Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Rhodium-catalyzed aminoacylation of alkenes *via* carbonylative C–H activation toward poly(hetero)cyclic alkylarylketones

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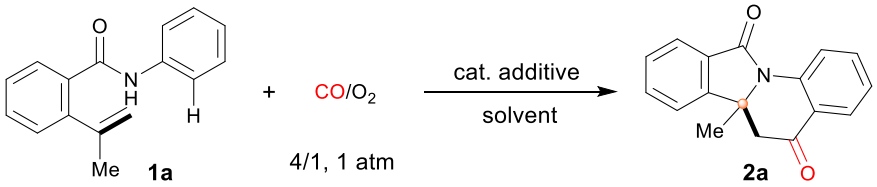
1. General information

Unless otherwise noted, all the reactions were carried out in standard Schlenk technique, and all reagents were used as supplied commercially without further purification from Aldrich, Alfa Aesar, Adamas-beta® or Bidepharm. An oil bath or aluminum heating module equipped with a magnetic stir bar was used for reactions requiring heating. ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded at 25 ^{o}C on a Varian Inova or Bruker Advance 400 M NMR spectrometers ($CDCl_3$ as solvent). Chemical shifts of ^{1}H, ^{19}F and ^{13}C NMR spectra are reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (δ 0.00) and relative to the signal of $SiMe_4$ (δ 0.00 singlet). Multiplicities were given as: s (singlet); d (doublet); t (triplet); q (quartet); p (pentet); m (multiplet); br (broad), *etc*. Coupling constants are reported as a *J* value in Hertz (Hz). The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale ($CDCl_3$: δ H = 7.26 ppm, δ C = 77.16 ppm). High resolution mass spectral analysis (HRMS) was performed on Agilent 6530 Accurate-Mass Q-TOF with ESI mode. Flash chromatography was performed using 200-300 mesh silica gel with the indicated eluent system. High performance liquid chromatography (HPLC) yields were recorded on the Agilent 1260A instrument and Agilent ZORBAX SB-C18 column, with a mixture of H_2O and acetonitrile as fluent. Single crystal X-ray diffraction data were collected on the Rigaku Oxford Diffraction (ROD) SuperNova Diffraction System.

2. Screening of the reaction conditions

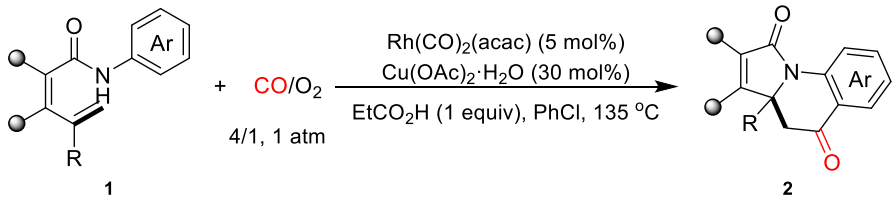
Table S1 Exploration and screening of the reaction conditions.[a]



Entry	Catalyst	Oxidant	Additive	Solvent	Yield (%)
1	$Pd(OAc)_2$	$Cu(OAc)_2·H_2O$	-	PhCl	0
2	$[Cp^*RhCl_2]_2$	$Cu(OAc)_2·H_2O$	-	PhCl	10
3	$[Cp^*RhCl_2]_2$	-	NaOAc	PhCl	0
4	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	-	PhCl	22
5	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	HOAc/NaOAc	PhCl	48
6	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	HOAc	PhCl	61
7	$[Cp^*RhCl_2]_2$	$Cu(OAc)_2·H_2O$	HOAc	PhCl	51
8	$[Rh(CO)_2Cl]_2$	$Cu(OAc)_2·H_2O$	HOAc	PhCl	53
9	$Rh(CO)_2(acac)$	-	HOAc	PhCl	0
10	$Rh(CO)_2(acac)$	$Cu(TFA)_2$	HOAc	PhCl	48
11	$Rh(CO)_2(acac)$	$Cu(acac)_2$	HOAc	PhCl	54
12	$Rh(CO)_2(acac)$	$CuCl_2$	HOAc	PhCl	2
13	$Rh(CO)_2(acac)$	AgOAc	HOAc	PhCl	trace
14	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	HOAc	PhMe	56
15	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	HOAc	THF	20
16	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	HOAc	DCE	9
17	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	PivOH	PhCl	57
18	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	TfOH	PhCl	0
19	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	$AdCO_2H$	PhCl	55
20	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	$EtCO_2H$	PhCl	65
21[b]	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	$EtCO_2H$	PhCl	71
22[c]	**$Rh(CO)_2(acac)$**	**$Cu(OAc)_2·H_2O$**	**$EtCO_2H$**	**PhCl**	**75 (73)**
23[d]	$Rh(CO)_2(acac)$	$Cu(OAc)_2·H_2O$	$EtCO_2H$	PhCl	75

[a] Reaction conditions: **1a** (0.3 mmol), catalyst (5 mol%), oxidant (10 mol%), additive (0.3 mmol), solvent (1 mL), CO/O_2 (4/1, v/v, 1 atm), 135 °C, 20 h. Yields were determined by HPLC analysis with biphenyl as an internal standard, with isolated yield in parentheses. [b] $Cu(OAc)_2·H_2O$ (20 mol%). [c] $Cu(OAc)_2·H_2O$ (30 mol%). [d] $Cu(OAc)_2·H_2O$ (50 mol%). acac = acetylacetone.

3. General procedure for the rhodium-catalyzed carbonylative assembly of poly(hetero)cyclic alkylarylketones

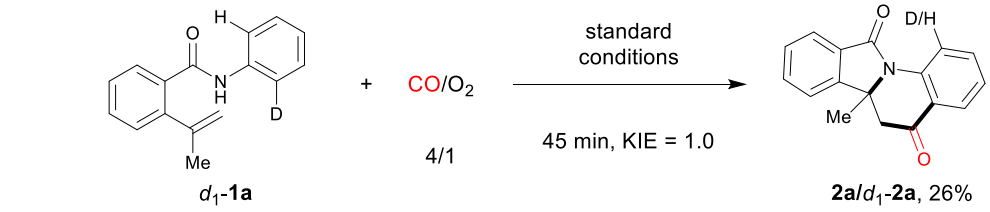


To an oven-dried 50 mL Schlenk tube with a magnetic stir bar, **1** (0.3 mmol), $Rh(CO)_2(acac)$ (3.9 mg, 5 mol%), $Cu(OAc)_2 \cdot H_2O$ (18 mg, 30 mol%), propionic acid (23 μL, 1 equiv) and PhCl (1 mL) were added under air atmosphere. Then the tube was purged with CO/O_2 (4/1, v/v) for 5 times and the mixture was stirred at 135 °C for 20 h. After cooling to room temperature, the reaction mixture was directly loaded onto a silica gel column and eluted with ethyl acetate/petroleum ether (v/v = 1:5) to afford the desired product **2**.

4. Mechanistic studies

We carried out some isotope labelling and KIE experiments under CO/O_2 (4/1, v/v). As shown in **Figures S1** and **S2**, small KIE values (26% yield, KIE = 1; 25% yield, KIE = 1) were obtained in the intra- and intermolecular reactions, respectively, suggesting that cyclometalation of the C–H bond is irreversible and C–H bond cleavage is not the rate-determining step. Meanwhile, the following investigation in **Figure S3** shows that the insertion of CO in the present carbonylative annulation is irreversible and **Figure S4** dedicates that the insertion of CO happened after the formation of the 6-membered rhodacycle.

4.1 Intramolecular kinetic isotope effect:



d_1-**1a** **2a**/d_1-**2a**, 26%

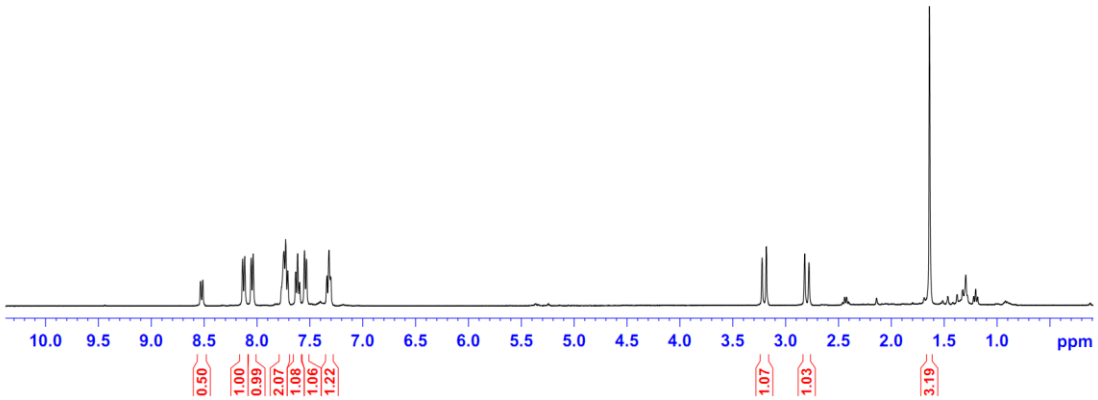


Figure S1 The ^{1}H-NMR spectrum of the product **2a**/d_1-**2a**.

4.2 Intermolecular kinetic isotope effect:

1a/d_5-**1a** **2a**/d_4-**2a**, 25%

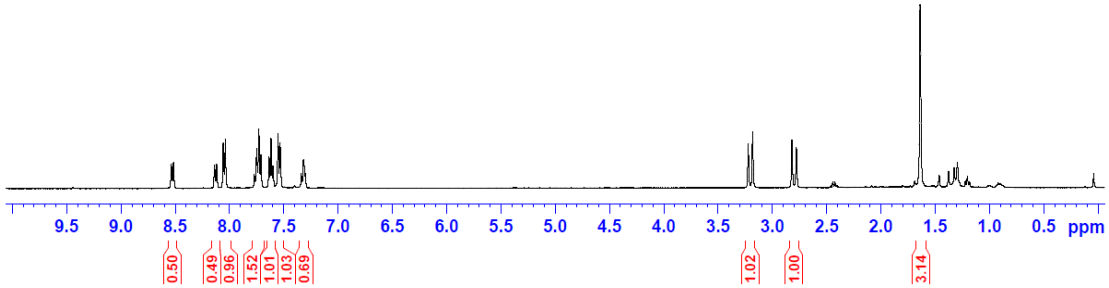


Figure S2 The ^{1}H-NMR spectrum of the product **2a**/d_4-**2a**.

4.3 Scrambling experiment using CD_3CO_2D:

To an oven-dried Schlenk tube equipped with a magnetic stir bar, **1a** (23.7 mg, 0.1 mmol), $Rh(CO)_2(acac)$ (1.3 mg, 5 mol%), $Cu(OAc)_2 \cdot H_2O$ (6 mg, 30 mol%), CD_3CO_2D (32.5 mg, 5 eq) and PhCl (0.5 mL) were added. Then the tube was purged with CO/O_2 (4/1, v/v) for 5 times and the mixture was stirred at 135 °C for 20 h. After cooling to room temperature, the slurry was purified directly by pre-TLC to afford *d*-**2a** in 63% yield. The deuterium incorporations in the products were determined by ^1H NMR spectroscopy, and the result shows that the insertion of CO into the six-membered rhodacycle **E** in such carbonylation is irreversible (**Figure S3**).

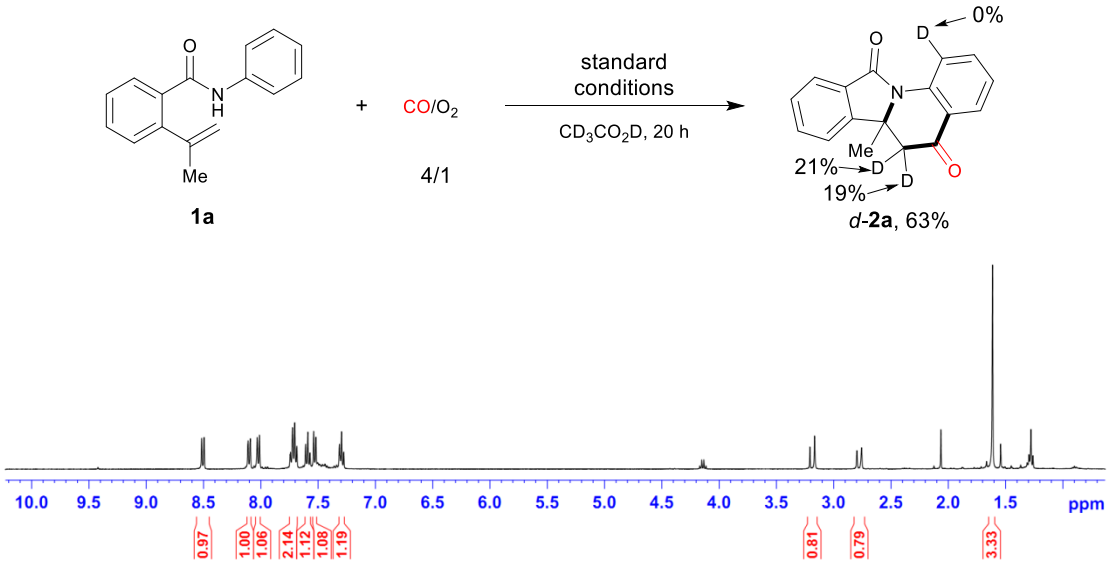
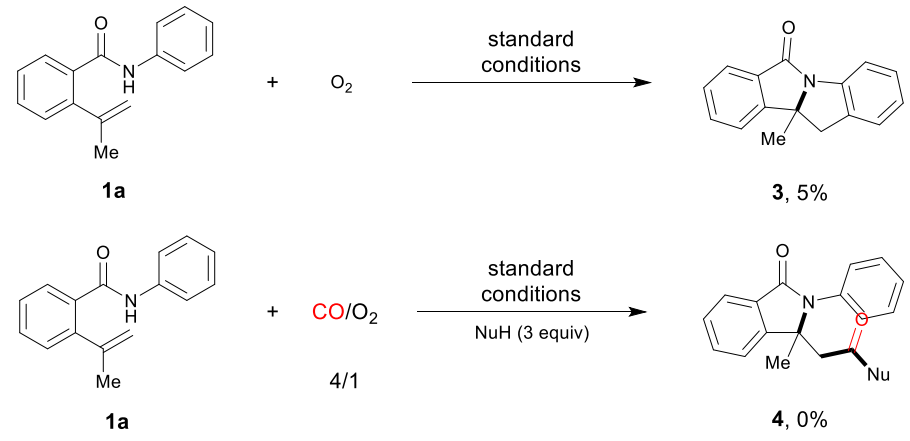


Figure S3 The ^1H-NMR spectrum of the product *d*-**2a**.

4.4 Control experiments without CO or with nucleophile



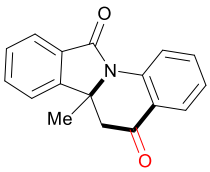
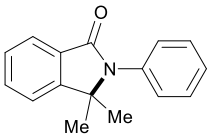
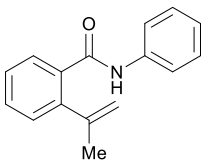
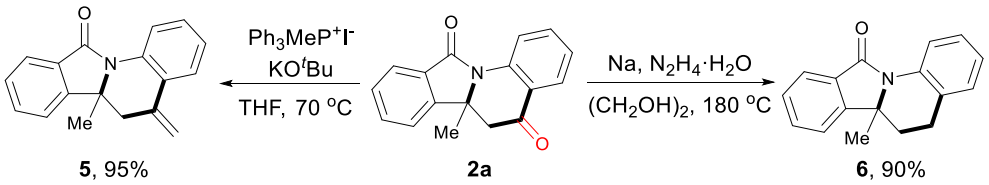
NuH	methanol	morpholine	aniline
reaction results	 71%	 40%, (**1a**, 60%)	 (**1a**, 92%)

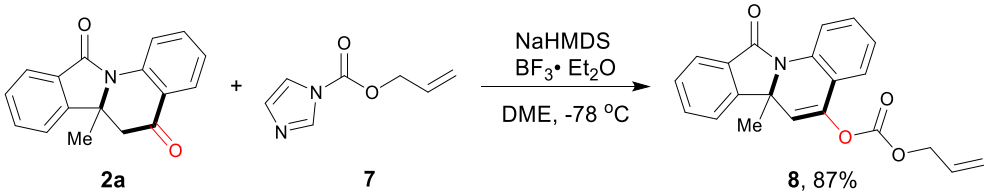
Figure S4 The results of the control experiments.

5. Synthetic utility of the product



Derived to compound 5: In the nitrogen filled glovebox, to a suspension of PPh_3MeI (97 mg, 1.2 equiv) in anhydrous THF (10 mL) was added KO^{t}Bu (34 mg, 1.5 equiv). The resulting bright yellow mixture was stirred at room temperature for 30 min. Then **2a** (52.6 mg, 0.2 mmol) in THF (10 mL) was added into the yellow mixture, then stirred at 70 °C for overnight. After cooling to room temperature, the reaction was quenched by H_2O (5 mL), extracted with ethyl acetate (5 mL×3) and washed with brine. The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated to give the crude product, which was subsequently purified by column chromatography using ethyl acetate/petroleum ether (v/v = 1:10) as eluent to afford the product **5** (49.6 mg, 95%) as white solid (m.p.: 110.5–112.0 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 5.81 (d, *J* = 2.1 Hz, 1H), 5.15 (d, *J* = 1.9 Hz, 1H), 2.93 (d, *J* = 14.0 Hz, 1H), 2.50 (d, *J* = 14.0 Hz, 1H), 1.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 150.5, 136.7, 133.7, 132.5, 131.3, 129.3, 128.7, 124.6, 124.3, 124.23, 124.18, 122.1, 120.8, 112.3, 62.3, 42.7, 22.9. HRMS (ESI) calcd for $C_{18}H_{15}NONa$ $[M+Na]^+$ 284.1046, found 284.1045.

Derived to compound 6[1]: Under argon atmosphere, to a solution of sodium (14 mg, 0.6 mmol, 3.0 equiv) in ethylene glycol was added **2a** (52.6 mg, 0.2 mmol) and $N_2H_4·H_2O$ (39 μL, 0.8 mmol, 4.0 equiv). The mixture was stirred at 180 °C for 5 h. After cooling to room temperature, the mixture was diluted with H_2O and extracted with CH_2Cl_2 for three times. The combined organic layers were dried over anhydrous Na_2SO_4, and concentrated to give the crude product, which was purified by column chromatography using ethyl acetate/petroleum ether (v/v = 1:10) as eluent to afford the desired product **6** (44.8 mg, 90%) as white solid (m.p.: 157.5–159.1 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.9 Hz, 1H), 7.91-7.89 (m, 1H), 7.58-7.56 (m, 1H), 7.48-7.45 (m, 2H), 7.28-7.27 (m, 1H), 7.21-7.20 (m, 1H), 7.08 (m, 1H), 3.11-3.08 (m, 1H), 2.97 (d, *J* = 16.8 Hz, 1H), 2.35-2.32 (m, 1H), 1.71-1.65 (m, 1H), 1.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 150.9, 134.9, 132.4, 131.2, 129.2, 128.5, 127.0, 125.5, 124.5, 124.2, 122.0, 120.8, 61.5, 32.4, 24.4, 22.2. HRMS (ESI) calcd for $C_{17}H_{15}NONa$ $[M+Na]^+$ 272.1046, found 272.1047.

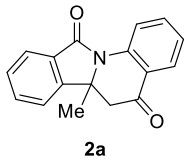


Derived to compound 8[2]: Under nitrogen atmosphere, a solution of **2a** (52.6 mg, 0.2 mol) in anhydrous 1,2-dimethoxyethane (DME) (3 mL) was added into an oven dried Schlenk tube and

cooled to -78 °C, then sodium bis(trimethylsilyl)amide (NaHMDS) (300 μL, 1 mol/L in THF, 1.5 equiv) was added dropwise. After stirring at this temperature for 1 h, to the mixture was added **7** (80 mg, 1.3 equiv) in DME (4 mL) followed by $BF_3 \cdot Et_2O$ (48% in Et_2O, 1.5 equiv). The mixture was further stirred at -78 °C for 3 h. After that the reaction was quenched by saturate NH_4Cl solution and warmed to room temperature. The mixture was extracted with Et_2O for 3 times and the combined organic layers were dried over anhydrous Na_2SO_4, concentrated under vacuum. The residue was purified by column chromatography using ethyl acetate/petroleum ether (v/v = 1:5) as eluent to afford the desired product **8** (62.5 mg, 87%) as white solid (m.p.: 76.2–77.3 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 1H), 7.94-7.91 (m, 1H), 7.63 (td, *J* = 7.5, 1.2 Hz, 1H), 7.52-7.43 (m, 3H), 7.39 (d, *J* = 7.8, 1.5 Hz, 1H), 7.21 (td, *J* = 7.6, 1.2 Hz, 1H), 6.18 (s, 1H), 6.01-5.91 (m, 1H), 5.43-5.38 (m, 1H), 5.34-5.31 (m, 1H), 4.70 (d, *J* = 5.8 Hz, 2H), 1.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 152.7, 148.3, 144.1, 133.6, 133.1, 131.1, 130.9, 130.1, 128.8, 124.94, 124.90, 122.9, 122.4, 122.2, 121.1, 119.8, 118.0, 69.5, 63.7, 27.4. HRMS (ESI) calcd for $C_{21}H_{17}NO_4Na$ $[M+Na]^+$ 370.1050, found 370.1050.

6. Experimental characterization data for products

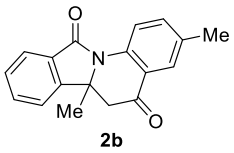
6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2a):



2a

White solid (57.9 mg, 73%, m.p.: 131.6–132.3 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.3 Hz, 1H), 8.08 (dd, *J* = 7.8, 0.9 Hz, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.73-7.66 (m, 2H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.30-7.26 (m, 1H), 3.16 (d, *J* = 16.2 Hz, 1H), 2.76 (d, *J* = 16.2 Hz, 1H), 1.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 165.4, 149.9, 139.2, 135.7, 133.3, 130.6, 129.3, 127.4, 125.1, 124.5, 122.4, 121.8, 121.0, 64.3, 48.7, 24.0. HRMS (ESI) calcd for $C_{17}H_{14}NO_2$ $[M+H]^+$ 264.1019, found 264.1019.

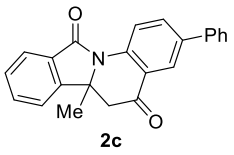
3,6a-dimethyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2b):



2b

White solid (59.3 mg, 71%, m.p.: 207.6–209.1 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 7.5 Hz, 1H), 7.85 (s, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.55-7.46 (m, 3H), 3.11 (d, *J* = 16.2 Hz, 1H), 2.71 (d, *J* = 16.2 Hz, 1H), 2.38 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.6, 165.2, 149.7, 136.8, 136.5, 134.3, 133.0, 130.7, 129.1, 127.2, 124.9, 122.0, 121.6, 120.9, 64.2, 48.6, 23.9, 20.9. HRMS (ESI) calcd for $C_{18}H_{15}NO_2Na$ $[M+Na]^+$ 300.0995, found 300.1011.

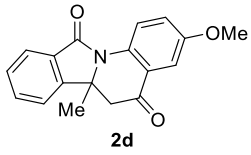
6a-methyl-3-phenyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2c):



2c

Pale yellow solid (63.1 mg, 62%, m.p.: 183.6–184.5 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 8.5 Hz, 1H), 8.32 (s, 1H), 8.02 (d, *J* = 7.6 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.71-7.64 (m, 3H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.52-7.45 (m, 3H), 7.38 (t, *J* = 7.3 Hz, 1H), 3.19 (d, *J* = 16.1 Hz, 1H), 2.79 (d, *J* = 16.1 Hz, 1H), 1.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 165.4, 149.8, 139.5, 138.3, 137.3, 134.2, 133.3, 130.6, 129.3, 129.1, 127.8, 127.0, 125.6, 125.1, 122.5, 122.2, 121.0, 64.3, 48.7, 24.1. HRMS (ESI) calcd for $C_{23}H_{17}NO_2Na$ $[M+Na]^+$ 362.1151, found 362.1143.

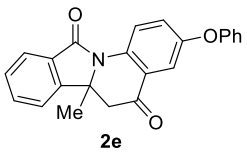
3-methoxy-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2d):



2d

White solid (64.3 mg, 73%, m.p.: 150.2–151.7 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.52-7.44 (m, 3H), 7.23-7.21 (m, 1H), 3.82 (s, 3H), 3.11 (d, *J* = 16.3 Hz, 1H), 2.69 (d, *J* = 16.2 Hz, 1H), 1.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 165.1, 156.3, 149.6, 132.98, 132.96, 130.7, 129.1, 124.9, 123.6, 123.3, 123.1, 120.9, 109.1, 64.3, 55.7, 48.7, 23.8. HRMS (ESI) calcd for $C_{18}H_{15}NO_3Na$ $[M+Na]^+$ 316.0944, found 316.0938.

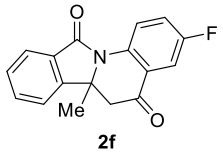
6a-methyl-3-phenoxy-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2e):



2e

Pale yellow solid (69.1 mg, 65%, m.p.: 179.7–181.2 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 9.0 Hz, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.70-7.66 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.41-7.35 (m, 3H), 7.15 (d, *J* = 7.4 Hz, 1H), 7.04 (d, *J* = 7.8 Hz, 2H), 3.15 (d, *J* = 16.3 Hz, 1H), 2.73 (d, *J* = 16.3 Hz, 1H), 1.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 165.3, 156.7, 154.1, 149.7, 134.7, 133.2, 130.6, 130.1, 129.3, 126.5, 125.0, 124.0, 123.6, 121.0, 119.2, 116.1, 64.3, 48.7, 23.9. HRMS (ESI) calcd for $C_{23}H_{17}NO_3Na$ $[M+Na]^+$ 378.1101, found 378.1102.

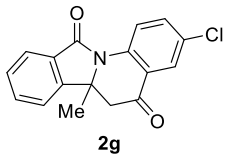
3-fluoro-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2f):



2f

White solid (54.8 mg, 65%, m.p.: 168.2–169.5 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 9.2, 4.6 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.72-7.65 (m, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.49 (d, *J* = 7.2 Hz, 1H), 7.41-7.36 (m, 1H), 3.16 (d, *J* = 16.3 Hz, 1H), 2.73 (d, *J* = 16.3 Hz, 1H), 1.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5 (d, *J* = 1.7 Hz), 165.3, 159.2 (d, *J* = 245.0 Hz), 149.5, 135.4 (d, *J* = 2.5 Hz), 133.3, 130.3, 129.3, 125.0, 123.8 (d, *J* = 7.1 Hz), 123.7 (d, *J* = 6.3 Hz), 122.9 (d, *J* = 23.2 Hz), 121.0, 113.1 (d, *J* = 23.3 Hz), 64.3, 48.5, 23.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.13. HRMS (ESI) calcd for $C_{17}H_{12}FNO_2Na$ $[M+Na]^+$ 304.0744, found 304.0749.

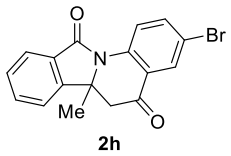
3-chloro-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2g):



2g

White solid (57.2 mg, 64%, m.p.: 217.6–219.2 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.45 (dd, *J* = 8.8, 1.0 Hz, 1H), 8.01 (dd, *J* = 2.6, 1.1 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.64-7.61 (m, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.50 (dd, *J* = 7.6, 0.6 Hz, 1H), 3.16 (d, *J* = 16.2 Hz, 1H), 2.75 (d, *J* = 16.2 Hz, 1H), 1.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 165.3, 149.6, 137.6, 135.4, 133.5, 130.24, 130.21, 129.4, 127.0, 125.1, 123.3, 123.2, 121.0, 64.2, 48.4, 24.0. HRMS (ESI) calcd for $C_{17}H_{12}ClNO_2Na$ $[M+Na]^+$ 320.0449, found 320.0447.

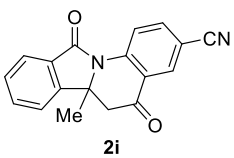
3-bromo-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2h):



2h

White solid (67.5 mg, 66%, m.p.: 175.2–177.5 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.8, 1H), 8.18 (s, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 3.16 (d, *J* = 16.2 Hz, 1H), 2.74 (d, *J* = 16.1 Hz, 1H), 1.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.2, 165.4, 149.7, 138.4, 138.1, 133.5, 130.3, 130.2, 129.4, 125.2, 123.6, 123.5, 121.0, 117.8, 64.2, 48.4, 24.0. HRMS (ESI) calcd for $C_{17}H_{12}BrNO_2Na$ $[M+Na]^+$ 363.9944, found 363.9945.

6a-methyl-5,11-dioxo-5,6,6a,11-tetrahydroisoindolo[2,1-*a*]quinoline-3-carbonitrile (2i):

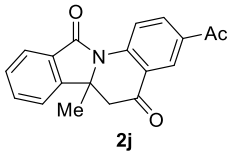


2i

White solid (46.1 mg, 53%, m.p.: 218.3–220.6 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.6 Hz, 1H), 8.36 (s, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.91 (d, *J* = 8.7 Hz, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 3.22 (d, *J* = 16.2 Hz, 1H), 2.78 (d, *J* = 16.2 Hz, 1H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.5, 165.7, 149.6, 142.3, 138.1, 134.1,

132.1, 129.72, 129.70, 125.5, 122.33, 122.31, 121.1, 118.0, 107.9, 64.3, 48.1, 24.3. HRMS (ESI) calcd for $C_{18}H_{12}N_2O_2Na$ $[M+Na]^+$ 311.0791, found 311.0782.

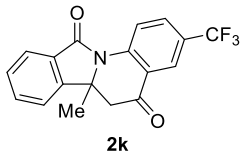
3-acetyl-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2j):



2j

White solid (50.2 mg, 55%, m.p.: 243.6–245.1 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.63-8.61 (m, 2H), 8.30 (d, *J* = 8.8 Hz, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.71 (t, *J* = 7.3 Hz, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.51 (d, *J* = 7.5 Hz, 1H), 3.21 (d, *J* = 16.3 Hz, 1H), 2.79 (d, *J* = 16.1 Hz, 1H), 2.65 (s, 3H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 191.7, 165.7, 149.7, 142.8, 134.9, 133.8, 132.9, 130.1, 129.5, 128.3, 125.3, 121.7, 121.1, 64.3, 48.3, 26.7, 24.3. HRMS (ESI) calcd for $C_{19}H_{15}NO_3Na$ $[M+Na]^+$ 328.0944, found 328.0948.

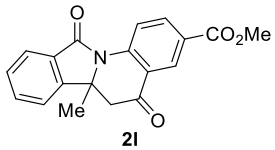
6a-methyl-3-(trifluoromethyl)-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2k):



2k

White solid (58.6 mg, 59%, m.p.: 180.7–182.5 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.6, Hz, 1H), 8.34 (s, 1H), 7.98 (d, *J* = 7.5 Hz, 1H), 7.90 (d, *J* = 8.6 Hz, 1H), 7.71 (t, *J* = 7.4 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 3.21 (d, *J* = 16.2 Hz, 1H), 2.79 (d, *J* = 16.2 Hz, 1H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.2, 165.6, 149.6, 141.7, 133.8, 132.0 (q, *J* = 3.6 Hz), 130.0, 129.5, 126.4 (q, *J* = 33.6 Hz), 125.3, 124.9 (q, *J* = 3.9 Hz), 123.7 (q, *J* = 270 Hz), 122.1, 122.0, 121.1, 64.3, 48.3, 24.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.54. HRMS (ESI) calcd for $C_{18}H_{12}F_3NO_2Na$ $[M+Na]^+$ 354.0712, found 354.0715.

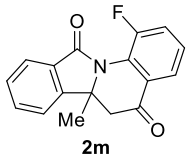
methyl 6a-methyl-5,11-dioxo-5,6,6a,11-tetrahydroisoindolo[2,1-*a*]quinoline-3-carboxylate (2l):



2l

White solid (66.5 mg, 69%, m.p.: 226.5–227.9 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.74 (s, 1H), 8.61 (d, *J* = 8.9 Hz, 1H), 8.34 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 7.7 Hz, 1H), 7.71 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.51 (d, *J* = 7.3 Hz, 1H), 3.94 (s, 3H), 3.20 (d, *J* = 16.3 Hz, 1H), 2.78 (d, *J* = 16.2 Hz, 1H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.6, 166.0, 165.7, 149.7, 142.6, 136.4, 133.8, 130.1, 129.5, 129.4, 126.1, 125.3, 121.9, 121.5, 121.1, 64.3, 52.5, 48.4, 24.3. HRMS (ESI) calcd for $C_{19}H_{15}NO_4Na$ $[M+Na]^+$ 344.0893, found 344.0893.

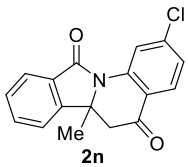
1-fluoro-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2m):



2m

White solid (59.0 mg, 70%, m.p.: 190.8–192.5 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.3 Hz, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.67 (t, *J* = 7.0 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.51-7.47 (m, 2H), 7.32-7.31 (m, 1H), 3.14 (d, *J* = 16.8 Hz, 1H), 2.68 (d, *J* = 16.9 Hz, 1H), 1.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.7 (d, *J* = 2.9 Hz), 164.4, 155.7 (d, *J* = 270 Hz), 150.2, 133.2, 130.0 (d, *J* = 1.3 Hz), 129.3, 126.9 (d, *J* = 13.8 Hz), 126.4 (d, *J* = 7.4 Hz), 125.7 (d, *J* = 1.8 Hz), 125.3, 123.4 (q, *J* = 20.3 Hz), 122.9 (d, *J* = 3.3 Hz), 121.0, 64.6, 50.7, 22.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.55. HRMS (ESI) calcd for $C_{17}H_{12}FNO_2Na$ $[M+Na]^+$ 304.0744, found 304.0753.

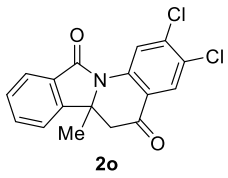
2-chloro-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2n):



2n

White solid (68.2 mg, 76%, m.p.: 196.1–197.6 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.54 (s, 1H), 8.00 (t, *J* = 8.0 Hz, 2H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 8.6 Hz, 1H), 3.16 (d, *J* = 16.0 Hz, 1H), 2.75 (d, *J* = 16.0 Hz, 1H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 165.4, 149.7, 142.1, 139.9, 133.6, 130.1, 129.4, 128.7, 125.2, 125.0, 121.6, 121.0, 120.6, 64.4, 48.3, 24.2. HRMS (ESI) calcd for $C_{17}H_{12}ClNO_2Na$ $[M+Na]^+$ 320.0449, found 320.0451.

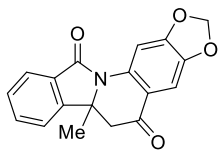
2,3-dichloro-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2o):



2o

White solid (64.8 mg, 65%, m.p.: 213.9–215.6 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.66 (s, 1H), 8.11 (s, 1H), 7.97 (d, *J* = 7.4 Hz, 1H), 7.70 (t, *J* = 7.1 Hz, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.49 (d, *J* = 7.4, 1H), 3.16 (d, *J* = 16.2 Hz, 1H), 2.75 (d, *J* = 16.4 Hz, 1H), 1.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.5, 165.3, 149.5, 140.1, 137.8, 133.7, 129.9, 129.5, 128.8, 125.3, 123.4, 121.7, 121.0, 64.3, 48.2, 24.2. HRMS (ESI) calcd for $C_{17}H_{11}Cl_2NO_2Na$ $[M+Na]^+$ 354.0059, found 354.0060.

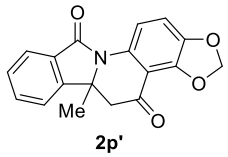
6a-methyl-6,6a-dihydro-[1,3]dioxolo[4,5-*g*]isoindolo[2,1-*a*]quinoline-5,11-dione (2p):



2p

White solid (35.2 mg, 38%, m.p.: 211.5–213.5 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 7.99-7.98 (m, 2H), 7.68 (t, *J* = 7.5, 1.2 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.49-7.47 (m, 2H), 6.09-6.08 (m, 2H), 3.08 (d, *J* = 16.4 Hz, 1H), 2.68 (d, *J* = 16.4 Hz, 1H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.8, 165.3, 153.8, 149.8, 145.2, 136.4, 133.2, 130.6, 129.2, 125.0, 121.0, 117.2, 105.6, 102.5, 102.3, 64.7, 48.3, 23.9. HRMS (ESI) calcd for $C_{18}H_{13}NO_4Na$ $[M+Na]^+$ 330.0737, found 330.0739.

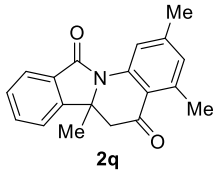
7a-methyl-7,7a-dihydro-[1,3]dioxolo[4,5-*f*]isoindolo[2,1-*a*]quinoline-6,12-dione (2p'):



2p'

White solid (34.7 mg, 38%, m.p.: 239.8–241.4 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.6 Hz, 1H), 7.93 (d *J* = 8.6 Hz, 1H), 7.67 (td, *J* = 7.5, 1.1 Hz, 1H), 7.56 (td, *J* = 7.5, 1.0 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.12 (d, *J* = 8.6 Hz, 1H), 6.18 (dd, *J* = 19.0, 1.2 Hz, 2H), 3.13 (d, *J* = 16.3 Hz, 1H), 2.71 (d, *J* = 16.3 Hz, 1H), 1.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 165.2, 149.4, 147.9, 145.4, 133.1, 132.0, 130.7, 129.2, 124.9, 120.9, 114.5, 114.0, 108.8, 103.1, 64.3, 49.4, 23.8. HRMS (ESI) calcd for $C_{18}H_{13}NO_4Na$ $[M+Na]^+$ 330.0737, found 330.0735.

2,4,6a-trimethyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2q):

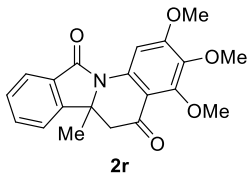


2q

White solid (56.9 mg, 65%, m.p.: 199.8–201.3 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 6.90 (s, 1H), 3.06 (d, *J* = 16.0 Hz, 1H), 2.73-2.68 (m, 4H), 2.43 (s, 3H), 1.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.7, 165.4, 150.0, 145.4, 142.2, 140.2, 133.1, 130.8,

129.7, 129.1, 125.0, 120.9, 120.6, 118.7, 64.0, 50.4, 23.52, 23.48, 22.1. HRMS (ESI) calcd for $C_{19}H_{17}NO_2Na$ $[M+Na]^+$ 314.1151, found 314.1152.

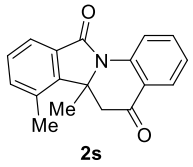
2,3,4-trimethoxy-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2r):



2r

White solid (68.9 mg, 65%, m.p.: 168.4–170.2 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 7.98-7.95 (m, 2H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 (d, *J* = 7.6, 1H), 4.03 (s, 3H), 3.95 (s, 3H), 3.89 (s, 3H), 3.04 (d, *J* = 16.0 Hz, 1H), 2.68 (d, *J* = 16.0 Hz, 1H), 1.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.0, 165.6, 158.7, 155.1, 149.9, 139.9, 137.0, 133.2, 130.5, 129.2, 124.8, 120.9, 110.7, 101.0, 64.3, 61.7, 61.3, 56.4, 49.9, 23.5. HRMS (ESI) calcd for $C_{20}H_{19}NO_5Na$ $[M+Na]^+$ 376.1155, found 376.1154.

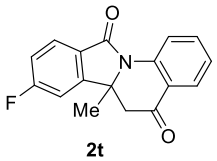
6a,7-dimethyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2s):



2s

White solid (63.7 mg, 77%, m.p.: 126.3–127.7 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.2 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 6.8 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.47-7.42 (m, 2H), 7.29-7.25 (m, 1H), 3.42 (d, *J* = 16.3 Hz, 1H), 2.88 (d, *J* = 16.2 Hz, 1H), 2.54 (s, 3H), 1.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 165.4, 147.0, 139.0, 135.7, 135.4, 132.1, 131.0, 129.2, 127.2, 124.4, 122.7, 122.3, 121.8, 65.2, 46.9, 21.7, 18.7. HRMS (ESI) calcd for $C_{18}H_{15}NO_2Na$ $[M+Na]^+$ 300.0995, found 300.1003.

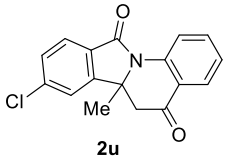
8-fluoro-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2t):



2t

White solid (66.1 mg, 78%, m.p.: 192.6–193.2 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.0 Hz, 1H), 8.08 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.99 (dd, *J* = 8.4, 4.9 Hz, 1H), 7.70 (td, *J* = 8.5, 8.0, 1.6 Hz, 1H), 7.30-7.24 (m, 2H), 7.19 (dd, *J* = 7.8, 2.1 Hz, 1H), 3.13 (d, *J* = 16.1 Hz, 1H), 2.78 (d, *J* = 16.1 Hz, 1H), 1.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.8, 166.1 (d, *J* = 254.7 Hz), 164.3, 152.3 (d, *J* = 9.5 Hz), 139.1, 135.7, 127.5, 127.4 (d, *J* = 10.3 Hz), 126.7 (d, *J* = 2.2 Hz), 124.6, 122.3, 121.6, 117.2 (d, *J* = 23.5 Hz), 108.6 (d, *J* = 24.3 Hz), 64.0 (d, *J* = 2.7 Hz), 48.5, 23.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.98. HRMS (ESI) calcd for $C_{17}H_{12}FNO_2Na$ $[M+Na]^+$ 304.0744, found 304.0753.

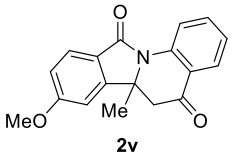
8-chloro-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2u):



2u

White solid (67.5 mg, 76%, m.p.: 197.4–199.2 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 8.5 Hz, 1H), 8.09 (d, *J* = 7.6 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.71 (t, *J* = 7.5 Hz, 1H), 7.55 (d, *J* = 8.2 Hz, 1H), 7.48 (s, 1H), 7.31-7.26 (m, 1H), 3.13 (d, *J* = 16.4 Hz, 1H), 2.77 (d, *J* = 16.1 Hz, 1H), 1.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.8, 164.3, 151.2, 139.6, 138.9, 135.8, 129.9, 129.1, 127.5, 126.3, 124.7, 122.2, 121.7, 121.6, 64.1, 48.4, 23.9. HRMS (ESI) calcd for $C_{17}H_{12}ClNO_2Na$ $[M+Na]^+$ 320.0449, found 320.0458.

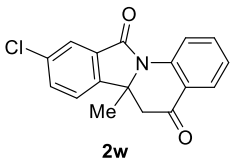
8-methoxy-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2v):



2v

White solid (58.1 mg, 66%, m.p.: 181.6–182.7 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 7.7 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 7.3 Hz, 1H), 7.07 (d, *J* = 8.4 Hz, 1H), 6.94 (s, 1H), 3.93 (s, 3H), 3.11 (d, *J* = 16.1 Hz, 1H), 2.77 (d, *J* = 16.2 Hz, 1H), 1.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 165.2, 164.1, 152.2, 139.4, 135.6, 127.3, 126.6, 124.1, 122.9, 122.1, 121.5, 115.7, 105.8, 63.8, 55.9, 48.6, 24.0. HRMS (ESI) calcd for $C_{18}H_{15}NO_3Na$ $[M+Na]^+$ 316.0944, found 316.0946.

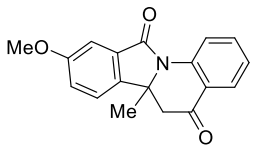
9-chloro-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2w):



2w

White solid (63.1 mg, 71%, m.p.: 178.1–179.3 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 8.1 Hz, 1H), 8.07 (d, *J* = 7.7 Hz, 1H), 7.92 (s, 1H), 7.72-7.63 (m, 2H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.31-7.27 (m, 1H), 3.15 (d, *J* = 16.2 Hz, 1H), 2.77 (d, *J* = 16.2 Hz, 1H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 163.9, 147.9, 138.8, 135.7, 135.5, 133.4, 132.3, 127.4, 125.0, 124.8, 122.3, 122.2, 121.7, 64.2, 48.4, 23.9. HRMS (ESI) calcd for $C_{17}H_{12}ClNO_2Na$ $[M+Na]^+$ 320.0449, found 320.0456.

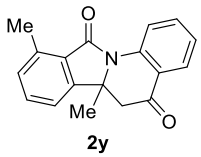
9-methoxy-6a-methyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2x):



2x

White solid (58.1 mg, 66%, m.p.: 198.3–199.6 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.2 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.44 (s, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.29-7.21 (m, 2H), 3.91 (s, 3H), 3.13 (d, *J* = 16.2 Hz, 1H), 2.72 (d, *J* = 16.1 Hz, 1H), 1.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 165.3, 160.7, 142.3, 139.2, 135.6, 131.9, 127.4, 124.4, 122.3, 121.9, 121.7, 121.6, 107.2, 64.0, 55.9, 48.9, 24.0. HRMS (ESI) calcd for $C_{18}H_{15}NO_3Na$ $[M+Na]^+$ 316.0944, found 316.0945.

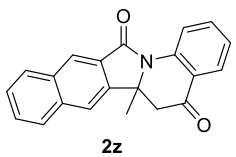
6a,10-dimethyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2y):



2y

White solid (60.7 mg, 73%, m.p.: 155.1–156.8 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.3 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.30-7.24 (m, 3H), 3.12 (d, *J* = 16.2 Hz, 1H), 2.80 (s, 3H), 2.73 (d, *J* = 16.5 Hz, 1H), 1.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.6, 166.3, 150.5, 139.4, 139.3, 135.6, 132.7, 131.1, 127.5, 127.4, 124.3, 122.3, 121.6, 118.3, 63.3, 48.8, 24.1, 17.7. HRMS (ESI) calcd for $C_{18}H_{15}NO_2Na$ $[M+Na]^+$ 300.0995, found 300.1002.

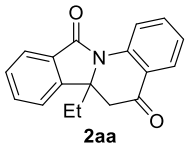
6a-methyl-6,6a-dihydrobenzo[5,6]isoindolo[2,1-*a*]quinoline-5,13-dione (2z):



2z

White solid (57.5 mg, 61%, m.p.: 221.2–223.4 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.56-8.54 (m, 2H), 8.12-8.06 (m, 2H), 7.98 (d, *J* = 7.7 Hz, 1H), 7.90 (s, 1H), 7.74-7.70 (m, 1H), 7.66-7.59 (m, 2H), 7.31-7.27 (m, 1H), 3.26 (d, *J* = 16.3 Hz, 1H), 2.86 (d, *J* = 16.3 Hz, 1H), 1.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ192.4, 165.3, 144.6, 139.3, 135.9, 135.7, 133.5, 129.9, 128.6, 128.5, 128.4, 127.5, 127.0, 125.9, 124.7, 122.5, 122.0, 120.0, 64.4, 49.3, 24.7. HRMS (ESI) calcd for $C_{21}H_{15}NO_2Na$ $[M+Na]^+$ 336.0995, found 336.0993.

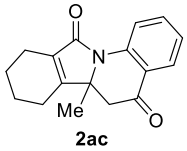
6a-ethyl-6,6a-dihydroisoindolo[2,1-*a*]quinoline-5,11-dione (2aa):



2aa

White solid (50.1 mg, 60%, m.p.: 156.4–160.1 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.2 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.74-7.60 (m, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.29-7.25 (m, 1H), 3.19 (d, *J* = 16.4 Hz, 1H), 2.82 (d, *J* = 16.4 Hz, 1H), 2.19-2.10 (m, 1H), 2.02-1.93 (m, 1H), 0.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 166.0, 147.6, 139.0, 135.6, 133.2, 131.8, 129.2, 127.4, 124.8, 124.5, 122.6, 121.6, 120.9, 67.3, 48.3, 28.6, 7.5. HRMS (ESI) calcd for $C_{18}H_{15}NO_2Na$ $[M+Na]^+$ 300.0995, found 300.1002.

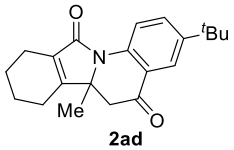
6a-methyl-6,6a,7,8,9,10-hexahydroisoindolo[2,1-*a*]quinoline-5,11-dione (2ac):



2ac

White solid (52.6 mg, 66%, m.p.: 148.5–150.3 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.3 Hz, 1H), 7.99 (d, *J* = 7.9 Hz, 1H), 7.65-7.61 (m, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 2.83 (d, *J* = 15.8 Hz, 1H), 2.53 (d, *J* = 15.8 Hz, 1H), 2.39-2.21 (m, 4H), 1.84-1.73 (m, 4H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.7, 168.3, 160.4, 139.5, 135.7, 131.2, 127.3, 123.6, 122.0, 121.0, 65.4, 46.9, 22.1, 21.9, 21.6, 21.4, 20.1. HRMS (ESI) calcd for $C_{17}H_{17}NO_2Na$ $[M+Na]^+$ 290.1151, found 290.1150.

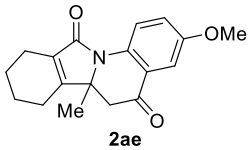
3-(*tert*-butyl)-6a-methyl-6,6a,7,8,9,10-hexahydroisoindolo[2,1-*a*]quinoline-5,11-dione (2ad):



2ad

White solid (60.3 mg, 62%, m.p.: 233.7–235.5 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.7 Hz, 1H), 8.00 (d, *J* = 2.5 Hz, 1H), 7.70 (dd, *J* = 8.7, 2.5 Hz, 1H), 2.83 (d, *J* = 15.8 Hz, 1H), 2.52 (d, *J* = 15.8 Hz, 1H), 2.34-2.20 (m, 4H), 1.90-1.71 (m, 4H), 1.36 (s, 3H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.98, 168.16, 160.14, 146.63, 137.13, 133.27, 131.18, 123.45, 121.44, 120.68, 65.40, 47.01, 34.67, 31.29, 22.07, 21.90, 21.63, 21.41, 20.12. HRMS (ESI) calcd for $C_{21}H_{25}NO_2Na$ $[M+Na]^+$ 346.1778, found 346.1779.

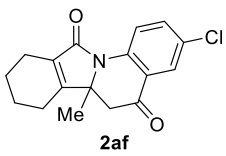
3-methoxy-6a-methyl-6,6a,7,8,9,10-hexahydroisoindolo[2,1-*a*]quinoline-5,11-dione (2ae):



2ae

White solid (56.5 mg, 63%, m.p.: 125.3–126.6 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 9.0 Hz, 1H), 7.45 (d, *J* = 3.1 Hz, 1H), 7.23 (dd, *J* = 9.1, 3.1 Hz, 1H), 3.84 (s, 3H), 2.83 (d, *J* = 15.9 Hz, 1H), 2.52 (d, *J* = 15.9 Hz, 1H), 2.37-2.20 (m, 4H), 1.88-1.72 (m, 4H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.58, 167.95, 159.79, 155.75, 133.49, 131.21, 123.77, 122.66, 122.57, 108.88, 65.44, 55.72, 46.94, 22.05, 21.88, 21.48, 21.38, 20.10. HRMS (ESI) calcd for $C_{18}H_{19}NO_3Na$ $[M+Na]^+$ 320.1257, found 320.1257.

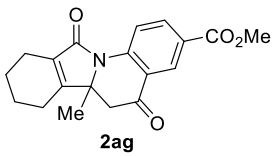
3-chloro-6a-methyl-6,6a,7,8,9,10-hexahydroisoindolo[2,1-*a*]quinoline-5,11-dione (2af):



2af

White solid (62.4 mg, 69%, m.p.: 168.6–170.1 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.8 Hz, 1H), 7.95 (d, *J* = 2.6 Hz, 1H), 7.57 (dd, *J* = 8.9, 2.6 Hz, 1H), 2.85 (d, *J* = 15.9 Hz, 1H), 2.53 (d, *J* = 15.9 Hz, 1H), 2.37-2.21 (m, 4H), 1.90-1.73 (m, 4H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.45, 168.07, 160.48, 137.82, 135.42, 131.13, 129.24, 126.79, 122.88, 122.45, 65.30, 46.60, 21.96, 21.78, 21.59, 21.43, 20.05. HRMS (ESI) calcd for $C_{17}H_{16}ClNO_2Na$ $[M+Na]^+$ 324.0762, found 324.0765.

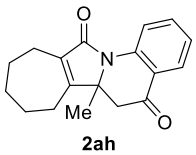
methyl 6a-methyl-5,11-dioxo-5,6,6a,7,8,9,10,11-octahydroisoindolo[2,1-*a*]quinoline-3-carboxylate (2ag):



2ag

White solid (47.7 mg, 49%, m.p.: 172.4–173.5 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (br, 1H), 8.43 (dd, *J* = 8.7, 1.6 Hz, 1H), 8.27 (m, 1H), 3.93 (s, 3H), 2.89 (d, *J* = 15.8 Hz, 1H), 2.57 (d, *J* = 15.8 Hz, 1H), 2.38-2.23 (m, 4H), 1.87-1.76 (m, 4H), 1.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.66, 168.28, 166.06, 161.01, 142.65, 136.30, 131.11, 129.26, 125.13, 121.38, 120.57, 65.36, 52.33, 46.49, 21.93, 21.76, 21.48, 20.04. HRMS (ESI) calcd for $C_{19}H_{19}NO_4Na$ $[M+Na]^+$ 348.1206, found 348.1207.

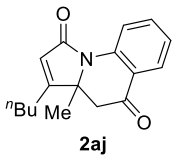
6a-methyl-6a,7,8,9,10,11-hexahydro-5*H*-cyclohepta[3,4]pyrrolo[1,2-*a*]quinoline-5,12(6*H*)-dione (2ah):



2ah

White solid (59.1 mg, 70%, m.p.: 151.5–153.2 °C). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.3 Hz, 1H), 7.99 (d, *J* = 7.9, 1.7 Hz, 1H), 7.65-7.61 (m, 1H), 7.20-7.16 (m, 1H), 2.87 (d, *J* = 15.8 Hz, 1H), 2.59-2.37 (m, 5H), 1.90-1.58 (m, 6H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.6, 168.4, 162.7, 139.5, 135.6, 134.3, 127.1, 123.6, 121.9, 120.8, 65.1, 46.3, 31.1, 27.2, 27.0, 26.8, 24.5, 21.1. HRMS (ESI) calcd for $C_{18}H_{19}NO_2Na$ $[M+Na]^+$ 304.1308, found 304.1309.

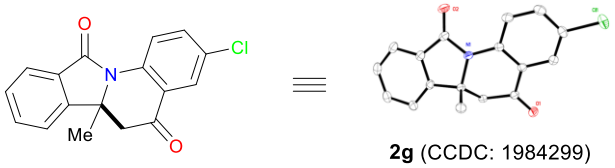
3-butyl-3a-methyl-3a,4-dihydropyrrolo[1,2-*a*]quinoline-1,5-dione (2aj):



2aj

White solid (14.3 mg, 18%, m.p.: 103.3–104.9 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.3 Hz, 1H), 8.01 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.66-7.62 (m, 1H), 7.22-7.18 (m, 1H), 6.00 (t, *J* = 1.7 Hz, 1H), 2.88 (d, *J* = 15.8 Hz, 1H), 2.59 (d, *J* = 15.8 Hz, 1H), 2.41-2.23 (m, 2H), 1.70-1.63 (m, 2H), 1.50-1.41 (m, 2H), 1.40 (s, 3H), 0.98 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.22, 169.76, 167.92, 139.23, 135.76, 127.29, 123.90, 121.91, 121.09, 120.74, 67.29, 46.85, 28.93, 26.34, 22.55, 21.79, 13.95. HRMS (ESI) calcd for $C_{17}H_{19}NO_2Na$ $[M+Na]^+$ 292.1308, found 292.1315.

7. X-Ray crystal structures of product 2g



2g (CCDC: 1984299)

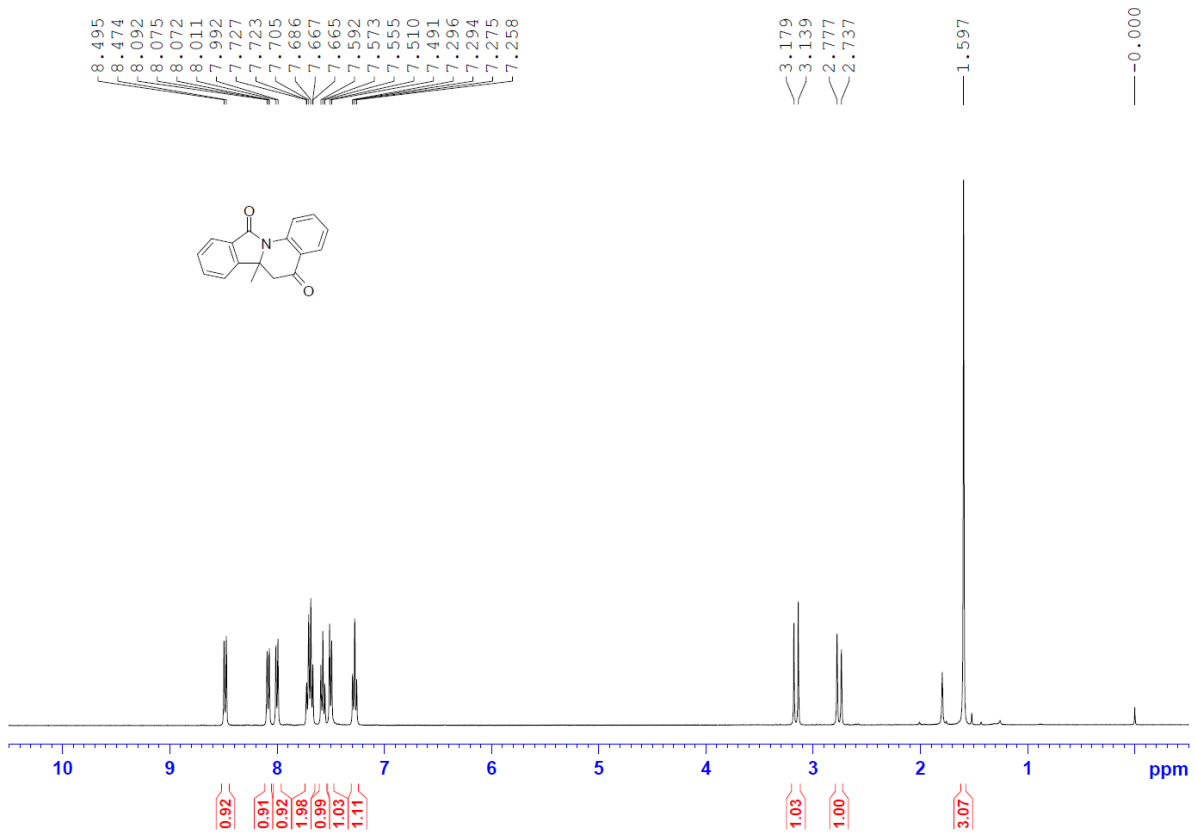
Empirical formula	$C_{17}H_{12}ClNO_2$
Formula weight	297.73
Temperature/K	180(2)
Crystal system	monoclinic
Space group	P 21/n
a/Å	7.0426(6)
b/Å	10.7671(10)
c/Å	18.0428(16)
α/°	90
β/°	98.613(3)
γ/°	90
Volume/Å^3	1352.7(2)
Z	4
ρ_{calc}g/cm^3	1.462
μ/mm^{-1}	0.286
F(000)	616.0
Crystal size/mm^3	0.20 × 0.15 × 0.15
Radiation	MoK\a
2Θ range for data collection/°	2.966 to 28.383
Index ranges	-9≤ h ≤ 9, -14 ≤ k ≤ 14, -24 ≤ l ≤ 24
Reflections collected	19441
Independent reflections	3402 [R(int) = 0.0390]
Data/restraints/parameters	3402/0/190
Goodness-of-fit on F^2	0.816
Final R indexes [I>=2σ (I)]	R_1 = 0.0435, wR_2 = 0.1147
Final R indexes [all data]	R_1 = 0.0536, wR_2 = 0.1259
Largest diff. peak/hole / e Å^{-3}	0.372/-0.261

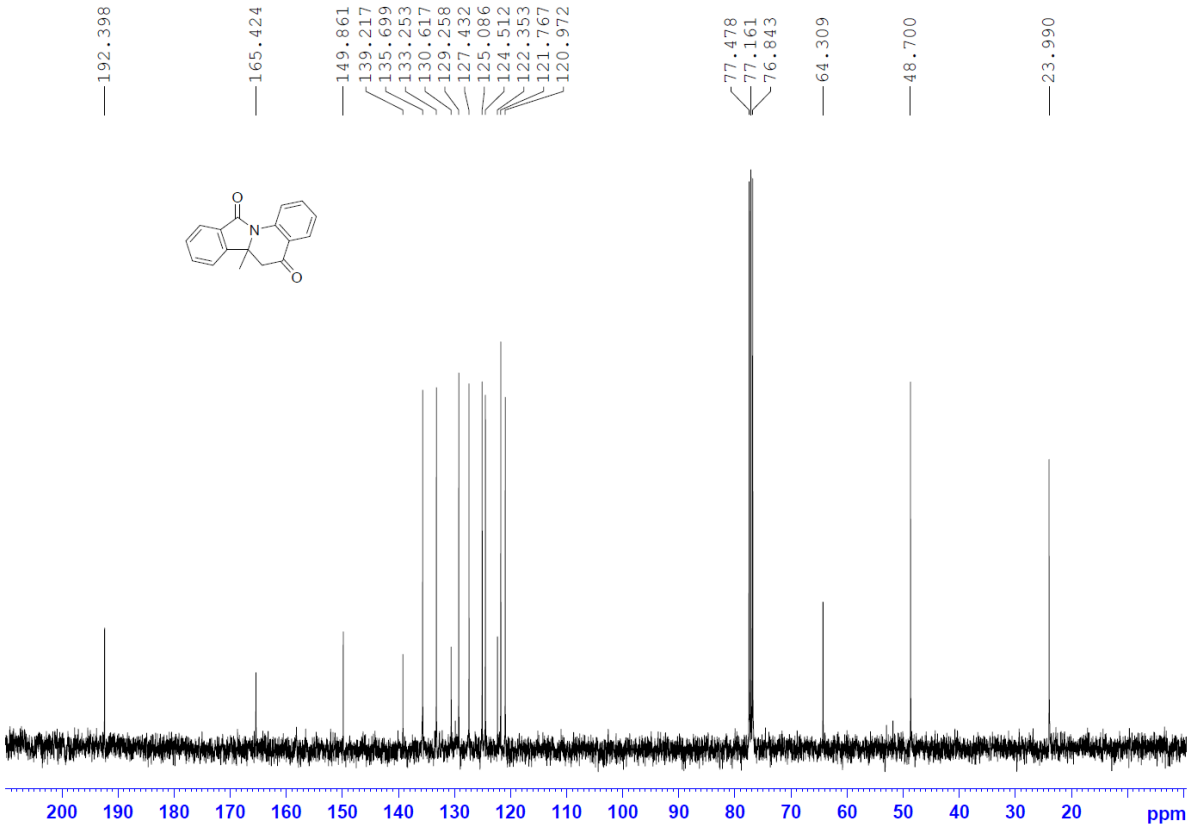
8. References

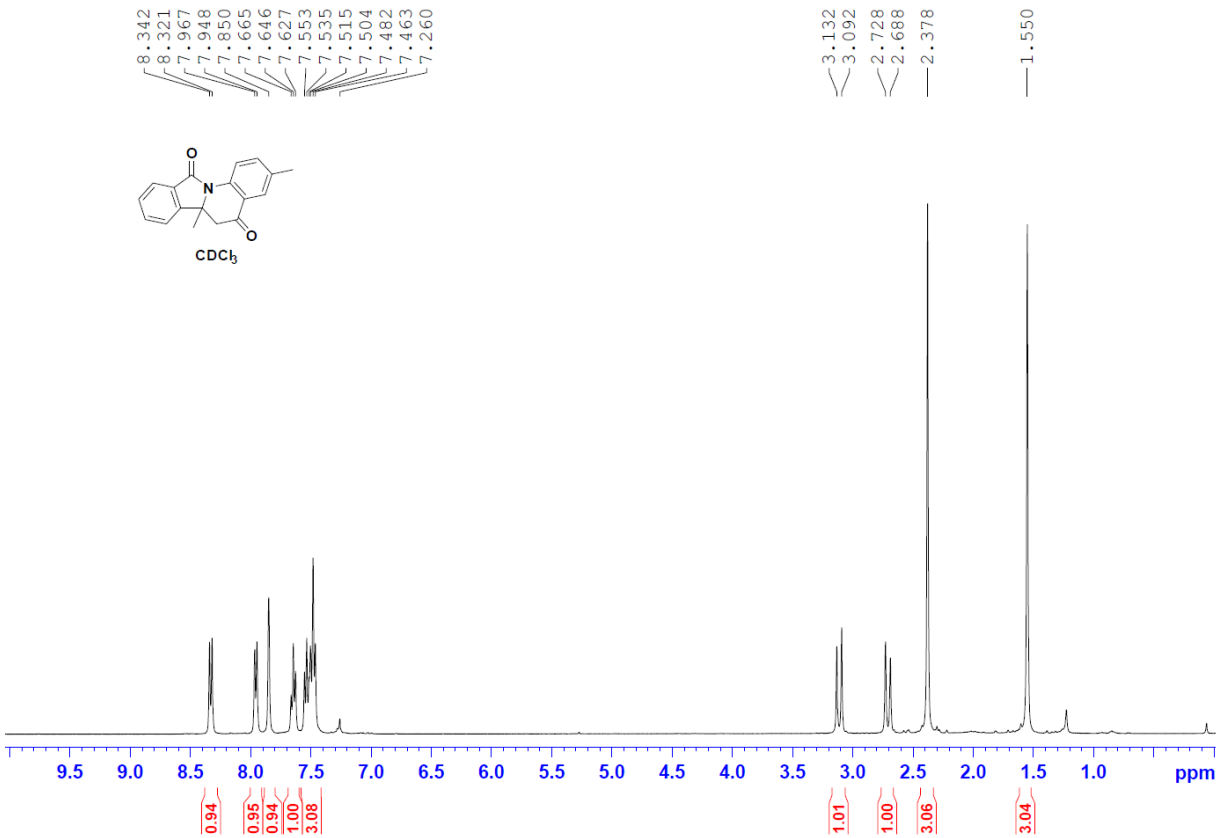
1. (a) Boulahjar, R.; Ouach, A.; Matteo, C.; Bourg, S.; Ravache, M.; Gueńel,R.L.; Marionneau,S.; Oullier,T.; Lozach,O.; Meijer,L.; Guguen-Guillouzo, C.; Lazar, S.; Akssira, M.; Troin, Y.; Guillaumet, G.; Routier, S. *J. Med. Chem.* **2012**, *55*, 9589; (b) Yada, A.; Okajima, S.; Murakami, M. *J. Am. Chem. Soc.* **2015,** *137*, 8708-8711.

2. (a) Trost, B. M.; Xu, J.; Schmidt, T. *J. Am. Chem. Soc.* **2009**, *131*, 18343-18357; (b) Trost, B. M.; Koller, R.; Schäffner, B. *Angew. Chem. Int. Ed*. **2012**, *51*, 8290-8293.

9. Copies of NMR spectra



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7.515
7.504
7.482
7.463
7.260
3.132
3.092
2.728
2.688
2.378
1.550
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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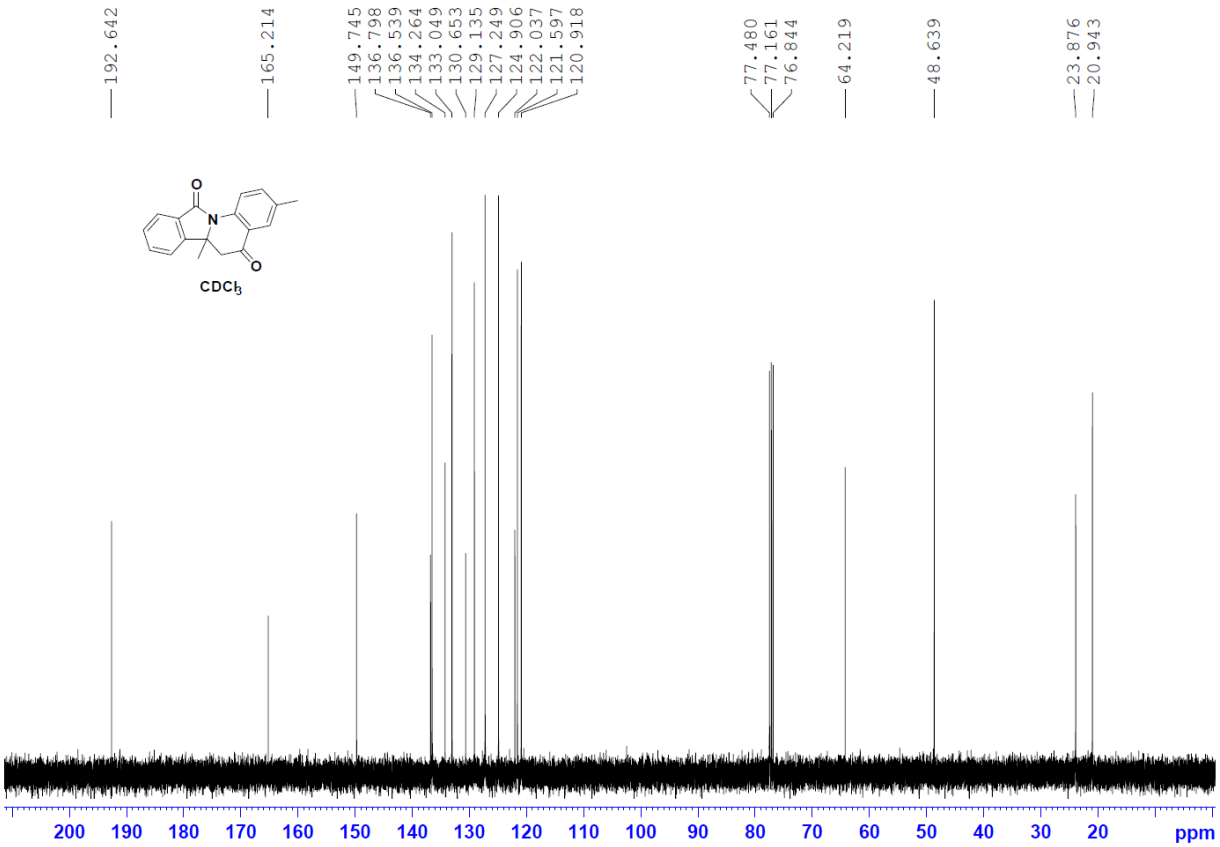
0.95
0.94
1.00
3.08
1.01
1.00
3.06
3.04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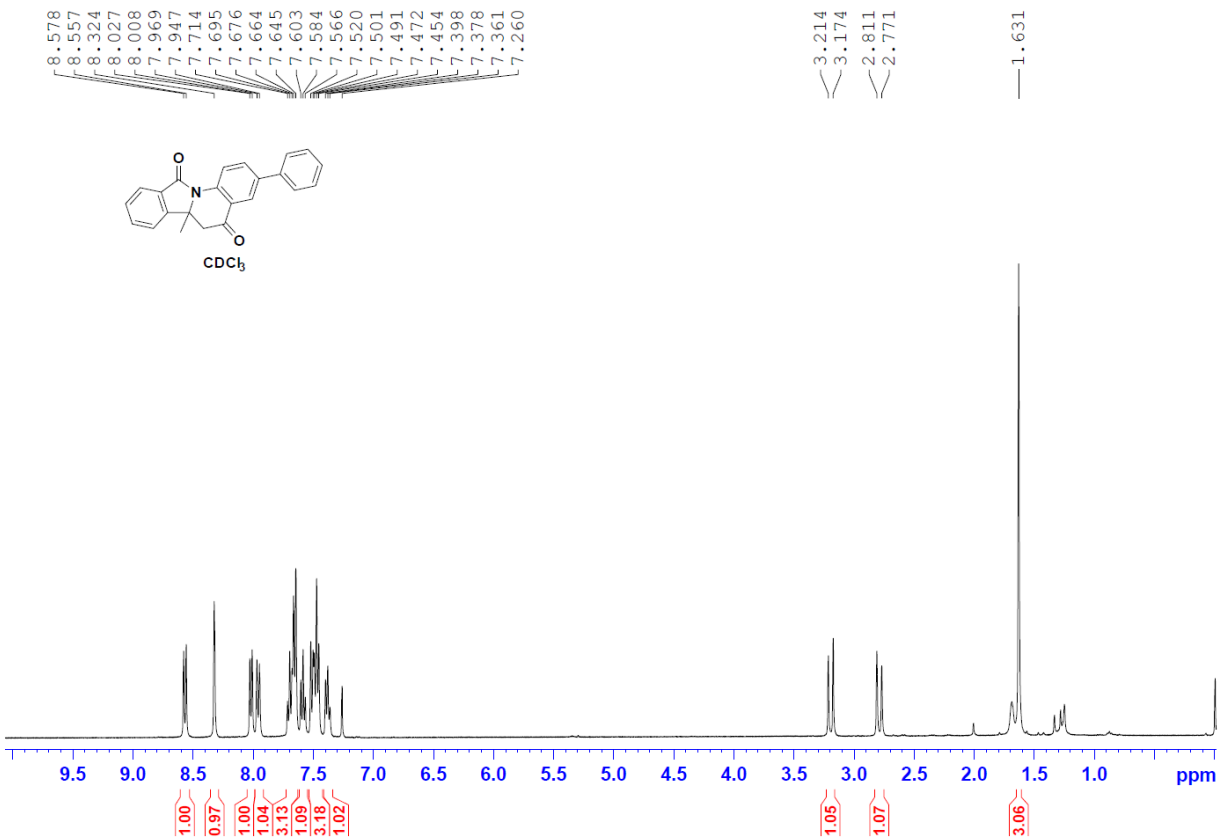
149.745
136.798
136.539
134.264
133.049
130.653
129.135
127.249
124.906
122.037
121.597
120.918
77.480
77.161
76.844
64.219
48.639
23.876
20.943
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.603
7.584
7.566
7.520
7.501
7.491
7.472
7.454
7.398
7.378
7.361
7.260
3.214
3.174
2.811
2.771
1.631
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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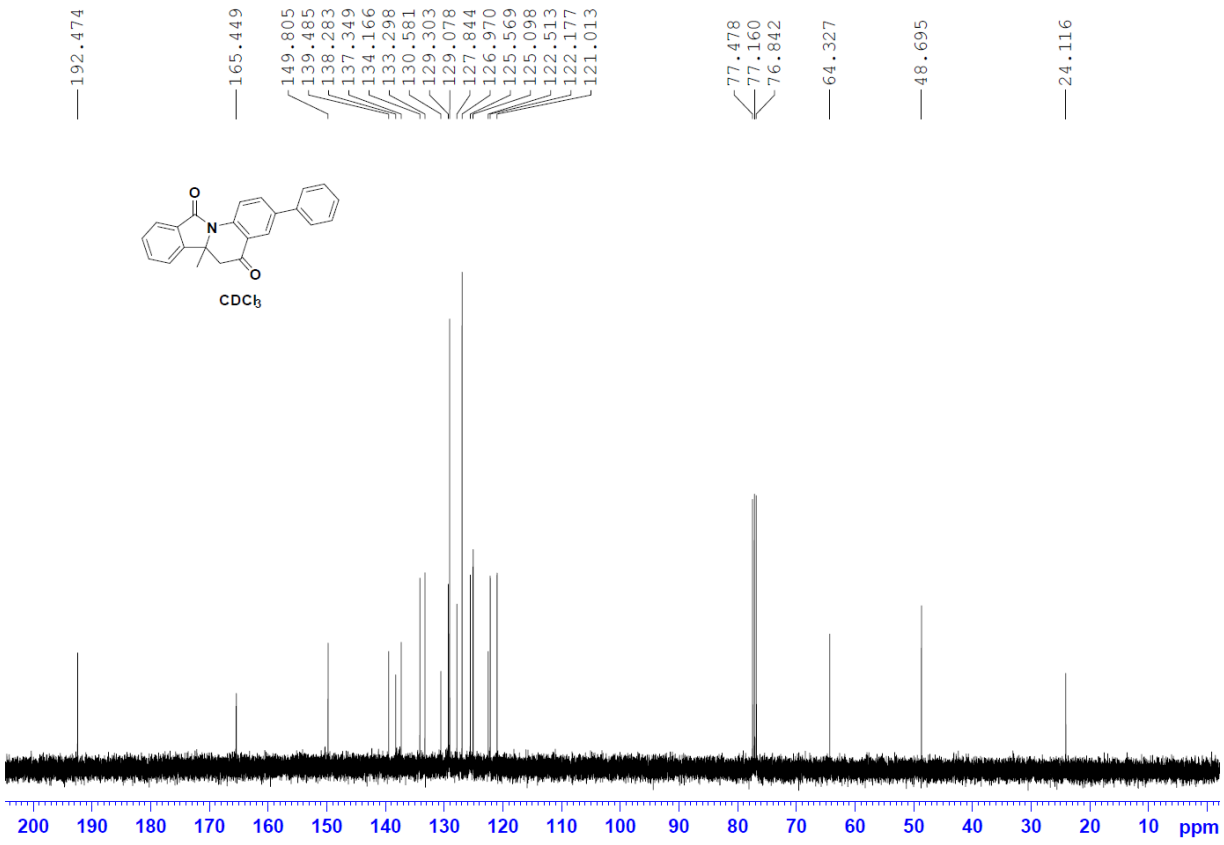
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133.298
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126.970
125.569
125.098
122.513
122.177
121.013
77.478
77.160
76.842
64.327
48.695
24.116
CDCl3
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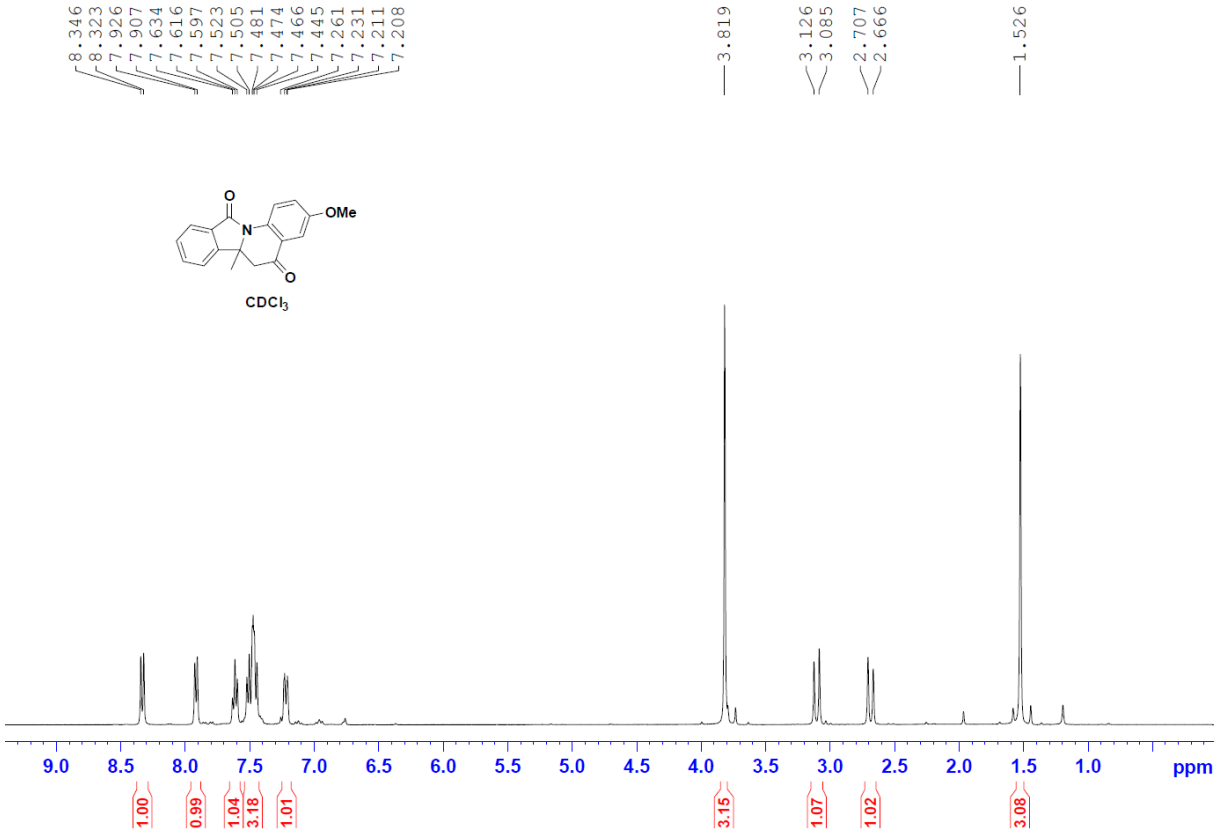
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7.445
7.261
7.231
7.211
7.208
3.819
3.126
3.085
2.707
2.666
1.526
OMe
CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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ppm
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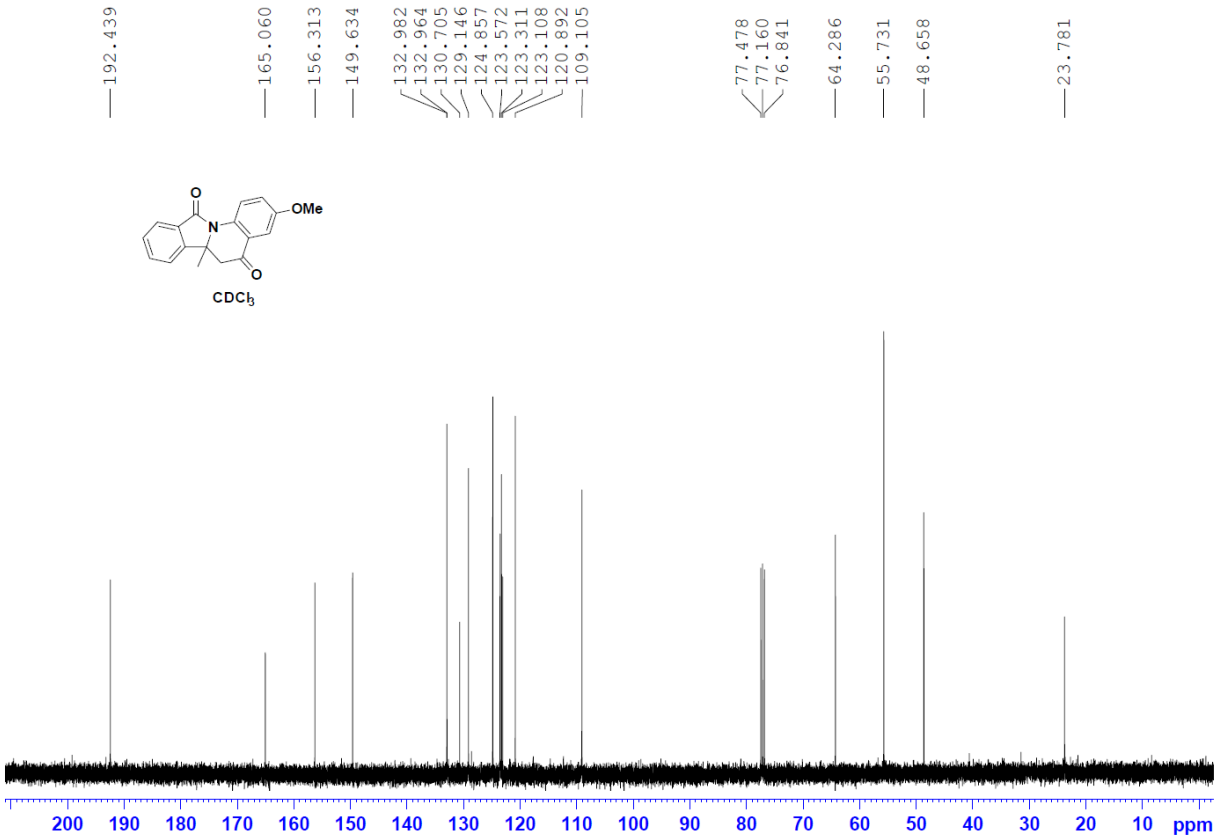
1.01
3.15
1.07
1.02
3.08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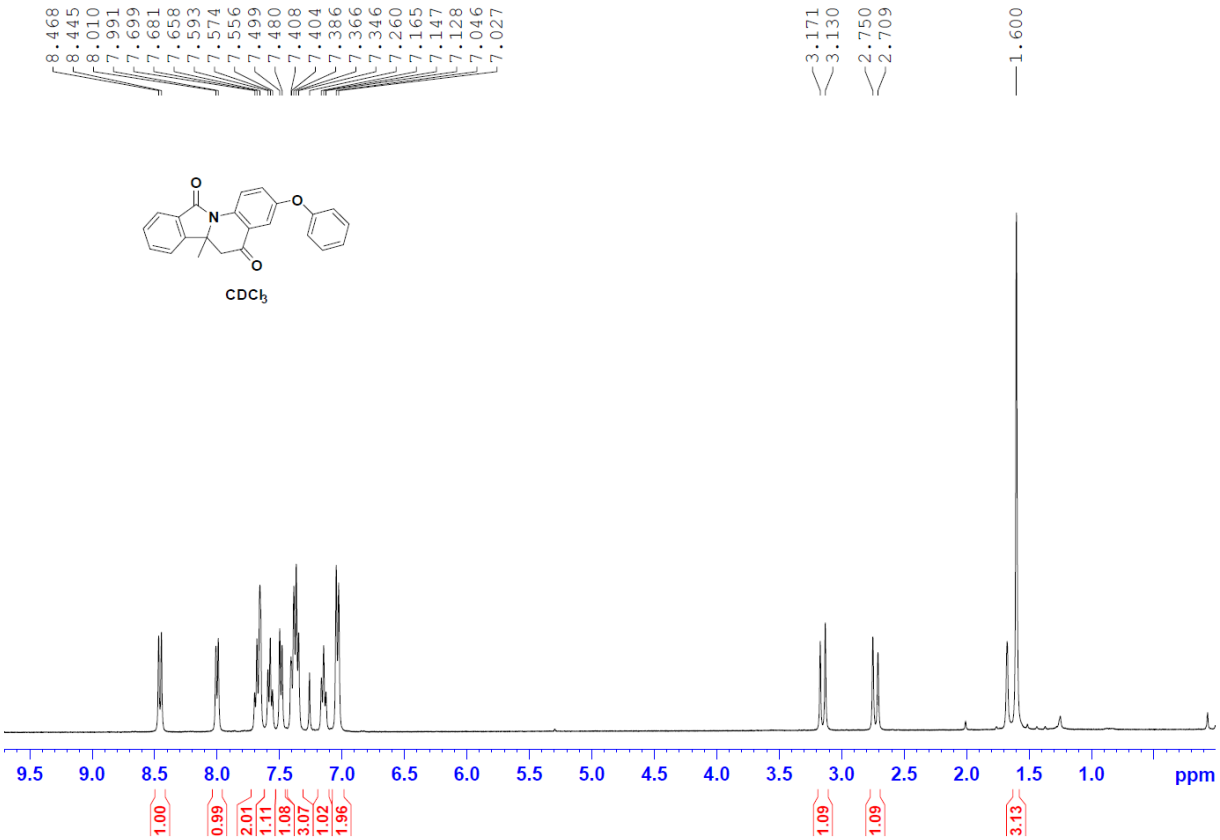
120.892
109.105
77.478
77.160
76.841
64.286
55.731
48.658
23.781
OMe
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.593
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7.499
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7.408
7.404
7.386
7.366
7.346
7.260
7.165
7.147
7.128
7.046
7.027
3.171
3.130
2.750
2.709
1.600
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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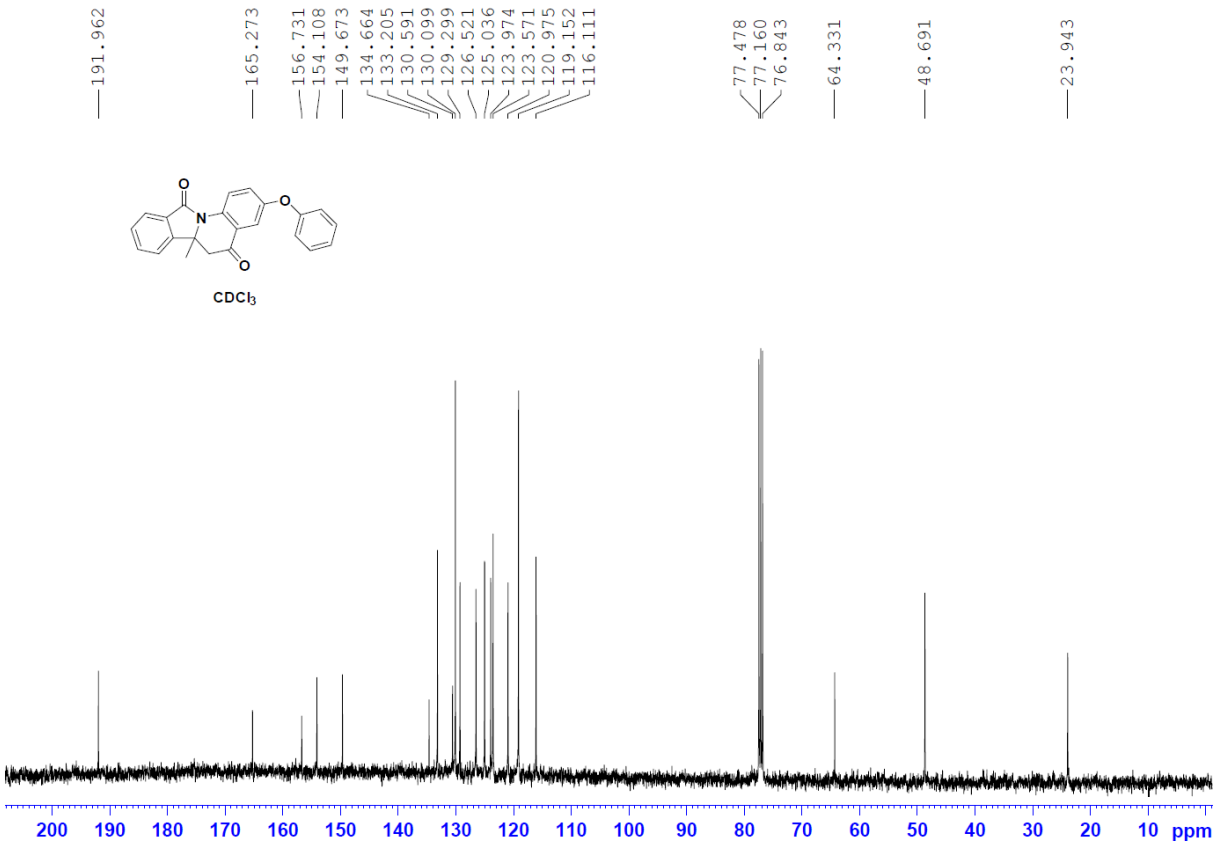
3.13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123.974
123.571
120.975
119.152
116.111
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64.331
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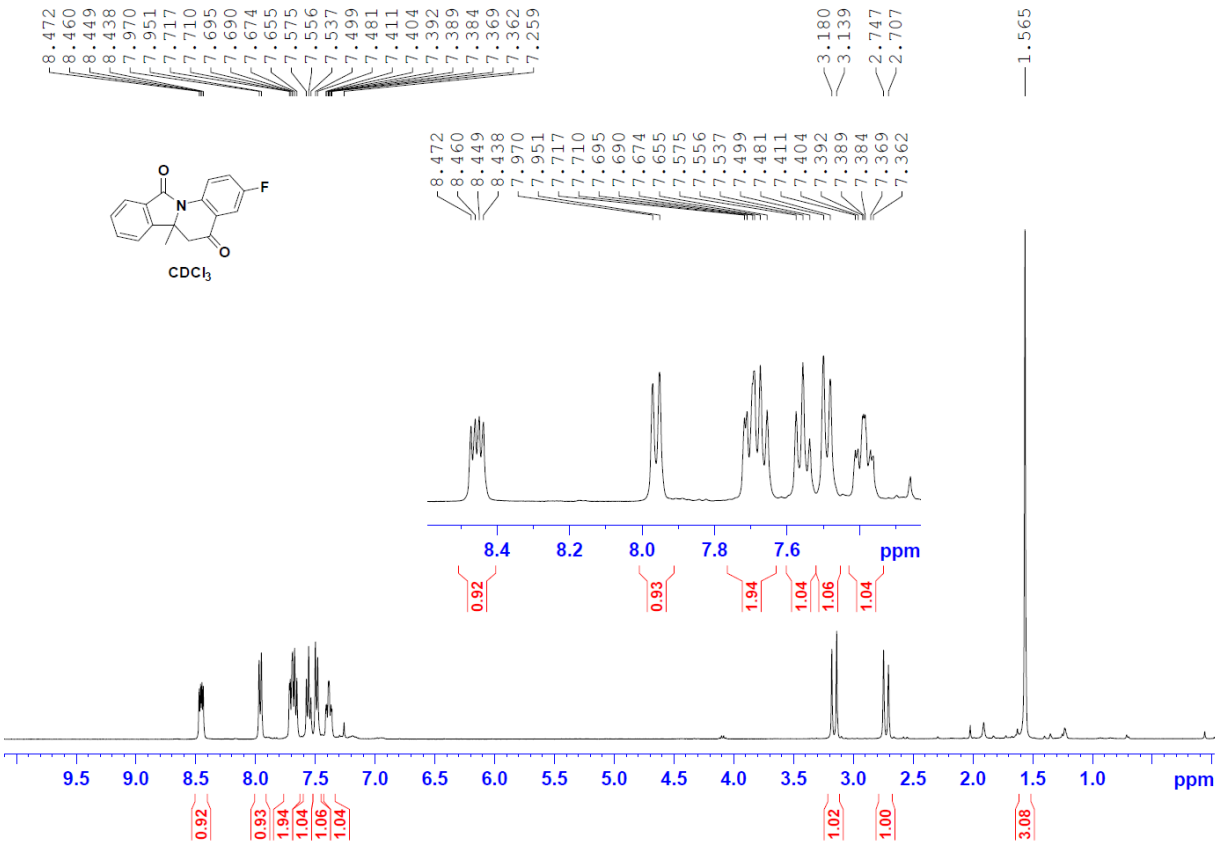
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.575
7.556
7.537
7.499
7.481
7.411
7.404
7.392
7.389
7.384
7.369
7.362
7.259
3.180
3.139
2.747
2.707
1.565
CDCl3
8.4
8.2
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7.8
7.6
ppm
0.92
0.93
1.94
1.04
1.06
1.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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ppm
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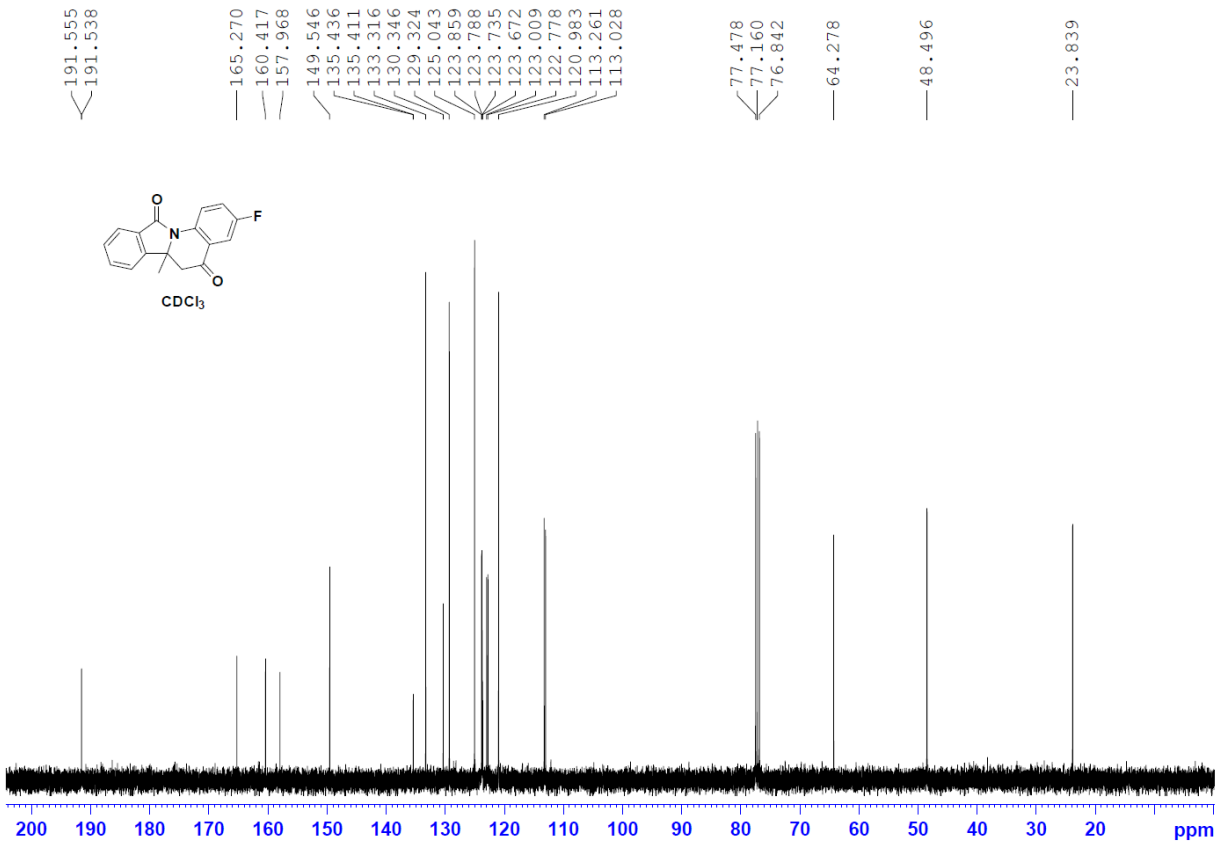
1.00
3.08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113.028
77.478
77.160
76.842
64.278
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23.839
CDCl3
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150
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130
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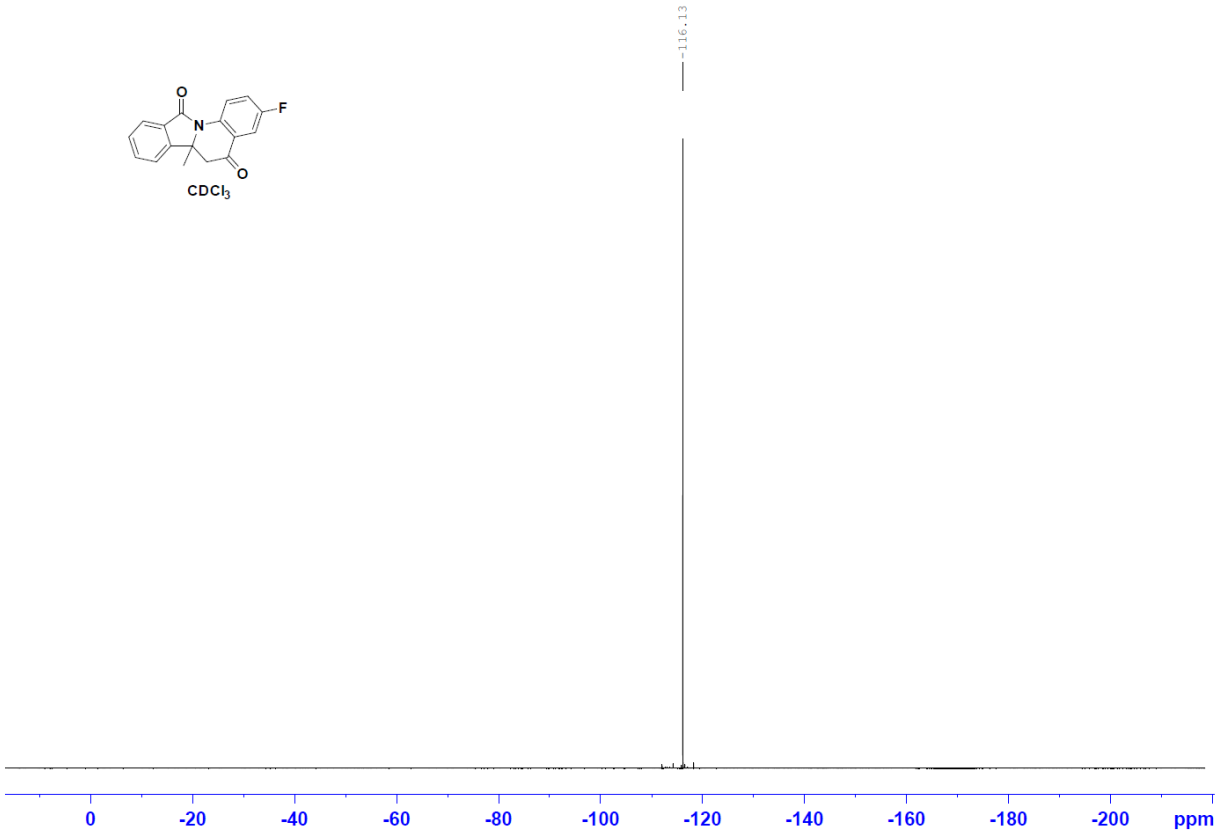
110
100
90
80
70
60
50
40
30
20
ppm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O
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F
O
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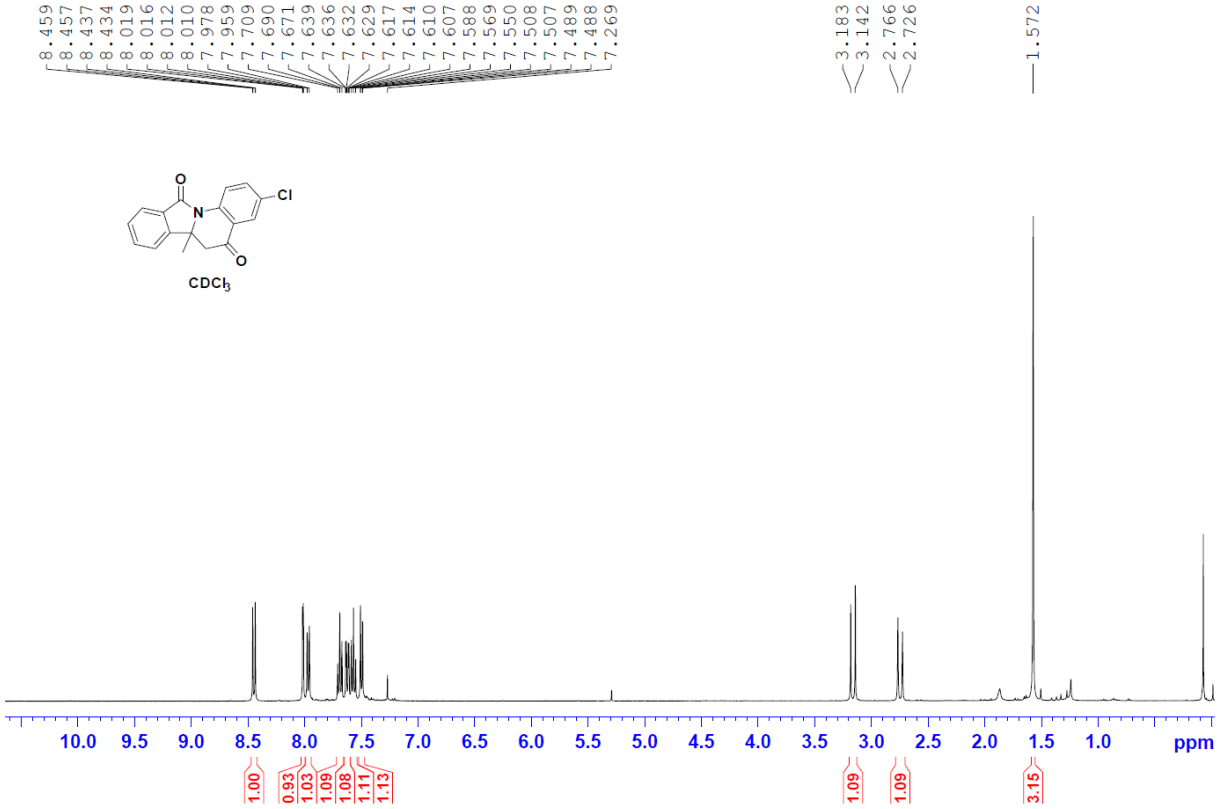
-200
ppm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7.610
7.607
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7.508
7.507
7.489
7.488
7.269
3.183
3.142
2.766
2.726
1.572
Cl
O
N
O
CDCl3
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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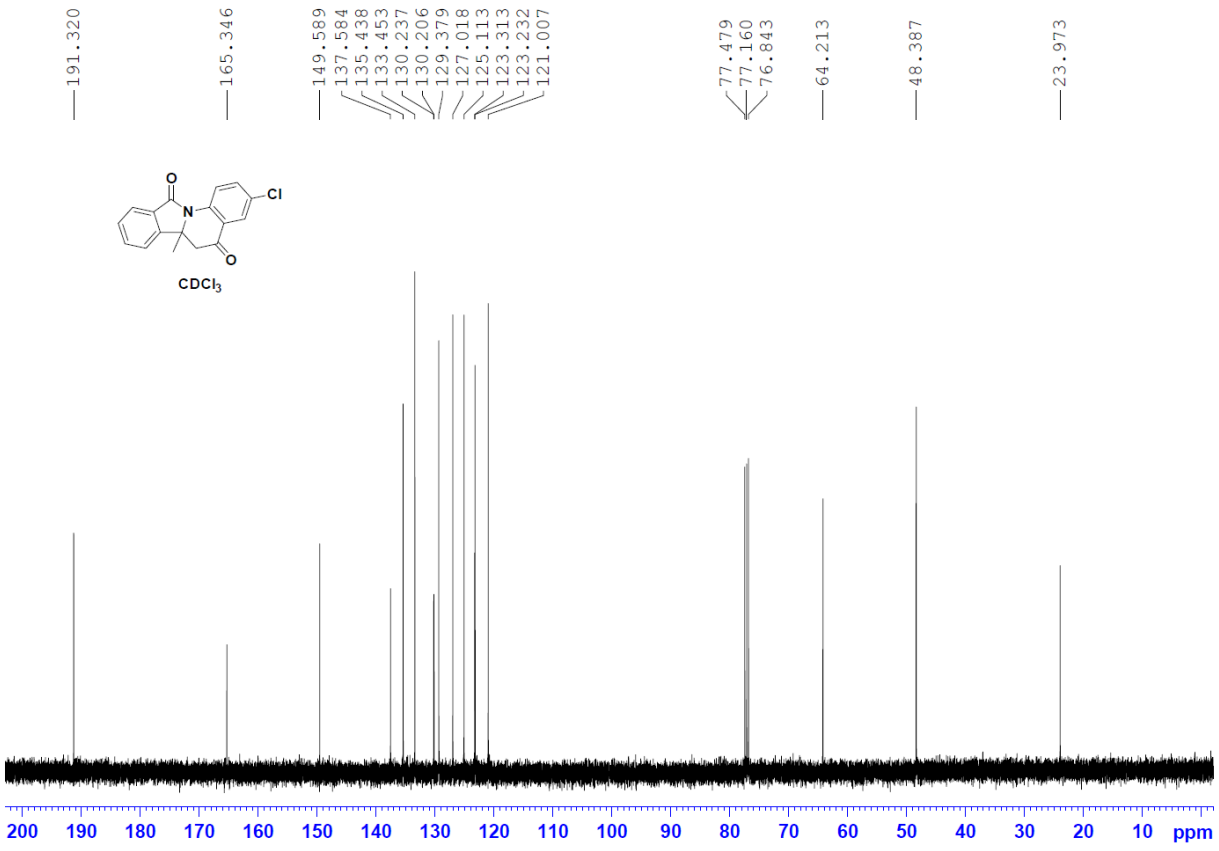
1.08
1.11
1.13
1.09
1.09
3.15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123.313
123.232
121.007
77.479
77.160
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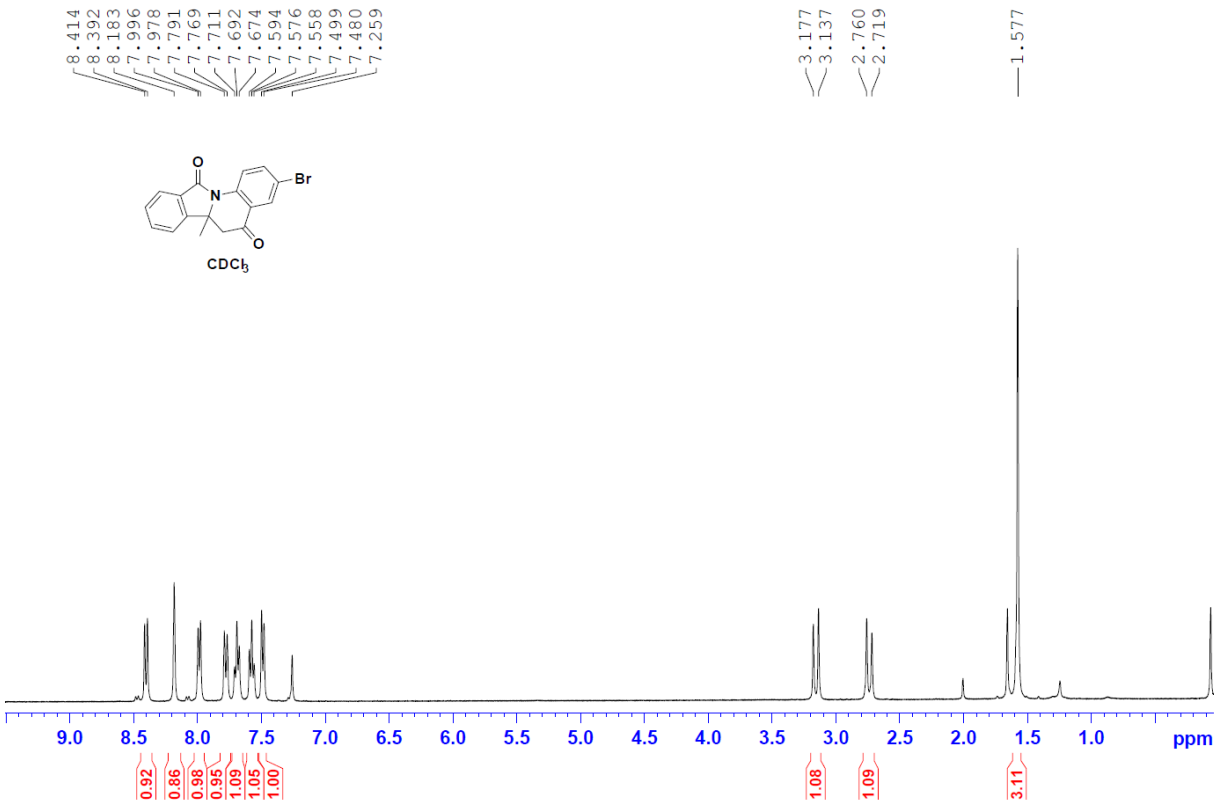
Cl
O
N
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.711
7.692
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7.576
7.558
7.499
7.480
7.259
3.177
3.137
2.760
2.719
1.577
Br
O
N
O
CDCl3
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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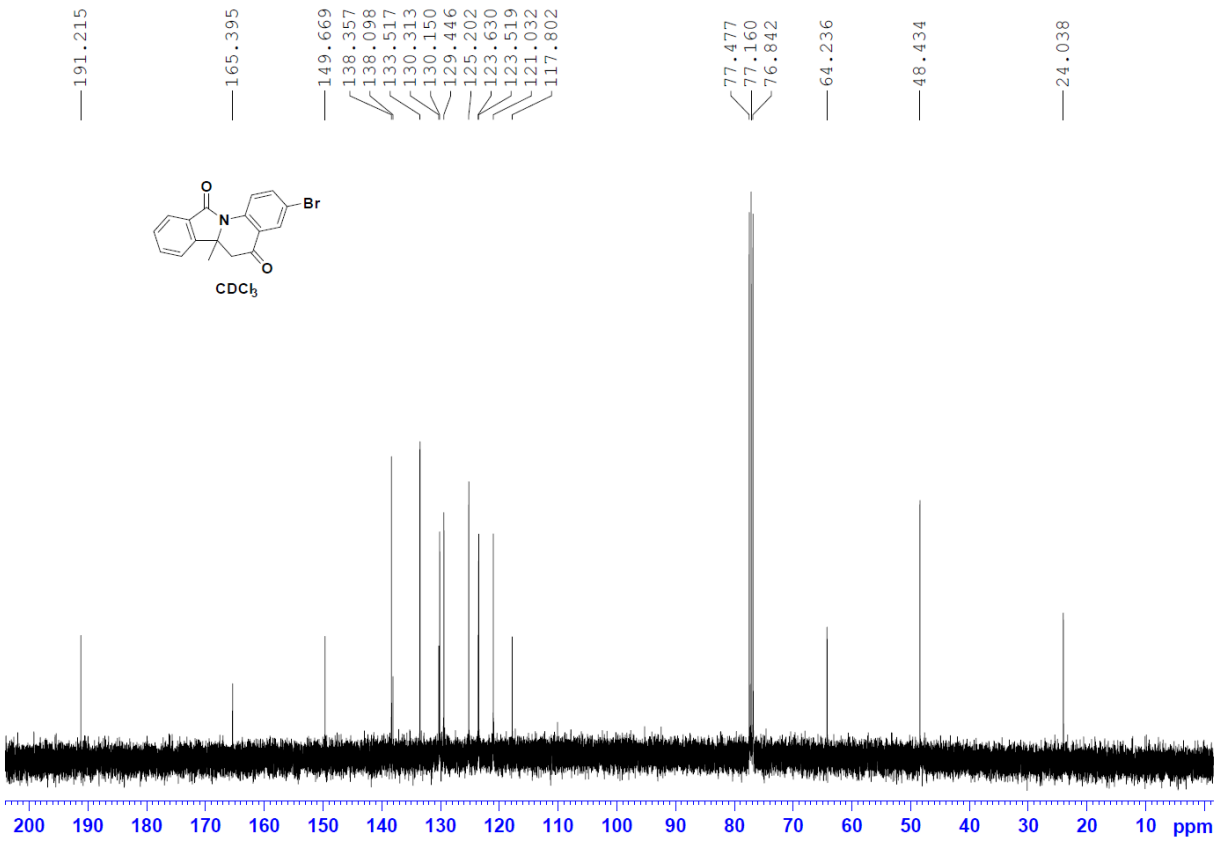
1.09
3.11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121.032
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77.477
77.160
76.842
64.236
48.434
24.038
Br
O
N
O
CDCl3
200
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180
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150
140
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90
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70
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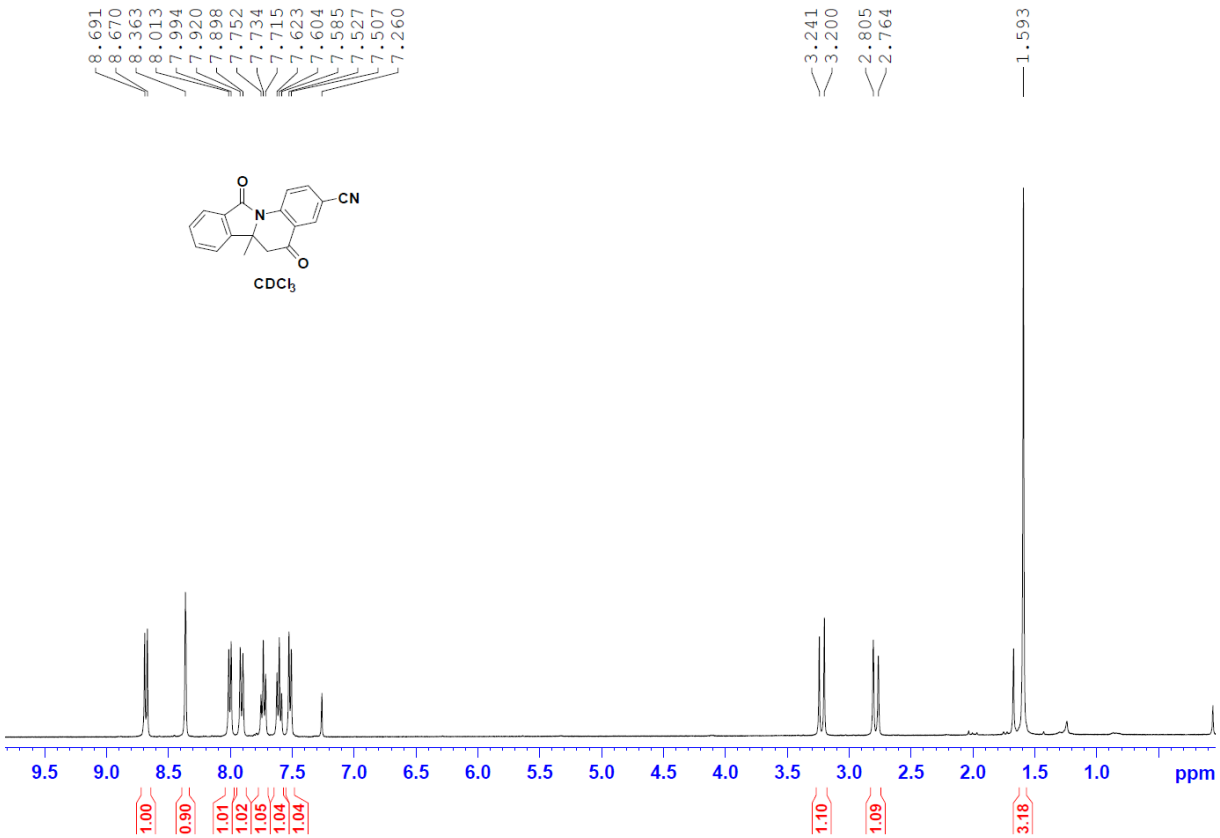
50
40
30
20
10
ppm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7.585
7.527
7.507
7.260
3.241
3.200
2.805
2.764
1.593
CN
O
N
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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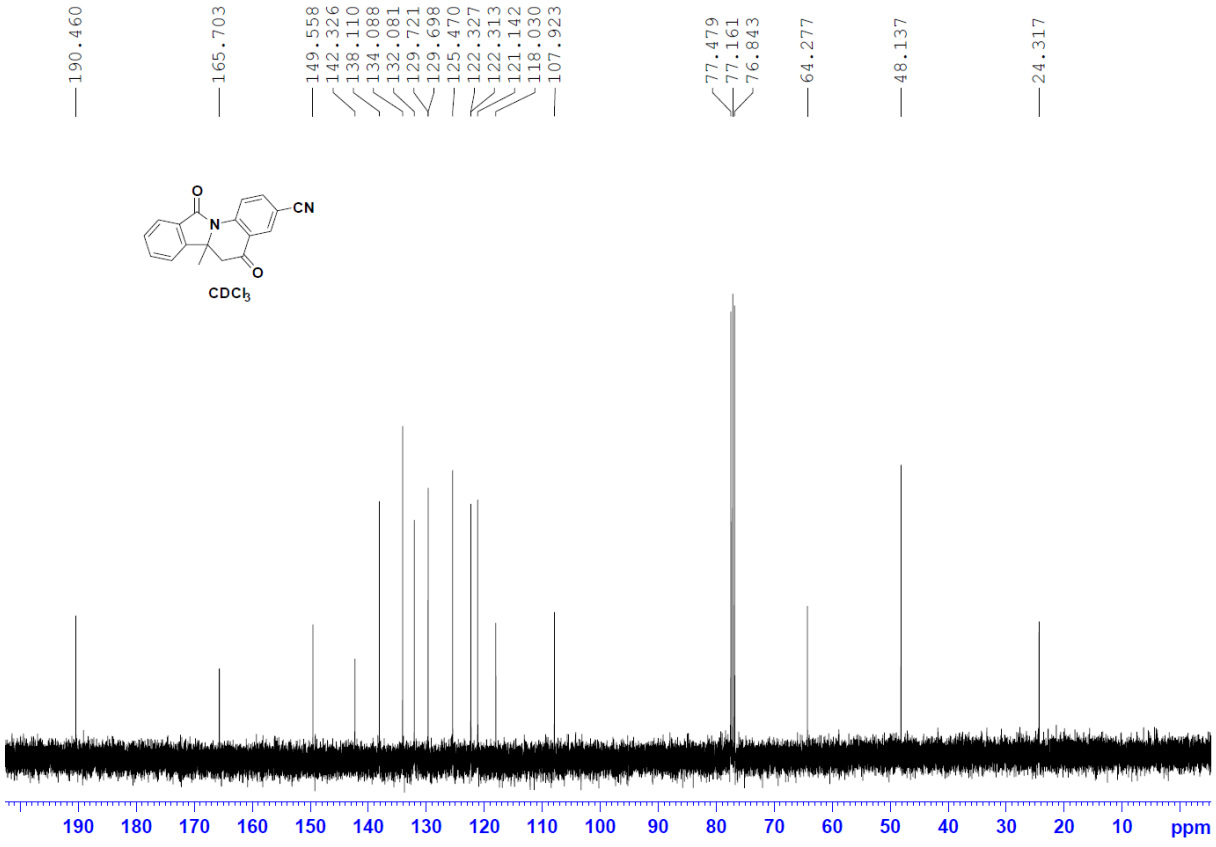
1.04
1.04
1.10
1.09
3.18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121.142
118.030
107.923
77.479
77.161
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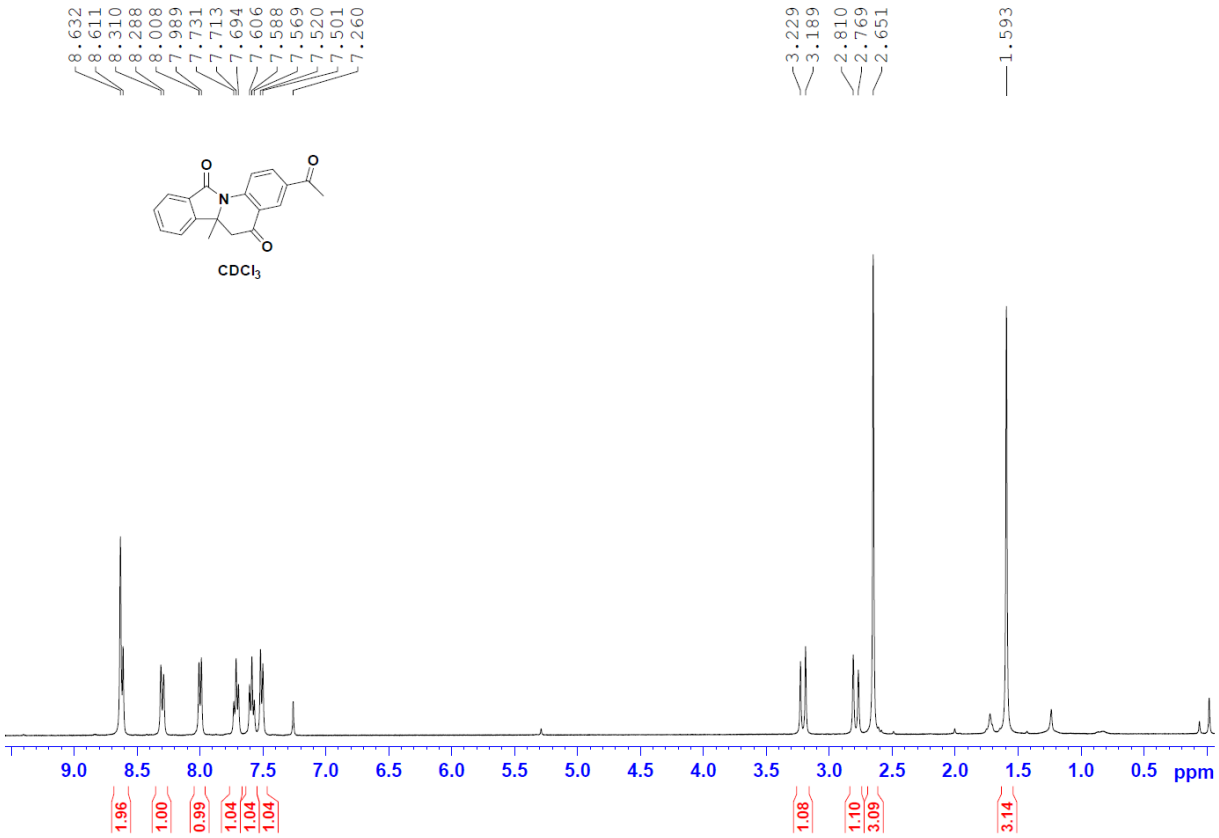
N
O
CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.606
7.588
7.569
7.520
7.501
7.260
3.229
3.189
2.810
2.769
2.651
1.593
CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.96
1.00
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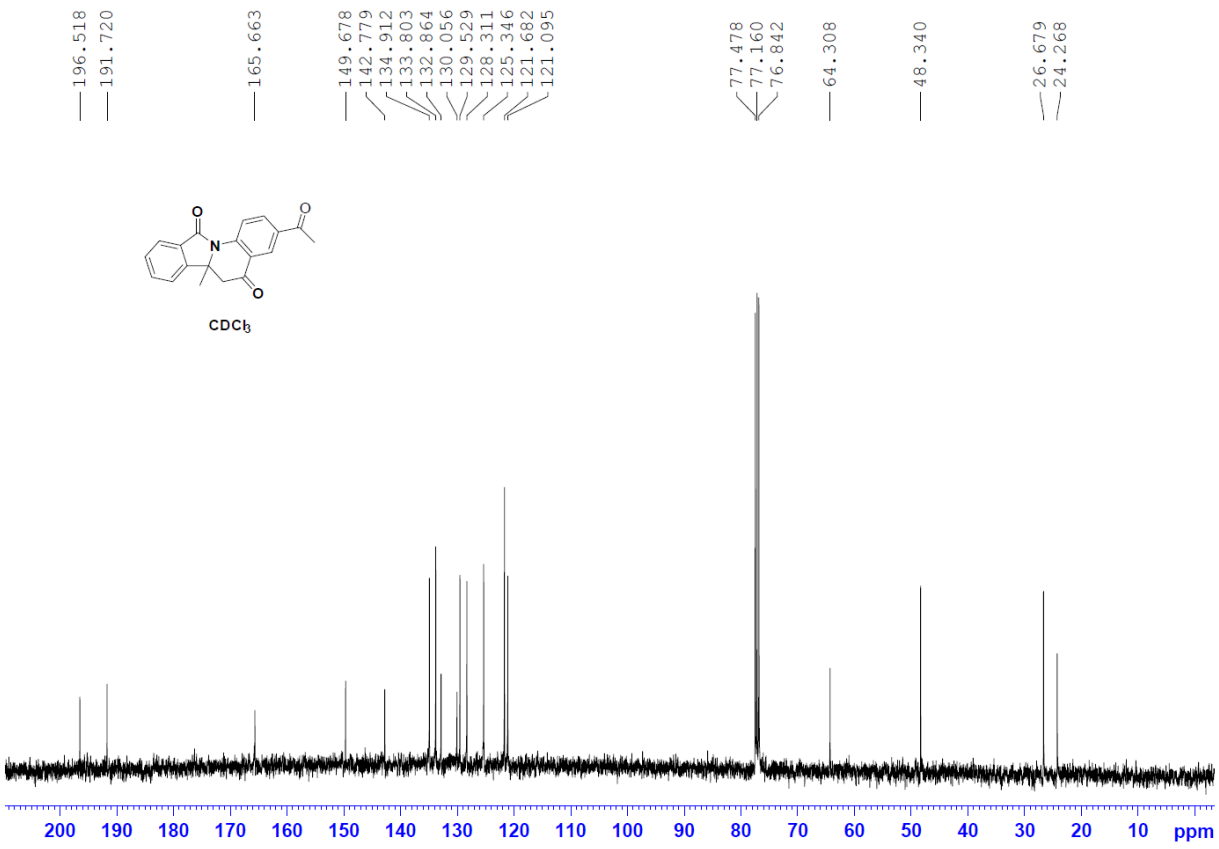
1.04
1.04
1.08
1.10
3.09
3.14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121.682
121.095
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64.308
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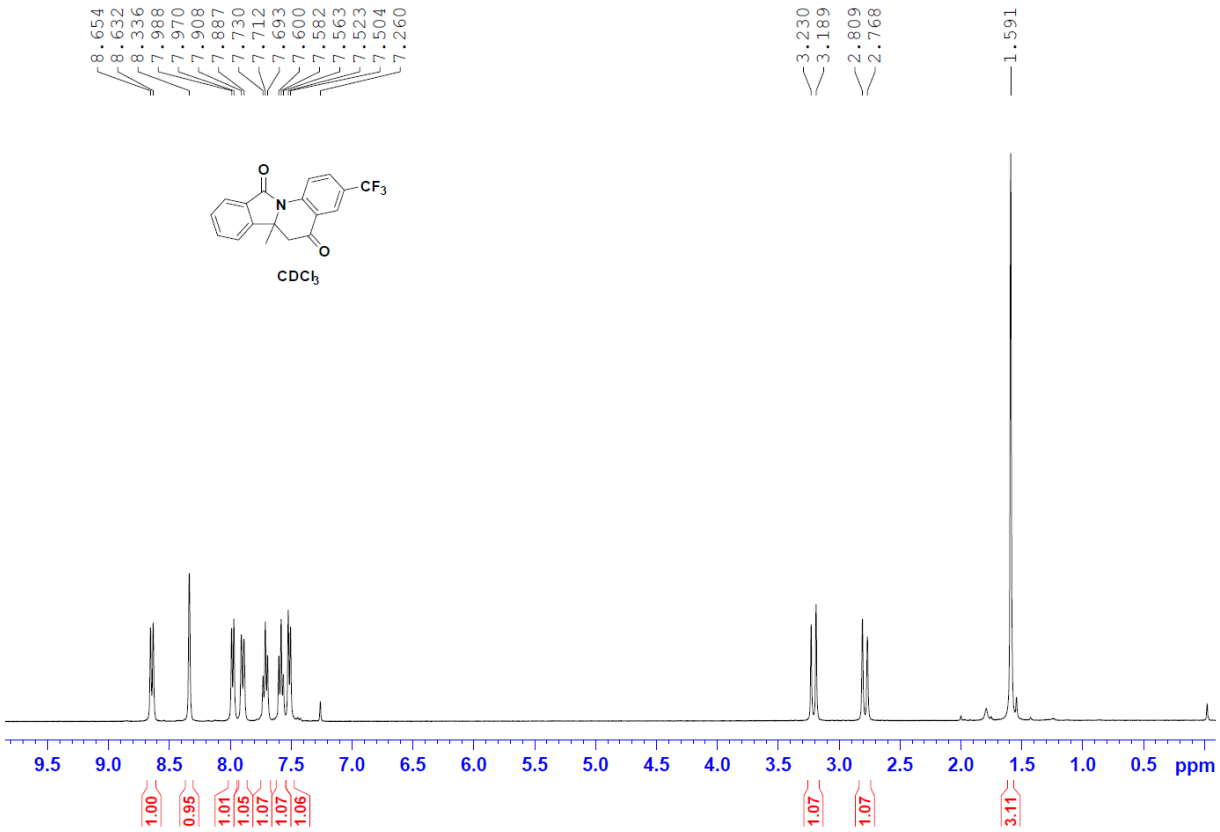
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.563
7.523
7.504
7.260
3.230
3.189
2.809
2.768
1.591
CF3
O
N
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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0.95
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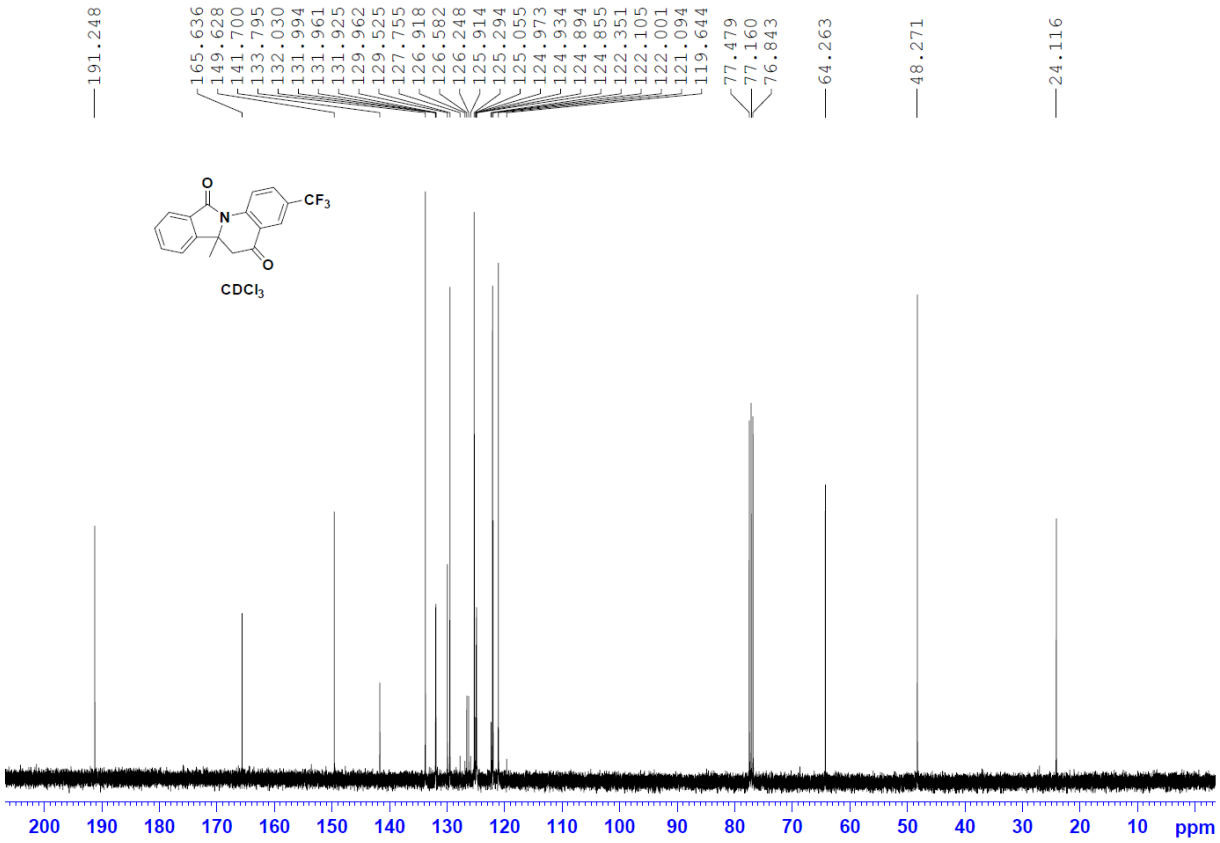
1.05
1.07
1.07
1.06
1.07
1.07
3.11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126.918
126.582
126.248
125.914
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125.055
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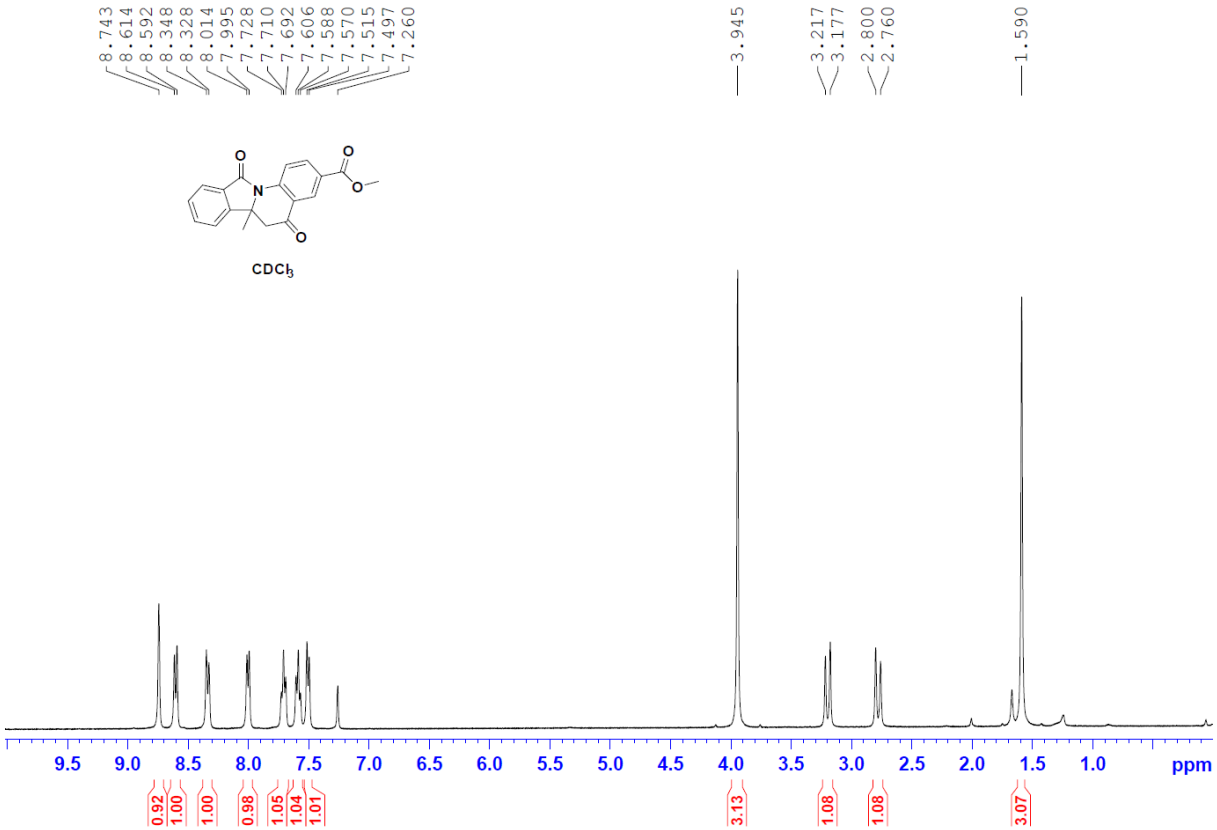
124.855
122.351
122.105
122.001
121.094
119.644
77.479
77.160
76.843
64.263
48.271
24.116
CF3
O
N
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


-62.54
O
N
CF3
O
CDCl3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm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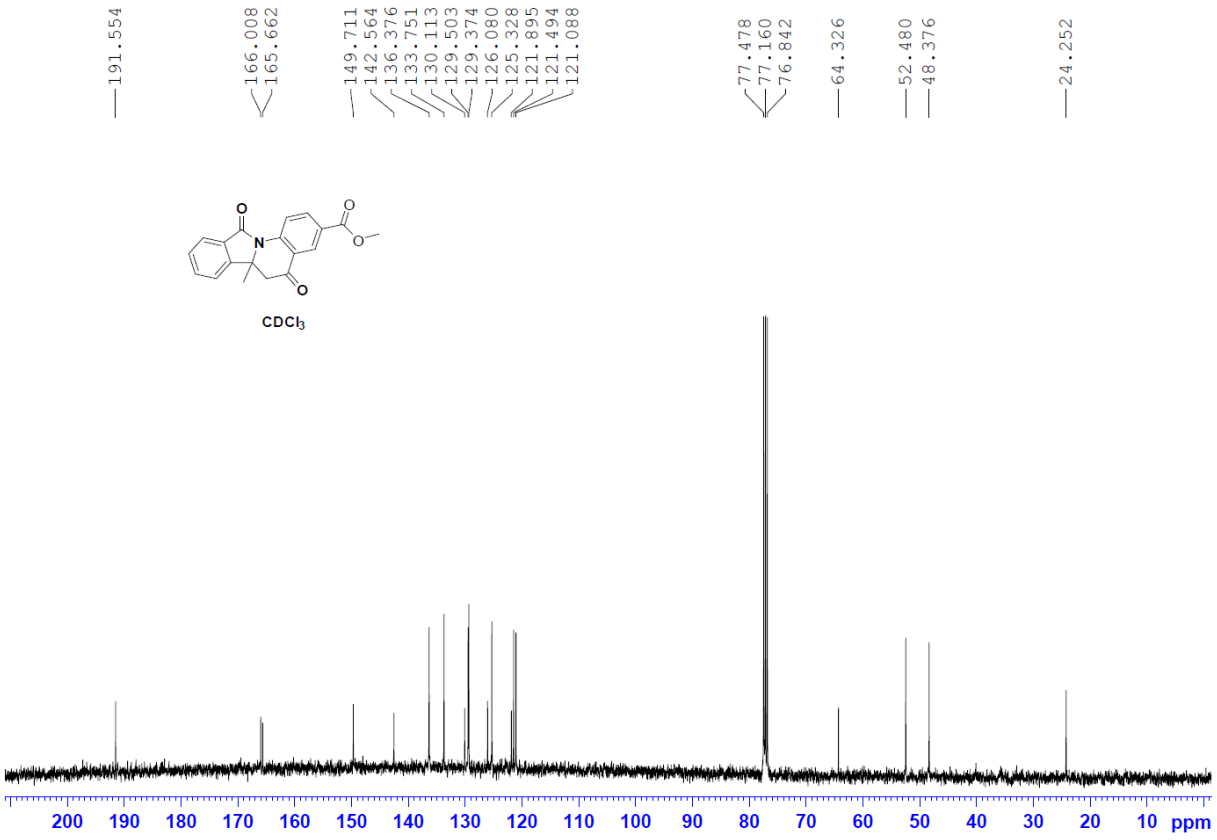
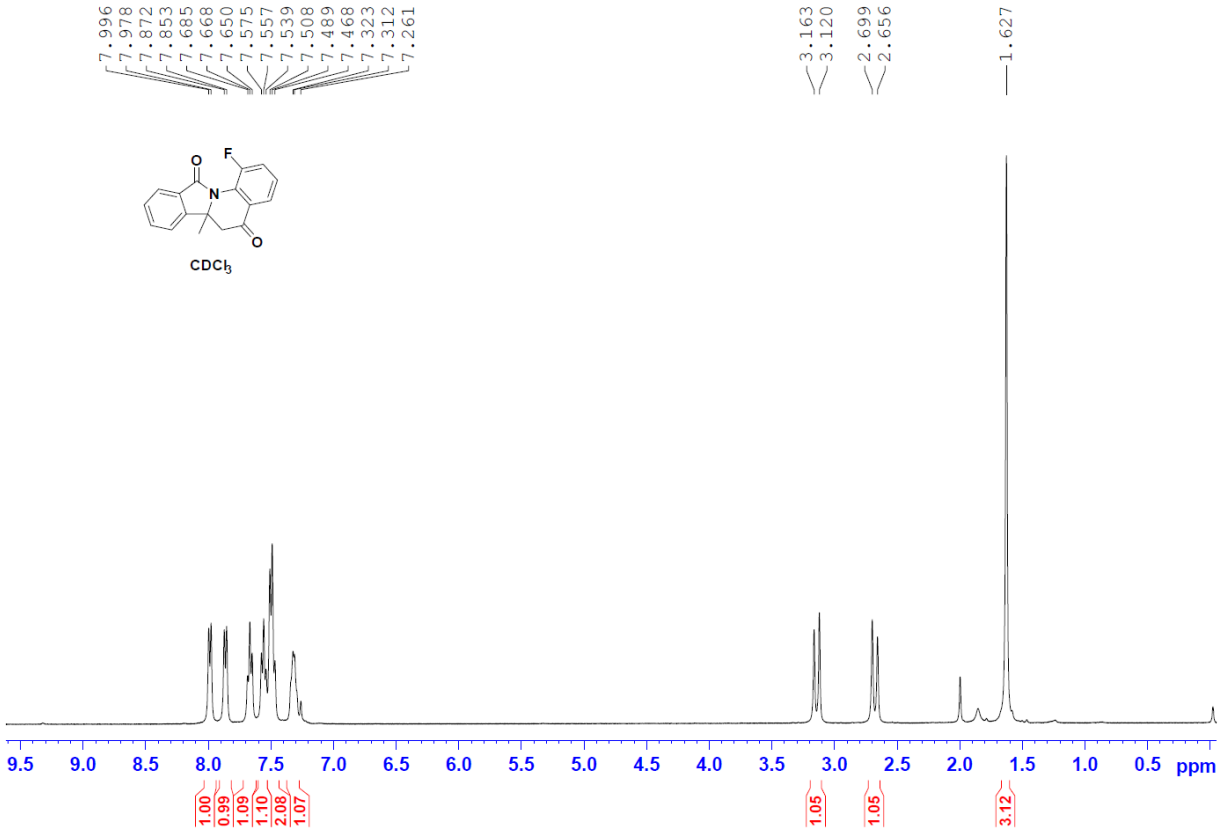
8.614
8.592
8.348
8.328
8.014
7.995
7.728
7.710
7.692
7.606
7.588
7.570
7.515
7.497
7.260
3.945
3.217
3.177
2.800
2.760
1.590
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.92
1.00
1.00
0.98
1.05
1.04
1.01
3.13
1.08
1.08
3.07


191.554
166.008
165.662
149.711
142.564
136.376
133.751
130.113
129.503
129.374
126.080
125.328
121.895
121.494
121.088
77.478
77.160
76.842
64.326
52.480
48.376
24.252
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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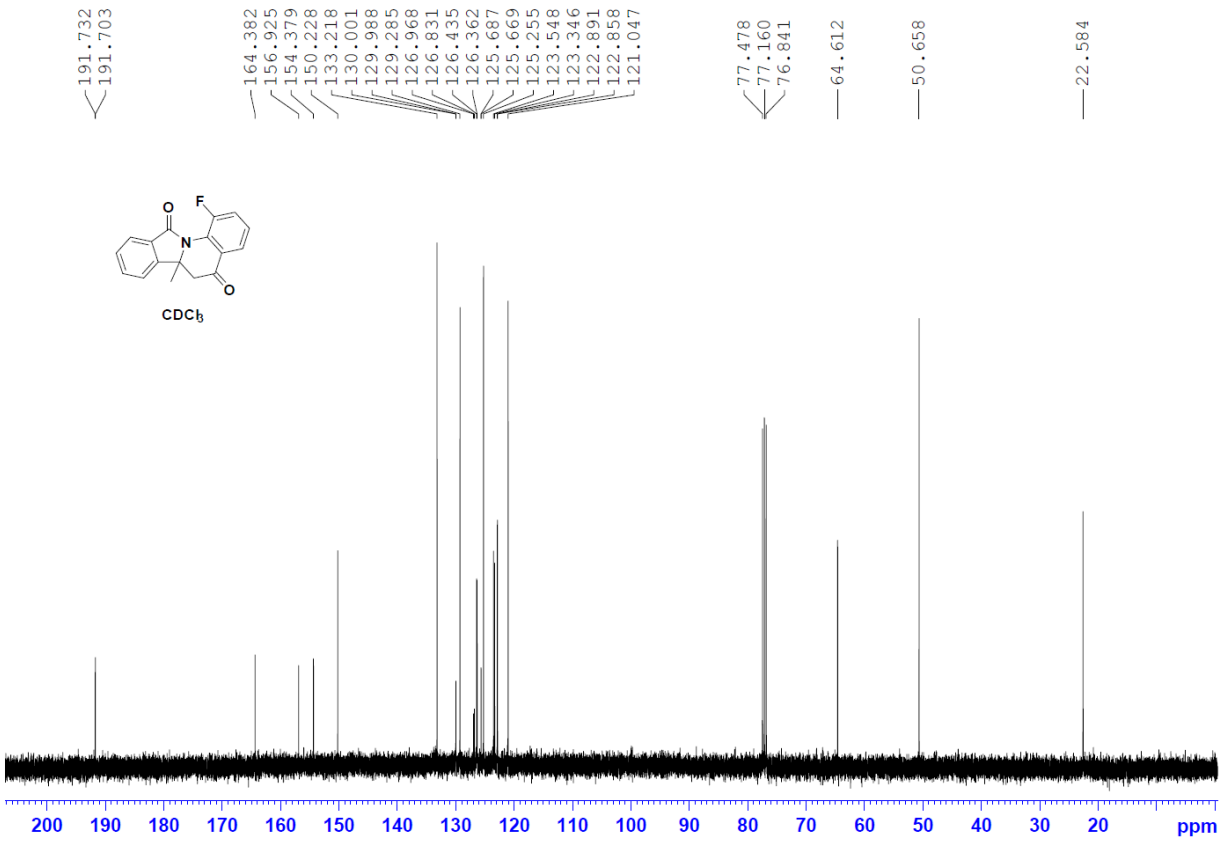
7.978
7.872
7.853
7.685
7.668
7.650
7.575
7.557
7.539
7.508
7.489
7.468
7.323
7.312
7.261
3.163
3.120
2.699
2.656
1.627
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00 0.99 1.09 1.10 2.08 1.07 1.05 1.05 3.12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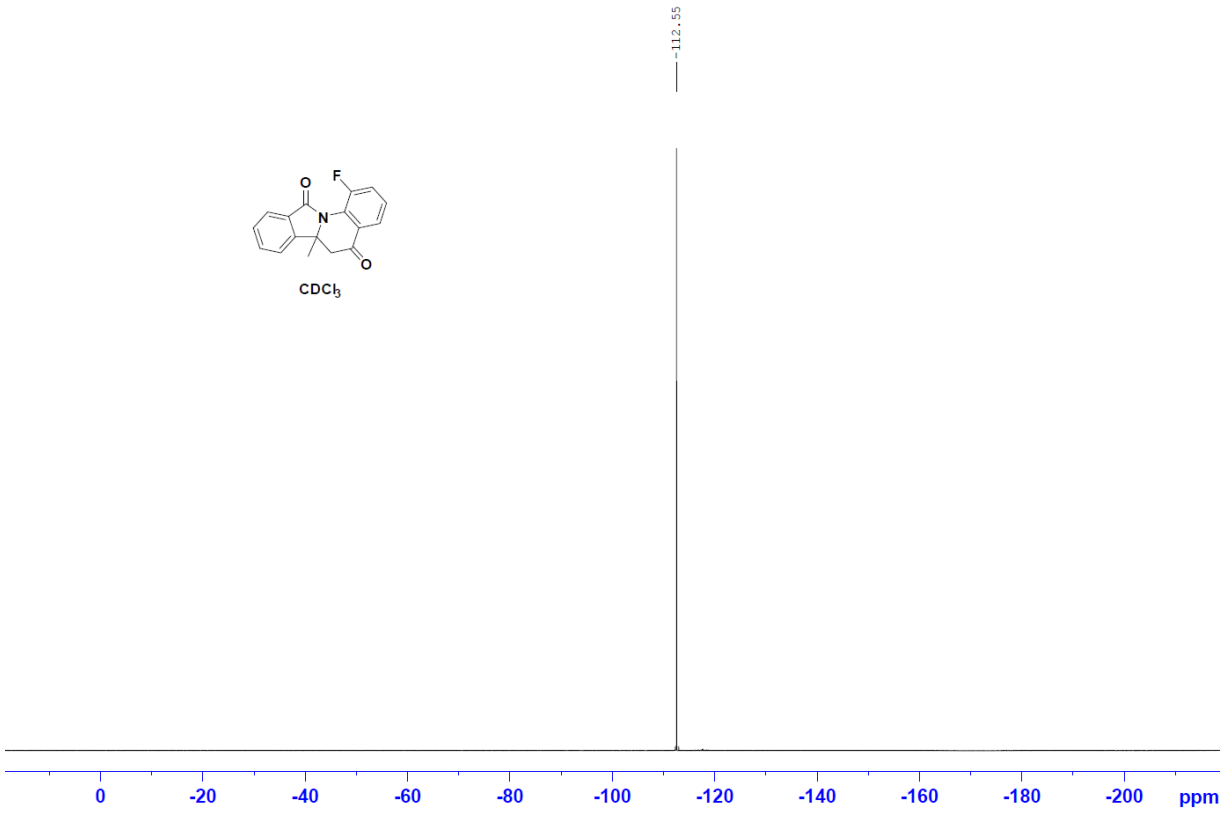
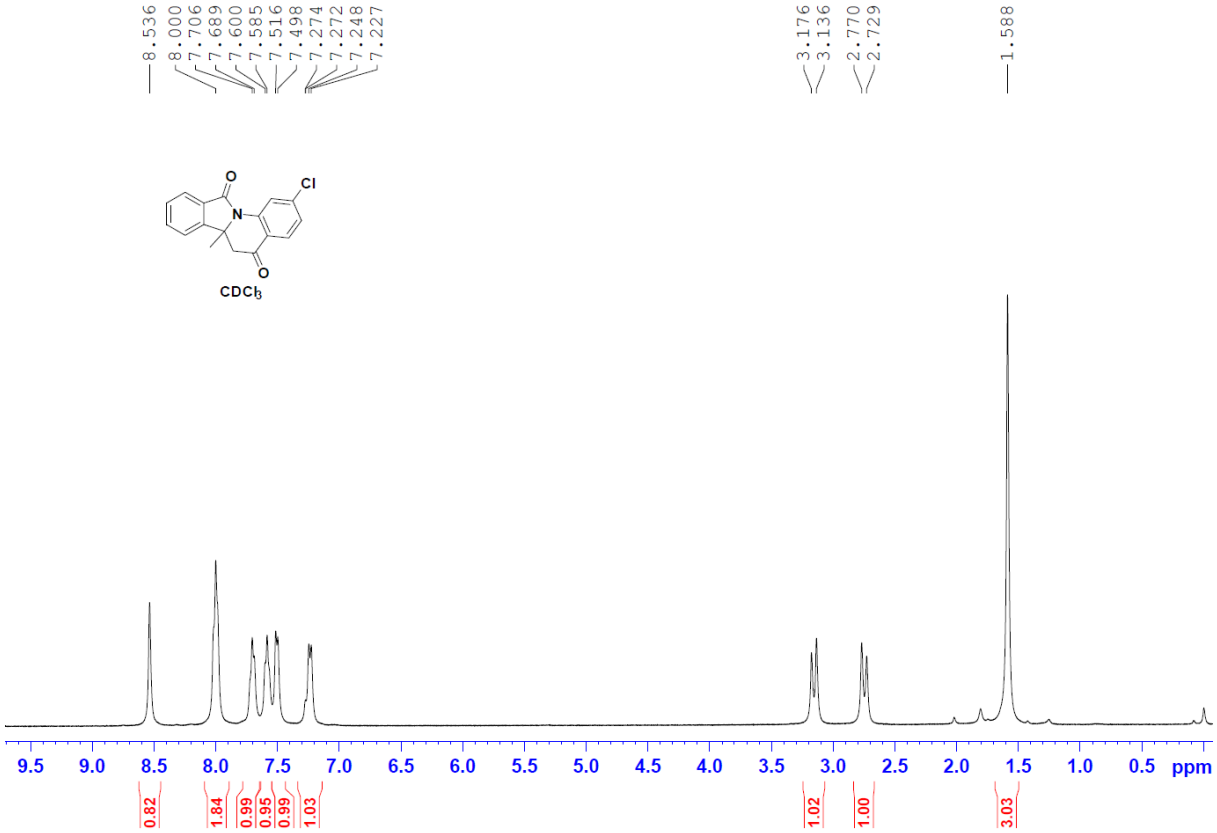
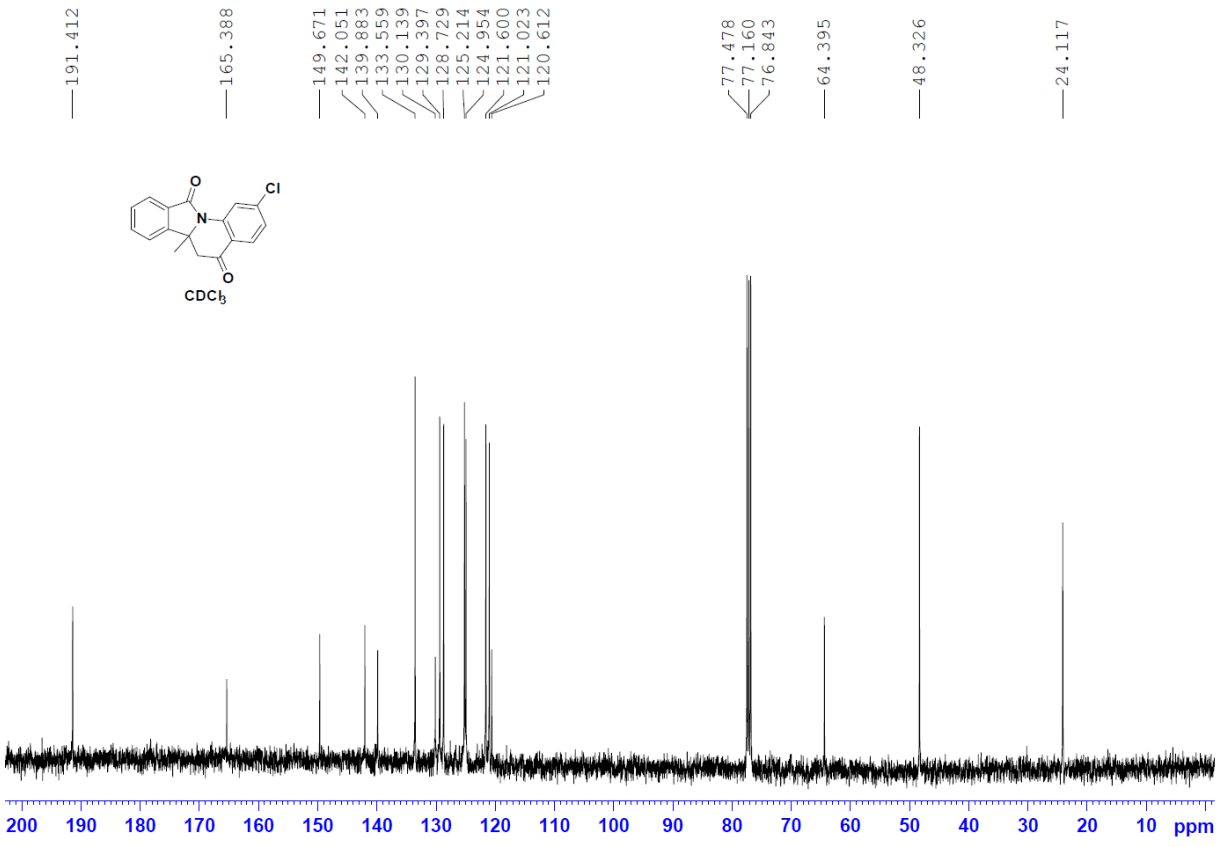
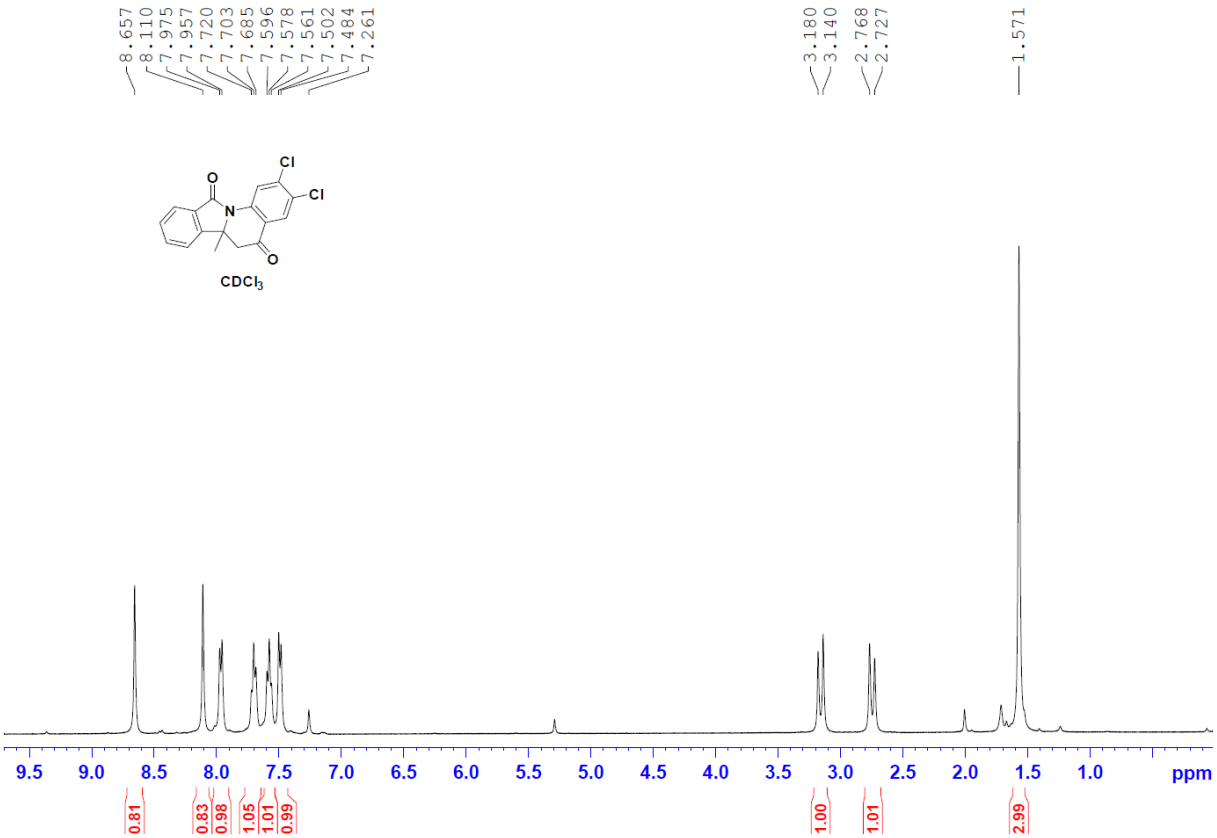
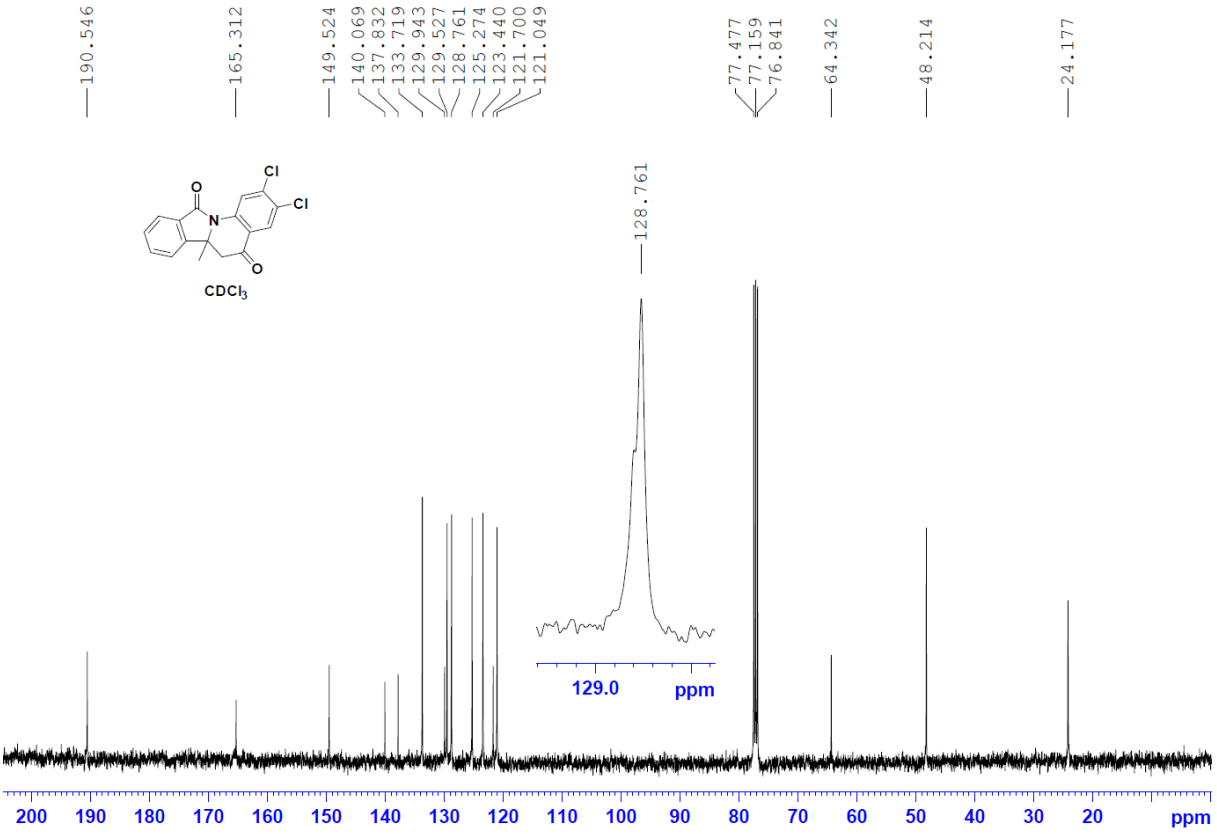
191.703
164.382
156.925
154.379
150.228
133.218
130.001
129.988
129.285
126.968
126.831
126.435
126.362
125.687
125.669
125.255
123.548
123.346
122.891
122.858
121.047
77.478
77.160
76.841
64.612
50.658
22.584
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

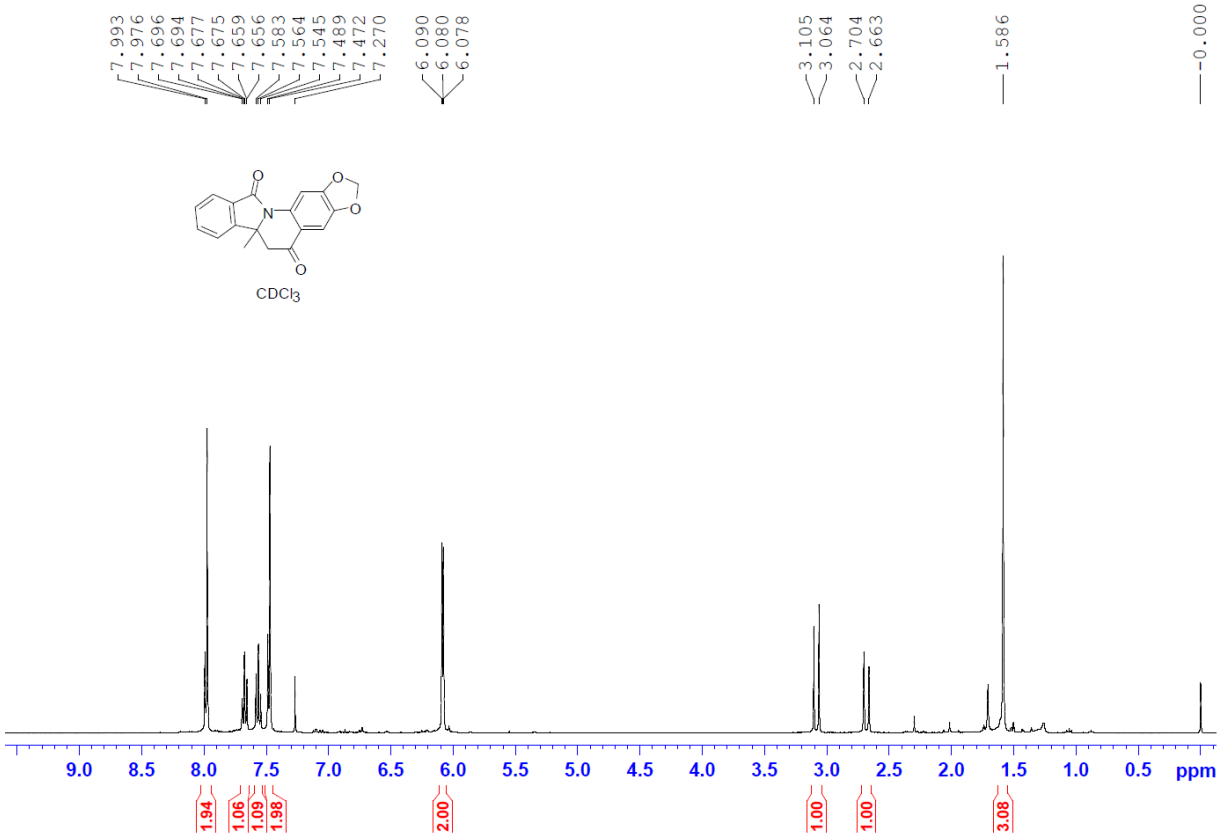

-112.55
F
O
N
O
CDCl3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

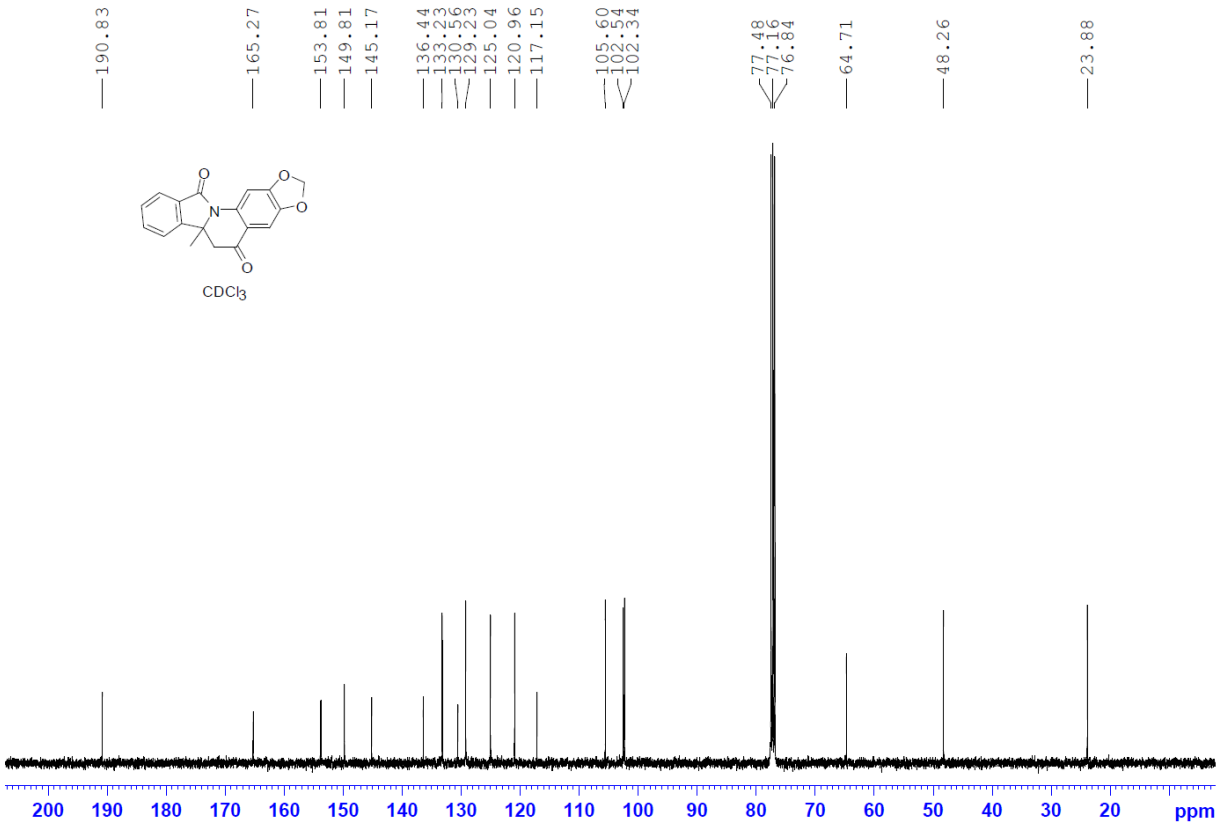

8.536
8.000
7.706
7.689
7.600
7.585
7.516
7.498
7.274
7.272
7.248
7.227
3.176
3.136
2.770
2.729
1.588
O
N
O
Cl
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.82
1.84
0.99
0.95
0.99
1.03
1.02
1.00
3.03

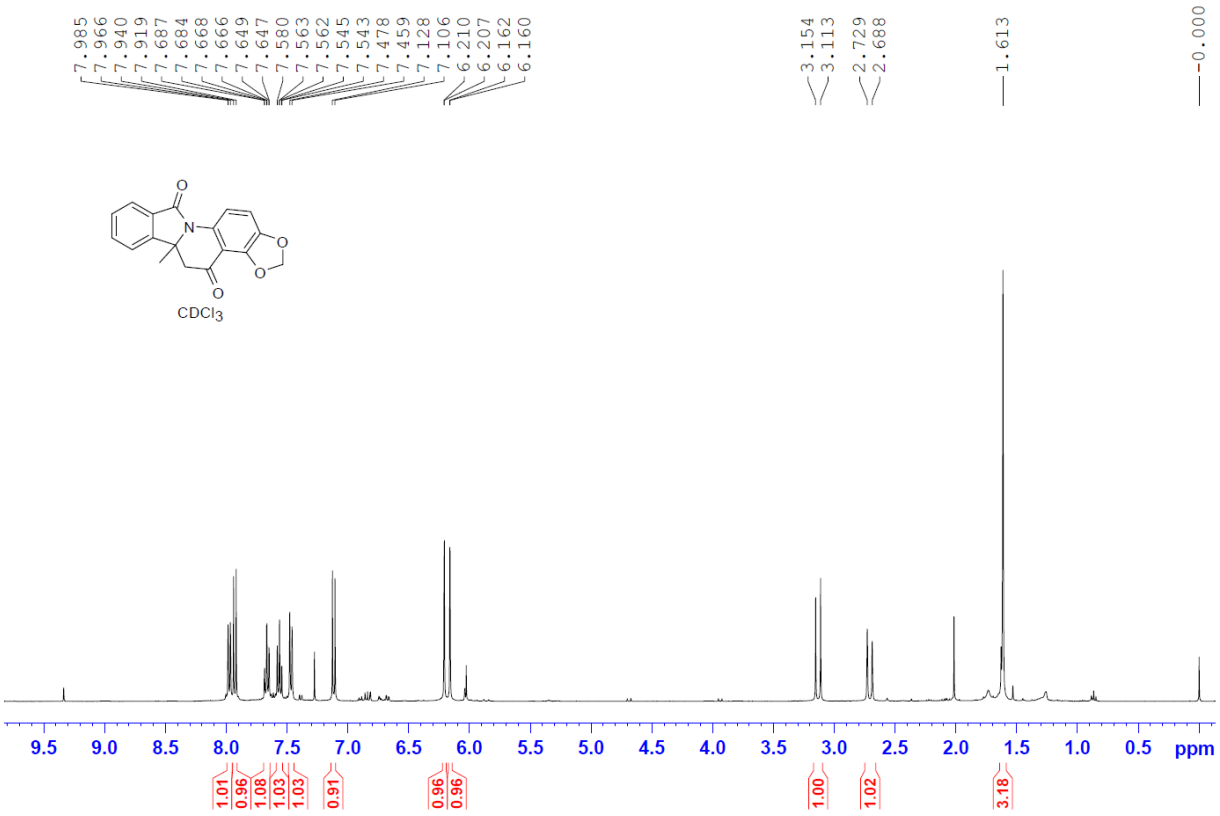

191.412
165.388
149.671
142.051
139.883
133.559
130.139
129.397
128.729
125.214
124.954
121.600
121.023
120.612
77.478
77.160
76.843
64.395
48.326
24.117
O
N
O
Cl
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

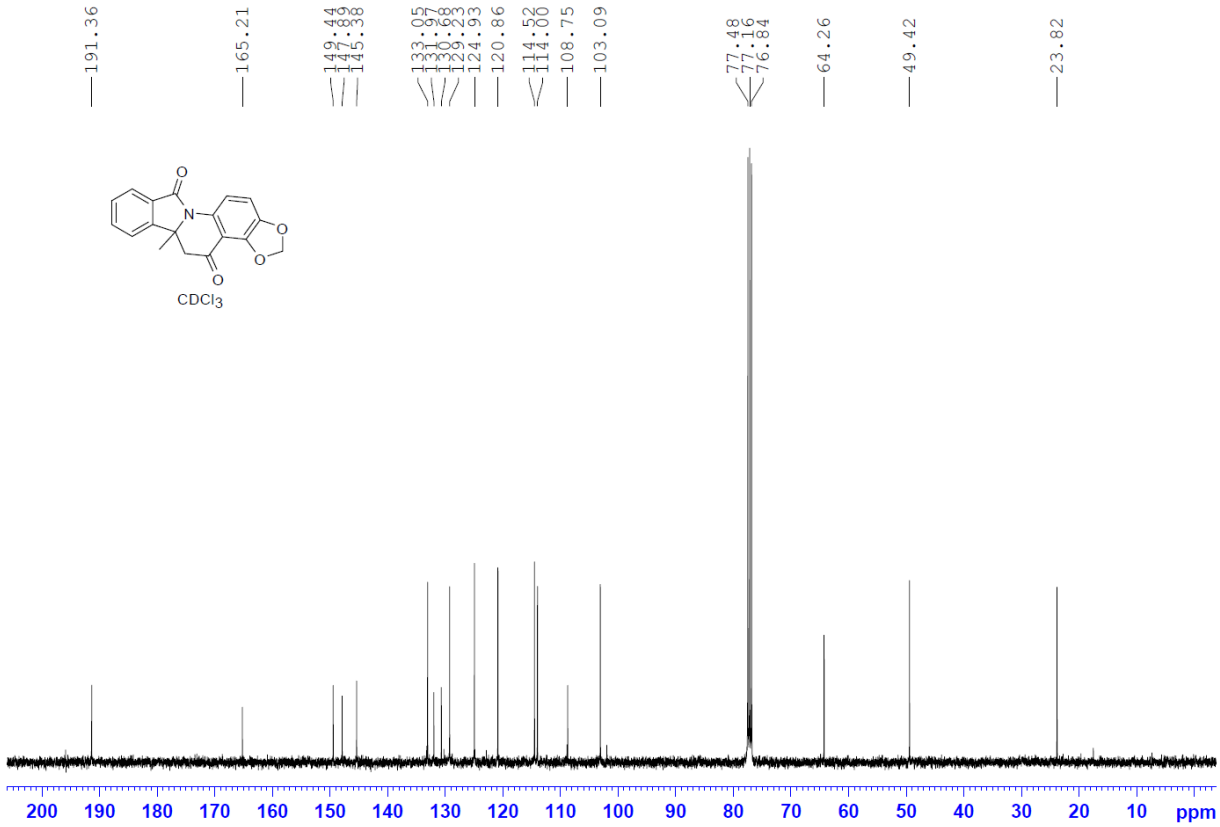

8.657
8.110
7.975
7.957
7.720
7.703
7.685
7.596
7.578
7.561
7.502
7.484
7.261
3.180
3.140
2.768
2.727
1.571
Cl
Cl
O
N
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.81
0.83
0.98
1.05
1.01
0.99
1.00
1.01
2.99

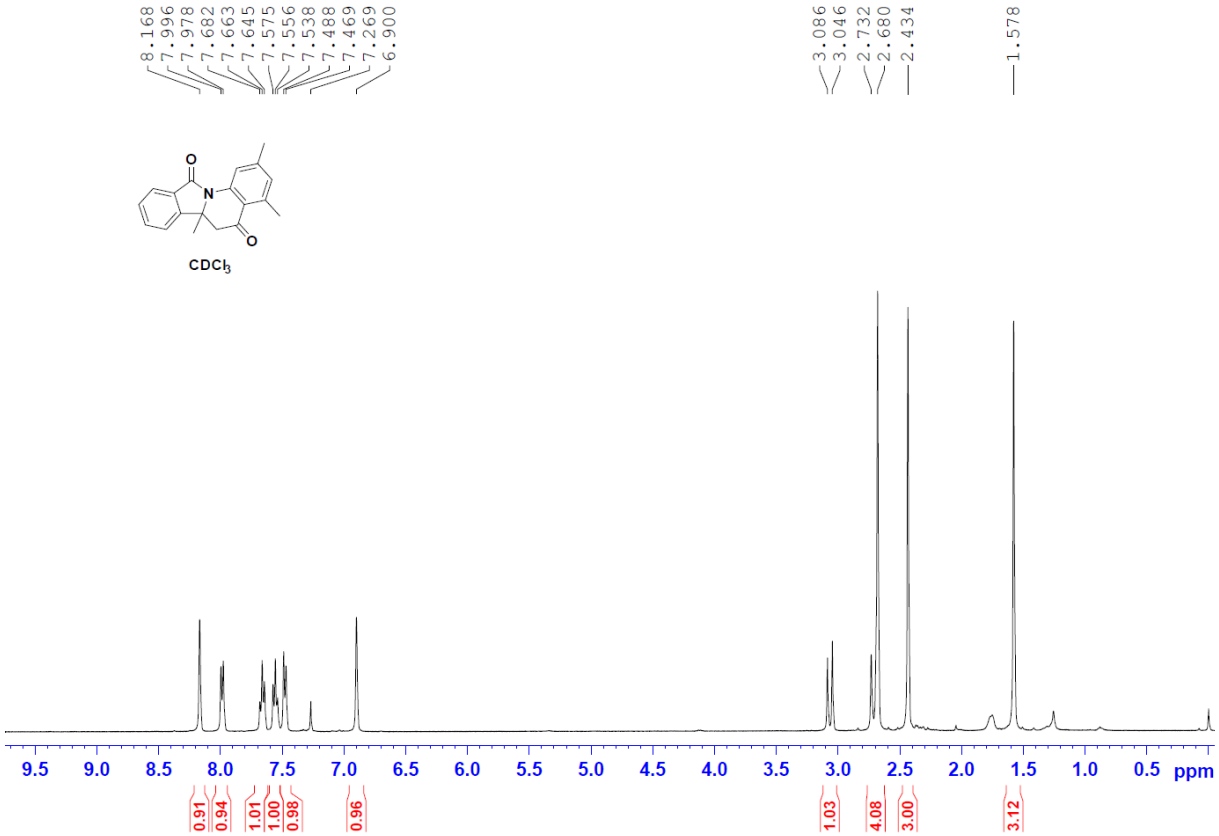

190.546
165.312
149.524
140.069
137.832
133.719
129.943
129.527
128.761
125.274
123.440
121.700
121.049
77.477
77.159
76.841
64.342
48.214
24.177
Cl
Cl
O
N
O
CDCl3
128.761
129.0 ppm
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

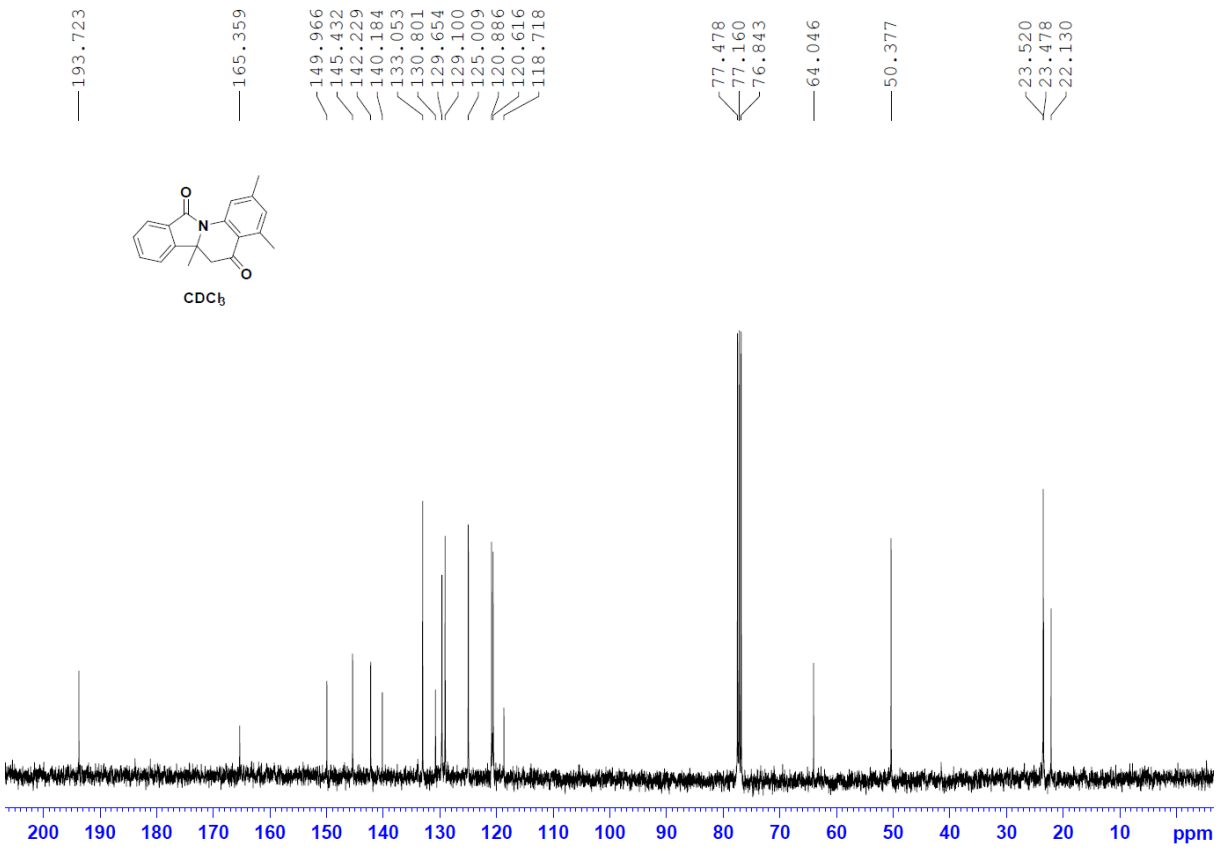

7.993
7.976
7.696
7.694
7.677
7.675
7.659
7.656
7.583
7.564
7.545
7.489
7.472
7.270
6.090
6.080
6.078
3.105
3.064
2.704
2.663
1.586
0.000
CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.94
1.06
1.09
1.98
2.00
1.00
1.00
3.08

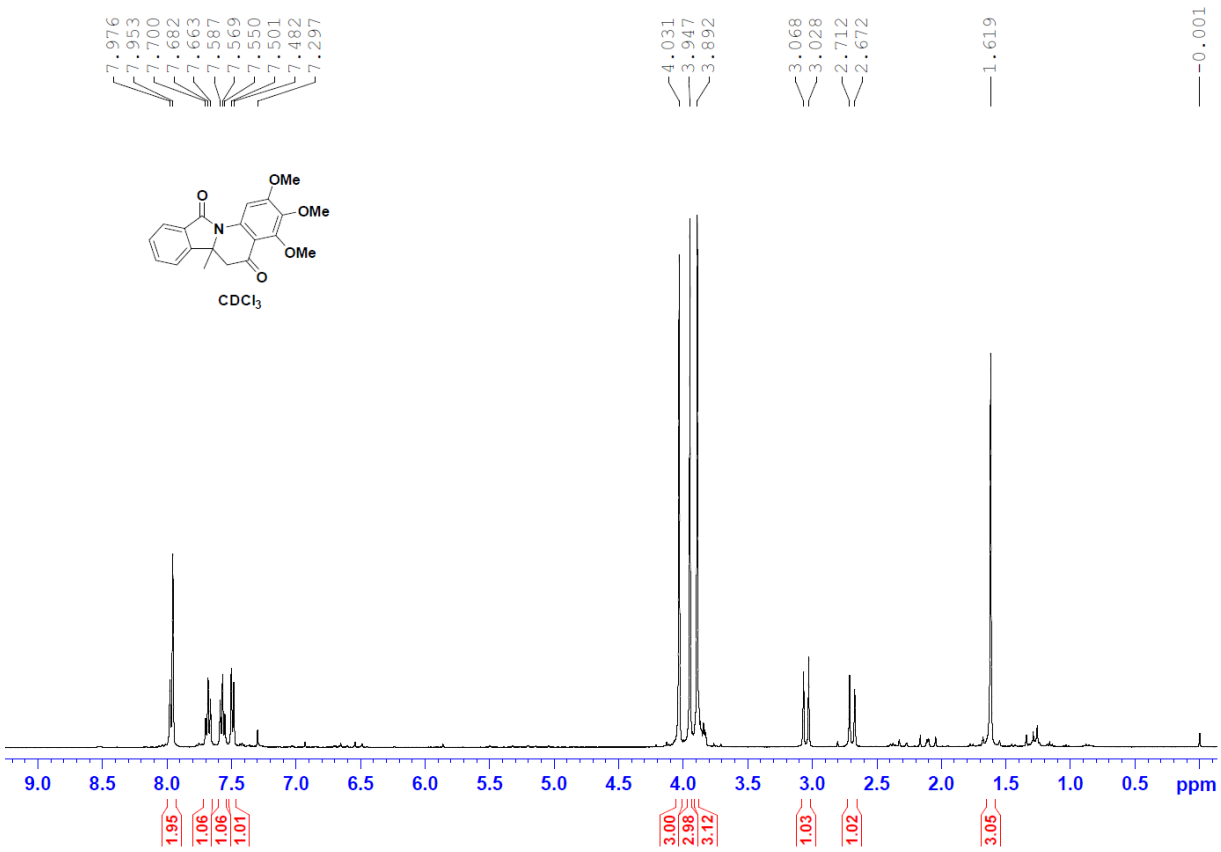

190.83
165.27
153.81
149.81
145.17
136.44
133.23
130.56
129.23
125.04
120.96
117.15
105.60
102.54
102.34
77.48
77.16
76.84
64.71
48.26
23.88
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

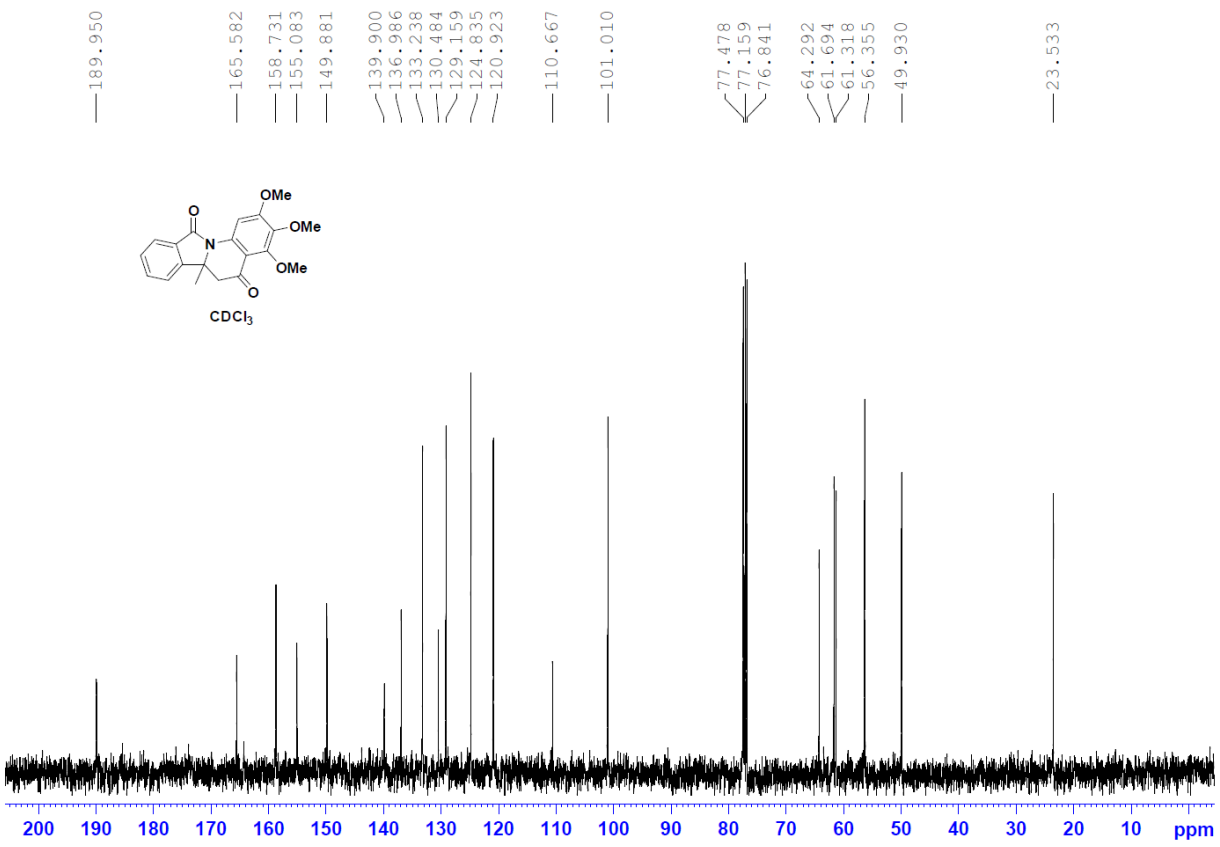

7.985
7.966
7.940
7.919
7.687
7.684
7.668
7.666
7.649
7.647
7.580
7.563
7.562
7.545
7.543
7.478
7.459
7.128
7.106
6.210
6.207
6.162
6.160
3.154
3.113
2.729
2.688
1.613
0.000
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.01
0.96
1.08
1.03
1.03
0.91
0.96
0.96
1.00
1.02
3.18

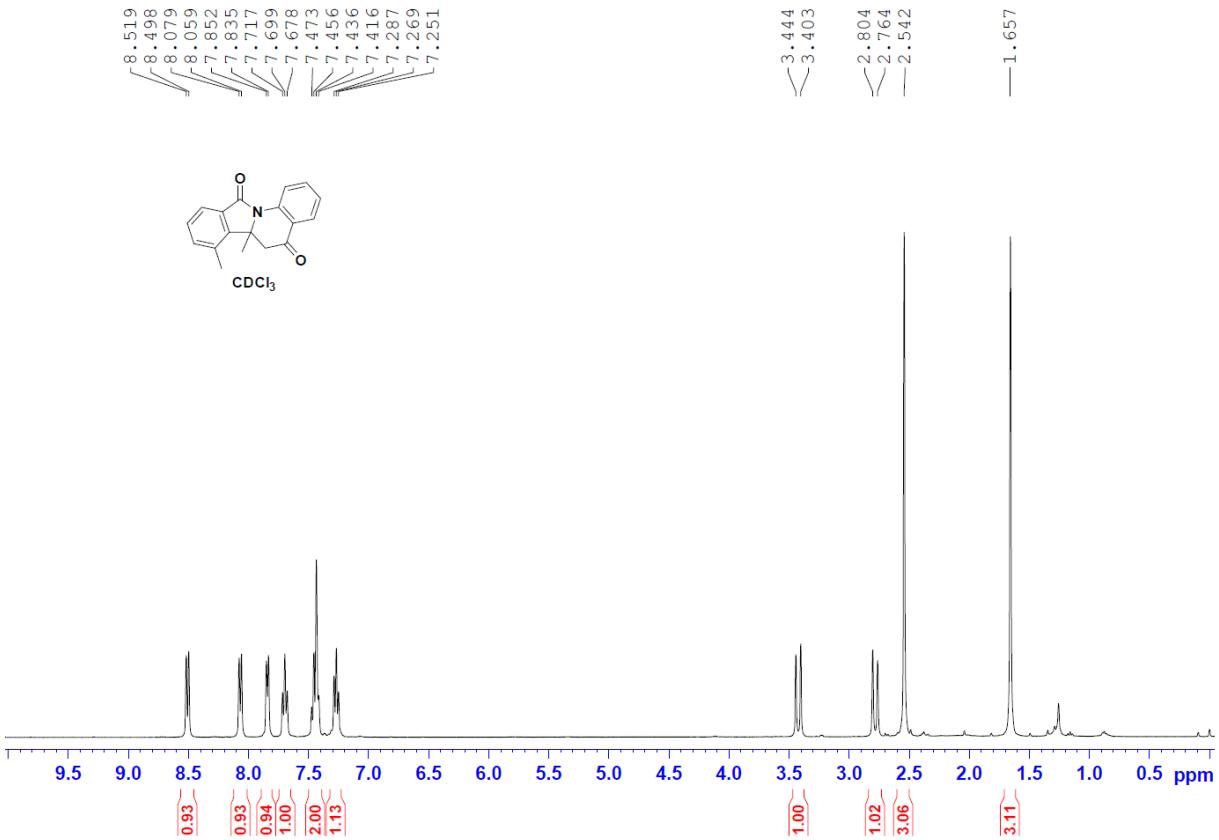

191.36
165.21
149.44
147.89
145.38
133.05
131.07
130.68
129.23
124.93
120.86
114.52
114.00
108.75
103.09
77.48
77.16
76.84
64.26
49.42
23.82
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.168
7.996
7.978
7.682
7.663
7.645
7.575
7.556
7.538
7.488
7.469
7.269
6.900
3.086
3.046
2.732
2.680
2.434
1.578
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.91
0.94
1.01
1.00
0.98
0.96
1.03
4.08
3.00
3.12


193.723
165.359
149.966
145.432
142.229
140.184
133.053
130.801
129.654
129.100
125.009
120.886
120.616
118.718
77.478
77.160
76.843
64.046
50.377
23.520
23.478
22.130
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.976
7.953
7.700
7.682
7.663
7.587
7.569
7.550
7.501
7.482
7.297
4.031
3.947
3.892
3.068
3.028
2.712
2.672
1.619
0.001
OMe
OMe
OMe
O
N
O
CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.95
1.06
1.06
1.01
3.00
2.98
3.12
1.03
1.02
3.05


189.950
165.582
158.731
155.083
149.881
139.900
136.986
133.238
130.484
129.159
124.835
120.923
110.667
101.010
77.478
77.159
76.841
64.292
61.694
61.318
56.355
49.930
23.533
OMe
OMe
OMe
O
N
O
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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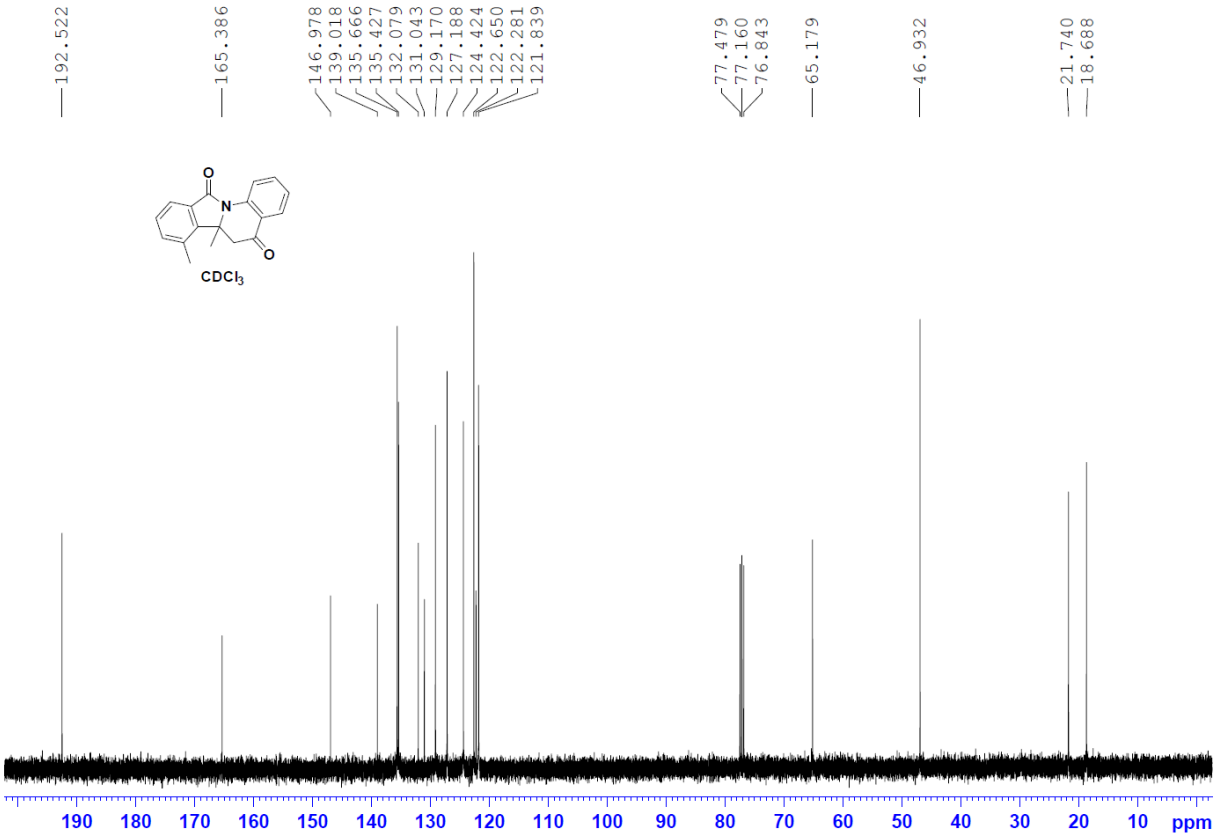
8.498
8.079
8.059
7.852
7.835
7.717
7.699
7.678
7.473
7.456
7.436
7.416
7.287
7.269
7.251
3.444
3.403
2.804
2.764
2.542
1.657
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.93
0.93
0.94
1.00
2.00
1.13
1.00
1.02
3.06
3.11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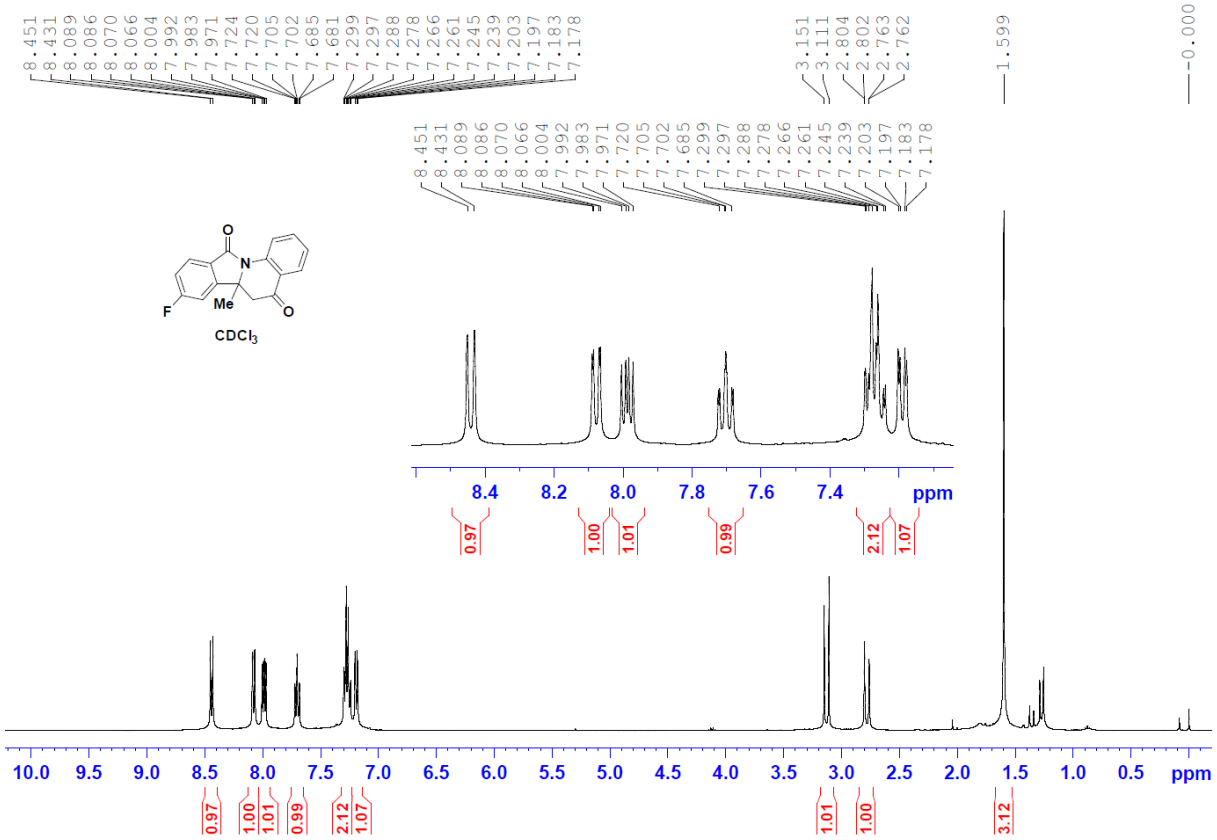
165.386
146.978
139.018
135.666
135.427
132.079
131.043
129.170
127.188
124.424
122.650
122.281
121.839
77.479
77.160
76.843
65.179
46.932
21.740
18.688
CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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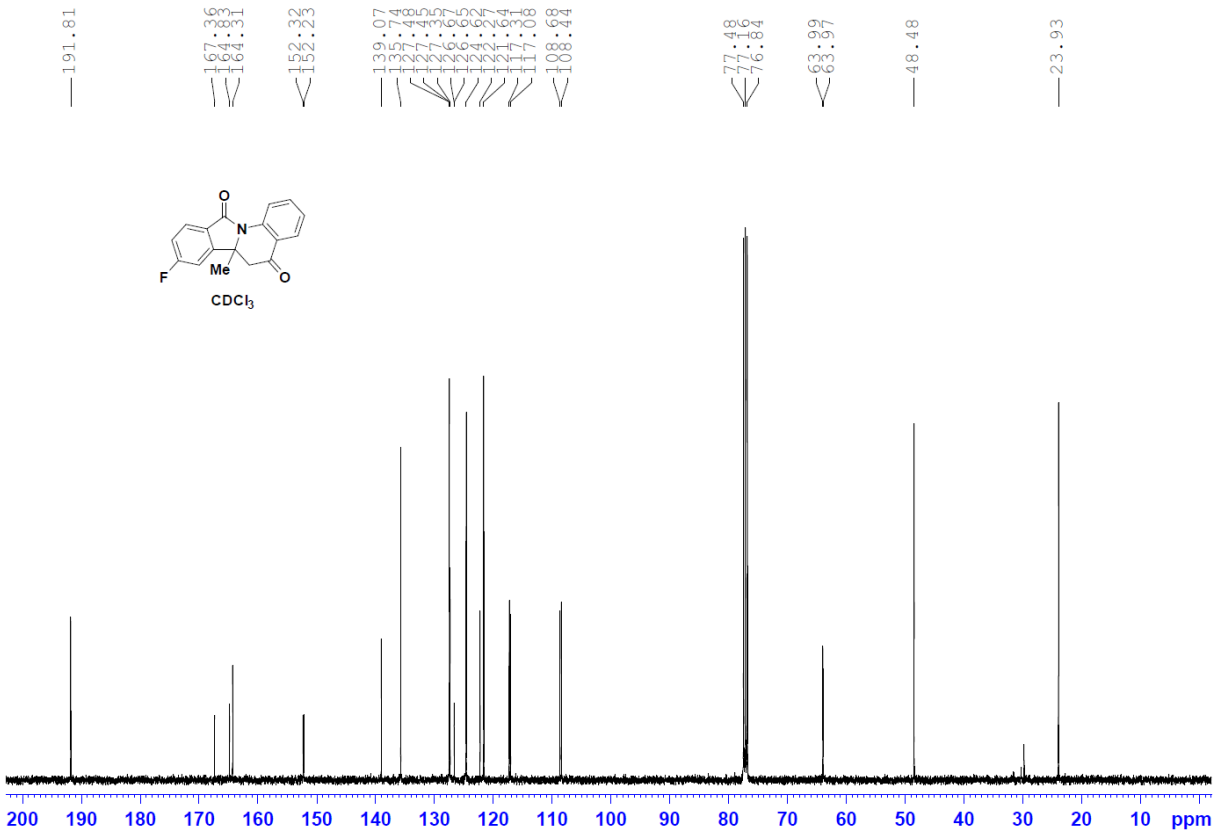
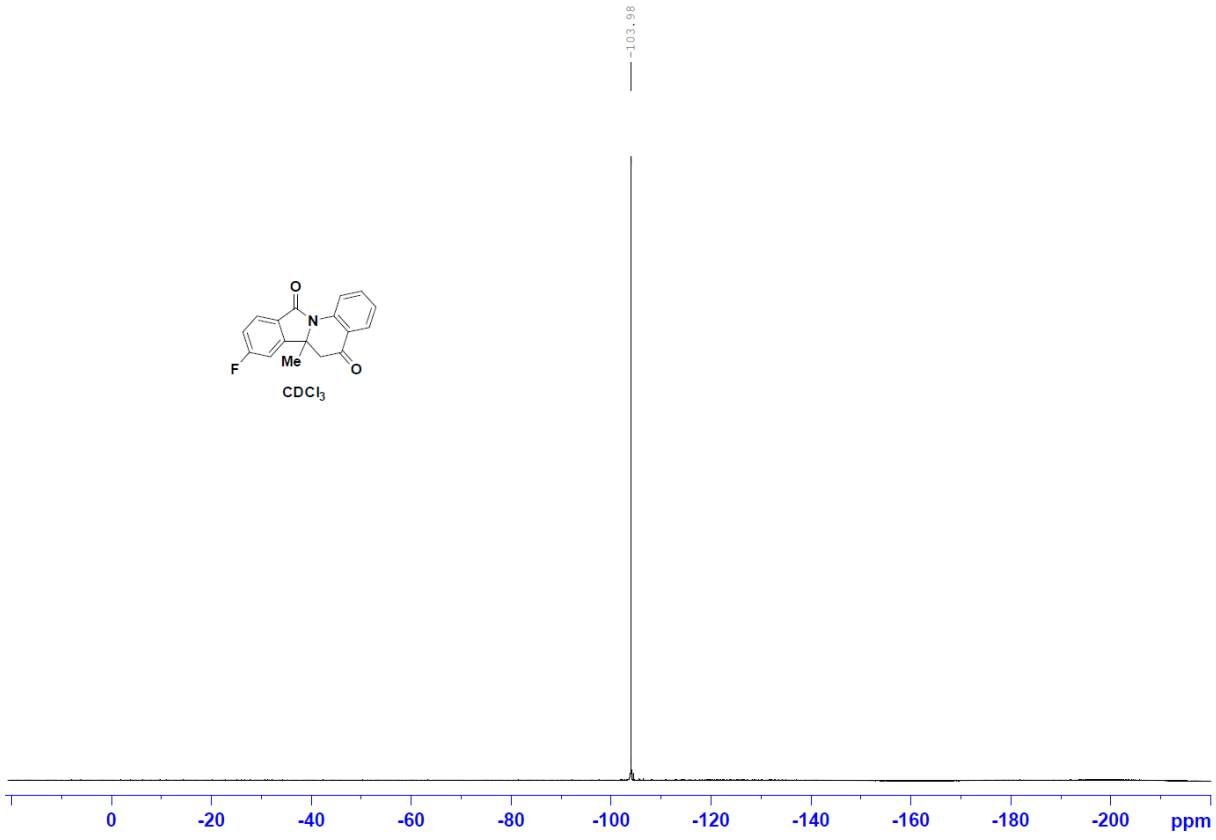
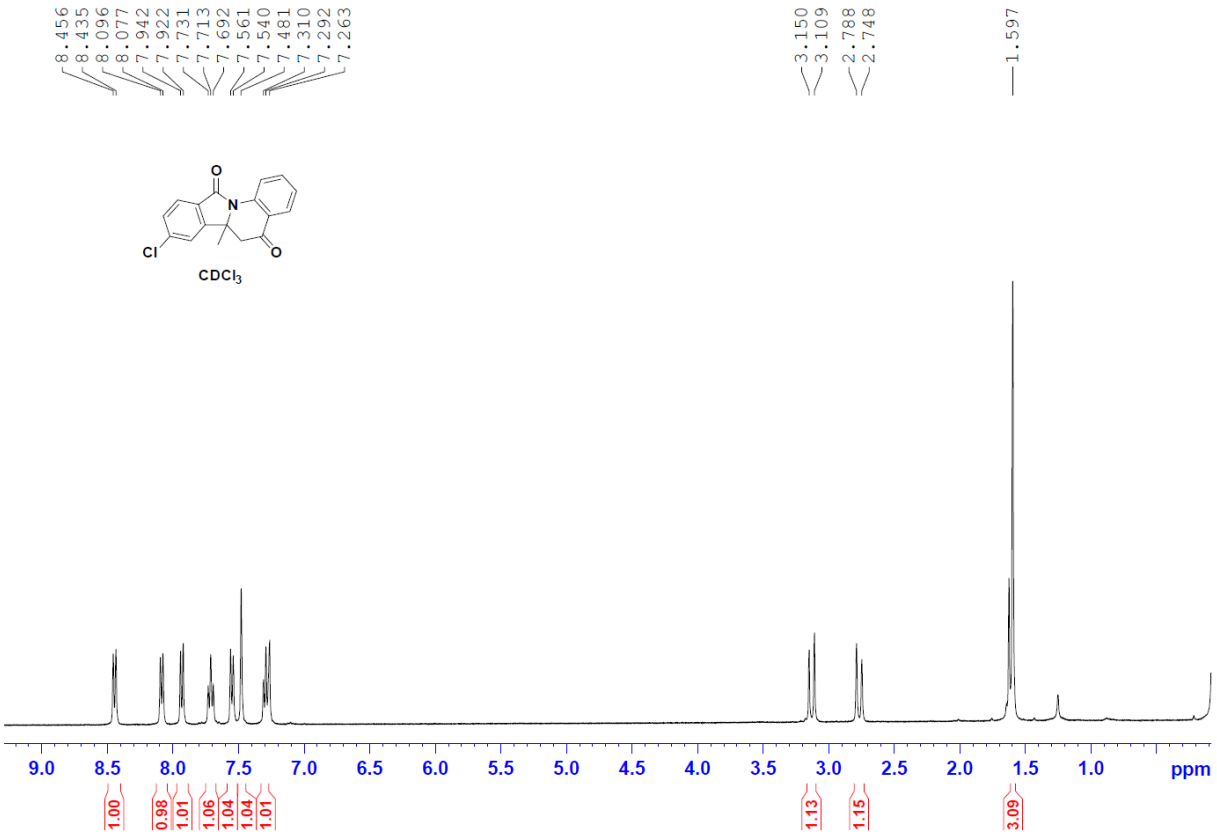
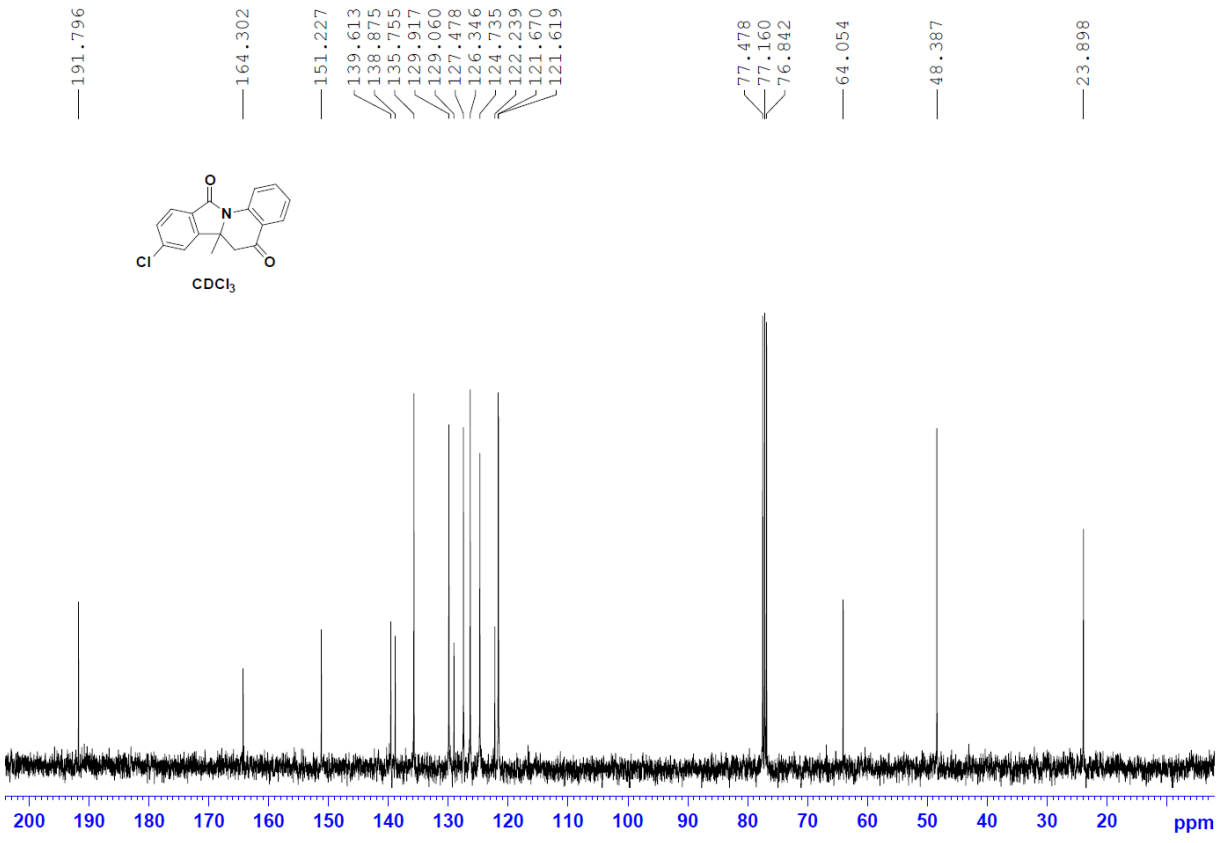
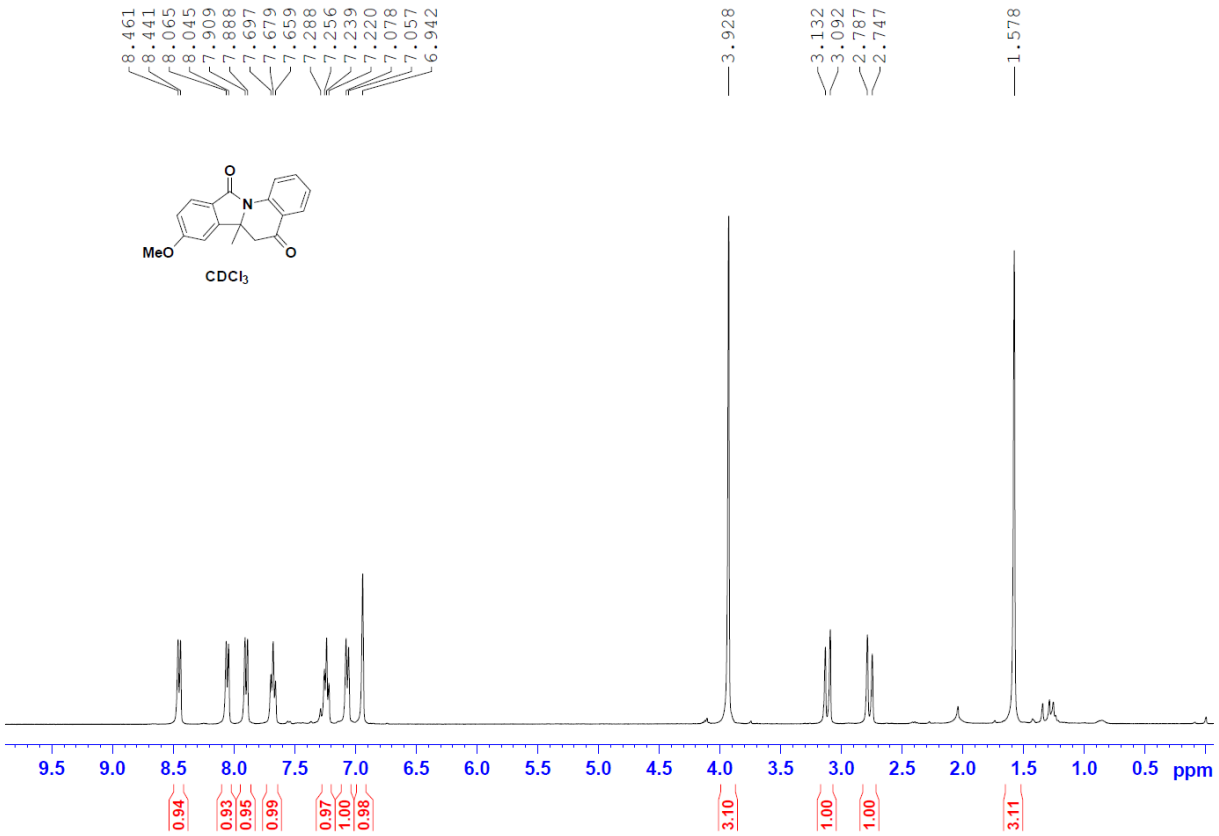
8.431
8.089
8.086
8.070
8.066
8.004
7.992
7.983
7.971
7.724
7.720
7.705
7.702
7.685
7.681
7.299
7.297
7.288
7.278
7.266
7.261
7.245
7.239
7.203
7.197
7.183
7.178
3.151
3.111
2.804
2.802
2.763
2.762
1.599
0.000
O
N
Me
F
O
CDCl3
8.4
8.2
8.0
7.8
7.6
7.4
ppm
0.97
1.00
1.01
0.99
2.12
1.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.97
1.00
1.01
0.99
2.12
1.07
1.01
1.00
3.12

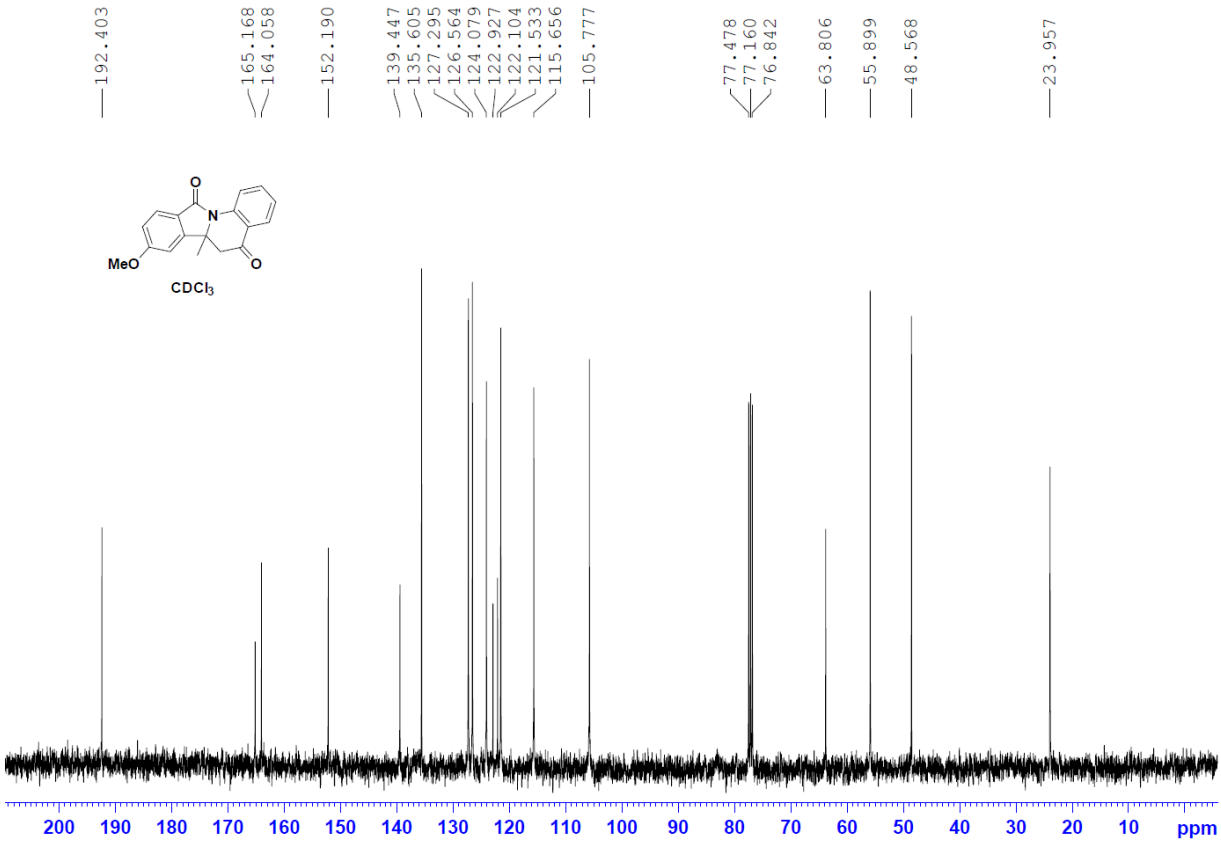

191.81
167.36
164.83
164.31
152.32
152.23
139.07
135.74
127.48
127.45
127.35
126.67
126.65
124.62
122.27
122.24
121.31
117.08
108.68
108.44
77.48
77.16
76.84
63.99
63.97
48.48
23.93
O
N
Me
F
O
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-103.98
O
N
F
Me
O
CDCl3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


8.456
8.435
8.096
8.077
7.942
7.922
7.731
7.713
7.692
7.561
7.540
7.481
7.310
7.292
7.263
3.150
3.109
2.788
2.748
1.597
O
N
Cl
O
CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
0.98
1.01
1.06
1.04
1.04
1.01
1.13
1.15
3.09


191.796
164.302
151.227
139.613
138.875
135.755
129.917
129.060
127.478
126.346
124.735
122.239
121.670
121.619
77.478
77.160
76.842
64.054
48.387
23.898
O
N
Cl
O
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.461
8.441
8.065
8.045
7.909
7.888
7.697
7.679
7.659
7.288
7.256
7.239
7.220
7.078
7.057
6.942
3.928
3.132
3.092
2.787
2.747
1.578
MeO
O
N
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.94
0.93
0.95
0.99
0.97
1.00
0.98
3.10
1.00
1.00
3.11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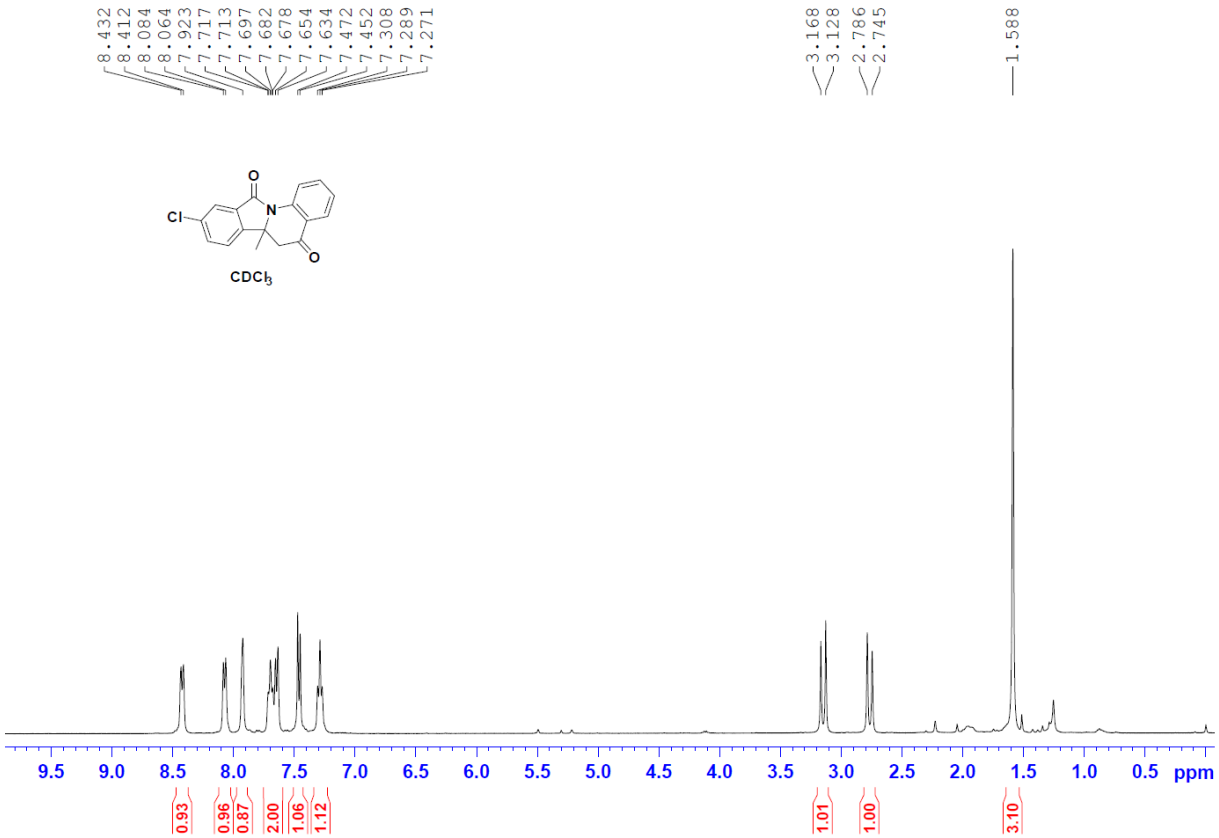
165.168
164.058
152.190
139.447
135.605
127.295
126.564
124.079
122.927
122.104
121.533
115.656
105.777
77.478
77.160
76.842
63.806
55.899
48.568
23.957
MeO
O
N
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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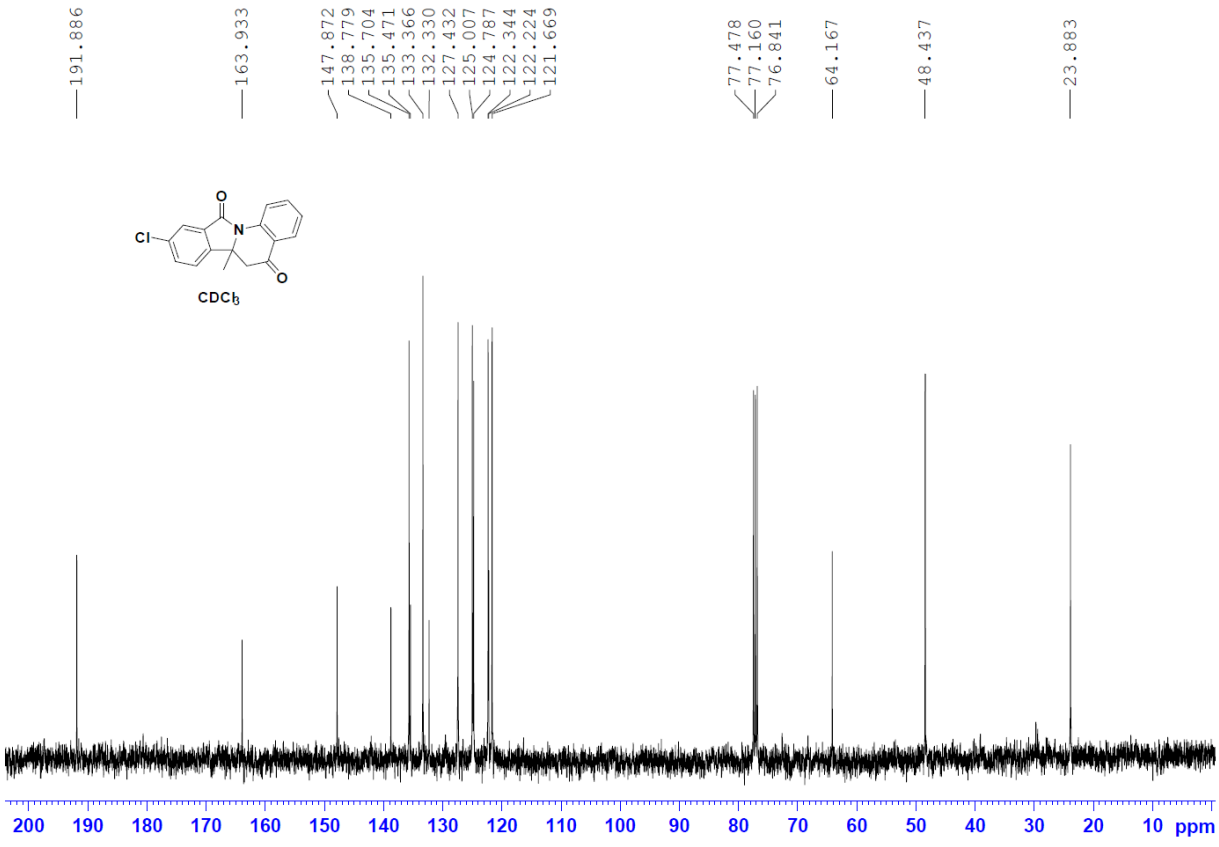
8.412
8.084
8.064
7.923
7.717
7.713
7.697
7.682
7.678
7.654
7.634
7.472
7.452
7.308
7.289
7.271
3.168
3.128
2.786
2.745
1.588
Cl
O
N
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.93
0.96
0.87
2.00
1.06
1.12
1.01
1.00
3.10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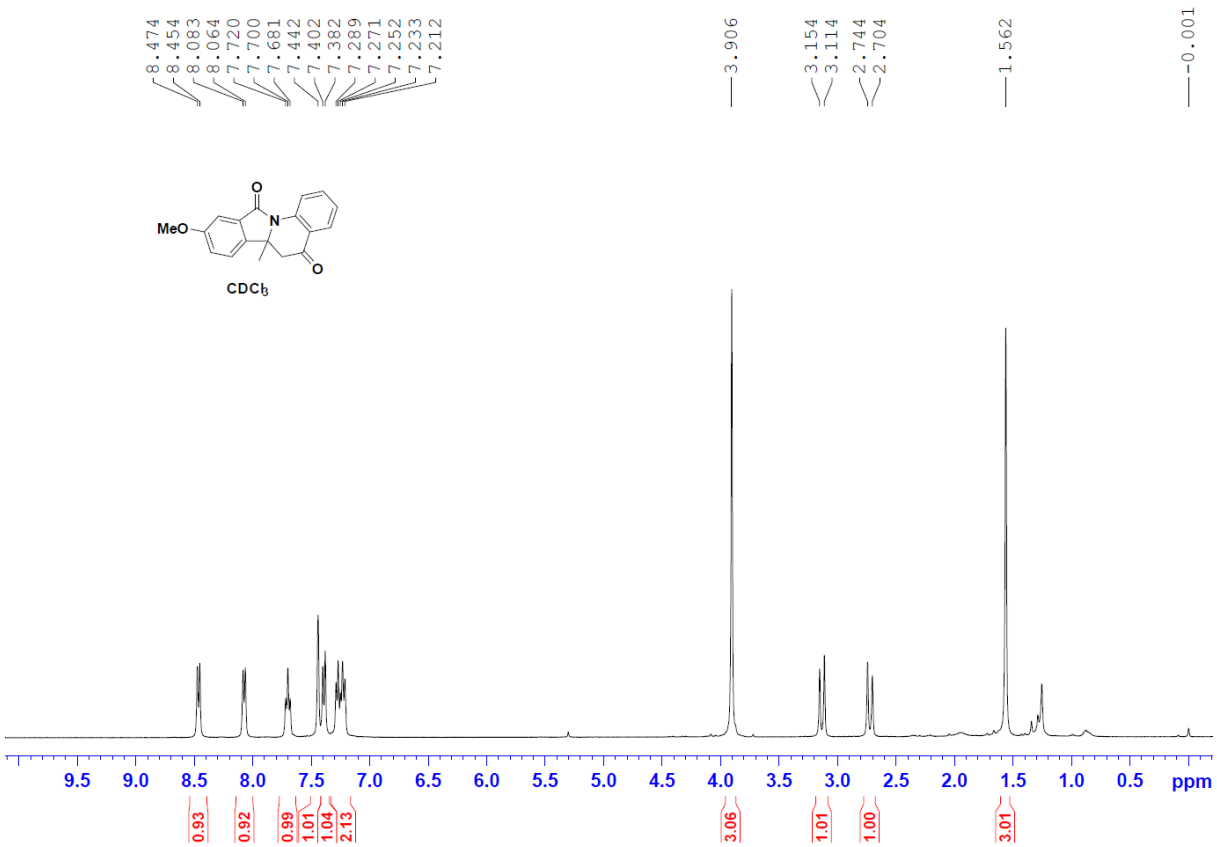
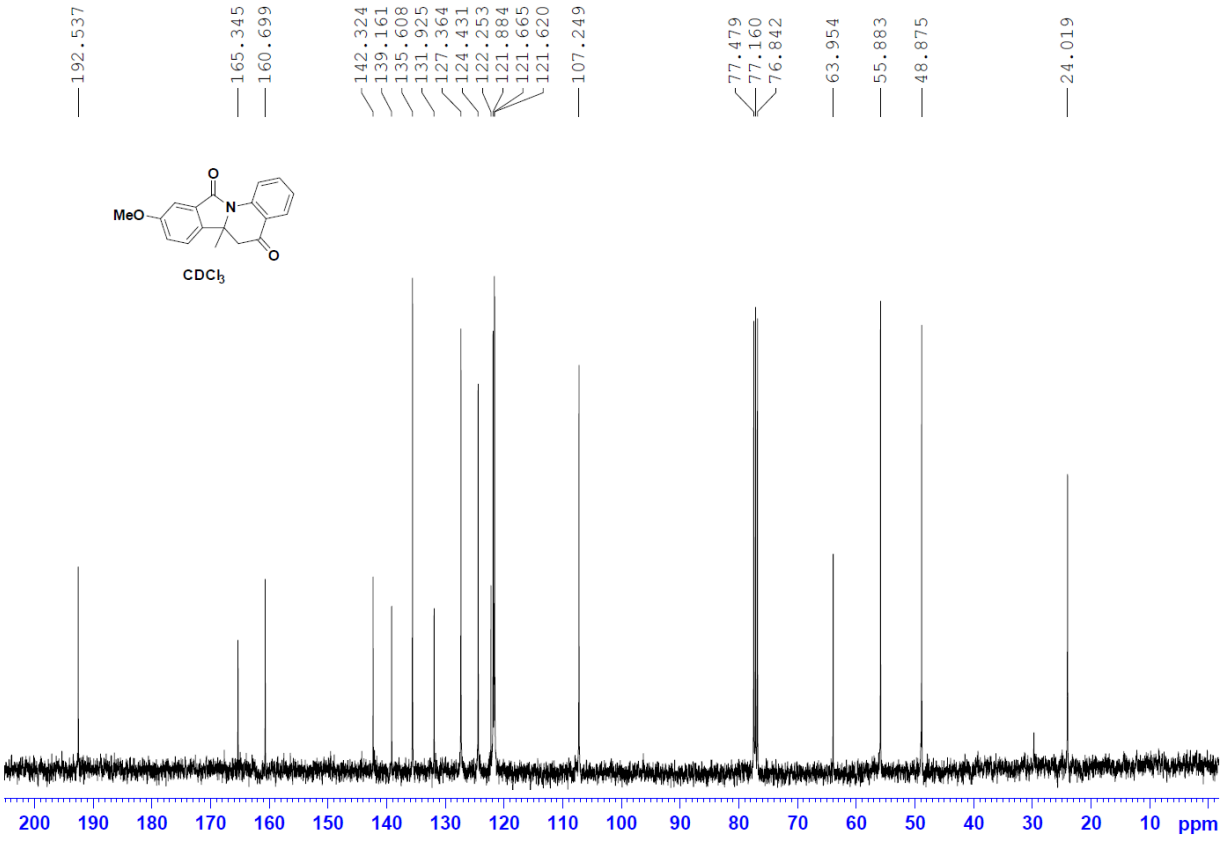
163.933
147.872
138.779
135.704
135.471
133.366
132.330
127.432
125.007
124.787
122.344
122.224
121.669
77.478
77.160
76.841
64.167
48.437
23.883
Cl
O
N
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.474
8.454
8.083
8.064
7.720
7.700
7.681
7.442
7.402
7.382
7.289
7.271
7.252
7.233
7.212
3.906
3.154
3.114
2.744
2.704
1.562
0.001
MeO
O
N
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.93
0.92
0.99
1.01
1.04
2.13
3.06
1.01
1.00
3.01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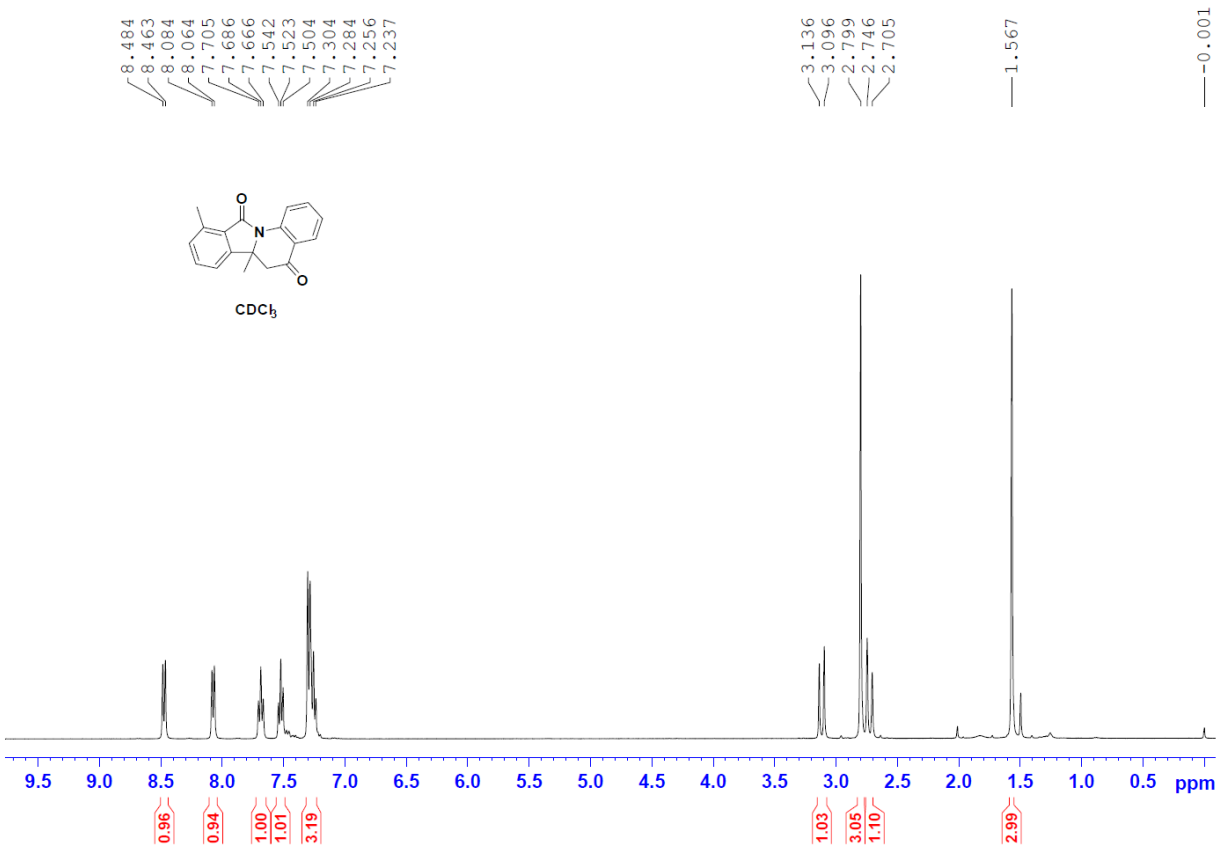
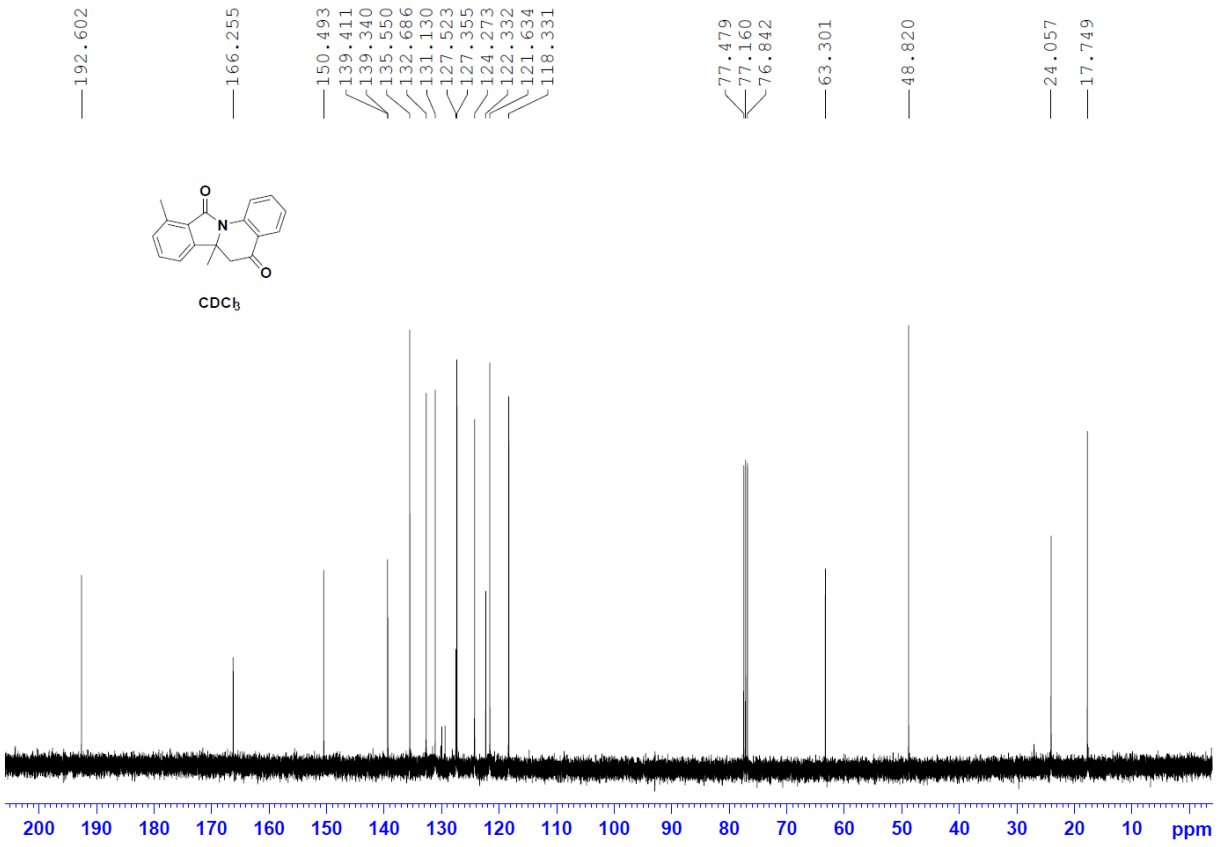
165.345
160.699
142.324
139.161
135.608
131.925
127.364
124.431
122.253
121.884
121.665
121.620
107.249
77.479
77.160
76.842
63.954
55.883
48.875
24.019
MeO
O
N
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.484
8.463
8.084
8.064
7.705
7.686
7.666
7.542
7.523
7.504
7.304
7.284
7.256
7.237
3.136
3.096
2.799
2.746
2.705
1.567
0.001
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.96
0.94
1.00
1.01
3.19
1.03
3.05
1.10
2.99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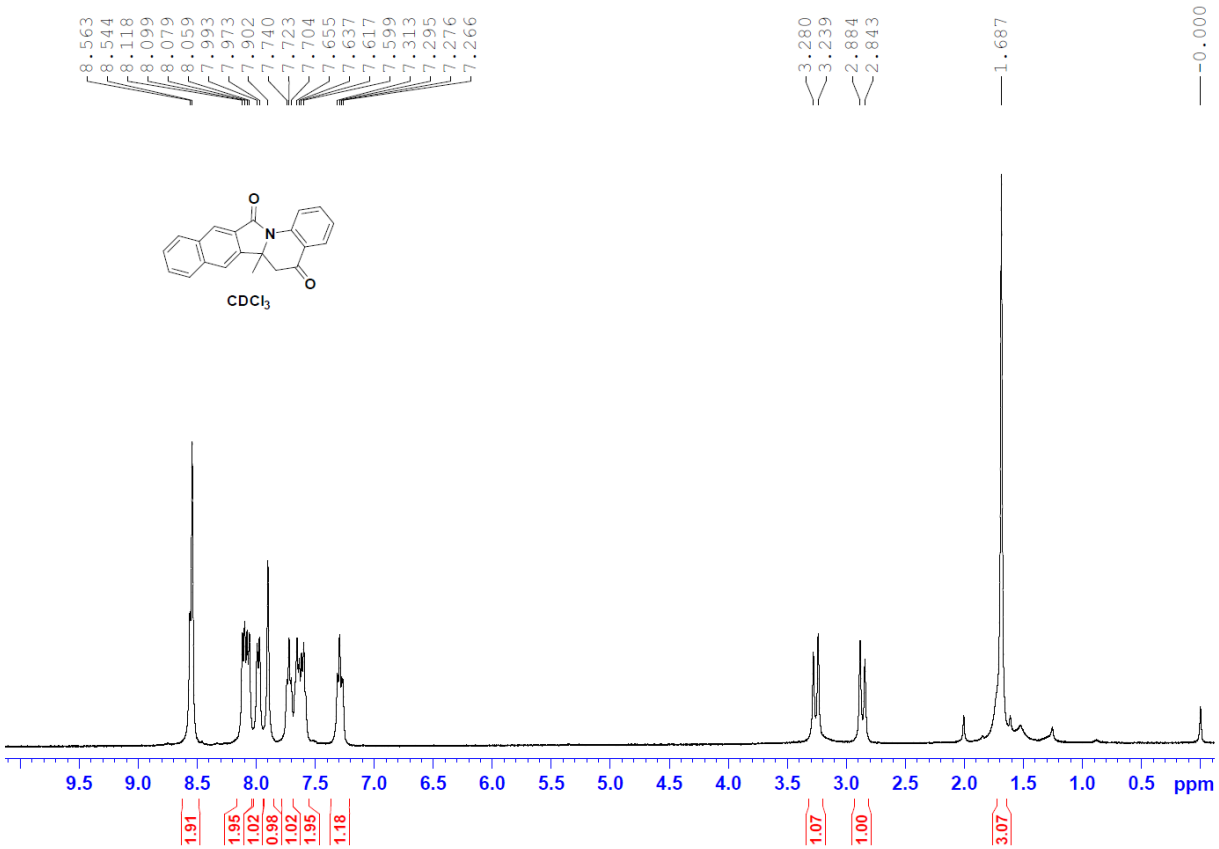
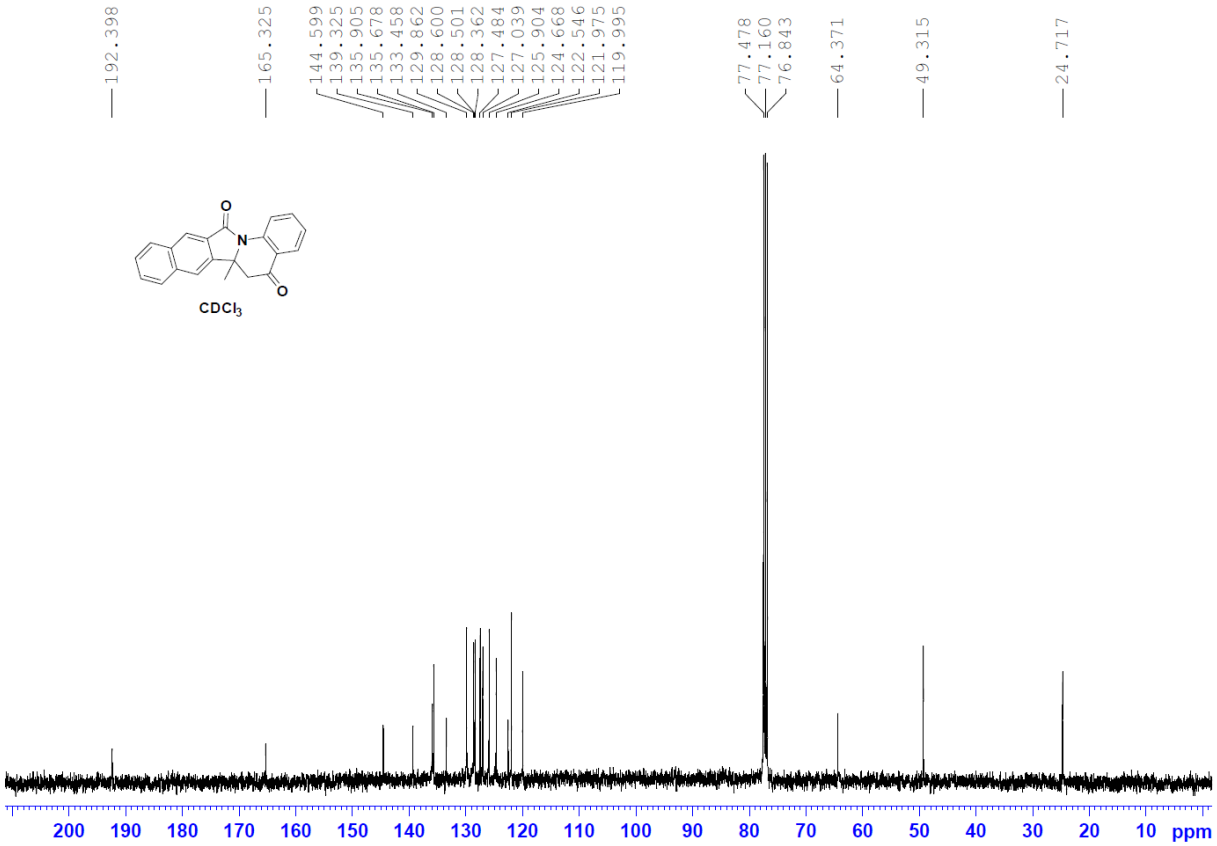
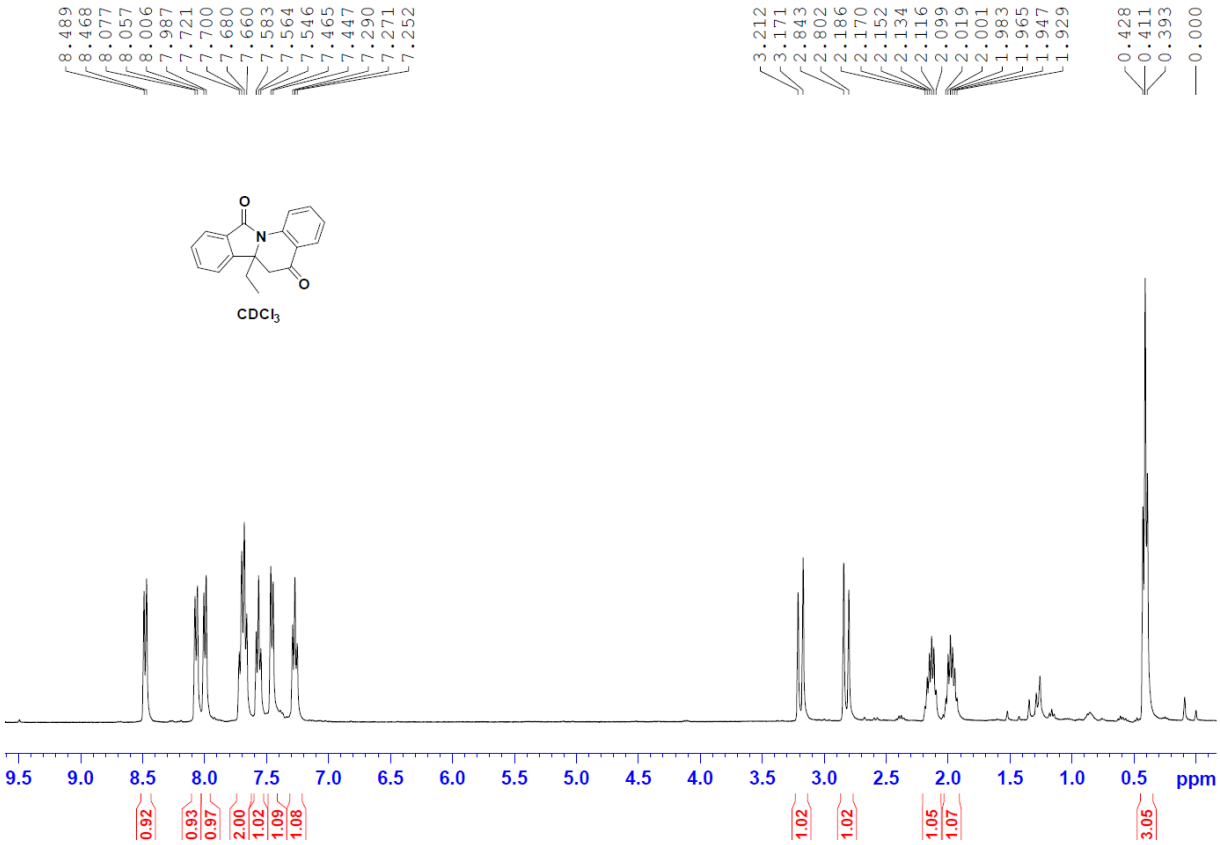
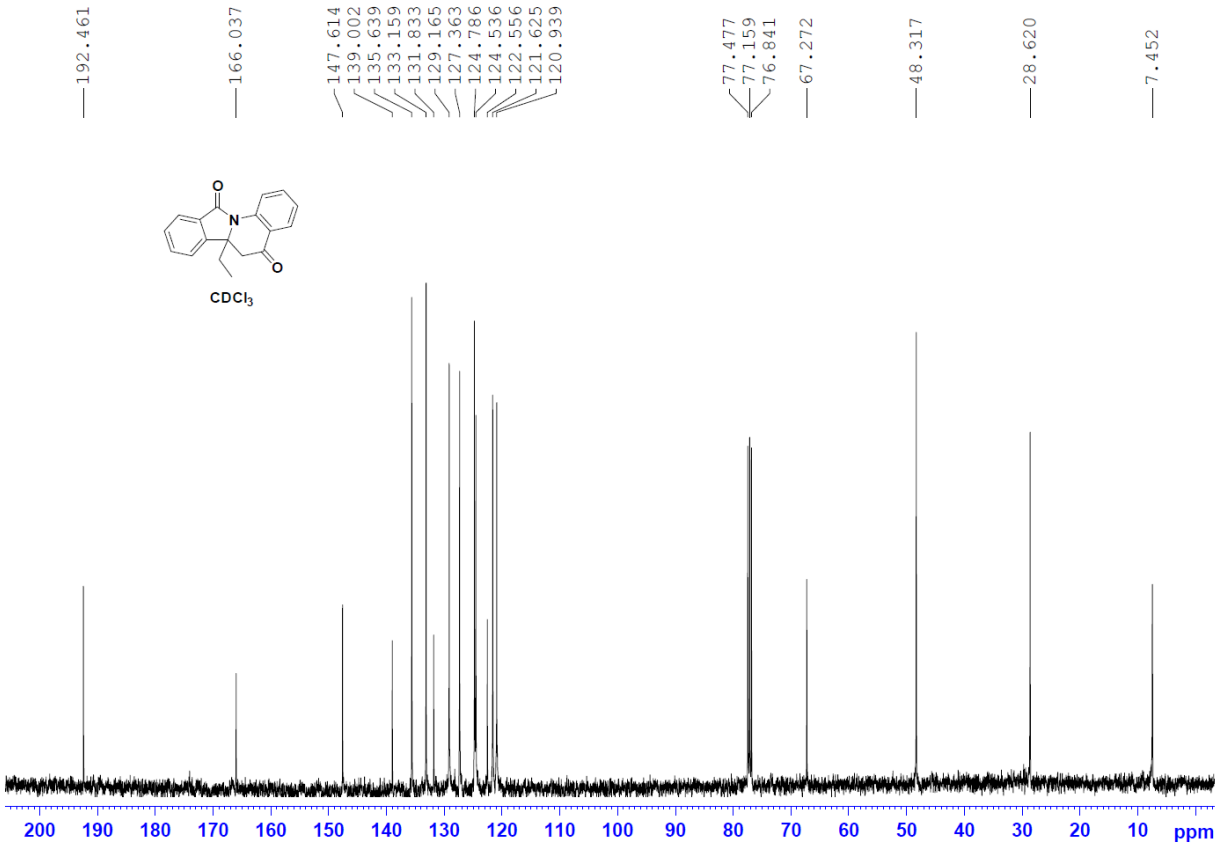
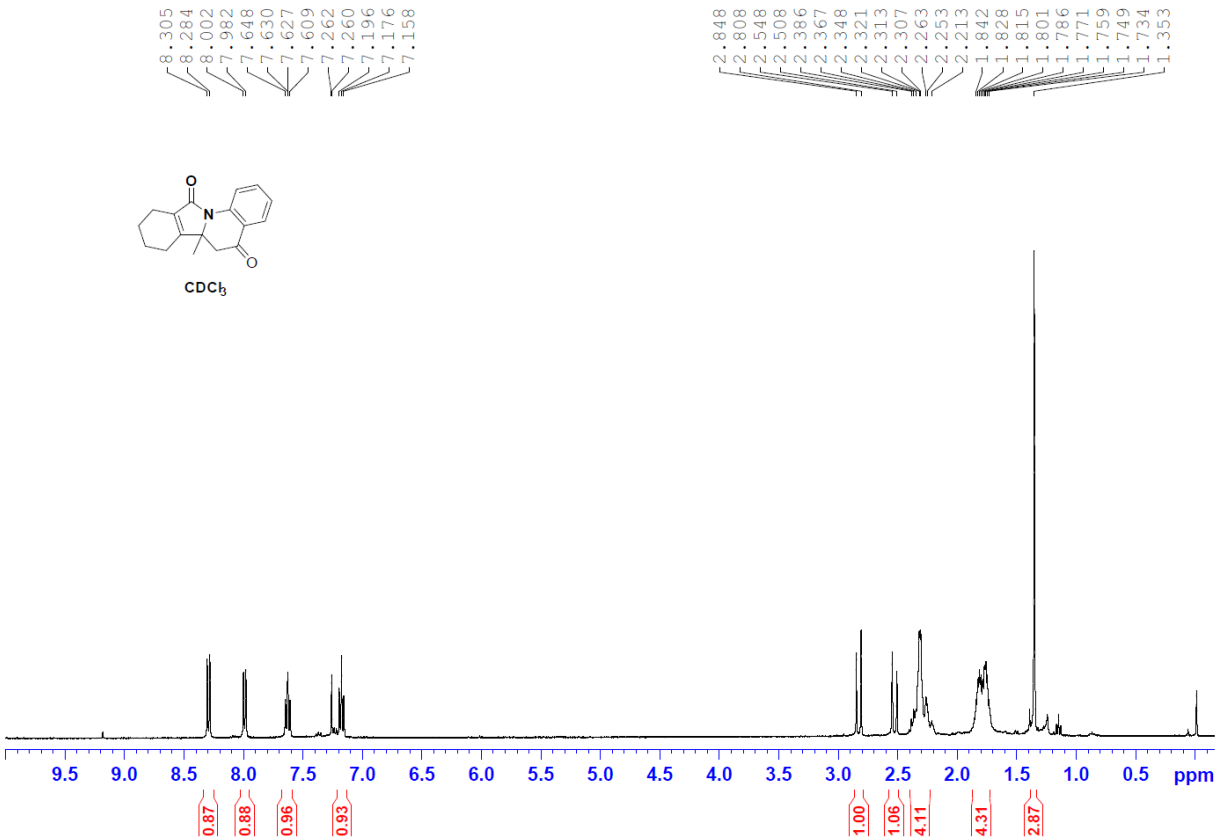
166.255
150.493
139.411
139.340
135.550
132.686
131.130
127.523
127.355
124.273
122.332
121.634
118.331
77.479
77.160
76.842
63.301
48.820
24.057
17.749
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

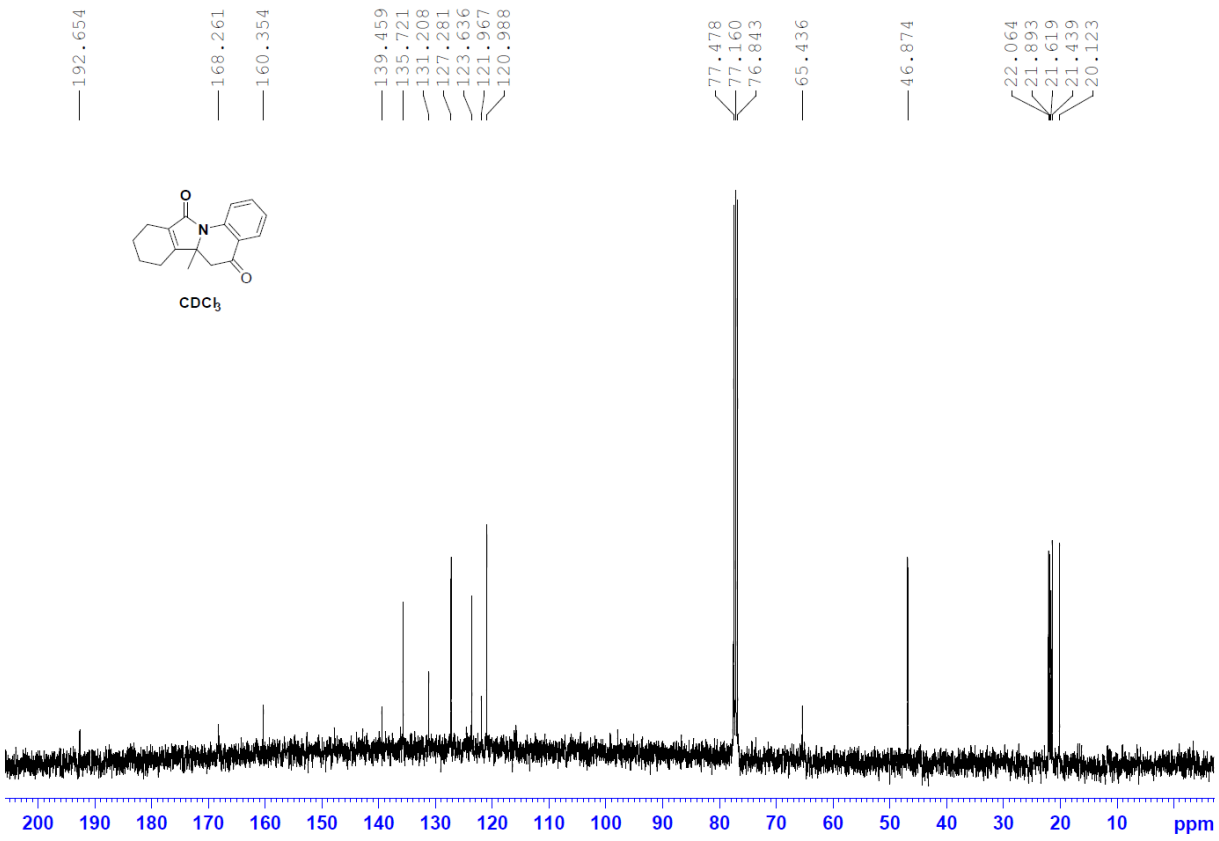

8.563
8.544
8.118
8.099
8.079
8.059
7.993
7.973
7.902
7.740
7.723
7.704
7.655
7.637
7.617
7.599
7.313
7.295
7.276
7.266
3.280
3.239
2.884
2.843
1.687
0.000
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.91
1.95
1.02
0.98
1.02
1.95
1.18
1.07
1.00
3.07

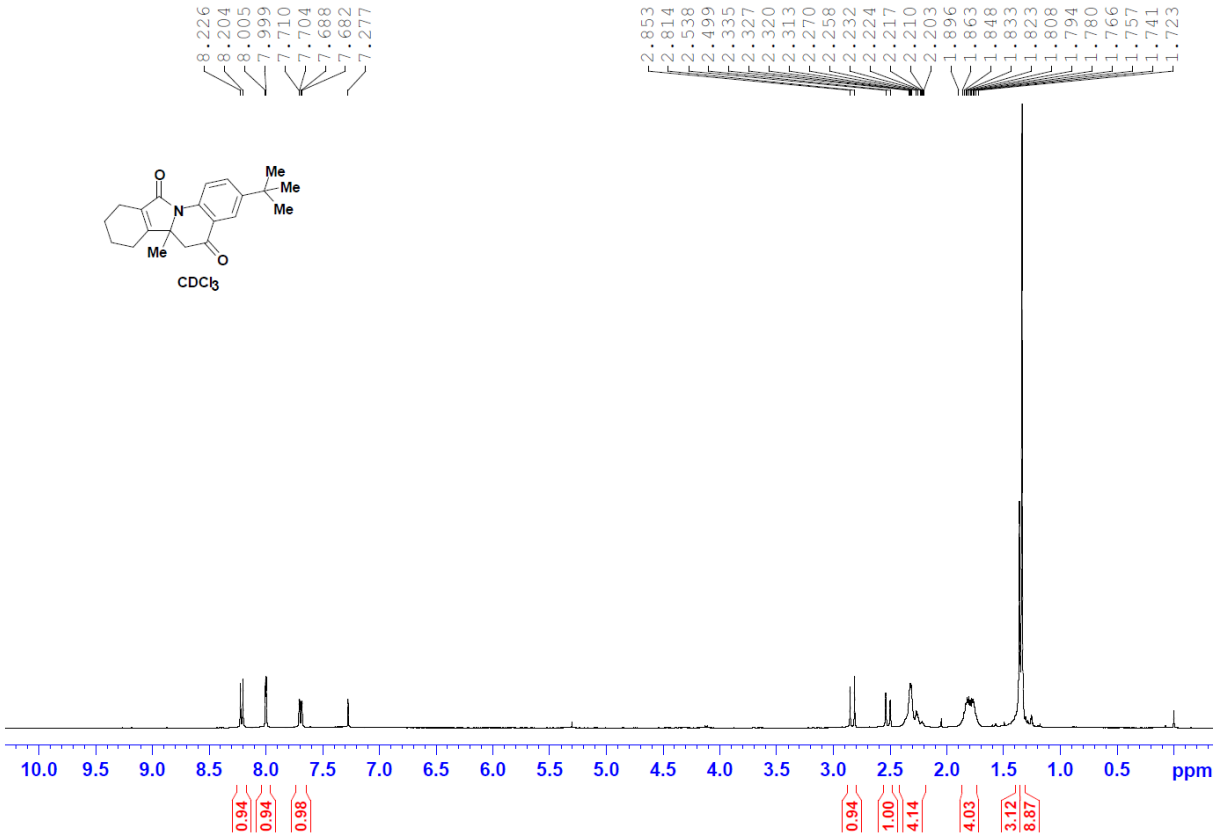

192.398
165.325
144.599
139.325
135.905
135.678
133.458
129.862
128.600
128.501
128.362
127.484
127.039
125.904
124.668
122.546
121.975
119.995
77.478
77.160
76.843
64.371
49.315
24.717
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

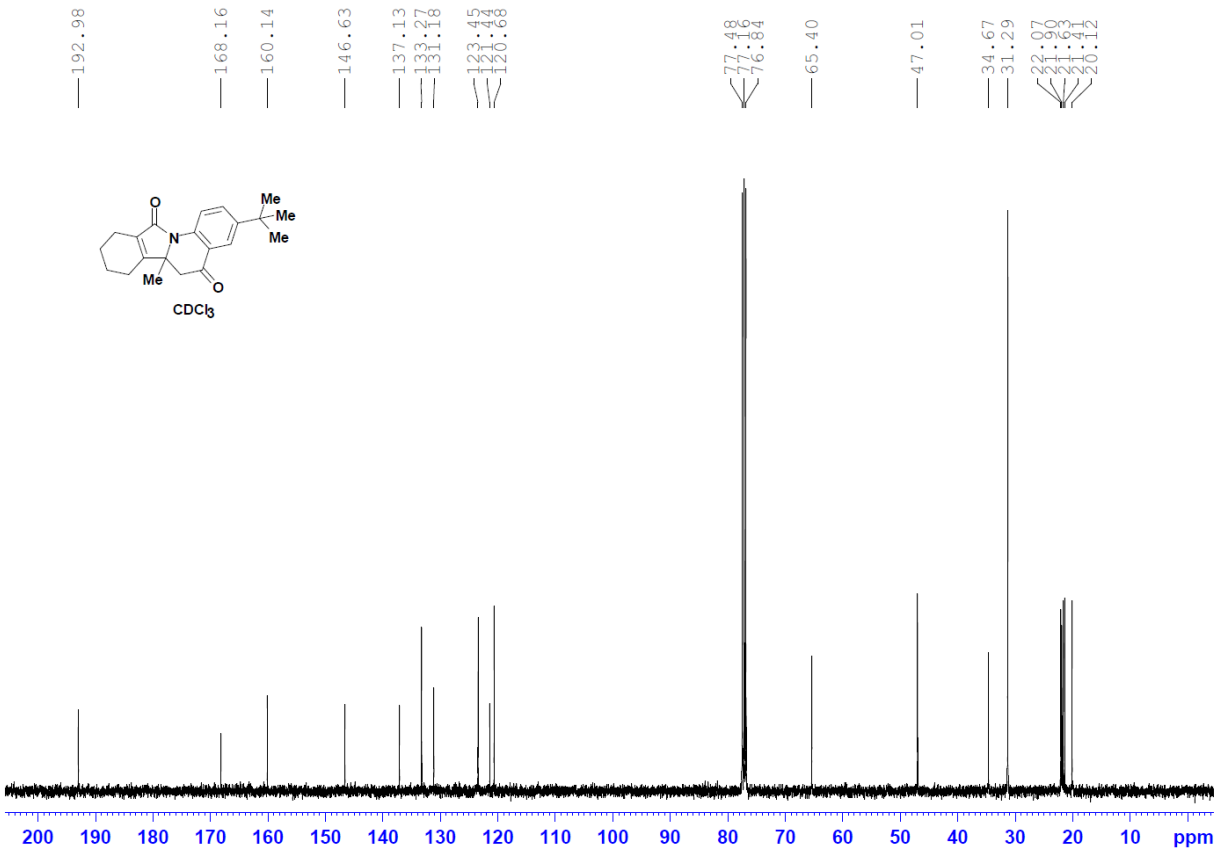

8.489
8.468
8.077
8.057
8.006
7.987
7.721
7.700
7.680
7.660
7.583
7.564
7.546
7.465
7.447
7.290
7.271
7.252
3.212
3.171
2.843
2.802
2.186
2.170
2.152
2.134
2.116
2.099
2.019
2.001
1.983
1.965
1.947
1.929
0.428
0.411
0.393
0.000
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.92 0.93 0.97 2.00 1.02 1.09 1.08 1.02 1.02 1.05 1.07 3.05

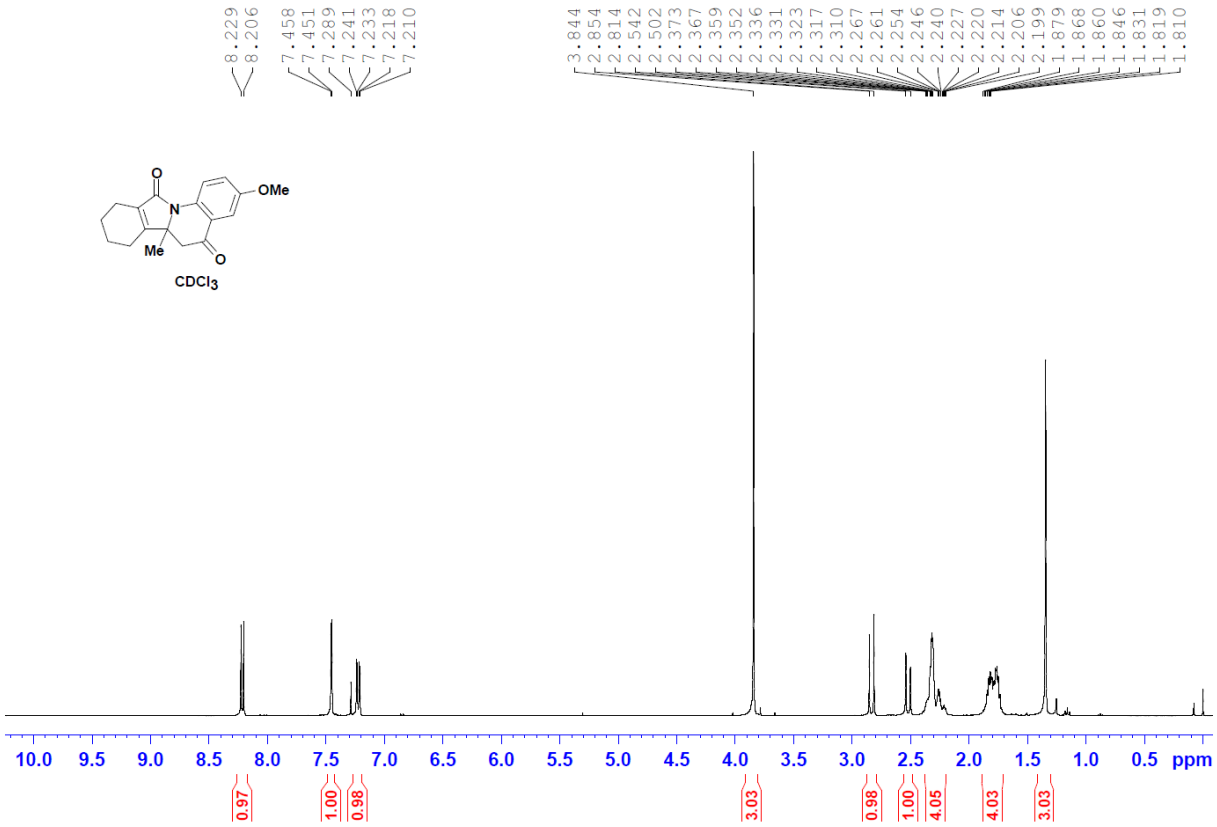

192.461
166.037
147.614
139.002
135.639
133.159
131.833
129.165
127.363
124.786
124.536
122.556
121.625
120.939
77.477
77.159
76.841
67.272
48.317
28.620
7.452
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.305
8.284
8.002
7.982
7.648
7.630
7.627
7.609
7.262
7.260
7.196
7.176
7.158
2.848
2.808
2.548
2.508
2.386
2.367
2.348
2.321
2.313
2.307
2.263
2.253
2.213
1.842
1.828
1.815
1.801
1.786
1.771
1.759
1.749
1.734
1.353
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.87
0.88
0.96
0.93
1.00
1.06
4.11
4.31
2.87


192.654
168.261
160.354
139.459
135.721
131.208
127.281
123.636
121.967
120.988
77.478
77.160
76.843
65.436
46.874
22.064
21.893
21.619
21.439
20.123
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.226
8.204
8.005
7.999
7.710
7.704
7.688
7.682
7.277
2.853
2.814
2.538
2.499
2.335
2.327
2.320
2.313
2.270
2.258
2.232
2.224
2.217
2.210
2.203
1.896
1.863
1.848
1.833
1.823
1.808
1.794
1.780
1.766
1.757
1.741
1.723
Me
Me
Me
Me
O
N
O
CDCl3
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.94
0.94
0.98
0.94
1.00
4.14
4.03
3.12
8.87


192.98
168.16
160.14
146.63
137.13
133.27
131.18
123.45
121.44
120.68
77.48
77.16
76.84
65.40
47.01
34.67
31.29
22.07
21.90
21.63
21.41
20.12
Me
Me
Me
Me
O
N
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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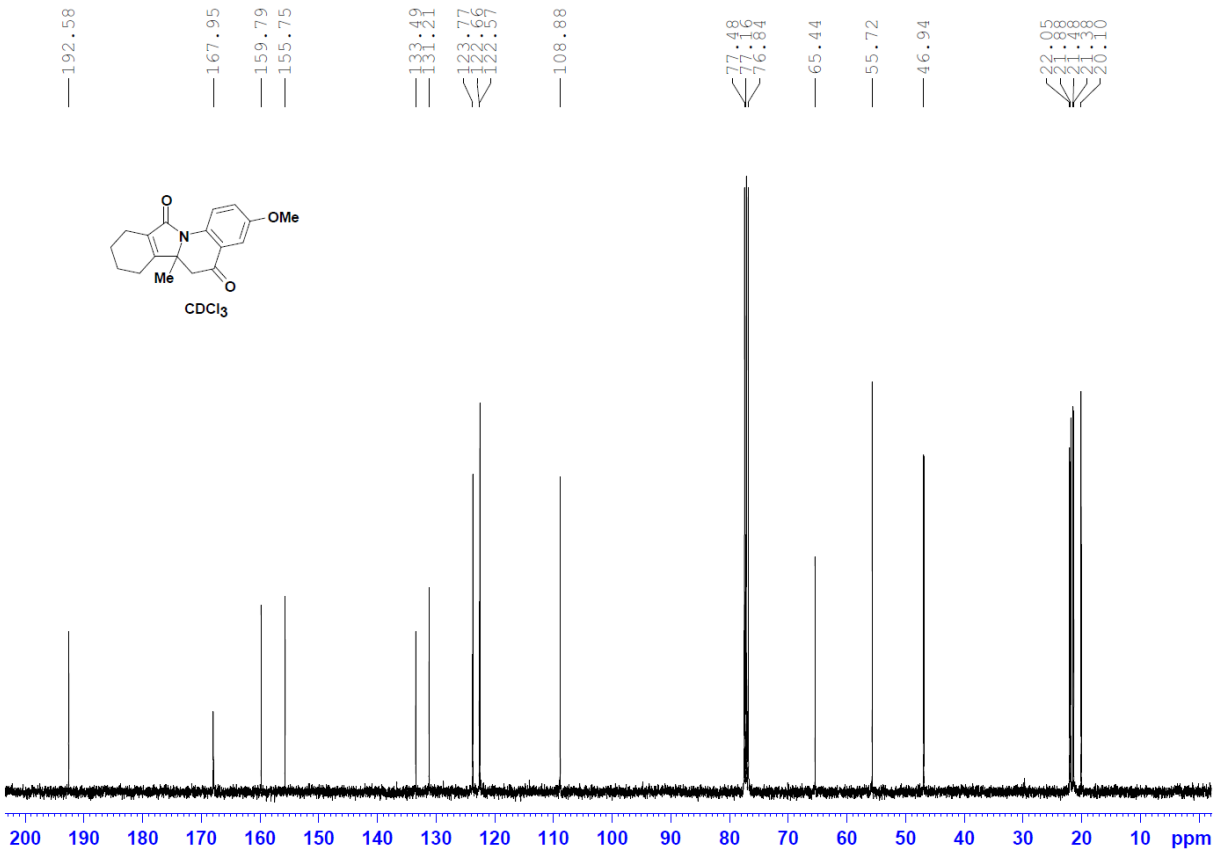
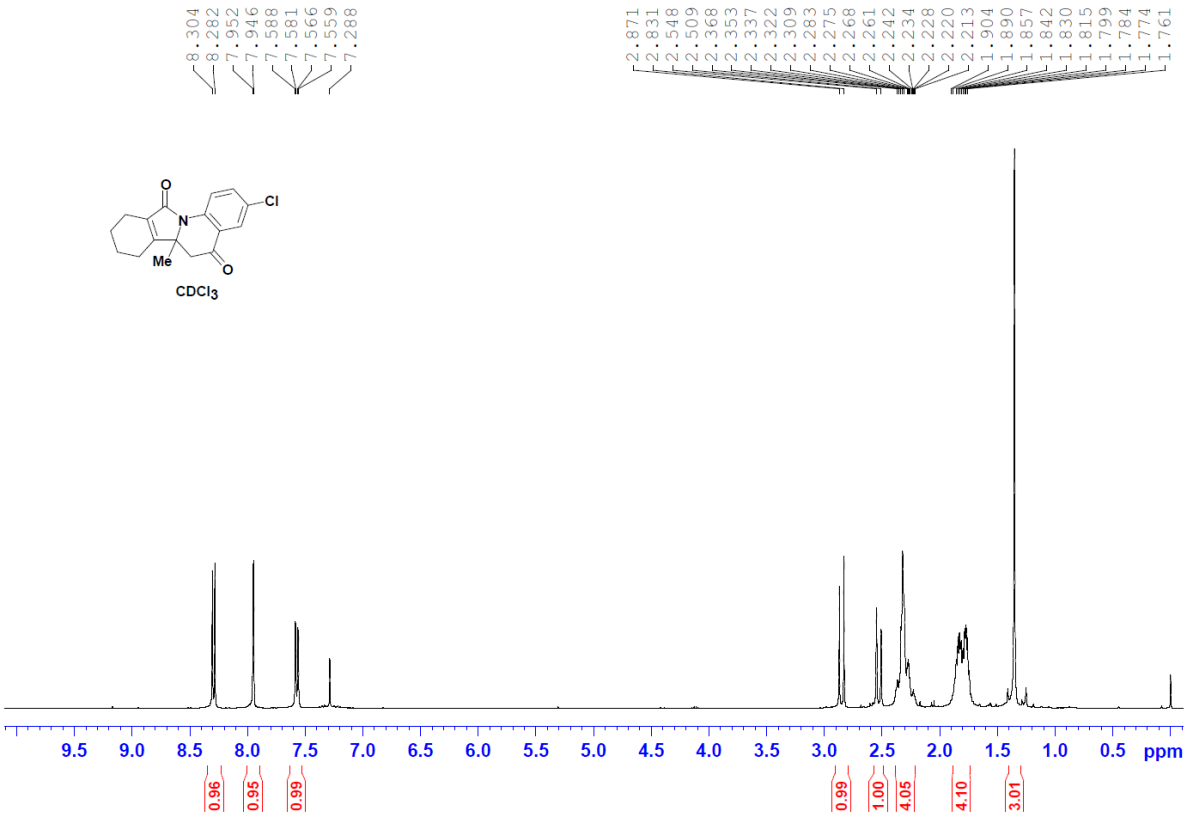
8.206
7.458
7.451
7.289
7.241
7.233
7.218
7.210
3.844
2.854
2.814
2.542
2.502
2.373
2.367
2.359
2.352
2.336
2.331
2.323
2.317
2.310
2.267
2.261
2.254
2.246
2.240
2.227
2.220
2.214
2.206
2.199
1.879
1.868
1.860
1.846
1.831
1.819
1.810
O
N
OMe
Me
O
CDCl3
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.97
1.00
0.98
3.03
0.98
1.00
4.05
4.03
3.03


192.58
167.95
159.79
155.75
133.49
131.21
123.77
122.66
122.57
108.88
77.48
77.16
76.84
65.44
55.72
46.94
22.05
21.88
21.48
21.38
20.10
O
N
OMe
Me
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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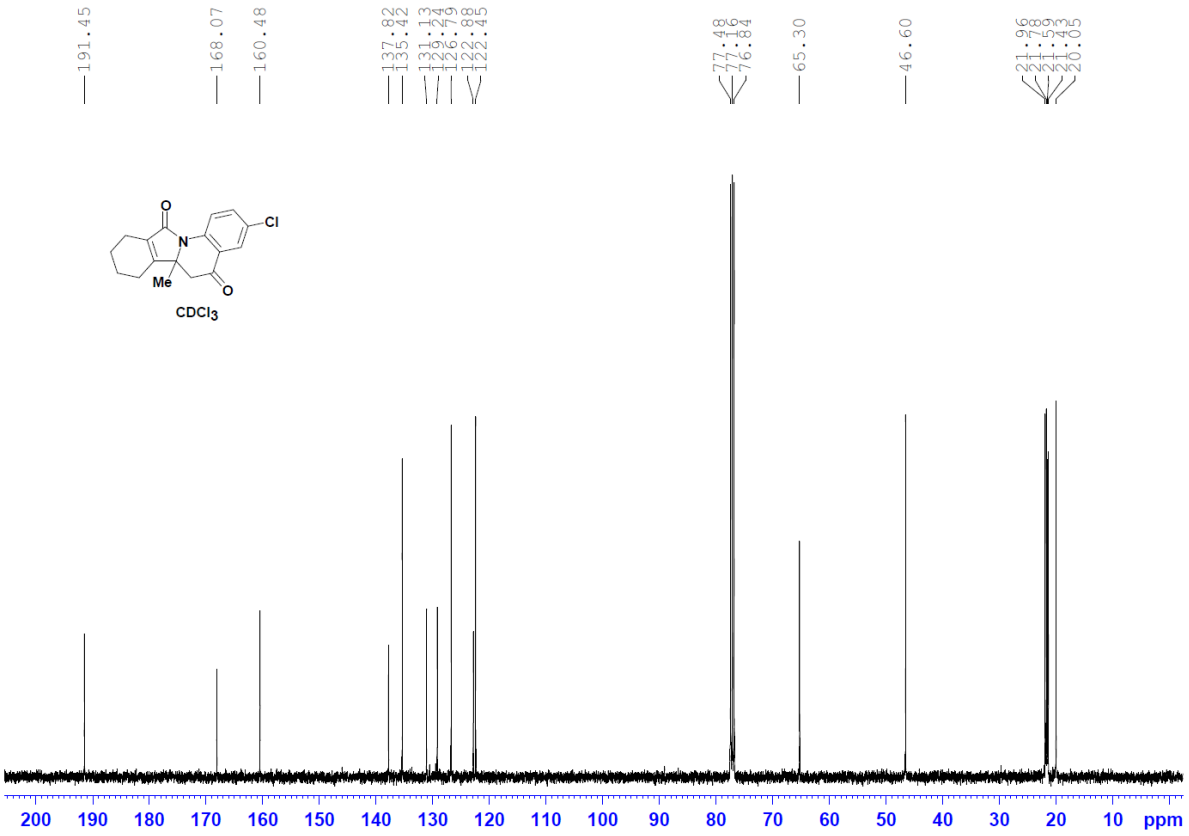
7.952
7.946
7.588
7.581
7.566
7.559
7.288
2.871
2.831
2.548
2.509
2.368
2.353
2.337
2.322
2.309
2.283
2.275
2.268
2.261
2.242
2.234
2.228
2.220
2.213
1.904
1.890
1.857
1.842
1.830
1.815
1.799
1.784
1.774
1.761
O
N
Cl
Me
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.96
0.95
0.99
0.99
1.00
4.05
4.10
3.01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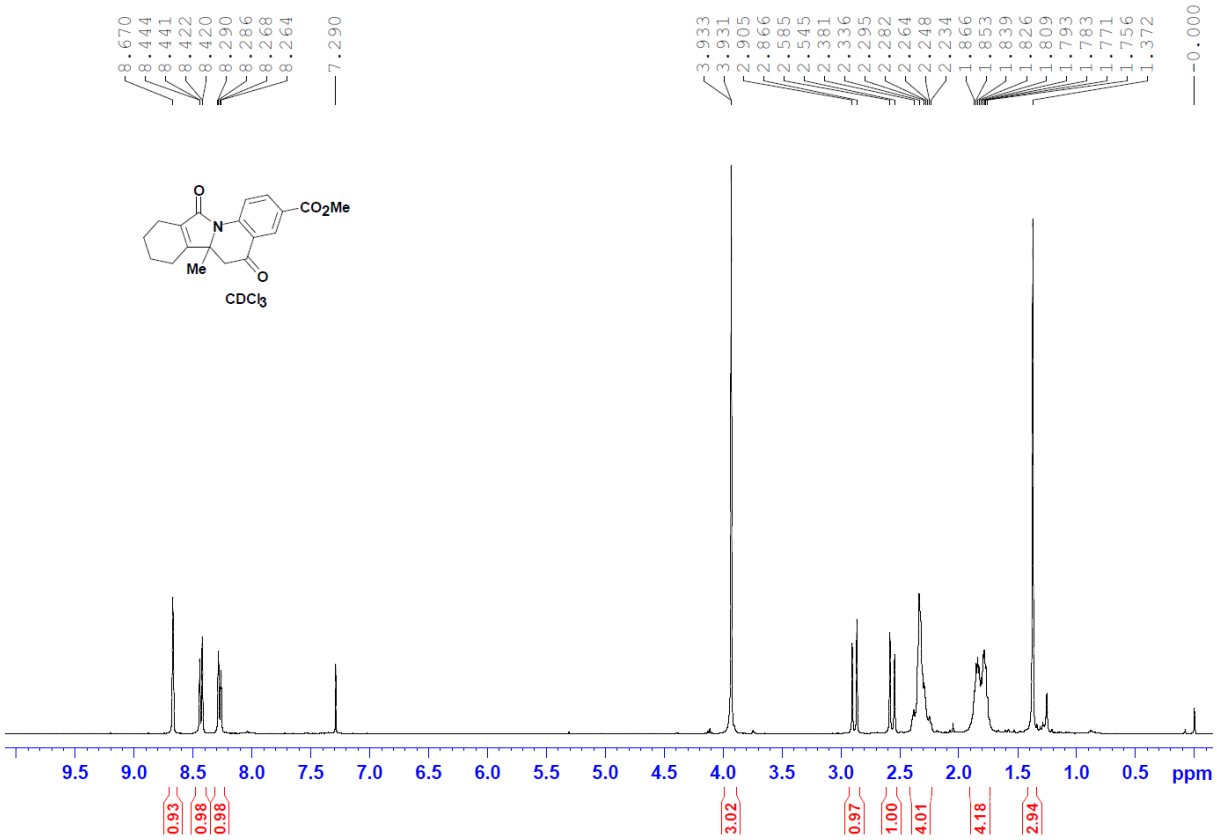
168.07
160.48
137.82
135.42
131.13
129.24
126.79
122.88
122.45
77.48
77.16
76.84
65.30
46.60
21.96
21.78
21.59
21.42
20.05
O
N
Cl
Me
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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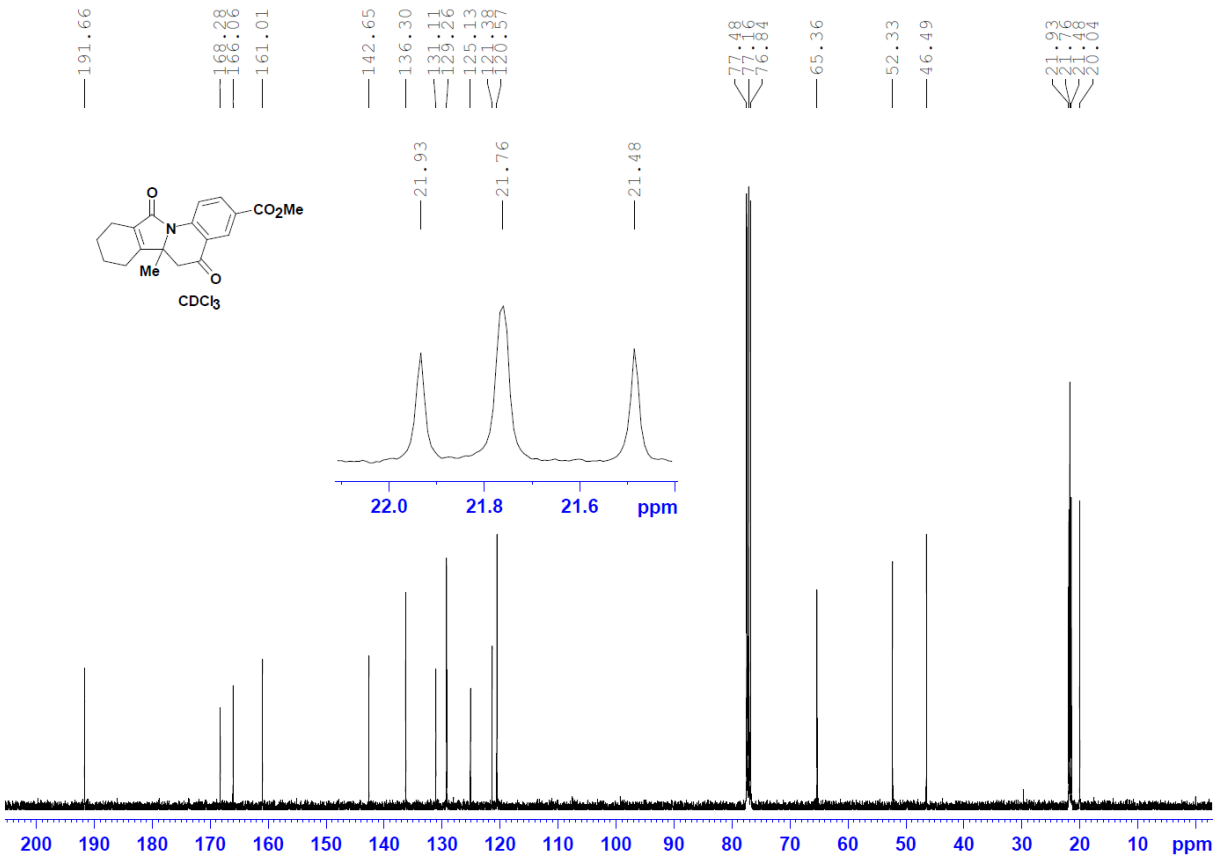
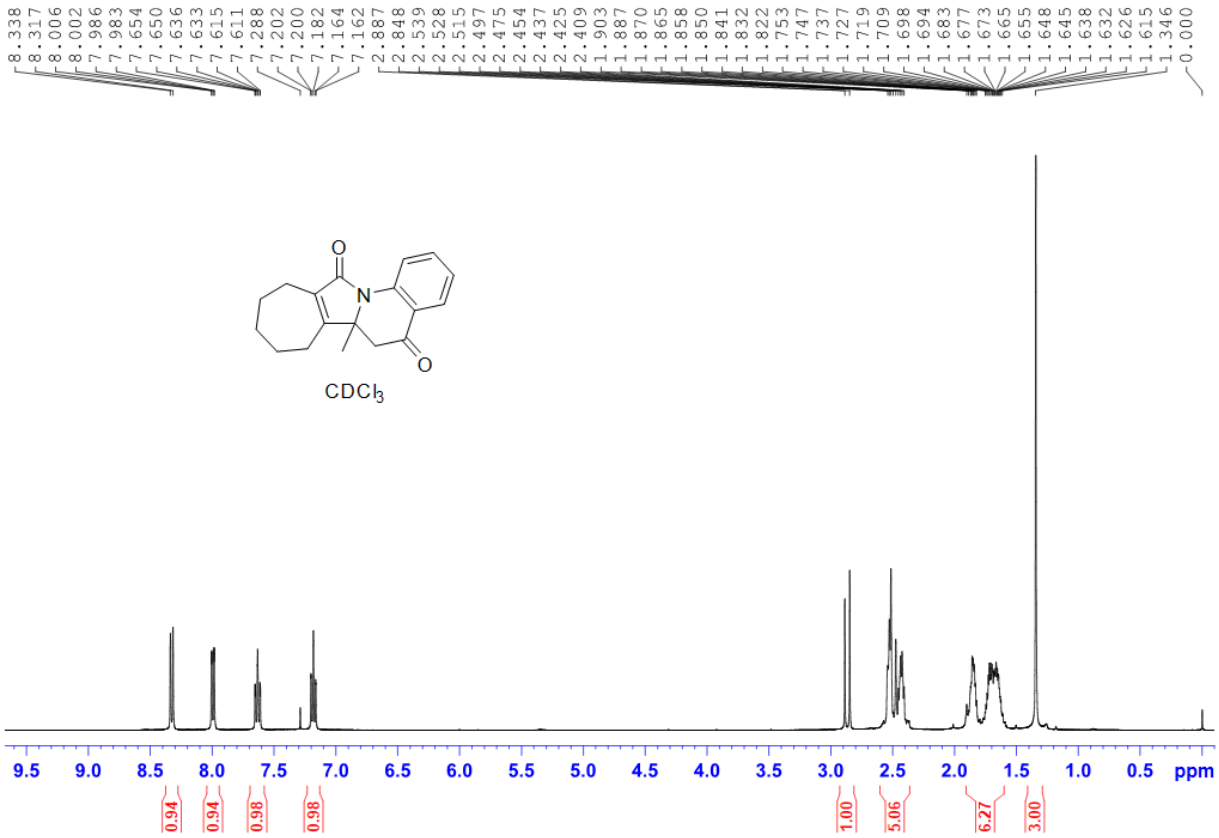
8.441
8.422
8.420
8.290
8.286
8.268
8.264
7.290
3.933
3.931
2.905
2.866
2.585
2.545
2.381
2.336
2.295
2.282
2.264
2.248
2.234
1.866
1.853
1.839
1.826
1.809
1.793
1.783
1.771
1.756
1.372
0.000
CO2Me
Me
O
N
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.93
0.98
0.98
3.02
0.97
1.00
4.01
4.18
2.94


191.66
168.28
166.06
161.01
142.65
136.30
131.11
129.26
125.13
121.38
120.57
77.48
77.16
76.84
65.36
52.33
46.49
21.93
21.76
21.48
20.04
CO2Me
Me
O
N
CDCl3
22.0 21.8 21.6 ppm
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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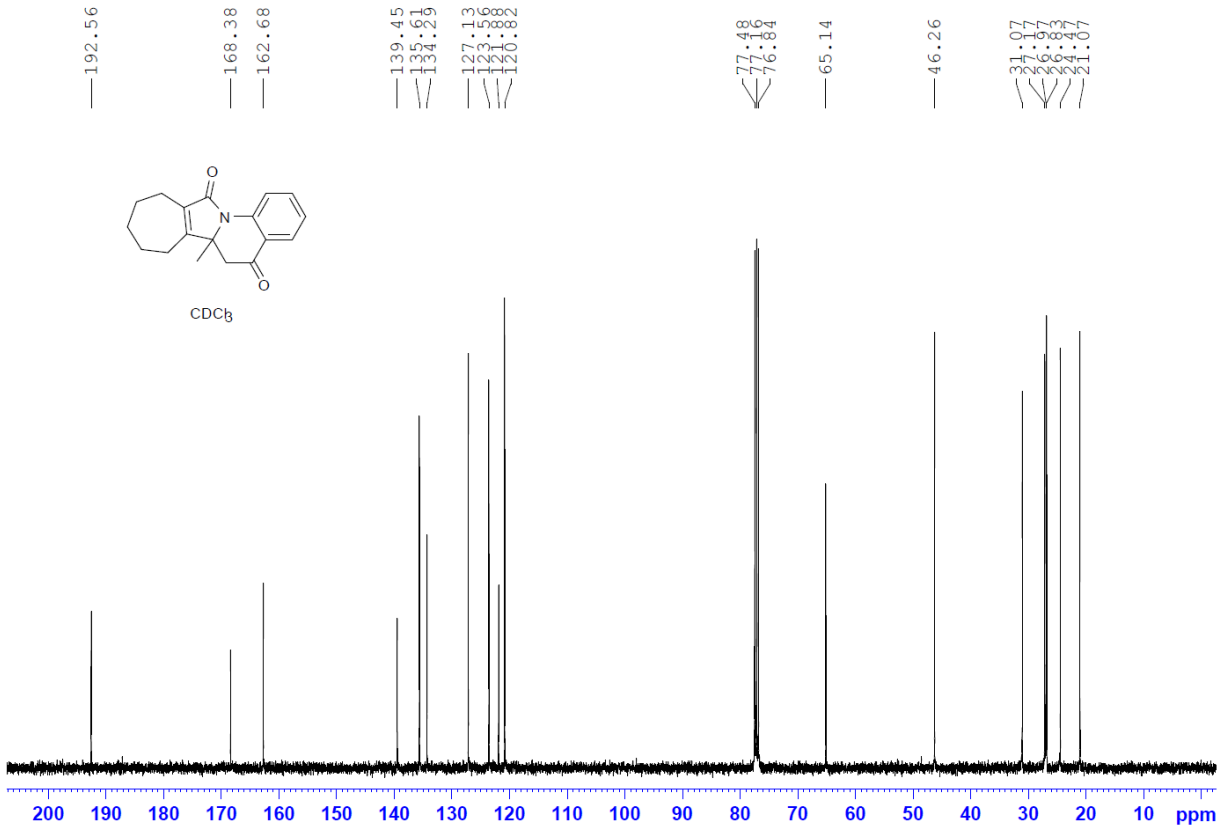
8.317
8.006
8.002
7.986
7.983
7.654
7.650
7.636
7.633
7.615
7.611
7.288
7.202
7.200
7.182
7.164
7.162
2.887
2.848
2.539
2.528
2.515
2.497
2.475
2.454
2.437
2.425
2.409
1.903
1.887
1.870
1.865
1.858
1.850
1.841
1.832
1.822
1.753
1.747
1.737
1.727
1.719
1.709
1.698
1.694
1.683
1.677
1.673
1.665
1.655
1.648
1.645
1.638
1.632
1.626
1.615
1.346
0.000
O
N
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.94
0.94
0.98
0.98
1.00
5.06
6.27
3.00


192.56
168.38
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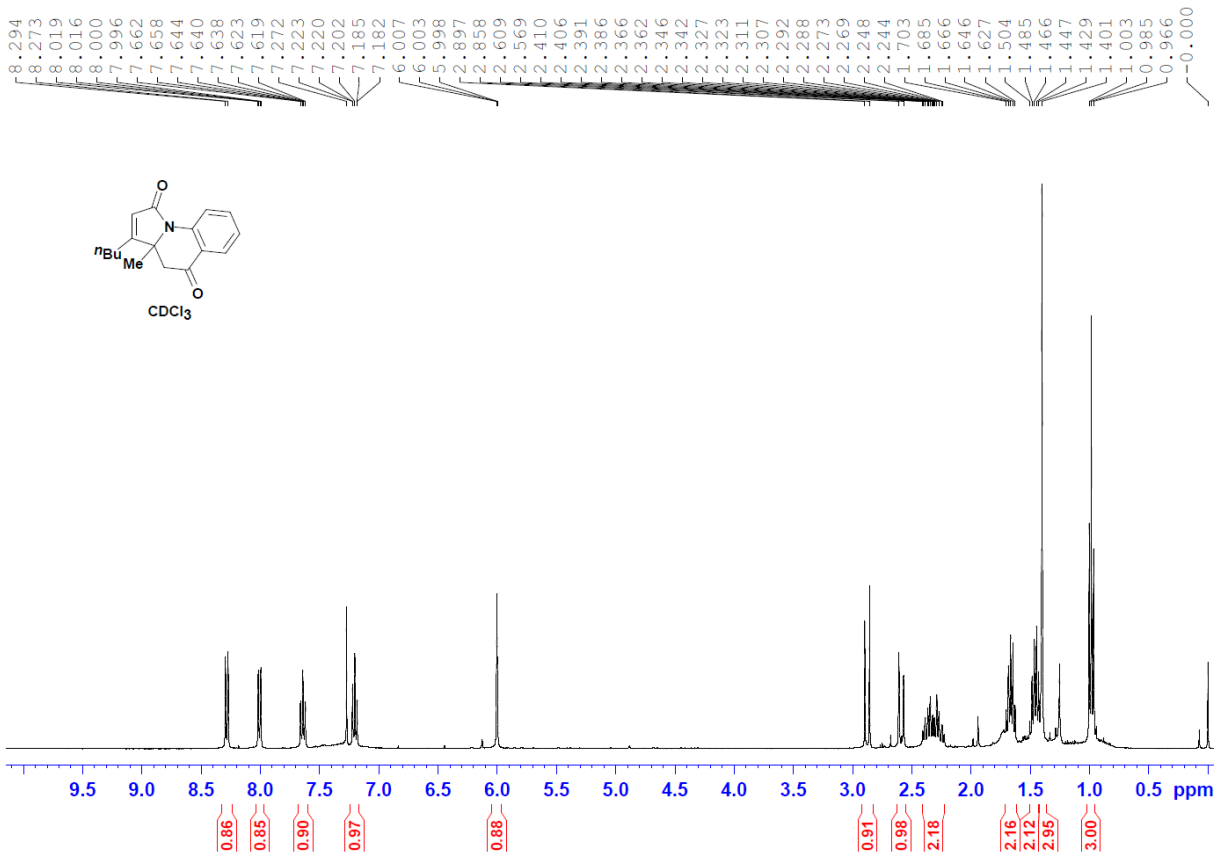
139.45
135.61
134.29
127.13
123.56
121.88
120.82
77.48
77.16
76.84
65.14
46.26
31.07
27.17
26.97
26.83
24.47
21.07
O
N
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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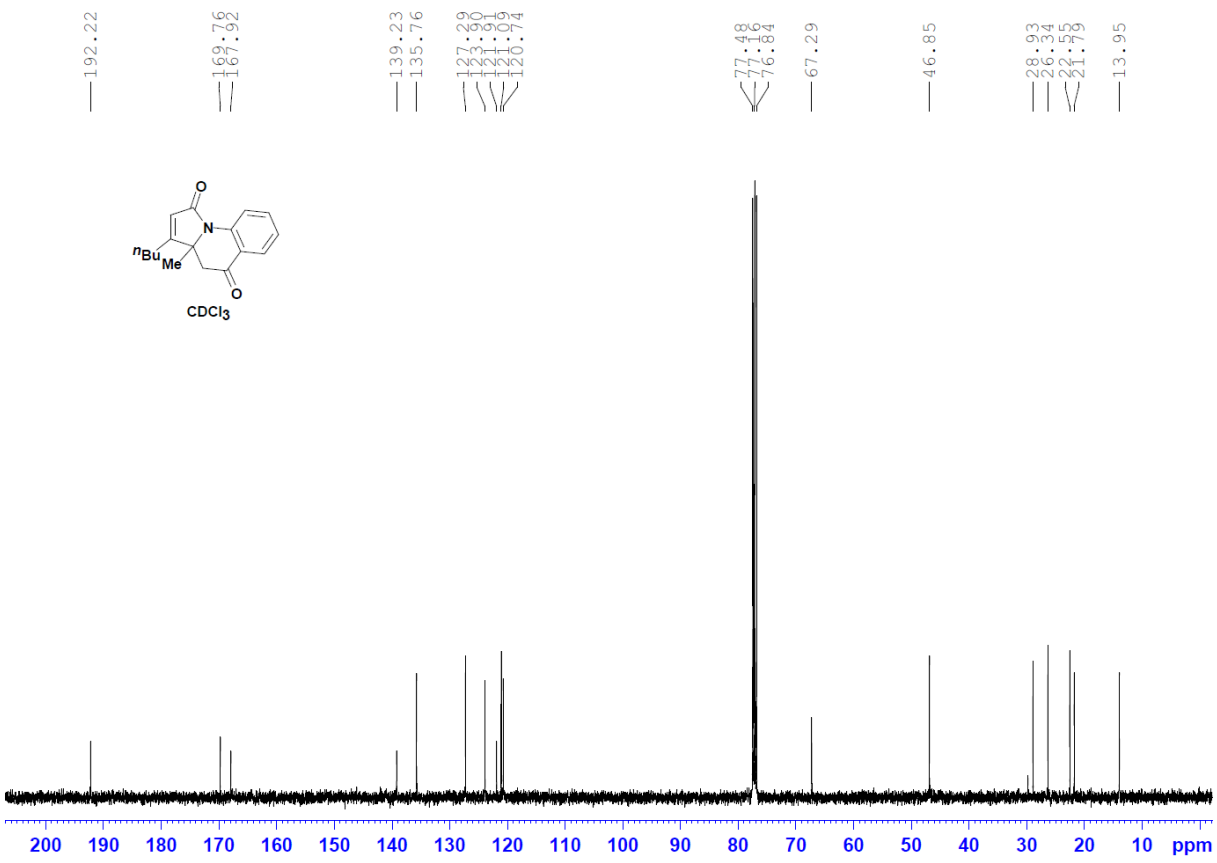
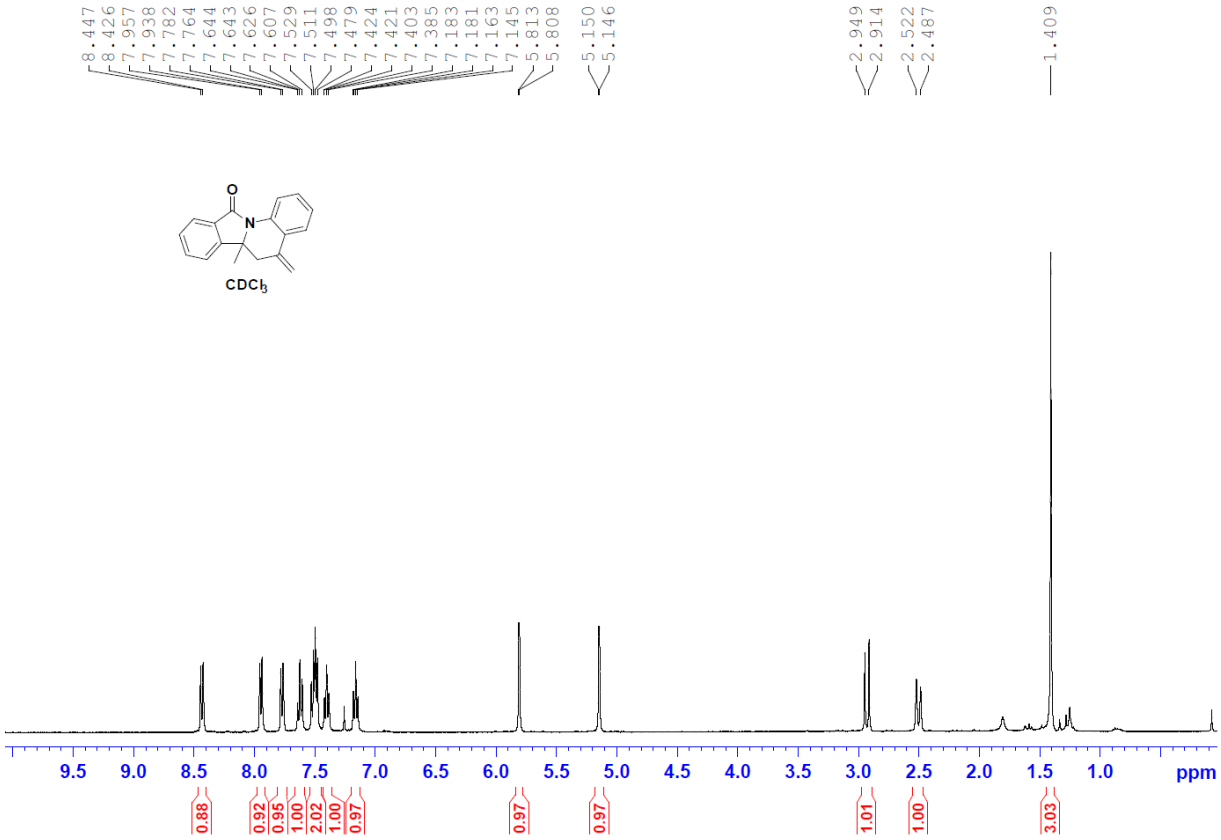
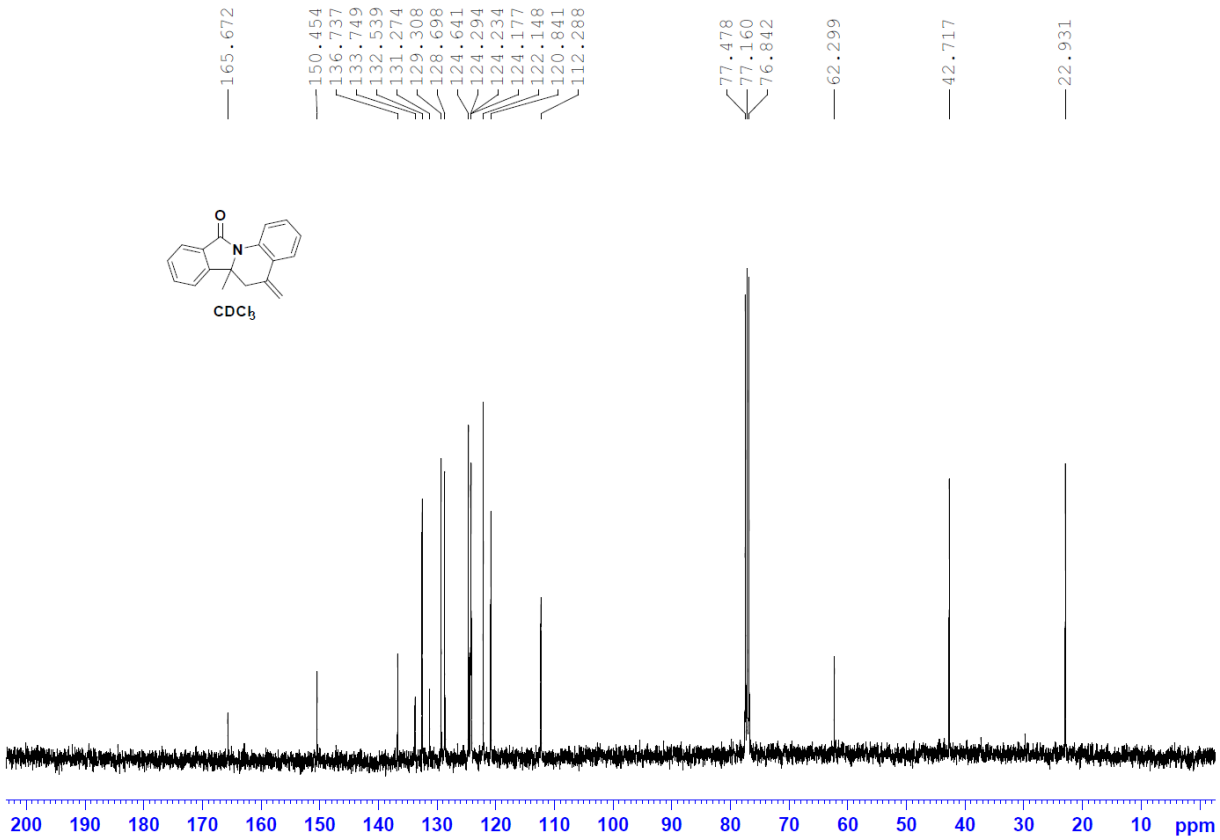
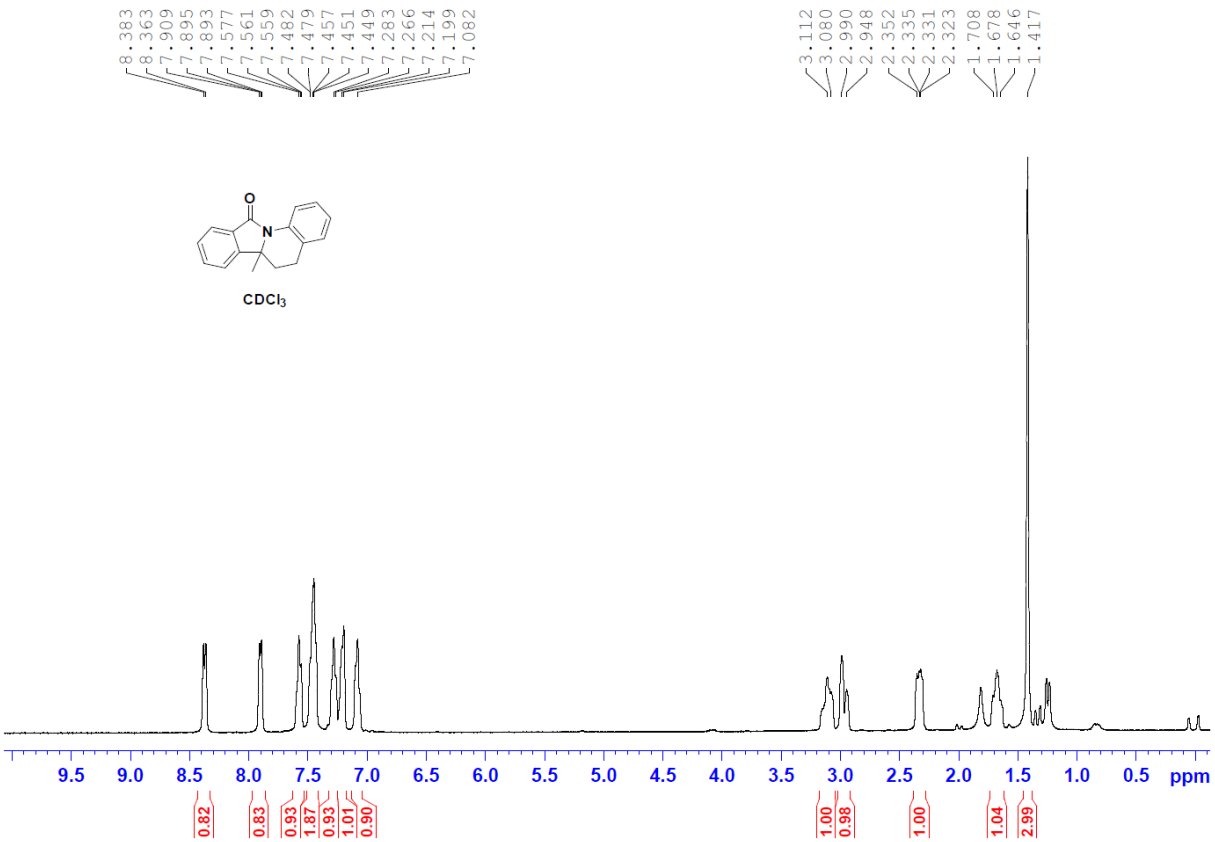
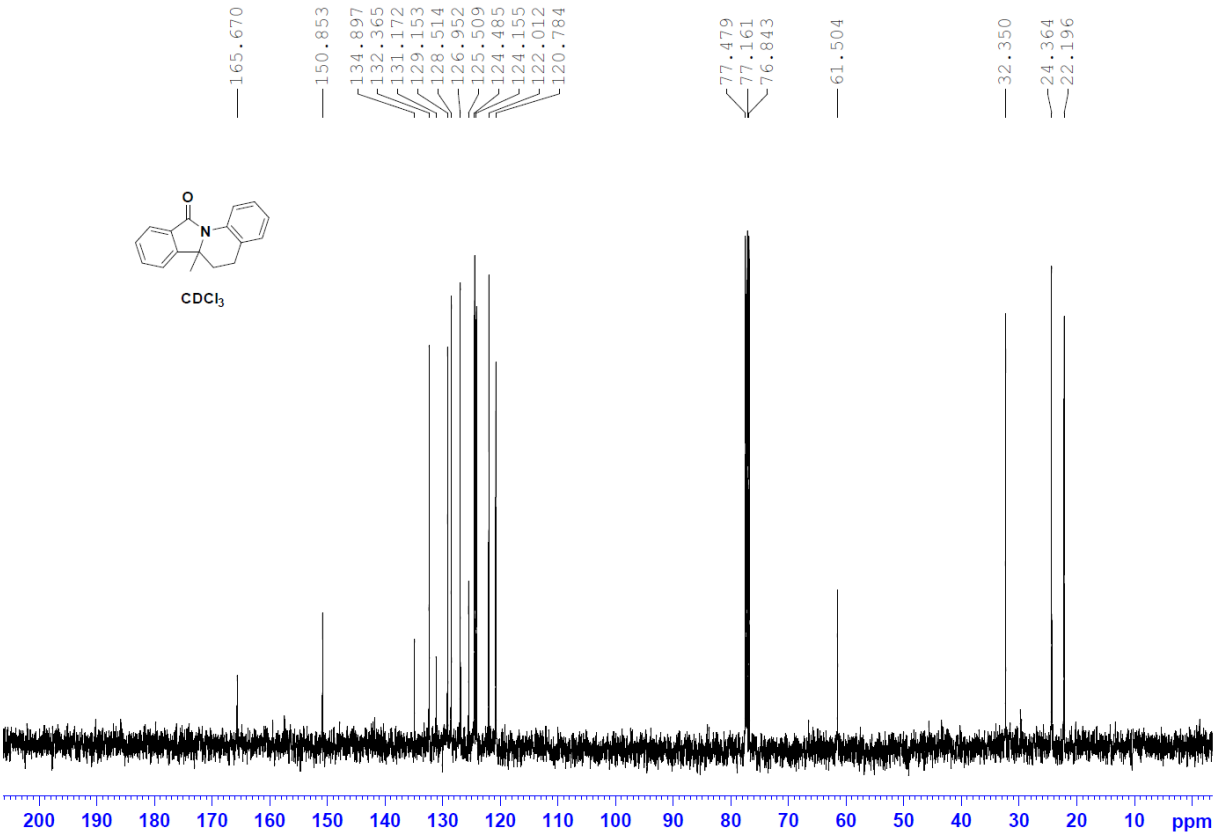
8.273
8.019
8.016
8.000
7.996
7.662
7.658
7.644
7.640
7.638
7.623
7.619
7.272
7.223
7.220
7.202
7.185
7.182
6.007
6.003
5.998
2.897
2.858
2.609
2.569
2.410
2.406
2.391
2.386
2.366
2.362
2.346
2.342
2.327
2.323
2.311
2.307
2.292
2.288
2.273
2.269
2.248
2.244
1.703
1.685
1.666
1.646
1.627
1.504
1.485
1.466
1.447
1.429
1.401
1.003
0.985
0.966
-0.000
O
N
nBu
Me
O
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.86
0.85
0.90
0.97
0.88
0.91
0.98
2.18
2.16
2.12
2.95
3.00

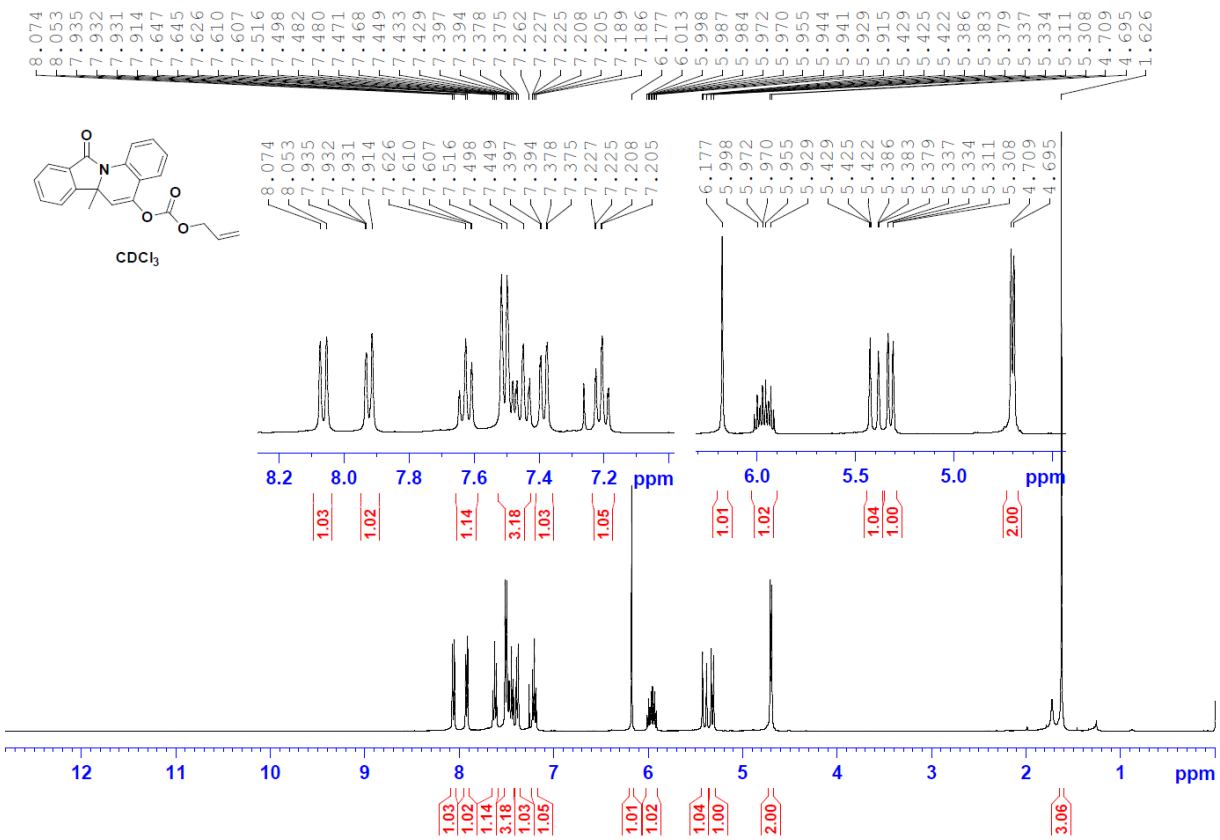

192.22
169.76
167.92
139.23
135.76
127.29
123.90
121.91
121.09
120.74
77.48
77.16
76.84
67.29
46.85
28.93
26.34
22.55
21.79
13.95
O
N
nBu
Me
O
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

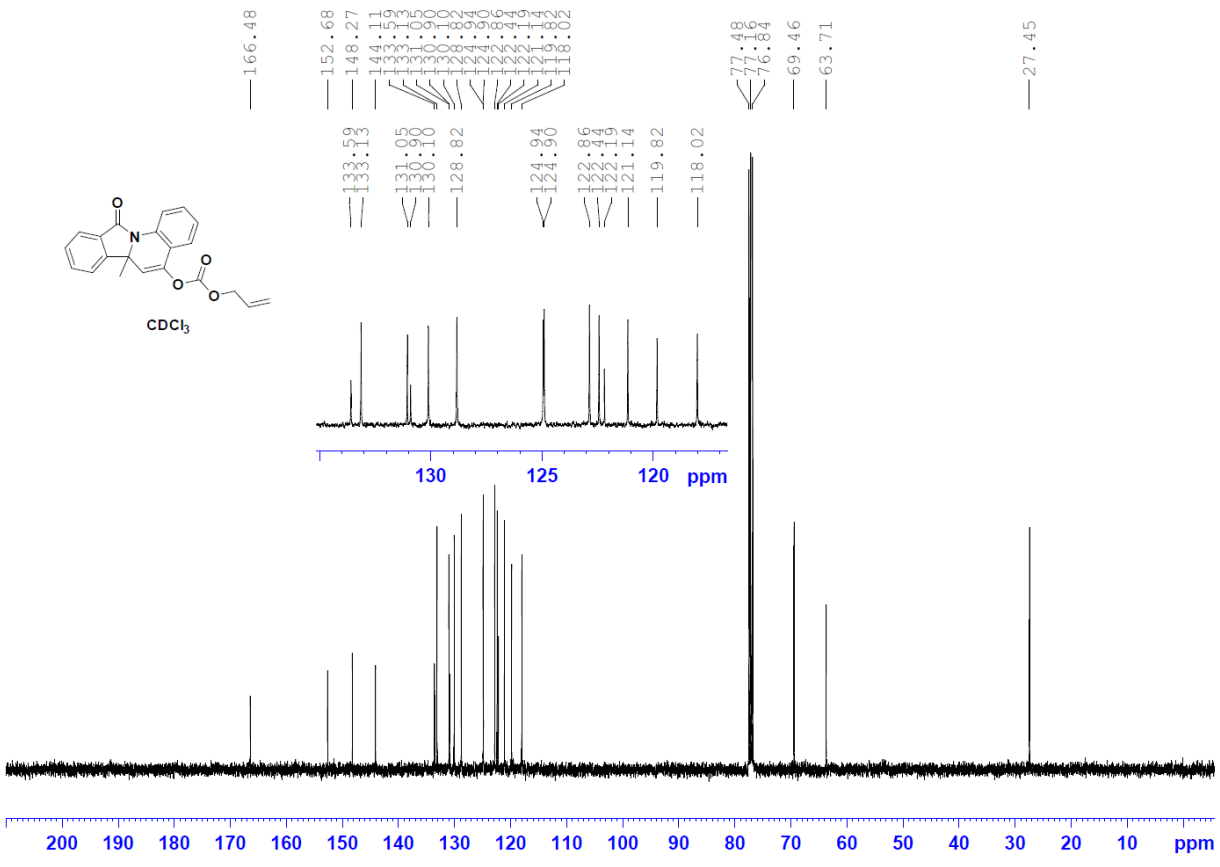

8.447
8.426
7.957
7.938
7.782
7.764
7.644
7.643
7.626
7.607
7.529
7.511
7.498
7.479
7.424
7.421
7.403
7.385
7.183
7.181
7.163
7.145
5.813
5.808
5.150
5.146
2.949
2.914
2.522
2.487
1.409
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.88
0.92
0.95
1.00
2.02
1.00
0.97
0.97
0.97
1.01
1.00
3.03


165.672
150.454
136.737
133.749
132.539
131.274
129.308
128.698
124.641
124.294
124.234
124.177
122.148
120.841
112.288
77.478
77.160
76.842
62.299
42.717
22.931
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.383
8.363
7.909
7.895
7.893
7.577
7.561
7.559
7.482
7.479
7.457
7.451
7.449
7.283
7.266
7.214
7.199
7.082
3.112
3.080
2.990
2.948
2.352
2.335
2.331
2.323
1.708
1.678
1.646
1.417
O
N
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.82
0.83
0.93
1.87
0.93
1.01
0.90
1.00
0.98
1.00
1.04
2.99


165.670
150.853
134.897
132.365
131.172
129.153
128.514
126.952
125.509
124.485
124.155
122.012
120.784
77.479
77.161
76.843
61.504
32.350
24.364
22.196
O
N
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.074
8.053
7.935
7.932
7.931
7.914
7.647
7.645
7.626
7.610
7.607
7.516
7.498
7.482
7.480
7.471
7.468
7.449
7.433
7.429
7.397
7.394
7.378
7.375
7.262
7.227
7.225
7.208
7.205
7.189
7.186
6.177
6.013
5.998
5.987
5.984
5.972
5.970
5.955
5.944
5.941
5.929
5.915
5.429
5.425
5.422
5.386
5.383
5.379
5.337
5.334
5.311
5.308
4.709
4.695
1.626
CDCl3
ppm
1.03
1.02
1.14
3.18
1.03
1.05
1.01
1.02
1.04
1.00
2.00
3.06


166.48
152.68
148.27
144.11
133.59
133.13
131.05
130.90
130.10
128.82
124.94
124.90
122.86
122.44
122.19
121.14
119.82
118.02
77.48
77.16
76.84
69.46
63.71
27.45
CDCl3
ppm