

## Supporting Information

### Light induced diversity-oriented synthesis (DOS) library of annulated indolizine fluorophores for imaging non-lysosomal lipid droplets (LDs)

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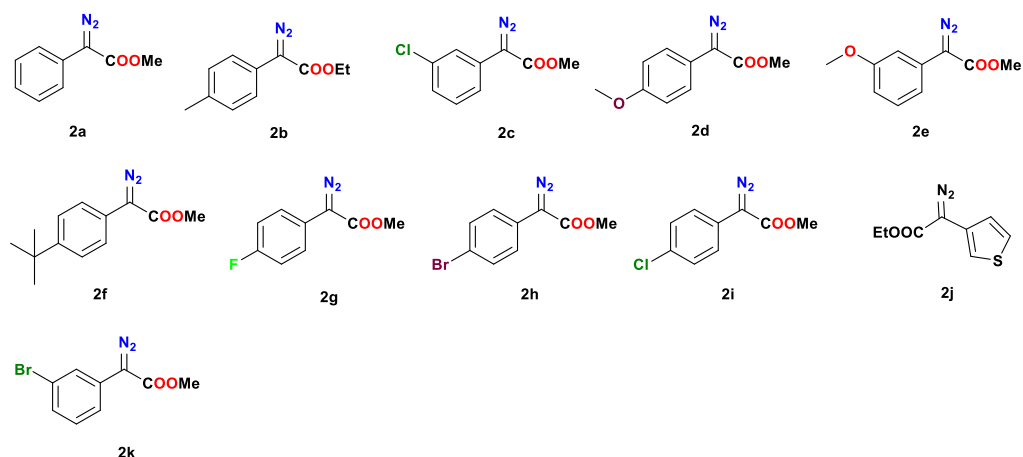
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## 1. General experimental Procedure:

All blue light reactions were carried out under air as specified unless otherwise mentioned. Photochemical Reactor Aldrich® Micro Photochemical Reactor, blue LED lights (ALDKIT001-1EA). LED light is IP68 double density 12V DC water proof blue light with spectral range of 435-445 nm with wall plug power supply 500mA with 5-6 watts. The irradiation vessel material is borosilicate glass. The distance of irradiation vessel from light source is 2 cm. Reactions were monitored through TLC by visualising in UV detector. All purifications were done in silica gel (100-200 mesh size) column chromatography. All  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded taking tetramethylsilane (TMS) as an internal standard at ambient temperature unless otherwise indicated with Bruker 400 MHz instruments at 400 MHz for  $^1\text{H}$  and 100 MHz for  $^{13}\text{C}$  NMR spectroscopy. Splitting patterns are designated as singlet (s), broad singlet (br s), doublet (d), triplet (t), quartet (q), quintet (quin) doublet of doublets (dd) and triplet of doublets (td). Splitting patterns that could not be interpreted or easily visualized are designated as multiplet (m). Ultra-performance liquid chromatography (UPLC) was carried out using an Agilent 6540 accurate-mass Q-TOF LC/MS (Agilent Technologies, U.S.A.). MS analyses were performed under the following operation parameters: dry gas temperature 350 °C, dry gas ( $\text{N}_2$ ) flow rate 10 L/min, nebulizer pressure 30 psi, Vcap 4000 and fragmentor voltage 100 V. Mass spectra were acquired in the positive ion mode by scanning from 100 to 1500 in the mass to charge ratio (m/z). The mobile phase composition used for UHPLC-QTOF MS comprised of  $\text{H}_2\text{O}$  (A) and ACN (B), with optimized linear gradient elution. The injection volume was 5  $\mu\text{L}$ . The flow rate was set at 0.3 mL/min. Accurate mass analysis calibration was carried out by ESI-low concentration tuning mix solution provided by Agilent technologies, U.S.A. The accuracy error threshold was set at 5 ppm. Steady state UV-vis(visible) absorption was measured by Shimadzu UV-26001 UV-Vis Spectrophotometer in a conventional quartz cell cuvette. Steady-state emissions were measured using HORIBA Fluorolog-3 spectrofluorometer (Model: FL3-2-IHR). Cyclic voltammetry was undertaken using BioLogic potentiostat that can be controlled by EC-Lab software.

## 2. Synthetic Procedure

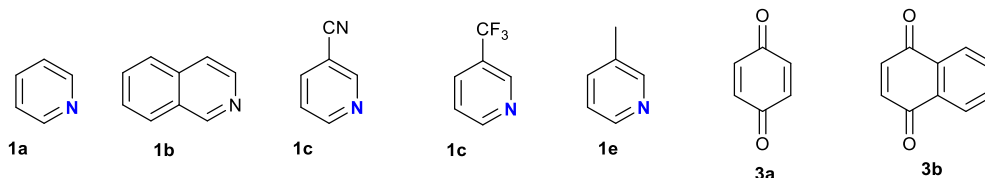
### 2.1 Synthesis of aryl diazo esters 2a-2k :



Scheme S1. Diazoesters used

All aryl diazo acetates were prepared by reported procedure. Aryl acetates (1 equivalent, 5 mmol) were dissolved in acetonitrile (10ml) in a clean oven dried round bottom flask, added DBU (1,8-Diazabicyclo[5.4.0]undec-7-ene) (1.2equivalent, 6 mmol), stirred for 10 minutes, pABSA (4-Acetamidobenzenesulfonyl azide) (1.2 equivalent, 6 mmol) was added, stirred for 4 hours in dark and r.t; after completion acetonitrile was removed under vacuum, diluted with ethyl acetate (25ml), washed with water and organic layer was dried with brine and sodium sulphate, purified with column chromatography in silica gel (100-200 mesh size) with 5% ethyl acetate in hexane to yield ~98%.<sup>S1</sup>

## 2.2 Synthesis of indolizines (4a-i, 5a-h, 6a-c, 7a-d) :



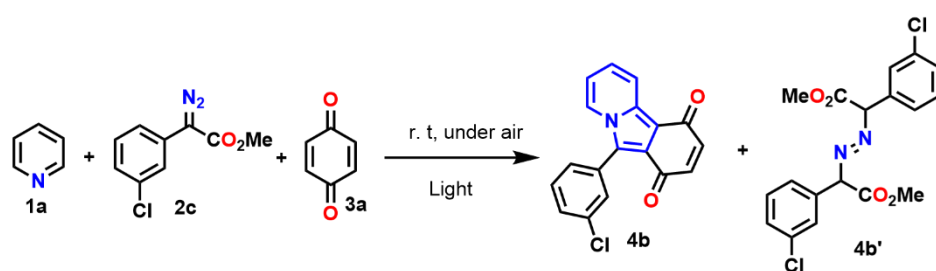
Scheme S2. Pyridines, Isoquinoline, benzoquinone and naphthaquinone used in this work

### 2.2.1 Optimisation of multicomponent indolizine synthesis

To optimize the blue LED induced DOS reaction, pyridine **1a** (2 eq.) was reacted with 3-chlorophenyldiazoacetate **2c** (1.2 eq.) and benzoquinone **3a** (1 eq.) in blue LED (5–6 W Micro Photochemical Reactor (ALDKIT001) with blue LED lights [435–445 nm] source) with tetrahydrofuran as a solvent at room temperature (r. t.) (Table 1, entry 1). The desired isoindolo[2, 1-a]pyridine **4b** was obtained in 31% yield in 6 h time. A considerable amount (60%) of the dimeric aryl methyl ester **4b'** was formed as the by product which could be because the resulting pyridine ylide **A** was slow enough to react with **3a** in THF that further facilitated the homo dimerization of **2c** to **4b'**. The similar thing happened with toluene as solvent were **4b** was obtained in 28% yield and the undesired **4b'** in 67% (Table 1, entry 2). However, the reaction in acetonitrile provided the desired compound **4a** in much improved yield of 67% with less formation of **4b'** (Table 1, entry 3). The reaction failed in water (Table 1, entry 4). The formation of pyridinium ylide was obtained in water but the subsequent [3+2] cycloaddition did not happen. Substantial improvement in the yield happened for reaction in

chlorinated solvents like dichloromethane (DCM) and dichloroethane (DCE), where the yield increased to nearly 75% (Table 1, entry 5 and 6). The reaction time was also shortened to 7h compared to 12h with acetonitrile. Since the reaction failed in water, in an effort to scout an alternate environmentally compatible strategy the reactions were performed in ethyl acetate and glycerol (Table 1, entry 7 and 8). Though the reaction in glycerol was comparable with that of acetonitrile, to our utmost gratification the reaction in ethyl acetate afforded **4b** in 78% yield in less than 12h time with no formation of the dimerized by-product. When the reaction in ethyl acetate as solvent was conducted in green and red LED there was no improvement in the yield (Table 1, entry 9 and 10).

**Table S1.** Reaction optimization of the isoindolo[2, 1-a]pyridine/ isoquinoline

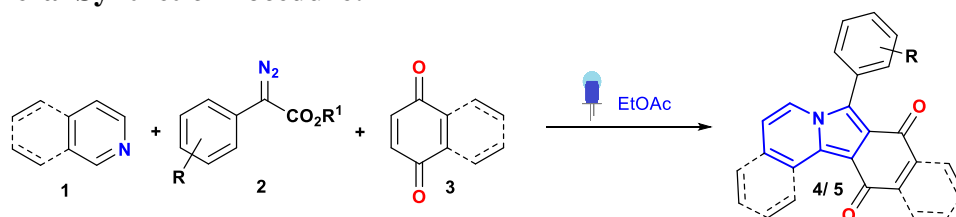


Entry	Solvent	Light source	Yield (%) <sup>a</sup> 4b/4b'
1	THF	Blue LED	31/60
2	Toluene	"	28/67
3	CH <sub>3</sub> CN	"	67/18
4	Water <sup>b</sup>	"	n.d <sup>c</sup>
5	DCM	"	75/7
6	DCE	"	73/5
7	Glycerol	"	71/n.d
8	Ethyl Acetate	"	78/n.d
9	"	Red LED	45/49
10	"	Green LED	66/21

<sup>a</sup> Isolated yield; <sup>b</sup> Only formation of pyridinium ylide **A** was detected;  
<sup>c</sup> n.d = not detected

<sup>a</sup> Isolated yield; <sup>b</sup> Only formation of pyridinium ylide **A** was detected

### 2.2.2 General Synthetic Procedure:



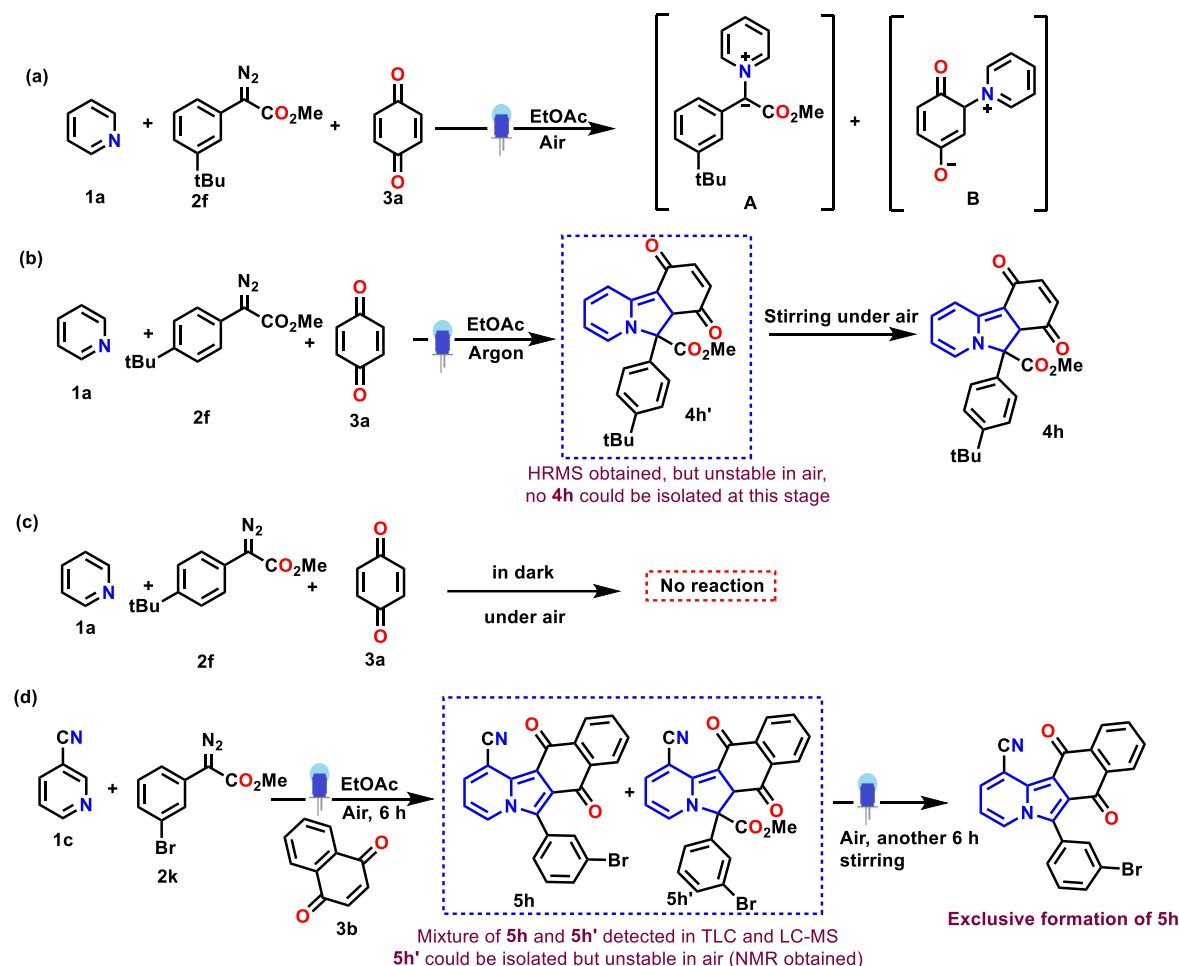
Scheme.S3

Pyridines/isoquinoline (**1a-d**) (2 equiv., 0.60 mmol) were added to a solution of aryl diazoesters (**2a-k**) (1.2 equiv., 0.36 mmol) in ethyl acetate, benzoquinone (**3a**) or naphthaquinone (**3b**) (1 equiv., 0.30 mmol) were added to the reaction mixture and stirred under blue light for 12 h. After completion of reaction (confirmed by TLC) direct column chromatography was done in EtOAc in hexane (10-30%) to get pure orange red or yellow coloured solids.

### 2.2.3 Scale up Synthesis:

In an oven dried 100 ml beaker tolyl diazo acetate, **2c** (1.2 equiv., 1.2 g, 5.5 mmol) solution in ethyl acetate (10ml) was taken with pyridine **1a** (2 equiv., 0.83 ml, 9.2 mmol). Then benzoquinone, **3a** (1 equiv., 0.5 g, 4.6 mmol) was added into the reaction mixture and continued stirring in blue light for 15 h. After completion of reaction (confirmed by TLC) direct column chromatography was done in ethyl acetate in hexane (10-30%) to get pure orange red solids (1.1 g, 76% yield).

### 2.2.4 Mechanistic studies



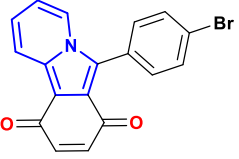
**Scheme S4.** Mechanistic studies

To begin with, the LCMS analysis of the reaction mixture for the reaction among pyridine **1a**, 4-tertbutyl phenyl diazoacetate **2f** and 1,4-benzoquinone **3a** in blue LED in ethyl acetate revealed the major formation of pyridinium ylide **[A]** (from the reaction of **1a** and **2a**) and a minor formation of ylide **[B]** (the reaction between **1a** and **3a**) (Scheme S4a). Next, the reaction of **1a** with **2f** and **3a** under argon atmosphere and blue light afforded **4h'**, which could only be

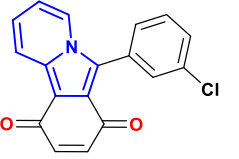
detected through a quick HRMS. Any effort to isolate it led to the formation of the final product **4h**. Hence, once the reaction in argon confirmed the formation of **4h'** (via HRMS), the reaction chamber was exposed to air to provide **4h** (Scheme S4b). Next, on stirring the same reaction mixture (**1a**, **2f** and **3a**) under air in absence of blue light, resulted in no reaction (scheme S4c). This confirmed that blue LED is essential for the generation of the carbene [A]. Finally, the reaction among **1c**, **2k** and **3b** under air and blue light when monitored through TLC and mass analysis indicated that after 6 h both **5h** and **5h'** were generated in ~1:1 ratio (Scheme 3d). <sup>1</sup>H-NMR spectra of **5h'** could be obtained here, with prompt purification and characterization. However similar to **4h'** it too got converted to **5h** when exposed to air. Stirring of the same reaction mixture for another 6 h under air, provided compound **5h** exclusively. These experiments depicted in scheme S4a-d revealed that our reaction could proceed via carbene generation, ylide formation and [3+2] cycloaddition followed by oxidation of the [3+2] intermediate to generate the desired product.

### 2.2.5 Characterisation data:

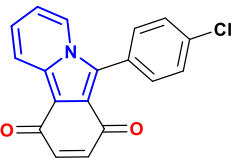
#### 6-(4-Bromophenyl)pyrido[2,1-a]isoindole-7,10-dione (**4a**):

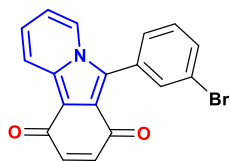
 Orange red solid, 79.24 mg, 75%, m.p. 215-217°C. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.34-8.31 (m, 1H), 8.03-8.00 (m, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.45(d, *J* = 8.8 Hz, 2H), 7.30-7.28 (m, 1H), 6.86-6.82 (m, 1H), 6.77(d, *J* = 10.4Hz, 1H), 6.62 (d, *J* = 10.4 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 183.6, 180.9, 141.3, 138.9, 134.9, 132.4, 132.1, 127.0, 126.9, 124.4, 124.3, 121.1, 115.8, 109.6; HRMS (ESI-TOF) *m/z* calcd for C<sub>18</sub>H<sub>11</sub>BrNO<sub>2</sub> [M+H]<sup>+</sup> 351.9968, found 351.9961. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3312.32, 2921.30, 2853.18, 1728.48, 1651.86, 1586.14, 1496.35, 1192..90, 1069.13, 1008.53, 796.58, 508.09.

#### 6-(3-chlorophenyl)pyrido[2,1-a]isoindole-7,10-dione (**4b**):

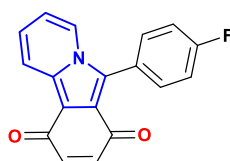
 Orange red solid, 71.9 mg, 78%, m.p. 227-229°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.33 (d, *J* = 9.2 Hz, 1H), 8.02 (d, *J* = 7.2 Hz, 1H), 7.56-7.45 (m, 4H), 7.32-7.27 (m, 1H), 6.86 (td, *J* = 6.8, 1.4 Hz, 1H), 6.79 (d, *J* = 10.4 Hz, 1H), 6.63 (d, *J* = 10.4 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 183.7, 180.9, 141.3, 138.9, 135.0, 134.8, 130.5, 130.4, 130.1, 129.8, 128.9, 127.1, 124.4, 121.1, 115.8, 109.8; HRMS (ESI-TOF) *m/z* calcd for C<sub>18</sub>H<sub>11</sub>ClNO<sub>2</sub> [M+H]<sup>+</sup> 308.0473, found 308.0477. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3039.08, 2918.89, 2855.25, 1731.03, 1636.05, 1582.62, 1504.80, 1430.91, 1224.73, 1082.85, 844.92, 791.99, 742.22, 684.81, 527.74.

#### 6-(4-chlorophenyl)pyrido[2,1-a]isoindole-7,10-dione (**4c**):

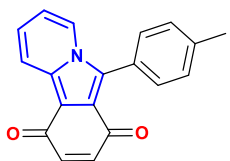
 Orange red solid, 64.5 mg, 70%, m.p. 205-207°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.34-8.32 (m, 1H), 8.03-8.00 (m, 1H), 7.56-7.50 (m, 4H), 7.30-7.26 (m, 1H), 6.84 (td, *J* = 6.9, 1.5 Hz, 1H), 6.78 (d, *J* = 10.4 Hz, 1H), 6.62 (d, *J* = 10.4 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 183.7, 180.9, 141.3, 138.9, 136.0, 131.9, 129.5, 127.0, 126.4, 124.4, 121.1, 115.7, 109.8; HRMS (ESI-TOF) *m/z* calcd for C<sub>18</sub>H<sub>11</sub>ClNO<sub>2</sub> [M+H]<sup>+</sup> 308.0473, found 308.0469. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 2919.89, 2855.32, 2355.28, 1735.21, 1636.37, 1581.47, 1500.12, 1428.20, 1228.20, 1228.15, 1065.67, 1012.31, 800.83, 734.86, 522.04.

**6-(3-bromophenyl)pyrido[2,1-a]isoindole-7,10-dione (4d):**

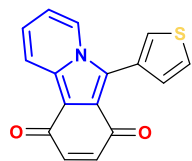
Orange red solid, 76.1 mg, 72%, m.p. 219-221°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.35-8.32 (m, 1H), 8.03 (d, *J* = 7.2 Hz, 1H), 7.72-7.65 (m, 2H), 7.53-7.50 (m, 1H), 7.45 (t, *J* = 7.8 Hz, 1H) 7.32-7.27 (m, 1H), , 6.86 (td, *J* = 6.9, 1.4 Hz, 1H), 6.78 (d, *J* = 10.0 Hz, 1H), 6.63 (d, *J* = 10.0 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 183.6, 180.9, 141.4, 138.9, 134.8, 133.3, 133.0, 130.7, 130.1, 129.4, 127.1, 124.4, 123.0, 121.1, 115.9, 109.8 HRMS (ESI-TOF) *m/z* calcd for C<sub>18</sub>H<sub>11</sub>BrNO<sub>2</sub> [M+H]<sup>+</sup> 351.9968, found 351.9969. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3058.80, 2956.91, 2117.13, 1942.63, 1740.14, 1632.06, 1496.08, 1427.16, 1254.25, 1016.52, 791.96, 685.11.

**6-(4-Fluorophenyl)pyrido[2,1-a]isoindole-7,10-dione (4e):**

Orange red solid, 45.9 mg, 80%, m.p. 220-222°C. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.34-8.32 (m, 1H), 8.02-8.00 (m, 1H), 7.57-7.54 (m, 2H), 7.30-7.28 (m, 2H), 7.07 (t, *J* = 8.6 Hz, 1H), 6.85-6.80 (m, 1H), 6.78 (d, *J* = 10.4 Hz, 1H), 6.62 (d, *J* = 10.4 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 190.9, 141.3, 138.8, 138.2, 132.6, 130.8, 120.9, 116.3, 115.6; <sup>19</sup>F NMR ((CDCl<sub>3</sub>, 376 MHz) δ<sub>F</sub> -115.7; HRMS (ESI-TOF) *m/z* calcd for C<sub>18</sub>H<sub>10</sub>FNO<sub>2</sub> [M+H]<sup>+</sup> 291.0696, found 291.0695. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 2956.55, 2917.95, 2852.71, 1723.45, 1457.52, 1256.09, 1020.06, 794.38.

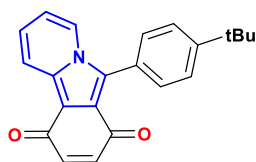
**6-(p-tolyl)pyrido[2,1-a]isoindole-7,10-dione (4f):**

Orange red solid, 70.7 mg, 82%, m.p. 230-232°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.34-8.32 (m, 1H), 8.03-8.00 (m, 1H), 7.56-7.50 (m, 4H), 7.30-7.26 (m, 1H), 6.84 (td, *J* = 6.9, 1.5 Hz, 1H), 6.78 (d, *J* = 10.4 Hz, 1H), 6.62 (d, *J* = 10.4 Hz, 1H), 1.25 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 183.7, 180.9, 141.3, 138.9, 136.0, 131.9, 129.5, 127.0, 126.4, 124.4, 121.1, 115.7, 109.8; C<sub>19</sub>H<sub>13</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 288.1019, found 288.1019. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3313.47, 2921.21, 1732.17, 1641.18, 1504.49, 1450.81, 1197.76, 1023.35, 802.64, 504.13.

**6-(thiophen-3-yl)pyrido[2,1-a]isoindole-7,10-dione (4g):**

Orange red solid, 76.3 mg, 91%, m.p. 220-222°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.36-8.34 (m, 1H), 8.24-8.21 (m, 1H), 7.80-7.79 (m, 1H), 7.57-7.55 (m, 1H), 7.44 (dd, *J* = 5.2, 1.4 Hz, 1H) 7.32-7.30 (m, 1H), , 6.88 (td, *J* = 6.9, 1.4 Hz, 1H), 6.80 (d, *J* = 10.4 Hz, 1H), 6.66 (d, *J* = 10.4 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 183.6, 180.9, 141.4, 138.9, 134.8, 133.3, 133.0, 130.7, 130.1, 129.4, 127.1, 124.4, 123.0, 121.1, 115.9, 109.8 HRMS (ESI-TOF) *m/z* calcd for C<sub>16</sub>H<sub>10</sub>NO<sub>2</sub>S [M+H]<sup>+</sup> 280.0427, found 280.0426. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3287.31, 3085.26, 2919.82, 2855.79, 1728.58, 1645.05, 1579.91, 1505.37, 1425.89, 1249.82, 1016.23, 792.34, 697.82.

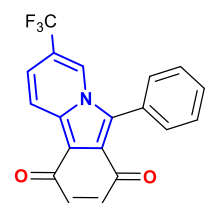
**6-(4-(tert-butyl)phenyl)pyrido[2,1-a]isoindole-7,10-dione (4h):**



Orange red solid, 84.9 mg, 86%, m.p. 235-237°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.32 (d, *J* = 8.8 Hz, 1H), 8.11 (d, *J* = 7.2 Hz, 1H), 7.59-7.49 (m, 4H), 6.82-6.80 (m, 1H), 6.77 (d, *J* = 10.4 Hz, 1H), 6.62 (d, *J* = 10.4 Hz, 1H), 1.40 (s, 9H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 183.8, 181.0, 141.3, 139.1, 130.2, 126.9, 126.0, 120.9, 115.4, 109.5, 31.4; HRMS (ESI-TOF) *m/z* calcd for C<sub>22</sub>H<sub>20</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 330.1489, found 330.1495. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3223.30, 3067.41, 2920.36, 2062.33, 1978.65, 1730.24, 1656.32, 1579.82, 1473.21, 1223.52, 1153.35, 1062.56, 725.50, 705.62, 512.52, 464.33.

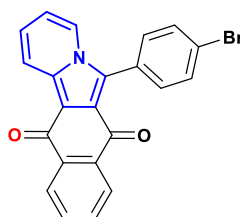
HRMS (ESI-TOF) for **4h'** *m/z* calcd for C<sub>24</sub>H<sub>23</sub>NO<sub>4</sub> [M+H]<sup>+</sup> 390.1700, found 390.1727.

#### 6-(2-(trifluoromethyl)phenyl)pyrido[2,1-a]isoindole-7,10-dione (**4i**):



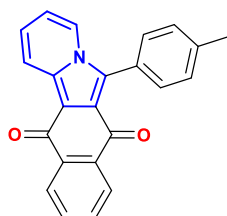
Orange red solid, 72.7 mg, 71%, m.p. 210-212°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.47-8.44 (m, 1H), 8.39-8.38 (m, 1H), 7.64-7.56 (m, 5H), 7.38 (dd, *J* = 9.2, 1.6 Hz, 1H), 6.85 (d, *J* = 10.0 Hz, 1H), 6.72 (d, *J* = 10.4 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 182.9, 181.2, 140.9, 139.4, 133.7, 130.4, 130.2, 129.6, 129.3, 126.9, 123.4-123.2 (m), 121.8, 110.5; <sup>19</sup>F NMR ((CDCl<sub>3</sub>, 376 MHz) δ<sub>F</sub> -62.7; HRMS (ESI-TOF) *m/z* calcd for C<sub>19</sub>H<sub>10</sub>F<sub>3</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 342.0736, found 342.0729. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 2922.55, 1729.73, 1636.84, 1555.18, 1439.01, 1326.33, 1125.51, 1054.50, 850.86, 695.41, 433.02.

#### 6-(4-bromophenyl)benzo[f]pyrido[2,1-a]isoindole-7,12-dione (**5a**):



Orange yellow solid, 90.5 mg, 75%, m.p. 241-243°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.54-8.52 (m, 1H), 8.31 (dd, *J* = 7.6, 0.9 Hz, 1H), 8.16 (dd, *J* = 7.6, 1.2 Hz, 1H), 8.05-8.04 (m, 1H), 7.75-7.71 (m, 3H), 7.66 (td, *J* = 7.4, 1.1 Hz, 1H), 7.52-7.49 (m, 2H), 7.34-7.29 (m, 1H), 6.88 (td, *J* = 6.9, 1.1 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 181.9, 179.5, 136.4, 135.4, 134.5, 133.7, 132.8, 132.5, 132.4, 132.3, 130.7, 127.5, 126.9, 26.8, 126.7, 126.6, 124.3, 121.7, 116.0; HRMS (ESI-TOF) *m/z* calcd for C<sub>22</sub>H<sub>13</sub>BrNO<sub>2</sub> [M+H]<sup>+</sup> 402.0124, found 402.0128. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 2919.54, 2855.14, 1732.02, 1678.53, 1590.59, 1443.79, 1232.86, 1076.85, 968.82, 817.81, 763.09, 763.09, 515.67.

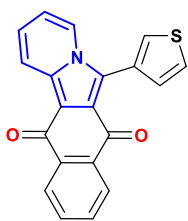
#### 6-(p-tolyl)-12a,12b-dihydrobenzo[f]pyrido[2,1-a]isoindole-7,12-dione (**5b**):



Orange yellow solid, 87.0 mg, 86%, m.p. 236-238°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.54-8.51 (m, 1H), 8.31 (dd, *J* = 7.8, 1.4 Hz, 1H), 8.16 (dd, *J* = 7.8, 1.4 Hz, 1H), 8.09-8.07 (m, 1H), 7.74-7.70 (m, 1H), 7.64 (td, *J* = 7.5, 1.5 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 7.6 Hz, 2H), 7.32-7.28 (m, 1H), 6.84 (d, *J* = 6.9, 1.5 Hz, 1H), 2.48 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 162.6, 161.1, 153.0, 139.9, 133.4, 132.5, 130.4, 129.7, 126.8, 126.4, 124.6, 121.4, 115.6, 21.6; HRMS (ESI-TOF) *m/z* calcd for C<sub>23</sub>H<sub>18</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 338.1176, found 338.1174. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 2921.81, 2858.65, 1662.48, 1594.43, 1501.96, 1436.62, 1230.89, 1089.64, 1089.64, 1019.68, 799.41, 710.82, 511.83.

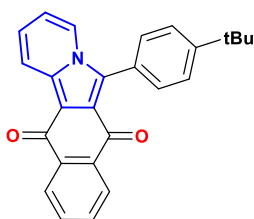
#### 6-(thiophen-3-yl)benzo[f]pyrido[2,1-a]isoindole-7,12-dione (**5c**):





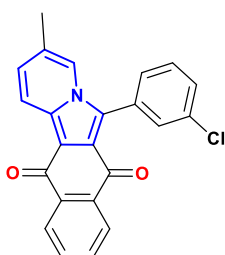
Orange yellow solid, 86.0 mg, 87%, m.p. 230-232°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.54-8.51 (m, 1H), 8.31 (dd, *J* = 7.86 1.6 Hz, 1H), 8.22-8.17 (m, 2H), 7.79-7.78 (m, 1H), 7.72 (td, *J* = 7.5, 1.6 Hz, 1H), 7.66 (td, *J* = 7.4, 1.5 Hz, 1H), 7.58-7.56 (m, 1H), 7.42 (dd, *J* = 4.8, 1.2 Hz, 1H), 7.32-7.28 (m, 1H), 6.89 (td, *J* = 6.8, 1.2 Hz, 1H);, <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 181.9, 179.2, 136.4, 135.6, 133.6, 132.6, 128.9, 128.2, 128.0, 126.9, 126.6, 126.5, 126.3, 124.9, 121.6, 115.8; HRMS (ESI-TOF) *m/z* calcd for C<sub>20</sub>H<sub>12</sub>NO<sub>2</sub>S [M+H]<sup>+</sup> 330.0583, found 330.0580. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3071.95, 2919.07, 2355.24, 2101.99, 1912.05, 1646.67, 1516.67, 1432.06, 1233.16, 1025.50, 705.41.

**6-(4-(tert-butyl)phenyl)benzo[f]pyrido[2,1-a]isoindole-7,12-dione (5d):**



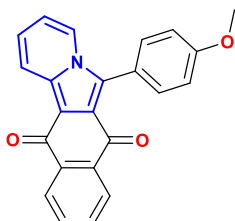
Orange yellow solid, 101.3 mg, 89%, m.p. 264-266°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.54-8.51 (m, 1H), 8.31 (dd, *J* = 7.8, 1.0 Hz, 1H), 8.19-8.12 (m, 2H), 7.72 (td, *J* = 7.5, 1.1 Hz, 1H), 7.67-7.63 (m, 1H), 7.62-7.60 (m, 2H), 7.58-7.55 (m, 2H), 7.32-7.27 (m, 1H), 6.84 (td, *J* = 6.9, 1.1 Hz, 1H), 1.42 (m, 9H);, <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 181.9, 179.2, 152.8, 136.4, 135.5, 135.2, 133.4, 132.5, 130.2, 126.8, 126.5, 126.4, 125.9, 124.7, 121.5, 115.5, 34.9, 31.3; HRMS (ESI-TOF) *m/z* calcd for C<sub>26</sub>H<sub>22</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 380.1645, found 380.1638. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 2951.10, 1749.48, 1655.17, 1591.84, 1445.48, 1226.86, 1106.57, 1007.57, 935.01, 771.85, 722.77, 558.03, 475.11.

**6-(3-chlorophenyl)-3-methylbenzo[f]pyrido[2,1-a]isoindole-7,12-dione (5e) :**



Orange red solid, 66.9 mg, 60%, m.p. 258-260°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 10.48 (d, *J* = 8.4 Hz, 1H), 8.44 (dd, *J* = 7.8, 1.1 Hz, 1H), 8.15 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.80-7.74 (m, 2H), 7.72-7.65 (m, 3H), 7.59-7.56 (m, 2H), 7.50-7.47 (m, 1H), 7.1 (d, *J* = 7.2 Hz, 1H), 1.56 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 181.4, 178.9, 136.9, 134.9, 133.6, 132.6, 130.8, 130.4, 130.0, 129.8, 129.3, 128.7, 128.5, 127.6, 127.0, 126.3, 121.3, 116.9, 29.7; HRMS (ESI-TOF) *m/z* calcd for C<sub>23</sub>H<sub>14</sub>ClNO<sub>2</sub> [M+H]<sup>+</sup> 372.0786, found 372.0782. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3064.72, 2915.71, 2250.00, 2657.12, 1587.63, 1463.59, 1258.43, 1463.59, 1258.43, 1015.90, 907.92, 795.58, 714.50.

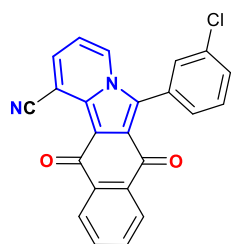
**6-(4-methoxyphenyl)benzo[f]pyrido[2,1-a]isoindole-7,12-dione (5f):**



Orange red solid, 75.3 mg, 71%, m.p. 222-224°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz) δ<sub>H</sub> 8.54-8.52 (m, 1H), 8.31 (dd, *J* = 7.8, 1.40Hz, 1H), 8.17 (dd, *J* = 7.6, 1.4 Hz, 1H), 8.11-8.08 (m, 1H), 7.72 (td, *J* = 7.5, 1.4 Hz, 1H), 7.65 (td, *J* = 7.6, 1.6 Hz, 1H), 7.57-7.54 (m, 2H), 7.32-7.27 (m, 1H), 7.13-7.11 (m, 2H), 6.85 (td, *J* = 6.9, 1.1 Hz, 1H), 3.92 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ<sub>C</sub> 184.7, 181.9, 136.4, 135.5, 133.4, 132.4, 126.8, 126.4, 121.5, 120.3, 115.5, 114.5, 55.4; HRMS (ESI-TOF) *m/z* calcd for C<sub>23</sub>H<sub>16</sub>NO<sub>3</sub> [M+H]<sup>+</sup> 354.1125, found 354.1124. FT-IR (Neat) ν<sub>max</sub> (cm<sup>-1</sup>) = 3294.89, 2919.40, 2853.54, 1637.53, 1498.32, 1426.79, 1329.66, 1169.29, 1088.98, 1018.98, 795.41, 705.54, 587.43, 477.45.

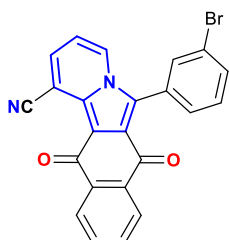
3079.35, 2957.30, 2919.65, 2854.00, 2234.70, 1721.56, 1658.47, 1530.78, 1427.91, 1245.62, 1019.13, 795.29, 718.09.

**6-(3-chlorophenyl)-7,12-dioxo-7,12-dihydrobenzo[f]pyrido[2,1-a]isoindole-3-carbonitrile (5g):**



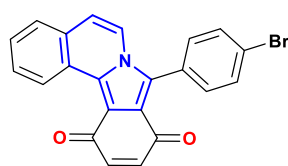
Orange yellow solid, 79.2 mg, 69%, m.p. 218-220°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz)  $\delta_{\text{H}}$  8.61 (d,  $J = 10.0$  Hz, 1H), 8.41-8.40 (m, 1H), 8.32 (dd,  $J = 7.6, 1.6$  Hz, 1H), 8.19 (dd,  $J = 7.6, 1.6$  Hz, 1H), 7.80-7.70 (m, 2H), 7.61-7.57 (m, 3H), 7.49-7.47 (m, 1H), 7.33 (dd,  $J = 9.8$  Hz, 1.4 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta_{\text{C}}$  179.5, 178.9, 133.6, 132.7, 132.5, 132.4, 129.8, 129.4, 128.6, 128.5, 127.6, 127.0, 126.3, 116.9; HRMS (ESI-TOF)  $m/z$  calcd for C<sub>23</sub>H<sub>12</sub>ClN<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> 383.0582, found 383.0585. FT-IR (Neat)  $\nu_{\text{max}}$  (cm<sup>-1</sup>) = 3294.99, 3093.23, 2917.08, 2852.18, 2235.92, 1729.37, 1650.44, 1575.56, 1462.32, 1252.94, 1013.91, 862.59, 794.27, 706.77.

**6-(3-bromophenyl)-7,12-dioxo-7,12-dihydrobenzo[f]pyrido[2,1-a]isoindole-1-carbonitrile (5h):**



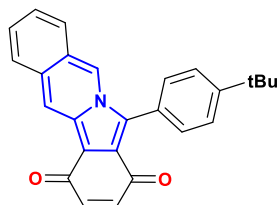
Yellow solid, 89.7 mg, 70 %, m.p. 233-235°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz)  $\delta_{\text{H}}$  8.59 (dd,  $J = 9.2, 1.2$  Hz, 1H), 8.40-8.39 (m, 1H), 8.30 (dd,  $J = 7.6, 1.6$  Hz, 1H), 8.18 (dd,  $J = 7.6, 1.6$  Hz, 1H), 7.79-7.70 (m, 4H), 7.54-7.53 (m, 2H), 7.32 (dd,  $J = 9.2$  Hz, 1.6 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta_{\text{C}}$  180.9, 179.4, 135.6, 135.0, 134.0, 133.7, 133.5, 133.4, 130.9, 130.4, 129.2, 129.0, 127.2, 126.7, 124.7, 123.4, 122.6, 115.9, 102.1; HRMS (ESI-TOF)  $m/z$  calcd for C<sub>23</sub>H<sub>12</sub>BrN<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> 427.0077, found 427.0078. FT-IR (Neat)  $\nu_{\text{max}}$  (cm<sup>-1</sup>) = 3324.55, 3052.08, 2915.01, 2229.41, 1665.51, 1623.33, 1535.55, 1485.18, 1425.69, 1233.19, 1013.23, 829.73, 790.74, 700.57, 599.30.

**7-(4-bromophenyl)isoindolo[2,1-b]isoquinoline-8,11-dione (6a):**



Orange red solid, 82.1 mg, 68%, m.p. 218-220°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz)  $\delta_{\text{H}}$  10.26-10.24(m, 1H), 7.75-7.63 (m, 6H), 7.71-7.67 (m, 2H), 7.42 (d,  $J = 6.8$  Hz, 2H), 7.07 (d,  $J = 6.0$  Hz, 1H), 6.93 (d,  $J = 8.0$  Hz, 1H), 6.68 (d,  $J = 8.0$  Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta_{\text{C}}$  183.3, 180.8, 153.1, 142.7, 138.2, 130.5, 130.1, 130.0, 128.6, 128.2, 126.9, 126.0, 125.8, 125.3, 121.9, 116.2, 35.1, 31.4; HRMS (ESI-TOF)  $m/z$  calcd for C<sub>22</sub>H<sub>13</sub>BrNO<sub>2</sub> [M+H]<sup>+</sup> 402.0124, found 402.0120. FT-IR (Neat)  $\nu_{\text{max}}$  (cm<sup>-1</sup>) = FT-IR (Neat)  $\nu_{\text{max}}$  (cm<sup>-1</sup>) = 3062.25, 2930.22, 2120.25, 1935.23, 1710.21, 1633.44, 1499.23, 1422.23, 1228.21, 1030.24, 718.23, 666.21.

**7-(4-(tert-butyl)phenyl)isoindolo[2,1-b]isoquinoline-8,11-dione (6b):**

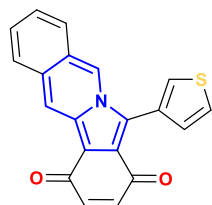


Orange red solid, 77.4 mg, 68%, m.p. 237-239°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz)  $\delta_{\text{H}}$  10.31-10.28 (m, 1H), 7.81 (d,  $J = 7.6$  Hz, 1H), 7.77-7.73 (m, 1H), 7.71-7.67 (m, 2H), 7.62 (d,  $J = 8.4$  Hz, 2H), 7.49 (d,  $J = 8.4$  Hz, 2H), 7.06-7.04 (m, 1H), 6.93 (d,  $J = 10.0$  Hz, 1H), 6.69 (d,  $J = 10.0$  Hz, 1H), 1.44 (s, 9H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta_{\text{C}}$  183.3, 180.8,

153.1, 142.7, 138.2, 130.5, 130.1, 130.0, 128.6, 128.2, 126.9, 126.0, 125.8, 125.3, 121.9, 116.2, 35.1, 31.4; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{26}H_{22}NO_2$   $[M+H]^+$  380.1645, found 380.1641. FT-IR (Neat)  $\nu_{max}$  (cm<sup>-1</sup>) = 3059.79, 2921.94, 1649.08, 1595.95, 1493.84, 1355.70, 1258.02, 1070.99, 1018.91, 831.68, 563.52.

### 7-(thiophen-3-yl)isoindolo[2,1-b]isoquinoline-8,11-dione (6c):

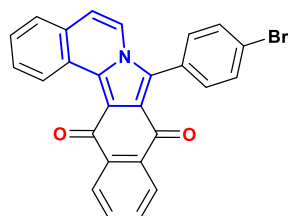
Orange red solid, 79.0 mg, 80%, m.p. 210-212°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz)  $\delta_H$  10.28-10.26



(m, 1H), 7.89 (d,  $J$  = 7.6 Hz, 1H), 7.76-7.66 (m, 4H), 7.58-7.56 (m, 1H), 7.31 (dd,  $J$  = 4.8, 1.2 Hz, 1H), 7.08 (d,  $J$  = 7.6 Hz, 1H), 6.91 (d,  $J$  = 10.4 Hz, 1H), 6.69 (d,  $J$  = 10.0 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta_C$  183.3, 180.8, 142.6, 138.1, 133.8, 130.1, 130.0, 129.1, 128.7, 128.6, 128.0, 127.0, 126.5, 121.9, 116.5; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{20}H_{12}NO_2S$   $[M+H]^+$

330.0583, found 331.0589. FT-IR (Neat)  $\nu_{max}$  (cm<sup>-1</sup>) = 3099.08, 2958.63, 2916.55, 2852.01, 2239.42, 1633.64, 1489.72, 1411.57, 1254.79, 1020.18, 914.00, 790.43, 719.13.

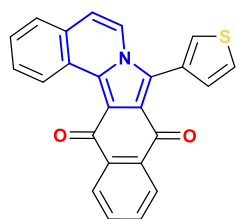
### 7-(4-bromophenyl)benzo[5,6]isoindolo[2,1-b]isoquinoline-8,13-dione (7a):



Yellow solid, 93.6 mg, 69%, m.p. 229-231°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz)  $\delta_H$  10.46-10.45 (m, 1H), 8.40 (dd,  $J$  = 6.2, 1.4 Hz, 1H), 8.14 (dd,  $J$  = 6.4, 1.2 Hz, 1H), 7.78-7.70 (m, 4H), 7.67-7.56 (m, 4H), 7.48-7.46 (m, 2H), 7.07 (d,  $J$  = 5.6 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta_C$  179.5, 178.9, 133.6, 132.7, 132.5, 132.4, 129.8, 129.4, 128.6, 128.5, 127.6, 127.0, 126.3, 116.9; HRMS (ESI-TOF)  $m/z$  calcd for

$C_{26}H_{15}BrNO_2$   $[M+H]^+$  452.0281, found 452.0287. FT-IR (Neat)  $\nu_{max}$  (cm<sup>-1</sup>) = 2933.84, 2889.22, 1711.21, 1640.21, 1423.10, 1405.90, 1211.11, 1001.23, 932.23, 805.52, 760.25, 753.23, 503.45.

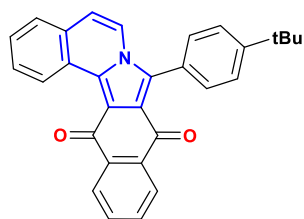
### 7-(thiophen-3-yl)benzo[5,6]isoindolo[2,1-b]isoquinoline-8,13-dione (7b):



Reddish yellow solid, 99.0 mg, 87%, m.p. 292-294°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz)  $\delta_H$  10.49 (d,  $J$  = 8.4 Hz, 1H), 8.45 (dd,  $J$  = 7.8, 1.4 Hz, 1H), 8.18 (dd,  $J$  = 7.6, 1.2 Hz, 1H), 7.91 (d,  $J$  = 7.6 Hz, 1H), 7.78-7.67 (m, 6H), 7.62-7.60 (m, 1H), 7.37 (dd,  $J$  = 4.8 Hz, 1.2 Hz, 1H), 7.12 (d,  $J$  = 7.2 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta_C$  181.5, 178.9, 133.5, 132.6, 129.8, 129.3, 128.4, 128.2, 127.5, 126.9, 126.4, 126.3, 121.8, 116.7; HRMS (ESI-

TOF)  $m/z$  calcd for  $C_{24}H_{14}NO_2S$   $[M+H]^+$  380.0740, found 380.0744. FT-IR (Neat)  $\nu_{max}$  (cm<sup>-1</sup>) = 3294.99, 3093.26, 2917.08, 2852.18, 2235.92, 1729.37, 1650.44, 1575.56, 1462.32, 1252.94, 1013.91, 862.59, 794.27, 706.77.

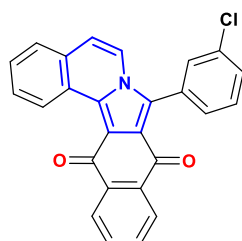
### 7-(4-(tert-butyl)phenyl)benzo[5,6]isoindolo[2,1-b]isoquinoline-8,13-dione (7c):



Yellow solid, 112.1 mg, 87%, m.p. 234-236°C. <sup>1</sup>H NMR ((CDCl<sub>3</sub>, 400 MHz)  $\delta_H$  10.48 (d,  $J$  = 8.0 Hz, 1H), 8.43 (dd,  $J$  = 7.8, 1.4 Hz, 1H), 8.16 (dd,  $J$  = 7.6, 1.2 Hz, 1H), 7.79 (d,  $J$  = 7.2 Hz, 1H), 7.77-7.72 (m, 2H), 7.67-7.62 (m, 5H), 7.53-7.51 (m, 2H), 7.04 (d,  $J$  = 7.2 Hz, 1H), 1.43 (s, 9H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta_C$  181.7, 179.1, 152.9, 137.1, 134.9, 133.9, 133.6, 132.6, 132.4, 130.6, 130.1,

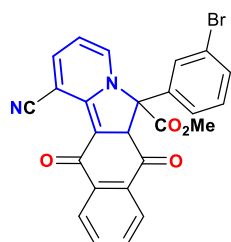
129.7, 128.6, 128.5, 127.6, 127.0, 126.4, 126.2, 126.1, 126.0, 122.0, 121.7, 116.5, 114.8, 35.1, 31.5; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{30}H_{24}NO_2$   $[M+H]^+$  430.1802, found 430.1803. FT-IR (Neat)  $\nu_{max}$  ( $cm^{-1}$ ) = 3220.73, 3066.31, 2916.36, 2852.35, 2557.26, 2346.05, 2155.54, 2062.33, 1978.65, 1730.24, 1656.32, 1569.71, 1471.18, 1254.42, 1102.95, 1003.64, 791.33, 711.57, 552.16, 463.67.

**8-(3-chlorophenyl)benzo[5,6]isoindolo[1,2-a]isoquinoline-9,14-dione (7d):**



Yellow solid, 84.3 mg, 69%, m.p. 223-225°C.  $\delta_H$  8.34-8.32 (m, 1H), 8.03-8.00 (m, 1H), 7.56-7.50 (m, 4H), 7.30-7.26 (m, 1H), 6.84 (td,  $J = 6.9, 1.5$  Hz, 1H), 6.78 (d,  $J = 10.4$  Hz, 1H), 6.62 (d,  $J = 10.4$  Hz, 1H), 1.25 (s, 3H);  $^{13}C$  NMR ( $CDCl_3$ , 100 MHz)  $\delta_C$  183.7, 180.9, 141.3, 138.9, 136.0, 131.9, 129.5, 127.0, 126.4, 124.4, 121.1, 115.7, 109.8; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{26}H_{14}ClNO_2$   $[M+H]^+$  408.0786, found 408.0781. FT-IR (Neat)  $\nu_{max}$  ( $cm^{-1}$ ) = 2929.30, 2870.52, 1755.21, 1613.23, 1399.21, 1428.90, 1222.32, 998.21, 901.23, 845.23, 746.52, 559.59.

**Methyl 6-(3-bromophenyl)-1-cyano-7,12-dioxo-6,6a,7,12-tetrahydrobenzo[f]pyrido[2,1-a]isoindole-6-carboxylate (5h’):**



$^1H$  NMR ( $CDCl_3$ , 400 MHz)  $\delta_H$  8.61 (dd,  $J = 9.2, 1.2$  Hz, 1H), 8.41-8.40 (m, 1H), 8.32 (dd,  $J = 7.8, 1.4$  Hz, 1H), 8.19 (dd,  $J = 7.8, 1.4$  Hz, 1H), 8.09-8.08 (m, 1H), 7.80-7.70 (m, 4H), 7.54-7.53 (m, 2H), 7.33 (dd,  $J = 9.4$  Hz, 1.4 Hz, 1H), 5.3 (s, 3H), 4.68 (s, 1H); HRMS (ESI-TOF)  $m/z$  calcd for  $C_{25}H_{15}BrN_2O_4$   $[M+H]^+$  487.0288, found 487.0281.

### 3. Quantum yield and molar extinction coefficient calculation

Relative fluorescence quantum yield of **7a** in DCM and water was measured using Rhodamine 6G as standard ( $\Phi_{st} = 0.95$  in ethanol)<sup>2</sup>. Quantum yields were calculated using the following equation:

$$\Phi_x = \Phi_{st} \left( \frac{grad_x}{grad_{st}} \right) \left( \frac{\eta_x^2}{\eta_{st}^2} \right) \dots \dots \dots \text{(Eq. 1)}$$

Where  $\Phi_x$  is the quantum yield to be determined,  $grad_x$  and  $grad_{st}$  are the gradient of the plot of emission vs absorption spectra of the sample and standard respectively.  $\eta$  represents refractive index of respective solutions. We found relative quantum yield of **7a** to be 0.82 (DCM), 0.48 (ACN), 0.26 (THF), 0.12 (hexane), 0.27 (toluene), 0.08 (methanol) and 0.05 (water).

Molar extinction coefficient ( $\mathcal{E}$ ) was calculated from the slope of absorbance vs concentration plot and were found to be,  $\mathcal{E} = 2.32 \times 10^4$  (DCM),  $1.55 \times 10^4$  (ACN),  $0.94 \times 10^4$  (THF),  $0.49 \times 10^4$  (hexane),  $0.97 \times 10^4$  (toluene),  $0.34 \times 10^4$  (methanol) and  $0.21 \times 10^4$  (water) in  $L \text{ Mol}^{-1} \text{ cm}^{-1}$ .

### 4. Theoretical calculation and crystal data

#### 4.1 Theoretical Calculation

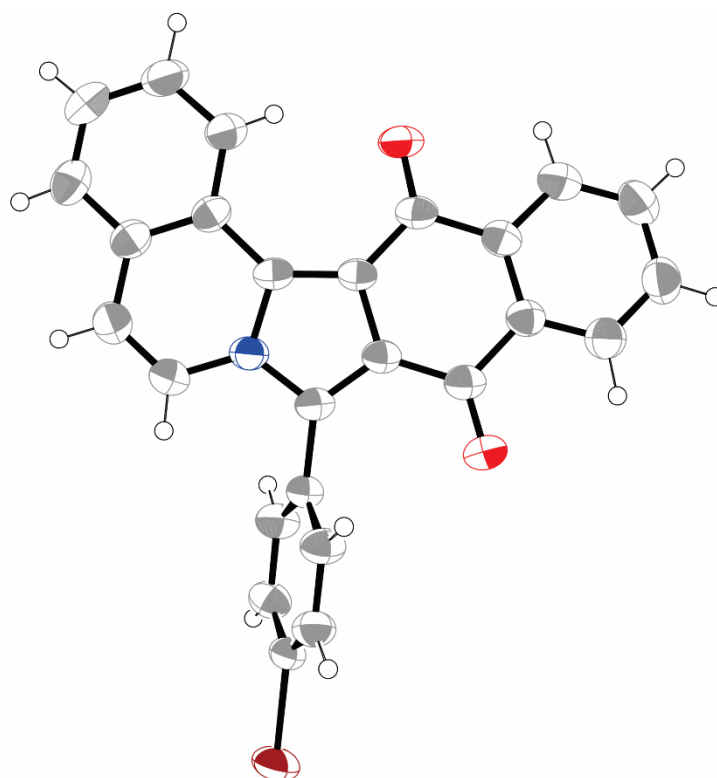
All the calculations are performed by using B3LYP<sup>S3</sup> level of theory as implemented in the Gaussians 09 package.<sup>S4</sup> For geometry optimizations, 6-311++G (d, p) basis set was used for all atoms.<sup>S5</sup> Frequency calculations of all the optimized structures were performed to ensure that the optimized structures were the local energy minima without any imaginary frequency, and to obtain zero-point corrections and the Gibbs free energies. All the HOMO and LUMO visualisation files were generated from FCHK file by the help of chemcraft software.

## 4.2 Single-crystal XRD analysis:

Single crystal data collections and corrections with D8 Venture Bruker AXS single-crystal X-ray diffractometer equipped with CMOS PHOTON 100 detector having monochromatized microfocus sources (Mo-K $\alpha$  = 0.71073 Å). Single crystals of **7a** (CCDC 214628) suitable for X-ray diffraction study were obtained from the slow evaporation process. The structure solution and refinement were performed by using the SHELX program implemented in APEX3.<sup>S6-10</sup> The non-H atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters. All the hydrogen atoms were placed at the hybridized positions and refined using a riding model with appropriate HFIX commands. The molecular structures were drawn by ORTEP.<sup>S10</sup> (Figure S1).

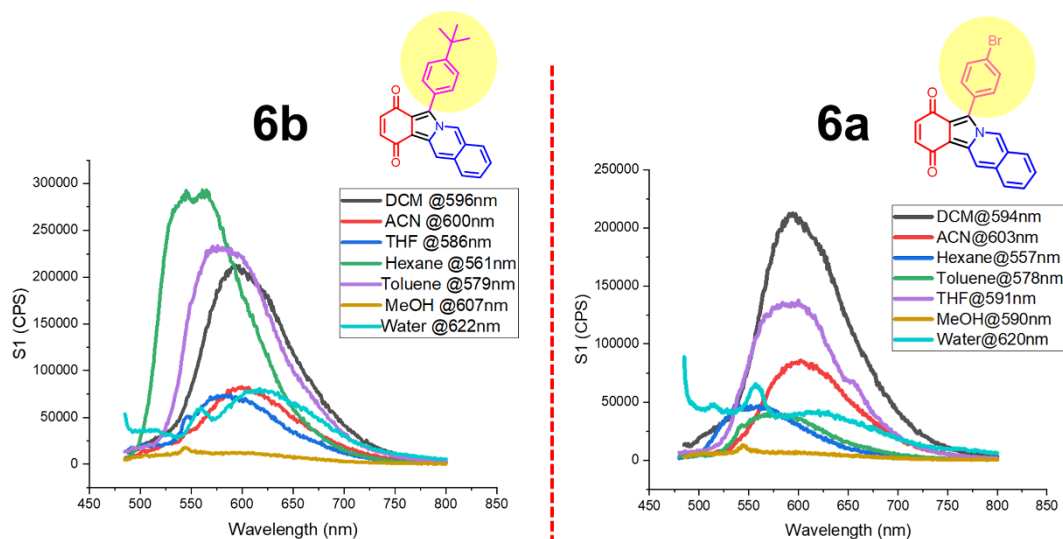
**Table S2:** Crystallographic data for **7a**.

<b>CCDC No</b>	2142628	<b>Radiation (<math>\lambda</math>)/Å<sup>o</sup></b>	0.71073
<b>Lattice</b>	monoclinic	<b><math>\rho</math> (g cm<sup>-3</sup>)</b>	1.568
<b>Formula</b>	C <sub>14</sub> H <sub>14</sub> BrNO <sub>2</sub>	<b><math>\mu</math> (Mo K<math>\alpha</math>) mm<sup>-1</sup></b>	0.0815
<b>Formula Weight</b>	452.28	<b><math>\theta_{\max}</math>/deg</b>	26.387
<b>Space Group</b>	<i>P</i> 21/ <i>c</i>	<b>Collected reflections</b>	3912
<b>a/ Å<sup>o</sup></b>	11.2943(4)	<b>Unique reflections</b>	3202
<b>b/ Å<sup>o</sup></b>	9.2072(5)	<b>No of parameters</b>	328
<b>c/ Å<sup>o</sup></b>	18.9546(9)	<b>R<sub>1</sub> [I &gt; 2<math>\sigma</math>I]</b>	0.0044
<b><math>\alpha</math>/ °</b>	90	<b>wR<sub>2</sub> [I &gt; 2<math>\sigma</math>I]</b>	0.0815
<b><math>\beta</math>/ °</b>	103.620	<b>R<sub>1</sub> [all data]</b>	0.0337
<b><math>\gamma</math>/ °</b>	90	<b>wR<sub>2</sub> [all data]</b>	0.0785
<b>V/ Å<sup>3</sup></b>	1915.64(15)	<b>R<sub>int</sub> [all data]</b>	0.033
<b>Z</b>	4	<b>GOF</b>	1.846



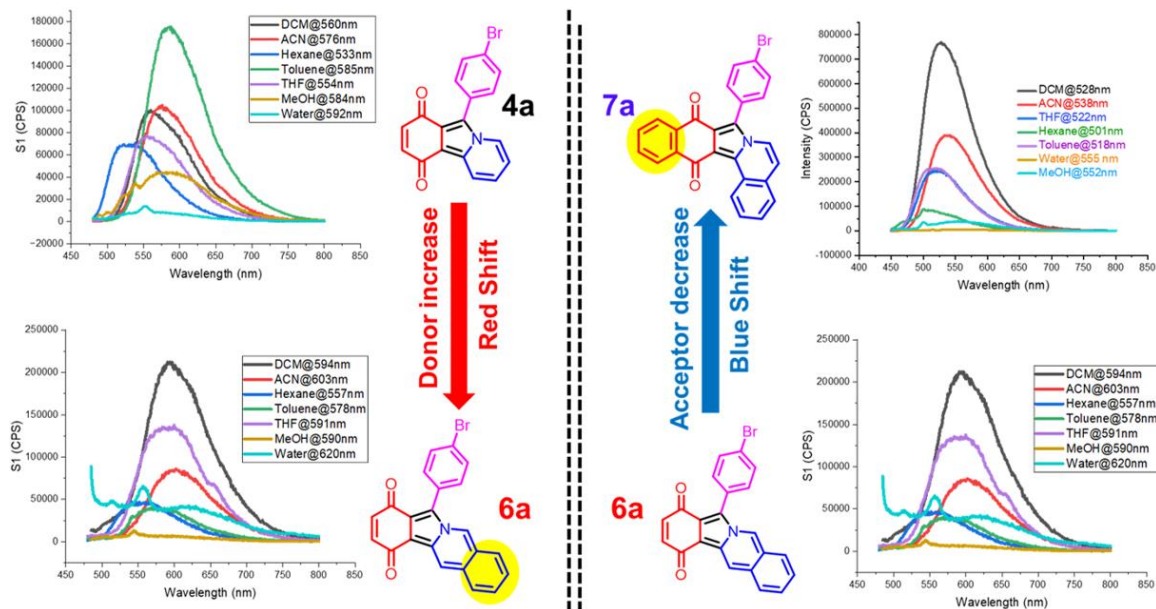
**Figure S1.** ORTEP diagram of **7a**.

### 4.3 Solvent dependent Emission spectra of **6a** & **6b**:



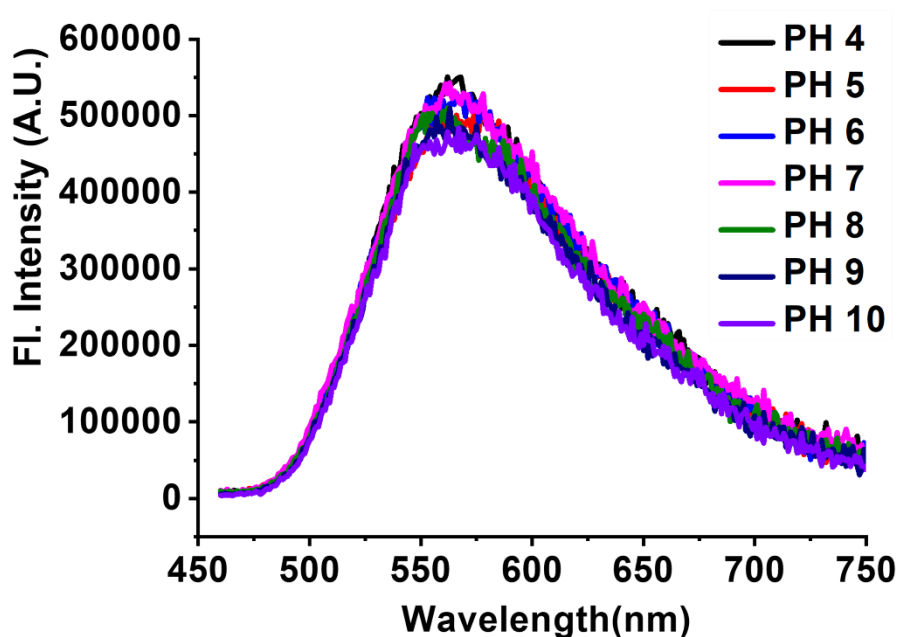
**Figure S2.** Photophysical investigation of indolizines: Solvent dependent emission spectra of **6b** [concentration 10 $\mu$ M,  $\lambda_{ex}$  = 472 nm (DCM), 469 nm (ACN), 458 nm (hexane), 468 nm (toluene), 465 nm (THF), 472 nm (methanol), 480 nm (water), Slit Width = 1/1nm] and **6a** [concentration 10 $\mu$ M,  $\lambda_{ex}$  = 465 nm (DCM), 464 nm (ACN), 452 nm (hexane), 459 nm (toluene), 457 nm (THF), 464 nm (methanol), 477 nm (water); Slit Width = 1/1nm].

#### 4.4 Solvent dependent Emission spectra of 4a, 6a, 6b & 7a:



**Figure S3.** Photophysical investigation of indolizines: Solvent dependent emission spectra of **4a** [concentration 10 $\mu$ M,  $\lambda_{\text{ex}}$  = 467 nm (DCM), 465 nm (ACN), 451 nm (hexane), 457 nm (toluene), 461 nm (THF), 470 nm (methanol), 476 nm (water); Slit Width = 1/1nm], **6a** [concentration 10 $\mu$ M,  $\lambda_{\text{ex}}$  = 465 nm (DCM), 464 nm (ACN), 452 nm (hexane), 459 nm (toluene), 457 nm (THF), 464 nm (methanol), 477 nm (water); Slit Width = 1/1nm], **6b** [concentration 10 $\mu$ M,  $\lambda_{\text{ex}}$  = 472 nm (DCM), 469 nm (ACN), 458 nm (hexane), 468 nm (toluene), 465 nm (THF), 472 nm (methanol), 480 nm (water), Slit Width = 1/1nm] and **7a** [concentration 10 $\mu$ M,  $\lambda_{\text{ex}}$  = 436 nm (DCM), 439 nm (ACN), 422 nm (hexane), 428 nm (toluene), 431 nm (THF), 465 nm (methanol), 467 nm (water); Slit Width = 1/1nm].

#### 4.5 pH dependent Emission spectra of 7a:



**Figure S4.** pH dependent emission spectra in pH = 4, 5, 6, 7, 8, 9, 10 in PBS (10 mM) solution of 30  $\mu$ M concentration of **7a** keeping excitation wavelength at 467 nm and slit width 2/2 nm.

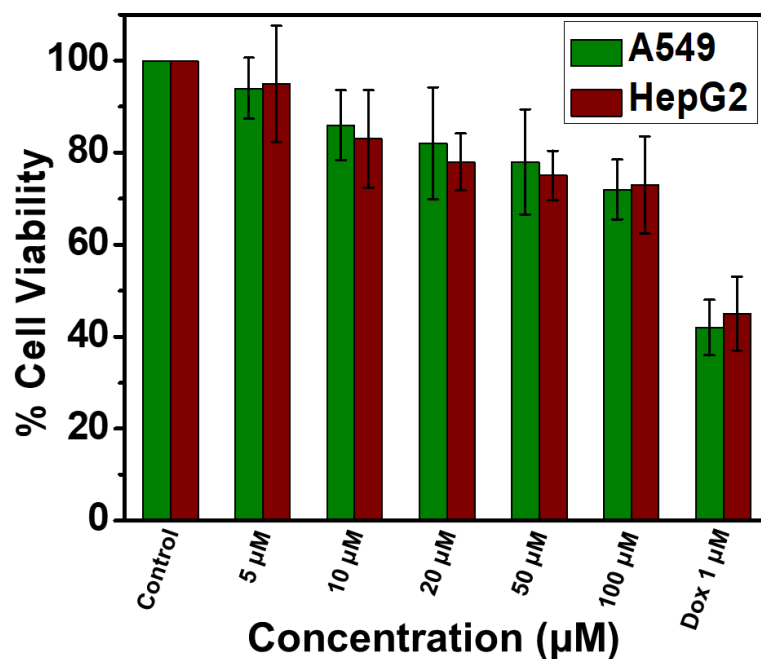
## 5. Cellular Biological Study:

### 5.1 Cell Viability Experiments

The cytotoxic nature of the compounds **7a (Probe)** was carried out on both human liver cancer cell line (HepG2) and human lung cancer cell line (A549) by colorimetric MTT (3-(4, 5- dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay. Here, cell suspension of  $5 \times 10^3$  cells/well (volume = 100  $\mu$ L) were seeded in a 96 well plate and cell lines are grown using DMEM culture media with 10% FBS, 2 mM glutamine and 100 U penicillin / 0.1 mg/ml streptomycin antibiotics for 24 hrs. in a CO<sub>2</sub> incubator. When the cells reached approximately 80% confluency, 100  $\mu$ L of **7a (Probe)** at various concentrations (5  $\mu$ M to 100  $\mu$ M) and doxorubicin (1  $\mu$ M) were added as a positive control. The plates were then incubated for 24 h in a 5% CO<sub>2</sub> incubator and later MTT solution in DMEM (0.5 mg/ml) was added to each well and incubation was continued for an additional 3 hrs. The insoluble formazan solid were solubilized by the addition of 100  $\mu$ L DMSO and the absorbance was measured at 570 nm using a microplate spectrophotometer (BioTek, Synergy H1; MST Lab in SNIoE, department of Chemistry).

$$\text{Cell Viability (\%)} = \frac{\text{Abs. sample}}{\text{Abs. control}} \times 100 \dots\dots\dots(\text{Eq. 2})$$

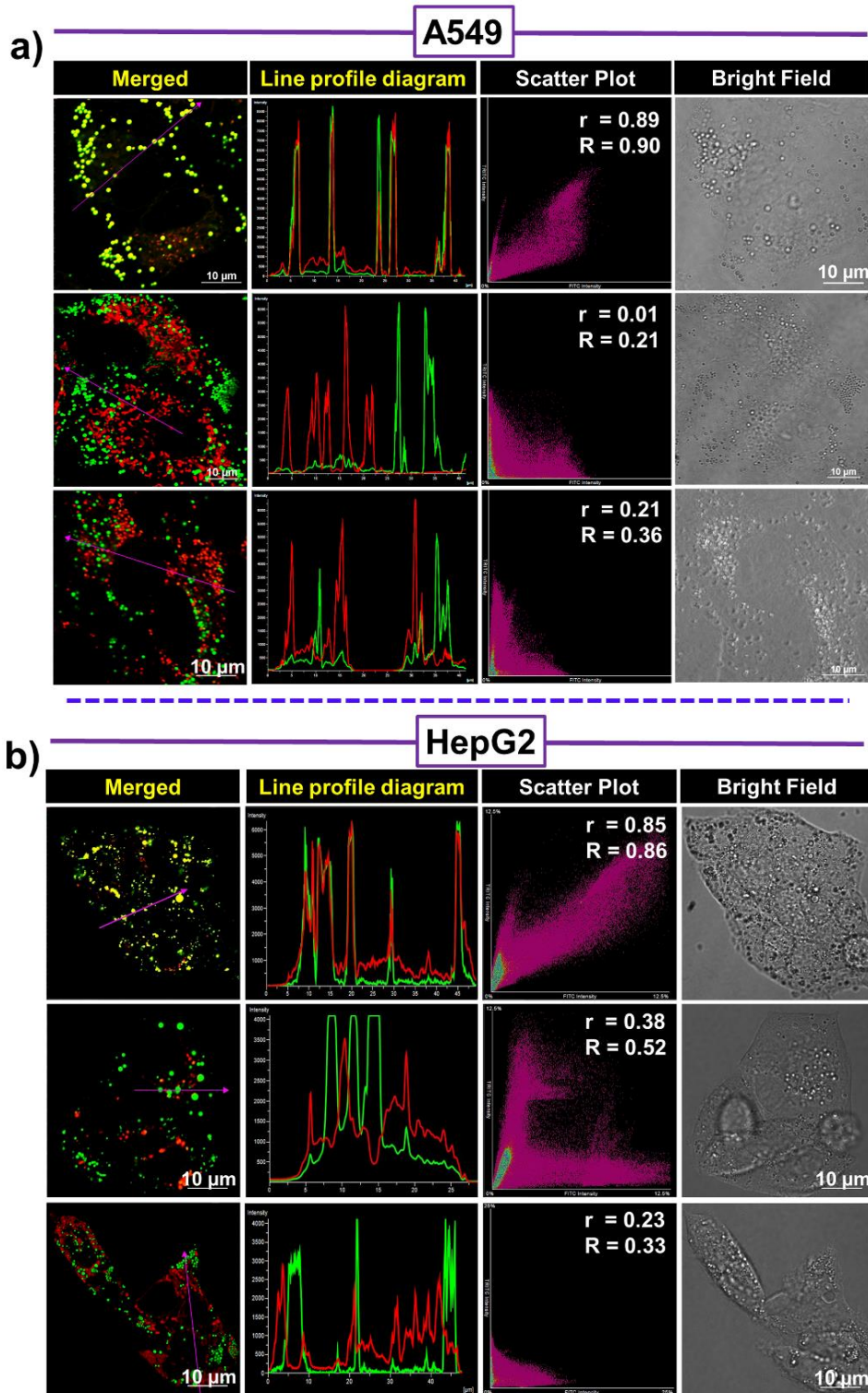




**Figure S5.** Cell viability studies of **7a (Probe)** with MTT assays in two cell lines (A549 and HepG2) with doxorubicin as a positive control.

## 5.2 Cellular Co-localization Experiment:

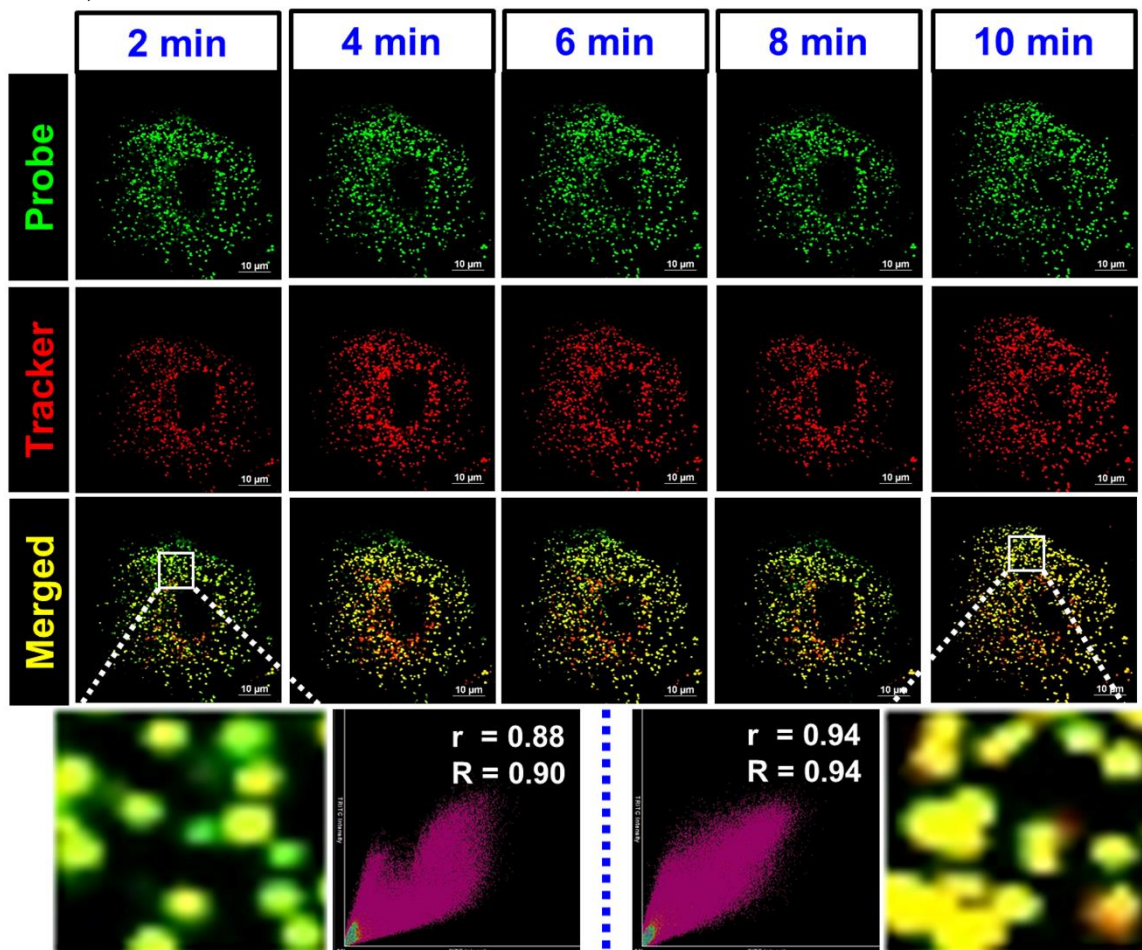
**Co-localization of 7a (Probe) with Nile red, MitoTracker-deep-red and LysoTracker-deep-red:** For labeling of lipid droplets, mitochondria and lysosome both the two cell lines (A549 and HepG2) were treated with Nile red (200 nM), MitoTracker-deep-red (200 nM) and LysoTracker deep red (200 nM) for 15 min respectively in serum free DMEM prior to imaging. The cells were also co-stained with the probe (**7a**) for 30 min and fluorescence images were acquired. The extent of co-localization was calculated using Pearson's correlation coefficient ( $r$ ) and Mander's overlap coefficients ( $R$ ).



**Figure S6:** Confocal imaging for intracellular co-localization of **7a (Probe)** was done in the green channel (em. 500–550 nm; ex. 488 nm), in the red channel (em. 580–620 nm) for the Nile red (ex. 560 nm) and in the deep-red channel (em. 650–720 nm) for MitoTracker deep red (ex. 640 nm) and LysoTracker deep red (ex. 640 nm). The cells were stained with the Trackers which was pre-treated with the probe for 20 min and the images were taken and the corresponding line profile diagram and scatter plot was plotted. The image scale bar is 10 μm.

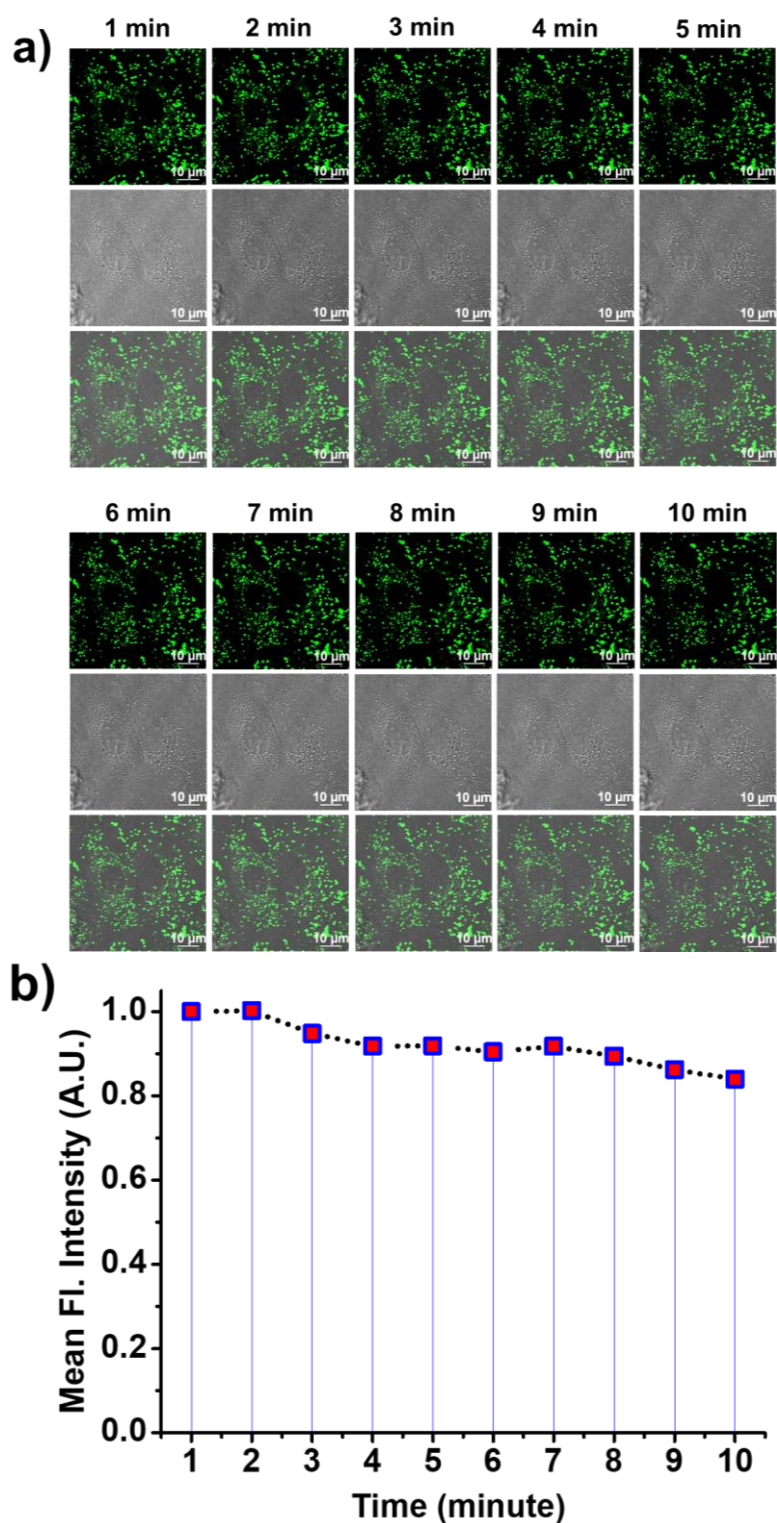
Images were captured using a 100X oil emersion lens with 2X zoom. The cell line was used here a) A549 and b) HepG2.

### 5.3 Time-dependent cross-talk between Lipid droplets: observed by 7a (Probe):



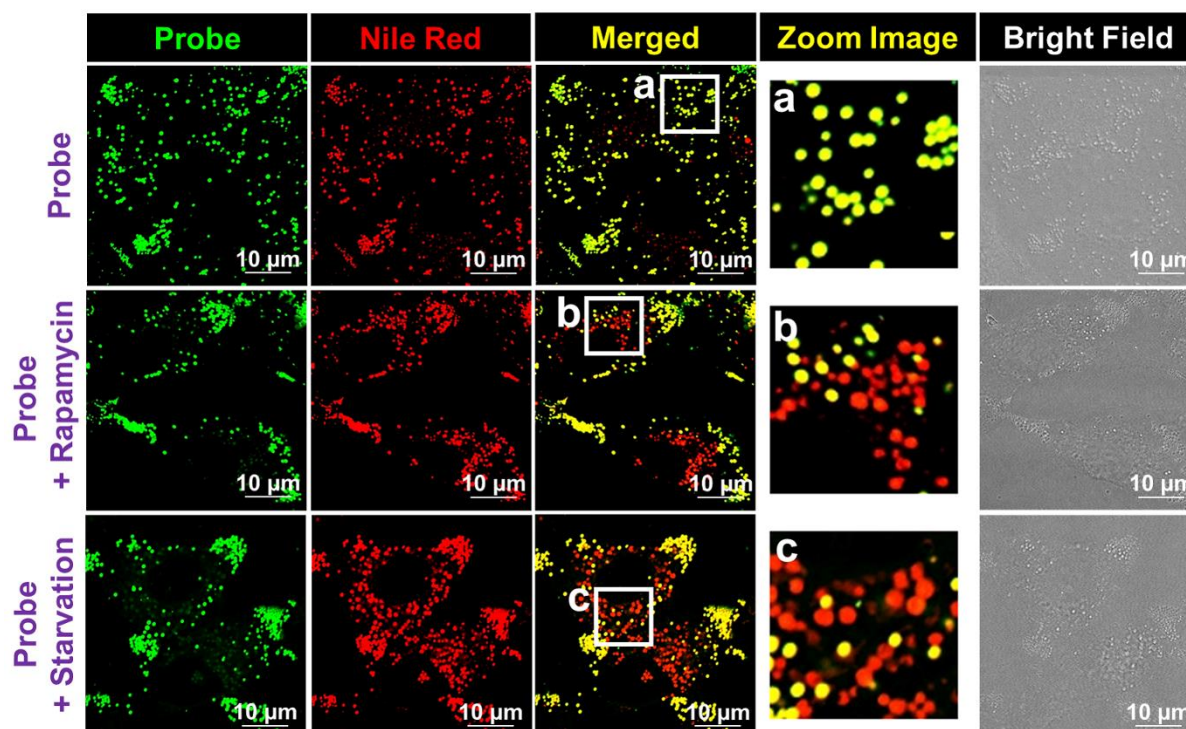
**Figure S7:** Confocal imaging for intra-cellular lipid droplets cross-talk. The images were taken with 2 min time interval up to 10 min for **7a (Probe)** in the green channel (em. 500–550 nm; ex. 488 nm) and in the red channel (em. 580–620 nm) for the Nile red (ex. 560 nm). The cells were pre-treated with the probe for 30 min and counter stained with the Nile red for 10 min and images were taken. The image scale bar is 10  $\mu\text{m}$ . Images were captured using a 100X oil emersion lens with 2X zoom. It was observed that with respect to time size of lipid droplets is increasing (Zoom image of 2 min and 10 min: Lipid droplets size for 10 min is bigger compared to 2 min).

## 5.4 Photo-stability and Photo-toxicity experiment of 7a (Probe):



**Figure S8:** Photo-stability and Photo-toxicity Study of **7a (Probe)**. A549 cells were treated with probe for 30 min at 37 °C and images were acquired with 1 min time intervals for 10 min in the green channel (em. 500–550 nm) with excitation 488 nm. **a)** It was found to be almost no photo-toxicity. **b)** In addition, under continuous laser irradiation for 10 min, the emission intensity of the probe still remaining >80%, suggesting the probe have good photo-stability. Image scale bar = 10  $\mu\text{m}$ . Images were captured using 100X oil emersion lens with 2X zoom.

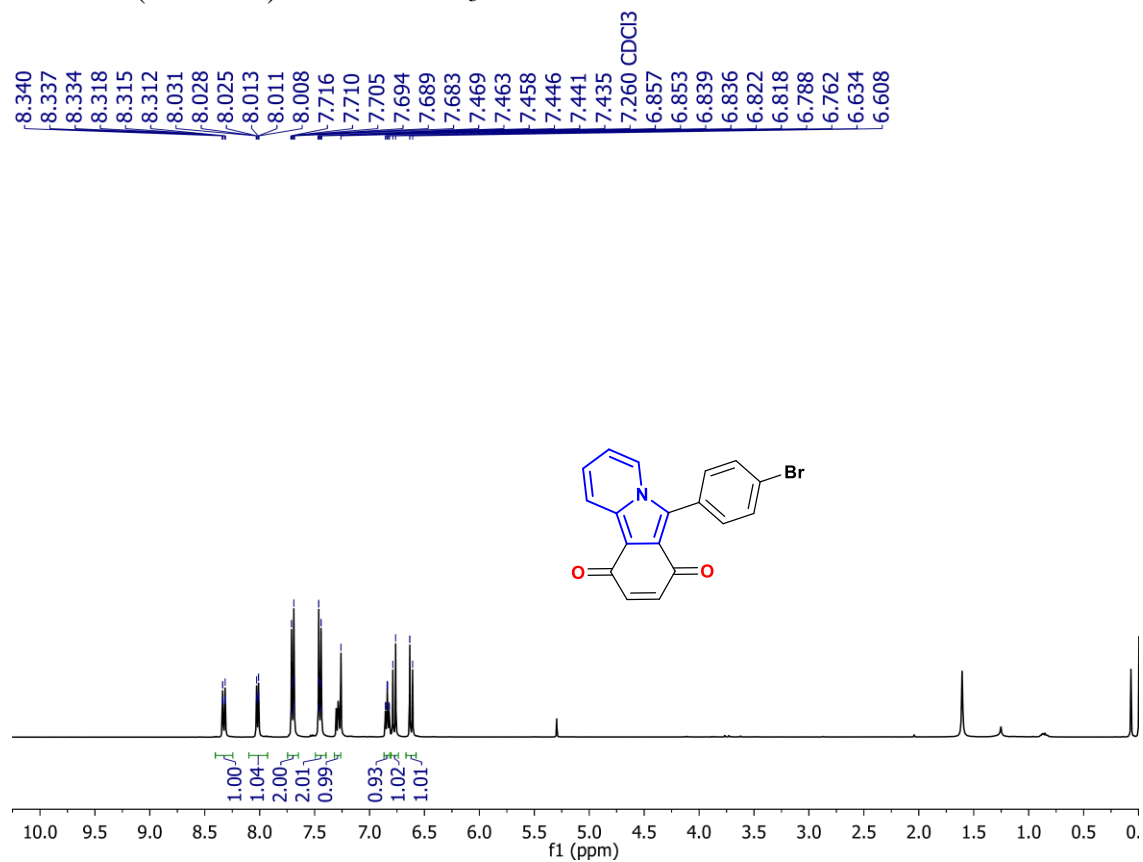
## 5.5 Detection of specific types of LDs Induced by Starvation and Rapamycin by 7a (Probe):



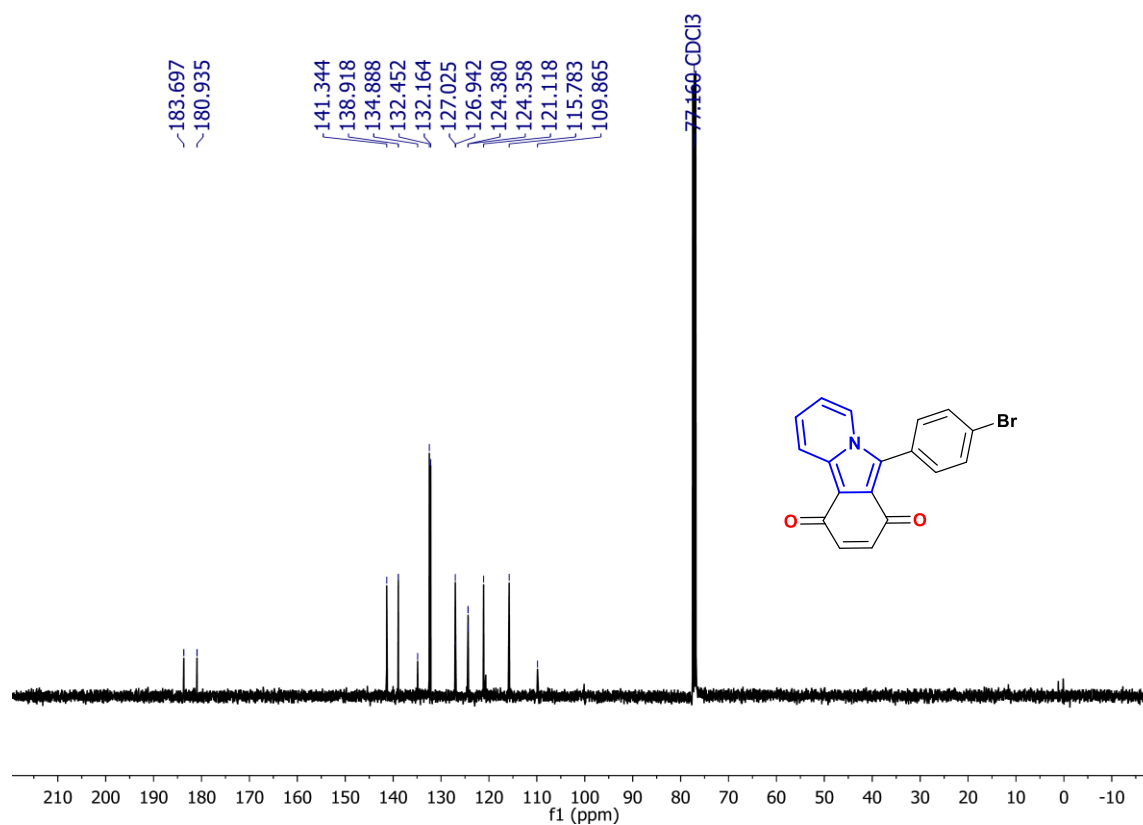
**Figure S9.** Confocal fluorescence images for A549 cells during the rapamycin-induced (200 nM) and nutrient-free starvation condition induced cellular stress. Images were acquired in the green channel (em. 500–550 nm) for the **7a** (ex. 488 nm), in the red channel (em. 580–620 nm) for the Nile red (ex. 560 nm). The image scale bar is 10  $\mu\text{m}$ . Images were captured using a 100X oil emersion lens with 2X zoom. “a”, “b” and “c” signify the zoomed-in picture of the respective merged images.

## 6. Characterization of NMR spectra

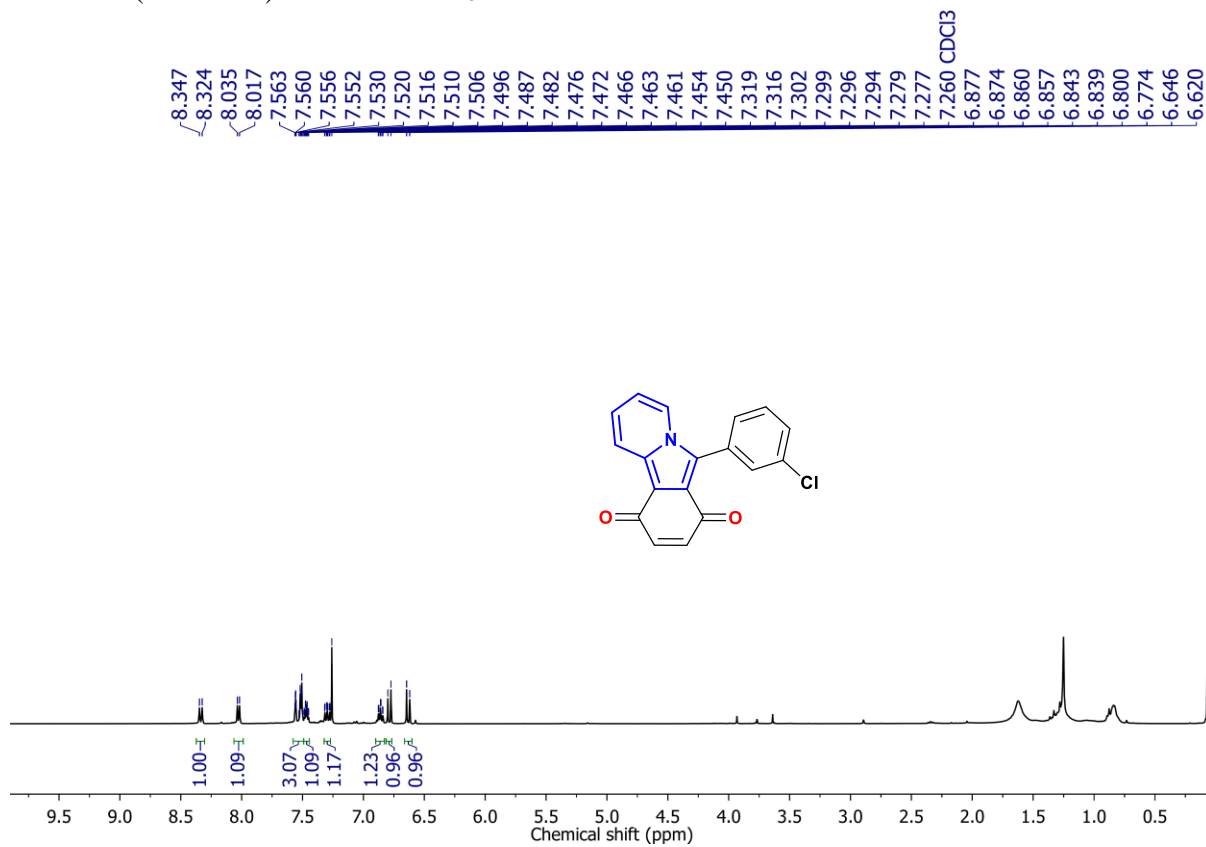
$^1\text{H}$  NMR (400 MHz) of **4a** in  $\text{CDCl}_3$



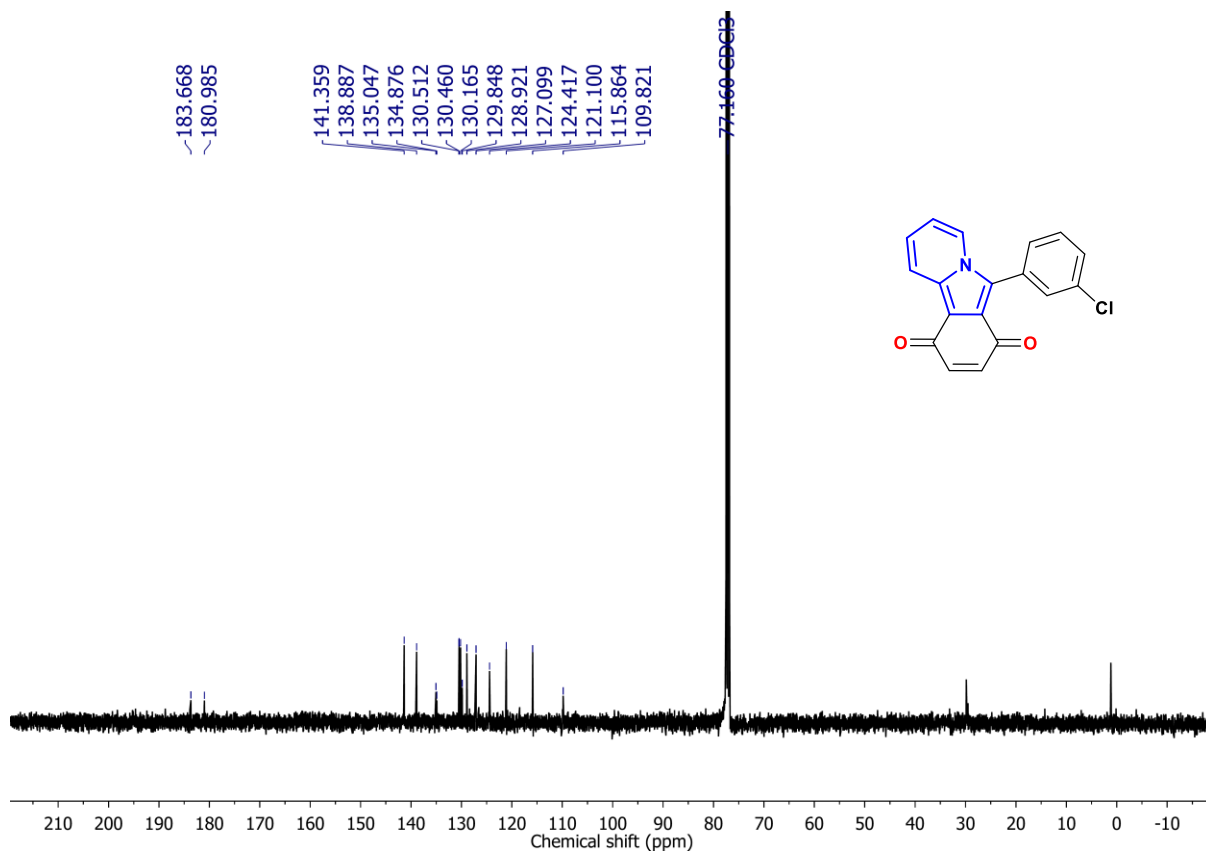
$^{13}\text{C}$  NMR (400 MHz) of **4a** in  $\text{CDCl}_3$



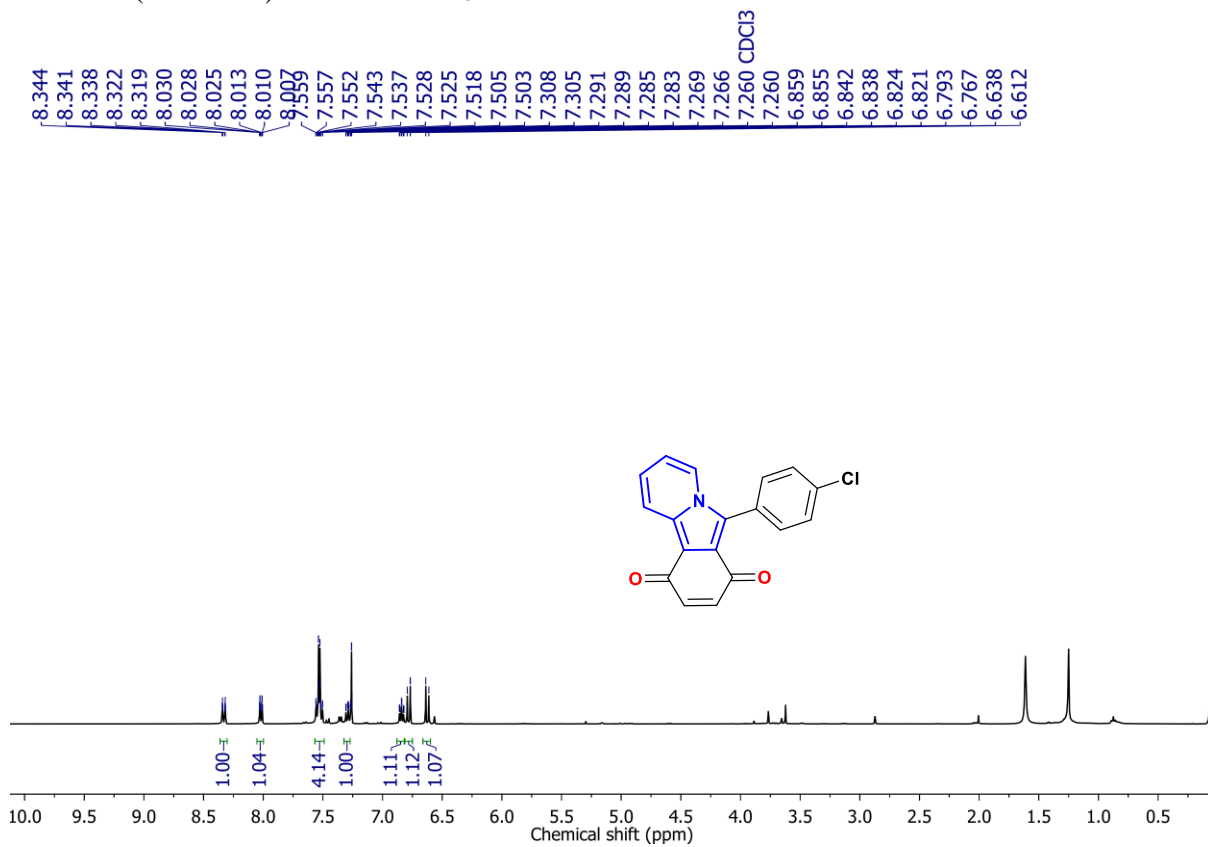
$^1\text{H}$  NMR (400 MHz) of **4b** in  $\text{CDCl}_3$



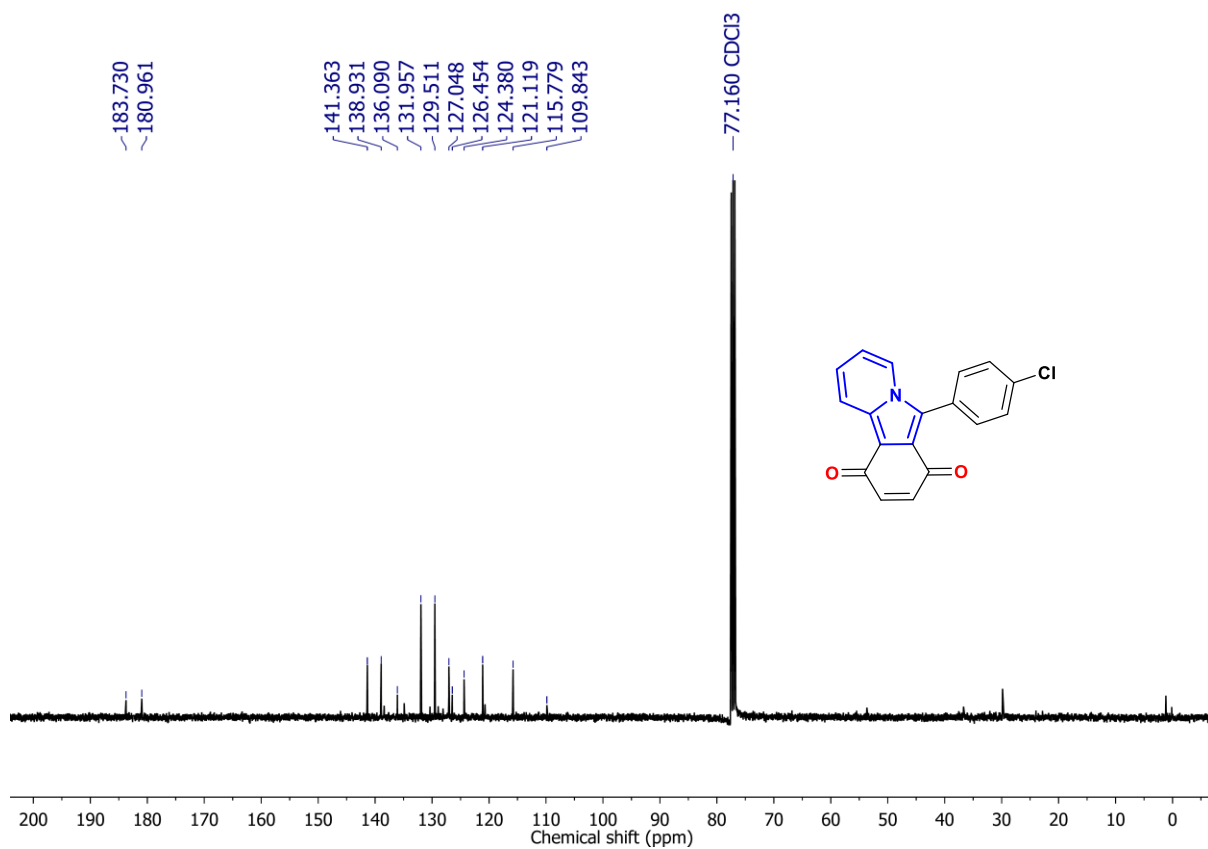
$^{13}\text{C}$  NMR (400 MHz) of **4b** in  $\text{CDCl}_3$



$^1\text{H}$  NMR (400 MHz) of **4c** in  $\text{CDCl}_3$

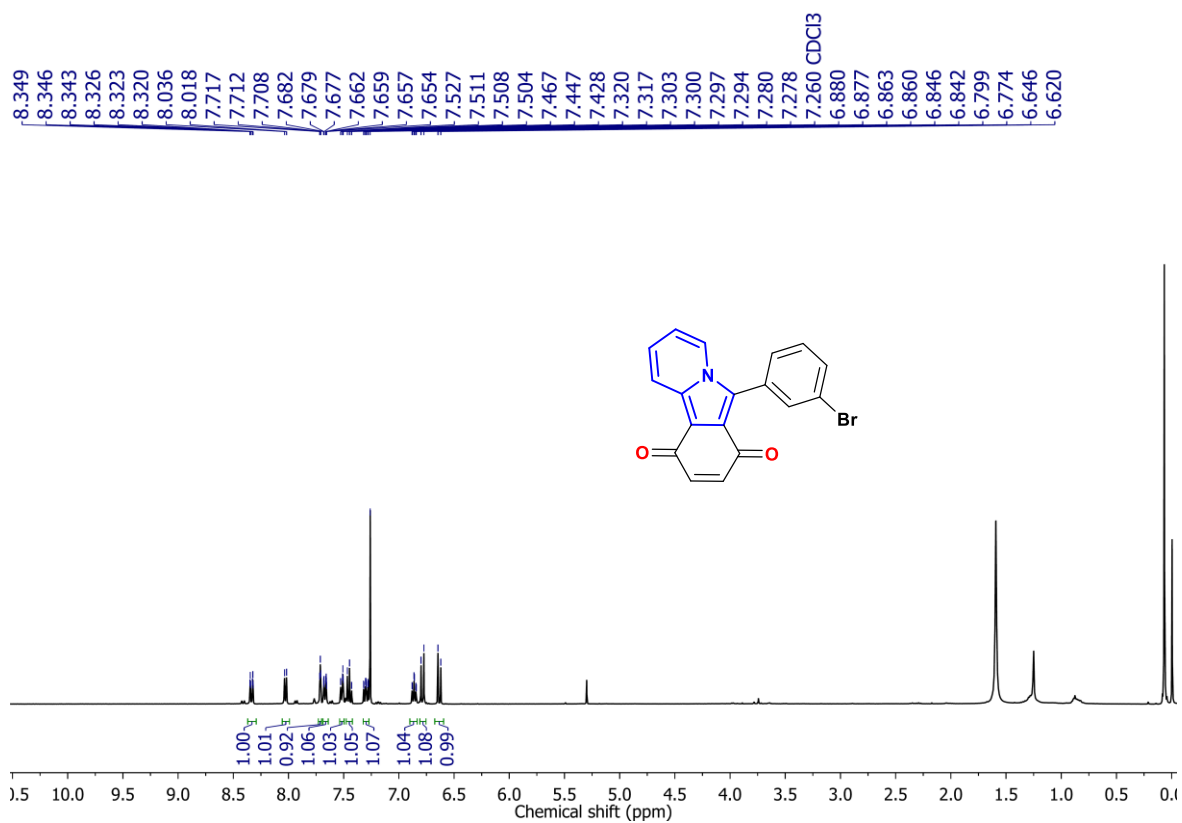


$^{13}\text{C}$  NMR (400 MHz) of **4c** in  $\text{CDCl}_3$

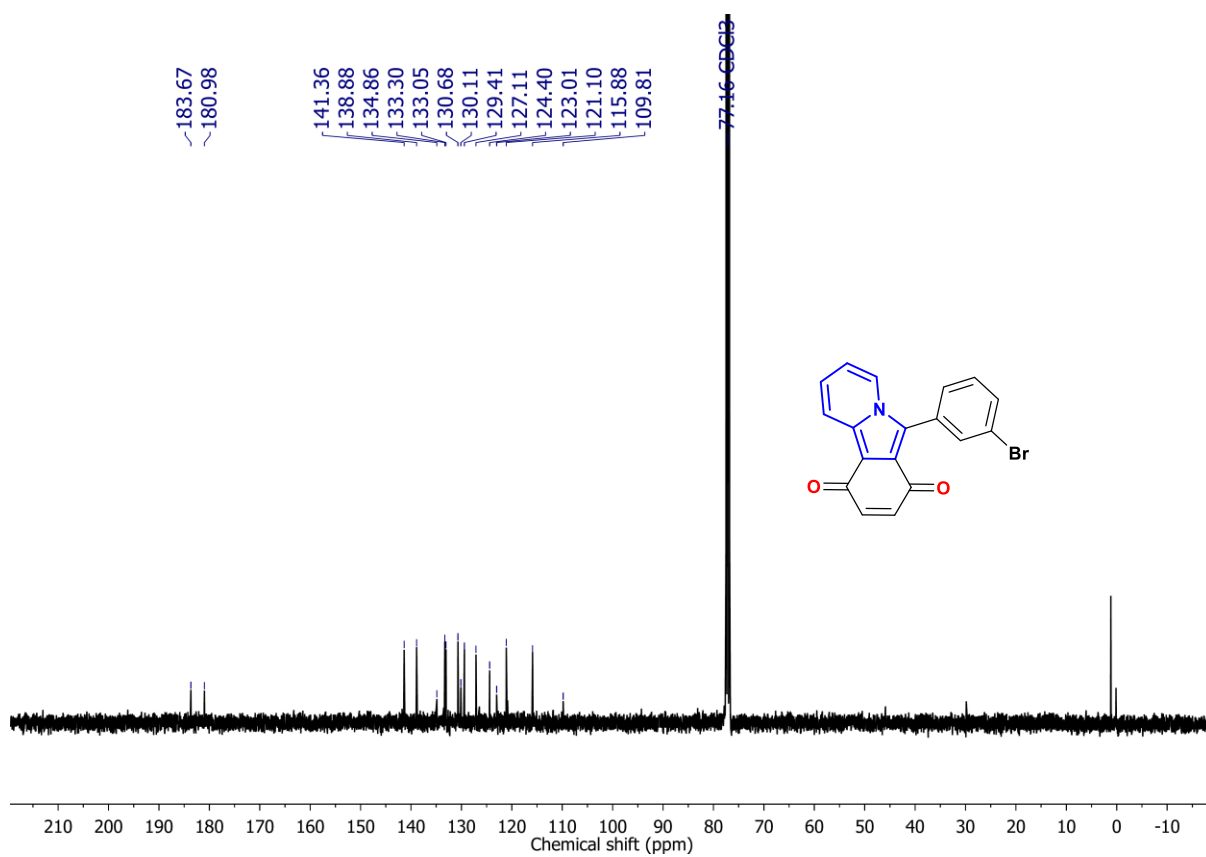




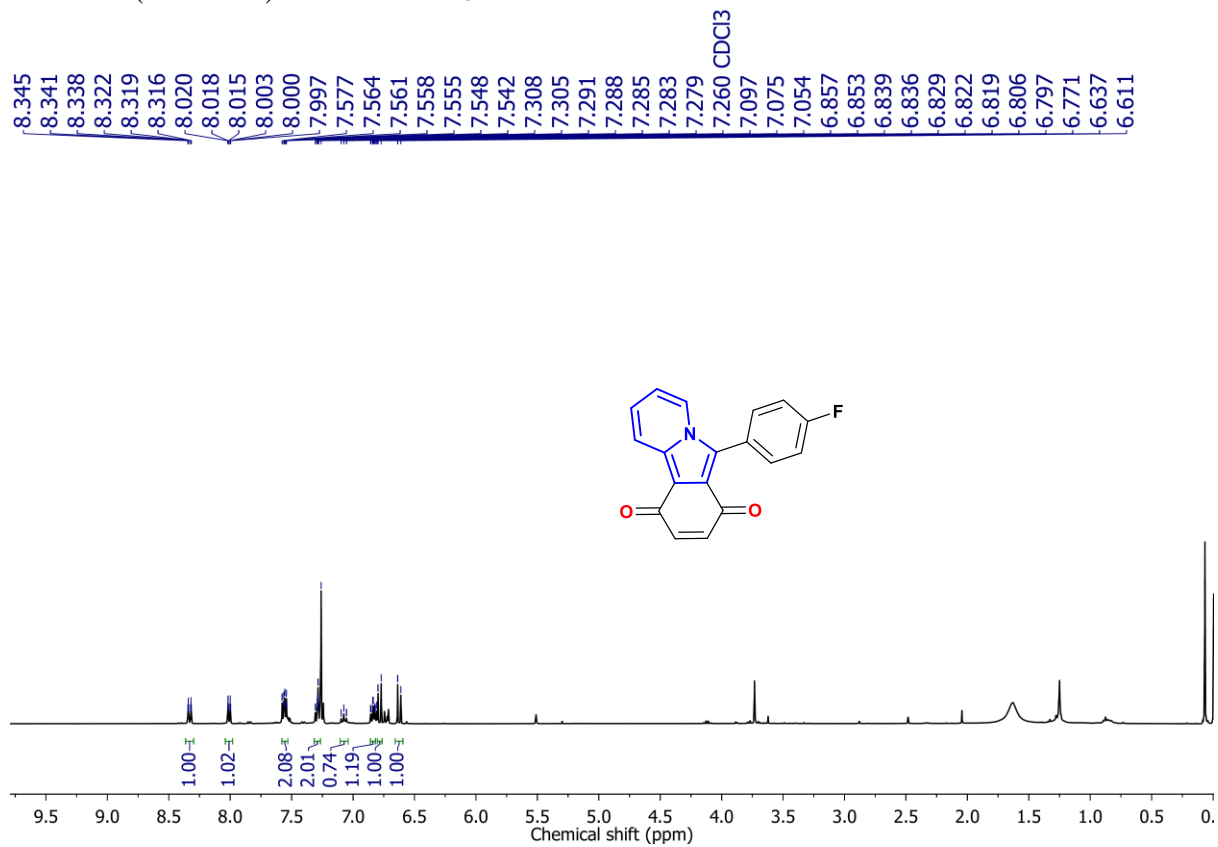
$^1\text{H}$  NMR (400 MHz) of **4d** in  $\text{CDCl}_3$



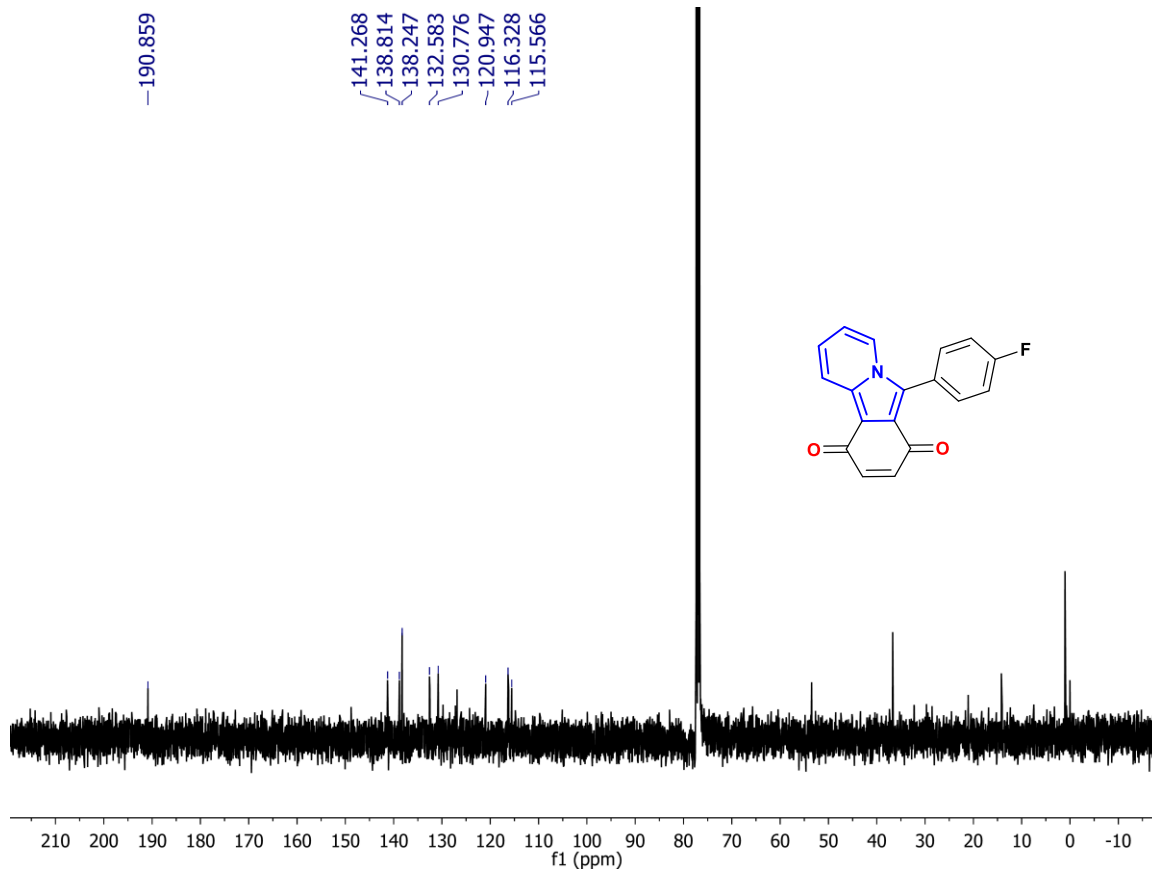
$^{13}\text{C}$  NMR (400 MHz) of **4d** in  $\text{CDCl}_3$



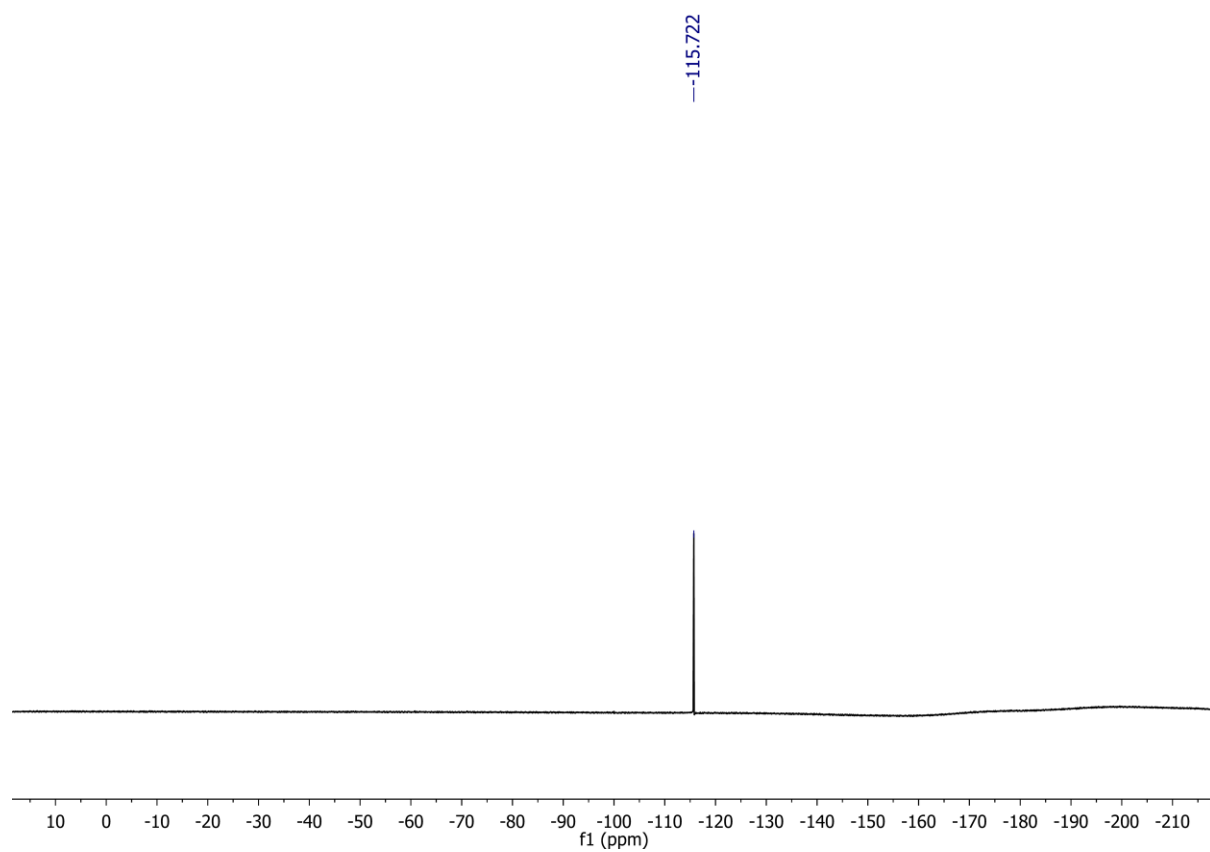
$^1\text{H}$  NMR (400 MHz) of **4e** in  $\text{CDCl}_3$



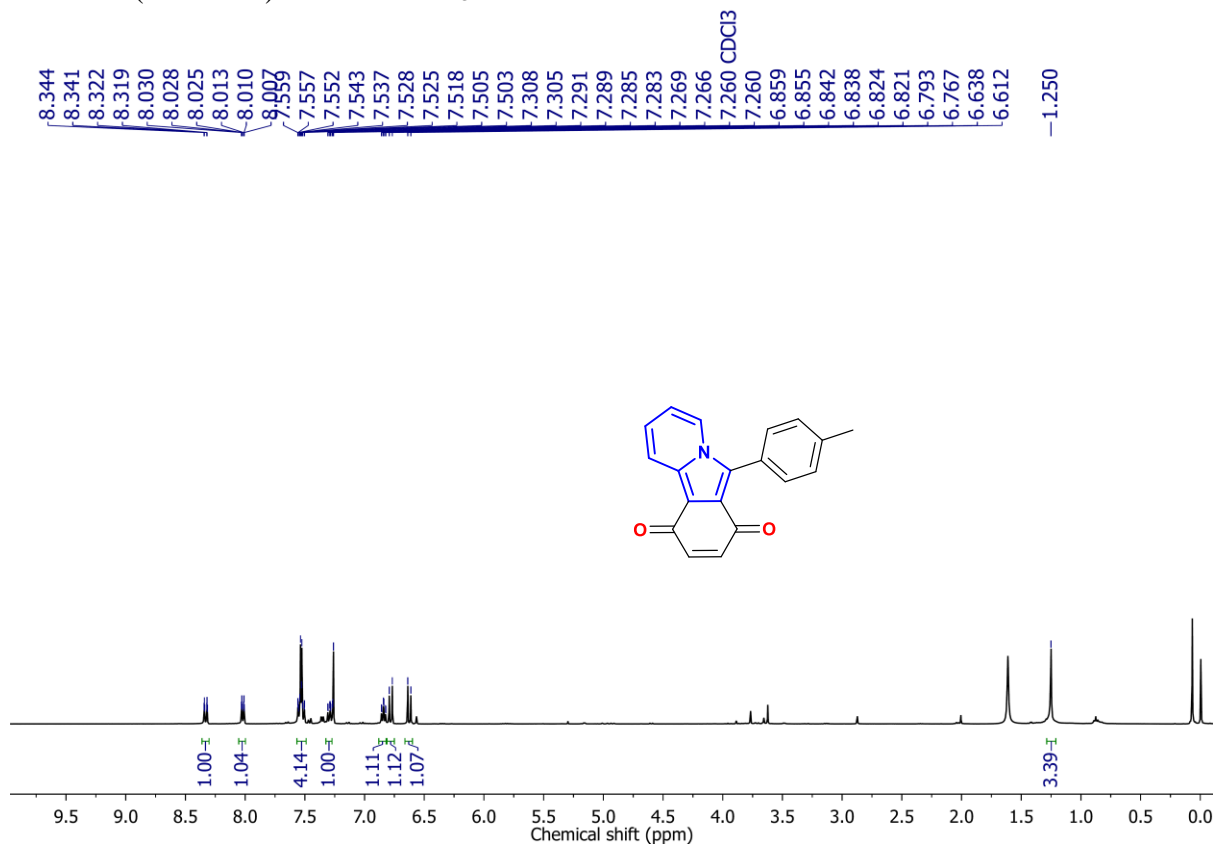
$^{13}\text{C}$  NMR (400 MHz) of **4e** in  $\text{CDCl}_3$



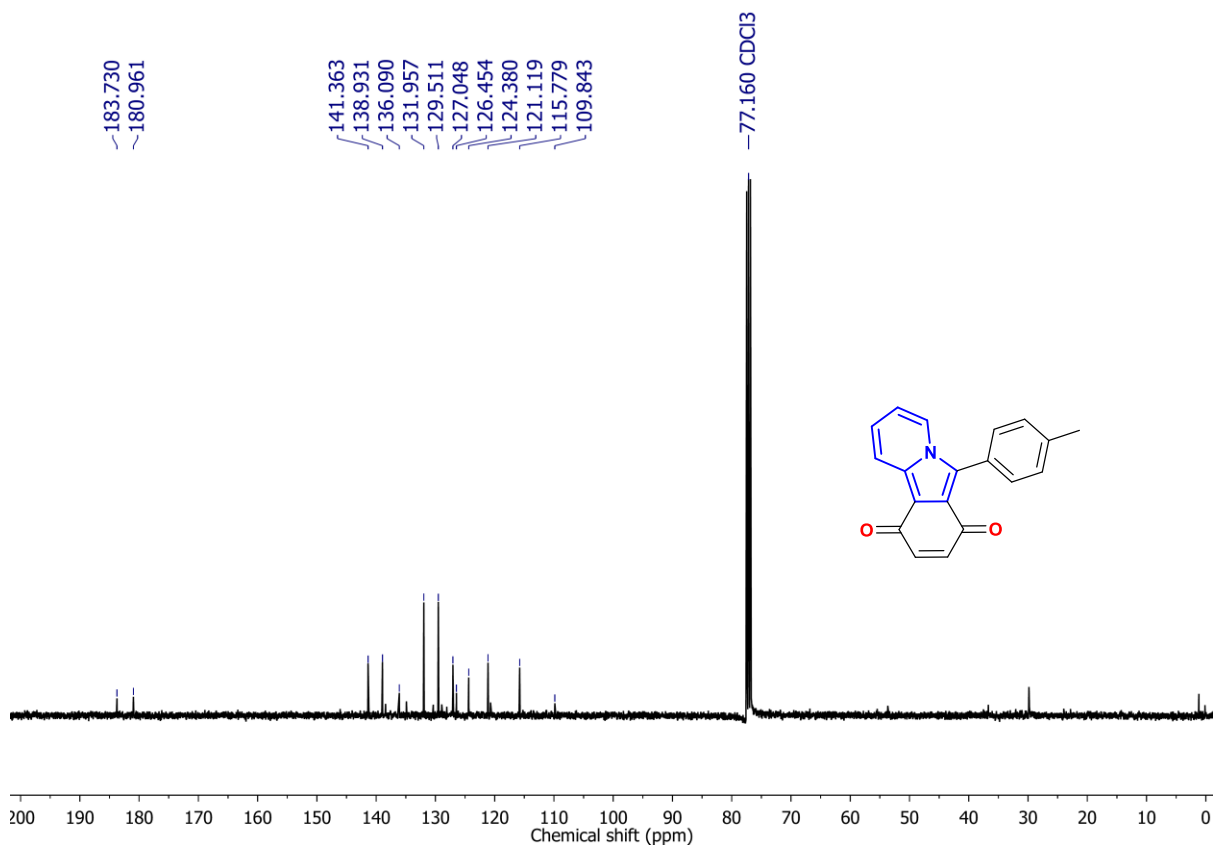
$^{19}\text{F}$  NMR (400 MHz) of **4e** in  $\text{CDCl}_3$



$^1\text{H}$  NMR (400 MHz) of **4f** in  $\text{CDCl}_3$

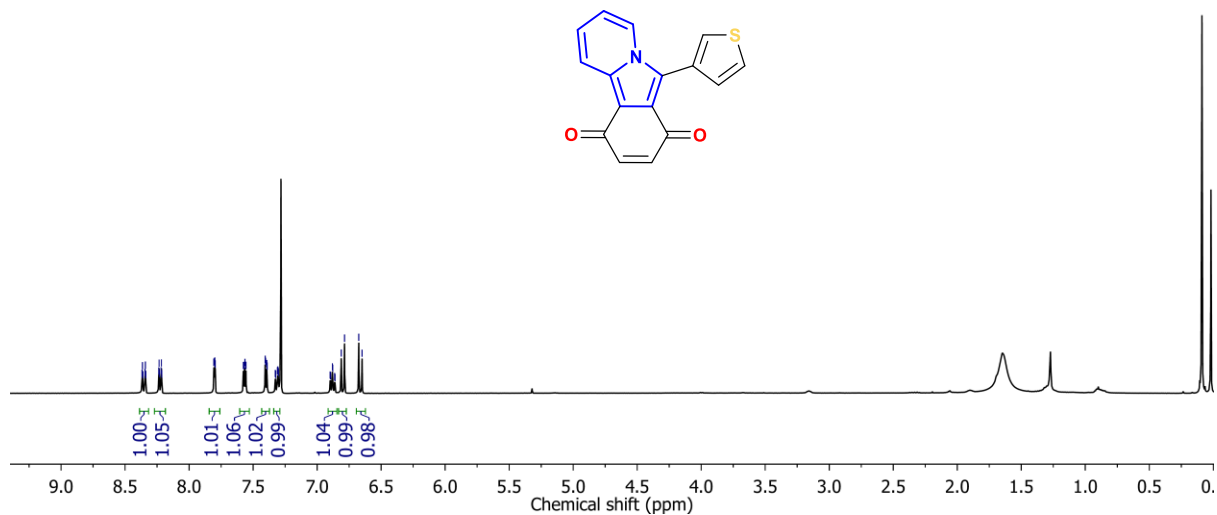


$^{13}\text{C}$  NMR (400 MHz) of **4f** in  $\text{CDCl}_3$

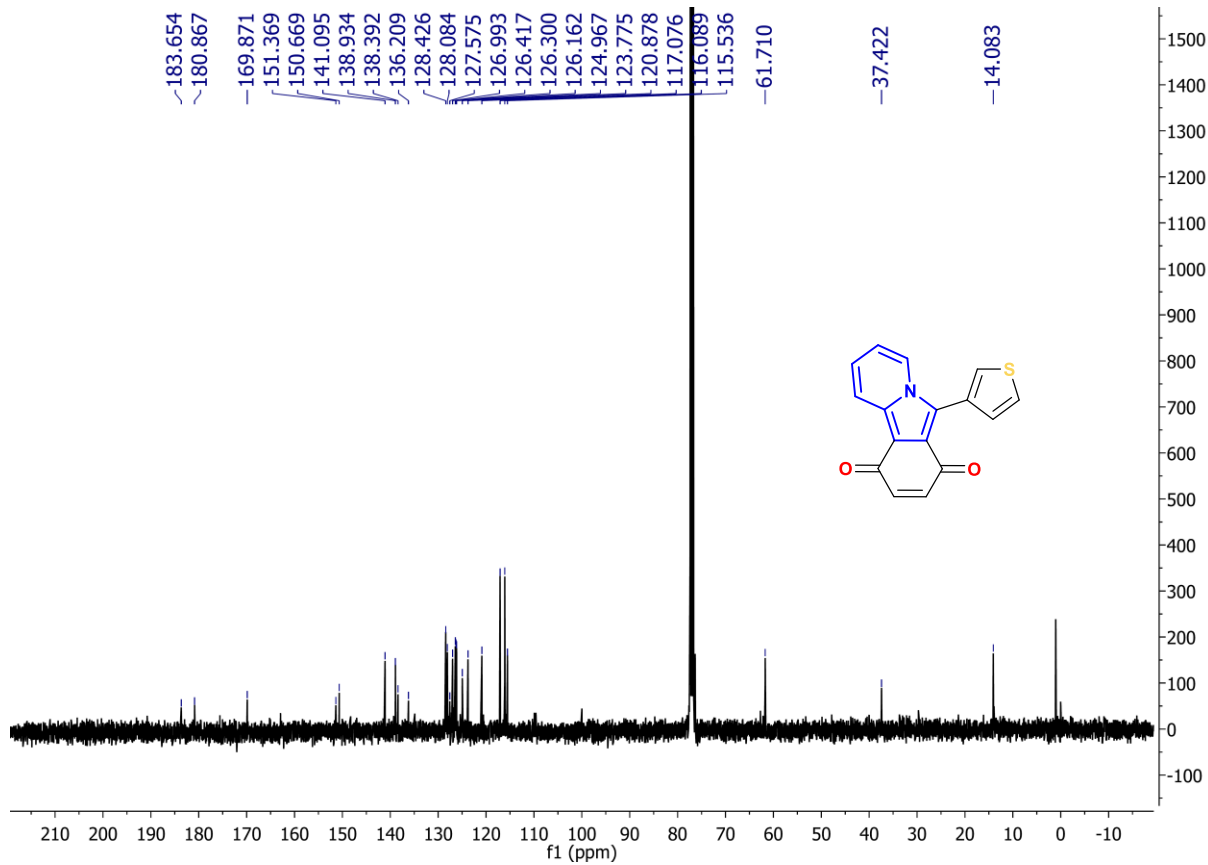


$^1\text{H}$  NMR (400 MHz) of **4g** in  $\text{CDCl}_3$

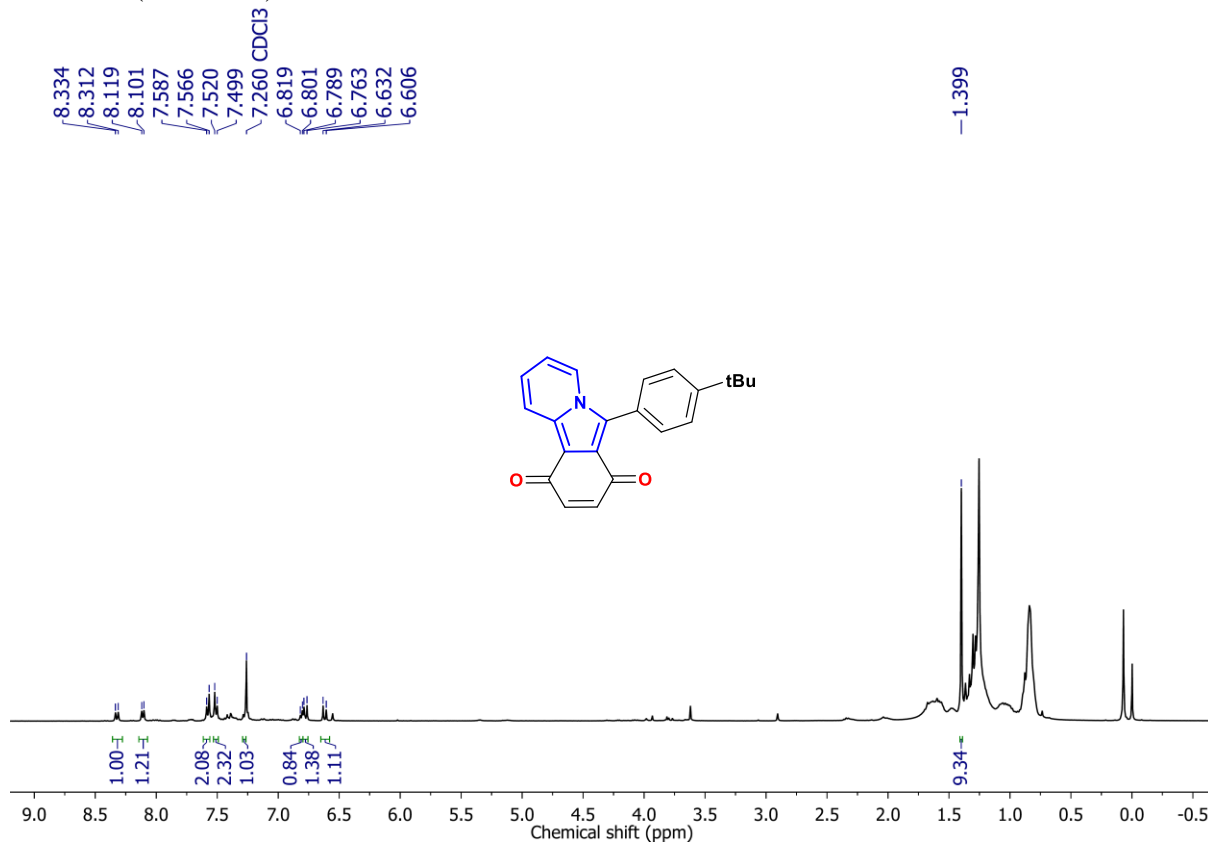
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6.649



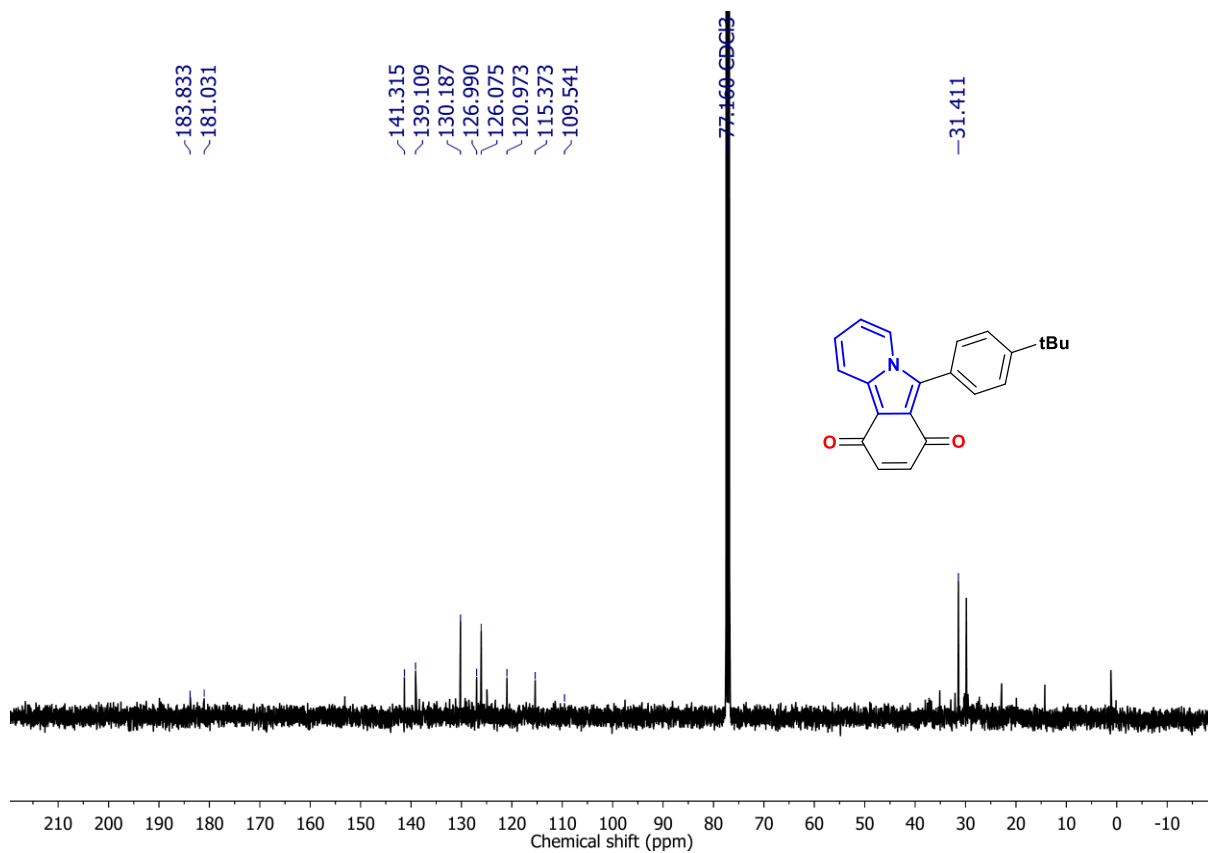
$^{13}\text{C}$  NMR (400 MHz) of **4g** in  $\text{CDCl}_3$



$^1\text{H}$  NMR (400 MHz) of **4h** in  $\text{CDCl}_3$

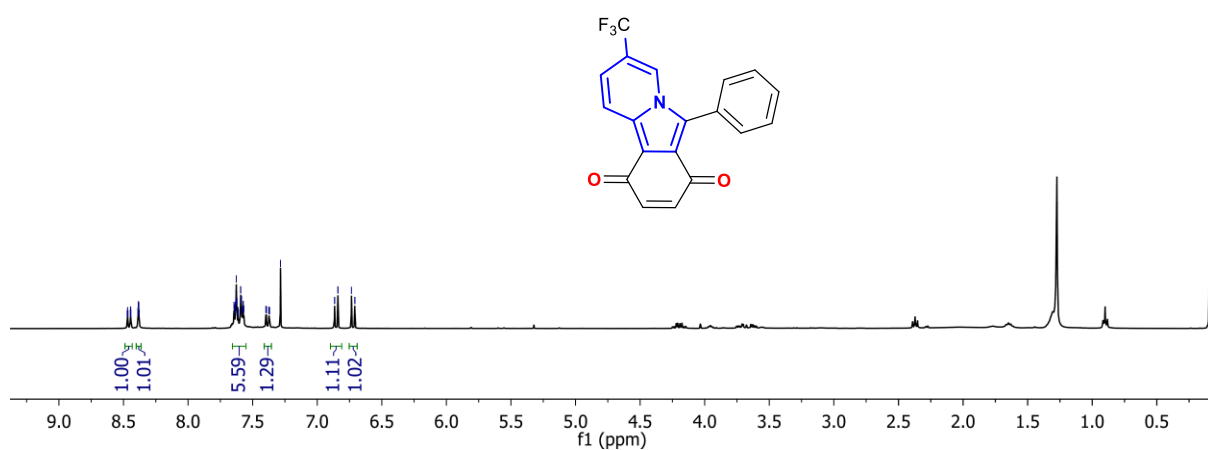


$^{13}\text{C}$  NMR (400 MHz) of **4h** in  $\text{CDCl}_3$

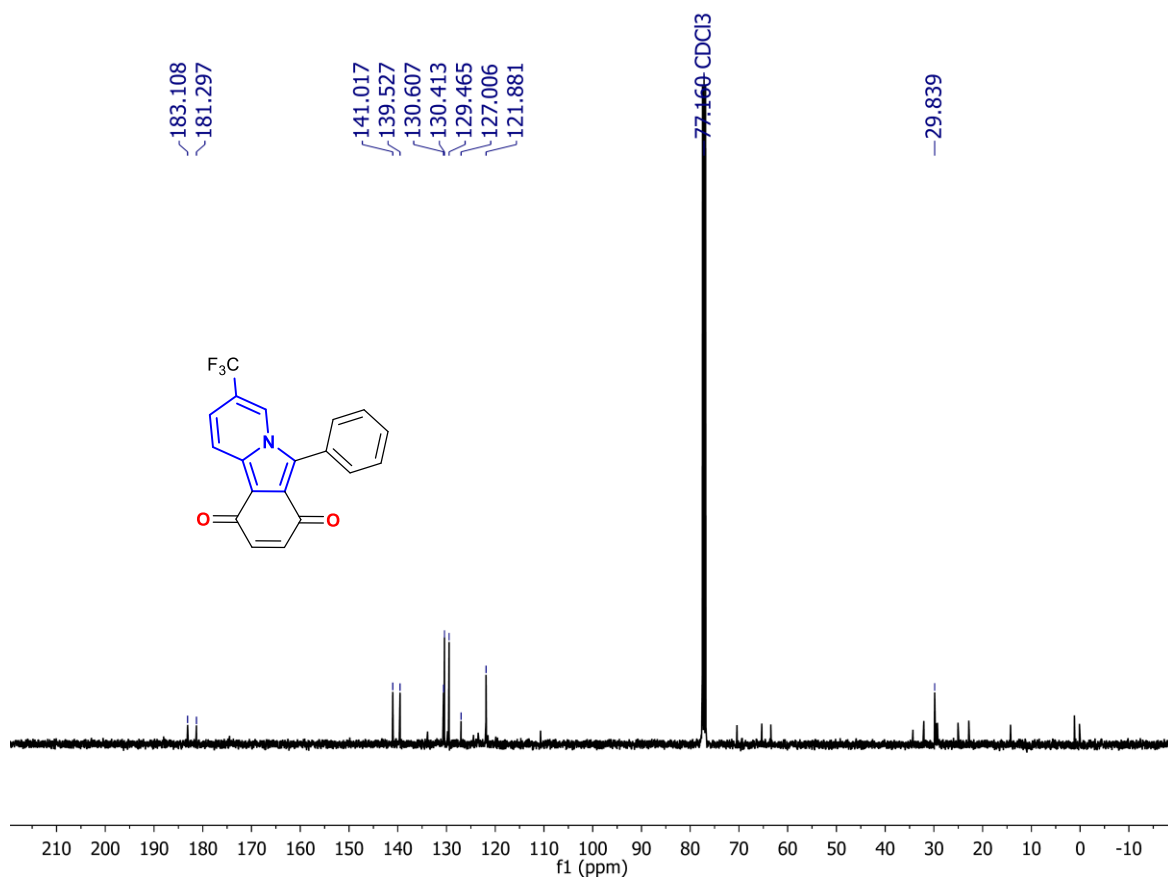


<sup>1</sup>H NMR (400 MHz) of **4i** in CDCl<sub>3</sub>

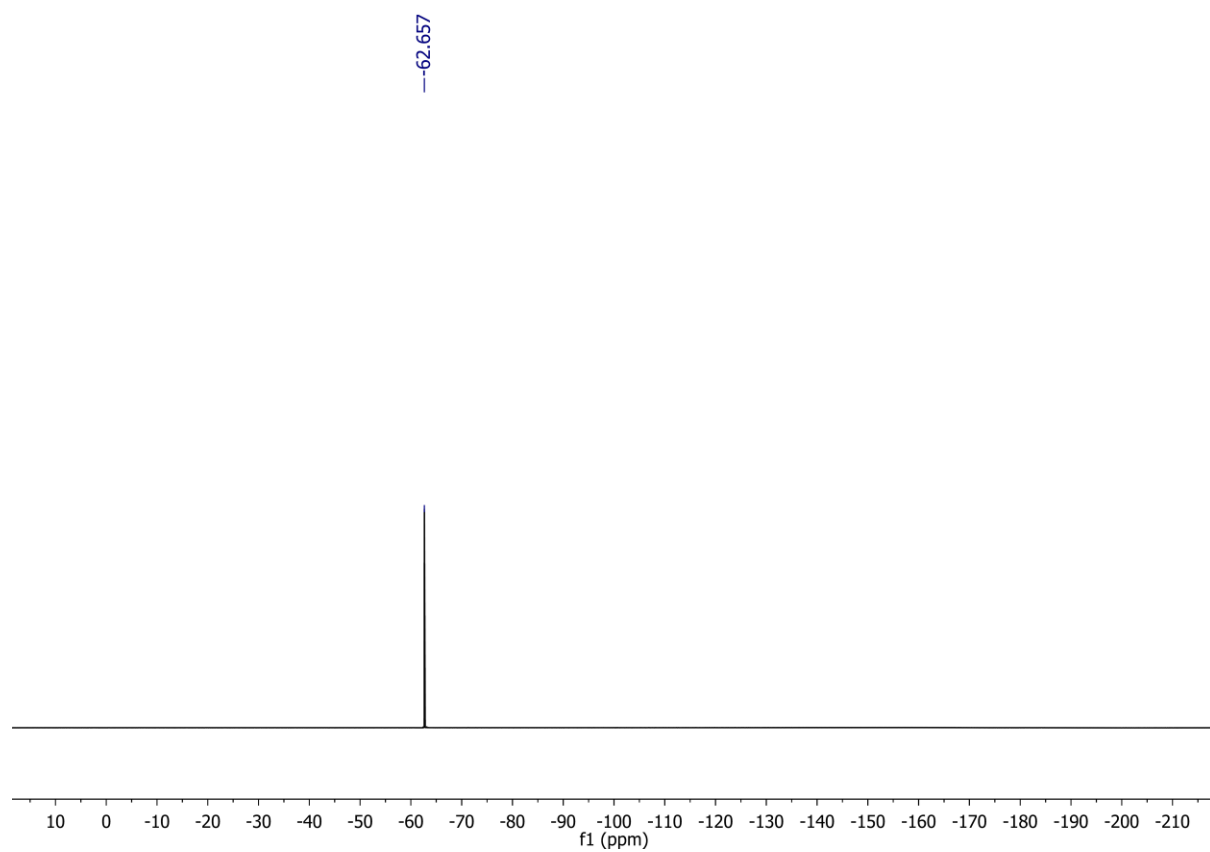
8.470  
8.468  
8.466  
8.447  
8.445  
8.442  
8.388  
8.385  
8.381  
8.378  
7.645  
7.642  
7.639  
7.634  
7.631  
7.626  
7.622  
7.614  
7.611  
7.592  
7.586  
7.580  
7.577  
7.573  
7.568  
7.397  
7.393  
7.374  
7.370  
7.284  
6.865  
6.840  
6.735  
6.709



<sup>13</sup>C NMR (400 MHz) of **4i** in CDCl<sub>3</sub>

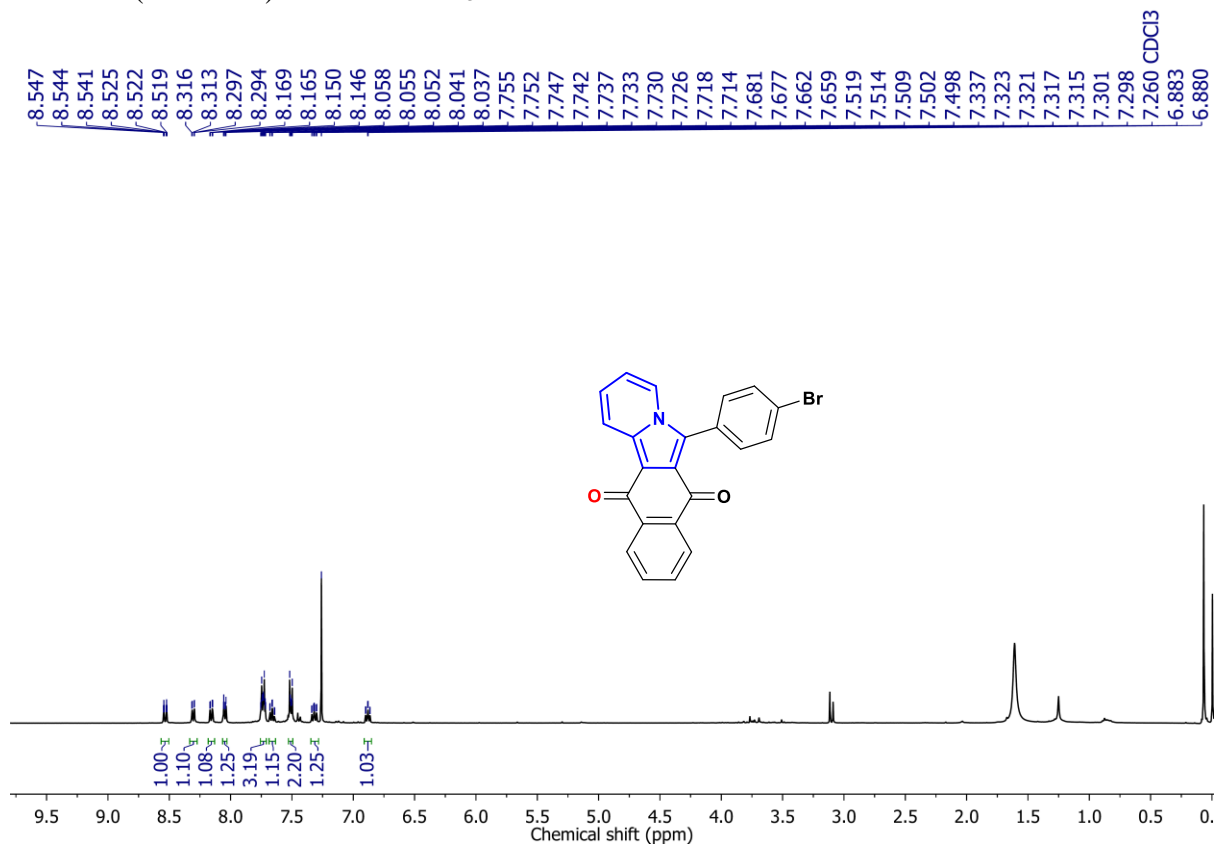


$^{19}\text{F}$  NMR (400 MHz) of **4i** in  $\text{CDCl}_3$

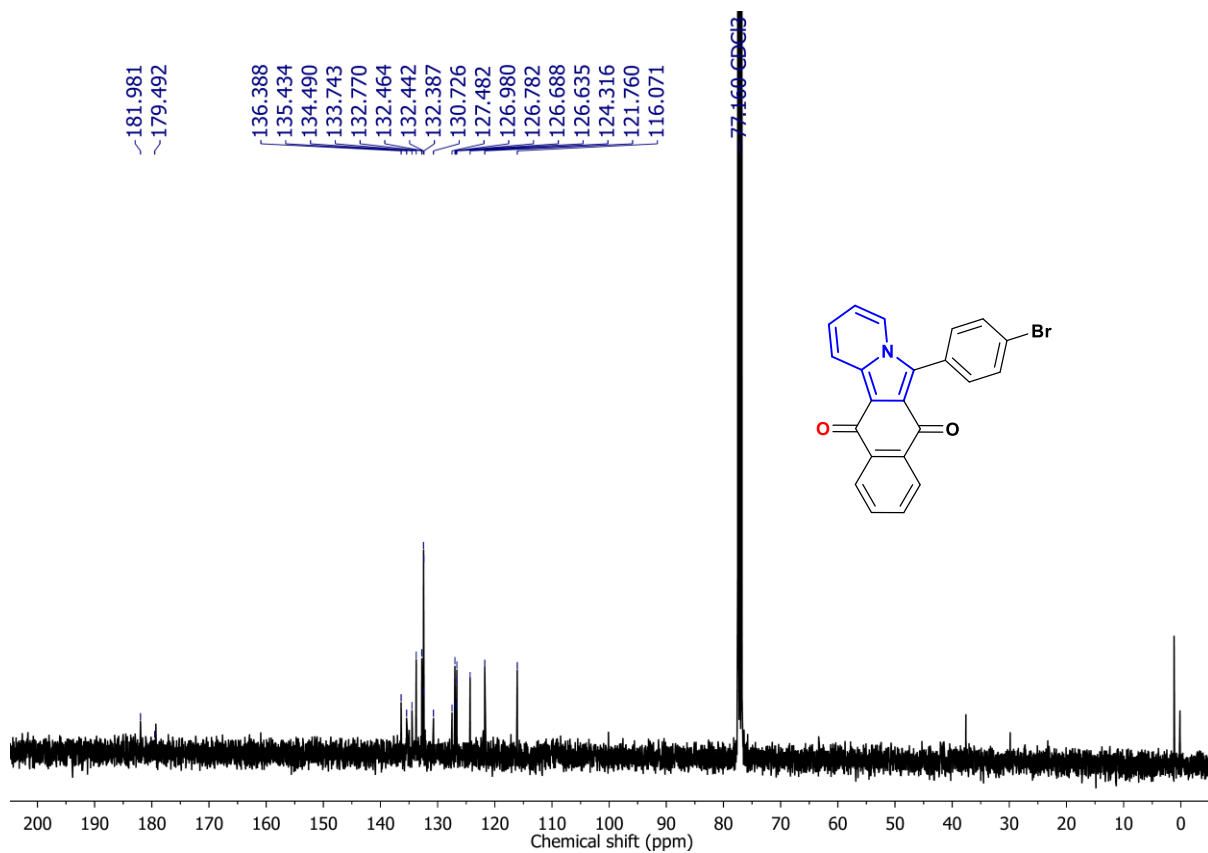




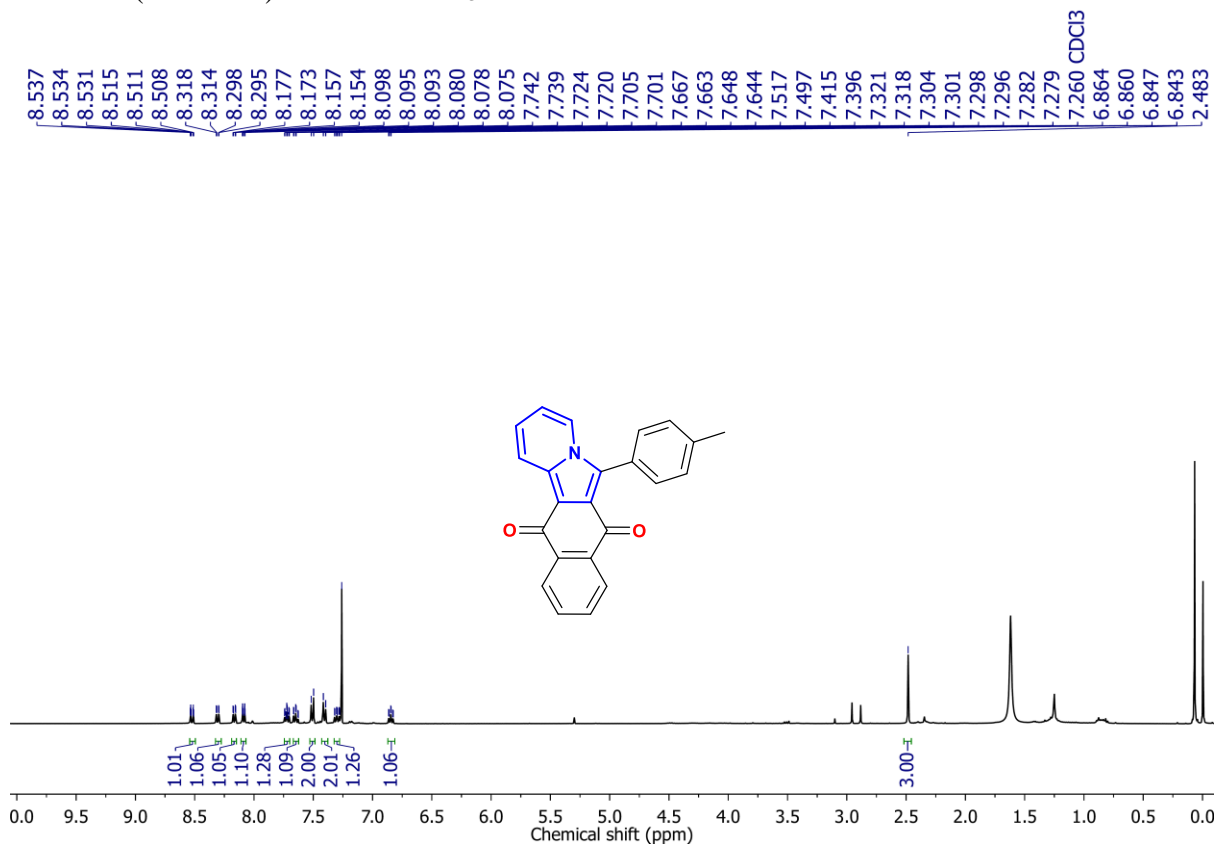
$^1\text{H}$  NMR (400 MHz) of **5a** in  $\text{CDCl}_3$



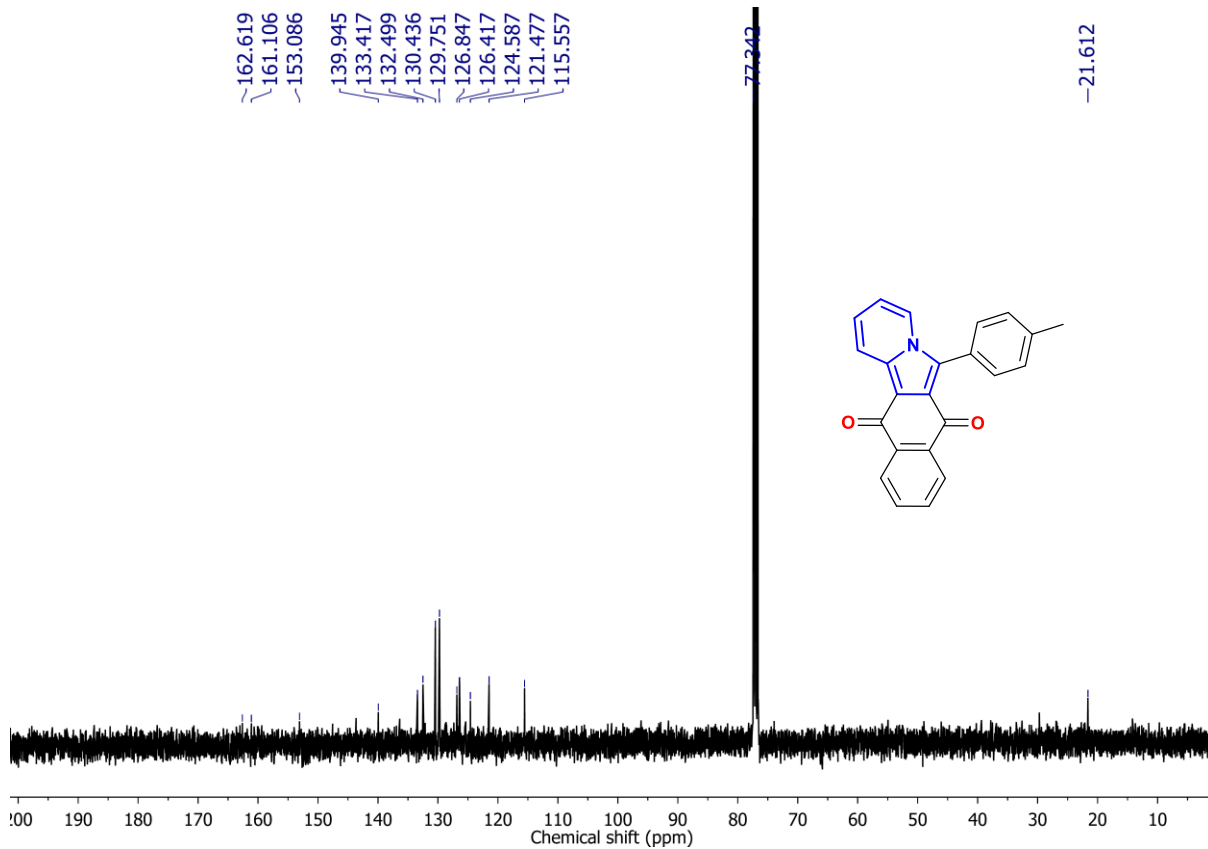
$^{13}\text{C}$  NMR (400 MHz) of **5a** in  $\text{CDCl}_3$



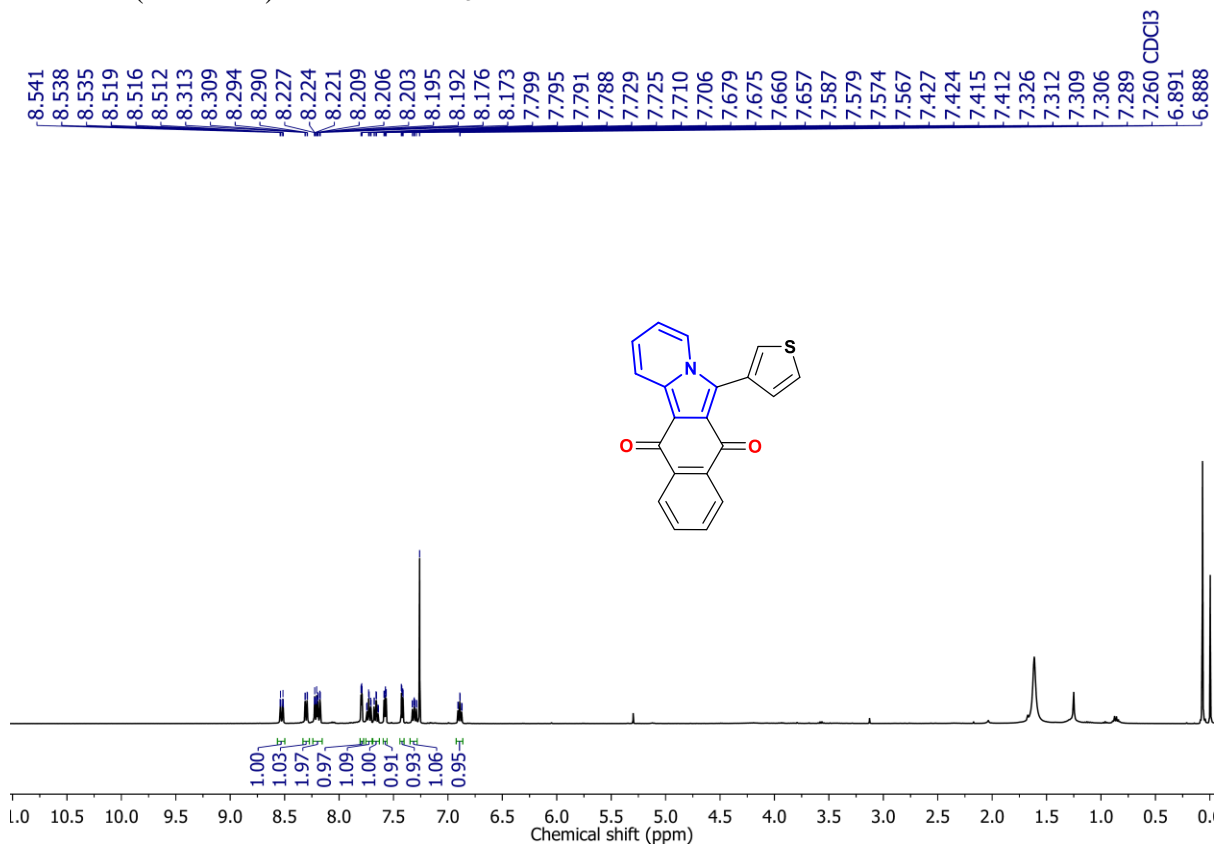
$^1\text{H}$  NMR (400 MHz) of **5b** in  $\text{CDCl}_3$



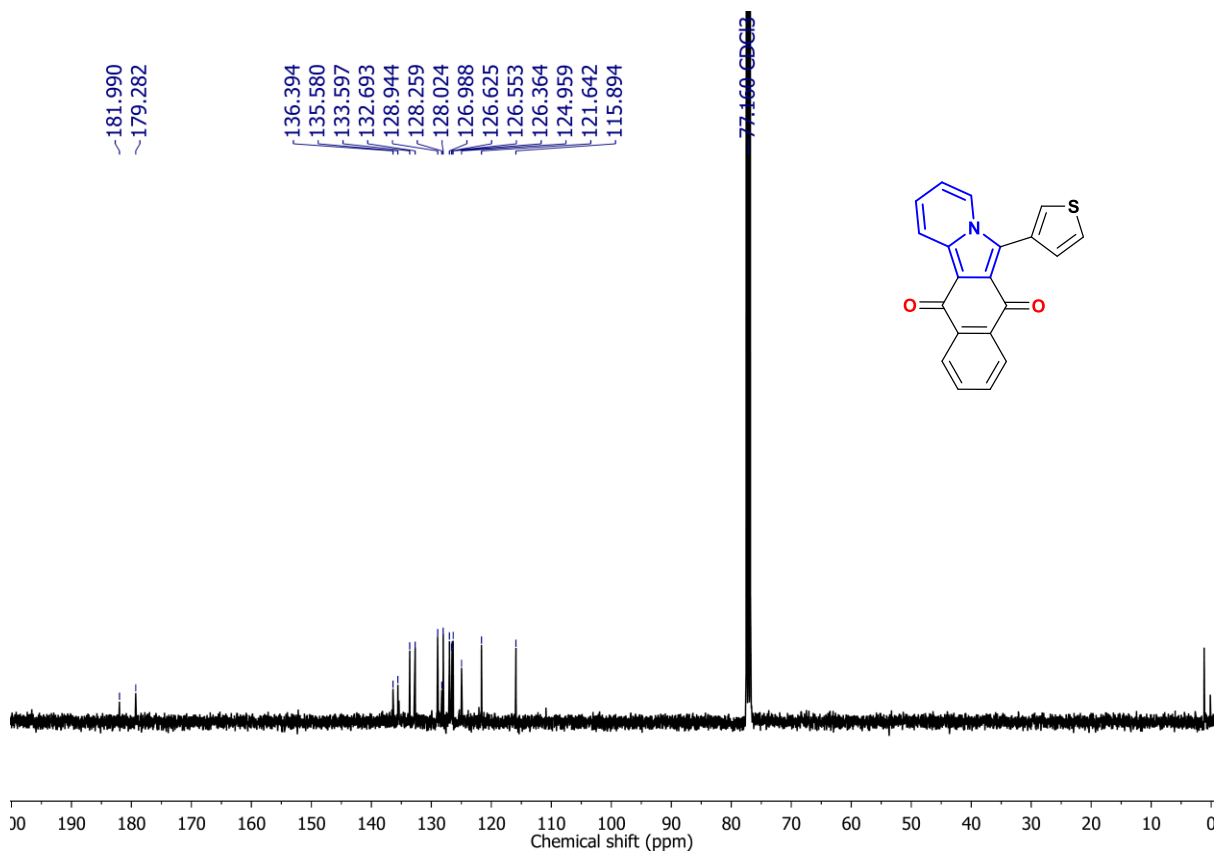
$^{13}\text{C}$  NMR (400 MHz) of **5b** in  $\text{CDCl}_3$



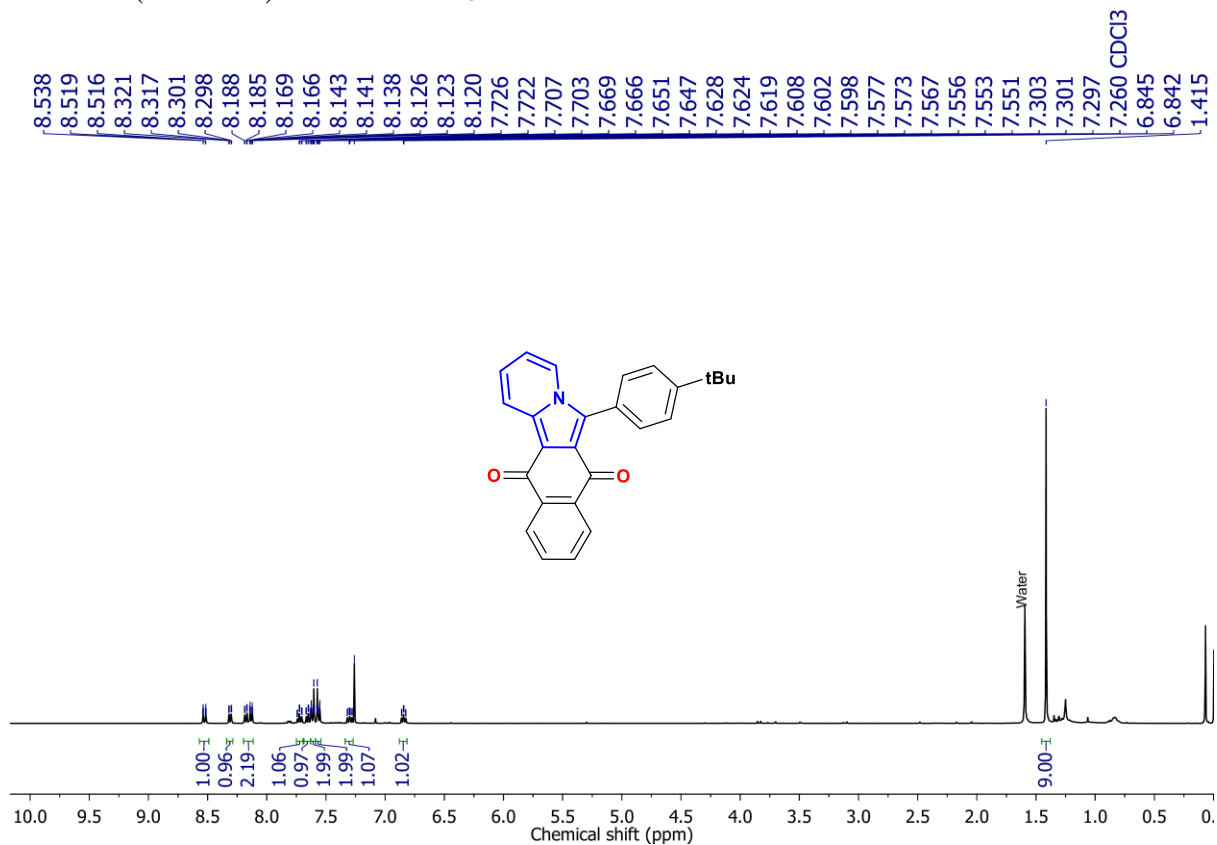
<sup>1</sup>H NMR (400 MHz) of **5c** in CDCl<sub>3</sub>



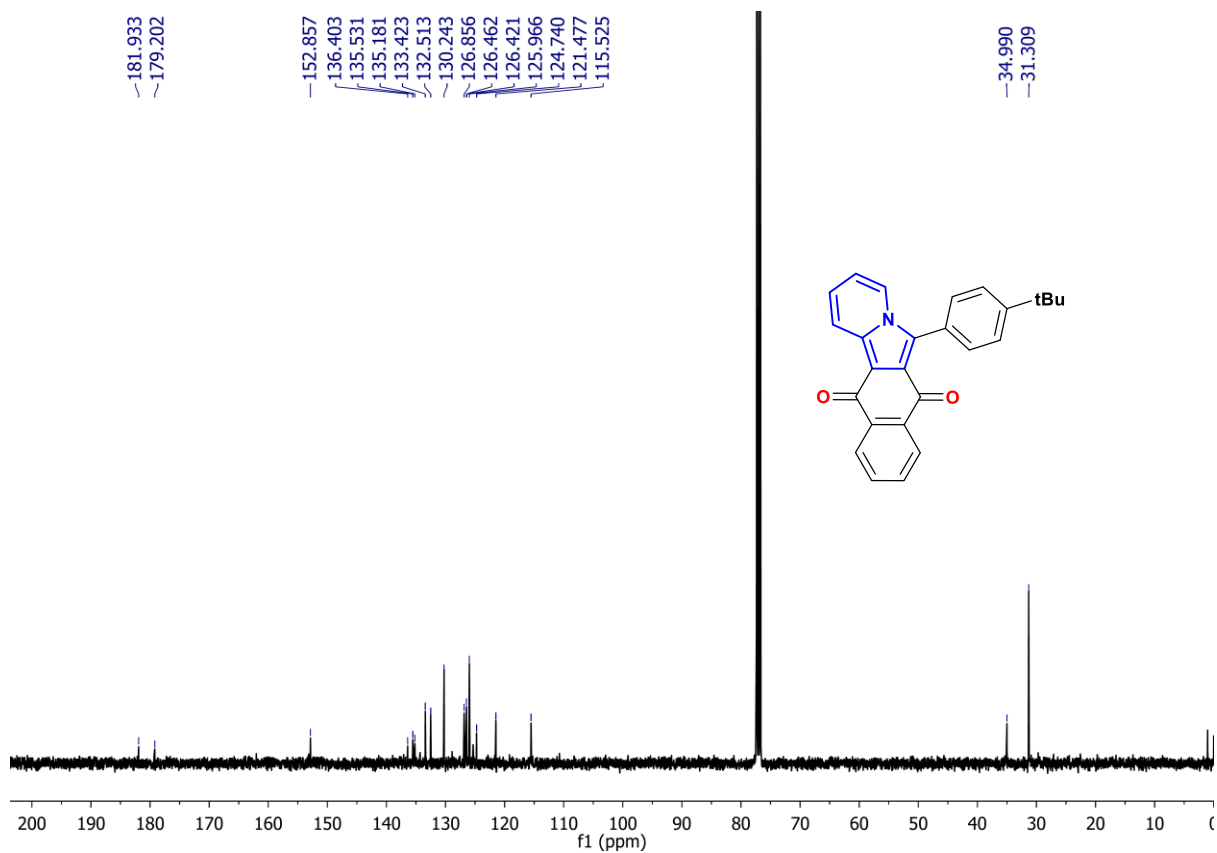
<sup>13</sup>C NMR (400 MHz) of **5c** in CDCl<sub>3</sub>



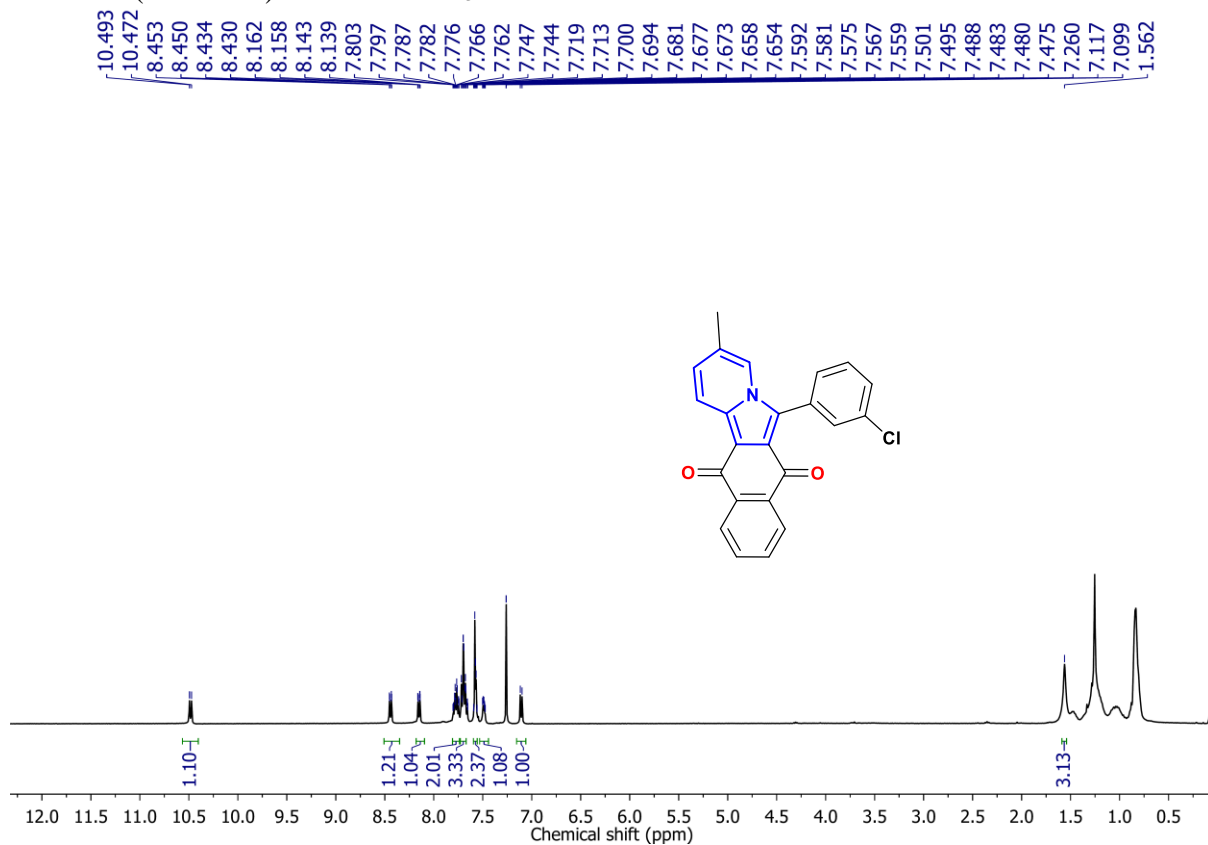
$^1\text{H}$  NMR (400 MHz) of **5d** in  $\text{CDCl}_3$



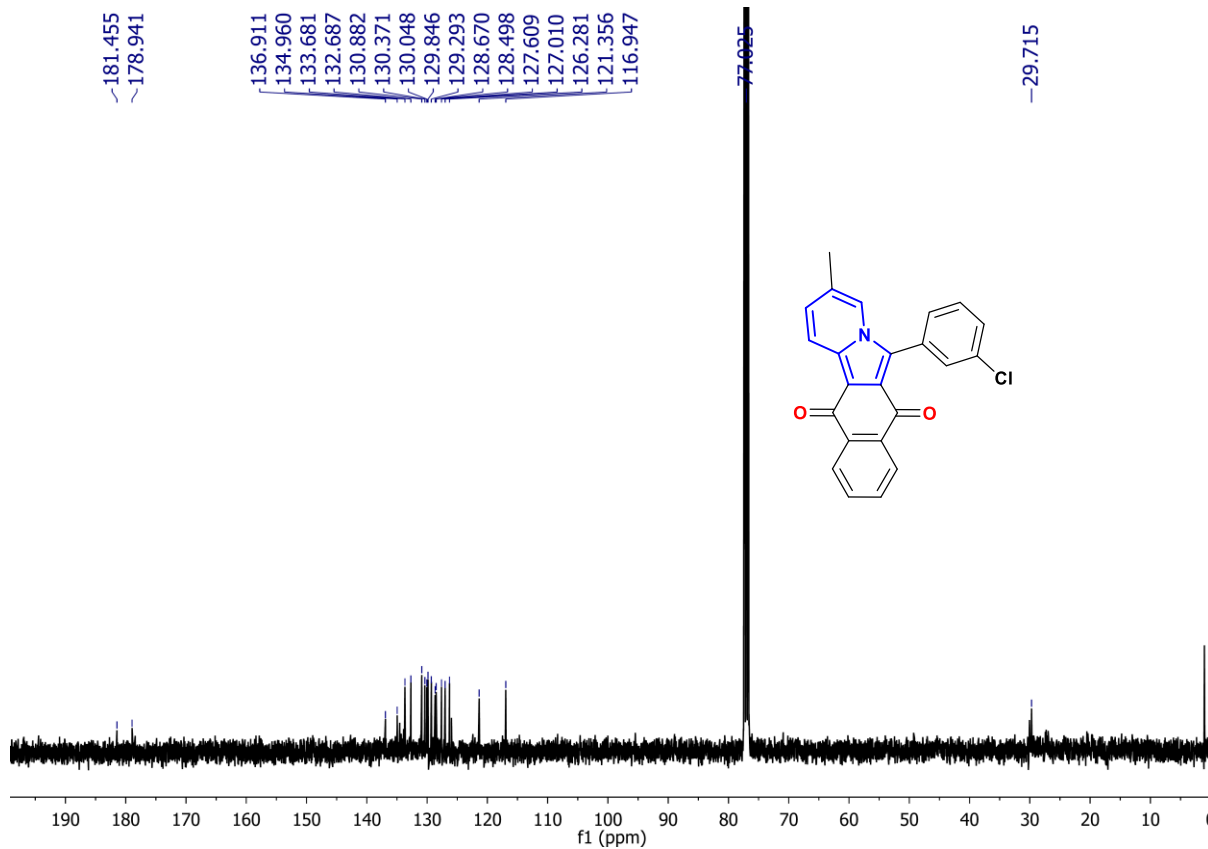
$^{13}\text{C}$  NMR (400 MHz) of **5d** in  $\text{CDCl}_3$



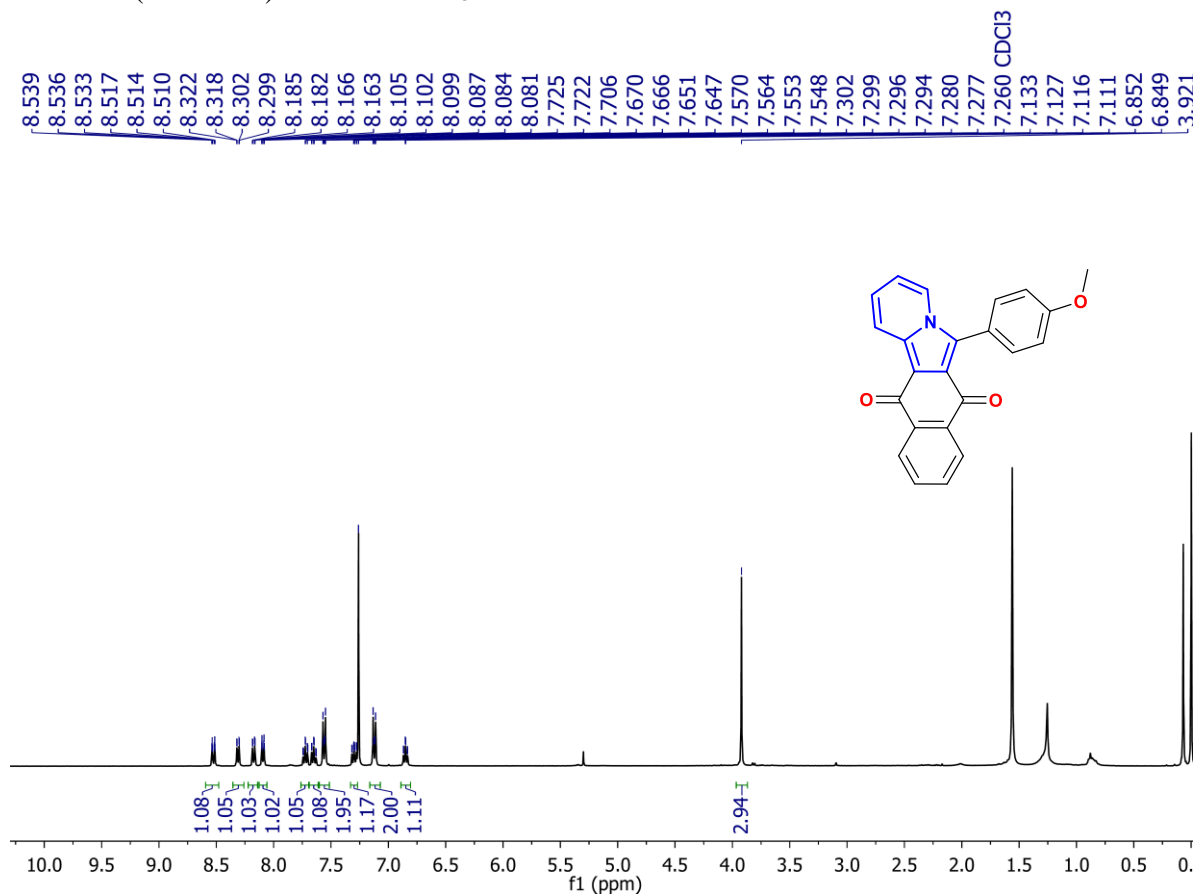
<sup>1</sup>H NMR (400 MHz) of **5e** in CDCl<sub>3</sub>



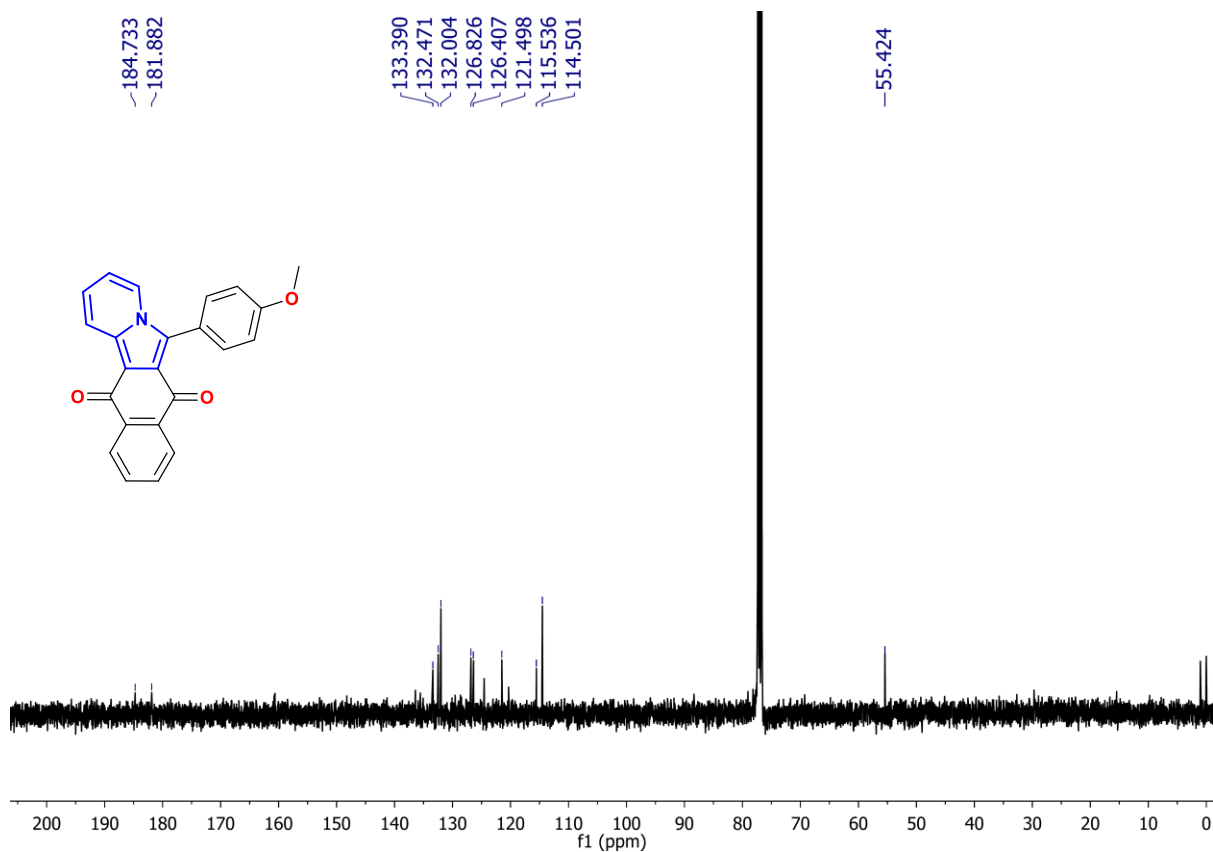
<sup>13</sup>C NMR (400 MHz) of **5e** in CDCl<sub>3</sub>



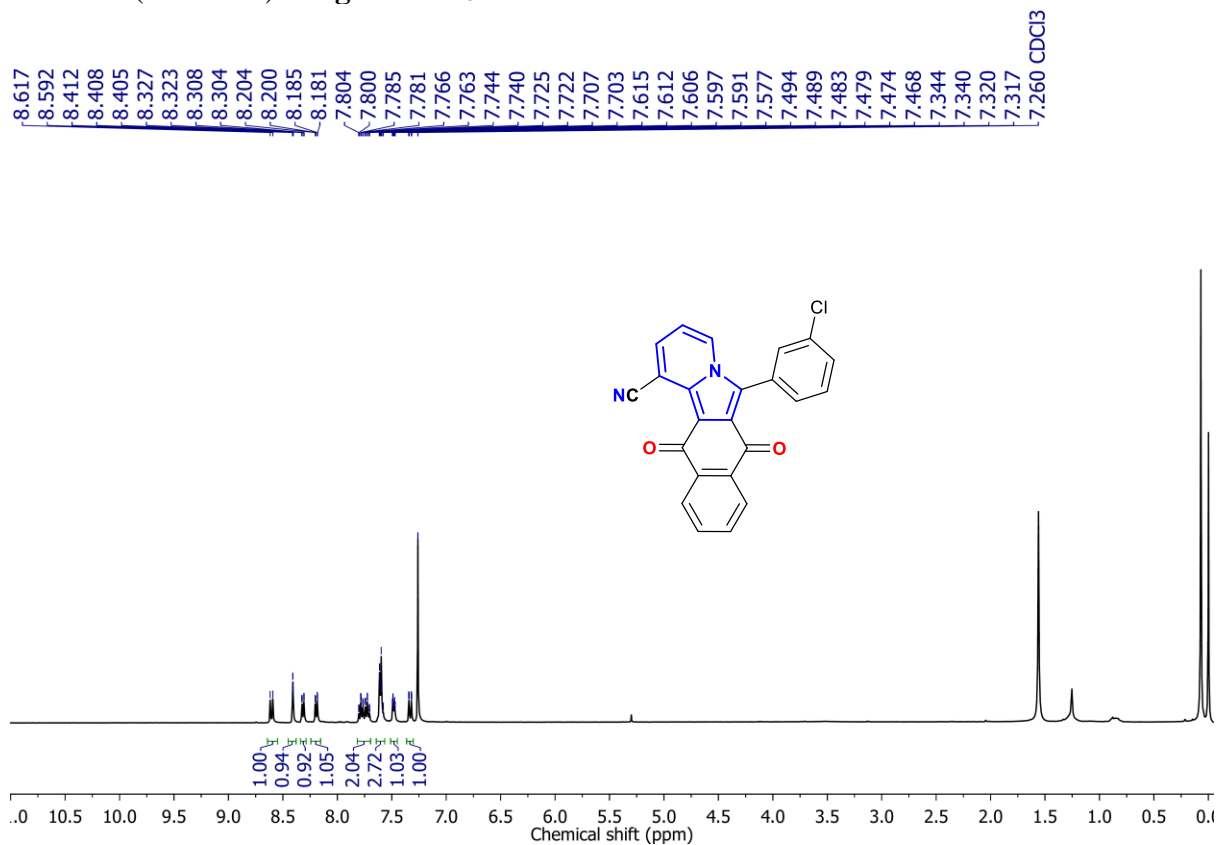
$^1\text{H}$  NMR (400 MHz) of **5f** in  $\text{CDCl}_3$



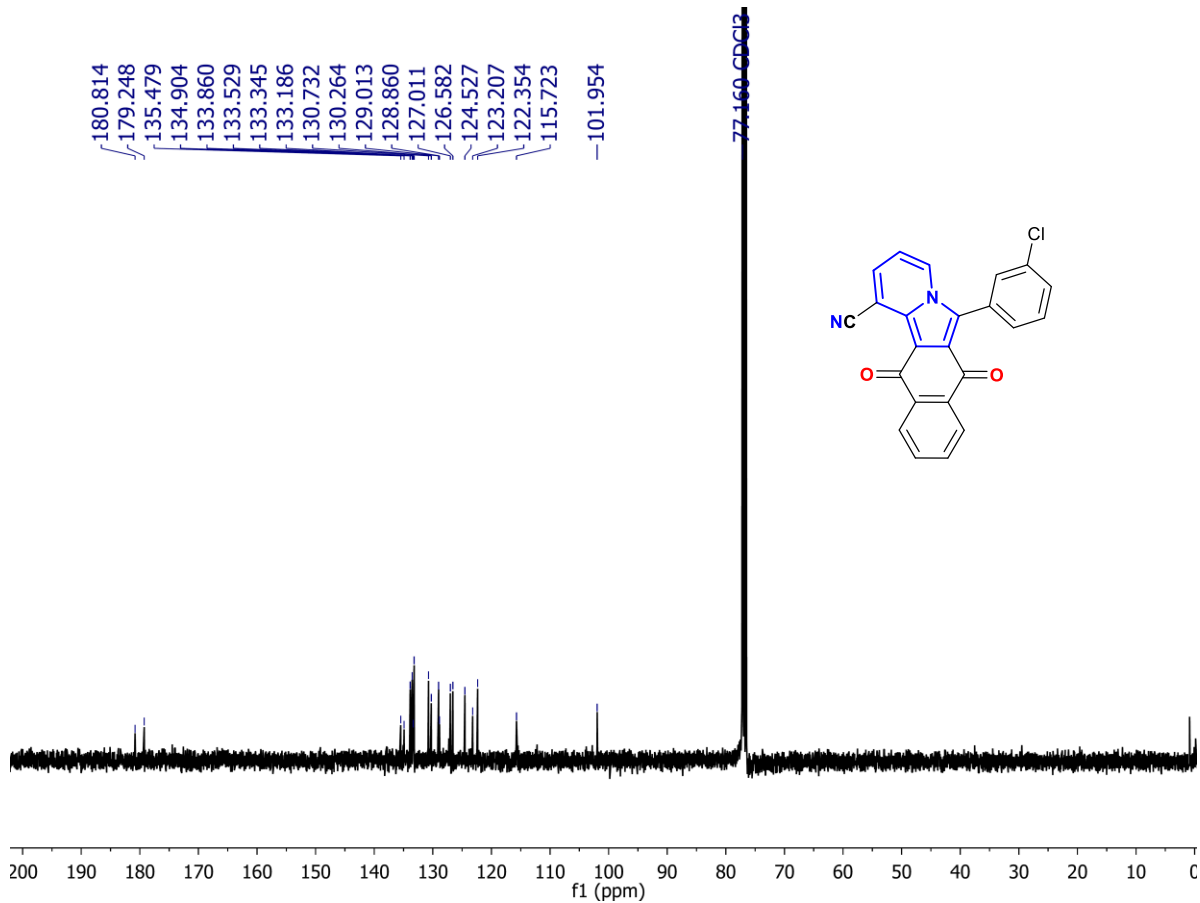
$^{13}\text{C}$  NMR (400 MHz) of **5f** in  $\text{CDCl}_3$



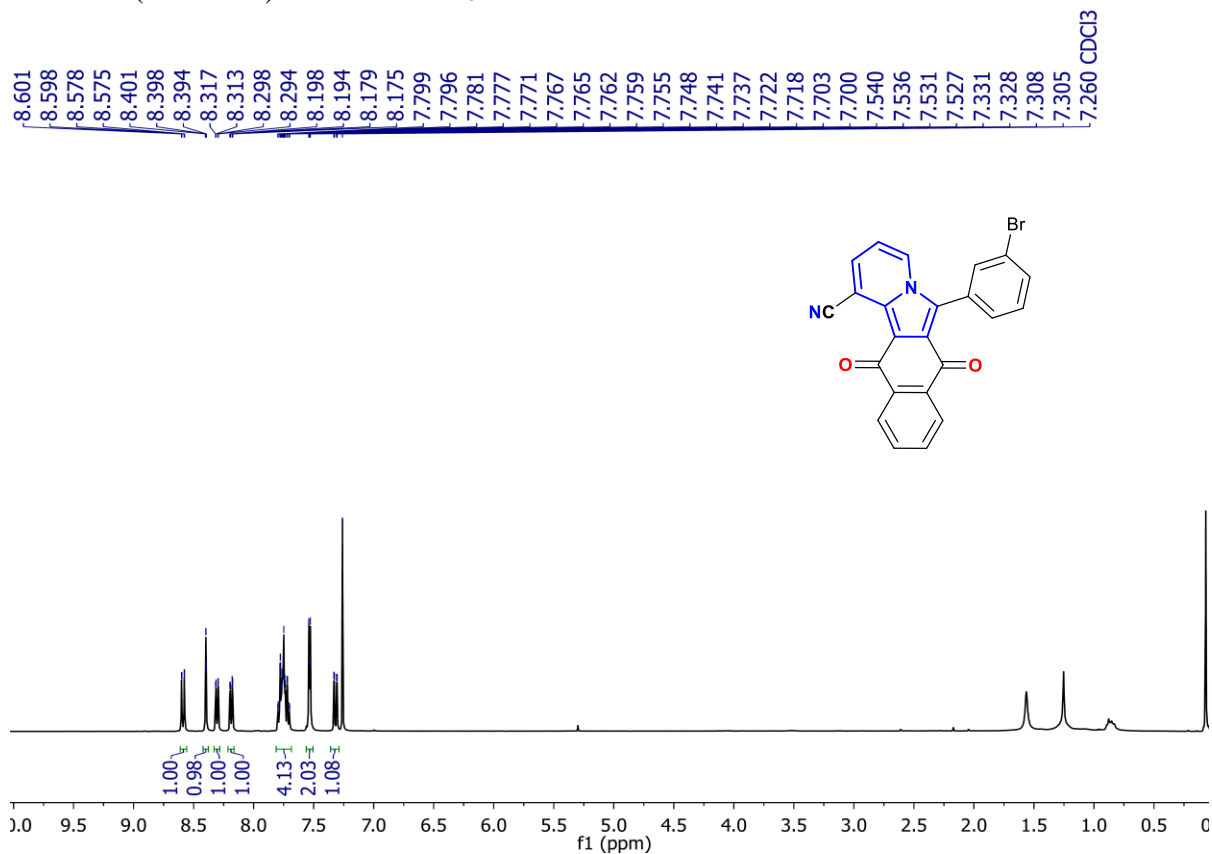
$^1\text{H}$  NMR (400 MHz) of **5g** in  $\text{CDCl}_3$



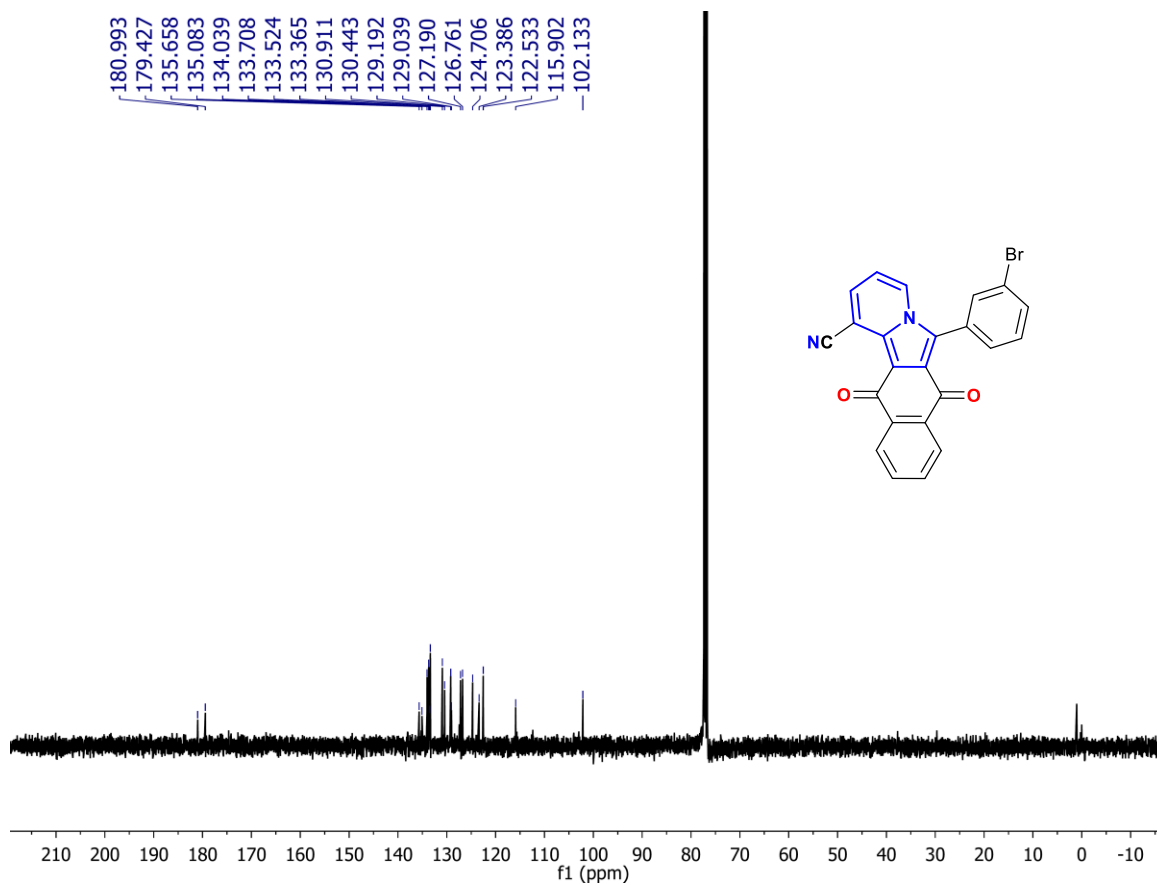
$^{13}\text{C}$  NMR (400 MHz) of **5g** in  $\text{CDCl}_3$



<sup>1</sup>H NMR (400 MHz) of **5h** in CDCl<sub>3</sub>

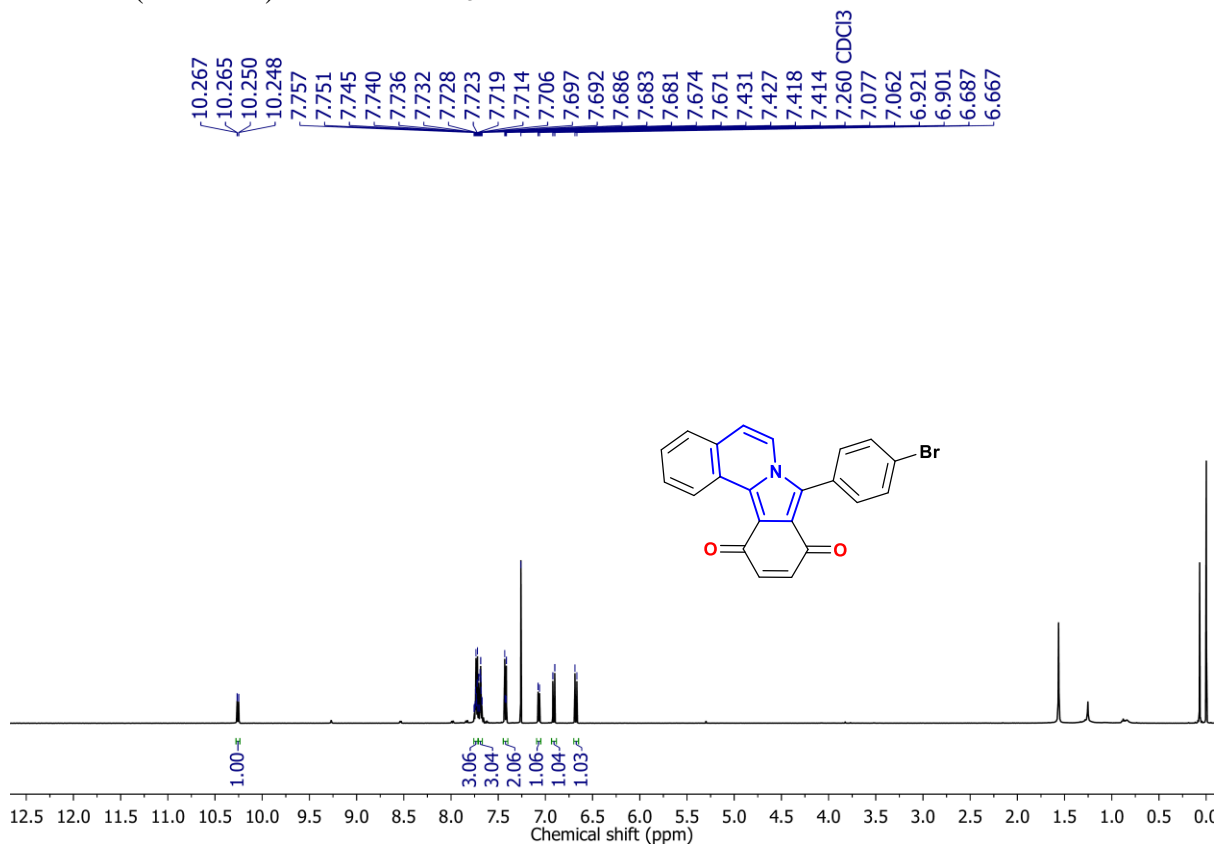


<sup>13</sup>C NMR (400 MHz) of **5h** in CDCl<sub>3</sub>

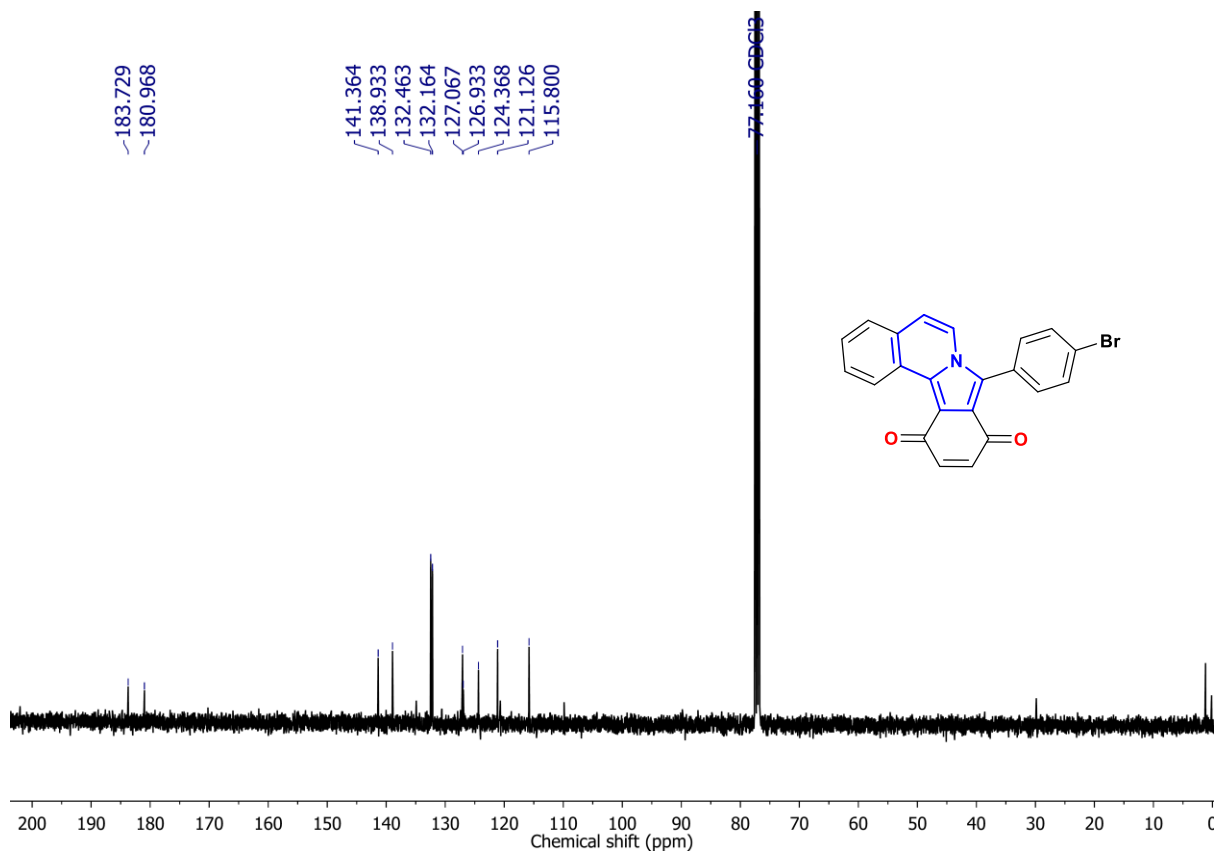




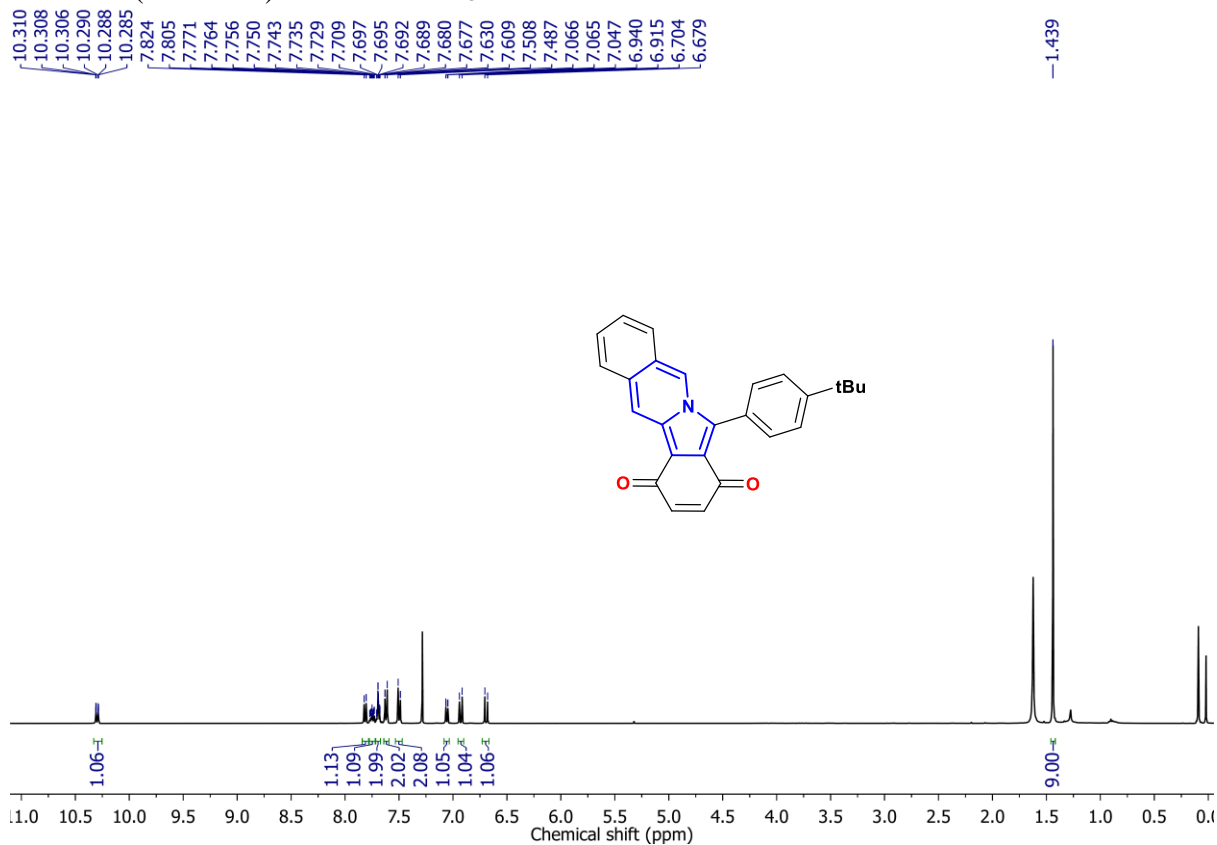
$^1\text{H}$  NMR (400 MHz) of **6a** in  $\text{CDCl}_3$



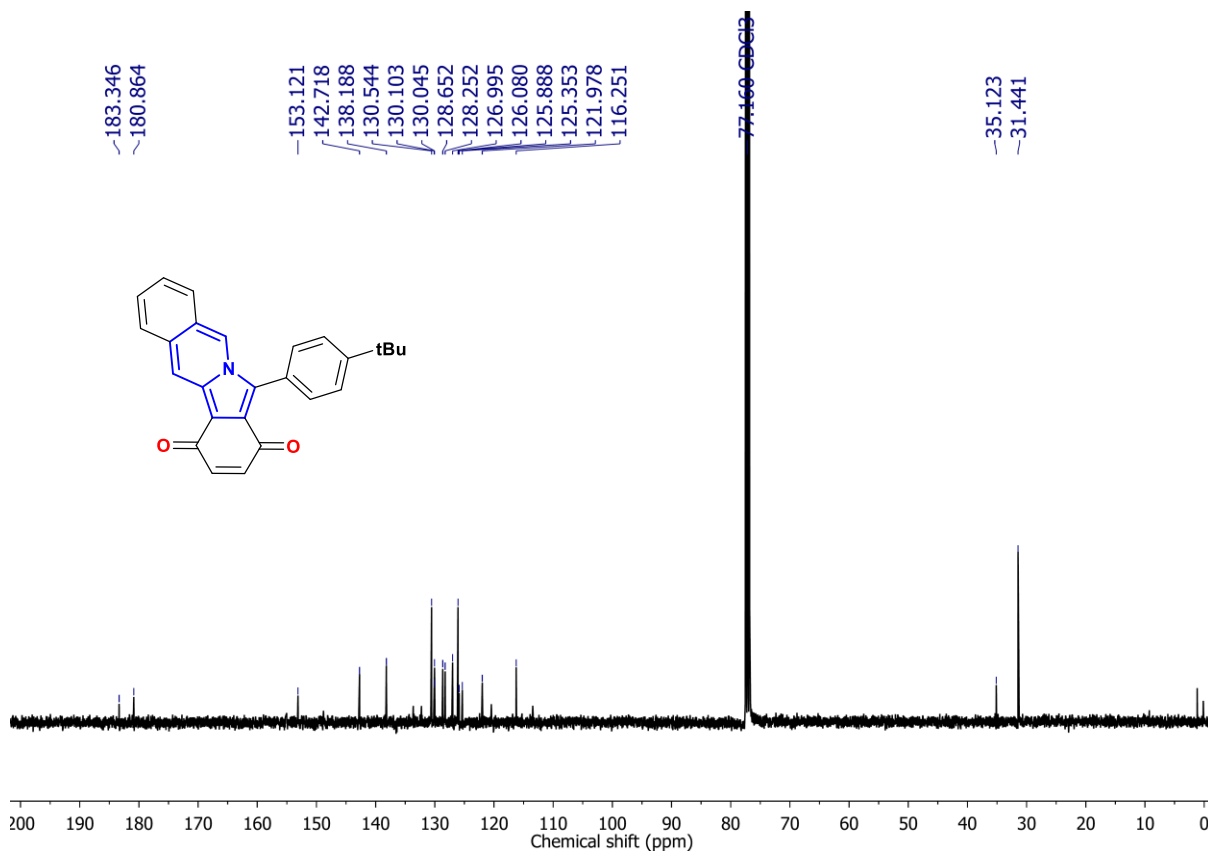
$^{13}\text{C}$  NMR (400 MHz) of **6a** in  $\text{CDCl}_3$



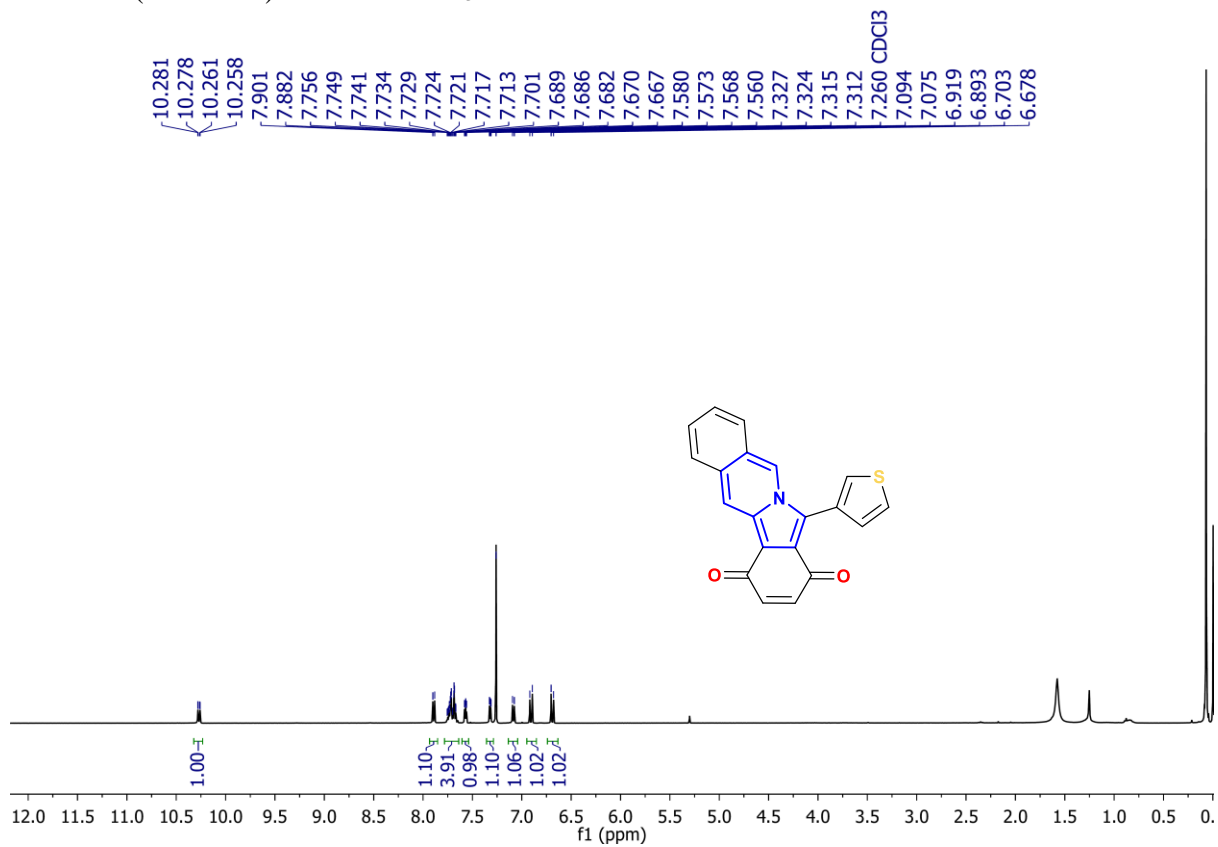
<sup>1</sup>H NMR (400 MHz) of **6b** in CDCl<sub>3</sub>



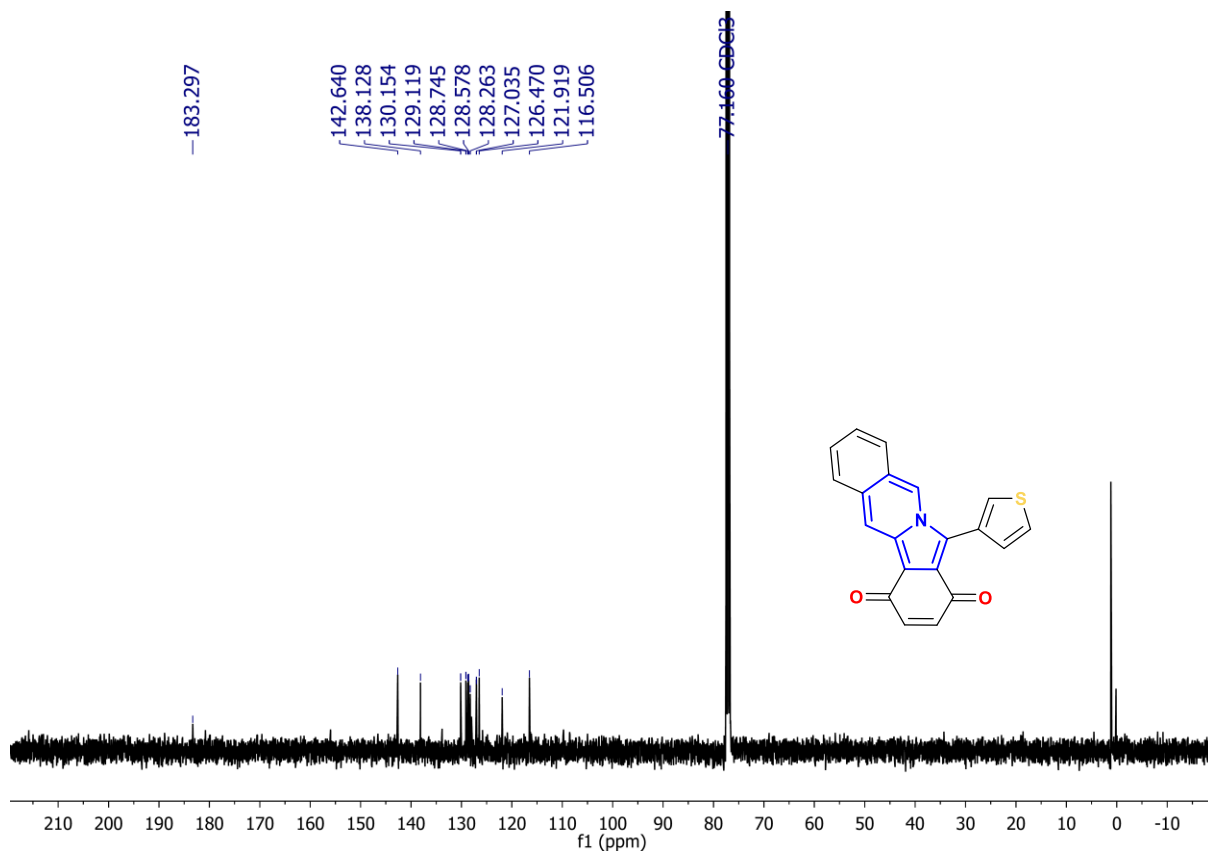
<sup>13</sup>C NMR (400 MHz) of **6b** in CDCl<sub>3</sub>



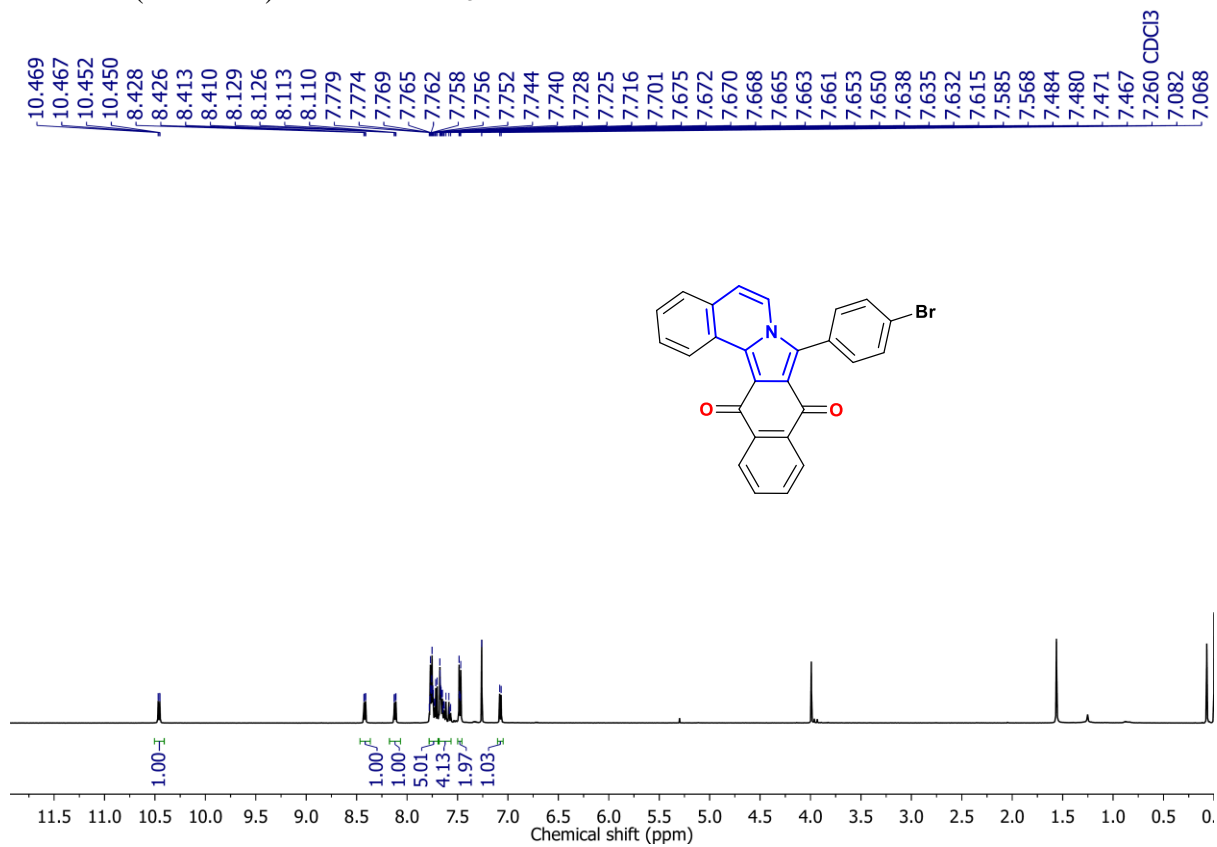
$^1\text{H}$  NMR (400 MHz) of **6c** in  $\text{CDCl}_3$



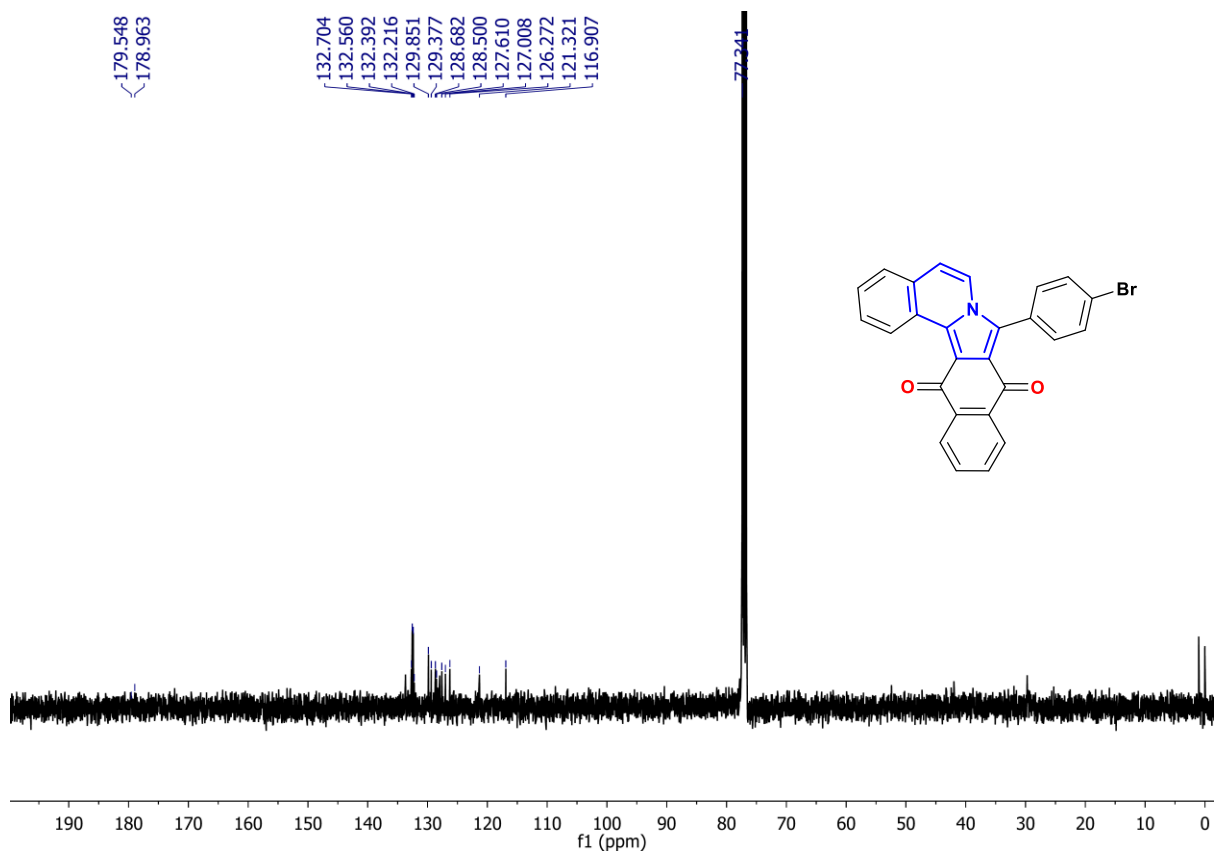
$^{13}\text{C}$  NMR (400 MHz) of **6c** in  $\text{CDCl}_3$



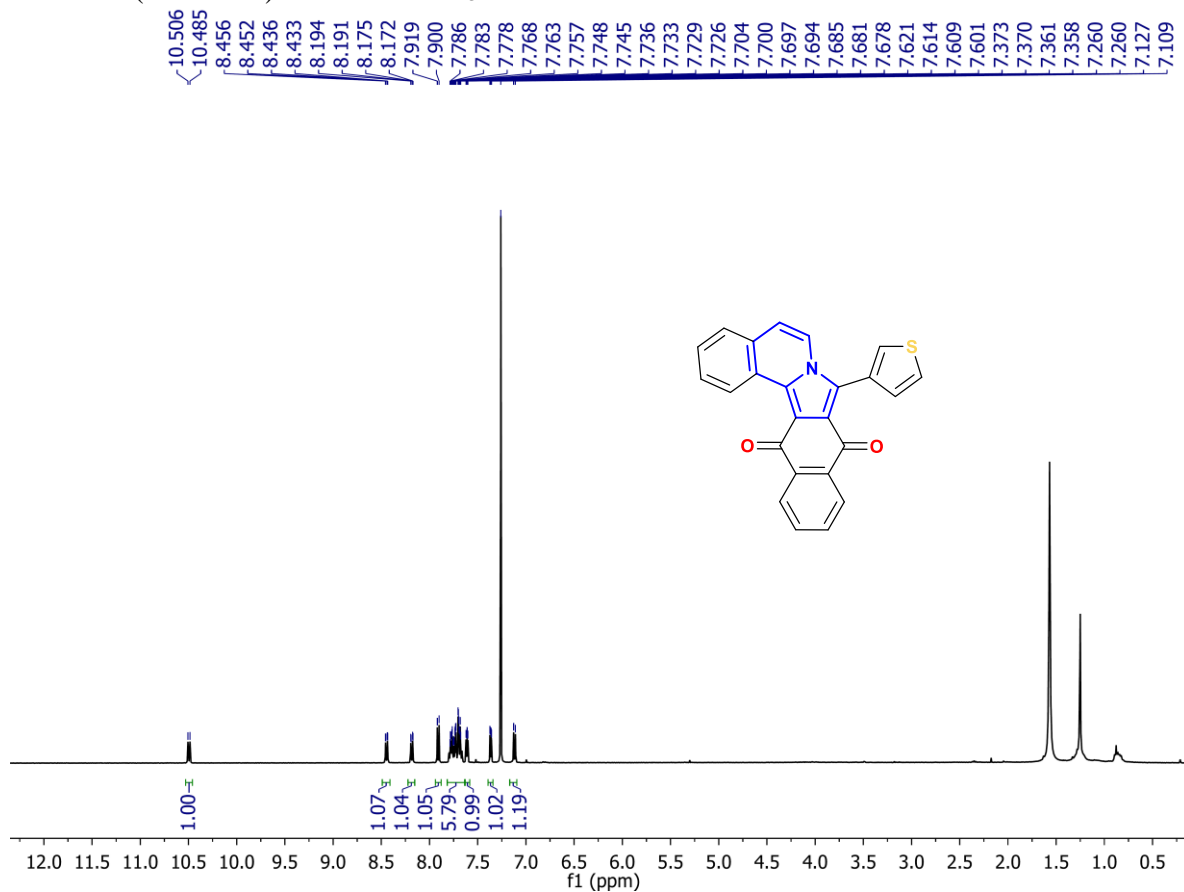
$^1\text{H}$  NMR (400 MHz) of **7a** in  $\text{CDCl}_3$



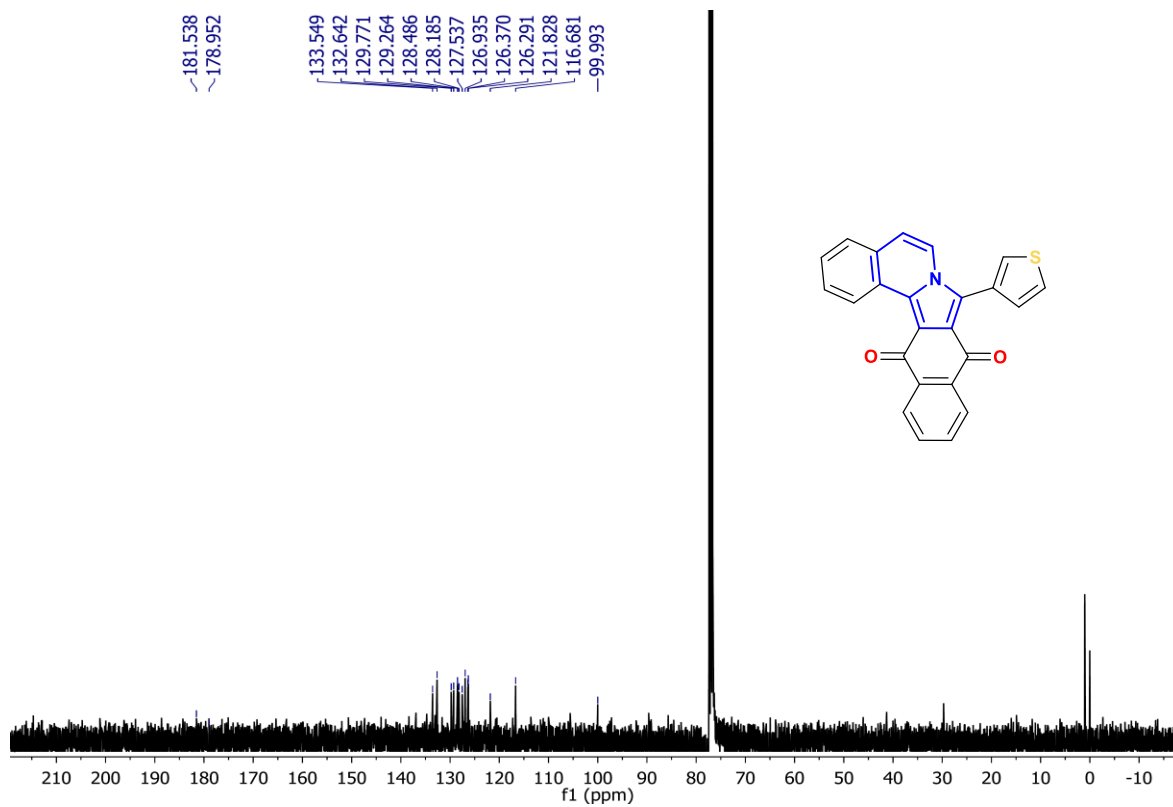
$^{13}\text{C}$  NMR (400 MHz) of **7a** in  $\text{CDCl}_3$



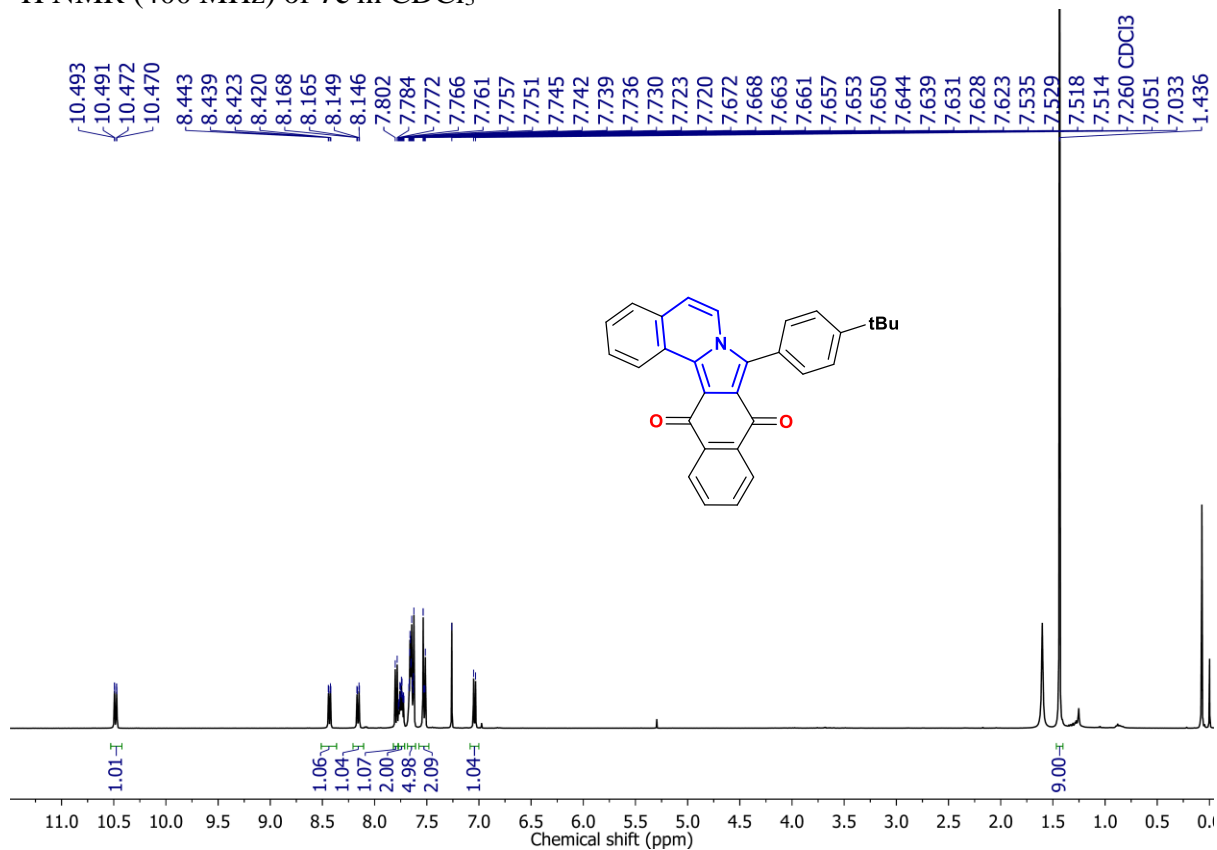
$^1\text{H}$  NMR (400 MHz) of **7b** in  $\text{CDCl}_3$



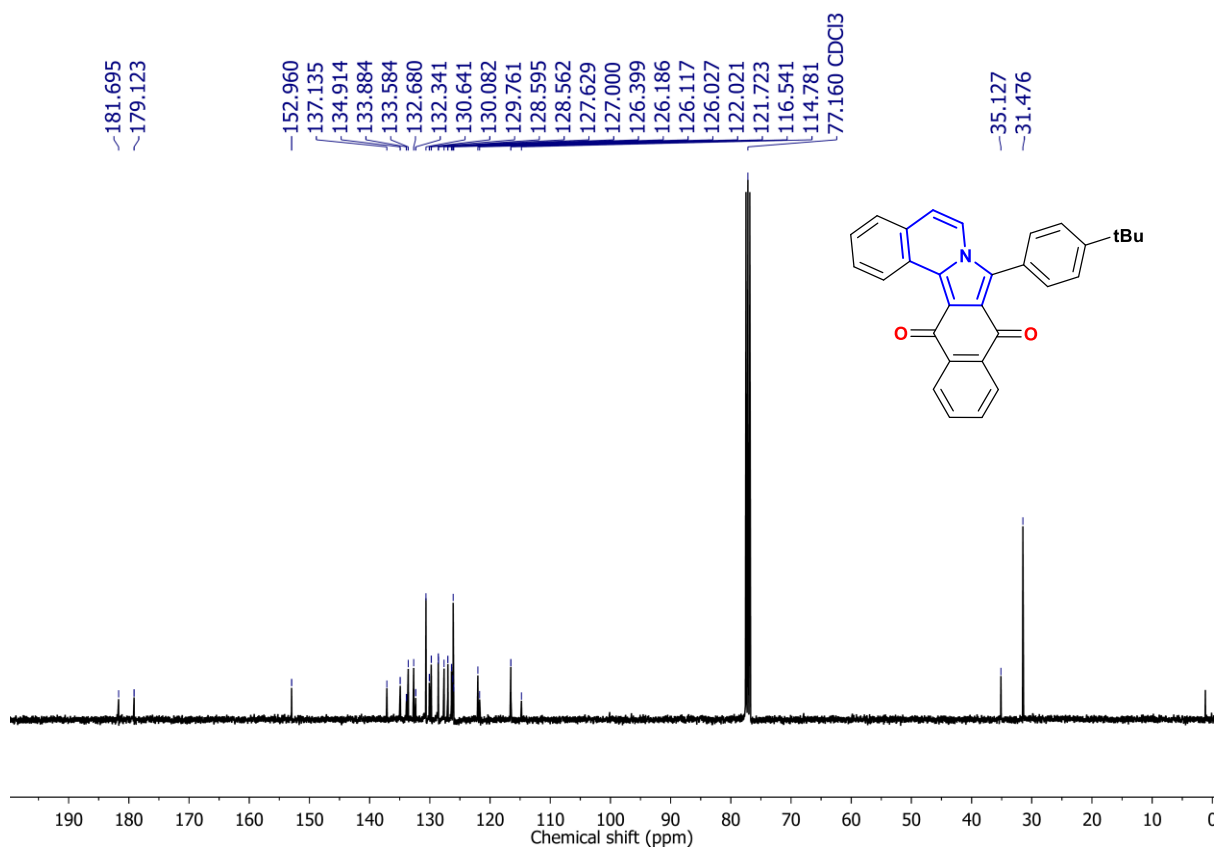
$^{13}\text{C}$  NMR (400 MHz) of **7b** in  $\text{CDCl}_3$



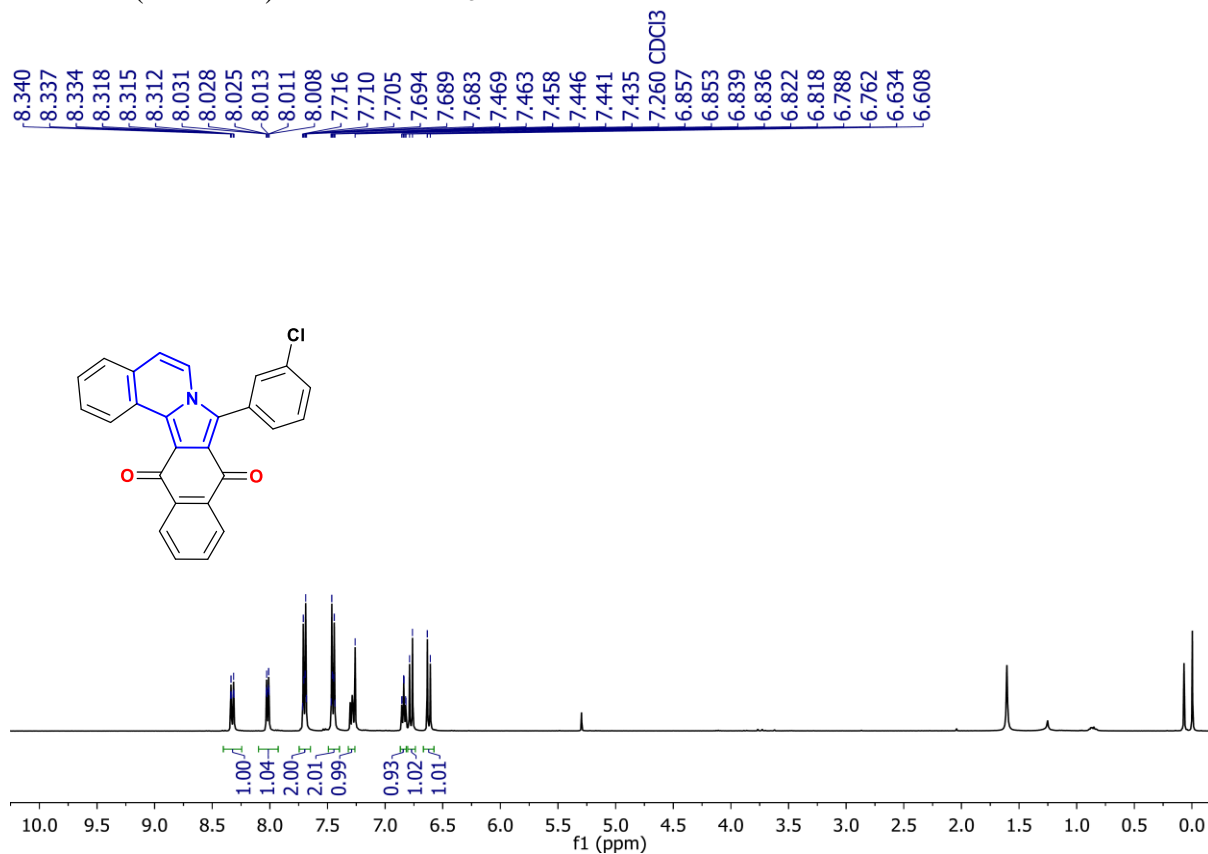
$^1\text{H}$  NMR (400 MHz) of **7c** in  $\text{CDCl}_3$



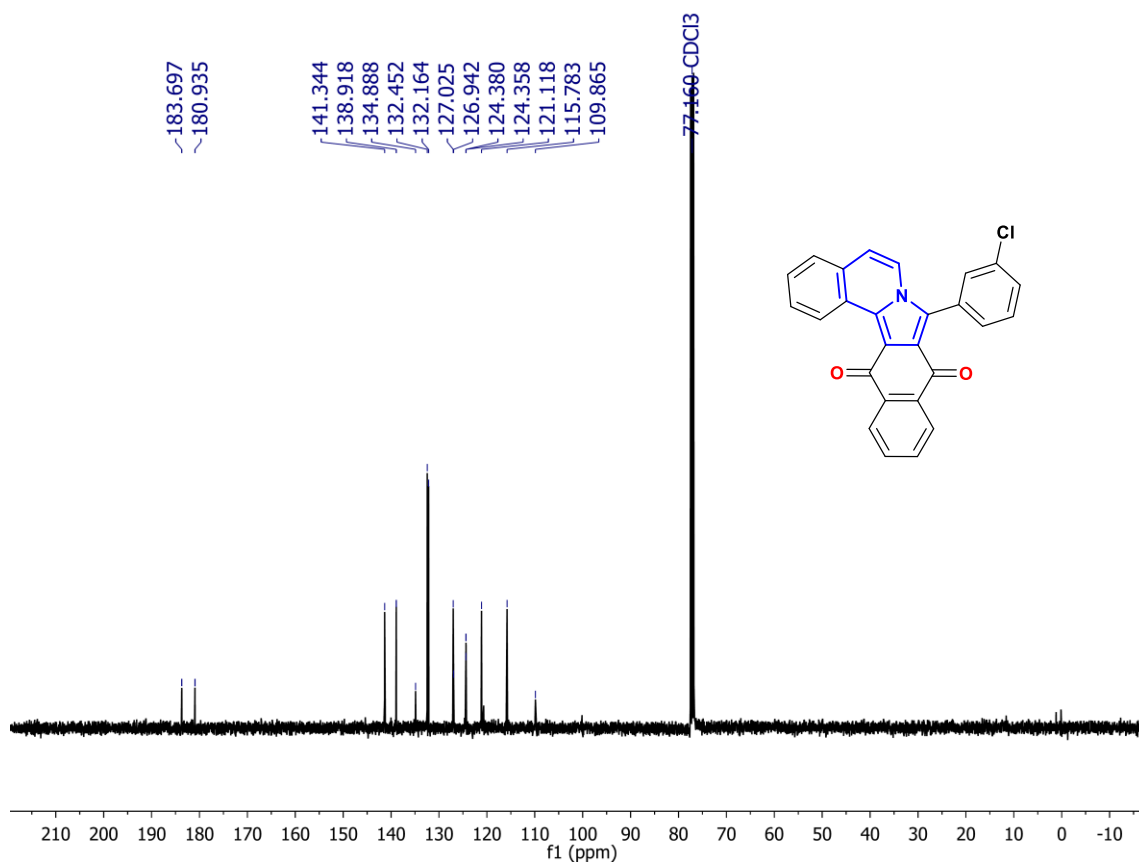
$^{13}\text{C}$  NMR (400 MHz) of **7c** in  $\text{CDCl}_3$



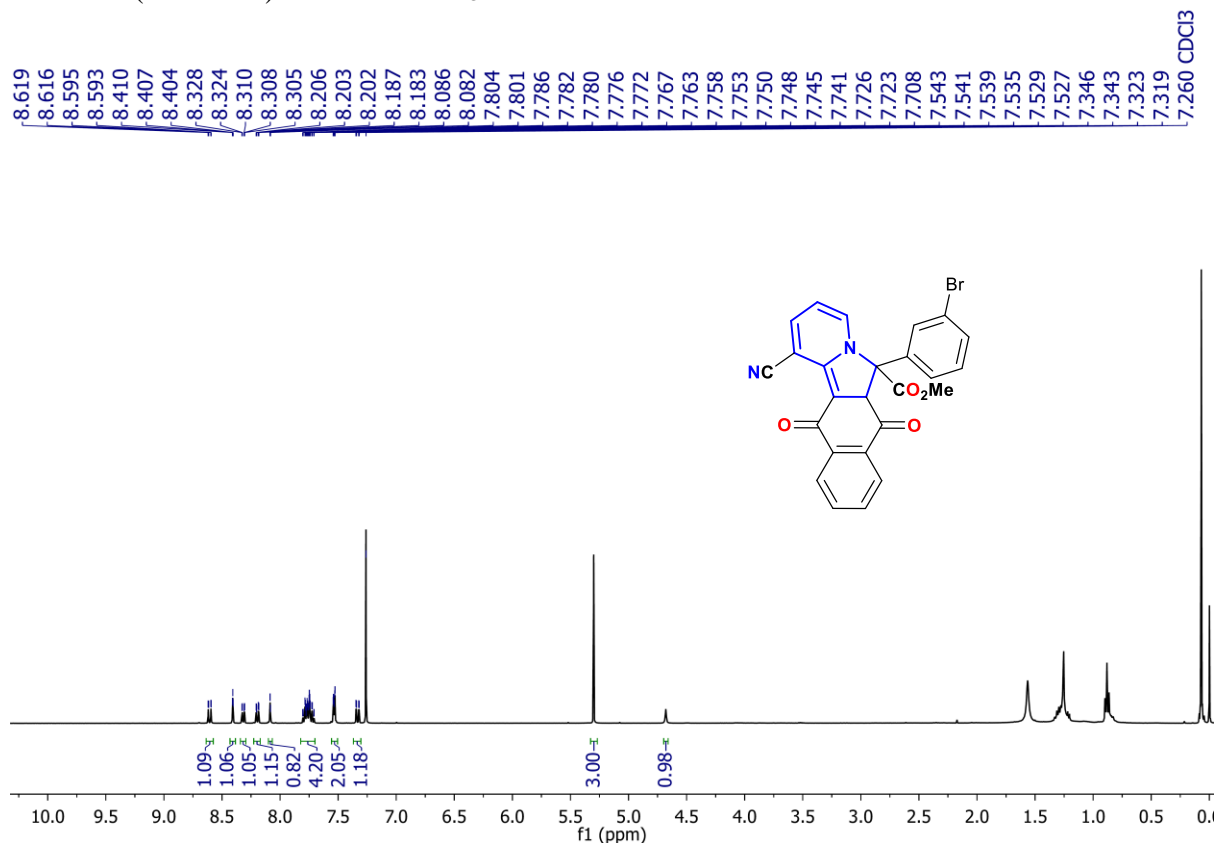
$^1\text{H}$  NMR (400 MHz) of **7d** in  $\text{CDCl}_3$



$^{13}\text{C}$  NMR (400 MHz) of **7d** in  $\text{CDCl}_3$



$^1\text{H}$  NMR (400 MHz) of **51'** in  $\text{CDCl}_3$



## 7. Catalog of Cartesian Co-ordinates ground state Optimized Geometries From B3LYP/6-311++G(d,p):

### 4a

6	-0.846381000	0.106424000	0.049156000
6	-1.793345000	-0.912942000	0.011456000
6	-2.942748000	1.049221000	0.039988000
6	-3.094738000	-0.338435000	-0.003146000
7	-1.559835000	1.307320000	0.074403000
6	0.624962000	0.072281000	0.033087000
6	1.350283000	0.775532000	-0.940538000
6	1.332893000	-0.681708000	0.977875000
6	2.741329000	0.740188000	-0.966614000
1	0.826103000	1.336177000	-1.706516000
6	2.722869000	-0.724425000	0.963680000
1	0.792366000	-1.248751000	1.724140000
6	3.416480000	-0.008667000	-0.007684000
1	3.289183000	1.277833000	-1.729550000
1	3.258077000	-1.311188000	1.698730000
6	-4.310778000	-1.124416000	-0.092698000
6	-1.612989000	-2.374863000	-0.064144000
6	-4.094532000	-2.598155000	-0.177824000
6	-2.874960000	-3.159348000	-0.174315000
8	-0.530287000	-2.941761000	-0.031774000
8	-5.446087000	-0.654129000	-0.109317000
6	-3.844318000	2.134254000	0.062292000

6	-3.359920000	3.413952000	0.140839000
6	-1.956991000	3.640529000	0.213405000
6	-1.083439000	2.596065000	0.183924000
1	-4.901161000	1.907963000	0.022527000
1	-0.011933000	2.707225000	0.250400000
35	5.330747000	-0.061644000	-0.031937000
1	-4.997221000	-3.196280000	-0.247456000
1	-2.739562000	-4.233867000	-0.238340000
1	-4.040162000	4.256367000	0.159219000
1	-1.564059000	4.645011000	0.300109000

### 6a

6	-0.272968000	0.709220000	-0.028562000
6	-0.893799000	1.956593000	-0.016663000
6	-2.559550000	0.404511000	0.012957000
6	-2.301101000	1.786181000	0.017966000
7	-1.298592000	-0.243695000	-0.019407000
6	1.146690000	0.322889000	-0.017828000
6	1.653290000	-0.526622000	0.977790000
6	2.029640000	0.810020000	-0.990398000
6	2.996532000	-0.889898000	0.999792000
1	1.000011000	-0.888828000	1.763954000
6	3.374019000	0.453686000	-0.980741000
1	1.665129000	1.482301000	-1.755832000
6	3.846061000	-0.397909000	0.013561000



1	3.376968000	-1.535760000	1.780509000
1	4.045272000	0.837575000	-1.737820000
6	-3.235007000	2.885716000	0.088458000
6	-0.296404000	3.308924000	0.013261000
6	-2.603423000	4.237863000	0.127600000
6	-1.274351000	4.426712000	0.103369000
8	0.904249000	3.531476000	-0.041275000
8	-4.460052000	2.764480000	0.124487000
6	-3.719630000	-0.362518000	0.022804000
6	-3.647696000	-1.753955000	-0.018765000
6	-2.346193000	-2.384868000	-0.087808000
6	-1.206694000	-1.600052000	-0.090202000
1	-4.667390000	0.159291000	0.054964000
1	-0.212275000	-2.016912000	-0.154390000
6	-4.807620000	-2.589348000	-0.011595000
6	-2.268555000	-3.814818000	-0.155483000
6	-4.690385000	-3.948405000	-0.073089000
1	-5.577957000	-4.570468000	-0.067404000
6	-3.404499000	-4.568840000	-0.147598000
1	-3.339297000	-5.649498000	-0.197511000
1	-5.783129000	-2.119008000	0.041877000
1	-1.292288000	-4.283987000	-0.211998000
35	5.695502000	-0.895900000	0.031000000
1	-3.296128000	5.071403000	0.181695000
1	-0.835064000	5.418107000	0.134130000

**6b**

6	0.237569000	0.704894000	0.020365000
6	0.849797000	1.956588000	0.012430000
6	2.528291000	0.417497000	-0.007947000
6	2.260093000	1.796756000	-0.012281000
7	1.271573000	-0.239450000	0.016393000
6	-1.177823000	0.304040000	0.006768000
6	-1.679405000	-0.549861000	-0.982803000
6	-2.072661000	0.777923000	0.975658000
6	-3.022494000	-0.921460000	-0.999267000
1	-1.024092000	-0.908830000	-1.769473000
6	-3.408237000	0.401718000	0.952148000
1	-1.719380000	1.454338000	1.743304000
6	-3.920902000	-0.458064000	-0.032130000
1	-3.361706000	-1.573586000	-1.793100000
1	-4.063985000	0.795856000	1.719813000
6	3.187286000	2.901352000	-0.074306000
6	0.243956000	3.304505000	-0.024666000
6	2.547097000	4.249061000	-0.115438000
6	1.216576000	4.428612000	-0.102324000
8	-0.958341000	3.522494000	0.012342000
8	4.414126000	2.788953000	-0.102272000
6	3.693704000	-0.341713000	-0.014943000
6	3.630785000	-1.733699000	0.021446000
6	2.333022000	-2.373487000	0.082376000
6	1.188320000	-1.596436000	0.082110000
1	4.637987000	0.186676000	-0.041652000
1	0.195511000	-2.018315000	0.137495000
6	4.796037000	-2.561839000	0.015333000
6	2.264847000	-3.804311000	0.143290000
6	4.687698000	-3.921959000	0.070122000
1	5.579463000	-4.538080000	0.065022000

6	3.405518000	-4.551205000	0.136501000
1	3.347105000	-5.632540000	0.180906000
1	5.768717000	-2.084937000	-0.032186000
1	1.291257000	-4.279840000	0.193234000
1	3.234523000	5.087521000	-0.161998000
1	0.771039000	5.417229000	-0.135328000
6	-5.411125000	-0.837689000	-0.024033000
6	-5.759618000	-1.529964000	1.314296000
1	-5.566644000	-0.880693000	2.171155000
1	-6.819431000	-1.801670000	1.334353000
1	-5.172397000	-2.443095000	1.446245000
6	-5.776973000	-1.798261000	-1.170492000
1	-5.587293000	-1.353980000	-2.151388000
1	-5.223934000	-2.739647000	-1.106521000
1	-6.842278000	-2.038513000	-1.119913000
6	-6.264399000	0.443742000	-0.176218000
1	-7.329361000	0.191762000	-0.170433000
1	-6.083814000	1.151040000	0.636386000
1	-6.040326000	0.953433000	-1.117198000

**7a**

6	0.018962000	0.005963000	-0.044952000
6	1.100159000	-0.873399000	-0.052060000
6	1.974474000	1.228299000	-0.013024000
6	2.311508000	-0.137364000	-0.024804000
7	0.558075000	1.296605000	-0.028491000
6	-1.434995000	-0.225252000	-0.026799000
6	-2.233536000	0.303725000	0.998243000
6	-2.052287000	-0.990627000	-1.024472000
6	-3.608316000	0.087207000	1.025306000
1	-1.776346000	0.870361000	1.802049000
6	-3.424885000	-1.215077000	-1.009638000
1	-1.452268000	-1.424471000	-1.813632000
6	-4.192871000	-0.669751000	0.014779000
1	-4.211332000	0.491555000	1.827939000
1	-3.889113000	-1.809547000	-1.785660000
6	3.625622000	-0.734481000	0.019152000
6	1.097113000	-2.349685000	-0.037556000
6	3.640821000	-2.236288000	0.041515000
6	2.450183000	-2.993122000	0.022110000
8	0.073689000	-3.015855000	-0.076393000
8	4.669581000	-0.082589000	0.044306000
6	2.712984000	2.406703000	0.000456000
6	2.070828000	3.644095000	-0.018258000
6	0.624479000	3.679886000	-0.067063000
6	-0.087964000	2.493380000	-0.074933000
1	3.791789000	2.322693000	0.018063000
1	-1.166568000	2.461527000	-0.123333000
6	2.781072000	4.884444000	-0.004838000
6	-0.039035000	4.949828000	-0.107853000
6	2.111088000	6.073895000	-0.040924000
1	2.661526000	7.007527000	-0.030543000
6	0.683003000	6.106589000	-0.094666000
1	0.175253000	7.063636000	-0.124539000
1	3.864430000	4.859240000	0.032966000
1	-1.122666000	4.973321000	-0.147961000
35	-6.084869000	-0.971291000	0.039540000
6	4.872148000	-2.893865000	0.088377000
6	2.519091000	-4.389548000	0.050818000

6	3.750567000	-5.033173000	0.098556000	1	1.592436000	-4.950148000	0.034143000
1	3.794498000	-6.116183000	0.121500000	1	5.772561000	-2.291843000	0.102170000
6	4.928738000	-4.283527000	0.116792000				
1	5.889807000	-4.784289000	0.153497000				

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