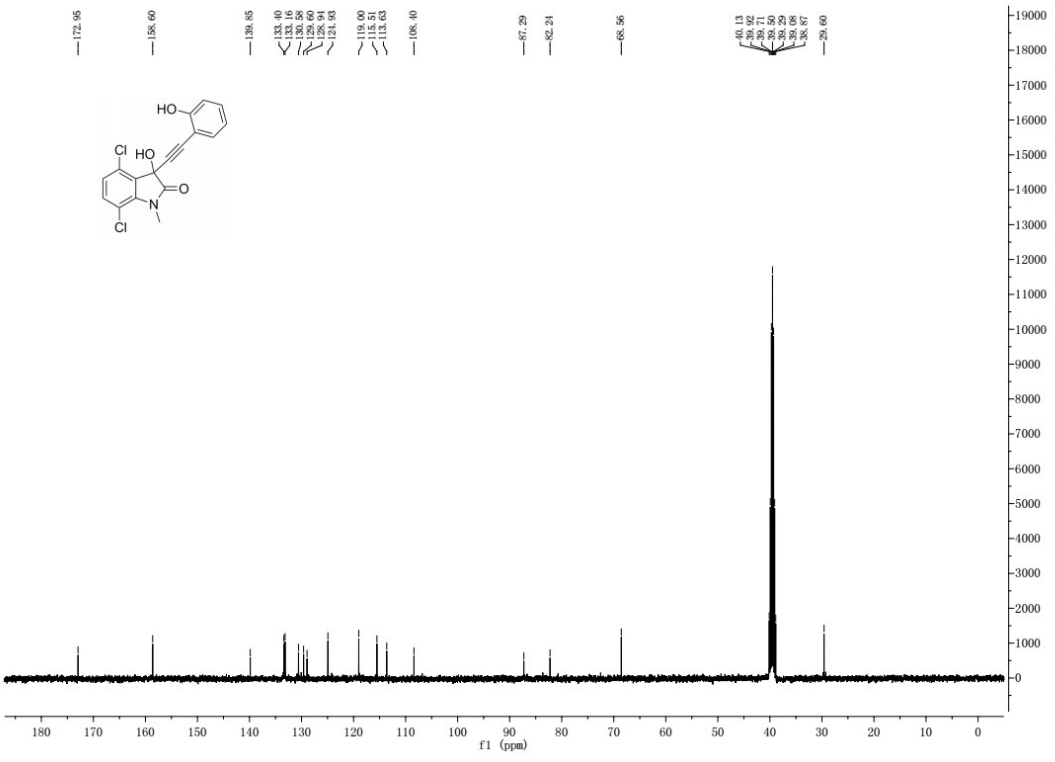
7.253
7.235
7.231
7.208
7.186
6.918
6.898
6.839
6.838
6.821
6.802
6.800
3.540
0.000
HO
Cl
HO
O
N
Cl
1.08
1.02
1.10
2.08
0.99
1.16
1.12
3.00
f1 (ppm)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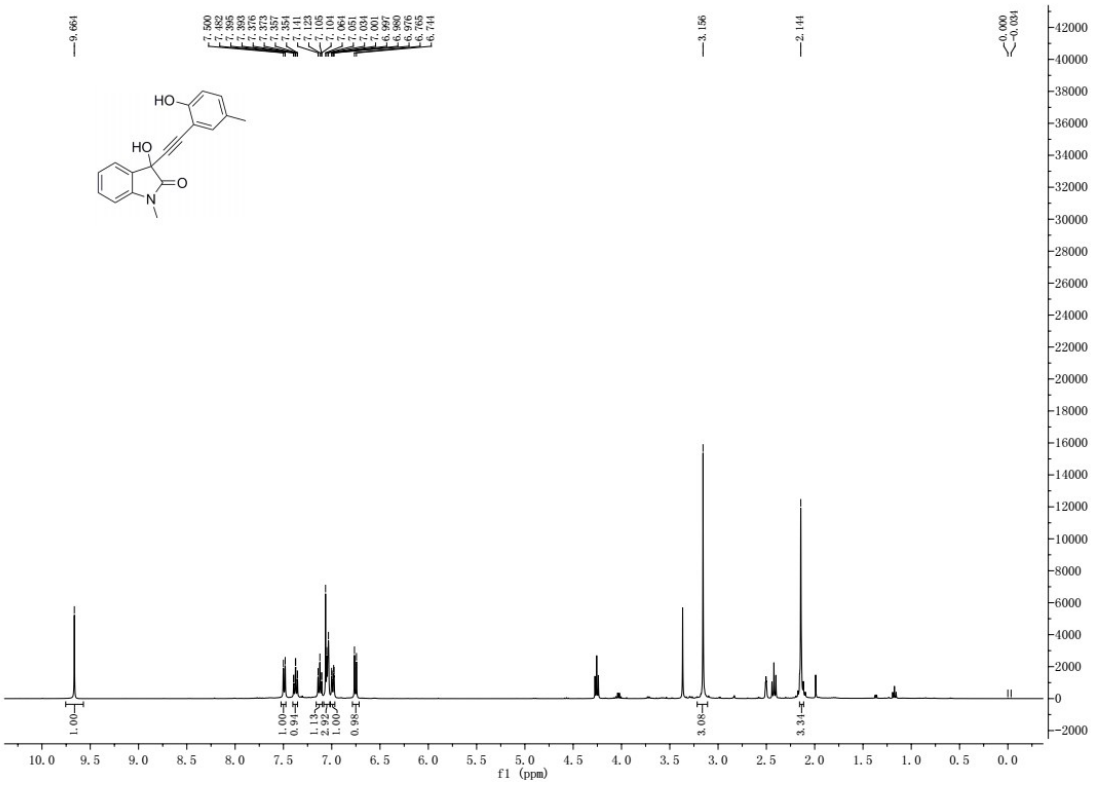
133.16
130.58
129.60
125.94
124.93
119.00
115.51
113.63
106.40
87.29
82.24
68.56
40.13
39.92
39.71
39.50
39.29
39.08
38.87
29.60
HO
Cl
HO
O
N
Cl
f1 (ppm)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7.376
7.373
7.357
7.354
7.111
7.105
7.104
7.061
7.061
7.034
7.001
6.997
6.980
6.765
6.744
3.156
2.144
0.000
-0.034
HO
HO
O
N
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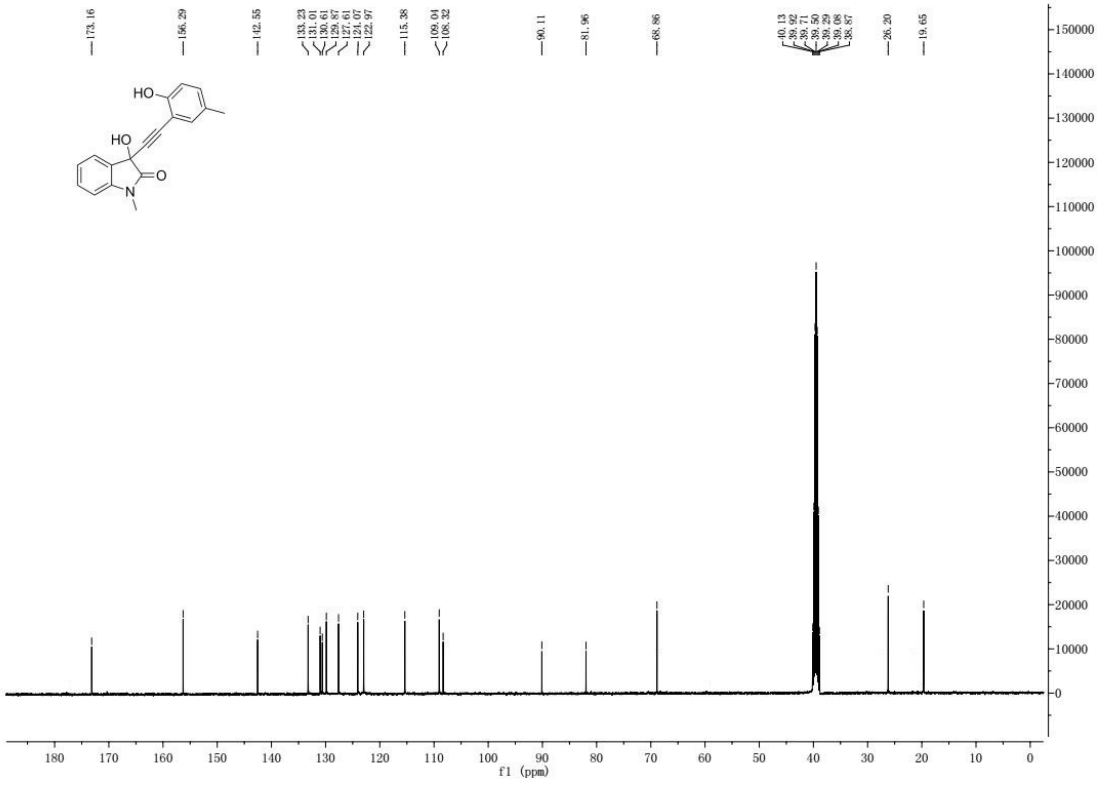
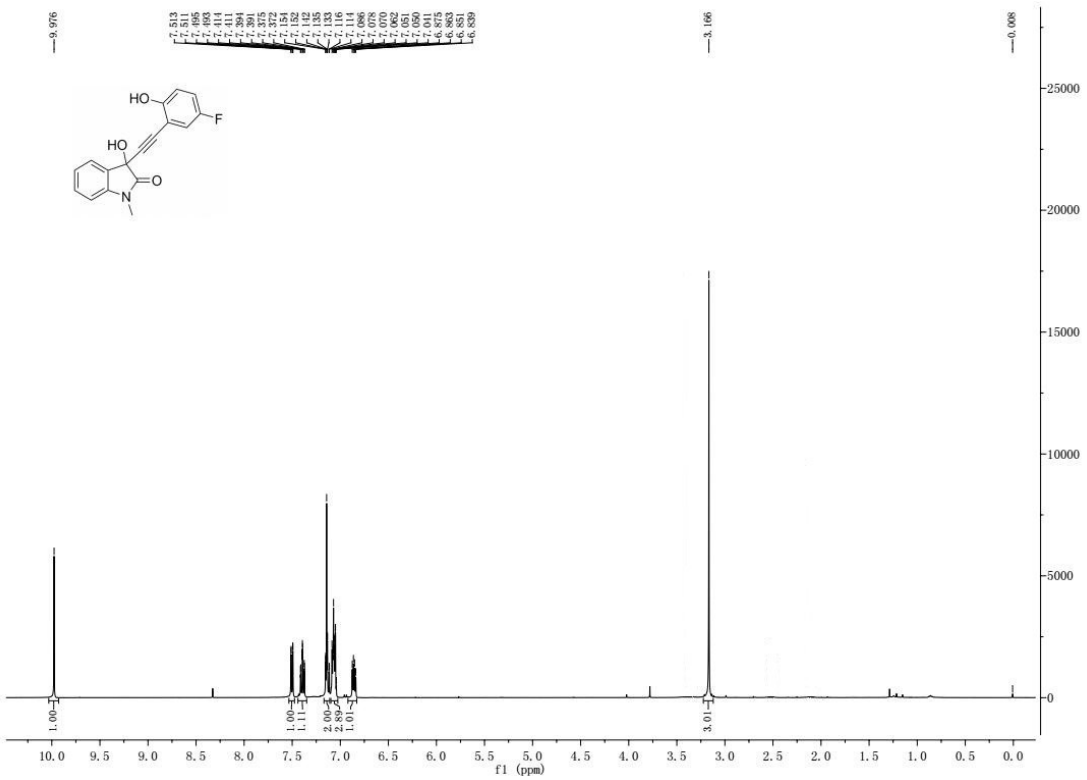
1.00
0.94
1.13
2.92
1.00
0.98
3.08
3.34
f1 (ppm)


173.16
156.29
142.55
133.23
131.01
130.64
129.87
127.61
124.07
122.97
115.38
109.04
108.32
90.11
81.96
68.86
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.20
19.65
HO
HO
O
N
f1 (ppm)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7.495
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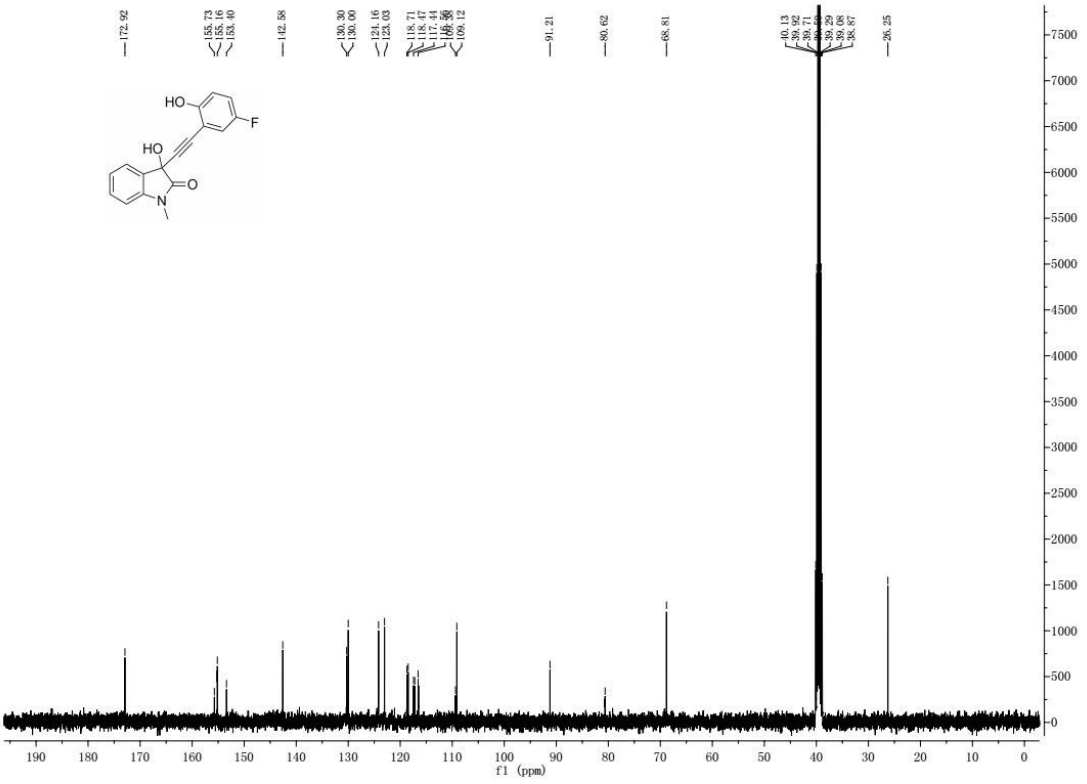
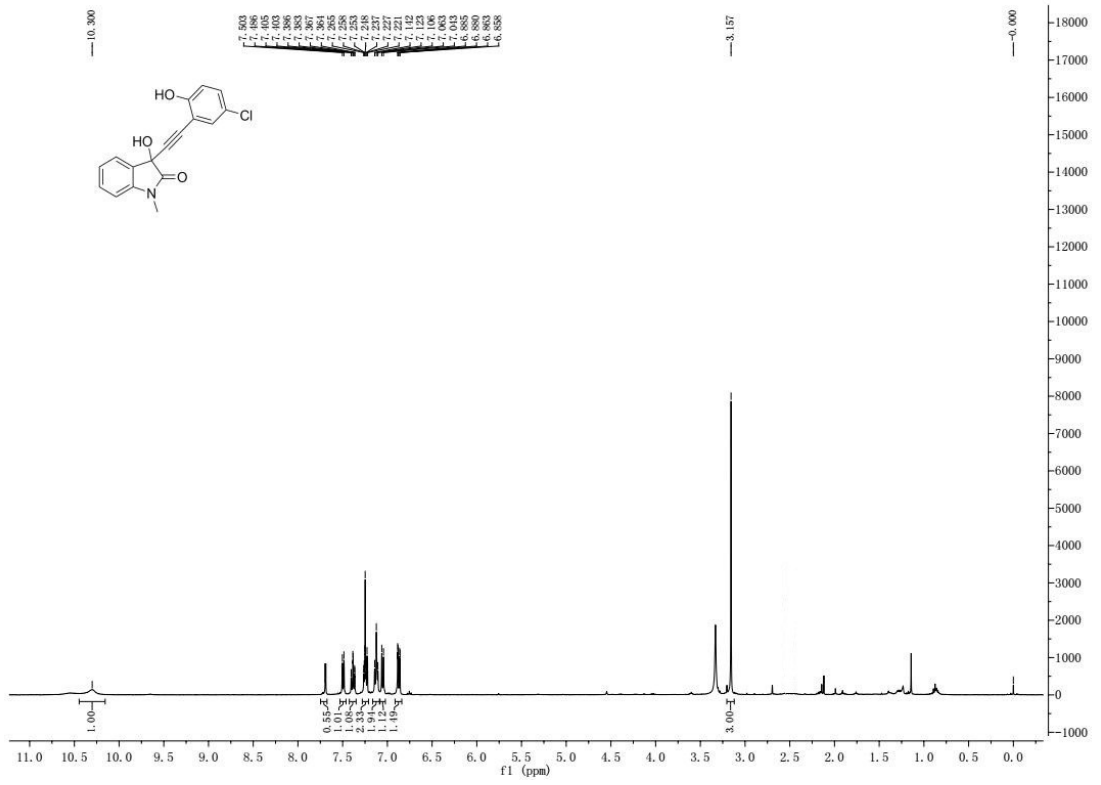
7.411
7.394
7.391
7.375
7.372
7.154
7.152
7.142
7.135
7.133
7.116
7.114
7.086
7.078
7.070
7.062
7.051
7.050
7.041
6.875
6.863
6.861
6.839
3.166
0.008
HO
F
HO
O
N
1.00
1.00
1.11
2.00
2.96
2.01
3.01
f1 (ppm)


172.92
155.73
155.16
153.40
142.58
130.30
130.00
124.16
123.03
118.71
118.57
117.44
116.86
116.66
109.12
91.21
80.62
68.81
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.25
HO
F
HO
O
N
f1 (ppm)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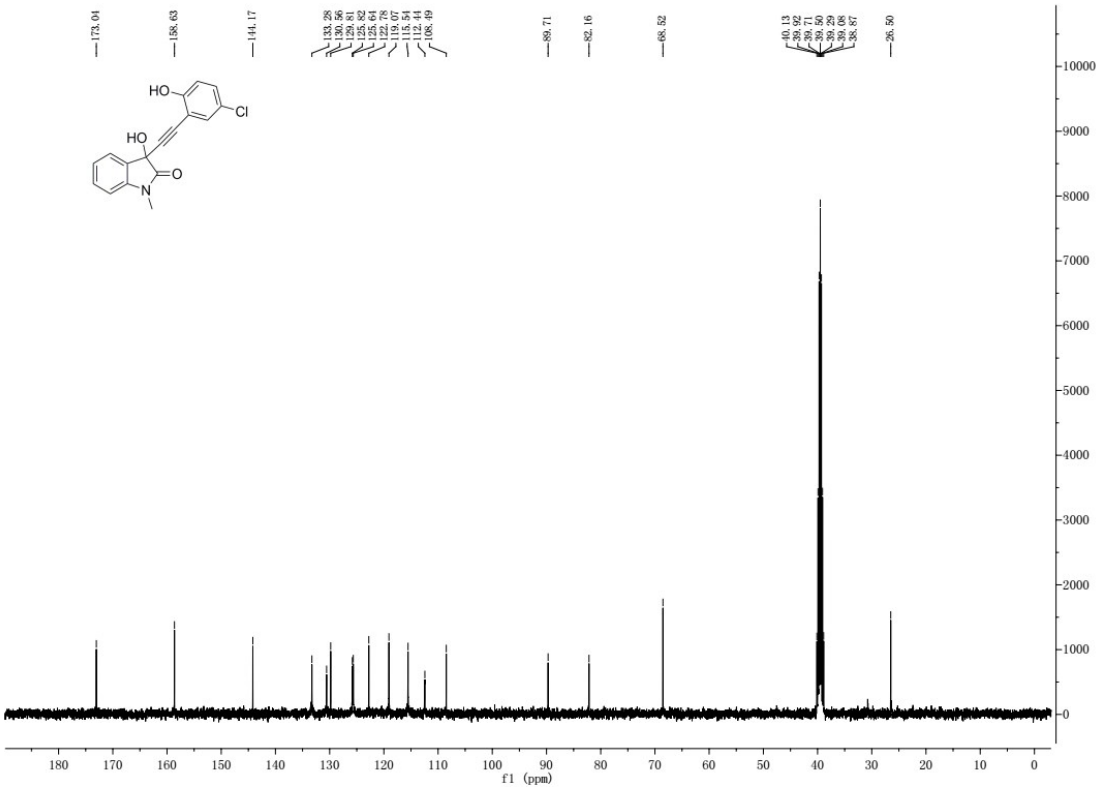
7.403
7.398
7.383
7.367
7.364
7.255
7.238
7.253
7.218
7.237
7.227
7.221
7.142
7.123
7.106
7.043
6.885
6.880
6.863
6.858
3.157
0.000
HO
Cl
HO
O
N
1.00
0.55
1.01
1.08
2.33
1.04
1.12
1.49
3.00
f1 (ppm)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144.17
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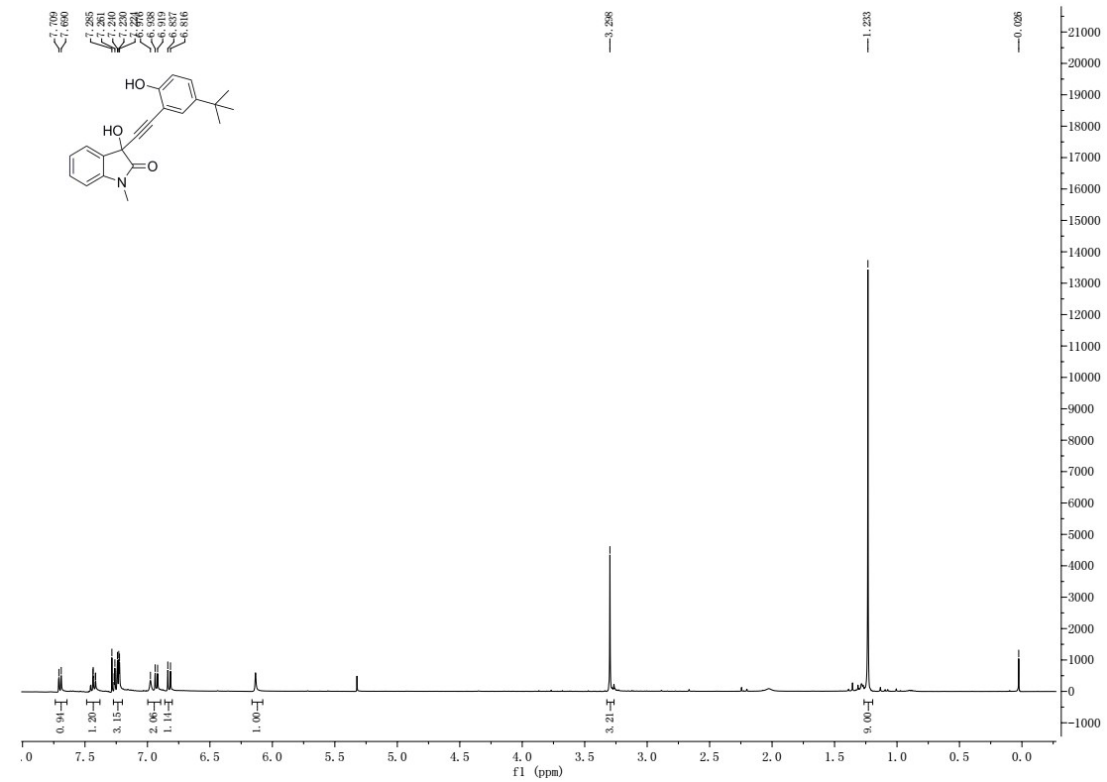
129.81
125.82
125.64
122.78
119.07
115.54
112.44
108.49
89.71
82.16
68.52
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.50
HO
Cl
HO
O
N
f1 (ppm)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7.285
7.261
7.250
7.230
7.224
7.218
7.208
6.938
6.919
6.837
6.816
3.298
1.233
0.026
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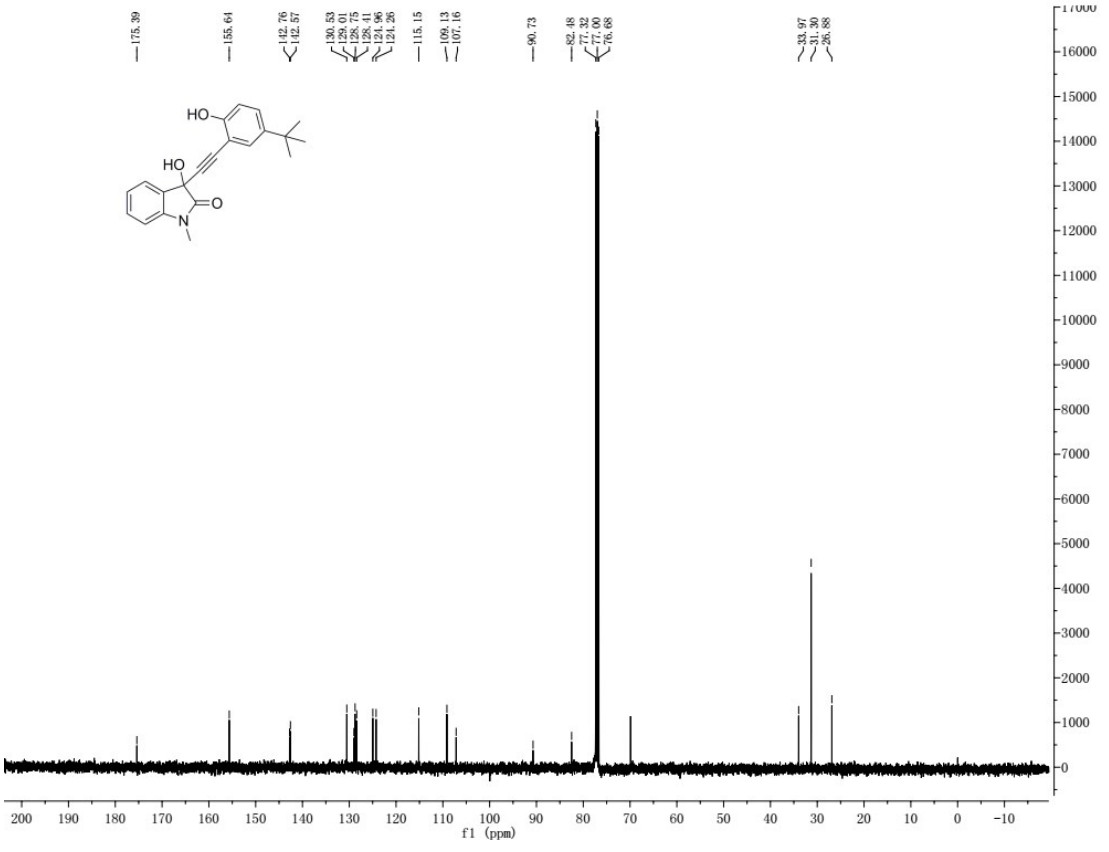
HO
O
N
0.94
1.20
3.15
2.06
1.14
1.00
3.21
9.00
f1 (ppm)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142.76
142.57
130.53
129.01
128.75
128.41
124.96
124.26
115.15
109.13
107.16
90.73
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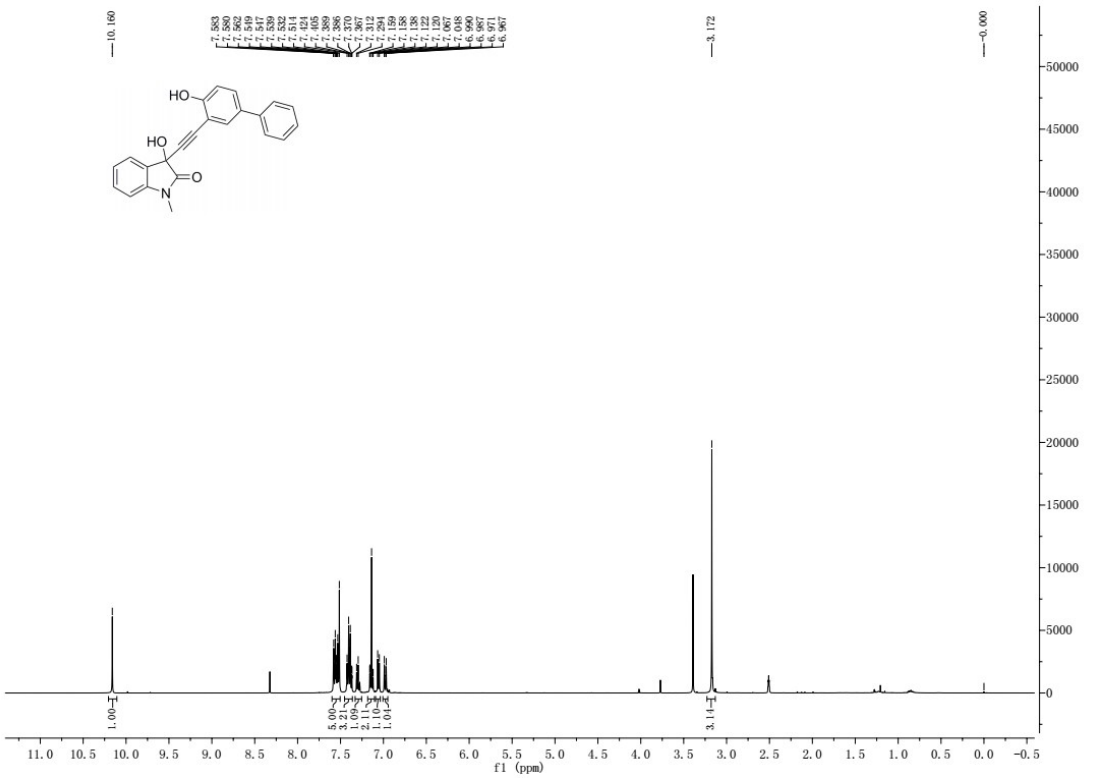
77.32
77.00
76.68
33.97
31.30
26.86
HO
HO
O
N
f1 (ppm)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7.532
7.514
7.424
7.405
7.389
7.386
7.370
7.367
7.312
7.294
7.159
7.158
7.138
7.122
7.120
7.067
7.048
6.990
6.987
6.971
6.967
3.172
0.000
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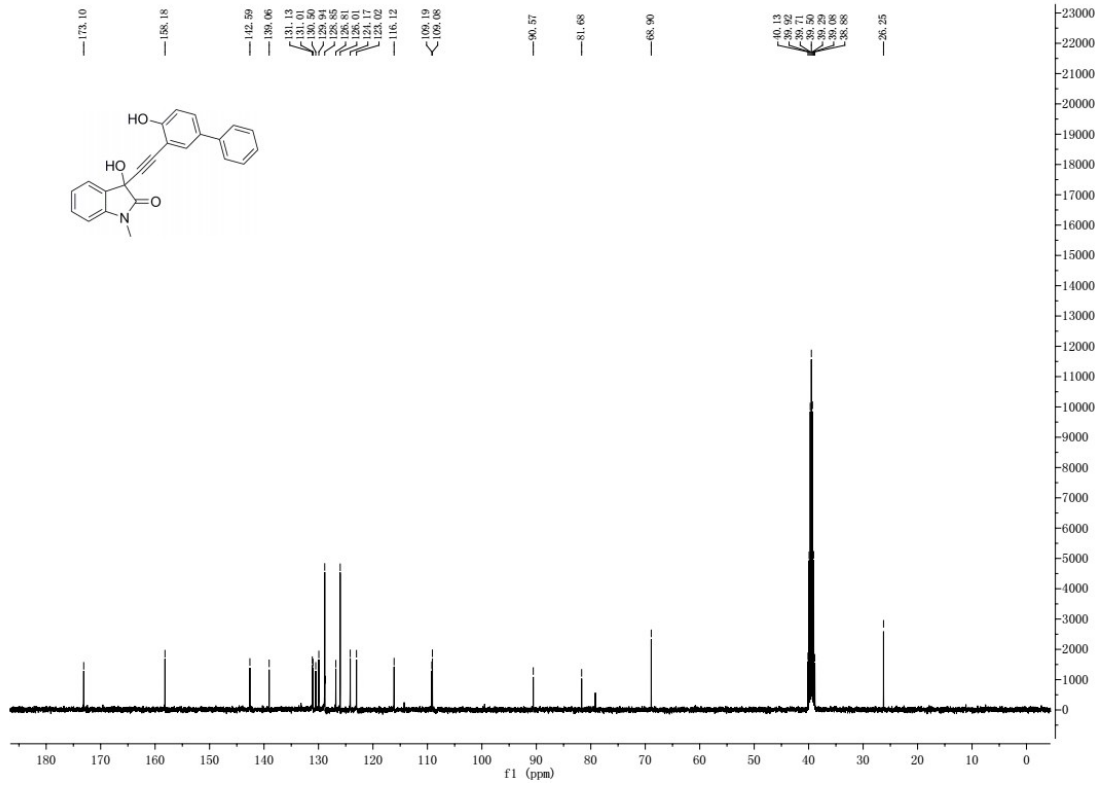
HO
O
N
1.00
5.09
3.21
1.09
2.11
1.10
1.04
3.14
f1 (ppm)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129.94
128.85
126.81
126.01
124.17
123.02
116.12
109.19
109.08
90.57
81.68
68.90
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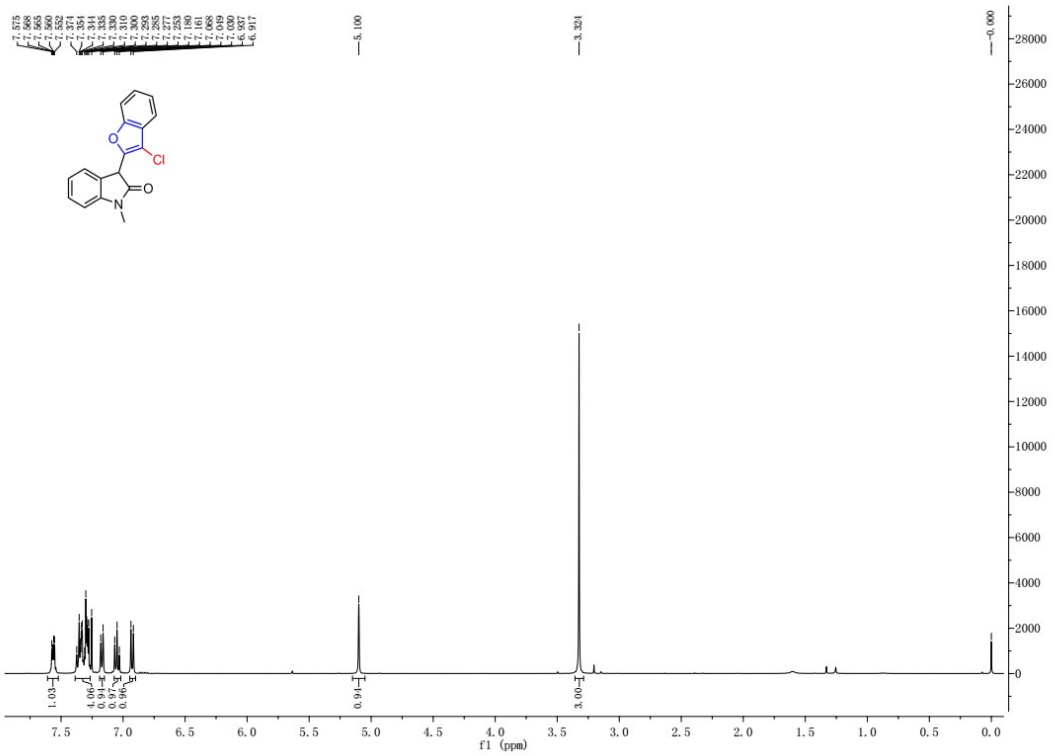
39.71
39.50
39.29
39.08
38.88
26.25
HO
HO
O
N
f1 (ppm)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7.560
7.552
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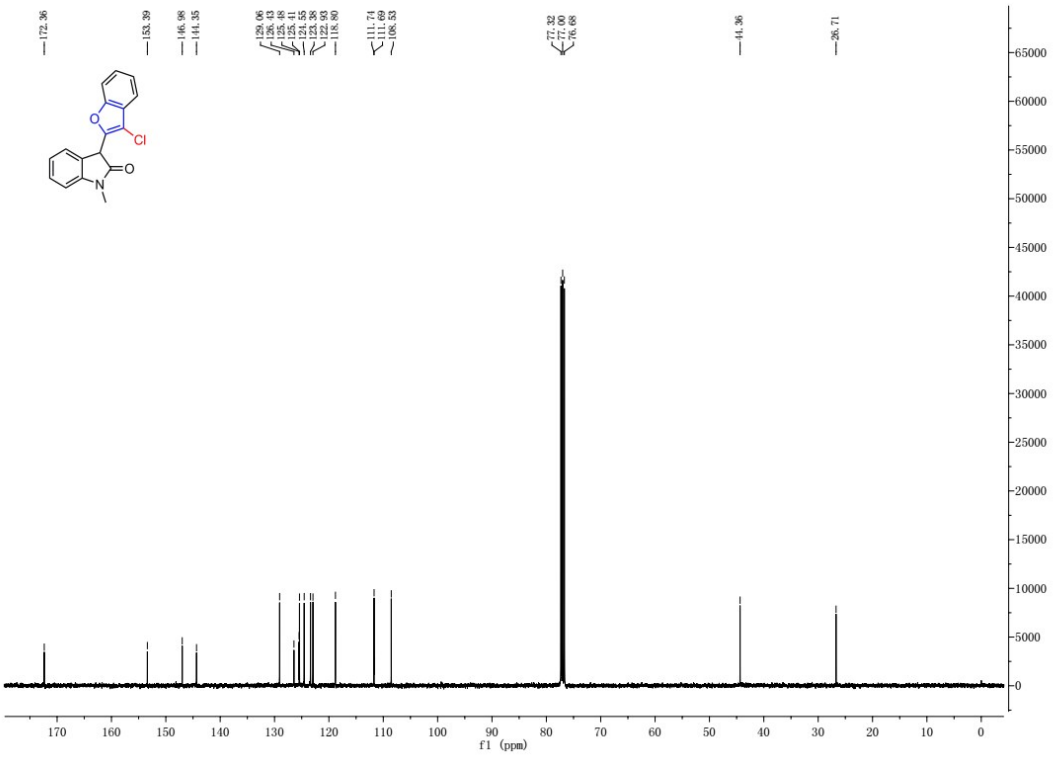
7.344
7.335
7.330
7.310
7.300
7.295
7.277
7.255
7.180
7.161
7.098
7.049
7.030
6.937
6.917
5.100
3.324
0.000
Cl
O
N
1.03
4.06
0.94
0.97
0.96
0.94
3.00
f1 (ppm)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126.43
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125.11
124.55
123.38
122.93
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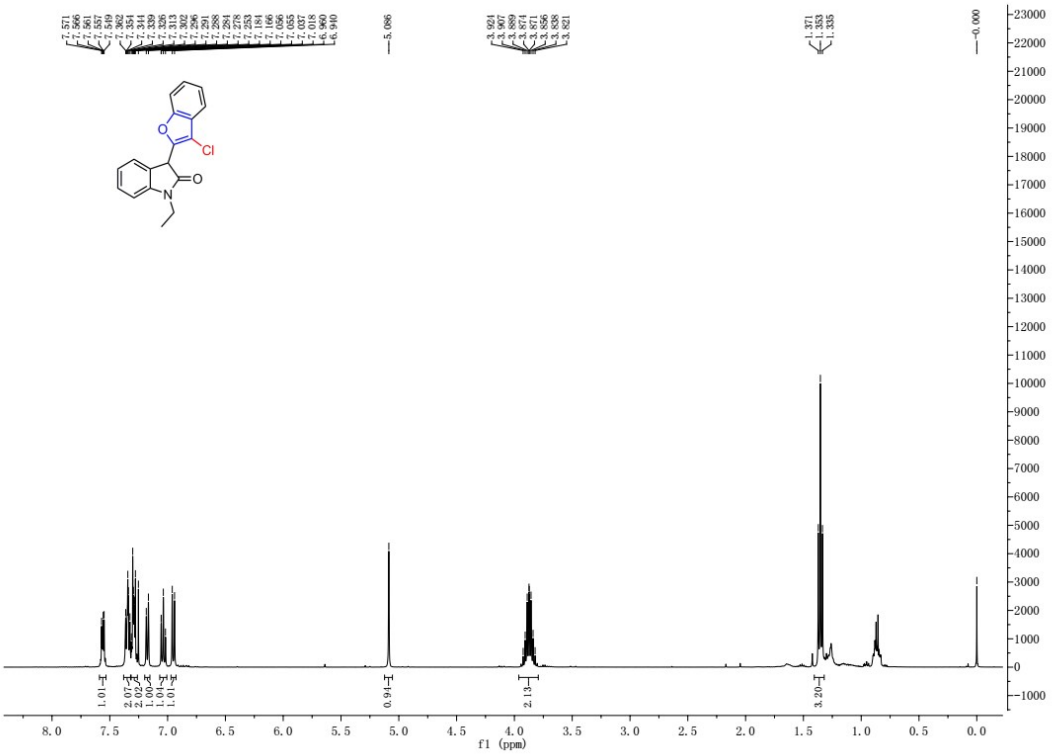
111.74
111.69
108.53
77.32
77.00
76.68
44.36
26.71
Cl
O
N
f1 (ppm)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7.561
7.557
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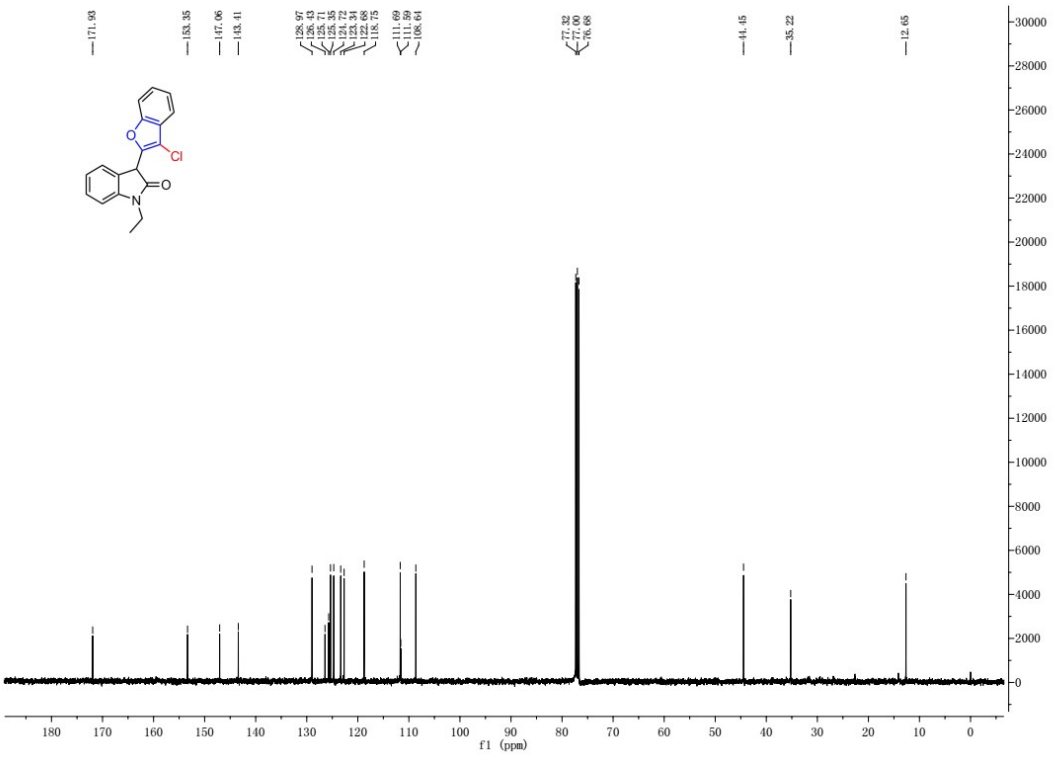
7.354
7.344
7.339
7.339
7.313
7.302
7.296
7.291
7.288
7.284
7.278
7.253
7.184
7.166
7.056
7.055
7.037
7.018
6.960
6.940
5.086
3.924
3.907
3.889
3.874
3.871
3.856
3.839
3.821
1.371
1.353
1.335
0.000
1.01
2.07
2.02
1.00
1.04
1.01
0.94
2.13
3.20
O
Cl
N
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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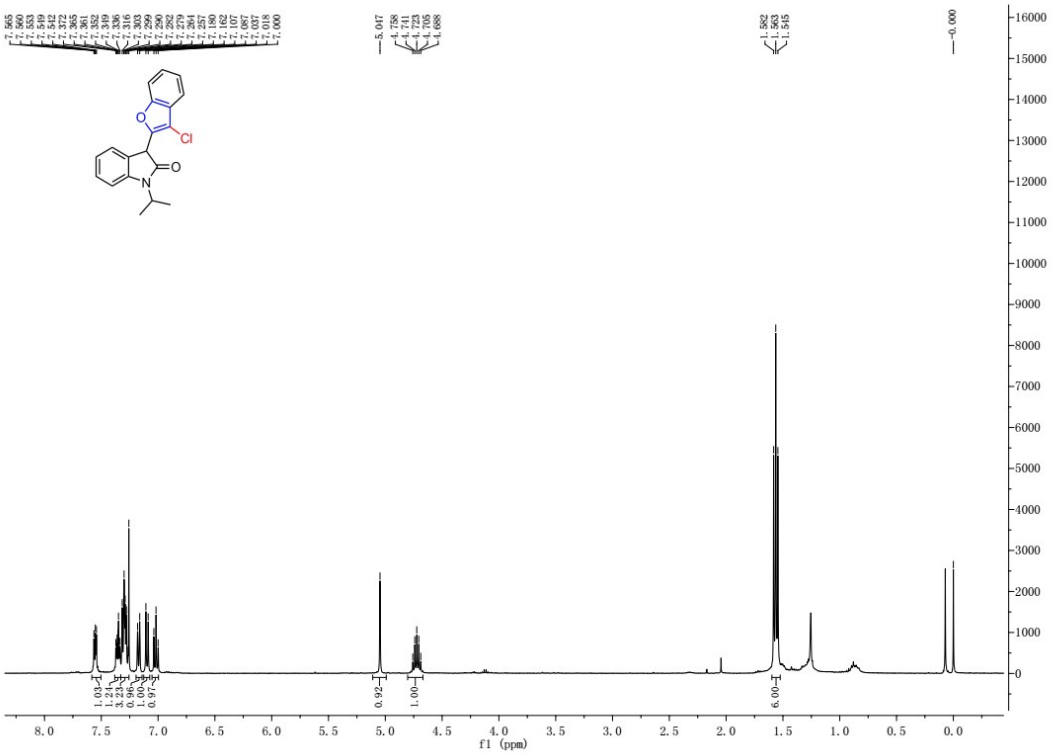
128.97
128.43
125.71
125.35
124.72
123.34
122.68
118.75
111.69
111.59
106.64
77.32
77.00
76.68
44.45
35.22
12.65
O
Cl
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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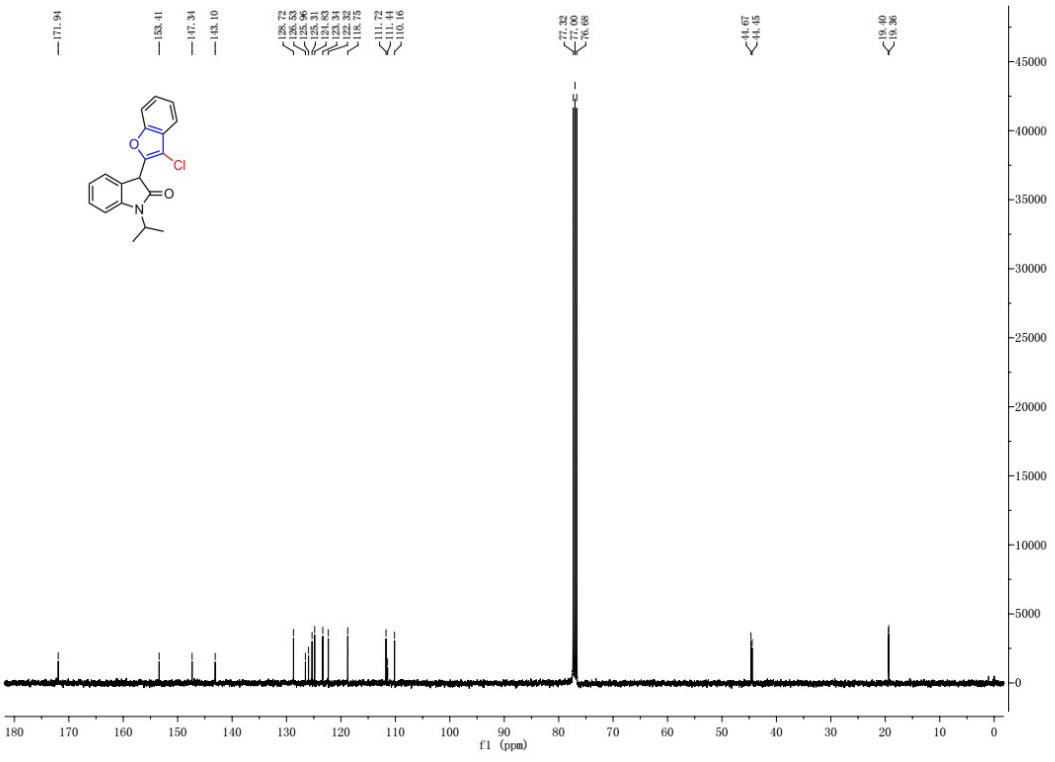
7.553
7.549
7.542
7.372
7.365
7.361
7.352
7.339
7.336
7.316
7.303
7.299
7.290
7.282
7.279
7.264
7.257
7.180
7.102
7.101
7.087
7.037
7.018
7.000
5.047
4.738
4.711
4.723
4.705
4.688
1.582
1.563
1.545
0.000
Cl
O
N
1.03
1.21
3.23
0.96
1.00
0.97
0.92
1.00
6.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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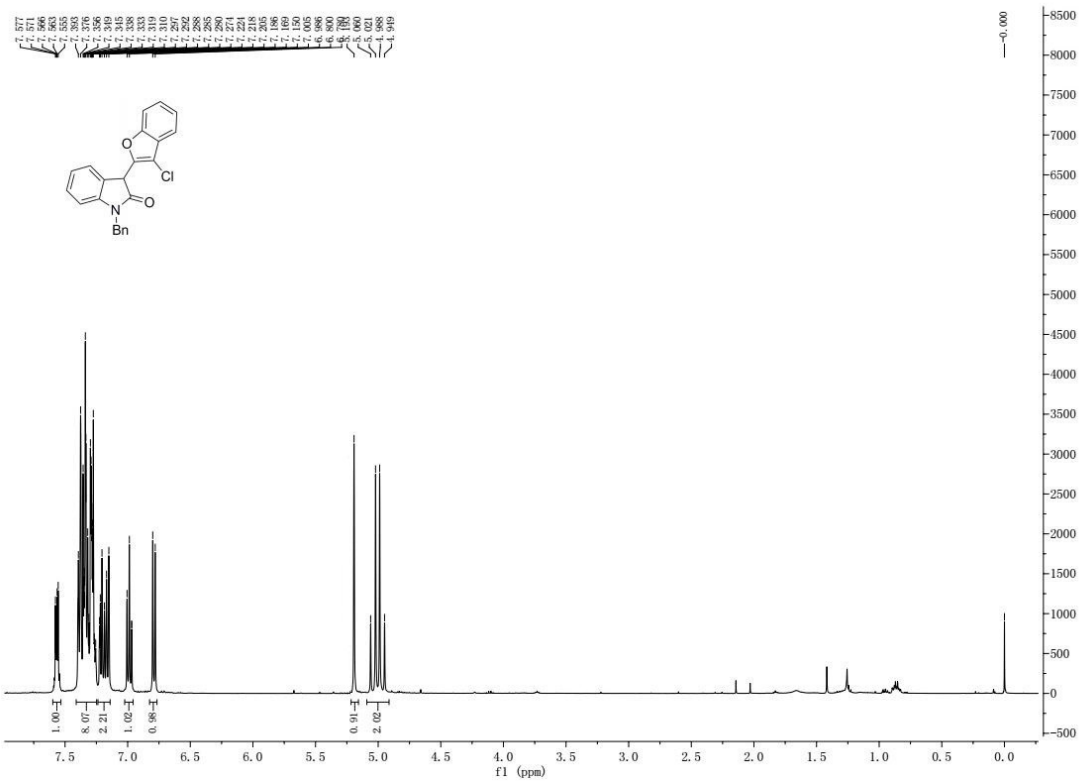
153.41
147.34
143.10
128.72
126.53
125.56
125.31
124.83
123.34
122.32
118.75
111.72
111.44
110.16
77.32
77.00
76.68
44.67
44.45
19.40
19.36
Cl
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.345
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7.333
7.319
7.310
7.297
7.292
7.288
7.285
7.280
7.274
7.271
7.218
7.205
7.196
7.169
7.159
7.005
6.986
6.800
5.060
5.051
4.988
4.949
-0.000
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Cl
N
O
Bn
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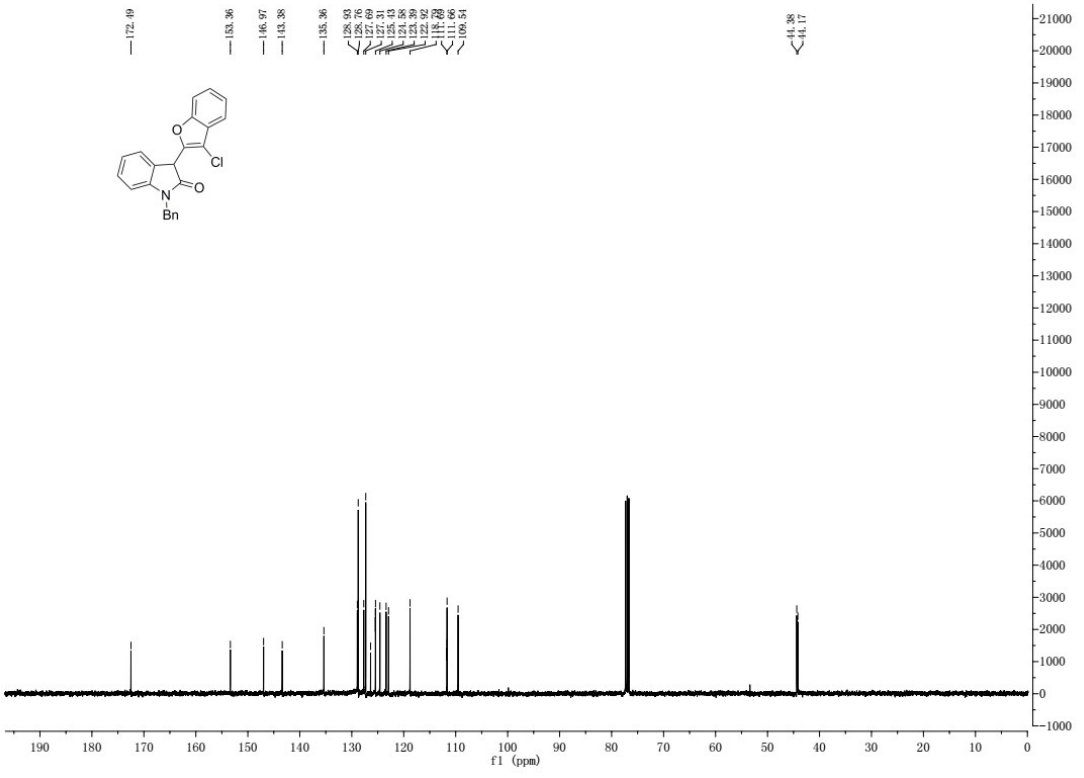
8.07
2.21
1.02
0.98
0.91
2.02
f1 (ppm)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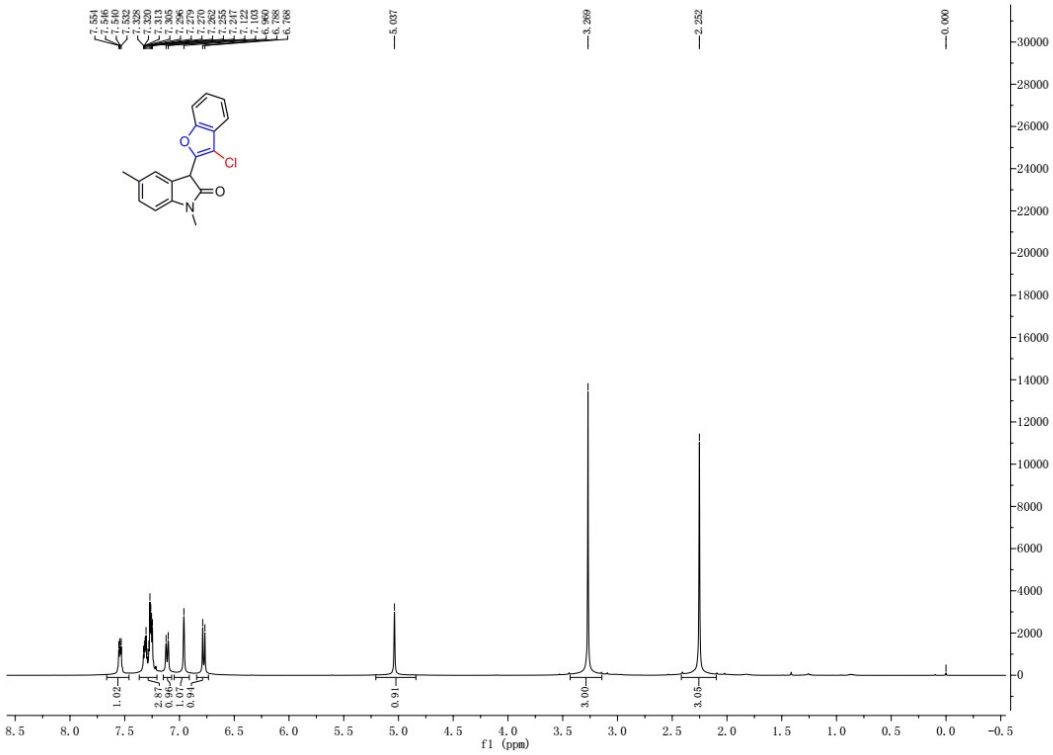
146.97
143.38
135.36
128.93
128.76
127.69
127.31
125.43
124.58
123.39
122.92
111.66
109.54
44.38
44.17
O
Cl
N
O
Bn
f1 (ppm)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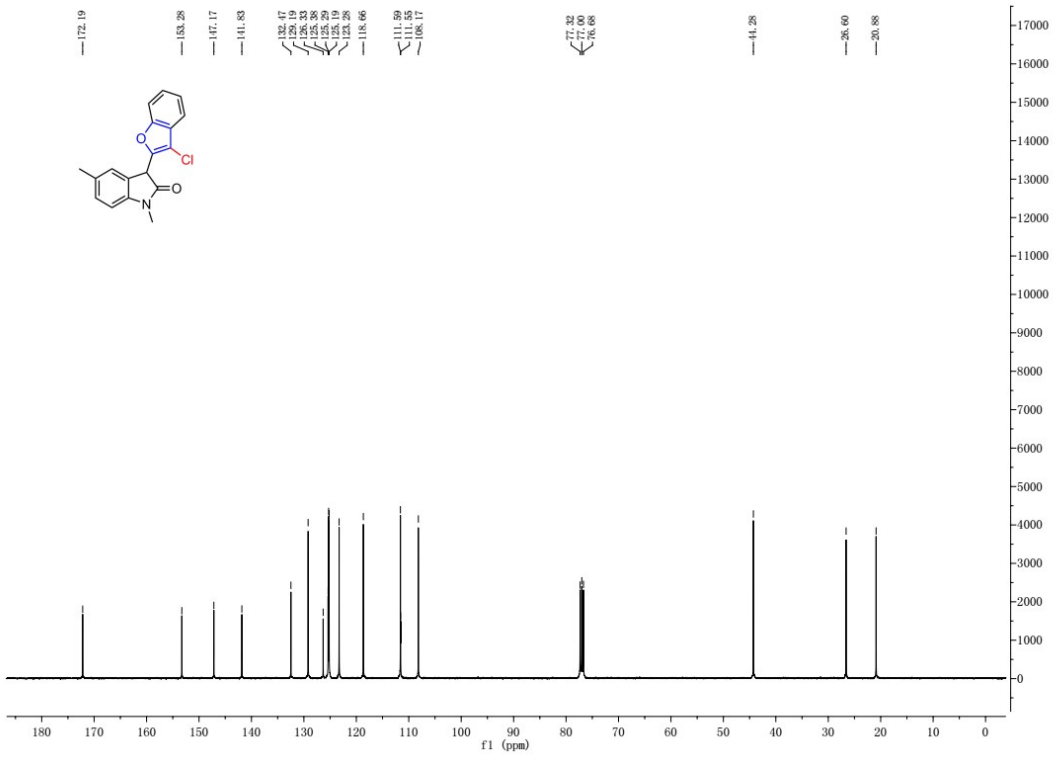
7.546
7.540
7.532
7.320
7.313
7.305
7.296
7.279
7.270
7.262
7.255
7.247
7.122
7.103
6.960
6.788
6.768
5.037
3.269
2.252
0.000
Cl
O
N
1.02
2.87
0.99
1.07
0.94
0.91
3.00
3.05
f1 (ppm)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129.19
126.33
125.38
125.29
125.19
123.28
118.66
111.59
111.55
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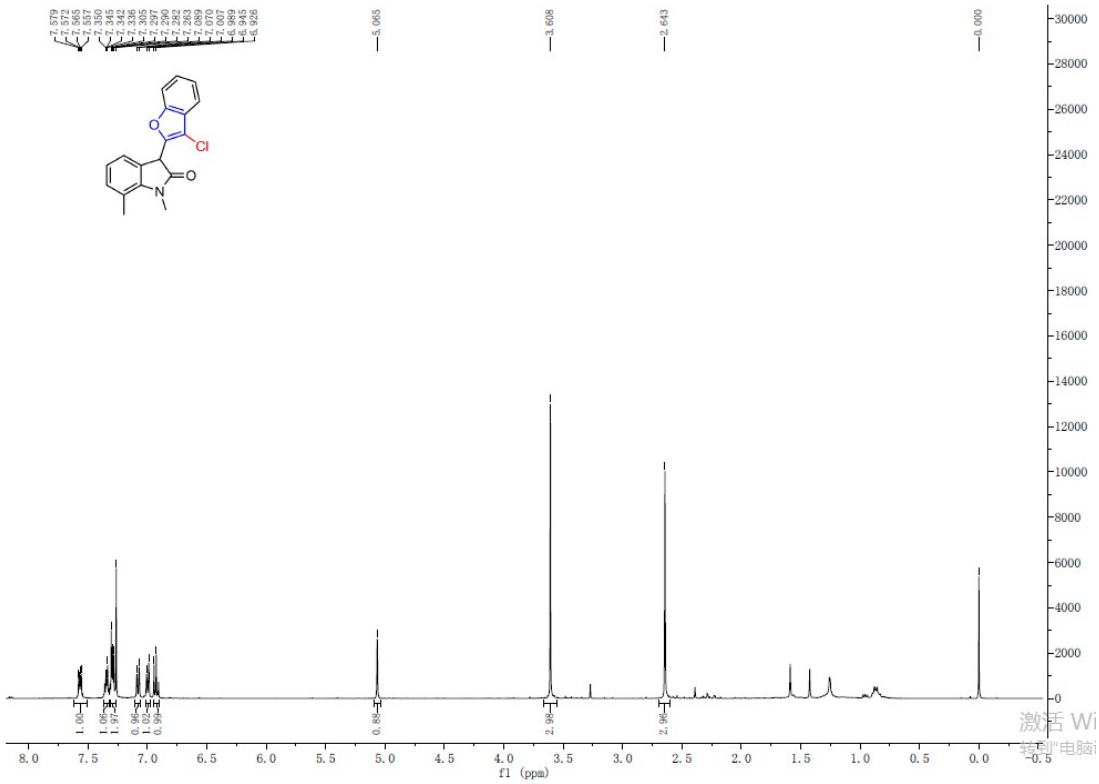
77.32
77.00
76.68
44.28
26.60
20.88
Cl
O
N
f1 (ppm)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7.342
7.336
7.305
7.297
7.290
7.282
7.263
7.089
7.070
7.007
6.989
6.945
6.926
5.065
3.608
2.643
0.000
1.00
1.04
1.97
0.96
1.02
0.99
0.88
2.98
2.96
O
Cl
N
O
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
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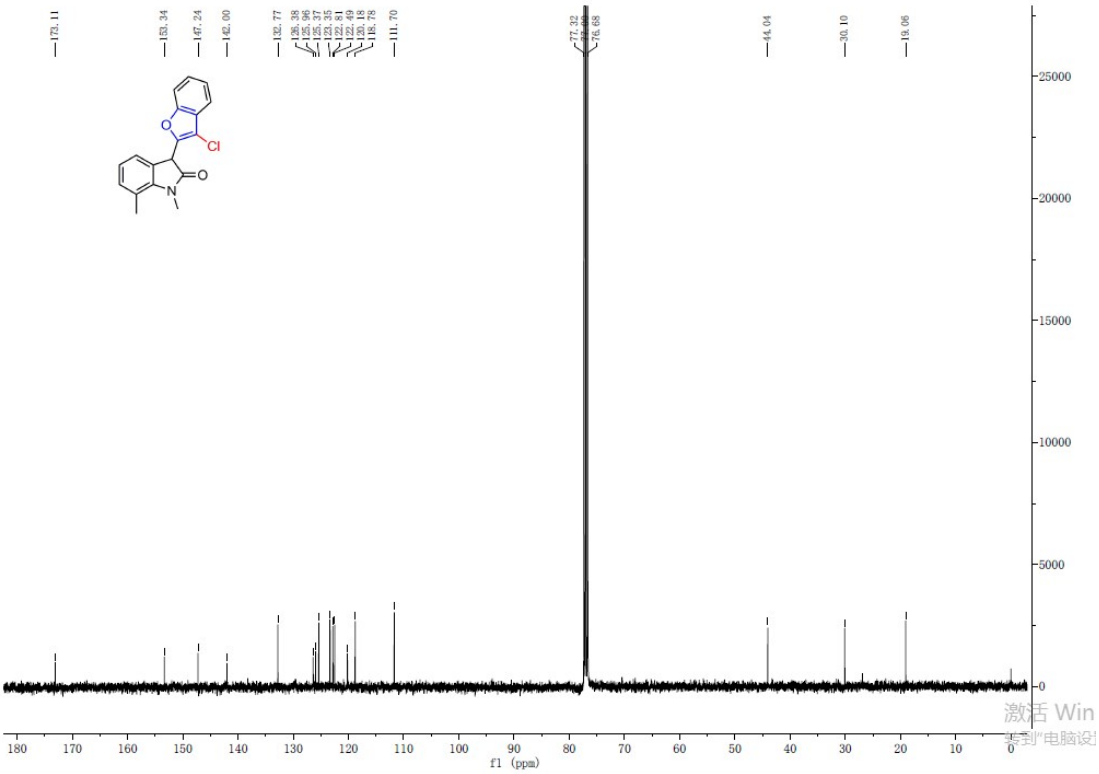
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0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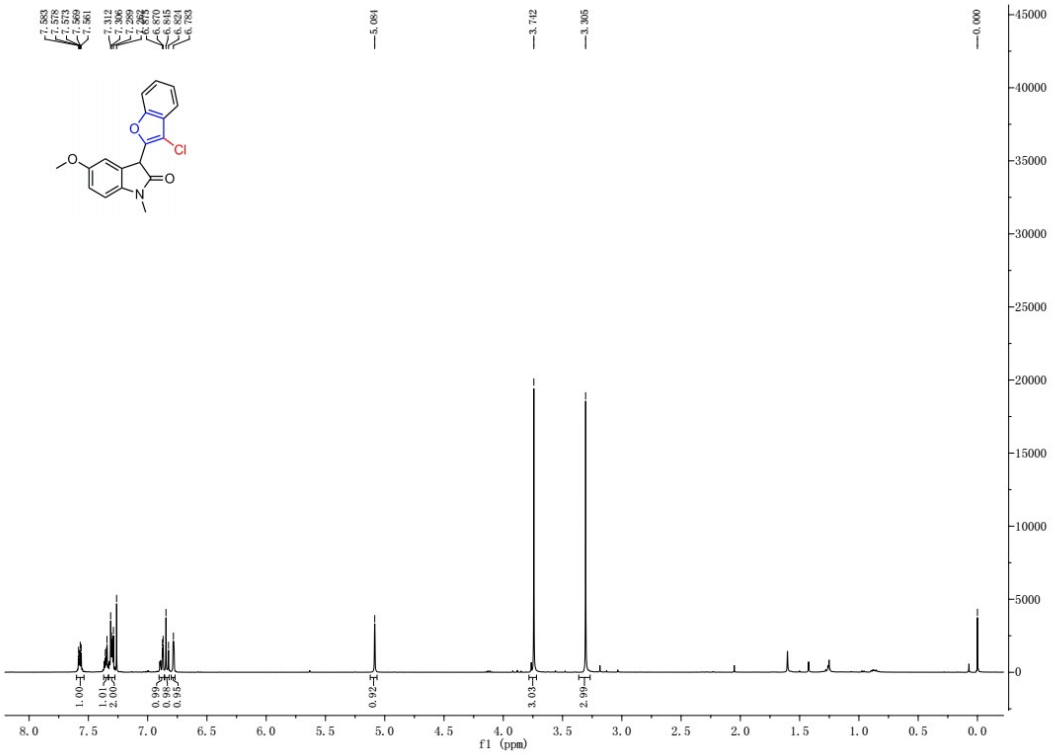
128.38
125.96
125.37
123.35
122.81
122.49
120.15
118.78
111.70
77.22
77.00
76.68
44.04
30.10
19.06
O
Cl
N
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
25000
20000
15000
10000
5000
0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7.561
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7.289
6.870
6.845
6.841
6.783
5.084
3.742
3.305
0.000
Cl
O
N
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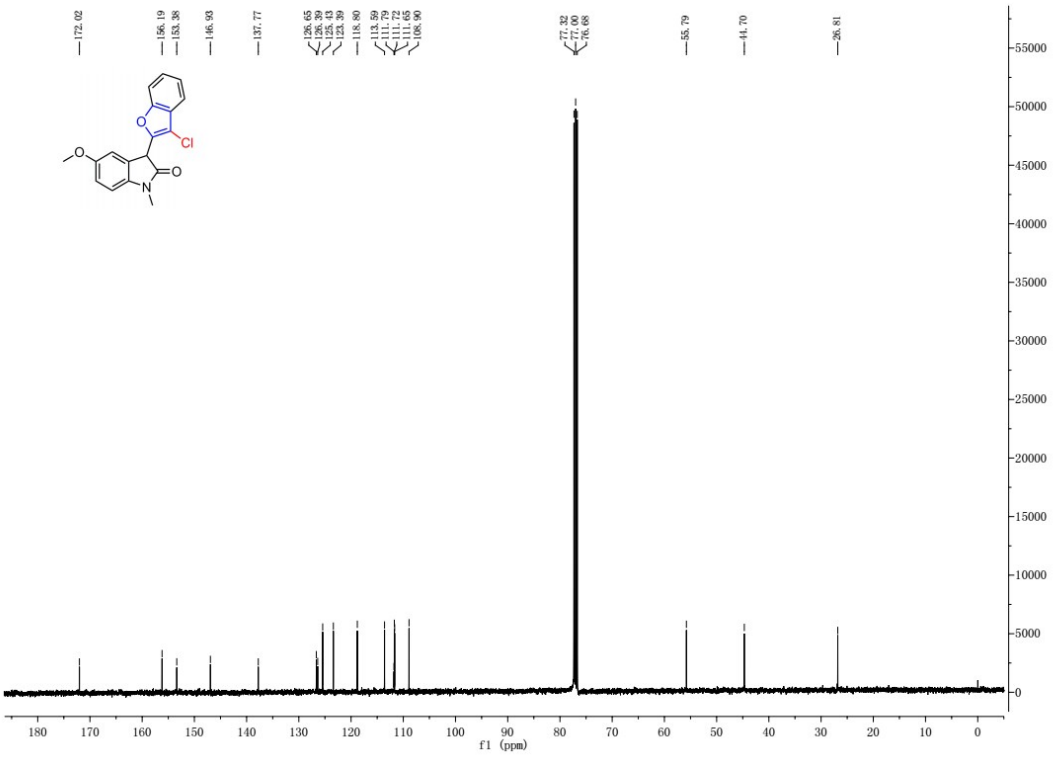
1.01
2.00
0.99
0.98
0.95
0.92
3.03
2.99
f1 (ppm)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125.39
125.43
123.39
118.80
113.59
111.79
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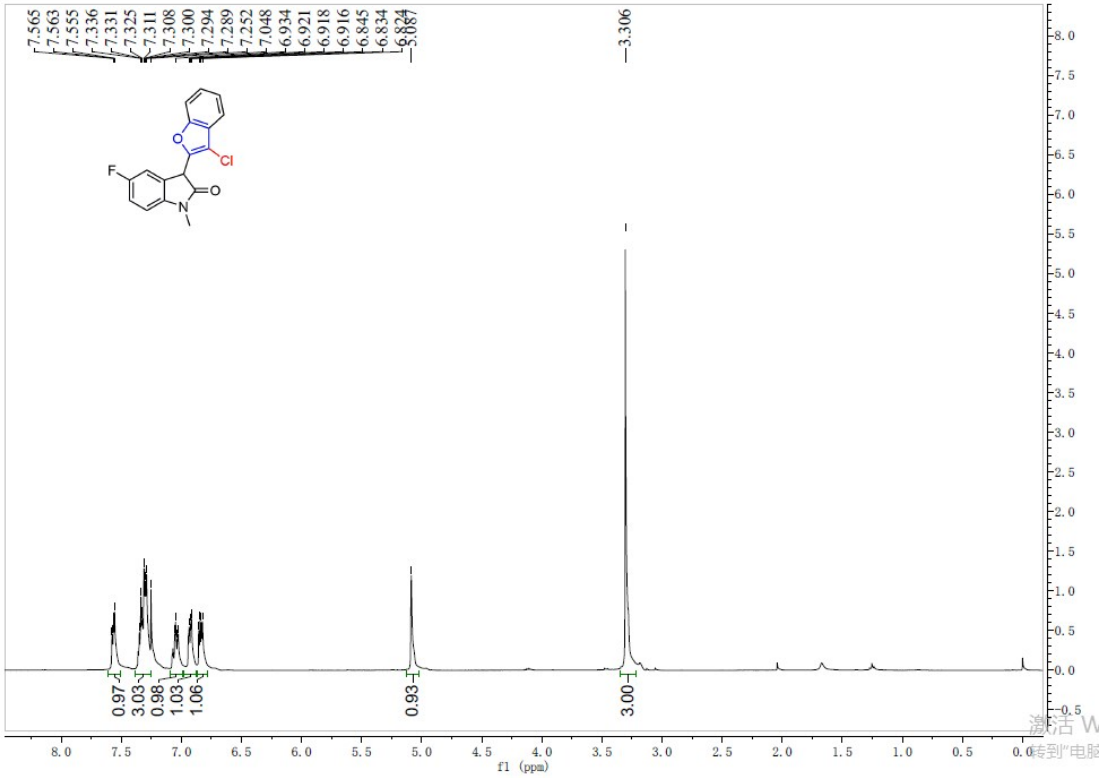
77.32
77.00
76.68
55.79
44.70
26.81
Cl
O
N
f1 (ppm)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7.308
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7.294
7.289
7.252
7.048
6.934
6.921
6.918
6.916
6.845
6.834
3.306
3.087
F
Cl
O
N
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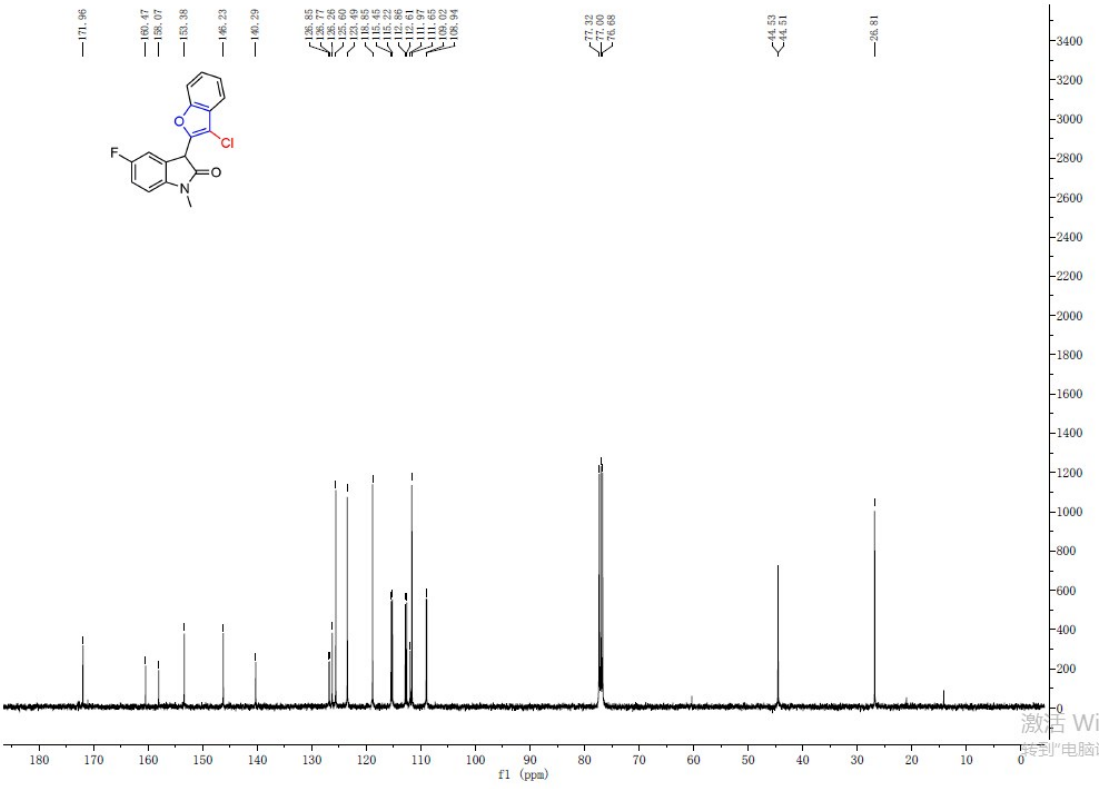
3.03
0.98
1.03
1.06
0.93
3.00
f1 (ppm)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158.07
153.38
146.23
140.29
126.85
126.77
126.26
125.60
125.49
116.65
115.45
115.22
112.86
112.61
111.97
111.65
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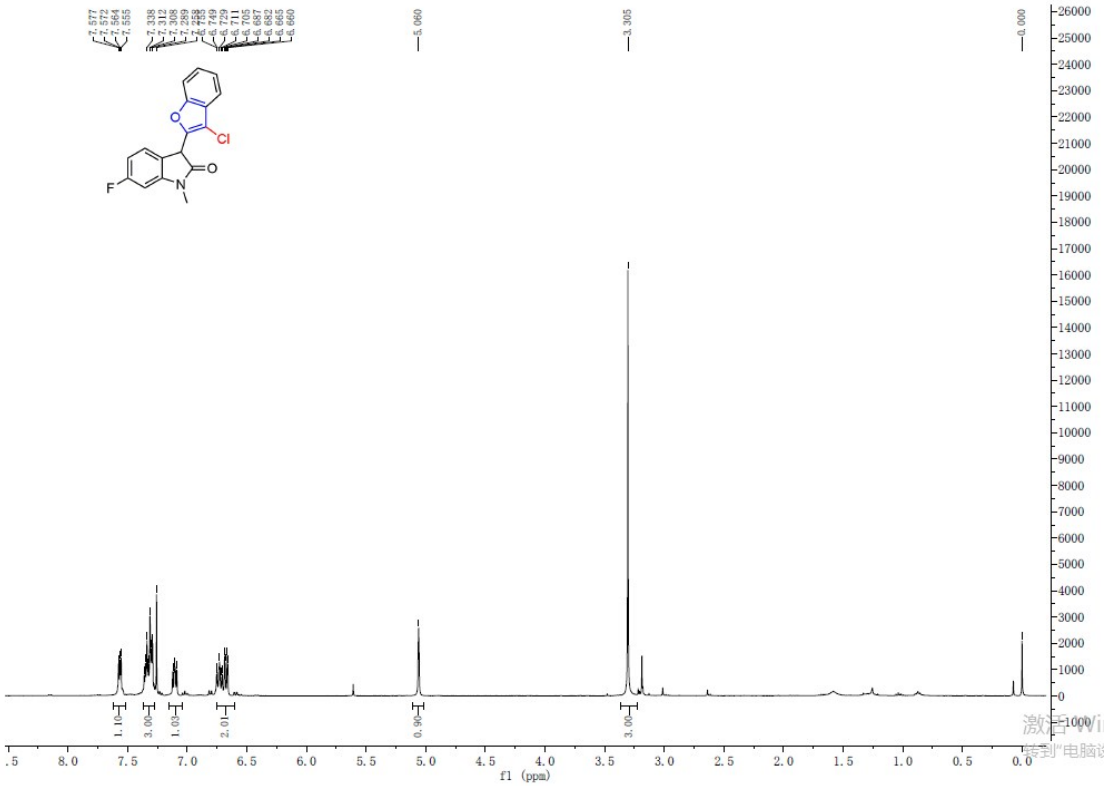
77.32
77.00
76.68
44.53
44.51
26.81
F
Cl
O
N
f1 (ppm)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7.555
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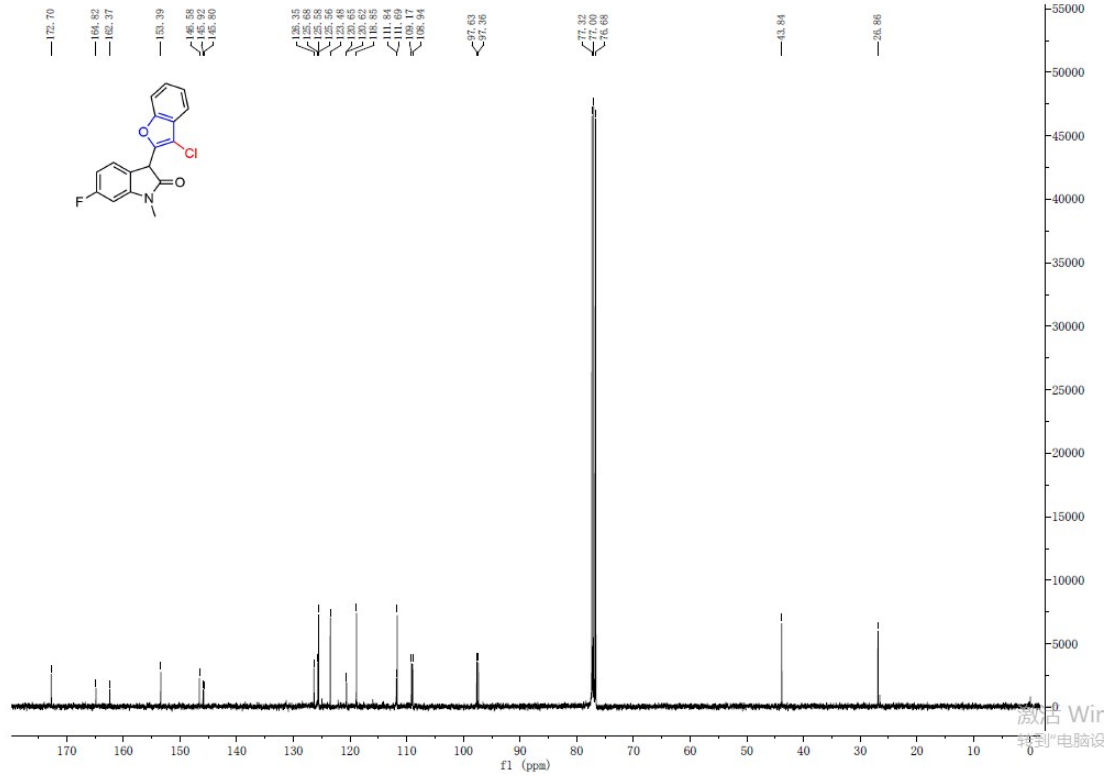
7.312
7.308
7.289
7.288
7.283
7.280
7.749
7.729
7.711
7.705
7.697
7.682
7.665
7.660
5.060
3.305
0.000
Cl
O
F
N
1.00
3.00
1.03
2.01
0.96
3.00
f1 (ppm)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145.92
145.80
126.35
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125.58
125.56
123.48
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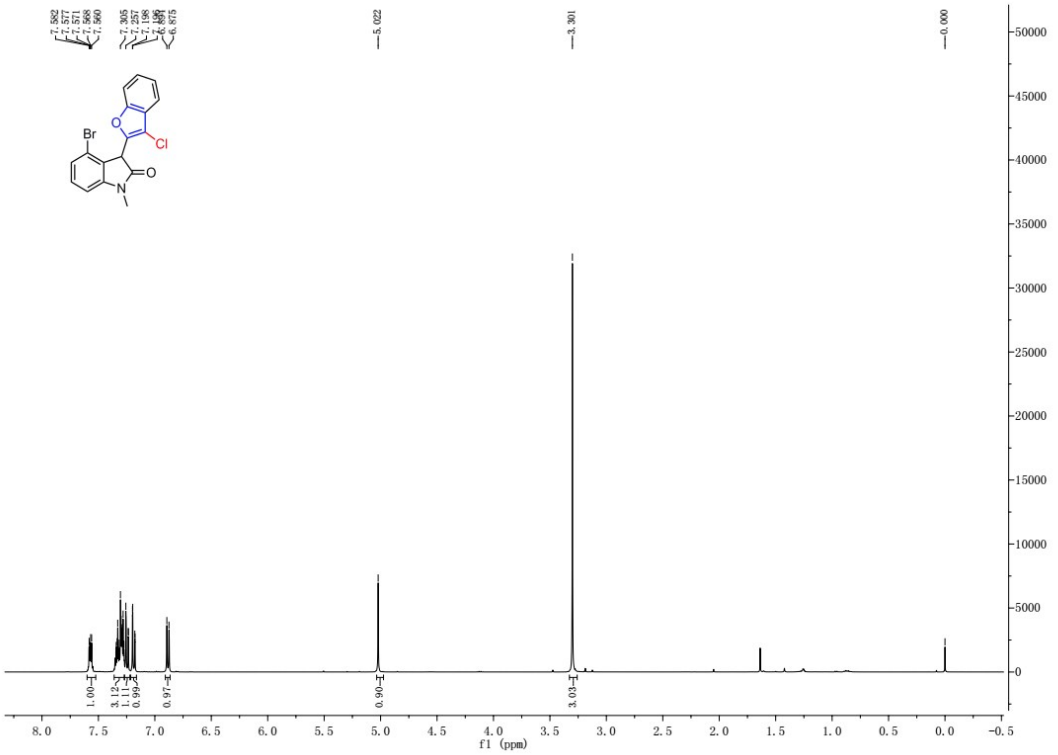
120.62
116.85
111.84
111.69
109.17
108.94
97.63
97.36
77.32
77.00
76.68
43.84
26.86
Cl
O
F
N
f1 (ppm)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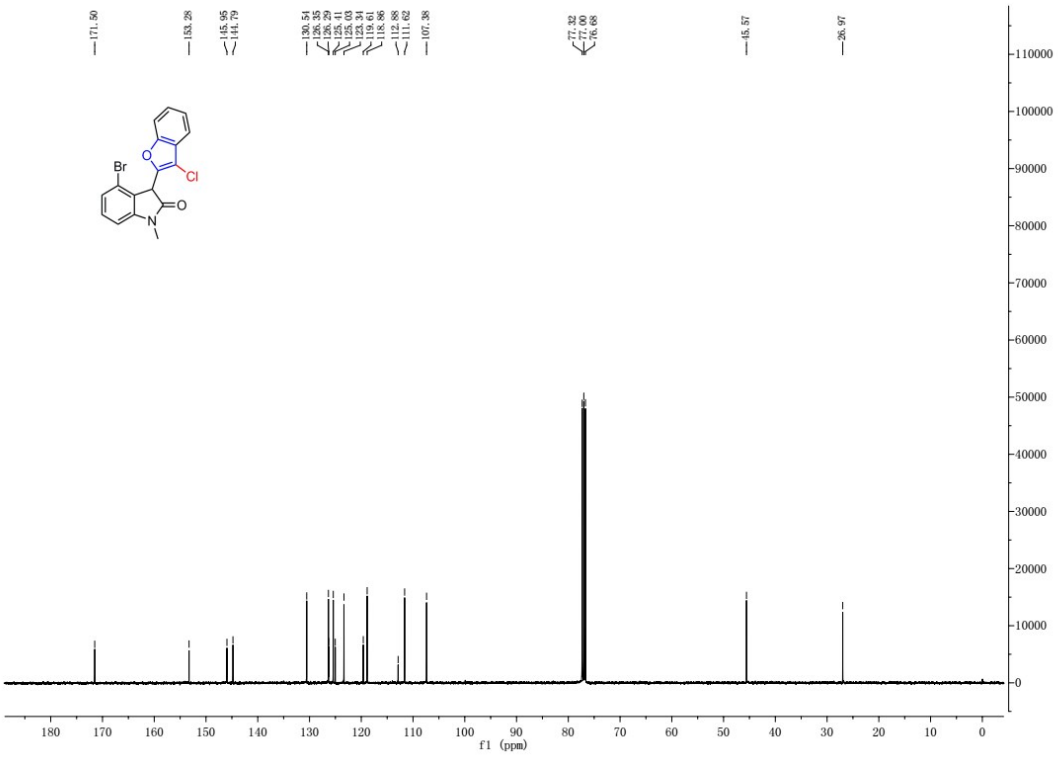
7.560
7.305
7.257
7.198
6.875
5.022
3.301
0.000
Br
Cl
O
N
1.00
3.12
1.01
0.99
0.97
0.90
3.03
f1 (ppm)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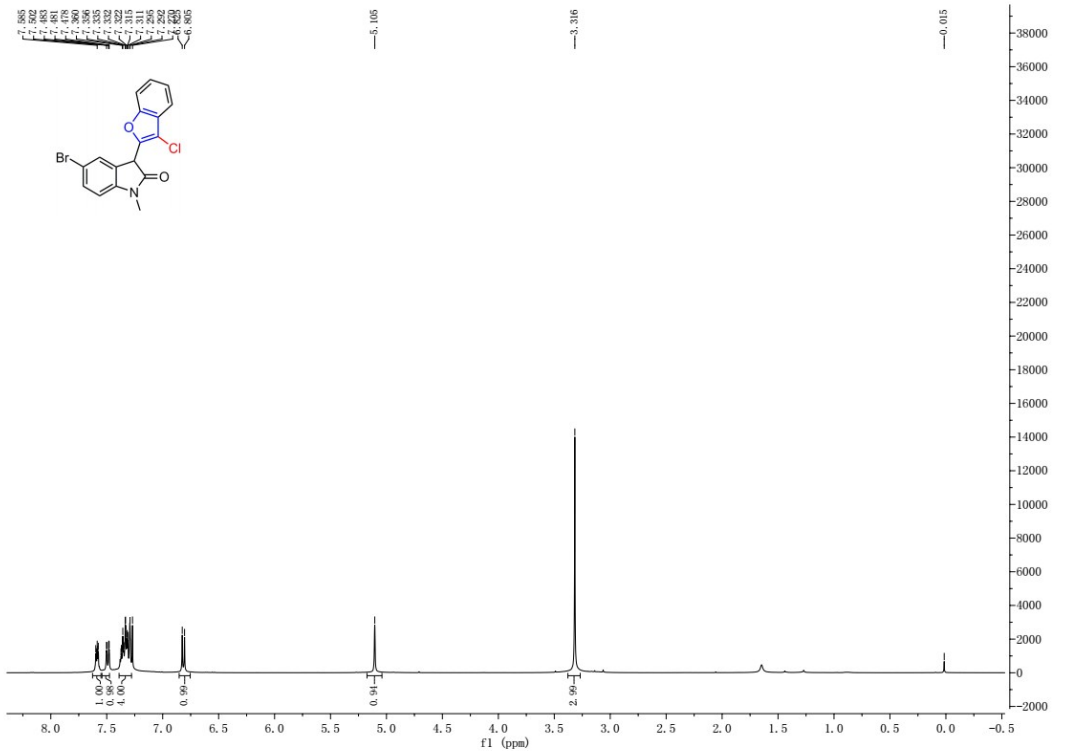
130.54
126.35
126.29
125.41
125.03
123.34
119.61
118.86
112.88
111.62
107.38
77.32
77.00
76.68
45.57
26.97
Br
Cl
O
N
f1 (ppm)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7.360
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7.335
7.332
7.322
7.315
7.311
7.291
7.292
6.820
6.805
5.105
3.316
0.015
Br
Cl
O
N
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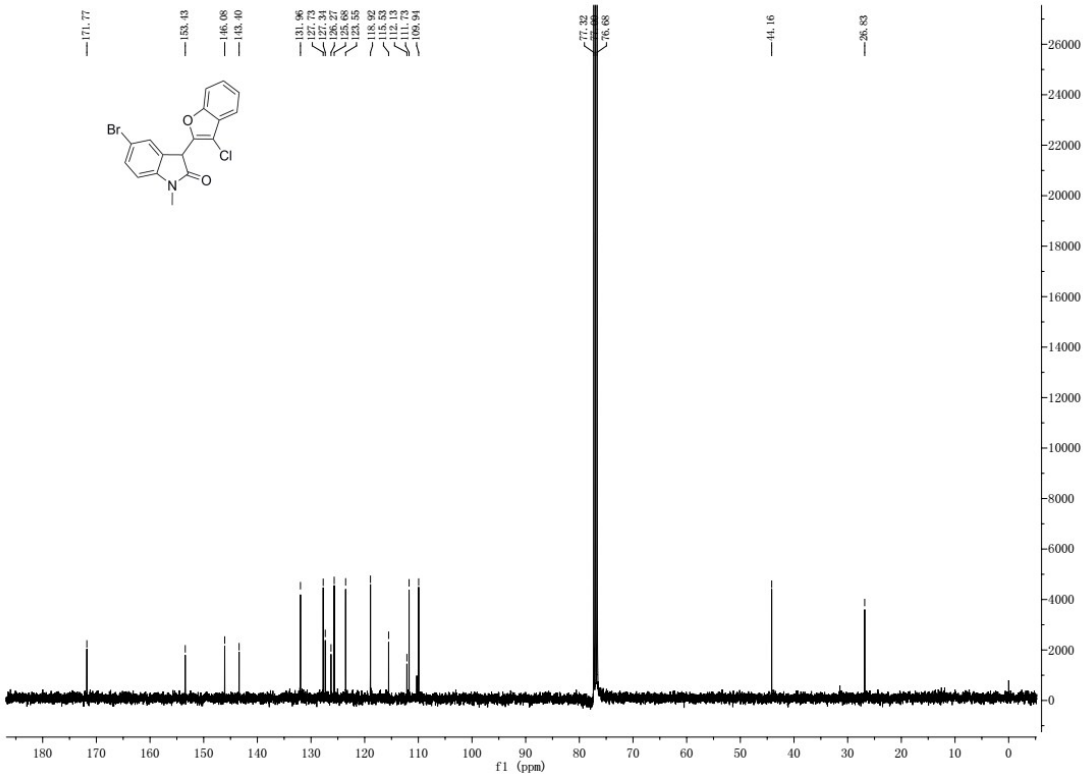
0.98
0.96
4.00
0.99
0.94
2.99
f1 (ppm)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127.34
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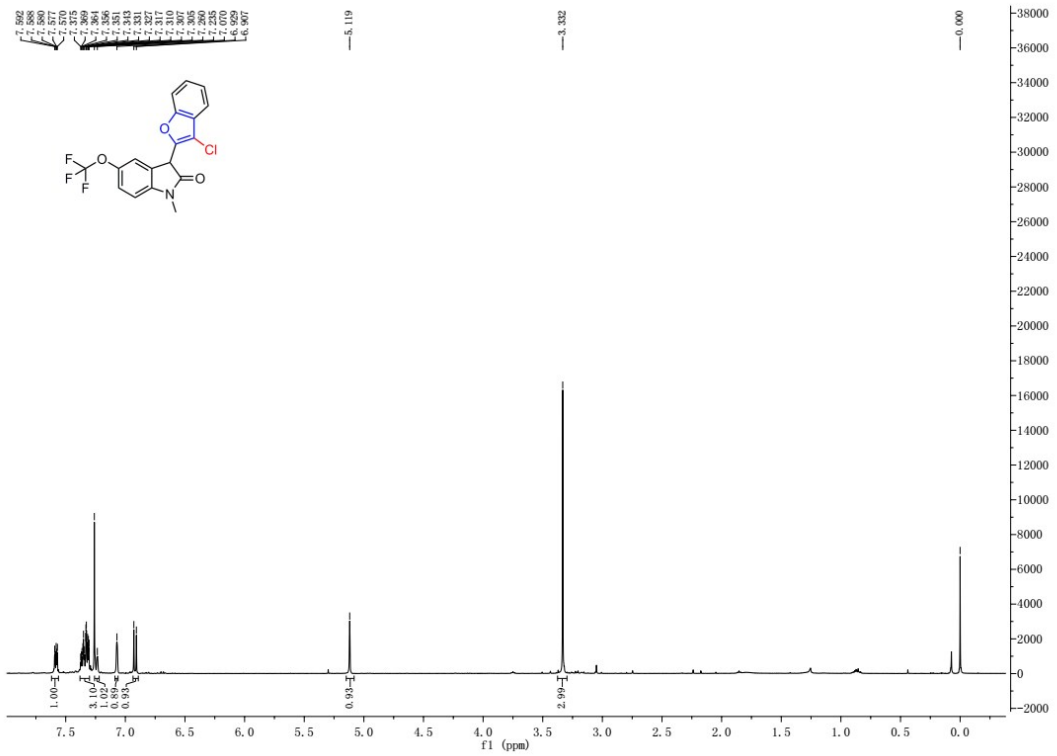
123.55
118.92
115.53
113.13
111.73
109.94
77.32
77.00
76.68
44.16
26.83
Br
Cl
O
N
f1 (ppm)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7.577
7.570
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7.369
7.364
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7.351
7.343
7.331
7.327
7.317
7.310
7.307
7.305
7.260
7.235
7.070
6.929
6.907
5.119
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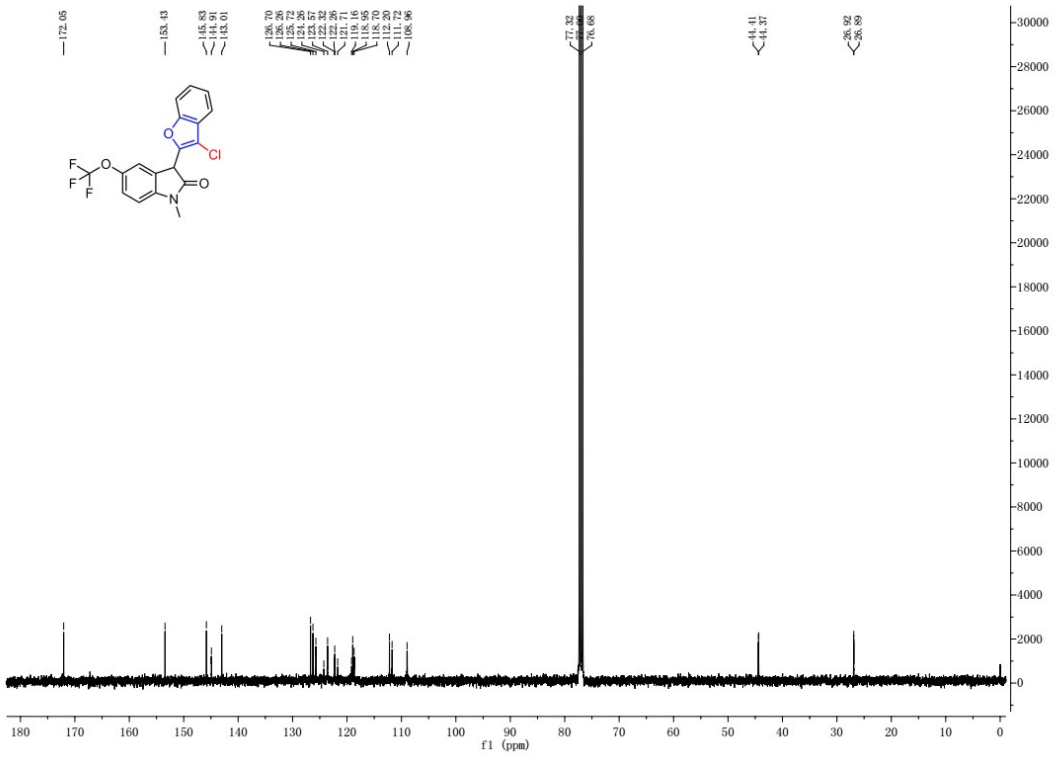
0.000
1.00
3.10
1.02
0.89
0.93
0.93
2.99
f1 (ppm)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125.36
125.72
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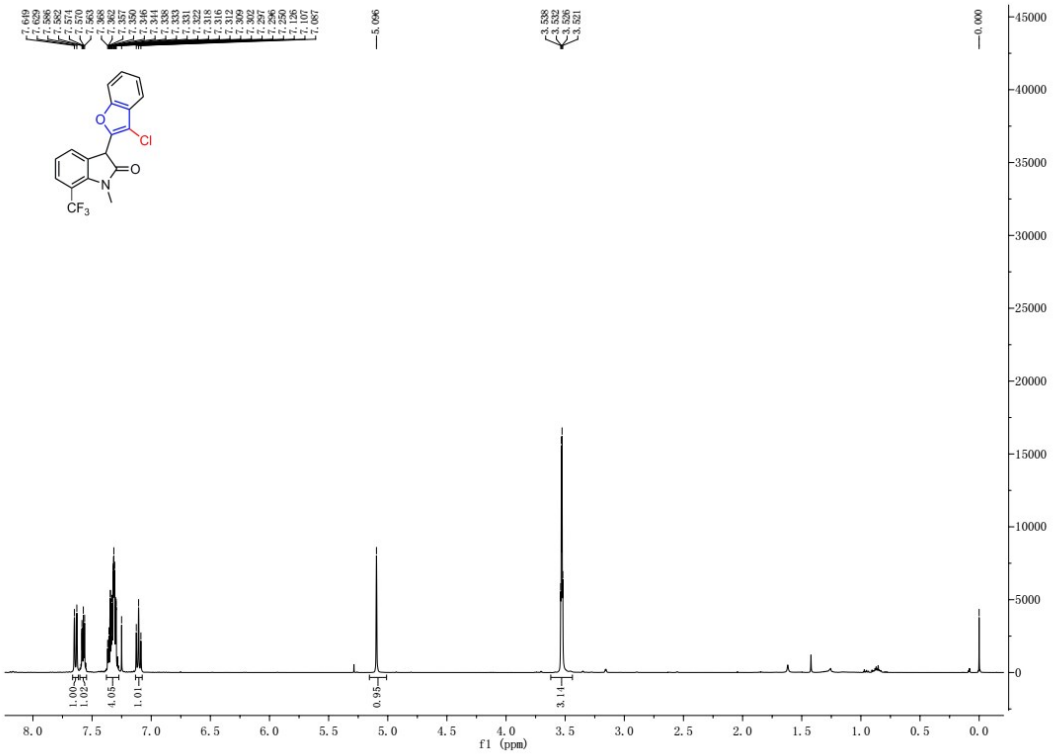
123.57
122.32
122.26
121.71
119.16
118.95
116.70
112.20
111.72
108.96
77.32
77.00
76.68
44.41
44.37
26.92
26.89
f1 (ppm)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7.346
7.341
7.338
7.333
7.331
7.322
7.318
7.316
7.312
7.309
7.302
7.297
7.296
7.250
7.126
7.107
7.087
5.096
3.538
3.532
3.526
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O
N
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1.02
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1.01
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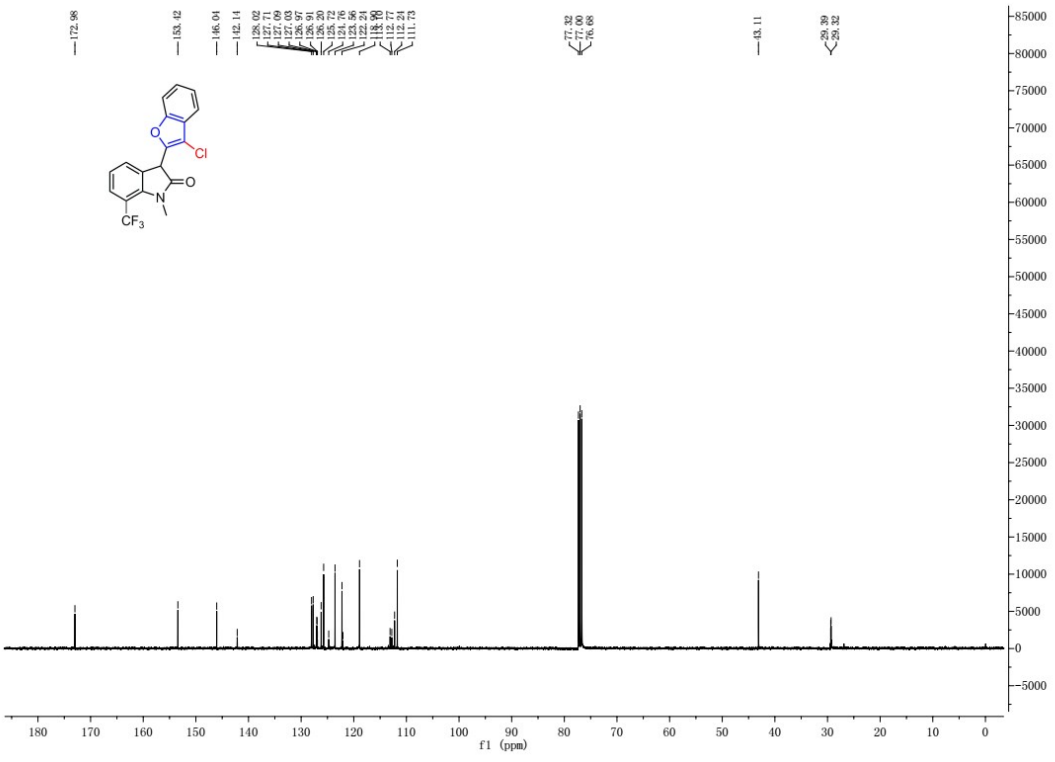
3.14
f1 (ppm)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142.14
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127.71
127.09
127.03
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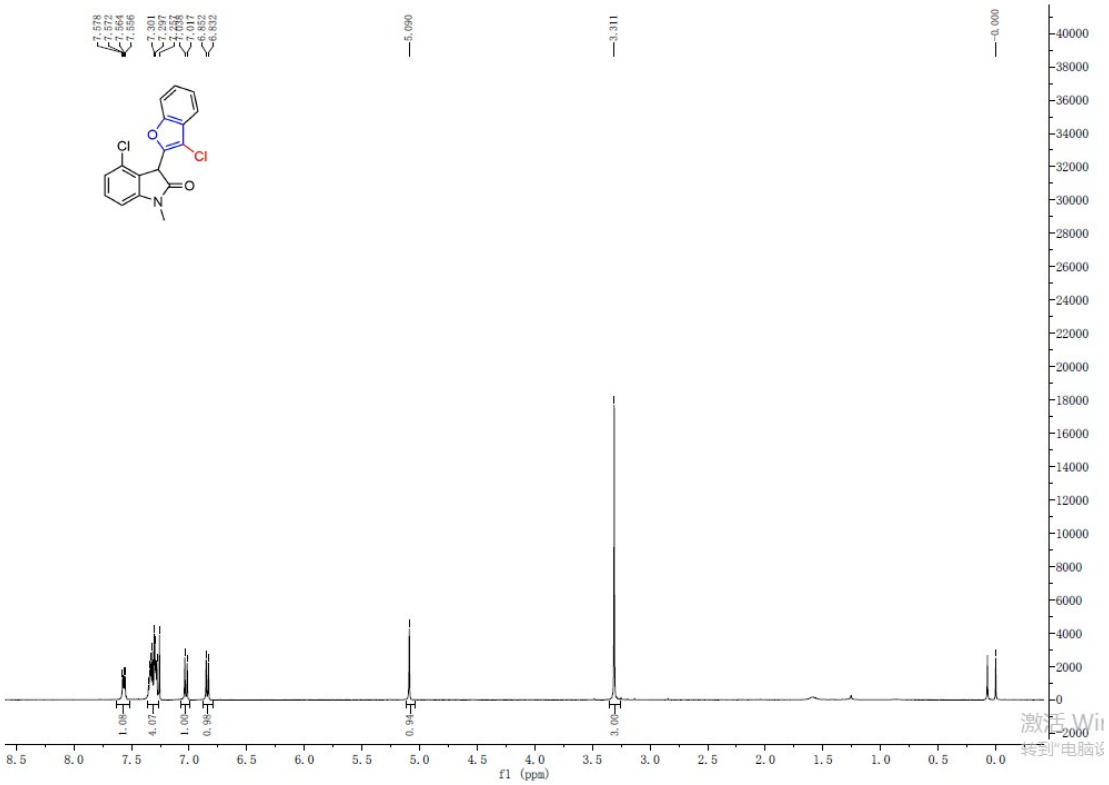
126.91
126.30
125.72
124.76
123.56
122.91
118.10
117.77
112.24
111.73
77.32
77.00
76.68
43.11
29.39
28.32
Cl
O
N
CF3
f1 (ppm)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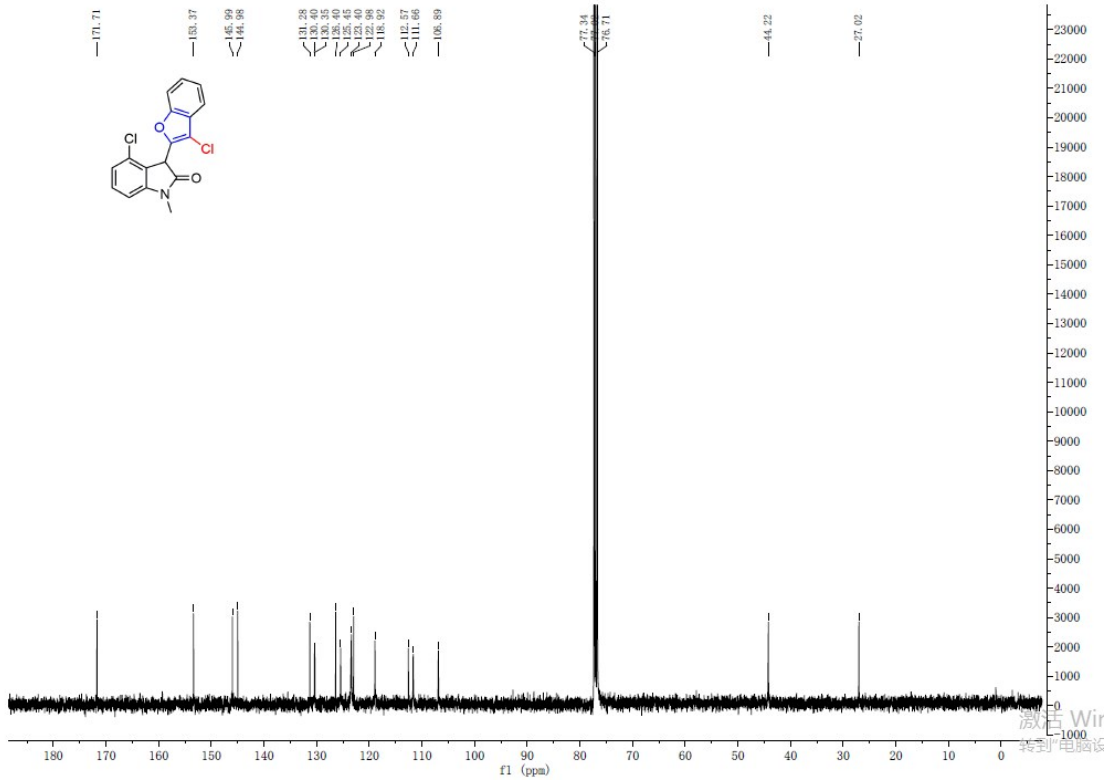
7.294
7.038
7.017
6.857
6.852
6.832
5.090
3.311
0.000
Cl
Cl
O
O
N
1.00
4.07
1.00
0.98
0.94
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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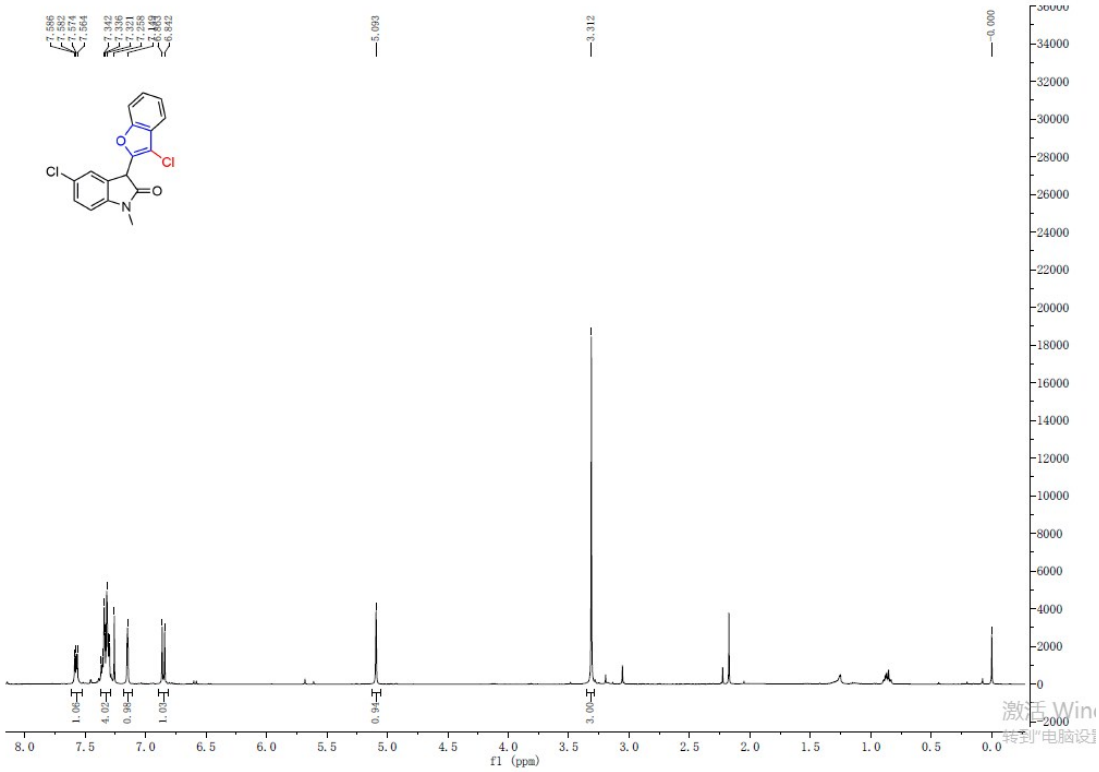
111.66
106.89
77.34
77.04
76.71
44.22
27.02
Cl
Cl
O
O
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.564
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7.321
5.093
3.312
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Cl
Cl
O
N
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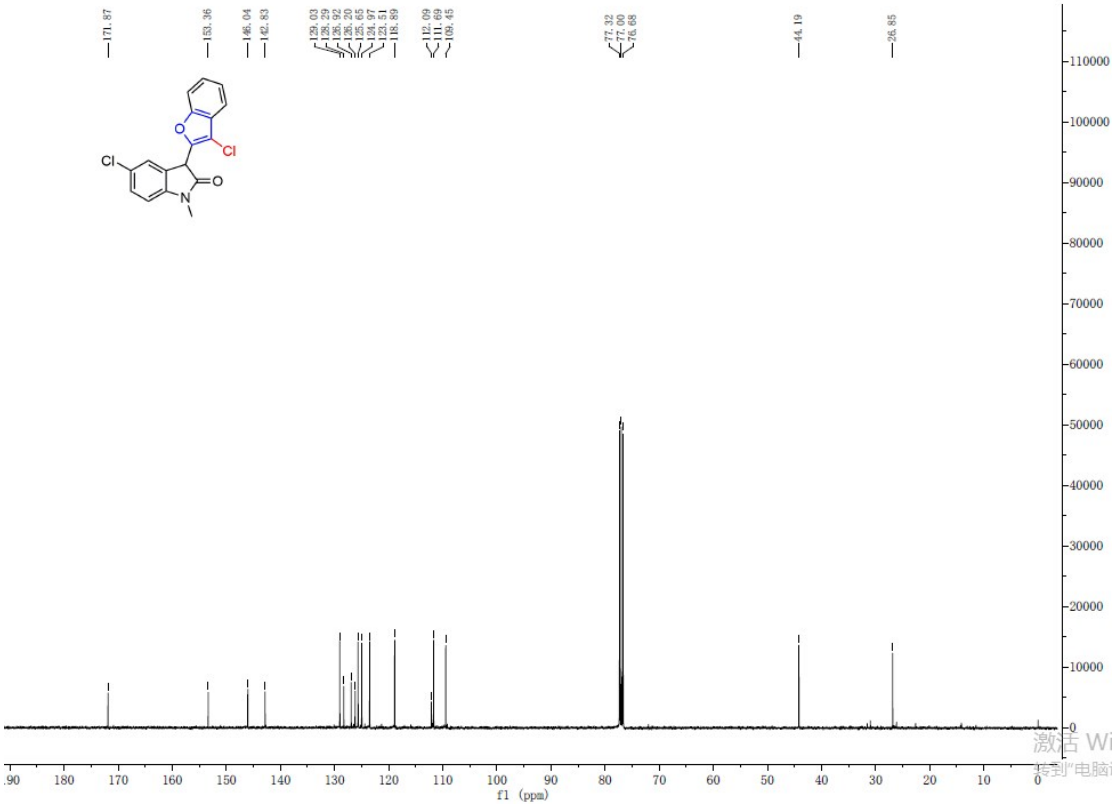
4.02
0.98
1.03
0.94
3.00
f1 (ppm)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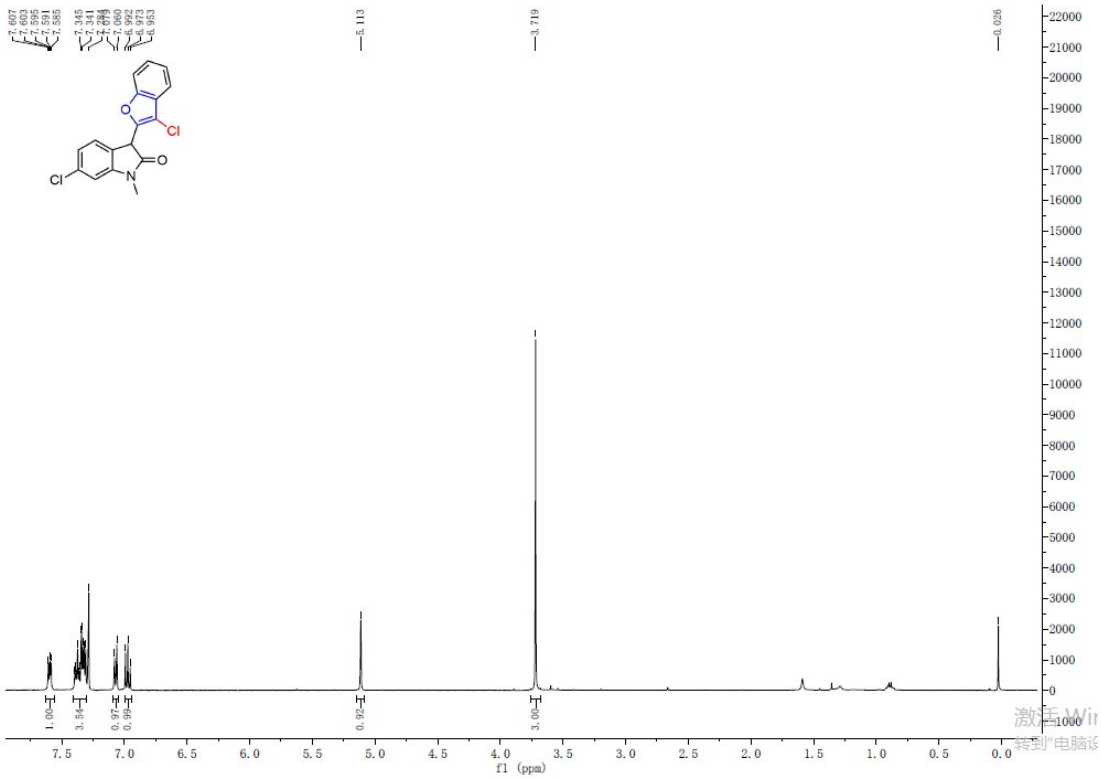
126.32
126.20
125.65
124.97
123.51
118.89
112.09
111.69
109.45
77.32
77.00
76.68
44.19
26.85
Cl
Cl
O
N
f1 (ppm)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7.595
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7.345
7.341
7.060
6.972
6.953
5.113
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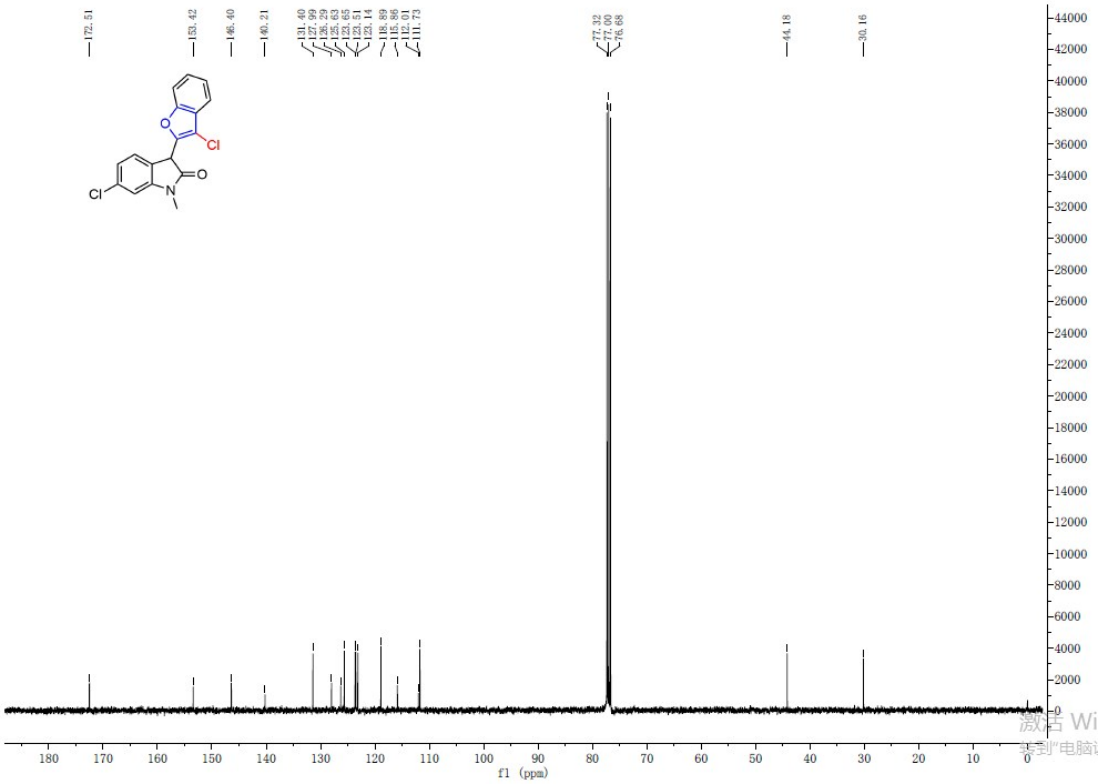
Cl
Cl
O
N
1.00
3.54
0.97
0.99
0.92
3.00
f1 (ppm)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127.99
126.39
125.63
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123.51
123.14
118.89
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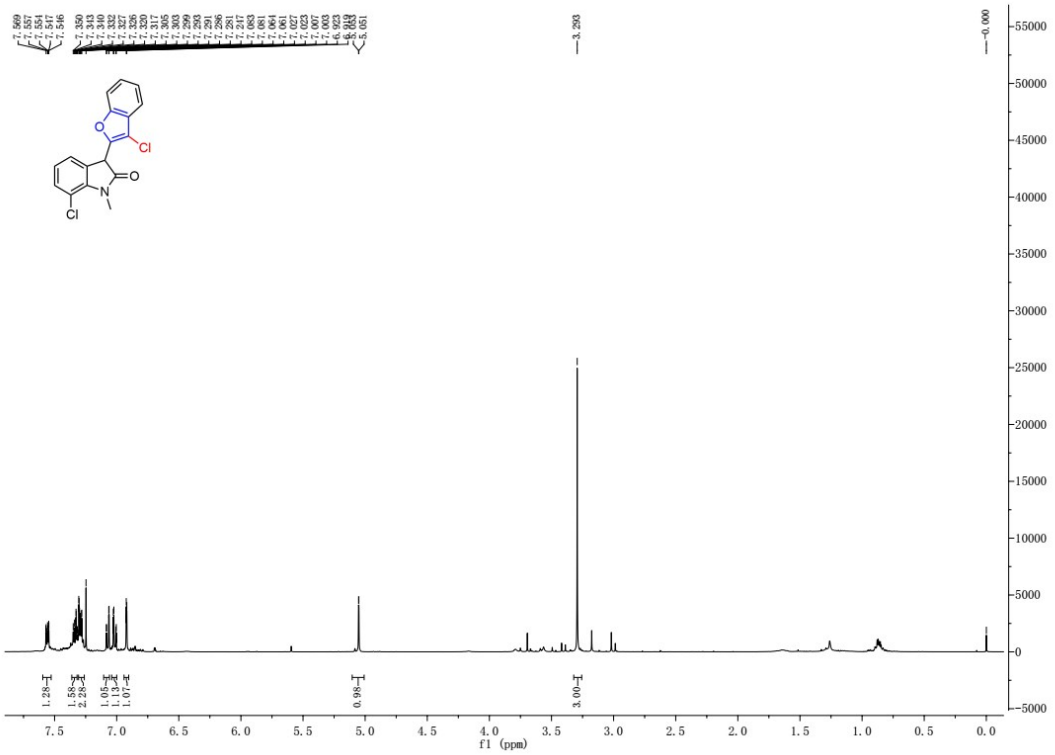
112.01
111.73
77.32
77.00
76.68
44.18
30.16
Cl
Cl
O
N
f1 (ppm)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7.547
7.546
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7.343
7.340
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7.326
7.320
7.317
7.305
7.303
7.299
7.293
7.291
7.286
7.281
7.247
7.083
7.081
7.064
7.061
7.027
7.025
7.007
7.003
6.923
6.921
6.834
6.832
5.651
3.293
0.000
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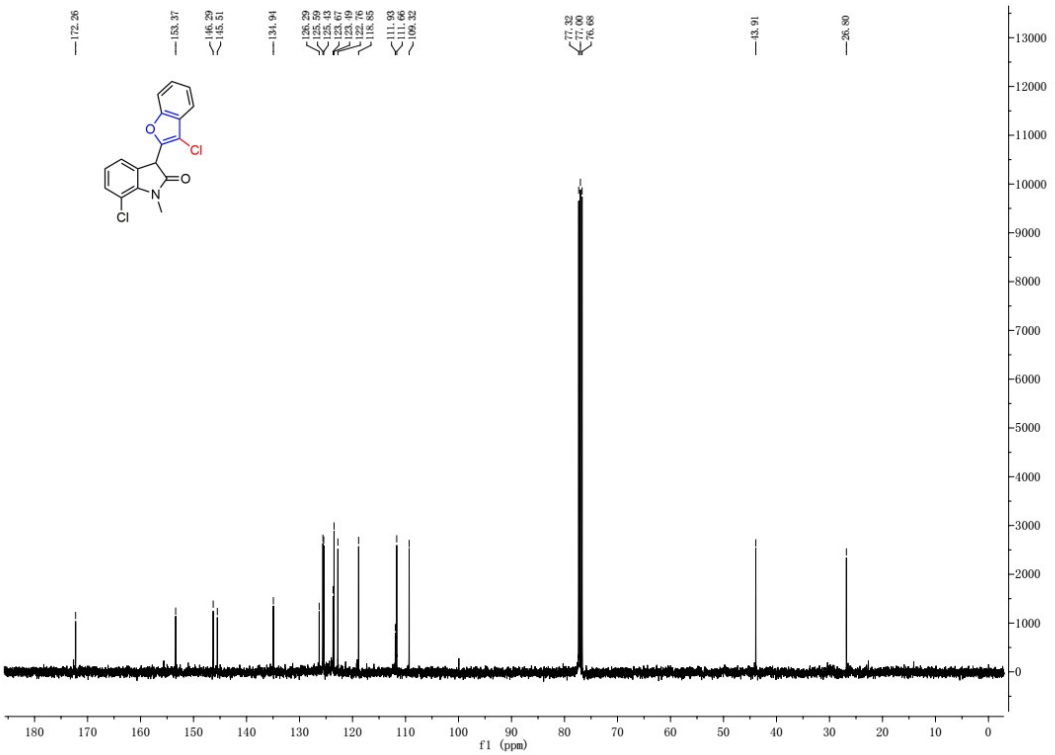
O
N
Cl
1.28
1.58
2.28
1.05
1.13
1.07
0.98
3.00
f1 (ppm)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125.43
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122.76
118.85
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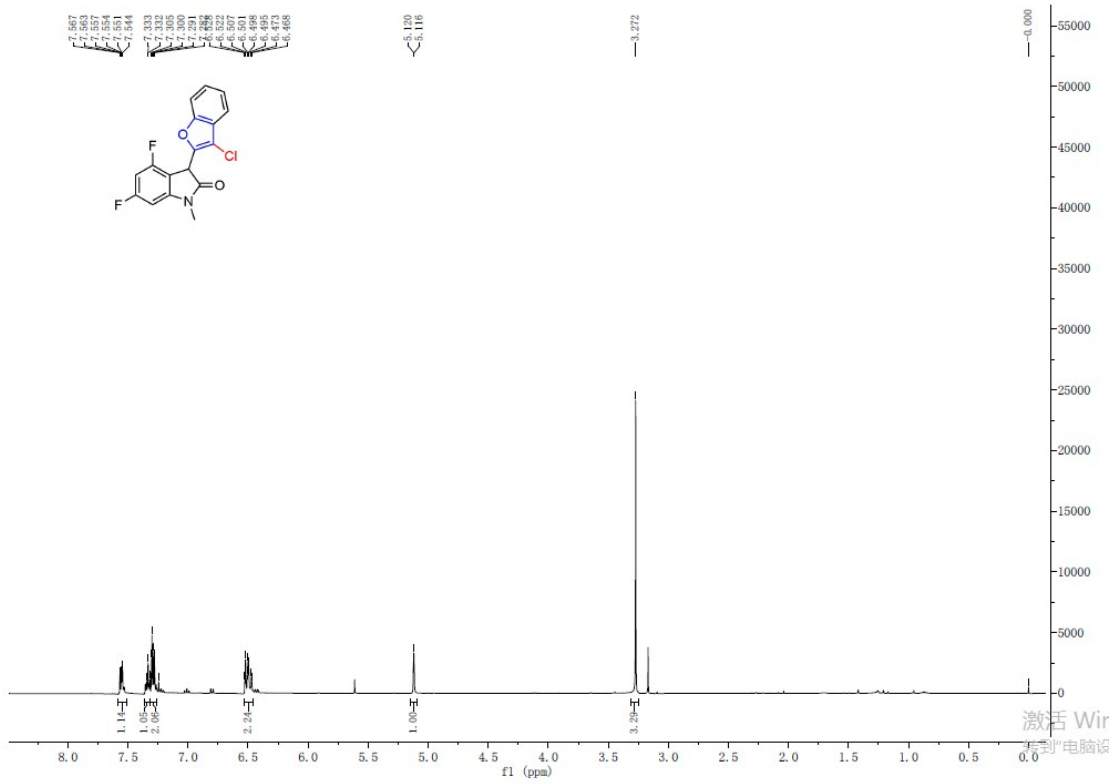
77.32
77.00
76.68
43.91
26.80
Cl
O
N
Cl
f1 (ppm)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7.544
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7.332
7.305
7.300
7.291
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6.507
6.501
6.498
6.495
6.473
6.468
5.120
5.116
3.272
0.000
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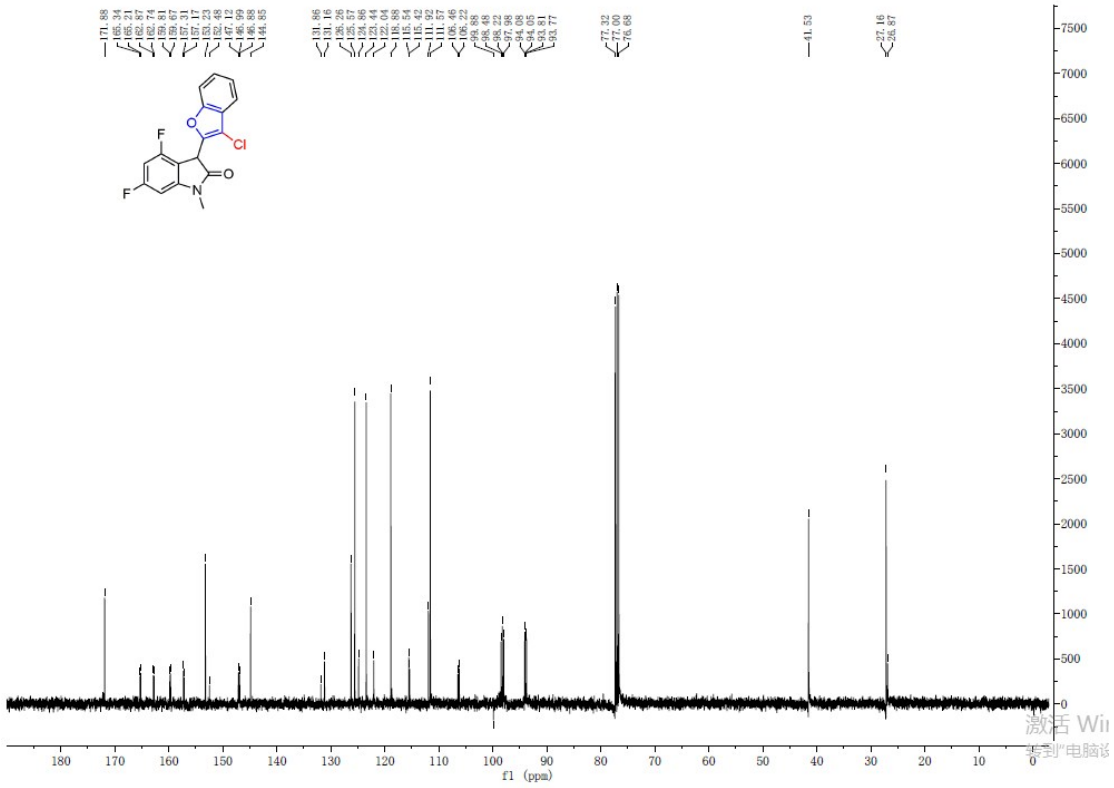
O
Cl
O
F
N
1.14
1.05
2.06
2.24
1.06
3.29
f1 (ppm)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162.87
162.74
159.81
159.67
137.31
137.17
132.23
132.48
147.12
146.99
146.88
144.85
131.86
131.16
126.26
125.67
124.96
123.44
122.04
118.88
115.54
115.42
111.92
111.57
106.46
106.22
98.88
98.49
98.22
97.98
94.08
94.05
93.81
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76.68
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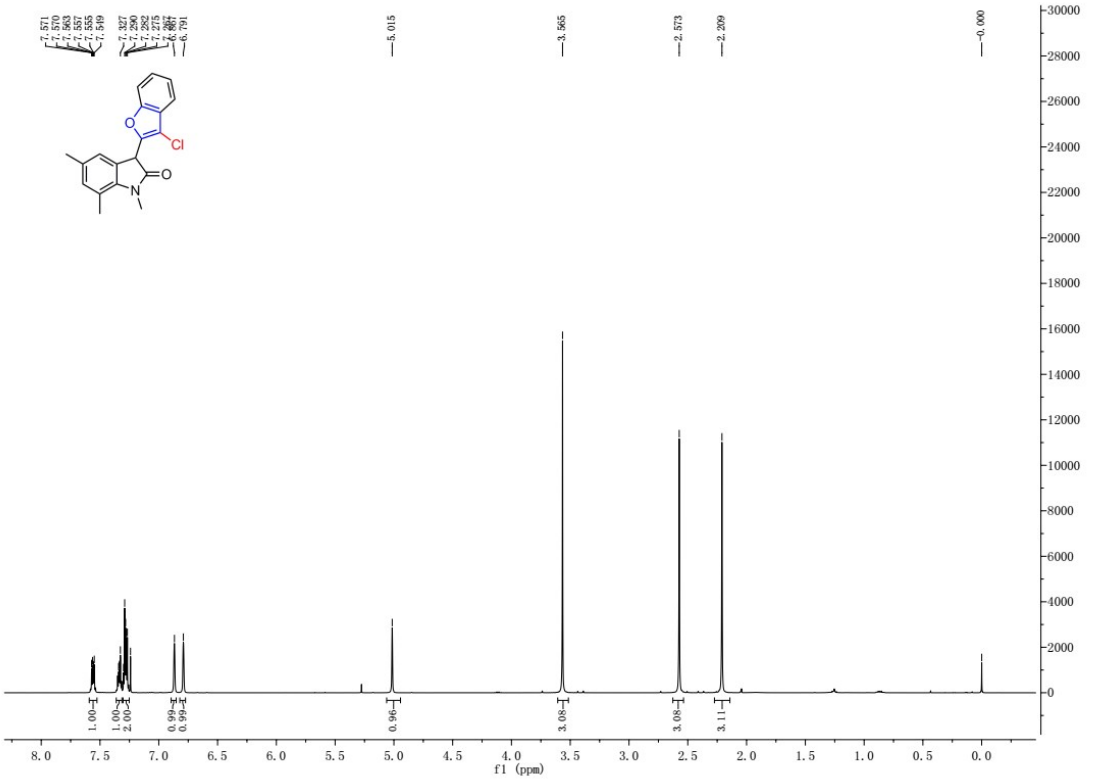
27.16
26.87
F
O
Cl
O
F
N
f1 (ppm)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5.015
3.565
2.573
2.209
0.000
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1.00
2.00
0.99
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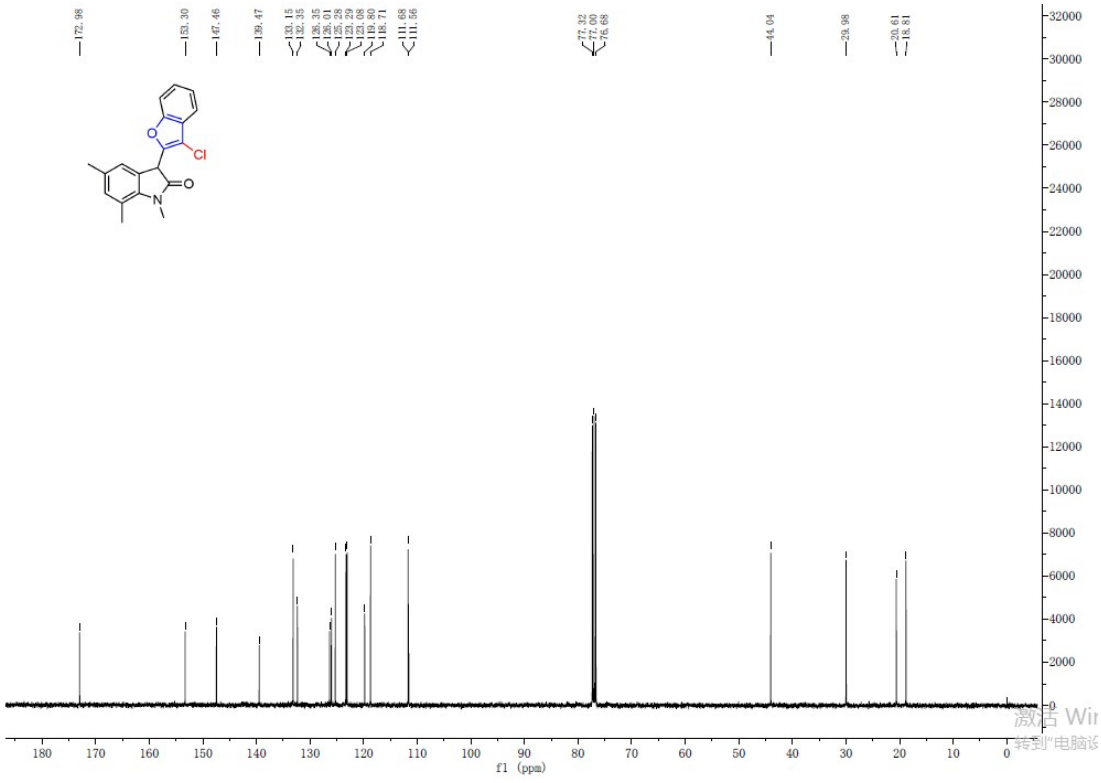
0.96
3.08
3.08
3.11
f1 (ppm)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126.01
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123.08
119.80
118.71
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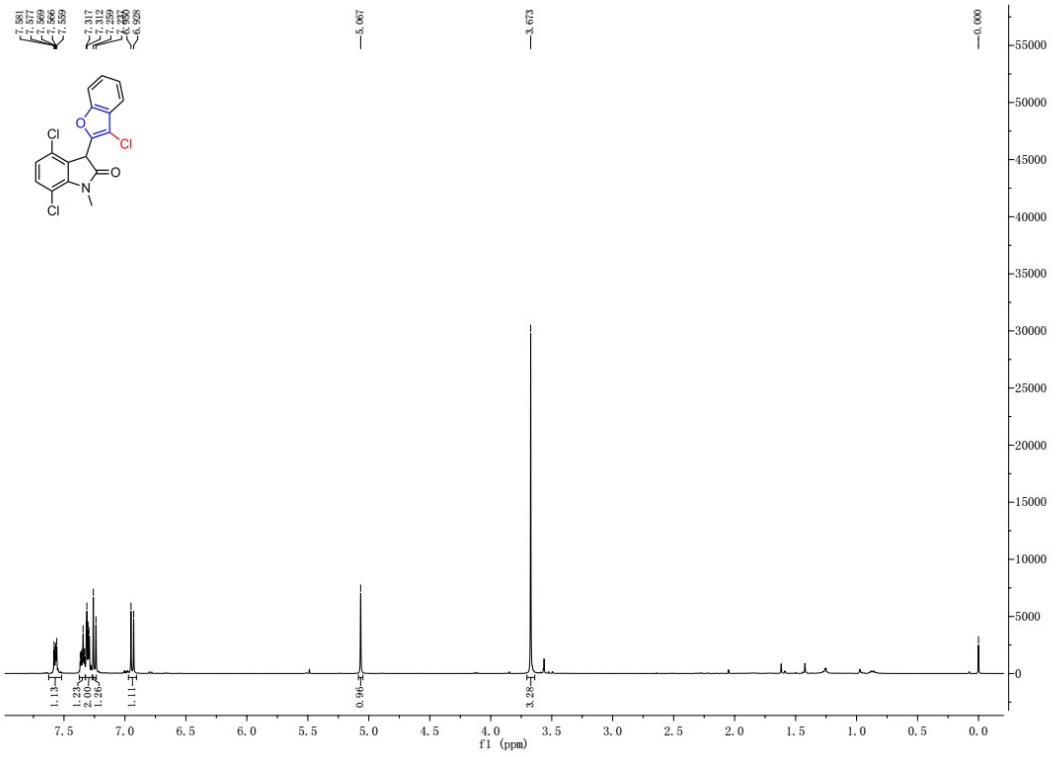
77.00
76.68
44.04
28.98
20.61
18.81
Cl
O
N
f1 (ppm)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7.309
7.299
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6.925
5.067
3.673
0.000
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Cl
O
N
Cl
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1.23
2.09
1.26
1.11
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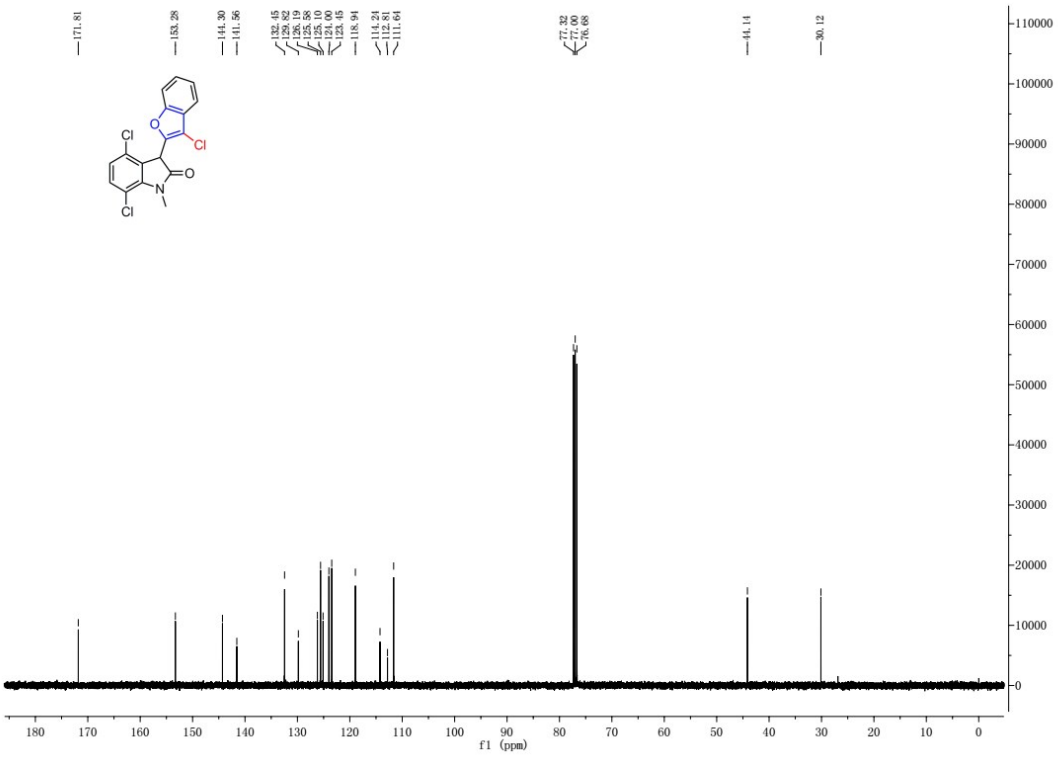
3.28
f1 (ppm)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123.45
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114.24
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77.00
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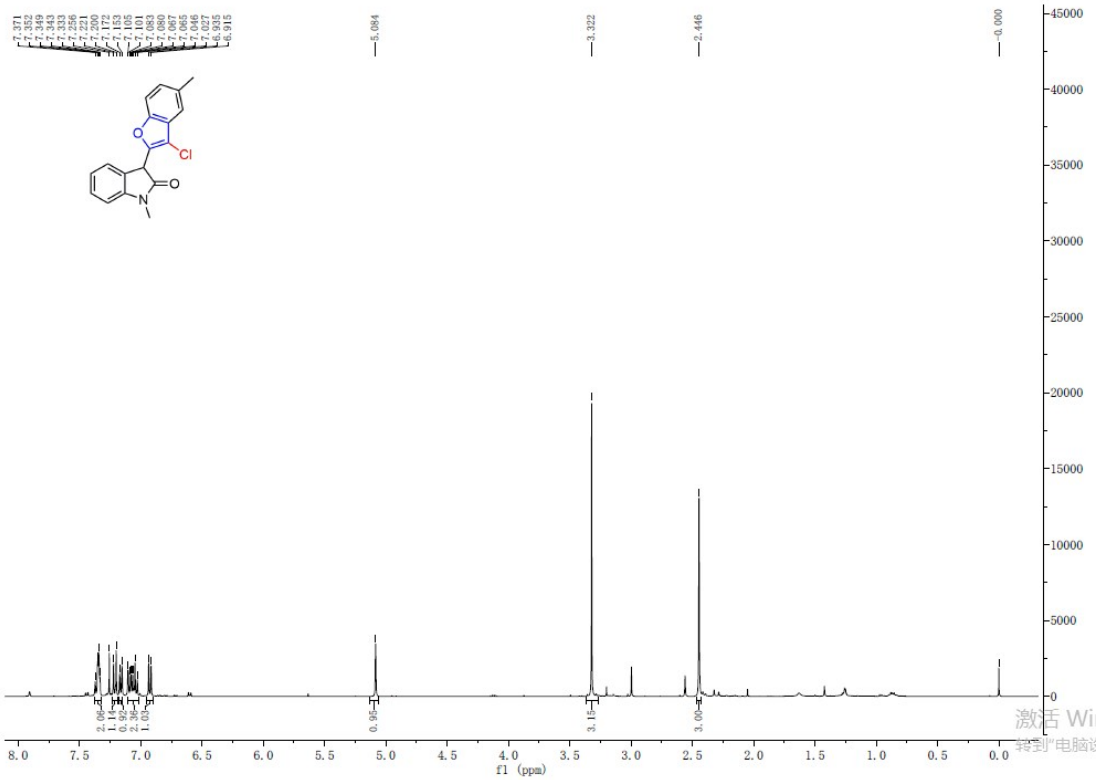
30.12
Cl
O
Cl
O
N
Cl
f1 (ppm)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7.153
7.105
7.101
7.083
7.080
7.067
7.065
7.046
7.027
6.935
6.915
5.084
3.322
2.446
0.000
Cl
O
N
2.00
1.14
0.92
2.36
1.03
0.96
3.18
3.00
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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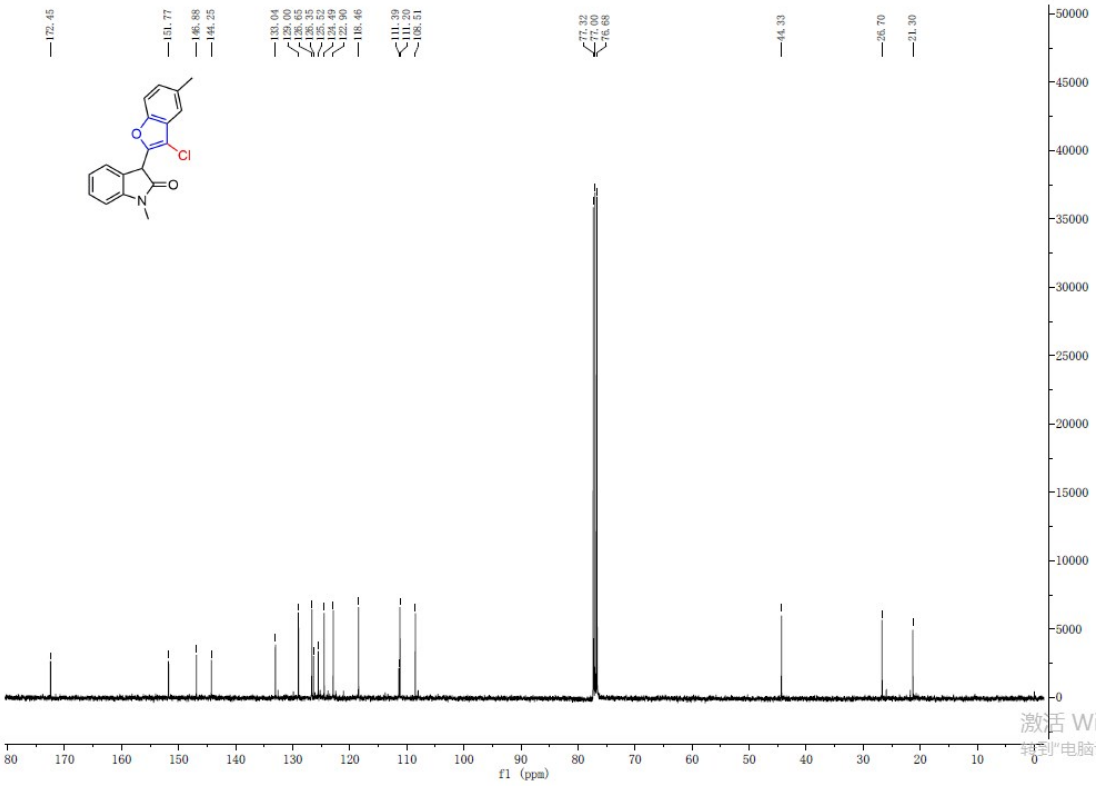
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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124.49
122.90
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111.39
111.20
108.51
77.32
77.00
76.68
44.33
26.70
21.30
Cl
O
N
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
80
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120
110
100
90
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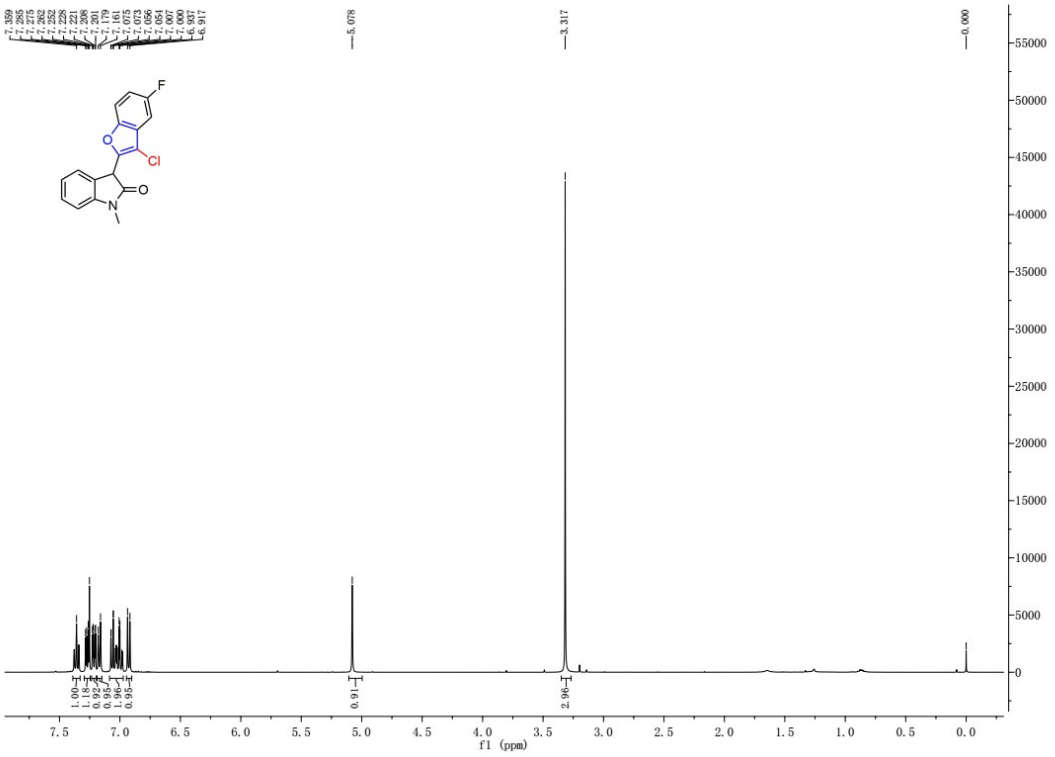
70
60
50
40
30
20
10
0
f1 (ppm)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7.161
7.075
7.073
7.056
7.054
7.007
7.000
6.937
6.917
5.078
3.317
0.000
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O
Cl
O
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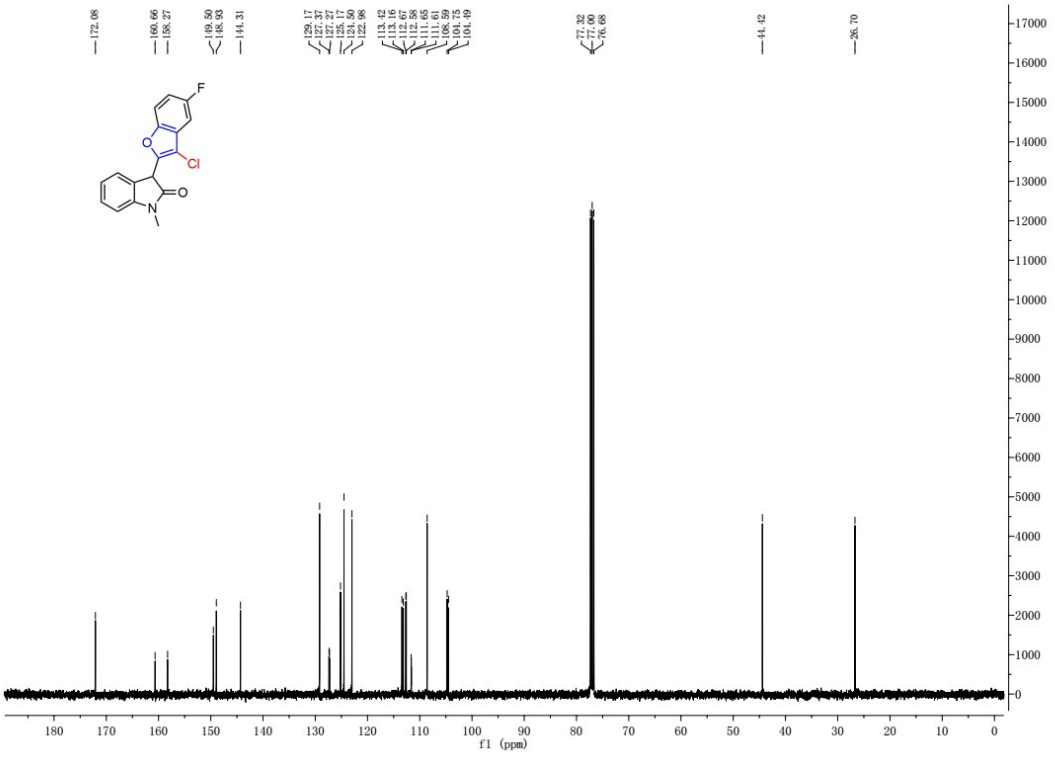
0.96
0.91
1.96
0.95
0.91
2.96
f1 (ppm)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127.37
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125.17
124.90
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113.16
112.67
112.58
111.65
111.61
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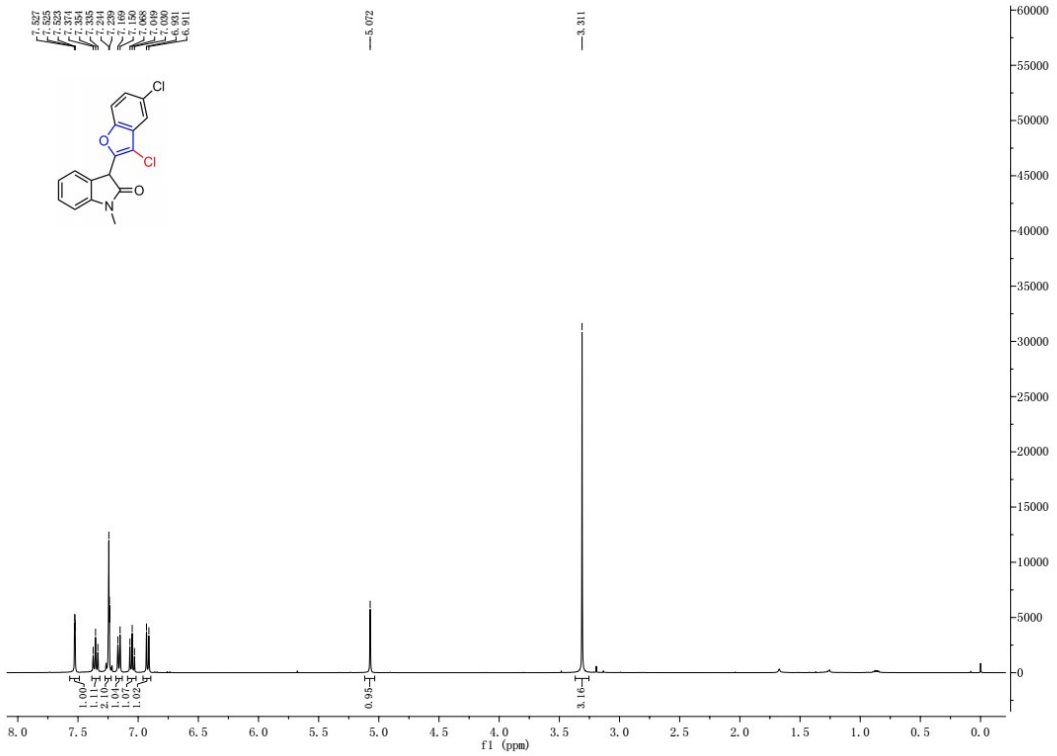
77.32
77.00
76.68
44.42
26.70
F
O
Cl
O
N
f1 (ppm)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6.931
6.911
5.072
3.311
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1.02
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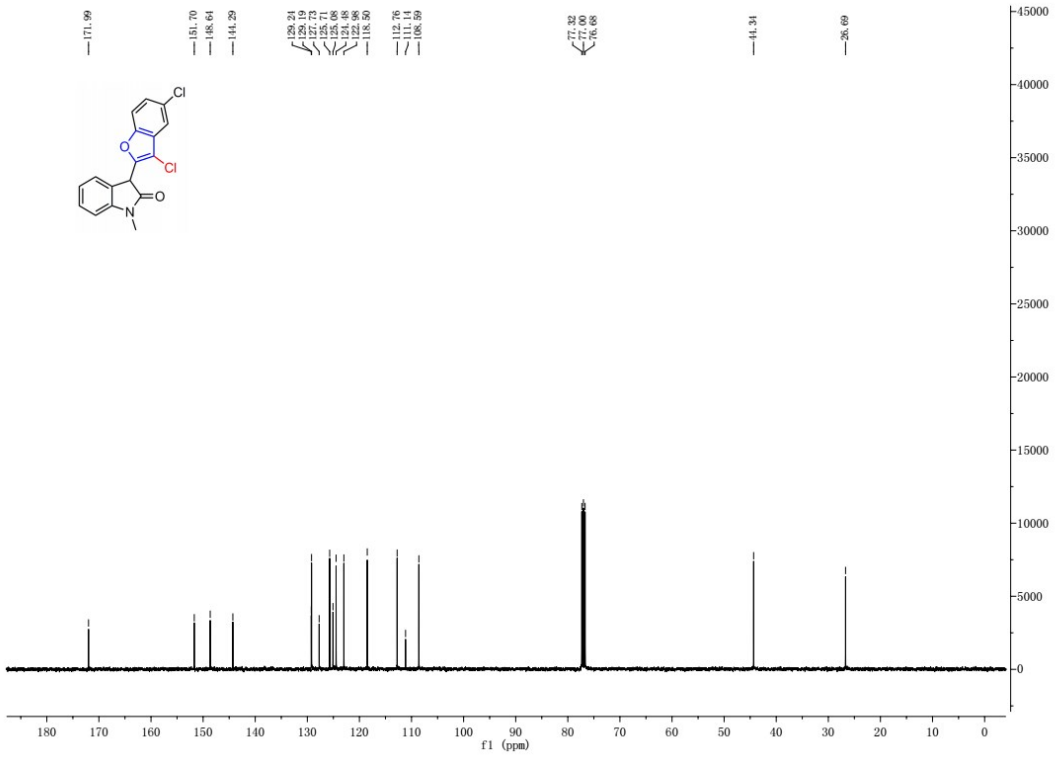
3.16
f1 (ppm)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129.19
127.73
125.71
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124.48
122.98
118.50
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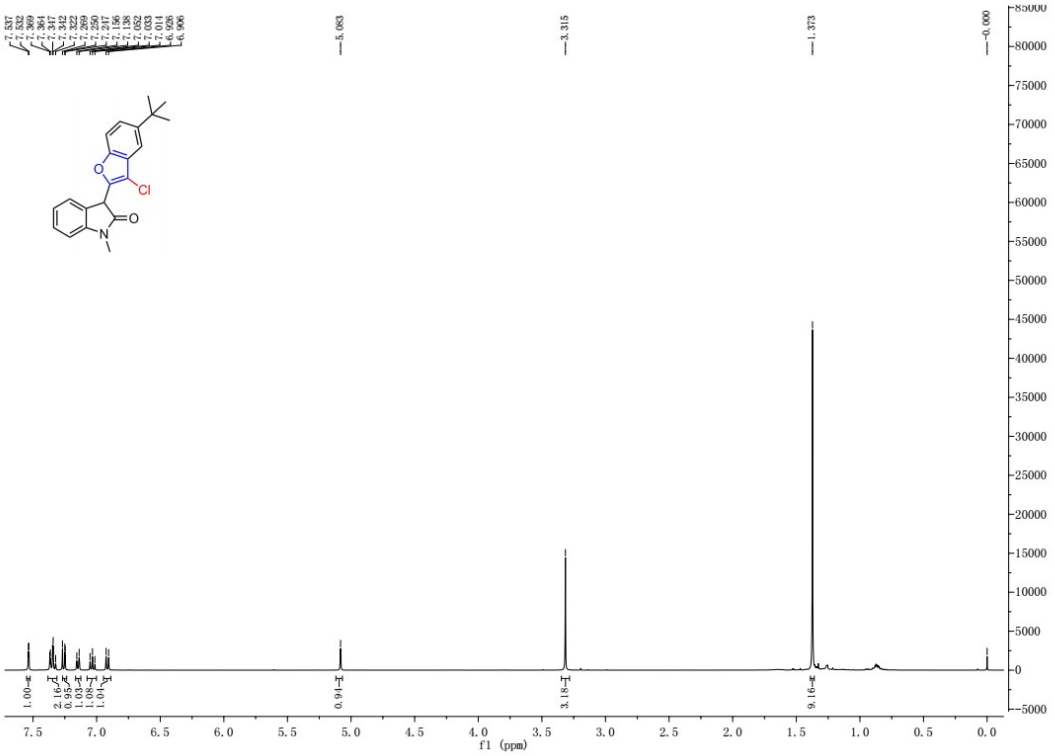
108.99
77.32
77.00
76.68
44.34
26.69
Cl
Cl
O
N
O
f1 (ppm)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7.032
7.033
7.014
6.926
6.906
5.083
3.315
1.373
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1.00
2.16
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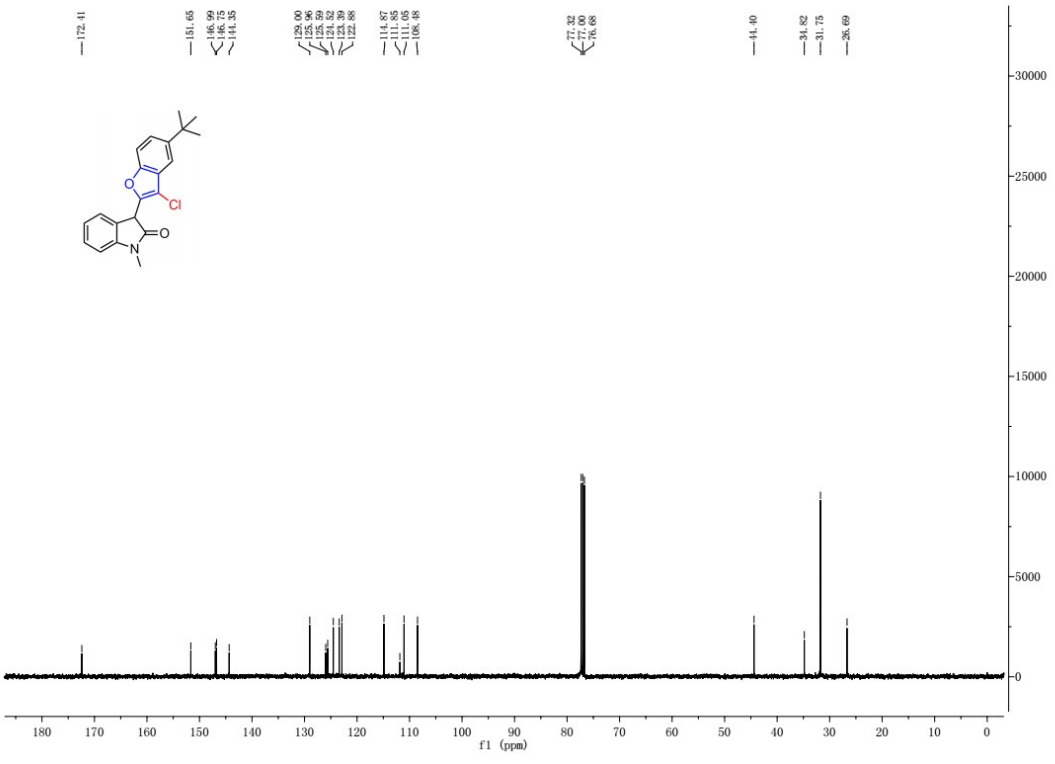
1.03
1.08
1.04
0.94
3.18
9.16
f1 (ppm)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122.88
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77.00
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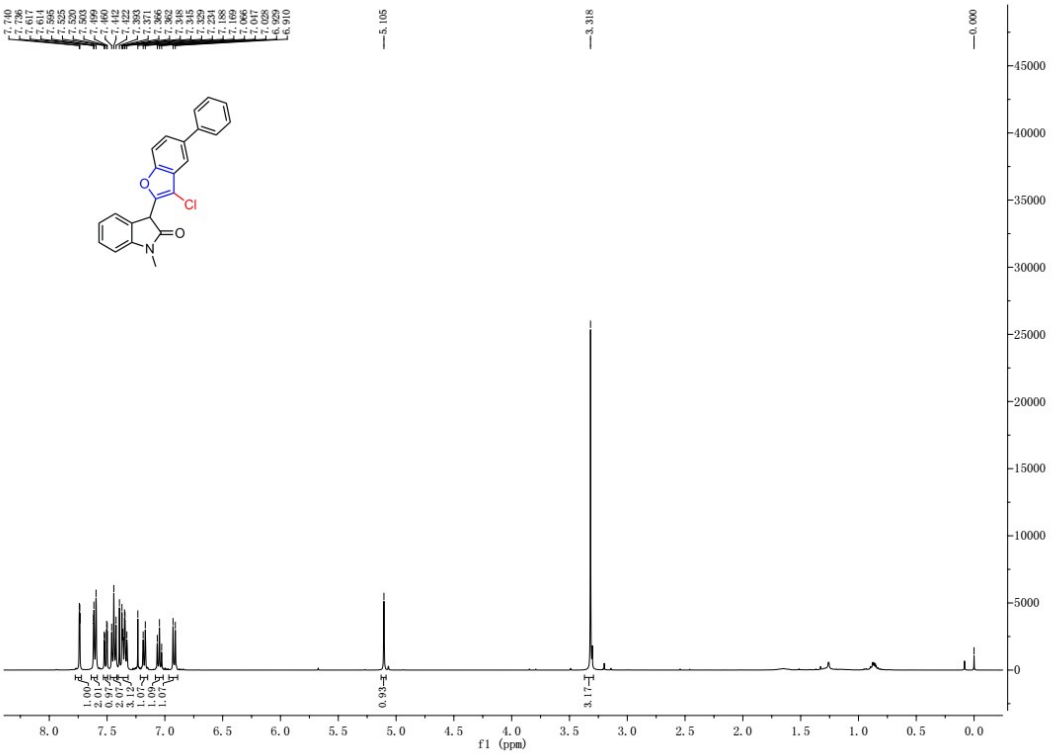
31.75
26.69
f1 (ppm)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7.329
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7.169
7.066
7.047
7.028
6.979
6.910
5.105
3.318
0.000
Cl
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2.07
3.12
1.07
1.09
1.07
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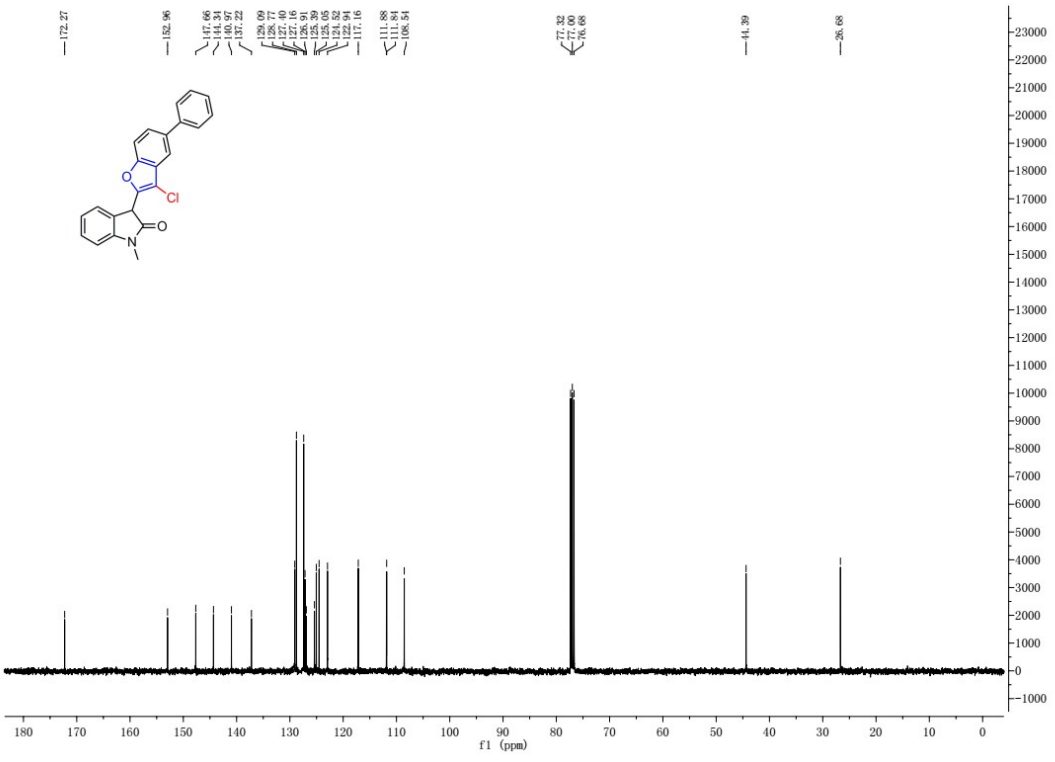
3.17
f1 (ppm)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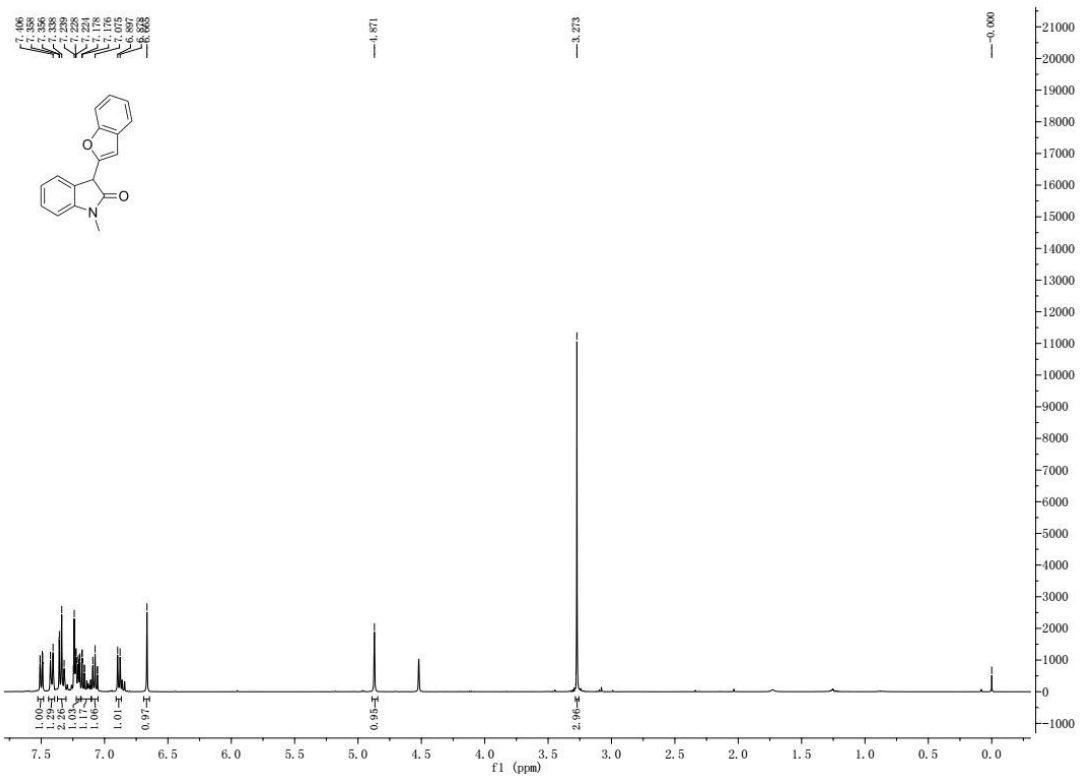
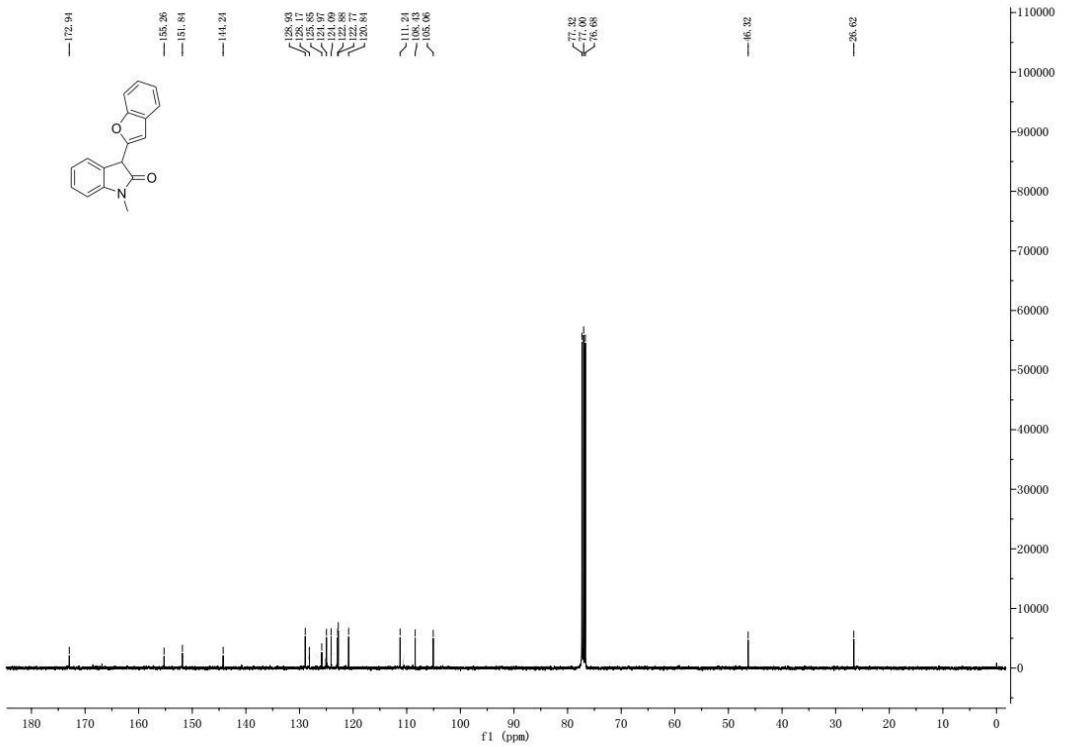
124.82
122.94
117.16
111.88
111.84
108.54
77.32
77.00
76.68
44.39
26.68
Cl
O
N
f1 (ppm)


7.406
7.358
7.356
7.338
7.239
7.228
7.224
7.178
7.176
7.075
6.897
6.893
4.871
3.273
0.000
1.00
1.29
2.26
1.03
1.17
1.06
1.01
0.97
0.95
2.96
f1 (ppm)


172.94
155.26
151.84
144.24
128.93
128.17
125.65
124.57
124.09
122.88
122.77
120.94
111.24
108.43
105.06
77.32
77.00
76.68
46.32
26.62
f1 (ppm)