Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Synthesis of maleimide fused benzocarbazoles and imidazo[1,2-*a*]pyridines via rhodium(III)-catalyzed [4 + 2] oxidative cycloaddition

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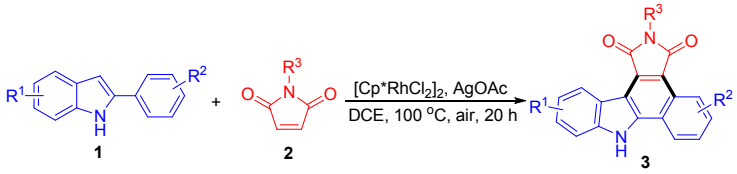
1. General Experimental Information

Reagents and solvents were purchased from commercial suppliers and used without further purification. 2-Arylindoles (**1**)[1], 2-arylimidazo[1,2-*a*]pyridine (**4**)[2], $[RhCp^*Cl_2]_2$[3] were prepared according to literature procedures. Melting points were recorded with a micro melting point apparatus and uncorrected. The ^1H NMR spectra were recorded at 400 MHz or 600 MHz. The ^{13}C NMR spectra were recorded at 100 MHz or 150 MHz. The ^{19}F NMR spectra were recorded at 376 MHz or 565 MHz. Chemical shifts were expressed in parts per million (δ), and were reported as s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublet), m (multiplet), etc. The coupling constants *J* were given in Hz. High resolution mass spectra (HRMS) were obtained *via* ESI mode by using a MicrOTOF mass spectrometer. The conversion of starting materials was monitored by thin layer chromatography (TLC) using silica gel plates (silica gel 60 F254 0.25 mm), and components were visualized by observation under UV light (254 and 365 nm).

2. General Procedure for the Preparation of 3, 5 and 6

2.1 General Procedure for the Preparation of 3

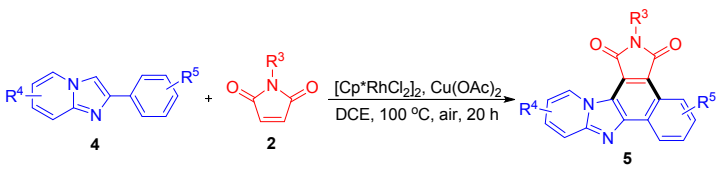


2-Arylindole (**1**, 0.75 mmol), *N*-substituted maleimide (**2**, 0.5 mmol), $[Cp^*RhCl_2]_2$ (0.025 mmol), AgOAc (1.25 mmol) and DCE (3 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C under air for 20 h. Upon completion, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/dichloromethane (1:1) as eluent to afford **3**.

2.1.1 Gram-Scale Synthesis of 3a

2-Phenylindole (**1a**, 15 mmol), *N*-methylmaleimide (**2a**, 10 mmol), $[Cp^*RhCl_2]_2$ (0.25 mmol), AgOAc (25 mmol) and DCE (30 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C under air for 20 h. Upon completion, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/dichloromethane (1:1) as eluent to afford **3a** (1.83 g) in 61% yield.

2.2 General Procedure for the Preparation of 5



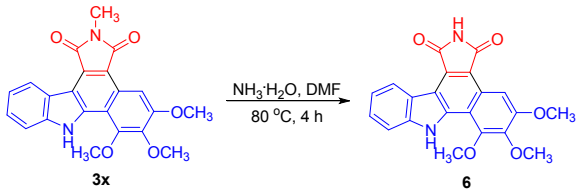
2-Arylimidazo[1,2-*a*]pyridine (**4**, 0.75 mmol), *N*-substituted maleimide (**2**, 0.5 mmol), $[Cp^*RhCl_2]_2$ (0.025 mmol), $Cu(OAc)_2$ (1.25 mmol) and DCE (3 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C under air for 20 h. Upon completion, the reaction mixture was cooled to room

temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/dichloromethane (1:1) as eluent to afford **5**.

2.2.1 Gram-Scale Synthesis of 5a

2-Phenylimidazo[1,2-*a*]pyridine (**4a**, 15 mmol), *N*-methylmaleimide (**2a**, 10 mmol), $[Cp^*RhCl_2]_2$ (0.25 mmol), $Cu(OAc)_2$ (25 mmol) and DCE (30 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C under air for 20 h. Upon completion, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/dichloromethane (1:1) as eluent to afford **5a** (2.77 g) in 92% yield.

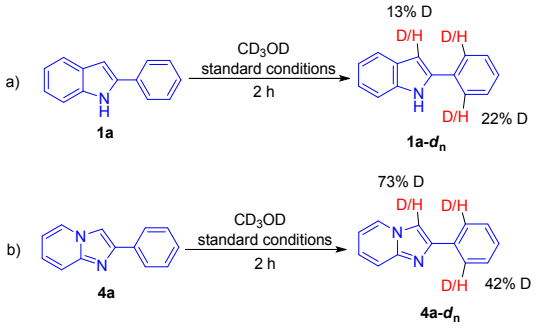
2.3 Synthesis of Compound 6



5,6,7-Trimethoxy-2-methyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (**3x**, 0.2 mmol), aqueous ammonia (26%, 2 mL) and DMF (2 mL) were charged into a sealed tube. The mixture was then stirred at 80 °C for 4h. Upon completion, it was cooled to room temperature and quenched with saturated NH_4Cl (15 mL) and extracted with DCM (5 mL × 3). The combined organic phase was dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel chromatography using petroleum ether/ethyl acetate (3:1) as eluent to afford 5,6,7-trimethoxy-2-methyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (**6**) in 93% yield.

3. Mechanistic Studies

3.1 Reversibility of C−H Bond Cleavage



(a) 2-Phenylindole (**1a**, 0.5 mmol), $[Cp^*RhCl_2]_2$ (0.025 mmol), AgOAc (1.25 mmol), CD_3OD (0.5 mL) and DCE (2 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C under air for 2 h. Then, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate (10:1) as eluent to afford **1a-*d*$_n$** in 87% yield. Upon analyzing the ^{1}H NMR spectra as shown in **Figure S1**, the rate of H/D exchange at the *ortho*-position of the 2-phenyl ring was 22% and at the C3-position of indole scaffold was 13%. This result implied that the phenyl C(sp^2)−H activation is reversible.

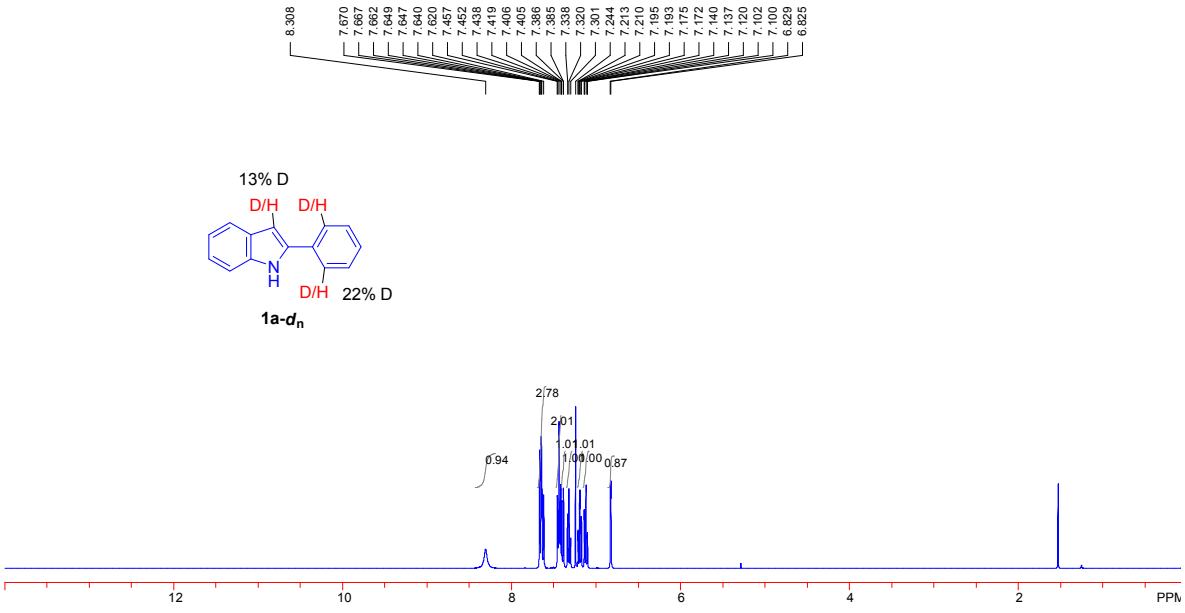


Figure S1. The ^{1}H NMR spectra of **1a-*d*$_n$**

(b) 2-Phenylimidazo[1,2-*a*]pyridine (**4a**, 0.5 mmol), $[Cp^*RhCl_2]_2$ (0.025 mmol), $Cu(OAc)_2$ (1.25 mmol), CD_3OD (0.5 mL) and DCE (2 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C under air for 2 h. Then, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate (3:1) as eluent to afford **4a-*d*$_n$** in 95% yield. Upon analyzing the ^{1}H NMR spectra as shown in **Figure S2**, the rate of H/D exchange at the *ortho*-position of the 2-phenyl ring was 42% and at the C3-position of imidazo[1,2-*a*]pyridine scaffold was 73%. This result implied that the phenyl C(sp^2)−H activation is reversible.

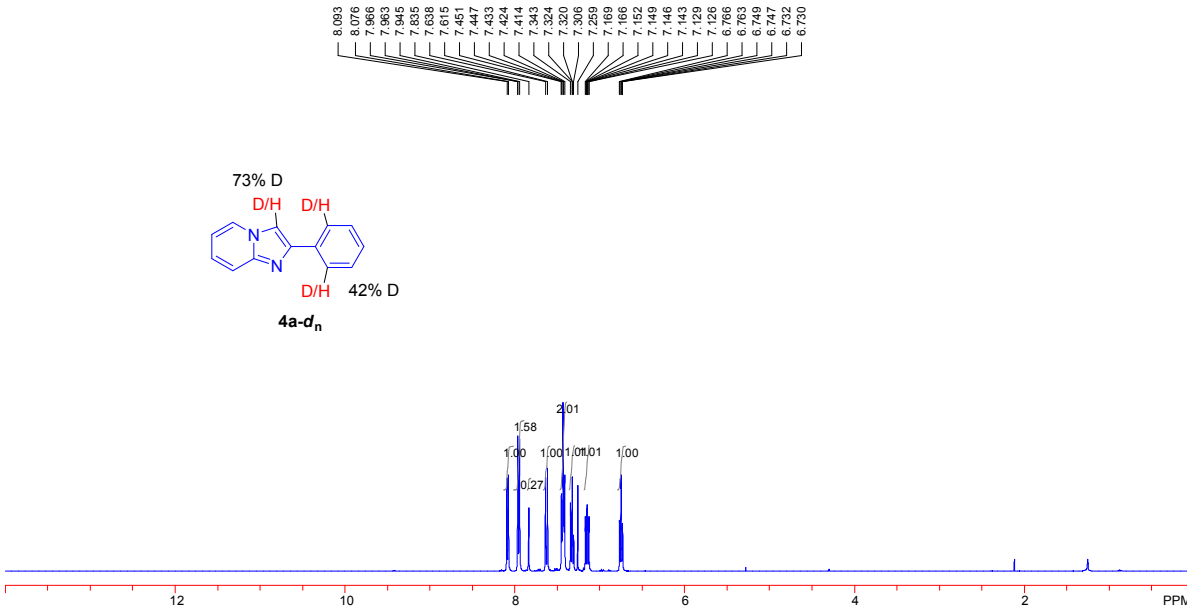
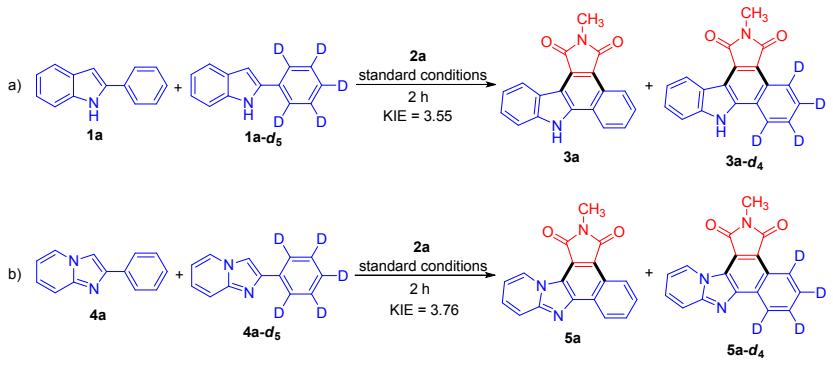


Figure S2. The ^{1}H NMR spectra of **4a-*d*$_n$**

3.2 Intermolecular Kinetic Isotope Effect Study



(a) 2-Phenylindole (**1a**, 0.375 mmol), deuterated substrate 2-Phenylindole (**1a-*d*$_5$**, 0.375 mmol), *N*-methylmaleimide (**2a**, 0.5 mmol), [Cp*RhCl$_2$]$_2$ (0.025 mmol), AgOAc (1.25 mmol) and DCE (3 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C for 2 h. Then, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/dichloromethane (1:1) as eluent to afford a mixture of **3a** and **3a-*d*$_4$**. Upon analyzing the ^{1}H NMR spectra as shown in **Figure S3**, the ratio of **3a** and **3a-*d*$_4$** was determined as 0.78:0.22 and a value of k_H/k_D = 3.55 was calculated, it seems that the C−H activation may be involved in the rate-determining step.

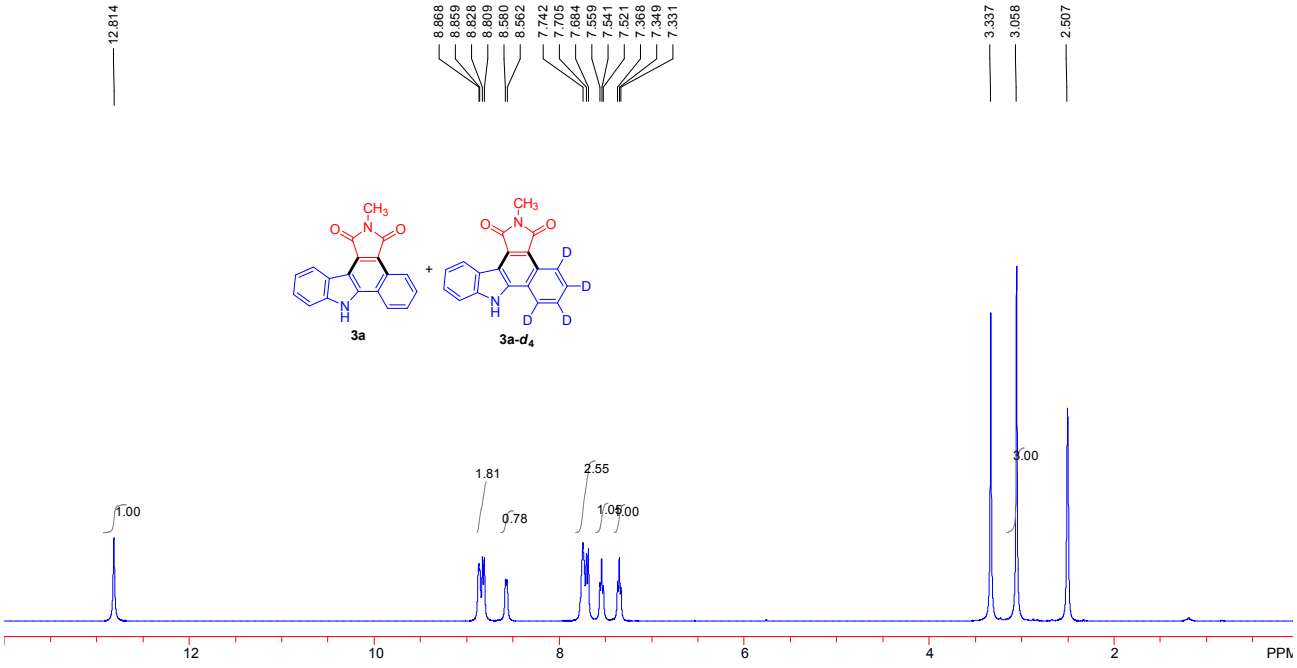


Figure S3. The ^{1}H NMR spectra of a mixture of **3a** and **3a-*d*$_4$**

(b) 2-Phenylimidazo[1,2-*a*]pyridine (**4a**, 0.375 mmol), deuterated substrate 2-phenylimidazo- [1,2-*a*]pyridine (**4a-*d*$_5$**, 0.375 mmol), *N*-methylmaleimide (**2a**, 0.5 mmol), [Cp*RhCl$_2$]$_2$ (0.025 mmol), Cu(OAc)$_2$ (1.25 mmol) and DCE (3 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C for 2 h. Then, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica

gel chromatography using petroleum ether/dichloromethane (1:1) as eluent to afford a mixture of **5a** and **5a-*d*$_4$**. Upon analyzing the ^{1}H NMR spectra as shown in **Figure S4**, the ratio of **5a** and **5a-*d*$_4$** was determined as 0.79:0.21 and a value of k_H/k_D = 3.76 was calculated, it seems that the C−H activation may be involved in the rate-determining step.

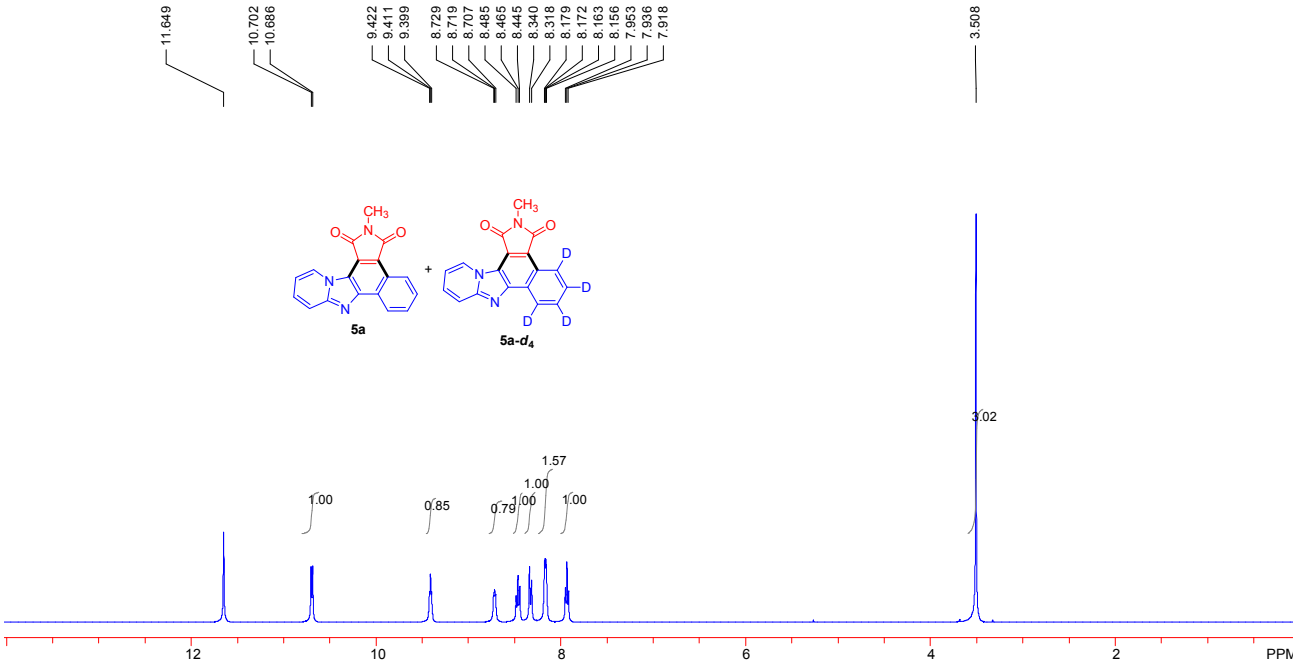
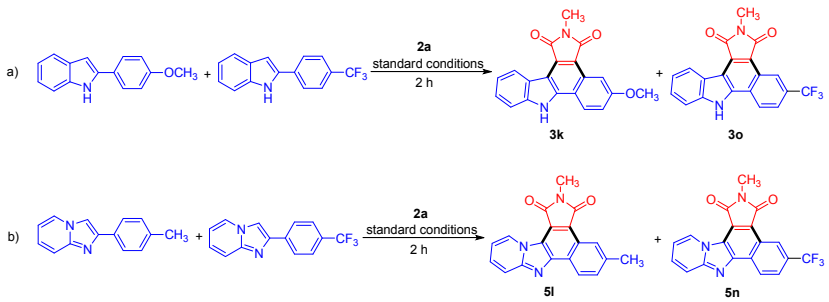


Figure S4. The ^{1}H NMR spectra of a mixture of **5a** and **5a-*d*$_4$**

3.3 Competitive Reaction



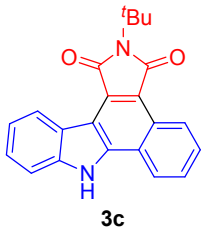
(a) 2-(4-Methoxyphenyl)-1*H*-indole (0.375 mmol), 2-(4-(trifluoromethyl)phenyl)-1*H*-indole (0.375 mmol), *N*-methylmaleimide (**2a**, 0.5 mmol), $[Cp^*RhCl_2]_2$ (0.025 mmol), AgOAc (1.25 mmol) and DCE (3 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C for 2 h. Then, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was

concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/dichloromethane (1:1) as eluent to afford **3k** and **3o** in 18% and 7% yields, respectively.

(b) 2-(*p*-Tolyl)imidazo[1,2-*a*]pyridine (0.375 mmol), 2-(4-(trifluoromethyl)phenyl)imidazo[1,2-*a*]-pyridine (0.375 mmol), *N*-methylmaleimide (**2a**, 0.5 mmol), $[Cp^*RhCl_2]_2$ (0.025 mmol), $Cu(OAc)_2$ (1.25 mmol) and DCE (3 mL) were charged into a sealed tube. The mixture was then stirred at 100 °C for 2 h. Then, the reaction mixture was cooled to room temperature and filtered through a plug of celite. The organic phase was concentrated under reduced pressure, and the residue was purified by silica gel chromatography using petroleum ether/dichloromethane (1:1) as eluent to afford **5l** and **5n** in 29% and 9% yields, respectively.

4. X-Ray Crystal Structure and Data of 3c

Compound 3c



3c

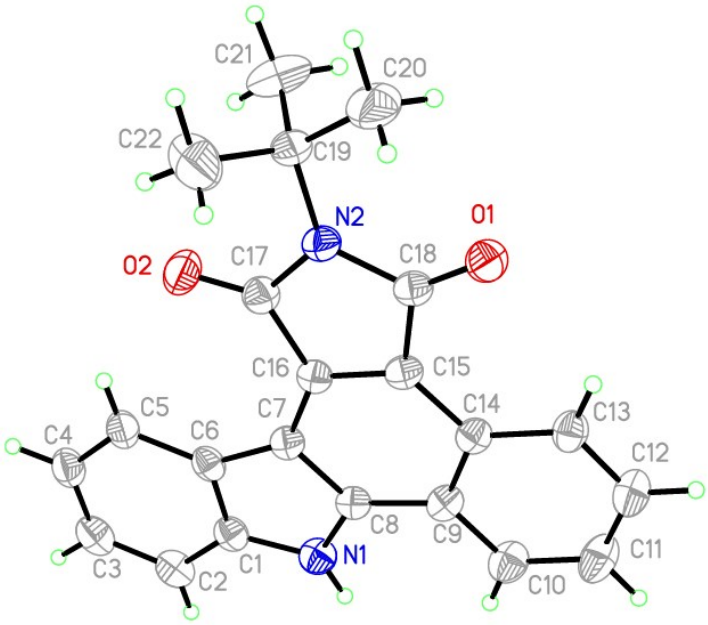


Figure S4. X-ray structure of **3c** with 30% ellipsoid probability

X-ray structure determination. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of the solvent from a trichloromethane solution of **3c**. Crystal data collection and refinement parameters of **3c** are summarized in Table S1. Intensity data were collected at 298 K on a SuperNova Dual diffractometer using mirror-monochromated Cu Kα radiation, λ = 1.54184 Å. The data were corrected for decay, Lorentz, and polarization effects as well as absorption and beam corrections based on the multi-scan technique. The structure was solved by a combination of direct methods in SHELXS and the difference Fourier technique, and refined by full-matrix least-squares procedures. Nonhydrogen atoms were refined with anisotropic displacement parameters. The H-atoms were either located or calculated and subsequently treated with a riding model.

Table S1 Crystallographic data and structure refinement results of **3c**

Empirical formula	$C_{22}H_{18}N_2O_2$
Formula weight	342.38
Temp, K	299.03(10)
Crystal system	monoclinic
Space group	$P2_1$
a, Å	6.1925(3)
b, Å	12.0017(6)
c, Å	11.9195(6)
α (°)	90
β (°)	97.588(4)
γ (°)	90
Volume, Å^3	878.11(8)
Z	2
d_{calc}, g cm^{-3}	1.295
λ, Å	1.54184
μ, mm^{-1}	0.670
No. of data collected	4154
No. of unique data	2613
R_{int}	0.0210
Goodness-of-fit on F^2	1.156
R_1, wR_2 ($I > 2\sigma(I)$)	0.0415, 0.1022
R_1, wR_2 (all data)	0.0482, 0.1074

5. Characterization Data of 3a-3y, 5a-5s and 6

2-Methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3a): yellow solid (117 mg, 78%); mp: >300 ºC (lit.[4] mp: 244 °C); ^{1}H NMR (600 MHz, DMSO-d_6): δ 3.04 (s, 3H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.70-7.75 (m, 2H), 8.55 (d, *J* = 7.8 Hz, 1H), 8.80 (d, *J* = 7.8 Hz, 1H), 8.84 (d, *J* = 7.8 Hz, 1H), 12.79 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 23.9, 112.2, 118.0, 121.1, 121.6, 122.8, 123.2, 124.4, 125.1, 125.2, 126.3, 127.0, 128.0, 128.1, 128.6, 140.3, 140.7, 169.5, 170.4. HRMS calcd for $C_{19}H_{13}N_2O_2^+$: 301.0972 $[M+H]^+$, found: 301.0962.

2-Ethylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3b): yellow solid (119 mg, 76%); mp: 293-294 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 1.26 (t, *J* = 7.2 Hz, 3H), 3.67 (q, *J* = 7.2 Hz, 2H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.74-7.80 (m, 2H), 8.59-8.61 (m, 1H), 8.86 (d, *J* = 8.0 Hz, 1H), 8.90-8.92 (m, 1H), 12.85 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 14.5, 32.6, 112.3, 112.3, 117.9, 121.2, 121.6, 122.9, 123.2, 124.4, 125.2, 126.3, 127.0, 128.0, 128.1, 128.6, 140.4, 140.8, 169.3, 170.2. HRMS calcd for $C_{20}H_{14}N_2NaO_2^+$: 337.0947 $[M+Na]^+$, found: 337.0945.

2-(*Tert*-butyl)benzo[*a*]pyrrolo[3,4-c]carbazole-1,3(2*H*,8*H*)-dione (3c): yellow solid (127 mg, 74%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 1.75 (s, 9 H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.78-7.85 (m, 2H), 8.68 (d, *J* = 8.0 Hz, 1H), 8.94 (d, *J* = 8.0 Hz, 1H), 9.03 (d, *J* = 7.6 Hz, 1H), 12.91 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 29.5, 57.3, 111.8, 112.3, 117.8, 121.2, 121.7, 123.2, 123.3, 124.7, 125.4, 126.2, 126.9, 128.2, 128.7, 140.4, 140.9, 170.8, 171.9. HRMS calcd for $C_{22}H_{18}N_2NaO_2^+$: 365.1260 $[M+Na]^+$, found: 365.1299.

2-Cyclohexylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3d): yellow solid (134 mg, 73%); mp: 275-276 ºC; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 1.23-1.28 (m, 1H), 1.36-1.43 (m, 2H), 1.70-1.72 (m, 1H), 1.82-1.89 (m, 4H), 2.19-2.26 (m, 2H), 4.08-4.14 (m, 1H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.79-7.83 (m, 2H), 8.65-8.68 (m, 1H), 8.92 (d, *J* = 7.8 Hz, 1H), 8.98-9.00 (m,

1H), 12.91 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 25.5, 26.2, 30.3, 50.4, 112.3, 112.3, 117.7, 121.2, 121.7, 123.0, 123.3, 124.5, 125.2, 126.4, 127.0, 128.0, 128.2, 128.7, 140.4, 140.9, 169.6, 170.5. HRMS calcd for $C_{24}H_{21}N_2O_2^+$: 369.1598 $[M+H]^+$, found: 369.1550.

2-Benzylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3e): yellow solid (150 mg, 80%); mp: 271-272 ºC; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 4.80 (s, 2H), 7.28 (t, J = 8.4 Hz, 1H), 7.33-7.37 (m, 3H), 7.40 (d, J = 7.8 Hz, 2H), 7.54 (t, J = 7.2 Hz, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.73-7.75 (m, 2H), 8.57 (d, J = 7.2 Hz, 1H), 8.82 (d, J = 8.4 Hz, 1H), 8.88 (d, J = 7.8 Hz, 1H), 12.83 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 41.1, 112.27, 112.32, 117.7, 121.2, 121.6, 122.9, 123.2, 124.4, 125.2, 126.3, 127.1, 127.8, 127.9, 128.2, 128.7, 129.1, 137.7, 140.4, 140.9, 169.2, 170.0. HRMS calcd for $C_{25}H_{17}N_2O_2^+$: 377.1285 $[M+H]^+$, found: 377.1260.

2-Phenylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3f): yellow solid (139 mg, 77%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.36 (t, J = 7.6 Hz, 1H), 7.44-7.51 (m, 1H), 7.54-7.61 (m, 5H), 7.72 (d, J = 8.4 Hz, 1H), 7.78-7.84 (m, 2H), 8.66 (d, J = 8.4 Hz, 1H), 8.88 (d, J = 8.0 Hz, 1H), 8.98 (d, J = 7.6 Hz, 1H), 12.94 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 112.35, 112.38, 117.7, 121.3, 121.7, 123.1, 123.3, 124.5, 125.4, 126.5, 127.1, 128.0, 128.0, 128.2, 128.4, 128.8, 129.3, 132.7, 140.4, 141.1, 168.6, 169.4. HRMS calcd for $C_{24}H_{15}N_2O_2^+$: 363.1128 $[M+H]^+$, found: 363.1120.

2,11-Dimethylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3g): yellow solid (112 mg, 71%); mp: 277-278 ºC; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 2.50 (s, 3H), 3.09 (s, 3H), 7.66 (s, 2H), 7.80-7.82 (m, 2H), 8.58-8.60 (m, 1H), 8.90-8.91 (m, 1H), 8.94 (s, 1H), 13.02 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 21.9, 23.9, 111.8, 112.0, 117.7, 121.8, 122.7, 123.1, 124.0, 125.1, 126.2, 127.9, 128.0, 128.3, 128.4, 129.8, 138.6, 140.9, 169.4, 170.4. HRMS calcd for $C_{20}H_{15}N_2O_2^+$: 315.1128 $[M+H]^+$, found: 315.1123.

11-Chloro-2-methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3h): yellow solid (120 mg, 72%); mp: >300 ºC; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 3.06 (s, 3H), 7.52 (dd, J_1 = 9.0 Hz, J_2 = 1.8 Hz, 1H),

7.67 (d, J = 8.4 Hz, 1H), 7.77-7.79 (m, 2H), 8.54 (d, J = 7.2 Hz, 1H), 8.73 (s, 1H), 8.86 (d, J = 8.4 Hz, 1H), 12.95 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 24.0, 111.2, 113.8, 118.6, 122.7, 122.9, 123.2, 123.3, 125.2, 125.3, 126.5, 126.8, 128.0, 128.4, 129.0, 138.7, 141.3, 169.4, 170.3. HRMS calcd for $C_{19}H_{11}ClN_2NaO_2^+$: 357.0401 $[M+Na]^+$, found: 357.0401.

11-Bromo-2-methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3i): yellow solid (142 mg, 75%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 2.97 (s, 3H), 7.53-7.59 (m, 2H), 7.67-7.73 (m, 2H), 8.42 (d, J = 6.8 Hz, 1H), 8.73 (s, 2H), 12.80 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 24.0, 111.2, 113.2, 114.3, 118.7, 122.9, 123.29, 123.31, 125.3, 126.3, 126.5, 128.0, 128.4, 129.0, 129.3, 139.0, 141.2, 169.5, 170.3. HRMS calcd for $C_{19}H_{11}BrN_2NaO_2^+$: 400.9896 $[M+Na]^+$, found: 400.9896.

2,9-Dimethylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3j): yellow solid (115 mg, 73%); mp: >300 ºC; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 3.09 (s, 3H), 3.10 (s, 3H), 7.38 (t, J = 7.2 Hz, 1H), 7.52-7.56 (m, 2H), 7.62 (t, J = 7.2 Hz, 1H), 7.92 (d, J = 7.8 Hz, 1H), 8.91 (d, J = 8.4 Hz, 1H), 8.98 (d, J = 7.8 Hz, 1H), 11.60 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 21.9, 24.0, 111.9, 112.1, 117.8, 121.9, 122.9, 123.2, 124.1, 125.2, 126.3, 128.0, 128.2, 128.4, 128.6, 130.0, 138.7, 140.9, 169.6, 170.6. HRMS calcd for $C_{20}H_{15}N_2O_2^+$: 315.1128 $[M+H]^+$, found: 315.1124.

5-Methoxy-2-methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3k): yellow solid (124 mg, 75%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 3.01 (s, 3H), 3.90 (s, 3H), 7.30-7.37 (m, 2H), 7.51 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.64 (d, J = 8.0 Hz, 1H), 8.15 (d, J = 2.8 Hz, 1H), 8.43 (d, J = 9.2 Hz, 1H), 8.77 (d, J = 8.0 Hz, 1H), 12.62 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 23.8, 55.7, 103.9, 111.4, 112.0, 116.6, 117.7, 119.8, 121.0, 121.7, 124.2, 124.8, 126.7, 128.1, 128.2, 140.4, 141.3, 159.5, 169.5, 170.5. HRMS calcd for $C_{20}H_{14}N_2NaO_3^+$: 353.0897 $[M+Na]^+$, found: 353.0861.

2,5-Dimethylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3l): yellow solid (113 mg, 72%); mp: >300 ºC; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 2.53 (s, 3H), 3.10 (s, 3H), 7.37 (d, J = 8.4 Hz, 1H), 7.60 (d,

J = 8.4 Hz, 1H), 7.75-7.80 (m, 2H), 8.61 (d, *J* = 7.8 Hz, 1H), 8.64 (s, 1H), 8.92-8.93 (m, 1H), 12.76 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 21.9, 24.0, 111.9, 112.1, 117.9, 121.9, 122.9, 123.2, 124.1, 125.2, 126.3, 128.0, 128.2, 128.4, 128.6, 130.0, 138.7, 141.0, 169.6, 170.6. HRMS calcd for $C_{20}H_{15}N_2O_2^+$: 315.1128. $[M+H]^+$, found: 315.1126.

5-Chloro-2-methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3m): yellow solid (114 mg, 68%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 2.98 (s, 3H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.72 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 1H), 8.50 (d, *J* = 8.8 Hz, 1H), 8.69 (d, *J* = 2.0 Hz, 1H), 8.74 (d, *J* = 8.0 Hz, 1H), 12.84 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 24.1, 112.4, 112.8, 117.1, 121.0, 121.47, 121.51, 123.8, 124.5, 125.5, 126.8, 127.4, 128.4, 129.1, 133.6, 140.5, 140.6, 169.3, 170.2. HRMS calcd for $C_{19}H_{11}ClN_2NaO_2^+$: 357.0401 $[M+Na]^+$, found: 357.0397.

5-Bromo-2-methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3n): yellow solid (145 mg, 77%); mp: 282-283 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 2.89 (s, 3H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.74 (d, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 8.32 (d, *J* = 8.8 Hz, 1H), 8.65 (d, *J* = 7.6 Hz, 1H), 8.74 (s, 1H), 12.72 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 24.1, 112.4, 112.8, 116.9, 121.2, 121.48, 121.50, 122.4, 124.5, 125.5, 127.0, 127.2, 127.4, 129.0, 130.9, 140.5, 140.7, 169.2, 170.2. HRMS calcd for $C_{19}H_{11}BrN_2NaO_2^+$: 400.9896 $[M+Na]^+$, found: 400.9897.

2-Methyl-5-(trifluoromethyl)benzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3o): yellow solid (120 mg, 65%); mp: >300 ºC. ^{1}H NMR (400 MHz, CF_3CO_2D) δ: 2.43 (s, 3H), 6.93-6.98 (m, 2H), 7.05 (t, *J* = 6.8 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 7.32 (t, *J* = 6.8 Hz, 1H), 7.74 (d, *J* = 7.2 Hz, 1H), 8.17 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 23.9, 112.3, 113.5, 118.1, 121.1, 121.5, 122.3 (q, $^3J_{C\text{-}F}$ = 4.8 Hz), 123.0 (q, $^3J_{C\text{-}F}$ = 2.7 Hz), 123.7, 124.5, 124.58, 124.64, 124.7 (q, $^1J_{C\text{-}F}$ = 271.35 Hz), 127.6, 128.1 (q, $^2J_{C\text{-}F}$ = 32.1 Hz), 128.8, 139.8, 140.5, 168.7, 169.8. ^{19}F NMR (565 MHz, DMSO-d_6) δ: -61.0. HRMS calcd for $C_{20}H_{11}F_3N_2NaO_2^+$: 391.0665 $[M+Na]^+$, found: 391.0652.

2,6-Dimethylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3p): yellow solid (130 mg, 79%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 3.07 (s, 3H), 4.00 (s, 3H), 7.33-7.40 (m, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 1.6 Hz, 1H), 8.79 (d, *J* = 9.2 Hz, 1H), 8.84 (d, *J* = 8.0 Hz, 1H), 12.64 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 23.9, 56.1, 102.6, 112.2, 112.5, 118.8, 120.7, 121.0, 121.2, 121.7, 124.4, 124.6, 125.3, 126.9, 127.0, 139.8, 140.3, 159.2, 169.8, 170.6. HRMS calcd for $C_{20}H_{15}N_2O_3^+$: 331.1077 $[M+H]^+$, found: 331.1069.

2,6-Dimethylbenzo[*a*]pyrrolo[3,4-c]carbazole-1,3(2*H*,8*H*)-dione (3q): yellow solid (121 mg, 77%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 2.51 (s, 3H), 3.02 (s, 3H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 1H), 8.28 (s, 1H), 8.68 (d, *J* = 8.4 Hz, 1H), 8.79 (d, *J* = 8.0 Hz, 1H), 12.66 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 22.2, 23.9, 112.2, 112.3, 118.2, 121.0, 121.7, 122.2, 123.0, 124.3, 124.9, 126.8, 127.0, 130.4, 137.8, 140.2, 140.3, 169.6, 170.4. HRMS calcd for $C_{20}H_{15}N_2O_2^+$: 315.1128 $[M+H]^+$, found: 315.1123.

6-Bromo-2-methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3r): yellow solid (144 mg, 76%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 2.88 (s, 3H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 8.46 (d, *J* = 8.8 Hz, 1H), 8.54 (s, 1H), 8.57 (d, *J* = 8.0 Hz, 1H), 12.5 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6): δ 23.7, 112.1, 112.7, 117.5, 121.09, 121.13, 121.4, 123.3, 124.2, 124.3, 125.2, 126.8, 127.1, 127.7, 130.9, 139.1, 140.1, 168.7, 169.6. HRMS calcd for $C_{19}H_{12}BrN_2O_2^+$: 379.0077 $[M+H]^+$, found: 379.0067.

7-Methoxy-2-methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3s): yellow solid (129 mg, 78%); mp: 243-244 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 3.09 (s, 3H), 4.18 (s, 3H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 8.51 (d, *J* = 8.4 Hz, 1H), 8.91 (d, *J* = 7.6 Hz, 1H), 11.99 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6): δ 19.0, 24.0, 56.5, 111.2, 113.2, 114.3, 118.7, 122.9, 123.3, 125.3, 126.3, 126.5, 128.1, 128.4, 129.1, 129.4, 139.0, 141.2,

169.5, 170.3. HRMS calcd for $C_{20}H_{14}N_2NaO_3^+$: 353.0897 $[M+Na]^+$, found: 353.0894.

2,7-Dimethylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3t): yellow solid (125 mg, 80%); mp: 269-270 ºC; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 3.08 (s, 6H), 7.37 (t, J = 7.2 Hz, 1H), 7.51 (d, J = 7.2 Hz, 1H), 7.54 (t, J = 7.2 Hz, 1H), 7.61 (d, J = 7.2 Hz, 1H), 7.92 (d, J = 8.4 Hz, 1H), 8.89 (d, J = 8.4 Hz, 1H), 8.97 (d, J = 7.8 Hz, 1H), 11.58 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6): δ 24.0, 24.5, 113.3, 113.6, 118.6, 120.7, 121.3, 123.0, 123.1, 124.1, 126.7, 127.6, 127.8, 128.0, 130.0, 134.2, 140.0, 140.6, 169.4, 170.4. HRMS calcd for $C_{20}H_{15}N_2O_2^+$: 315.1128 $[M+H]^+$, found: 315.1123.

8-Methylnaphtho[1,2-*a*]pyrrolo[3,4-*c*]carbazole-7,9(8*H*,14*H*)-dione (3u): red solid (144mg, 82%); mp: >300 ºC; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 3.13 (s, 3H), 7.40-7.42 (m, 1H), 7.62 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.82-7.84 (m, 1H), 7.92 (d, J = 7.8 Hz, 1H), 7.93-7.96 (m, 1H), 8.10 (d, J = 9.0 Hz, 1H), 8.15-8.16 (m ,1H), 9.03 (d, J = 9.0 Hz, 1H), 9.06 (d, J = 7.8 Hz, 1H), 9.21 (d, J = 8.4 Hz, 1H), 12.47 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 24.2, 113.1, 117.0, 118.4, 119.3, 120.8, 121.5, 122.5, 124.7, 126.4, 126.89, 126.94, 127.86, 127.94, 128.4, 128.7, 129.6, 129.9, 132.7, 140.2, 142.1, 169.3, 170.5. HRMS calcd for $C_{23}H_{14}N_2NaO_2^+$: 373.0947 $[M+Na]^+$, found: 373.0945.

6-Methylnaphtho[2,3-*a*]pyrrolo[3,4-*c*]carbazole-5,7(6*H*,14*H*)-dione (3v)[lit. 5]: red solid (135mg, 77%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 3.00 (s, 3H), 7.44 (t, J = 7.2 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.60-7.63 (m, 2H), 7.67 (d, J = 8.0 Hz, 1H), 8.04 (d, J = 7.2 Hz, 1H), 8.13 (d, J = 8.0 Hz, 1H), 8.77 (d, J = 8.0 Hz, 1H), 9.07 (s, 1H), 9.35 (s, 1H), 13.00 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 23.9, 109.9, 112.3, 118.4, 121.4, 121.5, 121.8, 122.1, 123.9, 124.0, 124.5, 126.2, 127.1, 127.4, 128.6, 129.1, 129.5, 131.8, 132.3, 139.7, 140.4, 169.5, 170.5. HRMS calcd for $C_{23}H_{14}N_2NaO_2^+$: 373.0947 $[M+Na]^+$, found: 373.0941.

3-Methoxy-6-methylnaphtho[2,3-*a*]pyrrolo[3,4-*c*]carbazole-5,7(6*H*,14*H*)-dione (3w): red solid (141mg, 74%); mp: >300 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 3.05 (s, 3H), 3.89 (s, 3H), 7.12 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 7.58 (d, J = 8.8 Hz, 1H), 7.60-7.66 (m, 2H), 8.06-8.08 (m, 1H), 8.15-8.17 (m, 1H),

8.32 (d, J = 2.4 Hz, 1H), 9.08 (s, 1H), 9.39 (s, 1H), 12.91 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ: 23.9, 55.8, 105.7, 110.0, 113.0, 115.9, 117.9, 121.65, 121.70, 122.7, 124.0, 124.5, 127.1, 127.4, 128.6, 129.2, 129.7, 131.8, 132.3, 134.5, 140.8, 154.9, 169.7, 170.5. HRMS calcd for $C_{24}H_{17}N_2O_3^+$: 381.1234 $[M+H]^+$, found: 381.1229.

5,6,7-Trimethoxy-2-methylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3x): yellow solid (121 mg, 62%); mp: 235-236 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.16 (s, 3H), 4.05 (s, 3H), 4.06 (s, 3H), 4.25 (s, 3H), 7.34-7.38 (m, 1H), 7.46-7.52 (m, 2H), 8.21 (s, 1H), 8.93 (d, J = 8.0 Hz, 1H), 10.03 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ: 23.5, 56.2, 61.3, 61.7, 100.7, 110.8, 112.5, 113.0, 117.0, 121.1, 121.2, 124.4, 124.7, 126.4, 127.2, 138.9, 139.1, 141.6, 148.4, 154.9, 169.4, 170.1. HRMS calcd for $C_{22}H_{19}N_2O_5^+$: 391.1288 $[M+H]^+$, found: 391.1294 .

5,6,7-Trimethoxy-2-phenylbenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (3y): yellow solid (146mg, 65%); mp: 257-258 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.05 (s, 3H), 4.06 (s, 3H), 4.28 (s, 3H), 7.36-7.43 (m, 2H), 7.50-7.60 (m, 6H), 8.40 (s, 1H), 9.05 (d, J = 8.0 Hz, 1H), 10.02 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ: 56.2, 61.4, 61.8, 101.1, 111.0, 112.8, 113.5, 116.5, 121.2, 121.4, 124.7, 124.9, 126.6, 126.7, 127.0, 127.6, 129.0, 132.3, 139.1, 139.6, 142.0, 148.6, 155.2, 168.4, 169.8. HRMS calcd for $C_{27}H_{21}N_2O_5^+$: 453.1445 $[M+H]^+$, found: 453.1440.

2-Methyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5a): yellow solid (145 mg, 96%); mp: >300 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 3.48 (s, 3H), 7.90 (t, J = 7.2 Hz, 1H), 8.13-8.16 (m, 2H), 8.30 (d, J = 9.0 Hz, 1H), 8.43 (t, J = 7.8 Hz, 1H), 8.69 (dd, J_1 = 6.6 Hz, J_2 = 3.0 Hz, 1H), 9.39 (dd, J_1 = 6.6 Hz, J_2 = 3.0 Hz, 1H), 10.67 (d, J = 6.6 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 23.3, 111.9, 117.7, 118.7, 119.7, 122.2, 123.0, 126.1, 126.3, 127.4, 131.9, 131.9, 132.6, 133.3, 139.2, 142.9, 167.5, 170.3. HRMS calcd for $C_{18}H_{12}N_3O_2^+$: 302.0924 $[M+H]^+$, found: 302.0909.

2-Ethyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5b): yellow solid (145

mg, 92%); mp: >300 ºC; ^{1}H NMR (400 MHz, CF_3CO_2D) δ: 1.57 (t, *J* = 7.2 Hz, 3H), 4.13 (q, *J* = 7.2 Hz, 2H), 7.98 (t, *J* = 7.2 Hz, 1H), 8.21-8.23 (m, 2H), 8.37 (d, *J* = 8.8 Hz, 1H), 8.50 (t, *J* = 8.0 Hz, 1H), 8.77 (d, *J* = 5.2 Hz, 1H), 9.46-9.48 (m, 1H), 10.76 (d, *J* = 6.4 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 12.1, 33.8, 111.9, 117.8, 118.7, 119.8, 122.2, 123.1, 126.2, 126.3, 127.5, 131.8, 131.9, 132.7, 133.3, 139.2, 142.8, 167.3, 170.0. HRMS calcd for $C_{19}H_{14}N_3O_2^+$: 316.1081 $[M+H]^+$, found: 316.1064.

2-(*Tert*-butyl)-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5c): yellow solid (151 mg, 88%); mp: 280-281 ºC; ^{1}H NMR (400 MHz, CF_3CO_2D) δ: 1.98 (s, 9H), 7.93 (t, *J* = 7.2 Hz, 1H), 8.13-8.19 (m, 2H), 8.33 (d, *J* = 8.8 Hz, 1H), 8.46 (t, *J* = 8.0 Hz, 1H), 8.71 (d, *J* = 8.4 Hz, 1H), 9.47 (d, *J* = 8.4 Hz, 1H), 10.85 (d, *J* = 6.8 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 27.7, 60.1, 111.7, 117.6, 118.4, 120.2, 122.0, 122.9, 126.0, 126.4, 127.2, 131.3, 131.6, 133.05, 133.14, 138.9, 142.7, 168.1, 171.0. HRMS calcd for $C_{21}H_{19}N_3O_2^+$: 344.1394 $[M+H]^+$, found: 344.1367.

2-Cyclohexyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-g]isoindole-1,3(2*H*)-dione (5d): yellow solid (168 mg, 91%); mp: 277-278 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 1.51-1.58 (m, 1H), 1.64-1.71 (m, 2H), 1.98-2.00 (m, 1H), 2.10-2.11 (m, 2H), 2.17-2.19 (m, 2H), 2.48-2.54 (m, 2H), 4.49-4.53 (m, 1H), 8.00 (t, *J* = 6.6 Hz, 1H), 8.24-8.26 (m, 2H), 8.40 (d, *J* = 9.6 Hz, 1H), 8.53 (t, *J* = 7.8 Hz, 1H), 8.79-8.80 (m, 1H), 9.51-9.53 (m, 1H), 10.84 (d, *J* = 6.6 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 24.5, 25.5, 29.6, 53.3, 111.9, 117.9, 118.7, 119.9, 122.2, 123.1, 126.0, 126.5, 127.6, 131.8, 132.0, 133.0, 133.3, 139.2, 142.9, 167.5, 170.3. HRMS calcd for $C_{23}H_{20}N_3O_2^+$: 370.1550 $[M+H]^+$, found: 370.1527.

2-Benzyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5e): yellow solid (174 mg, 92%); mp: >300 ºC; ^{1}H NMR (400 MHz, CF_3CO_2D) δ: 5.22 (s, 2H), 7.39-7.47 (m, 3H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.97 (t, *J* = 7.2 Hz, 1H), 8.22-8.23 (m, 2H), 8.38 (d, *J* = 8.0 Hz, 1H), 8.51 (t, *J* = 6.8 Hz, 1H), 8.78 (s, 1H), 9.47-9.49 (m, 1H), 10.77 (d, *J* = 6.4 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 42.3, 112.1, 118.0, 118.9, 120.0, 122.4, 123.3, 126.3, 126.6, 127.68, 127.72, 128.4, 128.9, 132.10, 132.14, 132.9, 133.6,

134.8, 139.5, 143.1, 167.4, 170.1. HRMS calcd for $C_{24}H_{16}N_3O_2^+$: 378.1237 $[M+H]^+$, found: 378.1231.

2-Phenyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-g]isoindole-1,3(2*H*)-dione (5f): yellow solid (171 mg, 94%); mp: 293-294 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 7.64 (d, *J* = 7.8 Hz, 2H), 7.76-7.79 (m, 3H), 7.99 (t, *J* = 7.2 Hz, 1H), 8.27-8.31 (m, 2H), 8.44 (d, *J* = 8.4 Hz, 1H), 8.55 (t, *J* = 7.8 Hz, 1H), 8.87 (d, *J* = 7.2 Hz, 1H), 9.54 (d, *J* = 8.4 Hz, 1H), 10.74 (d, *J* = 6.6 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 112.1, 117.9, 118.8, 119.6, 122.4, 123.4, 125.7, 126.6, 127.5, 127.6, 129.4, 129.8, 130.3, 132.2, 132.3, 132.6, 133.9, 139.5, 143.1, 167.6, 170.0. HRMS calcd for $C_{23}H_{14}N_3O_2^+$: 364.1081 $[M+H]^+$, found: 364.1071.

2,11-Dimethyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5g): yellow solid (131 mg, 83%); mp: >300 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 2.91 (s, 3H), 3.52 (s, 3H), 7.77 (d, *J* = 3.6 Hz, 1H), 8.09 (s, 1H), 8.170-8.173 (m, 2H), 8.90 (t, *J* = 1.8 Hz, 1H), 9.41 (d, *J* = 3.0 Hz, 1H), 10.52 (s, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 20.8, 23.3, 110.5, 117.5, 119.5, 120.9, 122.0, 123.0, 125.5, 126.2, 127.3, 131.4, 131.70, 131.73, 133.3, 143.1, 154.4, 167.7, 170.4. HRMS calcd for $C_{19}H_{14}N_3O_2^+$: 316.1081 $[M+H]^+$, found: 316.1077.

11-Chloro-2-methyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5h): yellow solid (138 mg, 82%); mp: >300 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 3.53 (s, 3H), 8.210-8.214 (m, 2H), 8.33 (d, *J* = 9.0 Hz, 1H), 8.41 (d, *J* = 8.4 Hz, 1H), 8.75 (s, 1H), 9.44 (d, *J* = 3.0 Hz, 1H), 10.78 (s, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 23.3, 112.4, 117.6, 119.5, 122.3, 123.0, 126.4, 126.6, 127.4, 127.9, 130.2, 132.05, 132.12, 133.6, 140.0, 141.2, 167.4, 170.0. HRMS calcd for $C_{18}H_{11}ClN_3O_2^+$: 336.0534 $[M+H]^+$, found: 336.0528.

2,10-Dimethyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5i): yellow solid (135 mg, 86%); mp: 291-292 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 2.91 (s, 3H), 3.52 (s, 3H), 7.78 (d, *J* = 6.6 Hz, 1H), 8.08 (s, 1H), 8.16-8.17 (m, 2H), 8.68-8.69 (m, 1H), 9.40 (dd, J_1 = 6.6 Hz, J_2 = 3.0 Hz, 1H), 10.51 (d, *J* = 7.2 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 20.8, 23.3, 110.5, 117.5, 119.5, 120.9, 122.0,

123.0, 125.5, 126.2, 127.3, 131.4, 131.7, 133.3, 143.1, 154.4, 167.7, 170.4. HRMS calcd for $C_{19}H_{14}N_3O_2^+$: 316.1081 $[M+H]^+$, found: 316.1080.

2,9-Dimethyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)–dione (5j): yellow solid (132 mg, 84%); mp: 287-288 ºC; ^{1}H NMR (400 MHz, CF_3CO_2D) δ: 2.97 (s, 3H), 3.48 (s, 3H), 7.82 (t, *J* = 6.8 Hz, 1H), 8.12-8.14 (m, 2H), 8.23 (d, *J* = 7.2 Hz, 1H), 8.77 (d, *J* = 5.2 Hz, 1H), 9.38-9.40 (m, 1H), 10.56 (d, *J* = 6.4 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 14.8, 23.3, 118.2, 118.7, 119.6, 122.3, 123.1, 123.3, 126.2, 126.3, 127.4, 130.2, 131.7, 131.8, 133.3, 138.8, 142.7, 167.5, 170.2. HRMS calcd for $C_{19}H_{14}N_3O_2^+$: 316.1081 $[M+H]^+$, found: 316.1073.

2-Methyl-5-phenyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5k): yellow solid (160 mg, 85%); mp: >300 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 3.55 (s, 3H), 7.48 (t, *J*= 7.8 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.81 (d, *J* = 7.2 Hz, 2H), 7.93 (t, *J* = 7.2 Hz, 1H), 8.33-8.37 (m, 2H), 8.48 (t, *J* = 7.8 Hz, 1H), 8.71 (d, *J* = 8.4 Hz, 1H), 9.44 (s, 1H), 10.63 (d, *J* = 6.6 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D): δ 23.4, 112.0, 117.6, 118.7, 120.1, 121.7, 122.77, 122.79, 125.7, 126.6, 127.8, 128.9, 129.0, 130.6, 132.5, 133.1, 137.6, 139.2, 142.8, 144.7, 167.3, 170.2. HRMS calcd for $C_{24}H_{16}N_3O_2^+$: 378.1237 $[M+H]^+$, found: 378.1228.

2,5-Dimethyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5l): yellow solid (150 mg, 95%); mp: 287-288 ºC; ^{1}H NMR (400 MHz, CF_3CO_2D) δ: 2.80 (s, 3H), 3.48 (s, 3H), 7.87 (t, *J* = 7.6 Hz, 1H), 8.02 (d, *J* = 8.8 Hz, 1H), 8.14 (t, *J*= 7.6 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 8.70 (d, *J* = 8.8 Hz, 1H), 9.16 (s, 1H), 9.30 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ: 21.6, 24.1, 116.9, 117.0, 117.5, 118.4, 121.6, 123.1, 123.4, 123.9, 125.3, 125.7, 129.1, 133.5, 138.2, 149.6, 167.4, 168.6. HRMS calcd for $C_{19}H_{14}N_3O_2^+$: 316.1081 $[M+H]^+$, found: 316.1073.

5-Chloro-2-methyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5m): yellow solid (148 mg, 88%); mp: >300 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D): δ 3.57 (s, 3H), 8.00 (t, *J* = 6.6

Hz, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 8.41 (d, *J* = 8.4 Hz, 1H), 8.54 (t, *J* = 7.2 Hz, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 9.47 (s, 1H), 10.75 (d, *J* = 6.0 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D): δ 23.4, 112.1, 117.9, 118.9, 120.9, 121.2, 123.7, 125.0, 125.4, 128.1, 132.67, 132.71, 133.4, 139.6, 139.7, 143.1, 167.1, 169.8. HRMS calcd for $C_{18}H_{11}ClN_3O_2^+$: 336.0534 $[M+H]^+$, found: 336.0525.

2-Methyl-5-(trifluoromethyl)-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5n): yellow solid (148 mg, 80%); mp: 292-293 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 3.55 (s, 3H), 7.99 (t, *J* = 6.6 Hz, 1H), 8.38-8.42 (m, 2H), 8.53 (t, *J* = 7.8 Hz, 1H), 8.94 (d, *J* = 8.4 Hz, 1H), 9.77 (s, 1H), 10.75 (d, *J* = 6.6 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 23.5, 112.2, 118.98, 119.02, 121.2, 123.0 (q, $^1J_{C\text{-}F}$ =270.3 Hz), 123.7, 123.9 (q, $^3J_{C\text{-}F}$ = 4.2 Hz), 124.4, 126.5, 126.7, 127.5 (q, $^4J_{C\text{-}F}$ = 3.15 Hz), 132.8, 133.0, 134.4 (q, $^2J_{C\text{-}F}$ = 34.05 Hz), 139.9, 143.3, 166.9, 169.5. ^{19}F NMR (565 MHz, CF_3CO_2D) δ: -78.1. HRMS calcd for $C_{19}H_{11}F_3N_3O_2^+$: 370.0798 $[M+H]^+$, found: 370.0789.

2,6–Dimethyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5o): yellow solid (151 mg, 96%); mp: 268-269 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 2.91 (s, 3H), 3.58 (s, 3H), 7.99 (t, *J* = 6.6 Hz,1H), 8.11 (d, *J* = 9.0 Hz, 1H), 8.43 (d, *J* = 7.2 Hz, 1H), 8.52 (d, *J* = 6.0 Hz, 1H), 8.58 (s, 1H), 9.37 (d, *J* = 8.4 Hz, 1H), 10.75 (d, *J* = 6.0 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 20.5, 23.3, 112.0, 117.9, 118.6, 121.3, 123.5, 125.6, 126.1, 126.3, 132.5, 132.7, 134.2, 139.1, 142.8, 144.6, 167.8, 170.5. HRMS calcd for $C_{19}H_{14}N_3O_2^+$: 316.1081 $[M+H]^+$, found: 316.1067.

6-Chloro-2-methyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5p): yellow solid (144 mg, 86%); mp: >300 ºC. ^{1}H NMR (400 MHz, CF_3CO_2D) δ: 3.53 (s, 3H), 7.97 (t, *J* = 7.6 Hz, 1H), 8.13 (d, *J* = 8.8 Hz, 1H), 8.37 (d, *J* = 8.8 Hz, 1H), 8.50 (t, *J* = 8.0 Hz, 1H), 8.74 (s, 1H), 9.39 (d, *J* = 9.2 Hz, 1H), 10.71 (d, *J* = 6.8 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 23.4, 112.1, 118.6, 118.9, 119.6, 121.7, 123.9, 125.6, 126.2, 127.7, 132.2, 132.7, 132.9, 139.60, 139.61, 143.0, 167.2, 169.8. HRMS calcd for $C_{18}H_{11}ClN_3O_2^+$: 336.0534 $[M+H]^+$, found: 336.0530.

2,7-Dimethyl-1*H*-benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-dione (5q): yellow solid (118 mg, 75%); mp: 284-285 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 3.33 (s, 3H), 3.51 (s, 3H), 7.96 (s, 1H), 8.00 (d, *J* = 6.0 Hz, 1H), 8.07 (t, *J* = 6.6 Hz, 1H), 8.44-8.46 (m, 2H), 9.42 (d, *J* = 7.8 Hz, 1H), 10.85 (d, *J* = 6.0 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 21.3, 23.4, 112.2, 118.3, 118.8, 119.3, 123.1, 124.5, 126.6, 128.7, 131.5, 132.4, 133.0, 134.0, 139.0, 142.3, 167.3, 170.2. HRMS calcd for $C_{19}H_{14}N_3O_2^+$: 316.1081 $[M+H]^+$, found: 316.1045.

8-Methyl-7*H*-naphtho[2,1-*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-7,9(8*H*)-dione (5r): yellow solid (119 mg, 68%); mp: >300 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 3.60 (s, 3H), 8.02 (t, *J* = 7.2 Hz, 1H), 8.05-8.06 (m, 1H), 8.08-8.10 (m, 1H), 8.31 (d, *J* = 7.8 Hz, 1H), 8.41 (d, *J* = 8.4 Hz, 1H), 8.47 (d, *J* = 9.0 Hz, 1H), 8.54-8.57 (m, 1H), 8.99 (d, *J* = 8.4 Hz, 1H), 9.36 (d, *J* = 9.0 Hz, 1H), 10.90 (d, *J* = 7.2 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D) δ: 23.5, 112.2, 118.9, 119.9, 121.1, 121.7, 124.0, 125.0, 127.0, 129.1, 129.4, 130.0, 130.1, 132.3, 132.8, 133.6, 133.8, 140.1, 143.6, 167.1, 170.1. HRMS calcd for $C_{22}H_{14}N_3O_2^+$: 352.1081 $[M+H]^+$, found: 352.1076.

5-Methyl-4*H*-pyrido[2',1':2,3]imidazo[4,5-*e*]thieno[2,3-*g*]isoindole-4,6(5*H*)-dione (5s): yellow solid (101 mg, 66%); mp: 283-284 ºC; ^{1}H NMR (600 MHz, CF_3CO_2D) δ: 3.60 (s, 3H), 8.02 (t, *J* = 7.2 Hz, 1H), 8.35-8.38 (m, 2H), 8.56-8.58 (m, 2H), 10.78 (d, *J* = 6.6 Hz, 1H). ^{13}C NMR (150 MHz, CF_3CO_2D): 23.4, 112.0, 117.7, 118.3, 118.7, 122.4, 123.5, 130.8, 131.0, 133.1, 134.7, 136.3, 140.1, 143.4, 167.7, 169.7. HRMS calcd for $C_{16}H_{10}N_3O_2S^+$: 308.0488 $[M+H]^+$, found: 308.0487.

5,6,7-Trimethoxybenzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-dione (6): yellow solid (35 mg, 93%); mp: >300 ºC (lit.[4] mp: 272 °C); ^{1}H NMR (400 MHz, DMSO-d_6) δ: 3.97 (s, 3H), 4.00 (s, 3H), 4.21 (s, 3H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 8.29 (s, 1H), 8.92 (d, *J* = 7.6 Hz, 1H), 11.09 (s, 1H), 11.91 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6): 56.4, 61.5, 62.1, 100.5, 112.1, 113.1, 113.7, 117.4, 120.9, 121.0, 124.0, 124.4, 126.5, 128.3, 138.9, 140.4, 141.9, 149.0, 155.1, 171.0, 172.2.

HRMS calcd for $C_{21}H_{17}N_2O_5^+$: 377.1132 $[M+H]^+$, found: 377.1128.

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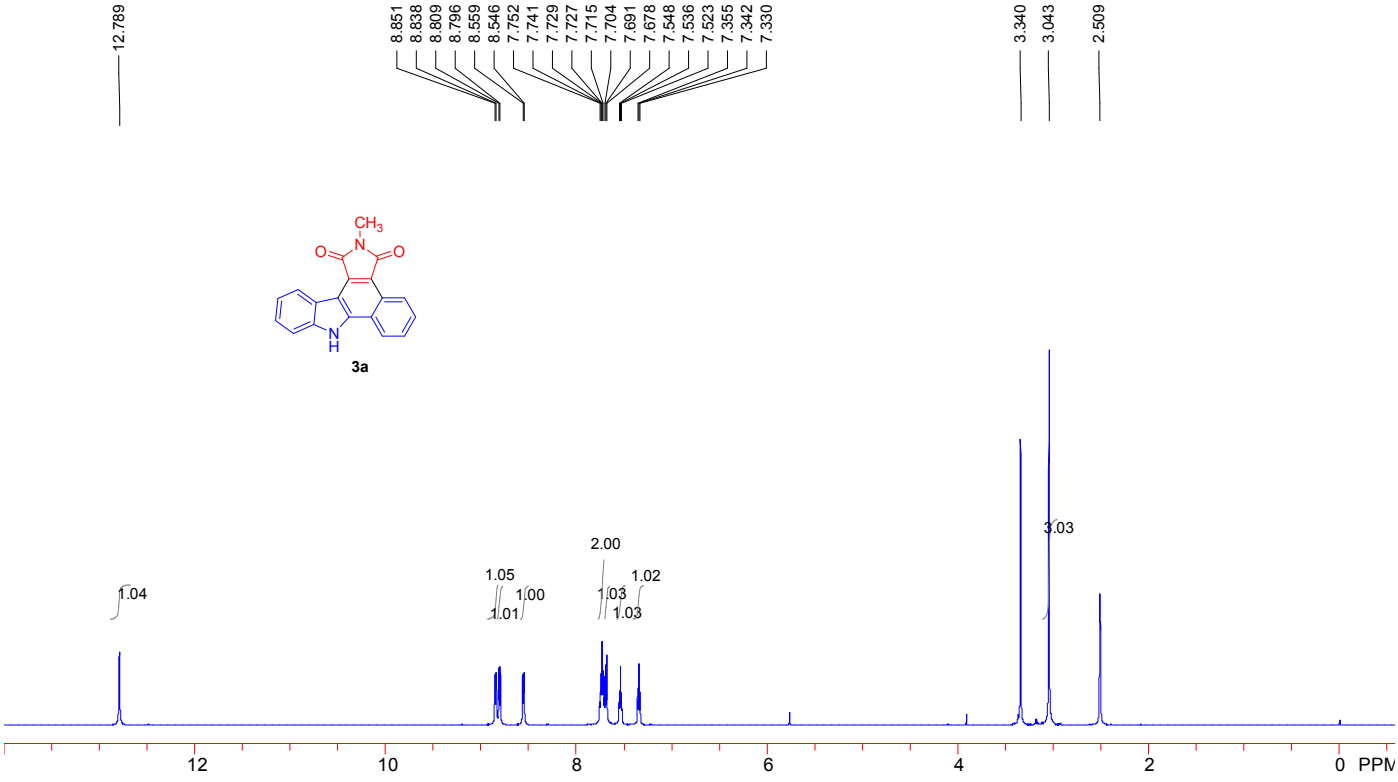
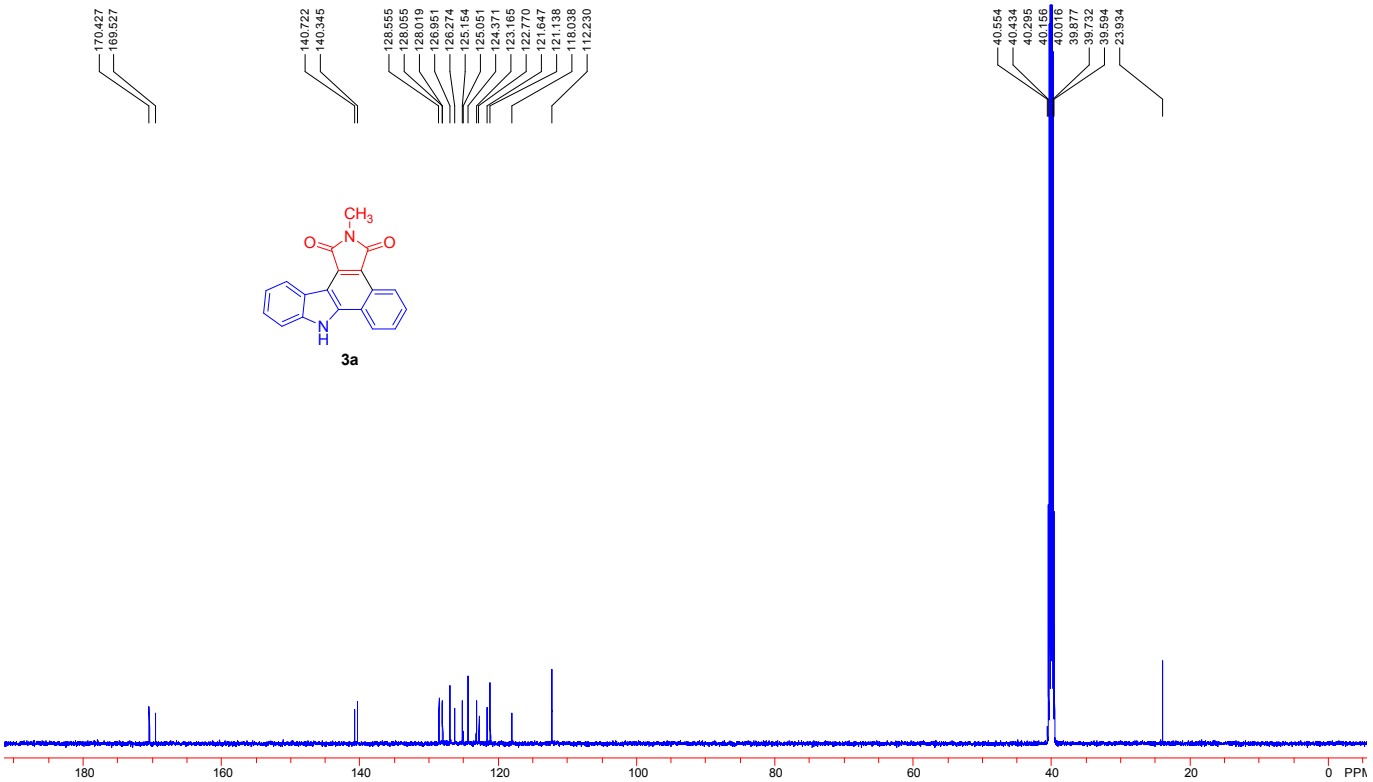
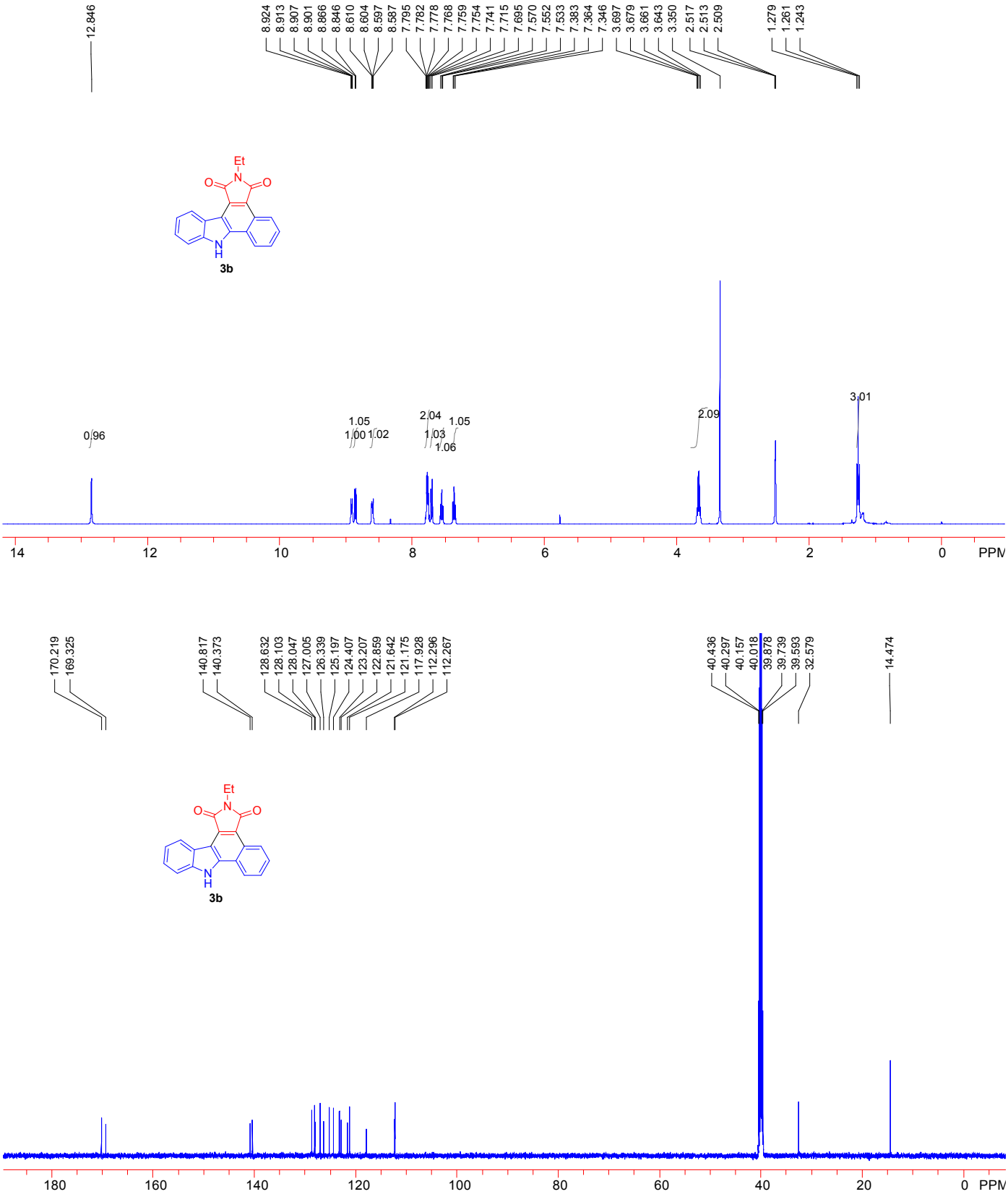
7. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra of 3a-3y, 5a-5s and 6



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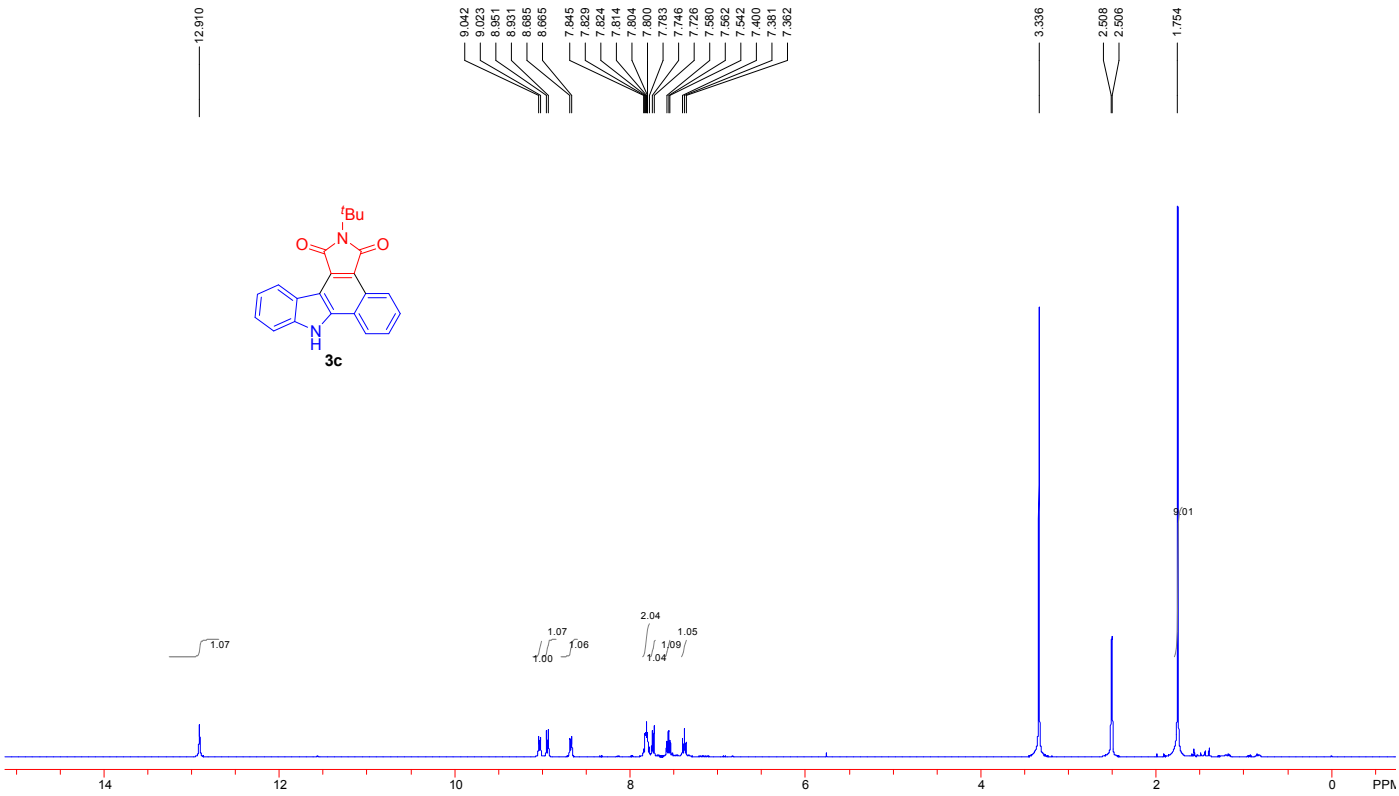
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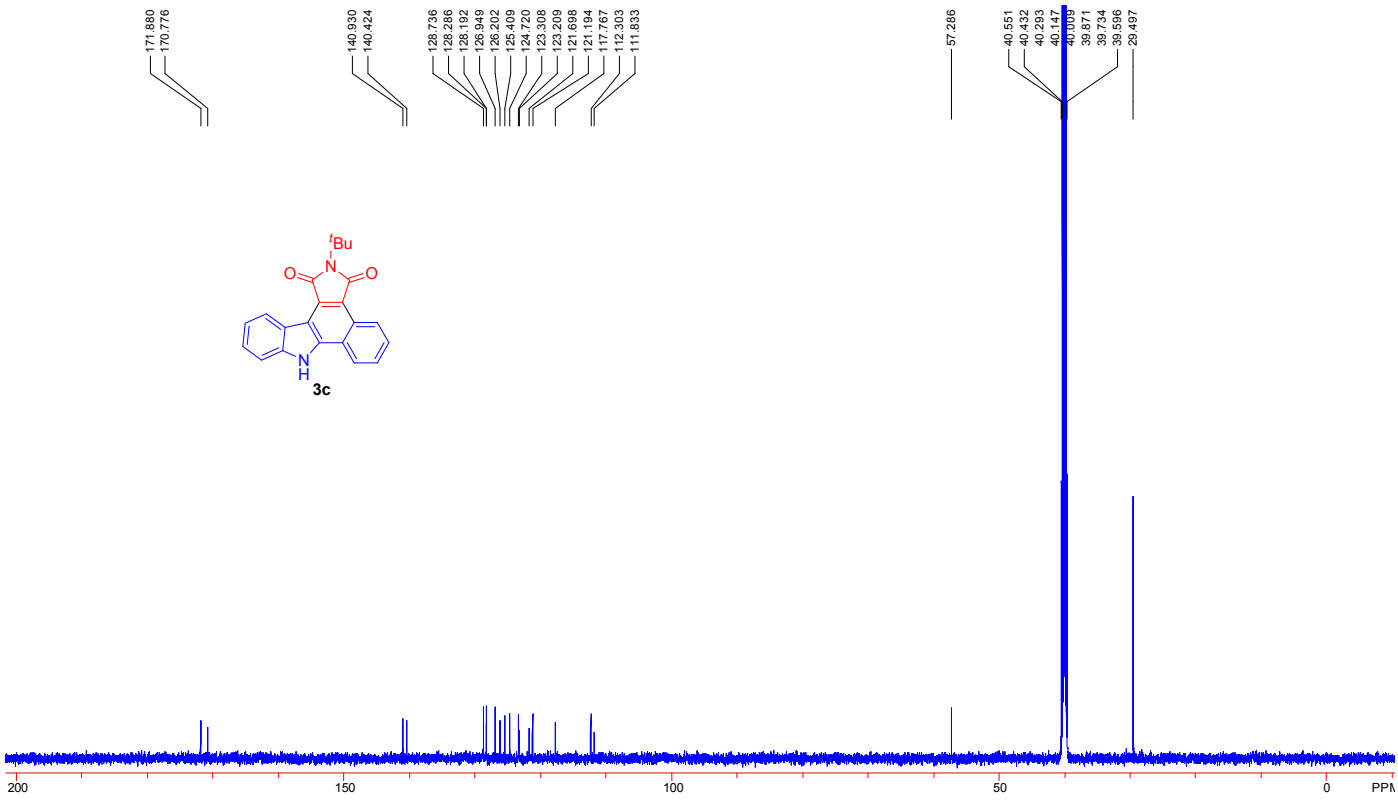
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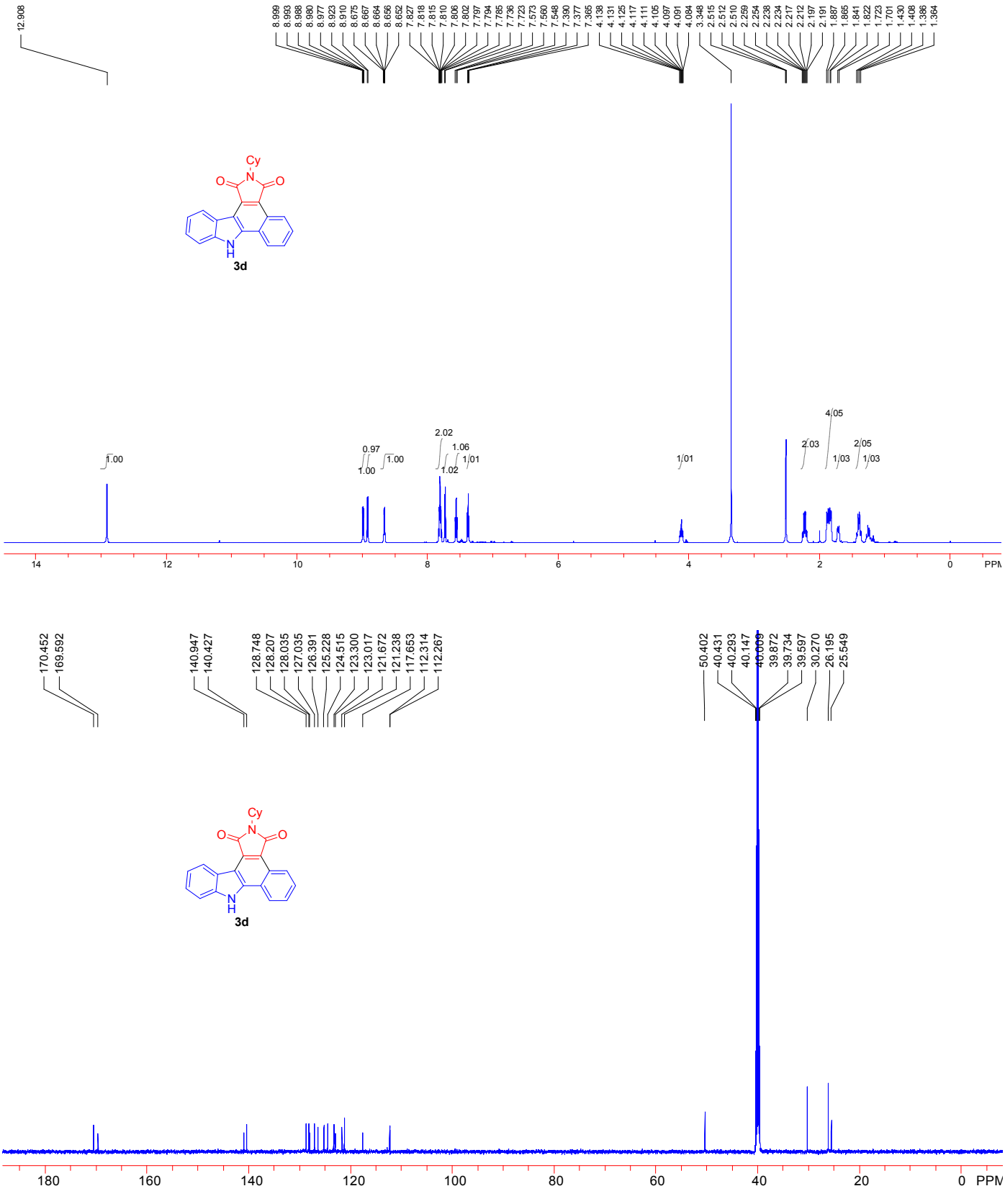
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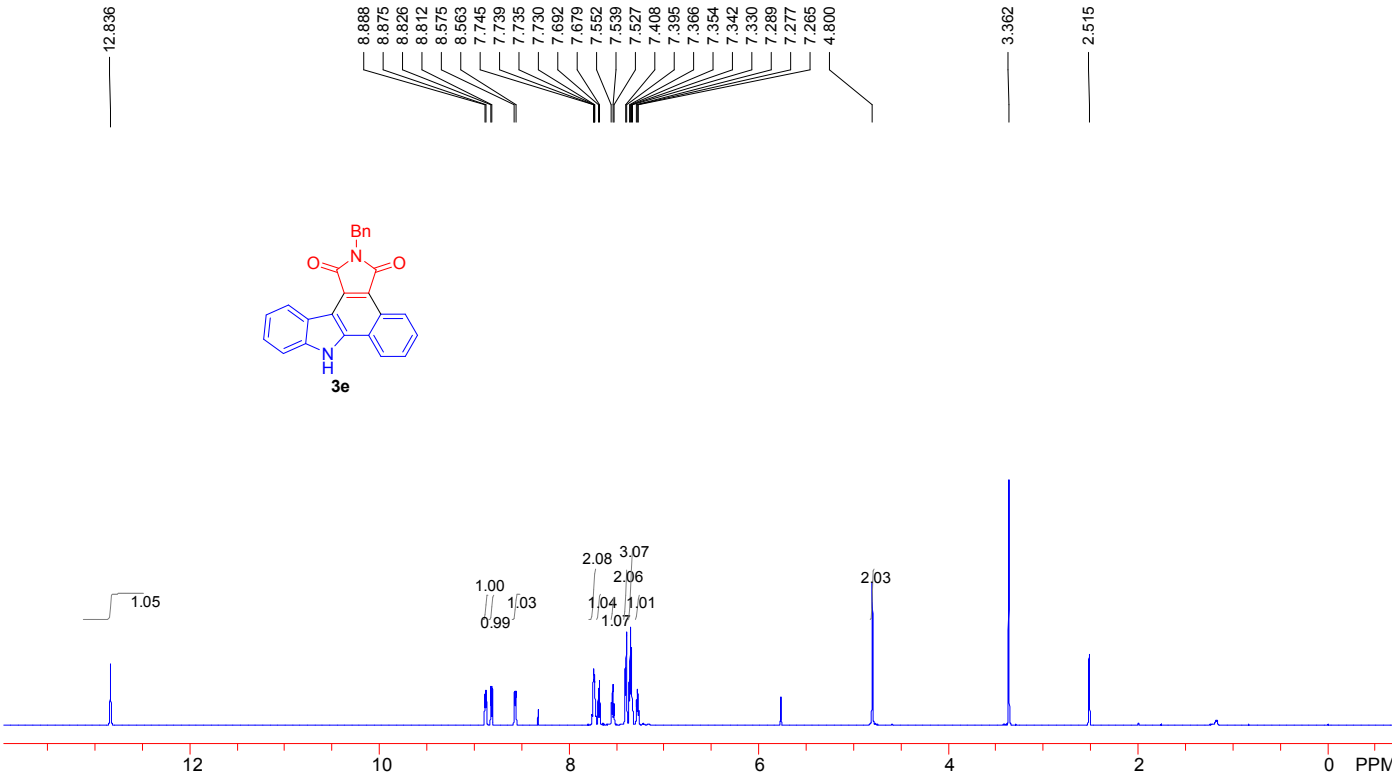
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O
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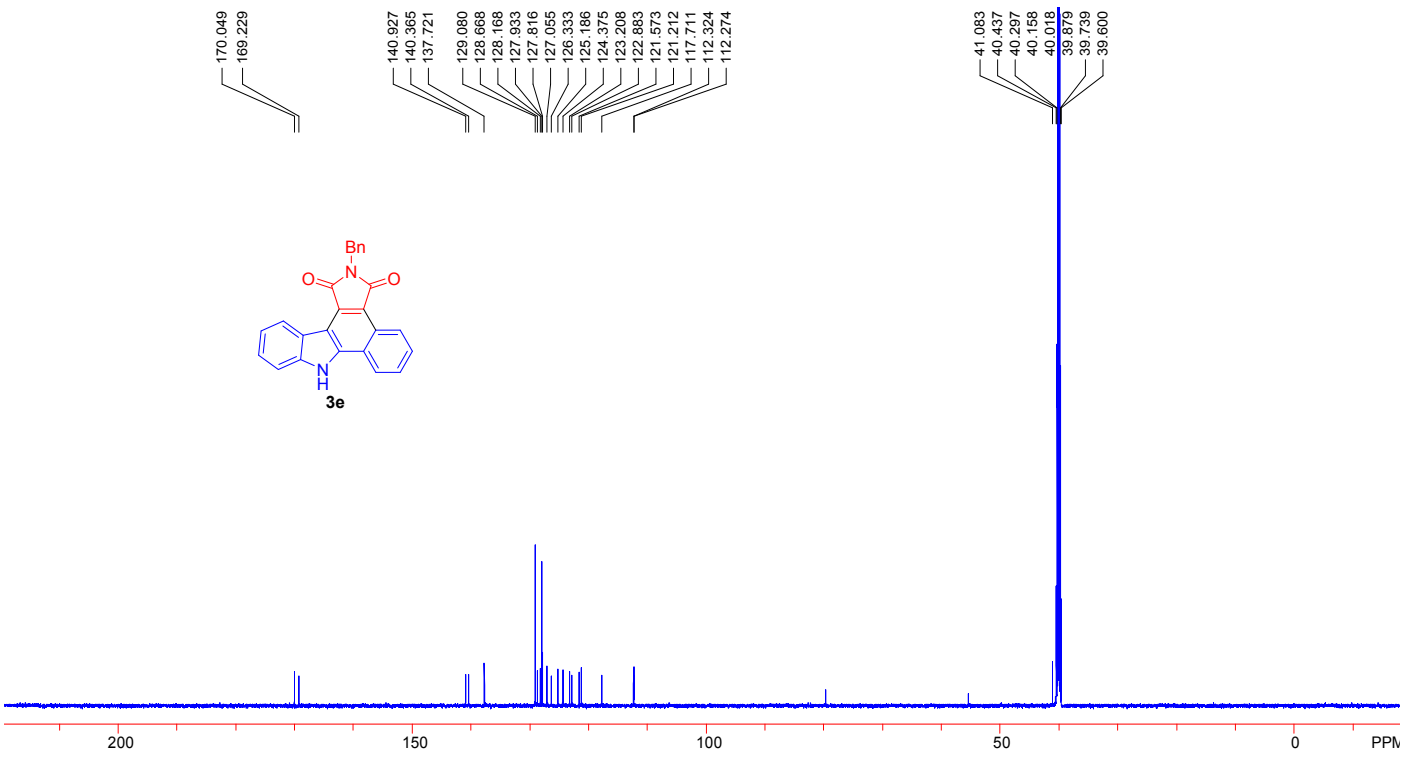
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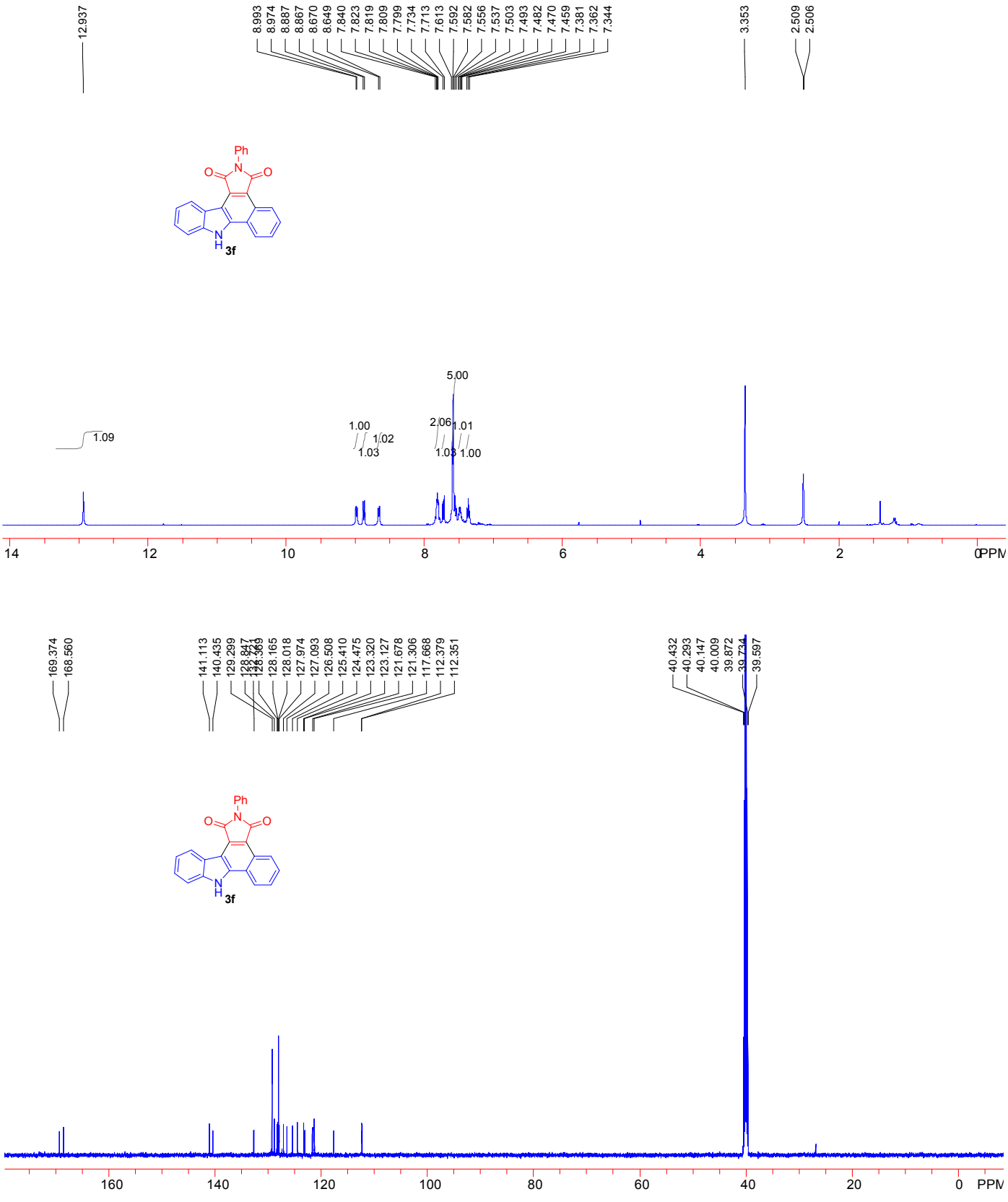
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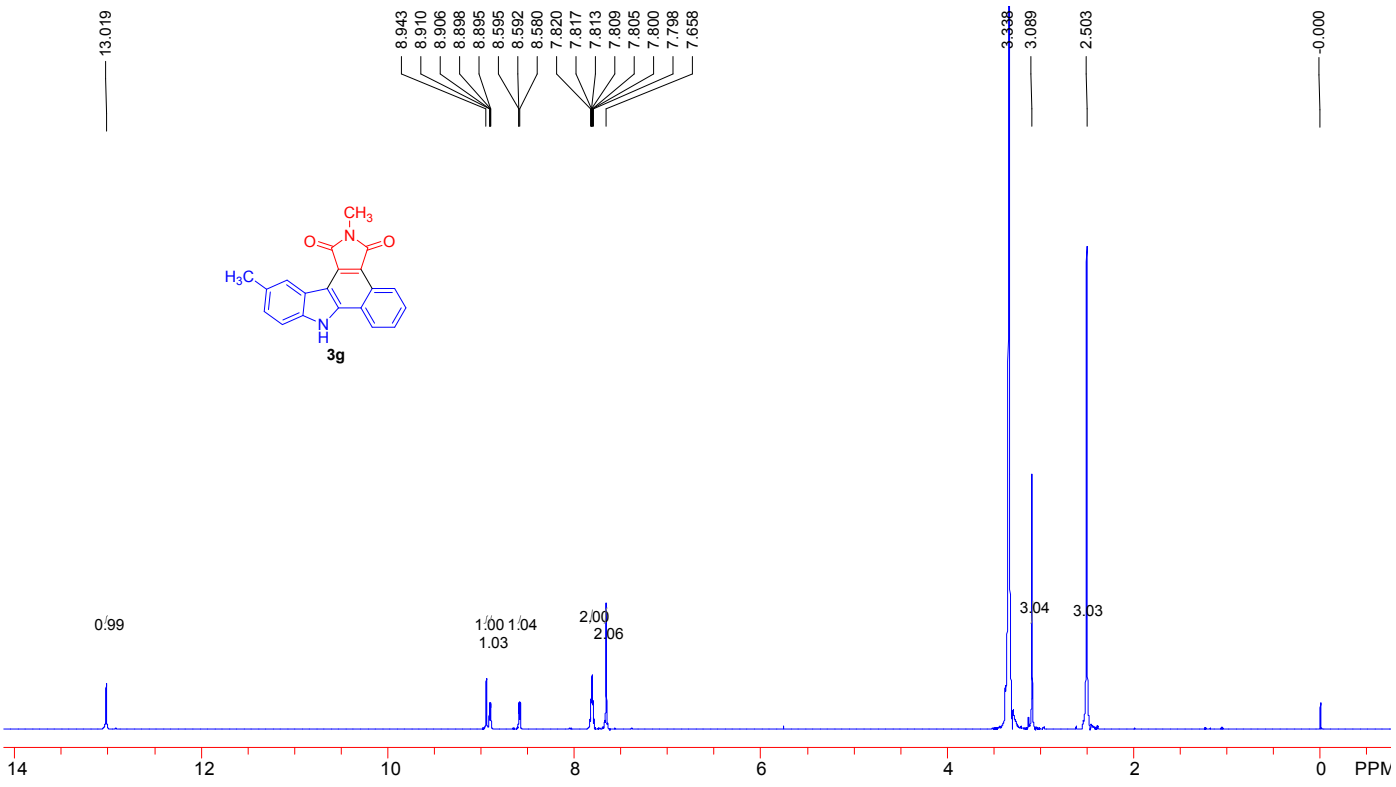
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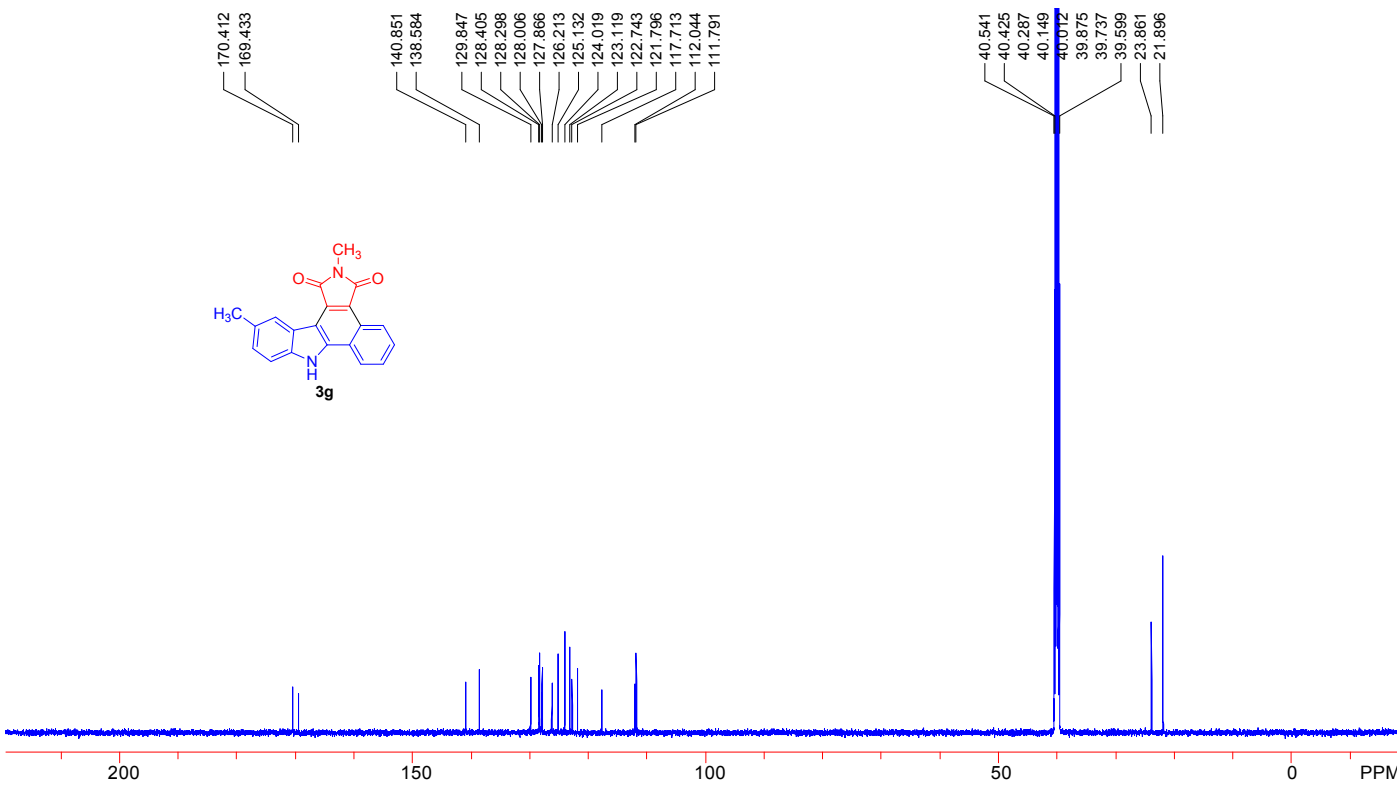
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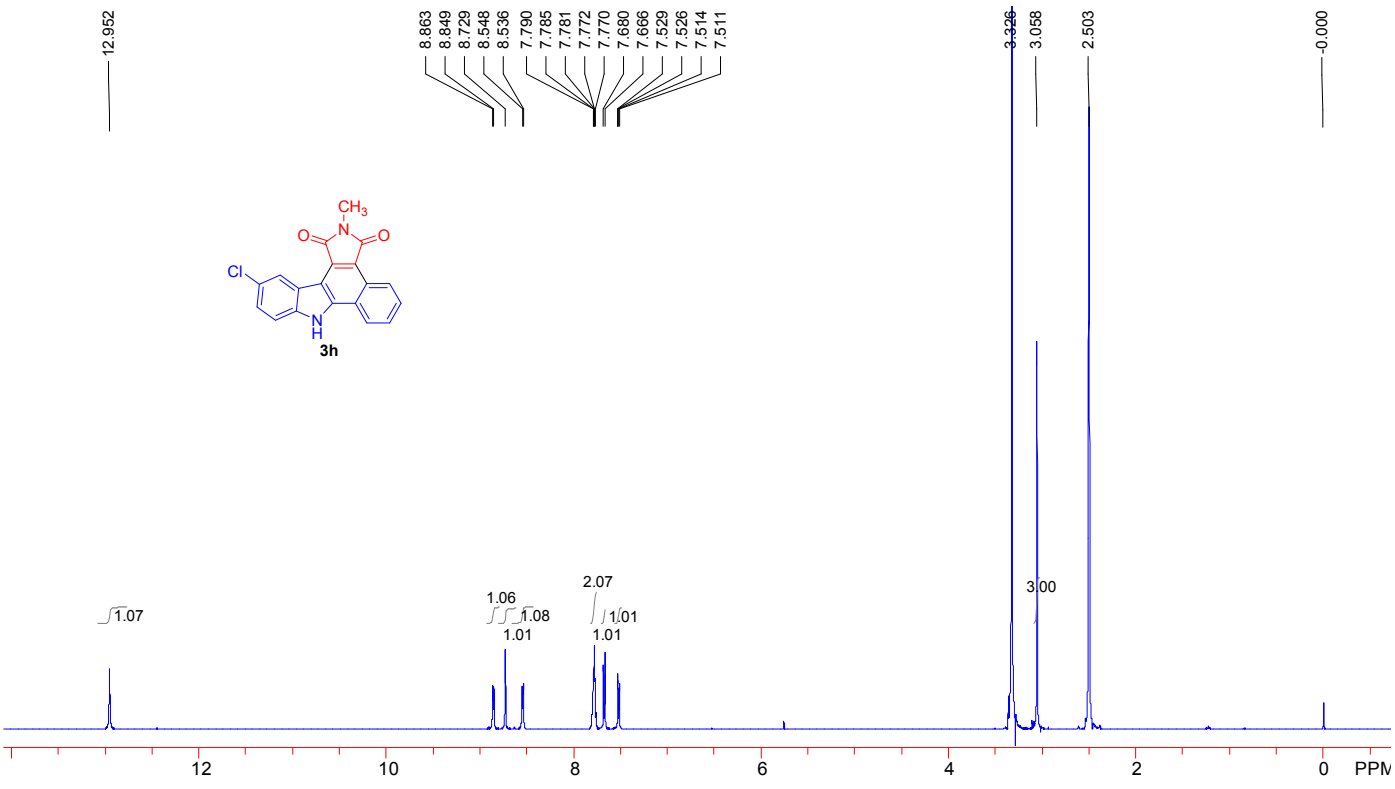
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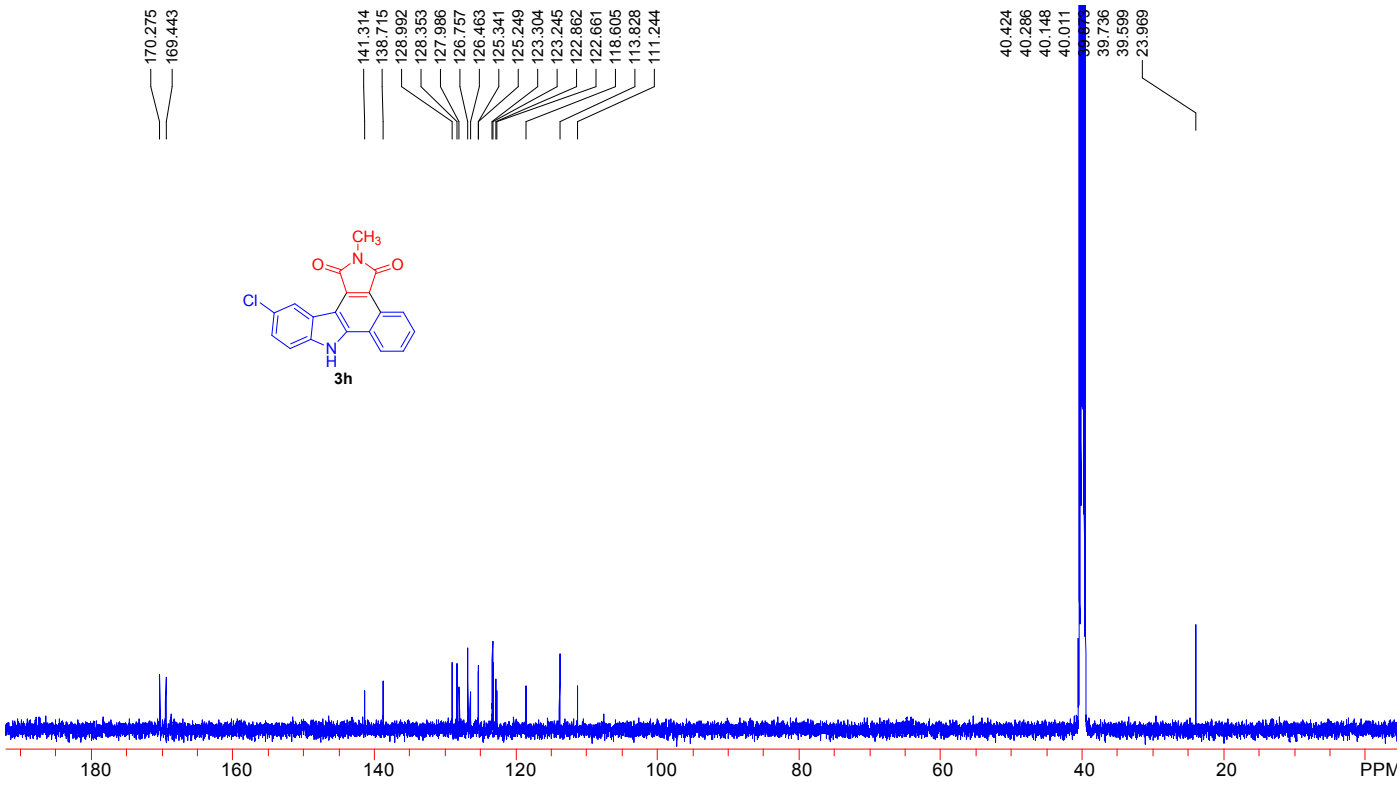
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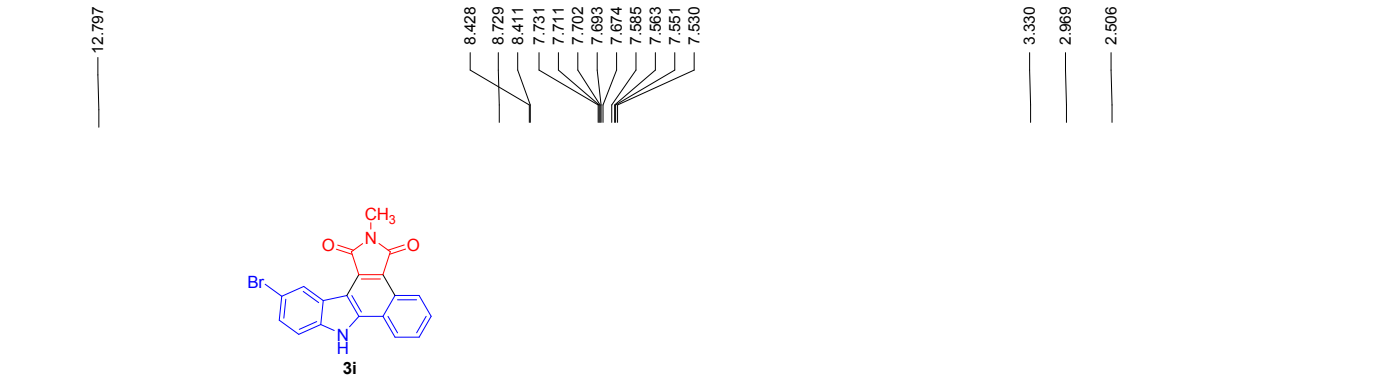
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N
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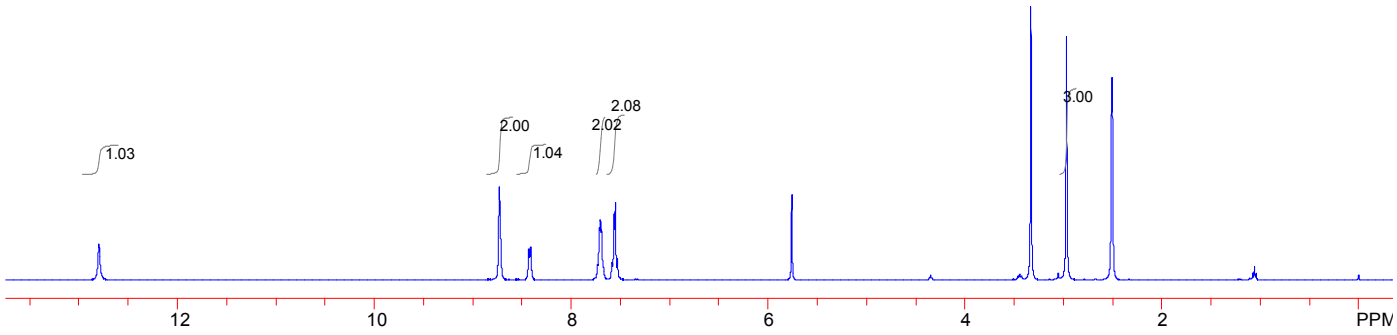
3i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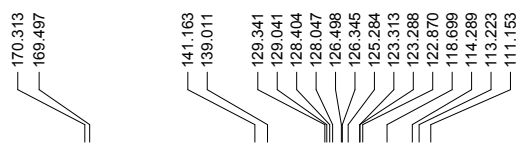
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H

3i

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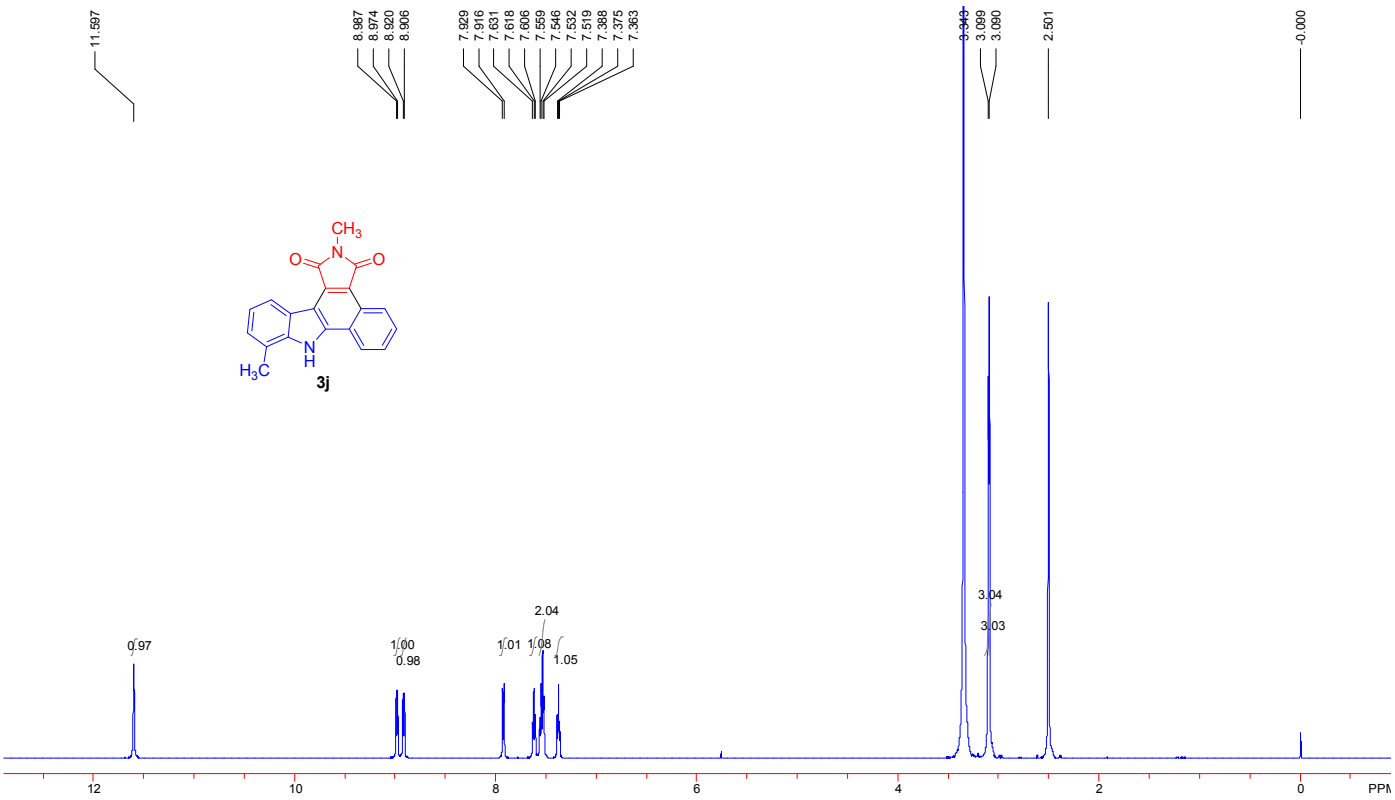
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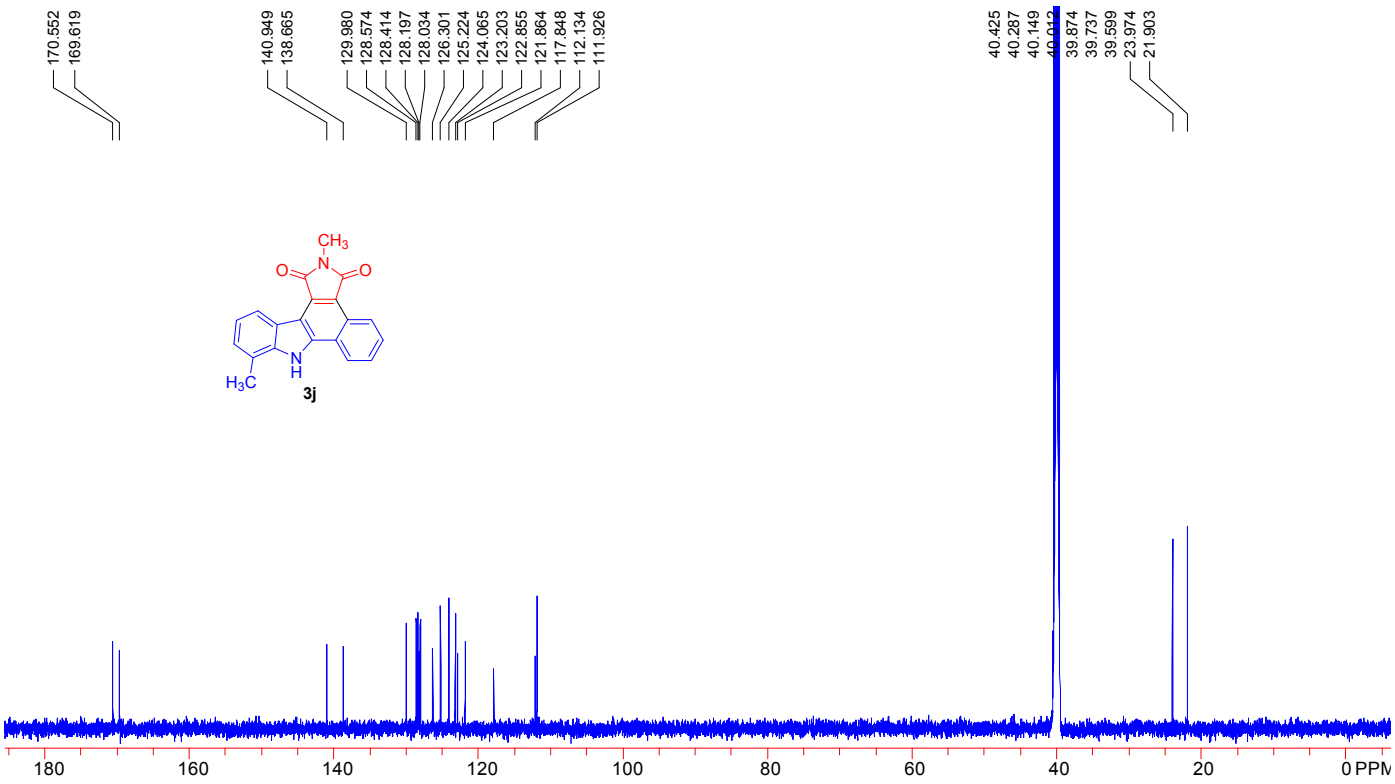
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H3C

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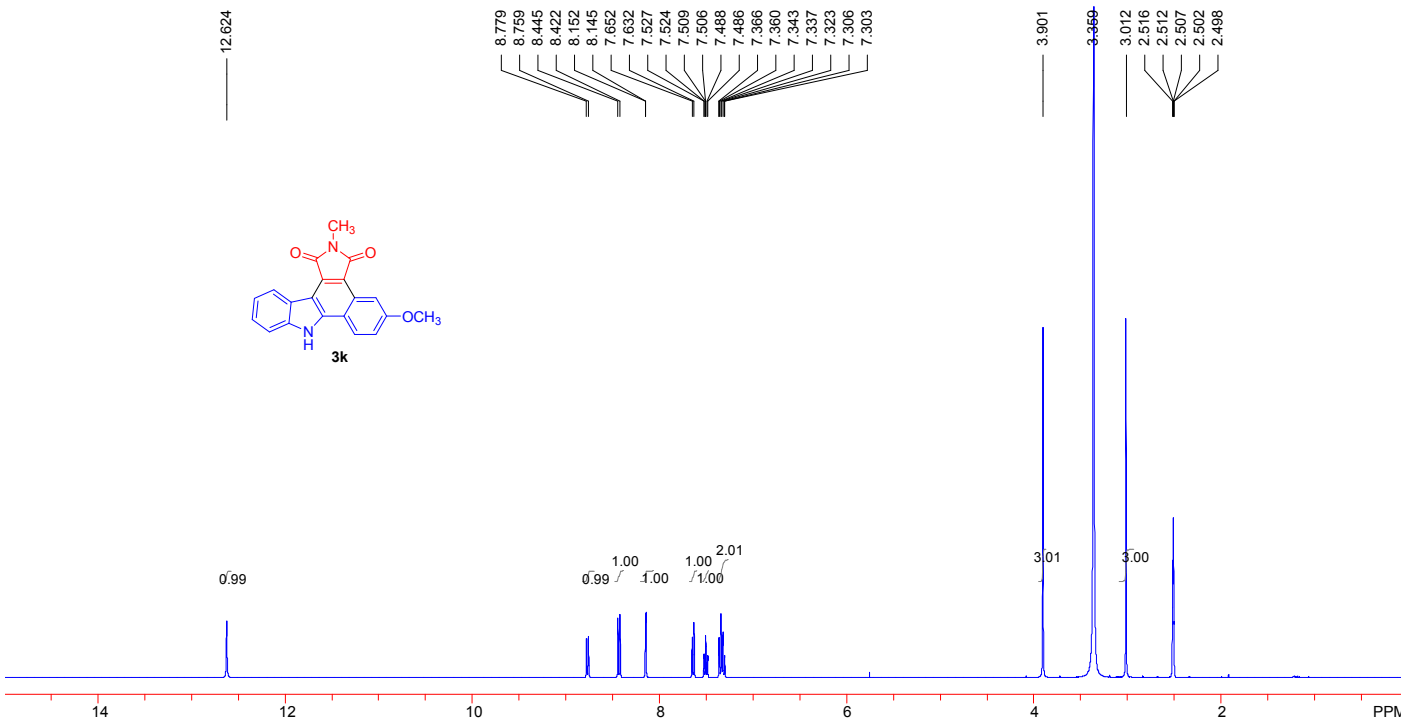
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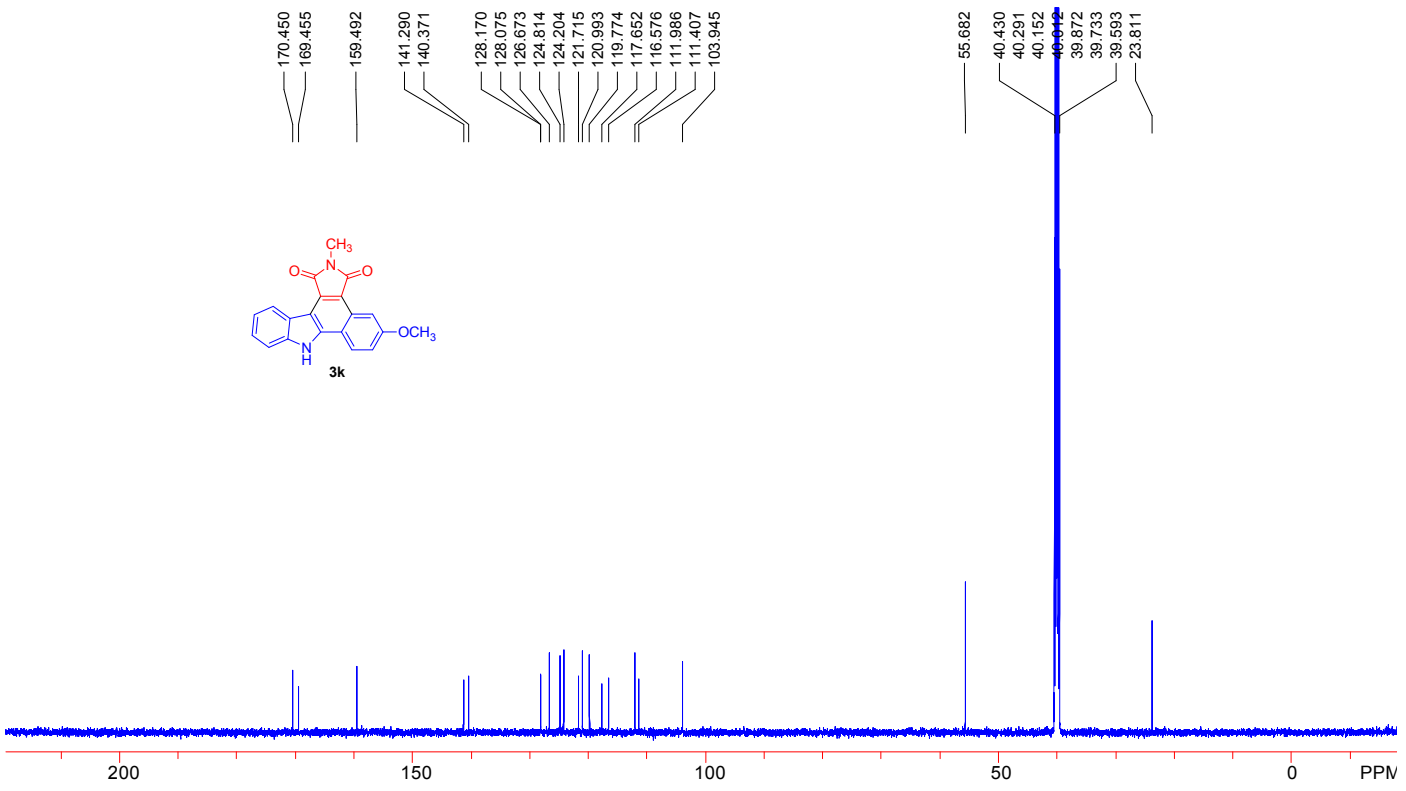
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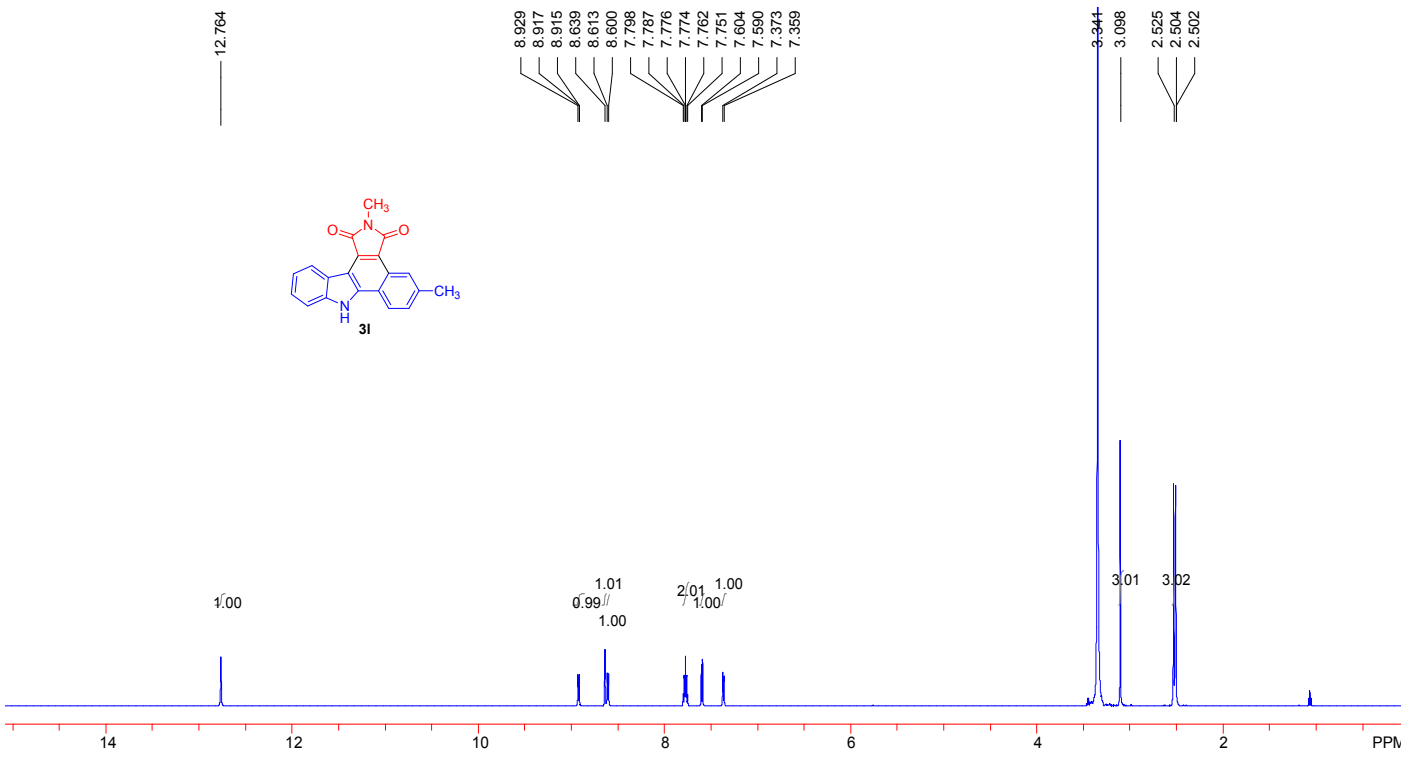
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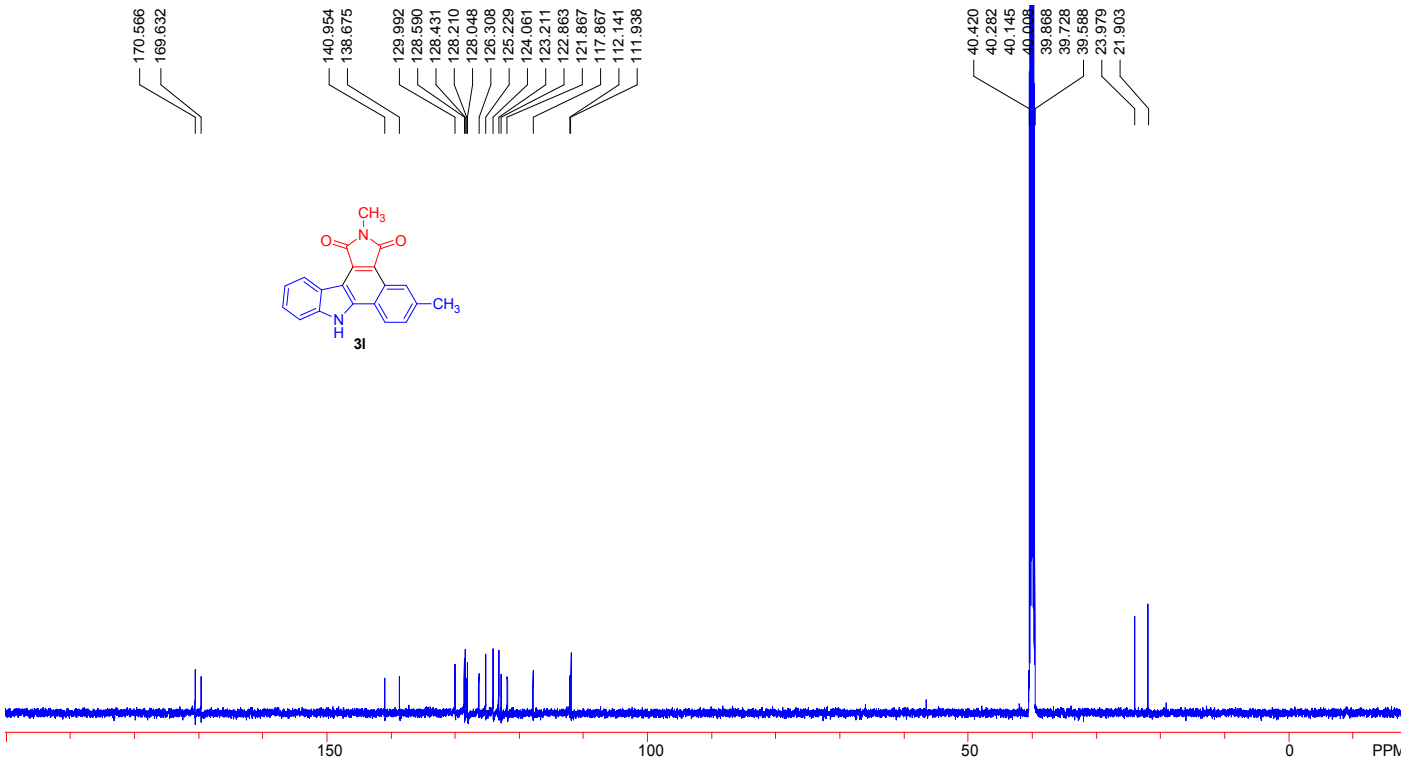
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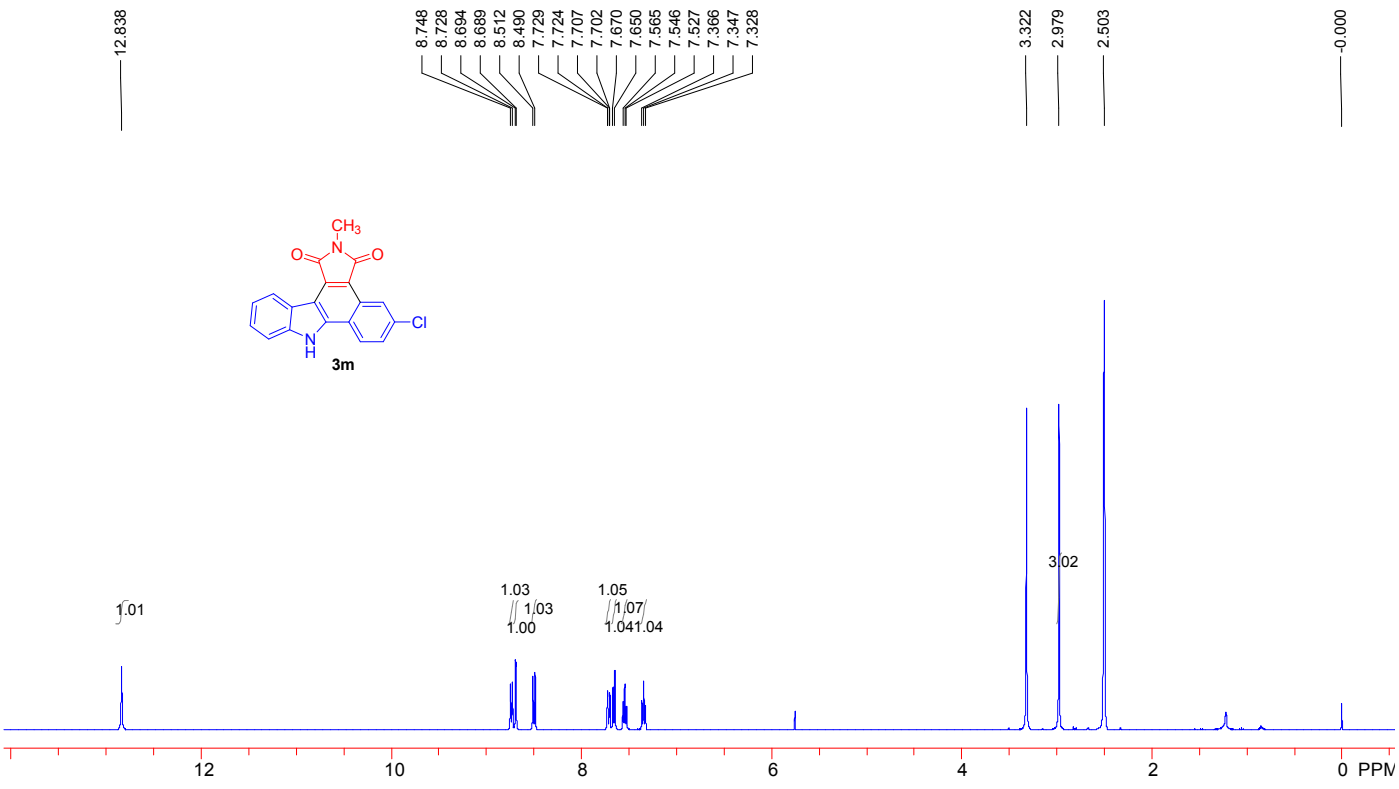
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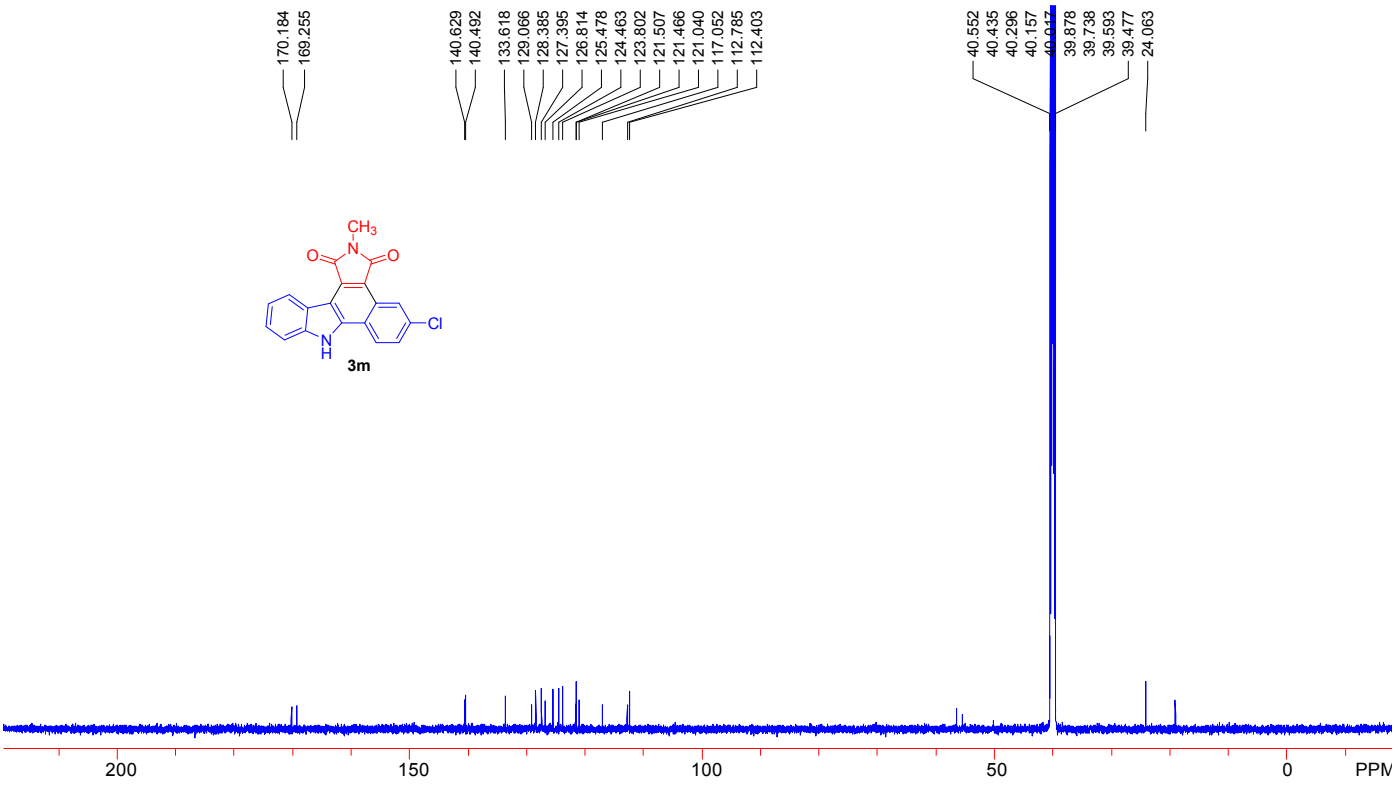
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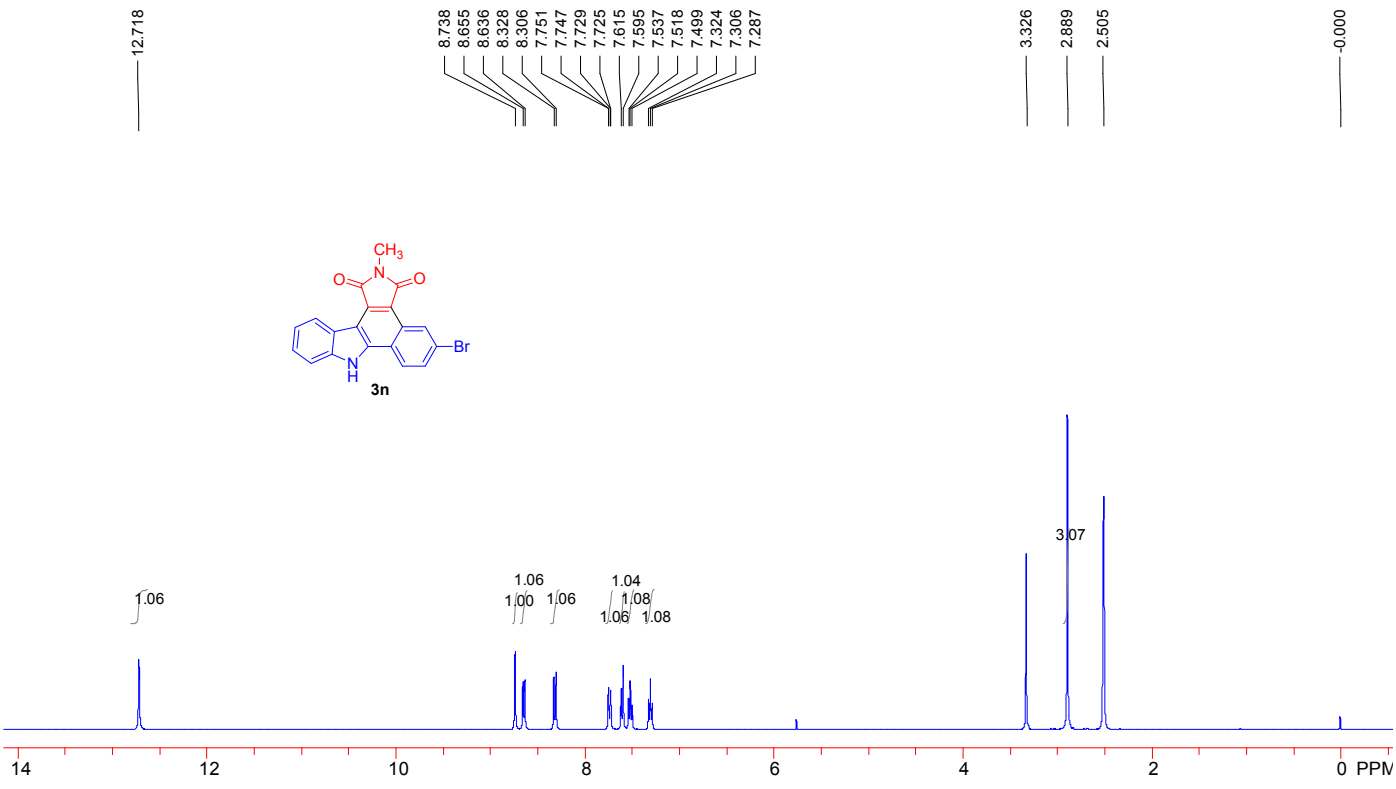
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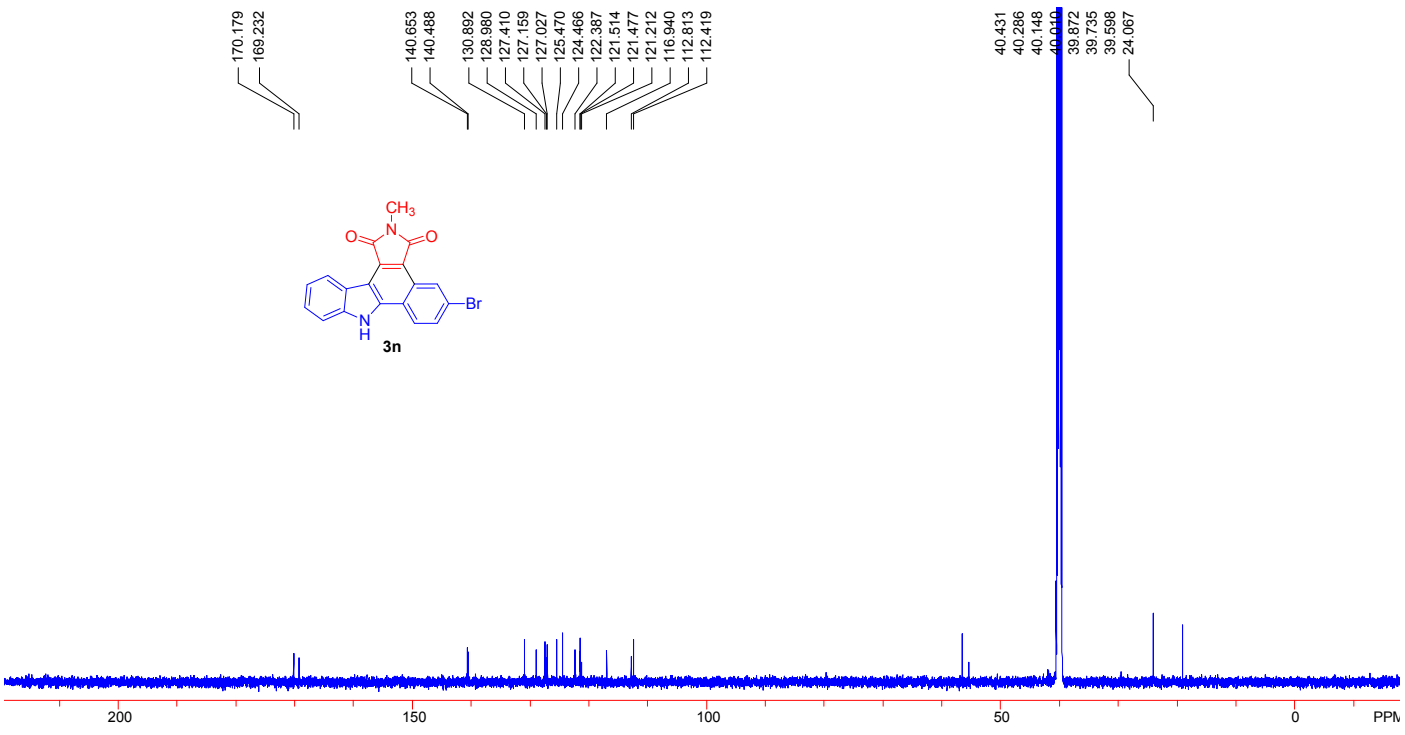
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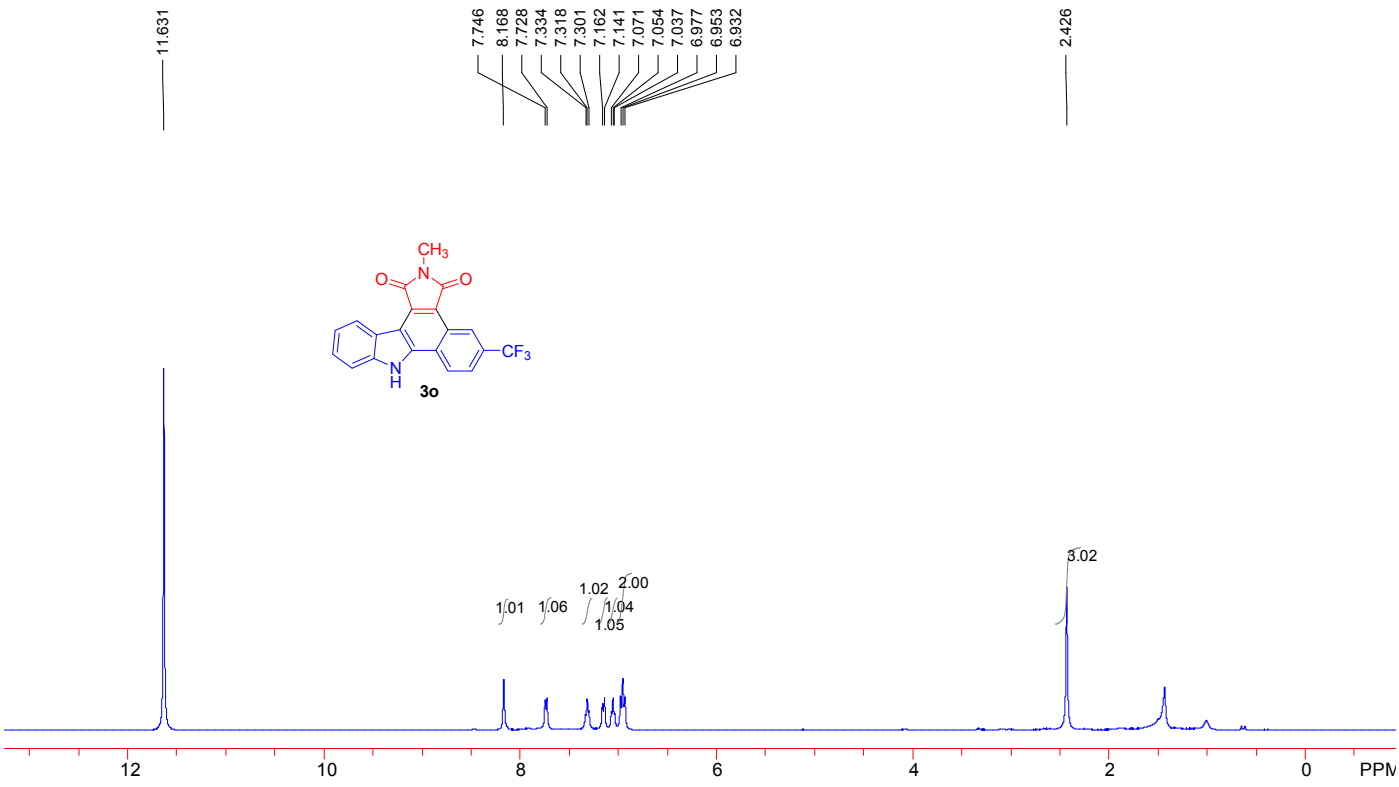
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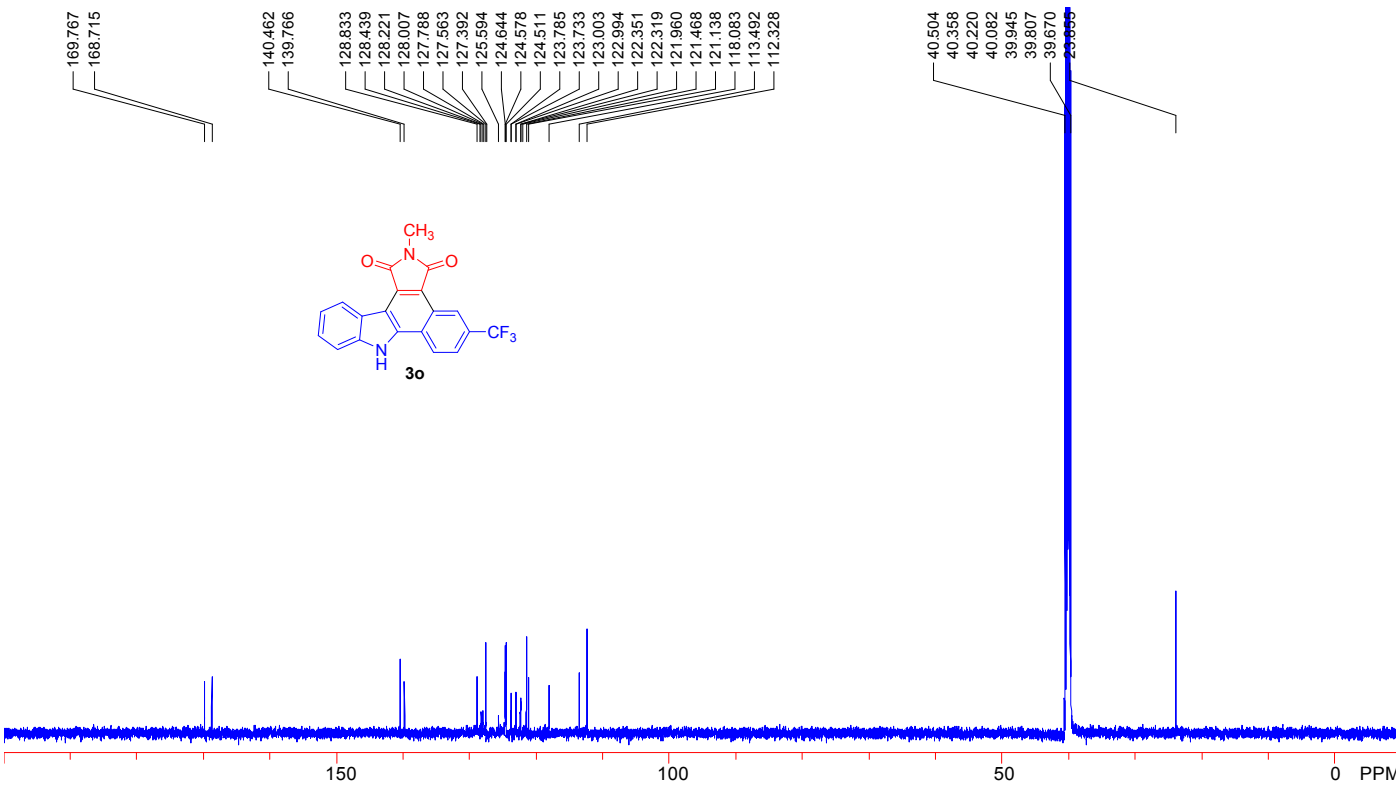
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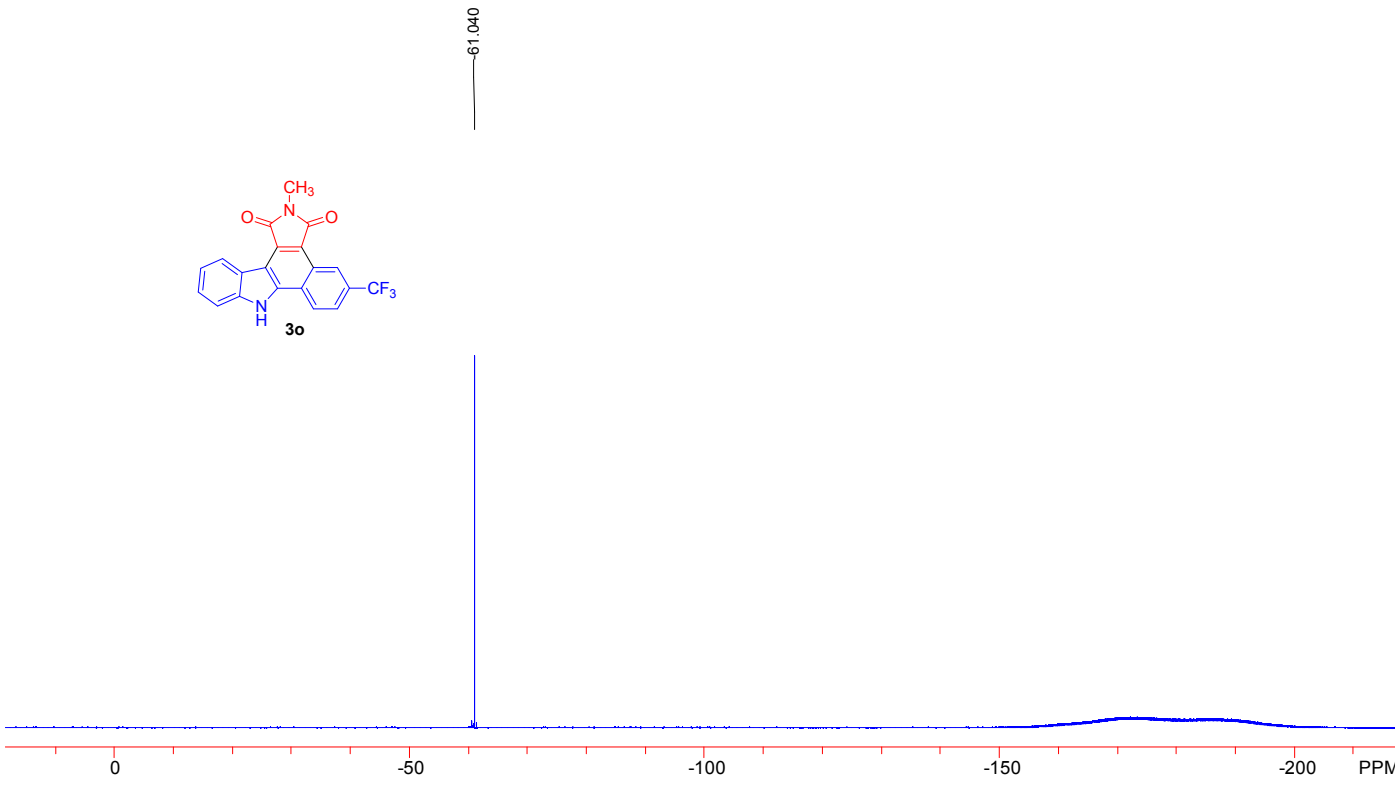
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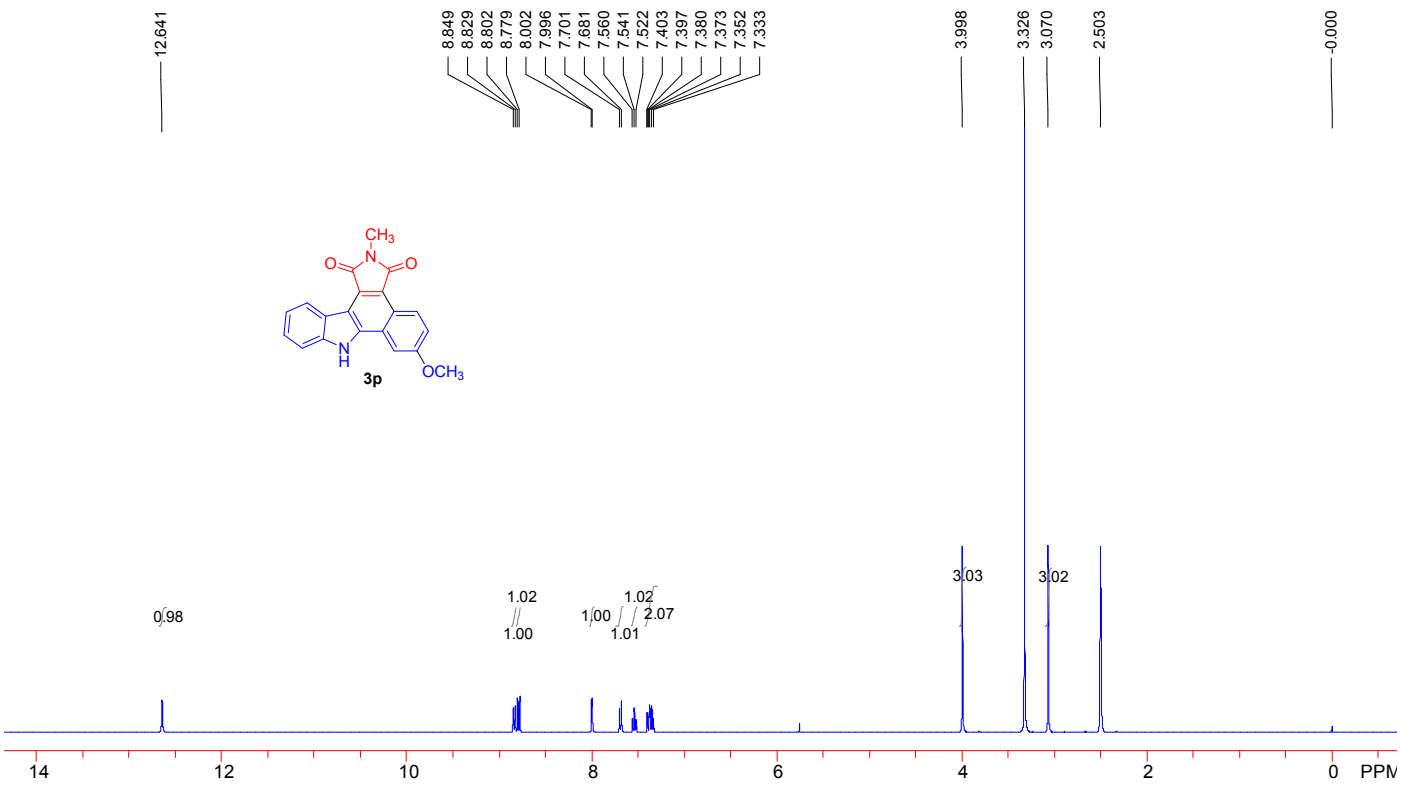
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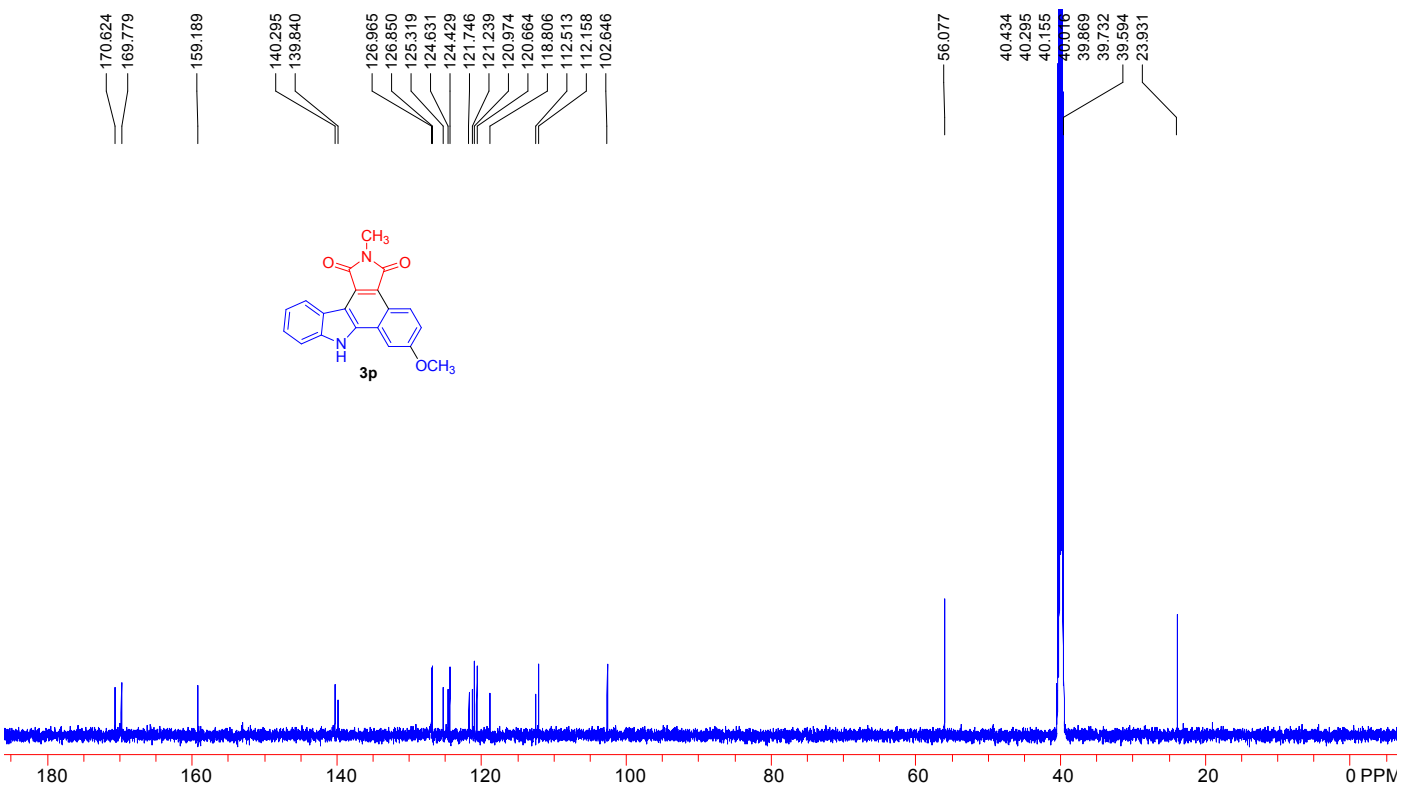
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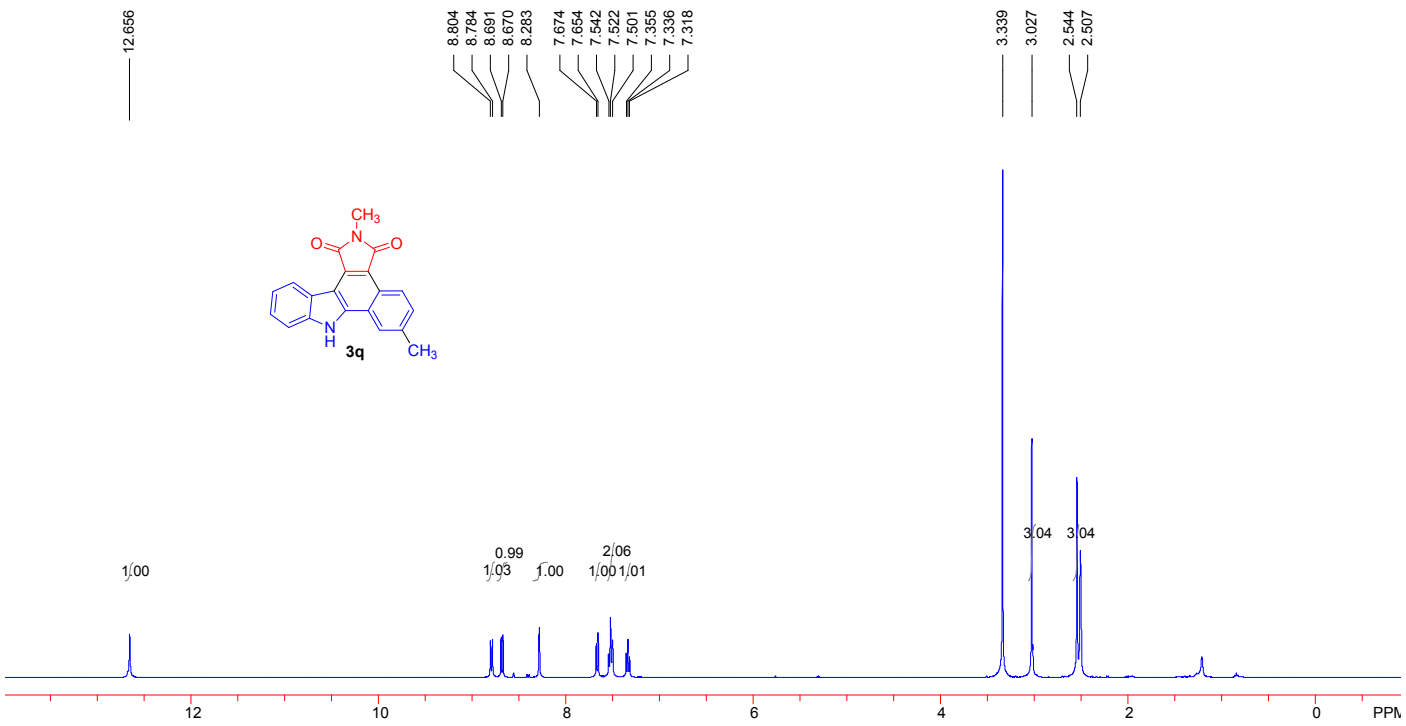
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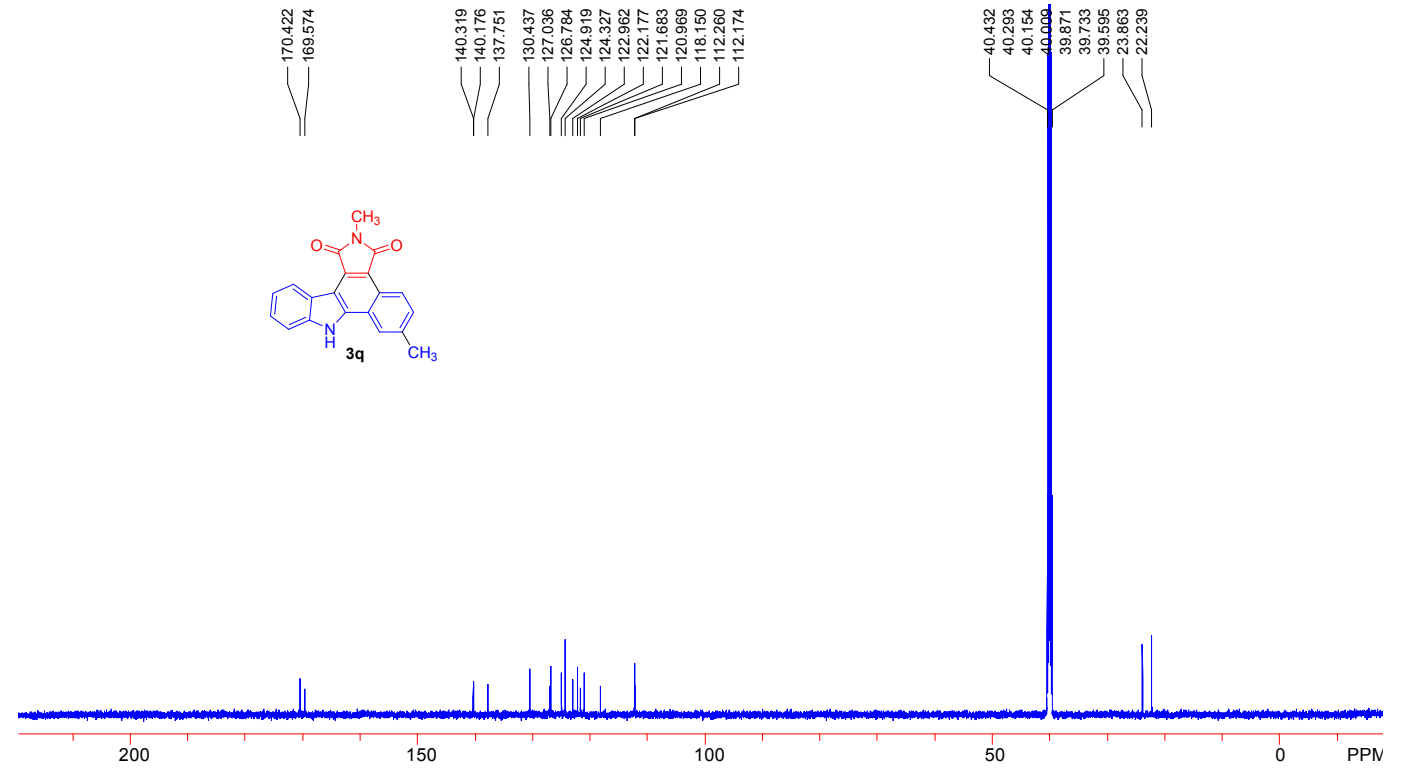
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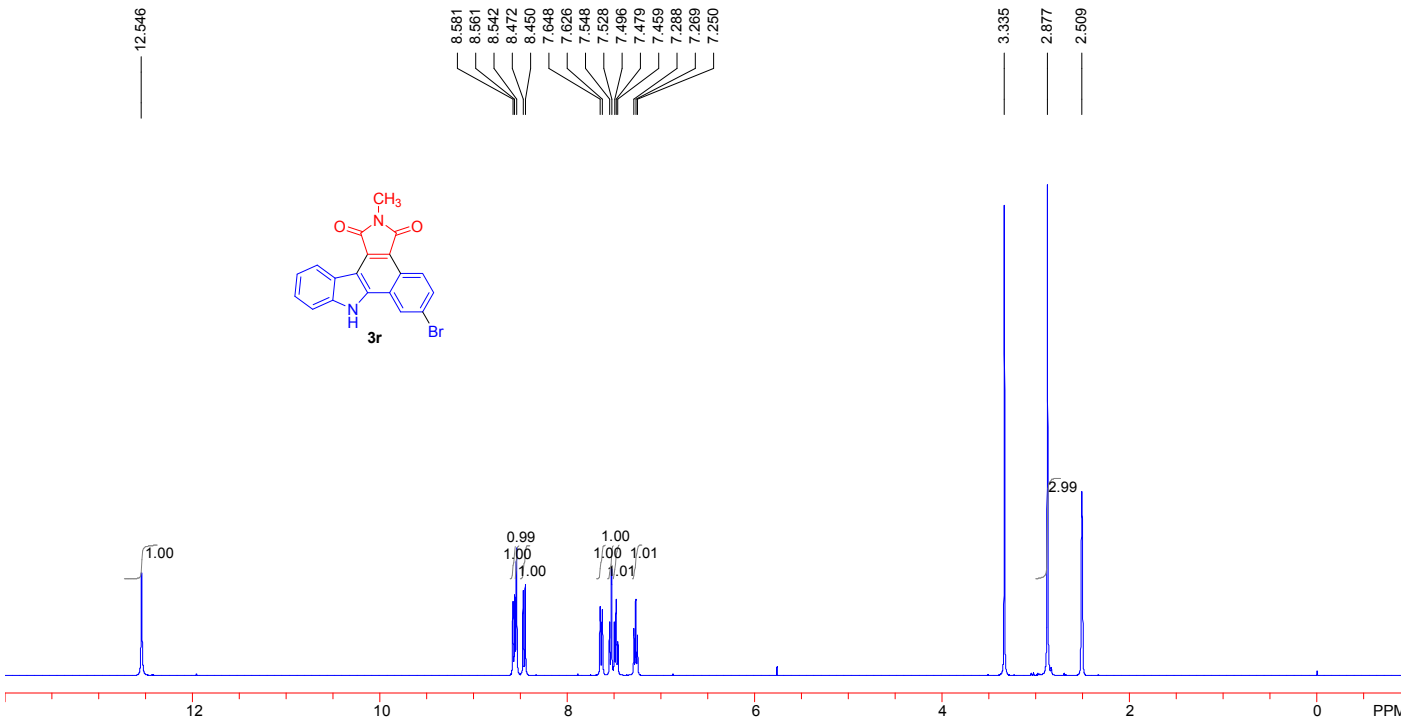
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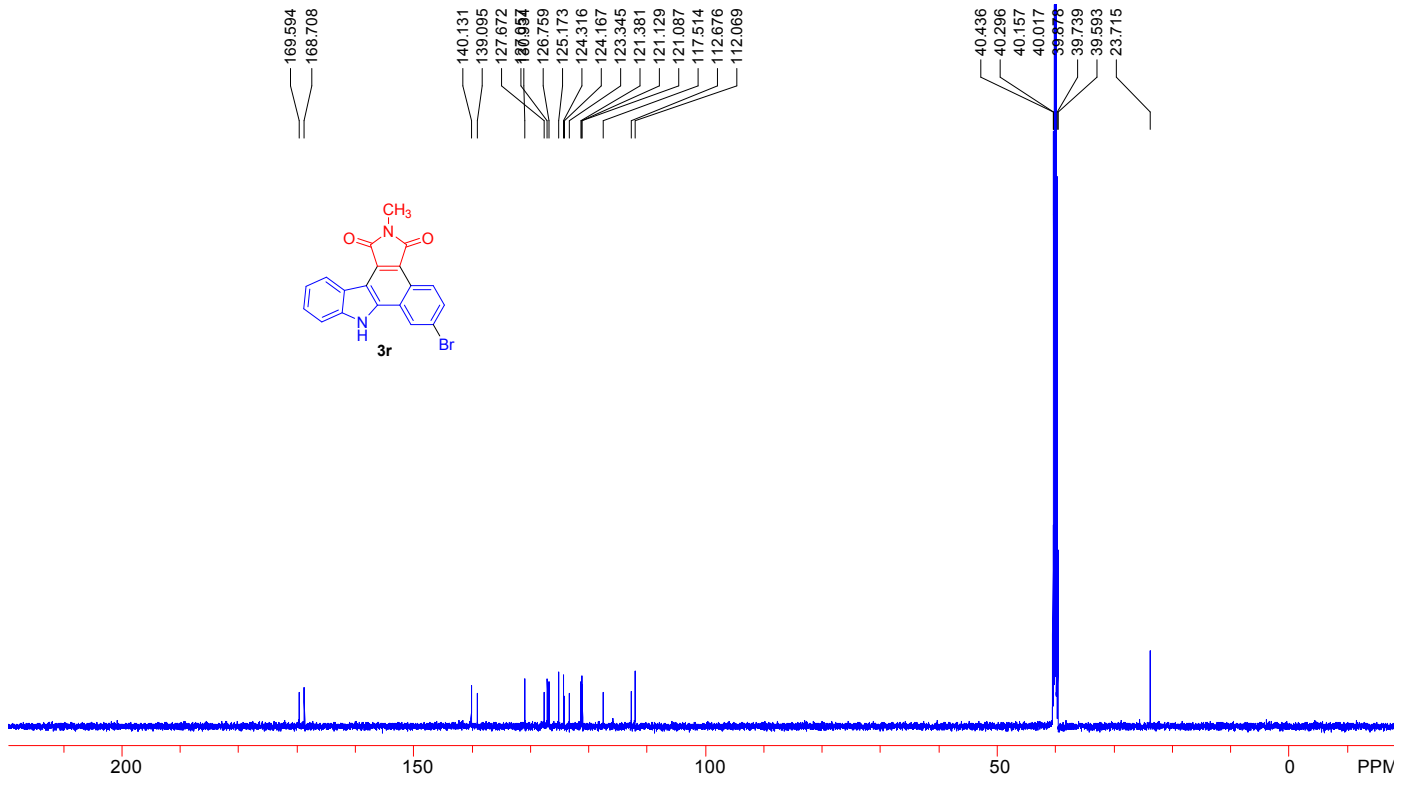
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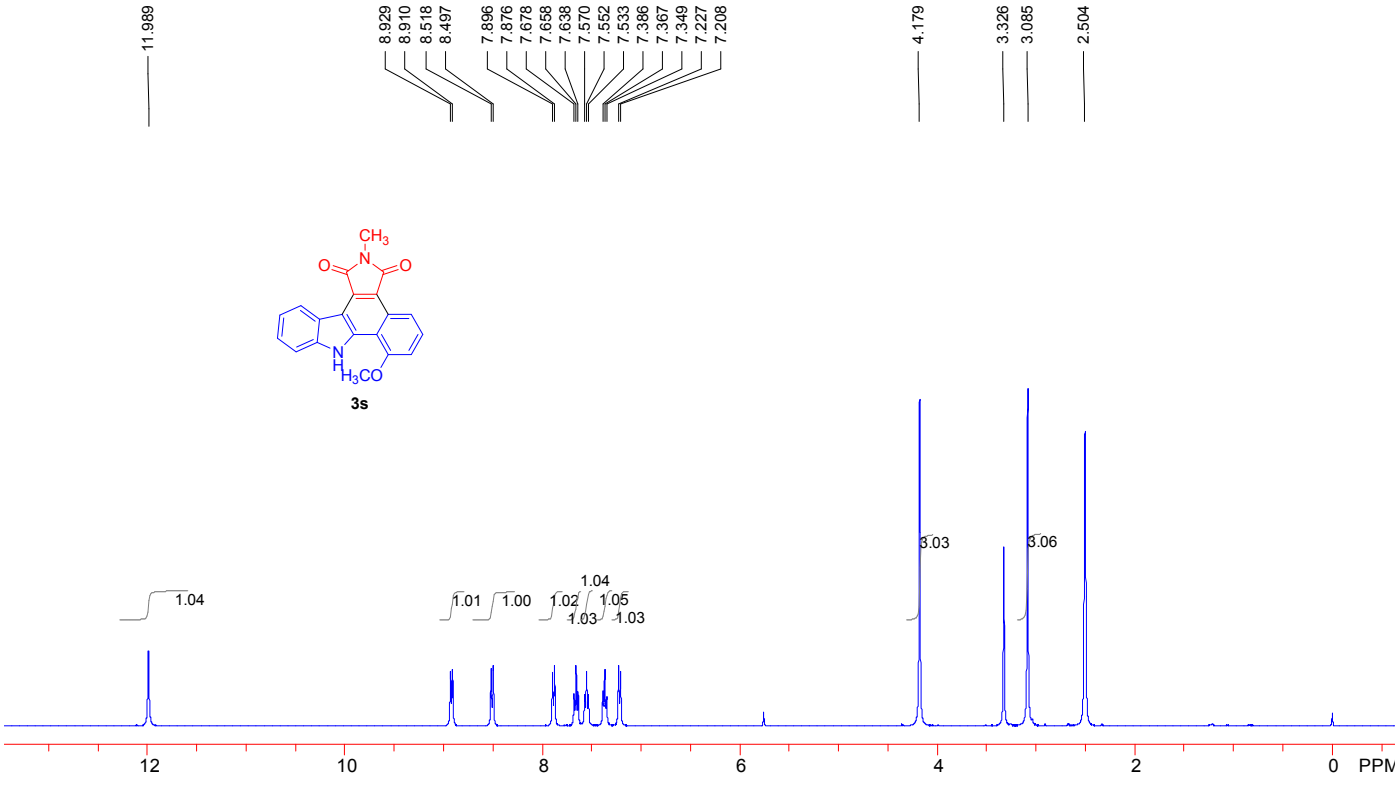
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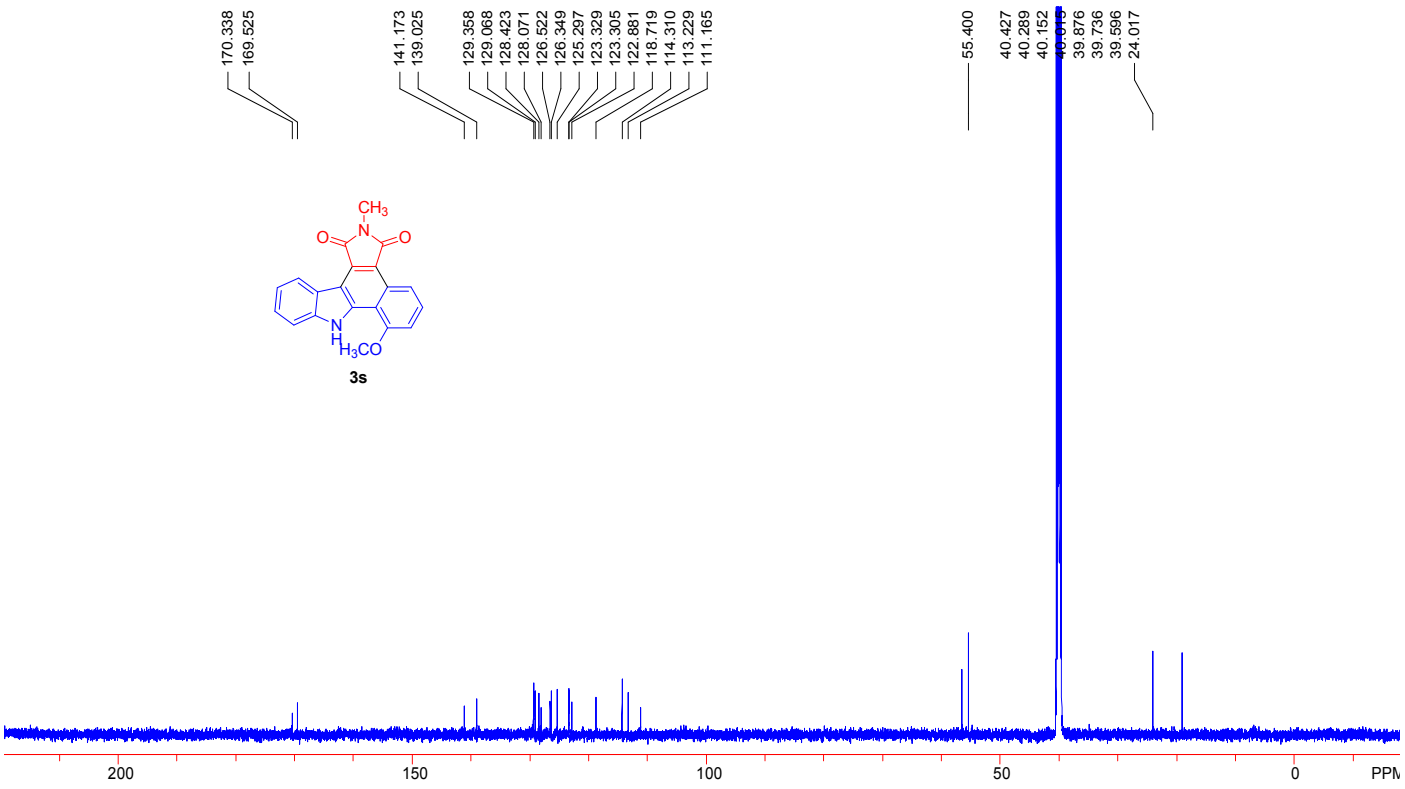
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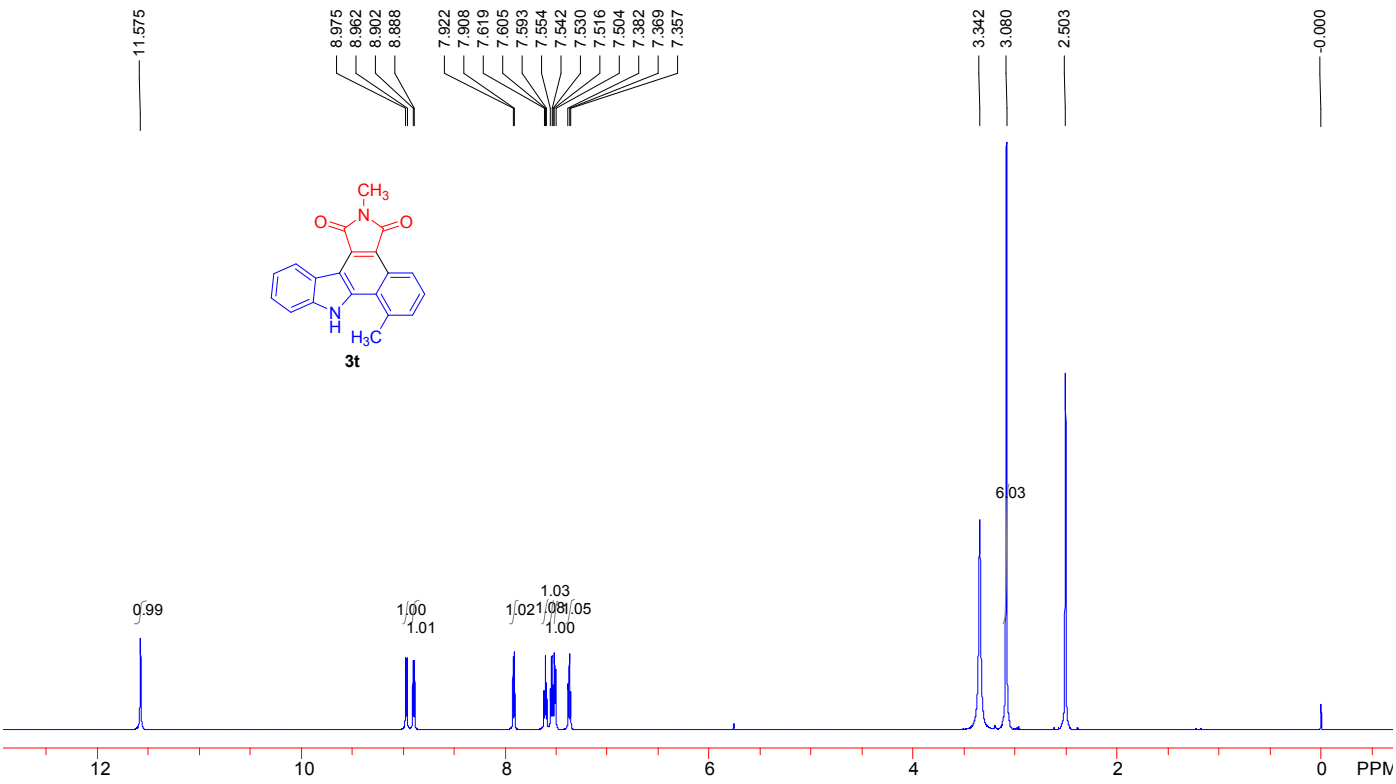
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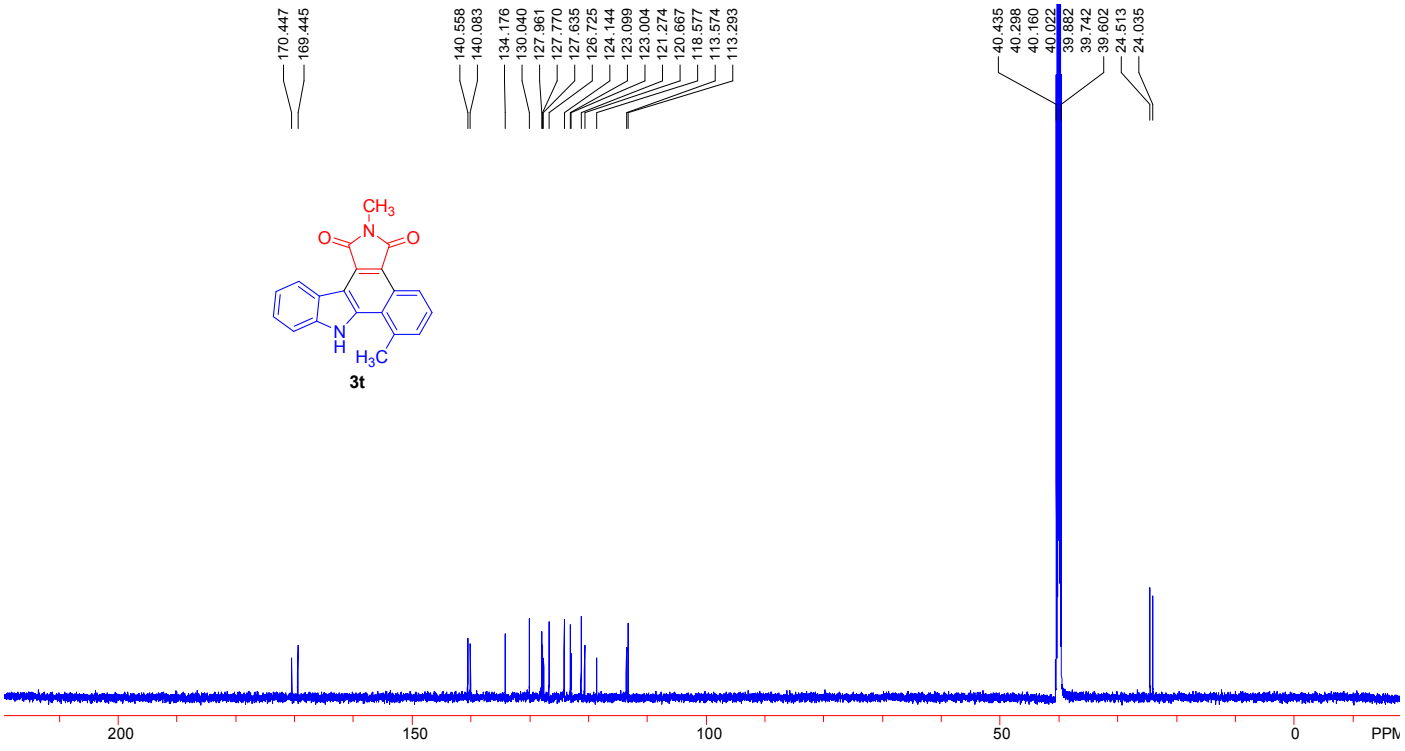
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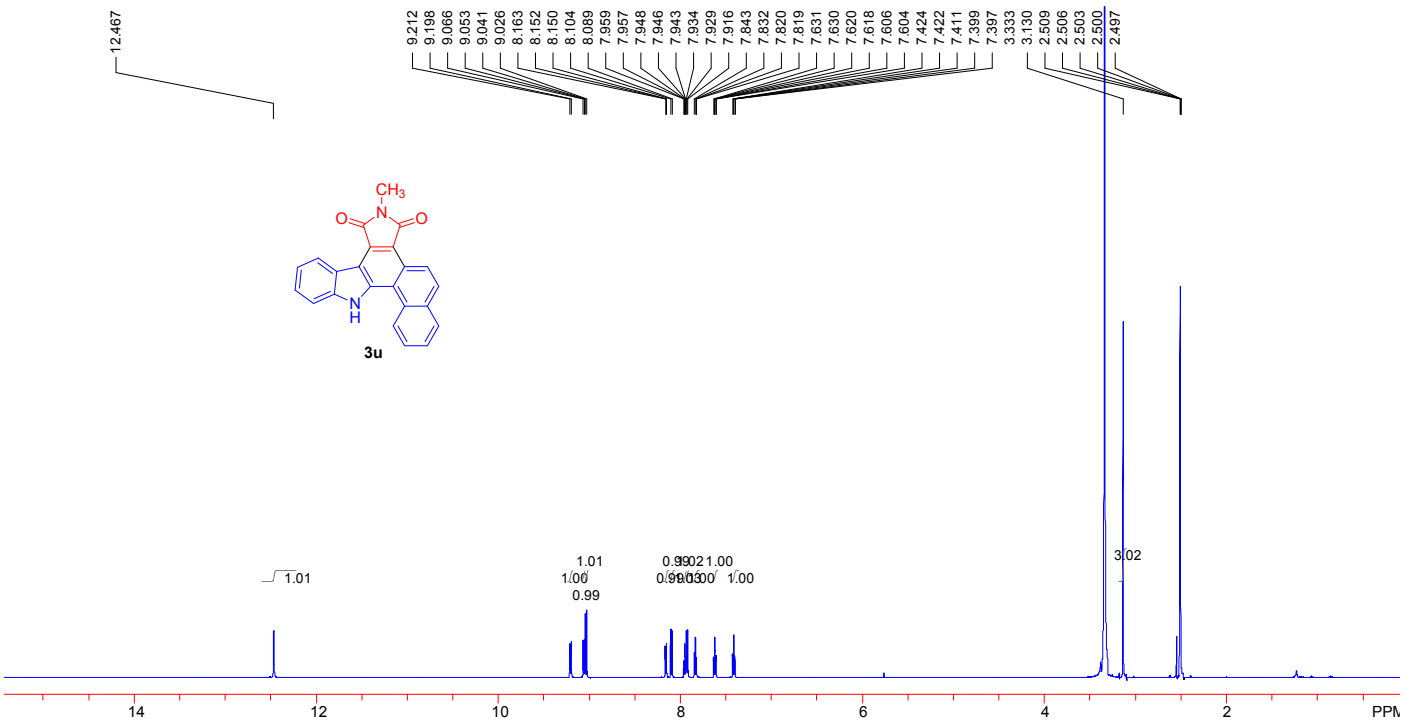
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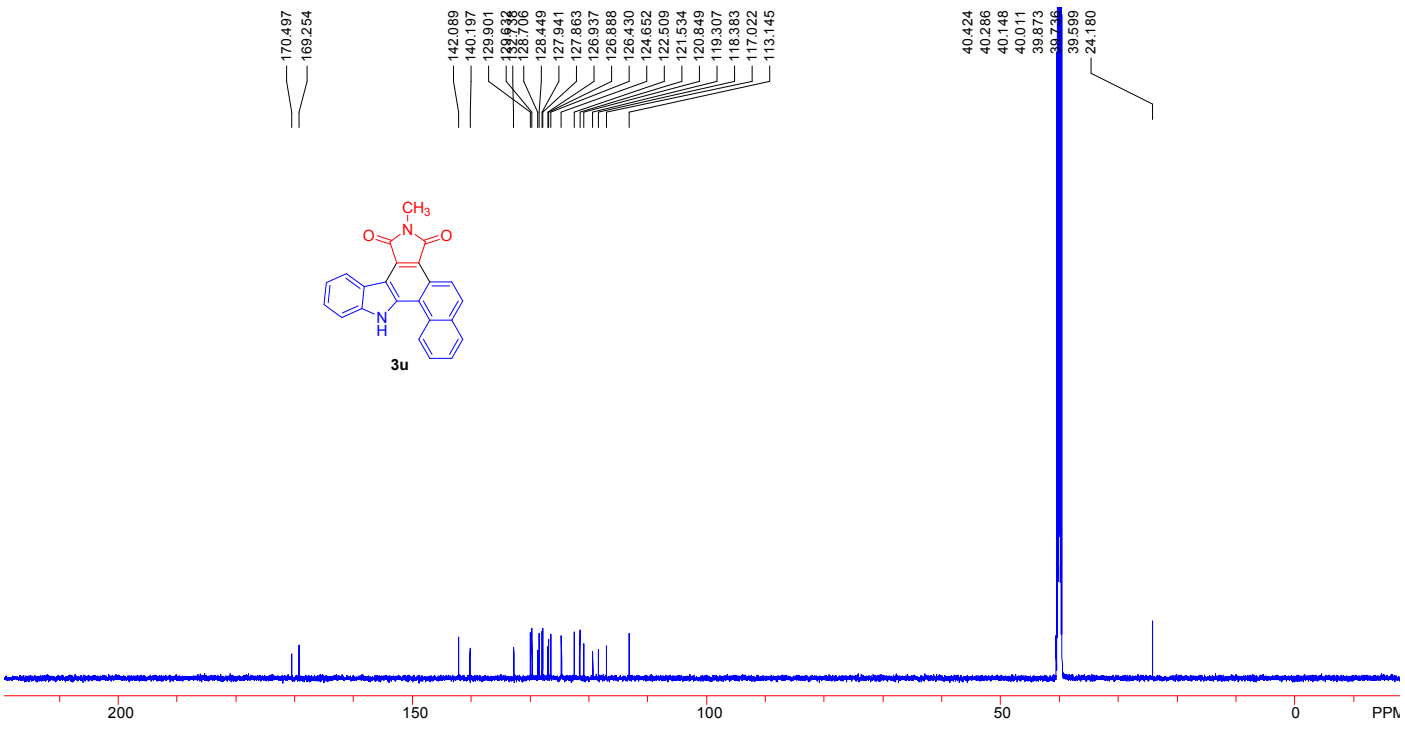
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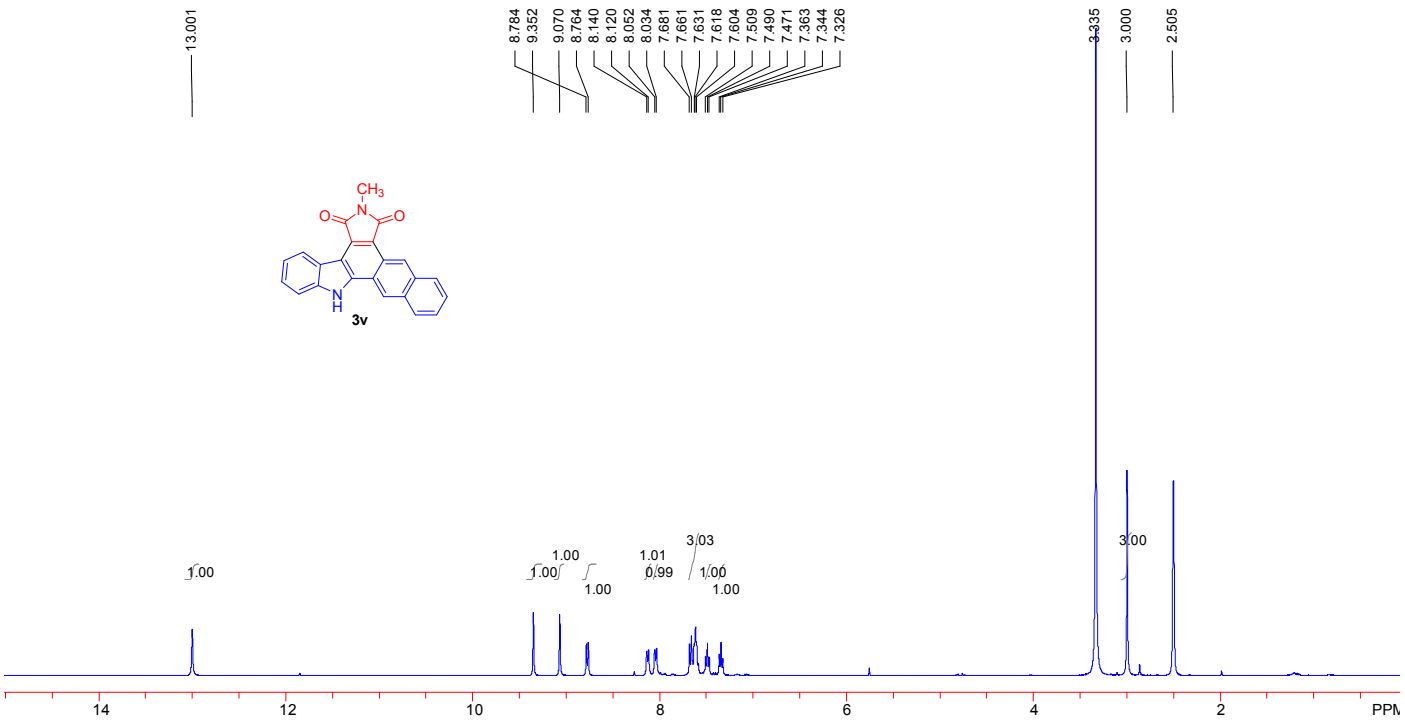
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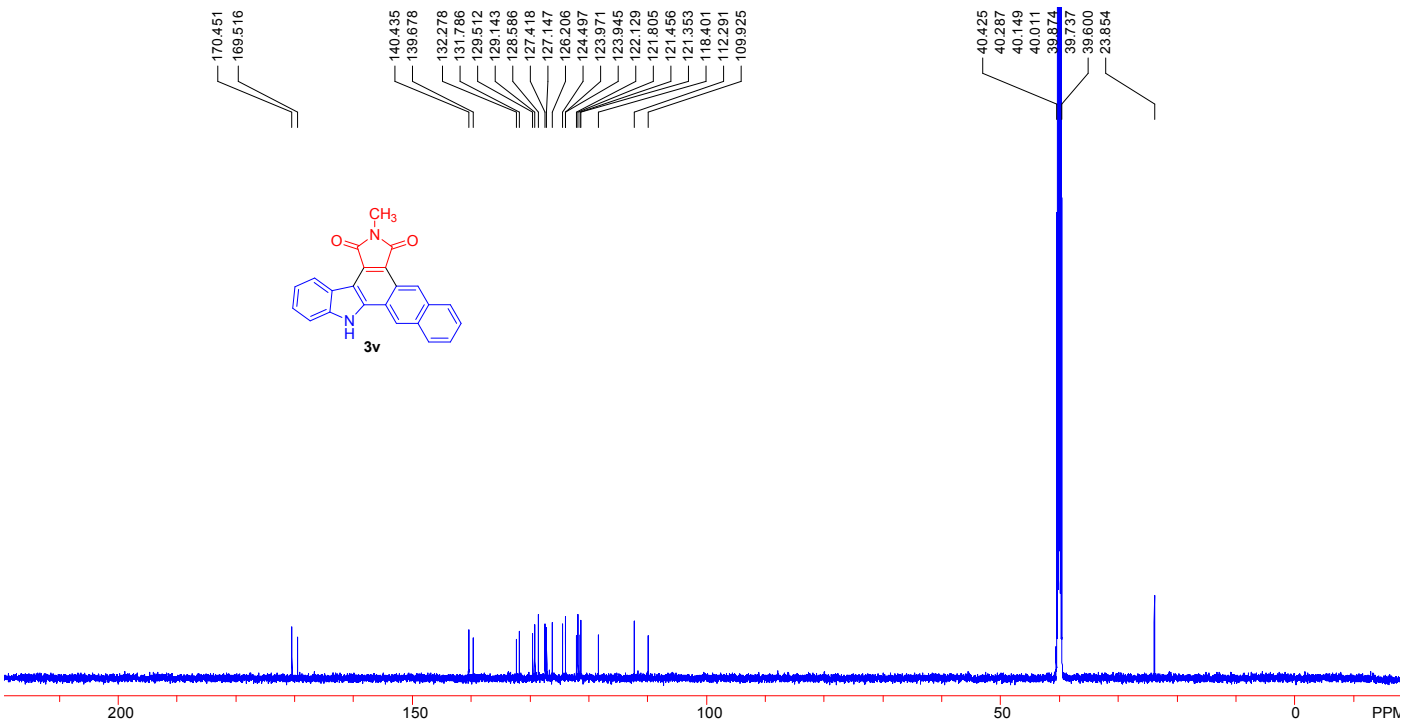
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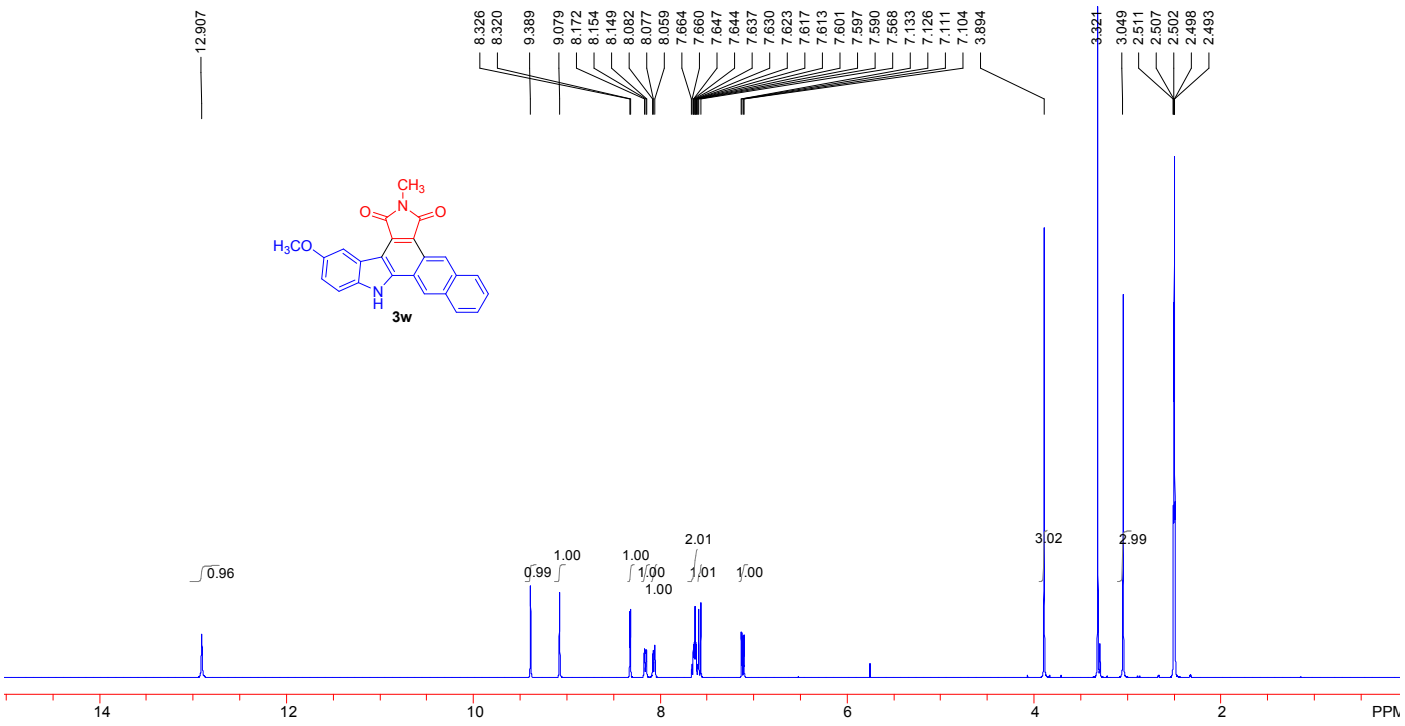
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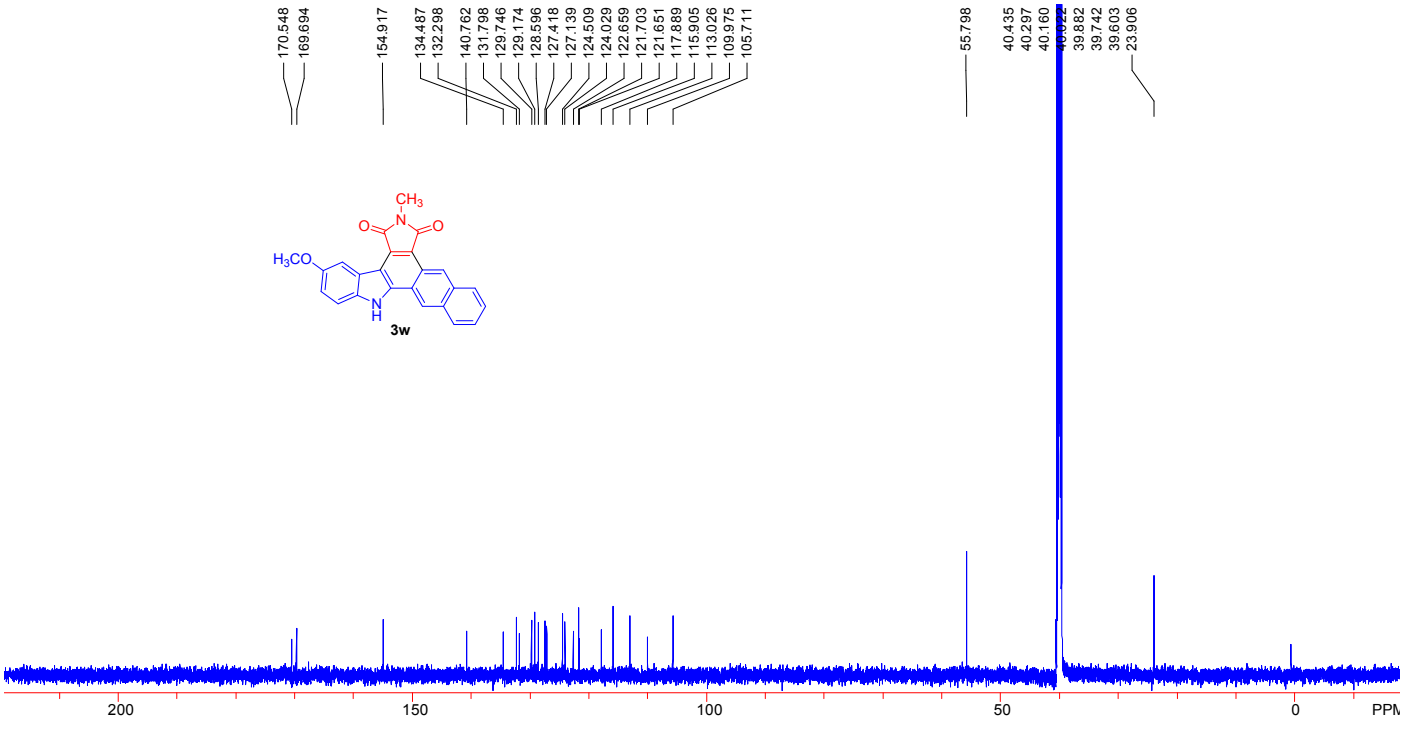
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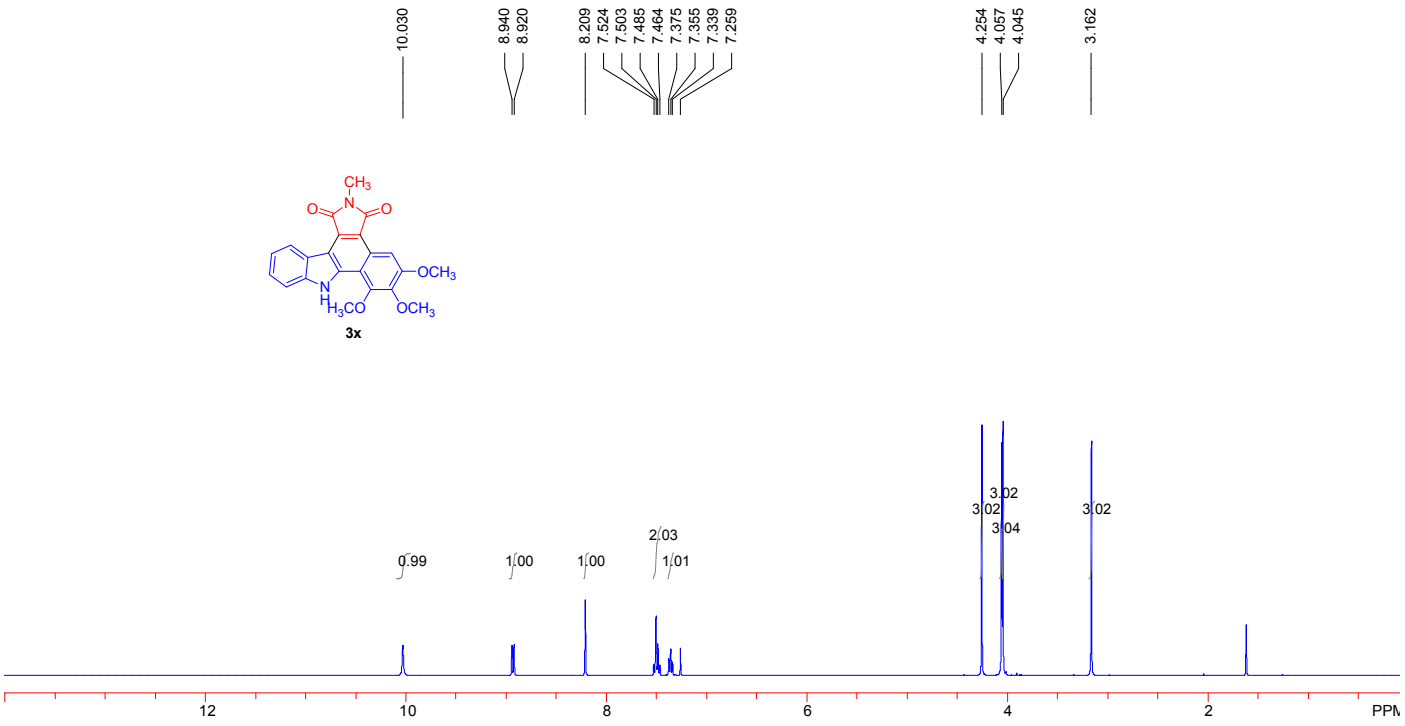
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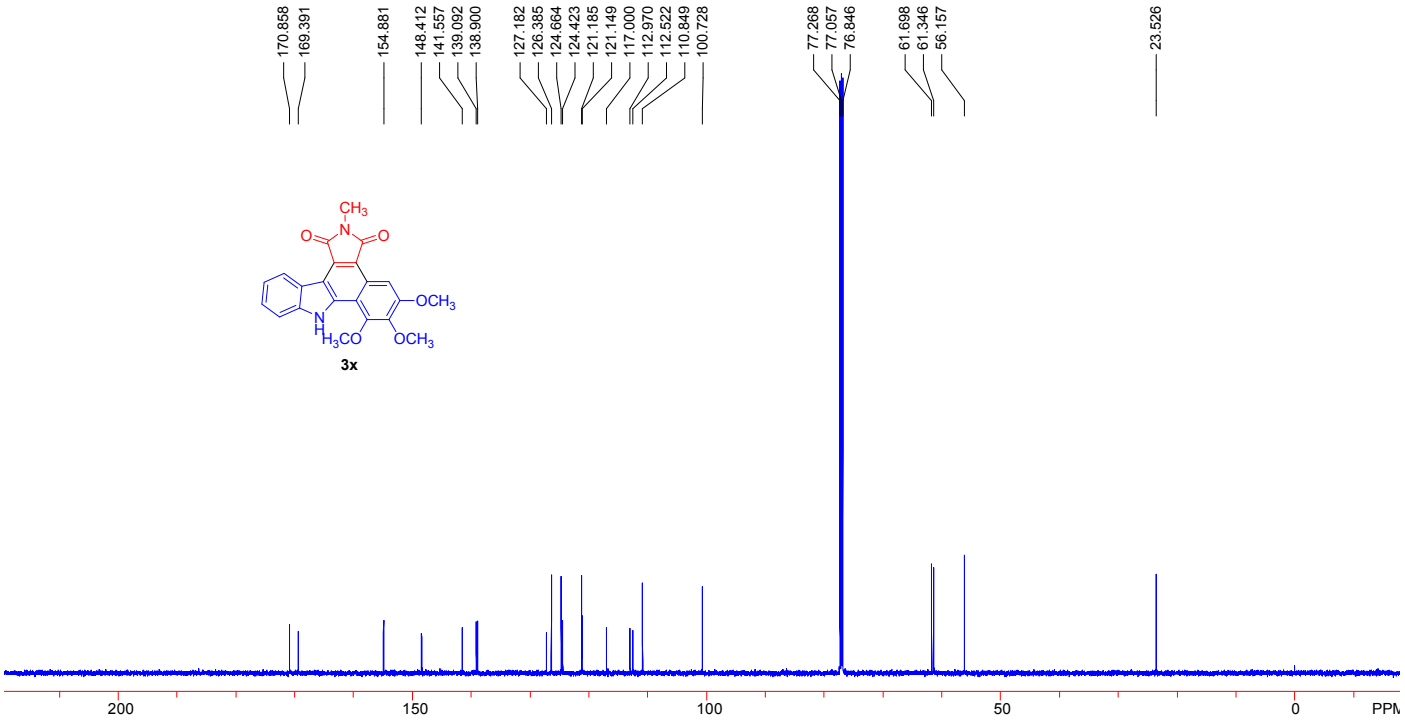
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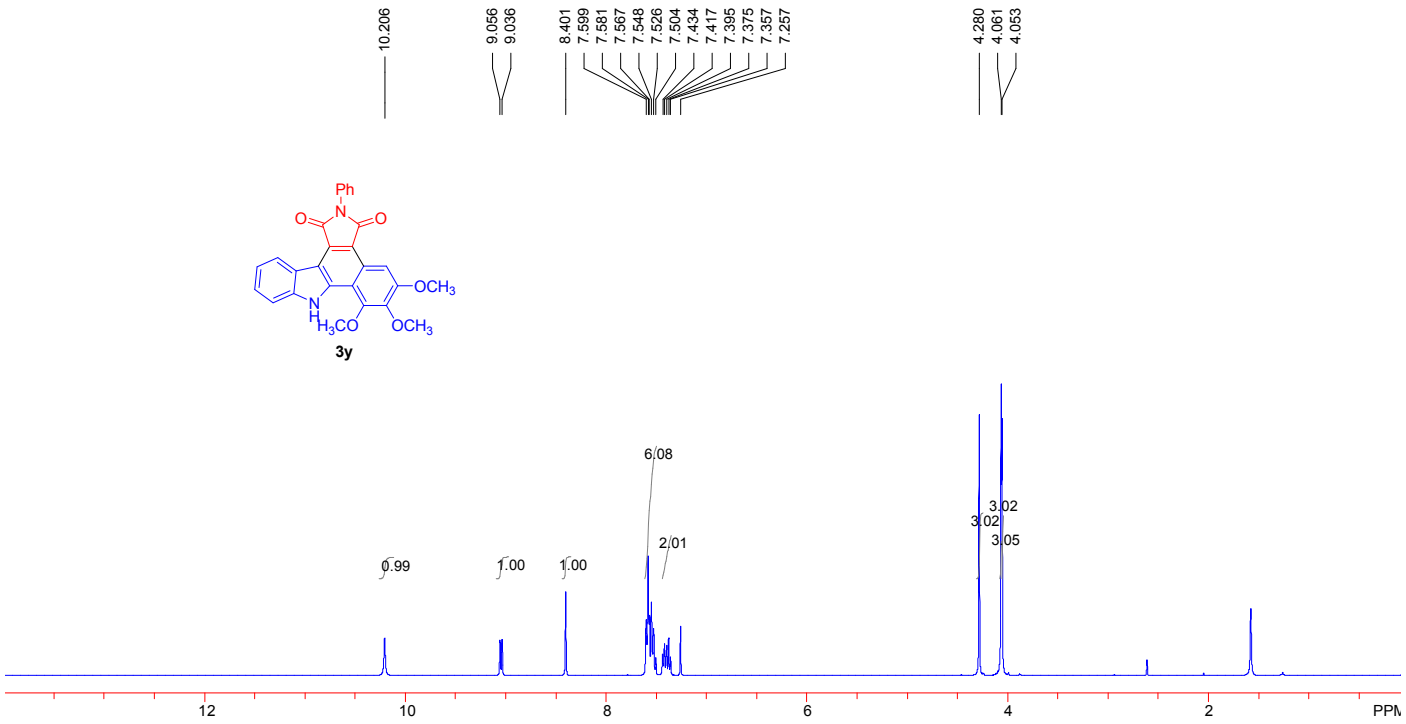
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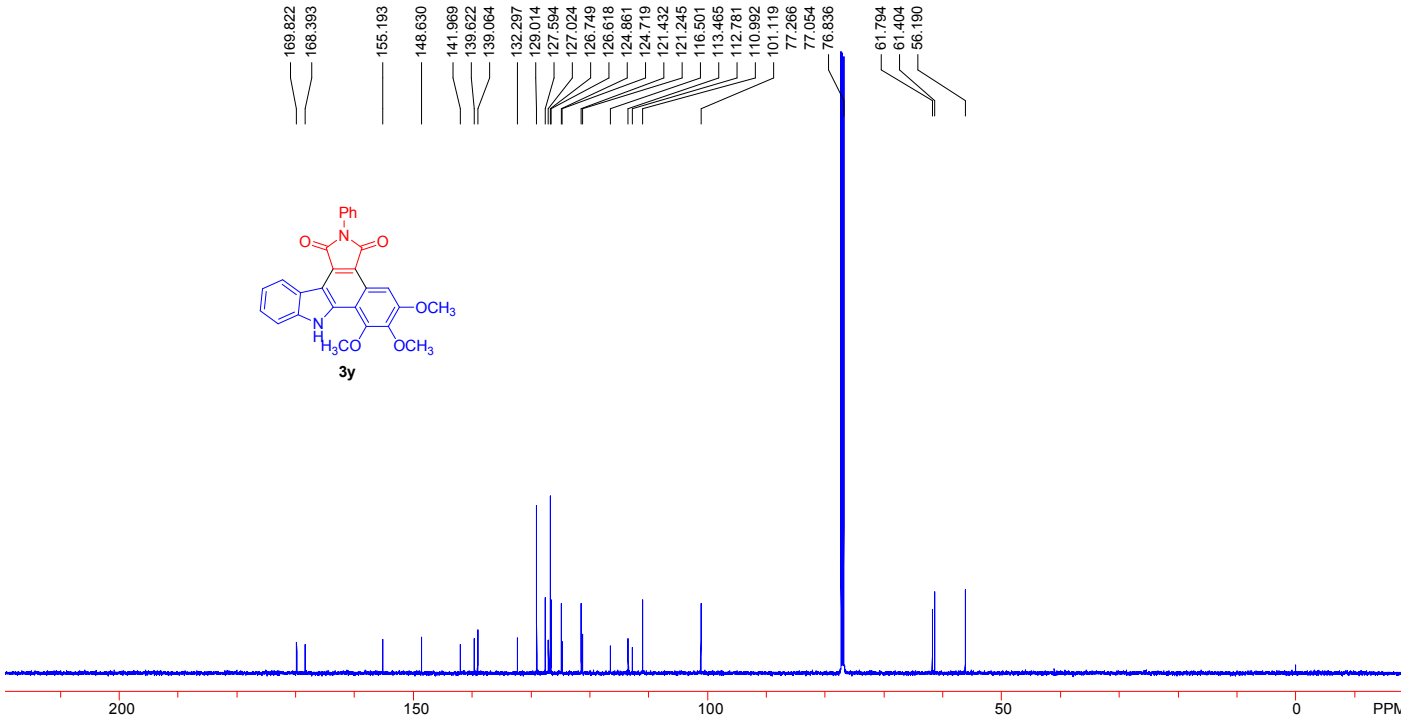
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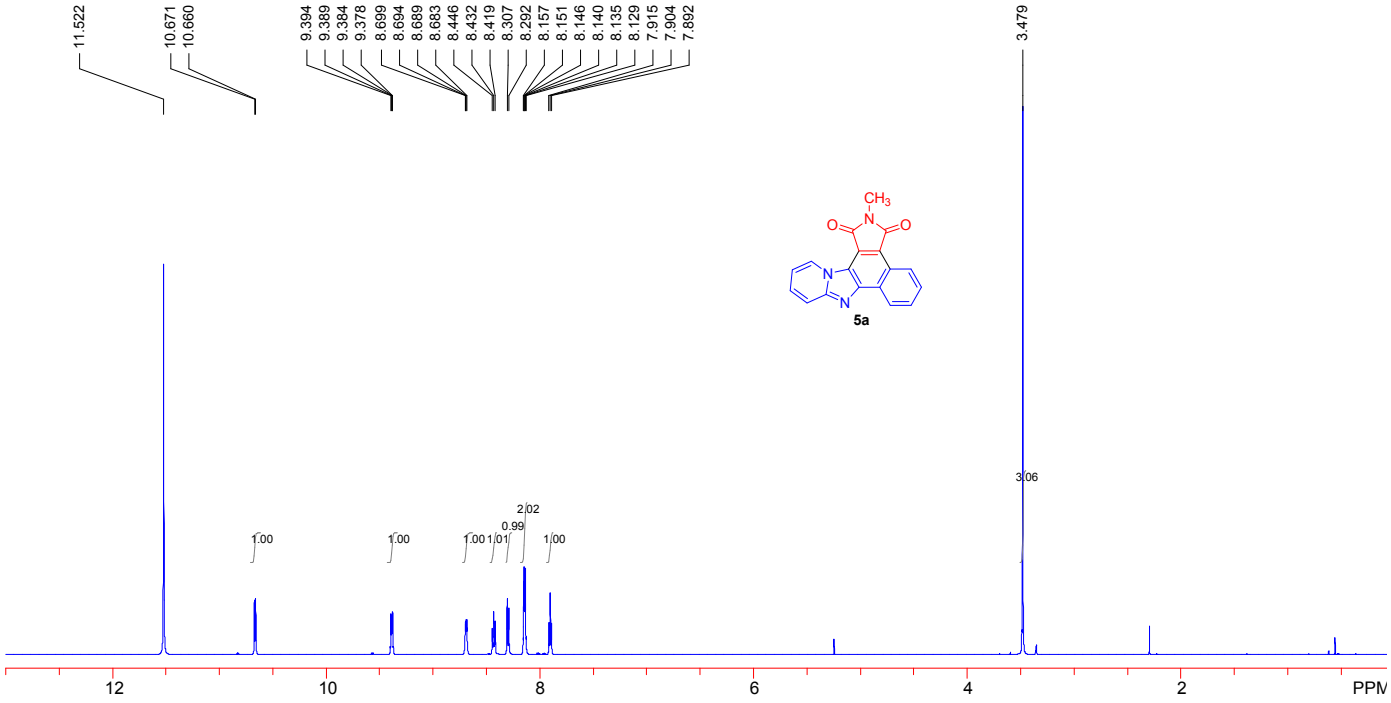
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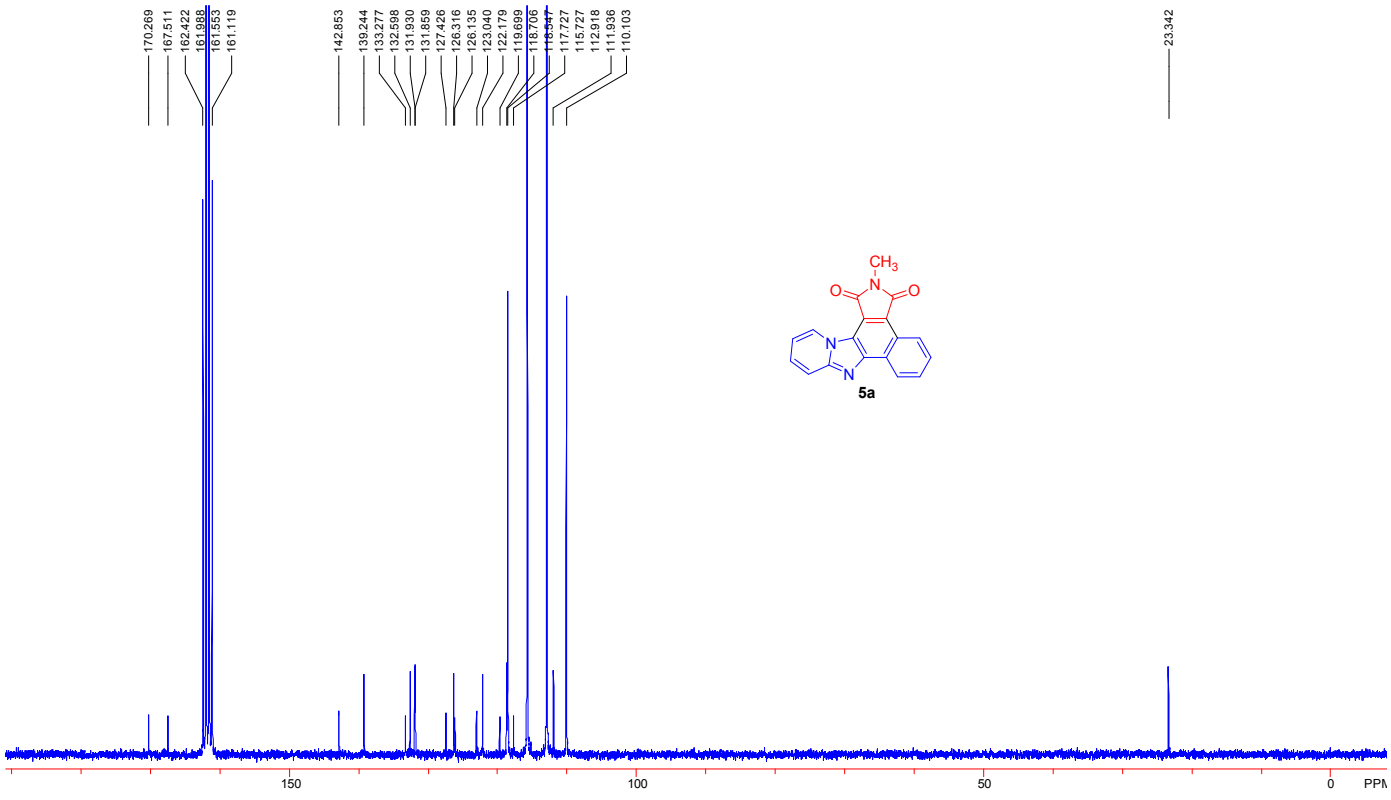
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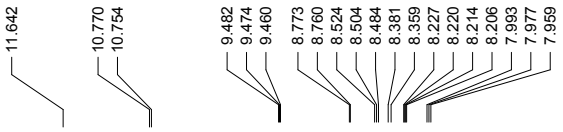
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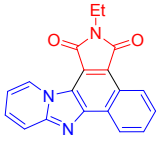
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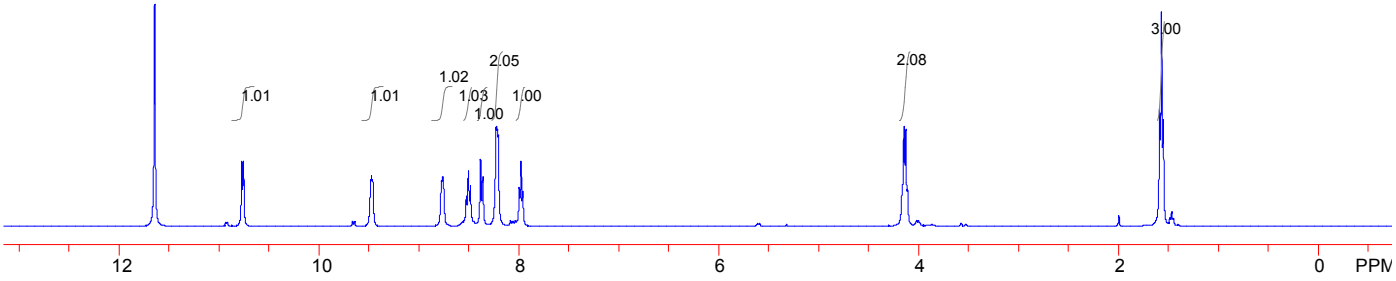
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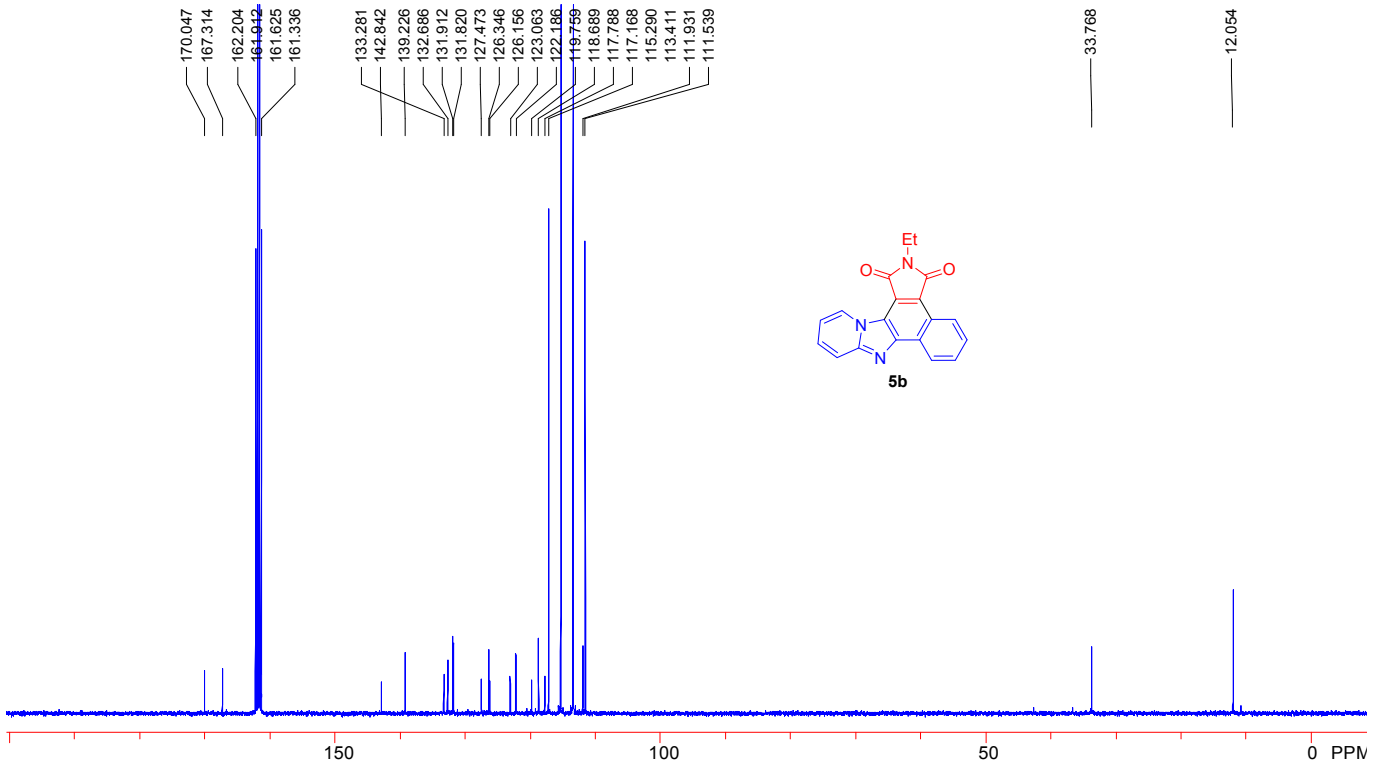
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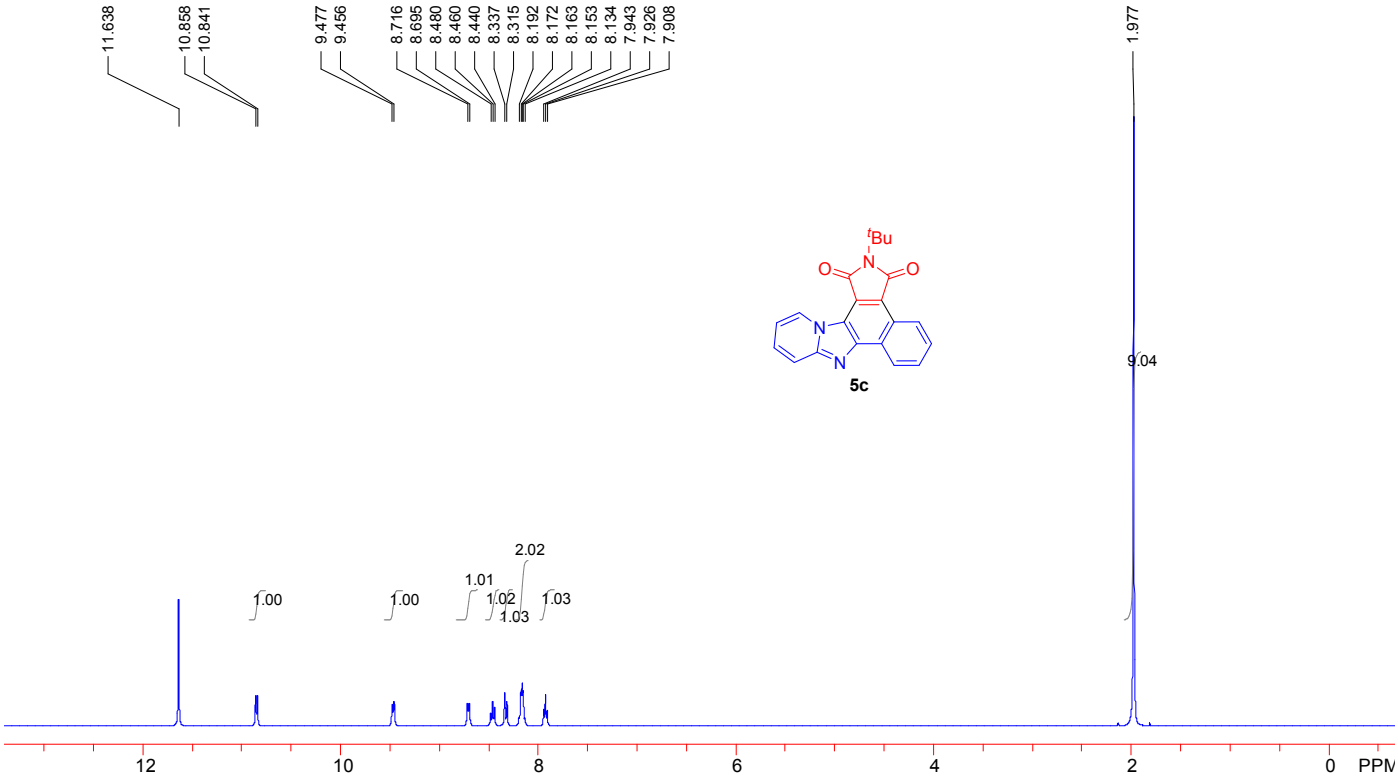
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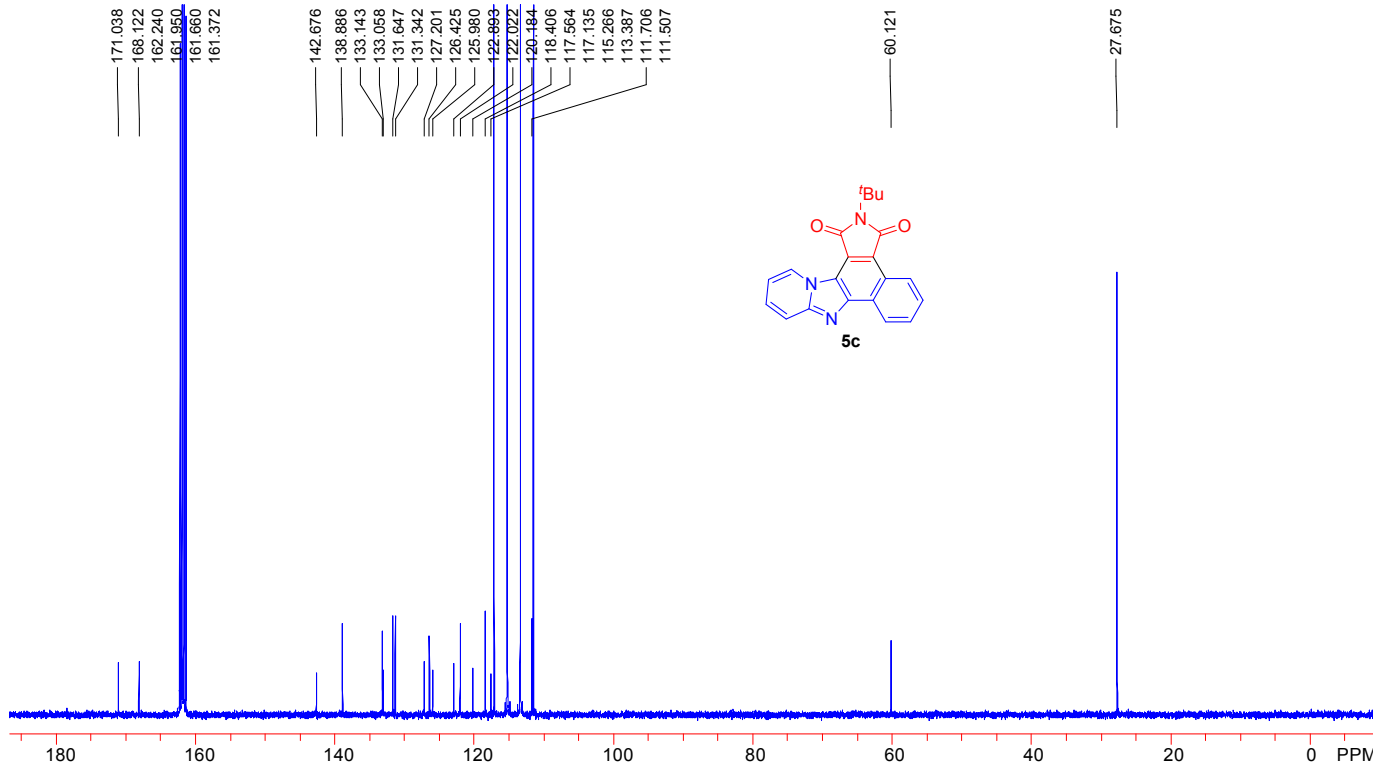
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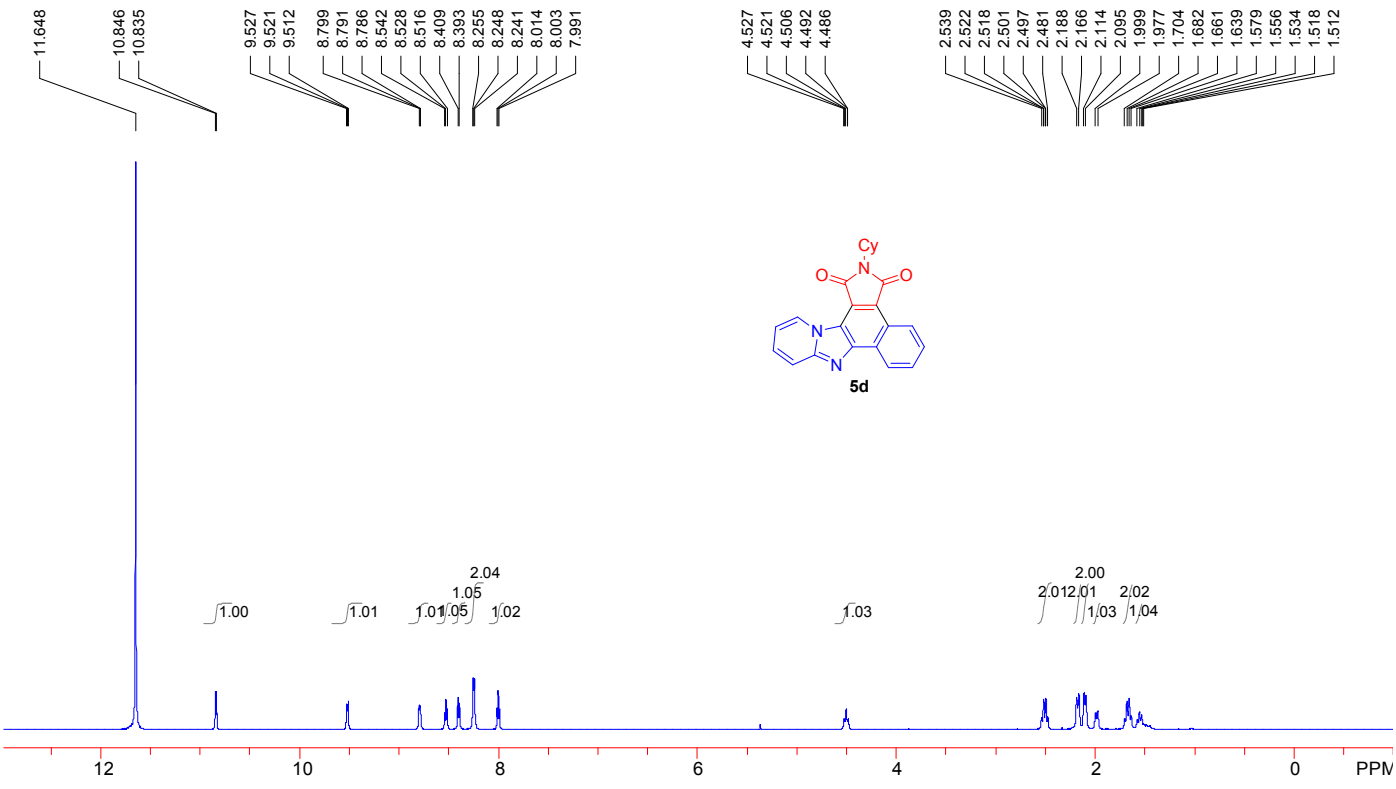
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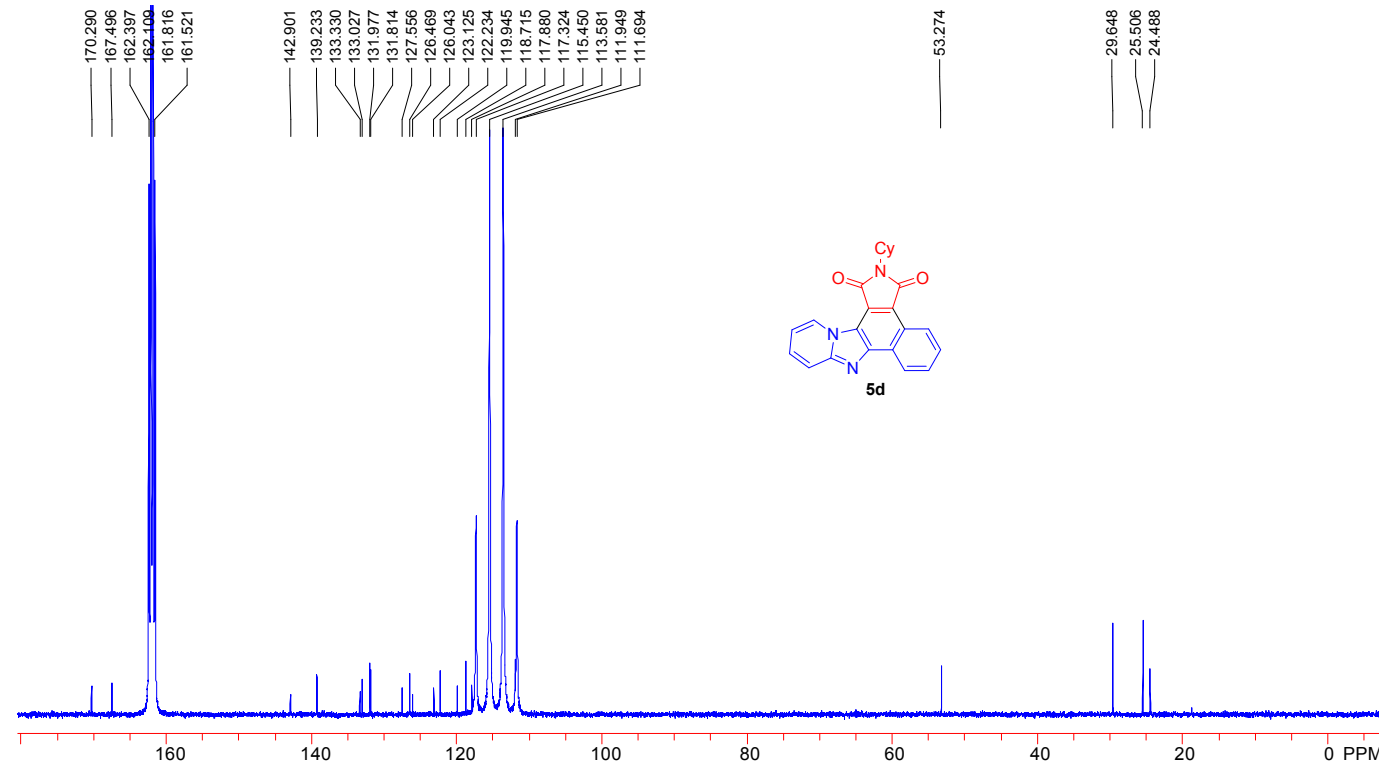
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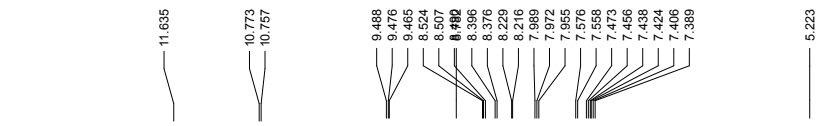
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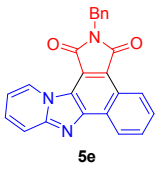
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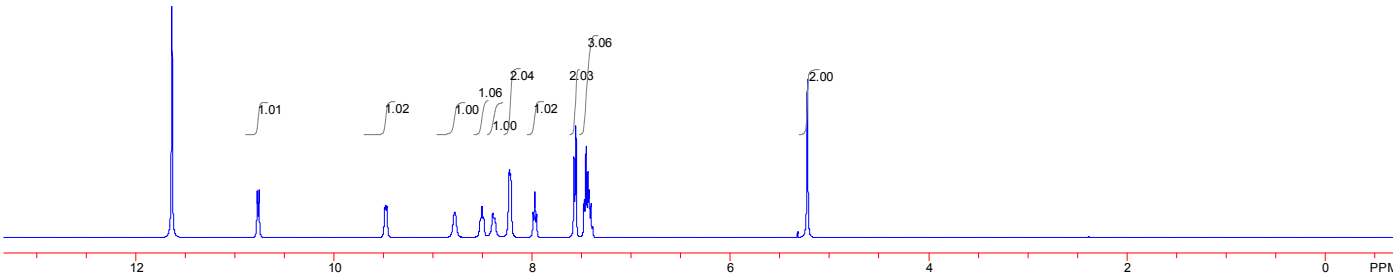
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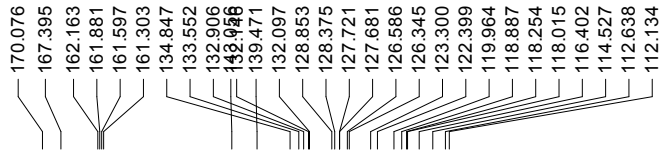
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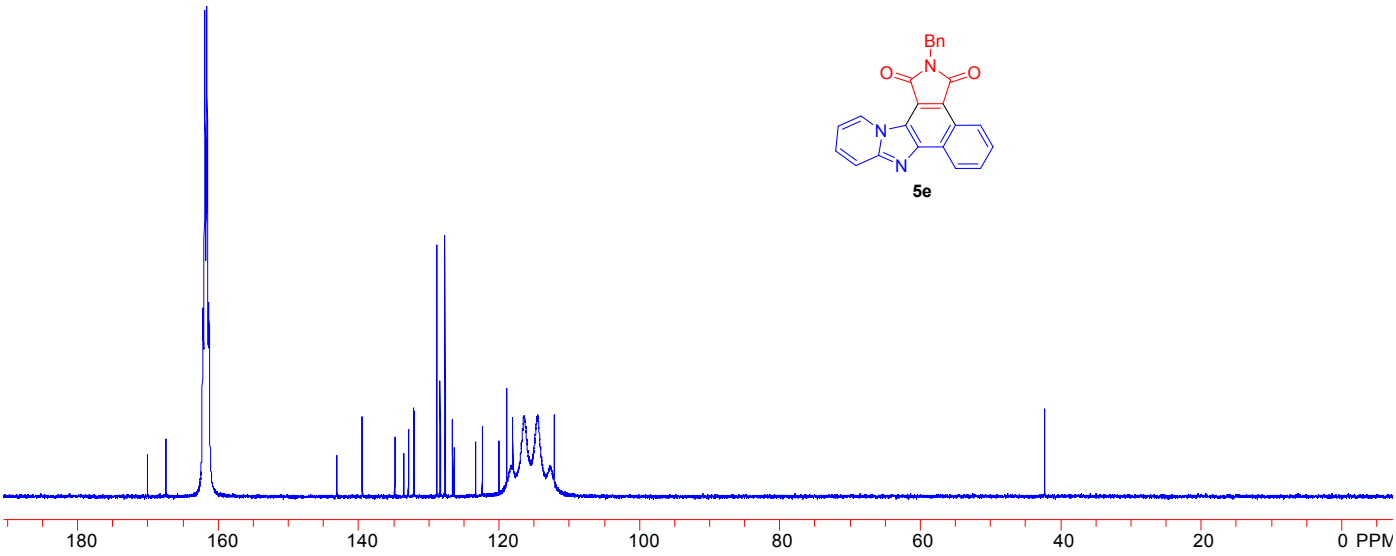
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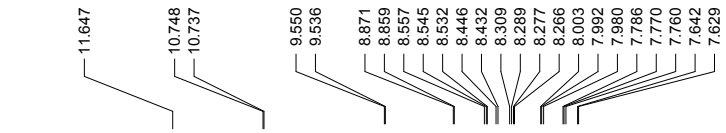
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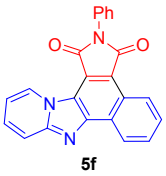
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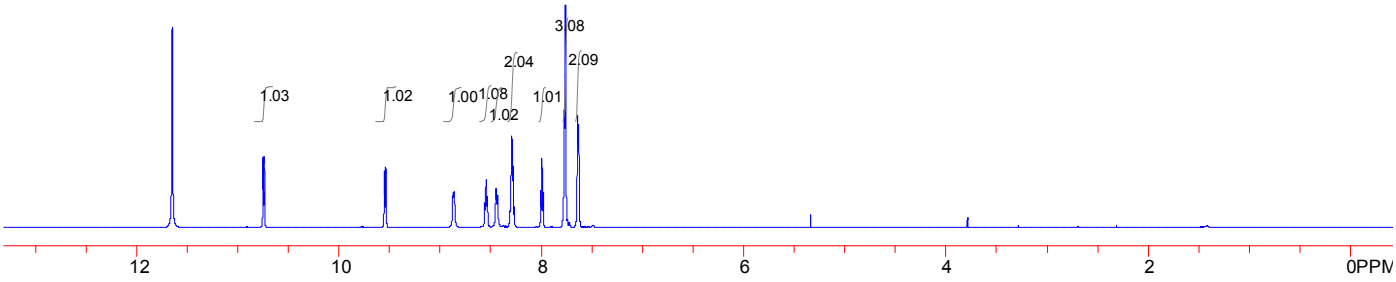
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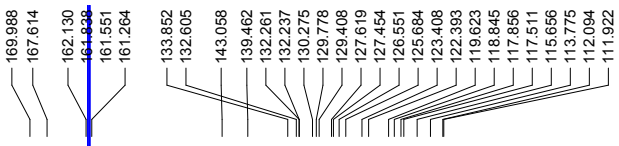
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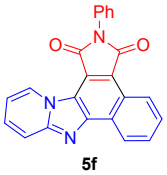
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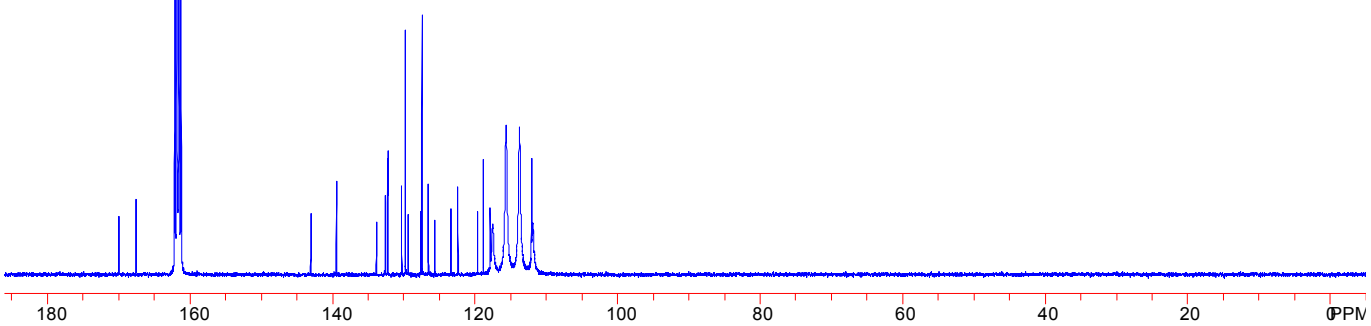
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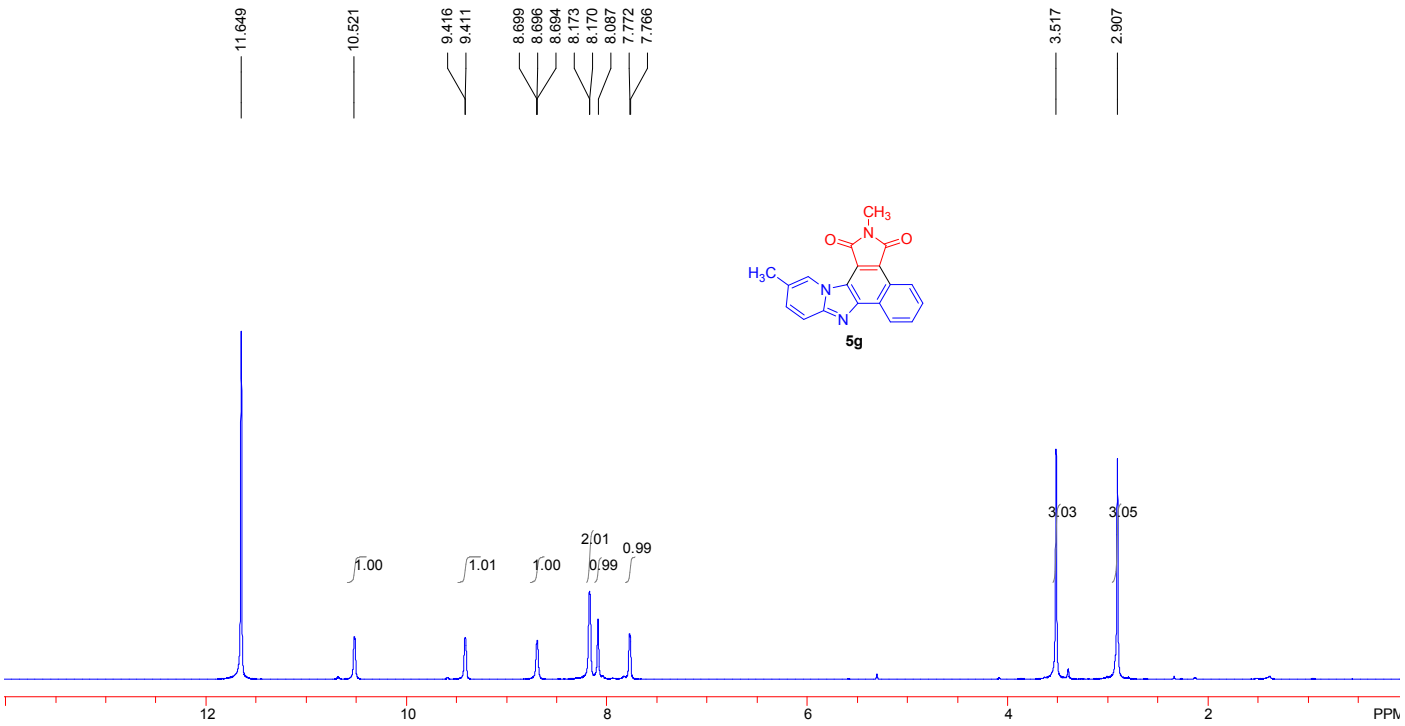
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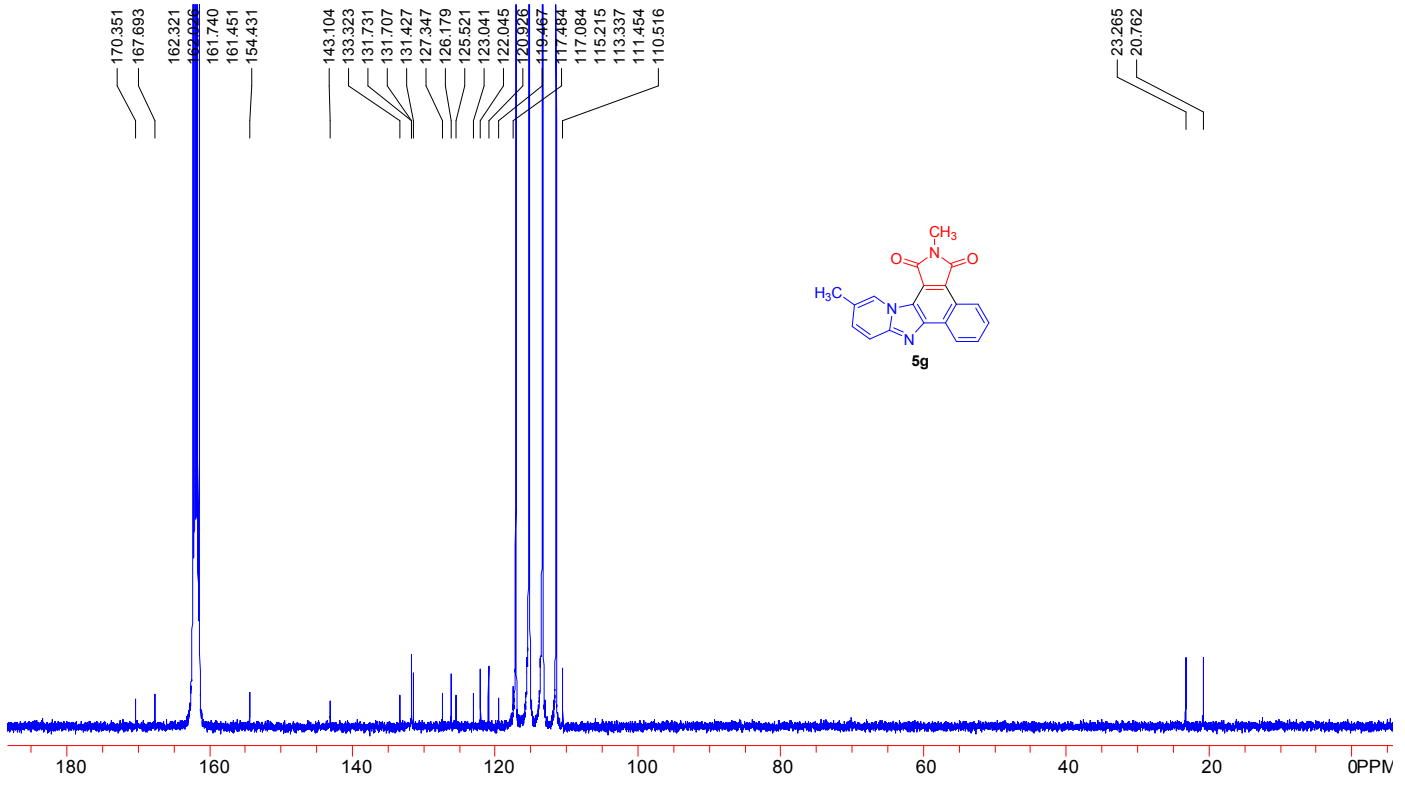
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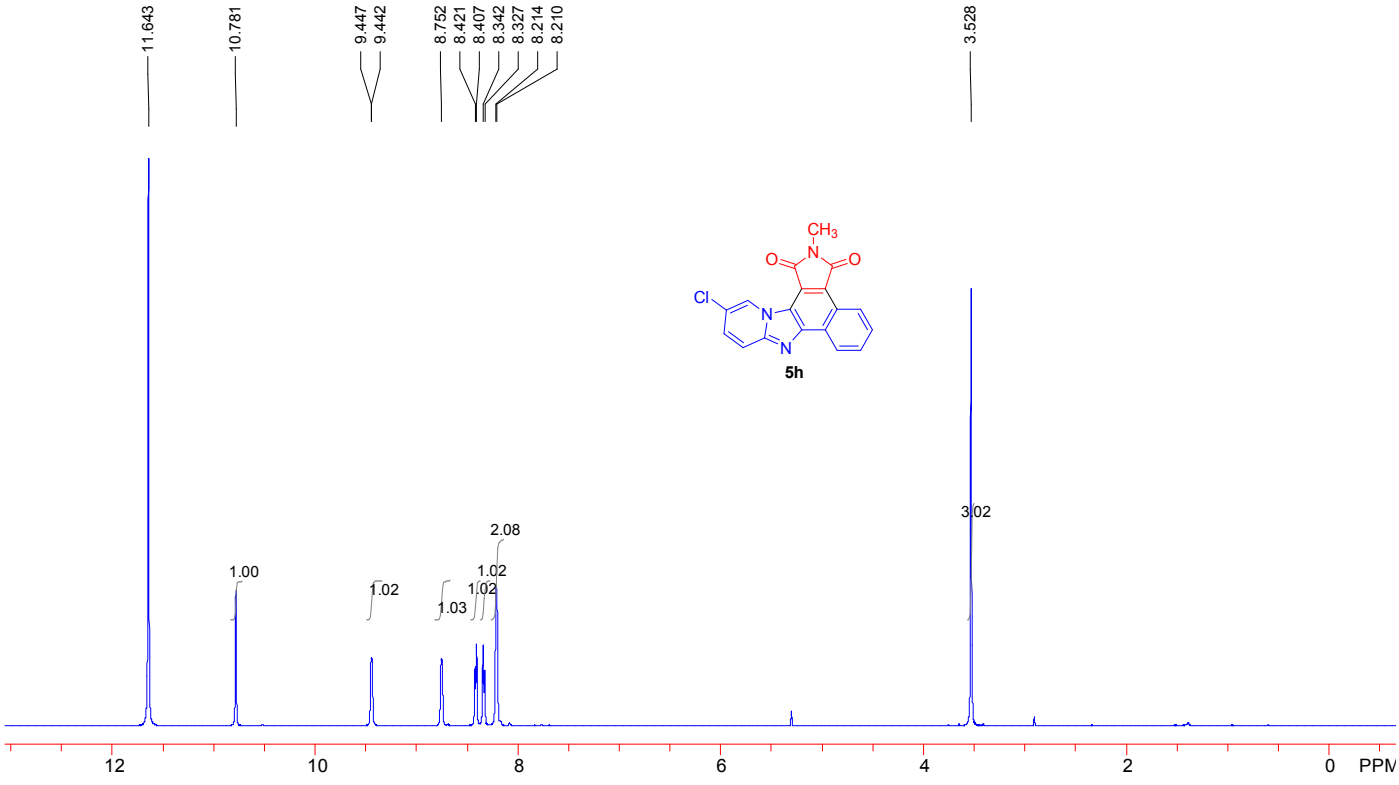
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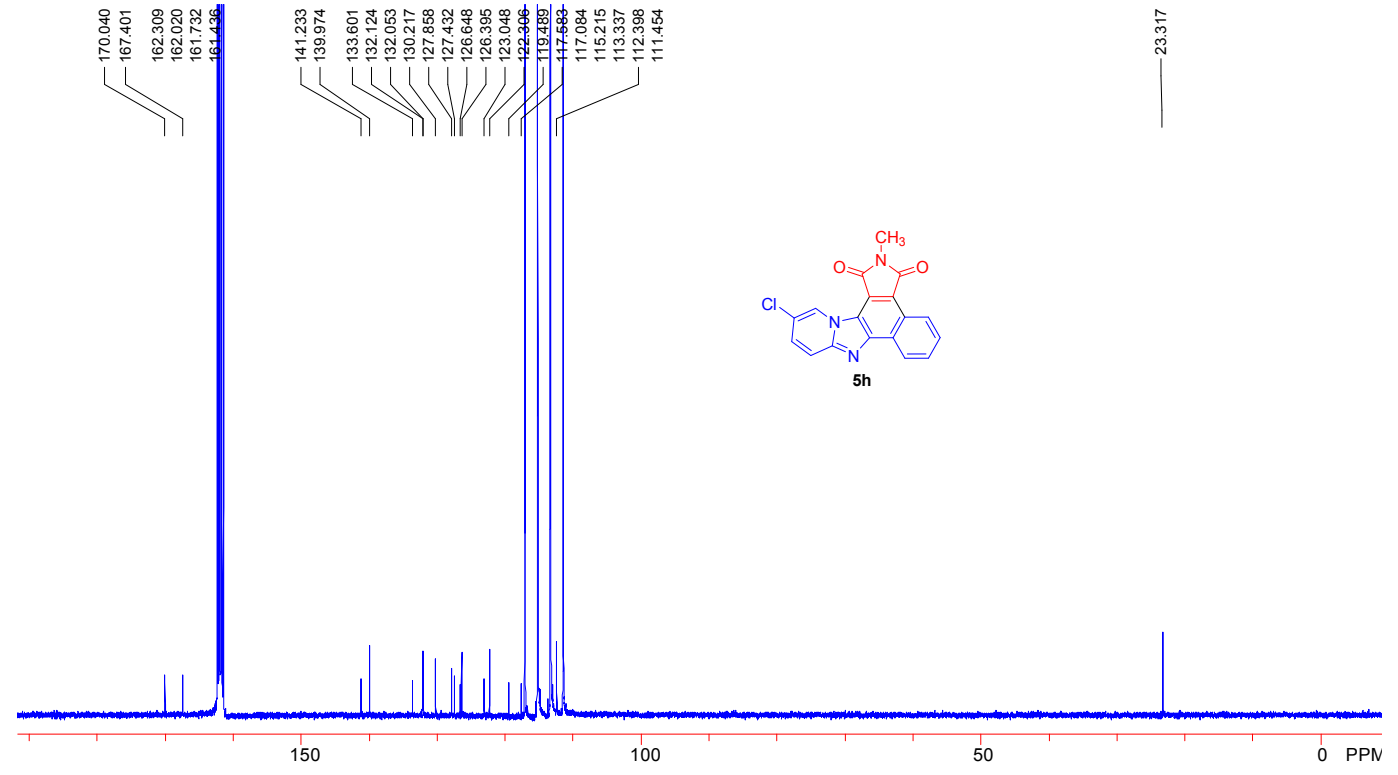
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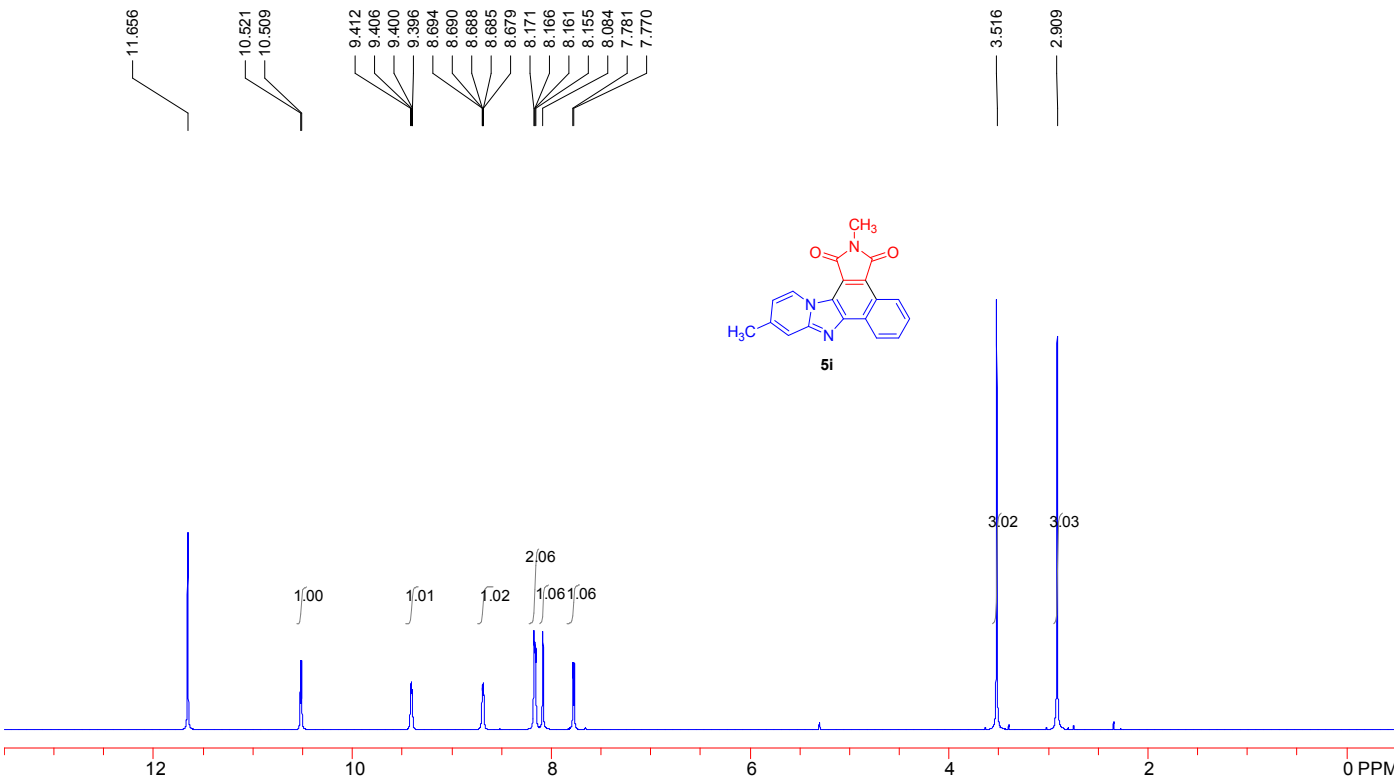
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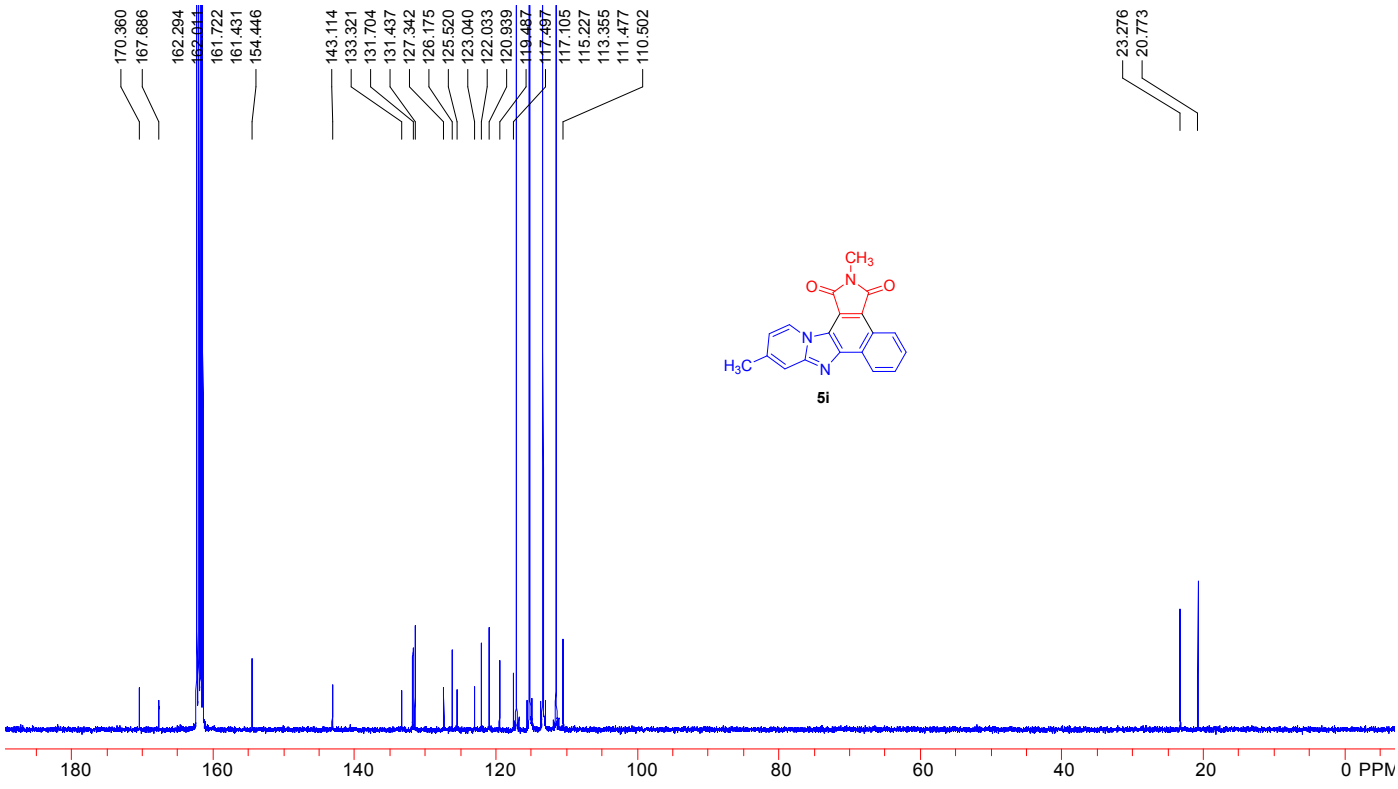
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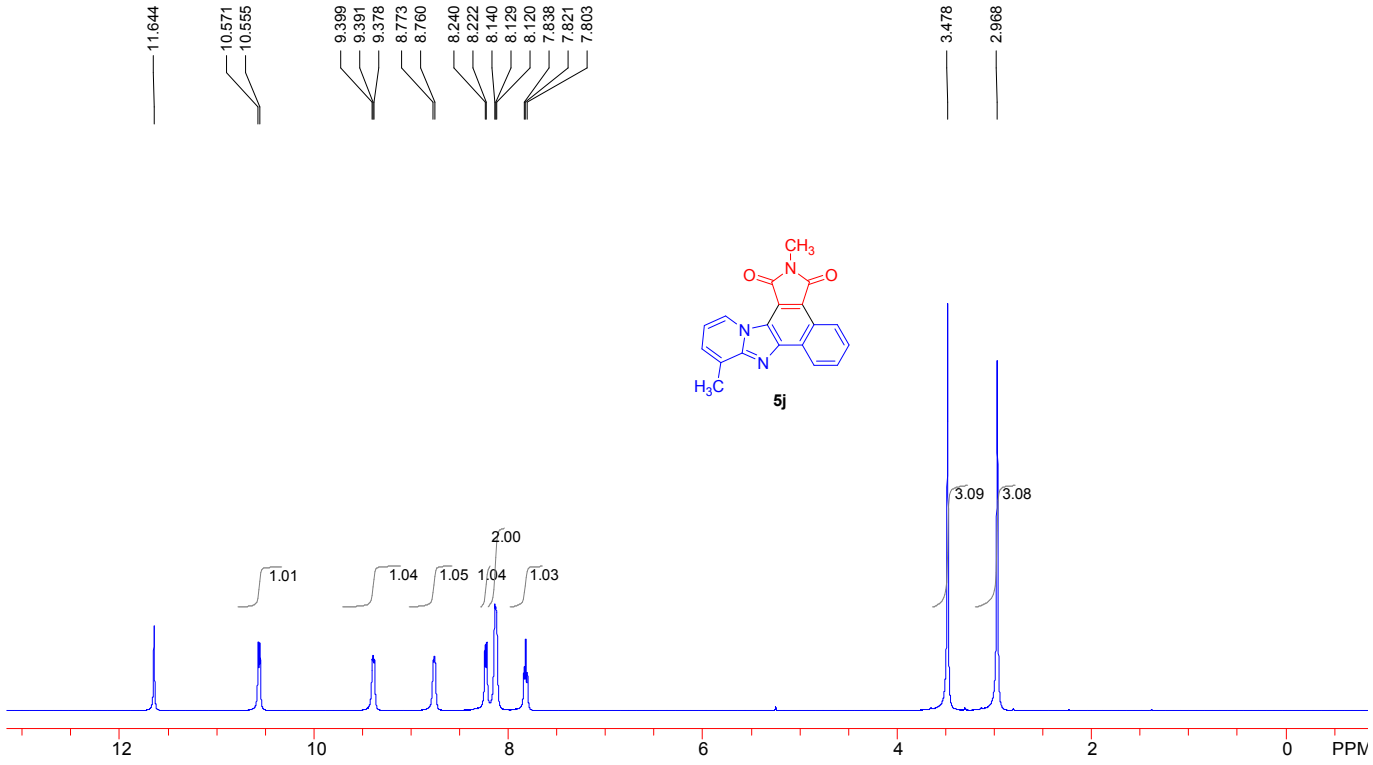
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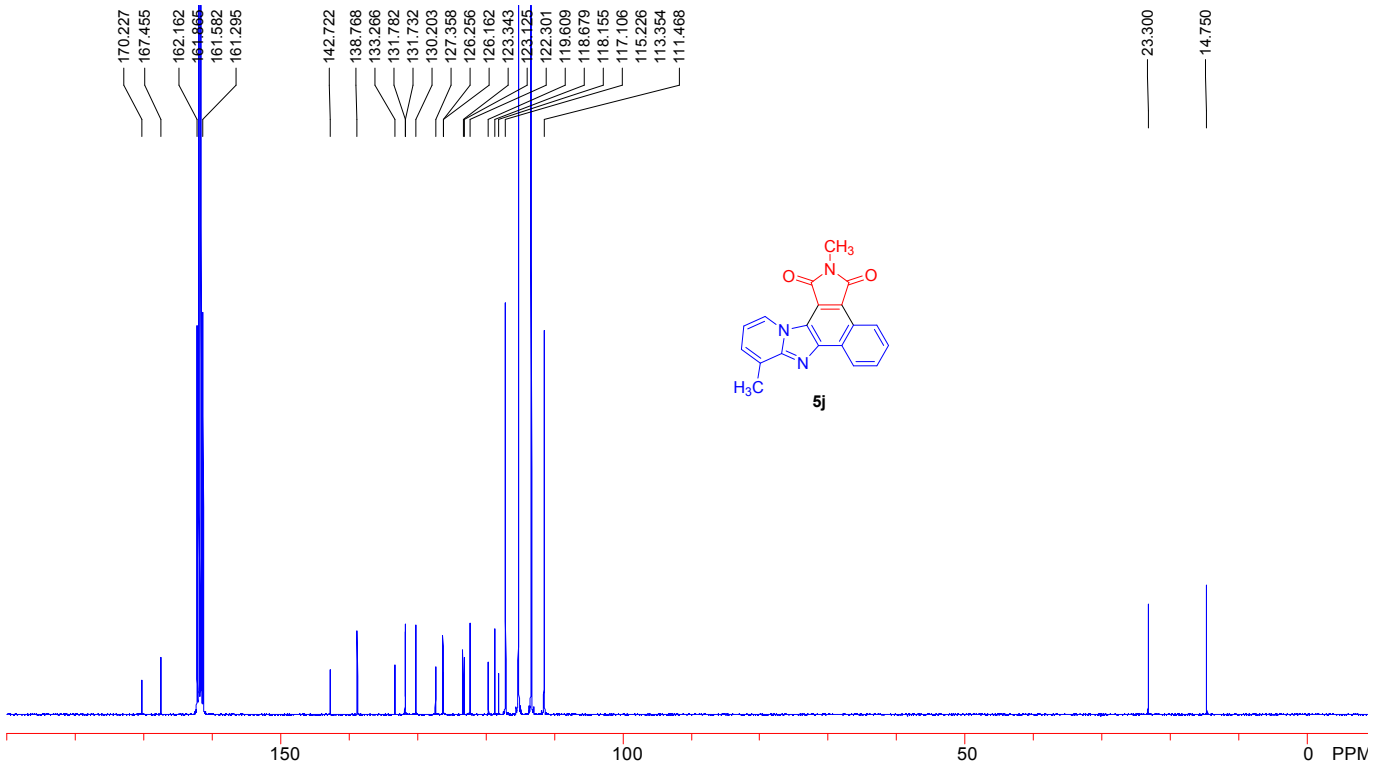
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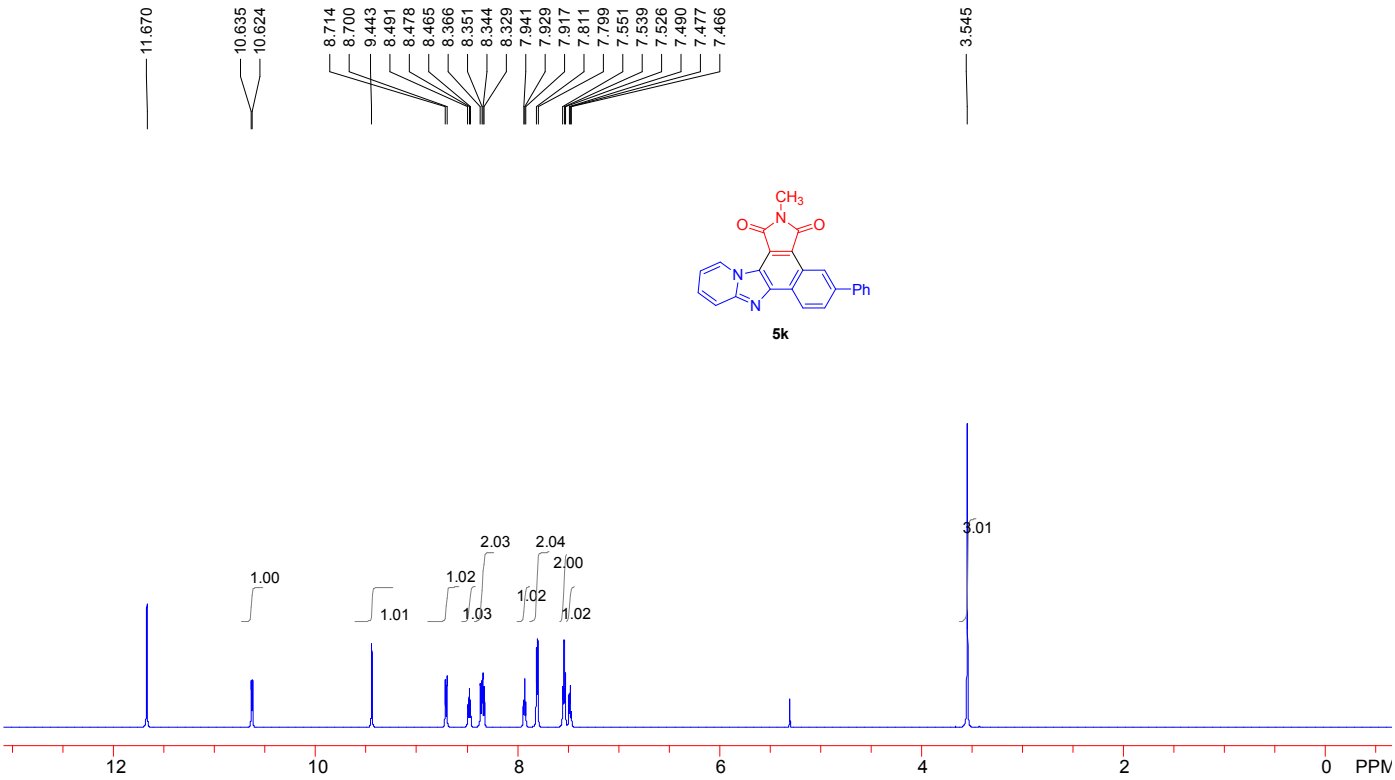
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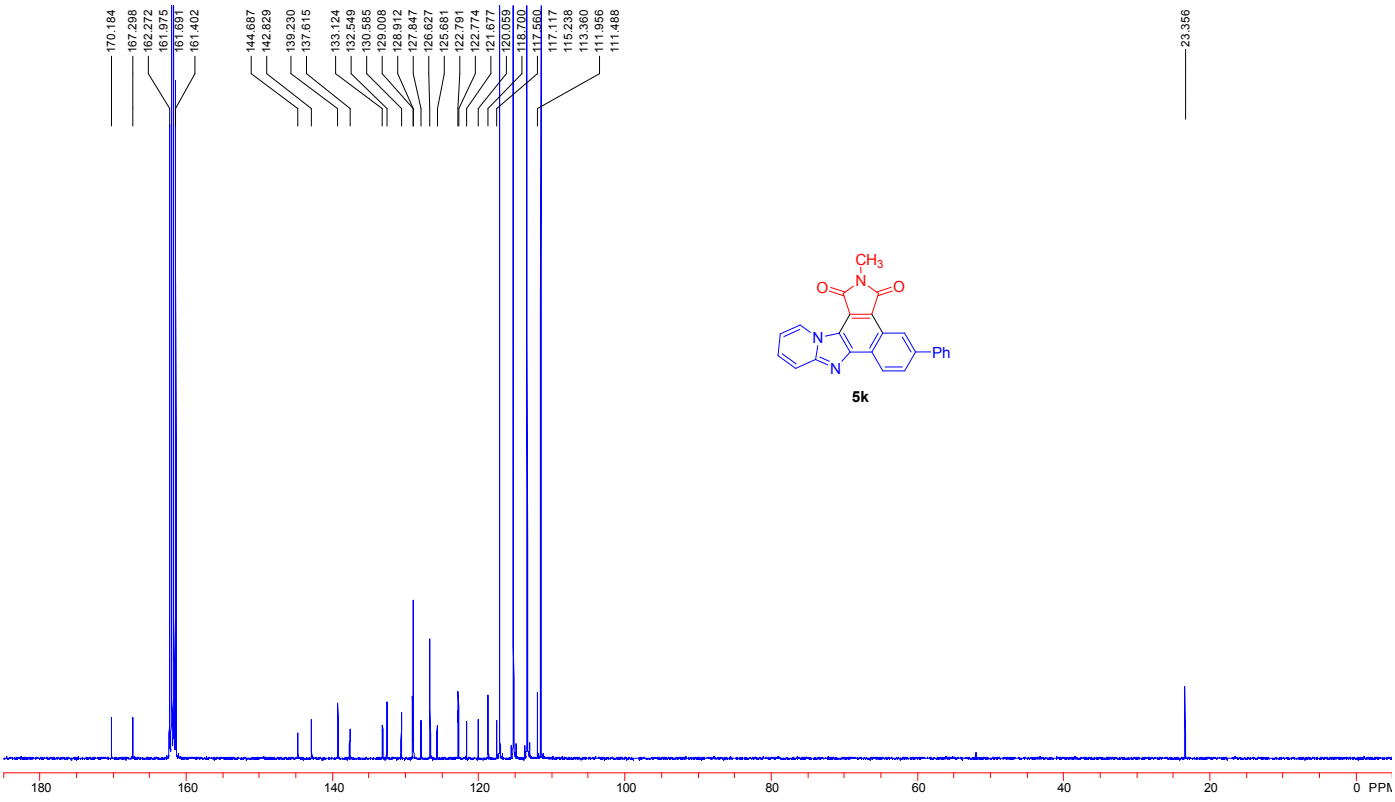
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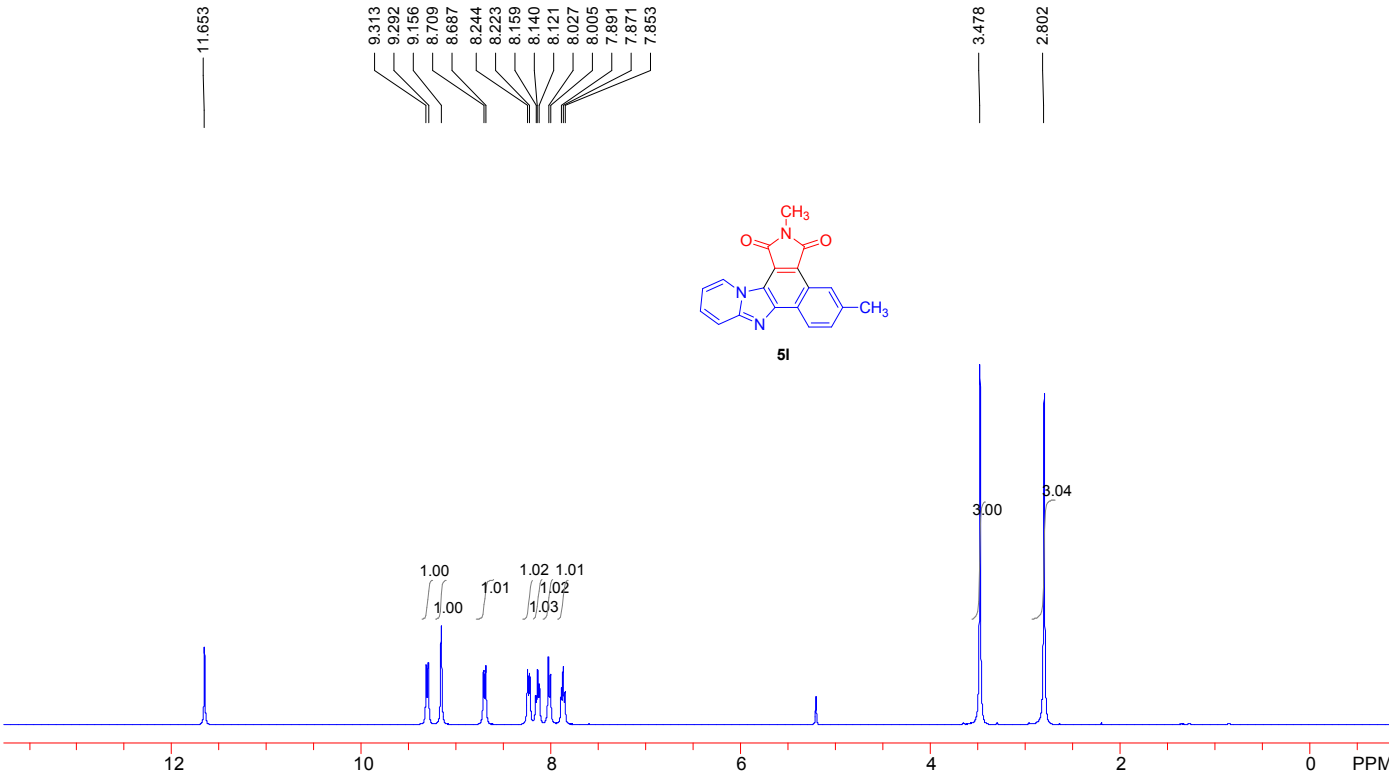
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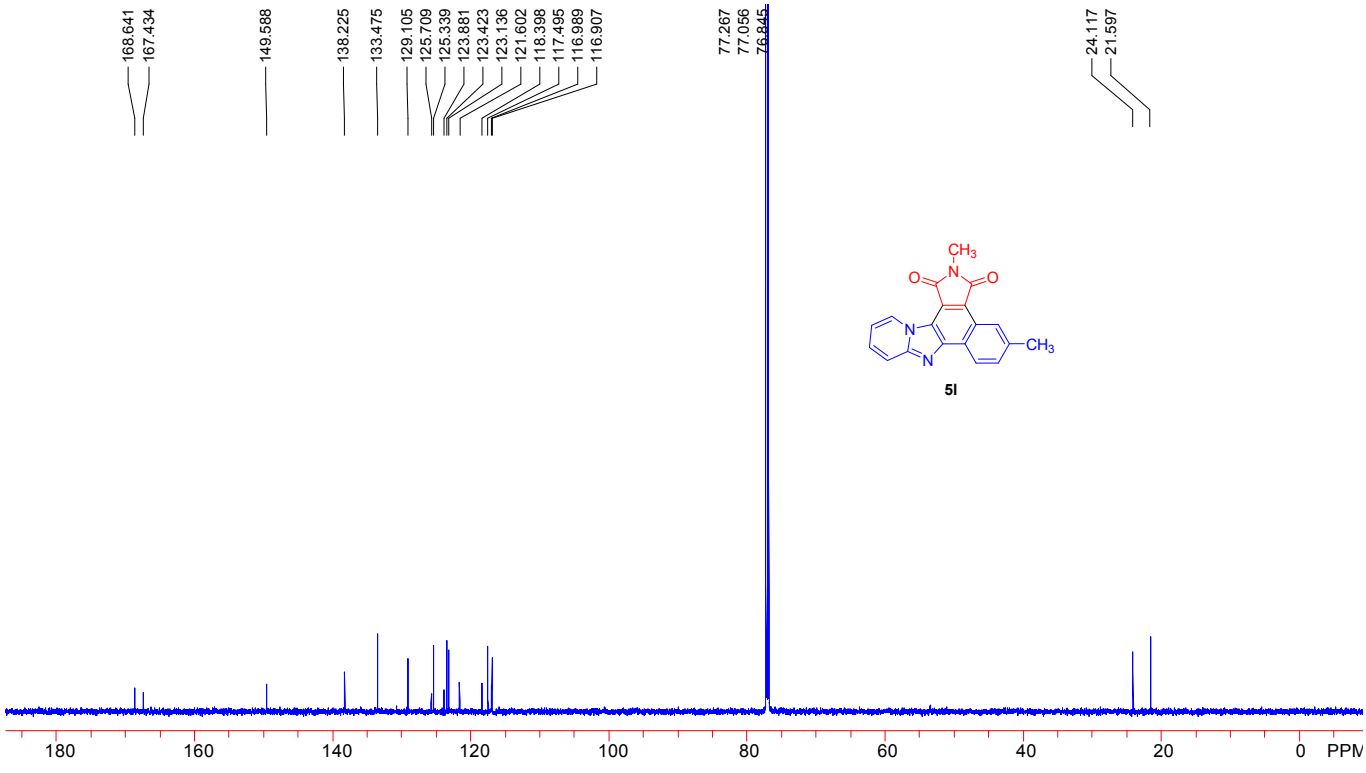
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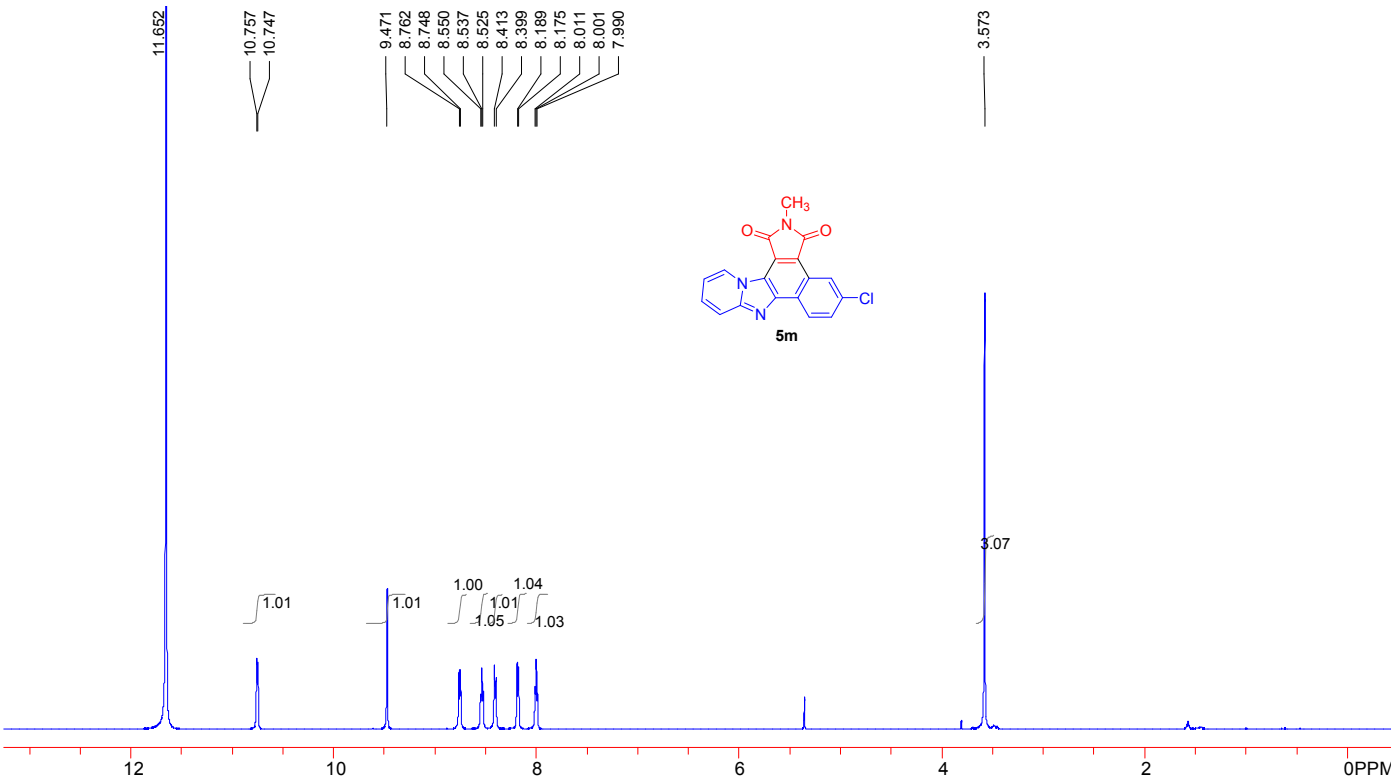
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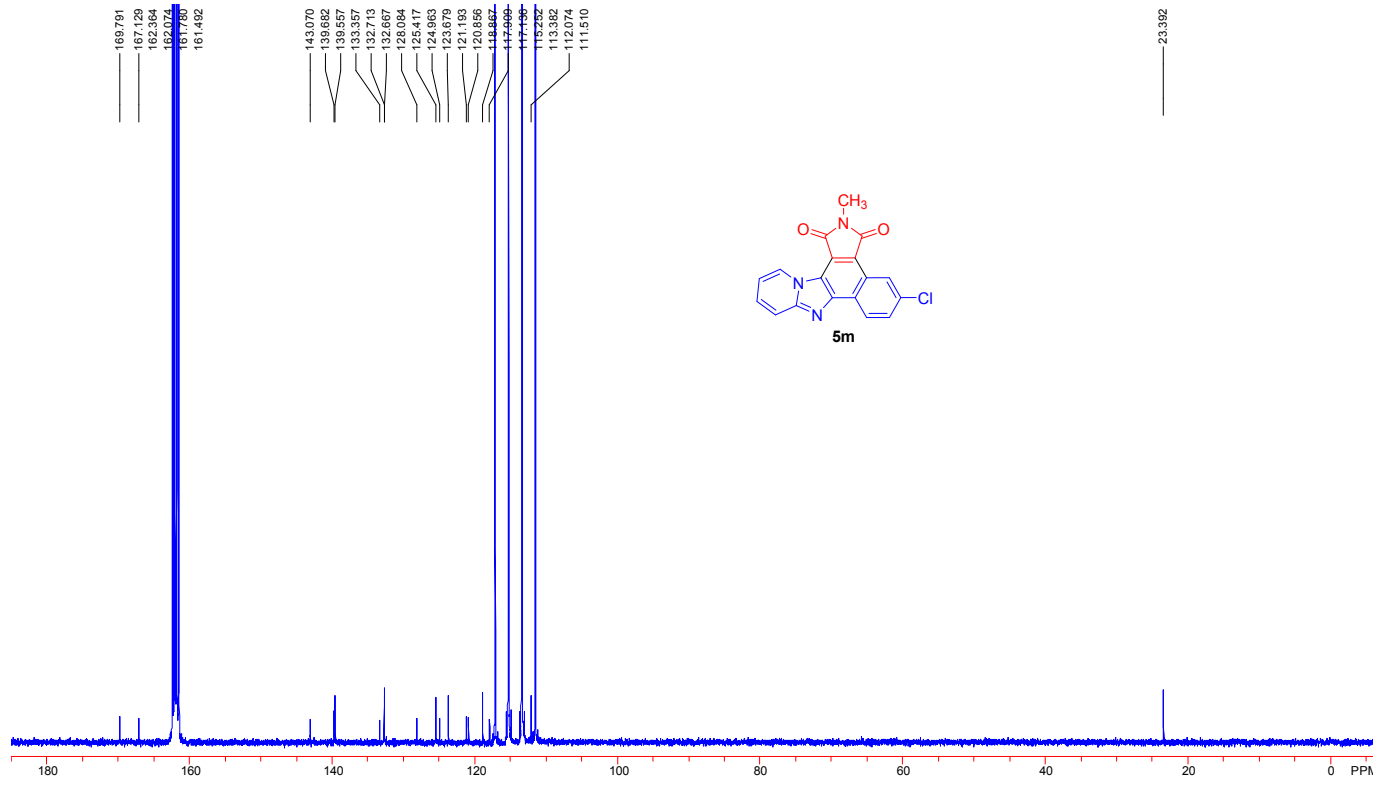
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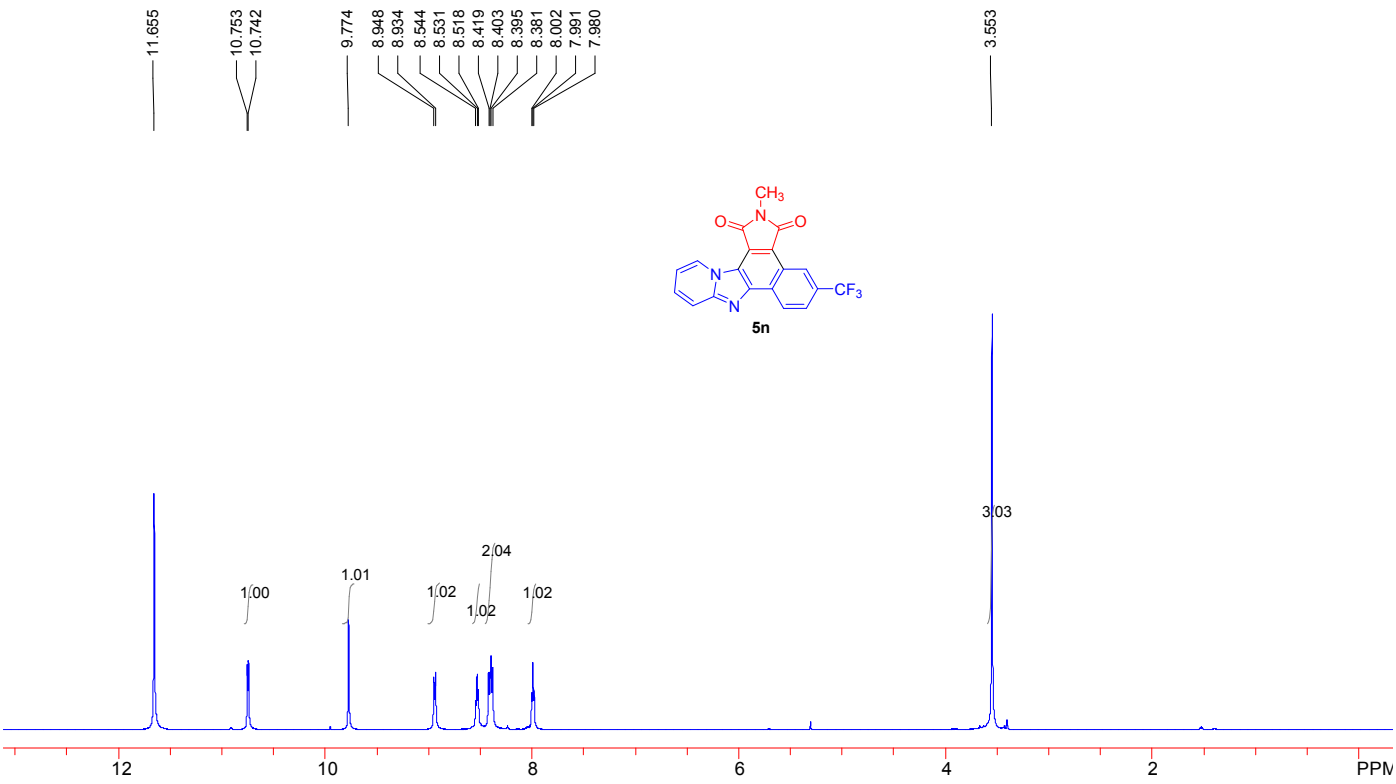
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8.395
8.381
8.002
7.991
7.980
3.553
CH3
O
N
O
N
N
CF3
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1.01
1.00
1.02
1.02
1.02
12
10
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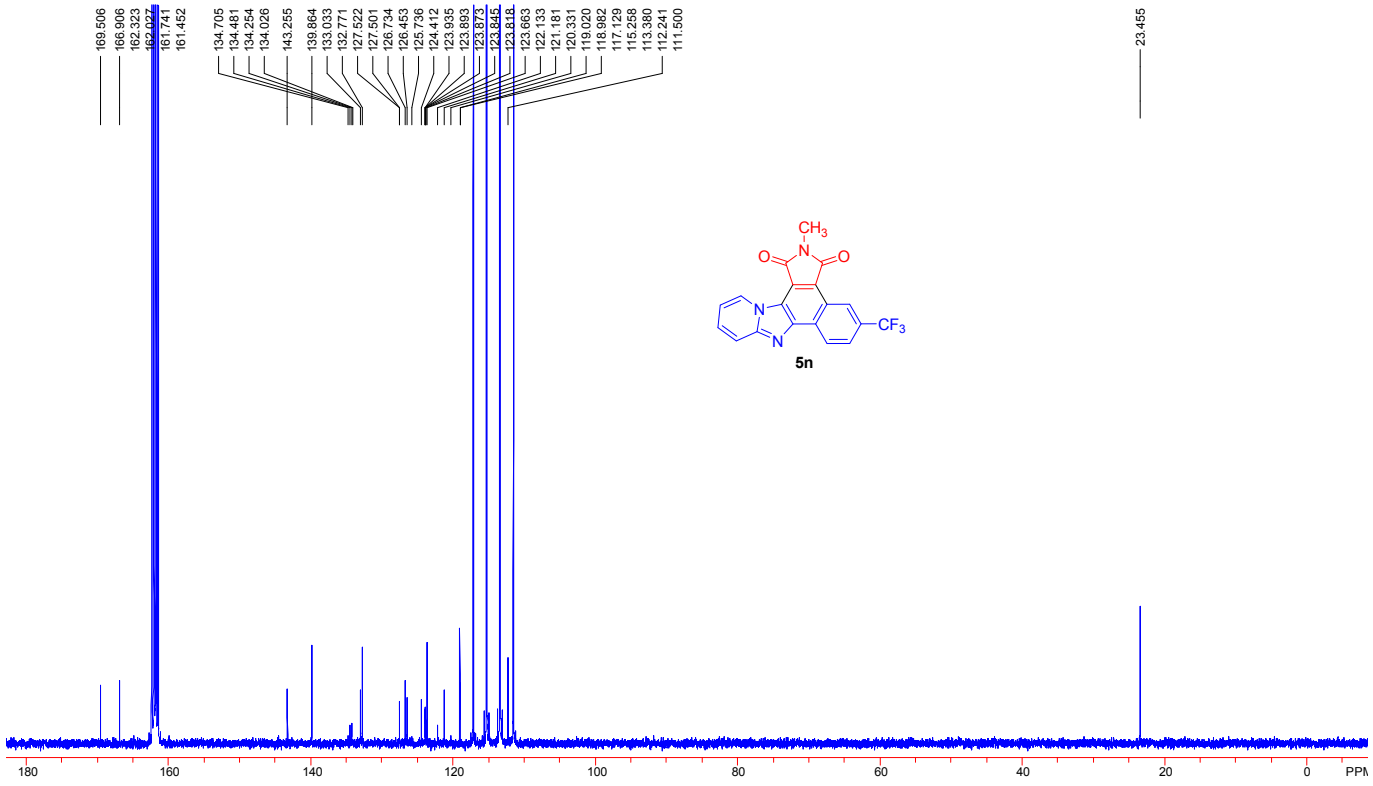
4
2
PPM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133.033
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127.501
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123.845
123.818
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122.133
121.181
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119.020
118.982
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115.258
113.380
112.241
111.500
23.455
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CF3
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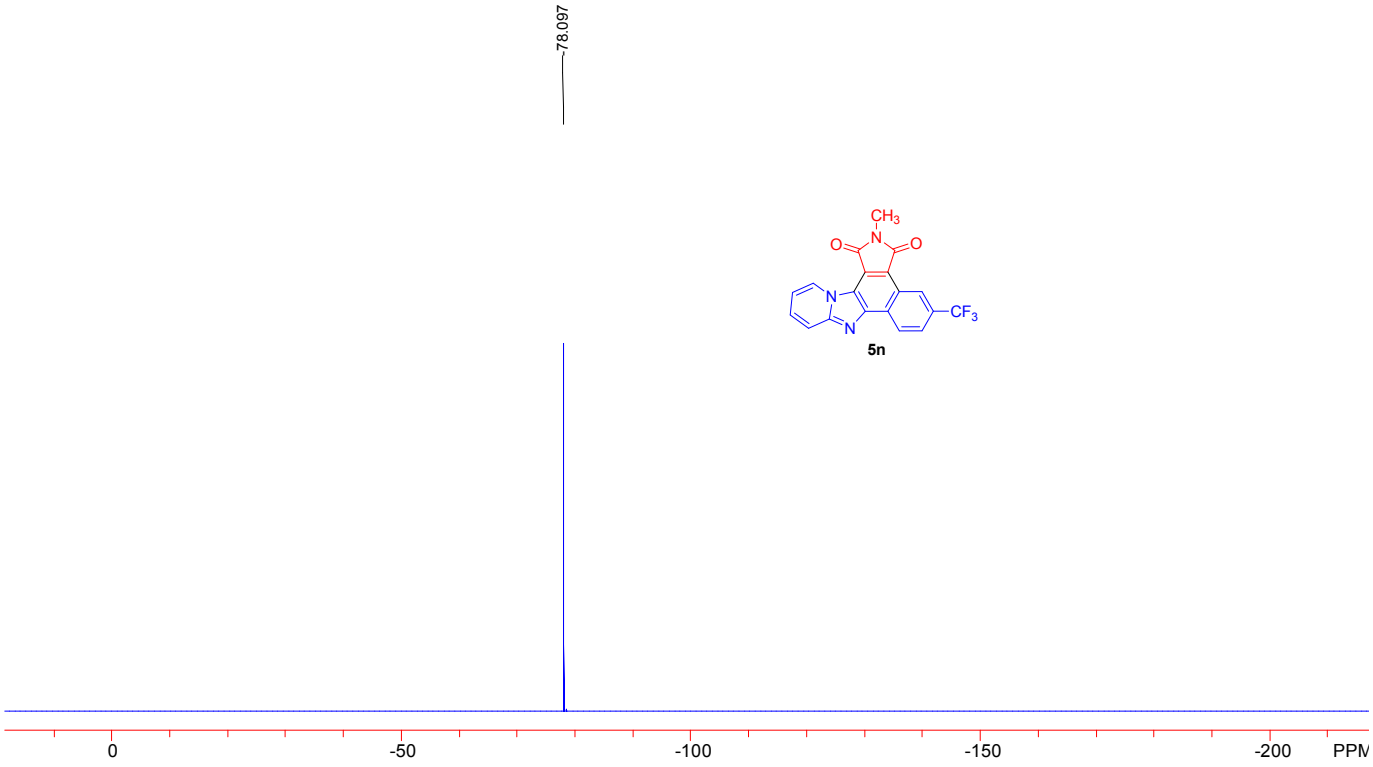
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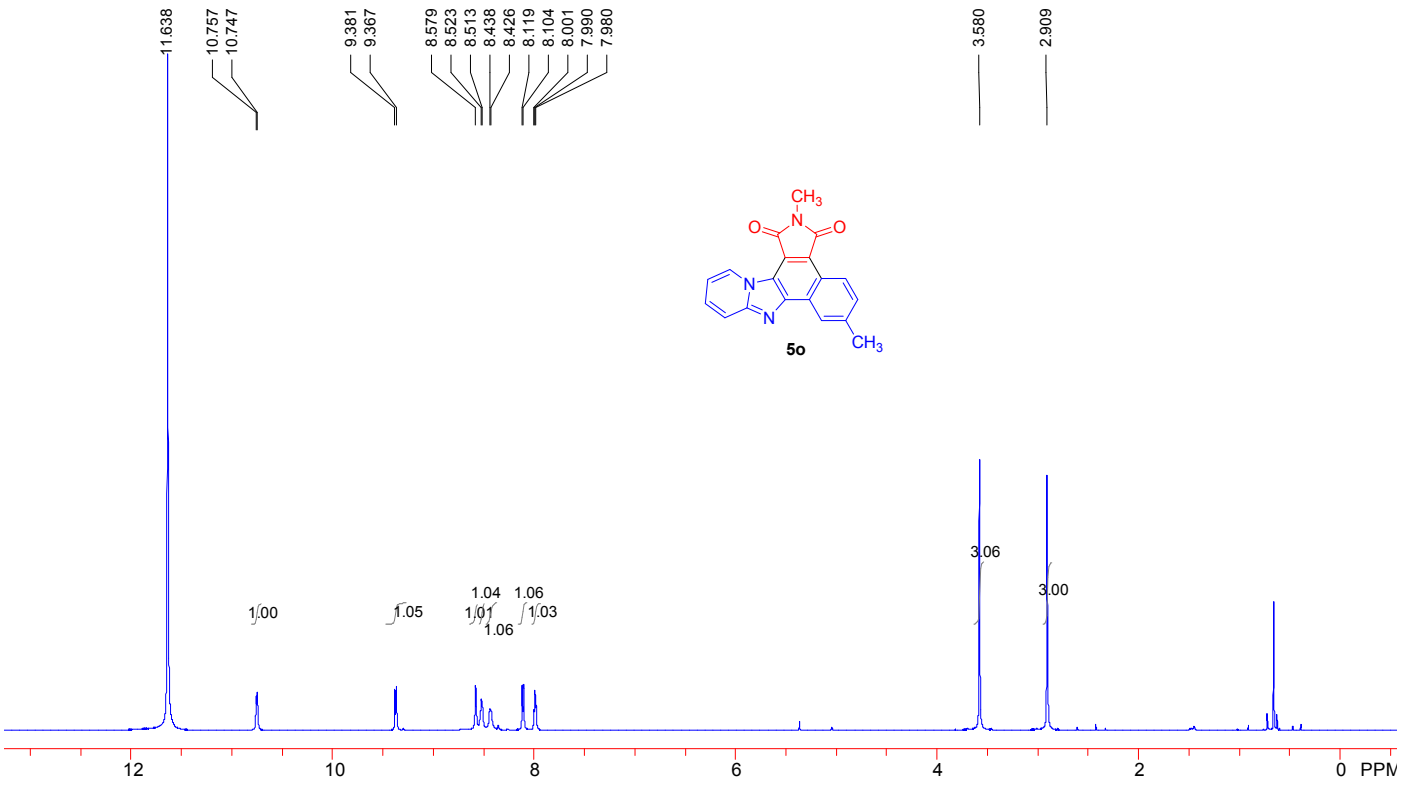
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7.980
3.580
2.909
CH3
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N
O
N
N
CH3
5o
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1.05
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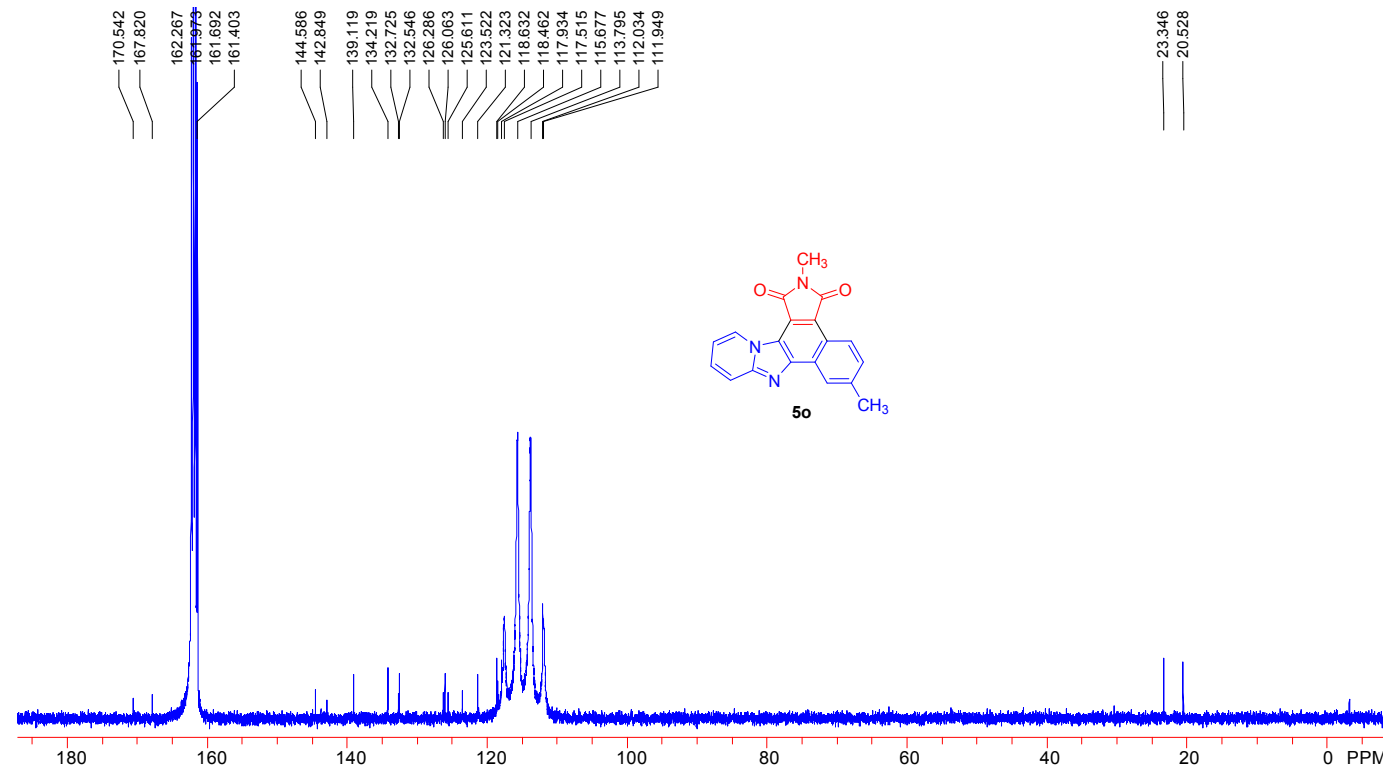
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125.611
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121.323
118.632
118.462
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117.515
115.677
113.795
112.034
111.949
23.346
20.528
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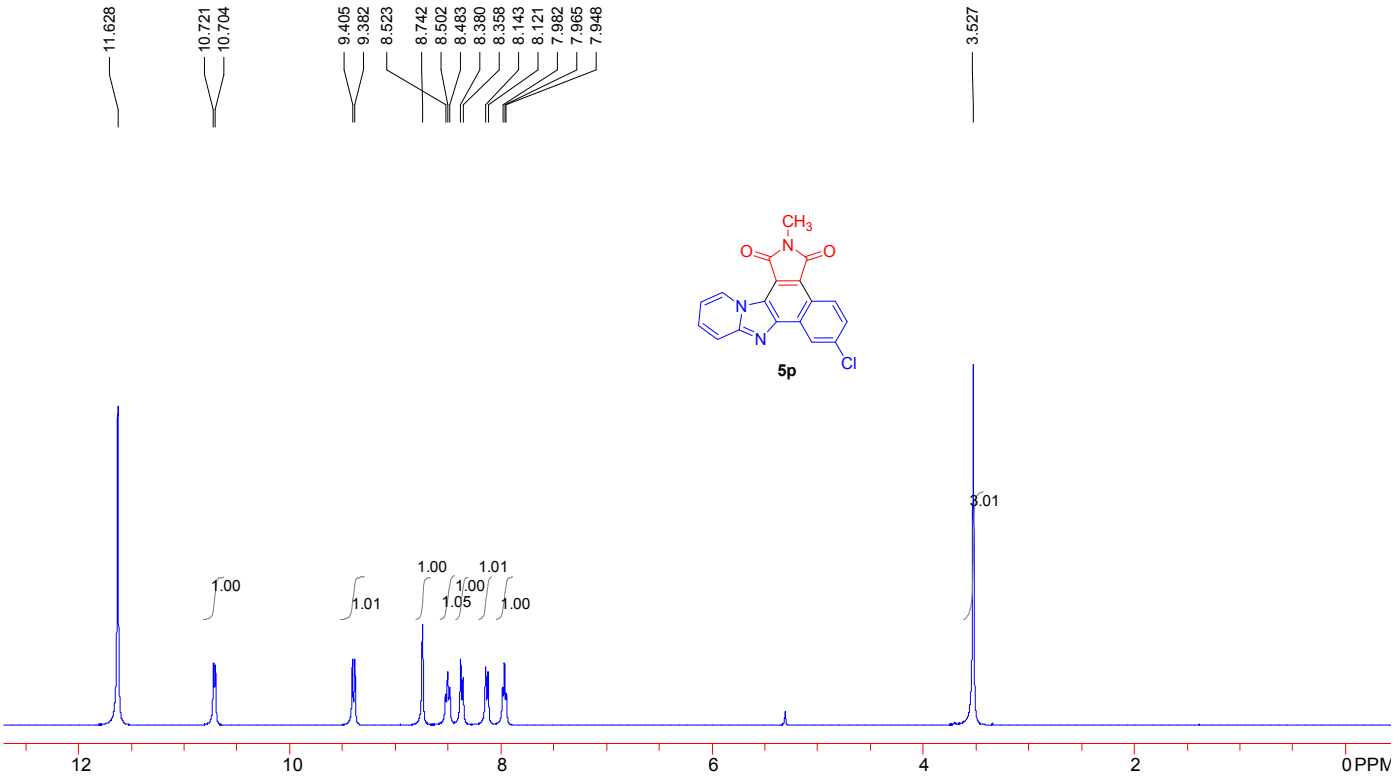
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7.982
7.965
7.948
3.527
CH3
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O
N
N
Cl
5p
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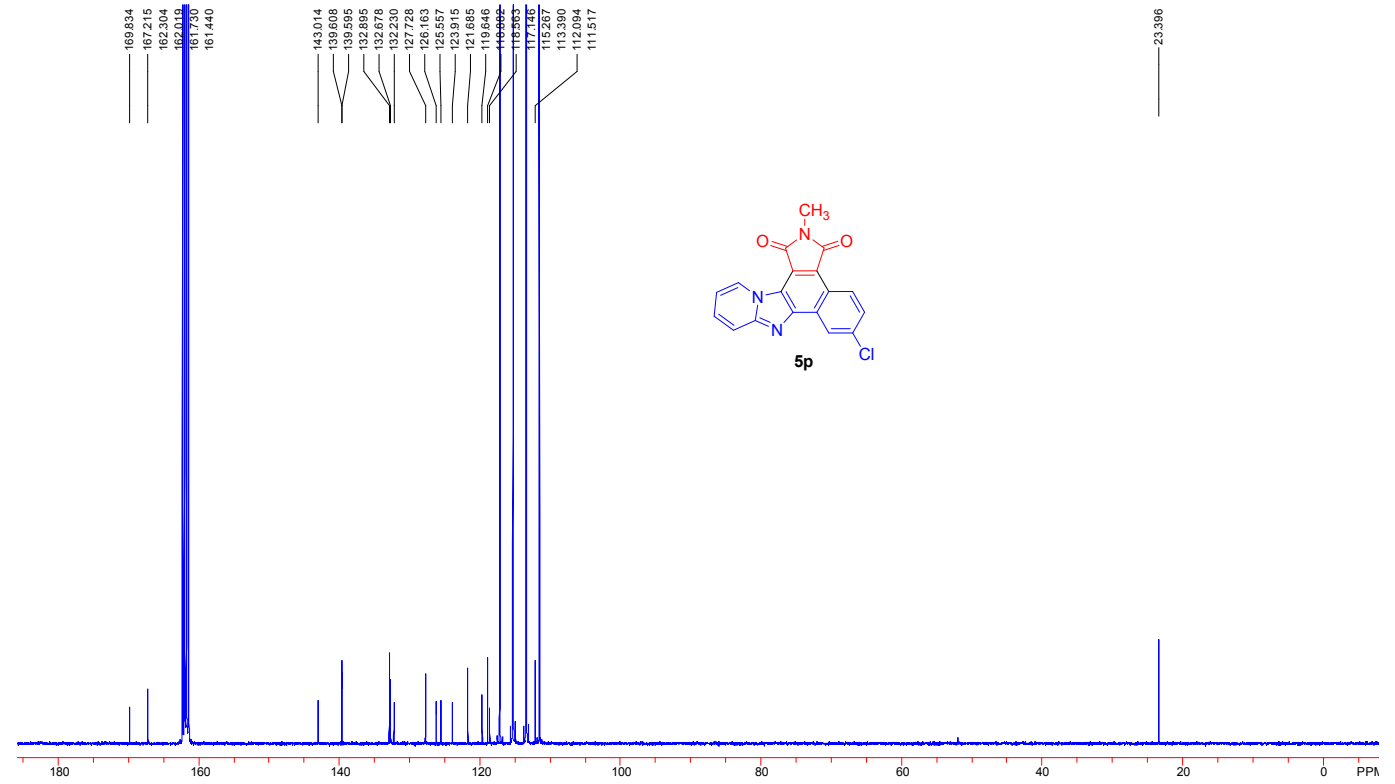
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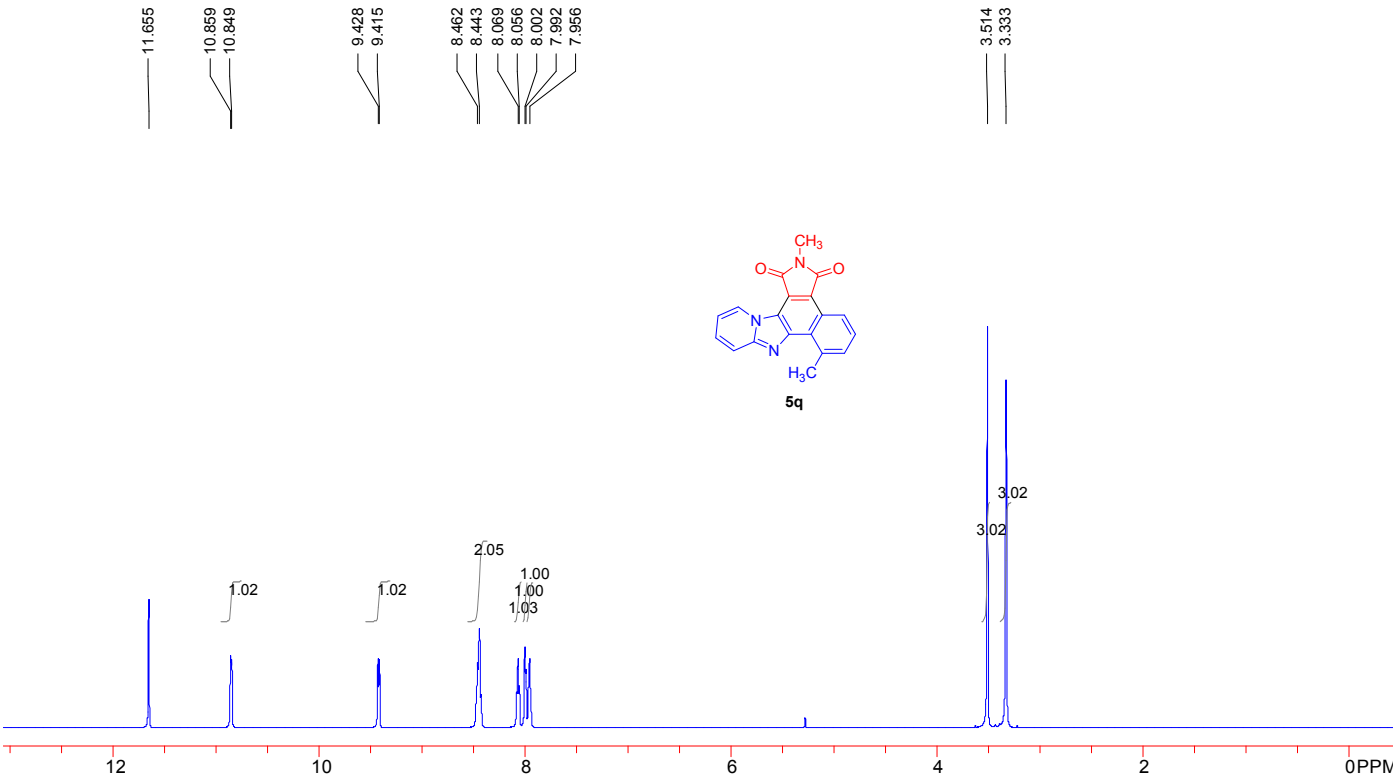
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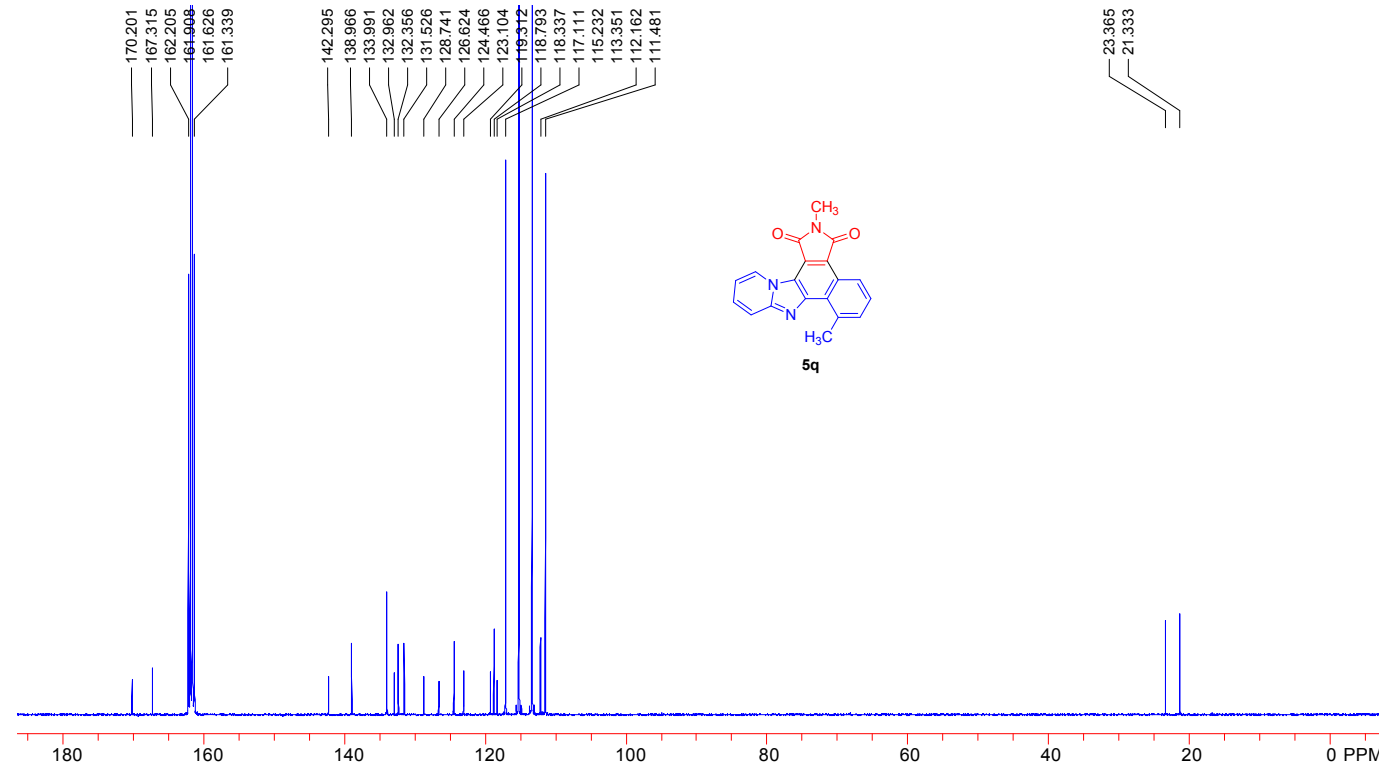
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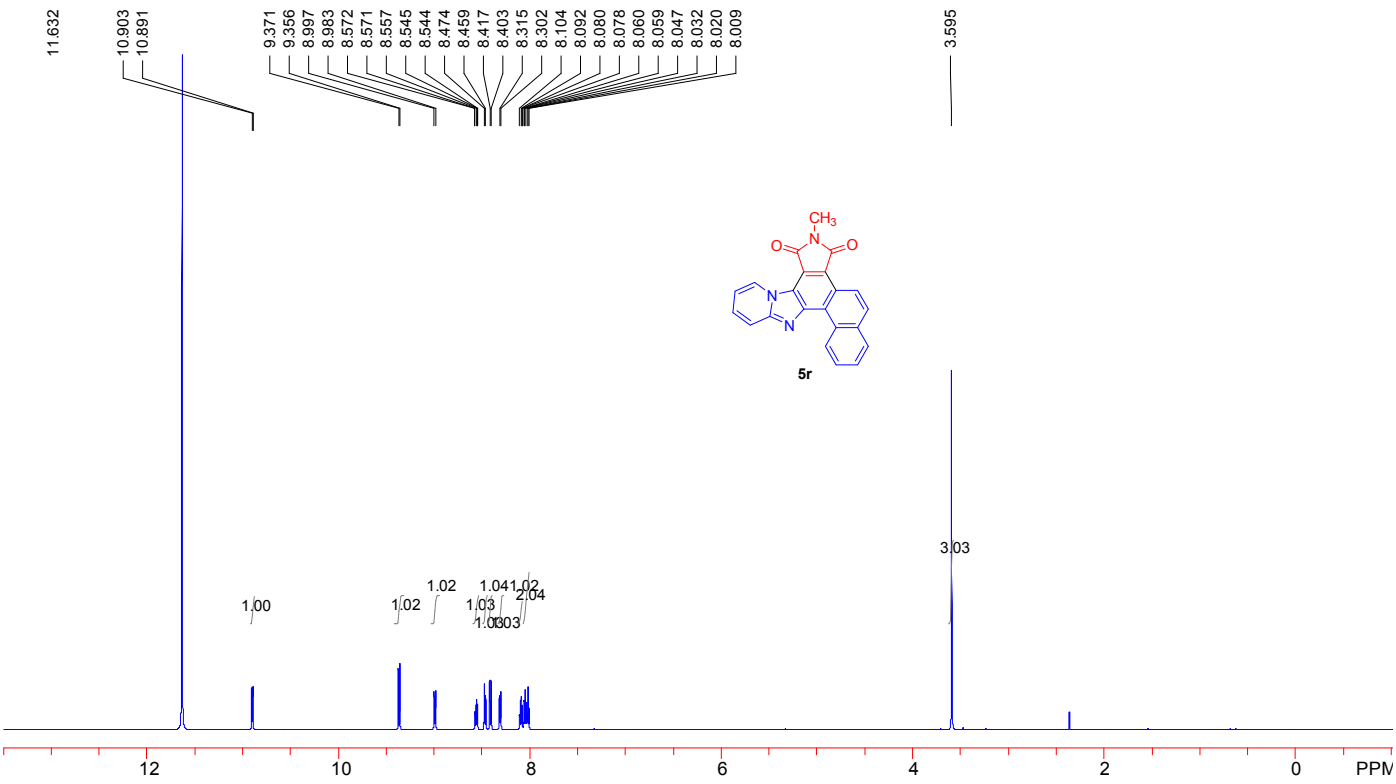
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8.059
8.047
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8.020
8.009
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N
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1.02
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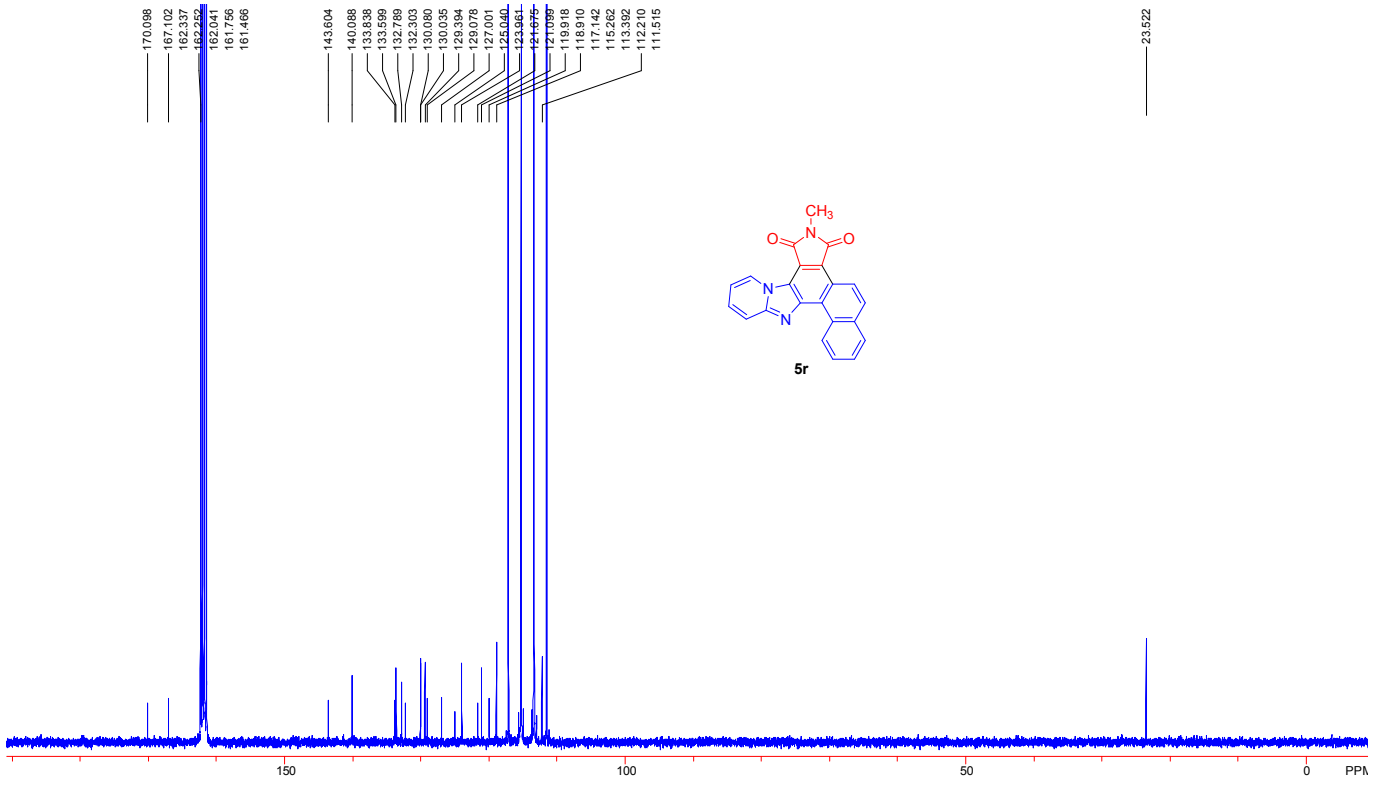
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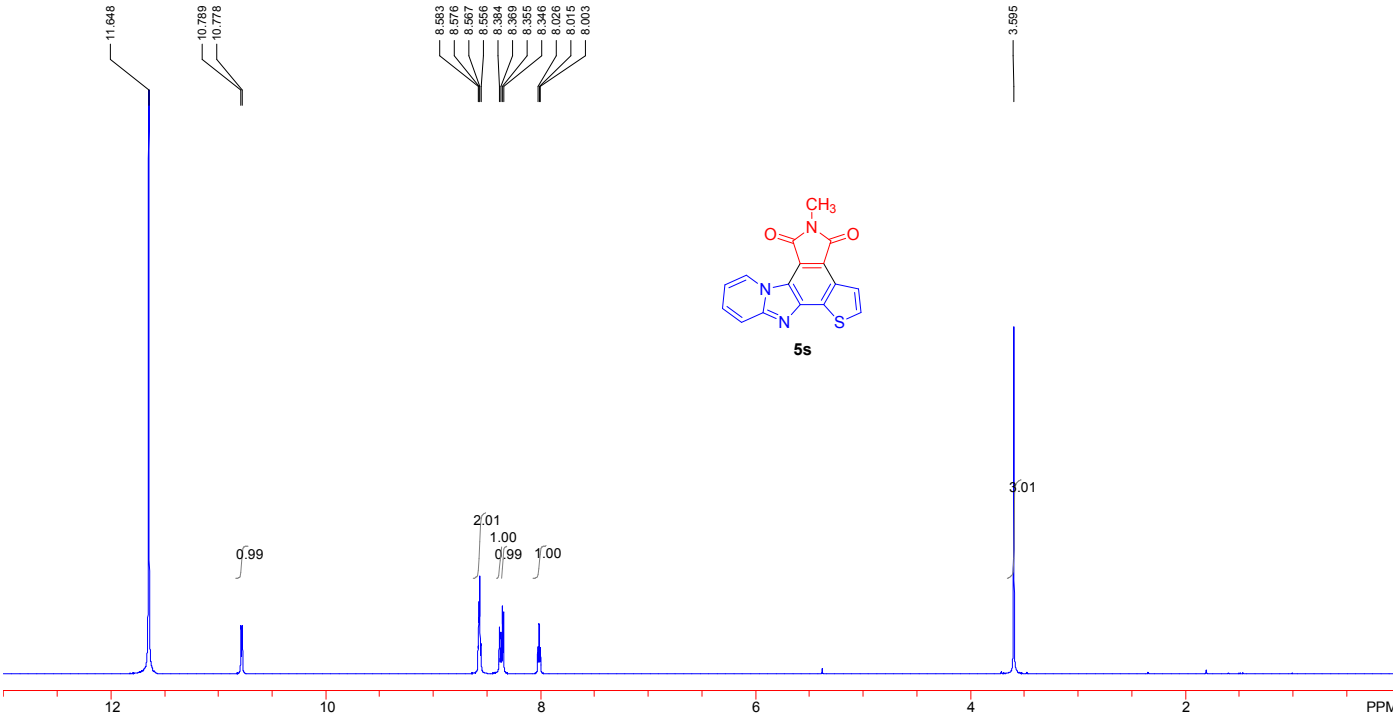
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2
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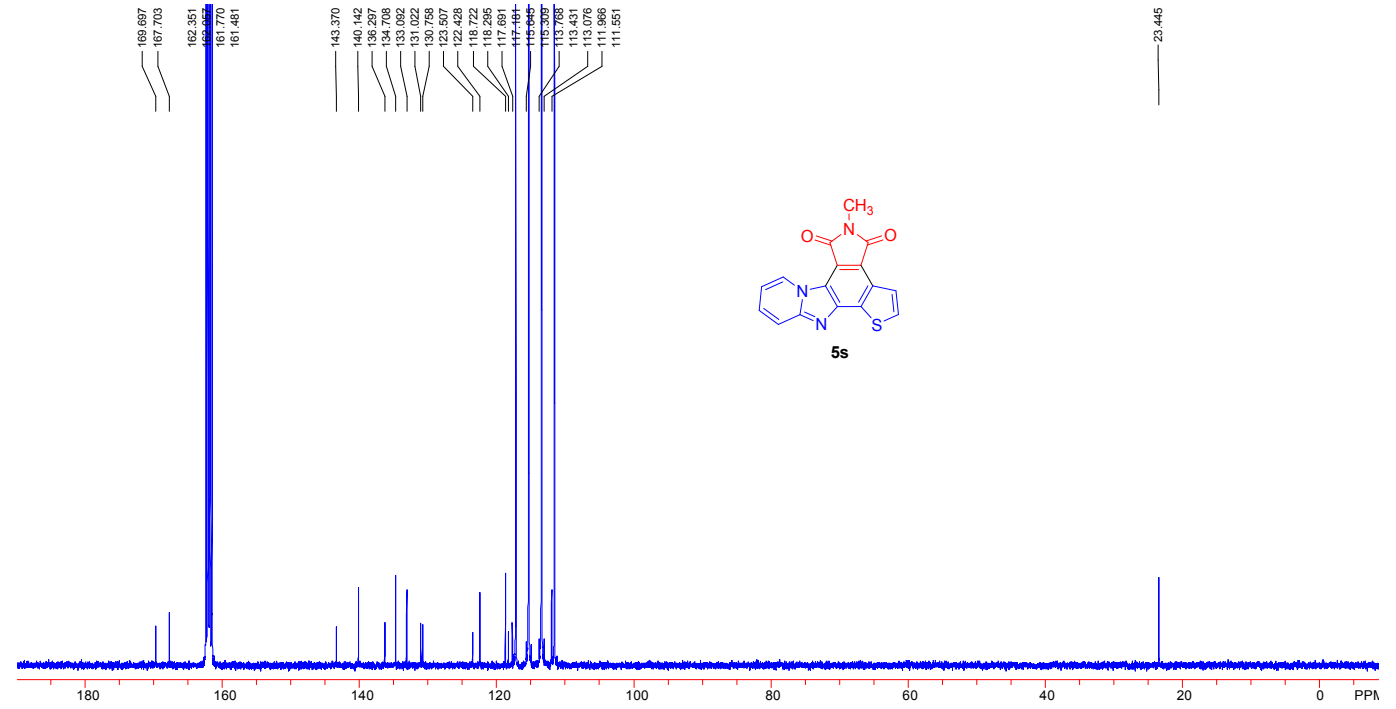
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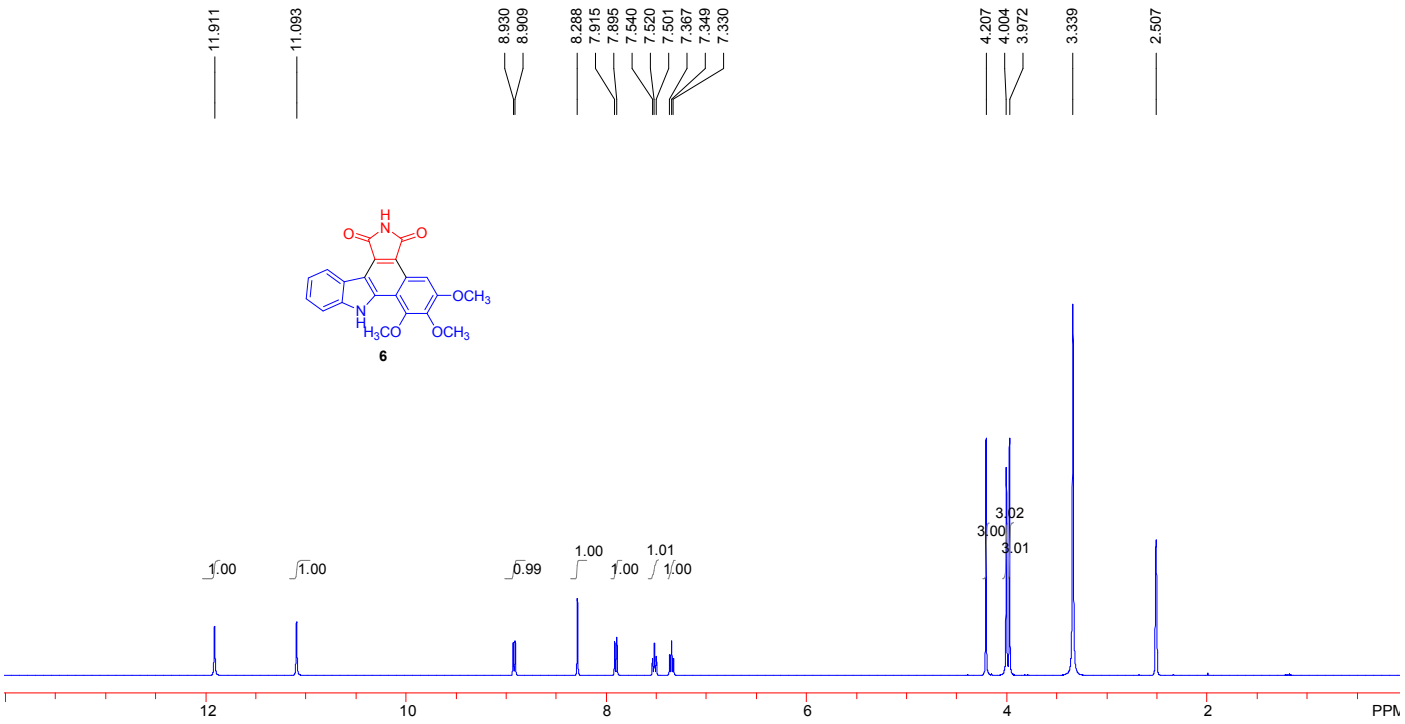
5s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OCH3
H3CO
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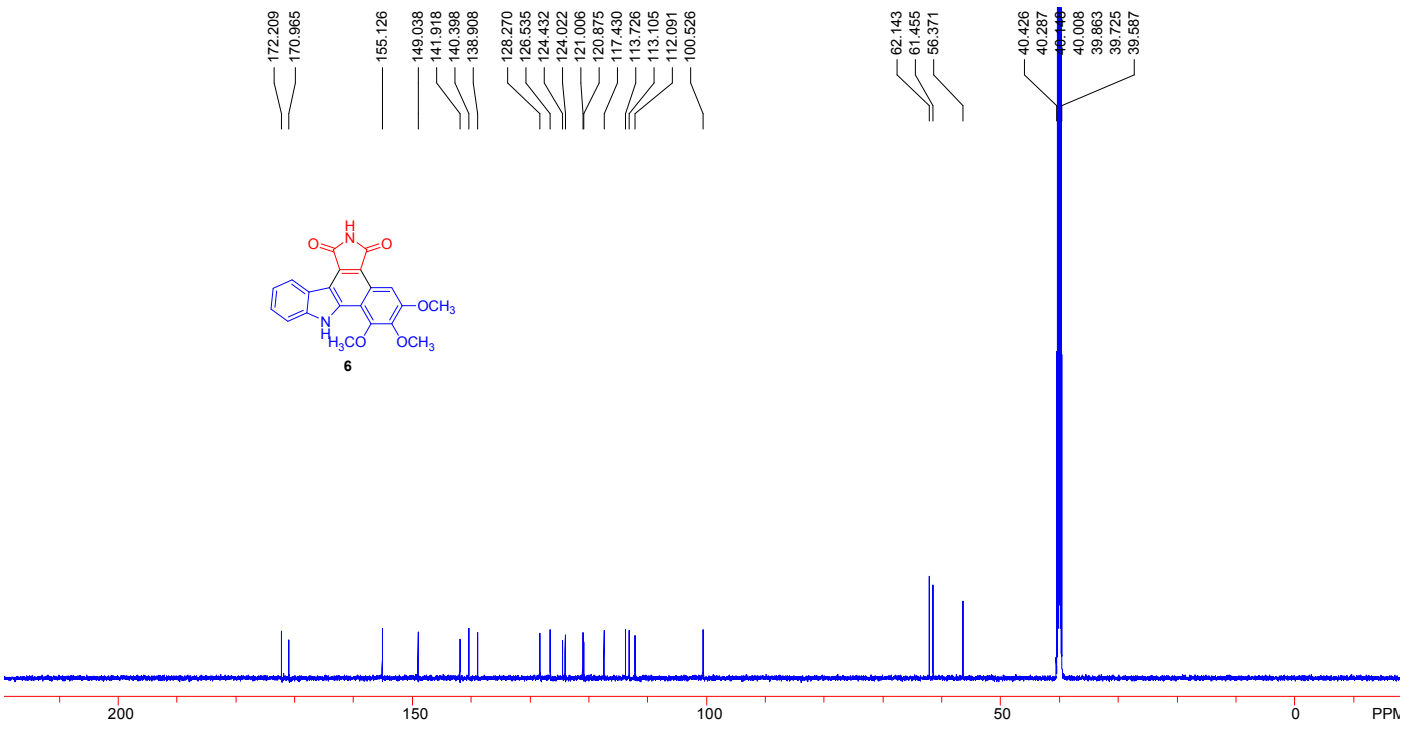
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