Supporting Information

Electron Donor-Acceptor Complex Enabled Cascade Reaction of Unprotected o-Anilide Aryl Chlorides for Heterocycle Synthesis

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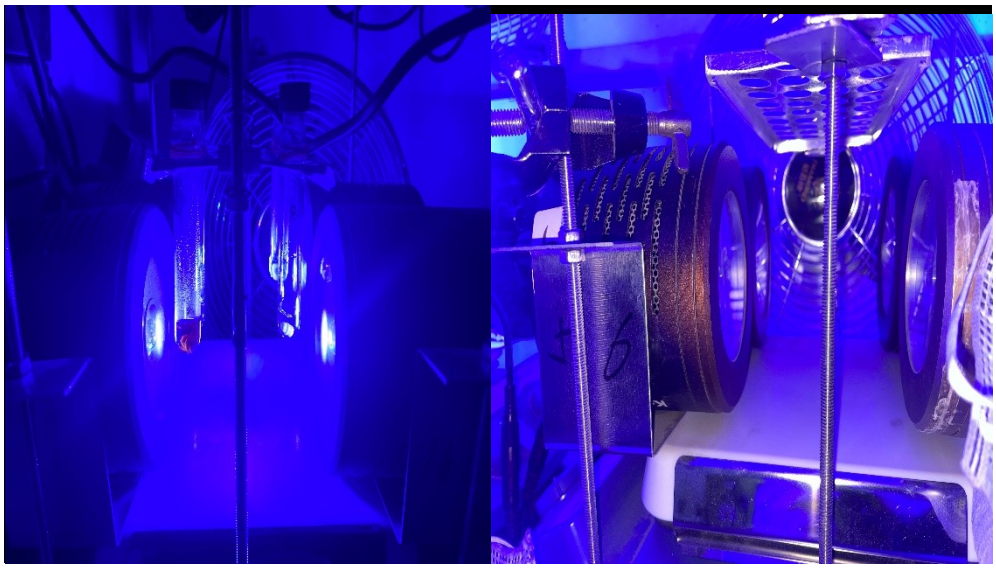
1. General Information

- Chemicals were purchased from Heowns, Innochem and Bidepharm, and they were used without further purification unless otherwise noted. The starting materials *o*-chloroanilines and *o*-chlorobenzamides were readily prepared according to the related literatures.[1] Solvents were purified using a solvent-purification system (VSPS-8, Vigor).
- Chromatographic purification of the products was performed on 200-300 mesh silica gel.
- IR spectra were taken on a Vertex 70 spectrophotometer and reported as wave numbers (cm^{-1}).
- UV/vis absorption spectra were acquired on a UV-5 spectrophotometer (METTLER TOLEDO).
- The GC-MS TQ8040 was used in the detection of the reaction mixture.
- The SGW X-4 was used to measure the melting point of solids.
- HRMS were obtained on an IonSpec FT-ICR mass spectrometer with ESI resource. The mass analysis mode of the HRMS was orbitrap.
- **^{1}H-, ^{19}F-** and **^{13}C- NMR** spectra were recorded at ambient temperature on JEOL JNM-LA400 Spectrometer and JEOL JNM-LA500 Spectrometer and The chemical shifts are reported in ppm downfield of tetramethylsilane (TMS) and referenced to residual solvent peaks resonance as the internal standard. The order of citation in parentheses is a) multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, m = multiplet), b) coupling constants, c) number of protons. Coupling constants (*J*) are reported in Hertz (Hz).
- Photochemical experiments were performed magnetically stirred in 10 mL glass tubes, sealed with a rubber septum. The tubes were irradiated with blue light (450 nm) using a LED lamp (kelo-A0100s blue LED). The distance from the light source to the irradiation vessel was 1 cm and a fan was used to keep the reaction temperature at 50 ± 5 °C. （The purchase link for LED lamp is https://item.jd.com/52714507033.html）



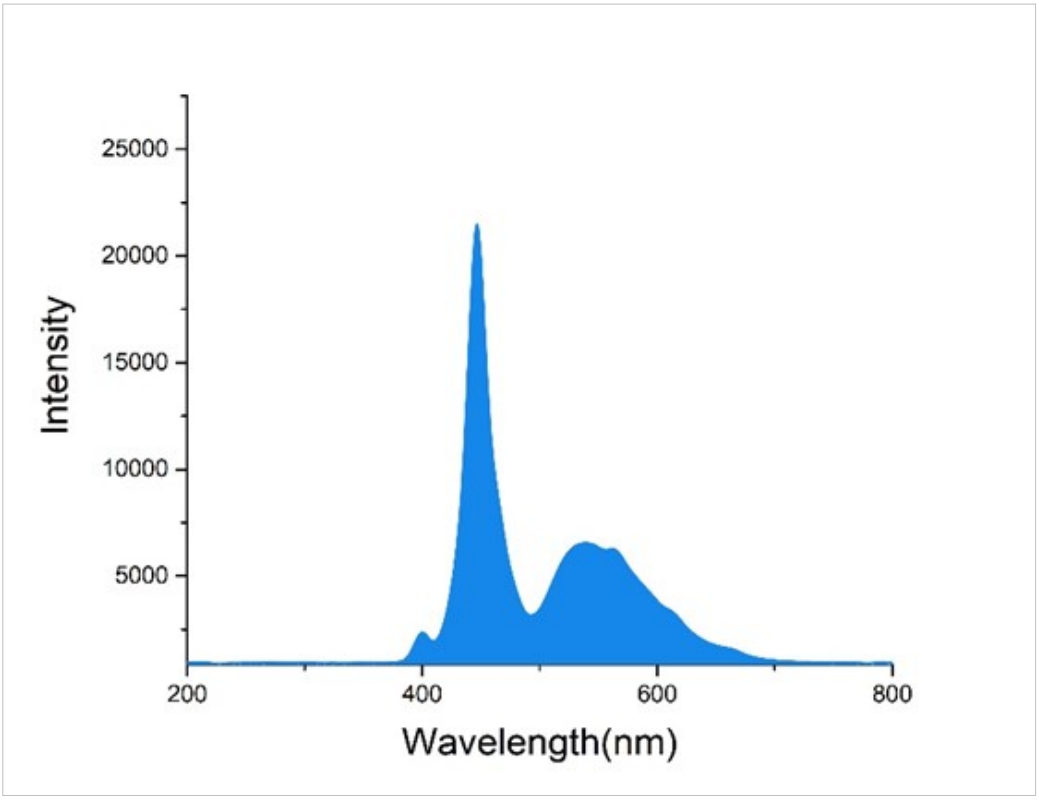
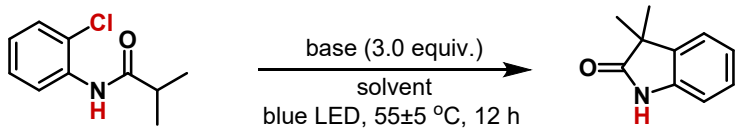


Figure S1. The spectra of blue LEDs employed in the reaction.

2. Experimental Procedures

Scheme S1. Optimization of the reaction conditions.

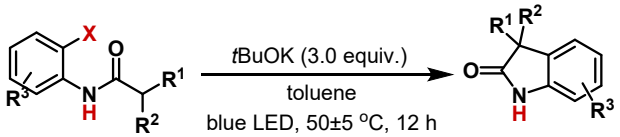


1 **2**

Entry	Base	Solvent	Yield (%)[a]
1	*t*BuOK	DMSO	trace
2	*t*BuOK	DMF	16
3	*t*BuOK	DCM	trace
4	*t*BuOK	Et_2O	24
5	*t*BuOK	toluene	68
6	*t*BuOK (2.0 equiv.)	toluene	38
7	*t*BuOK (1.0 equiv.)	toluene	trace
8	KOH	toluene	28
9	K_2CO_3	toluene	NR
10	NaH	toluene	32
11	/	toluene	NR
12[b]	*t*BuOK	toluene	NR

[a]Yield of isolated product after chromatography. [b]Without blue LED at 60 ℃

3. General Procedure



X = Cl, I

General procedure A: In a nitrogen atmosphere, to a dry tube equipped with a stirring bar, the *o*-iodobenzamides or *o*-chlorobenzamides (0.2 mmol), *t*BuOK (0.6 mmol, 67.2 mg, 3.0 equiv.) and toluene (2.0 mL) were added, the mixture was stirred under a 100 W blue LED (450 nm) lamp with an interval of 1 cm from the lamp and a fan was used to keep the reaction temperature at 50 ± 5 °C. After 12 hours, the reaction mixture was subjected to silica gel chromatography to afford the desired product (PE/EA = 3:1 – 1:1).

4. Mechanism Studies

4.1 UV/Vis absorption spectrometry

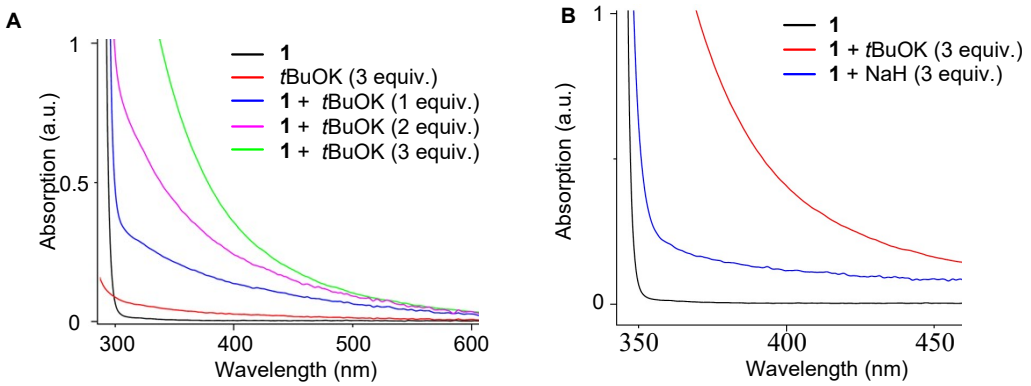
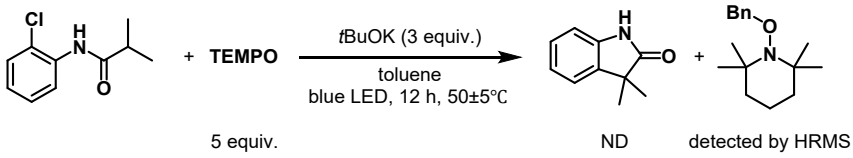
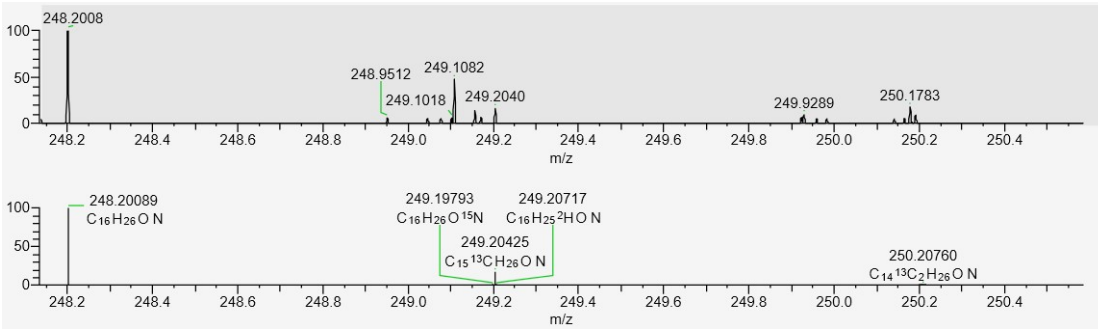


Figure S2: (A). Absorption spectra of substrate **1**, *t*BuOK and their mixture. The UV/vis spectra of *N*-(2-chlorophenyl)isobutyramide **1** (10^{-2} M in toluene), *t*BuOK (3×10^{-2} M in toluene), **1** (10^{-2} M in toluene) and *t*BuOK (10^{-2} M in toluene), **1** (10^{-2} M in toluene) and *t*BuOK (2×10^{-2} M in toluene), **1** (10^{-2} M in toluene) and *t*BuOK (3×10^{-2} M in toluene). (B). Absorption spectra of substrate **1**, mixture of **1** and *t*BuOK, and mixture of **1** and NaH. The UV/vis spectra of *N*-(2-chlorophenyl)isobutyramide **1** (10^{-2} M in toluene), **1** (10^{-2} M in toluene) and *t*BuOK (3×10^{-2} M in toluene), **1** (10^{-2} M in toluene) and NaH (3×10^{-2} M in toluene).

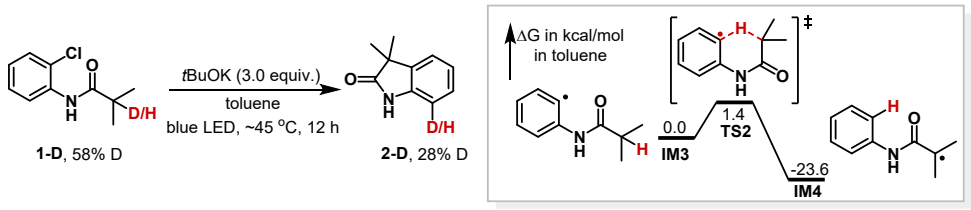
4.2 TEMPO trapping experiment



In a nitrogen atmosphere, to a dry tube equipped with a stirring bar, *N*-(2-chlorophenyl)isobutyramide **1** (0.2 mmol), TEMPO (1.0 mmol, 5.0 equiv.), *t*BuOK (0.6 mmol, 67.2 mg, 3.0 equiv.) and toluene (2.0 mL) were added, the mixture was stirred under a 100 W blue LED (450 nm) lamp for 12 hours. The benzyl radical trapped by TEMPO was detected by HRMS. **HRMS** (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{25}ON^+$: 248.2008; found: 248.2008.


248.2008
248.9512
249.1082
249.1018
249.2040
249.9289
250.1783
m/z
248.20089
C16H26O N
249.19793
C16H26O15N
249.20717
C16H252HO N
249.20425
C15 13CH26O N
250.20760
C14 13C2H26O N
m/z

4.3 Evidence for 1,5-HAT



The experiment with **1-D** as the substrate afforded the desired oxindole **2-D** with 28% deuterium incorporation at the aromatic ring.

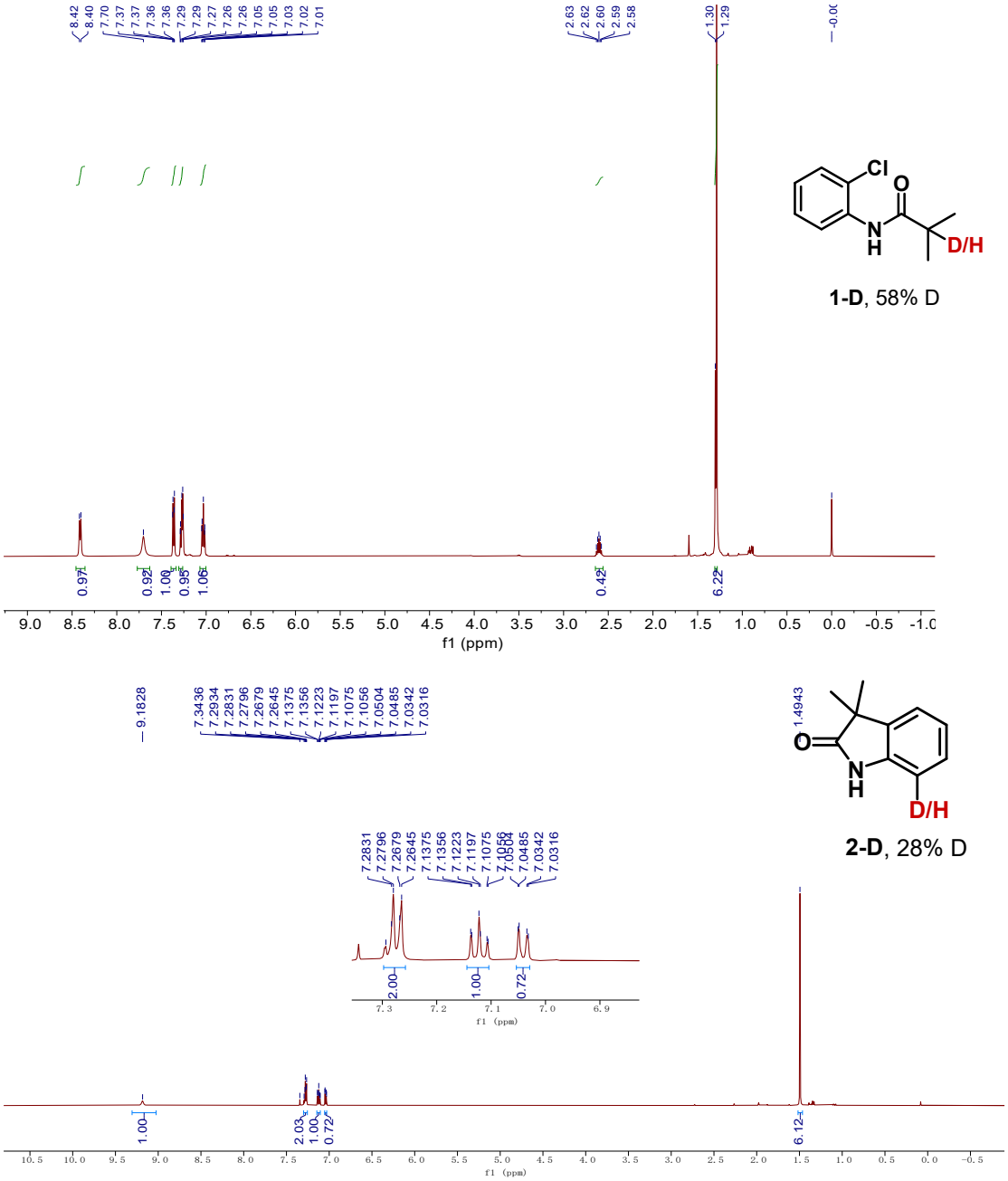


Figure S3. Evidence for 1,5-HAT.

4.4 Density functional theory (DFT) studies

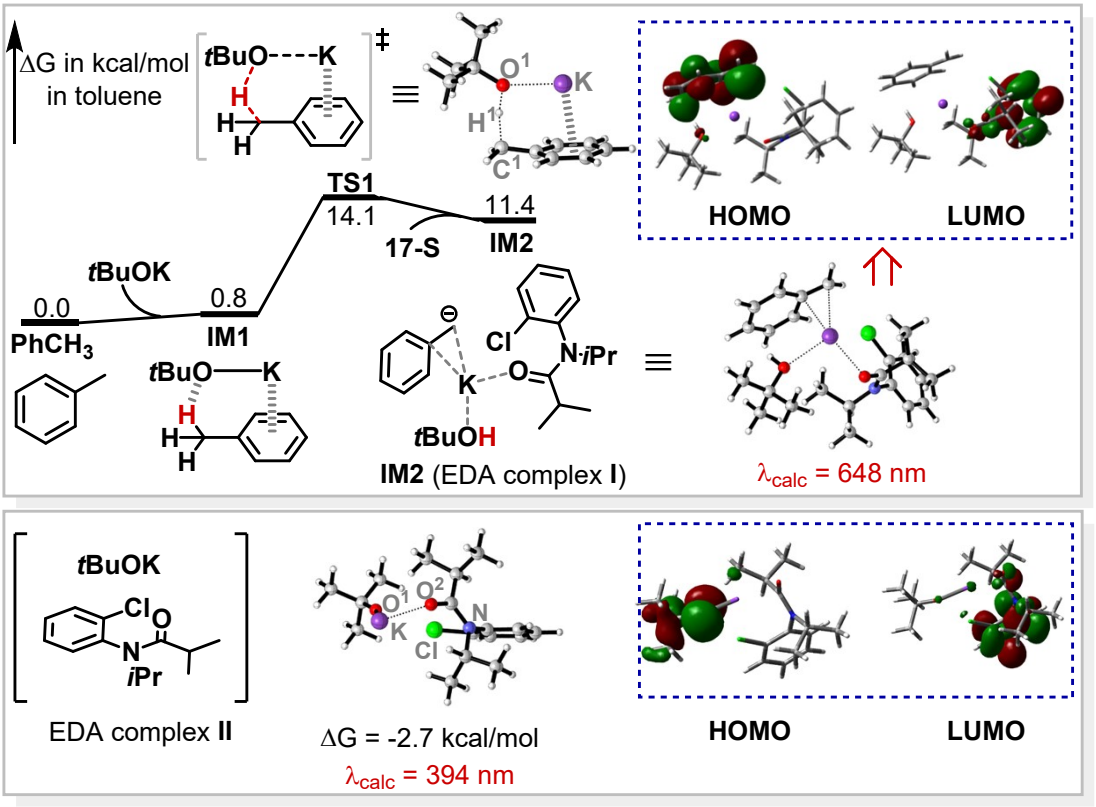


Figure S4. DFT studies.

We carried out density functional theory (DFT) and time-dependent DFT (TDDFT) calculations to further study the possible EDA complexes. We successfully located the possible EDA complexes **I** and **II**, showing that complex **I** has a λ_{calc} = 648 nm, much longer than complex **II** (λ_{calc} = 394 nm).

4.5 Quantum yield determination

According to the procedure of Xu[2]: To an oven-dried 10 mL glass tubes sealed with rubber septum, *N*-(2-chlorophenyl)isobutyramide **1** (0.2 mmol) were combined in toluene (2 mL) under nitrogen atmosphere. The reaction mixture was stirred and irradiated (λ = 450 nm, PLS-LED100C) for 2.0 h. After irradiation, the solution was measured the unit area photon flux (MQ-500 photosynthetic active radiation meter). And the yield of product formed was isolated. The quantum yield is calculated using the following equation:

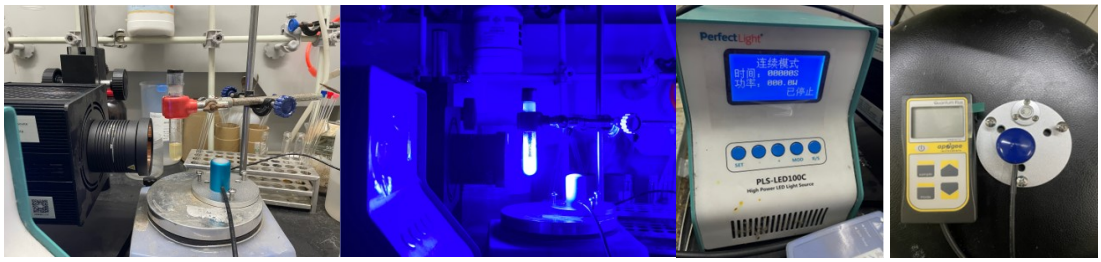
$$\phi = \frac{mol\ product}{flux \cdot S \cdot t}$$

Where, Φ is quantum yield, S (m^2) is the irradiation area and t (s) is the photoreaction time.

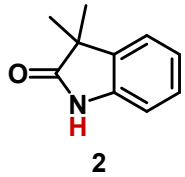
Experiment: the unit photon flux was 665 $\mu mol \cdot s^{-1} \cdot m^{-2}$ (average of three experiments), the irradiation area was 2.2×10^{-4} m^2, and the product yield was 9% after 2.0 h (7200 s).

Quantum yield calculation:

$$\phi = \frac{mol\ product}{flux \cdot S \cdot t} = \frac{0.09 \times 0.2 \times 10^{3}}{665 \times 2.2 \times 10^{-4} \times 7200} = 0.017$$

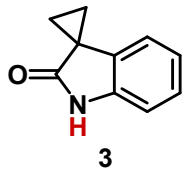


5. Compound Characterization Data



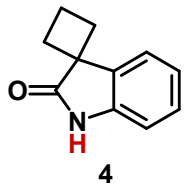
2

3,3-Dimethylindolin-2-one (2): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (36 mg, 0.177 mmol, 88%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 7.19 (d, *J* = 7.5 Hz, 2H), 7.03 – 7.06 (m, 1H), 6.96 (d, *J* = 8.3 Hz, 1H), 1.41 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.4, 140.0, 136.4, 127.7, 122.7, 122.5, 110.0, 44.8, 24.4. These data are in agreement with those reported previously in the literature.[3]



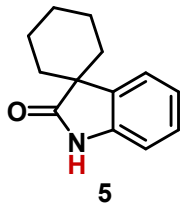
3

Spiro[cyclopropane-1,3'-indolin]-2'-one (3): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (29 mg, 0.166 mmol, 83%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.76 (s, 1H), 7.21 – 7.21 (m, 1H), 7.04 – 6.94 (m, 2H), 6.88 – 6.72 (m, 1H), 1.78 – 1.75 (m, 2H), 1.56 – 1.53 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 179.6, 140.7, 131.4, 126.9, 122.1, 118.7, 109.9, 27.6, 19.6. These data are in agreement with those reported previously in the literature.[4]



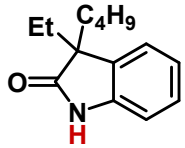
4

Spiro[cyclobutane-1,3'-indolin]-2'-one (4): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (31 mg, 0.166 mmol, 83%).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.67 (s, 1H), 7.48 (d, *J* = 7.4 Hz, 1H), 7.21 – 7.16 (m, 1H), 7.08 – 7.04 (m, 1H), 6.89 (d, *J* = 7.7 Hz, 1H), 2.72 – 2.63 (m, 2H), 2.39 – 2.32 (m, 3H), 2.28 – 2.21 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 183.0, 140.3, 135.0, 127.9, 122.8, 122.7, 109.6, 48.7, 31.4, 16.9. These data are in agreement with those reported previously in the literature.[5]



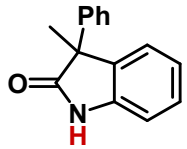
5

Spiro[cyclohexane-1,3'-indolin]-2'-one (5): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (33 mg, 0.142 mmol, 71%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.69 (s, 1H), 7.45 (d, *J* = 7.4 Hz, 1H), 7.22 – 7.18 (m, 1H), 7.03 – 6.99 (m, 1H), 6.93 (d, *J* = 7.7 Hz, 1H), 1.94 – 1.89 (m, 2H), 1.87 – 1.83 (m, 2H), 1.78 – 1.71 (m, 3H), 1.64 – 1.58 (m, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 183.4, 140.1, 135.9, 127.5, 124.4, 122.0, 109.8, 48.1, 33.0, 25.3, 21.2. These data are in agreement with those reported previously in the literature.[3]



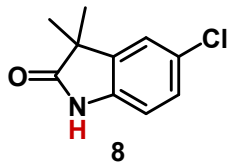
6

3-Butyl-3-ethylindolin-2-one (6): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid M.P. 95 – 96 °C. (42 mg, 0.144 mmol, 72%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.25 – 7.15 (m, 1H), 7.12 (d, *J* = 7.4 Hz, 1H), 7.09 – 6.99 (m, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 2.00 – 1.85 (m, 2H), 1.83 – 1.73 (m, 2H), 1.32 – 1.13 (m, 2H), 1.11 – 0.99 (m, 1H), 0.89 – 0.80 (m, 1H), 0.76 (t, *J* = 7.3 Hz, 3H), 0.63 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 182.9, 141.4, 133.0, 127.6, 123.2, 122.5, 109.6, 54.4, 37.7, 31.2, 26.5, 23.0, 14.0, 8.7. **IR (ATR)** ν 3205, 2959, 2929, 1700, 1619, 1470, 1192, 748, 652 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+H]^+$ calcd for $C_{14}H_{20}ON^+$: 218.1539; found: 218.1532.



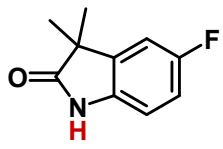
7

3-Methyl-3-phenylindolin-2-one (7): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid M.P. 132 – 133 °C. (27 mg, 0.126 mmol, 63%).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.70 (s, 1H), 7.33 – 7.31 (m, 3H), 7.31 – 7.28 (m, 1H), 7.27 – 7.26 (m, 1H), 7.24 – 7.22 (m, 1H), 7.13 (d, *J* = 7.4 Hz, 1H), 7.10 – 7.02 (m, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 1.82 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 182.1, 140.6, 140.4, 135.7, 128.7, 128.2, 127.4, 126.7, 124.5, 122.9, 110.2, 52.8, 23.5. **IR (ATR)** ν 3213, 2928, 1706, 1619, 1472, 1215, 715, 696 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+H]^+$ calcd for $C_{15}H_{14}ON^+$: 224.1069; found: 224.1062.



8

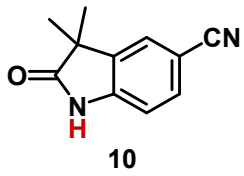
5-Chloro-3,3-dimethylindolin-2-one (8): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a colorless oil (36 mg, 0.166 mmol, 83%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.02 (s, 1H), 7.19 – 7.11 (m, 2H), 6.87 (d, *J* = 8.0 Hz, 1H), 1.38 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 183.7, 138.4, 138.1, 128.0, 127.8, 123.4, 111.0, 45.2, 24.3. These data are in agreement with those reported previously in the literature.[3]



9

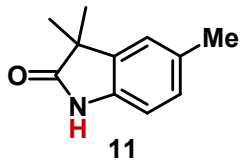
5-Fluoro-3,3-dimethylindolin-2-one (9): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (29 mg, 0.124 mmol, 62%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.52 (s, 1H), 6.94 – 6.82 (m, 3H), 1.39 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.6, 159.4 (d, *J* = 239.9 Hz), 138.0 (d, *J* = 7.7 Hz), 114.0 (d, *J* = 23.6 Hz), 110.8 (d, *J* = 3.9 Hz), 110.6 (d, *J* = 12.5 Hz), 45.5, 24.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -

120.6 (q, *J* = 7.3 Hz). These data are in agreement with those reported previously in the literature.[6]



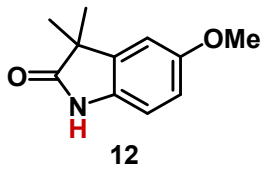
10

3,3-Dimethyl-2-oxoindoline-5-carbonitrile (10) Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a yellow solid (22 mg, 0.114 mmol, 57%). **^{1}H NMR**(400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 7.55 (d, *J* = 9.7 Hz, 1H), 7.47 (s, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 1.43 (s, 6H). **^{13}C NMR**(101 MHz, $CDCl_3$) δ 183.8, 144.1, 137.3, 133.1, 126.4, 119.3, 110.6, 105.9, 44.8, 24.2. These data are in agreement with those reported previously in the literature.[7]



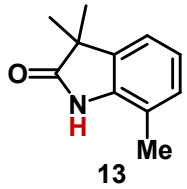
11

3,3,5-Trimethylindolin-2-one (11): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (35 mg, 0.150 mmol, 75%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.01 – 6.99 (m, 2H), 6.82 (d, *J* = 7.4 Hz, 1H), 2.32 (s, 3H), 1.38 (s, 6H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.3, 137.5, 136.5, 132.0, 128.0, 123.5, 109.7, 44.8, 24.5, 21.3. These data are in agreement with those reported previously in the literature.[3]



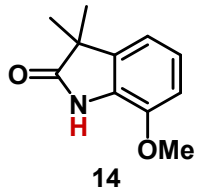
12

5-Methoxy-3,3-dimethylindolin-2-one (12): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (33 mg, 0.142 mmol, 71%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.61 (s, 1H), 6.83 (d, *J* = 8.3 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 6.74 – 6.71 (m, 1H), 3.80 (s, 3H), 1.40 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.1, 156.0, 137.9, 133.3, 112.0, 110.3, 110.2, 55.9, 45.3, 24.5. These data are in agreement with those reported previously in the literature.[3]



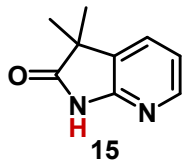
13

3,3,7-Trimethylindolin-2-one (13): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (25 mg, 0.116 mmol, 58%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.77 (s, 1H), 7.04 – 7.02 (m, 2H), 6.97 (d, *J* = 7.1 Hz, 1H), 2.31 (s, 3H), 1.40 (s, 6H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.3, 138.7, 136.0, 129.1, 122.5, 120.1, 119.3, 45.1, 24.5, 16.6. These data are in agreement with those reported previously in the literature.[8]



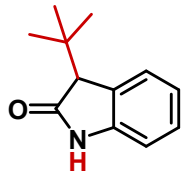
14

7-Methoxy-3,3-dimethylindolin-2-one (14): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a yellow solid M.P. 120 – 121 °C. (30 mg, 0.124 mmol, 62%).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.05 – 6.97 (m, 1H), 6.83 (d, *J* = 7.5 Hz, 1H), 6.79 (d, *J* = 8.2 Hz, 1H), 3.88 (s, 3H), 1.39 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 182.6, 143.8, 137.1, 128.3, 123.1, 115.1, 110.1, 55.7, 45.4, 24.4. **IR (ATR)** ν 3219, 2965, 2927, 1703, 1461, 1260, 1053, 731 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+H]^+$ calcd for $C_{11}H_{14}O_2N^+$: 192.1019; found: 192.1012.



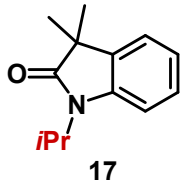
15

3,3-Dimethyl-1,3-dihydro-2H-pyrrolo[2,3-b]pyridin-2-one (15): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a colorless oil (45 mg, 0.167 mmol, 84%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.84 (s, 1H), 8.17 – 8.16 (m, 1H), 7.48 – 7.43 (m, 1H), 7.03 – 6.90 (m, 1H), 1.40 (s, 6H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 182.2, 155.6, 146.3, 130.59, 130.56, 118.3, 44.8, 24.0. These data are in agreement with those reported previously in the literature.[3]



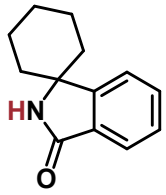
16

3-(*tert*-Butyl)indolin-2-one (16): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (32 mg, 0.119 mmol, 59%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.30 (s, 1H), 7.21 – 7.17 (m, 1H), 6.99 – 6.95 (m, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 3.13 (s, 1H), 1.12 (s, 9H). **^{13}C NMR**(126 MHz, $CDCl_3$) δ 179.0, 142.1, 128.4, 128.0, 126.6, 121.7, 109.3, 56.0, 35.1, 27.5. These data are in agreement with those reported previously in the literature.[9]



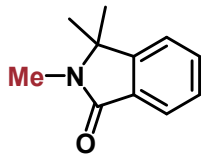
17

1-Isopropyl-3,3-dimethylindolin-2-one (17): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (32 mg, 0.112 mmol, 57%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 – 7.15 (m, 2H), 7.09 – 6.95 (m, 2H), 4.71 – 4.61 (m, 1H), 1.46 (d, *J* = 7.1 Hz, 6H), 1.33 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 181.2, 141.3, 136.5, 127.5, 122.7, 122.0, 110.0, 44.0, 43.5, 24.6, 19.6. These data are in agreement with those reported previously in the literature.[10]



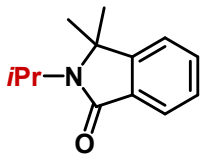
18

Spiro[cyclohexane-1,1'-isoindolin]-3'-one (18): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (33 mg, 0.142 mmol, 71%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.57 – 7.53 (m, 1H), 7.50 – 7.36 (m, 2H), 1.93 – 1.84 (m, 5H), 1.60 – 1.56 (m, 4H), 1.44 – 1.41 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.3, 153.2, 131.9, 131.1, 128.1, 124.1, 121.4, 62.0, 36.8, 25.2, 23.4. These data are in agreement with those reported previously in the literature.[10]



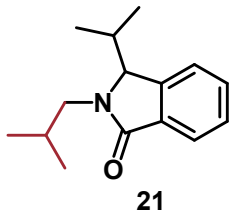
19

1'–Methylspiro[cyclobutane–1,3'–indolin]–2'–one (19): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) a colorless oil (29 mg, 0.155 mmol, 78%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 – 7.82 (m, 1H), 7.56 – 7.52 (m, 1H), 7.45 – 7.41 (m, 2H), 3.01 (s, 3H), 1.44 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.4, 151.6, 131.6, 131.0, 128.1, 123.7, 120.8, 62.2, 25.0, 24.0. These data are in agreement with those reported previously in the literature.[10]



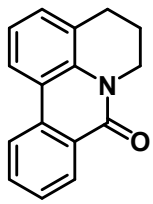
20

2-Isopropyl-3,3-dimethylisoindolin-1-one (20): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (18 mg, 0.090 mmol, 45%).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.4 Hz, 1H), 7.54 – 7.46 (m, 1H), 7.44 – 7.36 (m, 1H), 7.34 (d, *J* = 7.5 Hz, 1H), 3.72 – 3.58 (m, 1H), 1.56 (d, *J* = 6.9 Hz, 6H), 1.48 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.3, 151.4, 132.1, 131.3, 127.9, 123.2, 120.7, 63.3, 44.6, 25.5, 20.6. These data are in agreement with those reported previously in the literature.[10]



21

2-Isobutyl-3-isopropylisoindolin-1-one (21): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (23 mg, 0.106 mmol, 53%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.1 Hz, 1H), 7.50 – 7.43 (m, 3H), 4.47 (d, *J* = 3.4 Hz, 1H), 3.89 (dd, *J* = 14.0, 10.1 Hz, 1H), 2.92 (dd, *J* = 14.0, 5.3 Hz, 1H), 2.41 – 2.37 (m, 1H), 2.07 – 1.97 (m, 1H), 1.24 (d, *J* = 7.1 Hz, 3H), 1.00 (d, *J* = 6.6 Hz, 3H), 0.86 (d, *J* = 6.6 Hz, 3H), 0.48 (d, *J* = 6.9 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.8, 143.4, 133.5, 130.8, 128.1, 123.8, 123.2, 64.3, 47.1, 28.8, 27.4, 20.7, 19.9, 19.2, 14.9. These data are in agreement with those reported previously in the literature.[10]

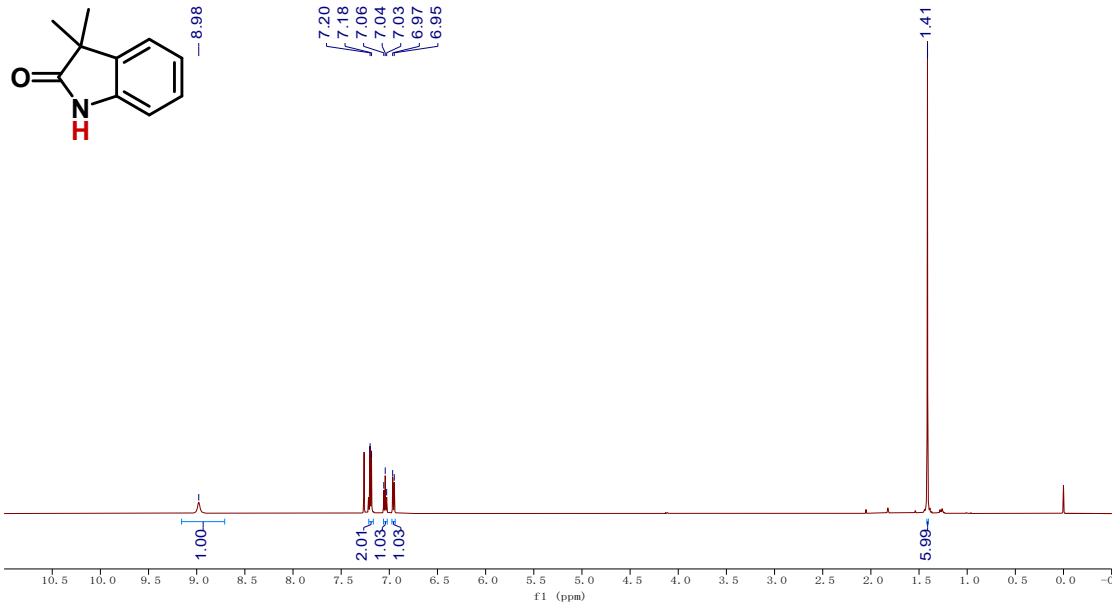


22

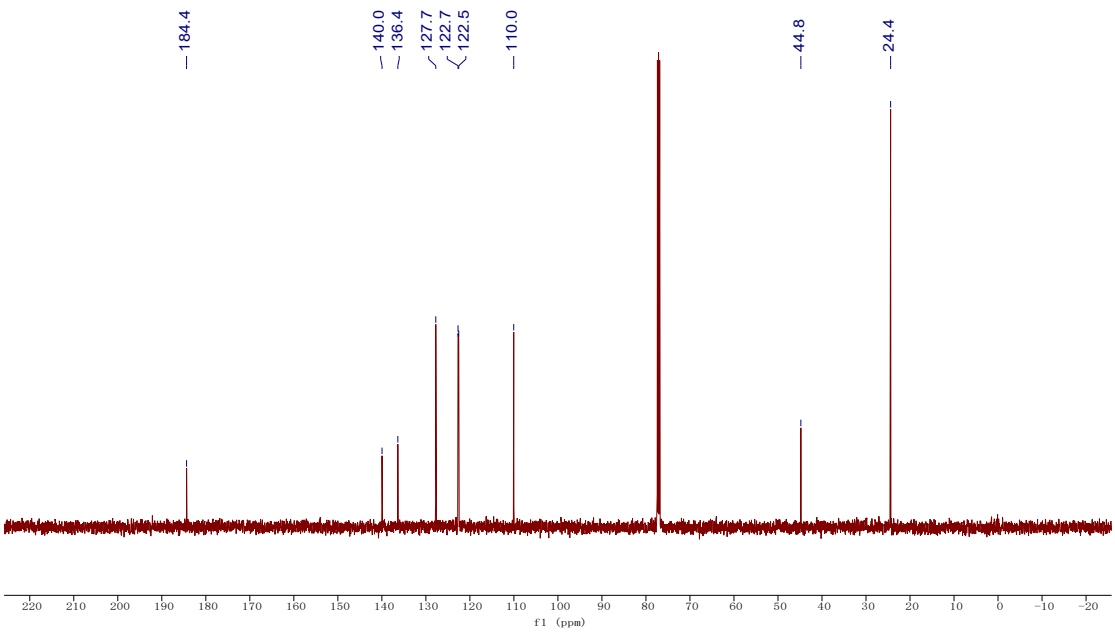
5,6-Dihydro-4*H*,8*H*-pyrido[3,2,1-*de*]phenanthridin-8-one (22): Following the general procedure, the title product was obtained after purification by column chromatography (PE/EA = 3:1-1:1) as a white solid (34 mg, 0.156 mmol, 78%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.54 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.27 (d, *J* = 9.0 Hz, 1H), 8.13 (d, *J* = 8.9 Hz, 1H), 7.79 – 7.70 (m, 1H), 7.61 – 7.53 (m, 1H), 7.32 – 7.25 (m, 1H), 7.23 – 7.19 (m, 1H), 4.35 – 4.29 (m, 2H), 3.05 – 2.99 (m, 2H), 2.20 – 2.10 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.3, 134.6, 133.7, 132.4, 129.6, 128.6, 127.9, 125.7, 125.4, 122.0, 121.9, 121.4, 119.2, 42.9, 28.3, 20.8. These data are in agreement with those reported previously in the literature.[10]

6. NMR Spectra

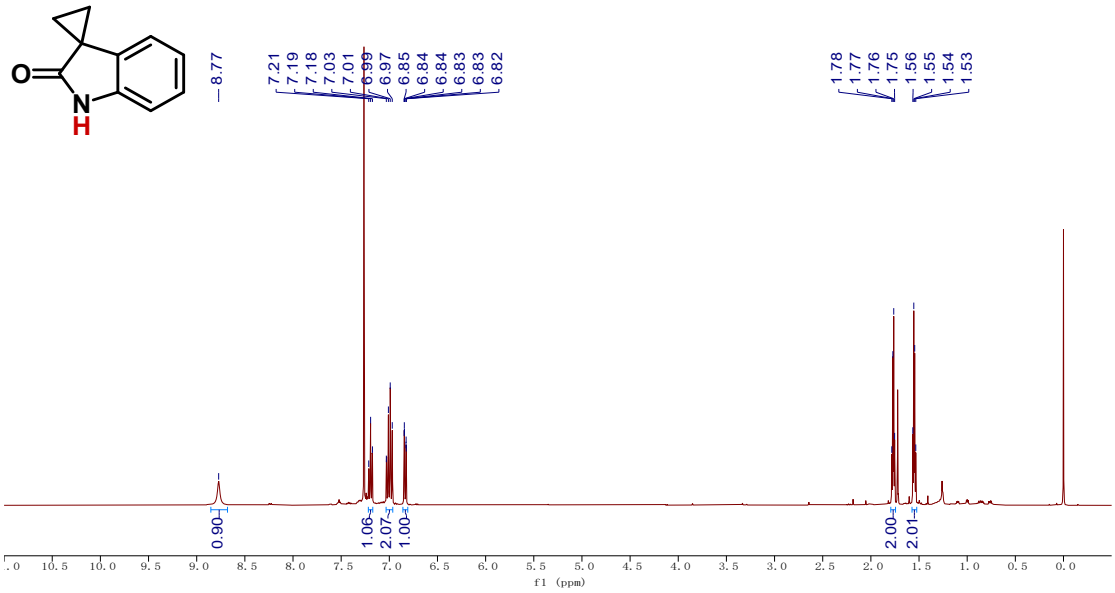
^{1}H NMR of compound **2** (500 MHz in $CDCl_3$)



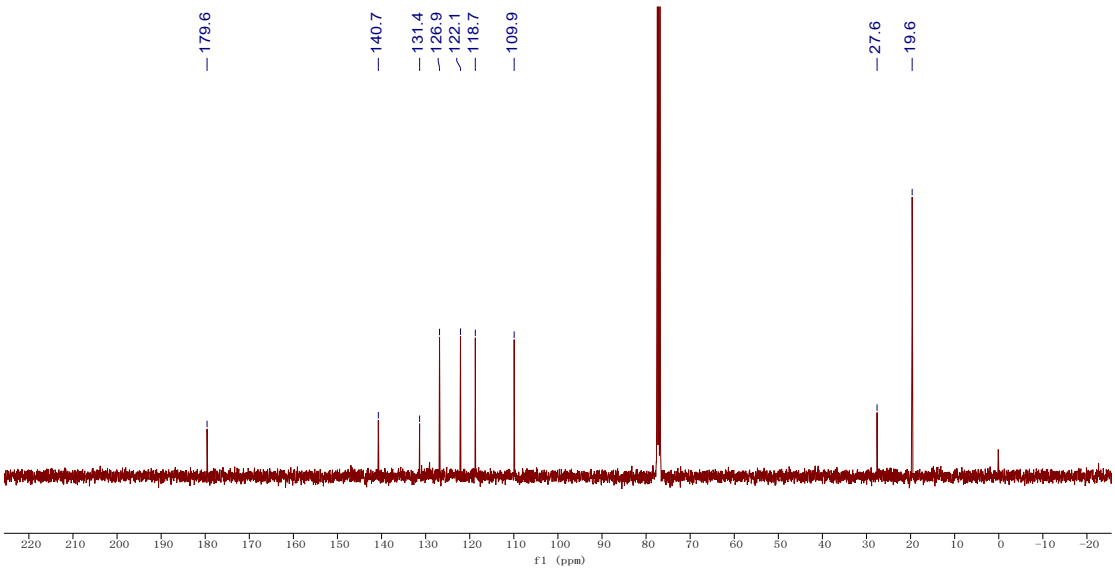
^{13}C NMR of compound **2** (126 MHz in $CDCl_3$)



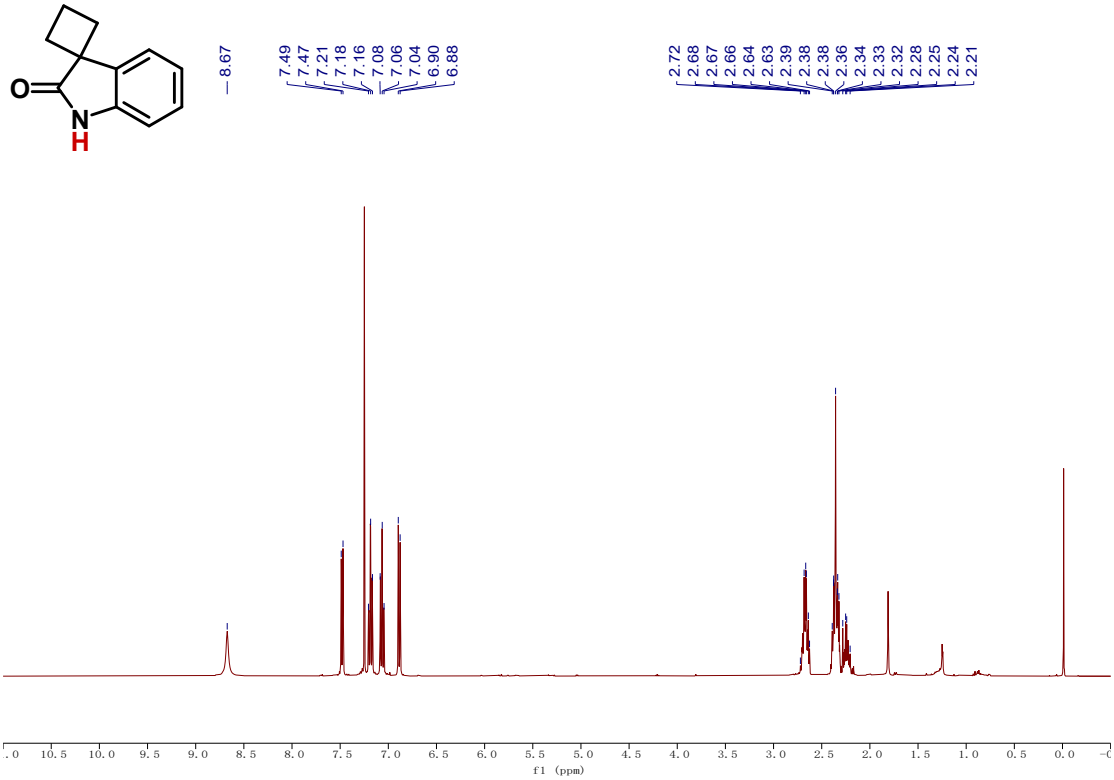
^{1}H NMR of compound **3** (400 MHz in $CDCl_3$)



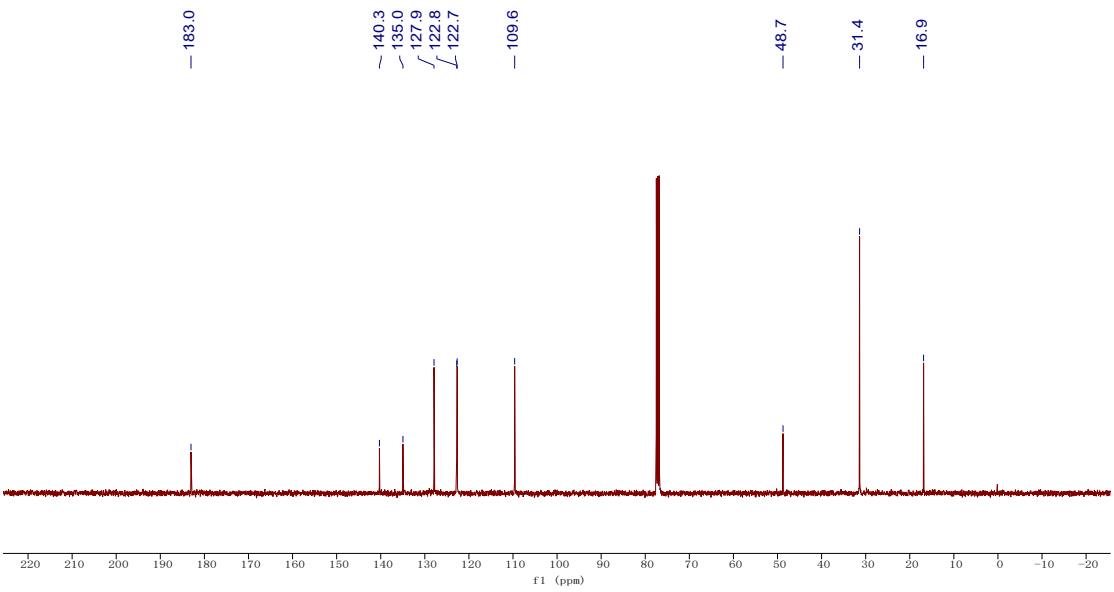
^{13}C NMR of compound **3** (101 MHz in $CDCl_3$)



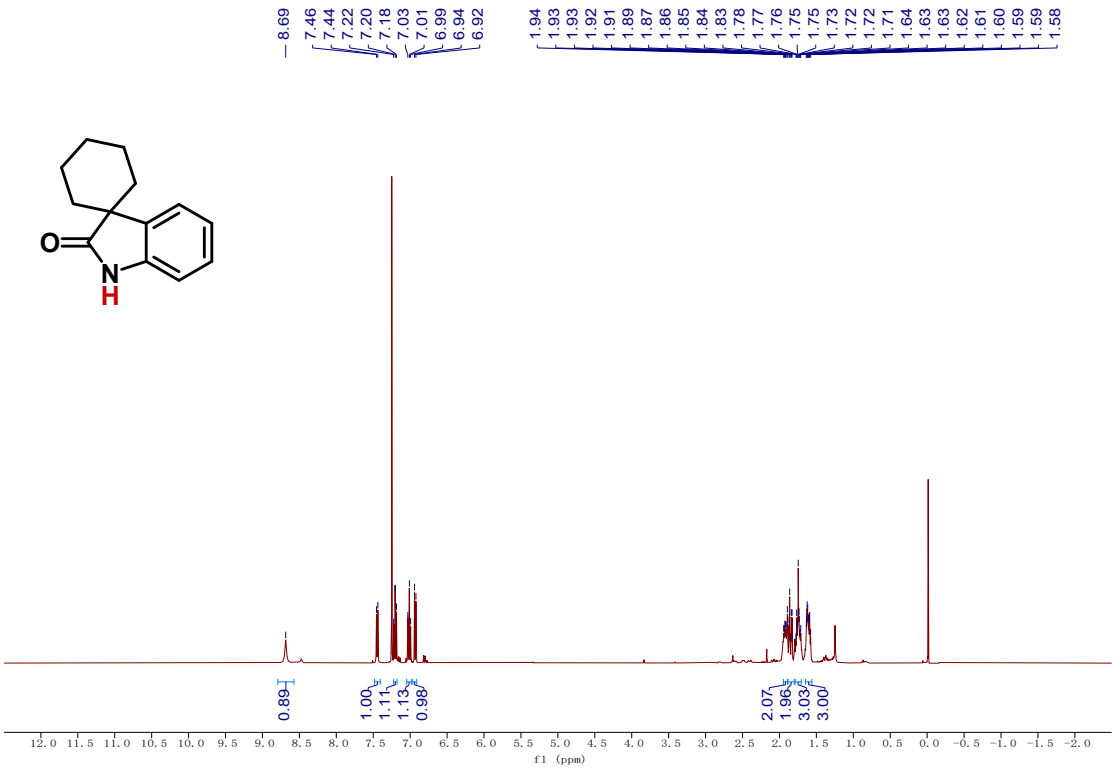
^{1}H NMR of compound **4** (400 MHz in $CDCl_3$)



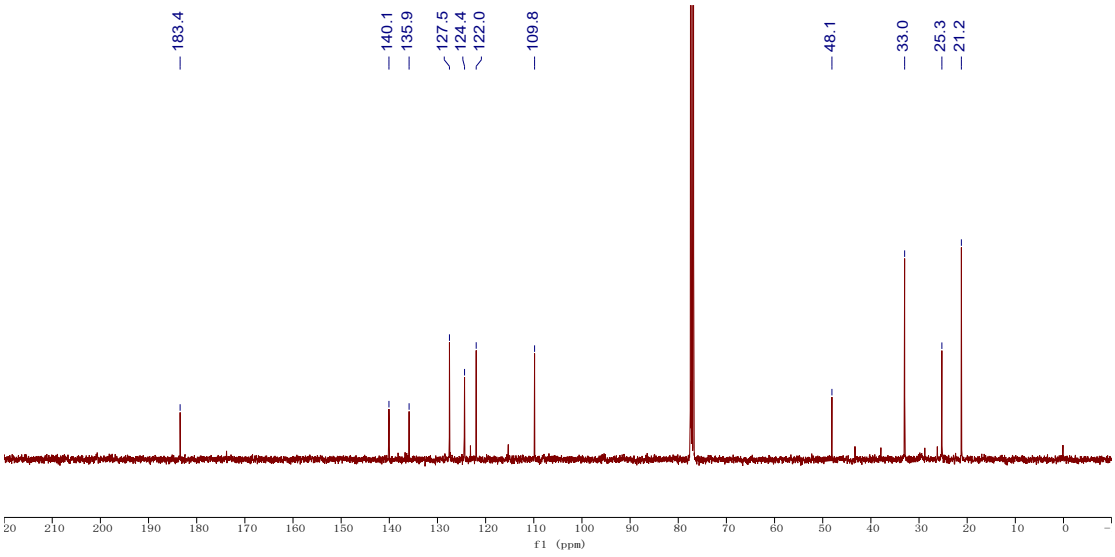
^{13}C NMR of compound **4** (101 MHz in $CDCl_3$)



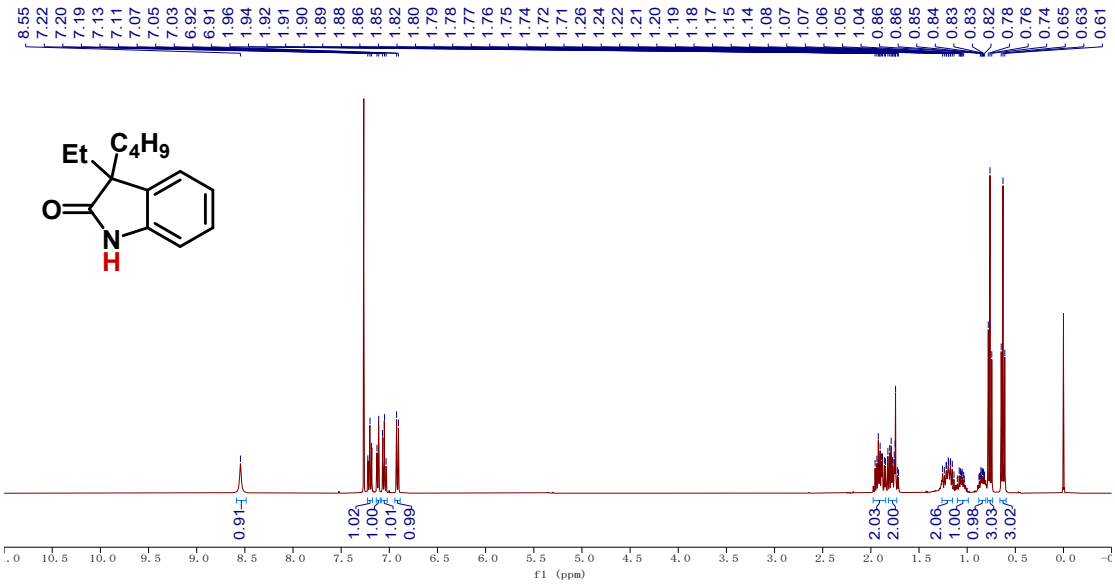
^{1}H NMR of compound **5** (400 MHz in $CDCl_3$)



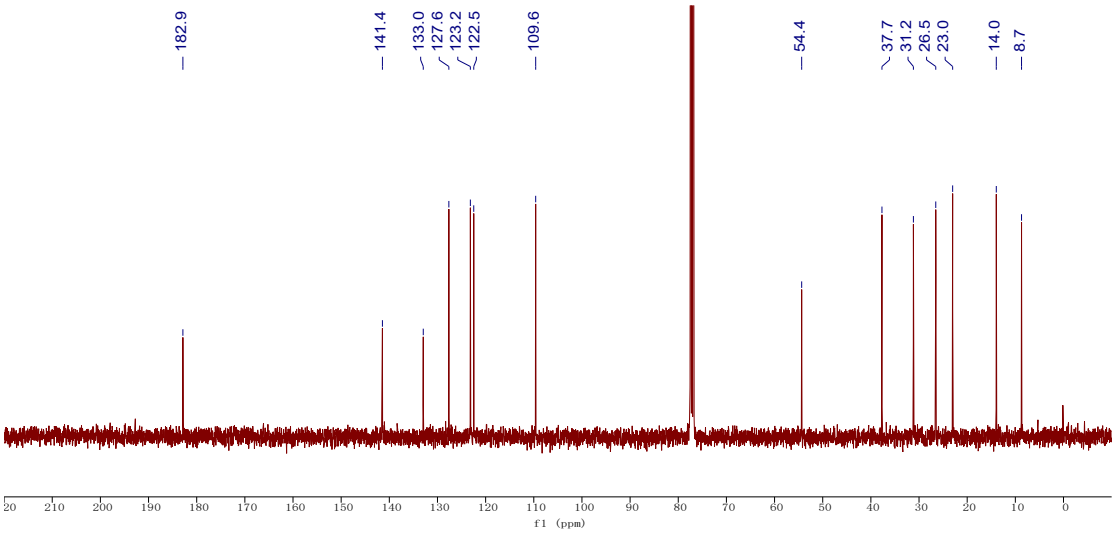
^{13}C NMR of compound **5** (101 MHz in $CDCl_3$)



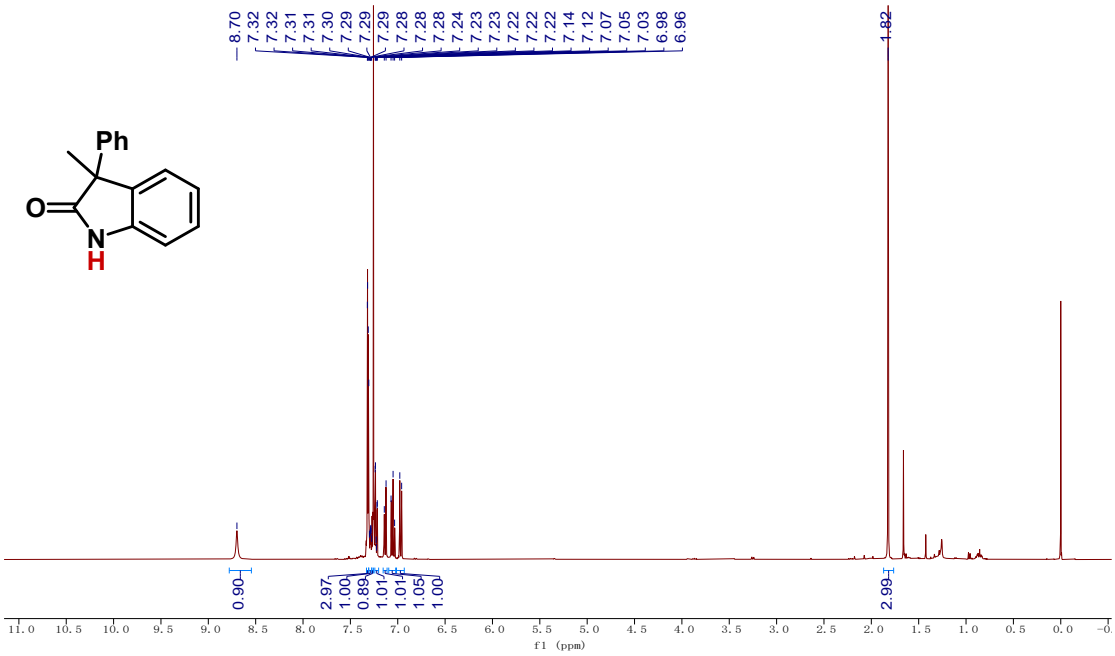
^{1}H NMR of compound **6** (400 MHz in $CDCl_3$)



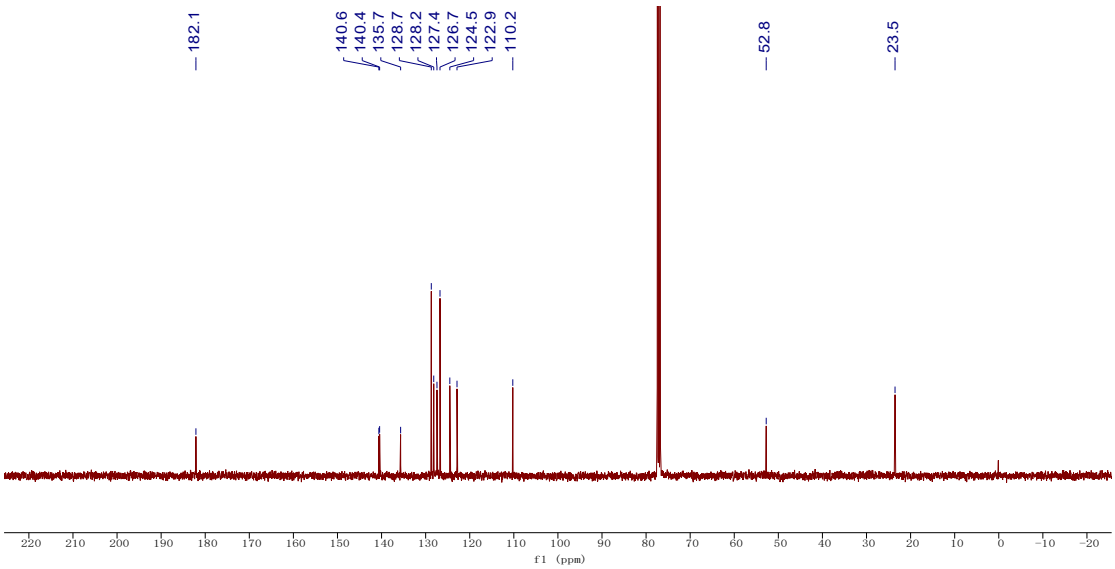
^{13}C NMR of compound **6** (101 MHz in $CDCl_3$)



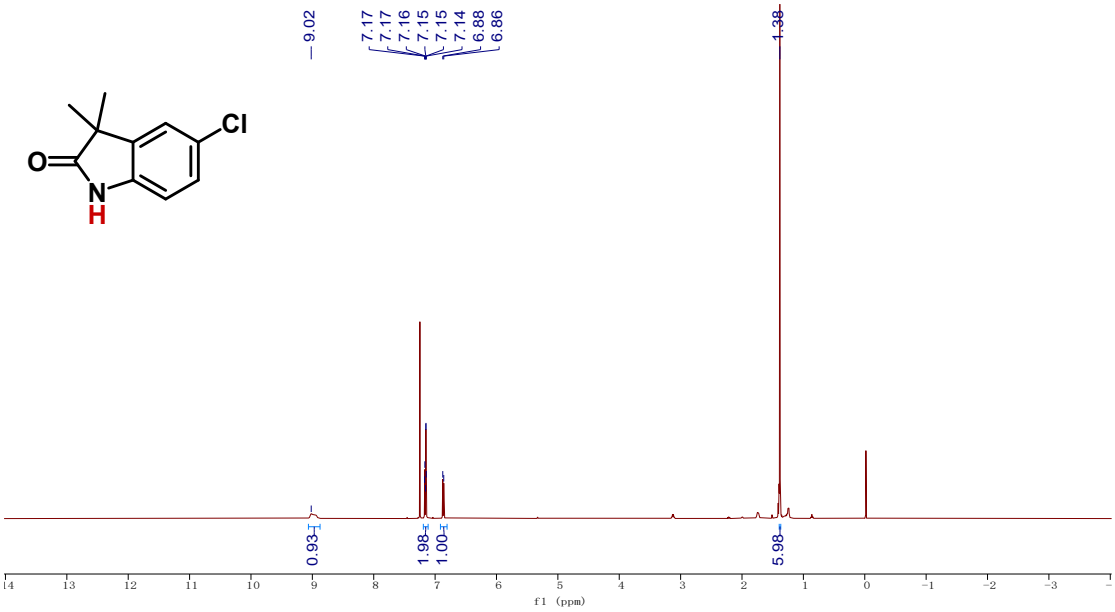
^{1}H NMR of compound **7** (400 MHz in $CDCl_3$)



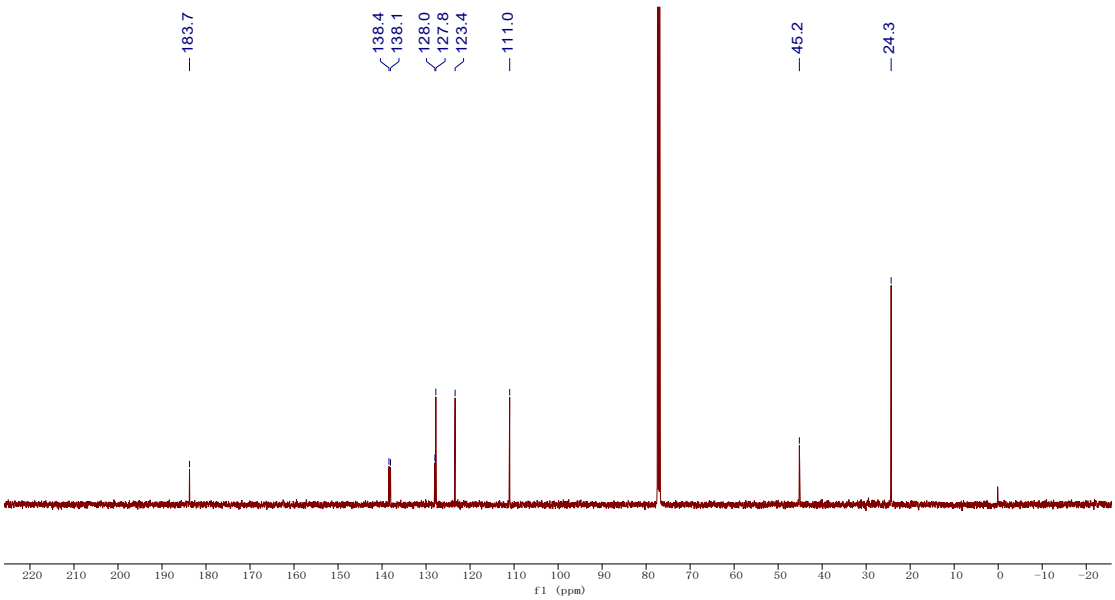
^{13}C NMR of compound **7** (101 MHz in $CDCl_3$)



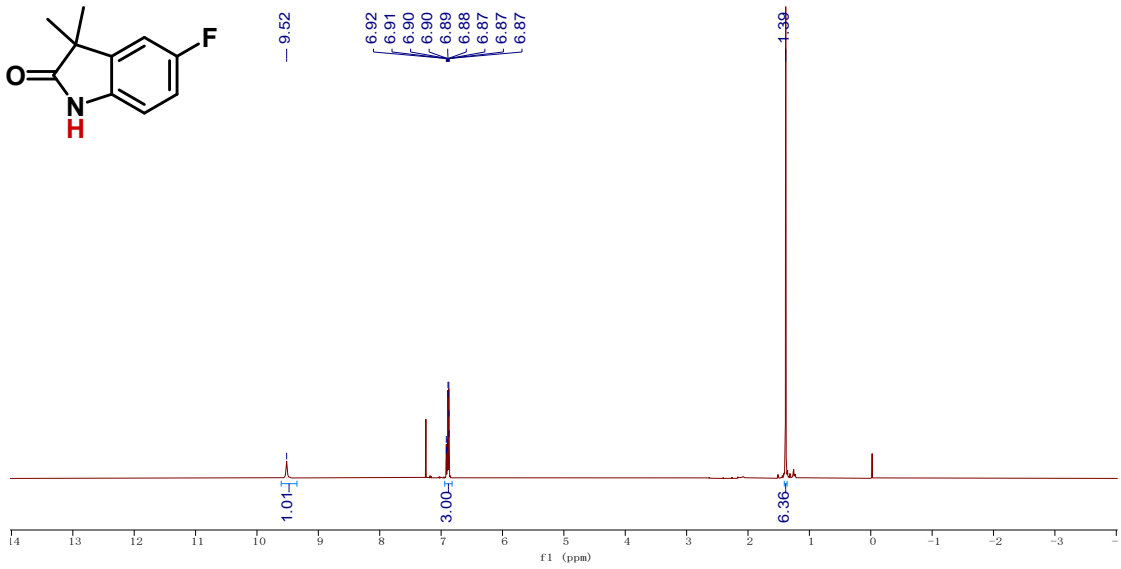
^{1}H NMR of compound **8** (500 MHz in $CDCl_3$)



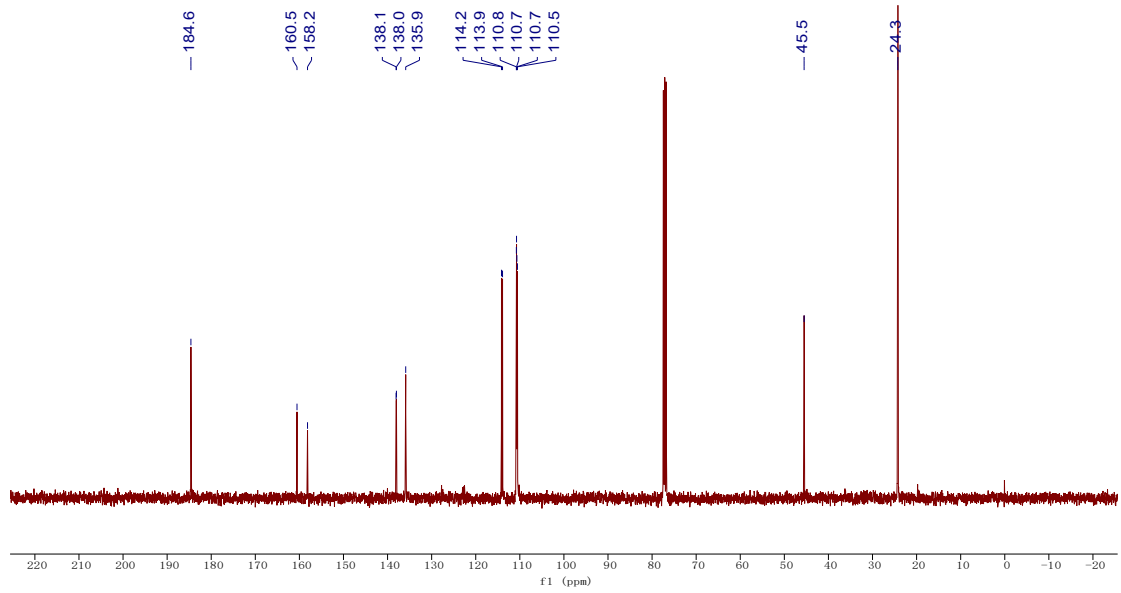
^{13}C NMR of compound **8** (126 MHz in $CDCl_3$)



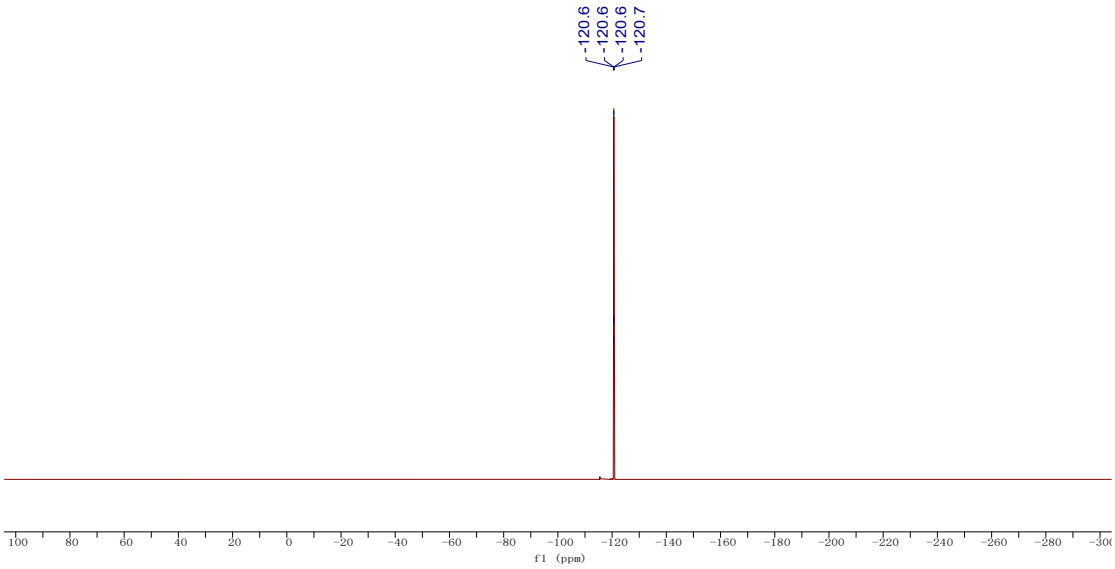
^{1}H NMR of compound **9** (500 MHz in $CDCl_3$)



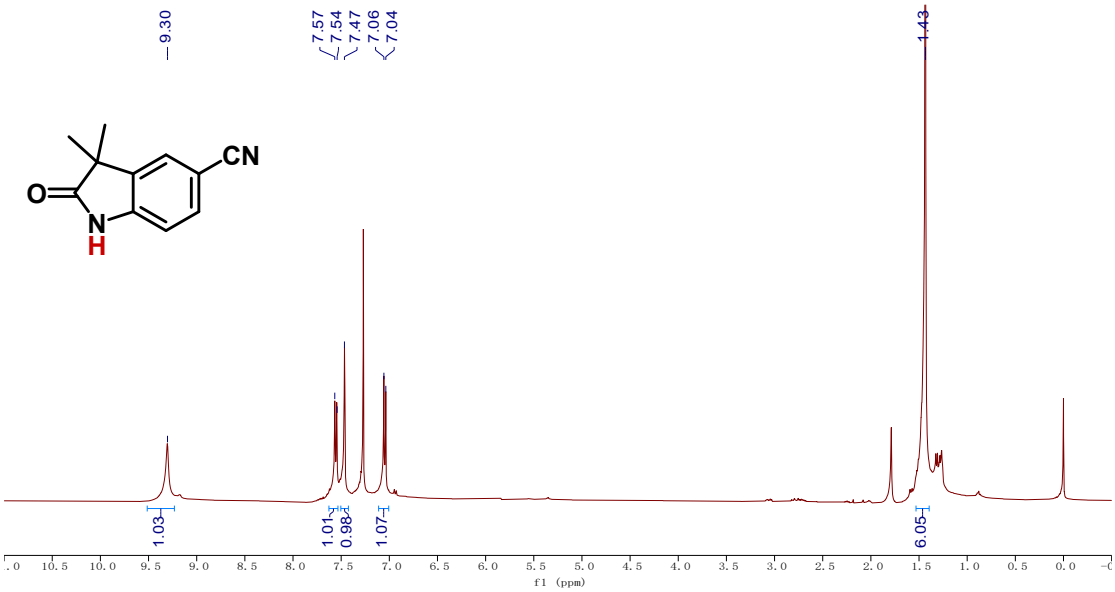
^{13}C NMR of compound **9** (126 MHz in $CDCl_3$)



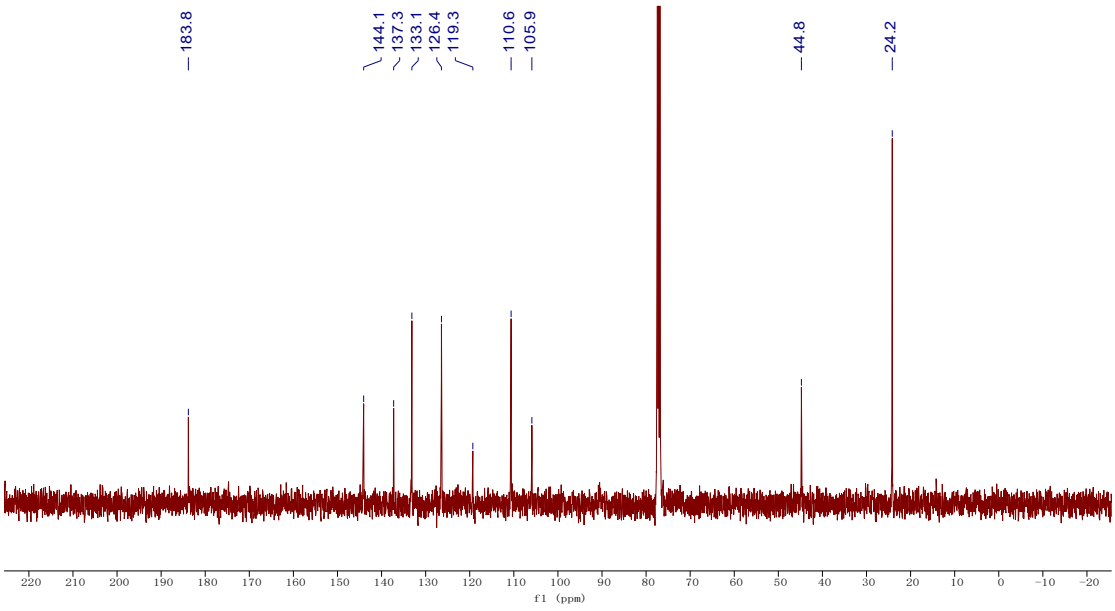
^{19}F NMR of compound **9** (471 MHz in $CDCl_3$)



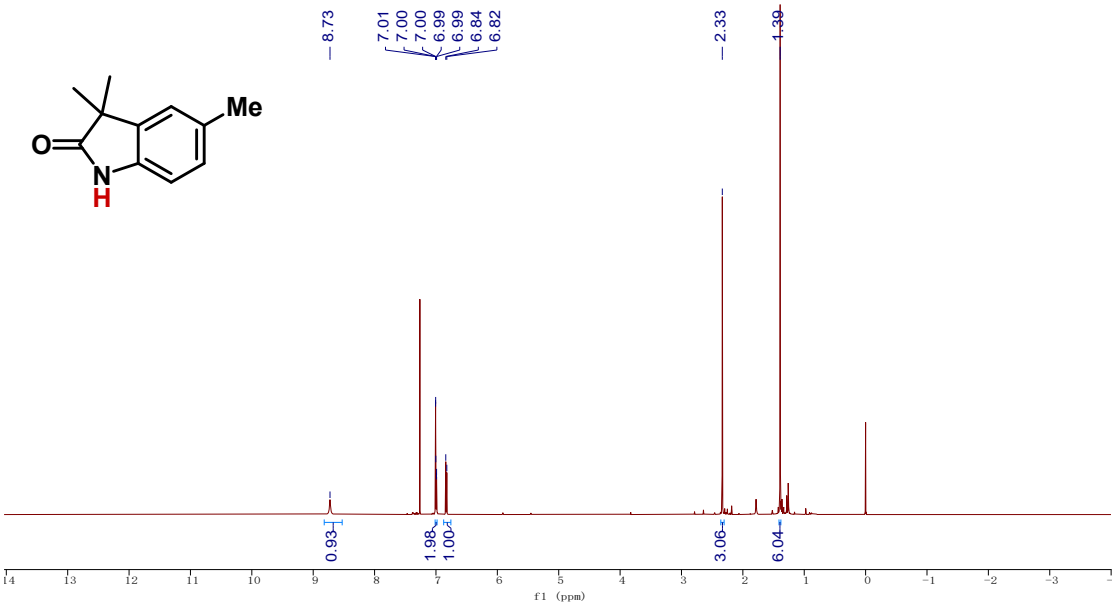
^{1}H NMR of compound **10**(400 MHz in $CDCl_3$)



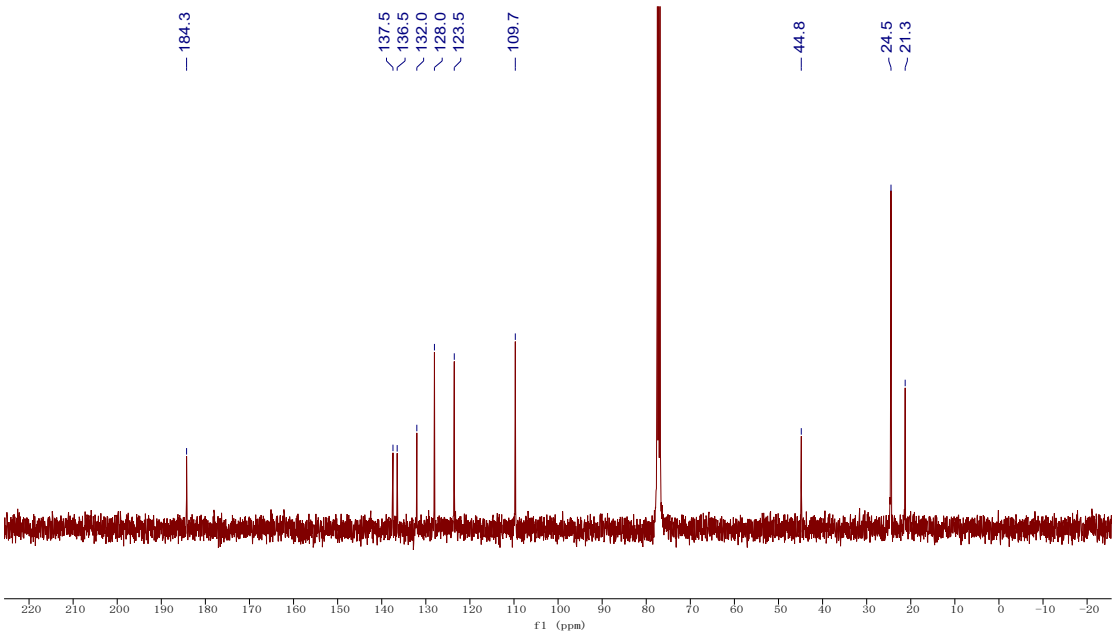
^{13}C NMR of compound **10** (101 MHz in $CDCl_3$)



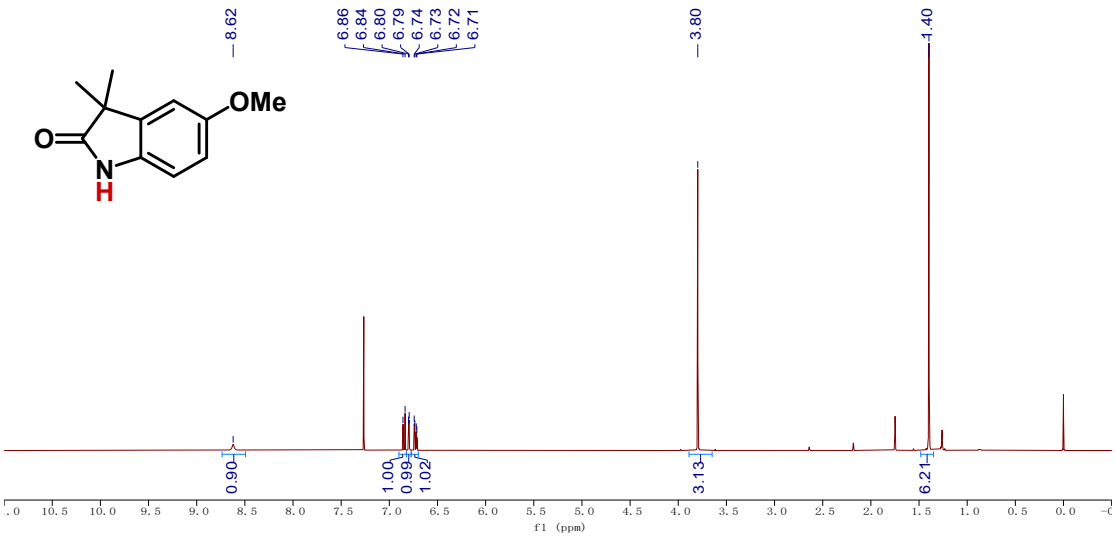
^{1}H NMR of compound **11** (500 MHz in $CDCl_3$)



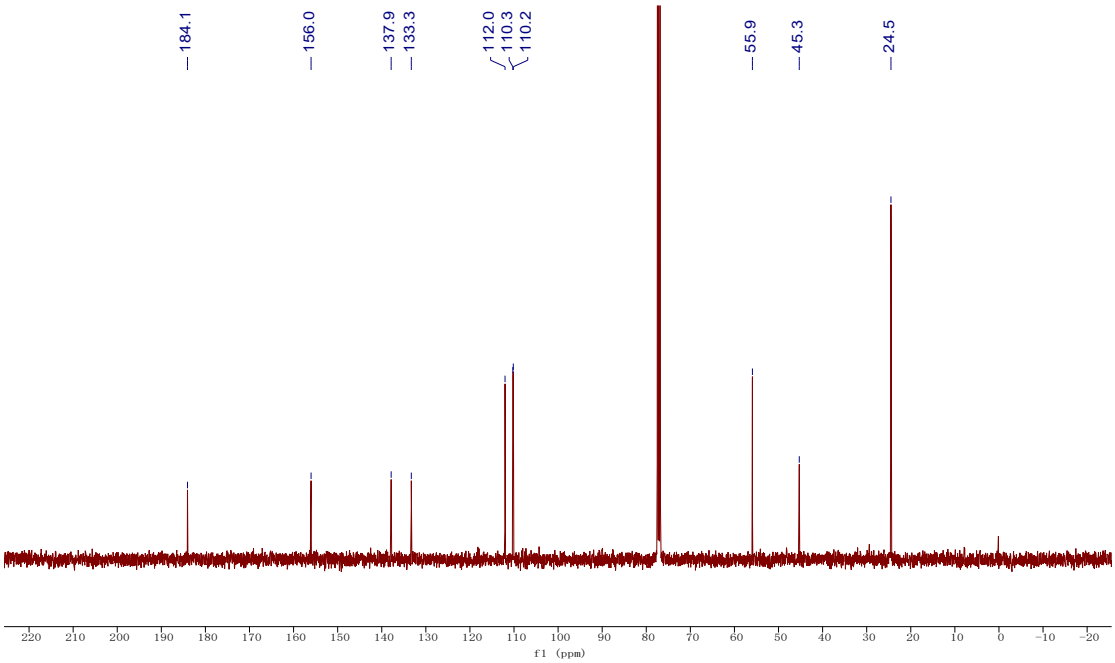
^{13}C NMR of compound **11** (101 MHz in $CDCl_3$)



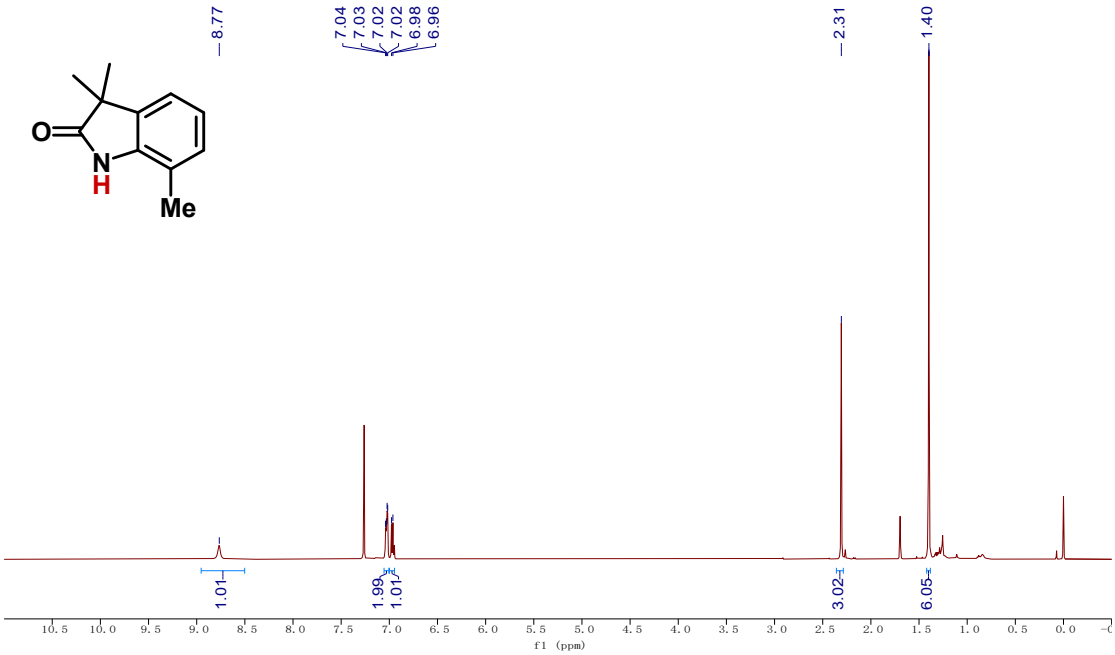
^{1}H NMR of compound **12** (400 MHz in $CDCl_3$)



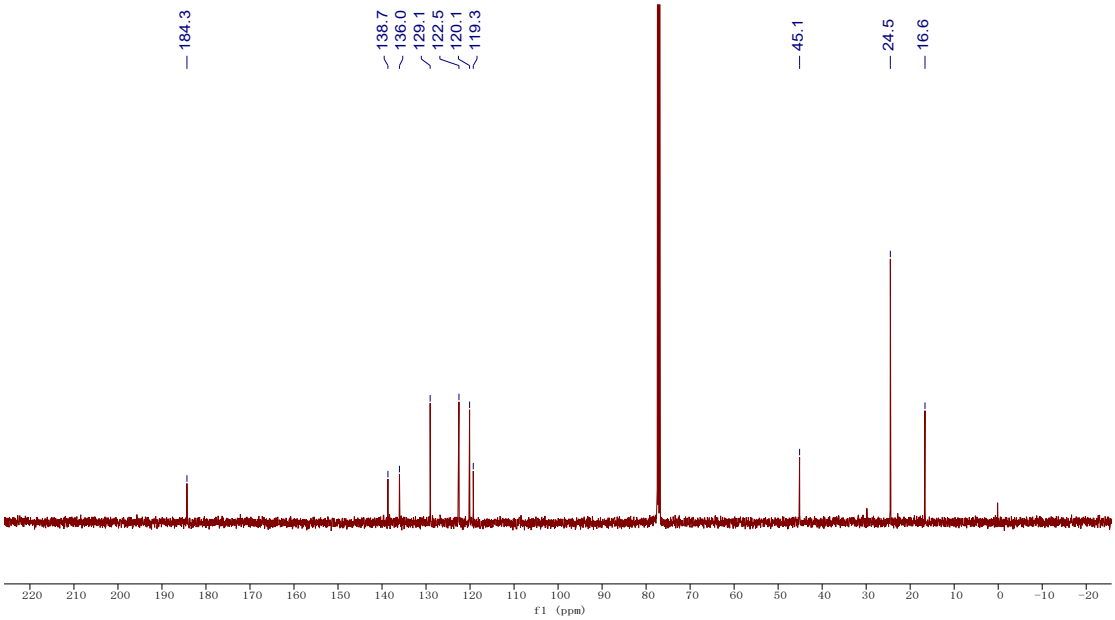
^{13}C NMR of compound **12** (101 MHz in $CDCl_3$)



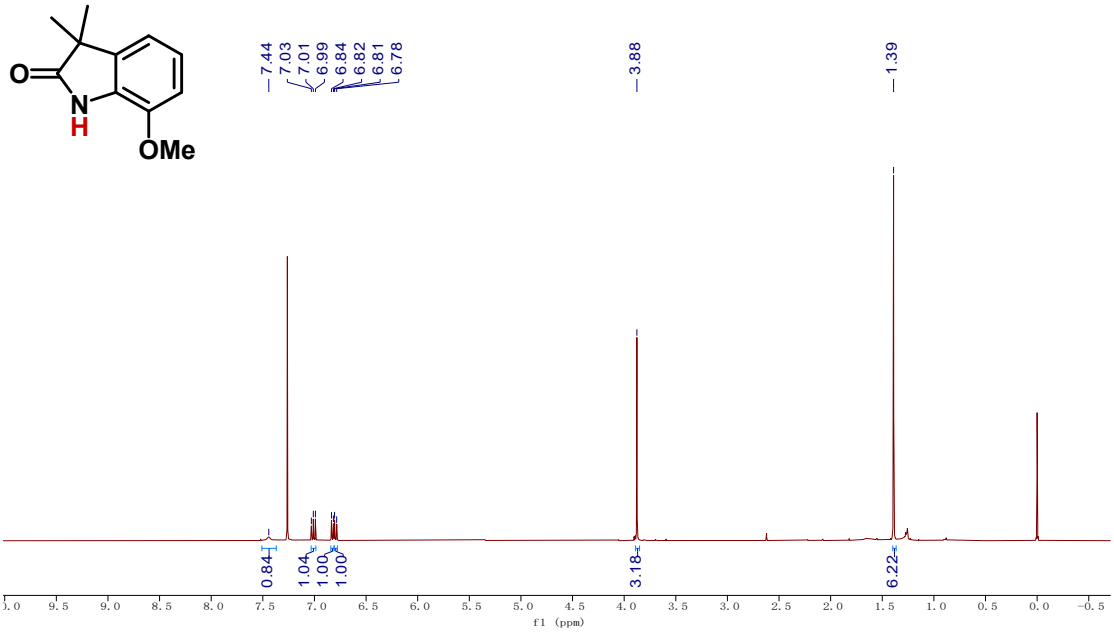
^{1}H NMR of compound **13** (500 MHz in $CDCl_3$)



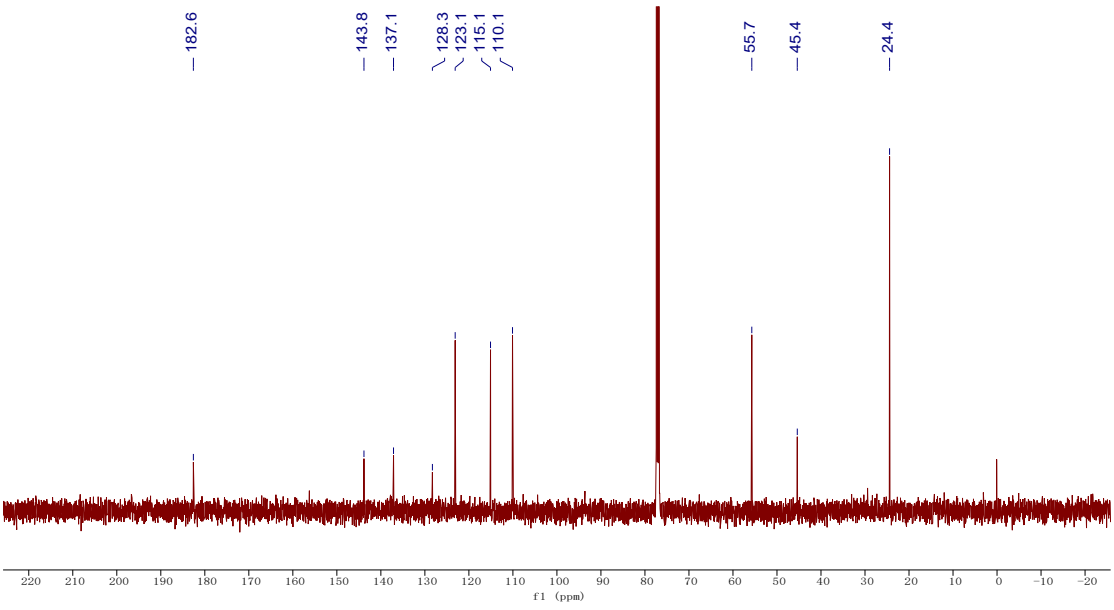
^{13}C NMR of compound **13** (126 MHz in $CDCl_3$)



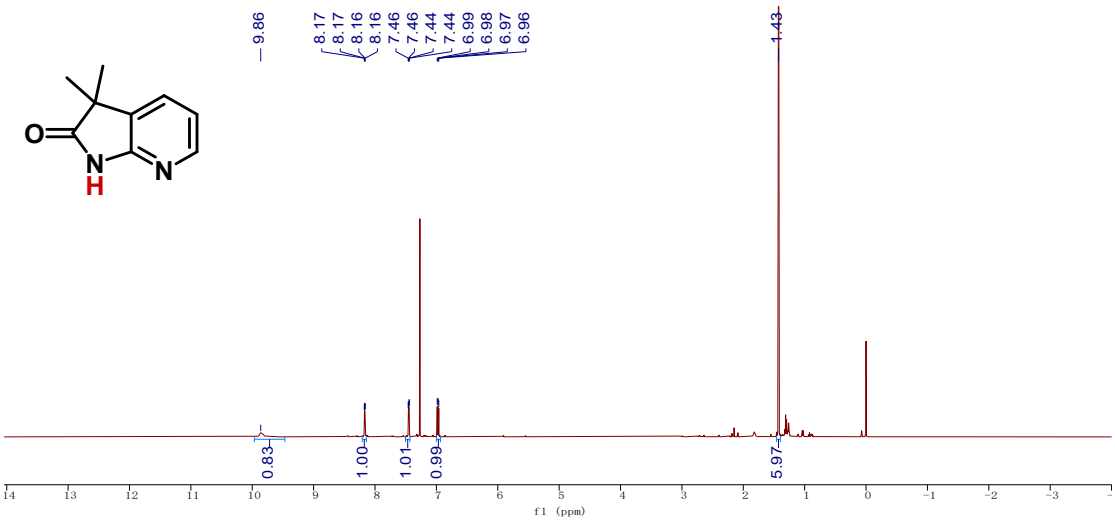
^{1}H NMR of compound **14** (400 MHz in $CDCl_3$)



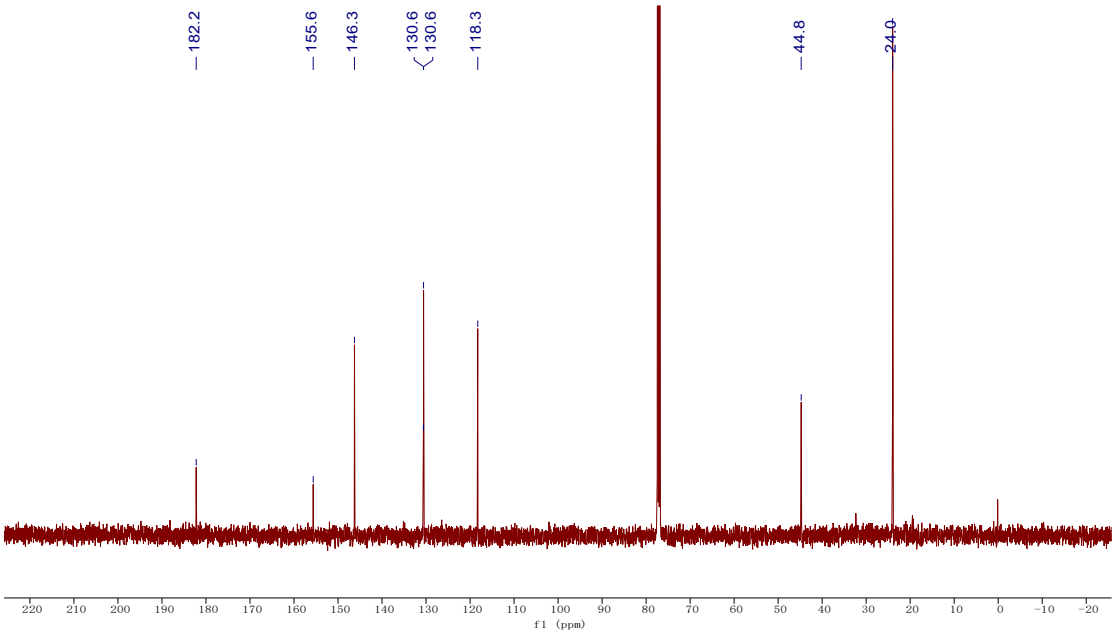
^{13}C NMR of compound **14** (126 MHz in $CDCl_3$)



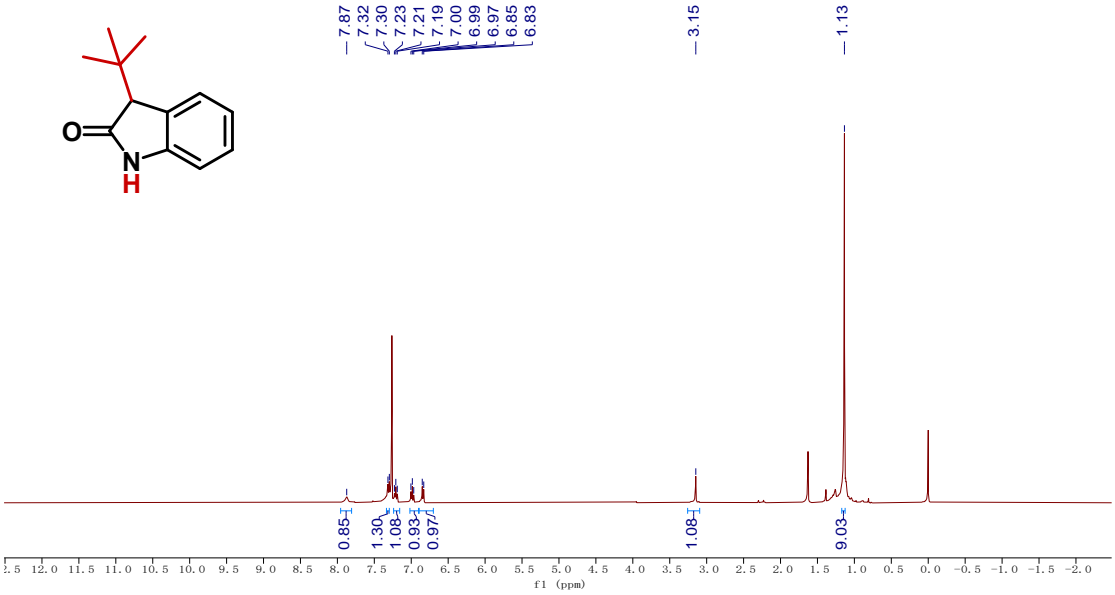
^{1}H NMR of compound **15** (500 MHz in $CDCl_3$)



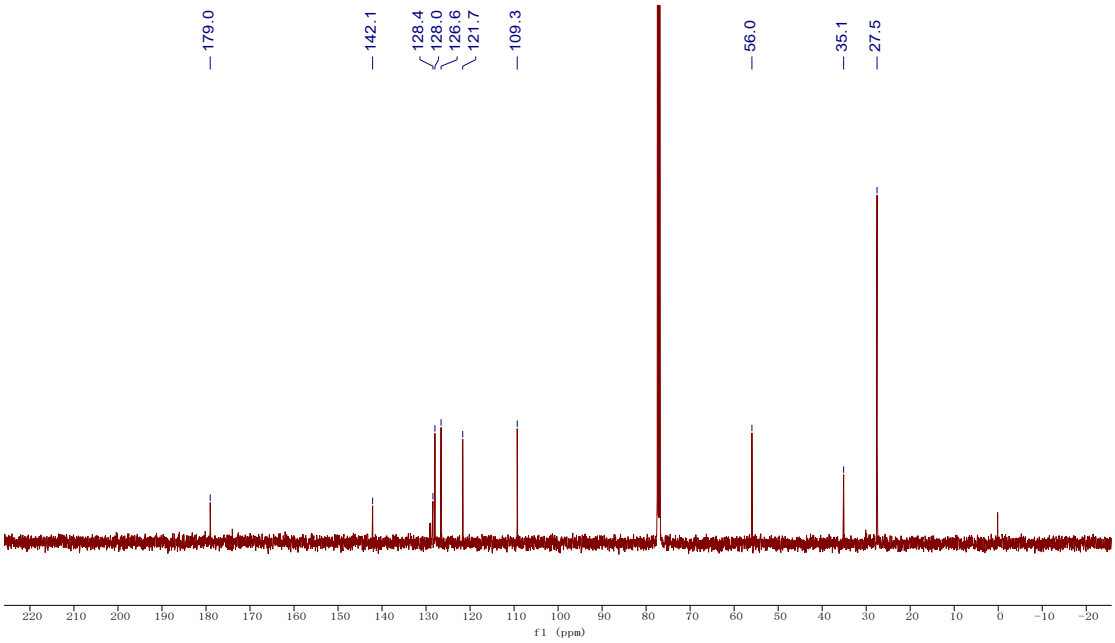
^{13}C NMR of compound **15** (126 MHz in $CDCl_3$)



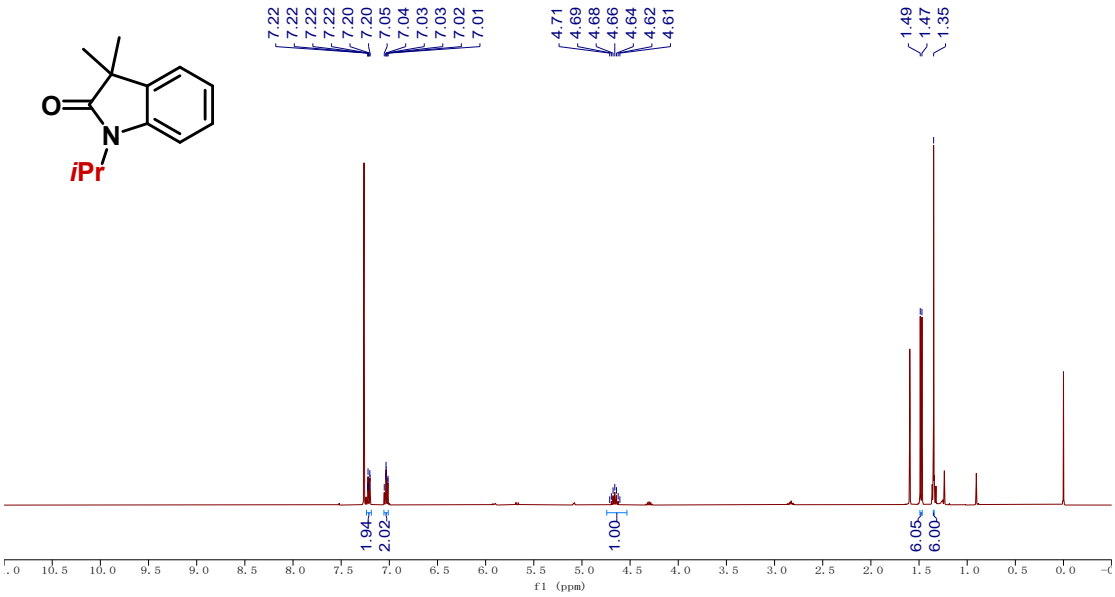
^{1}H NMR of compound **16** (400 MHz in $CDCl_3$)



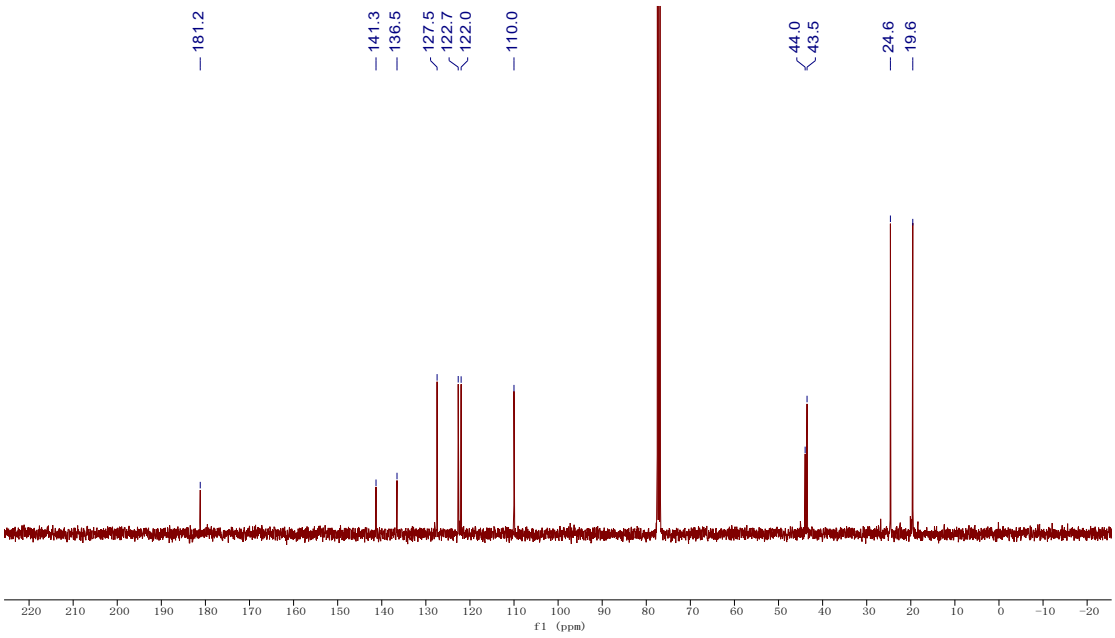
^{13}C NMR of compound **16** (126 MHz in $CDCl_3$)



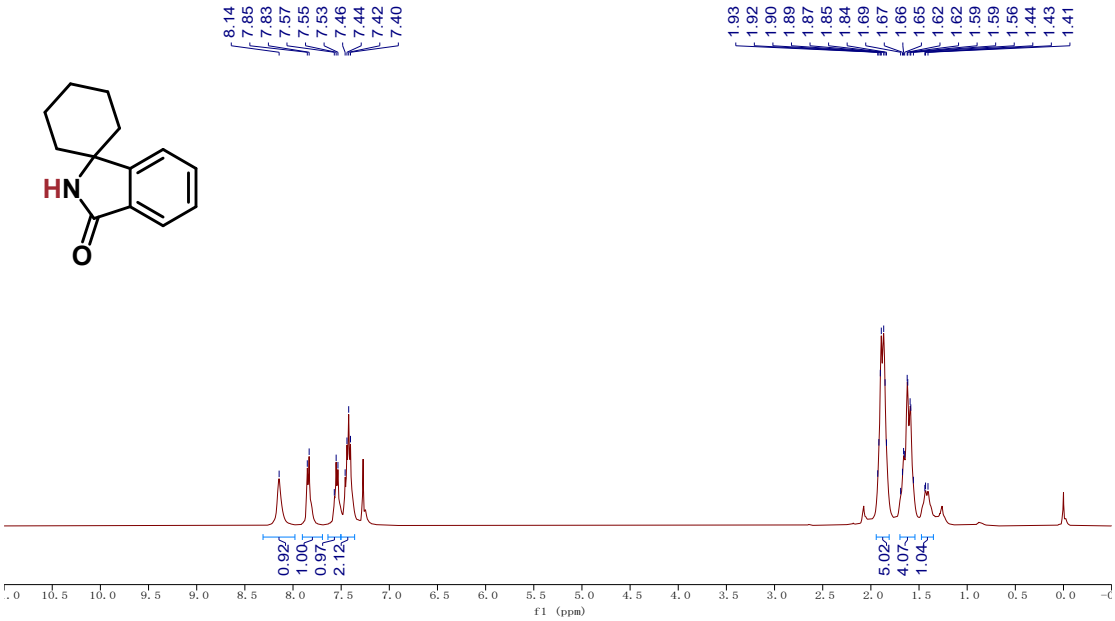
^{1}H NMR of compound **17** (400 MHz in $CDCl_3$)



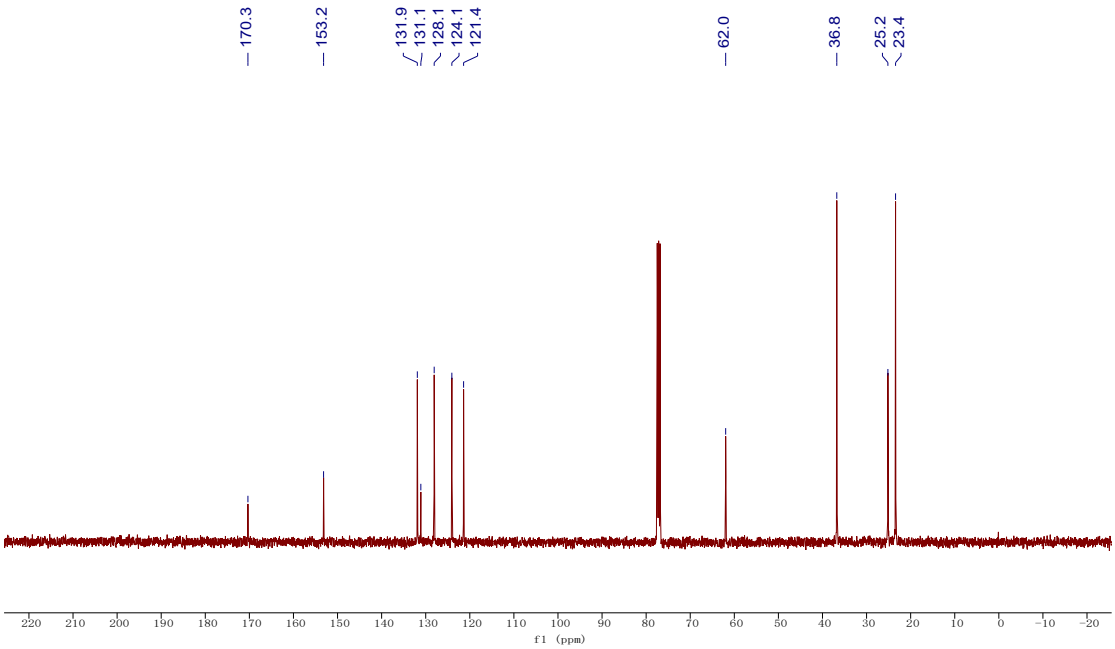
^{13}C NMR of compound **17** (101 MHz in $CDCl_3$)



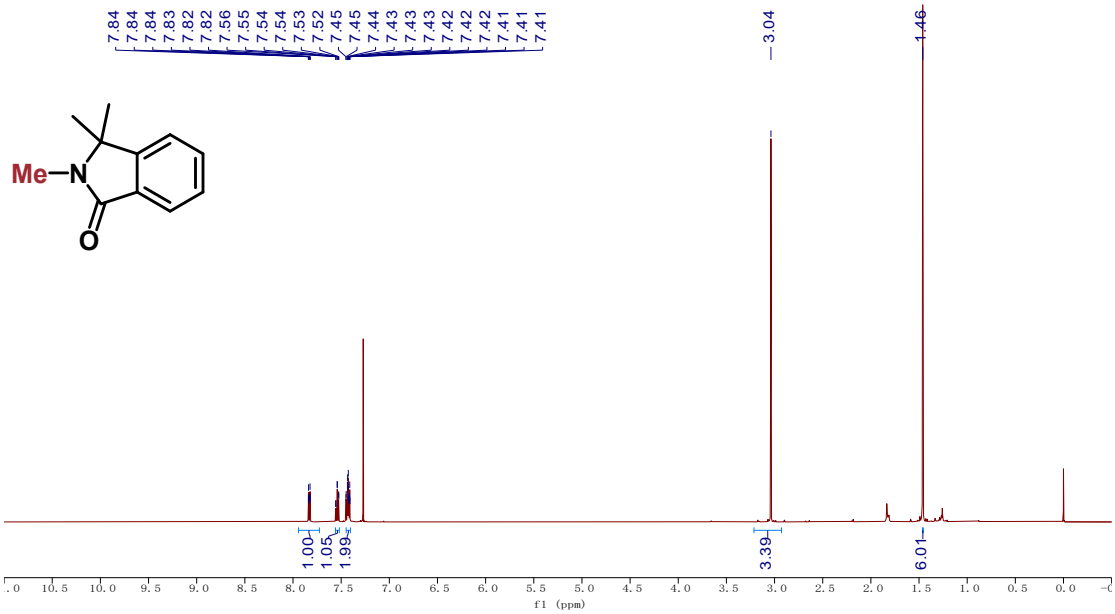
^{1}H NMR of compound **18** (400 MHz in $CDCl_3$)



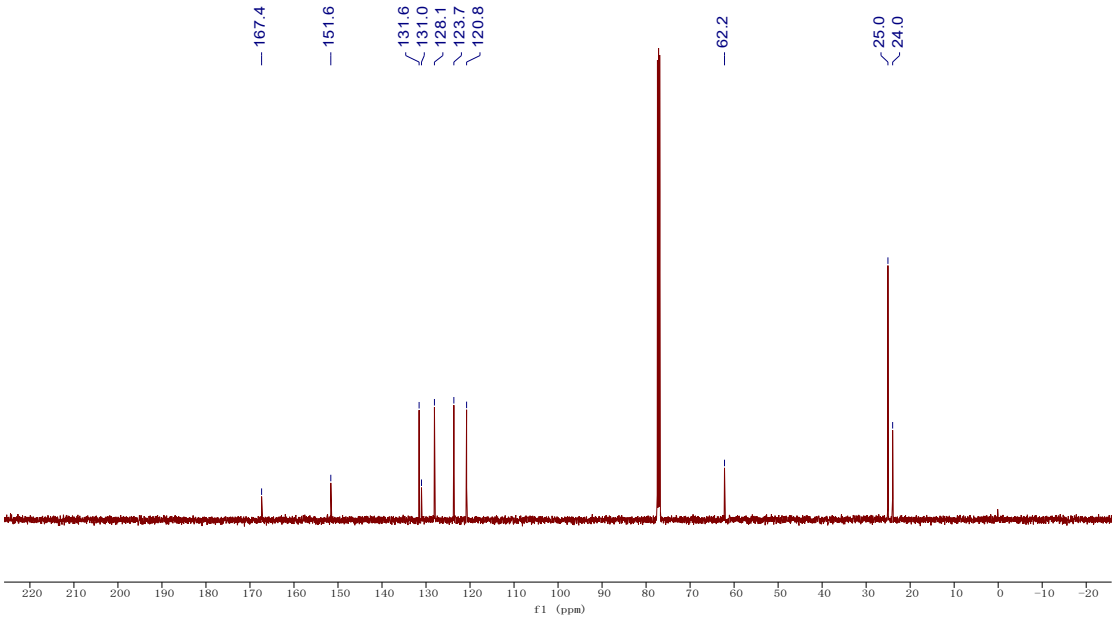
^{13}C NMR of compound **18** (101 MHz in $CDCl_3$)



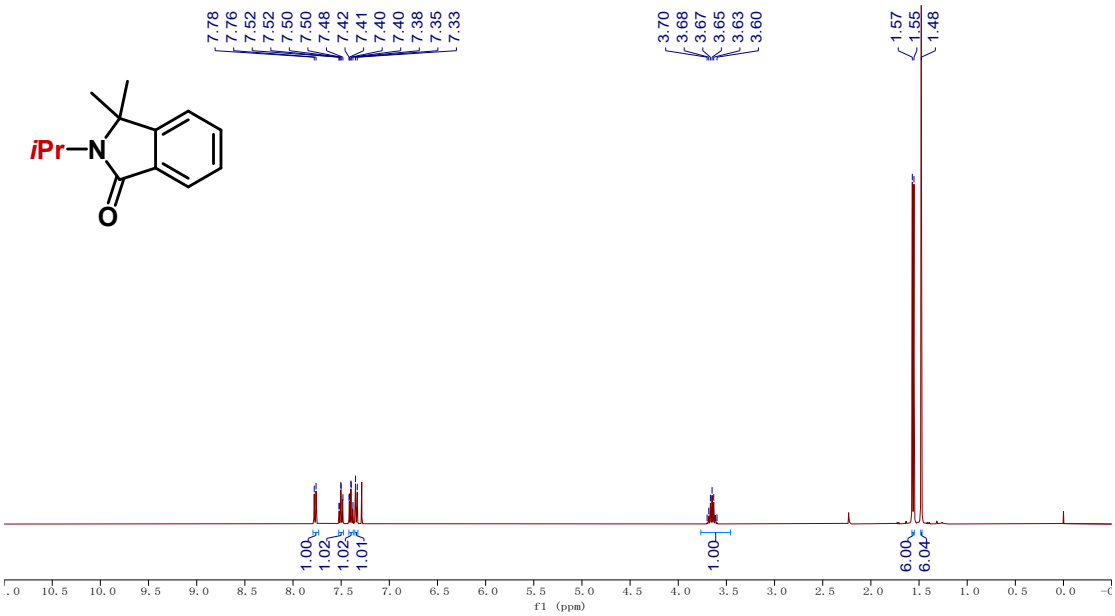
^{1}H NMR of compound **19** (500 MHz in $CDCl_3$)



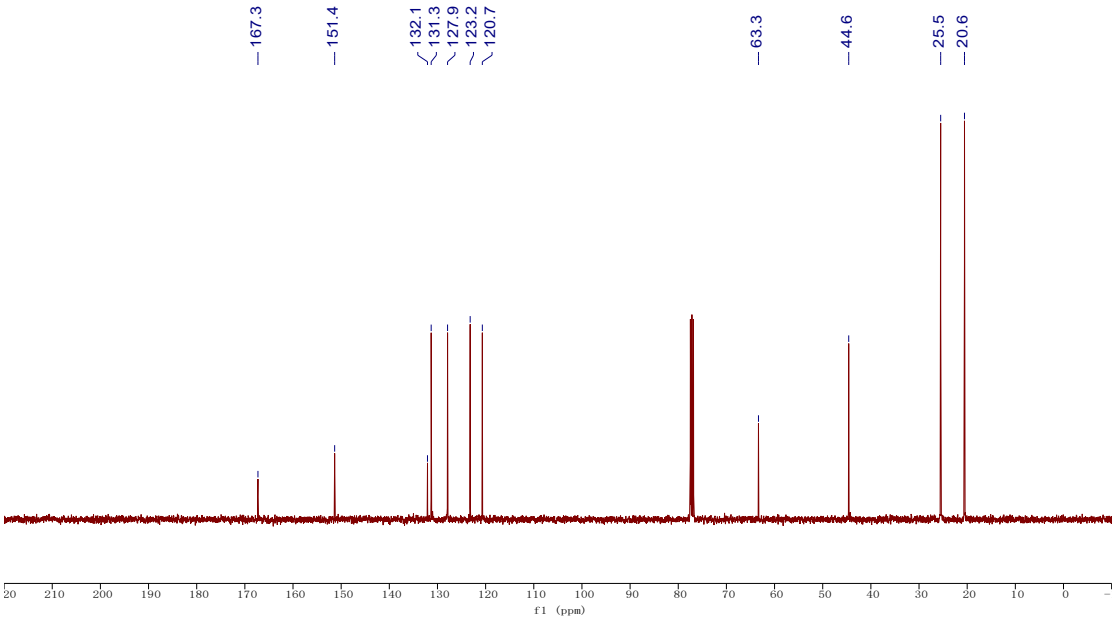
^{13}C NMR of compound **19** (126 MHz in $CDCl_3$)



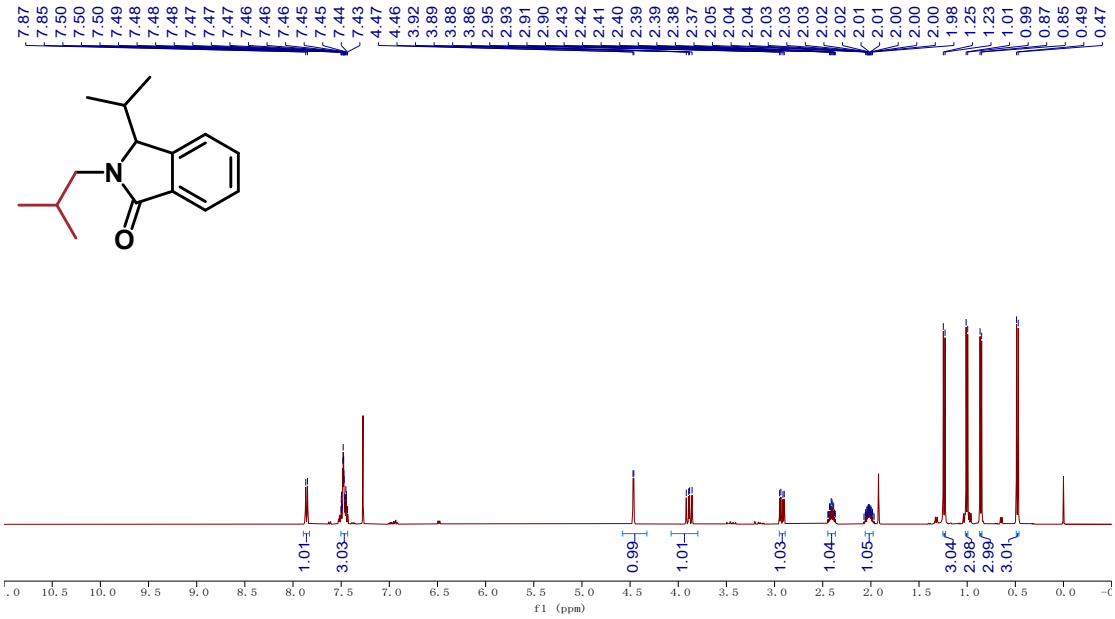
^{1}H NMR of compound **20** (400 MHz in $CDCl_3$)



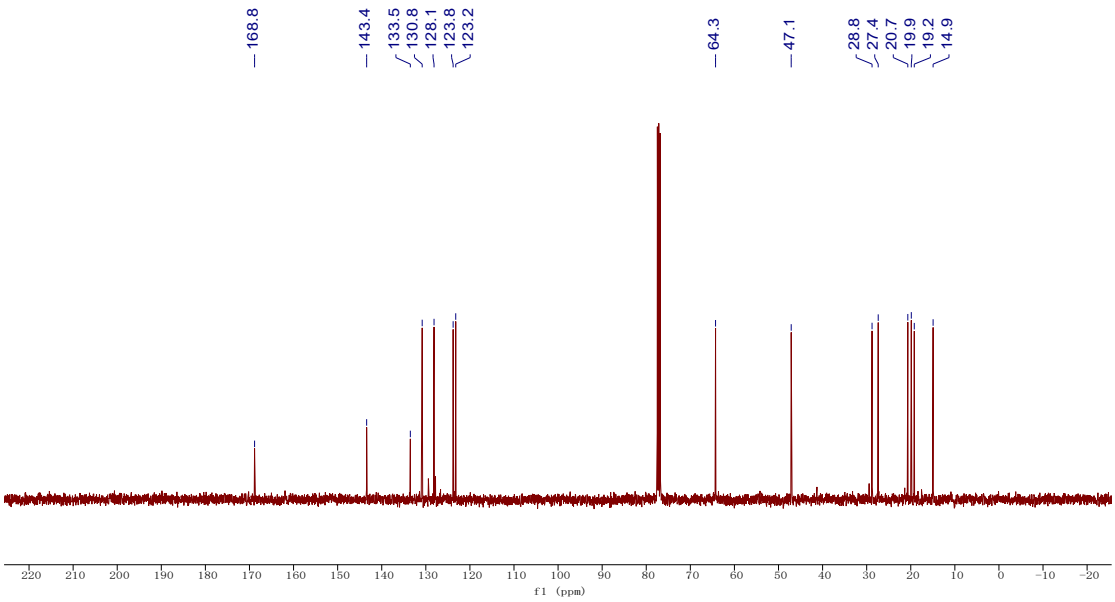
^{13}C NMR of compound **20** (101 MHz in $CDCl_3$)



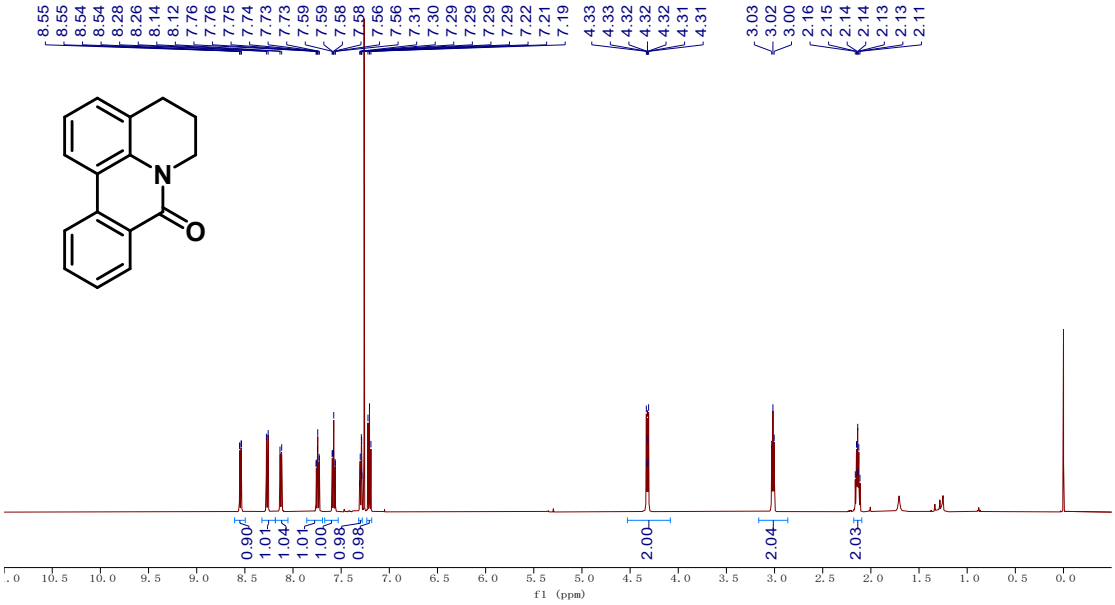
^{1}H NMR of compound **21** (400 MHz in $CDCl_3$)



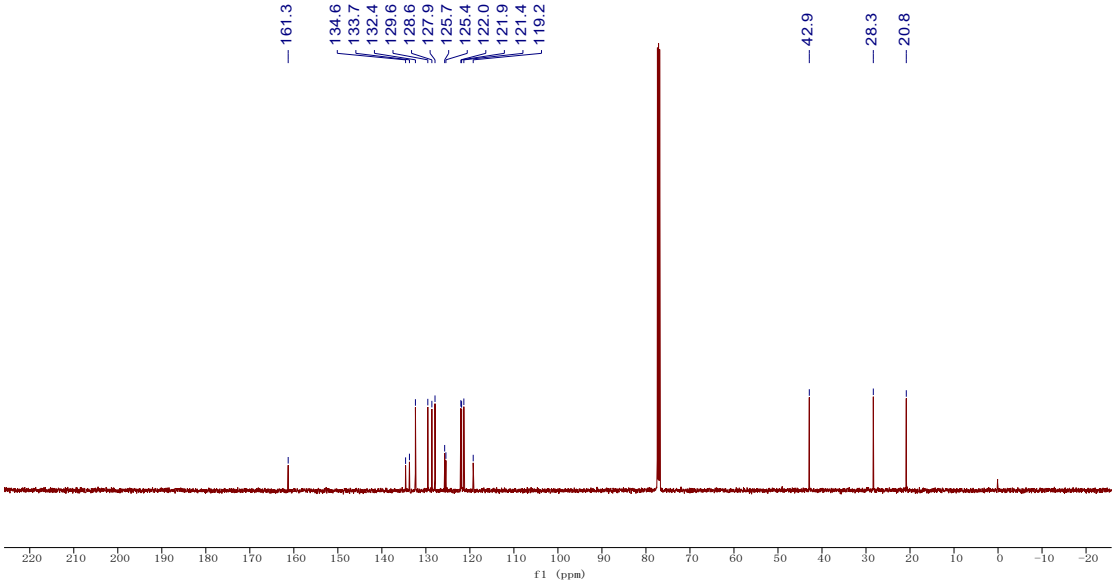
^{13}C NMR of compound **21** (101 MHz in $CDCl_3$)



^{1}H NMR of compound **22**(500 MHz in $CDCl_3$)



^{13}C NMR of compound **3e** (126 MHz in $CDCl_3$)



7. Computational Details

All calculations were carried out by using Gaussian 16 program.[11] The structures were optimized at B3LYP[12]-D3(BJ)[13]/6-31G(d,p) level in toluene solvent with SMD[14] solvation model. To confirm that the minima have no imaginary frequency and the transition states have unique one imaginary frequency, harmonic frequency analysis calculations were performed at the same level. Using the optimized geometries, the energies were further refined by single-point energy calculations at B3LYP-D3(BJ)/6-311++G(d,p) level with SMD solvation model. A correction factor of 1.89 kcal/mol was employed for the standard state change from 1 atm to 1 M. The vertical excitation energies were calculated at TD[15]-B3LYP-D3(BJ)/6-311++G(d,p) level with the optimized geometries in the ground state. Selected structures were illustrated by using the CYLview[16] visualization software.

Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K for the Optimized Structures [BSI=6-31G(d,p), BSII=6-311++G(d,p)]

$PhCH_3$

B3LYP-D3BJ/BSI SCF energy in toluene:

-271.605318 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-271.671546 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-271.570993 a.u.

C	-1.200535	1.205388	0.002262
C	0.194797	1.202908	-0.009144
C	0.913785	0.000301	-0.012267
C	0.195165	-1.202688	-0.009145
C	-1.200032	-1.205665	0.002261
C	-1.903915	-0.000213	0.008445
H	-1.738408	2.149281	0.002119
H	0.735745	2.145928	-0.017207
H	0.736491	-2.145511	-0.017223
H	-1.737629	-2.149716	0.002117
H	-2.989964	-0.000449	0.014041
C	2.422349	0.000120	0.009371
H	2.802687	-0.013031	1.038908
H	2.830718	-0.879567	-0.497825
H	2.830676	0.892162	-0.475627

*t*BuOK

B3LYP-D3BJ/BSI SCF energy in toluene:

-833.022658 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-833.142665 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-833.050769 a.u.

C	1.617211	-1.437286	0.211126
C	1.074103	0.000016	0.000164
H	1.245286	-1.832654	1.164344
H	1.244234	-2.090059	-0.587627
H	2.714376	-1.497915	0.219259
C	1.615472	0.534423	-1.351219
C	1.621072	0.901740	1.137164
H	1.241615	1.552119	-1.517851
H	2.712581	0.557932	-1.409243
H	1.242755	-0.094451	-2.169025
H	2.718406	0.938114	1.182683
H	1.249949	1.925201	1.003288
H	1.250343	0.537840	2.103228
O	-0.292385	0.001035	0.002621
K	-2.570927	0.000118	0.000346

IM1

B3LYP-D3BJ/BSI SCF energy in toluene:

-1104.651761 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-1104.828735 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-1104.620562 a.u.

C	-3.232132	0.178018	1.276075
C	-2.189388	-0.751528	1.211225
C	-1.711453	-1.224853	-0.024116
C	-2.328615	-0.748122	-1.194361
C	-3.372113	0.181609	-1.135665
C	-3.823577	0.656241	0.101023
H	-3.584110	0.526734	2.243023
H	-1.729164	-1.111380	2.127772
H	-1.978672	-1.106186	-2.159160
H	-3.834156	0.532240	-2.054415
H	-4.636341	1.374810	0.149180
C	-0.498280	-2.110727	-0.093700
H	-0.430681	-2.767966	0.778812
H	-0.502966	-2.728644	-0.996888
H	0.399467	-1.463719	-0.112888
C	3.380746	-0.841647	-1.217983
C	2.937804	-0.014151	0.015200
H	2.793982	-1.765934	-1.276108
H	3.186931	-0.267498	-2.132043
H	4.445036	-1.114102	-1.202667
C	3.812533	1.264352	0.083295
C	3.201914	-0.852344	1.291970
H	3.519295	1.863129	0.954911
H	4.889353	1.059036	0.158131
H	3.643867	1.872460	-0.814297
H	4.258196	-1.122877	1.427003
H	2.877688	-0.286536	2.173969
H	2.615886	-1.778276	1.257916
O	1.610351	0.317460	-0.077578
K	-0.309529	1.648628	-0.093653

TS1

B3LYP-D3BJ/BSI SCF energy in toluene:

-1104.632431 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-1104.805562 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-1104.599295 a.u.

C	3.075160	0.037056	-1.204915
C	1.996406	-0.844705	-1.206575
C	1.391911	-1.309080	0.000138
C	1.996968	-0.844637	1.206543
C	3.075728	0.037120	1.204326
C	3.621360	0.512110	-0.000435
H	3.499677	0.359506	-2.153271
H	1.586933	-1.186491	-2.154427
H	1.587948	-1.186375	2.154608
H	3.500706	0.359602	2.152465
H	4.470243	1.188554	-0.000651
C	0.140205	-2.030196	0.000446
H	-0.049006	-2.612902	0.906027
H	-0.800037	-0.892897	0.000526
H	-0.049395	-2.613019	-0.904980
C	-3.216162	-0.731353	1.260390
C	-2.760091	0.025514	-0.000067
H	-2.789032	-1.739072	1.273356
H	-2.868671	-0.207602	2.157896
H	-4.307617	-0.821947	1.314302
C	-3.358054	1.440280	0.000006
C	-3.215298	-0.730851	-1.261142
H	-3.027730	1.990839	-0.889095
H	-4.454344	1.424293	-0.000548
H	-3.028602	1.990397	0.889699
H	-4.306742	-0.820909	-1.316150
H	-2.866659	-0.207044	-2.158169
H	-2.788636	-1.738774	-1.273950
O	-1.356829	0.154207	0.000446
K	0.581936	1.690139	0.000343

17-S

B3LYP-D3BJ/BSI SCF energy in toluene:

-1096.513931 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-1096.705402 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-1096.460219 a.u.

C	2.745381	0.330156	-1.815252
C	1.379643	0.514693	-1.610664
C	0.806472	0.338983	-0.345595
C	1.650016	-0.024267	0.717001
C	3.015941	-0.222046	0.522530
C	3.562599	-0.040787	-0.747299
H	3.167147	0.469574	-2.805347
H	0.729311	0.796345	-2.431965
H	3.639972	-0.510472	1.360794
H	4.626912	-0.192040	-0.896572
Cl	0.980623	-0.267739	2.321187
N	-0.584309	0.583356	-0.155429
C	-1.516906	-0.429505	-0.101882
O	-2.713550	-0.194556	0.053940
C	-1.025591	-1.864066	-0.317068
H	0.033610	-1.940749	-0.062330
C	-1.821288	-2.824081	0.569998
H	-2.890338	-2.741104	0.359530
H	-1.505643	-3.856828	0.389980
H	-1.669097	-2.601442	1.630725
C	-1.188084	-2.207007	-1.808446
H	-0.580860	-1.551428	-2.440650
H	-0.878415	-3.239802	-1.997955
H	-2.234548	-2.101369	-2.111915
C	-1.002329	2.014314	-0.069721
C	-1.640781	2.342934	1.282323
C	-1.887631	2.414331	-1.252829
H	-0.064052	2.571344	-0.143434
H	-0.972810	2.068363	2.102988
H	-1.834130	3.419339	1.342929
H	-2.583686	1.808827	1.403627
H	-1.390089	2.202171	-2.204764
H	-2.834358	1.873214	-1.225307
H	-2.095612	3.488671	-1.212604

IM2 (**I**)

B3LYP-D3BJ/BSI SCF energy in toluene:

-2201.175146 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-2201.535067 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-2201.063805 a.u.

C	-4.442992	2.101493	-0.417370
C	-3.563319	2.699526	0.469560
C	-2.152579	2.851061	0.181841
C	-1.762232	2.377826	-1.128785
C	-2.654439	1.775491	-1.996205
C	-4.014029	1.589464	-1.659737
H	-5.492393	2.017126	-0.138856
H	-3.937413	3.078132	1.420156
H	-0.721895	2.491789	-1.425371
H	-2.292582	1.430917	-2.963761
H	-4.719663	1.176266	-2.373435
C	-1.231773	3.315551	1.129126
H	-0.217311	3.557132	0.819824
H	-3.482402	-0.160058	-0.642472
H	-1.591312	3.824531	2.022026
C	-3.525779	-2.609869	-1.625680
C	-3.869800	-2.070984	-0.232561
H	-3.799913	-1.881133	-2.396018
H	-2.452317	-2.802851	-1.706018
H	-4.062368	-3.541667	-1.833703
C	-3.378791	-3.023976	0.856511
C	-5.374601	-1.813205	-0.101802
H	-3.633323	-2.636810	1.849679
H	-3.838528	-4.011299	0.750102
H	-2.292015	-3.141142	0.797803
H	-5.946954	-2.739284	-0.219923
H	-5.604272	-1.386590	0.879826
H	-5.712265	-1.105955	-0.866469
O	-3.158321	-0.842460	-0.012532
K	-1.665104	0.394545	1.705943
C	5.667550	-0.830801	-1.176944
C	4.430860	-1.302032	-0.741263
C	3.348341	-0.432264	-0.576123
C	3.533089	0.930066	-0.863709
C	4.769675	1.412095	-1.289620
C	5.835505	0.527226	-1.448927
H	6.496254	-1.520775	-1.297571
H	4.283530	-2.354106	-0.520446
H	4.888873	2.469591	-1.496596
H	6.795801	0.904829	-1.784986

Cl	2.206786	2.056039	-0.649666
N	2.076465	-0.948718	-0.181389
C	1.576357	-0.767826	1.074624
O	0.430479	-1.139431	1.369595
C	2.485168	-0.161231	2.144707
H	3.248617	0.460049	1.673888
C	1.671265	0.709087	3.106733
H	0.923633	0.108387	3.634564
H	2.331711	1.156085	3.856113
H	1.164046	1.525197	2.580305
C	3.193027	-1.313983	2.880056
H	3.817056	-1.900250	2.198418
H	3.836117	-0.917814	3.671907
H	2.459462	-1.985938	3.337432
C	1.286495	-1.646233	-1.246791
C	0.024214	-0.875974	-1.643668
C	0.999492	-3.100060	-0.868418
H	1.962362	-1.646627	-2.105622
H	0.241457	0.181921	-1.800213
H	-0.361298	-1.282931	-2.584649
H	-0.764235	-0.964969	-0.897129
H	1.924036	-3.636910	-0.632493
H	0.335398	-3.152008	-0.004408
H	0.518983	-3.608380	-1.710588

II

B3LYP-D3BJ/BSI SCF energy in toluene:

-1929.573538 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-1929.872846 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-1929.515230 a.u.

C	3.916085	2.259474	0.482889
C	3.538882	0.920702	0.389172
C	2.235871	0.567699	0.025139
C	1.297822	1.589481	-0.218444
C	1.671901	2.929164	-0.118287
C	2.983165	3.262449	0.219969
H	4.931728	2.515158	0.766799
H	4.249283	0.131689	0.606497
H	0.932396	3.701526	-0.299294
H	3.267709	4.307608	0.291007
Cl	-0.382945	1.176346	-0.515673
N	1.880912	-0.807942	-0.144031
C	0.993124	-1.441754	0.686699
O	0.502796	-2.541680	0.381407
C	0.666795	-0.807161	2.034857
H	0.874444	0.263178	1.997114
C	-0.811885	-1.015372	2.384119
H	-1.034858	-2.083545	2.476540
H	-1.031523	-0.543357	3.347264
H	-1.480930	-0.572464	1.635263
C	1.599749	-1.437149	3.085680
H	2.652974	-1.251782	2.850234
H	1.392589	-1.012562	4.072768
H	1.444786	-2.519552	3.138393
C	-3.743852	1.651868	1.144622
C	-3.971217	0.768509	-0.108256
H	-3.592813	1.014650	2.023982
H	-2.839873	2.256168	1.012840
H	-4.583186	2.329452	1.353613
C	-4.205416	1.696092	-1.326573
C	-5.254045	-0.072594	0.119385
H	-4.365215	1.088249	-2.225740
H	-5.069886	2.363832	-1.207169
H	-3.316905	2.314633	-1.497413
H	-6.149047	0.533028	0.318849
H	-5.453032	-0.689575	-0.766315
H	-5.100359	-0.746229	0.971365
O	-2.894892	-0.055613	-0.326629
K	-1.801227	-2.085021	-0.838476
C	2.273854	-1.477911	-1.415758
C	3.790350	-1.635031	-1.530350
C	1.685984	-0.767849	-2.636990
H	1.828152	-2.469244	-1.332069
H	4.204162	-2.119079	-0.640645
H	4.024309	-2.261786	-2.396864
H	4.291654	-0.673379	-1.672804
H	0.597017	-0.689763	-2.578087
H	2.084808	0.245784	-2.742266
H	1.942380	-1.324900	-3.543632

IM3

B3LYP-D3BJ/BSI SCF energy in toluene:

-518.269038 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-518.405681 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-518.242331 a.u.

C	-3.358733	0.588565	0.029090
C	-2.136889	1.255330	0.090924
C	-0.922076	0.544731	-0.012969
C	-1.045676	-0.825871	-0.175682
C	-2.224825	-1.526608	-0.242201
C	-3.419724	-0.797172	-0.137060
H	-4.276116	1.163196	0.111823
H	-2.107509	2.334854	0.222558
H	-2.237794	-2.605284	-0.371833
H	-4.376033	-1.308835	-0.184943
N	0.284622	1.249270	0.054881
H	0.202887	2.253188	0.165392
C	1.604966	0.845067	-0.038812
O	2.484358	1.697717	0.013721
C	1.907694	-0.642053	-0.152605
H	1.107142	-1.119931	-0.732104
C	3.245944	-0.859529	-0.859615
H	4.053768	-0.365899	-0.313429
H	3.468247	-1.929317	-0.923460
H	3.232635	-0.451691	-1.874911
C	1.904943	-1.257273	1.259944
H	0.941162	-1.124163	1.759769
H	2.110048	-2.330798	1.203216
H	2.680607	-0.793076	1.877902

TS2

B3LYP-D3BJ/BSI SCF energy in toluene:

-518.261352 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-518.398184 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-518.240169 a.u.

C	-3.308904	0.493958	-0.000057
C	-2.151249	1.273976	-0.000121
C	-0.899100	0.643793	0.000017
C	-0.850365	-0.747173	0.000223
C	-1.985820	-1.532623	0.000282
C	-3.239054	-0.901060	0.000139
H	-4.277071	0.985643	-0.000166
H	-2.215136	2.359339	-0.000283
H	-1.916668	-2.617231	0.000450
H	-4.148162	-1.495124	0.000186
N	0.291842	1.388598	-0.000059
H	0.224567	2.399268	-0.000010
C	1.577577	0.896925	0.000147
O	2.543167	1.653237	0.000337
C	1.738075	-0.614708	-0.000020
H	0.552578	-1.037477	0.000276
C	2.392248	-1.104514	-1.282181
H	3.395080	-0.671799	-1.381336
H	2.487116	-2.194679	-1.275583
H	1.812023	-0.814460	-2.164191
C	2.393198	-1.104819	1.281523
H	1.813606	-0.815032	2.164036
H	2.488121	-2.194977	1.274565
H	3.396077	-0.672076	1.380068

IM4

B3LYP-D3BJ/BSI SCF energy in toluene:

-518.304335 a.u.

B3LYP-D3BJ/BSII SCF energy in toluene:

-518.441994 a.u.

B3LYP-D3BJ/BSII free energy in toluene:

-518.279913 a.u.

C	-3.179228	0.457024	0.515580
C	-1.953404	1.111778	0.608332
C	-0.829486	0.606681	-0.061636
C	-0.957327	-0.556569	-0.834565
C	-2.181534	-1.219566	-0.899621
C	-3.298605	-0.718598	-0.228907
H	-4.041359	0.861442	1.037788
H	-1.851956	2.013009	1.206199
H	-2.265392	-2.122412	-1.497525
H	-4.252090	-1.233453	-0.291597
N	0.390057	1.308235	0.039470

H	0.335389	2.311531	-0.090272	H	3.141880	-2.164072	-0.512461
C	1.682278	0.826323	-0.163077	H	3.702938	-0.551970	-1.047965
O	2.543513	1.584831	-0.631087	C	1.248632	-1.270546	1.322839
C	2.016050	-0.522843	0.280654	H	0.510532	-0.650216	1.833373
H	-0.103218	-0.928702	-1.389800	H	0.717518	-2.133375	0.896519
C	3.291960	-1.118469	-0.211555	H	1.942774	-1.673728	2.072099
H	4.048472	-1.135637	0.587784				

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