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


# Supporting Information

for

# Iron-catalyzed Selective Construction of Indole Derivatives via Oxidative C(sp3)-H Functionalization of Indolin-2-ones

Wei Chen, Lang-Qi Wen, Xiao-Bing Lu and Hui Zhou*

zhouhui@dlut.edu.cn

State Key Laboratory of Fine Chemicals, Dalian University of Technology, 116024

Dalian, China.

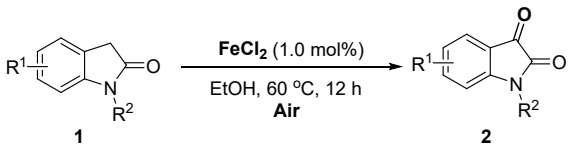
# Table of Contents

## 1. General Procedure

NMR spectrum were recorded on Varian Inova 400, Bruker 400M, 500M and 600 M spectrometers in $CDCl_3$ or DMSO-$d_6$ and chemical shifts are expressed in parts per million ($\delta$, ppm). Proton chemical shifts are referenced to 7.26 ppm ($CHCl_3$) or 2.50 ppm (DMSO-$d_6$) and carbon chemical shifts are referenced to 77.2 ppm ($CHCl_3$) or 39.5 ppm (DMSO-$d_6$). High resolution mass spectrum (HRMS) were recorded on a Q-TOF mass spectrometry equipped with Z-spray ionization source. Infrared spectrum (IR) were measured using a Nicolet NEXUS FT-IR spectrophotometer. Commercially available chemicals were purchased from TCI, Sigma-Aldrich, Alfa Aesar, Acros, adamas, Energy Chemicalor Innochem and used directly without further purification.

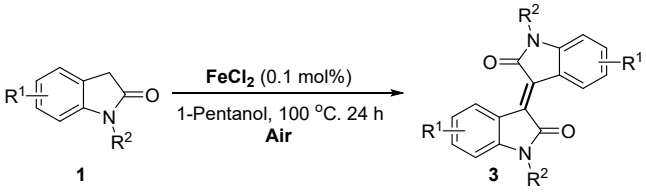
## 2. Iron-catalyzed oxidative reaction of indolin-2-ones to isatins.

A 10 mL flask containing a stir bar was charged with oxindolin-2-one (1.0 mmol), $FeCl_2$ (0.01 mmol, 1.0 mmol%) and EtOH (1.0 mL), respectively. The reaction mixture was stirred at 60 °C in open air for 12 h, then cooled to room temperature. The solvent was evaporated at reduced pressure and the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc: 10/1-3/1) to give desired products.




## 3. Iron-catalyzed oxidative coupling of indolin-2-ones to symmetrical isoindigos.

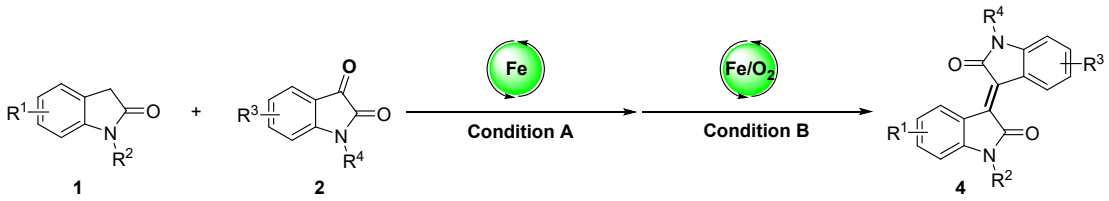
A 10 mL flask containing a stir bar was charged with oxindolin-2-one (1.0 mmol), $FeCl_2$ (0.001 mmol, 0.1 mmol%) and 1-pentanol (1.0 mL), respectively. The reaction mixture was stirred at 100 °C in open air for 24 h, then cooled to room temperature. The solvent was evaporated at reduced pressure and the crude product was purified by washing with dichloromethane or column chromatography on silica gel (petroleum ether/EtOAc: 10/1-5/1 or dichloromethane) to give desired products.




## 4. Iron-catalyzed cascade reaction of indolin-2-ones to non-symmetrical isoindigos.

In an argon atmosphere, a 10 mL oven-dried flask containing a stir bar was charged with oxindolin-2-one (0.5 mmol), isatin (0.5 mmol), $FeCl_2$ (0.0005 mmol, 0.1 mmol%) and 1-pentanol (1.0 mL), respectively. The reaction mixture was stirred at 100 °C in argon for 2 h, then stirred for 1 h in open air.

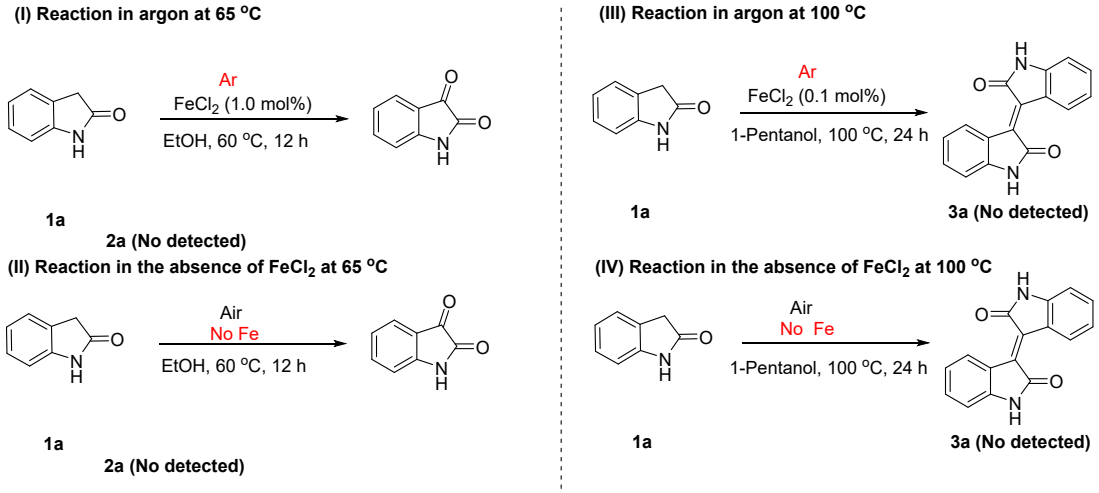
Subsequently, the reaction mixture was cooled to room temperature. The solvent was evaporated at reduced pressure and the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc: 10/1-1/1) to give desired product.




## 5. Mechanistic studies

### 5.1 Control experiments

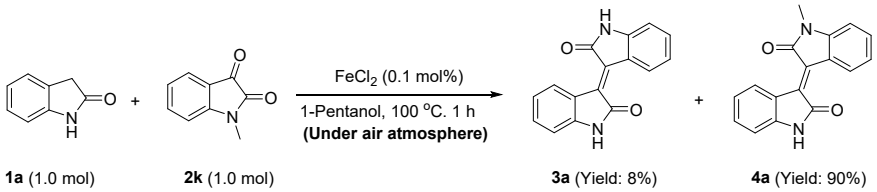
In order to investigate reaction mechanism, several control experiments were performed as depicted in Scheme S1. In the absence of $FeCl_2$ or air, no desired product **2a** or **3a** was observed (Scheme S1. **I**, **II**, **III** and **IV**), which indicated iron salts and air were essential for this process.



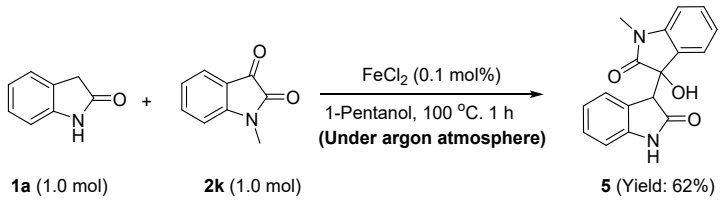

Scheme S1. Control experiments

### 5.2 Intermediate capture experiments

In air atmosphere, a 10 mL flask containing a stir bar was charged with oxindolin-2-one **1a** (1.0 mmol), isatin **2k** (1.0 mmol), $FeCl_2$ (0.001 mmol 0.1 mmol%) and 1-pentanol (1.0 mL), respectively. The reaction mixture was stirred at 100 °C for 1 h under open air. Then the reaction mixture was cooled to room temperature, and the solvent was evaporated under reduced pressure. The crude product was filtered and the residue was washed with dichloromethane to give **3a** in 8% yield. The filtrate was further purified by column chromatography on silica gel (dichloromethane) to gain **4a** in 90% yield.



In argon atmosphere, a 10 mL oven-dried flask containing a stir bar was charged with oxindolin-2-one **1a** (1.0 mmol), isatin **2k** (1.0 mmol), $FeCl_2$ (0.001 mmol 0.1 mmol%) and 1-pentanol (1.0 mL), respectively. The reaction mixture was stirred at 100 °C for 1 h under argon atmosphere. Then the reaction mixture was cooled to room temperature. The solvent was evaporated under reduced pressure and the crude product was purified by washing with dichloromethane to give aldol product **5** in 62% yield.




**Aldol product (5)**. White solid. **$^1$H NMR** (600 MHz, DMSO-$d_6$) $\delta$ 10.12 (s, 1H), 7.56 (t, $J$ = 13.1 Hz, 1H), 7.24 (m, 2H), 7.02 (t, $J$ = 7.5 Hz, 1H), 6.93 (d, $J$ = 7.7 Hz, 1H), 6.77 – 6.68 (m, 2H), 6.66 (s, 1H), 6.15 (d, $J$ = 7.2 Hz, 1H), 4.02 (d, $J$ = 10.8 Hz, 1H), 3.09 (d, $J$ = 6.2 Hz, 3H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 175.6, 173.9, 144.1, 143.3, 129.7, 128.5, 127.6, 126.6, 125.7, 123.1, 121.7, 121.1, 109.1, 108.4; **IR** (KBr cm$^{-1}$): 3250, 1705, 1686, 1614, 1472, 1380, 1336, 1105, 750; **HRMS**(ESI): calcd. for $C_{17}H_{15}N_2O_3$: $[M+H]^+$ m/z 295.1083, found: 295.1084.

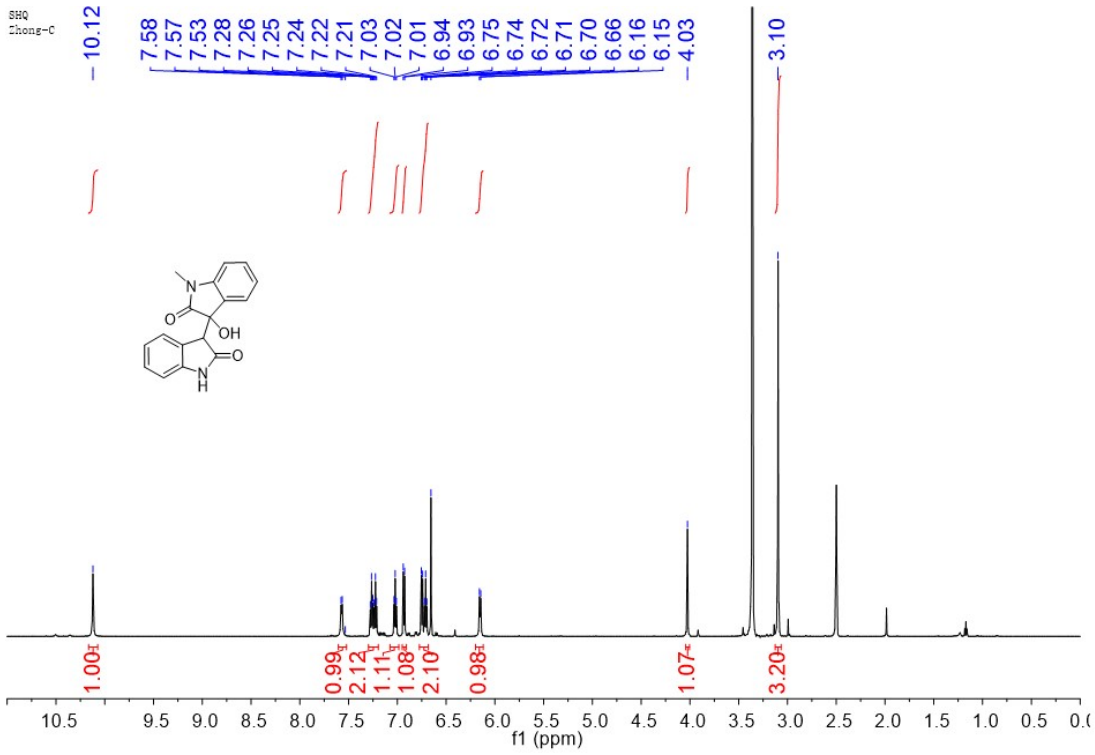



Figure S1. **$^1$H NMR** spectrum of **5**

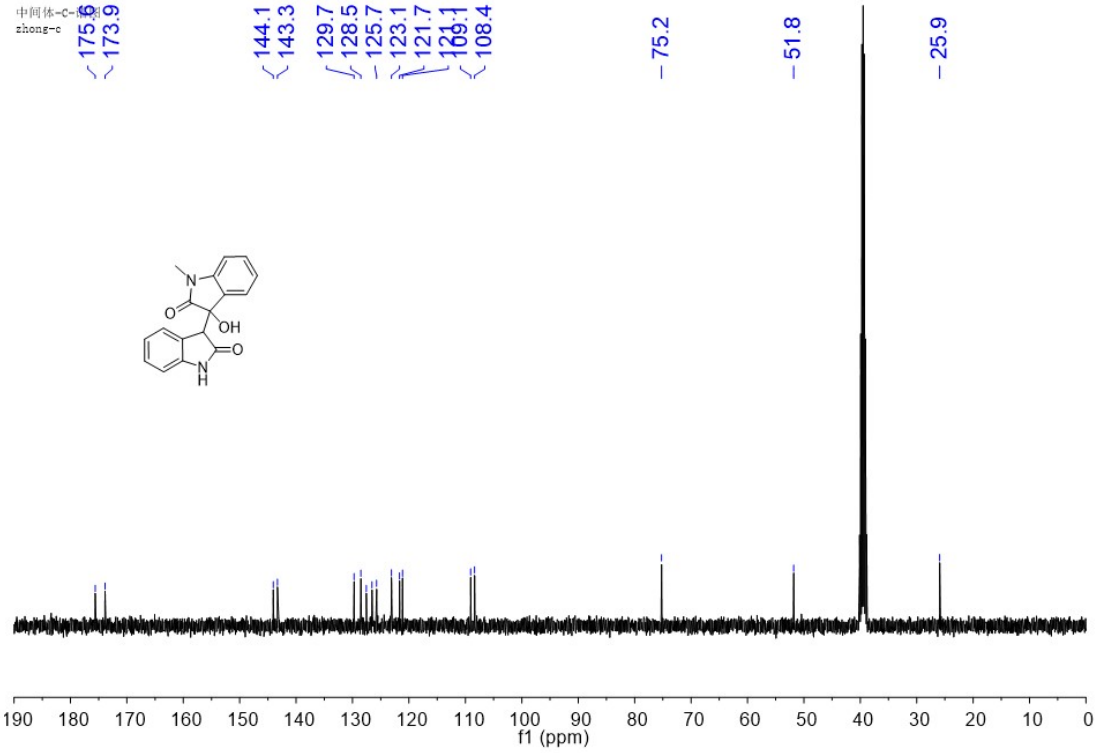
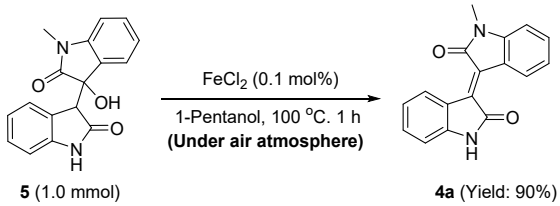
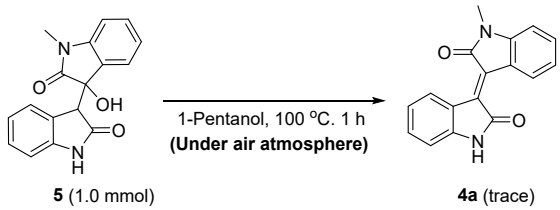



Figure S2. **$^{13}$C NMR** spectrum of **5**

A 10 mL flask containing a stir bar was charged with aldol product **5** (1.0 mmol) , $FeCl_2$ (0.001 mmol 0.1 mmol%) and 1-pentanol (1.0 mL), respectively. The reaction mixture was stirred at 100 °C under open air for 1 h. Then the reaction mixture was cooled to room temperature. The solvent was evaporated at reduced pressure and the crude product was purified by column chromatography on silica gel (dichloromethane) to gain **4a** in 90% yield.



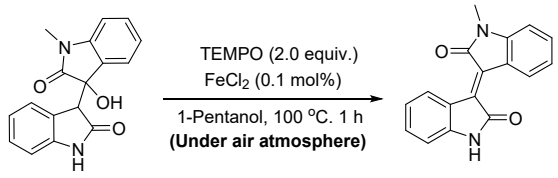

When the same experiment was conducted in absence of $FeCl_2$, only trace amounts of **4a** was detected in reaction mixture.




In order to further verify whether a free-radical process was involved in the dehydration of aldol product **5**, 2, 2, 6, 6-tetramethylpiperdiny-l-oxy (TEMPO) was introduced. The results showed that no **4a** was formed during this process. The detailed experimental process is as follows.

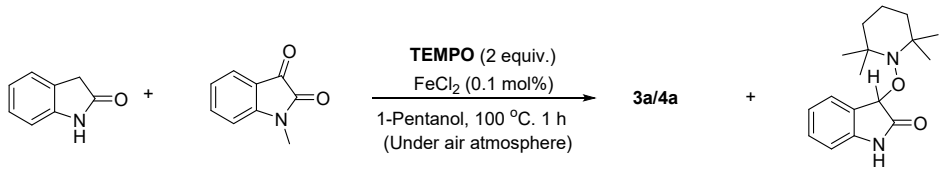
A 10 mL flask containing a stir bar was charged with aldol product **5** (1.0 mmol), TEMPO (2.0 mmol),

$FeCl_2$ (0.001 mmol, 0.1 mmol%) and 1-pentanol (1 mL), respectively. The reaction mixture was stirred at 100 °C in open air for 1 h. Then the reaction mixture was cooled to room temperature. The solvent was evaporated at reduced pressure, and the crude mixture was detected by $^1$H-NMR spectrum.




**5** (1.0 mmol) **4a** (No detected)

A 10 mL oven-dried flask containing a stir bar was charged with oxindolin-2-one **1a** (1.0 mmol), isatin **2k** (1.0 mmol), $FeCl_2$ (0.001 mmol, 0.1 mmol%), TEMPO (2.0 mmol) and 1-pentanol (1 mL), respectively. The reaction mixture was stirred at 100 °C in open air for 1 h. Then the reaction mixture was cooled to room temperature. The solvent was evaporated at reduced pressure and the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc: 5/1) to obtain the radical adduct **6** in 10% yield.




**1a** (1.0 mol) **2k** (1.0 mol) (No detected) **6** (Yield: 10%)

**Radical adduct (6)**. Pale yellow solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.91 (dd, $J$ = 8.0, 1.3 Hz, 1H), 7.29 (dd, $J$ = 11.6, 4.6 Hz, 1H), 6.73 – 6.55 (m, 2H), 5.77 (s, 1H), 1.82 – 1.62 (m, 4H), 1.58 (d, $J$ = 2.6 Hz, 1H), 1.49 – 1.42 (m, 1H), 1.27 (s, 6H), 1.12 (s, 6H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 167.1, 150.1, 133.1, 129.5, 116.0, 115.3, 108.9, 59.5, 38.3, 31.1, 20.1; **IR** (neat): 2930, 1703, 1619, 1589,1487, 1455, 1381, 1231, 1042, 749, 700; **HRMS**(ESI): calcd. for $C_{17}H_{25}N_2O_2$: $[M+H]^+$ m/z 288.1916, found: 288.1901.

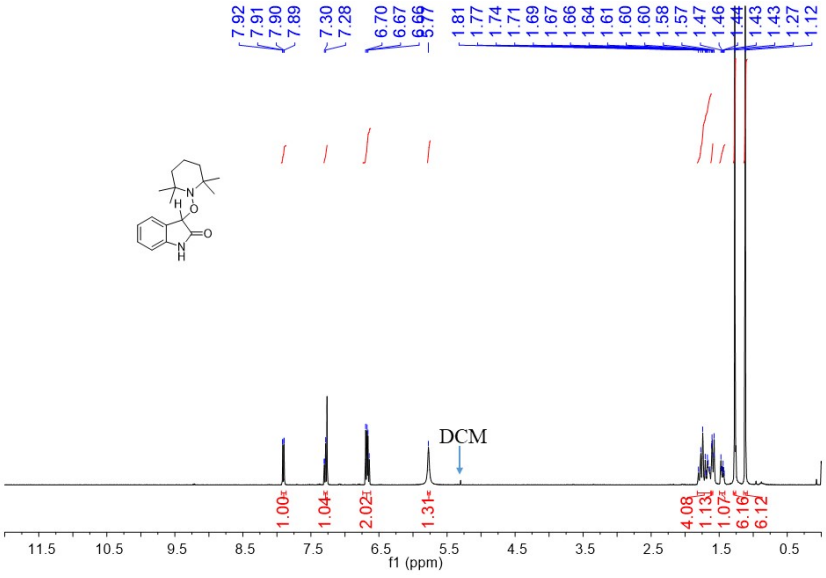



Figure S3. **$^1$H NMR** spectrumof **6**

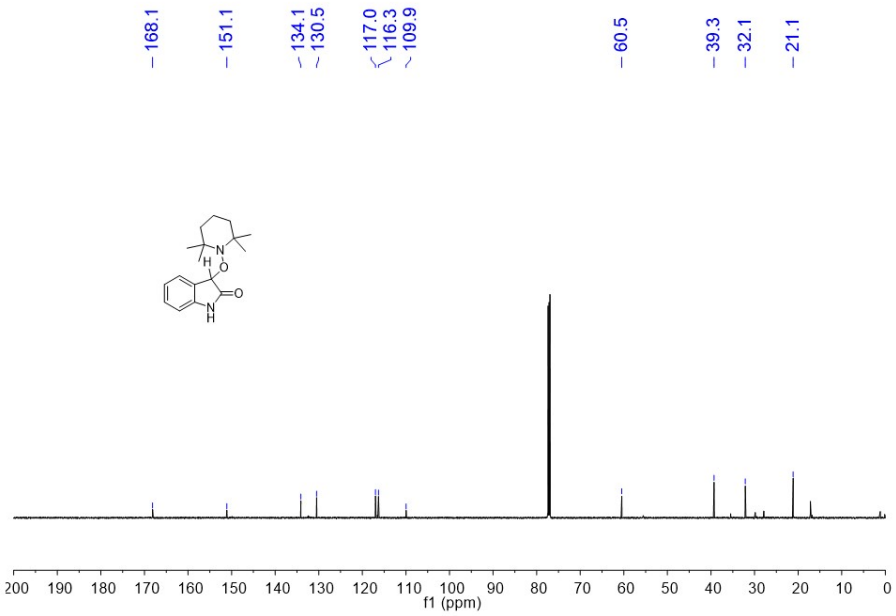
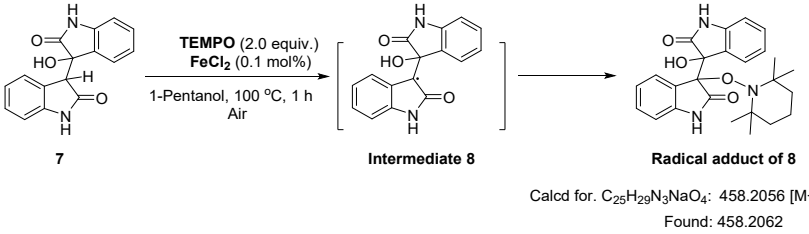



Figure S4. **$^{13}$C NMR** spectrum of **6**

## 5.3 Control experiment on dehydration mechanism

In order to gain insight of the dehydration mechanism, the corresponding control experiment was conducted. A 10 mL flask containing a stir bar was charged with **7** (1.0 mmol), TEMPO (2.0 mmol), $FeCl_2$ (0.001 mmol, 0.1 mmol%) and 1-pentanol (1.0 mL), respectively. The reaction mixture was stirred at 100 °C in open air for 1 h. Meanwhile, the reaction process was investigated by high-resolution mass spectrometry every 5 min. To our delight, the radical adduct of **8** was detected, as shown in Figure S5, which further suggested a free radical process could be involved in the process of dehydration.



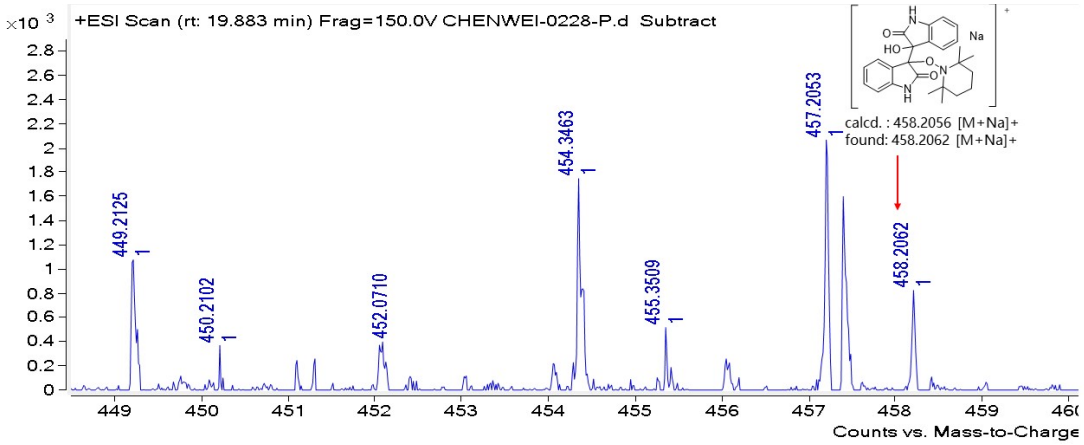
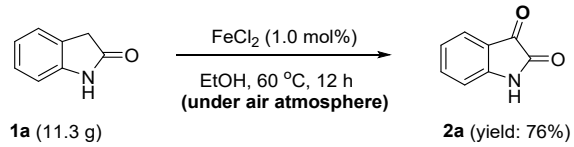




Figure S5. The HRMS spectrum of control experiment

## 6. Large-scale synthesis of valuable indole derivatives

### 6.1 Large-scale synthesis of 2a

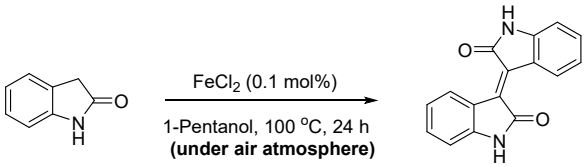
A 250 mL round-bottom flask containing a stir bar was charged with indolin-2-ones **1a** (100 mmol, 13.3 g), $FeCl_2$ (1 mmol, 126 mg) and EtOH (100 mL), The reaction mixture was stirred at 60 °C in air for 12 h. Then the reaction mixture was cooled to room temperature. The solvent was evaporated at reduced pressure and the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc: 3/1) to give red solid 11.3 g in 76% yield.




**1a** (11.3 g) **2a** (yield: 76%)

### 6.2 Large-scale synthesis of 3a

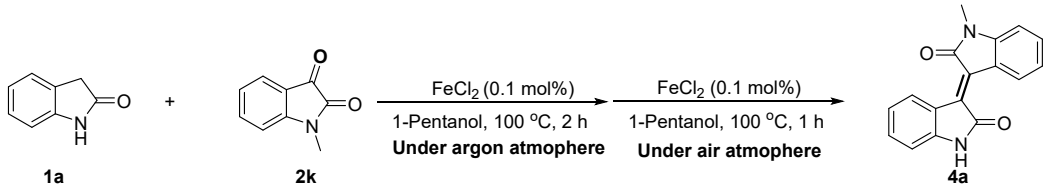
A 250 mL round-bottom flask containing a stir bar was charged with indolin-2-ones **1a** (100 mmol, 13.3 g), $FeCl_2$ (0.1 mmol, 13 mg) and 1-pentanol (100 mL), respectively. The reaction mixture was stirred at 100 °C in air for 24 h. Then the reaction mixture was cooled to room temperature. The solvent was evaporated at reduced pressure and the crude product was washed by dichloromethane to give dark red solid 11.8 g in 90% yield.




**1a** **3a** (yield: 90%)

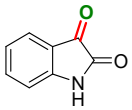
### 6.3 Large-scale synthesis of 4a

A 500 mL round-bottom flask containing a stir bar was charged with indolin-2-ones **1a** (50 mmol, 6.7 g), 1-methylisatin **2k** (50 mmol, 8.0 g), $FeCl_2$ (0.05 mmol, 6 mg) and 1-pentanol (100 mL), respectively. The reaction mixture was stirred at 100 °C in argon for 2 h, then stirred at 100 °C in air for 1 h. Then the reaction mixture was cooled to room temperature. The solvent was evaporated at reduced pressure and the crude product was purified by column chromatography on silica gel (dichloromethane) to give dark red solid 10.1 g in 73% yield .



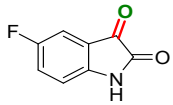

**1a** **2k** **4a**

## 7. Characterization data of isatins



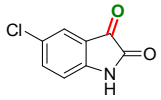
**2a**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.04 (s, 1H), 7.58 (t, $J$ = 7.7, 1H), 7.50 (d, $J$ = 7.5 Hz, 1H), 7.06 (t, $J$ = 7.5 Hz, 1H), 6.90 (d, $J$ = 7.9 Hz, 1H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 185.0, 160.0, 151.1, 139.1, 125.3, 123.5, 118.2, 112.8. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



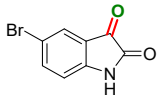
**2b**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.04 (s, 1H), 7.52 – 7.37 (m, 2H), 6.91 (dd, $J$ = 8.5, 3.9 Hz, 1H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 184.1 (d, $J$ = 2.0 Hz), 159.4 (d, $J$ = 92.6 Hz), 157.5, 147.1, 124.7 (d, $J$ = 24.2 Hz), 118.6 (d, $J$ = 7.5 Hz), 113.7 (d, $J$ = 6.0 Hz), 111.6 (d, $J$ = 24 Hz). All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



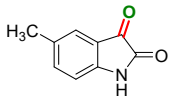
**2c**

Orange-red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.13 (s, 1H), 7.61 (dd, $J$ = 8.4, 2.2 Hz, 1H), 7.56 (d, $J$ = 2.1 Hz, 1H), 6.92 (d, $J$ = 8.4 Hz, 1H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 183.6, 159.4, 149.4, 137.5, 127.1, 124.3, 119.2, 114.1. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



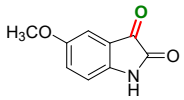
**2d**

Yellow solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.17 (s, 1H), 7.72 (d, $J$ = 8.4 Hz, 1H), 7.62 (s, 1H), 6.88 (d, $J$ = 8.3 Hz, 1H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 183.7, 159.5, 149.9, 140.7, 127.4, 119.9, 114.9, 114.9. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



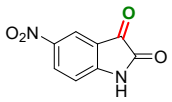
**2e**

Orange solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.93 (s, 1H), 7.40 (d, $J$ = 7.9 Hz, 1H), 7.32 (s, 1H), 6.81 (d, $J$ = 8.0 Hz, 1H), 2.25 (s, 3H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 184.8, 159.7, 148.7, 139.2, 132.4, 125.1, 117.9, 112.3, 20.3. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



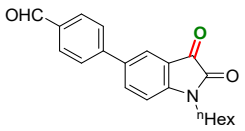
**2f**

Orange solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.84 (s, 1H), 7.18 (dd, $J$ = 8.5, 2.7 Hz, 1H), 7.08 (d, $J$ = 2.5 Hz, 1H), 6.85 (d, $J$ = 8.5 Hz, 1H), 3.75 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 184.9, 159.8, 155.5, 144.8, 125.1, 118.3, 113.4, 108.9, 55.9. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



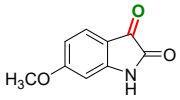
**2g**

Orange solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.66 (s, 1H), 8.44 (dd, $J$ = 8.7, 2.4 Hz, 1H), 8.21 (d, $J$ = 2.3 Hz, 1H), 7.09 (d, $J$ = 8.7 Hz, 1H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 182.8, 160.4, 155.6, 143.1, 133.6, 131.5, 120.1, 118.6, 113.0. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



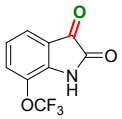
**2h**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 10.07 (s, 1H), 7.97 (d, $J$ = 8.2 Hz, 2H), 7.92 – 7.82 (m, 2H), 7.70 (d, $J$ = 8.1 Hz, 2H), 7.01 (t, $J$ = 10.5 Hz, 1H), 3.77 (t, $J$ = 7.3 Hz, 2H), 1.73 (dd, $J$ = 14.6, 7.5 Hz, 2H), 1.41 – 1.26 (m, 6H), 0.91 – 0.85 (m, 3H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ $^{13}$C NMR (101 MHz, $CDCl_3$) $\delta$ 191.7, 183.5, 158.3, 151.1, 145.1, 137.1, 135.7, 135.7, 130.7, 127.2, 124.2, 118.3, 110.9, 77.5, 77.2, 76.8, 40.7, 31.5, 27.4, 26.7, 22.65, 14.12; **IR** (neat cm$^{-1}$): 2921 1738 1698 1620 1602 1483 1384 1344 1215 1170 820 737; **HRMS**(ESI): calcd. for $C_{21}H_{21}NNaO_3$: 358.1419 $[M+Na]^+$, found: 358.1412.



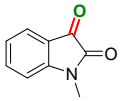
**2i**

Yellow solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.96 (s, 1H), 7.48 (d, $J$ = 8.5 Hz, 1H), 6.59 (d, $J$ = 8.5 Hz, 1H), 6.40 (s, 1H), 3.87 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 181.7, 168.0, 160.8, 153.7, 127.5, 111.3, 109.1, 98.0, 56.3. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[2]



**2j**

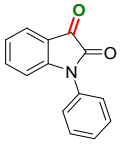
Yellow solid. **$^1$H NMR** (600 MHz, $CDCl_3$) $\delta$ 7.86 (s, 1H), 7.60 (d, $J$ = 7.5 Hz, 1H), 7.51 (d, $J$ = 8.4 Hz, 1H), 7.18 (t, $J$ = 7.9 Hz, 1H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 181.6, 158.1, 141.6, 133.7, 131.1, 124.6, 124.4, 121.5, 120.0; **IR** (neat cm$^{-1}$): 3212 1751 1633 1593 1491 1385 1279 1255 1234 1198 692; **HRMS**(ESI): calcd. for $C_9H_3F_3NO_3$: 230.0065 $[M-H]^-$, found: 230.0065.



**2k**

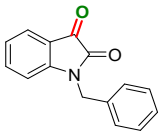
Orange solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.66 – 7.53 (m, 2H), 7.13 (t, $J$ = 7.5 Hz, 1H), 6.94 – 6.85

(m, 1H), 3.26 (s, 3H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ $^{13}$C NMR (151 MHz, $CDCl_3$) $\delta$ 183.5, 158.3, 151.6, 138.6, 125.4, 124.0, 117.5, 110.1, 26.4. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



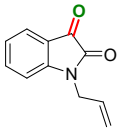
**2l**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.70 (d, $J$ = 7.4 Hz, 1H), 7.60 – 7.51 (m, 3H), 7.46 (t, $J$ = 6.3 Hz, 1H), 7.44 – 7.40 (m, 2H), 7.18 (t, $J$ = 7.5 Hz, 1H), 6.90 (d, $J$ = 8.0 Hz, 1H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 183.0, 157.4, 151.7, 138.5, 132.9, 130.1, 128.9, 126.1, 125.7, 124.4, 117.5, 111.4. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



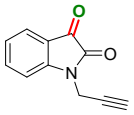
**2m**

Orange solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.61 (dd, $J$ = 7.5, 0.8 Hz, 1H), 7.48 (m, 1.3 Hz, 1H), 7.39 – 7.29 (m, 5H), 7.09 (t, $J$ = 7.5 Hz, 1H), 6.77 (d, $J$ = 8.0 Hz, 1H), 4.93 (s, 2H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 183.4, 158.4, 150.8, 138.8, 134.6, 129.1, 128.3, 127.5, 125.5, 124.0, 117.7, 111.1, 44.1. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



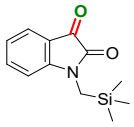
**2n**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.57 (dd, $J$ = 18.4, 7.7 Hz, 2H), 7.11 (t, $J$ = 7.5 Hz, 1H), 6.89 (d, $J$ = 7.9 Hz, 1H), 5.83 (m, 1H), 5.30 (t, $J$ = 12.7 Hz, 2H), 4.36 (d, $J$ = 5.2 Hz, 2H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 183.3, 157.9, 150.8, 138.4, 130.4, 125.3, 123.8, 118.6, 117.5, 111.0, 42.5. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



**2o**

Orange solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.67 – 7.62 (m, 2H), 7.18 (t, $J$ = 7.6 Hz, 1H), 7.13 (d, $J$ = 8.3 Hz, 1H), 4.54 (d, $J$ = 2.5 Hz, 2H), 2.31 (t, $J$ = 2.5 Hz, 1H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 182.7, 157.3, 149.7, 138.6, 125.7, 124.4, 117.8, 111.2, 75.8, 73.5, 29.6. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[3]

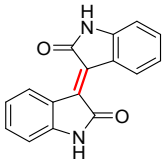


**2p**

Orange solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.55 (t, $J$ = 7.3 Hz, 2H), 7.08 (t, $J$ = 7.5 Hz, 1H), 6.80 (d, $J$

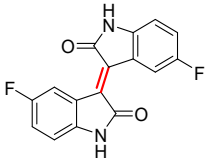
= 8.1 Hz, 1H), 3.20 (s, 2H), 0.15 (s, 9H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 183.8, 158.0, 152.0, 138.2, 125.3, 123.6, 118.0, 110.3, 31.8, -1.3. All the resonances in $^{1}$H and $^{13}$C NMR spectrum were in good agreement with literature values.[4]

## 8. Characterization data of symmetrical isoindigos



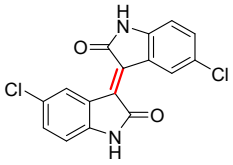
**3a**

Red solid. **$^{1}$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.90 (s, 2H), 9.05 (d, $J$ = 7.1 Hz, 2H), 7.38 – 7.30 (m, 2H), 6.96 (t, $J$ = 7.5 Hz, 2H), 6.84 (d, $J$ = 6.6 Hz, 2H); **$^{13}$C NMR** (126 MHz, DMSO-$d_6$) $\delta$ 169.0, 144.1, 133.3, 132.6, 129.3, 121.7, 121.1, 109.5. All the resonances in $^{1}$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



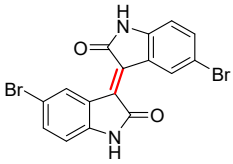
**3b**

Red solid. **$^{1}$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.99 (s, 1H), 8.99 (dd, $J$ = 11.3, 2.4 Hz, 1H), 7.24 (td, $J$ = 8.6, 2.4 Hz, 1H), 6.84 (dd, $J$ = 8.5, 4.9 Hz, 1H); **$^{13}$C NMR** (126 MHz, DMSO-$d_6$) $\delta$ 169.0, 156.1 (d, $J$ = 233.2 Hz), 140.8, 133.9 (d, $J$ = 2.5 Hz), 122.1 (d, $J$ = 10.2 Hz), 119.6 (d, $J$ = 24.2 Hz), 116.3 (d, $J$ = 28.2 Hz), 110.2 (d, $J$ = 8.3 Hz). All the resonances in $^{1}$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



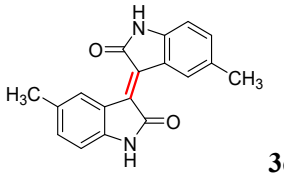
**3c**

Red solid. **$^{1}$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.11 (s, 2H), 9.18 (d, $J$ = 1.7 Hz, 2H), 7.42 (dd, $J$ = 8.3, 2.0 Hz, 2H), 6.87 (d, $J$ = 8.3 Hz, 2H); **$^{13}$C NMR** (126 MHz, DMSO-$d_6$) $\delta$ 168.7, 143.1, 133.5, 132.5, 129.0, 125.2, 122.7, 111.1. All the resonances in $^{1}$H and $^{13}$C NMR spectrum were in good agreement with literature values.[5]



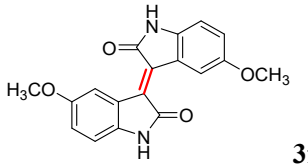
**3d**

Red solid. **$^{1}$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.06 (s, 2H), 9.31 (s, 2H), 7.54 (d, $J$ = 6.5 Hz, 2H), 6.83 (d, $J$ = 5.7 Hz, 2H). All the resonances in $^{1}$H spectrum were in good agreement with literature values.[6]



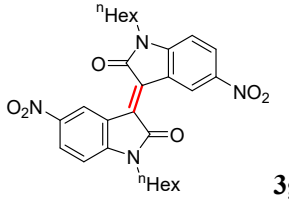
**3e**

Dark red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.73 (s, 2H), 8.89 (s, 2H), 7.15 (d, $J$ = 7.9 Hz, 2H), 6.73 (d, $J$ = 7.9 Hz, 2H), 2.26 (s, 6H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 168.6, 141.4, 132.8, 132.2, 129.1, 121.5, 108.6, 20.2. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[6]



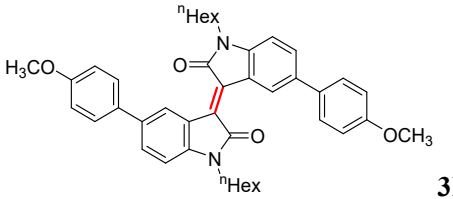
**3f**

Blue-green solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.69 (s, 2H), 8.85 (d, $J$ = 2.2 Hz, 2H), 6.97 (dd, $J$ = 8.4, 2.4 Hz, 2H), 6.75 (d, $J$ = 8.5 Hz, 2H), 3.73 (s, 6H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 168.6, 153.8, 137.7, 133.5, 122.0, 118.3, 115.3, 109.1, 55.3. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[6]



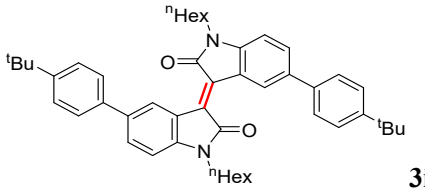
**3g**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.18 (d, $J$ = 8.0 Hz, 2H), 7.35 (t, $J$ = 7.8 Hz, 2H), 7.04 (t, $J$ = 7.8 Hz, 2H), 6.79 (d, $J$ = 7.9 Hz, 2H), 3.77 (t, $J$ = 7.4 Hz, 4H), 1.75 – 1.66 (m, 4H), 1.35 (dt, $J$ = 42.6, 15.9 Hz, 16H), 0.88 (t, $J$ = 6.5 Hz, 6H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 168.0, 144.9, 133.7, 132.5, 130.1, 122.3, 121.9, 108.0, 40.2, 31.7, 27.6, 26.9, 22.7, 14.2; **IR** (neat cm$^{-1}$): 2921 1733 1694 1609 1468 1384 1356 1099 776 748; **HRMS**(ESI): calcd. for $C_{28}H_{33}N_4O_6$: 521.2400 $[M+H]^+$, found: 521.2332.



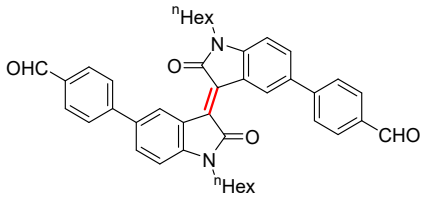
**3h**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.45 (s, 2H), 7.59 (d, $J$ = 8.5 Hz, 4H), 7.53 (d, $J$ = 8.1 Hz, 2H), 6.99 (d, $J$ = 8.5 Hz, 4H), 6.81 (d, $J$ = 8.1 Hz, 2H), 3.86 (s, 6H), 3.77 (dd, $J$ = 15.1, 7.7 Hz, 4H), 1.70 (dd, $J$ = 14.8, 7.5 Hz, 4H), 1.46 – 1.23 (m, 12H), 0.89 (t, $J$ = 6.7 Hz, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 167.9, 159.0, 143.7, 135.1, 134.0, 133.8, 130.7, 128.5, 128.0, 122.2, 114.4, 108.1, 55.5, 40.2, 31.7, 27.6, 26.8, 22.7, 14.2. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[7]



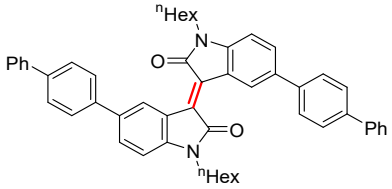
**3i**

Red solid. **$^1$H NMR** (600 MHz, $CDCl_3$) $\delta$ 9.49 (s, 2H), 7.59 (t, $J$ = 7.7 Hz, 6H), 7.48 (d, $J$ = 8.2 Hz, 4H), 6.84 (d, $J$ = 8.1 Hz, 2H), 3.80 (t, $J$ = 7.4 Hz, 4H), 1.77 – 1.65 (m, 4H), 1.41 (dd, $J$ = 14.3, 6.7 Hz, 4H), 1.37 (s, 18H), 1.35 – 1.29 (m, 8H), 0.89 (t, $J$ = 6.8 Hz, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 168.0, 149.9, 144.1, 138.4, 135.4, 134.1, 131.1, 128.9, 126.7, 125.9, 122.3, 108.2, 40.3, 34.7, 31.7, 31.6, 27.7, 26.9, 22.7, 14.2; **IR** (neat cm$^{-1}$): 2922 1694 1609 1481 1384 1333 1116 811 743; **HRMS**(ESI): calcd. for $C_{48}H_{59}N_2O_2$: 695.4577 $[M+H]^+$, found: 695.4561.



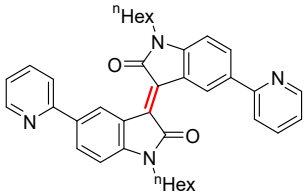
**3j**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 10.06 (s, 2H), 9.63 (d, $J$ = 1.6 Hz, 2H), 7.98 (d, $J$ = 8.2 Hz, 4H), 7.83 (d, $J$ = 8.2 Hz, 4H), 7.68 (dd, $J$ = 8.2, 1.7 Hz, 2H), 6.92 (d, $J$ = 8.2 Hz, 2H), 3.90 – 3.75 (m, 4H), 1.80 – 1.67 (m, 4H), 1.37 (dd, $J$ = 28.9, 9.4 Hz, 12H), 0.89 (t, $J$ = 6.9 Hz, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 191.9, 167.8, 147.0, 145.1, 134.9, 133.9, 133.8, 131.5, 130.4, 129.2, 127.3, 122.2, 108.4, 40.3, 31.5, 27.5, 26.7, 22.6, 14.0; **IR** (neat cm$^{-1}$): 2922 1687 1601 1482 1385 1349 1319 1273 1224 1166 1113 809; **HRMS**(ESI): calcd. for $C_{42}H_{43}N_2O_4$: 639.3223 $[M+H]^+$, found: 639.3212.



**3k**

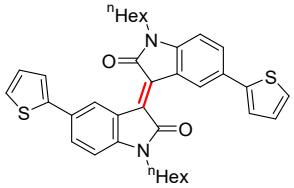
Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.58 (s, 2H), 7.75 (d, $J$ = 8.1 Hz, 4H), 7.68 (dd, $J$ = 15.1, 8.1 Hz, 10H), 7.47 (t, $J$ = 7.6 Hz, 4H), 7.36 (t, $J$ = 7.6 Hz, 2H), 6.89 (d, $J$ = 8.0 Hz, 2H), 3.84 (t, $J$ = 7.2 Hz, 4H), 1.74 (d, $J$ = 7.5 Hz, 4H), 1.35 (t, $J$ = 34.6 Hz, 16H), 0.90 (t, $J$ = 6.6 Hz, 6H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 167.9, 144.2, 140.9, 140.0, 139.7, 134.8, 134.0, 131.0, 128.8, 128.7, 127.6, 127.2, 127.0, 122.2, 108.2, 40.2, 39.8, 31.6, 27.5, 26.7, 22.6, 14.1; **IR** (neat cm$^{-1}$): 2928 1693 1609 1487 1385 1110 810 770; **HRMS**(ESI): calcd. for $C_{52}H_{51}N_2O_2$: 735.3951 $[M+H]^+$, found: 735.3942.



**3l**

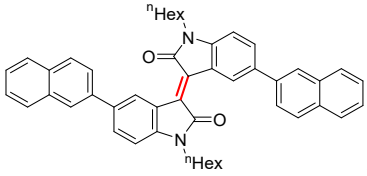
Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.55 (s, 1H), 8.91 (s, 1H), 8.58 (d, $J$ = 3.8 Hz, 1H), 7.96 (d, $J$

= 7.3 Hz, 1H), 7.61 (d, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 24.0 Hz, 1H), 6.91 (d, *J* = 7.9 Hz, 1H), 3.81 (t, *J* = 6.6 Hz, 2H), 1.73 (s, 2H), 1.38 (d, *J* = 33.4 Hz, 6H), 0.89 (s, 3H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 168.0, 156.7, 143.9, 133.8, 132.5, 131.0, 130.9, 130.8, 128.4, 121.7, 121.1, 111.4, 107.5, 40.2, 31.7, 27.7, 26.8, 22.7, 14.2. **IR** (neat cm$^{-1}$): 2951 1687 1609 1747 1396 1349 1177 1113 826 794; **HRMS**(ESI): calcd. for $C_{38}H_{41}N_4O_2$: 585.3230 $[M+H]^+$, found: 585.3216.



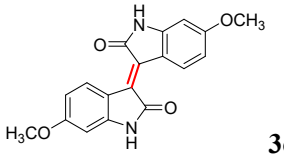

**3m**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.59 (d, *J* = 1.7 Hz), 7.60 (dd, *J* = 8.1, 1.8 Hz), 7.34 (dd, *J* = 3.5, 1.0 Hz), 7.24 (dd, *J* = 5.1, 0.9 Hz), 7.09 (dd, *J* = 5.1, 3.6 Hz), 6.79 (d, *J* = 8.2 Hz), 3.80 (t, *J* = 7.4 Hz), 1.77 – 1.65 (m), 1.45 – 1.27 (m), 0.89 (t, *J* = 7.0 Hz); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 167.9, 144.7, 144.3, 134.0, 130.2, 129.0, 128.1, 128.0, 124.1, 122.8, 122.3, 108.2, 40.3, 31.7, 27.6, 26.8, 22.7, 14.2; **IR** (neat cm$^{-1}$): 2921 1686 1607 1385 1352 1114 801 682; **HRMS**(ESI): calcd. for $C_{36}H_{39}N_2O_2S_2$: 595.2453 $[M+H]^+$, found: 595.2444.



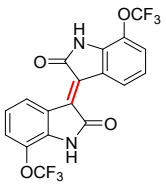

**3n**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.65 (s, 2H), 8.10 (s, 2H), 7.94 (d, *J* = 8.1 Hz, 4H), 7.86 (dd, *J* = 13.8, 8.2 Hz, 4H), 7.73 (d, *J* = 7.7 Hz, 2H), 7.50 (t, *J* = 7.2 Hz, 4H), 6.90 (d, *J* = 8.0 Hz, 2H), 3.83 (s, 4H), 1.75 (s, 4H), 1.39 (d, *J* = 35.7 Hz, 12H), 0.89 (s, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 167.9, 144.3, 138.5, 135.3, 132.5, 131.4, 129.1, 128.5, 128.2, 127.6, 126.2, 125.7, 125.6, 125.2, 122.3, 108.2, 40.2, 31.5, 27.5, 26.7, 22.6, 14.0; **IR** (neat cm$^{-1}$): 2920 1697 1636 1558 1458 1385 1075 761; **HRMS**(ESI): calcd. for $C_{48}H_{47}N_2O_2$: 683.3638 $[M+H]^+$, found: 683.3622.



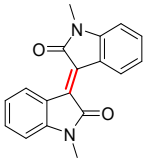

**3o**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.79 (s, 2H), 9.00 (d, *J* = 6.3 Hz, 2H), 6.45 (d, *J* = 58.2 Hz, 4H), 3.81 (s, 6H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 170.0, 162.4, 145.7, 130.8, 129.7, 115.1, 106.6, 95.4, 55.4. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[7]



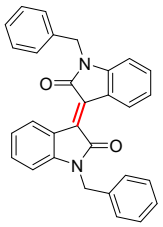
**3p**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.65 (s, 2H), 9.06 (d, $J$ = 8.1 Hz, 2H), 7.43 (d, $J$ = 8.3 Hz, 2H), 7.09 (t, $J$ = 8.2 Hz, 1H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 168.5, 137.3, 133.6, 131.1, 128.5, 125.6, 123.9, 121.6, 120.3 (d, $J$ = 257.6 Hz). All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[7]



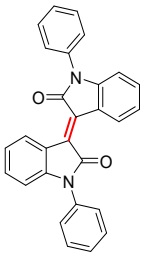
**3q**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.22 (d, $J$ = 7.4 Hz, 2H), 7.38 (td, $J$ = 7.7, 1.1 Hz, 2H), 7.07 (td, $J$ = 7.9, 1.0 Hz, 2H), 6.79 (d, $J$ = 7.7 Hz, 2H), 3.29 (s, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 168.1, 145.3, 133.5, 132.5, 130.0, 122.5, 121.7, 107.8, 26.2. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



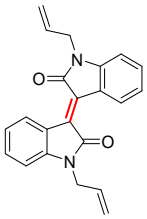
**3r**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.23 (d, $J$ = 7.4 Hz, 2H), 7.36 – 7.26 (m, 12H), 7.09 – 7.01 (m, 2H), 6.72 (d, $J$ = 7.8 Hz, 2H), 5.02 (s, 4H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 168.0, 144.5, 135.7, 133.5, 132.5, 130.0, 128.8, 127.7, 127.2, 122.5, 121.7, 108.7, 43.7. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



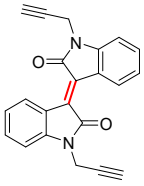
**3s**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.22 (d, $J$ = 8.0 Hz, 2H), 7.57 (dd, $J$ = 9.9, 5.6 Hz, 4H), 7.49 – 7.42 (m, 6H), 7.30 – 7.24 (m, 2H), 7.08 – 7.01 (m, 2H), 6.74 (d, $J$ = 7.8 Hz, 2H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 167.6, 145.5, 134.3, 133.9, 132.7, 130.4, 129.9, 128.5, 127.3, 123.0, 121.7, 109.2. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[1]



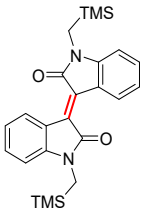
**3t**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.20 (d, $J$ = 8.0 Hz, 2H), 7.34 (t, $J$ = 7.6 Hz, 2H), 7.06 (t, $J$ = 7.6 Hz, 2H), 6.79 (d, $J$ = 7.8 Hz, 2H), 5.88 (m, 2H), 5.25 (t, $J$ = 13.0 Hz, 4H), 4.44 (d, $J$ = 5.1 Hz, 4H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 167.8, 144.6, 133.5, 132.5, 131.3, 130.1, 122.5, 121.7, 117.7, 108.6, 42.4. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[7]



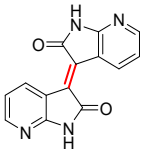
**3u**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 9.08 (d, $J$ = 8.0 Hz, 2H), 7.48 (t, $J$ = 7.7 Hz, 2H), 7.14 – 7.06 (m, 4H), 4.63 (d, $J$ = 2.1 Hz, 4H), 3.27 (s, 2H); $^{13}$C NMR (151 MHz, DMSO-$d_6$) $\delta$ 166.4, 143.3, 133.1, 132.6, 129.3, 122.4, 120.8, 109.3, 77.9, 74.5, 29.0. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[7]



**3v**

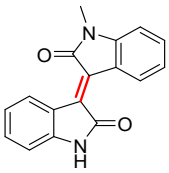
Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.19 (d, $J$ = 8.0 Hz, 1H), 7.34 (t, $J$ = 7.7 Hz, 1H), 7.04 (t, $J$ = 7.8 Hz, 1H), 6.72 (d, $J$ = 7.8 Hz, 1H), 3.32 (s, 2H), 0.16 (s, 9H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 166.6, 144.6, 132.6, 131.2, 128.6, 121.3, 121.1, 107.3, 30.6, -2.2. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[6]



**3w**

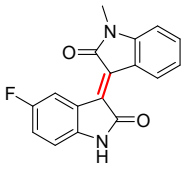
Red solid. **$^1$H NMR** (600 MHz, DMSO-$d_6$) $\delta$ 11.59 (s, 2H), 9.31 (d, $J$ = 7.7 Hz, 2H), 8.21 (d, $J$ = 4.7 Hz, 2H), 7.12 – 7.03 (m, 2H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 168.7, 168.7, 158.1, 150.6, 136.8, 132.5, 118.0, 116.1. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[7]

## 9. Characterization data of non-symmetrical isoindigos



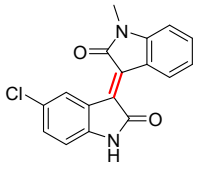
**4a**

Dark red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.89 (s, 1H), 9.07 (d, $J$ = 7.7 Hz, 2H), 7.41 (t, $J$ = 7.4 Hz, 1H), 7.34 (t, $J$ = 7.4 Hz, 1H), 7.06 – 6.92 (m, 3H), 6.83 (d, $J$ = 7.6 Hz, 1H), 3.21 (s, 3H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 168.9, 167.2, 145.0, 144.2, 133.8, 132.9, 132.6, 132.3, 129.5, 129.0, 121.8, 121.7, 121.2, 120.8, 109.6, 108.5, 26.1. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[5]



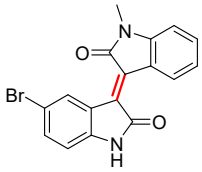
**4b**

Dark red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.89 (s, 1H), 9.08 (d, J = 7.9 Hz, 1H), 8.94 (dd, J = 11.4, 2.4 Hz, 1H), 7.41 (t, J = 7.6 Hz, 1H), 7.18 (td, J = 8.7, 2.5 Hz, 1H), 7.04 – 6.90 (m, 2H), 6.78 (dd, J = 8.5, 4.9 Hz, 1H), 3.18 (s, 3H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 168.7, 167.2, 158.1, 155.8, 145.2, 140.6, 133.4, 133.0, 129.3, 122.3, 121.9, 120.6, 119.1, 118.9, 116.2, 115.9, 110.0, 110.0, 108.5, 26.0. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[8]



**4c**

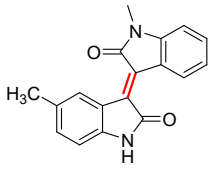
Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.06 (s, 1H), 9.20 (s, 1H), 9.10 (d, J = 8.0 Hz, 1H), 7.49 – 7.33 (m, 2H), 7.04 (dd, J = 11.5, 7.8 Hz, 2H), 6.85 (d, J = 8.3 Hz, 1H), 3.22 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 168.6, 167.2, 145.3, 142.9, 133.7, 133.2, 132.4, 132.0, 129.3, 128.7, 125.1, 122.9, 121.9, 120.6, 110.9, 108.6, 26.1. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[5]



**4d**

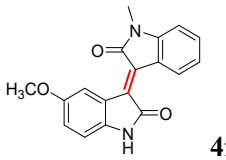
Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.07 (s, 1H), 9.35 (d, J = 2.0 Hz, 1H), 9.11 (d, J = 7.8 Hz, 1H), 7.53 (dd, J = 8.3, 2.1 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.08 – 7.02 (m, 2H), 6.82 (d, J = 8.3 Hz, 1H), 3.23 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 168.5, 167.3, 145.4, 143.3, 134.9, 133.8, 133.3, 132.3,

131.5, 129.3, 123.4, 122.0, 120.7, 112.9, 111.5, 108.7, 26.2. All the resonances in $^{1}H$ and $^{13}C$ NMR spectrum were in good agreement with literature values.[8]



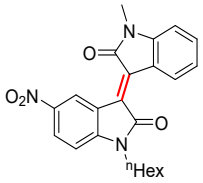
**4e**

Red solid. **$^{1}$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.79 (s, 1H), 9.08 (d, $J$ = 7.0 Hz, 1H), 7.50 – 7.30 (m, 1H), 7.23 – 6.95 (m, 3H), 6.72 (d, $J$ = 6.5 Hz, 1H), 3.22 (s, 3H), 2.27 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 168.9, 167.2, 144.9, 142.0, 134.1, 133.3, 132.4, 132.0, 129.8, 129.7, 128.9, 121.7, 120.8, 109.3, 108.4, 26.0, 21.0; **IR** (neat cm$^{-1}$): 2927 1688 1610 1472 1375 1343 1159 1095 814 772 751; **HRMS**(ESI): calcd. for $C_{18}H_{15}N_2O_2$: 291.1134 $[M+H]^+$, found: 291.1130.



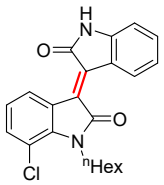
**4f**

Red solid. **$^{1}$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.72 (s, 1H), 9.11 (d, $J$ = 7.7 Hz, 1H), 8.86 (d, $J$ = 2.5 Hz, 1H), 7.43 (td, $J$ = 7.7, 1.0 Hz, 1H), 7.03 (t, $J$ = 8.4 Hz, 2H), 6.97 (dd, $J$ = 8.5, 2.6 Hz, 1H), 6.74 (d, $J$ = 8.5 Hz, 1H), 3.74 (s, 3H), 3.23 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 168.9, 167.3, 154.0, 145.0, 138.2, 134.4, 132.6, 132.4, 129.0, 122.3, 121.8, 120.8, 118.8, 115.2, 109.8, 108.5, 55.5, 26.1. All the resonances in $^{1}H$ and $^{13}C$ NMR spectrum were in good agreement with literature values.[8]



**4g**

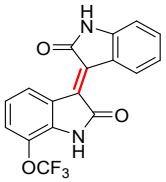
Red solid. **$^{1}$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.84 – 11.44 (m, 1H), 10.13 (d, J = 2.3 Hz, 1H), 9.11 (d, J = 7.7 Hz, 1H), 8.29 (dd, J = 8.7, 2.3 Hz, 1H), 7.48 (t, J = 7.7 Hz, 1H), 7.14 – 6.97 (m, 3H), 3.79 (t, J = 7.0 Hz, 2H), 1.63 (s, 2H), 1.30 (s, 6H), 0.85 (t, J = 6.9 Hz, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 169.5, 167.6, 150.0, 145.5, 142.0, 135.3, 134.3, 131.7, 130.1, 128.9, 125.5, 122.5, 121.9, 121.0, 110.2, 109.4, 31.4, 31.2, 27.3, 26.4, 22.5, 19.7, 14.3; **IR** (neat cm$^{-1}$): 2929 1697 1626 1529 1401 1339 1164 771; **HRMS**(ESI): calcd. for $C_{22}H_{22}N_3O_4$: 392.1610 $[M+H]^+$, found: 392.1607.



**4h**

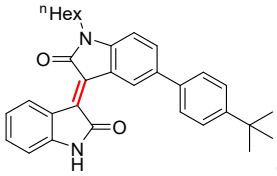
Red solid. **$^{1}$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.07 (t, $J$ = 8.3 Hz, 2H), 7.80 (s, 1H), 7.31 (dd, $J$ = 16.0, 7.8 Hz, 2H), 7.00 (dt, $J$ = 34.4, 7.9 Hz, 2H), 6.79 (d, $J$ = 7.8 Hz, 1H), 4.26 – 4.10 (m, 2H), 1.74 (s, 2H), 1.33

(s, 4H), 0.89 (s, 3H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 169.2, 168.1, 142.7, 140.5, 134.8, 134.5, 133.2, 132.7, 130.4, 128.1, 124.6, 122.9, 122.6, 122.6, 114.8, 109.5, 42.2, 31.6, 29.7, 26.6, 22.7, 14.2; **IR** (neat $cm^{-1}$): 2926 1728 1691 1620 1484 1467 1384 1332 1102 804 745; **HRMS**(ESI): calcd. for $C_{22}H_{20}ClN_2O_2$: 379.1213 $[M-H]^-$, found: 379.1219.



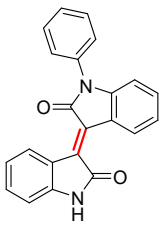
**4i**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.59 (s, 1H), 10.96 (s, 1H), 9.11 – 8.98 (m, 2H), 7.48 – 7.25 (m, 2H), 7.05 (t, $J$ = 8.2 Hz, 1H), 7.01 – 6.95 (m, 1H), 6.84 (d, $J$ = 7.5 Hz, 1H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 168.8, 144.6, 137.0, 135.2, 133.4, 131.8, 131.1, 129.7, 128.2, 125.1, 124.2, 121.5, 121.4, 121.3, 119.6, 109.8; **IR** (neat $cm^{-1}$): 3084 1697 1637 1620 1489 1465 1325 1255 1201 1176 789; **HRMS**(ESI): calcd. for $C_{17}H_8F_3N_2O_3$: 345.0487 $[M-H]^-$, found: 345.0491.



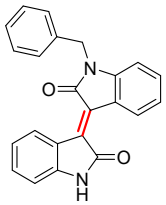
**4j**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.53 (d, $J$ = 1.7 Hz, 1H), 9.29 (s, 1H), 9.19 (d, $J$ = 8.0 Hz, 1H), 7.63 – 7.58 (m, 3H), 7.46 (d, $J$ = 8.4 Hz, 2H), 7.26 (m, 1H), 7.08 – 6.98 (m, 1H), 6.88 – 6.75 (m, 2H), 3.76 (t, $J$ = 7.4 Hz, 2H), 1.72 (dt, $J$ = 15.0, 7.6 Hz, 2H), 1.41 – 1.33 (m, 12H), 0.89 (t, $J$ = 7.0 Hz, 3H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 170.6, 167.9, 150.0, 144.0, 143.0, 138.2, 135.1, 134.2, 133.9, 132.6, 131.0, 130.4, 128.9, 126.5, 125.9, 122.6, 122.5, 122.1, 109.7, 108.2, 40.4, 34.6, 31.7, 31.5, 27.6, 26.9, 22.7, 14.2; **IR** (neat $cm^{-1}$): 2922 1691 1618 1608 1482 1385 1353 1333 1116 1020 811 744; **HRMS**(ESI): calcd. for $C_{32}H_{35}N_2O_2$: 479.2699 $[M+H]^+$, found: 479.2702.



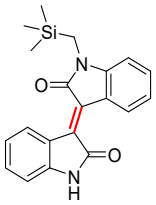
**4k**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.97 (s, 1H), 9.17 (d, $J$ = 8.0 Hz, 1H), 8.98 (d, $J$ = 8.0 Hz, 1H), 7.66 – 7.57 (m, 2H), 7.55 – 7.47 (m, 3H), 7.36 (dd, $J$ = 13.6, 7.1 Hz, 2H), 7.10 (t, $J$ = 7.8 Hz, 1H), 6.95 (t, $J$ = 7.8 Hz, 1H), 6.86 (d, $J$ = 7.8 Hz, 1H), 6.69 (d, $J$ = 7.9 Hz, 1H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 169.3, 167.7, 145.5, 142.6, 134.3, 134.0, 133.5, 132.9, 132.6, 130.6, 130.0, 129.9, 128.6, 127.3, 123.0, 122.6, 122.6, 121.7, 109.4, 109.2. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[5]



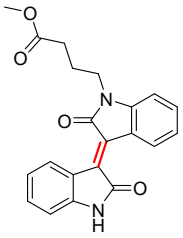
**4l**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.95 (s, 1H), 9.11 (dd, $J$ = 7.9, 4.6 Hz, 2H), 7.42 – 7.30 (m, 6H), 7.30 – 7.22 (m, 1H), 7.00 (m, 3H), 6.85 (d, $J$ = 7.8 Hz, 1H), 5.02 (s, 2H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 168.8, 167.4, 144.4, 143.9, 136.3, 134.3, 133.1, 132.5, 131.8, 129.6, 129.2, 128.7, 127.5, 127.3, 121.9, 121.6, 121.2, 120.9, 109.7, 109.0, 42.7. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[5]



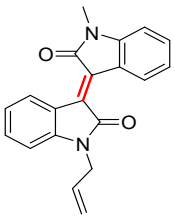
**4m**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.19 (d, $J$ = 8.0 Hz, 1H), 9.09 (d, $J$ = 8.0 Hz, 1H), 7.81 (s, 1H), 7.32 (dt, $J$ = 11.5, 7.7 Hz, 2H), 7.04 (dd, $J$ = 17.4, 8.1 Hz, 2H), 6.81 (d, $J$ = 7.7 Hz, 1H), 6.71 (d, $J$ = 7.8 Hz, 1H), 3.30 (s, 2H), 0.14 (s, 9H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 169.6, 167.4, 145.7, 142.4, 134.2, 133.1, 132.5, 132.5, 130.1, 129.6, 122.7, 122.6, 122.3, 121.9, 109.4, 108.3, 31.5, -1.2; **IR** (neat cm$^{-1}$): 2916 1691 1608 1464 1384 1354 1330 1103 1049 855 742; **HRMS**(ESI): calcd. for $C_{20}H_{21}N_2O_2Si$: 349.1372 $[M+H]^+$, found: 349.1367.



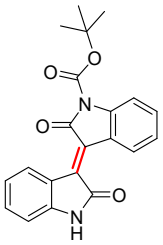
**4n**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.91 (s, 1H), 9.07 (dd, $J$ = 16.7, 7.5 Hz, 2H), 7.42 (td, $J$ = 7.7, 1.1 Hz, 1H), 7.34 (m, 1H), 7.08 (d, $J$ = 7.7 Hz, 1H), 7.06 – 7.00 (m, 1H), 6.99 – 6.94 (m, 1H), 6.84 (d, $J$ = 7.5 Hz, 1H), 3.79 (t, $J$ = 7.0 Hz, 2H), 3.54 (s, 3H), 2.41 (t, $J$ = 7.2 Hz, 2H), 1.88 (m, 2H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 172.9, 168.9, 167.2, 144.3, 144.2, 133.9, 132.9, 132.6, 132.2, 129.5, 129.1, 121.7, 121.7, 121.2, 120.9, 109.6, 108.5, 51.3, 38.6, 30.5, 22.3; **IR** (neat cm$^{-1}$): 2916 1728 1693 1608 1464 1384 1366 1329 1199 1107 776; **HRMS**(ESI): calcd. for $C_{21}H_{19}N_2O_4$: 363.1345 $[M+H]^+$, found: 363.1342.



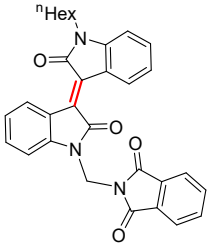
**4o**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.20 (td, $J$ = 8.0, 0.7 Hz, 2H), 7.34 (m, 2H), 7.12 – 6.99 (m, 2H), 6.77 (d, $J$ = 7.8 Hz, 2H), 5.88 (m, 1H), 5.31 – 5.15 (m, 2H), 4.41 (dt, $J$ = 5.2, 1.6 Hz, 2H), 3.27 (d, $J$ = 2.2 Hz, 3H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 168.1, 167.8, 145.4, 144.5, 133.7, 133.3, 132.6, 132.4, 131.3, 130.1, 130.0, 122.5, 122.5, 121.7, 121.7, 117.7, 108.5, 107.8, 42.4, 26.3; **IR** (neat cm$^{-1}$): 3282 1692 1608 1468 1358 1108 772; **HRMS**(ESI): calcd. for $C_{20}H_{17}N_2O_2$: 317.1290 $[M+H]^+$, found: 317.1285.



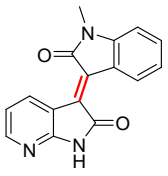
**4p**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.14 (d, $J$ = 8.1 Hz, 1H), 8.94 (d, $J$ = 8.0 Hz, 1H), 7.82 (d, $J$ = 8.4 Hz, 2H), 7.43 (t, $J$ = 7.9 Hz, 1H), 7.32 (t, $J$ = 7.6 Hz, 1H), 7.18 (t, $J$ = 7.8 Hz, 1H), 7.04 (t, $J$ = 7.8 Hz, 1H), 6.80 (d, $J$ = 7.8 Hz, 1H), 1.68 (s, 9H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 169.0, 166.2, 148.9, 142.8, 141.1, 136.3, 134.1, 133.1, 133.0, 130.4, 129.1, 124.2, 122.6, 122.4, 122.0, 114.3, 109.6, 84.9, 28.3; **IR** (neat cm$^{-1}$): 2920 1698 1619 1462 1385 1254 1099 774 742; **HRMS**(ESI): calcd. for $C_{21}H_{18}N_2NaO_4$: 385.1164 $[M+Na]^+$, found: 385.1159.



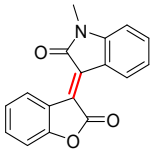
**4q**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.22 (m, 2H), 7.91 – 7.85 (m, 2H), 7.78 – 7.72 (m, 2H), 7.42 – 7.34 (m, 2H), 7.28 (s, 1H), 7.13 – 7.04 (m, 2H), 6.80 (t, $J$ = 6.0 Hz, 1H), 5.77 (d, $J$ = 5.6 Hz, 2H), 3.79 – 3.74 (m, 2H), 1.71 (dd, $J$ = 14.6, 7.1 Hz, 2H), 1.35 – 1.31 (m, 4H), 0.91 – 0.87 (m, 3H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 167.7, 167.5, 144.9, 142.8, 134.6, 134.5, 134.4, 132.7, 132.7, 132.4, 131.8, 130.4, 130.0, 123.9, 123.0, 122.4, 121.8, 121.7, 108.9, 107.9, 42.4, 40.2, 31.6, 27.5, 26.8, 22.6, 14.1; **IR** (neat cm$^{-1}$): 2928 1725 1694 1609 1467 1328 1098 776 749; **HRMS**(ESI): calcd. for $C_{31}H_{28}N_3O_4$: 506.2080 $[M+H]^+$, found: 506.2074.



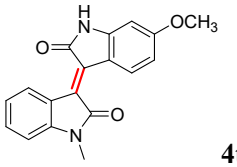
**4r**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.53 (s, 1H), 9.32 (d, $J$ = 7.2 Hz, 1H), 9.10 (d, $J$ = 7.1 Hz, 1H), 8.18 (s, 1H), 7.45 (s, 1H), 7.03 (s, 3H), 3.21 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 168.5, 167.2, 157.7, 150.1, 145.4, 136.6, 133.6, 133.2, 131.4, 129.3, 122.0, 120.5, 117.7, 116.2, 108.6, 26.1. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[8]



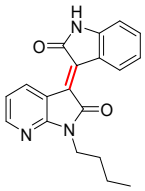
**4s**

Red solid. **$^1$H NMR** (600 MHz, $CDCl_3$) $\delta$ 9.32 – 9.24 (m, 1H), 9.03 (d, $J$ = 8.0 Hz, 1H), 7.50 – 7.43 (m, 1H), 7.43 – 7.36 (m, 1H), 7.24 – 7.19 (m, 1H), 7.15 – 7.02 (m, 2H), 6.80 (dd, $J$ = 15.3, 7.9 Hz, 1H), 3.29 (d, $J$ = 5.3 Hz, 3H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 167.6, 167.6, 155.6, 145.9, 135.5, 133.7, 133.5, 130.1, 130.0, 127.3, 124.3, 122.9, 110.6, 108.2, 26.3. **IR** (neat cm$^{-1}$): 3132 1779 1699 1613 1474 1457 1326 1078 774 744; **HRMS**(ESI): calcd. for $C_{20}H_{17}N_2O_2$: 278.0817 $[M+H]^+$, found: 278.0811.



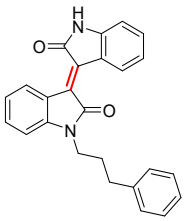
**4t**

Red solid. **$^1$H NMR** (600 MHz, DMSO-$d_6$) $\delta$ 10.87 (s, 1H), 9.07 (dd, $J$ = 30.7, 8.4 Hz, 2H), 7.39 (t, $J$ = 7.7 Hz, 1H), 7.02 (dd, $J$ = 13.3, 7.7 Hz, 2H), 6.54 (dd, $J$ = 9.0, 2.5 Hz, 1H), 6.39 (d, $J$ = 2.4 Hz, 1H), 3.83 (s, 3H), 3.23 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 169.7, 167.5, 163.3, 146.6, 144.2, 133.5, 131.6, 128.6, 128.3, 121.6, 121.0, 114.8, 108.3, 106.9, 95.6, 55.6, 26.0. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[8]



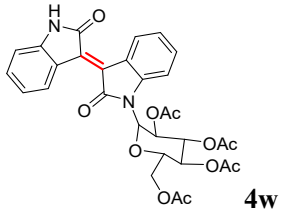
**4u**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 10.97 (s, 1H), 9.32 (d, $J$ = 7.8 Hz, 1H), 9.11 (d, $J$ = 8.0 Hz, 1H), 8.25 (d, $J$ = 4.9 Hz, 1H), 7.38 (t, $J$ = 7.6 Hz, 1H), 7.11 – 7.05 (m, 1H), 6.99 (d, $J$ = 7.5 Hz, 1H), 6.86 (d, $J$ = 7.7 Hz, 1H), 3.82 (t, $J$ = 7.0 Hz, 2H), 1.68 (dd, $J$ = 14.7, 7.3 Hz, 2H), 1.33 (dd, $J$ = 14.0, 6.7 Hz, 2H), 0.92 (t, $J$ = 6.9 Hz, 3H); **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ 168.9, 167.0, 156.7, 149.5, 144.7, 136.3, 135.2, 133.5, 129.8, 129.6, 121.4, 121.3, 118.0, 115.7, 109.8, 29.2, 19.6, 13.6. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[9]



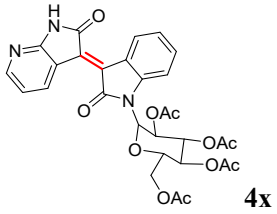
**4v**

Red solid. **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 9.18 (d, $J$ = 8.2 Hz, 1H), 9.10 (d, $J$ = 8.0 Hz, 1H), 7.61 (d, $J$ = 11.1 Hz, 1H), 7.36 – 7.26 (m, 4H), 7.22 – 7.18 (m, 3H), 7.05 (ddd, $J$ = 7.9, 5.6, 1.1 Hz, 2H), 6.81 (d, $J$ = 7.3 Hz, 1H), 6.69 (d, $J$ = 7.5 Hz, 1H), 3.88 – 3.80 (m, 2H), 2.80 – 2.71 (m, 2H), 2.11 – 2.03 (m, 2H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 169.5, 167.9, 144.6, 142.5, 141.0, 133.8, 133.4, 132.5, 132.5, 130.1, 129.9, 128.5, 128.3, 126.1, 122.5, 122.4, 122.3, 121.7, 109.4, 107.9, 39.7, 33.3, 28.9. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[8]



**4w**

Red solid. **$^1$H NMR** (600 MHz, $CDCl_3$) $\delta$ 9.14 (d, $J$ = 8.1 Hz, 1H), 9.02 (d, $J$ = 8.1 Hz, 1H), 7.57 (s, 1H), 7.40 (t, $J$ = 7.7 Hz, 1H), 7.33 (t, $J$ = 7.6 Hz, 1H), 7.19 (d, $J$ = 7.5 Hz, 1H), 7.12 (t, $J$ = 7.8 Hz, 1H), 7.05 (t, $J$ = 7.8 Hz, 1H), 6.81 (d, $J$ = 7.7 Hz, 1H), 5.80 (d, $J$ = 69.0 Hz, 2H), 5.42 (t, $J$ = 9.4 Hz, 1H), 5.36 – 5.24 (m, 1H), 4.29 – 4.20 (m, 2H), 4.02 – 3.86 (m, 1H), 2.10 (d, $J$ = 6.8 Hz, 6H), 2.02 (s, 3H), 1.86 (s, 3H); **$^{13}$C NMR** (151 MHz, $CDCl_3$) $\delta$ 170.7, 170.2, 169.7, 169.3, 169.1, 167.7, 142.8, 134.4, 133.1, 132.8, 132.3, 130.1, 129.8, 123.3, 122.5, 122.5, 121.7, 109.6, 79.7, 74.9, 73.7, 68.1, 67.7, 61.9, 31.1, 20.9, 20.8, 20.7, 20.5. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[10]



**4x**

Red solid. **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ 11.56 (s, 1H), 9.15 (t, $J$ = 9.0 Hz, 2H), 8.20 (d, $J$ = 4.5 Hz, 1H), 7.49 (d, $J$ = 6.9 Hz, 2H), 7.09 (dt, $J$ = 12.7, 7.2 Hz, 2H), 6.09 (s, 1H), 5.58 (d, $J$ = 9.0 Hz, 2H), 5.32 (s, 1H), 4.37 (s, 1H), 4.15 (s, 2H), 2.03 (d, $J$ = 8.9 Hz, 6H), 1.97 (d, $J$ = 9.8 Hz, 3H), 1.77 (s, 3H); **$^{13}$C NMR** (151 MHz, DMSO-$d_6$) $\delta$ 170.1, 169.6, 169.4, 168.9, 168.3, 167.0, 157.9, 150.5, 136.5, 133.2, 132.5, 132.2, 129.1, 122.6, 120.7, 117.8, 116.1, 78.4, 73.1, 72.6, 67.8, 67.3, 61.9, 20.5, 20.5, 20.3, 20.0. All the resonances in $^1$H and $^{13}$C NMR spectrum were in good agreement with literature values.[11]

## 10. References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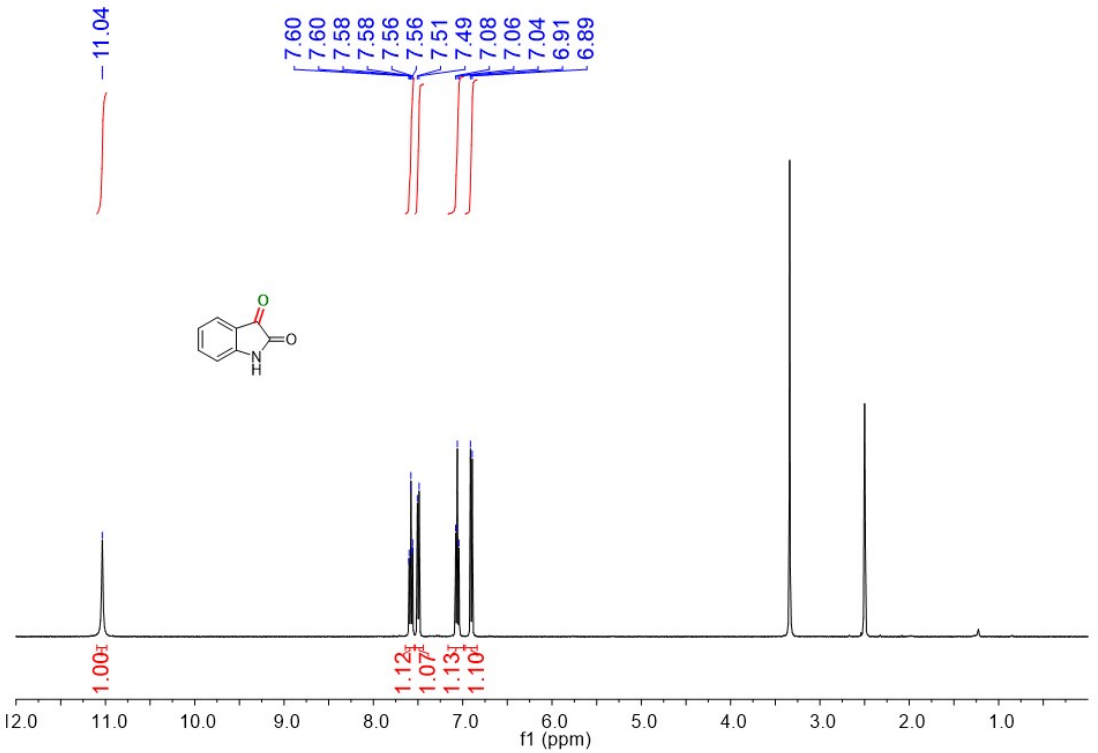
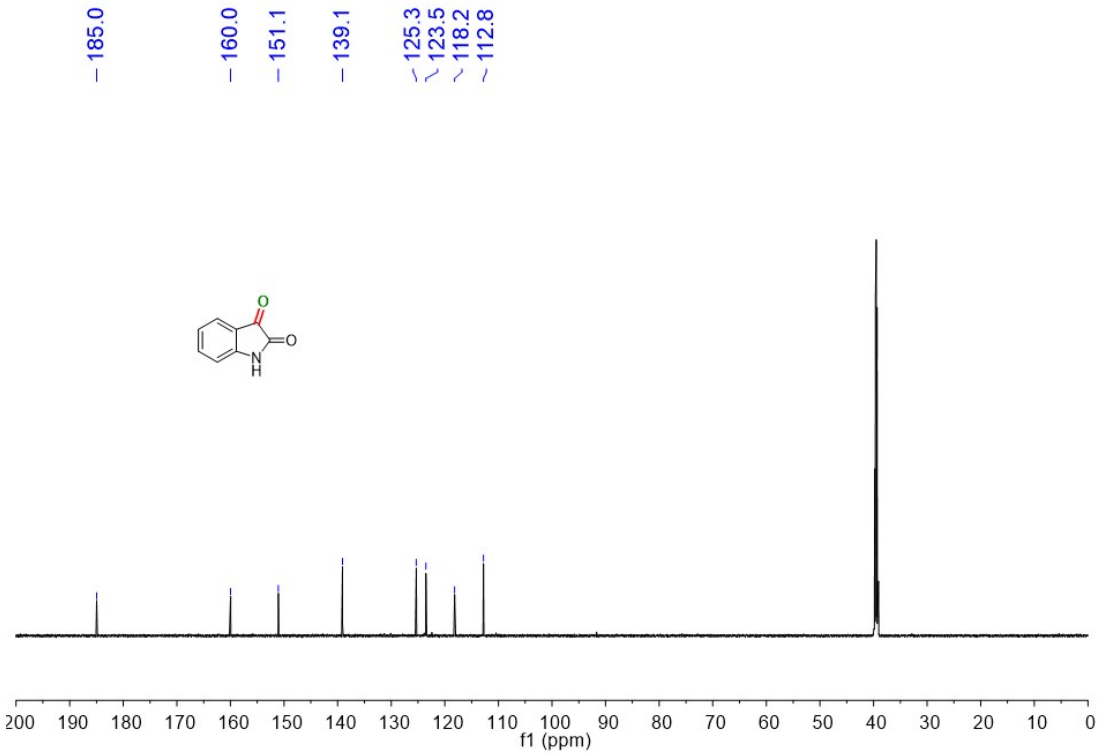
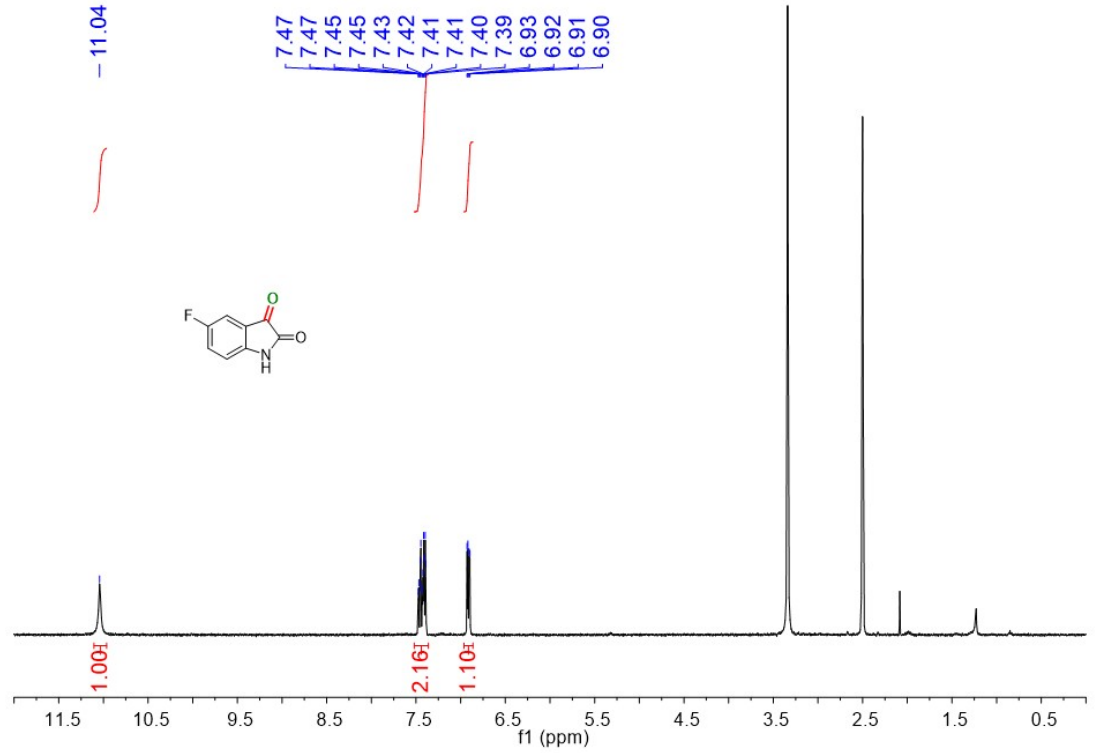
## 11. NMR spectrum




11.04
7.47
7.47
7.45
7.45
7.43
7.42
7.41
7.41
7.40
7.39
6.93
6.92
6.91
6.90
F
O
O
N
H
1.00
2.16
1.10
11.5
10.5
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7.5
6.5
5.5
4.5
3.5
2.5
1.5
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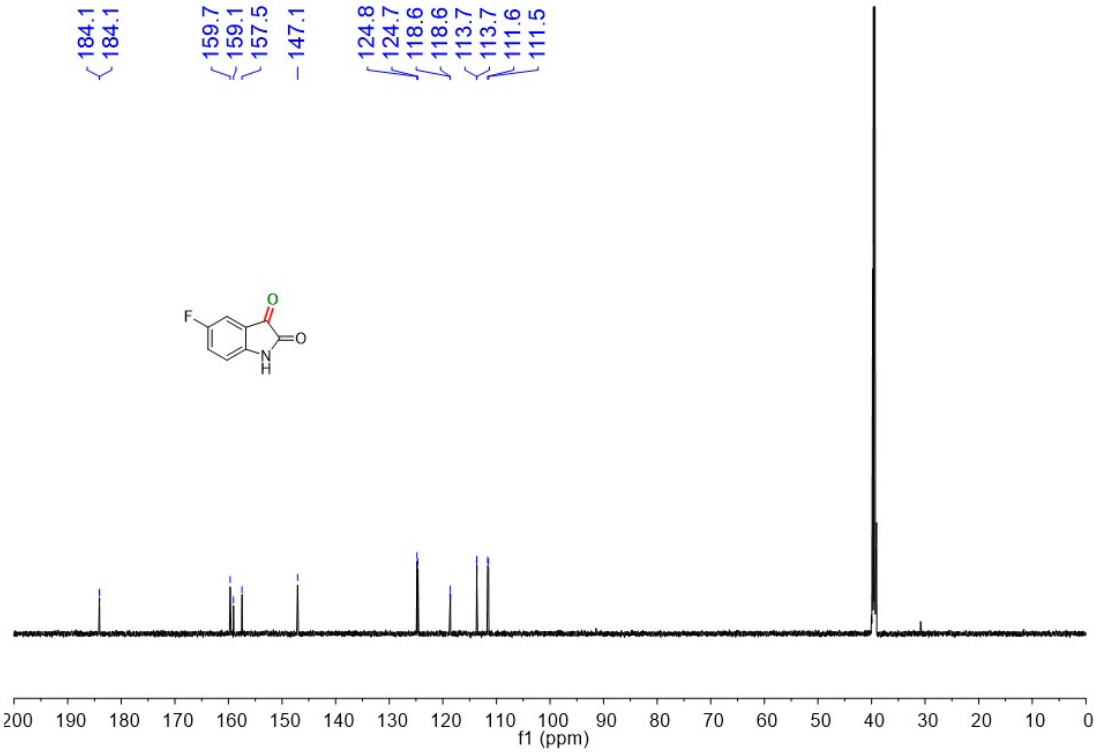
f1 (ppm)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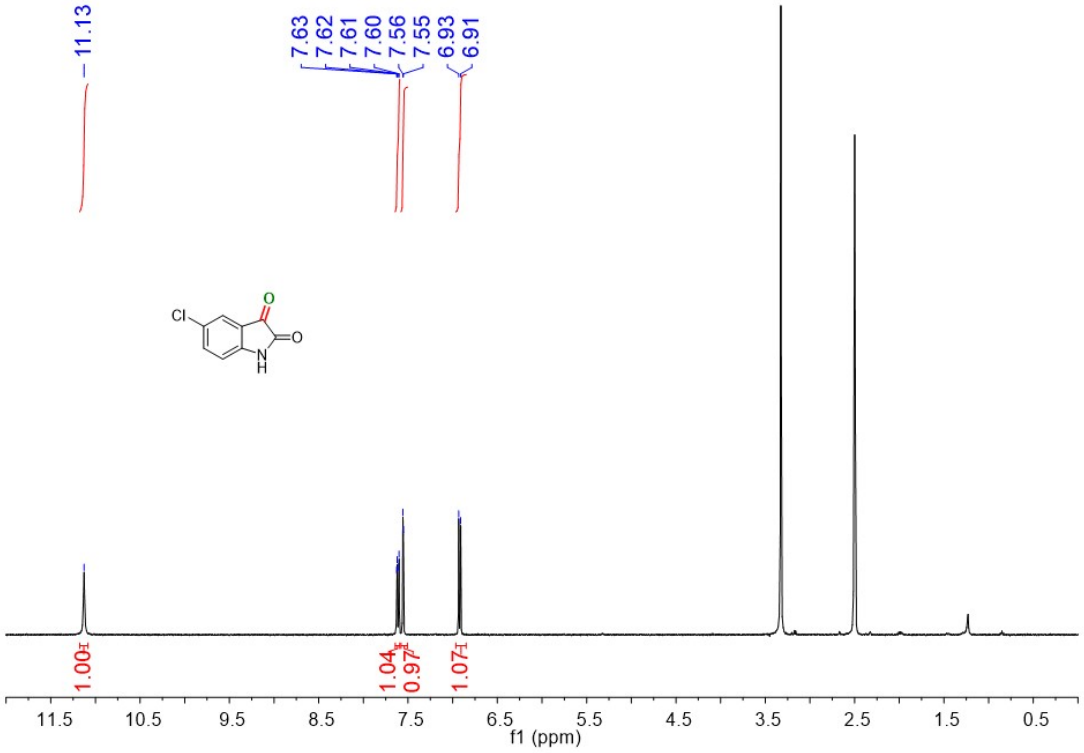
184.1
159.7
159.1
157.5
147.1
124.8
124.7
118.6
118.6
113.7
113.7
111.6
111.5
F
O
O
N
H
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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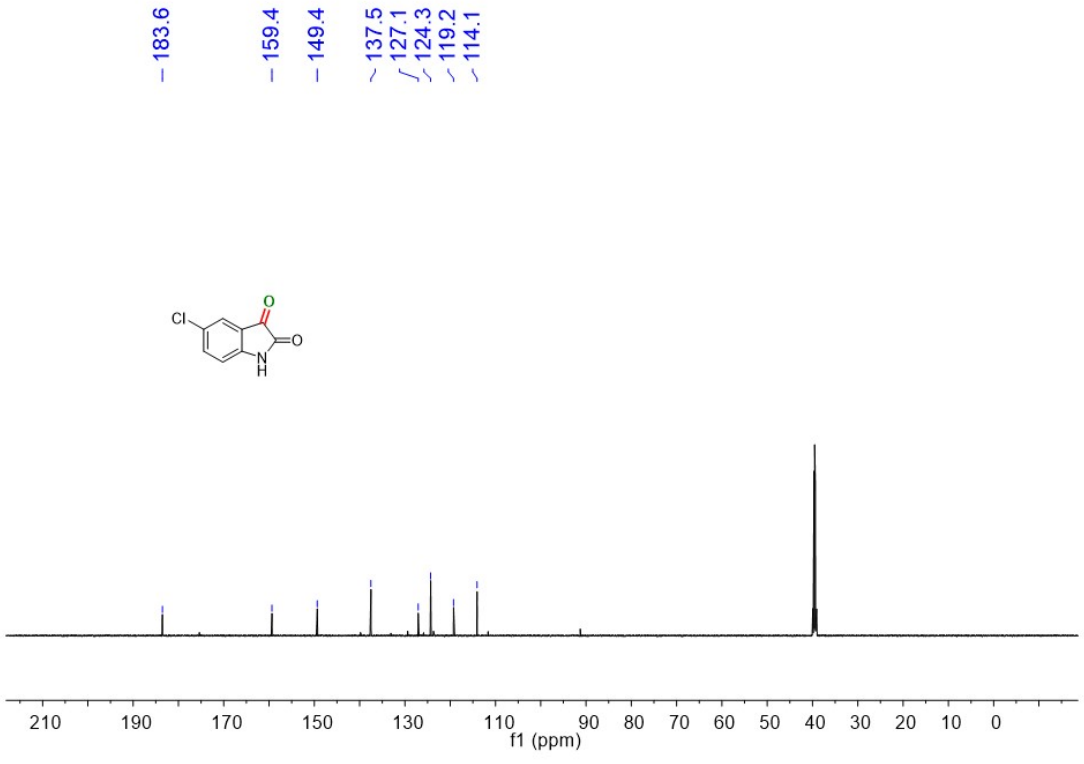
7.60
7.56
7.55
6.93
6.91
Cl
O
O
N
H
1.00
1.04
0.97
1.07
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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149.4
137.5
127.1
124.3
119.2
114.1
Cl
O
O
N
H
210
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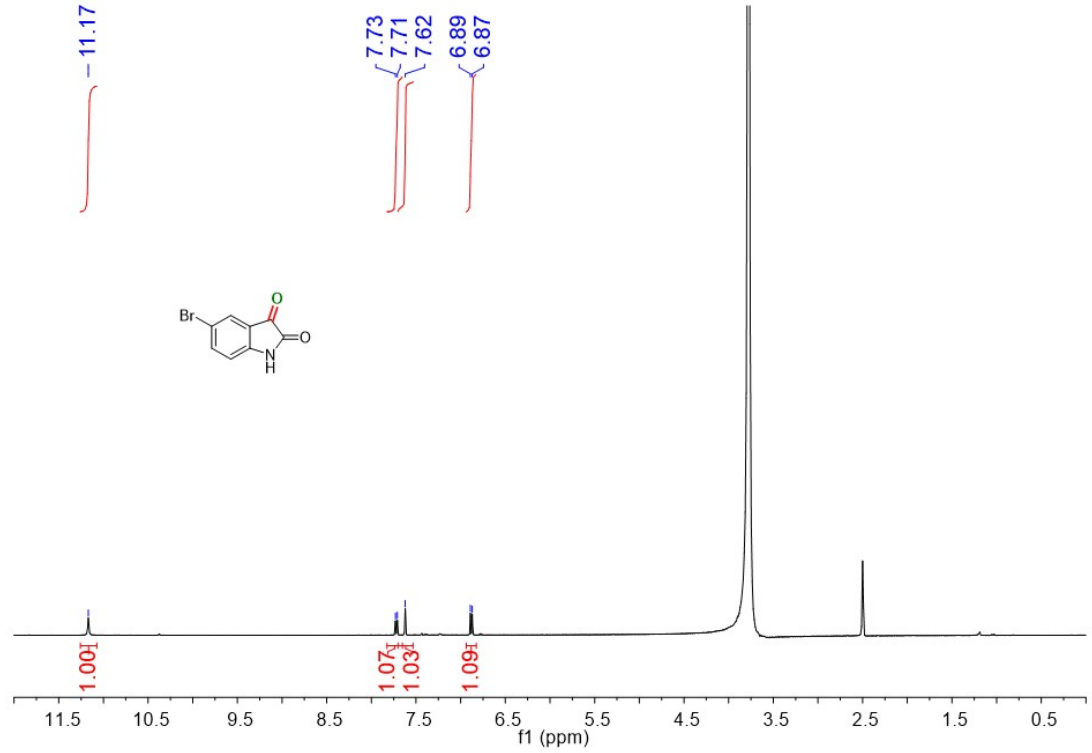
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.71
7.62
6.89
6.87
Br
O
O
N
H
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1.07
1.03
1.09
11.5
10.5
9.5
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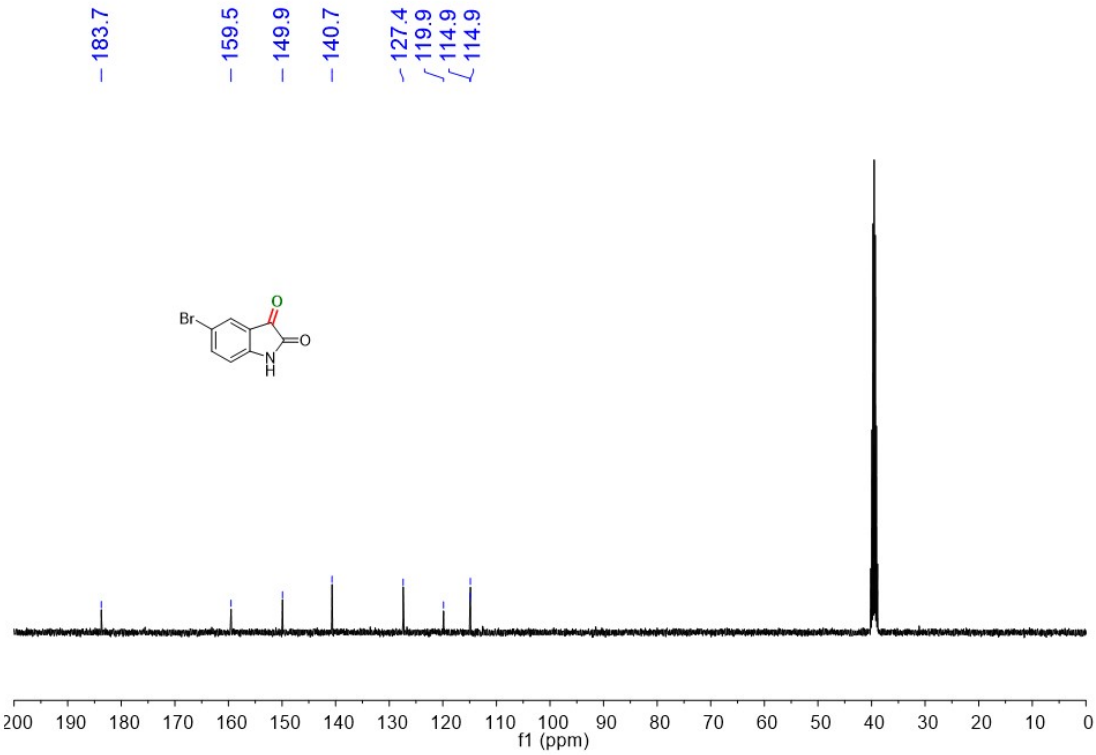
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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149.9
140.7
127.4
119.9
114.9
114.9
Br
O
O
N
H
200
190
180
170
160
150
140
130
120
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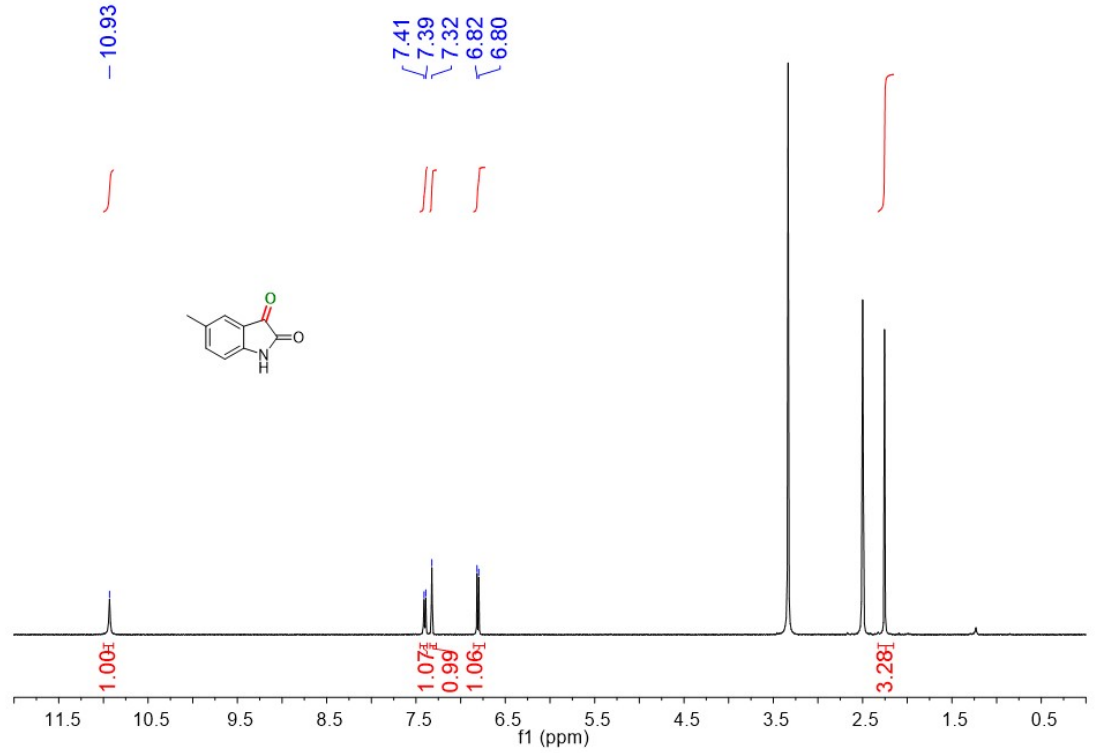
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.41
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6.82
6.80
1.00
1.07
0.99
1.06
3.28
11.5
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9.5
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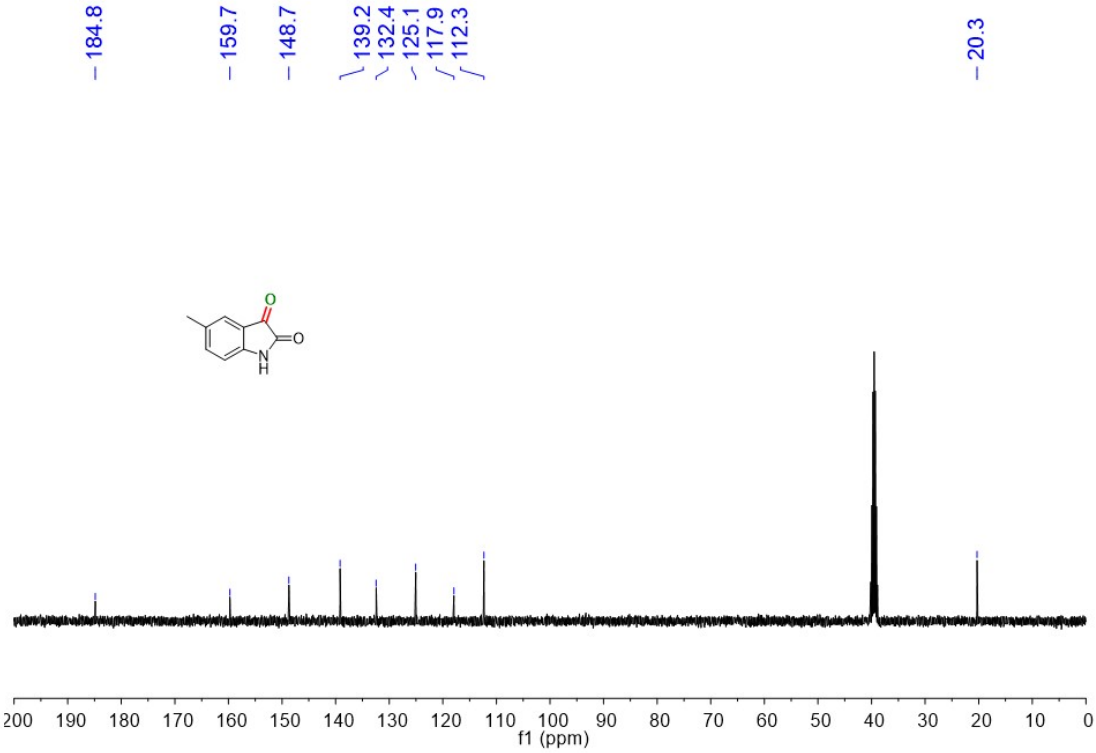
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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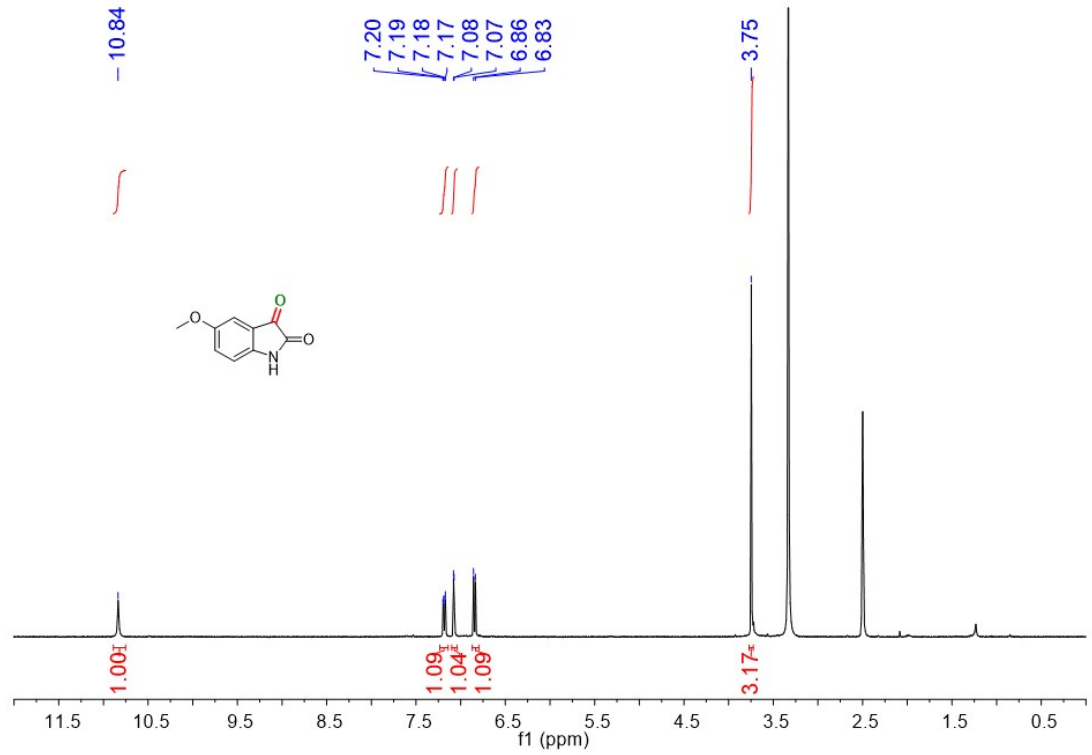
159.7
148.7
139.2
132.4
125.1
117.9
112.3
20.3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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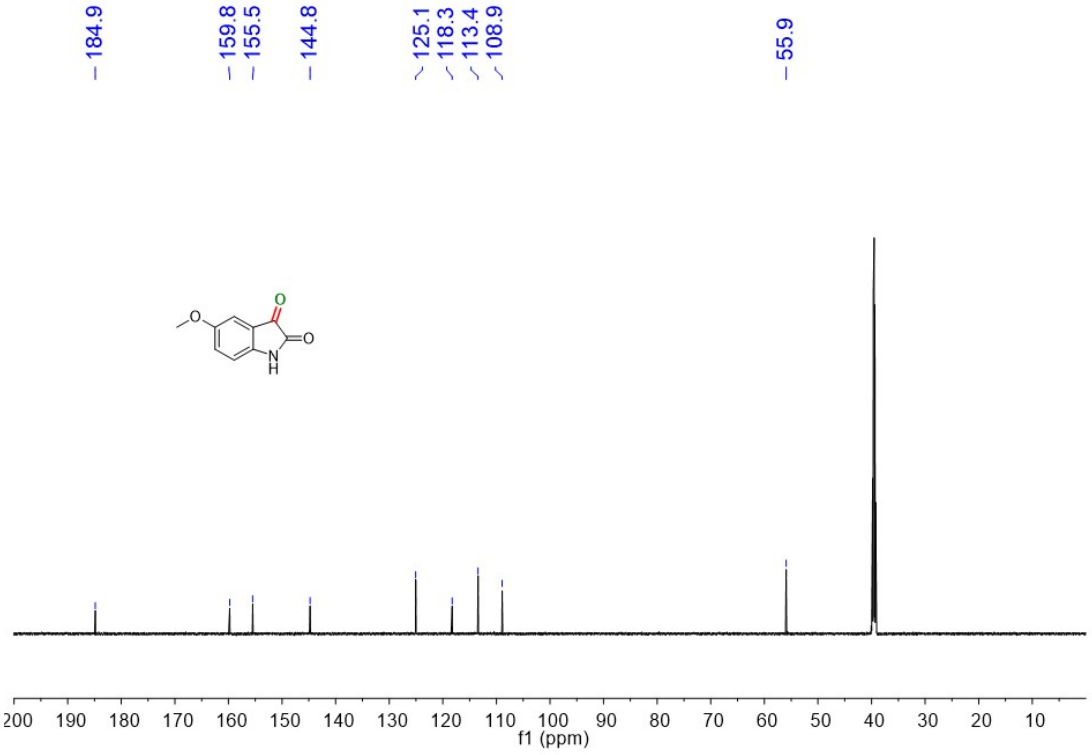
7.19
7.18
7.17
7.08
7.07
6.86
6.83
3.75
1.00
1.09
1.04
1.09
3.17
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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159.8
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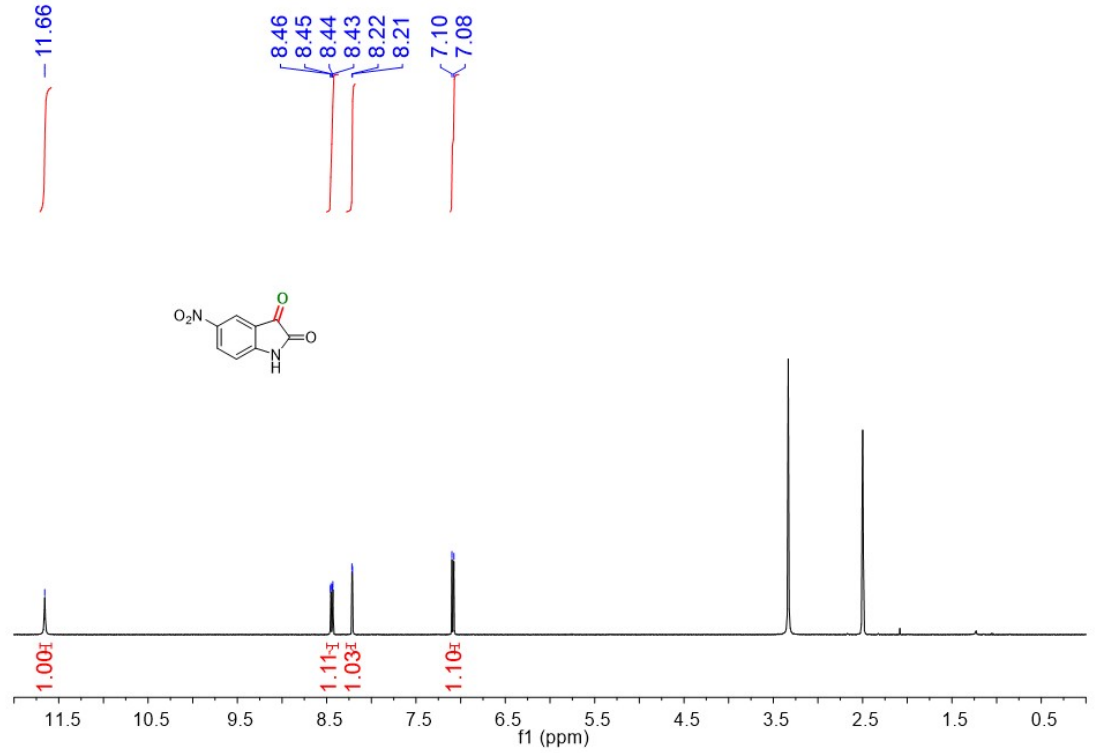
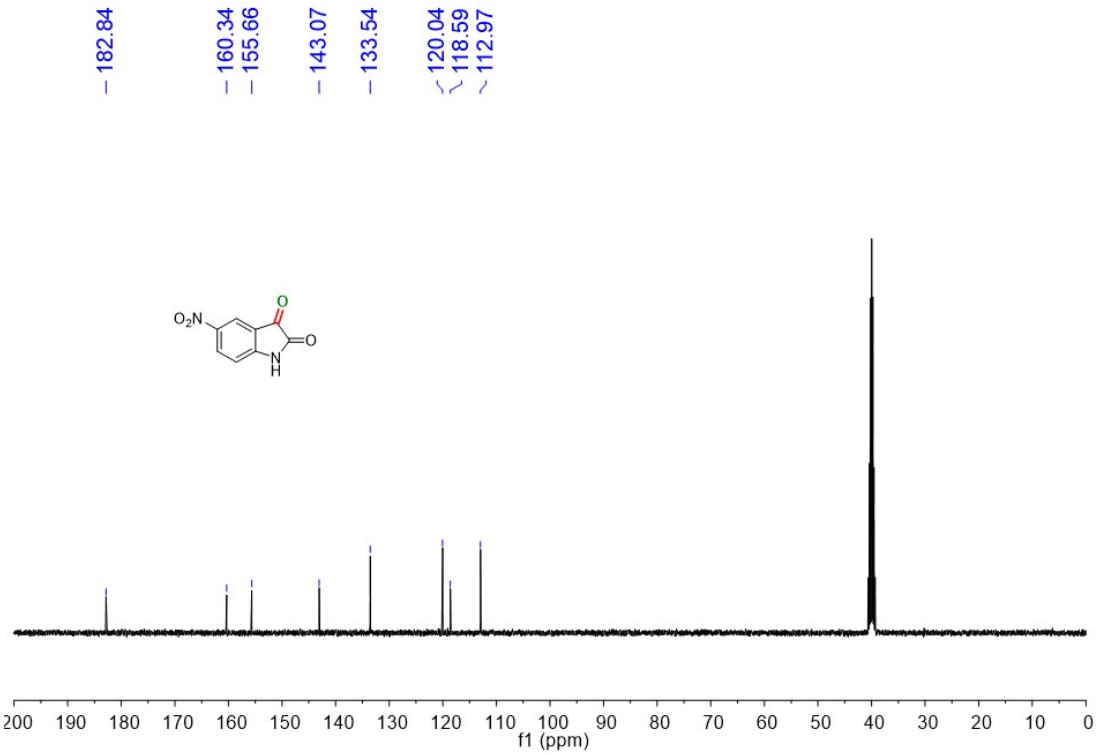
144.8
125.1
118.3
113.4
108.9
55.9
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


11.66
8.46
8.45
8.44
8.43
8.22
8.21
7.10
7.08
O2N
O
O
N
H
1.00
1.11
1.03
1.10
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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160.34
155.66
143.07
133.54
120.04
118.59
112.97
O2N
O
O
N
H
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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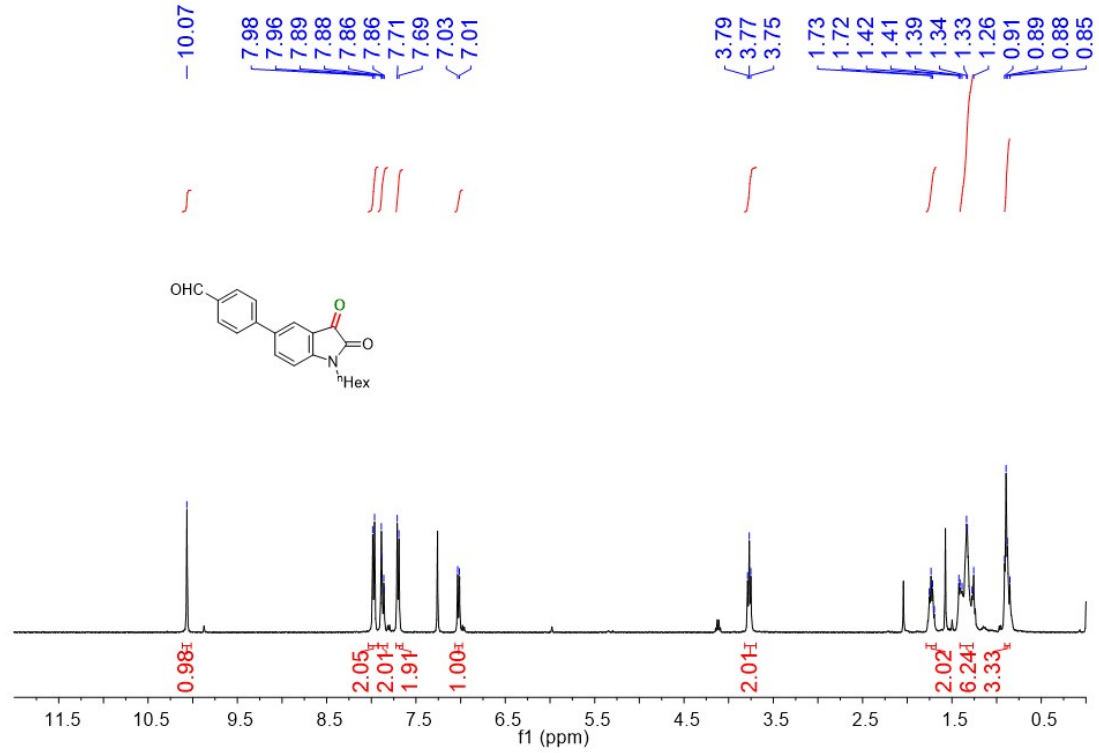
50
40
30
20
10
0
f1 (ppm)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7.96
7.89
7.88
7.86
7.86
7.71
7.69
7.03
7.01
3.79
3.77
3.75
1.73
1.72
1.42
1.41
1.39
1.34
1.33
1.26
0.91
0.89
0.88
0.85
OHC
O
O
N
nHex
0.98
2.05
2.01
1.91
1.00
2.01
2.02
6.24
3.33
11.5
10.5
9.5
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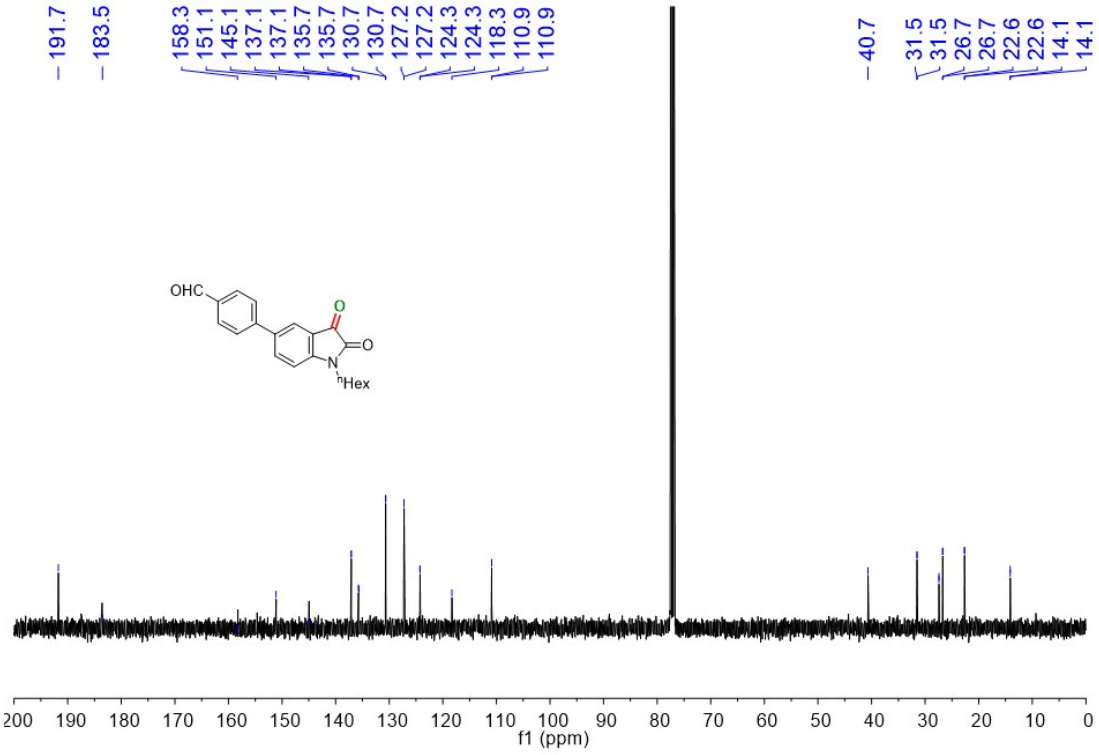
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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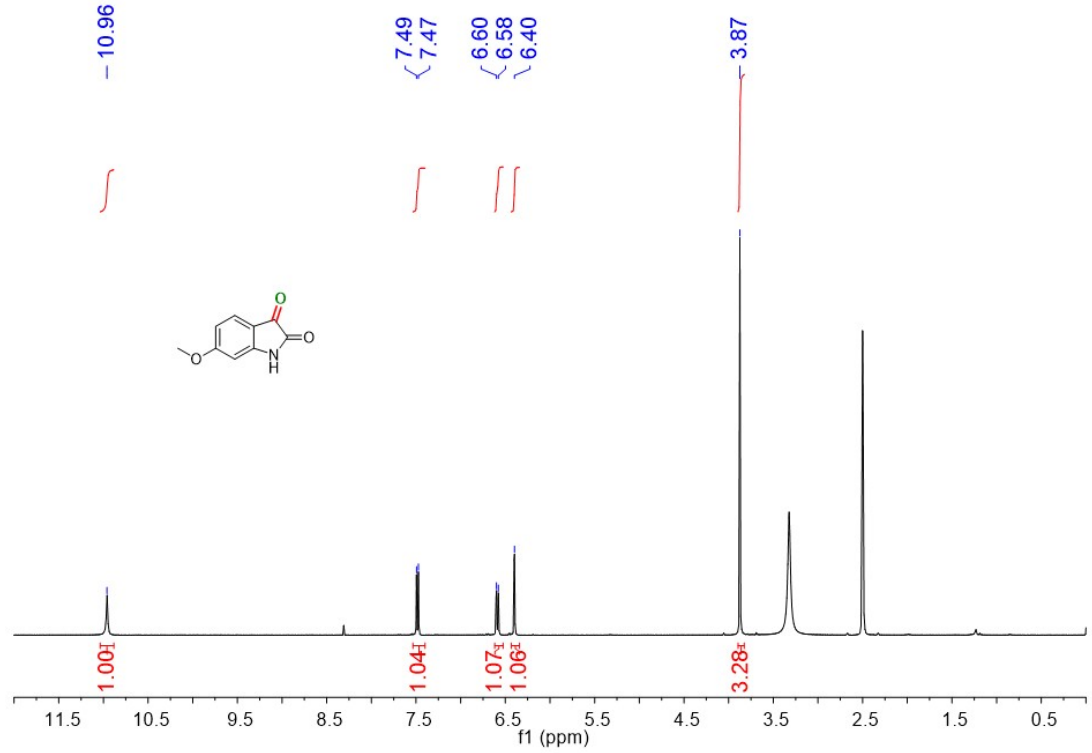
183.5
158.3
151.1
145.1
137.1
137.1
135.7
135.7
130.7
130.7
127.2
127.2
124.3
124.3
118.3
110.9
110.9
40.7
31.5
31.5
26.7
26.7
22.6
22.6
14.1
14.1
OHC
O
O
N
nHex
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.40
3.87
1.00
1.04
1.07
1.06
3.28
11.5
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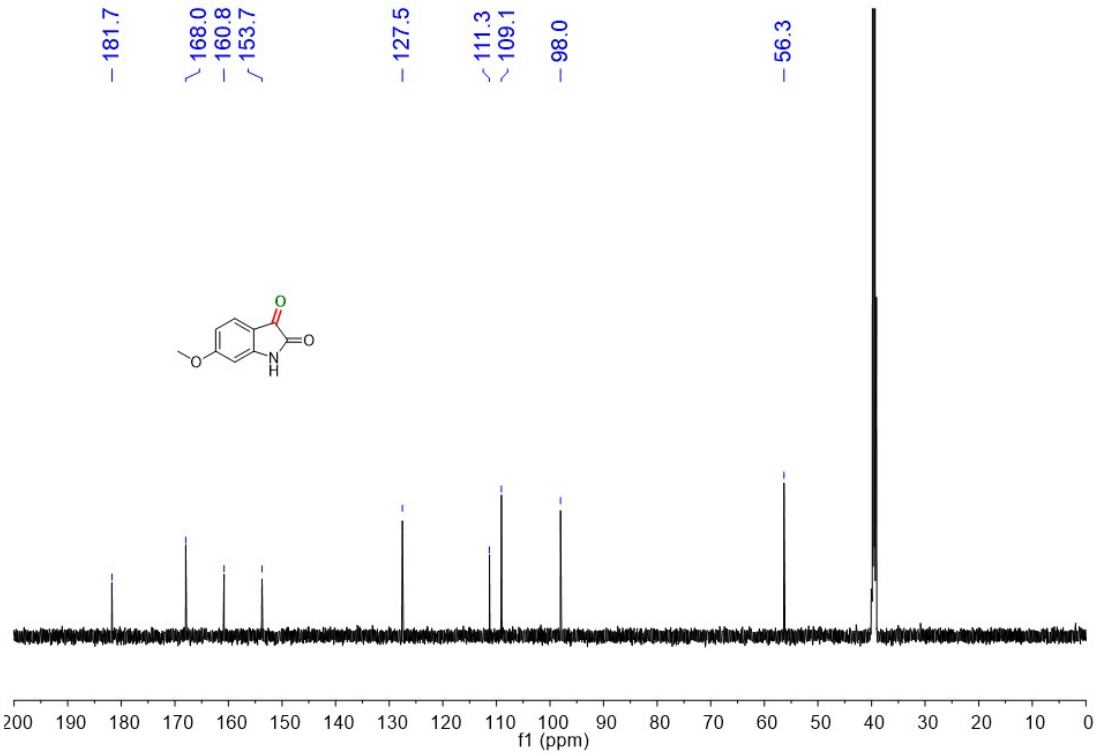
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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160.8
153.7
127.5
111.3
109.1
98.0
56.3
200
190
180
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160
150
140
130
120
110
100
90
80
70
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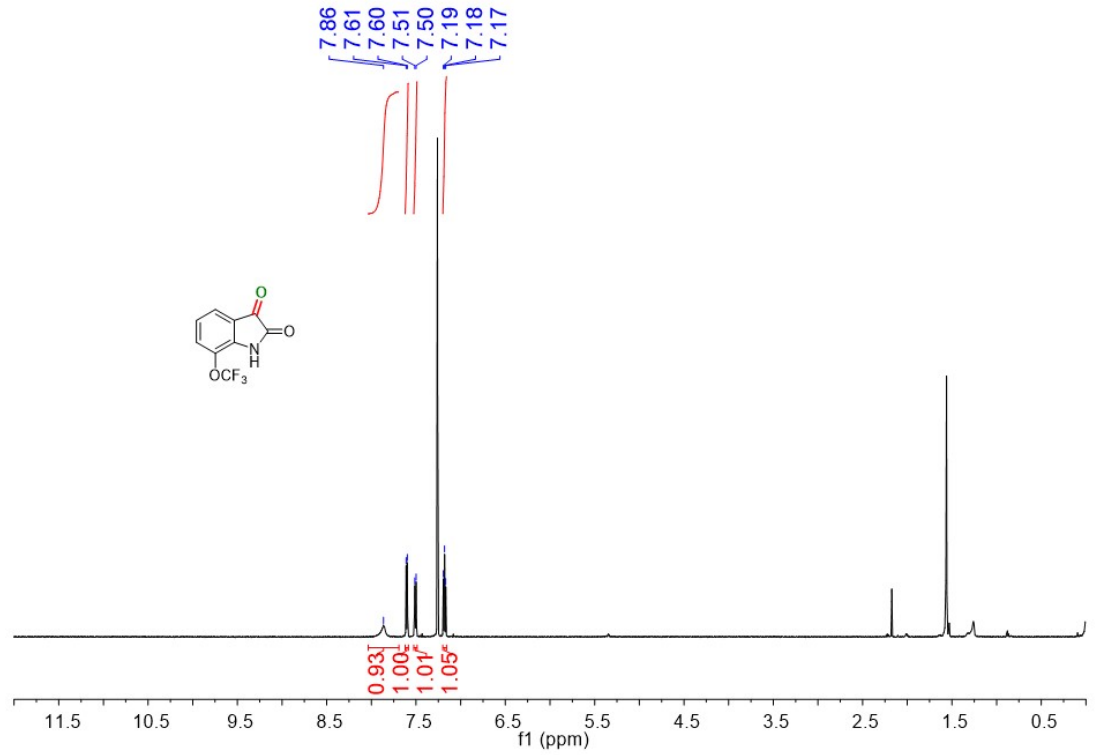
50
40
30
20
10
0
f1 (ppm)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7.50
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7.17
O
O
N
H
OCF3
0.93
1.00
1.01
1.05
11.5
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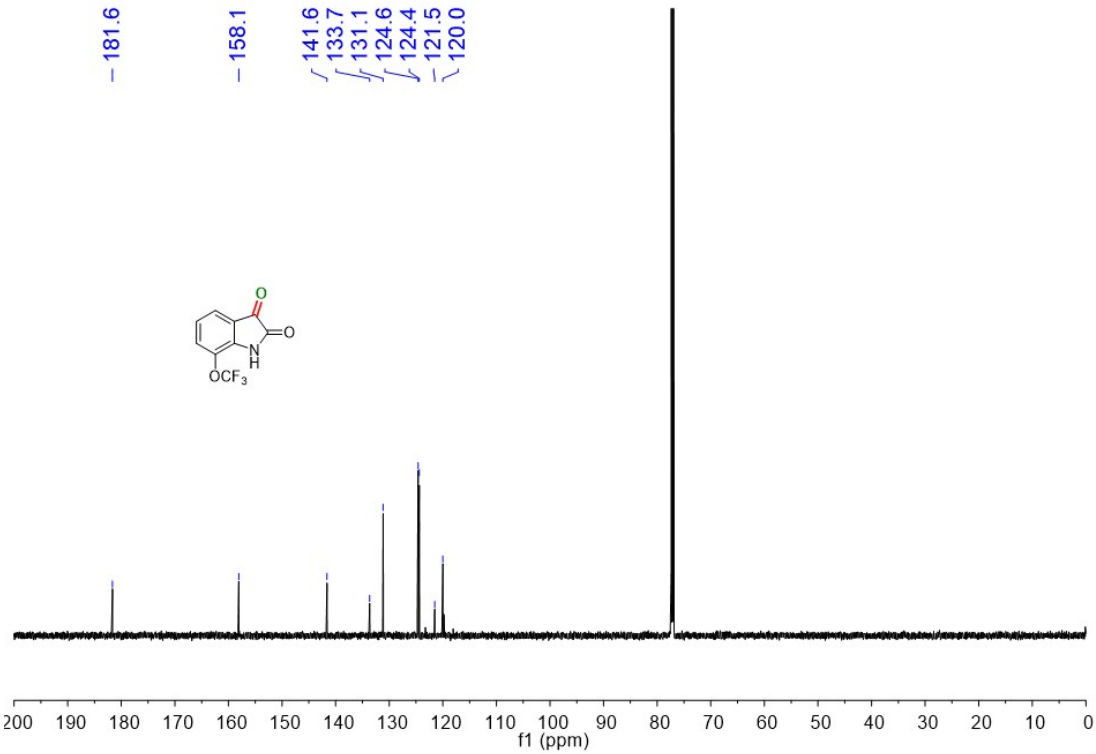
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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158.1
141.6
133.7
131.1
124.6
124.4
121.5
120.0
O
O
N
H
OCF3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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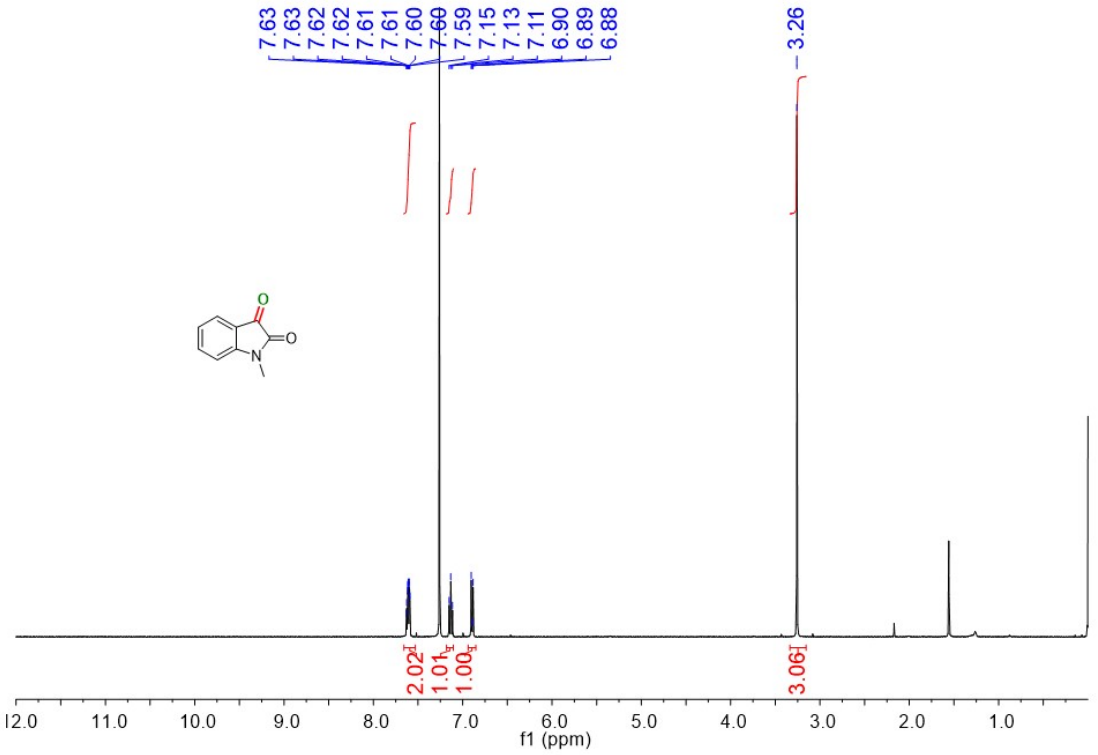
50
40
30
20
10
0
f1 (ppm)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7.63
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7.61
7.60
7.60
7.59
7.15
7.13
7.11
6.90
6.89
6.88
3.26
2.02
1.01
1.00
3.06
12.0
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10.0
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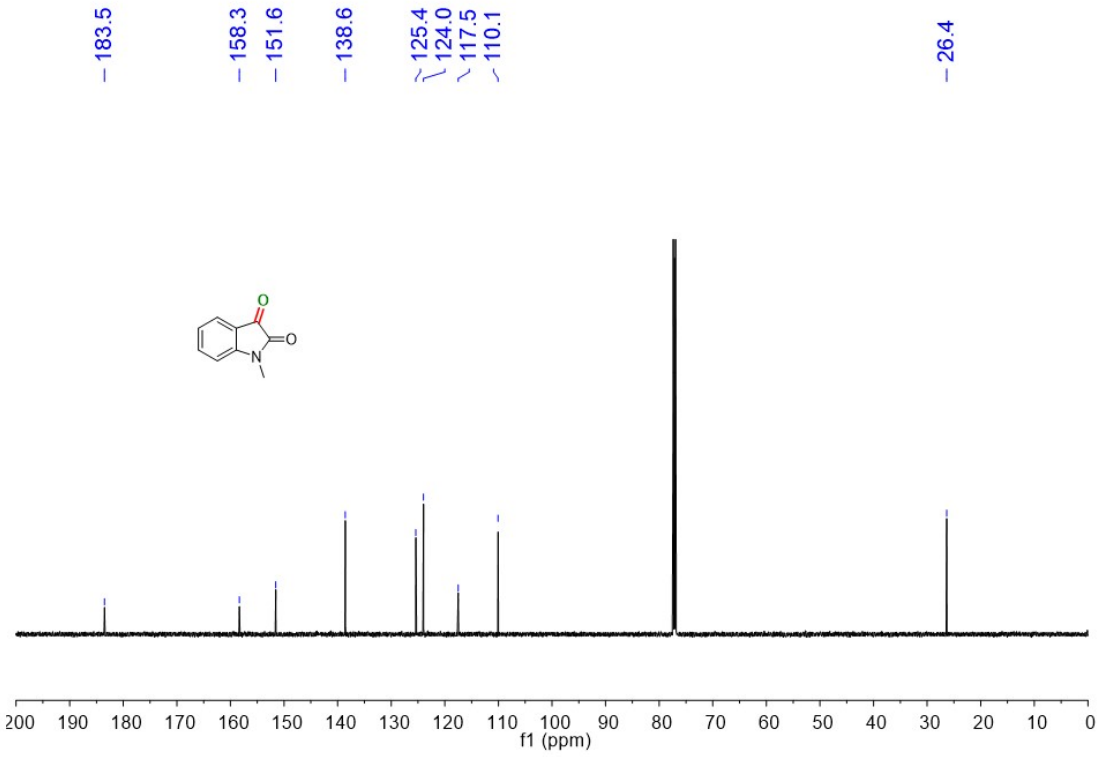
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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151.6
138.6
125.4
124.0
117.5
110.1
26.4
200
190
180
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110
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90
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50
40
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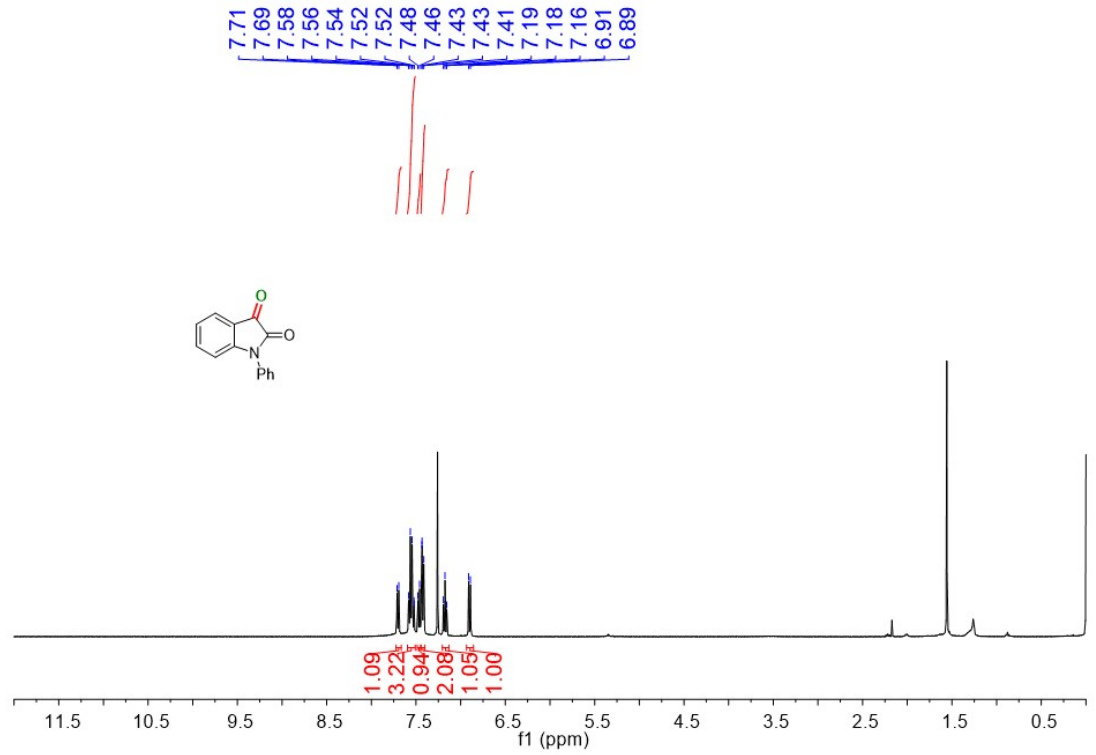
20
10
0
f1 (ppm)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7.43
7.41
7.19
7.18
7.16
6.91
6.89
O
O
N
Ph
1.09
3.22
0.94
2.08
1.05
1.00
11.5
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9.5
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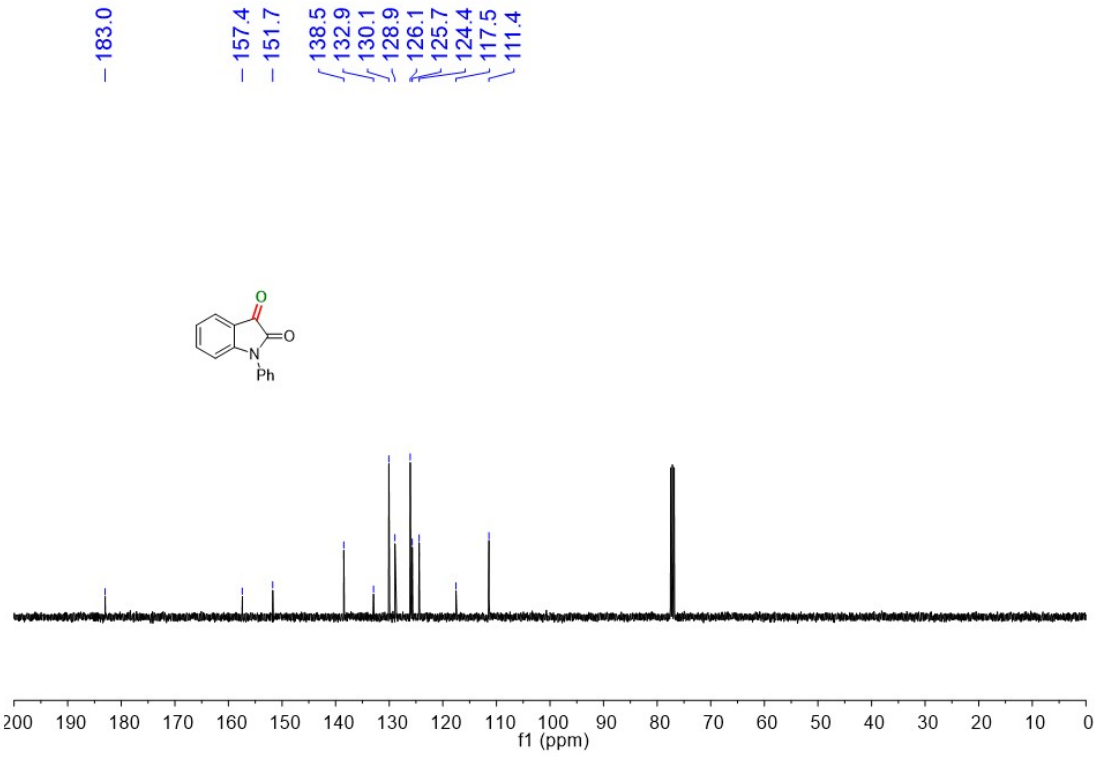
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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151.7
138.5
132.9
130.1
128.9
126.1
125.7
124.4
117.5
111.4
O
O
N
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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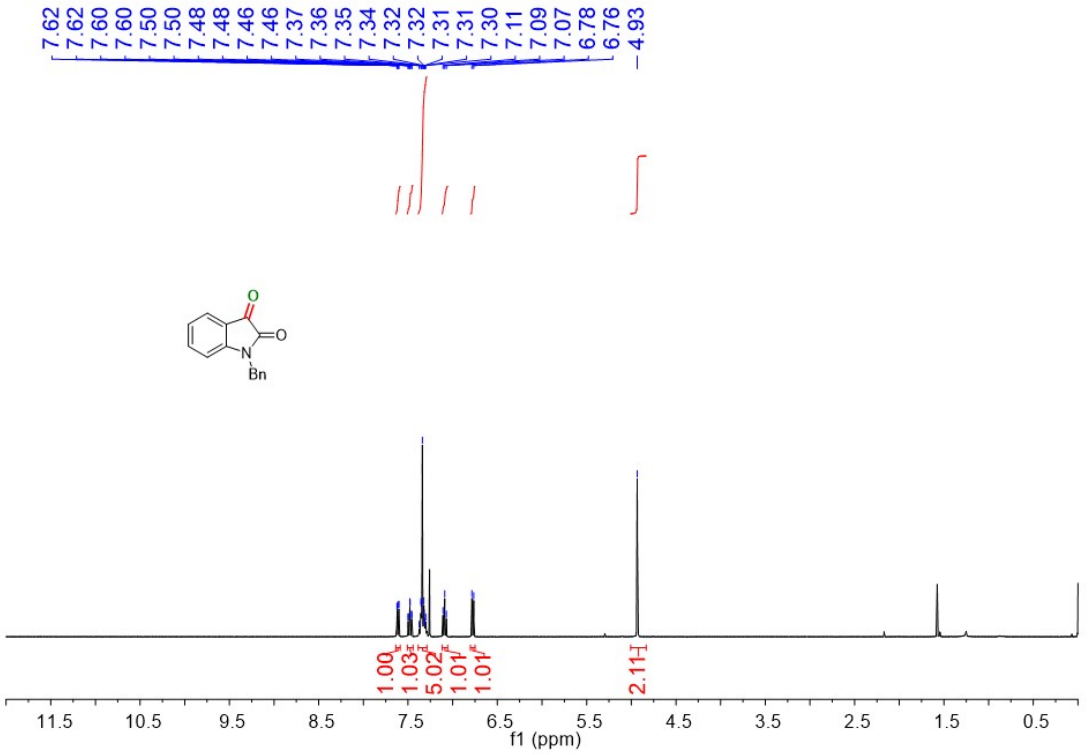
50
40
30
20
10
0
f1 (ppm)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7.48
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7.35
7.34
7.32
7.32
7.31
7.31
7.30
7.11
7.09
7.07
6.78
6.76
4.93
O
O
N
Bn
1.00
1.03
5.02
1.01
1.01
2.11
11.5
10.5
9.5
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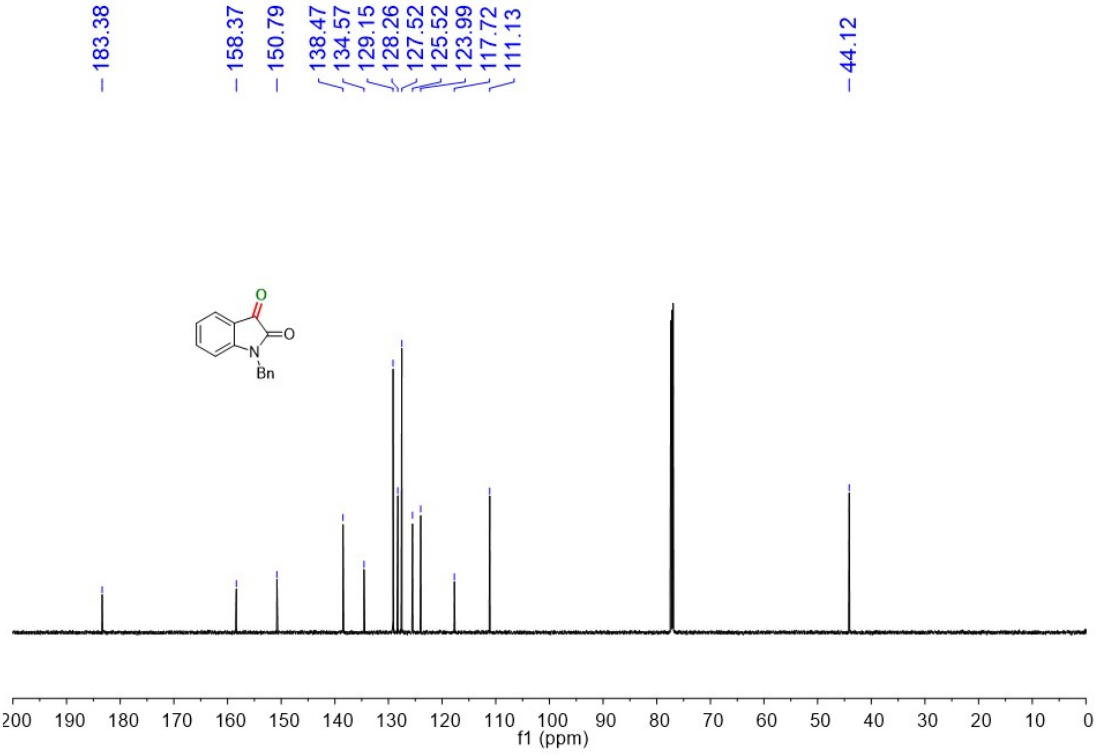
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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127.52
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123.99
117.72
111.13
44.12
O
O
N
Bn
200
190
180
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130
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110
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50
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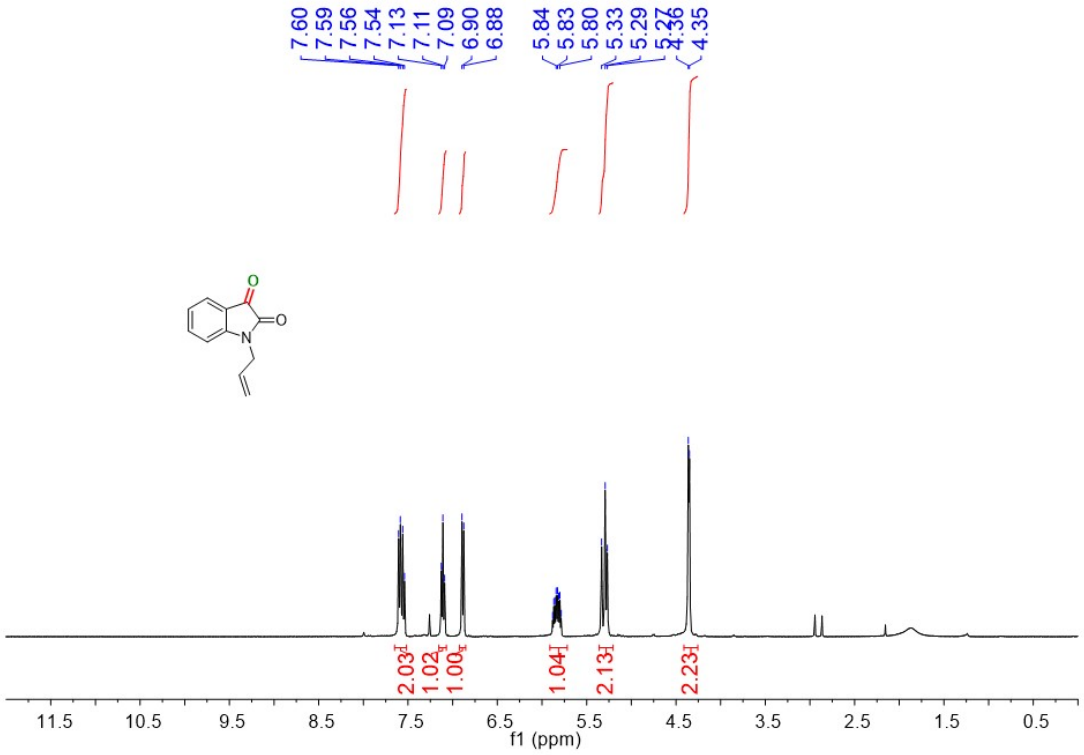
10
0
f1 (ppm)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7.59
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7.13
7.11
7.09
6.90
6.88
5.84
5.83
5.80
5.33
5.29
4.36
4.35
O
O
N
2.03
1.02
1.00
1.04
2.13
2.23
11.5
10.5
9.5
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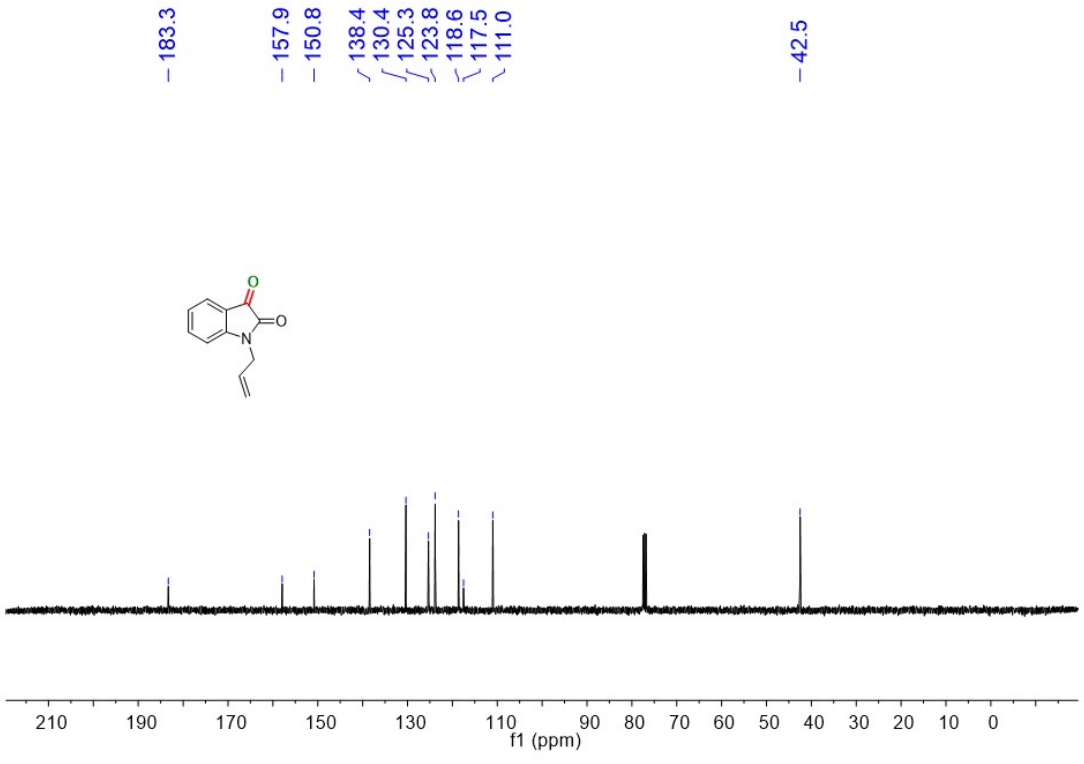
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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125.3
123.8
118.6
117.5
111.0
42.5
O
O
N
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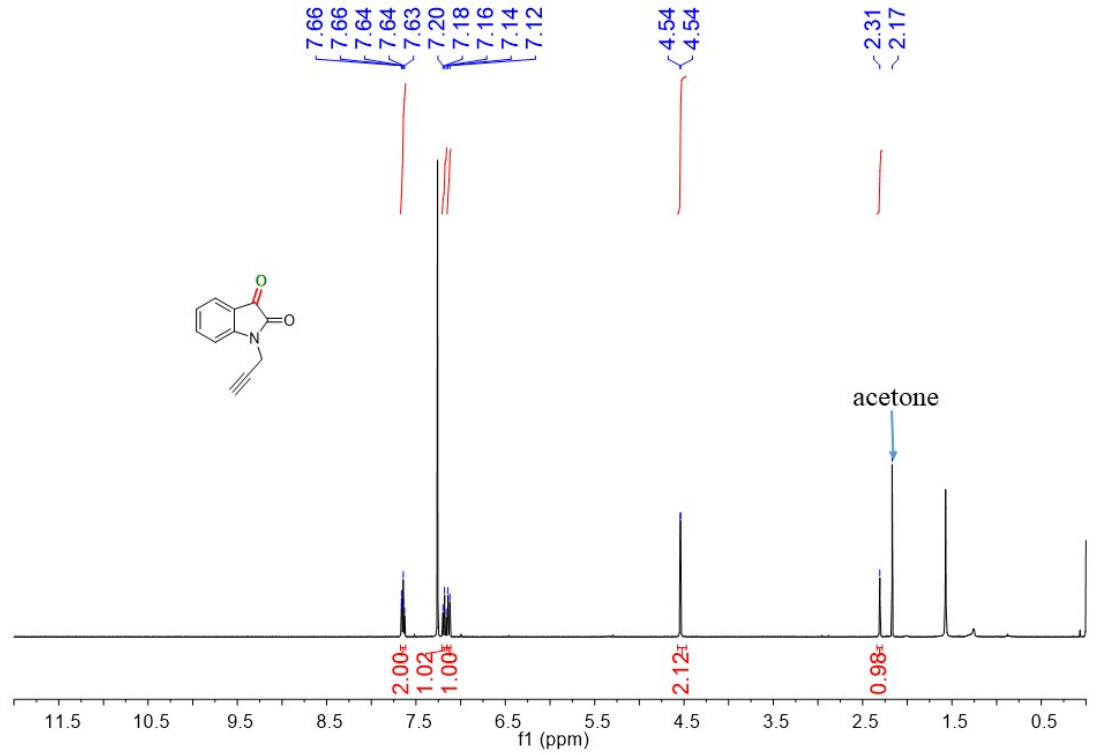
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.66
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7.64
7.63
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7.16
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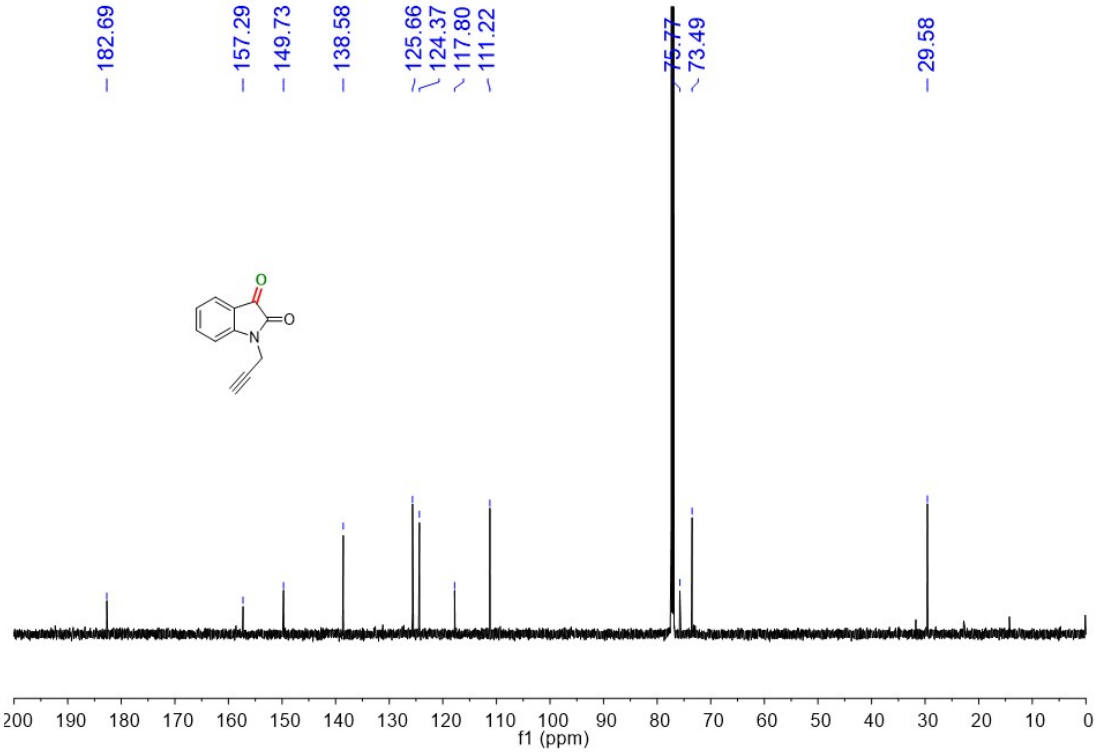
7.12
4.54
4.54
2.31
2.17
acetone
2.00
1.02
1.00
2.12
0.98
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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124.37
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111.22
77.77
73.49
29.58
200
190
180
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130
120
110
100
90
80
70
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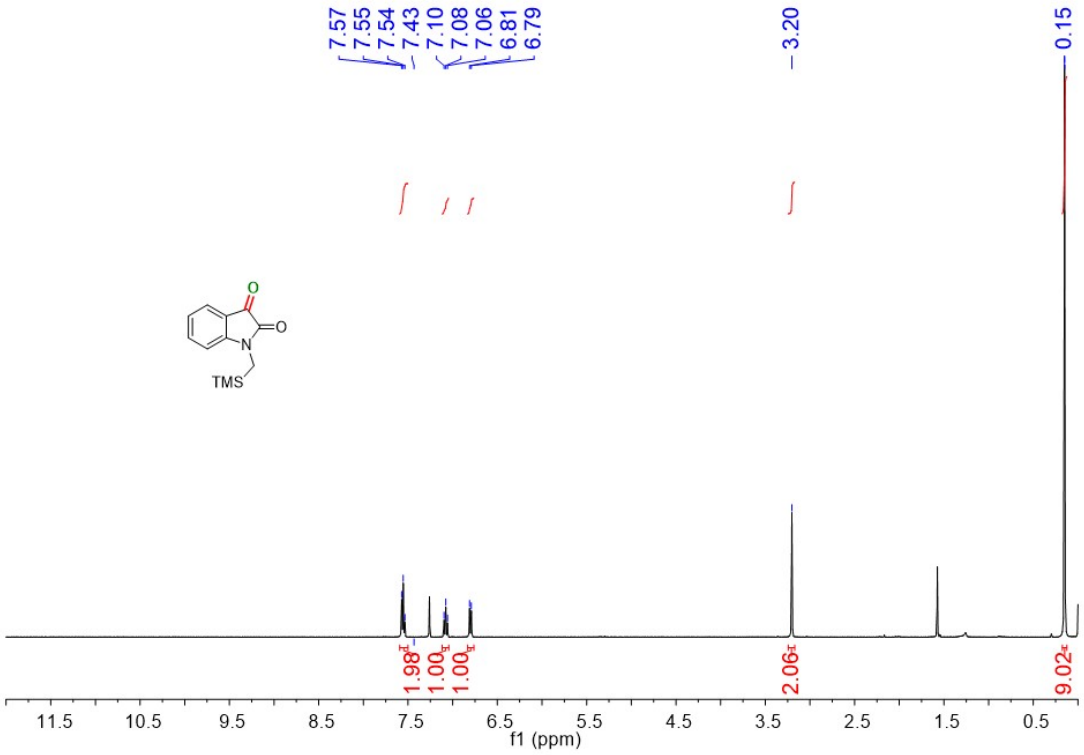
50
40
30
20
10
0
f1 (ppm)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7.54
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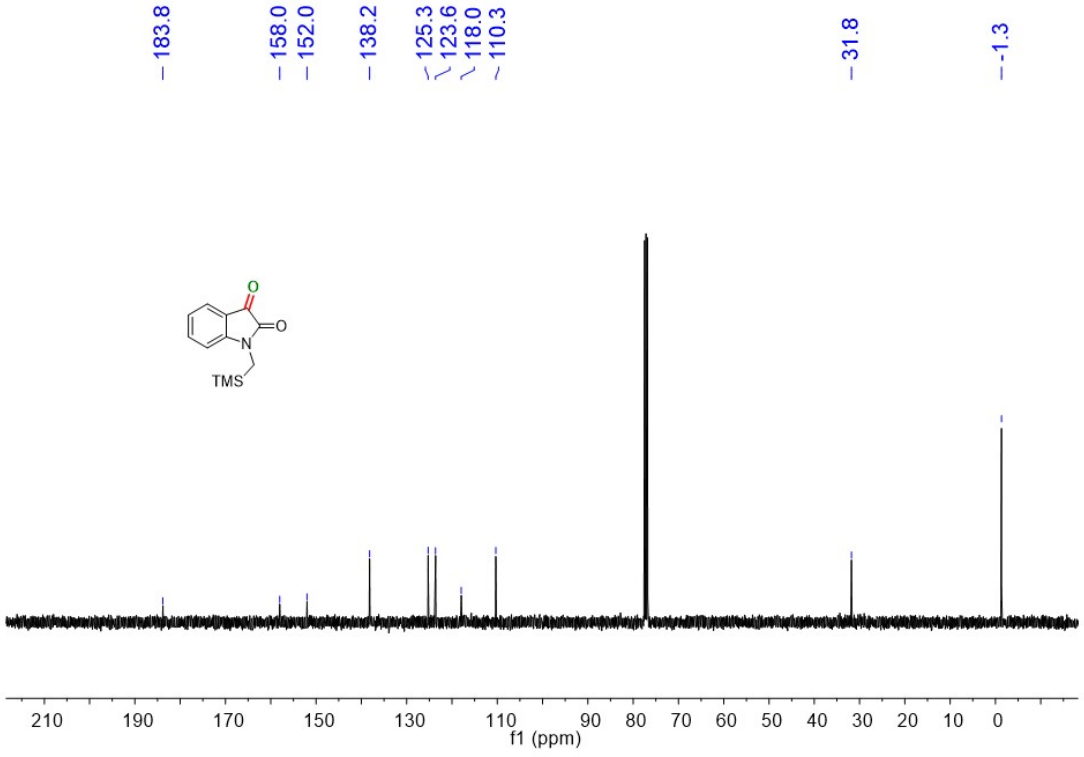
7.06
6.81
6.79
3.20
0.15
O
O
N
TMS
1.98
1.00
1.00
2.06
9.02
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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152.0
138.2
125.3
123.6
118.0
110.3
31.8
1.3
O
O
N
TMS
210
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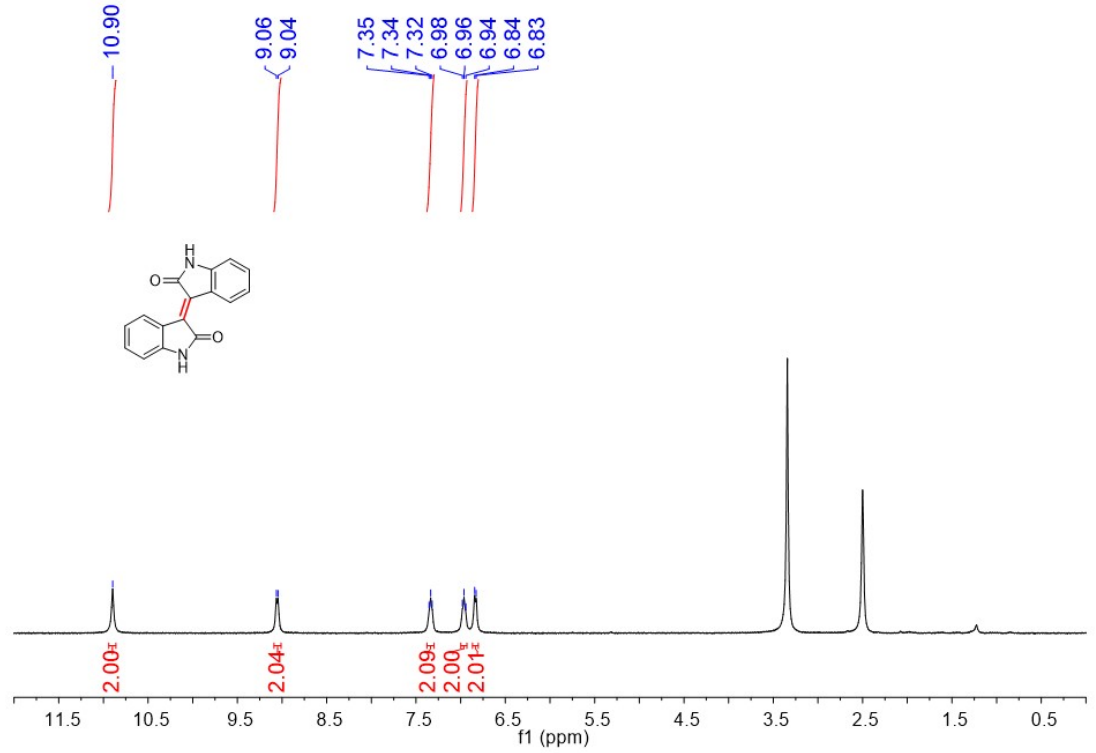
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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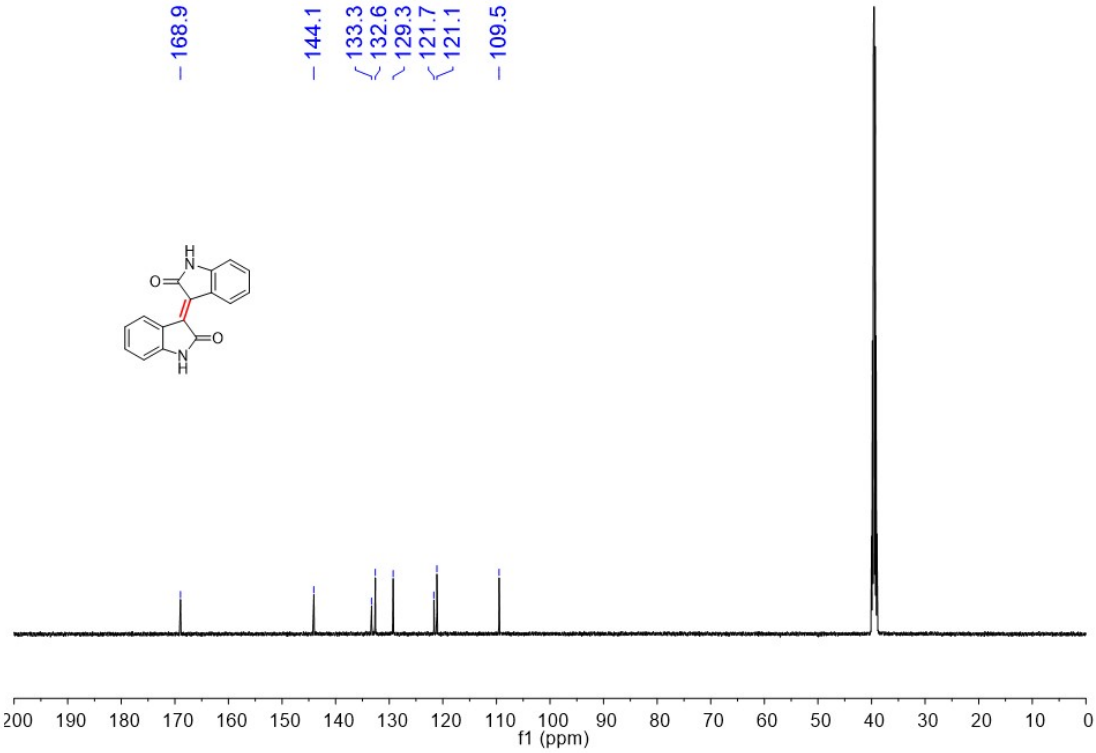
9.06
9.04
7.35
7.34
7.32
6.98
6.96
6.94
6.84
6.83
2.00
2.04
2.09
2.00
2.01
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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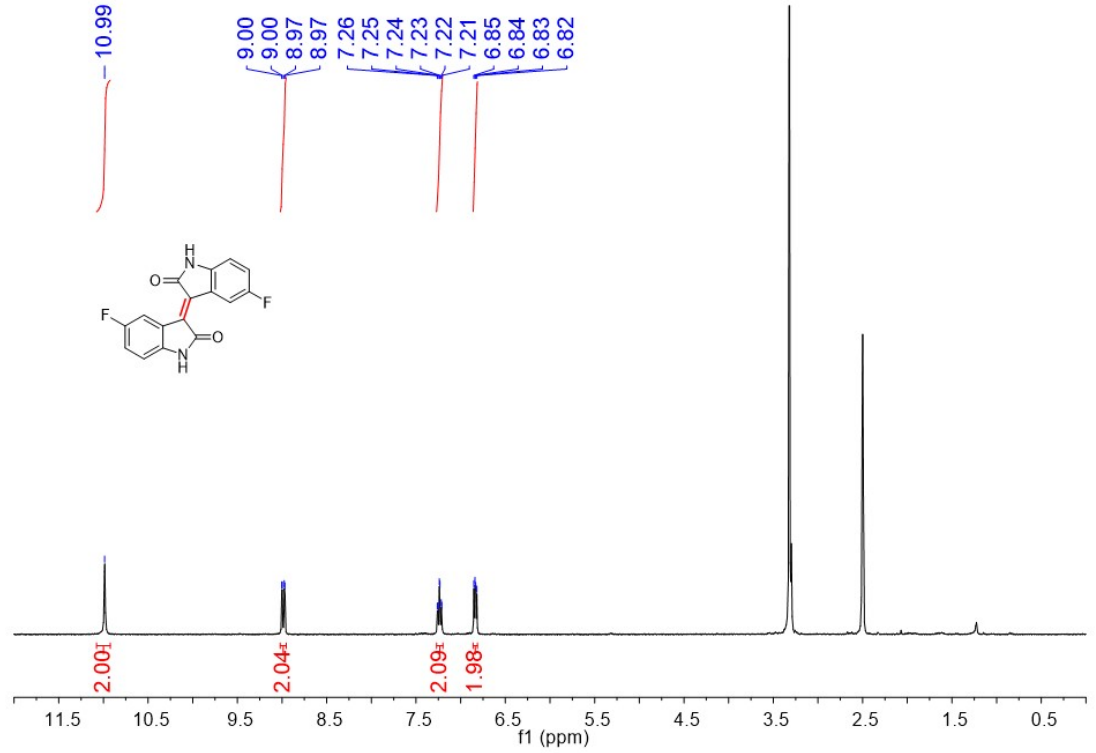
144.1
133.3
132.6
129.3
121.7
121.1
109.5
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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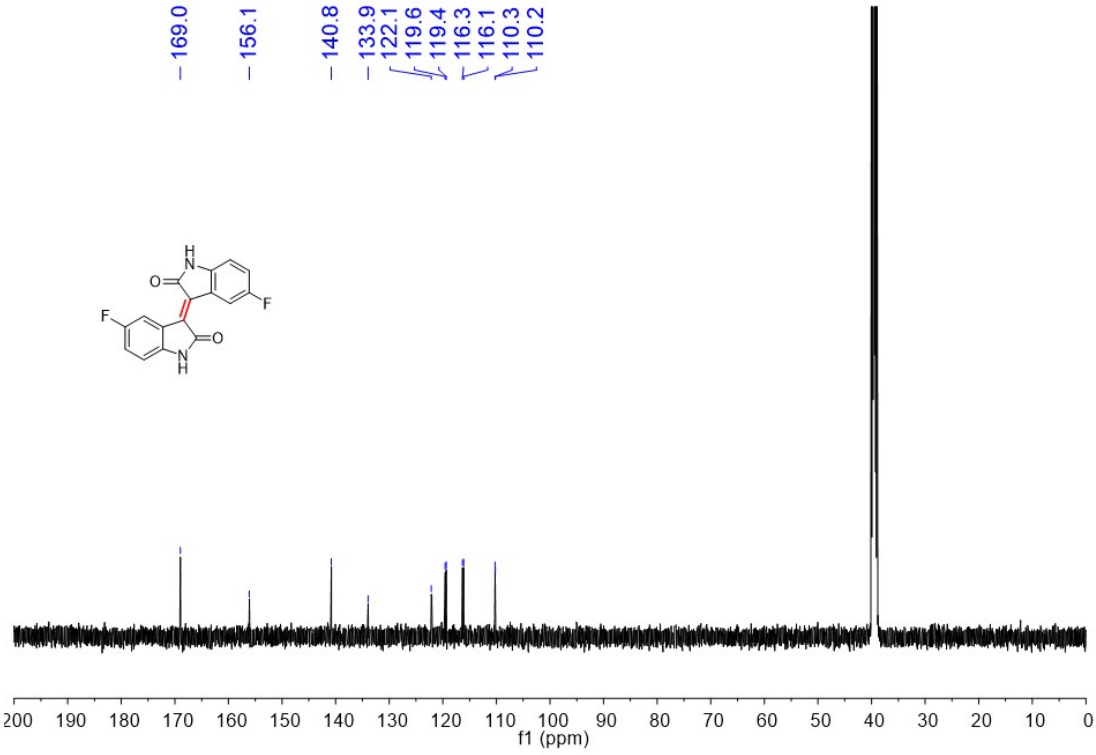
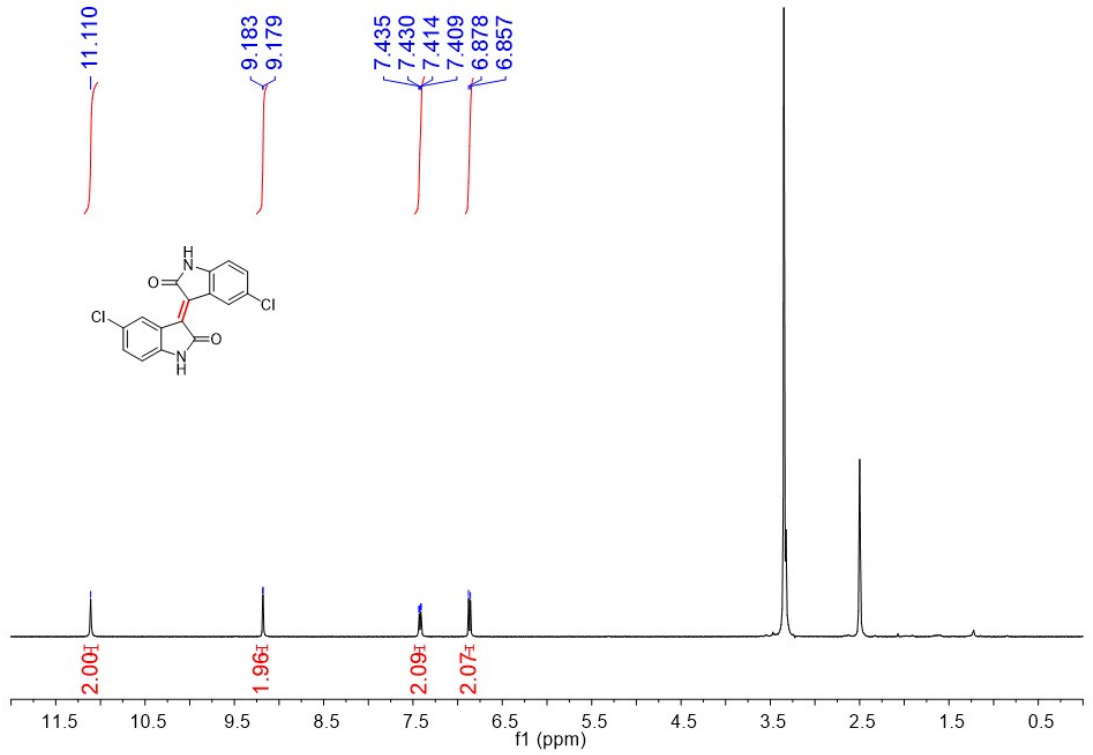
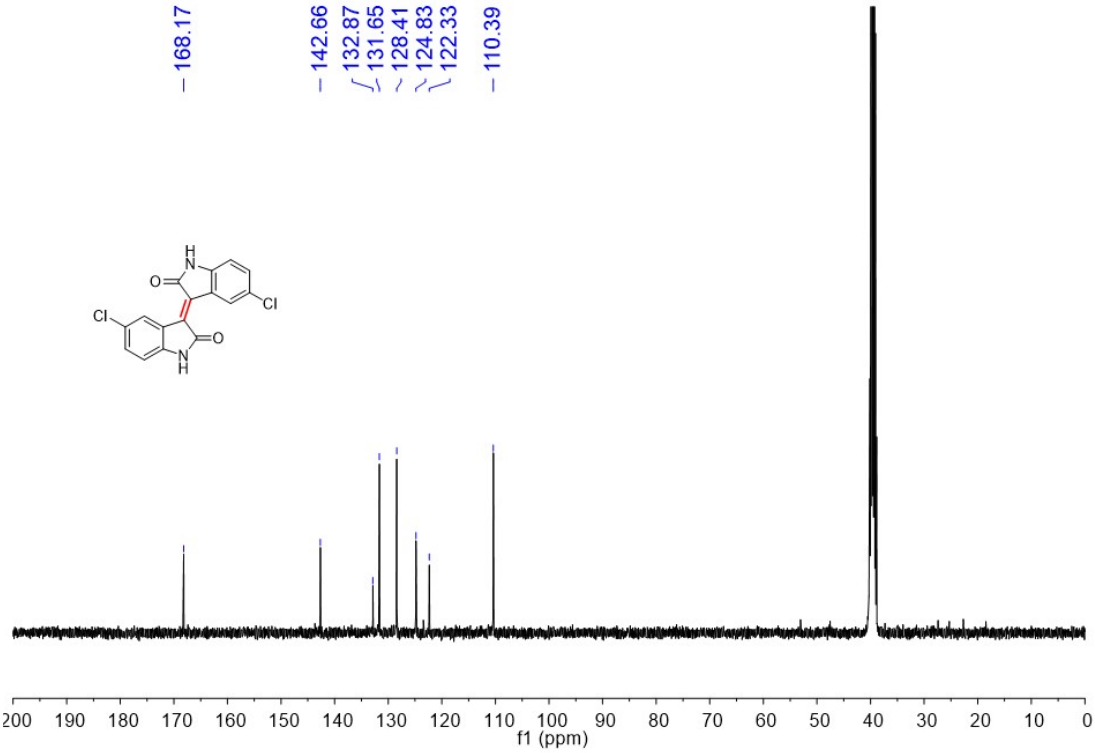
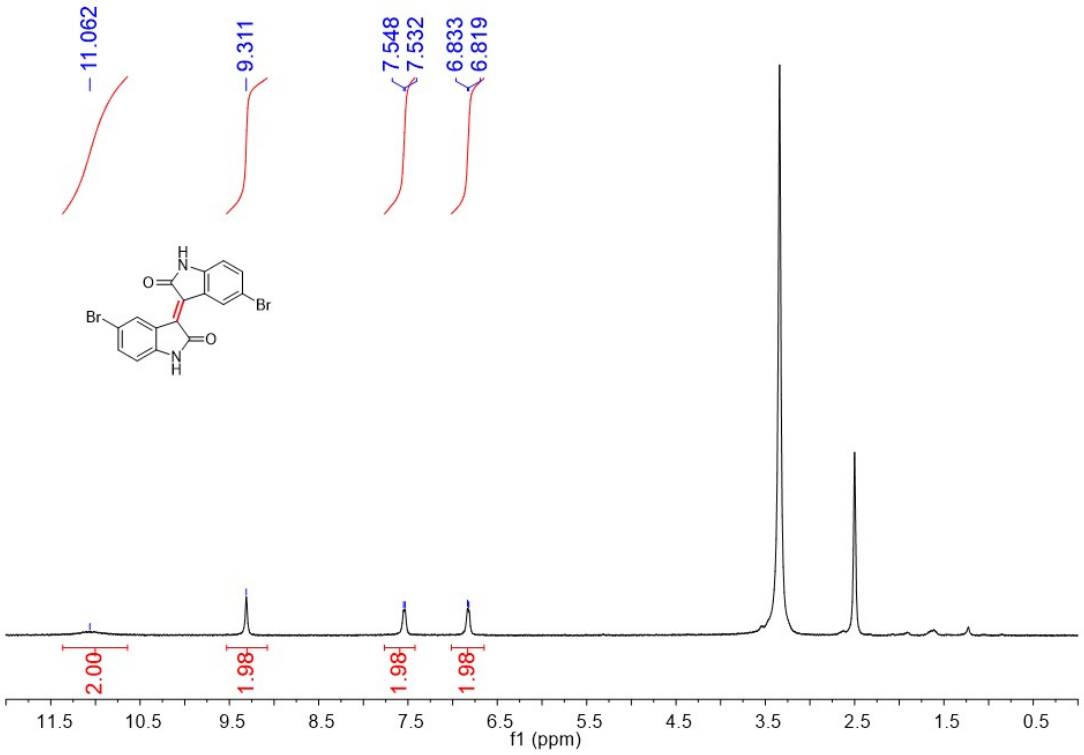
9.00
9.00
8.97
8.97
7.26
7.25
7.24
7.23
7.22
7.21
6.85
6.84
6.83
6.82
2.00
2.04
2.09
1.98
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


169.0
156.1
140.8
133.9
122.1
119.6
119.4
116.3
116.1
110.3
110.2
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.110
9.183
9.179
7.435
7.430
7.414
7.409
6.878
6.857
2.00
1.96
2.09
2.07
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


168.17
142.66
132.87
131.65
128.41
124.83
122.33
110.39
200
190
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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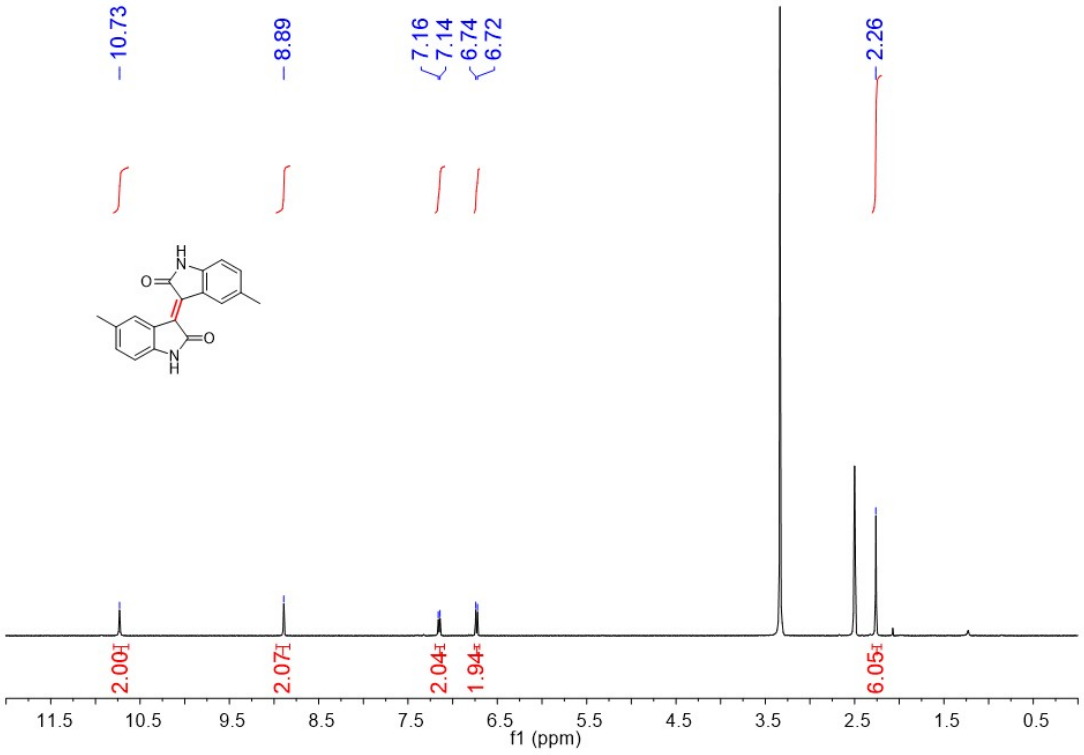
9.311
7.548
7.532
6.833
6.819
Br
Br
2.00
1.98
1.98
1.98
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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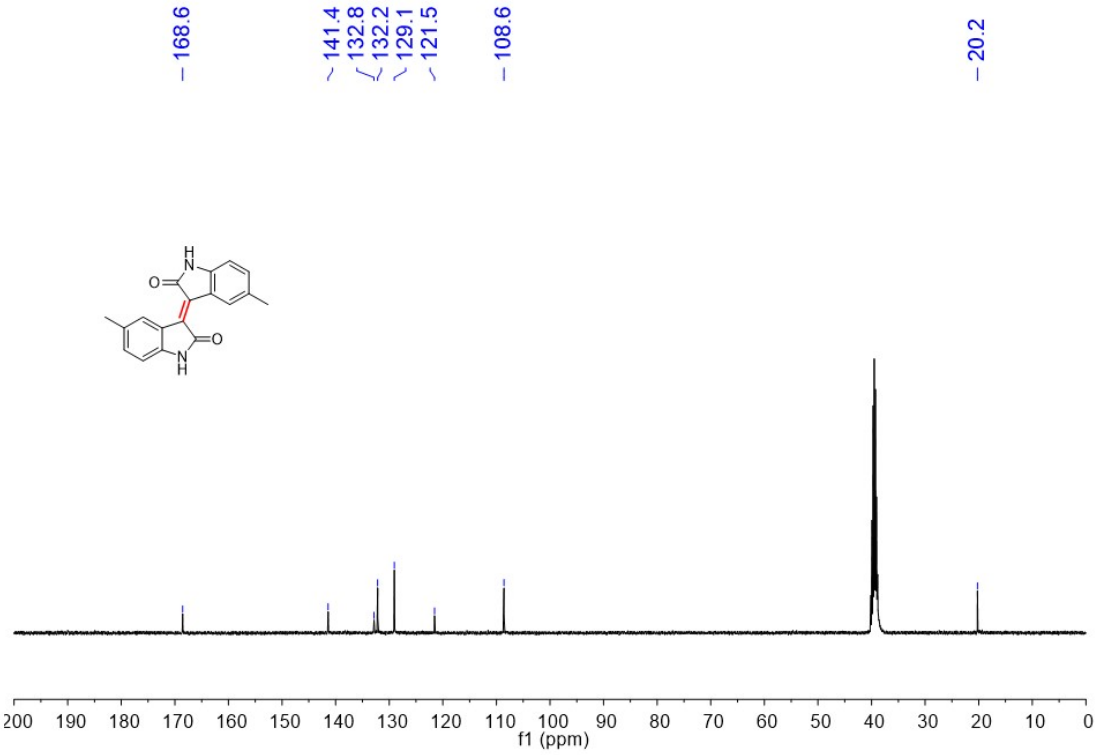
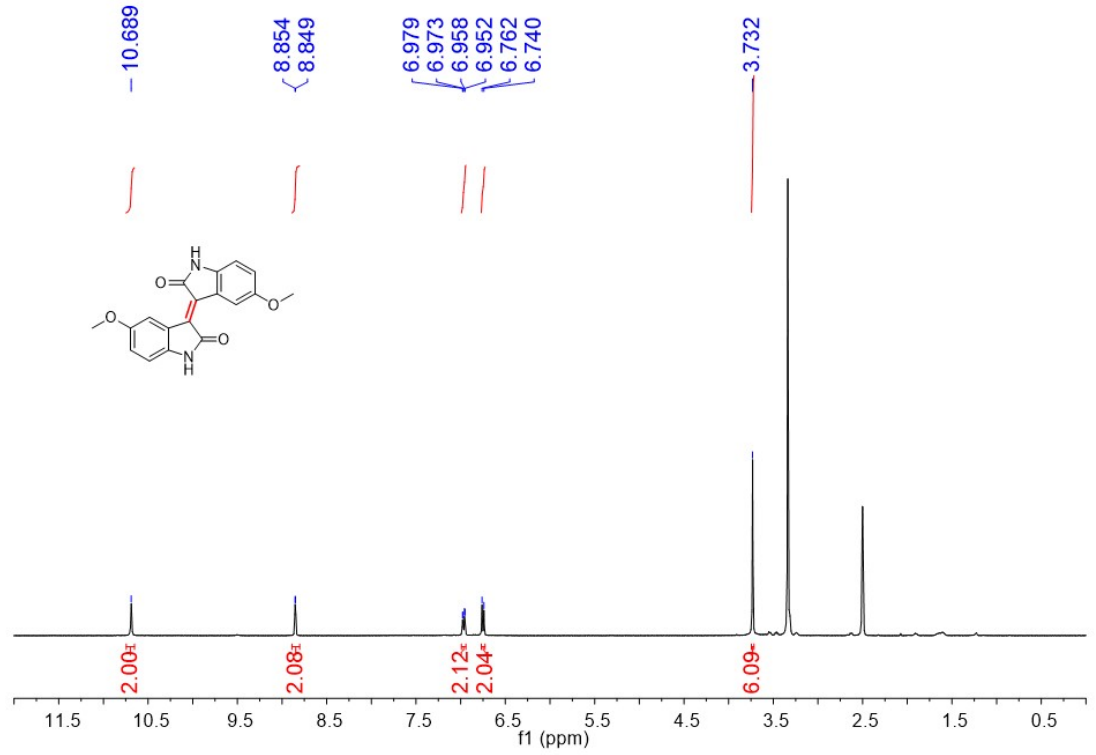
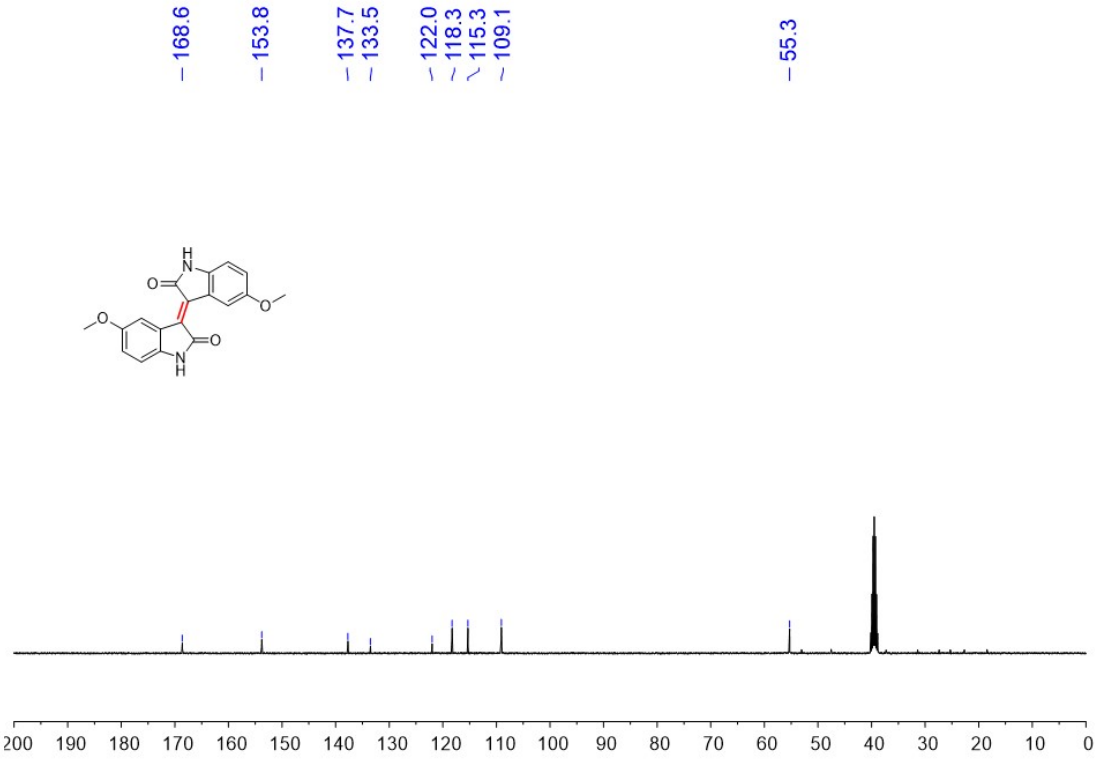
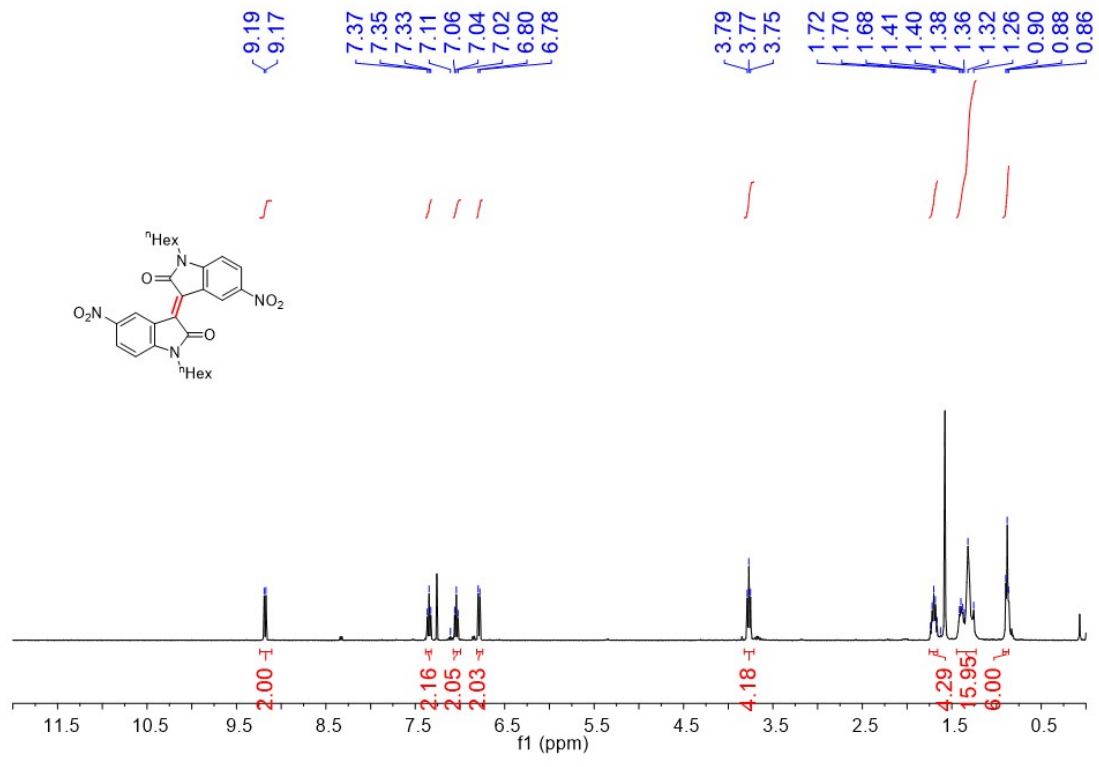
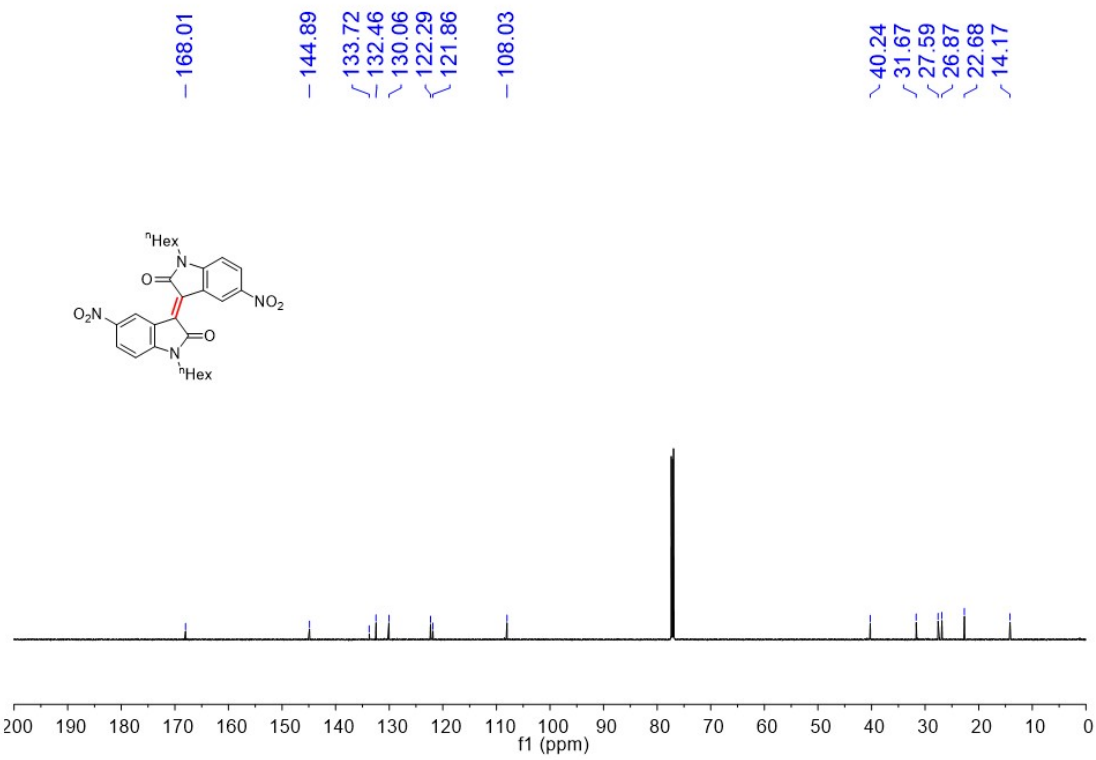
8.89
7.16
7.14
6.74
6.72
2.26
2.00
2.07
2.04
1.94
6.05
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

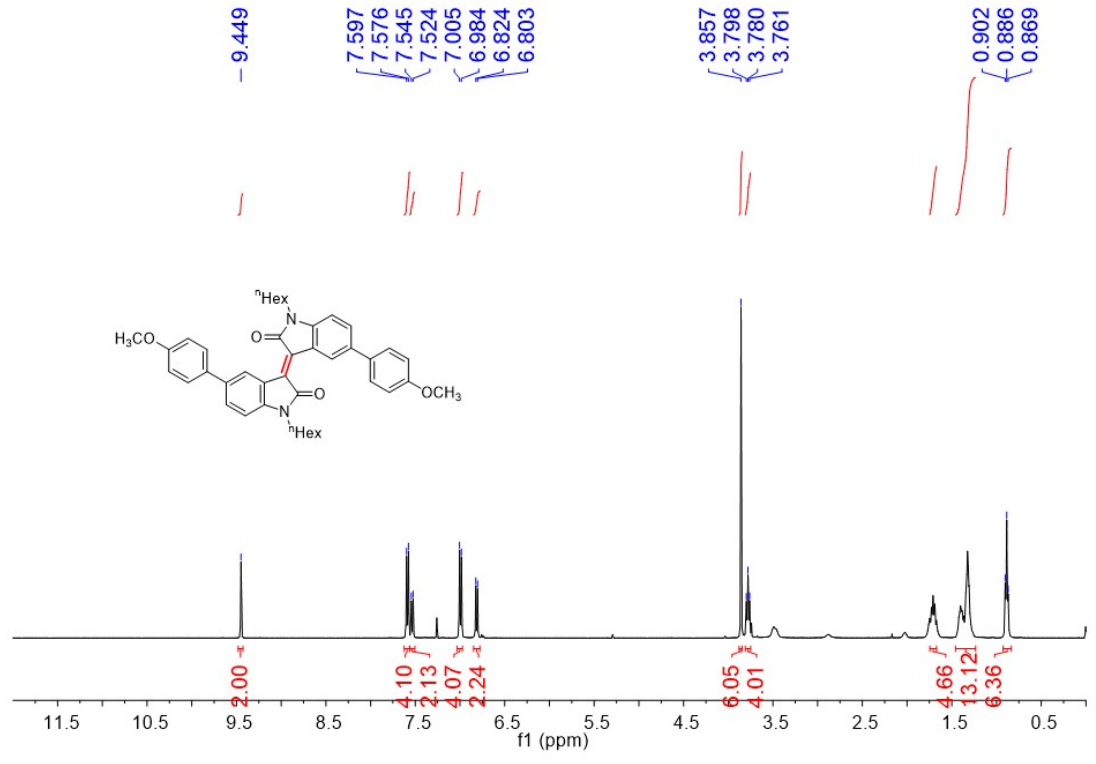

168.6
141.4
132.8
132.2
129.1
121.5
108.6
20.2
f1 (ppm)

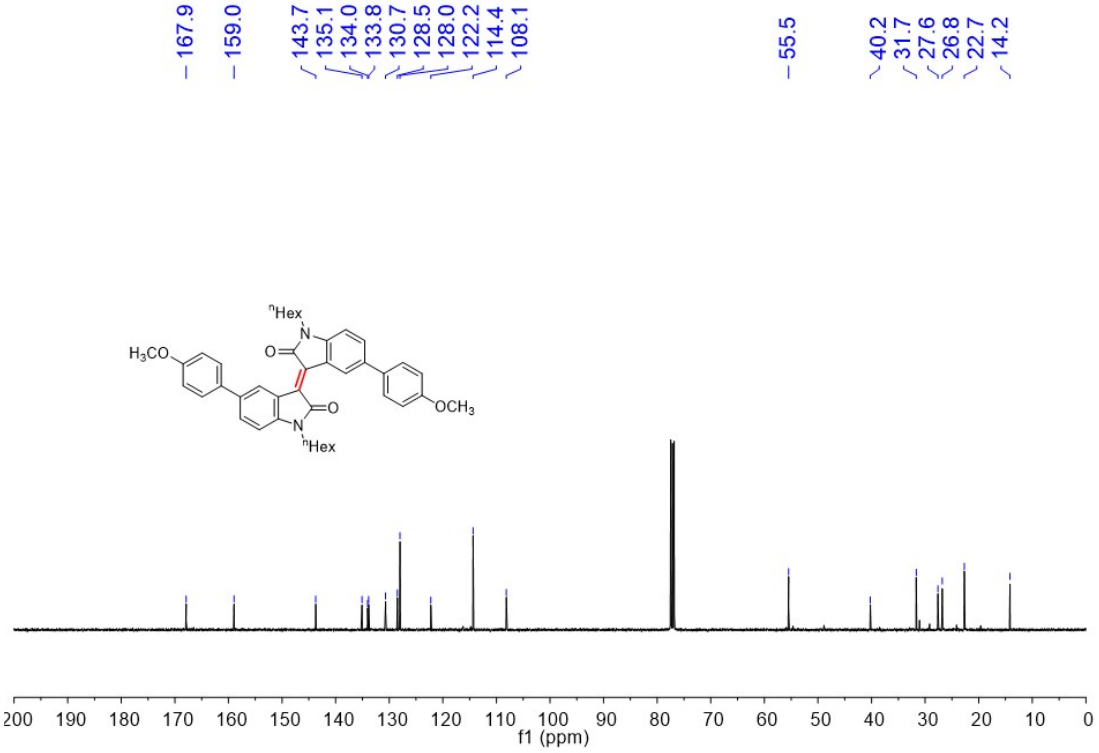

10.689
8.854
8.849
6.979
6.973
6.958
6.952
6.762
6.740
3.732
2.00
2.08
2.12
2.04
6.09
f1 (ppm)

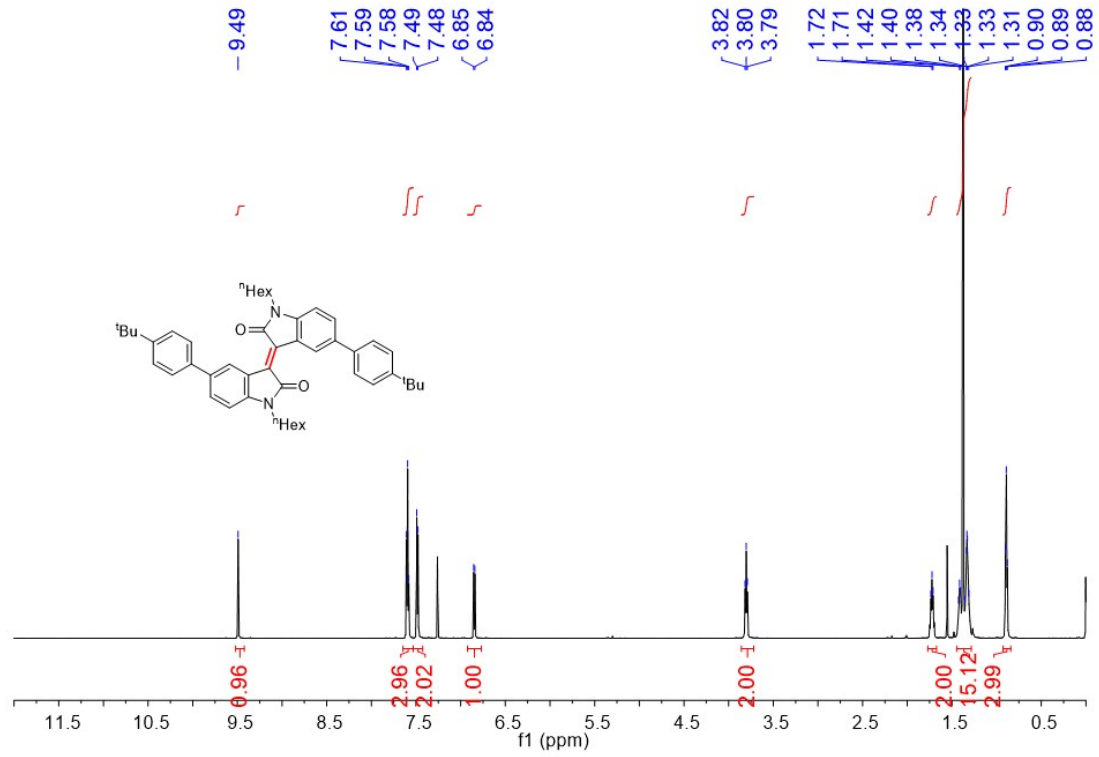

168.6
153.8
137.7
133.5
122.0
118.3
115.3
109.1
55.3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

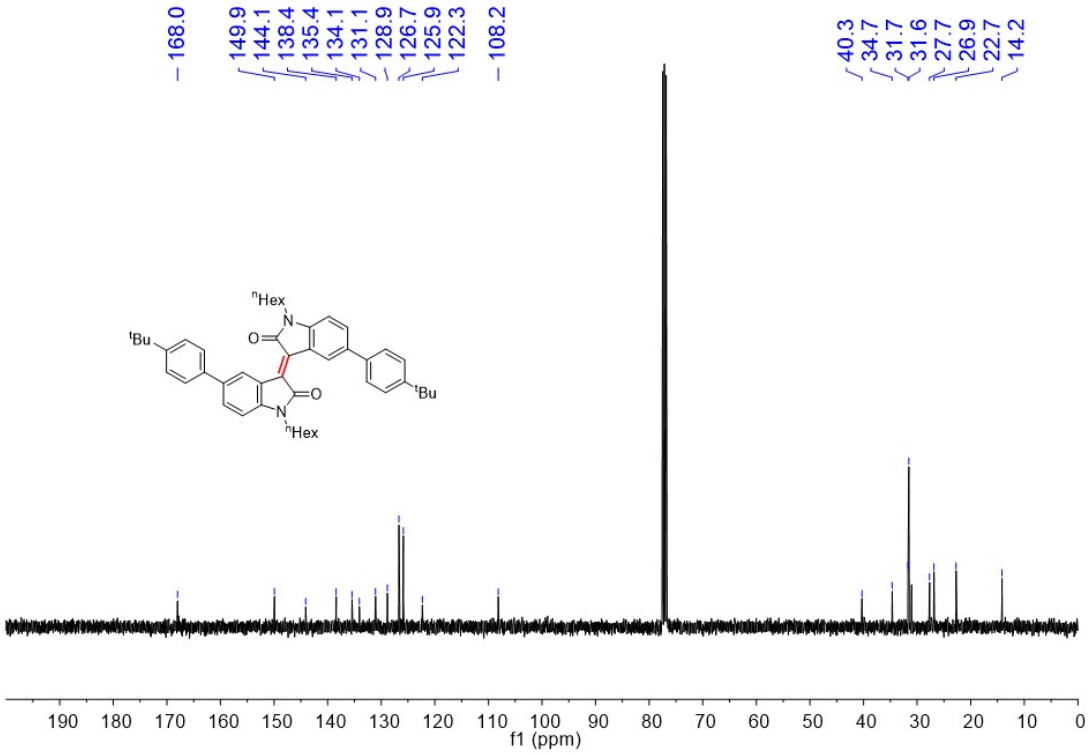

9.19
9.17
7.37
7.35
7.33
7.11
7.06
7.04
7.02
6.80
6.78
3.79
3.77
3.75
1.72
1.70
1.68
1.41
1.40
1.38
1.36
1.32
1.26
0.90
0.88
0.86
2.00
2.16
2.05
2.03
4.18
4.29
15.95
6.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)


168.01
144.89
133.72
132.46
130.06
122.29
121.86
108.03
40.24
31.67
27.59
26.87
22.68
14.17
nHex
N
O
NO2
O2N
O
N
nHex
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.449
7.597
7.576
7.545
7.524
7.005
6.984
6.824
6.803
3.857
3.798
3.780
3.761
0.902
0.886
0.869
nHex
N
O
H3CO
OCH3
O
N
nHex
2.00
4.10
2.13
4.07
2.24
6.05
4.01
4.66
13.12
6.36
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)


167.9
159.0
143.7
135.1
134.0
133.8
130.7
128.5
128.0
122.2
114.4
108.1
55.5
40.2
31.7
27.6
26.8
22.7
14.2
nHex
N
O
H3CO
OCH3
O
N
nHex
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.49
7.61
7.59
7.58
7.49
7.48
6.85
6.84
3.82
3.80
3.79
1.72
1.71
1.42
1.40
1.38
1.34
1.33
1.33
1.31
0.90
0.89
0.88
nHex
N
O
tBu
O
N
tBu
nHex
0.96
2.96
2.02
1.00
2.00
2.00
15.12
2.99
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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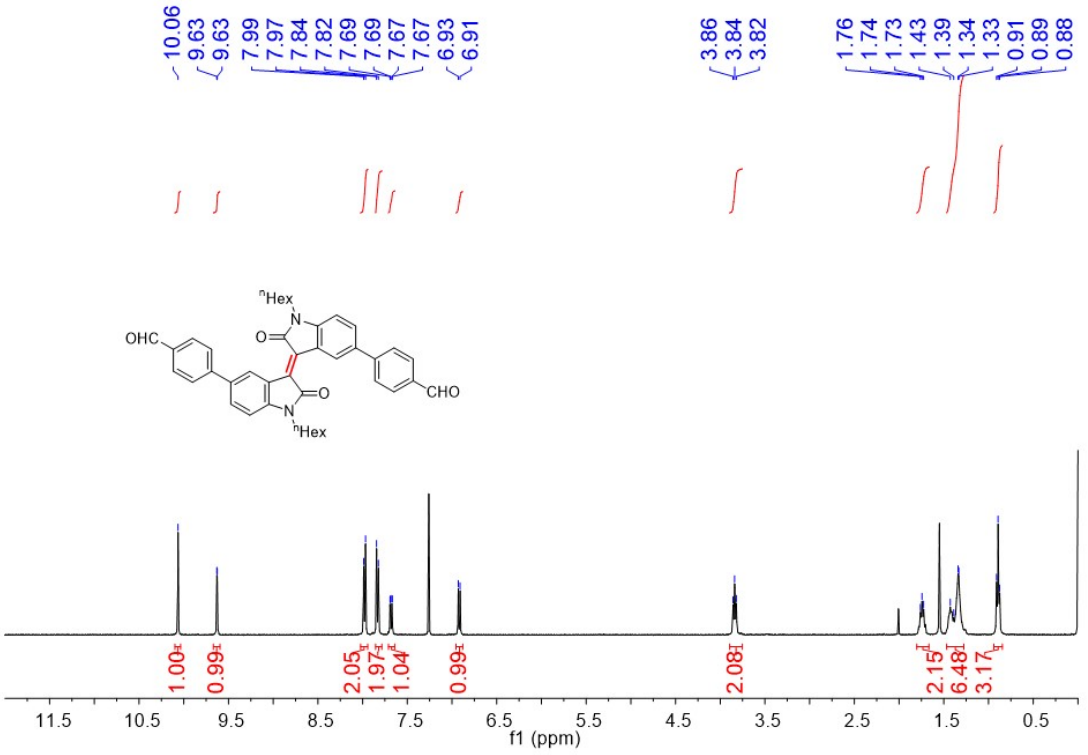
149.9
144.1
138.4
135.4
134.1
131.1
128.9
126.7
125.9
122.3
108.2
40.3
34.7
31.7
31.6
27.7
26.9
22.7
14.2
nHex
tBu
tBu
nHex
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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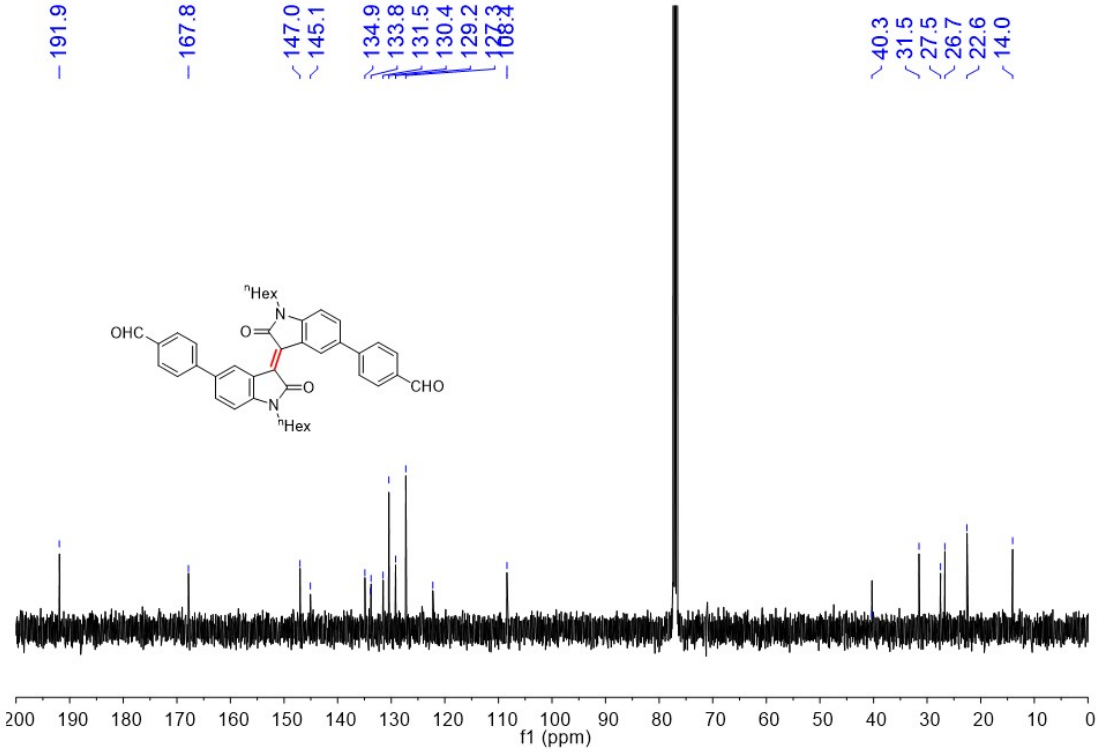
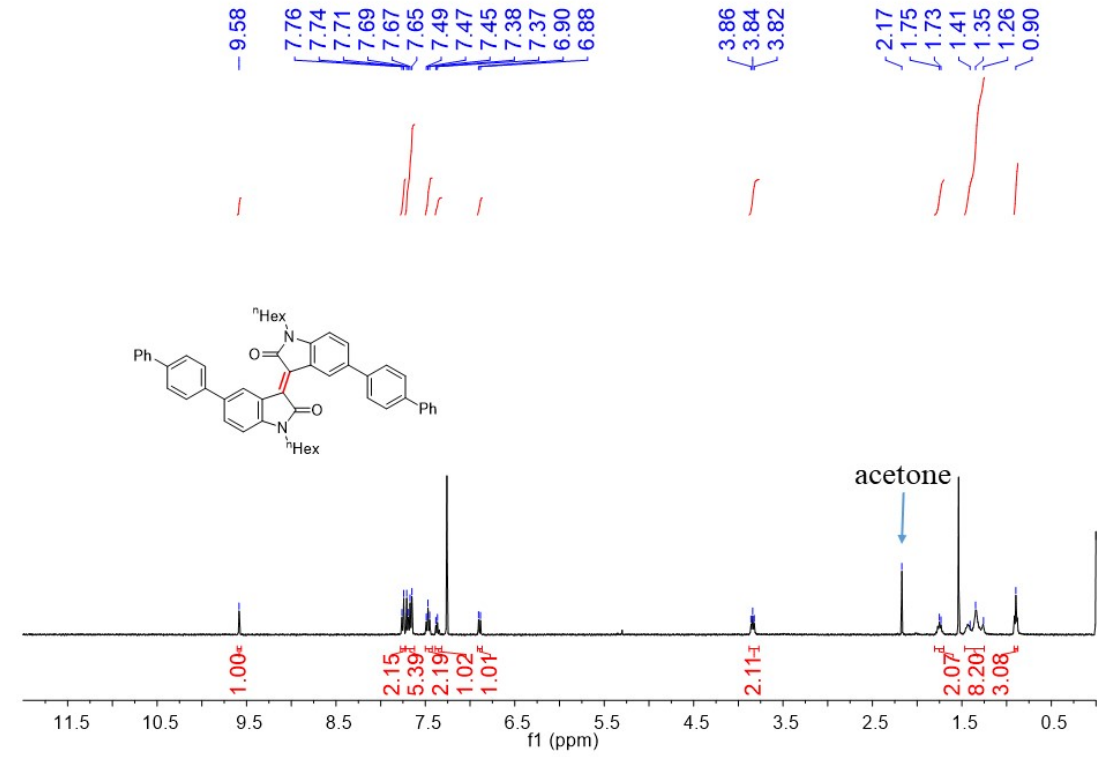
9.63
9.63
7.99
7.97
7.84
7.82
7.69
7.69
7.67
7.67
6.93
6.91
3.86
3.84
3.82
1.76
1.74
1.73
1.43
1.39
1.34
1.33
0.91
0.89
0.88
nHex
OHC
CHO
nHex
1.00
0.99
2.05
1.97
1.04
0.99
2.08
2.15
6.48
3.17
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)


191.9
167.8
147.0
145.1
134.9
133.8
131.5
130.4
129.2
127.3
108.4
40.3
31.5
27.5
26.7
22.6
14.0
nHex
OHC
CHO
nHex
f1 (ppm)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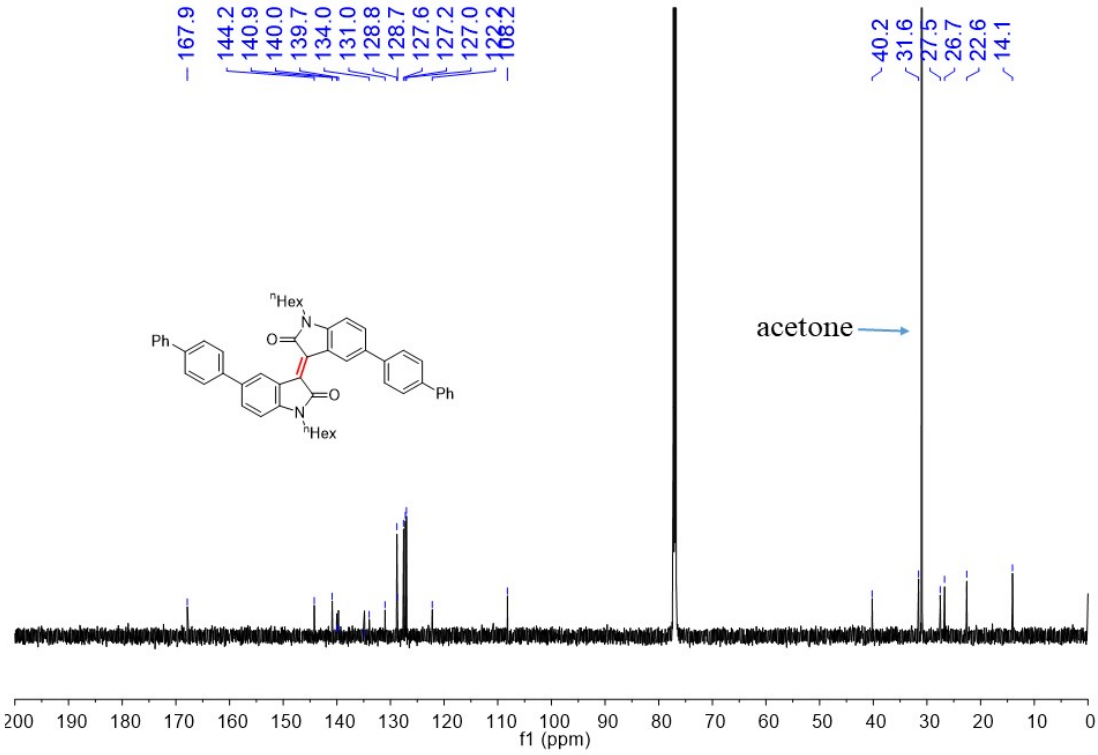
7.76
7.74
7.71
7.69
7.67
7.65
7.49
7.47
7.45
7.38
7.37
6.90
6.88
3.86
3.84
3.82
2.17
1.75
1.73
1.41
1.35
1.26
0.90
nHex
Ph
Ph
nHex
acetone
1.00
2.15
5.39
2.15
1.02
1.01
2.11
2.07
8.20
3.08
f1 (ppm)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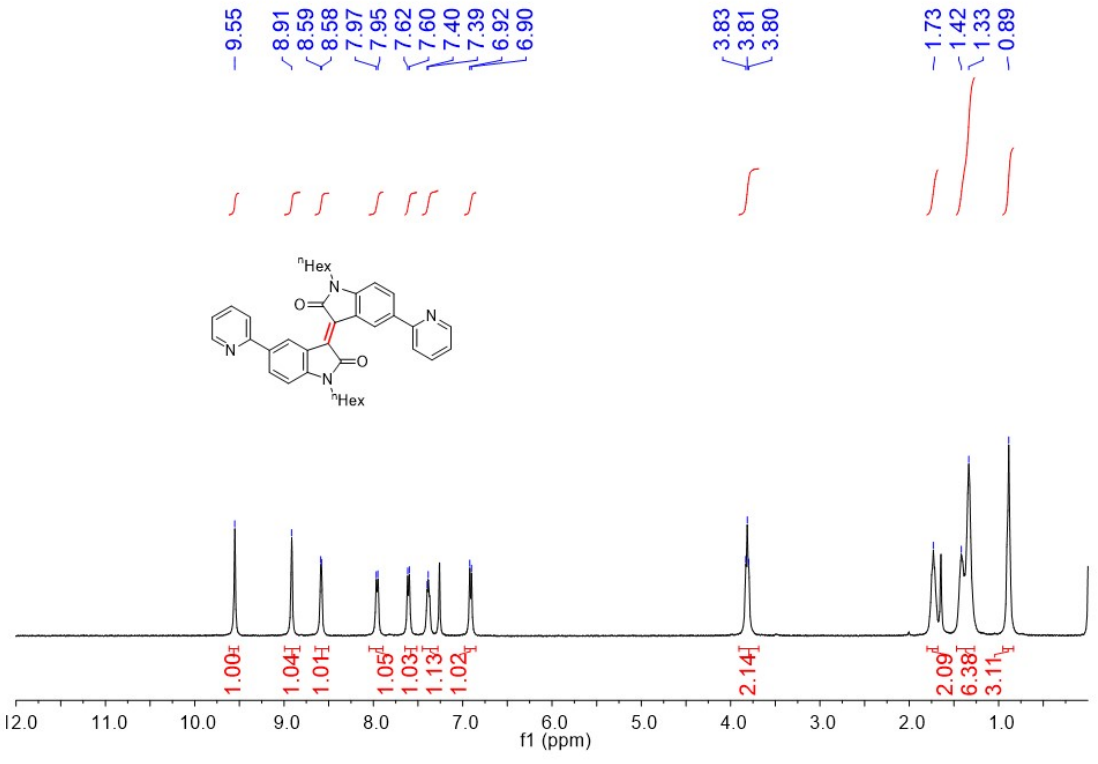
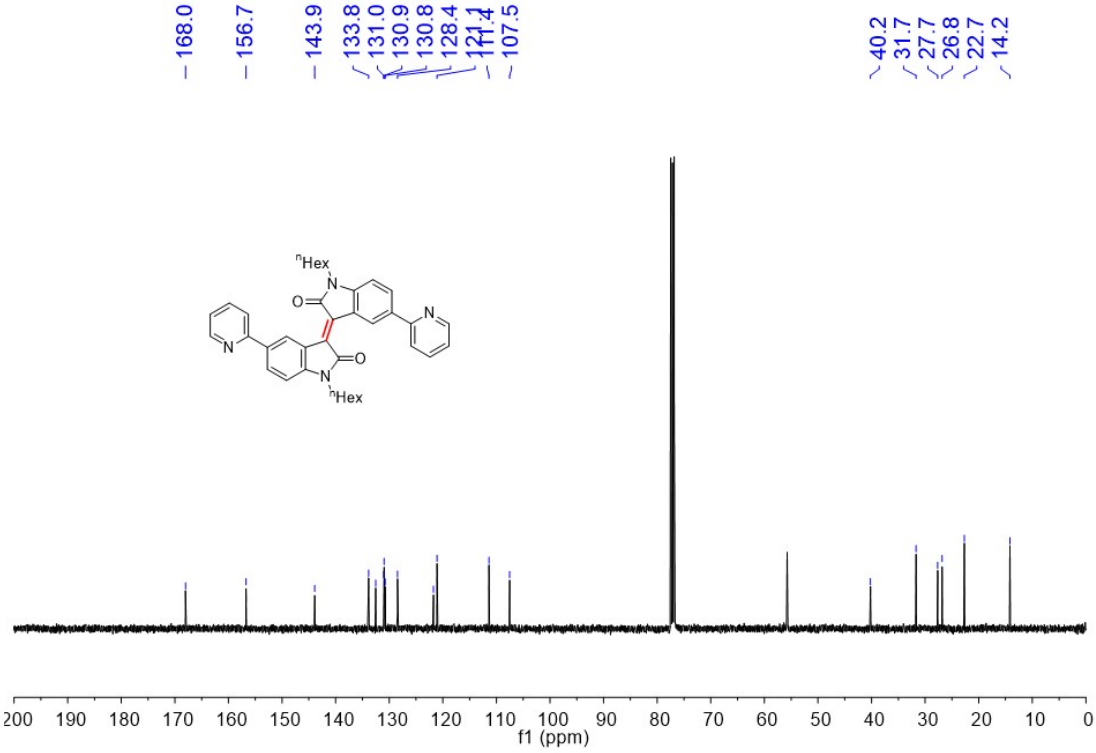
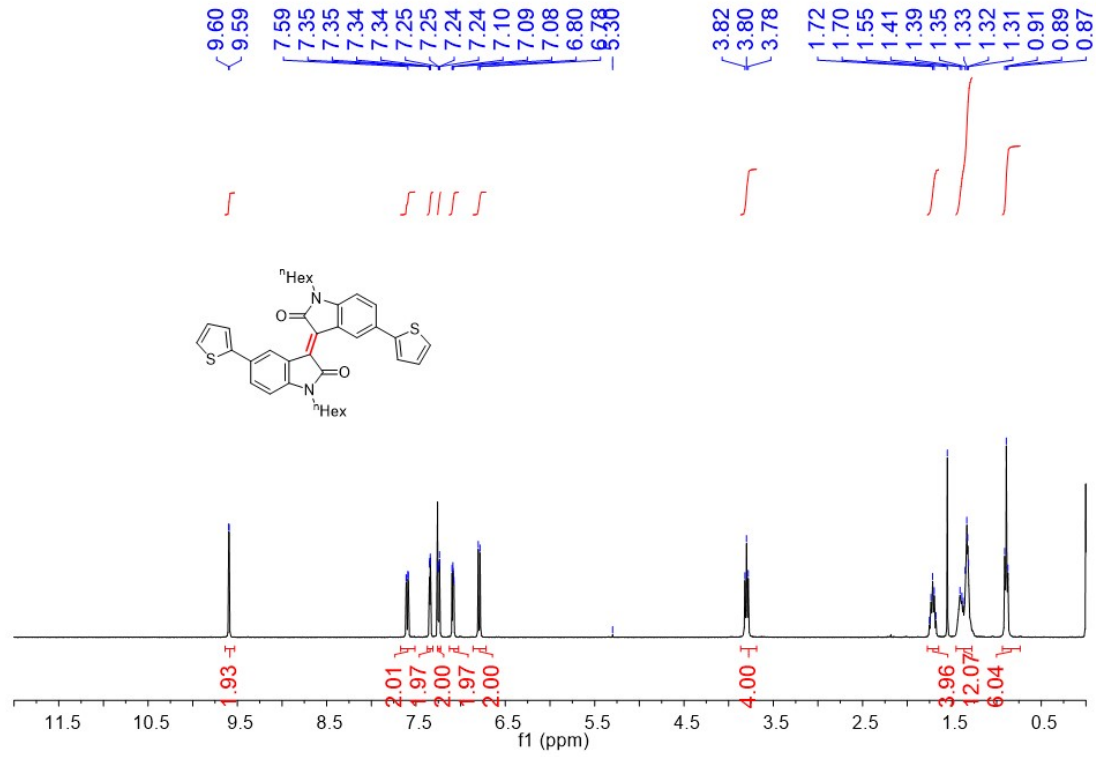
144.2
140.9
140.0
139.7
134.0
131.0
128.8
128.7
127.6
127.2
127.0
122.2
108.2
40.2
31.6
27.5
26.7
22.6
14.1
acetone
nHex
Ph
Ph
nHex
f1 (ppm)


9.55
8.91
8.59
8.58
7.97
7.95
7.62
7.60
7.40
7.39
6.92
6.90
3.83
3.81
3.80
1.73
1.42
1.33
0.89
nHex
nHex
1.00
1.04
1.01
1.05
1.03
1.13
1.02
2.14
2.09
6.38
3.11
f1 (ppm)


168.0
156.7
143.9
133.8
131.0
130.9
130.8
128.4
121.1
111.4
107.5
40.2
31.7
27.7
26.8
22.7
14.2
nHex
nHex
f1 (ppm)


9.60
9.59
7.59
7.35
7.35
7.34
7.34
7.25
7.25
7.24
7.24
7.10
7.09
7.08
6.80
3.82
3.80
3.78
1.72
1.70
1.55
1.41
1.39
1.35
1.33
1.32
1.31
0.91
0.89
0.87
nHex
nHex
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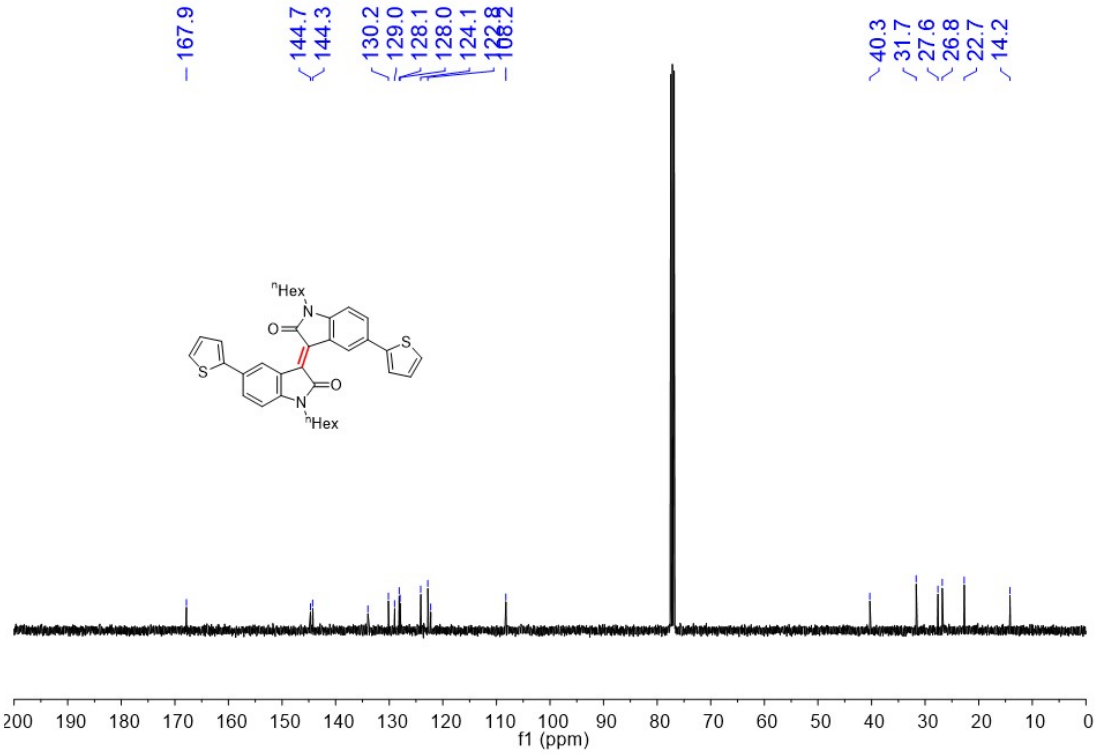
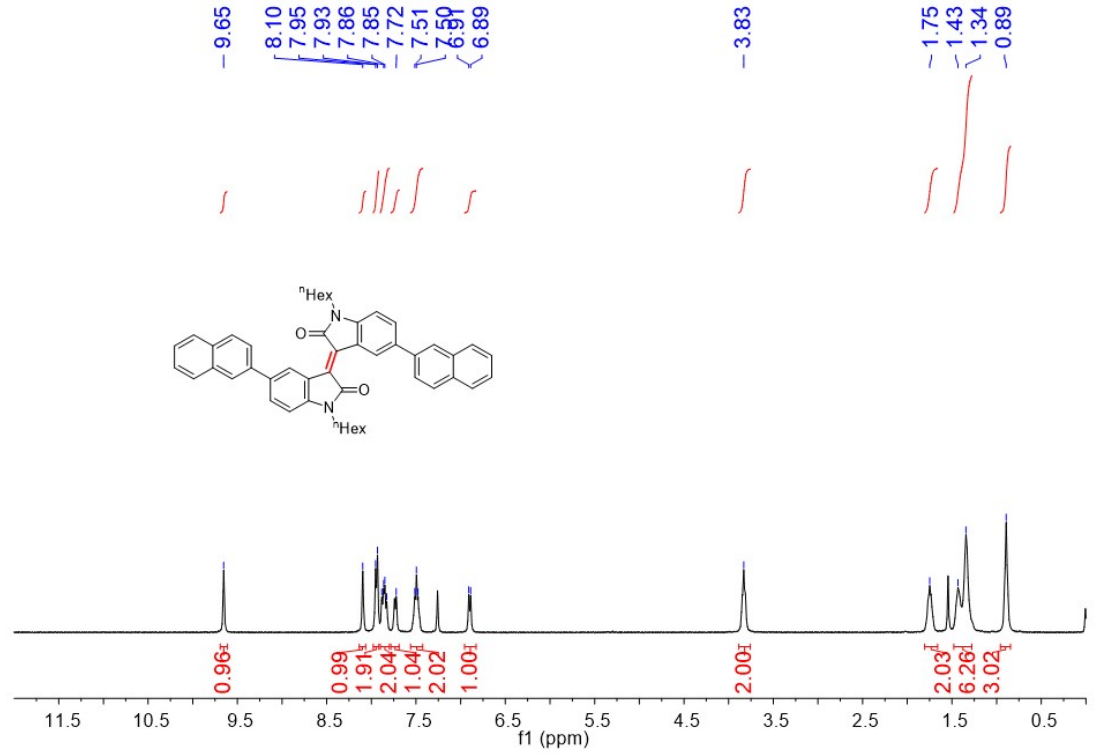
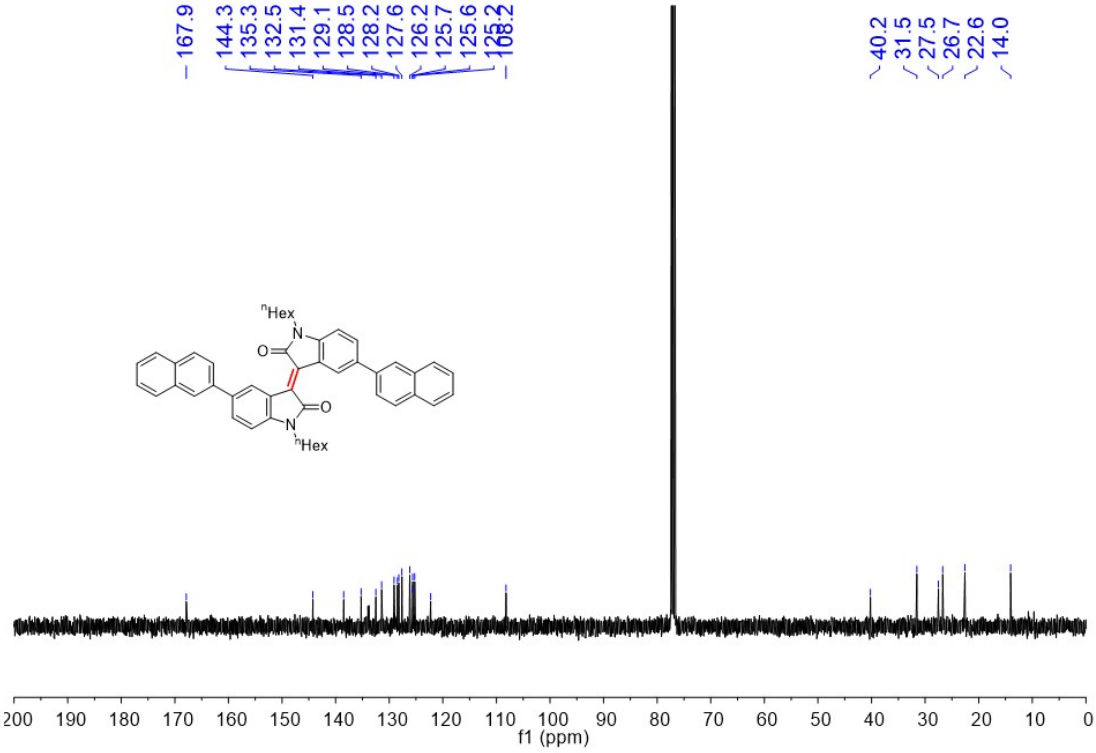
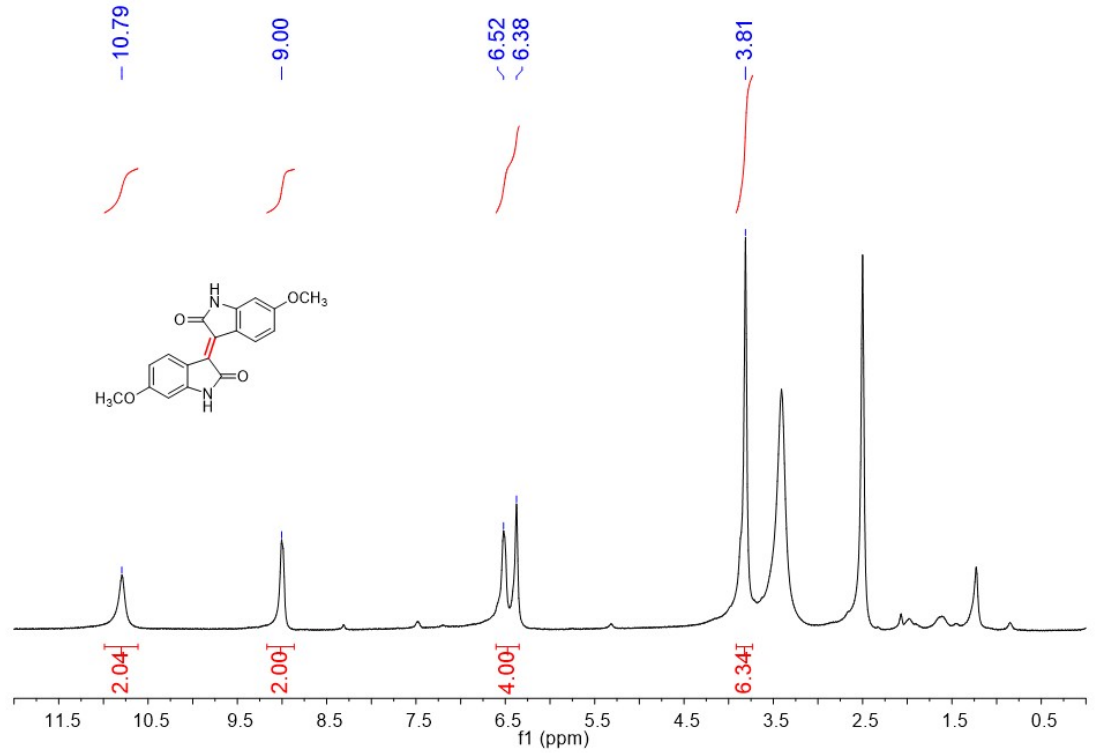
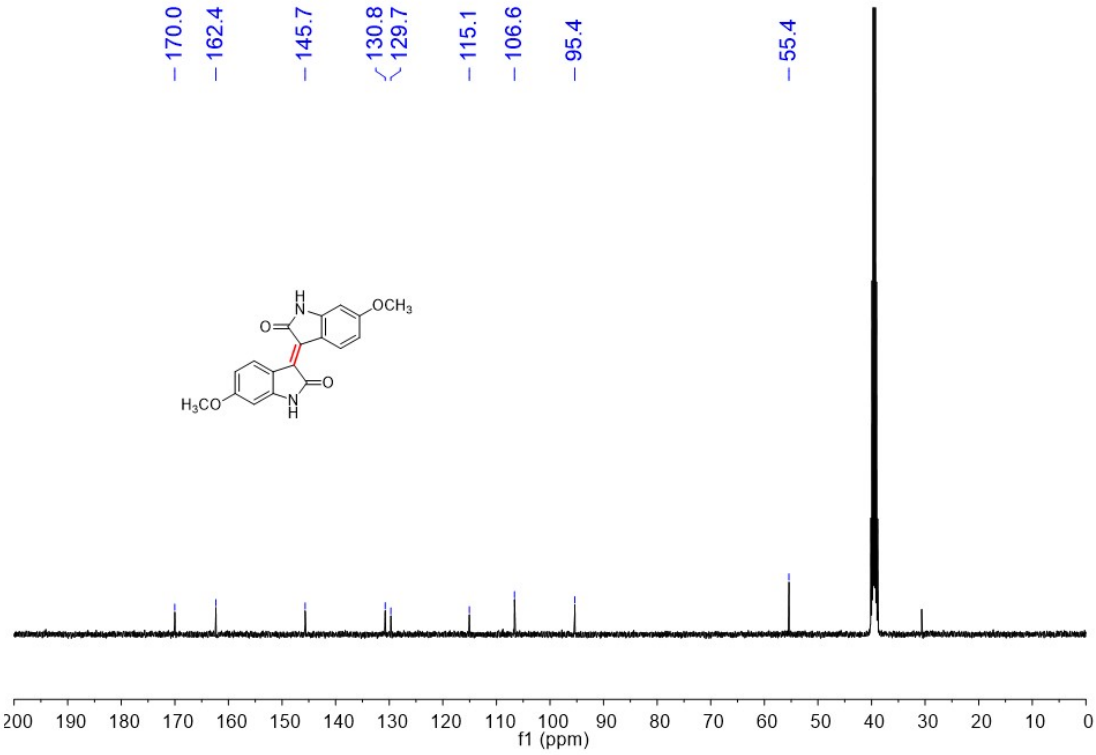
1.97
2.00
1.97
2.00
4.00
3.96
12.07
6.04
f1 (ppm)

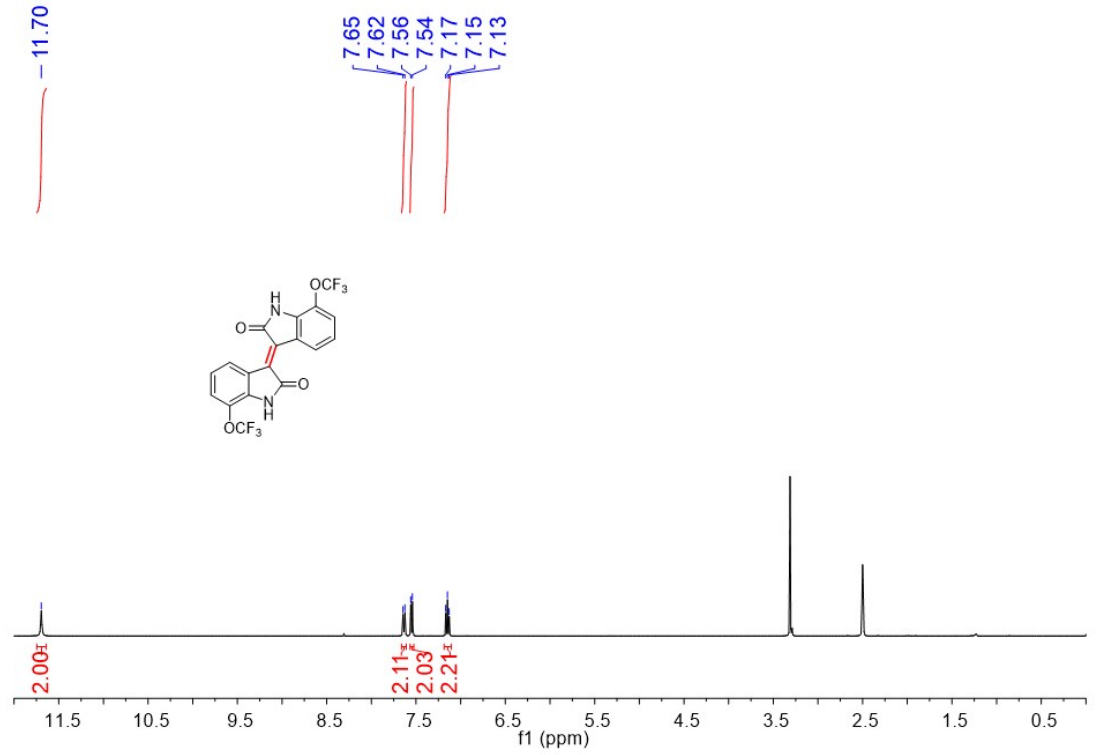

167.9
144.7
144.3
130.2
129.0
128.1
128.0
124.1
40.3
31.7
27.6
26.8
22.7
14.2
nHex
N
O
S
O
N
nHex
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

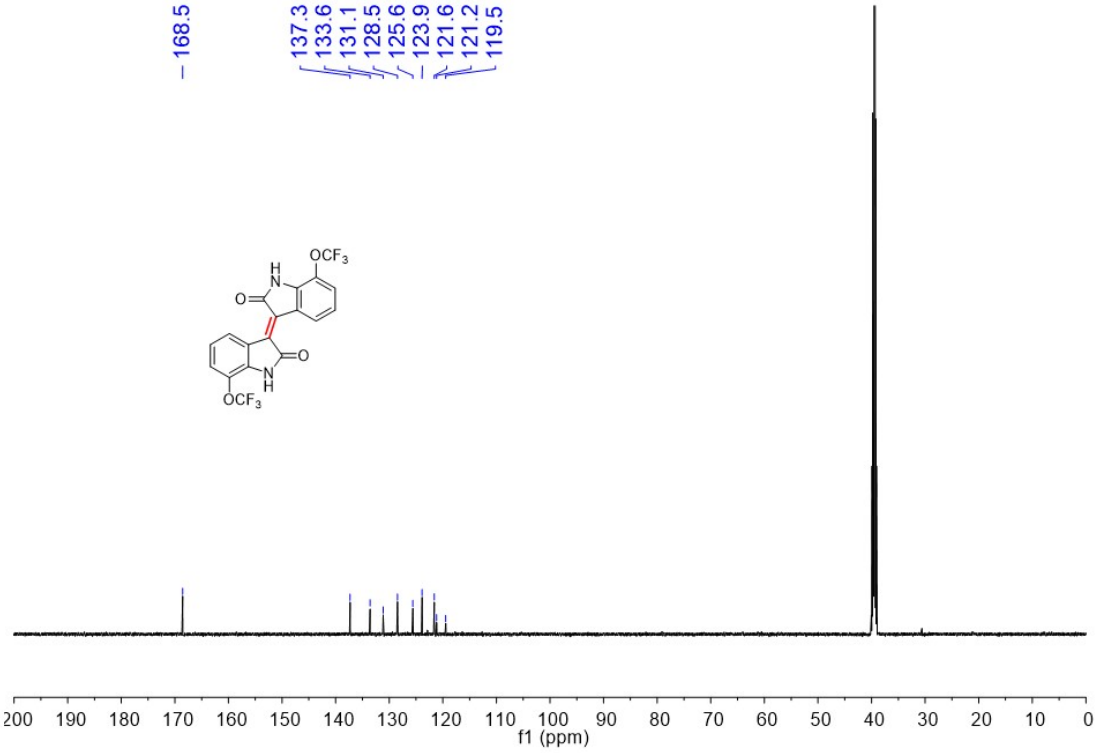

9.65
8.10
7.95
7.93
7.86
7.85
7.72
7.51
6.91
6.89
3.83
1.75
1.43
1.34
0.89
nHex
N
O
O
N
nHex
0.96
0.99
1.91
2.04
1.04
2.02
1.00
2.00
2.03
6.26
3.02
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

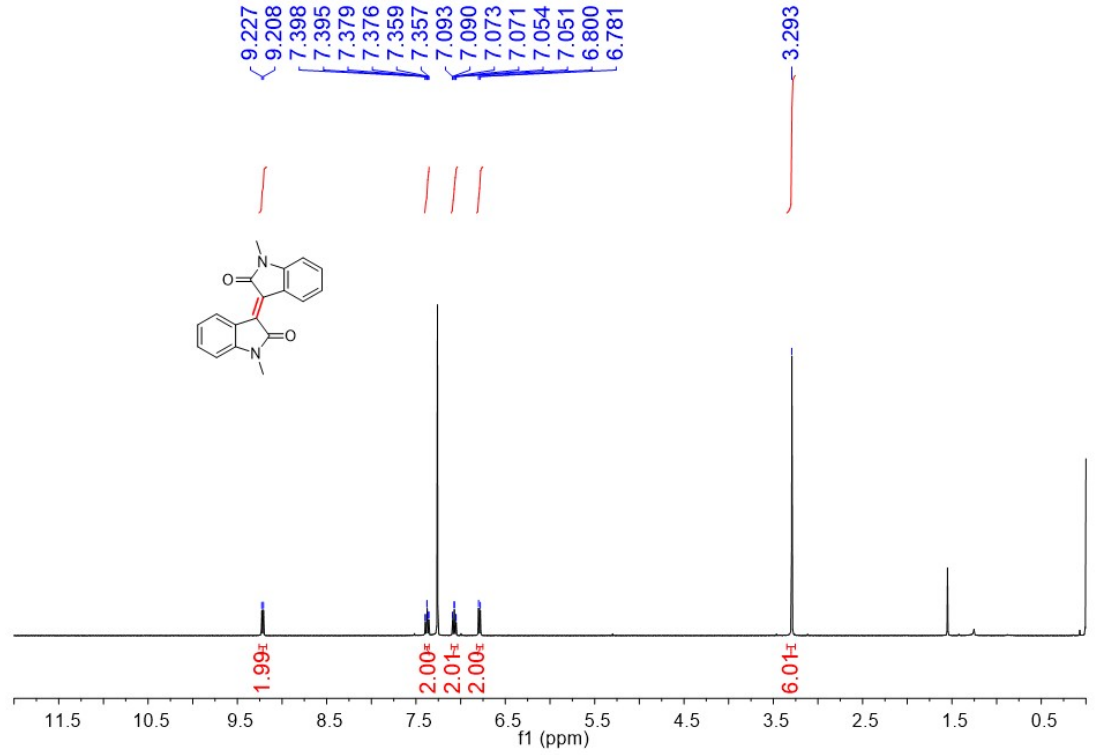

167.9
144.3
135.3
132.5
131.4
129.1
128.5
128.2
127.6
126.2
125.7
125.6
40.2
31.5
27.5
26.7
22.6
14.0
nHex
N
O
O
N
nHex
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


10.79
9.00
6.52
6.38
3.81
H
N
OCH3
O
O
H3CO
N
H
2.04
2.00
4.00
6.34
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)


170.0
162.4
145.7
130.8
129.7
115.1
106.6
95.4
55.4
OCH3
H3CO
f1 (ppm)


11.70
7.65
7.62
7.56
7.54
7.17
7.15
7.13
OCF3
OCF3
2.00
2.11
2.03
2.21
f1 (ppm)


168.5
137.3
133.6
131.1
128.5
125.6
123.9
121.6
121.2
119.5
OCF3
OCF3
f1 (ppm)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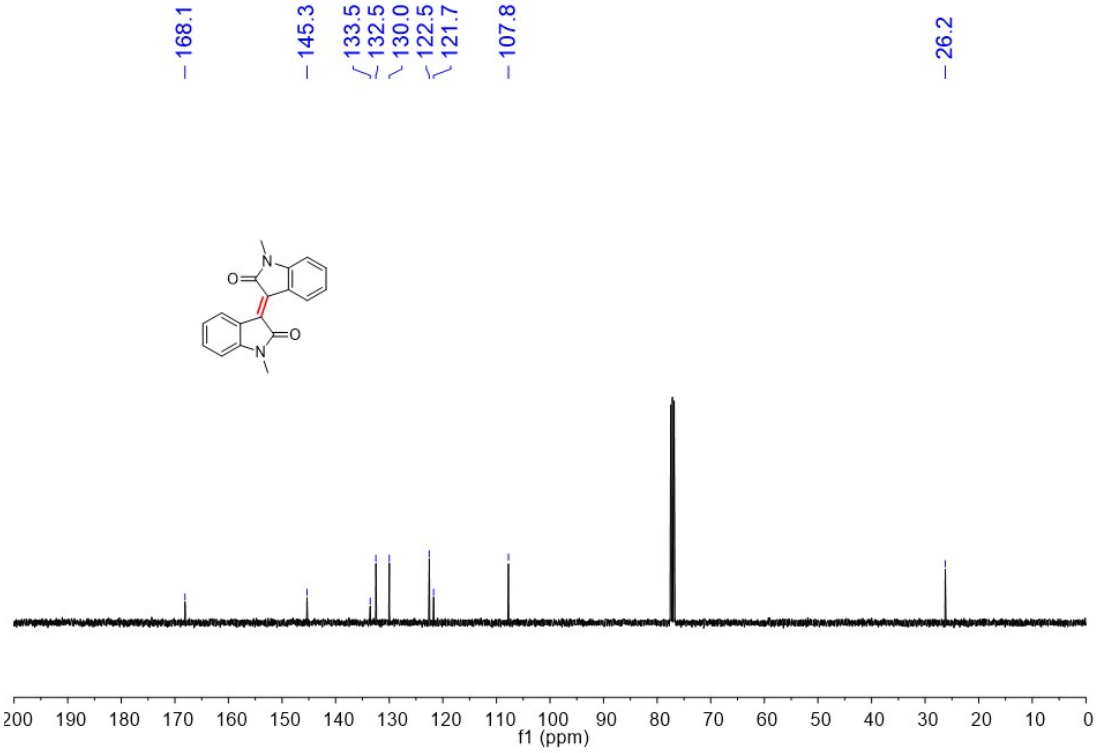
9.208
7.398
7.395
7.379
7.376
7.359
7.357
7.093
7.090
7.073
7.071
7.054
7.051
6.800
6.781
3.293
1.99
2.00
2.01
2.00
6.01
f1 (ppm)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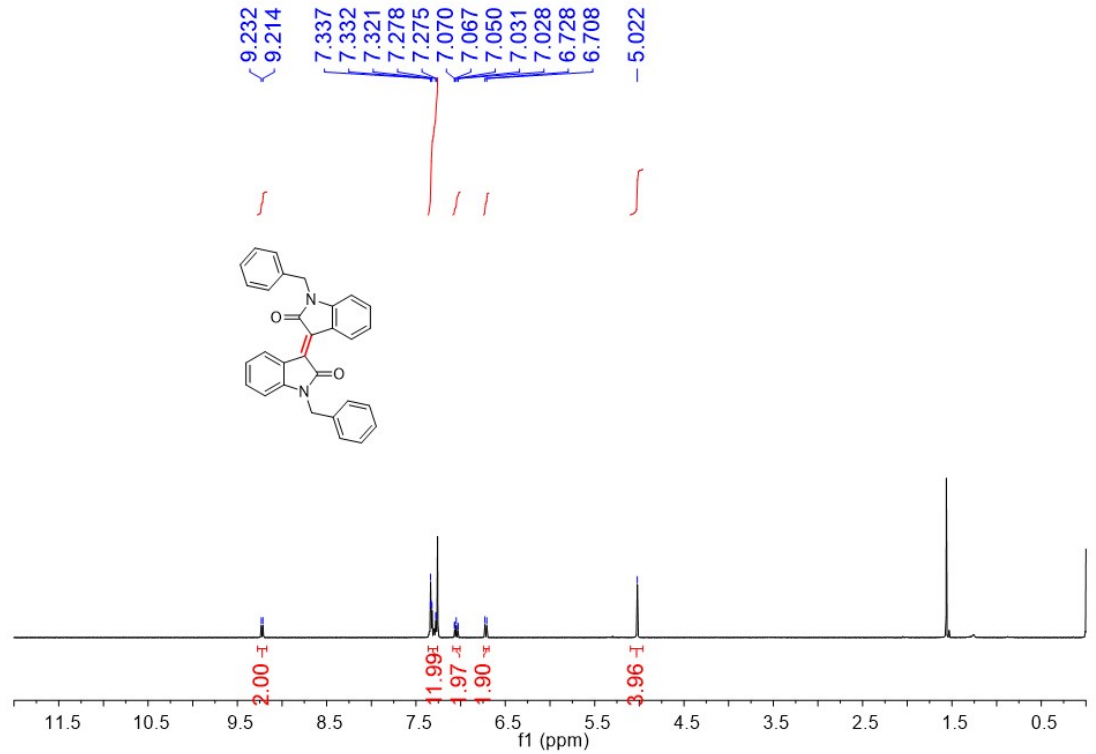
145.3
133.5
132.5
130.0
122.5
121.7
107.8
26.2
f1 (ppm)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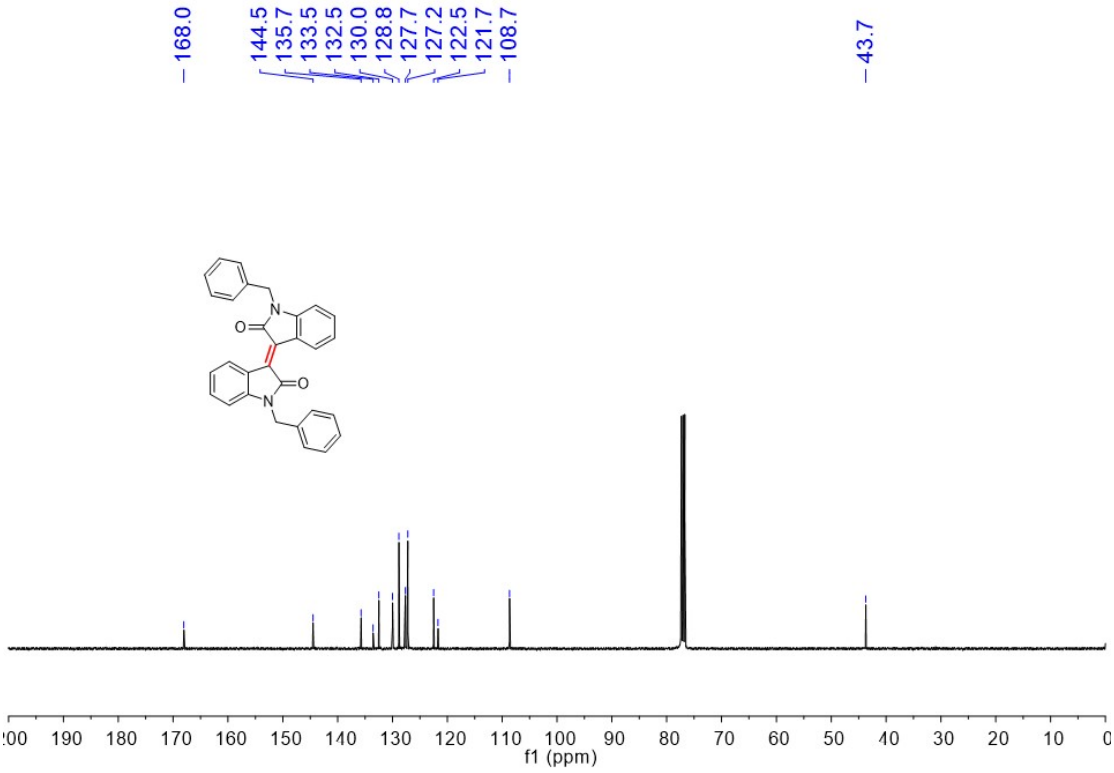
9.214
7.337
7.332
7.321
7.278
7.275
7.070
7.067
7.050
7.031
7.028
6.728
6.708
5.022
2.00
11.99
1.97
1.90
3.96
f1 (ppm)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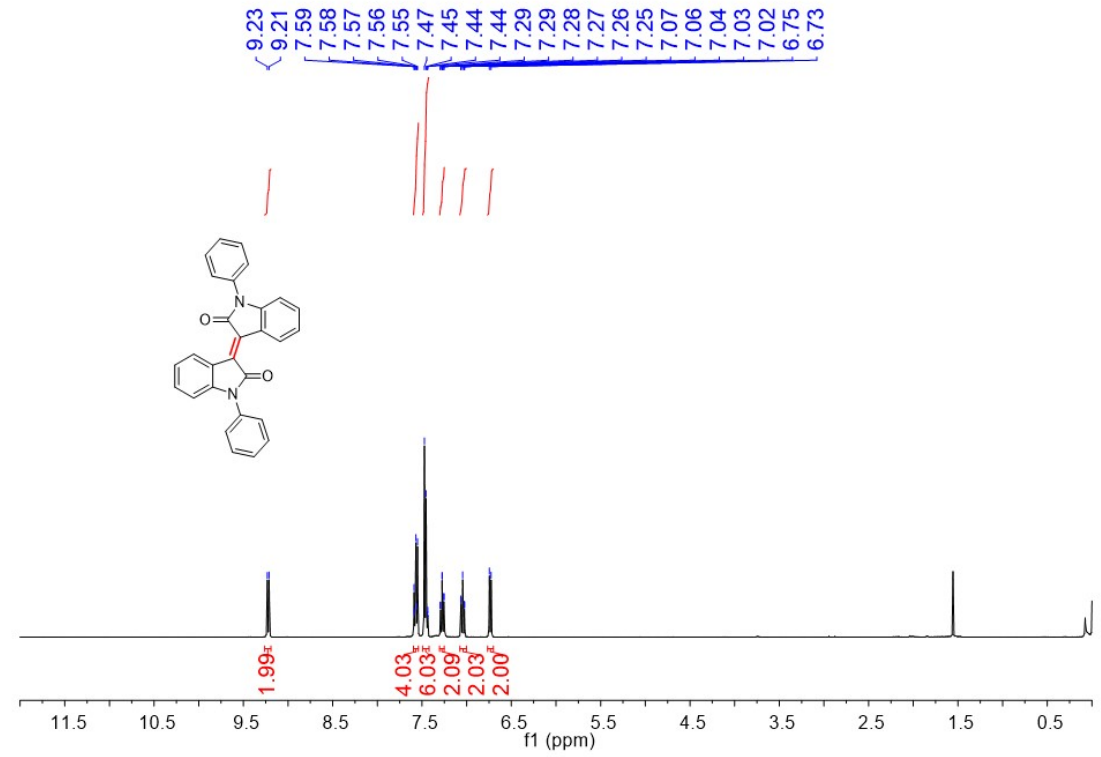
135.7
133.5
132.5
130.0
128.8
127.7
127.2
122.5
121.7
108.7
43.7
O
N
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.23
9.21
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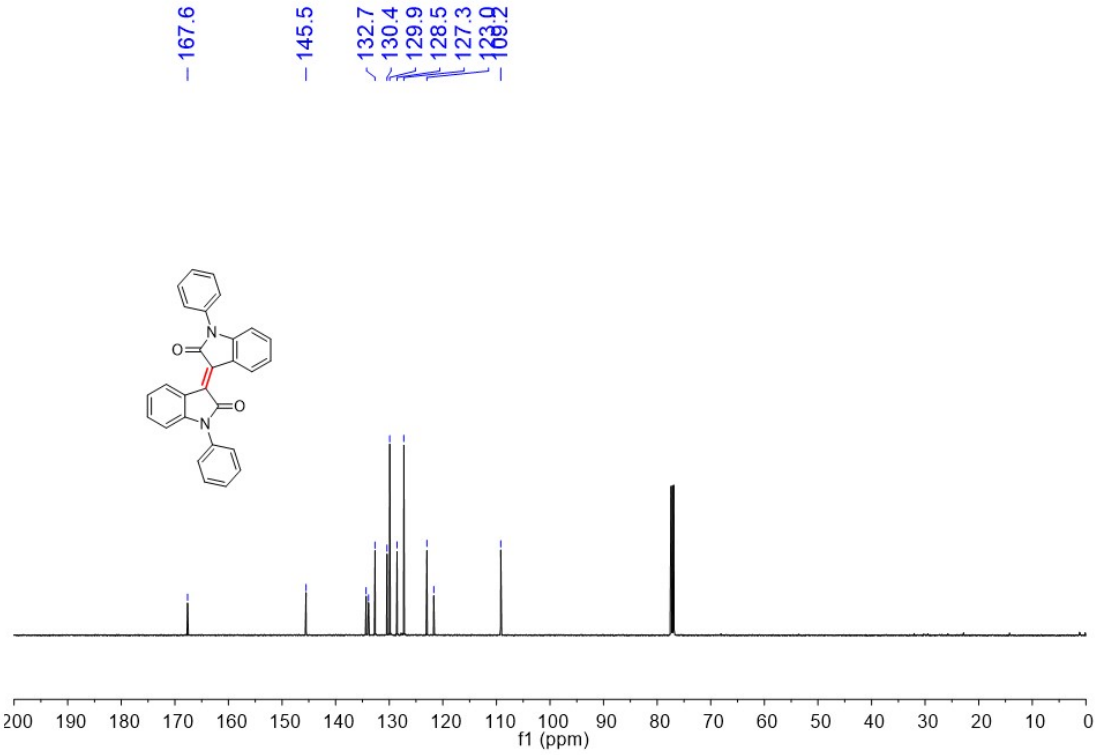
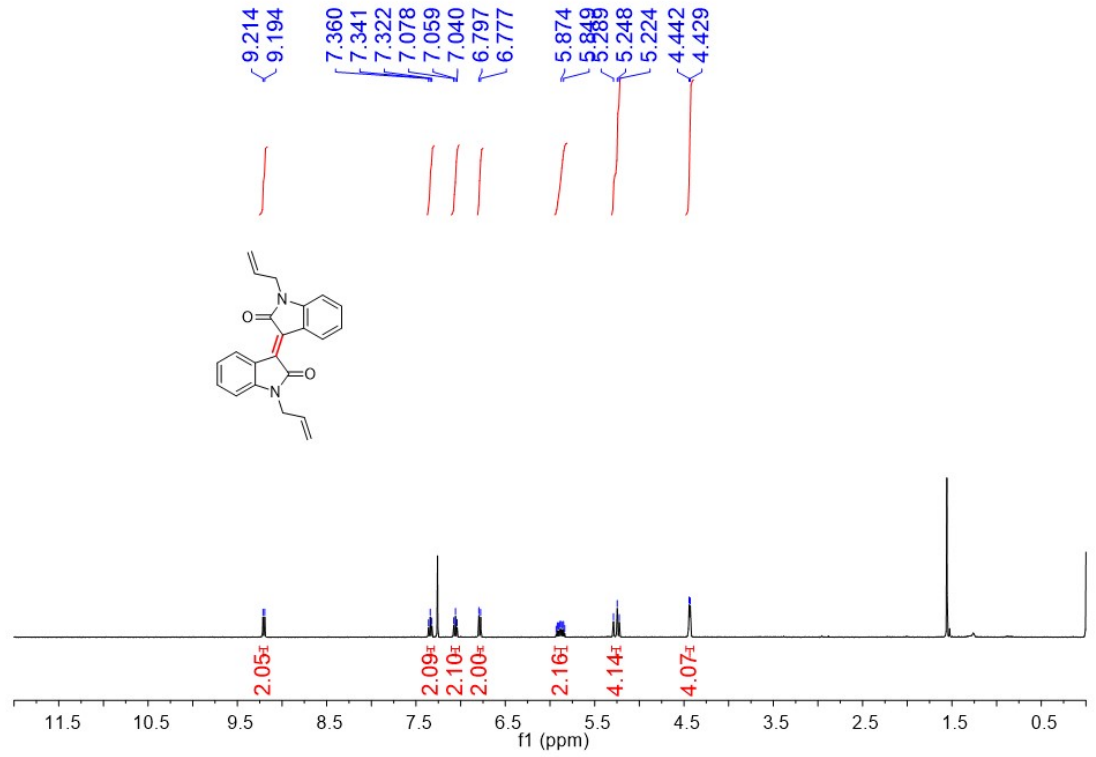
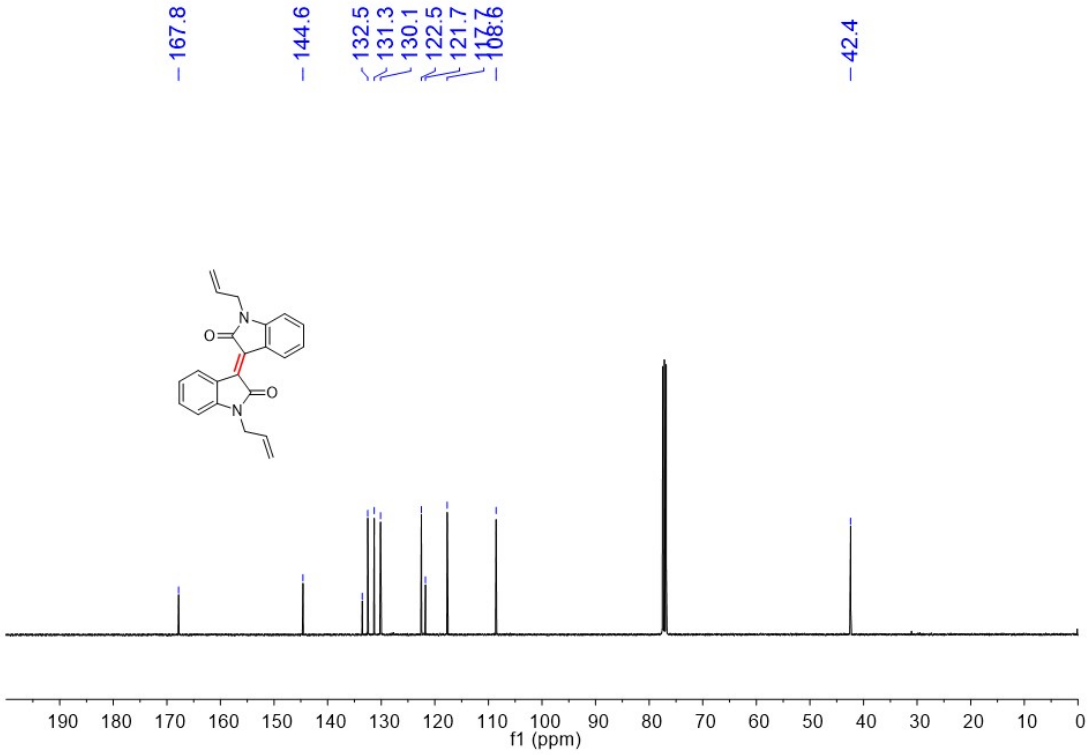
7.47
7.45
7.44
7.44
7.29
7.29
7.28
7.27
7.26
7.25
7.07
7.06
7.04
7.03
7.02
6.75
6.73
O
N
O
N
1.99
4.03
6.03
2.09
2.03
2.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)


167.6
145.5
132.7
130.4
129.9
128.5
127.3
123.9
109.2
O
N
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.214
9.194
7.360
7.341
7.322
7.078
7.059
7.040
6.797
6.777
5.874
5.289
5.248
5.224
4.442
4.429
N
O
O
N
2.05
2.09
2.10
2.00
2.16
4.14
4.07
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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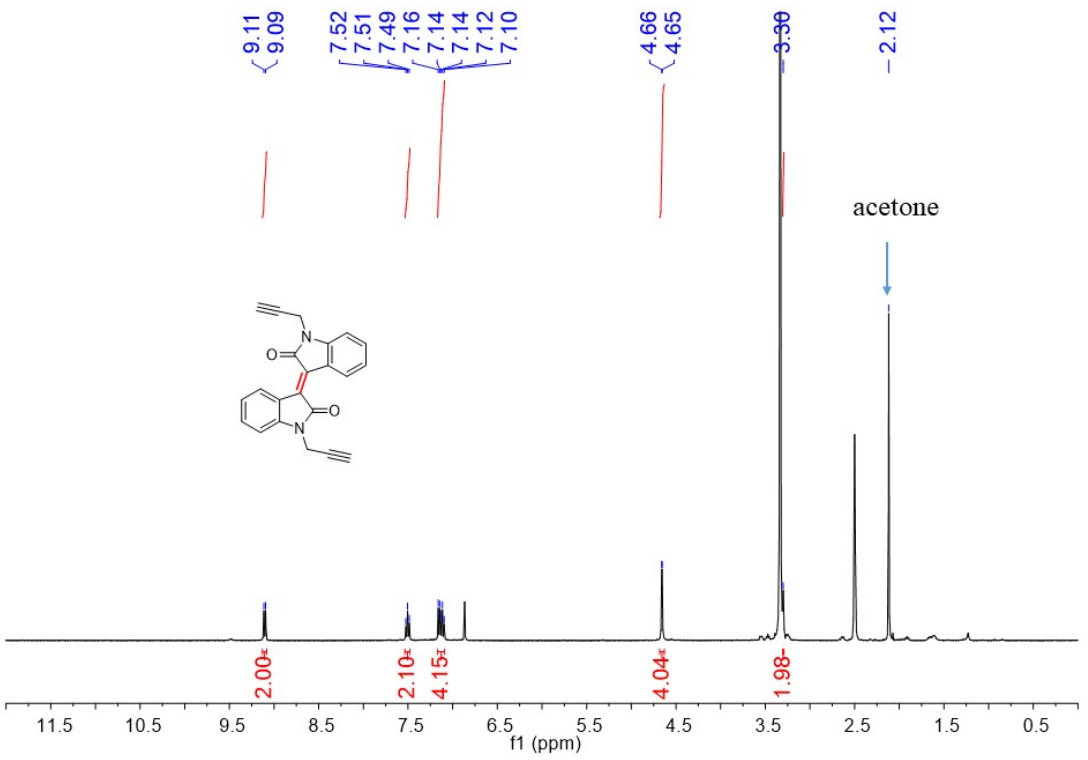
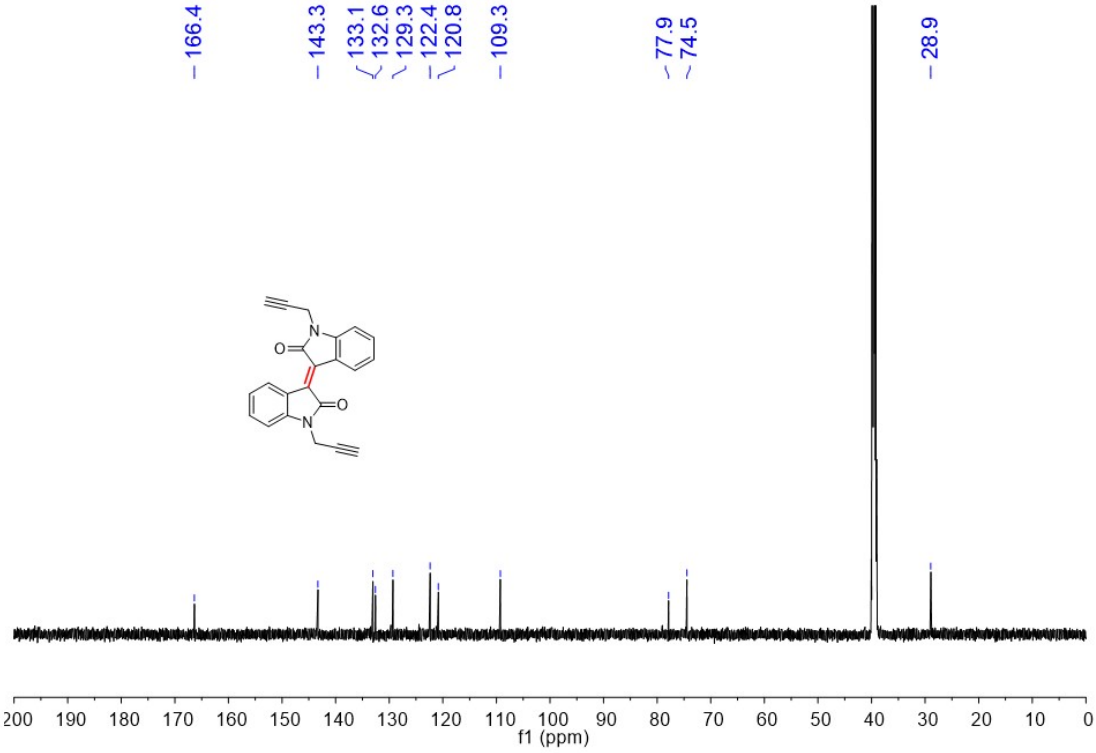
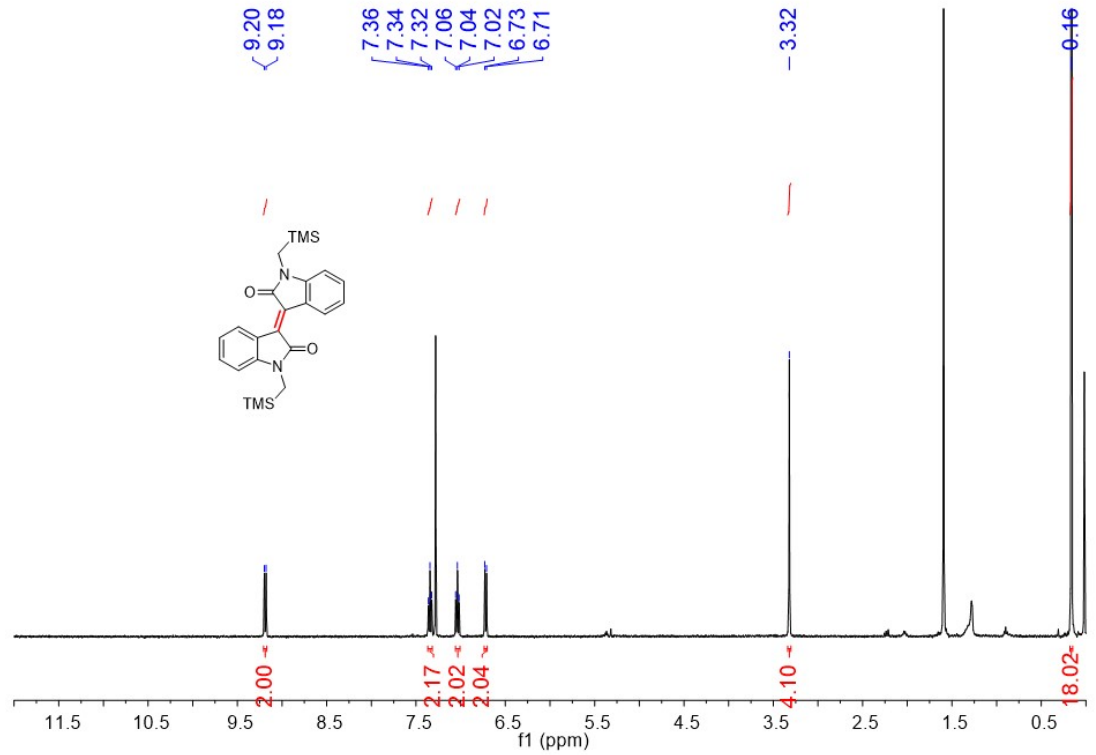
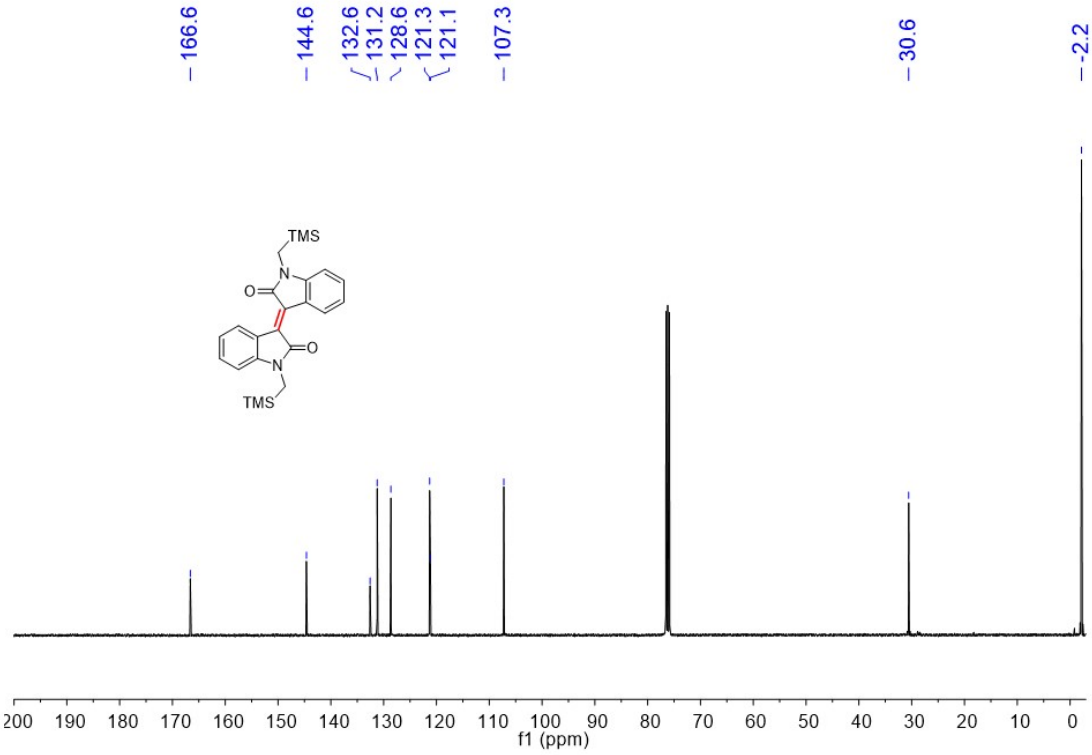
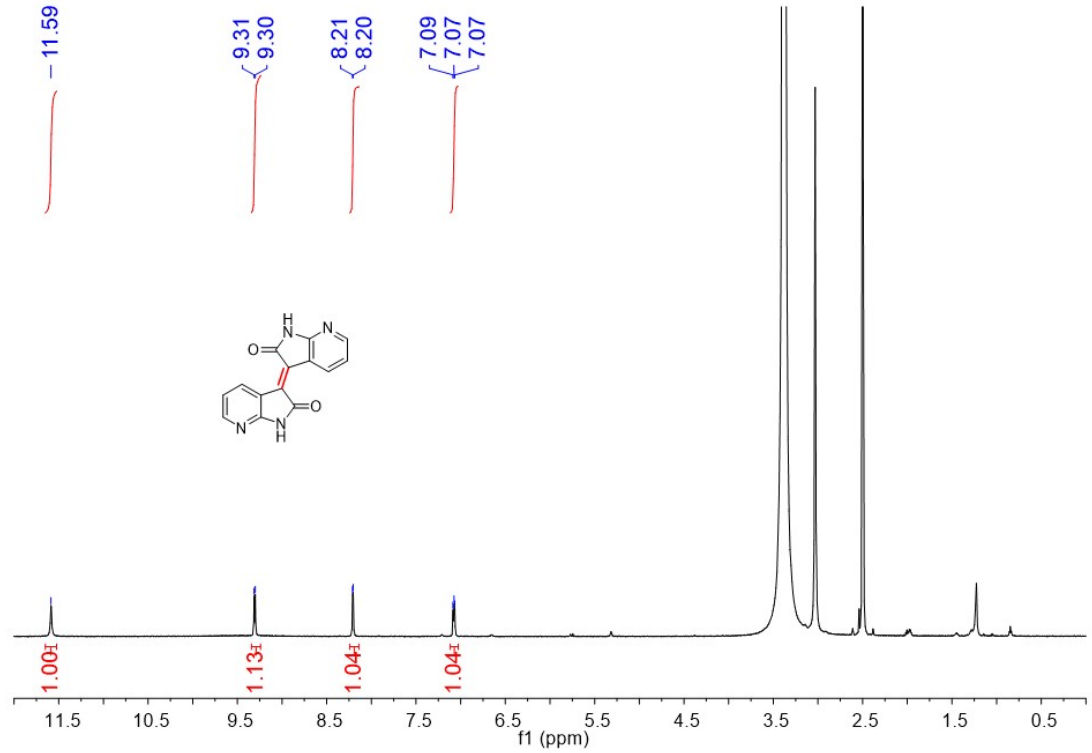
144.6
132.5
131.3
130.1
122.5
121.7
117.7
108.6
42.4
f1 (ppm)

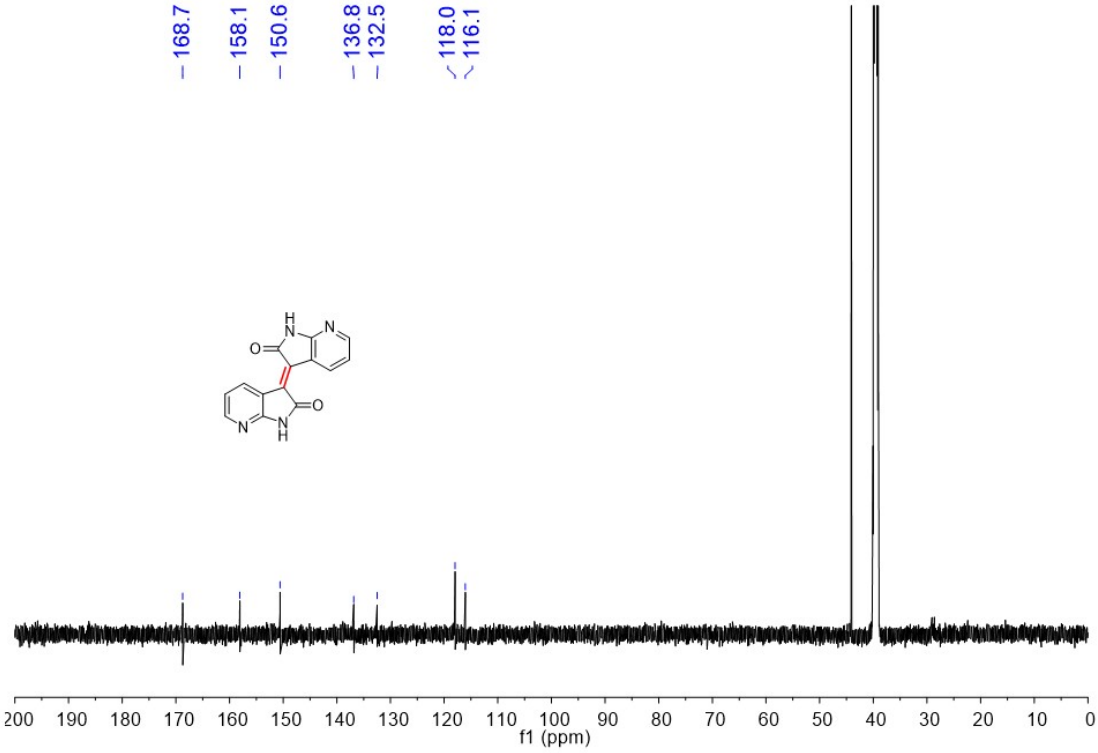

9.11
9.09
7.52
7.51
7.49
7.16
7.14
7.14
7.12
7.10
4.66
4.65
3.30
2.12
acetone
2.00
2.10
4.15
4.04
1.98
f1 (ppm)

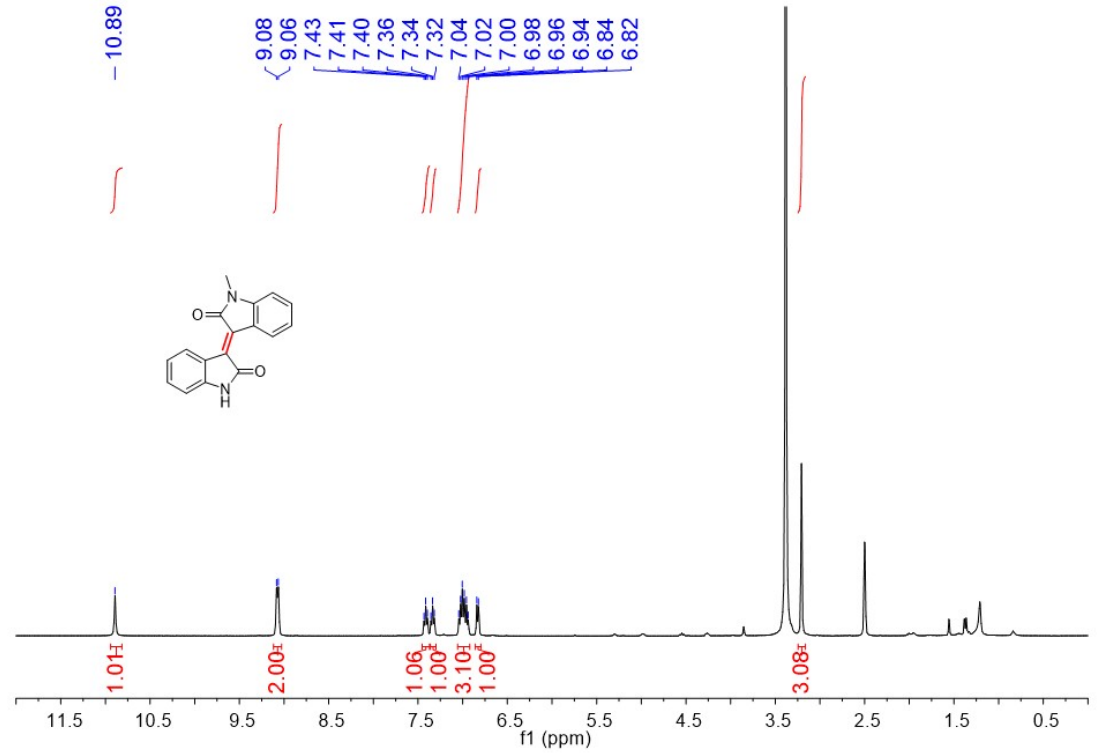

166.4
143.3
133.1
132.6
129.3
122.4
120.8
109.3
77.9
74.5
28.9
O
N
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

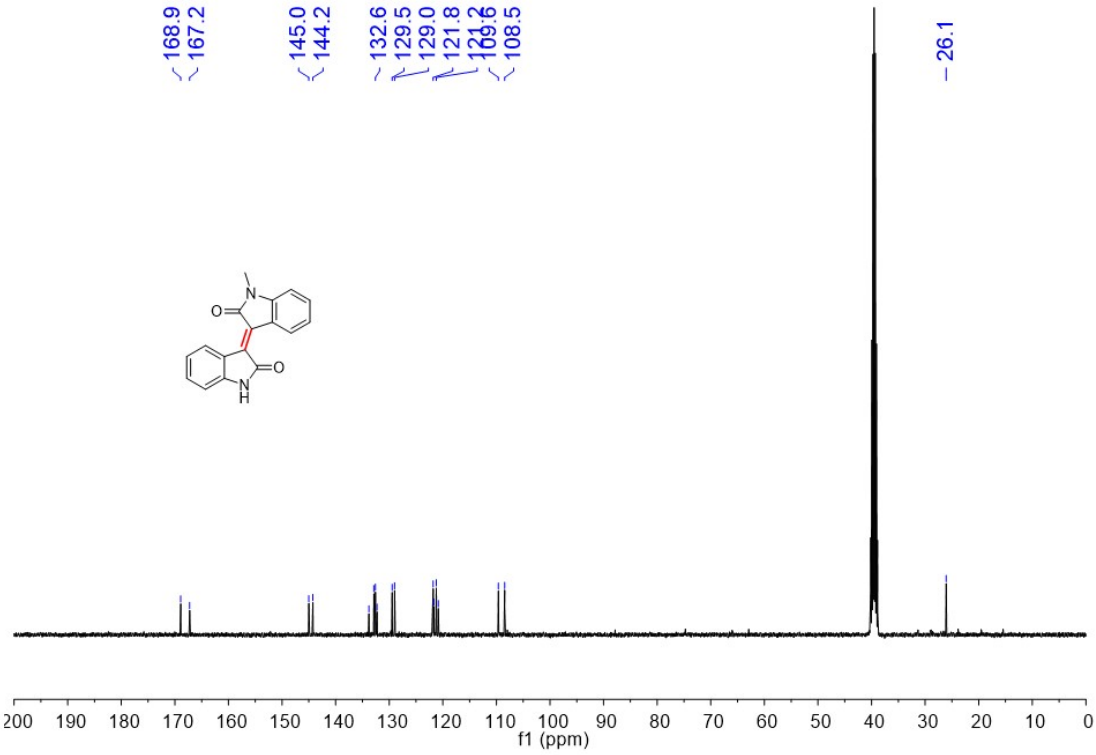

9.20
9.18
7.36
7.34
7.32
7.06
7.04
7.02
6.73
6.71
3.32
0.16
TMS
O
N
O
N
TMS
2.00
2.17
2.02
2.04
4.10
18.02
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)


166.6
144.6
132.6
131.2
128.6
121.3
121.1
107.3
30.6
-2.2
TMS
TMS
f1 (ppm)


11.59
9.31
9.30
8.21
8.20
7.09
7.07
7.07
1.00
1.13
1.04
1.04
f1 (ppm)


168.7
158.1
150.6
136.8
132.5
118.0
116.1
f1 (ppm)


10.89
9.08
9.06
7.43
7.41
7.40
7.36
7.34
7.32
7.04
7.02
7.00
6.98
6.96
6.94
6.84
6.82
1.01
2.00
1.06
1.00
3.10
1.00
3.08
f1 (ppm)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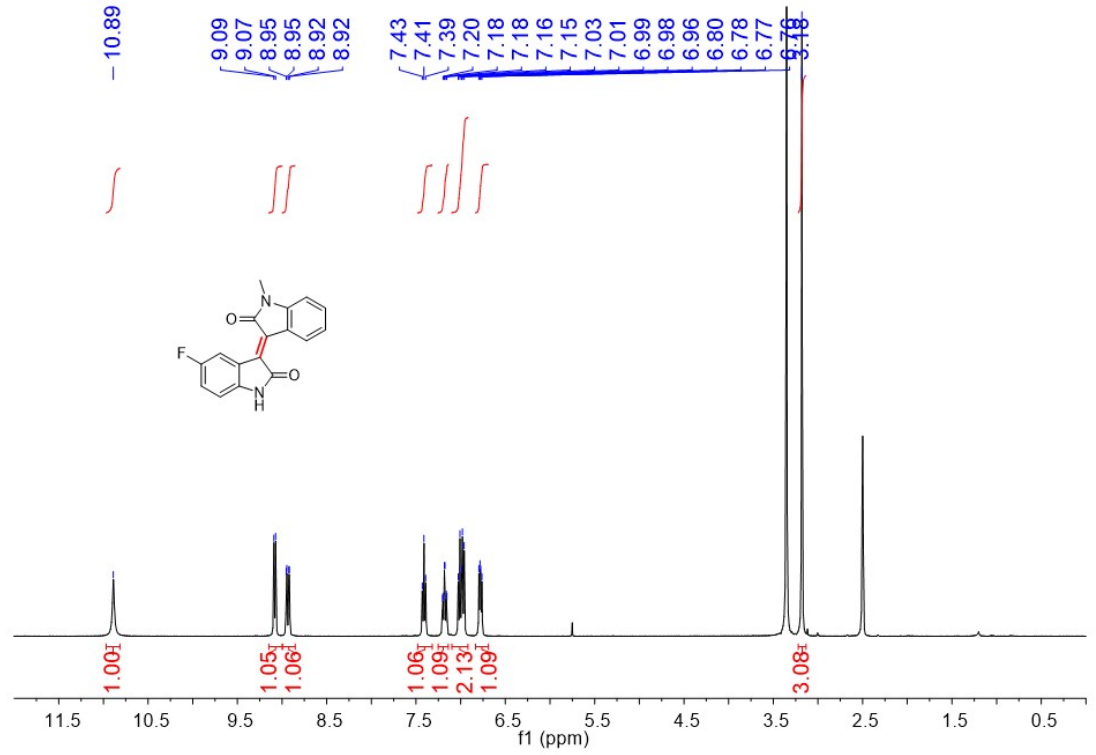
167.2
145.0
144.2
132.6
129.5
129.0
121.8
121.2
109.6
108.5
26.1
O
N
O
O
H
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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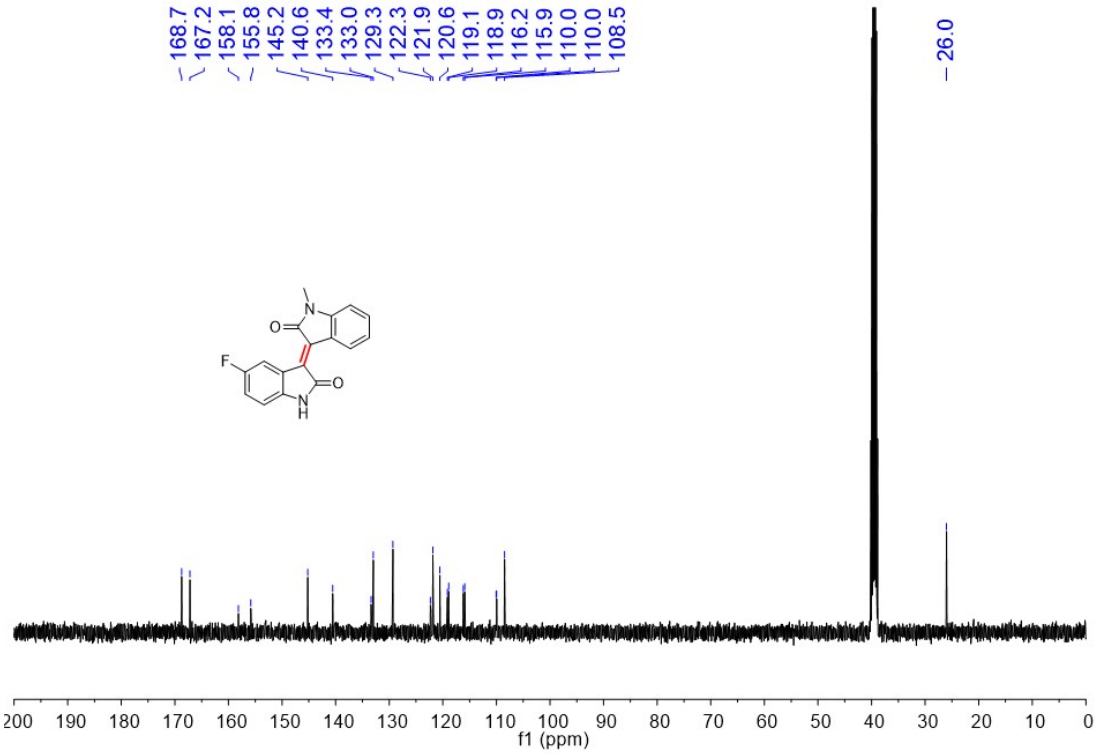
8.95
8.92
8.92
7.43
7.41
7.39
7.20
7.18
7.18
7.16
7.15
7.03
7.01
6.99
6.98
6.96
6.80
6.78
6.77
6.76
3.18
O
N
F
O
H
1.00
1.05
1.06
1.06
1.09
2.13
1.09
3.08
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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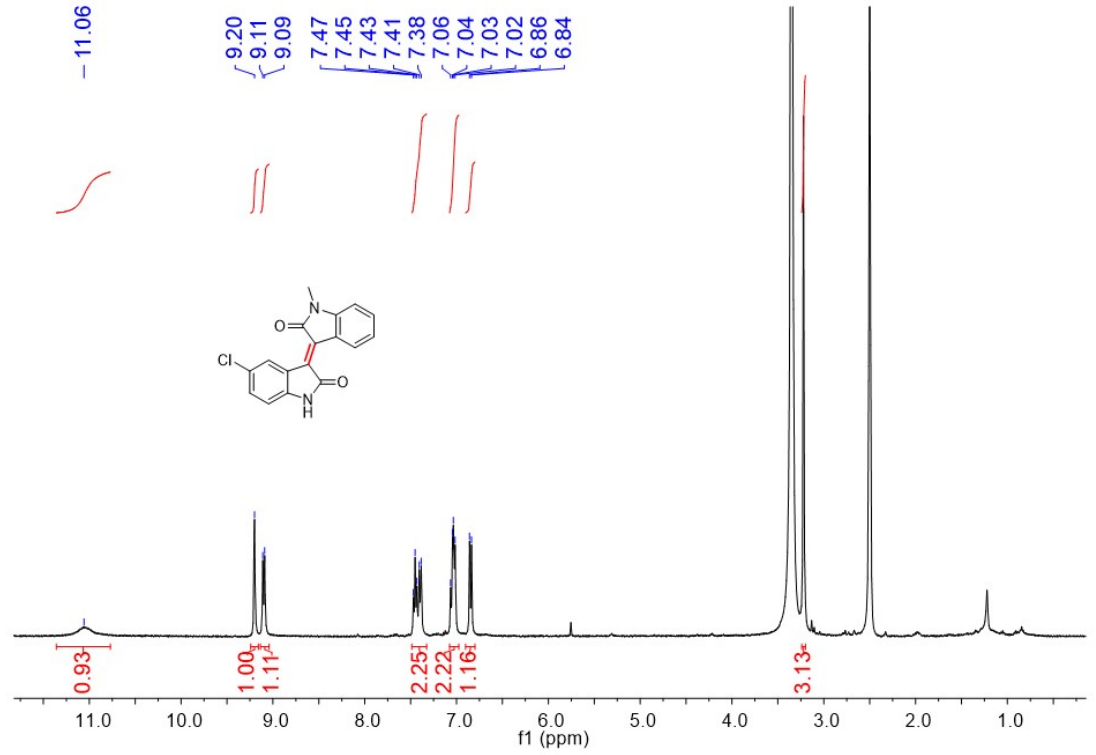
167.2
158.1
155.8
145.2
140.6
133.4
133.0
129.3
122.3
121.9
120.6
119.1
118.9
116.2
115.9
110.0
110.0
108.5
26.0
f1 (ppm)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9.11
9.09
7.47
7.45
7.43
7.41
7.38
7.06
7.04
7.03
7.02
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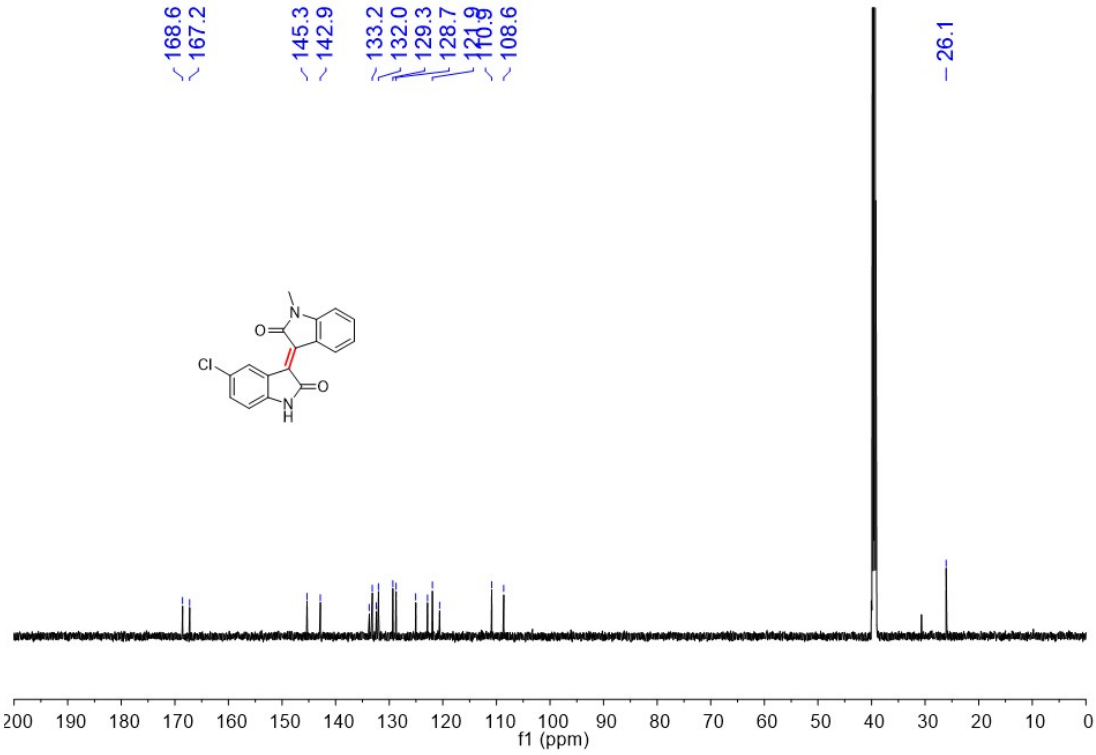
6.84
0.93
1.00
1.11
2.25
2.22
1.16
3.13
f1 (ppm)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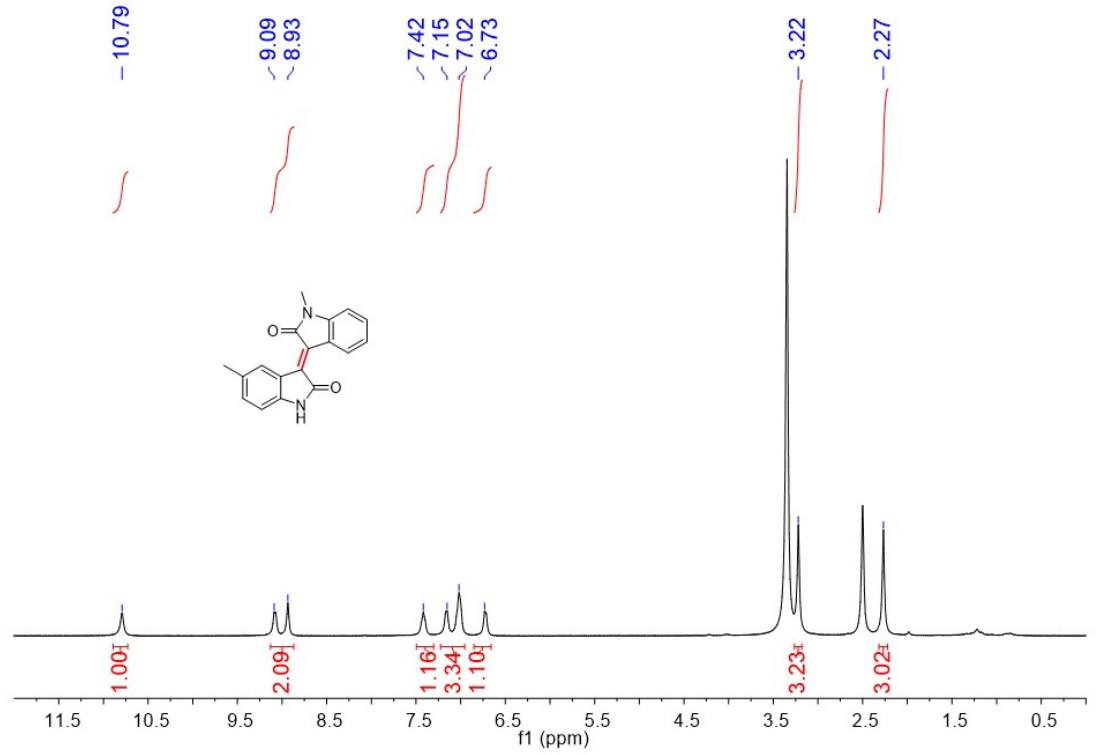
167.2
145.3
142.9
133.2
132.0
129.3
128.7
121.9
110.9
108.6
26.1
Cl
O
N
H
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.42
7.15
7.02
6.73
3.22
2.27
O
N
H
1.00
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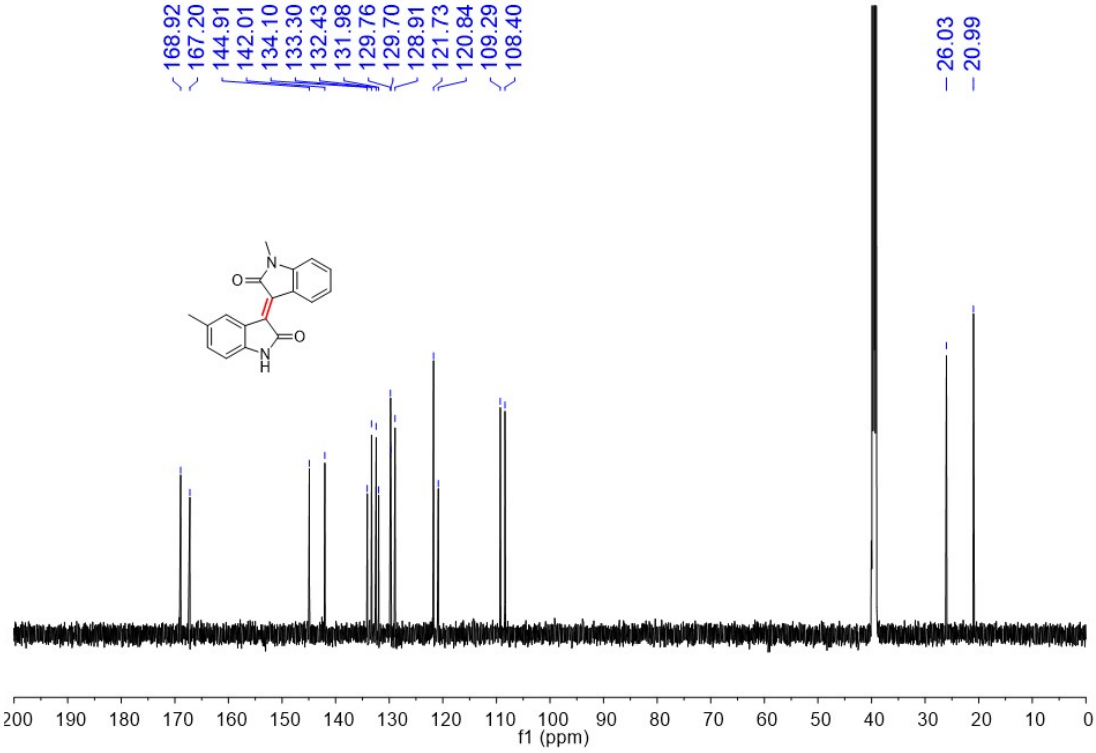
1.16
3.34
1.10
3.23
3.02
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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133.30
132.43
131.98
129.76
129.70
128.91
121.73
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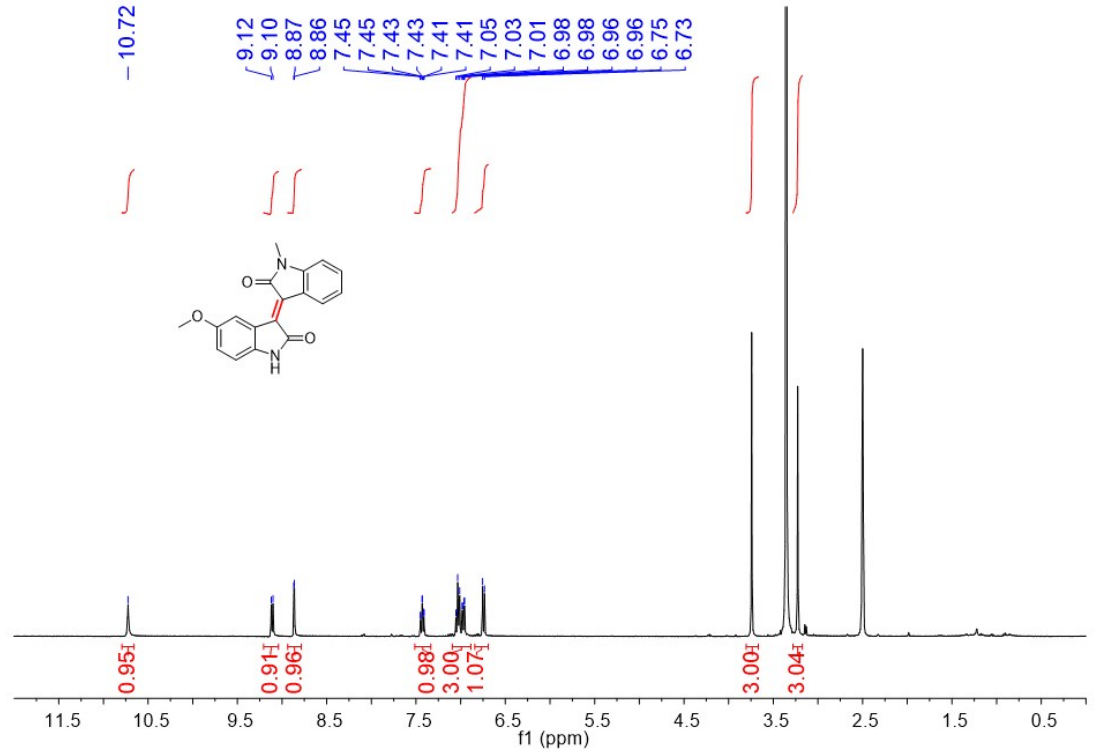
109.29
108.40
26.03
20.99
f1 (ppm)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8.86
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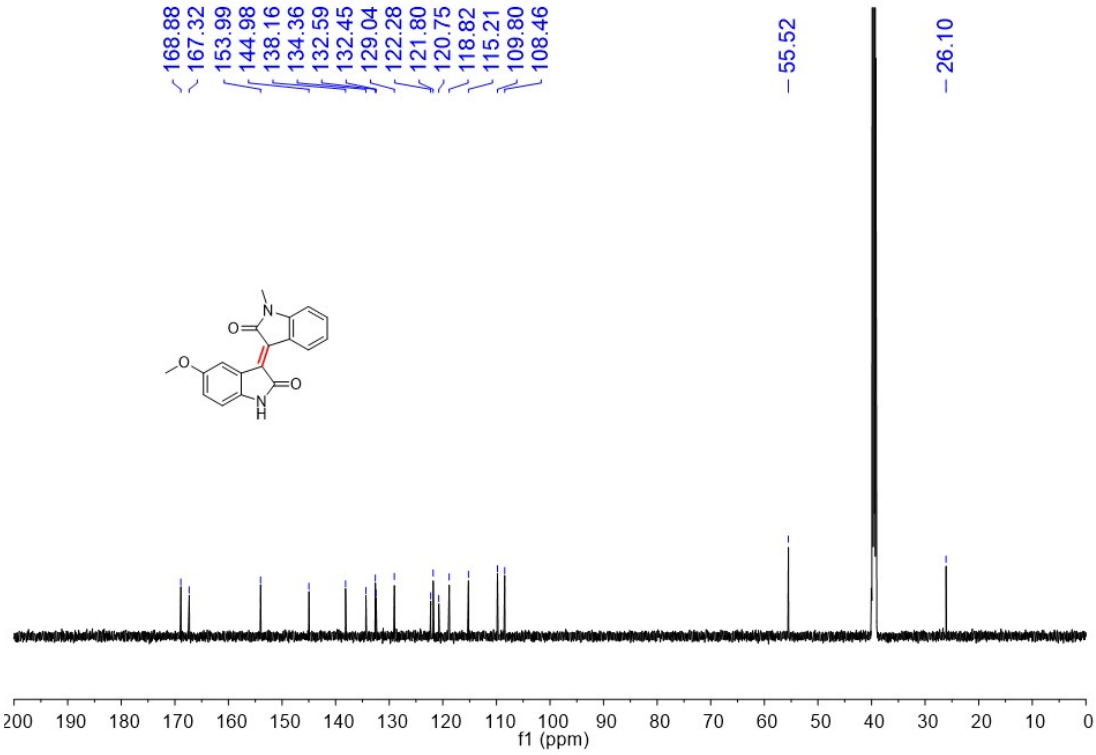
7.45
7.43
7.43
7.41
7.41
7.05
7.03
7.01
6.98
6.98
6.96
6.96
6.75
6.73
0.95
0.91
0.96
0.98
3.00
1.07
3.00
3.04
f1 (ppm)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121.80
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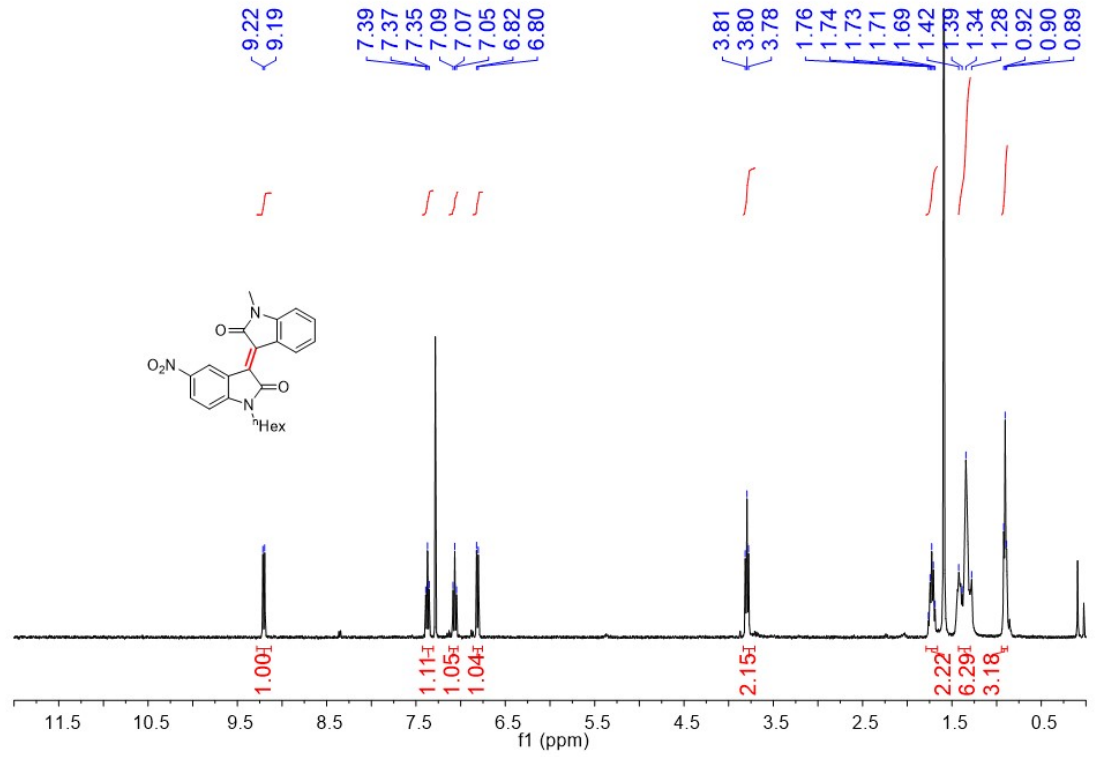
109.80
108.46
55.52
26.10
f1 (ppm)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9.19
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7.37
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7.09
7.07
7.05
6.82
6.80
3.81
3.80
3.78
1.76
1.74
1.73
1.71
1.69
1.42
1.39
1.34
1.28
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0.90
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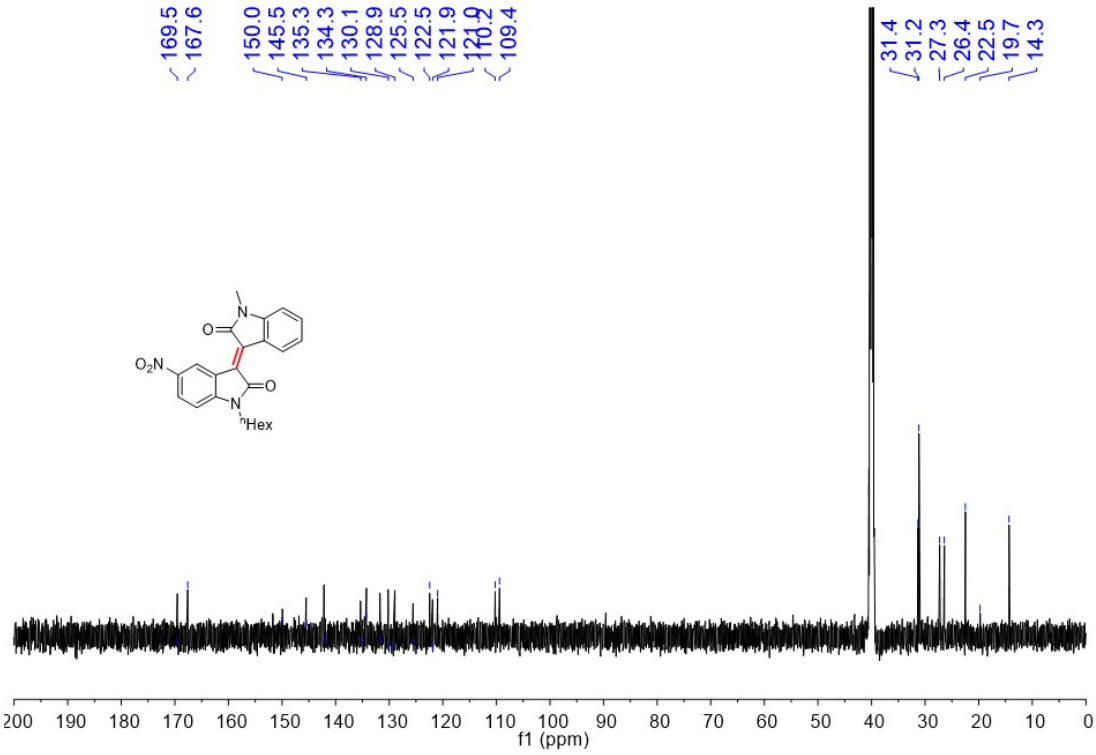
1.00
1.11
1.05
1.04
2.15
2.22
6.29
3.18
f1 (ppm)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167.6
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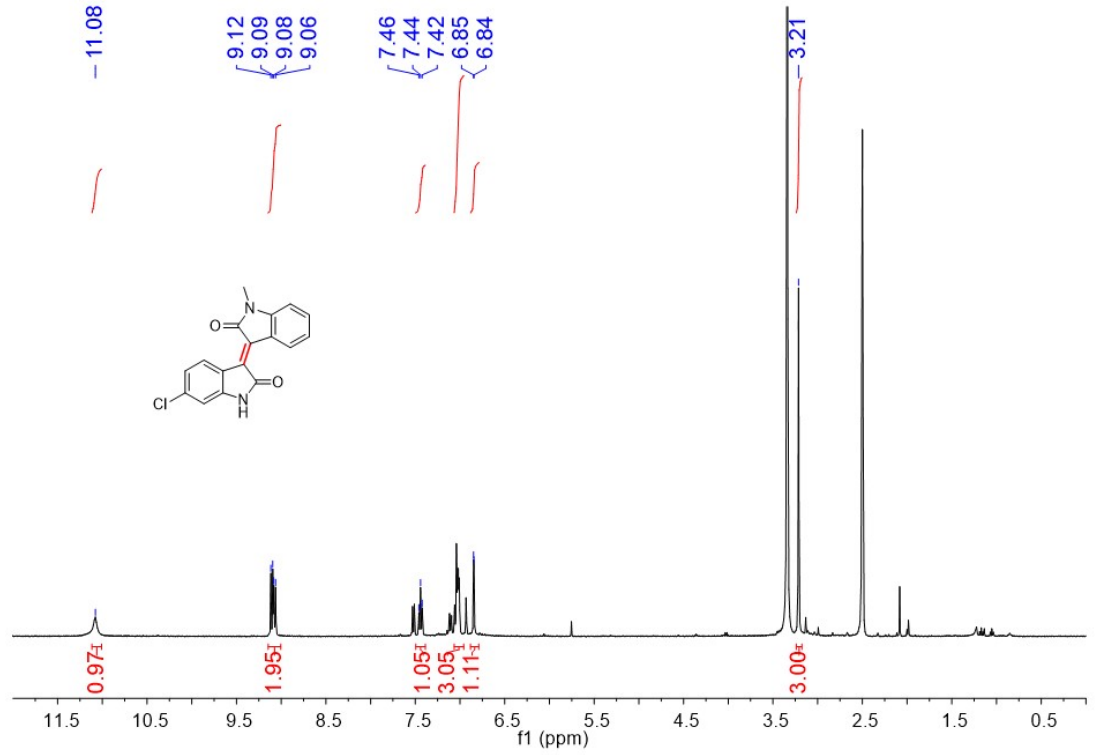
145.5
135.3
134.3
130.1
128.9
125.5
122.5
121.9
109.4
31.4
31.2
27.3
26.4
22.5
19.7
14.3
O2N
O
O
N
nHex
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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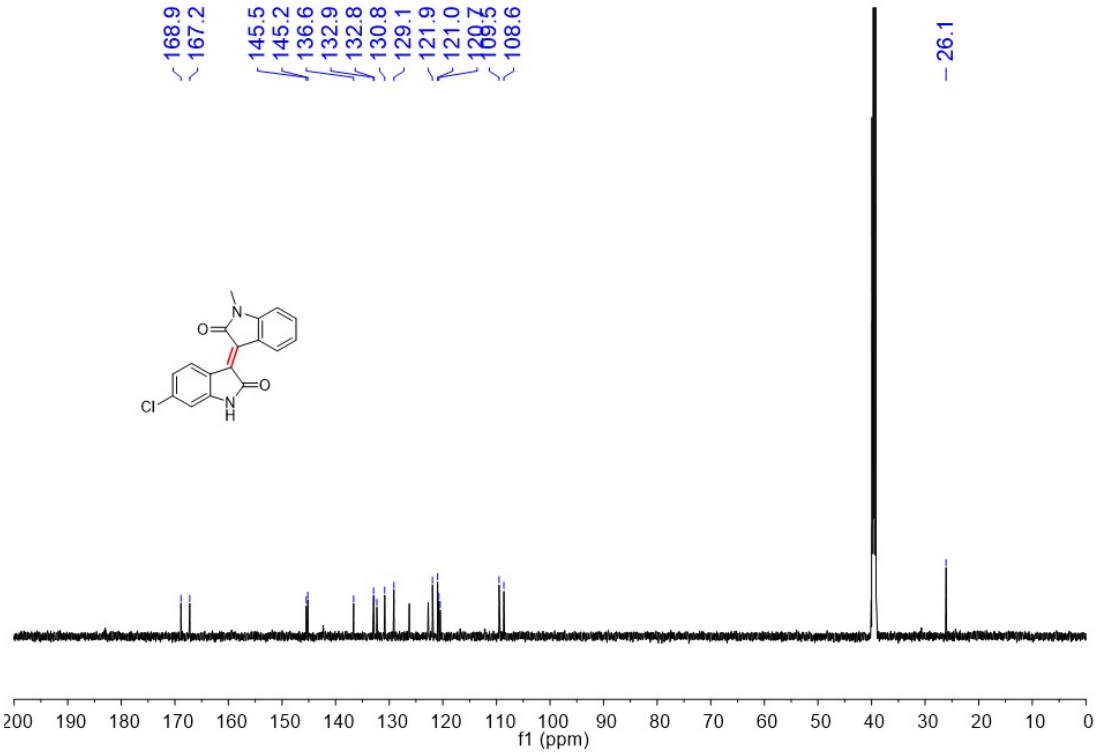
9.08
9.06
7.46
7.44
7.42
6.85
6.84
3.21
Cl
O
N
H
0.97
1.95
1.05
3.05
1.11
3.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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145.2
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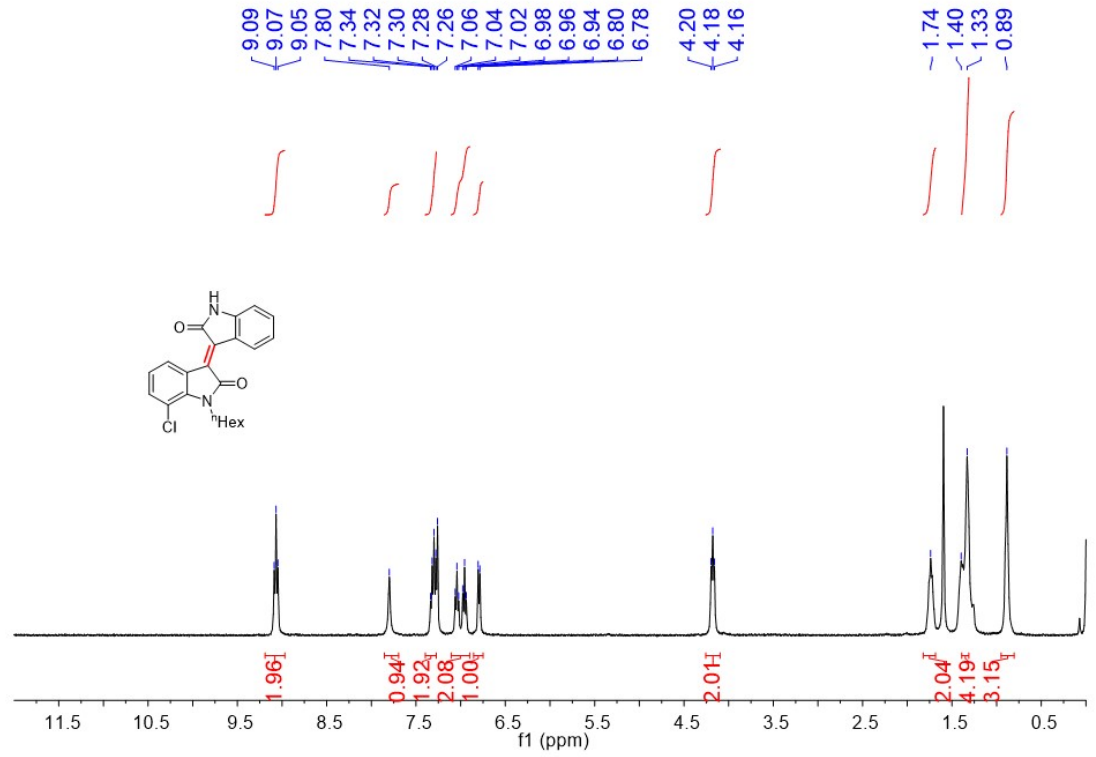
132.9
132.8
130.8
129.1
121.9
121.0
108.6
26.1
f1 (ppm)


9.09
9.07
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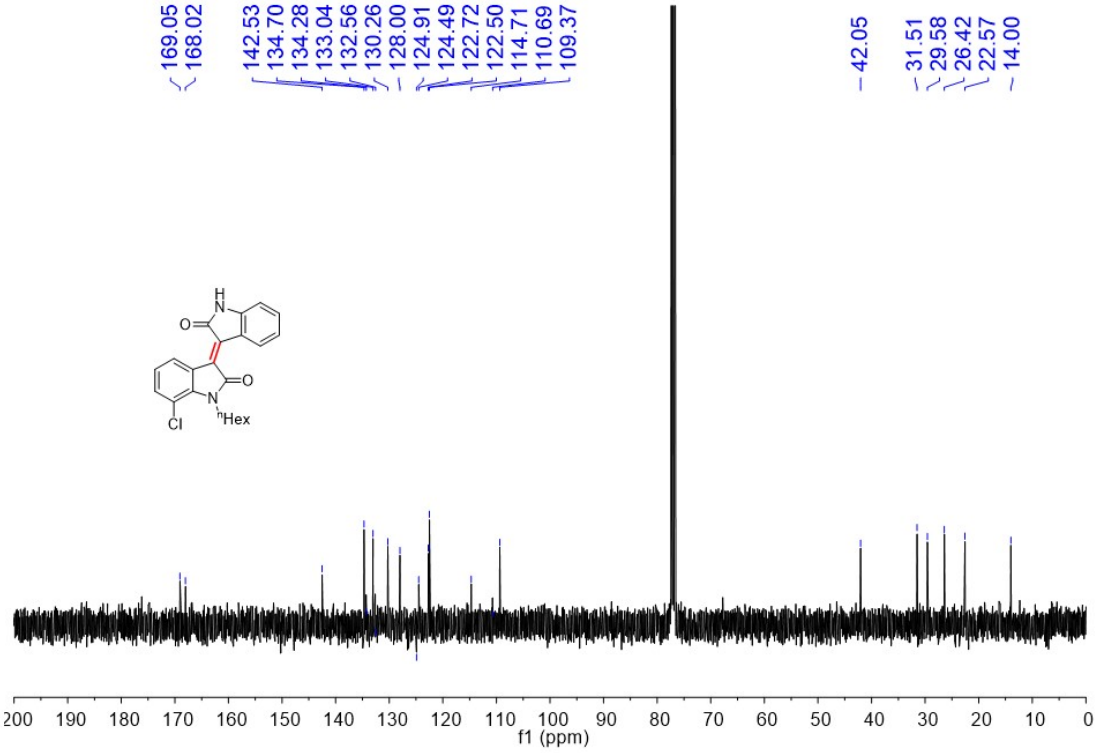
7.32
7.30
7.28
7.26
7.06
7.04
7.02
6.98
6.96
6.94
6.80
6.78
4.20
4.18
4.16
1.74
1.40
1.33
0.89
1.96
0.94
1.92
2.08
1.00
2.01
2.04
4.19
3.15
f1 (ppm)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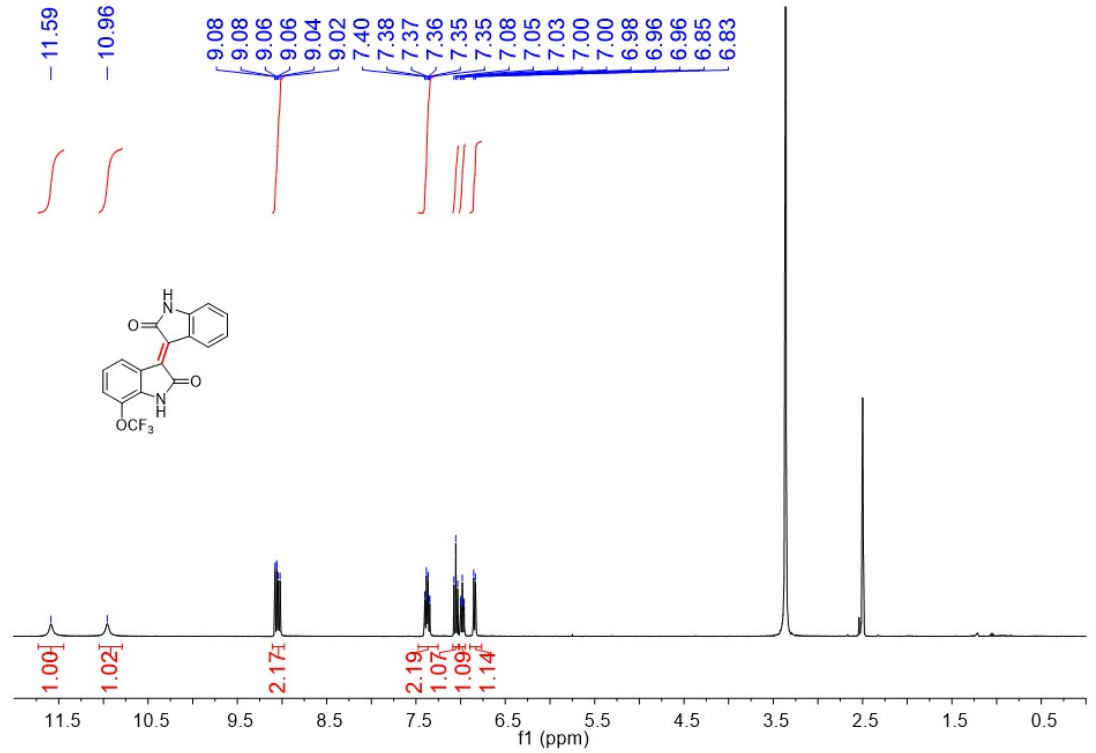
26.42
22.57
14.00
Cl
nHex
f1 (ppm)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9.08
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9.06
9.04
9.02
7.40
7.38
7.37
7.36
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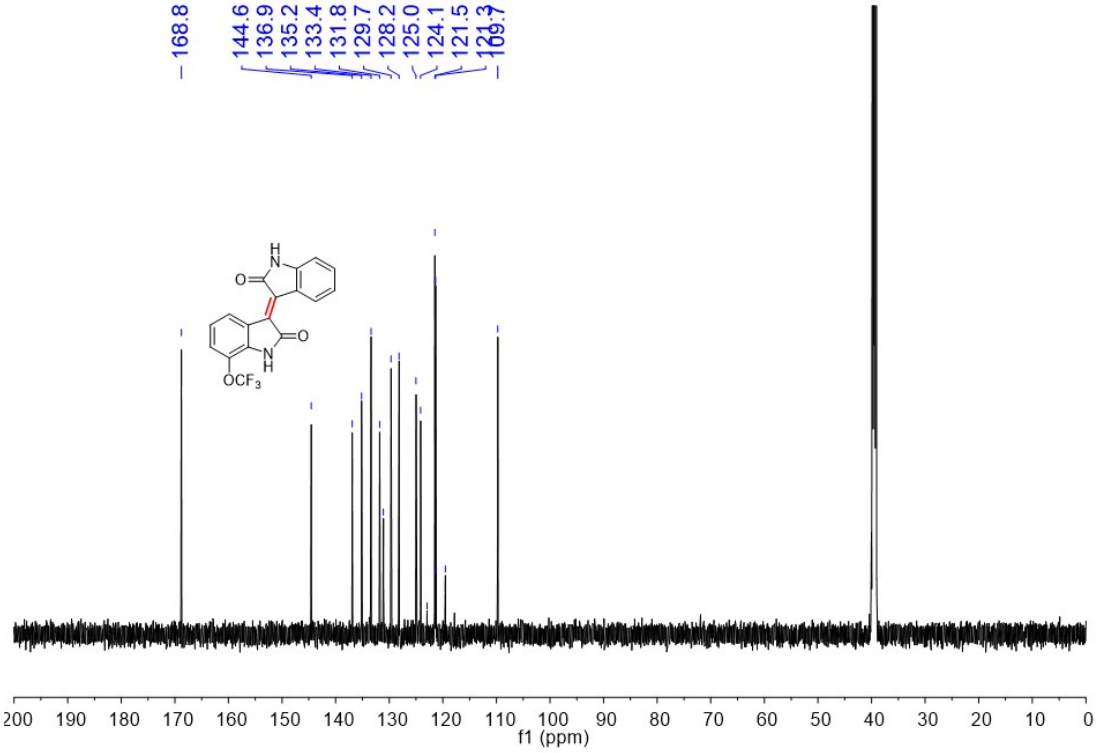
7.35
7.08
7.05
7.03
7.00
7.00
6.98
6.96
6.96
6.85
6.83
OCF3
1.00
1.02
2.17
2.19
1.07
1.09
1.14
f1 (ppm)


168.8
144.6
136.9
135.2
133.4
131.8
129.7
128.2
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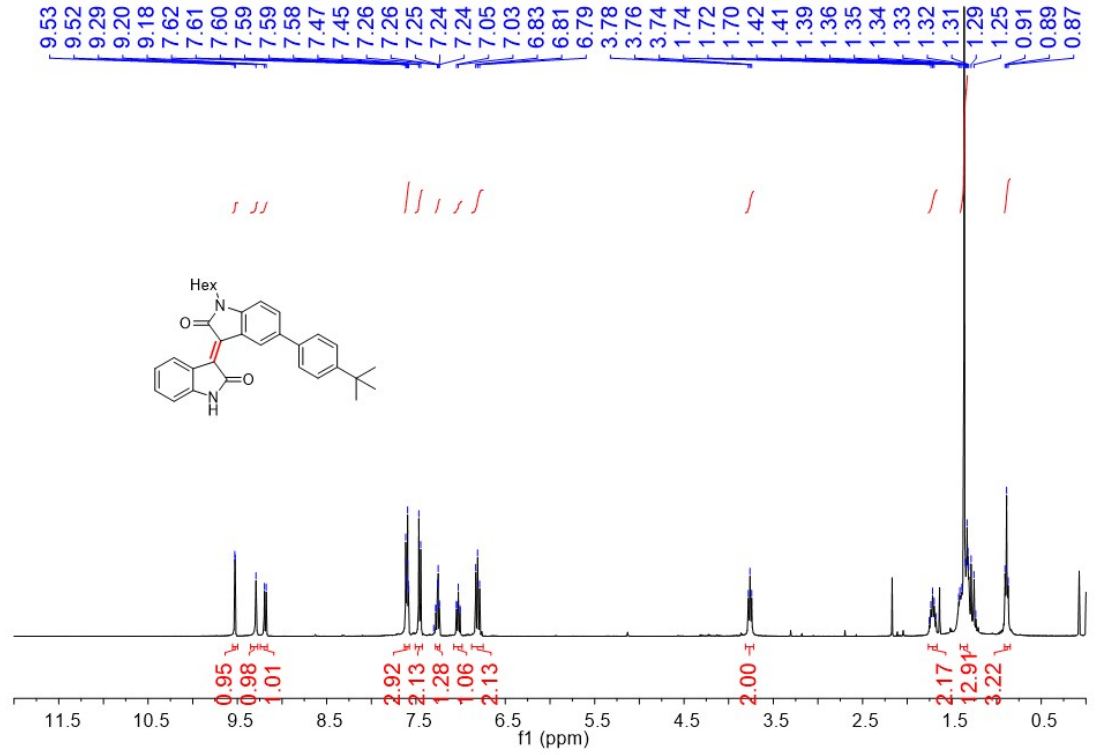
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0.89
0.87
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0.98
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2.92
2.13
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1.06
2.13
2.00
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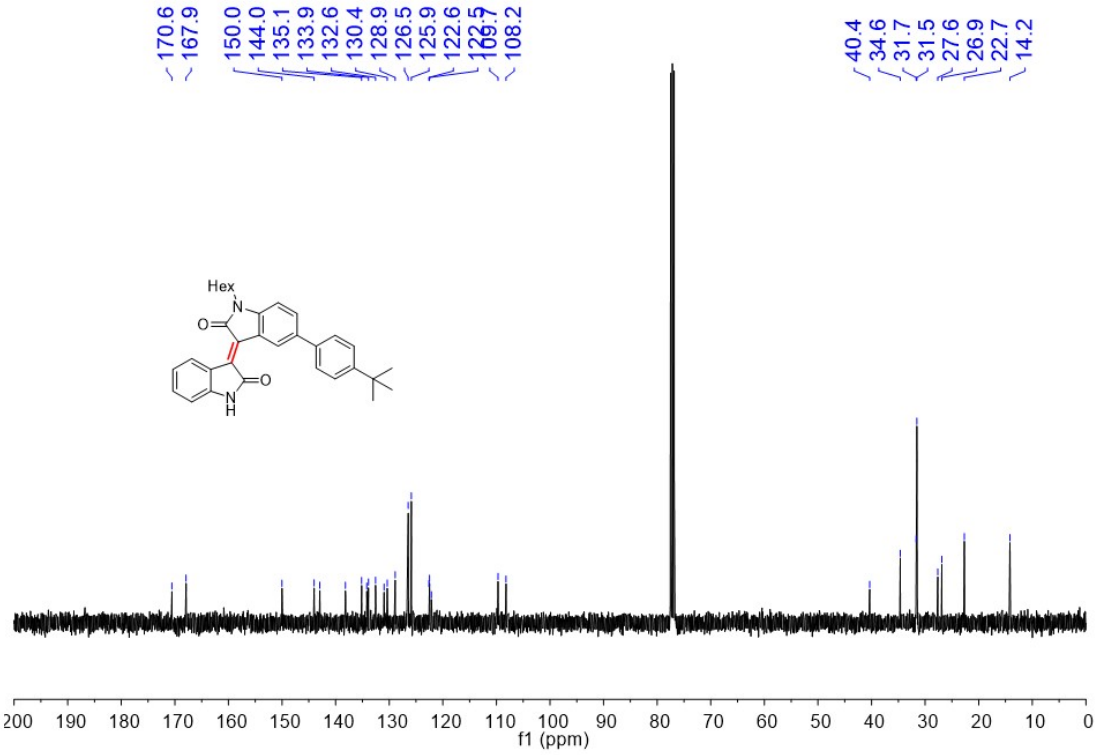
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31.5
27.6
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N
H
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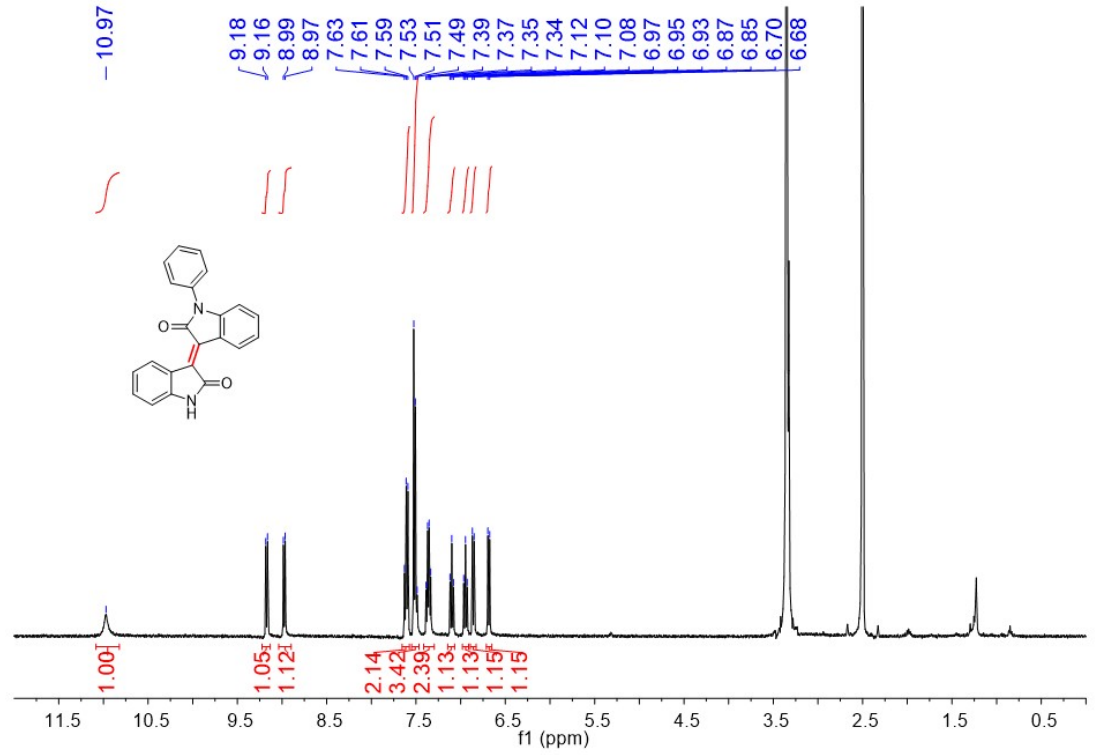
f1 (ppm)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7.34
7.12
7.10
7.08
6.97
6.95
6.93
6.87
6.85
6.70
6.68
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O
O
N
H
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1.05
1.12
2.14
3.42
2.39
1.13
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1.15
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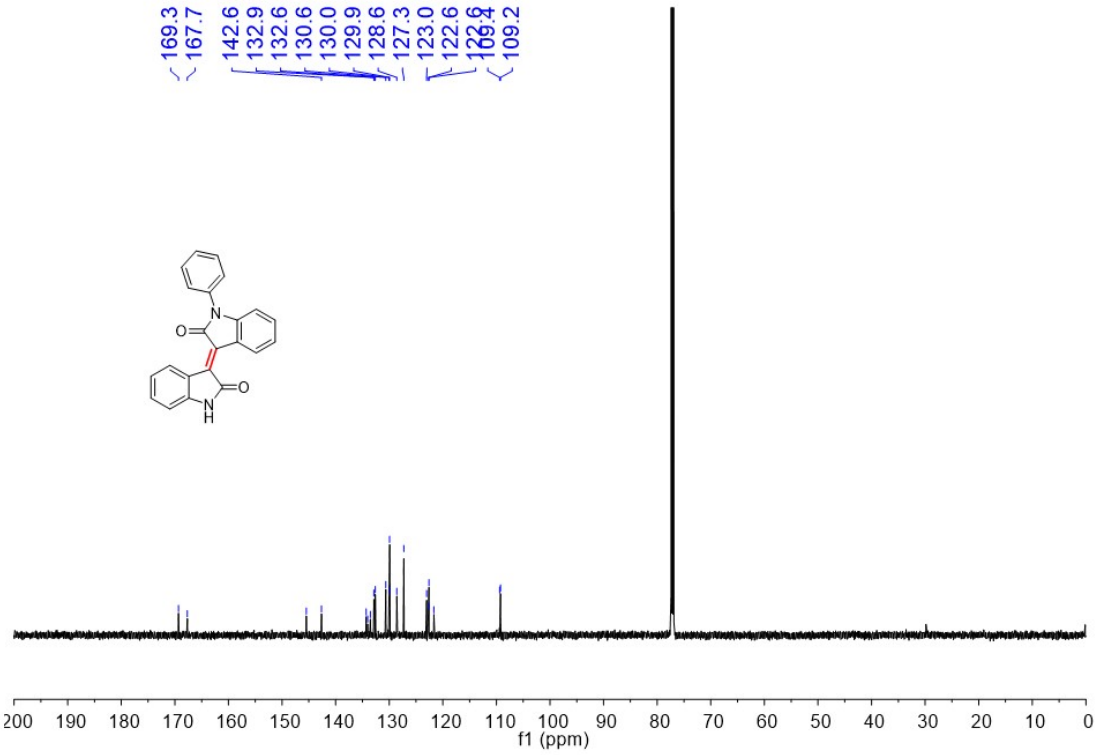
f1 (ppm)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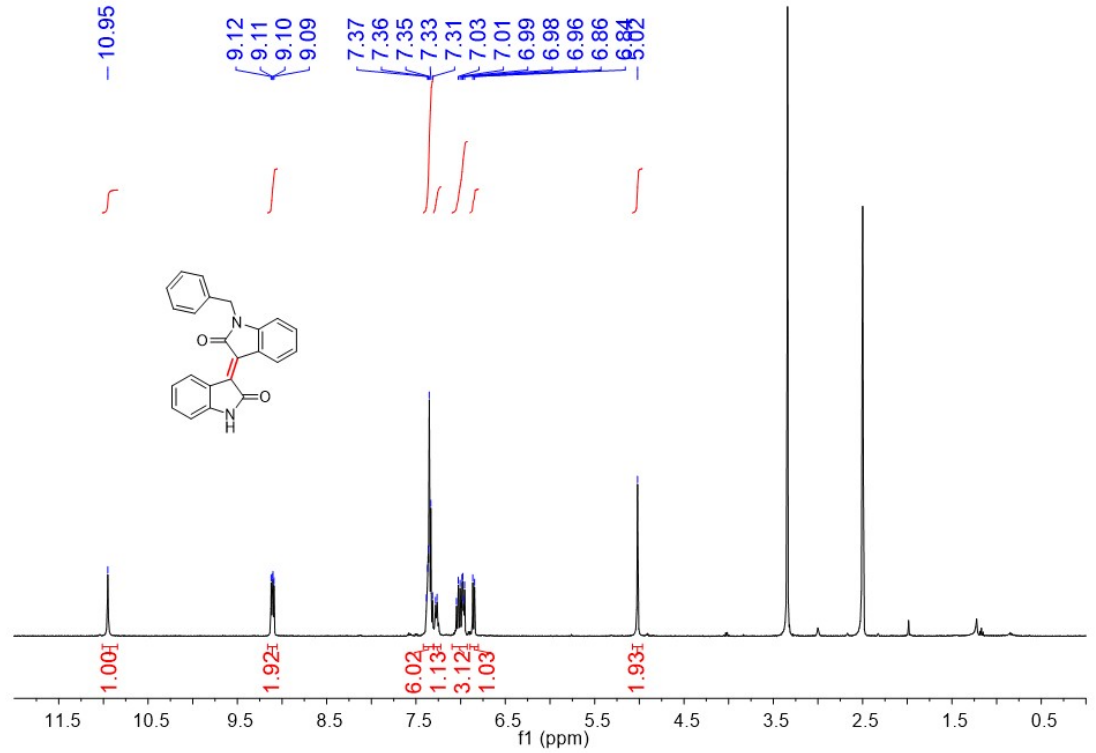
109.2
f1 (ppm)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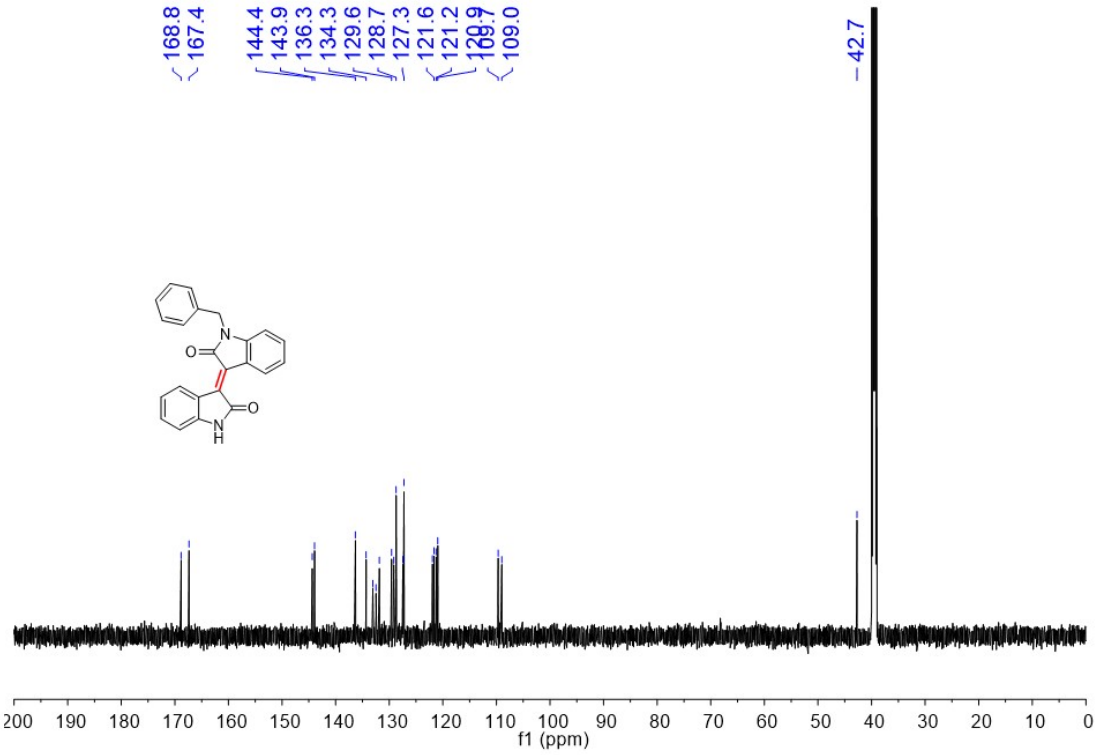
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127.3
121.6
121.2
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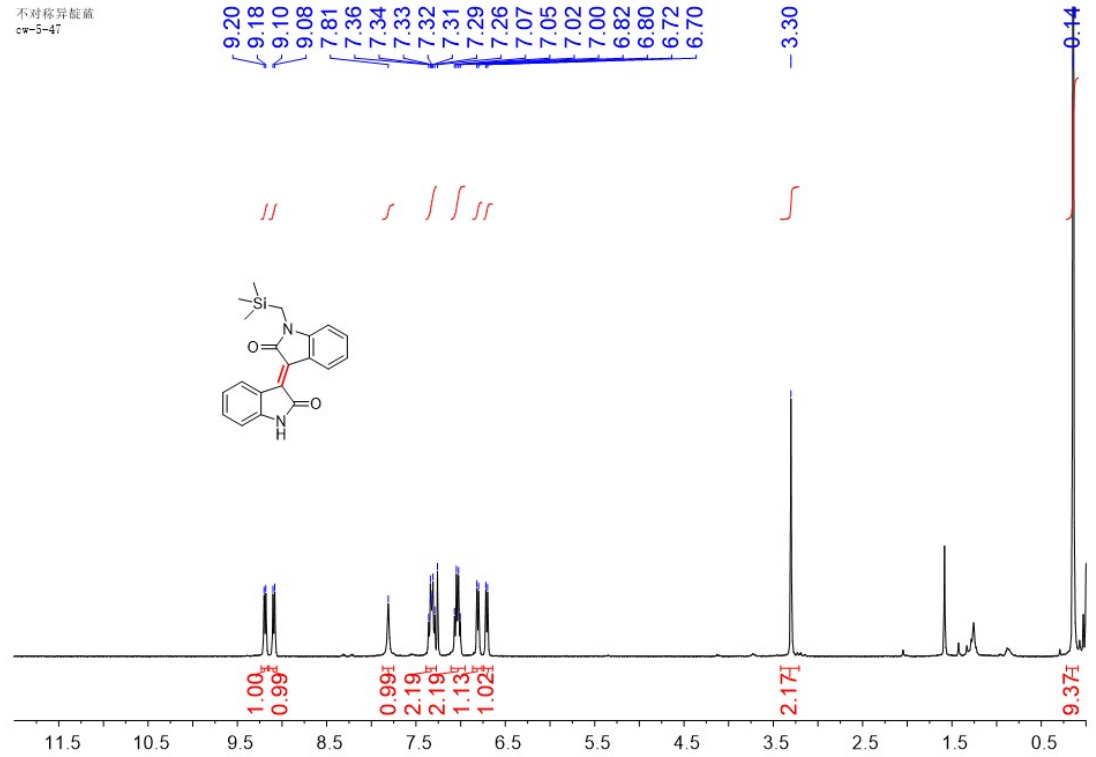
f1 (ppm)


不对称异靛蓝
cw-5-47
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7.31
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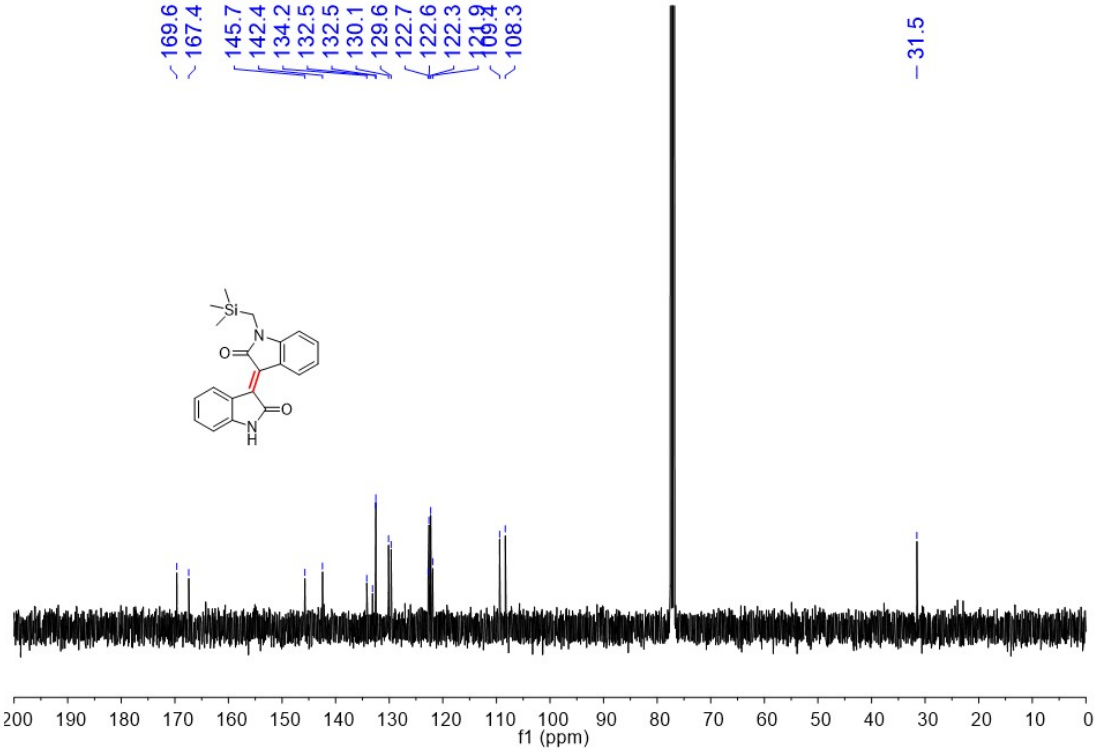
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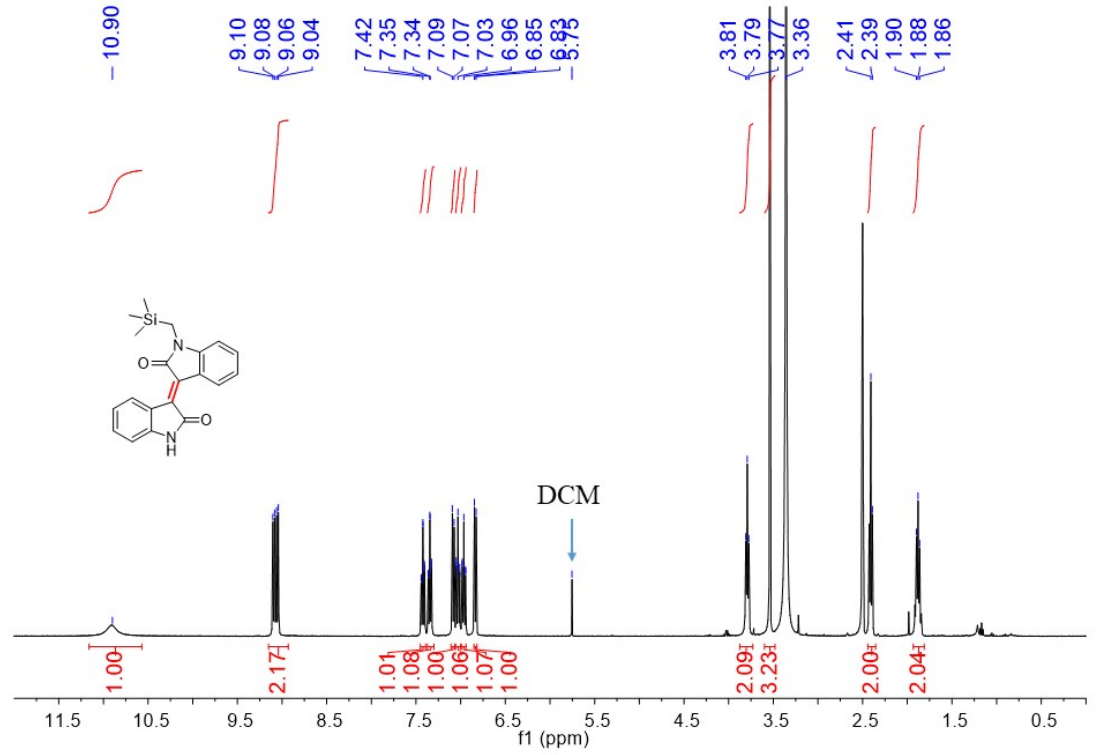
122.6
122.3
108.3
31.5
f1 (ppm)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3.79
3.77
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2.41
2.39
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DCM
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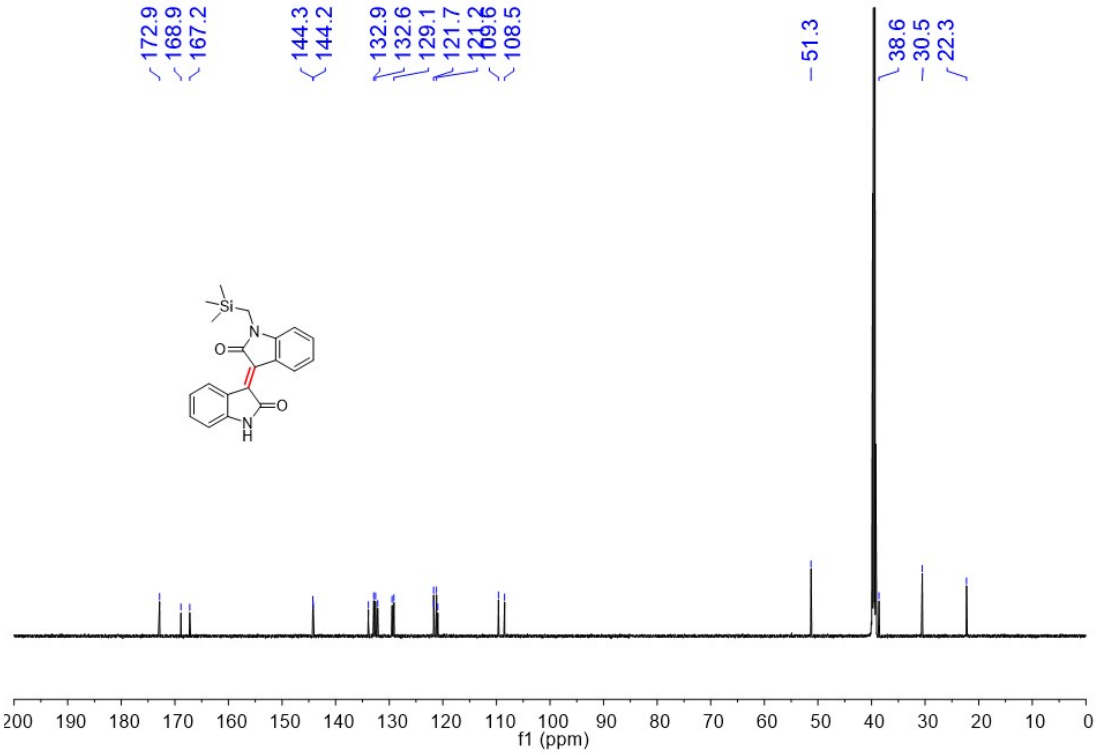
2.09
3.23
2.00
2.04
f1 (ppm)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N
H
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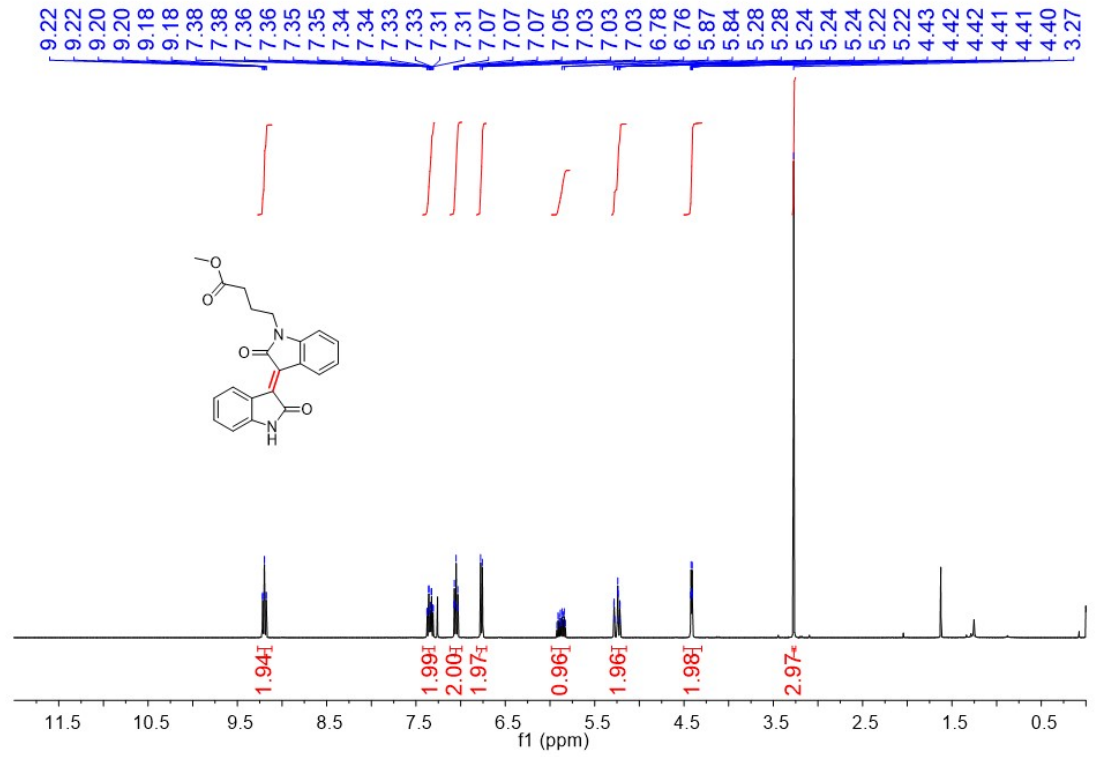
f1 (ppm)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6.76
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5.28
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5.24
5.24
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4.43
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N
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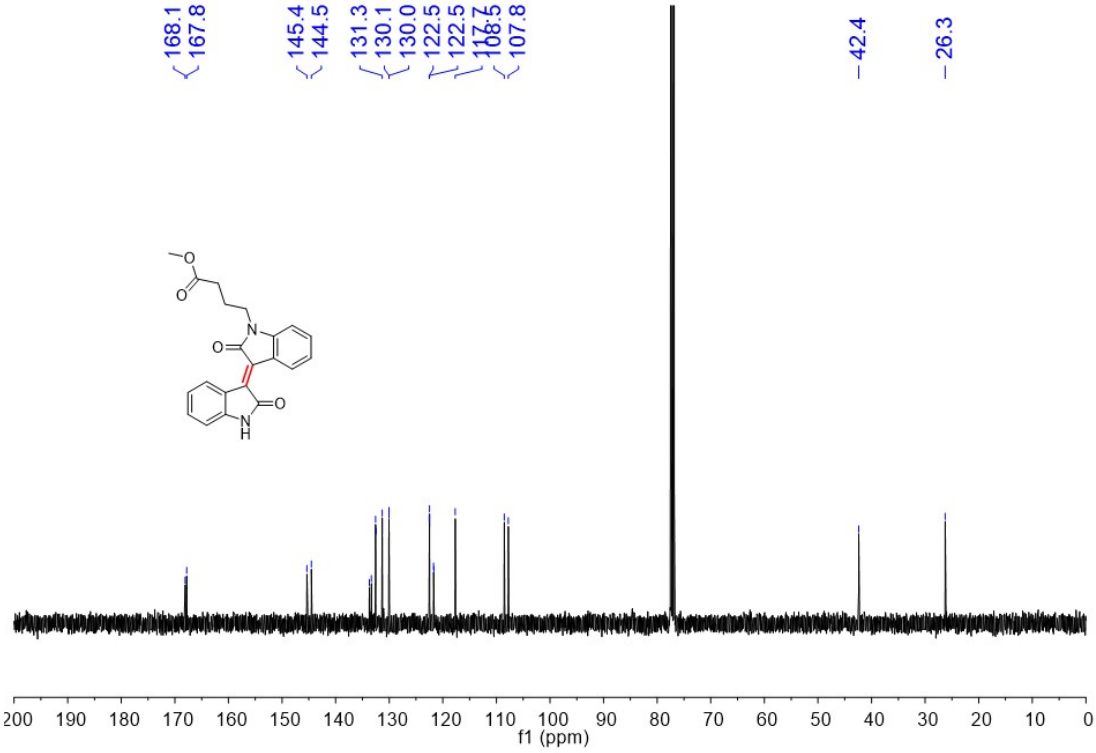
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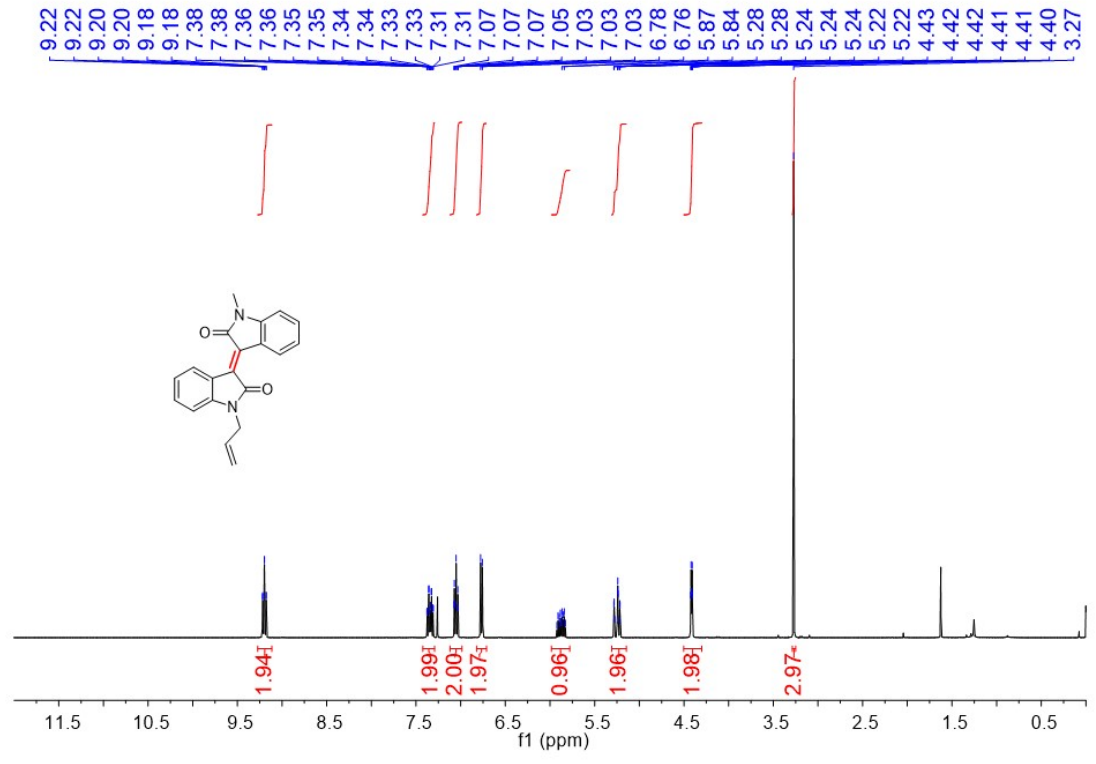
108.5
107.8
42.4
26.3
f1 (ppm)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7.31
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2.97
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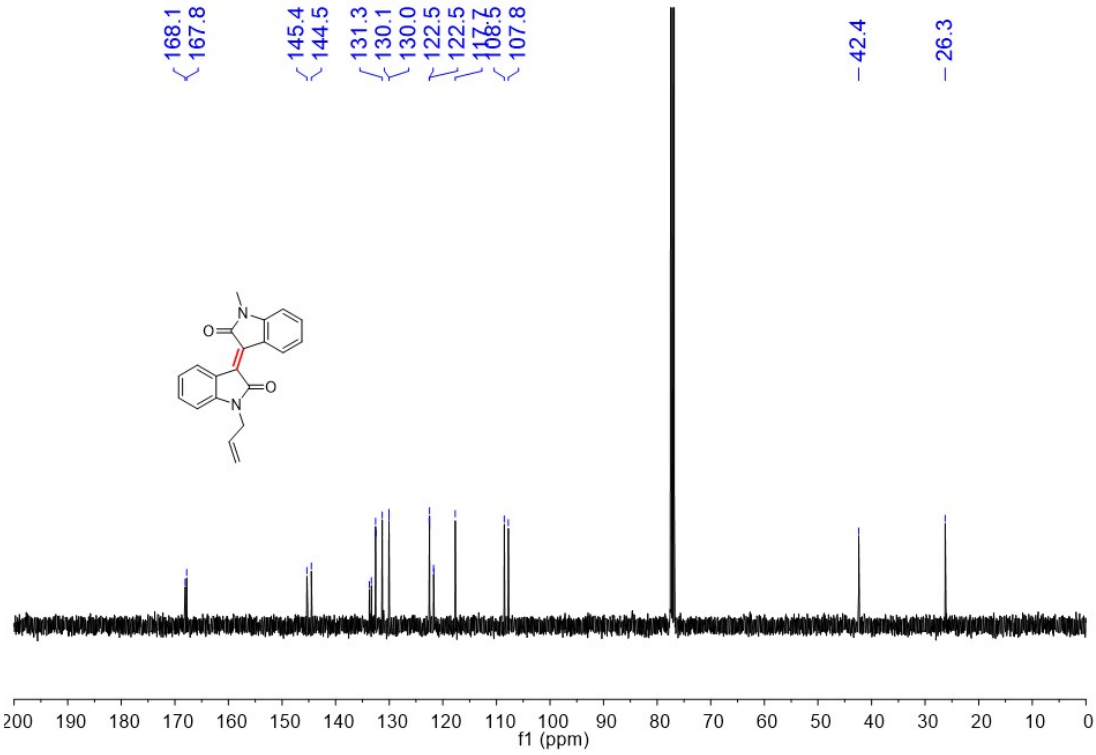
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107.8
42.4
26.3
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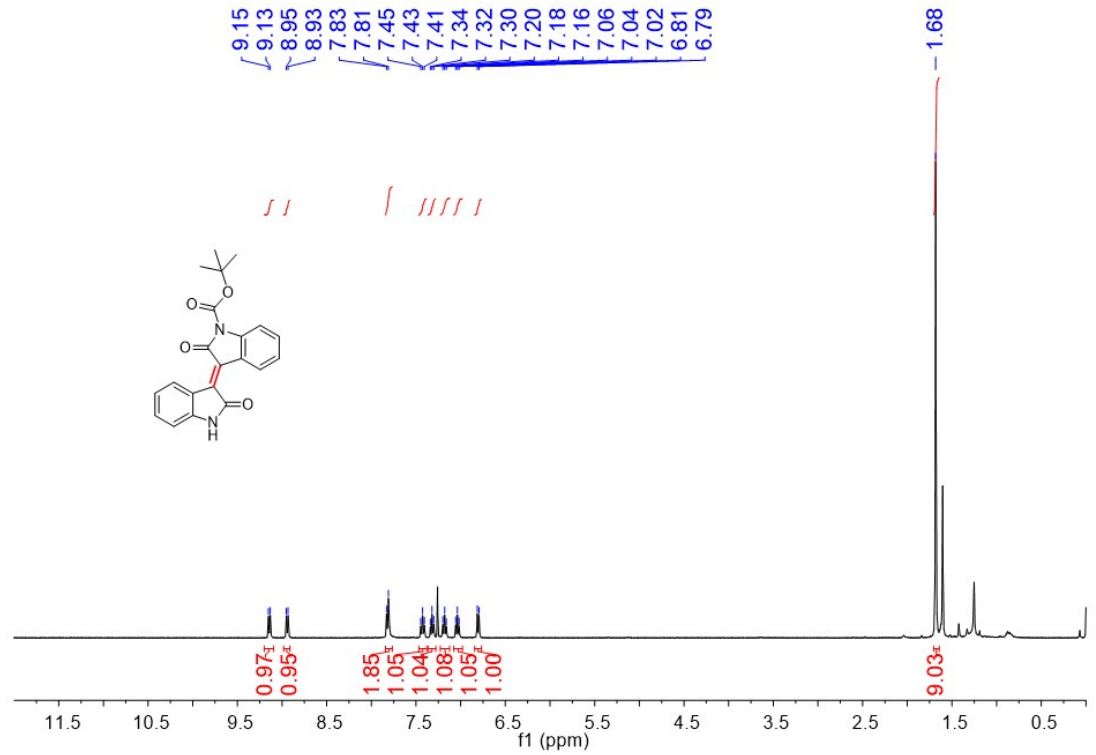
f1 (ppm)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7.06
7.04
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6.81
6.79
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1.05
1.04
1.08
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11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
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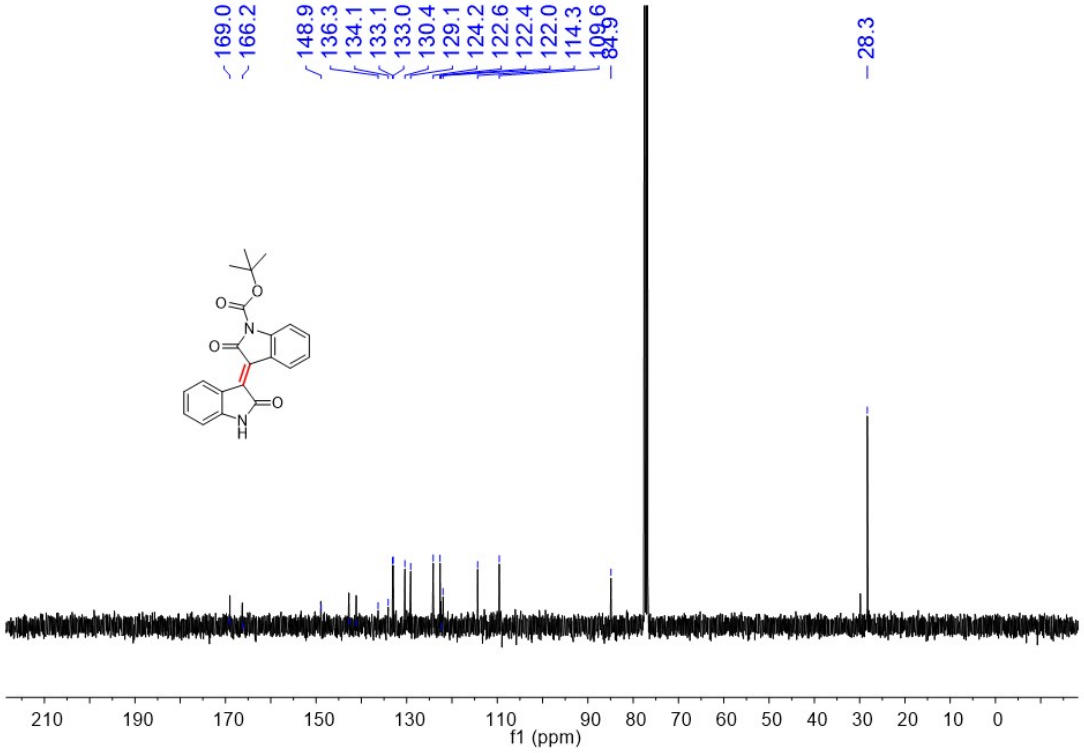
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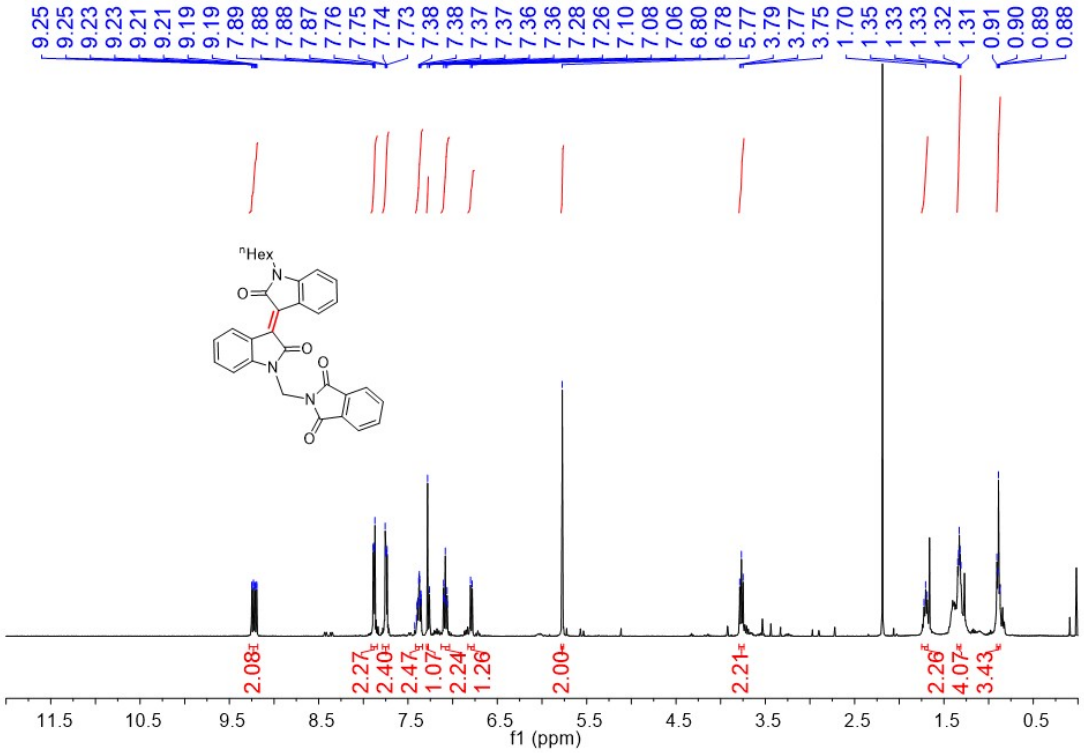
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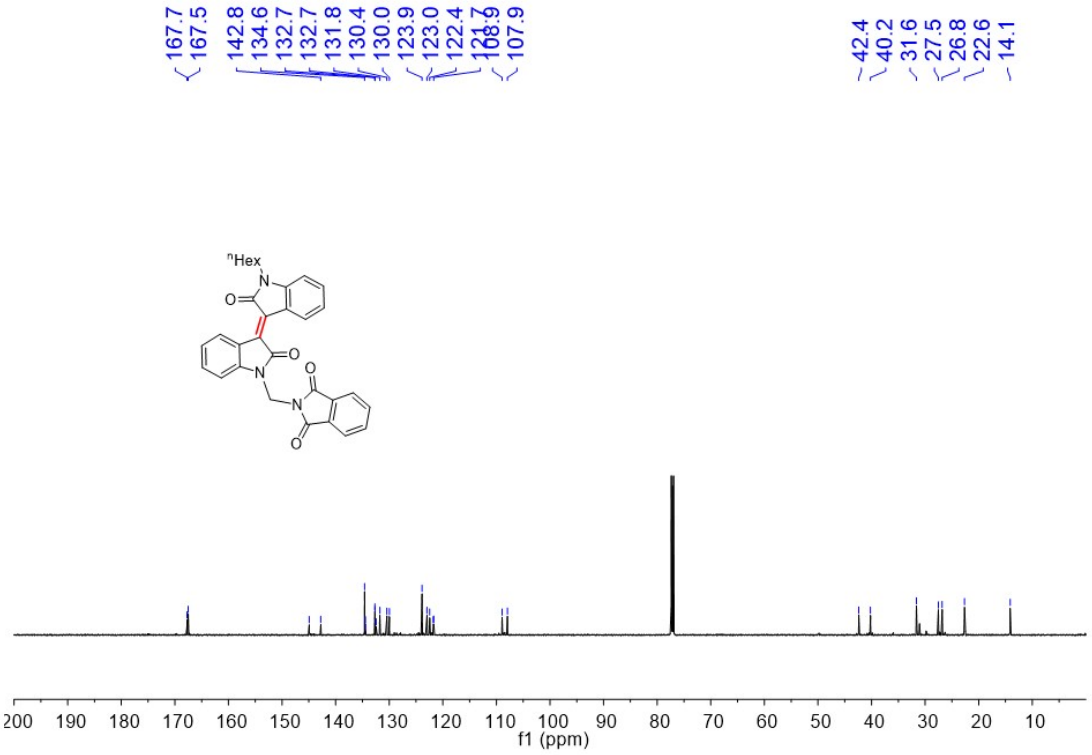
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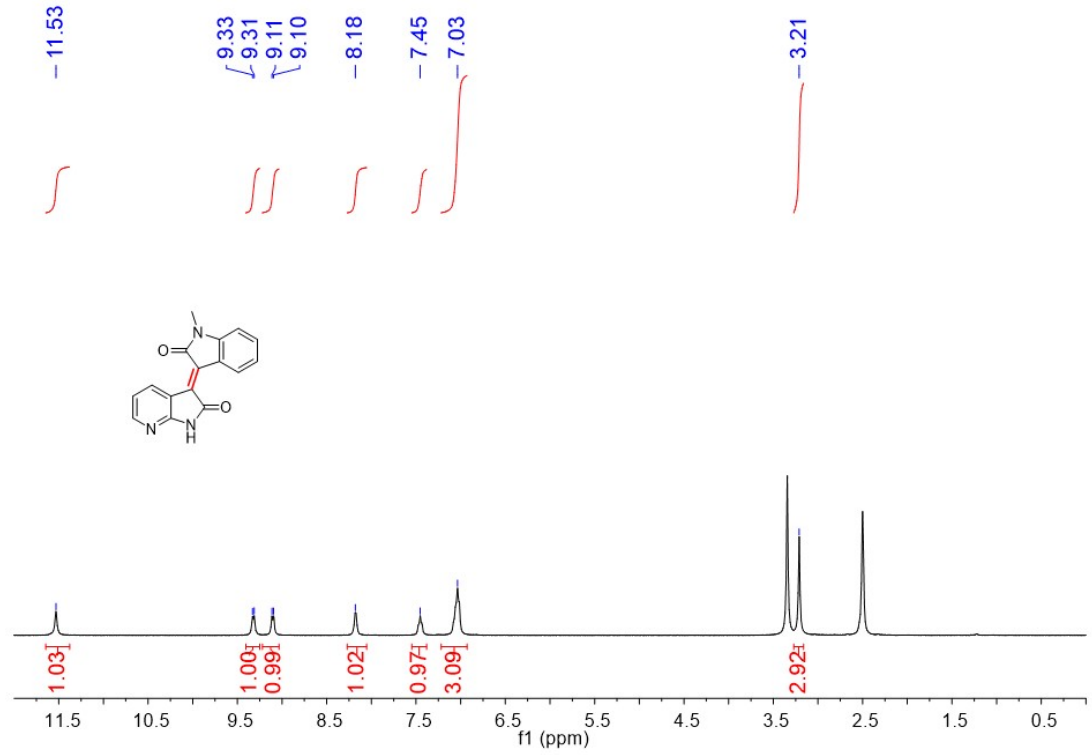
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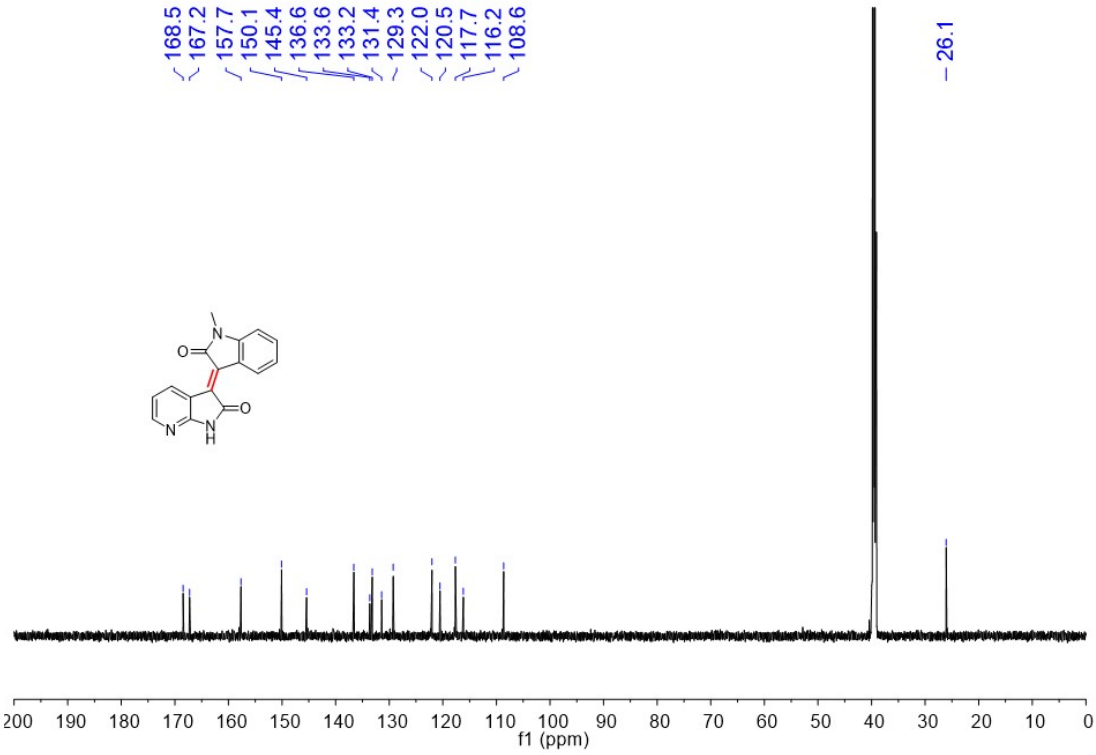
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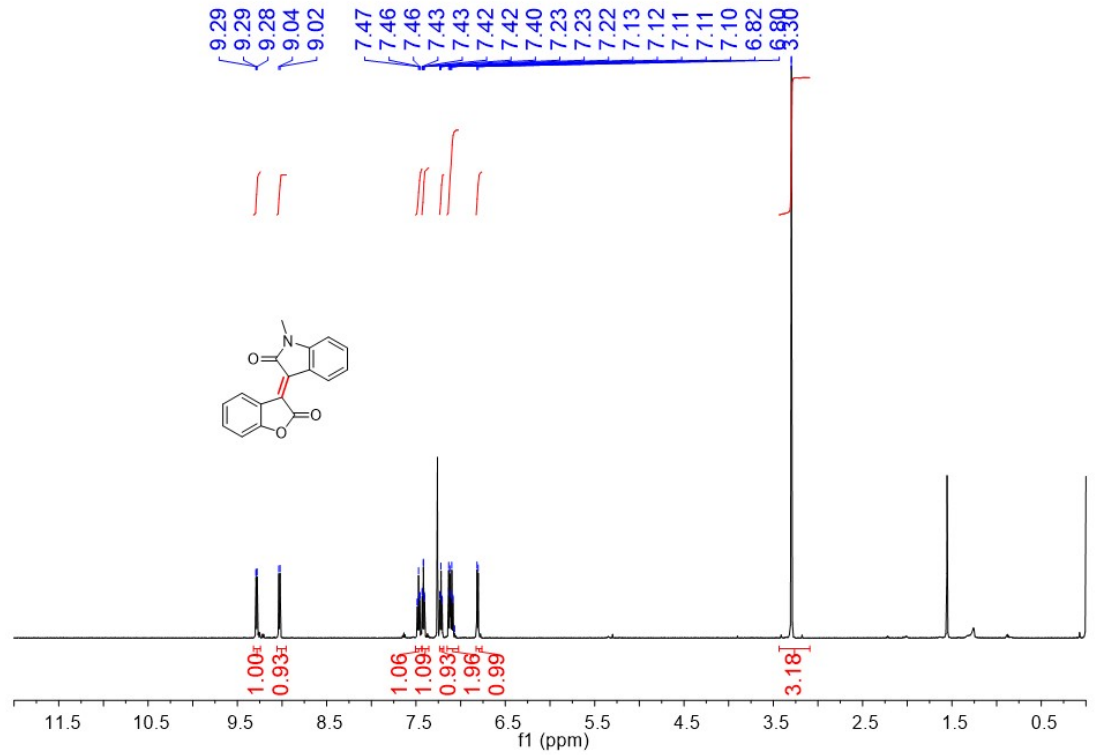
116.2
108.6
26.1
f1 (ppm)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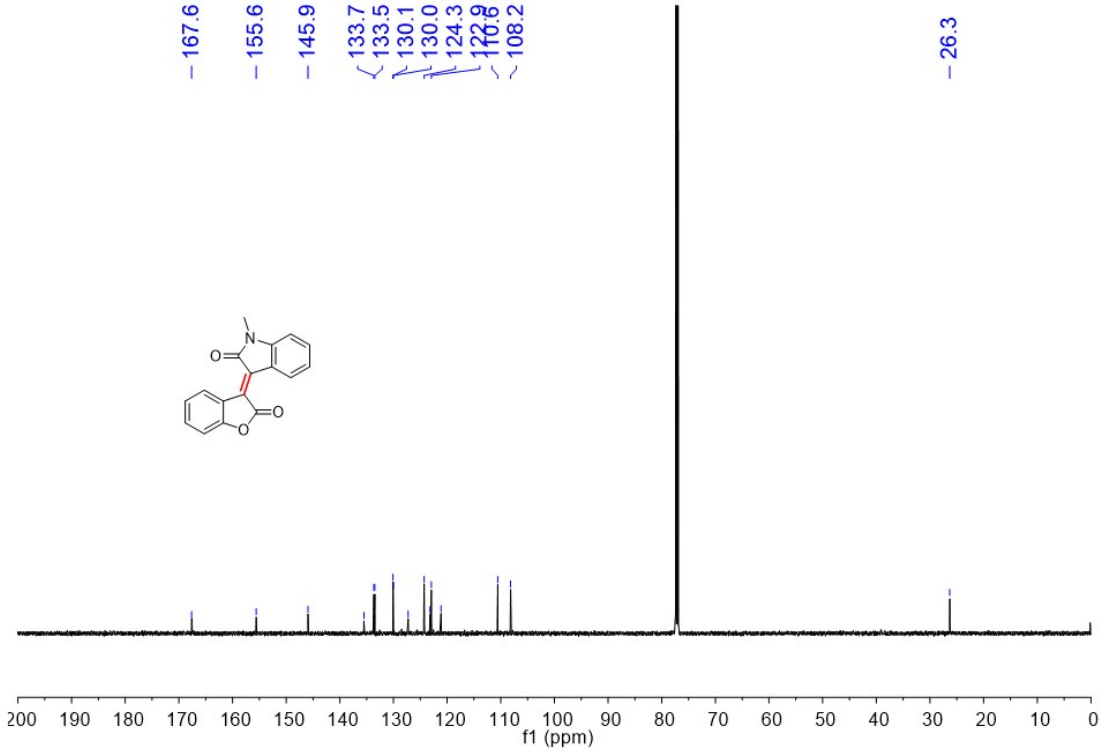
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110.6
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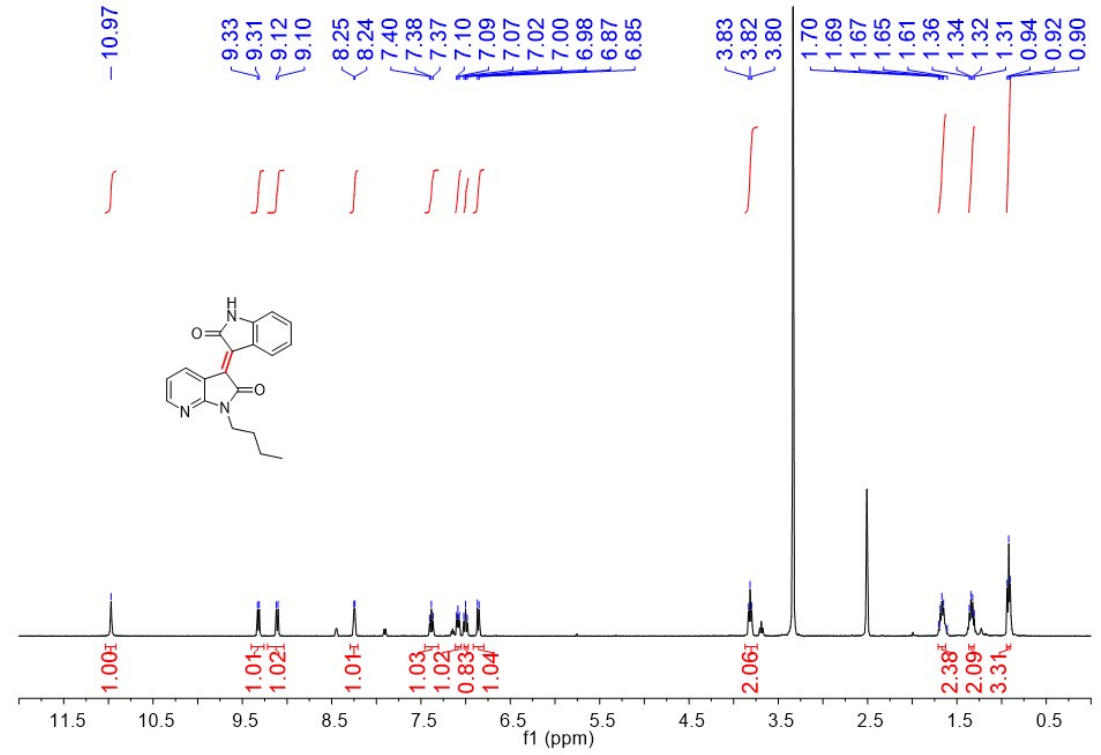
26.3
f1 (ppm)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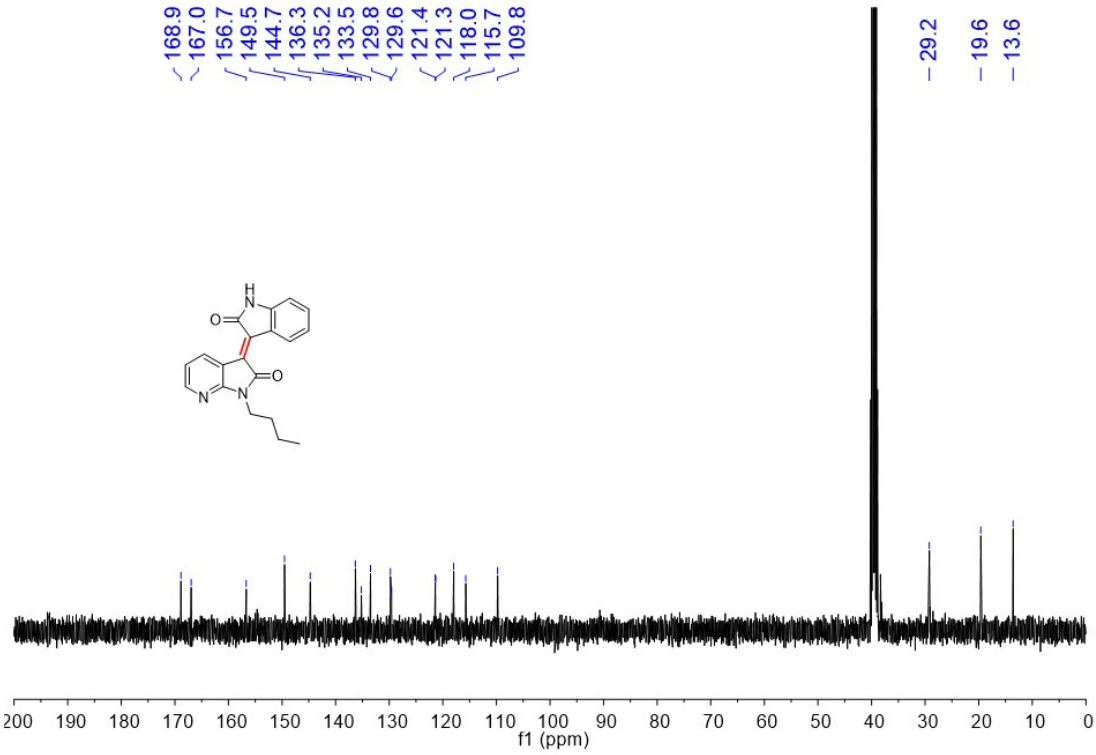
f1 (ppm)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13.6
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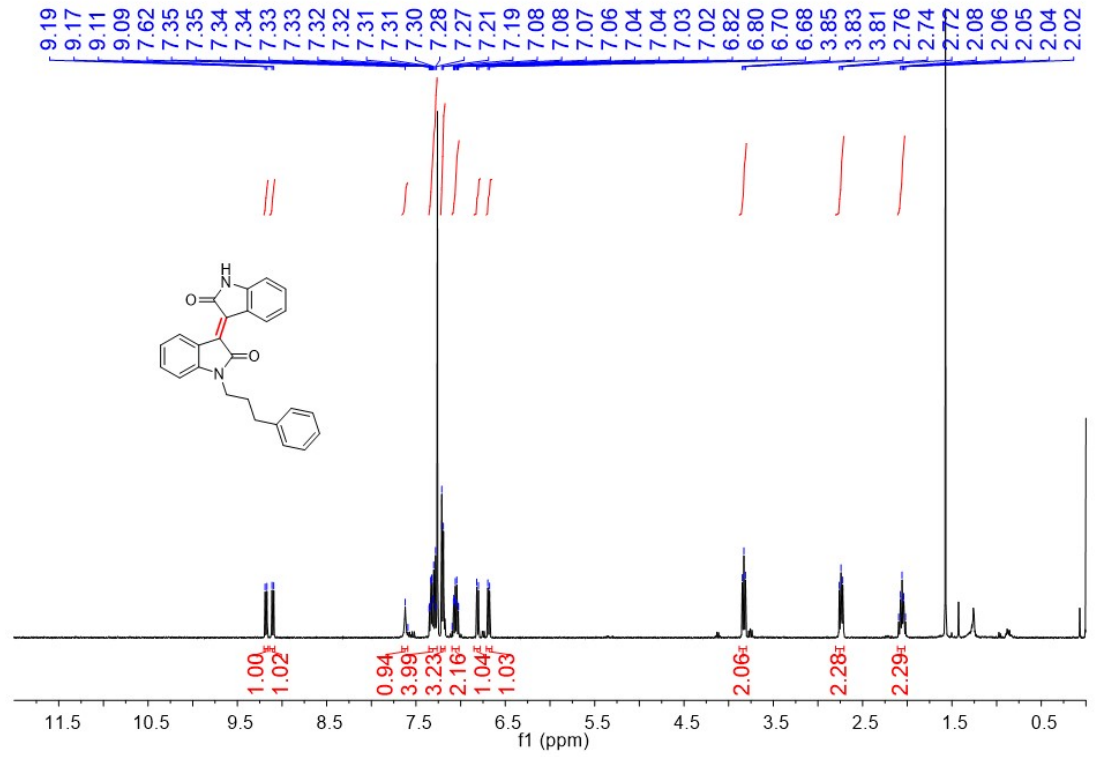
f1 (ppm)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1.03
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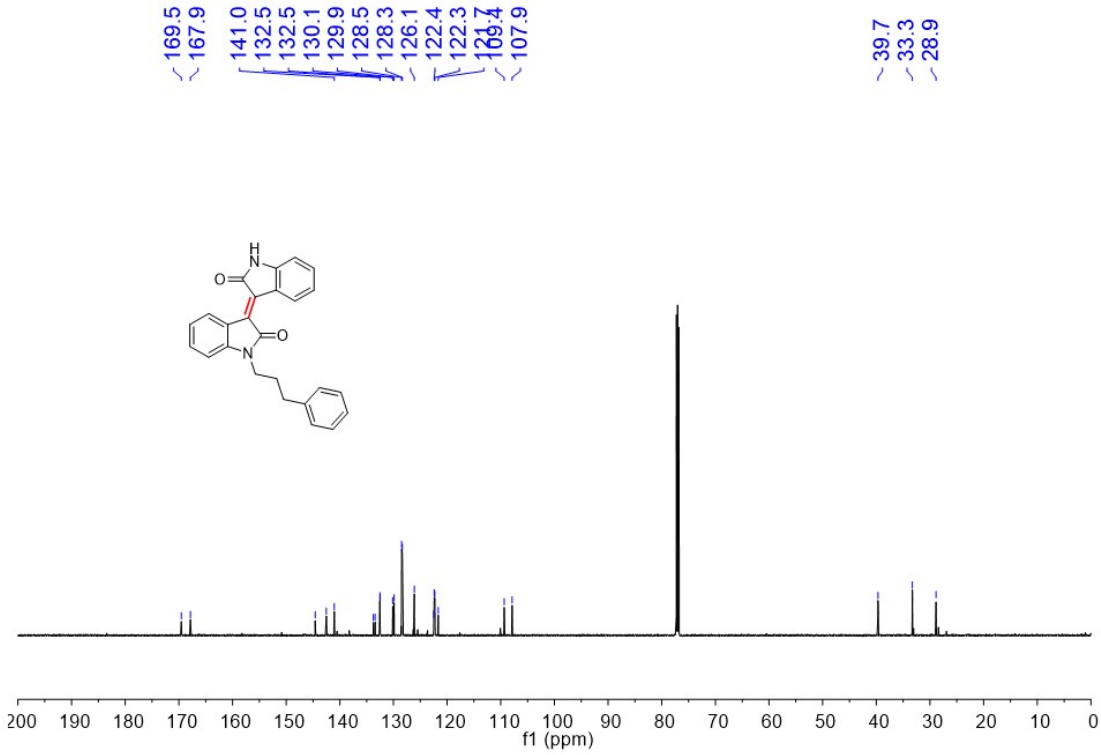
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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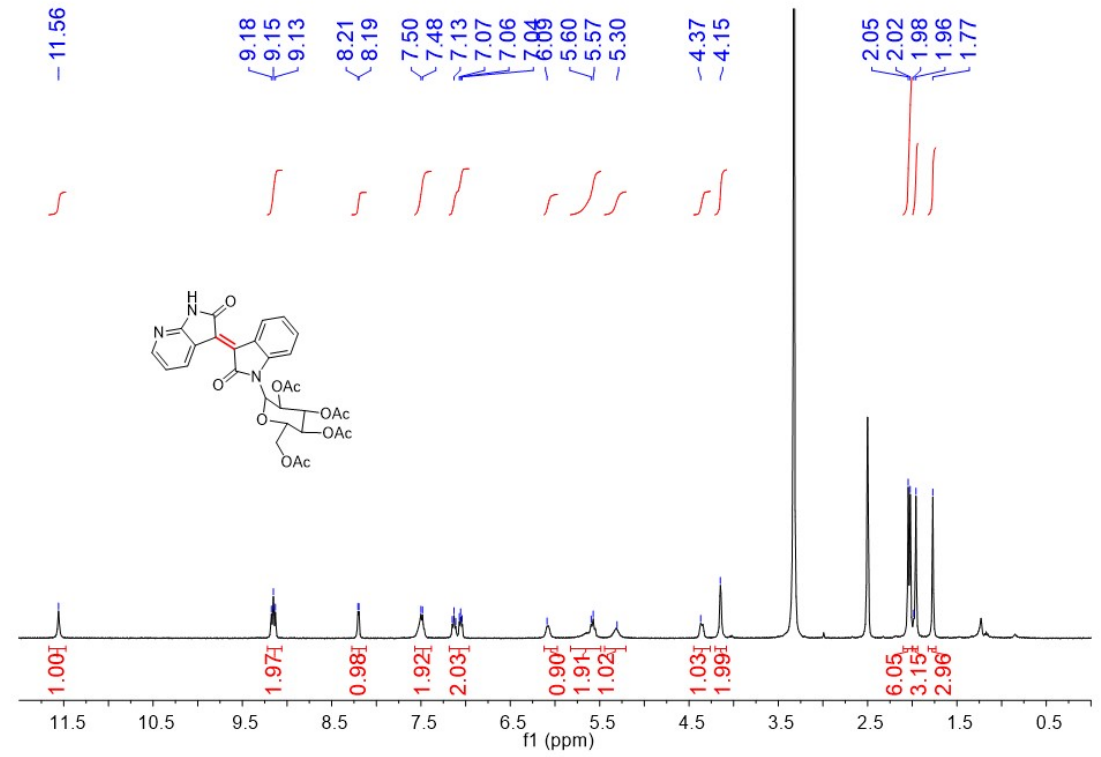
39.7
33.3
28.9
f1 (ppm)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OAc
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1.03
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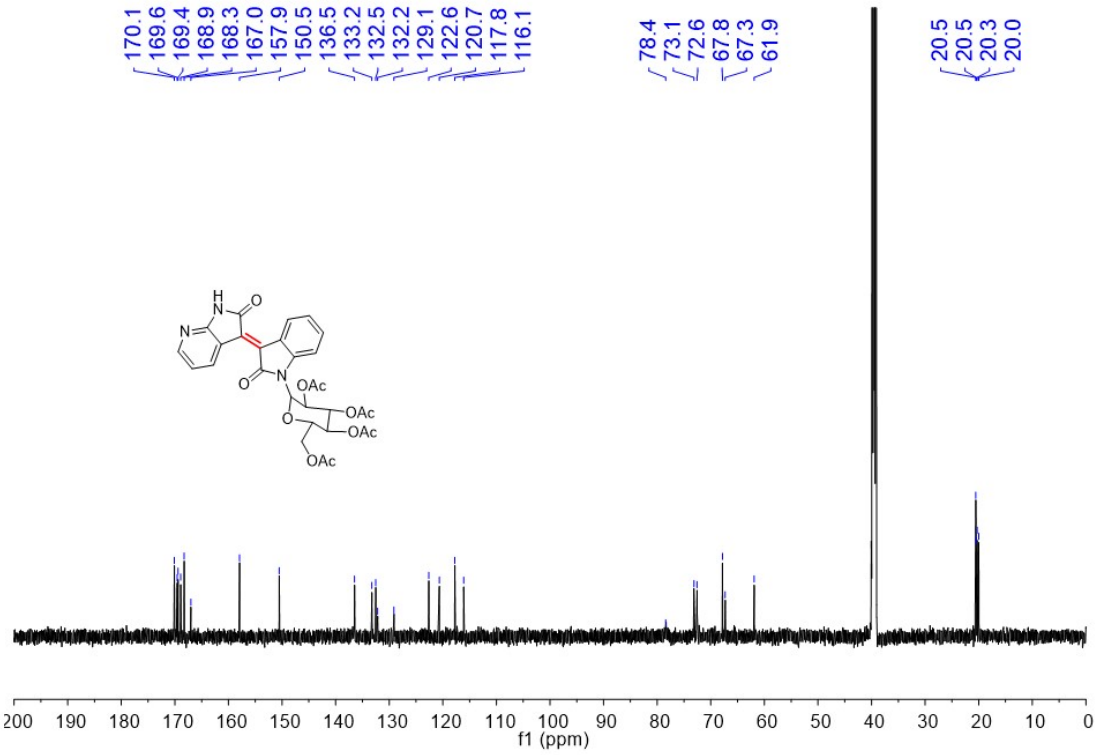
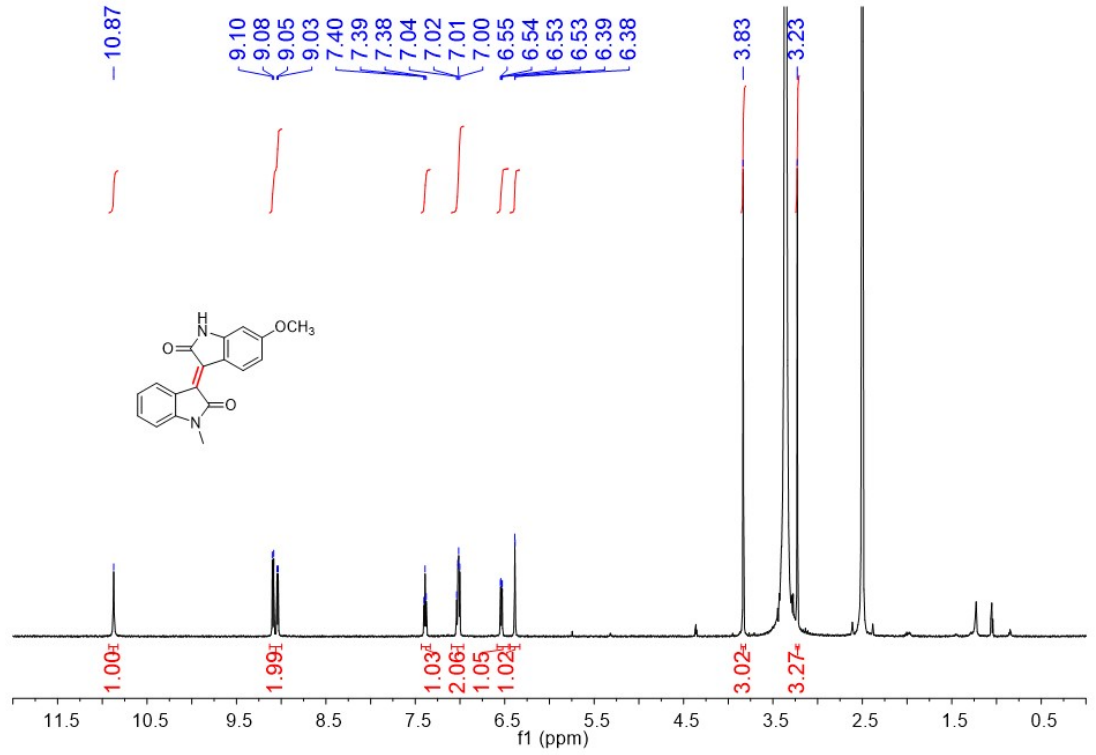
6.05
3.15
2.96
f1 (ppm)


170.1
169.6
169.4
168.9
168.3
167.0
157.9
150.5
136.5
133.2
132.5
132.2
129.1
122.6
120.7
117.8
116.1
78.4
73.1
72.6
67.8
67.3
61.9
20.5
20.5
20.3
20.0
OAc
OAc
OAc
OAc
f1 (ppm)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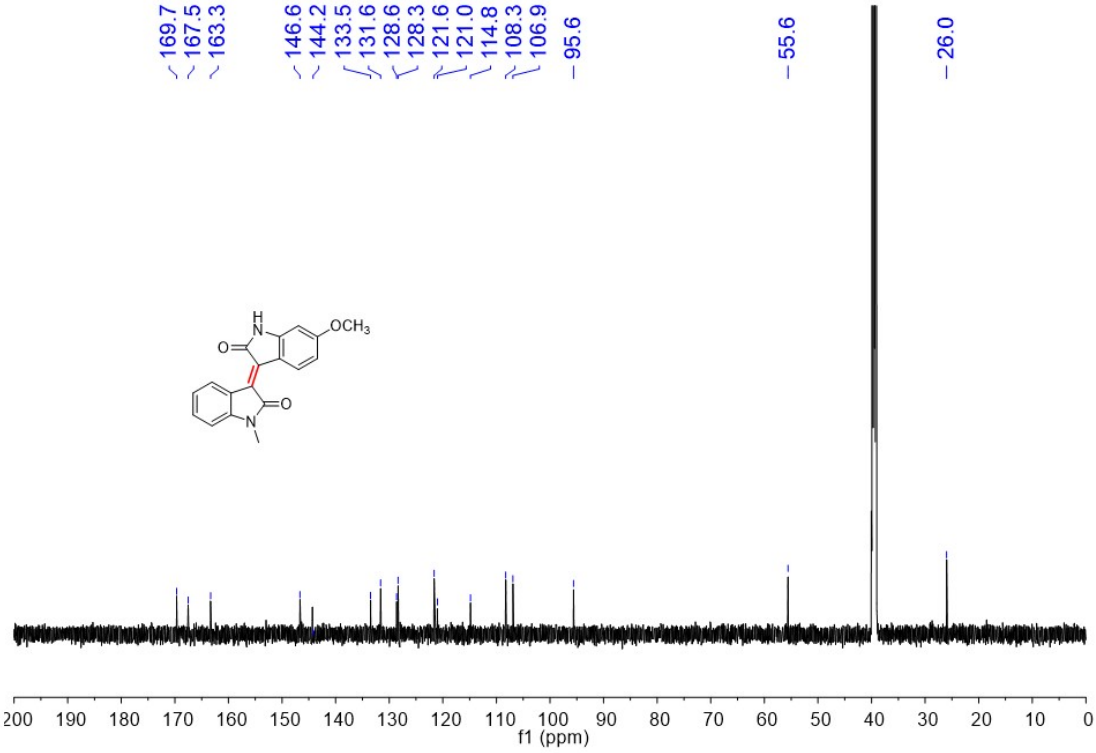
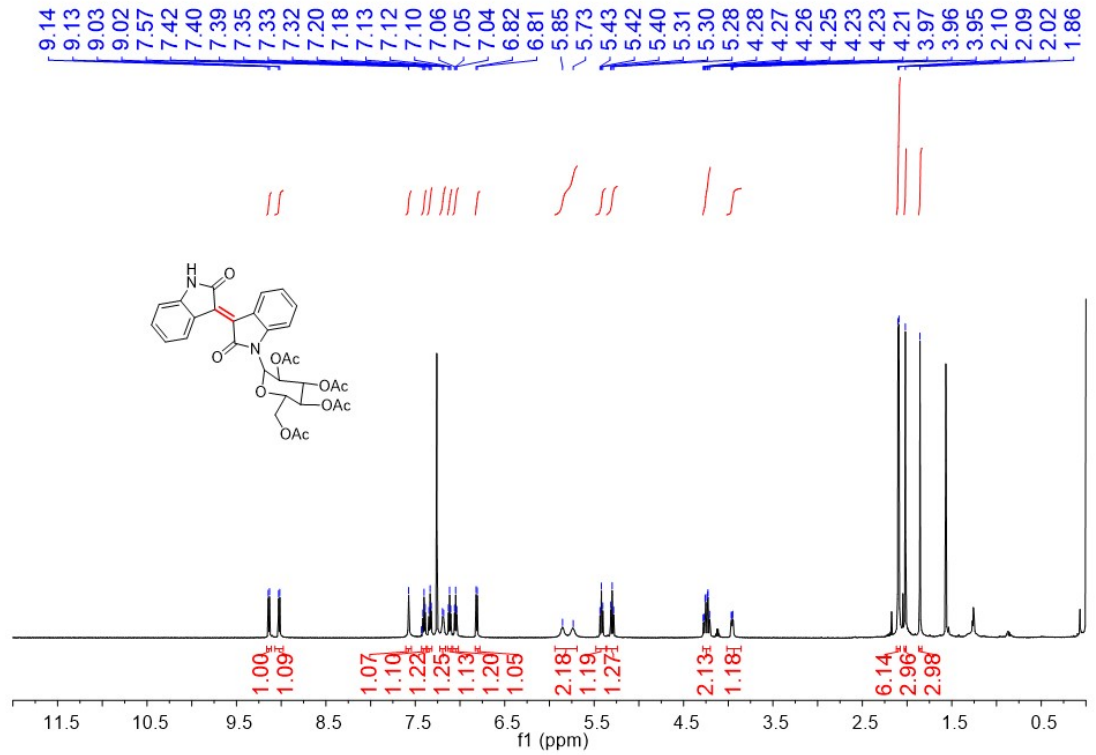
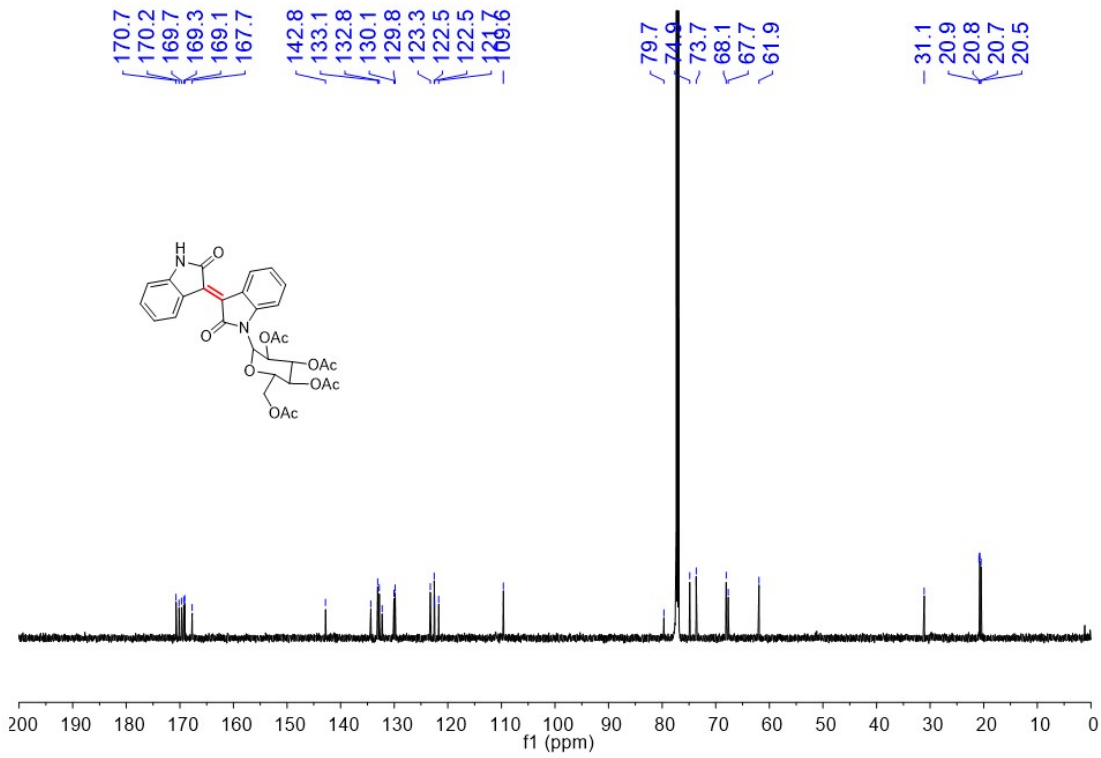
9.10
9.08
9.05
9.03
7.40
7.39
7.38
7.04
7.02
7.01
7.00
6.55
6.54
6.53
6.53
6.39
6.38
3.83
3.23
OCH3
1.00
1.99
1.03
2.06
1.05
1.02
3.02
3.27
f1 (ppm)


169.7
167.5
163.3
146.6
144.2
133.5
131.6
128.6
128.3
121.6
121.0
114.8
108.3
106.9
95.6
55.6
26.0
OCH3
f1 (ppm)


9.14
9.13
9.03
9.02
7.57
7.42
7.40
7.39
7.35
7.33
7.32
7.20
7.18
7.13
7.12
7.10
7.06
7.05
7.04
6.82
6.81
5.85
5.73
5.43
5.42
5.40
5.31
5.30
5.28
4.28
4.27
4.26
4.25
4.23
4.23
4.21
3.97
3.96
3.95
2.10
2.09
2.02
1.86
OAc
OAc
OAc
OAc
1.00
1.09
1.07
1.10
1.22
1.25
1.13
1.20
1.05
2.18
1.19
1.27
2.13
1.18
6.14
2.96
2.98
f1 (ppm)


170.7
170.2
169.7
169.3
169.1
167.7
142.8
133.1
132.8
130.1
129.8
123.3
122.5
122.5
79.7
74.9
73.7
68.1
67.7
61.9
31.1
20.9
20.8
20.7
20.5
H
N
O
O
N
OAc
O
OAc
OAc
OAc
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)