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Microwave-Assisted Cu(I)-Catalyzed One-Pot Tandem Synthesis of Pyridoimidazole Fused Quinolines as New Antimycobacterial Agents: DFT and ESI-HRMS Study

Gaurav Pawar,[a] Shaikh Mohammad Ghouse,[a] Swanand Vinayak Joshi,[a] Md Naiyaz Ahmad,[b] Arunava Dasgupta,[b] Y. V. Madhavi,[a] Siddharth Chopra,[b,c] Srinivas Nanduri,*[a]

[a]Department of Chemical Sciences, National Institute of Pharmaceutical Education and Research (NIPER) Balanagar, 500037, Hyderabad, Telangana, India.
E-mail: Prof. Srinivas Nanduri, nandurisrini92@gmail.com
[b]Division of Molecular Microbiology and Immunology, Council of Scientific and Industrial Research–Central Drug Research Institute, Sitapur Road, Sector 10, Janakipuram Extension, Lucknow, Uttar Pradesh, 226031, India
[c]Academy of Scientific and Innovative Research, Ghaziabad, 201002, India.

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1. General information:

All chemicals and solvents were received from commercial suppliers and used without purification. Catalyst Copper(I) iodide was purchased from Sigma-Aldrich. The reaction mixture was analyzed by TLC silica gel plates (MERCK precoated silica gel 60F-254) with a thickness of 0.5 mm under UV chamber (λ = 254 nm). Compound purification was done by Biotage flash chromatography using SNAP KP-Sil Cartridge, 10 g under gradient elution technique. NMR spectra were recorded on Bruker 500 and 125 MHz spectrophotometer in the deuterated solvent. ^{1}H spectral data include chemical shift (δ) in parts per million (ppm) and coupling constant (J) in Hz, while all the multiplicities represented by standard abbreviation: s (singlet), d (doublet), dd (double doublet), t (triplet), and m (multiplet). HRMS data were recorded on Agilent (LC/TOF) system. Reactions were carried out in a Monowave 300 single-mode microwave reactor using G10 reaction vessels (10 mL).

1.1. General procedure for the synthesis of 2-(-2-bromophenyl)imidazo[1,2-*a*]pyridine: [1]

In a clean oven-dried 10-mL RB flask, acetophenone (1 mmol), 2-aminopyridine (1.2 mmol), CuI (0.2 mmol), and 3.0 mL of 1,4-dioxane were added. After stirring for 14 hours at 100 °C under ambient air, the resulting solution was cooled to room temperature. The reaction mass was evaporated to dryness after completion. Purification of the crude residue by column chromatography (EtOAc: Hexanes, 1:2) yielded 2-(-2-bromophenyl)imidazo[1,2-*a*]pyridine.

1.2 General procedure for the synthesis of compounds 3a-3y and 3aa-3ab:

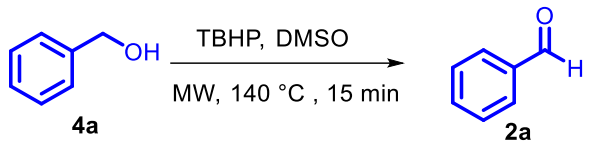
Procedure A: In 10 mL oven-dried G10 reaction vial, a solution of compound **1** (1 mmol) and aldehyde 2 (1.2 mmol) in DMSO were added, followed by $TMSN_3$ (2 mmol) and CuI (0.1 mmol). The reaction vial was then kept in a microwave reactor and the microwave irradiation was carried out at 140 °C for 15 min. After monitoring the completion of the reaction monitored by TLC, 3 mL of water was added into the reaction mixture to obtain the precipitate which was extracted with ethyl acetate (50 mL x 3). The combined organic layer was passed through a plug of sodium sulfate (Na_2SO_4) and evaporated *in vacuo*. The residue was purified by flash chromatography using a gradient of hexane /EtOAc (eluent system) to afford the pure products.

Procedure B: In 10 mL oven-dried G10 reaction vial, a solution of compound **1** (1 mmol) and alcohol **4** (1.2 mmol) in DMSO were added, followed by $TMSN_3$ (2 mmol), TBHP (2 mmol), and CuI (0.1 mmol). The reaction vial was then kept in the reactor and microwave irradiation was carried out at 140 °C for 15 min. After completion of the reaction monitored by TLC, 3mL of water was added into the reaction mixture to obtain precipitate which was extracted with ethyl acetate (50 mL x 3). The combined organic layer was passed through a plug of sodium sulfate (Na_2SO_4) and evaporated *in vacuo*. The residue was purified by flash chromatography using a gradient of hexane /EtOAc (eluent system) to afford the pure products.

Procedure C: In 10 mL oven dried G10 reaction vial, a solution of compound **1** (1 mmol) and methyl arene **5** (2 mL) in DMSO were added, followed by $TMSN_3$ (2 mmol), TBHP (4 mmol), and CuI (0.1 mmol). Then, the reaction vial was kept in a microwave reactor and microwave irradiation was carried out at 140 °C for 15 min. After completion of the reaction monitored by TLC, 3mL of water was added into the reaction mixture to obtain precipitate which was extracted with ethyl acetate (50 mL x 3). The combined organic layer was passed through a plug of sodium sulfate (Na_2SO_4) and evaporated *in vacuo*. The residue was purified by flash chromatography using a gradient of hexane/EtOAc (eluent system) to afford the pure products.

2. Control experiments:

Scheme S1:



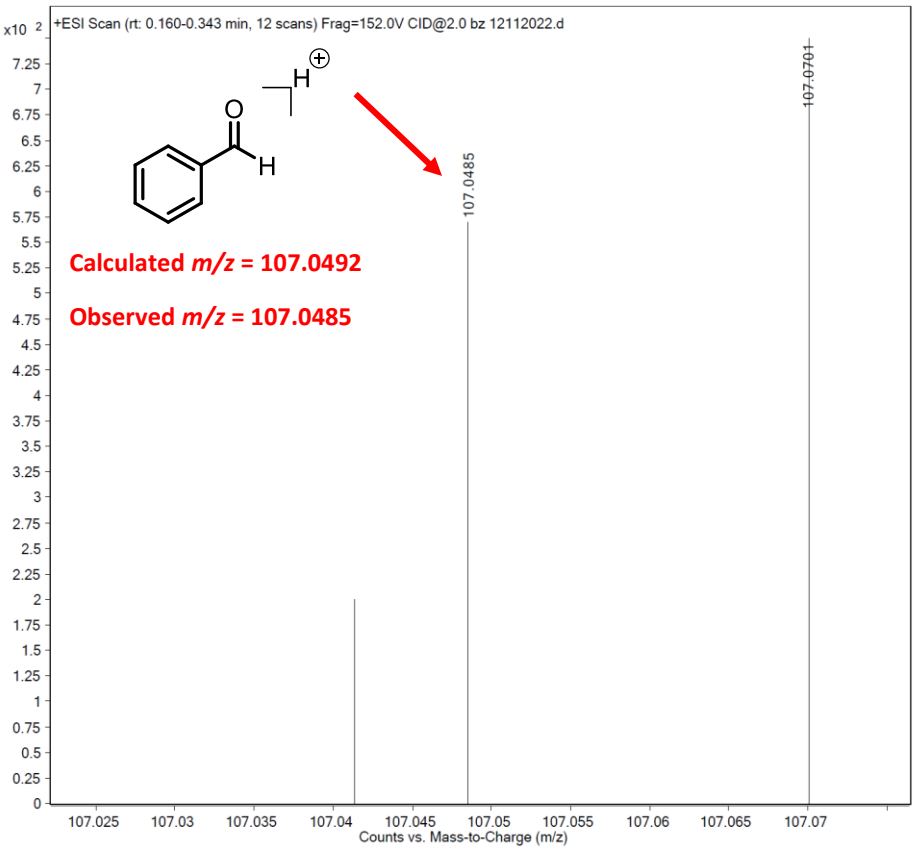


Figure S1. HRMS spectra of scheme S1.

Scheme S2:

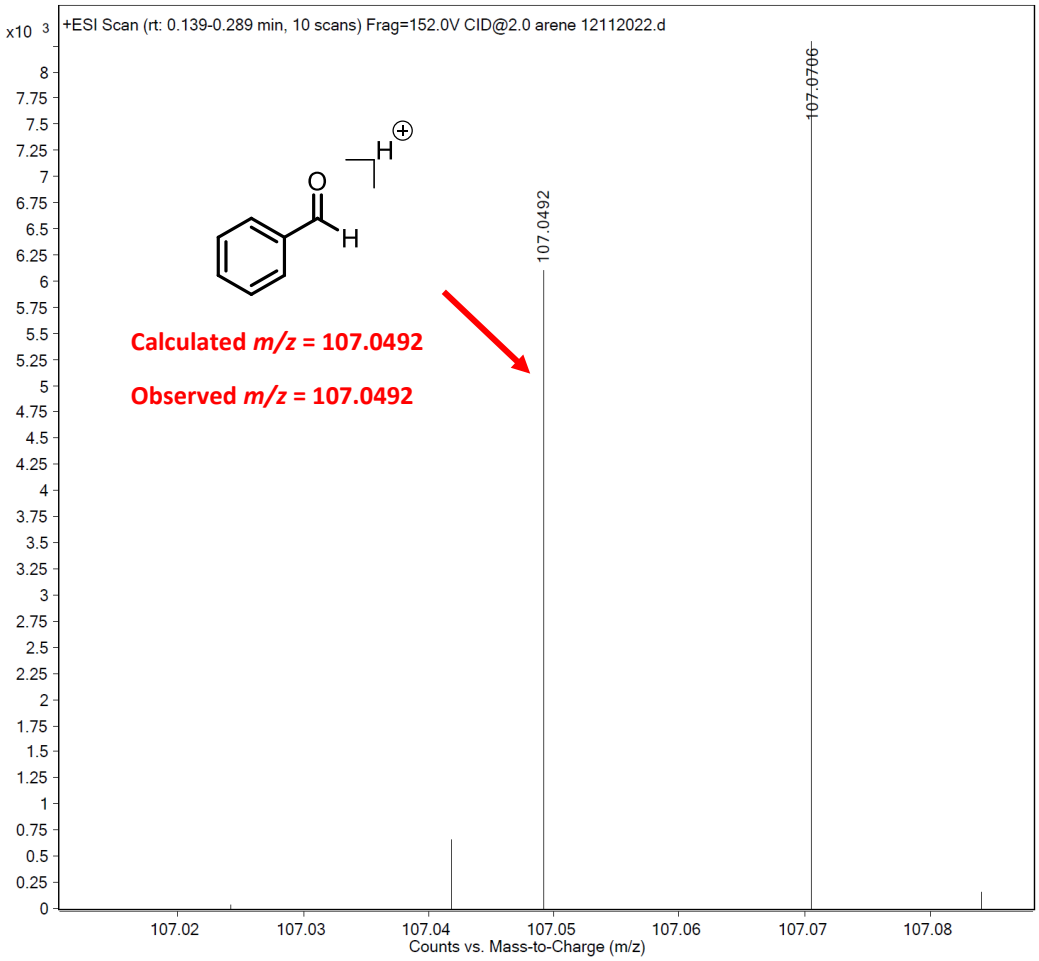
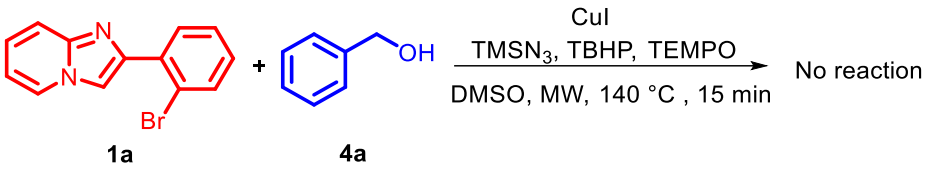


Figure S2. HRMS spectra of scheme S2.

Scheme S3:



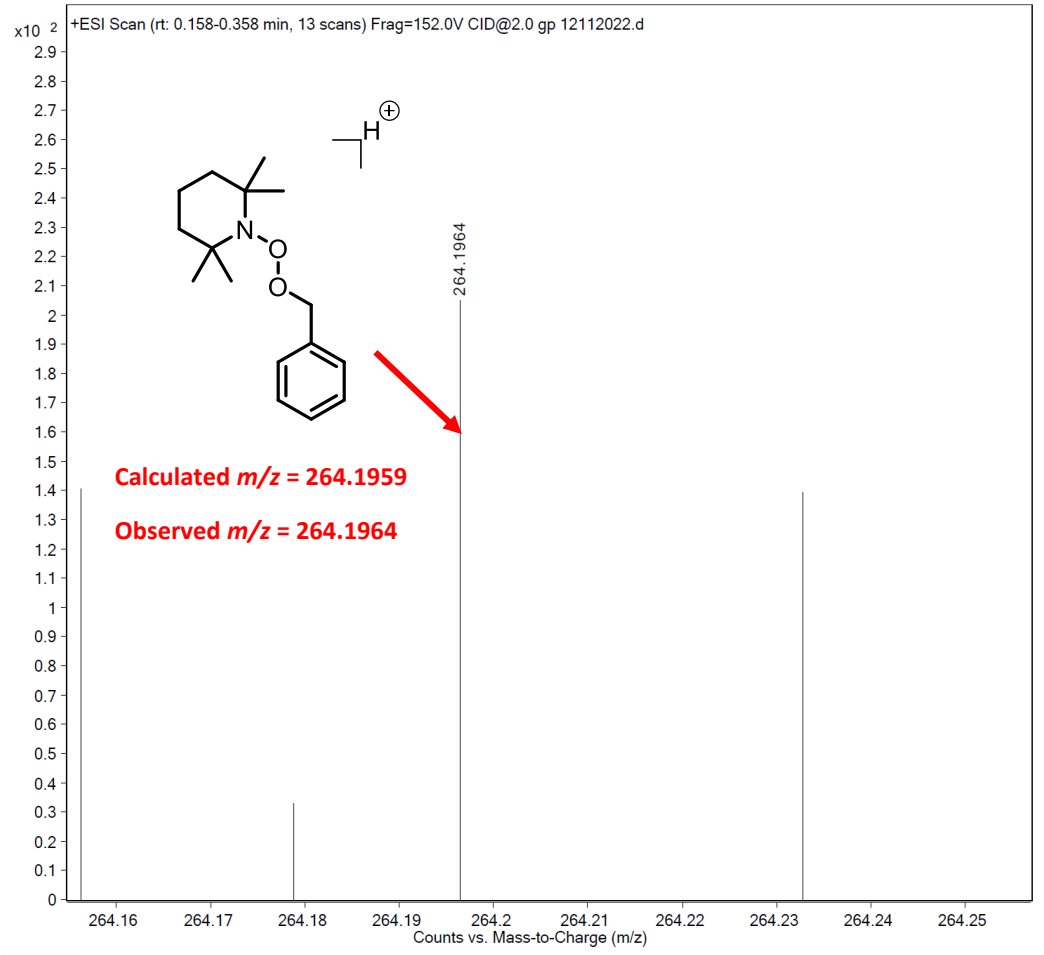
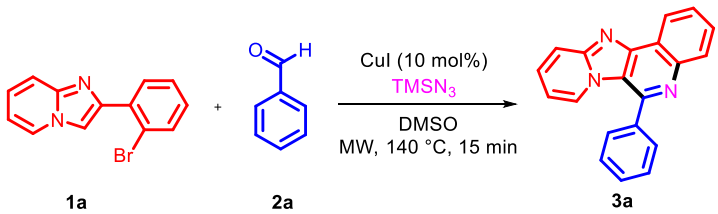


Figure S3. HRMS spectra of scheme S3.

3. Gram scale reaction:



Scheme S4: Gram-scale synthesis of compound **3a**.

In 30 mL oven dried G30 reaction vial, a solution of compound **1** (5.491 mmol) and benzaldehyde (6.59 mmol) in DMSO were added, followed by $TMSN_3$ (10.98 mmol) and CuI

(0.54 mmol). Then, the reaction vial was kept in a microwave reactor and microwave irradiation was carried out at 140 °C for 15 min. After completion of the reaction monitored by TLC, 10 mL of water was added into the reaction mixture to obtain precipitate which was extracted with ethyl acetate (50 mL x 3). The combined organic layer was passed through a plug of sodium sulfate (Na_2SO_4) and evaporated *in vacuo*. The residue was purified by flash chromatography using a gradient of hexane /EtOAc (eluent system) to afford the pure products **3a** (1.08 g, 72%)

4. DFT study:

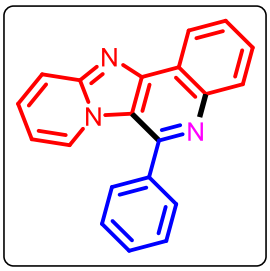
The patterns of free energy change as recorded in Table S1 (SI), show a negative change in the energy for most of the steps, which confirms the thermodynamic spntaneity in the forward direction. Interestingly, the maximum free energy observed in step 4 (-658.666). This can be attributed to the loss of CuI.

Structure	**E_0+G_{corr} (au)**
Reactant	-617.1650
I	-821.6400
II	-974.8030
III	-864.4720
IV	-658.6660
V	-924.9600
VI	-925.3400
VII	-925.1170
Product	-925.1470

Table S1. Total energy of intermediates

5. Analytical data:

6-phenylpyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3a):[2]



Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 92% (300 mg);

Following the general **procedure (B)**, the title product was obtained as a white solid; Yield 79% (233 mg);

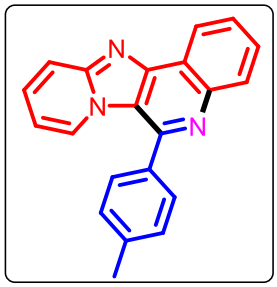
Following the general **procedure (C)**, the title product was obtained as a white solid; Yield 77% (227 mg); mp: 215-217 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (dd, J = 8.1, 1.2 Hz, 1H), 8.31 (d, J = 8.2 Hz, 1H), 8.05 (d, J = 7.0 Hz, 1H), 7.94 (d, J = 9.1 Hz, 1H), 7.81 (ddd, J = 8.4, 7.0, 1.5 Hz, 1H), 7.77 – 7.72 (m, 3H), 7.67 – 7.62 (m, 3H), 7.57 – 7.51 (m, 1H), 6.81 – 6.77 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 148.2, 147.4, 145.0, 138.3, 130.0, 129.6, 129.6, 129.3, 128.9, 128.7, 127.2, 126.6, 122.7, 121.5, 120.5, 118.1, 112.0.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{14}N_3O$ 296.1183; found 296.1190.

6-(*p*-tolyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3b):[2]



Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 75% (233 mg);

Following the general **procedure (B)**, the title product was obtained as a white solid; Yield 66% (204 mg); mp: 238-240 °C

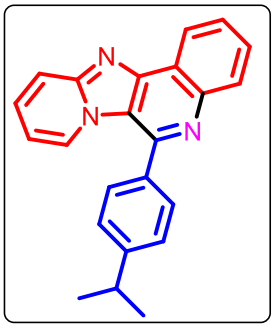
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (dd, J = 8.1, 1.1 Hz, 1H), 8.30 (d, J = 8.0 Hz, 1H), 8.13 (dd, J = 7.0, 1.0 Hz, 1H), 7.92 (d, J = 9.1 Hz, 1H), 7.80 (ddd, J = 8.4, 7.0, 1.5 Hz, 1H), 7.76 – 7.69 (m, 1H),

7.62 (d, *J* = 8.0 Hz, 2H), 7.53 (ddd, *J* = 9.1, 6.7, 1.2 Hz, 1H), 7.45 (d, *J* = 7.7 Hz, 2H), 6.79 (td, *J* = 6.9, 1.2 Hz, 1H), 2.53 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 148.4, 147.4, 145.1, 139.6, 135.4, 130.0, 129.9, 129.6, 128.9, 128.6, 127.3, 126.5, 122.6, 121.5, 120.5, 118.0, 111.9, 21.5.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{16}N_3$ 310.1339; found 310.1336.

6-(4-isopropylphenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3c):[3]



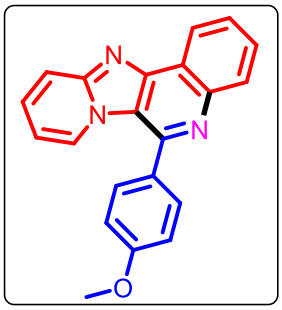
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 72% (243 mg); mp: 220-222 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.84 – 8.73 (m, 1H), 8.30 (dd, J = 8.3, 0.5 Hz, 1H), 8.18 (dt, J = 7.0, 1.1 Hz, 1H), 7.93 (dt, J = 9.1, 1.0 Hz, 1H), 7.82 – 7.70 (m, 2H), 7.68 – 7.63 (m, 2H), 7.56 – 7.47 (m, 3H), 6.81 (td, J = 6.9, 1.2 Hz, 1H), 3.14 – 3.00 (m, 1H), 1.37 (d, J = 6.9 Hz, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 150.6, 149.7, 148.4, 147.4, 145.1, 135.8, 129.9, 129.6, 128.9, 128.7, 127.4, 127.3, 126.5, 122.6, 121.4, 120.5, 118.0, 111.9, 34.2, 24.0.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{23}H_{20}N_3$ 338.1652; found 338.1653.

6-(4-methoxyphenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3d):[2]



Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 80% (261 mg);

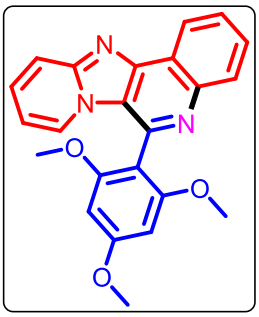
Following the general **procedure (B)**, the title product was obtained as a white solid; Yield 71% (231 mg); mp: 224-226 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (ddd, J = 8.0, 1.5, 0.4 Hz, 1H), 8.29 (dd, J = 8.3, 0.5 Hz, 1H), 8.18 (dt, J = 7.0, 1.1 Hz, 1H), 7.92 (dt, J = 9.1, 1.1 Hz, 1H), 7.83 – 7.76 (m, 1H), 7.75 – 7.64 (m, 3H), 7.53 (ddd, J = 9.1, 6.7, 1.3 Hz, 1H), 7.19 – 7.13 (m, 2H), 6.81 (td, J = 6.9, 1.2 Hz, 1H), 3.95 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 160.7, 149.7, 148.1, 147.5, 145.1, 130.7, 130.2, 129.9, 129.5, 128.9, 127.3, 126.4, 122.6, 121.4, 120.6, 118.1, 114.7, 111.9, 55.5.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{16}N_3O$ 326.1288; found 326.1292.

6-(2,4,6-trimethoxyphenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3e):[4]



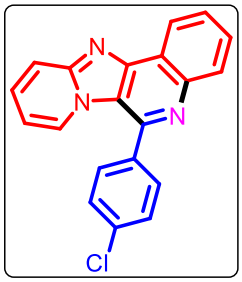
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 76% (293 mg); mp: 208-210 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (d, *J* = 7.2 Hz, 1H), 8.31 (d, *J* = 8.1 Hz, 1H), 8.13 (d, *J* = 7.0 Hz, 1H), 7.94 (d, *J* = 9.1 Hz, 1H), 7.86 – 7.69 (m, 2H), 7.56 (ddd, *J* = 9.0, 6.8, 1.1 Hz, 1H), 6.93 (s, 2H), 6.86 (td, *J* = 6.9, 1.0 Hz, 1H), 3.94 (d, *J* = 31.2 Hz, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 154.1, 149.8, 148.0, 147.5, 144.9, 139.0, 133.7, 130.1, 129.6, 129.0, 127.4, 126.7, 122.7, 121.6, 120.3, 118.1, 112.1, 105.6, 61.1, 56.3.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{23}H_{20}N_3O_3$ 386.1500; found 386.1499.

6-(4-chlorophenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3f):[5]



Following the general **procedure (A)**, the title product was obtained as an off white solid; Yield 71% (234 mg);

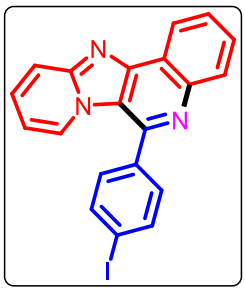
Following the general **procedure (B)**, the title product was obtained as an off white solid; Yield 61% (201 mg); mp: 282-284 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 7.9 Hz, 1H), 8.22 (d, *J* = 8.3 Hz, 1H), 8.03 (d, *J* = 7.0 Hz, 1H), 7.87 (d, *J* = 9.1 Hz, 1H), 7.74 (t, *J* = 7.3 Hz, 1H), 7.71 – 7.54 (m, 5H), 7.52 – 7.44 (m, 1H), 6.78 (t, *J* = 6.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.7, 146.9, 146.6, 145.8, 144.0, 135.8, 134.8, 129.2, 129.1, 128.6, 128.1, 126.0, 125.8, 121.7, 120.5, 119.3, 117.2, 111.2.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{13}ClN_3$ 330.0793 found 330.0774.

6-(4-iodophenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3g):



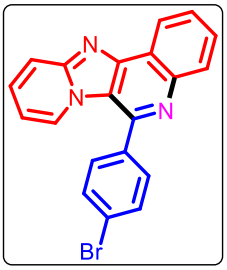
Following the general **procedure (A)**, the title product was obtained as a yellow solid; Yield 63% (266 mg); mp: 275-277 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 7.9 Hz, 1H), 8.28 (d, *J* = 8.3 Hz, 1H), 8.12 (t, *J* = 7.7 Hz, 1H), 7.97 (dd, *J* = 32.1, 8.6 Hz, 3H), 7.78 (dt, *J* = 31.8, 7.6 Hz, 2H), 7.60 – 7.46 (m, 3H), 6.86 (t, *J* = 6.6 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.8, 147.6, 147.0, 145.0, 138.5, 137.8, 132.5, 130.6, 130.1, 129.6, 129.1, 127.1, 126.8, 122.7, 121.5, 120.2, 118.2, 112.2.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{13}IN_3$ 422.0143 found 422.0122.

6-(4-bromophenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3h):[5]



Following the general **procedure (A)**, the title product was obtained as an off white solid; Yield 68% (254 mg);

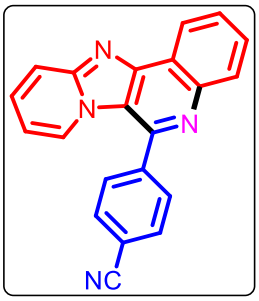
Following the general **procedure (B)**, the title product was obtained as an off white solid; Yield 63% (235 mg); mp: 230-232 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 7.2 Hz, 1H), 8.29 (d, *J* = 8.2 Hz, 1H), 8.11 (d, *J* = 6.9 Hz, 1H), 7.94 (d, *J* = 9.1 Hz, 1H), 7.81 (t, *J* = 8.3 Hz, 3H), 7.74 (t, *J* = 7.0 Hz, 1H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.59 – 7.53 (m, 1H), 6.85 (t, *J* = 6.5 Hz, 1H).

^{13}C NMR (125 MHz, CDCl3) δ 149.8, 147.6, 146.9, 145.0, 137.3, 132.5, 130.5, 130.1, 129.6, 129.1, 127.0, 126.8, 124.1, 122.7, 121.5, 119.9, 118.2, 112.2.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{13}BrN_3$ 374.0288; found 374.0272

4-(pyrido[2',1':2,3]imidazo[4,5-*c*]quinolin-6-yl)benzonitrile (3i):[2]



Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 56% (180 mg);

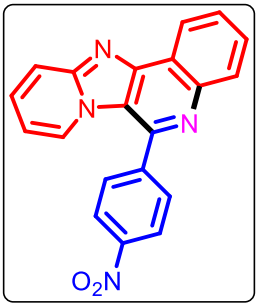
Following the general **procedure (B)**, the title product was obtained as a white solid; Yield 45% (144 mg); mp: 280-282 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 (dd, *J* = 8.1, 1.5 Hz, 1H), 8.31 – 8.26 (m, 1H), 8.01 (dt, *J* = 7.0, 1.2 Hz, 1H), 7.99 – 7.94 (m, 3H), 7.94 – 7.89 (m, 2H), 7.86 – 7.81 (m, 1H), 7.80 – 7.75 (m, 1H), 7.63 – 7.53 (m, 1H), 6.87 (td, *J* = 6.9, 1.3 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.9, 147.8, 145.8, 144.9, 142.9, 133.1, 130.3, 129.8, 129.6, 129.3, 127.2, 126.7, 122.8, 121.6, 120.0, 118.4, 118.3, 113.6, 112.5.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{13}N_4$ 321.1135; found 321.1190.

6-(4-nitrophenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3j):[3]



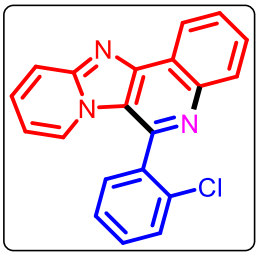
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 58% (198 mg); mp: 255-258 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.82 (d, *J* = 7.9 Hz, 1H), 8.51 (t, *J* = 14.2 Hz, 2H), 8.29 (d, *J* = 8.1 Hz, 1H), 8.07 – 7.93 (m, 4H), 7.80 (ddd, *J* = 28.2, 17.8, 10.3 Hz, 2H), 7.58 (dd, *J* = 19.8, 11.6 Hz, 1H), 6.87 (t, *J* = 6.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.9, 148.6, 147.9, 145.4, 144.9, 144.7, 130.3, 130.2, 129.7, 129.4, 127.3, 126.7, 124.5, 122.8, 121.7, 120.0, 118.5, 112.6.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{13}N_4O_2$ 341.1034; found 341.1020.

6-(2-chlorophenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3k):[2]



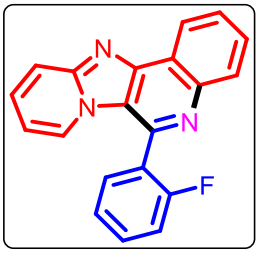
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 68% (239 mg); mp: 256-258 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.82 (dt, *J* = 14.9, 7.4 Hz, 1H), 8.32 (t, *J* = 10.3 Hz, 1H), 7.93 (t, *J* = 11.0 Hz, 1H), 7.83 (ddd, *J* = 8.4, 7.0, 1.6 Hz, 1H), 7.79 – 7.72 (m, 2H), 7.71 – 7.68 (m, 1H), 7.67 – 7.64 (m, 1H), 7.61 – 7.53 (m, 3H), 6.88 – 6.79 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 147.1, 145.3, 145.1, 137.1, 133.3, 131.2, 131.1, 130.0, 130.0, 129.7, 129.0, 128.0, 126.9, 126.6, 122.7, 121.8, 120.9, 118.0, 112.5.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{13}ClN_3$ 330.0793 found 330.0794.

6-(2-fluorophenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3l):



Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 60% (188 mg); mp: 271-273 °C

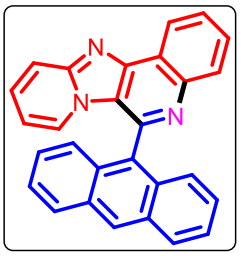
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.82 (dd, J = 8.0, 1.1 Hz, 1H), 8.35 – 8.27 (m, 1H), 7.97 (ddd, J = 28.7, 15.0, 5.2 Hz, 2H), 7.79 (dddd, J = 17.8, 15.1, 7.0, 1.3 Hz, 3H), 7.67 – 7.51 (m, 2H), 7.47 (td, J = 7.5, 1.0 Hz, 1H), 7.38 – 7.29 (m, 1H), 6.84 (td, J = 6.9, 1.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 160.9, 159.0, 149.7, 147.2, 145.2, 142.4, 131.9, 131.8, 131.5, 131.5, 130.0, 129.7, 128.9, 126.9, 126.7, 126.4, 126.3, 125.5, 125.5, 122.7, 121.7, 121.2, 118.1, 116.4, 116.2, 112.4.

^{19}F NMR (470 MHz, $CDCl_3$) δ -115.97.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{13}FN_3$ 314.1089 found 314.1089.

6-(anthracen-9-yl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3m):



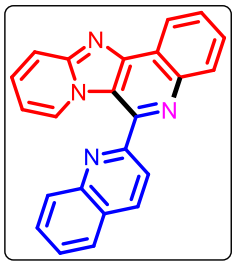
Following the general **procedure (A)**, the title product was obtained as a yellow solid; Yield 82% (317 mg); mp: 245-246 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.95 (dd, J = 7.9, 1.3 Hz, 1H), 8.74 (s, 1H), 8.39 (d, J = 7.6 Hz, 1H), 8.16 (d, J = 8.6 Hz, 2H), 7.87 (ddd, J = 15.2, 11.4, 5.1 Hz, 3H), 7.52 – 7.42 (m, 4H), 7.40 – 7.35 (m, 1H), 7.29 (dd, J = 11.0, 4.2 Hz, 2H), 6.72 (d, J = 7.0 Hz, 1H), 6.34 (dd, J = 9.9, 3.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 147.2, 146.0, 145.7, 131.6, 130.5, 130.1, 130.0, 130.0, 129.1, 128.9, 128.8, 127.1, 127.0, 126.5, 125.8, 125.2, 122.8, 122.5, 121.8, 117.8, 112.4.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{28}H_{18}N_3$ 386.1496 found 386.1482.

6-(quinolin-2-yl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3n):[6]



Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 52% (180 mg);

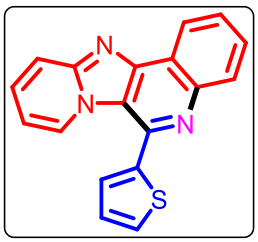
Following the general **procedure (C)**, the title product was obtained as a white solid; Yield 38% (131 mg); mp: 160-162 °C

^{1}H NMR (500 MHz, $CDCl_3$) *δ* 9.44 (d, *J* = 6.9 Hz, 1H), 8.85 (d, *J* = 7.9 Hz, 1H), 8.53 (dd, *J* = 26.7, 8.4 Hz, 2H), 8.34 (d, *J* = 8.0 Hz, 1H), 8.21 (d, *J* = 8.2 Hz, 1H), 7.99 (dd, *J* = 23.2, 8.4 Hz, 2H), 7.92 – 7.66 (m, 4H), 7.64 – 7.54 (m, 1H), 6.90 (t, *J* = 6.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) *δ* 157.0, 150.1, 148.5, 146.9, 146.8, 144.7, 137.7, 130.6, 130.4, 130.3, 129.7, 129.2, 128.9, 128.3, 128.0, 127.6, 127.1, 122.8, 122.5, 122.0, 121.3, 117.7, 111.3.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{23}H_{15}N_4$ 347.1292 found 347.1277.

6-(thiophen-2-yl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3o):[2]



Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 55% (181 mg); mp: 218-220 °C

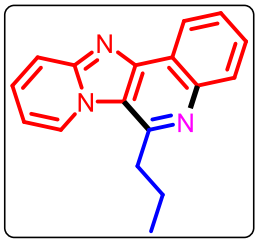
^{1}H NMR (500 MHz, $CDCl_3$) *δ* 8.78 (dd, *J* = 8.1, 1.1 Hz, 1H), 8.38 (dt, *J* = 7.0, 1.1 Hz, 1H), 8.33 – 8.25 (m, 1H), 7.93 (d, *J* = 9.1 Hz, 1H), 7.84 – 7.70 (m, 2H), 7.65 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.56

(ddd, *J* = 9.1, 6.7, 1.2 Hz, 1H), 7.49 (dt, *J* = 10.0, 5.0 Hz, 1H), 7.31 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.88 (td, *J* = 6.9, 1.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.8, 147.6, 144.9, 141.5, 139.7, 130.1, 129.7, 129.0, 128.4, 128.2, 127.7, 127.2, 126.9, 122.7, 121.6, 120.8, 118.3, 112.1.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{12}N_3S$ 330.0747 found 330.0782.

6-propylpyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3p):[2]



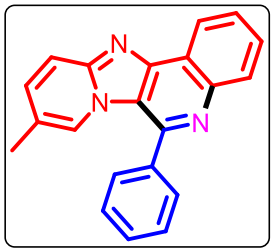
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 71% (186 mg); mp: 120-122 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (dd, *J* = 12.9, 4.4 Hz, 2H), 8.21 (d, *J* = 8.3 Hz, 1H), 7.97 (d, *J* = 9.1 Hz, 1H), 7.81 – 7.73 (m, 1H), 7.68 (t, *J* = 7.1 Hz, 1H), 7.63 – 7.56 (m, 1H), 7.12 (t, *J* = 6.4 Hz, 1H), 3.56 – 3.32 (m, 2H), 2.00 (dq, *J* = 15.0, 7.4 Hz, 2H), 1.21 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.8, 149.3, 147.0, 144.8, 129.3, 128.8, 128.7, 127.3, 126.0, 122.6, 121.4, 121.3, 118.4, 112.8, 39.0, 21.5, 14.1.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}N_3$ 262.1339 found 262.1339.

9-methyl-6-phenylpyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3q):[5]



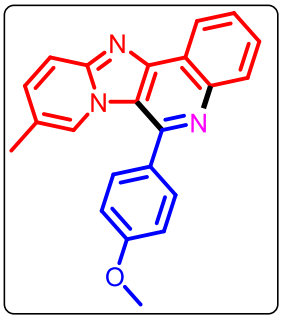
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 82% (239 mg); mp: 160-162 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.78 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.30 (d, *J* = 8.2 Hz, 1H), 7.81 (dd, *J* = 8.4, 5.4 Hz, 1H), 7.79 – 7.77 (m, 2H), 7.75 – 7.70 (m, 3H), 7.67 – 7.62 (m, 3H), 7.37 (dd, *J* = 9.2, 1.5 Hz, 1H), 2.21 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.8, 148.3, 147.3, 144.9, 138.4, 133.1, 129.6, 129.8, 129.2, 128.8, 126.5, 125.0, 122.5, 121.7, 121.6, 120.4, 117.3, 18.4.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}N_3$ 310.1339 found 310.1359.

6-(4-methoxyphenyl)-9-methylpyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3r):[5]



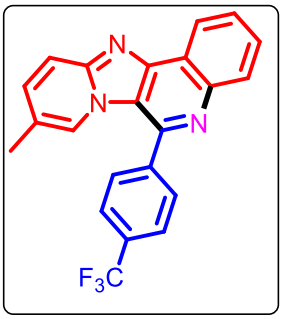
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 79% (268 mg); mp: 278-280 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 7.9 Hz, 1H), 8.28 (d, *J* = 8.2 Hz, 1H), 7.95 (s, 1H), 7.79 (dd, *J* = 19.9, 8.5 Hz, 2H), 7.69 (t, *J* = 7.9 Hz, 3H), 7.37 (d, *J* = 9.1 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 3.95 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 160.7, 148.7, 148.1, 147.3, 144.9, 133.0, 130.7, 130.3, 129.4, 128.6, 126.3, 125.0, 122.5, 121.6, 121.5, 120.4, 117.2, 114.5, 55.6, 18.5.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}N_3$ 340.1445 found 340.1420.

9-methyl-6-(4-(trifluoromethyl)phenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3s):[5]



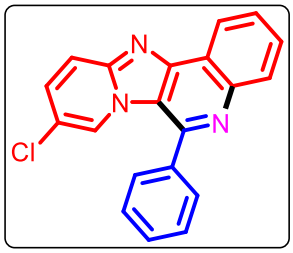
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 62% (210 mg); mp: 282-284 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.78 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.27 (d, *J* = 8.2 Hz, 1H), 7.92 (q, *J* = 8.4 Hz, 4H), 7.82 (ddd, *J* = 12.3, 9.7, 5.4 Hz, 2H), 7.78 – 7.70 (m, 2H), 7.40 (dd, *J* = 9.2, 1.5 Hz, 1H), 2.24 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.9, 147.6, 146.4, 144.8, 142.1, 133.3, 131.9, 131.6, 129.6, 129.5, 129.0, 126.9, 126.2, 126.1, 125.4, 124.5, 122.6, 122.1, 121.6, 120.0, 117.5, 18.5.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}N_3$ 340.1445 found 340.1420.

9-chloro-6-phenylpyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3t):[2]



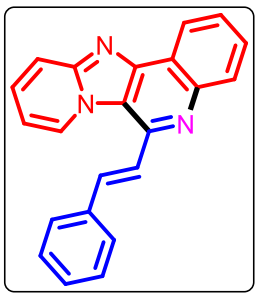
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 64% (211 mg); mp: 158-160 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 7.9 Hz, 1H), 8.31 (d, *J* = 8.3 Hz, 1H), 8.04 (d, *J* = 1.0 Hz, 1H), 7.90 – 7.79 (m, 2H), 7.77 – 7.63 (m, 6H), 7.47 (dd, *J* = 9.6, 1.9 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 146.4, 145.1, 137.5, 131.2, 130.0, 129.7, 129.5, 129.2, 128.6, 126.9, 125.1, 122.6, 121.4, 121.0, 120.0, 118.3, 109.4.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}N_3$ 330.0793 found 330.0788

(*E*)-6-styrylpyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3u):[2]



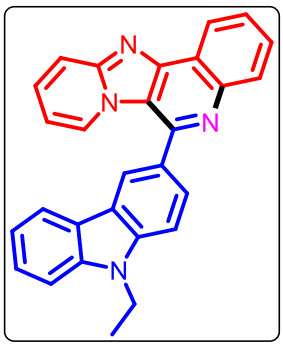
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 48% (154 mg); mp: 190-192 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.92 (d, *J* = 6.6 Hz, 1H), 8.72 (d, *J* = 7.2 Hz, 1H), 8.25 (d, *J* = 8.1 Hz, 1H), 7.93 (d, *J* = 15.4 Hz, 2H), 7.85 – 7.64 (m, 5H), 7.60 – 7.51 (m, 1H), 7.50 – 7.35 (m, 3H), 7.04 (t, *J* = 6.6 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.5, 147.2, 145.1, 144.6, 138.1, 136.2, 129.6, 129.3, 129.2, 128.9, 128.9, 127.8, 127.5, 126.3, 123.1, 122.6, 121.5, 120.8, 118.3, 112.7.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{22}H_{16}N_3$ 322.1339 found 322.1337.

6-(9-ethyl-9*H*-carbazol-3-yl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3v):



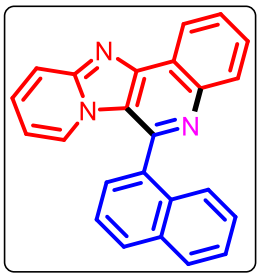
Following the general **procedure (A)**, the title product was obtained as a white solid; Yield 35% (144-mg); mp: 288-290 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.82 (d, *J* = 7.3 Hz, 1H), 8.52 – 8.32 (m, 2H), 8.12 (dd, *J* = 16.9, 8.7 Hz, 2H), 7.94 (d, *J* = 9.1 Hz, 1H), 7.87 – 7.62 (m, 4H), 7.58 – 7.47 (m, 3H), 7.26 (dd, *J* = 8.4, 5.3 Hz, 1H), 6.69 (t, *J* = 6.4 Hz, 1H), 4.49 (q, *J* = 7.2 Hz, 2H), 1.53 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.8, 149.3, 147.5, 145.0, 140.6, 130.0, 129.4, 128.9, 128.5, 127.3, 126.4, 126.4, 126.3, 123.5, 122.9, 122.7, 121.4, 121.1, 120.9, 119.4, 118.0, 112.0, 109.3, 108.8, 37.8, 13.9.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{28}H_{21}N_4$ 413.1761 found 413.1743.

6-(naphthalen-1-yl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3w):[2]



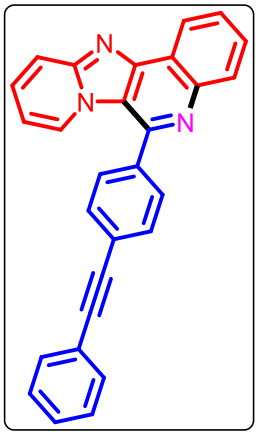
Following the general **procedure (B)**, the title product was obtained as a white solid; Yield 75% (259 mg); mp: 245-247 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.87 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.35 (dd, *J* = 8.2, 0.6 Hz, 1H), 8.11 (t, *J* = 11.5 Hz, 1H), 8.02 (d, *J* = 8.3 Hz, 1H), 7.95 – 7.87 (m, 1H), 7.87 – 7.67 (m, 4H), 7.58 – 7.49 (m, 1H), 7.49 – 7.37 (m, 2H), 7.32 (ddd, *J* = 8.3, 6.8, 1.2 Hz, 1H), 7.29 – 7.21 (m, 1H), 6.53 (td, *J* = 6.9, 1.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 147.1, 147.0, 145.3, 135.3, 133.8, 131.3, 130.0, 129.9, 129.8, 129.0, 128.7, 127.5, 127.1, 126.9, 126.8, 126.7, 125.9, 124.8, 122.7, 121.7, 121.6, 117.9, 112.2.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{16}N_3$ 346.1339 found 346.1334.

6-(4-(phenylethynyl)phenyl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3x):



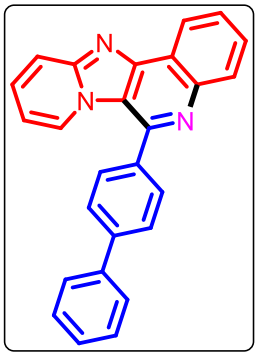
The title product was obtained as a white solid; Yield 48% (45 mg); mp: 145-146 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (d, *J* = 7.9 Hz, 1H), 8.30 (d, *J* = 8.2 Hz, 1H), 8.12 (d, *J* = 7.0 Hz, 1H), 7.93 (d, *J* = 9.1 Hz, 1H), 7.86 – 7.71 (m, 6H), 7.65 – 7.50 (m, 3H), 7.45 – 7.35 (m, 3H), 6.82 (t, *J* = 6.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 147.6, 147.5, 145.1, 138.0, 132.5, 131.7, 130.1, 129.6, 129.0, 128.9, 128.7, 128.5, 127.2, 126.8, 124.7, 122.9, 122.7, 121.5, 120.3, 118.1, 112.2, 91.2, 88.8.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{28}H_{18}N_3$ 396.1496 found 396.1483.

6-([1,1'-biphenyl]-4-yl)pyrido[2',1':2,3]imidazo[4,5-*c*]quinoline (3y):



The title product was obtained as a white solid; Yield 54% (53 mg); mp: 235-238 °C

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 (d, *J* = 8.0 Hz, 1H), 8.28 (dd, *J* = 42.7, 7.6 Hz, 2H), 7.91 (dd, *J* = 26.6, 8.6 Hz, 3H), 7.85 – 7.79 (m, 3H), 7.77 – 7.71 (m, 3H), 7.57 – 7.49 (m, 3H), 7.43 (t, *J* = 7.4 Hz, 1H), 6.86 – 6.77 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 147.9, 147.5, 145.1, 142.5, 140.3, 137.2, 130.0, 129.6, 129.3, 129.0, 129.0, 128.0, 127.9, 127.3, 127.2, 126.6, 122.7, 121.5, 120.5, 118.1, 112.0.

HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{26}H_{18}N_3$ 372.1496 found 372.1497.

6. Antibiotic susceptibility testing against pathogenic mycobacteria:[8]

The newly synthesized compounds were tested for antimycobacterial susceptibility using a broth microdilution assay. Test and control compound stock solutions were prepared in DMSO at 1 g/100 mL and kept at -20°C. Mycobacterial cultures were inoculated in Middlebrook 7H9 enriched (Difco, Becton, NJ, USA) media supplemented with 10% ADC-Tween-80 (Bovine Serum Albumin, Dextrose, 0.2% glycerol and 0.05% Tween-80) and OD600 of the cultures was measured, followed by dilution to achieve ~106 cfu/mL. Assays were performed on newly synthesized compounds between 0.0064 and 0.00005 g/100 mL diluted two-fold in 96-well micro-titre plates, 2.5 µL of each concentration was added per well. To each well containing the test compound, 97.5 µL of bacterial suspension were added, along with appropriate controls. For the visual identification of active compounds, presto blue resazurin dye (Thermo Fisher, USA) was used. After incubation, the MIC of an active compound was determined as the lowest concentration that inhibits visible growth. MIC determinations were replicated three times using duplicate samples for each compound. The MIC plates were incubated at 37°C for 7 days for Mtb.

7. References:

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3 X.-S. Fan, J. Zhang, B. Li and X.-Y. Zhang, *Chem. - An Asian J.*, 2015, **10**, 1281–1285.

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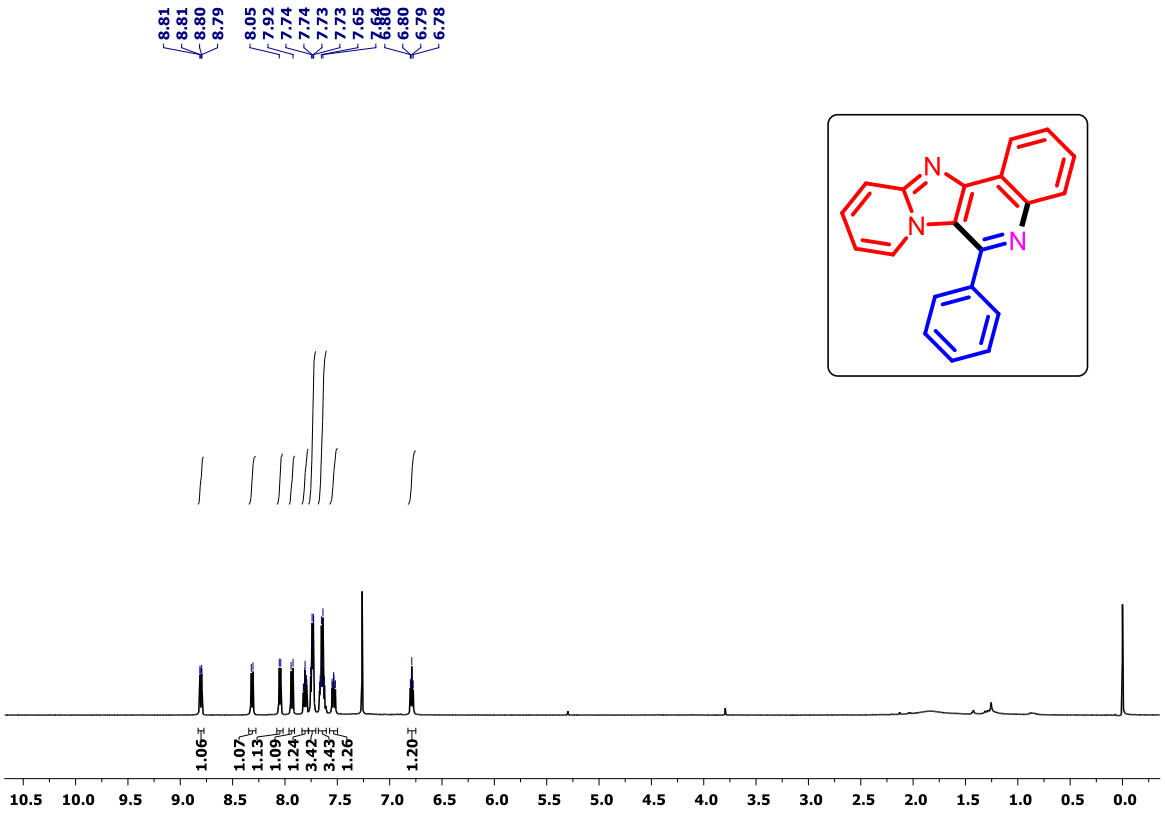
6 G. Sai Mani, A. V. Subba Rao, Y. Tangella, S. Sunkari, F. Sultana, H. Krishna Namballa, N. Shankaraiah and A. Kamal, *New J. Chem.*, 2018, **42**, 15820–15829.

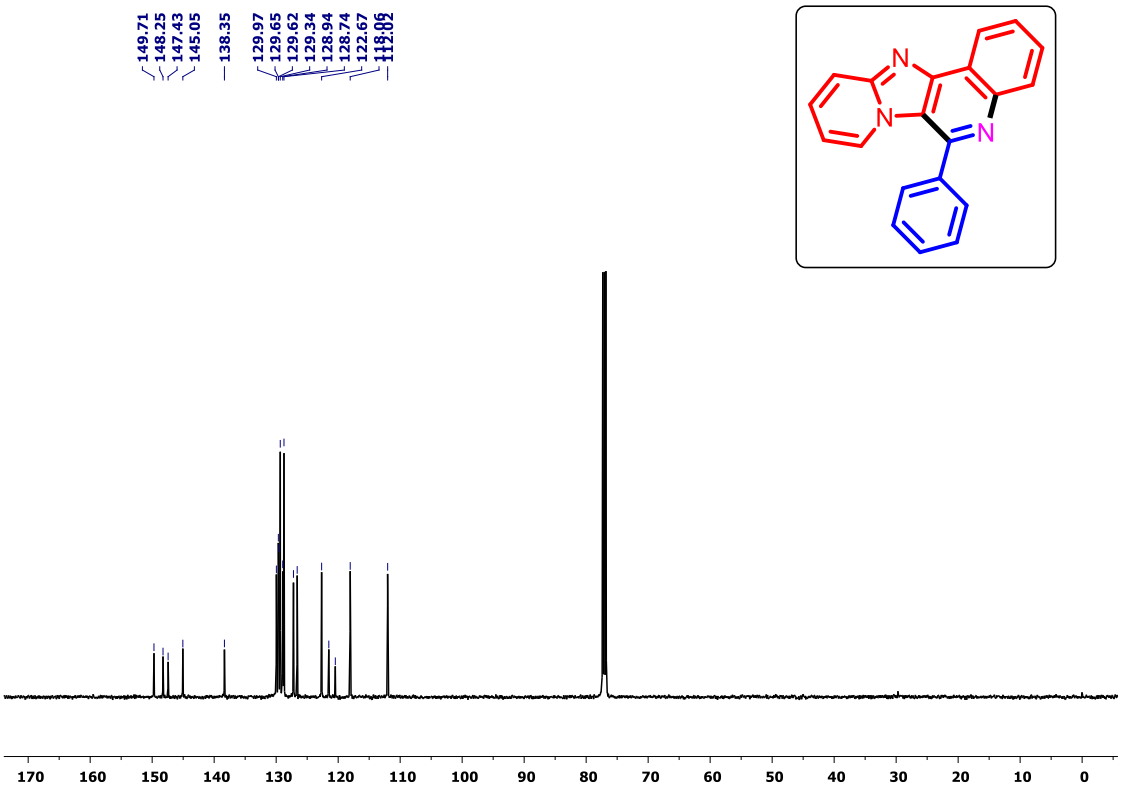
7 B. Sridevi, S. Reddy Kandimalla and B. V Subba Reddy, *European J. Org. Chem.*, 2019, **2019**, 6800–6806.

8. S. Malasala, M. N. Ahmad, R. Akunuri, M. Shukla, G. Kaul, A. Dasgupta, Y. V. Madhavi, S. Chopra, and S. Nanduri. Eur. J. Med. Chem. 2021, 212, 112996.

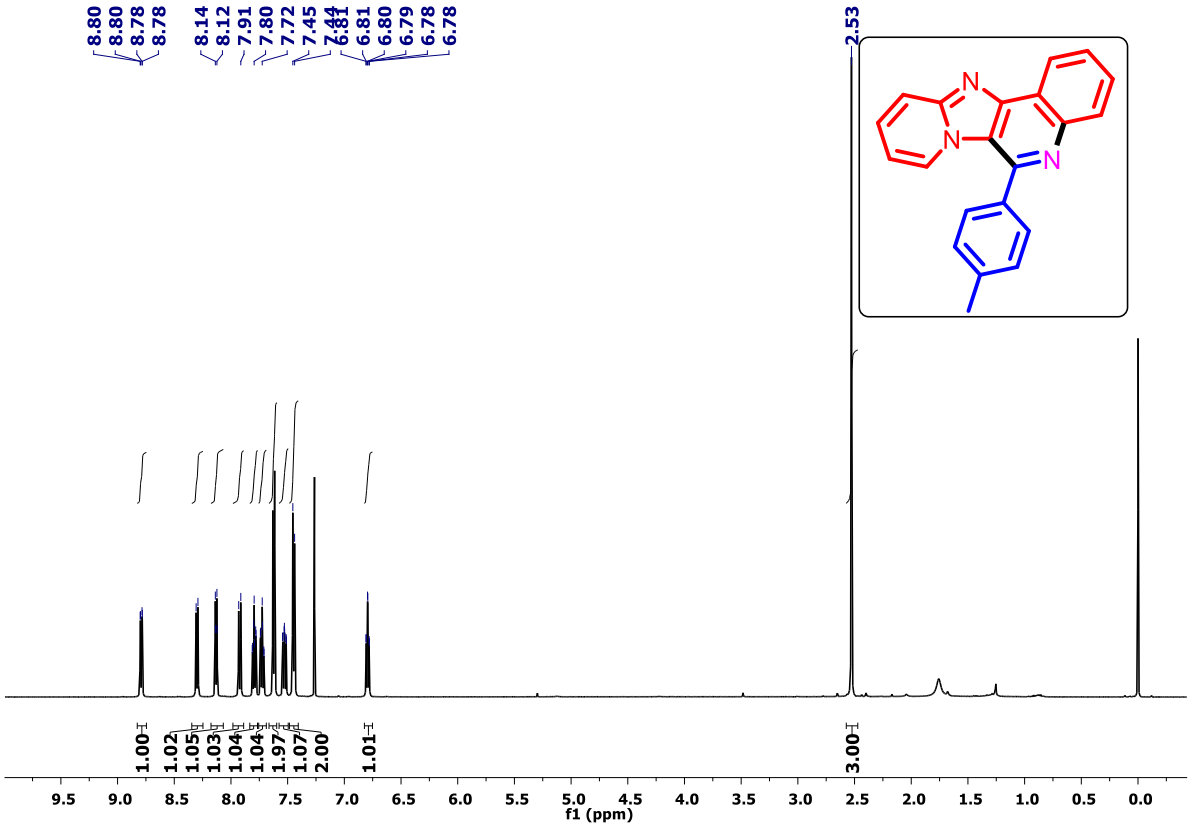
8. ^{1}H NMR, ^{13}C NMR Spectra of the compounds:



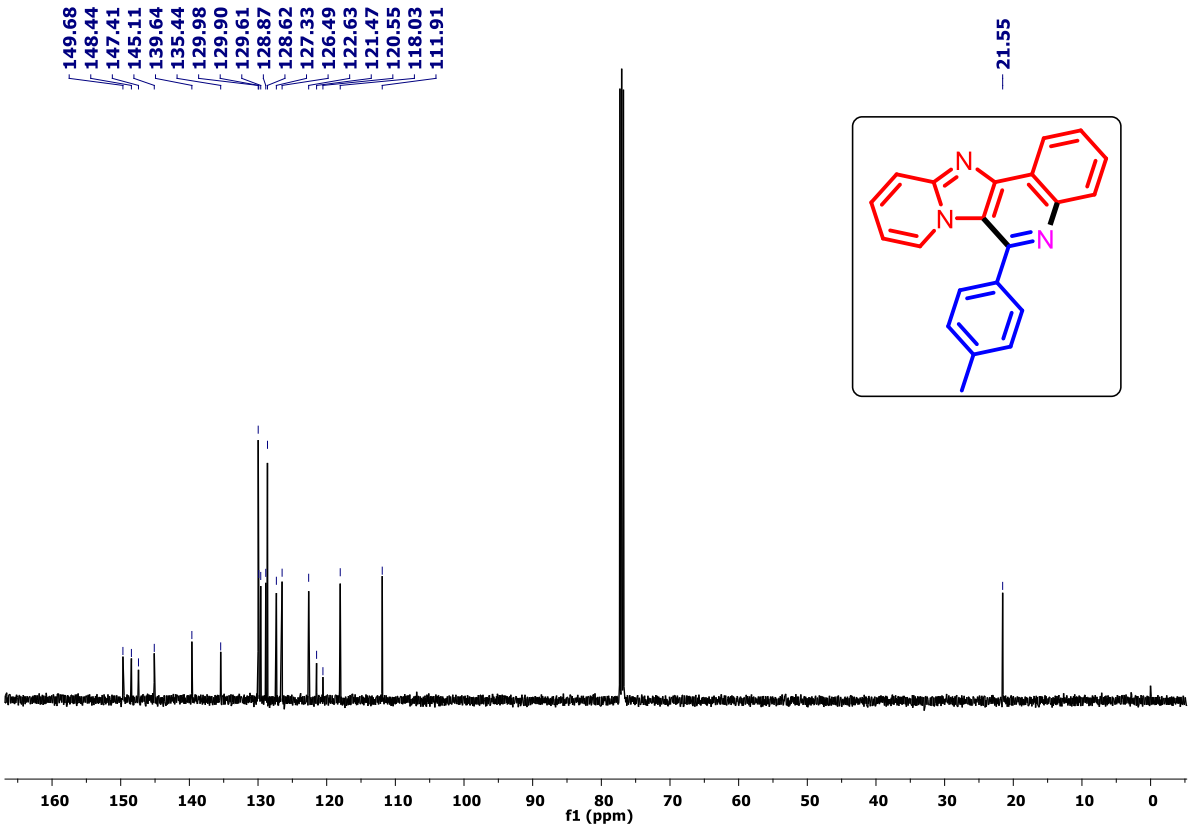
^{1}H NMR spectrum of compound **3a** ($CDCl_3$, 500 MHz)



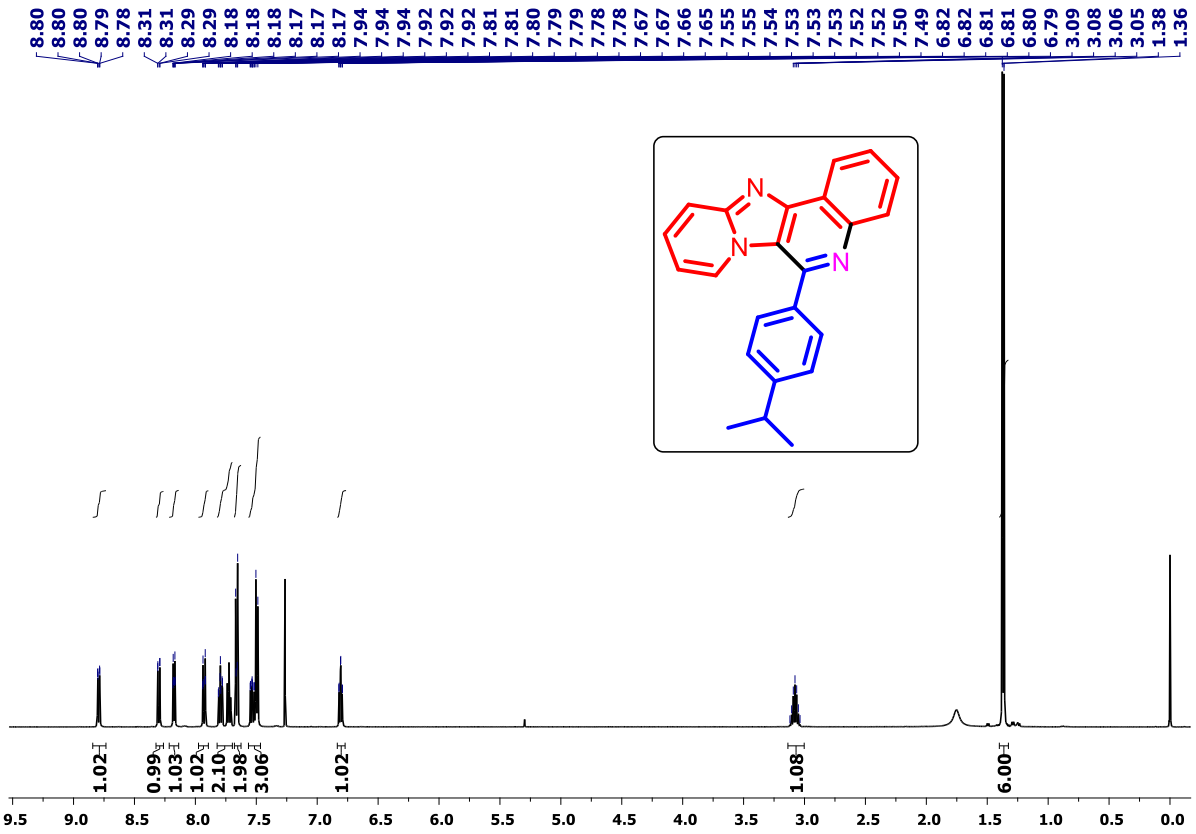
^{13}C NMR spectrum of compound **3a** ($CDCl_3$, 125 MHz)



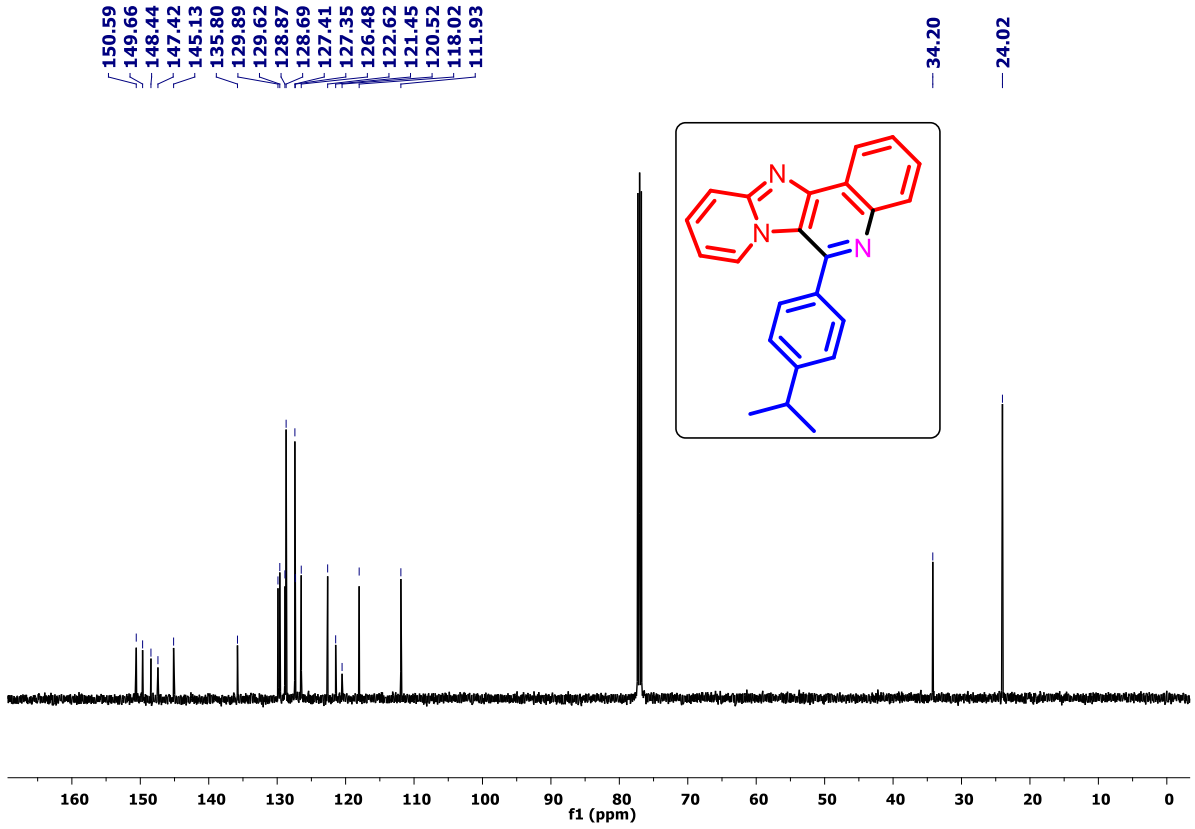
^{1}H NMR spectrum of compound **3b** ($CDCl_3$, 500 MHz)



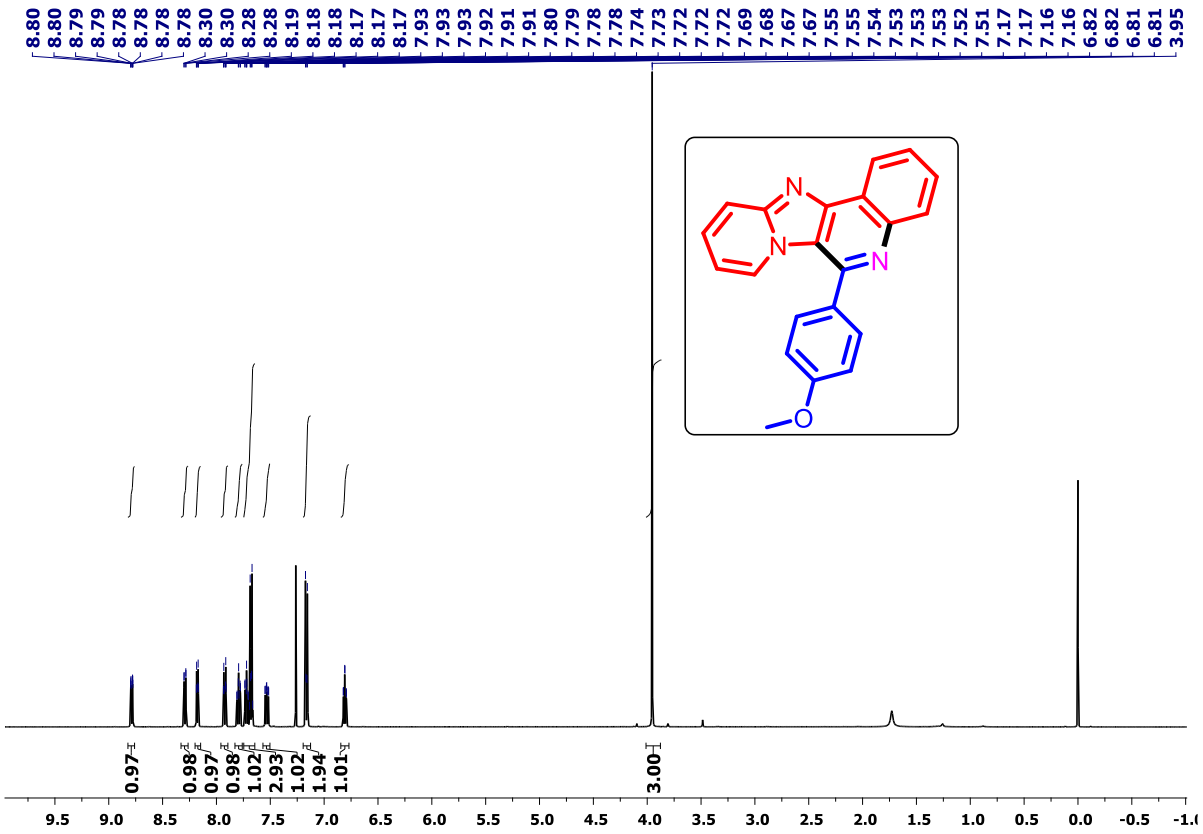
^{13}C NMR spectrum of compound **3b** ($CDCl_3$, 125 MHz)



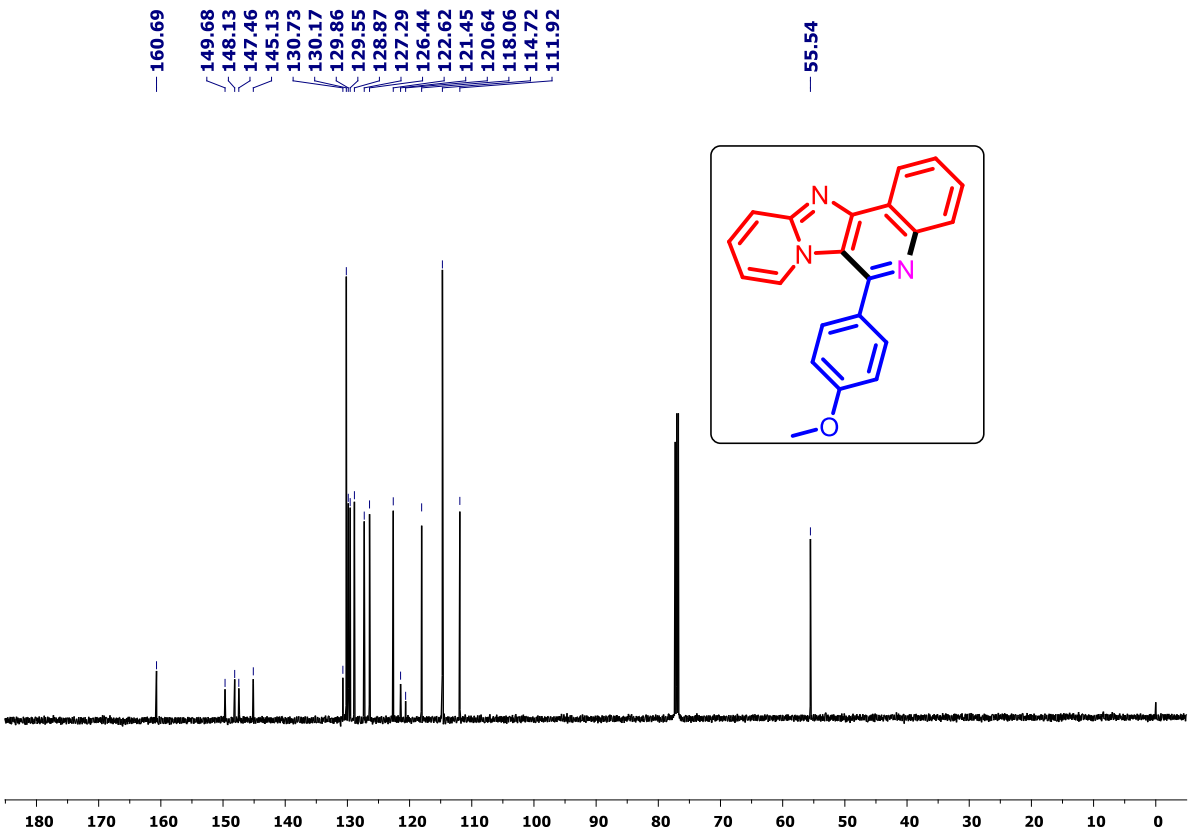
^{1}H NMR spectrum of compound **3c** ($CDCl_3$, 500 MHz)



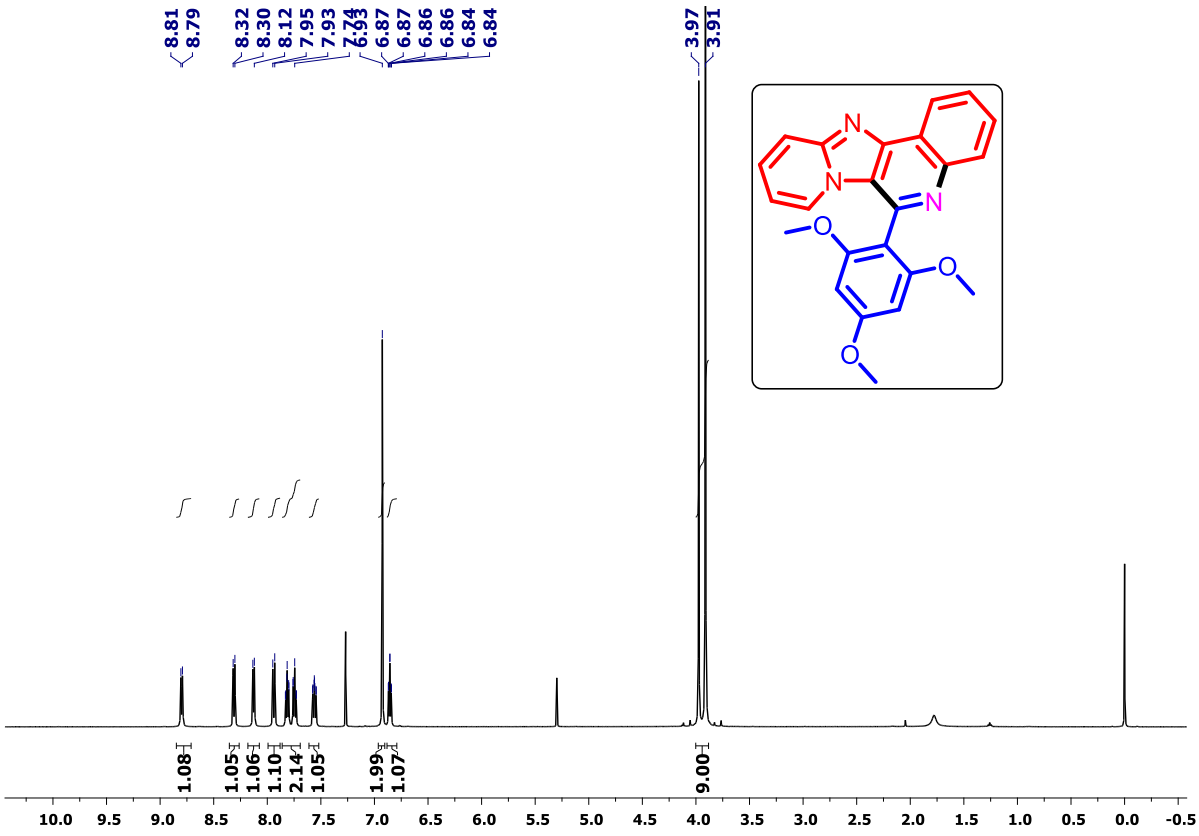
^{13}C NMR spectrum of compound **3c** ($CDCl_3$, 500 MHz)



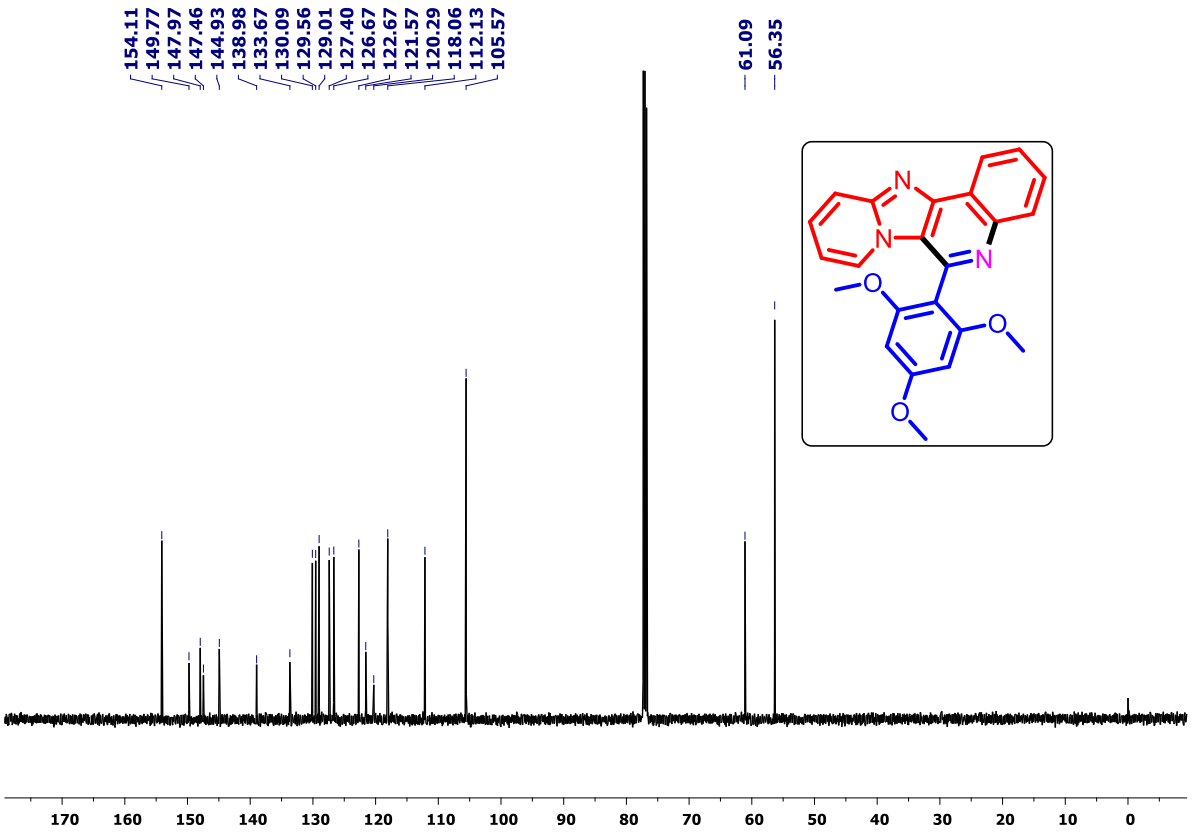
^{1}H NMR spectrum of compound **3d** ($CDCl_3$, 500 MHz)



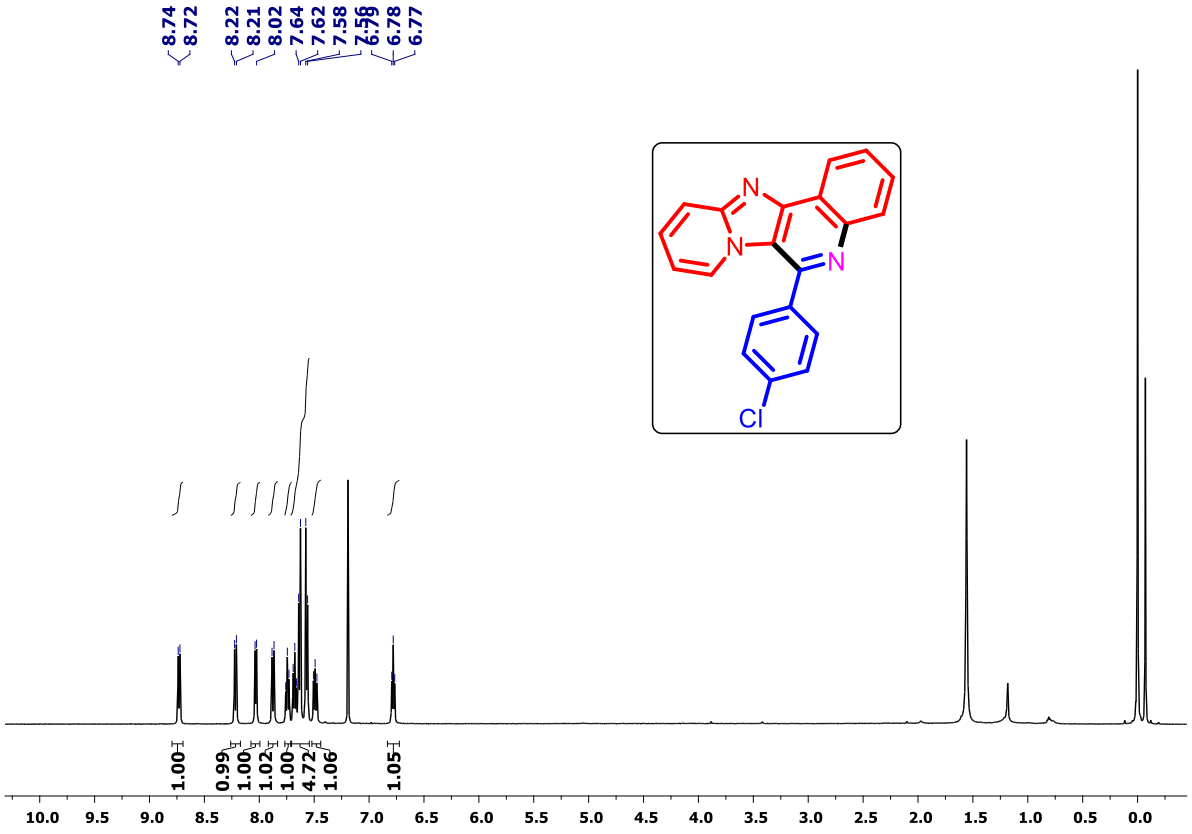
^{13}C NMR spectrum of compound **3d** ($CDCl_3$, 125 MHz)



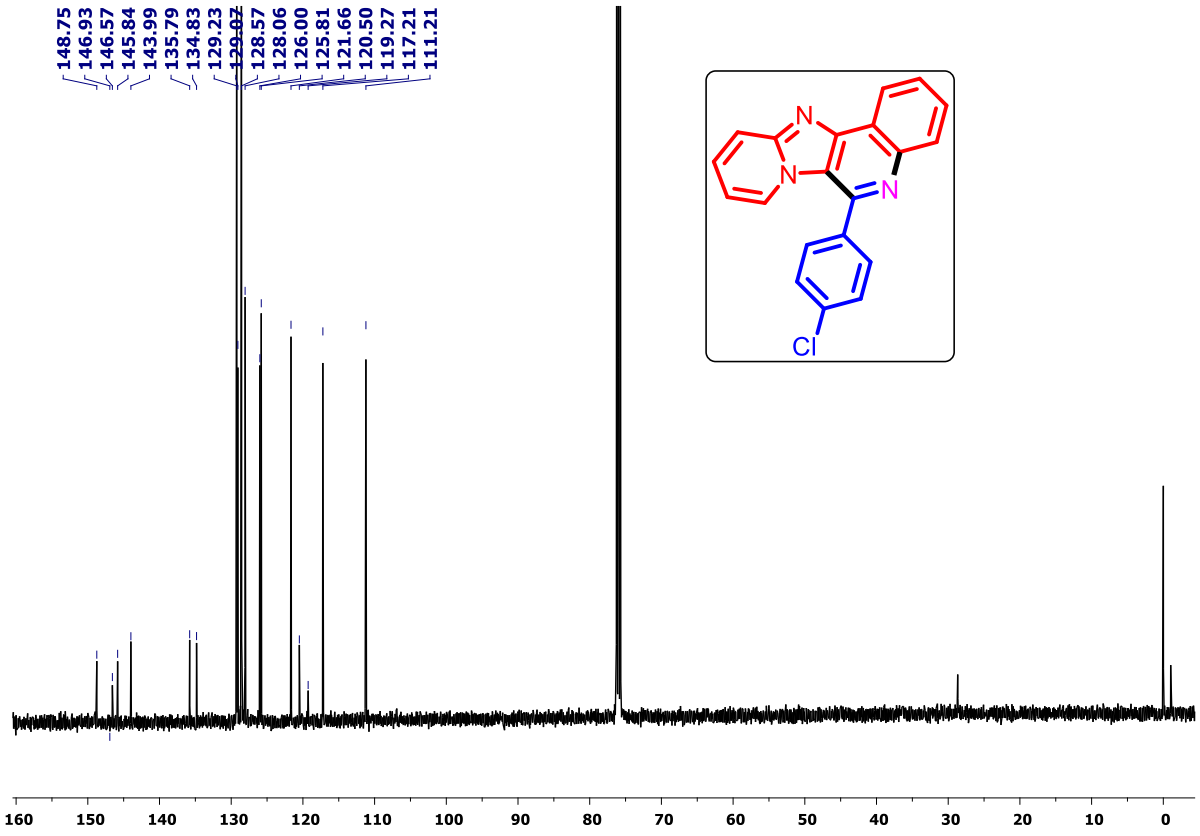
^{1}H NMR spectrum of compound **3e** ($CDCl_3$, 500 MHz)



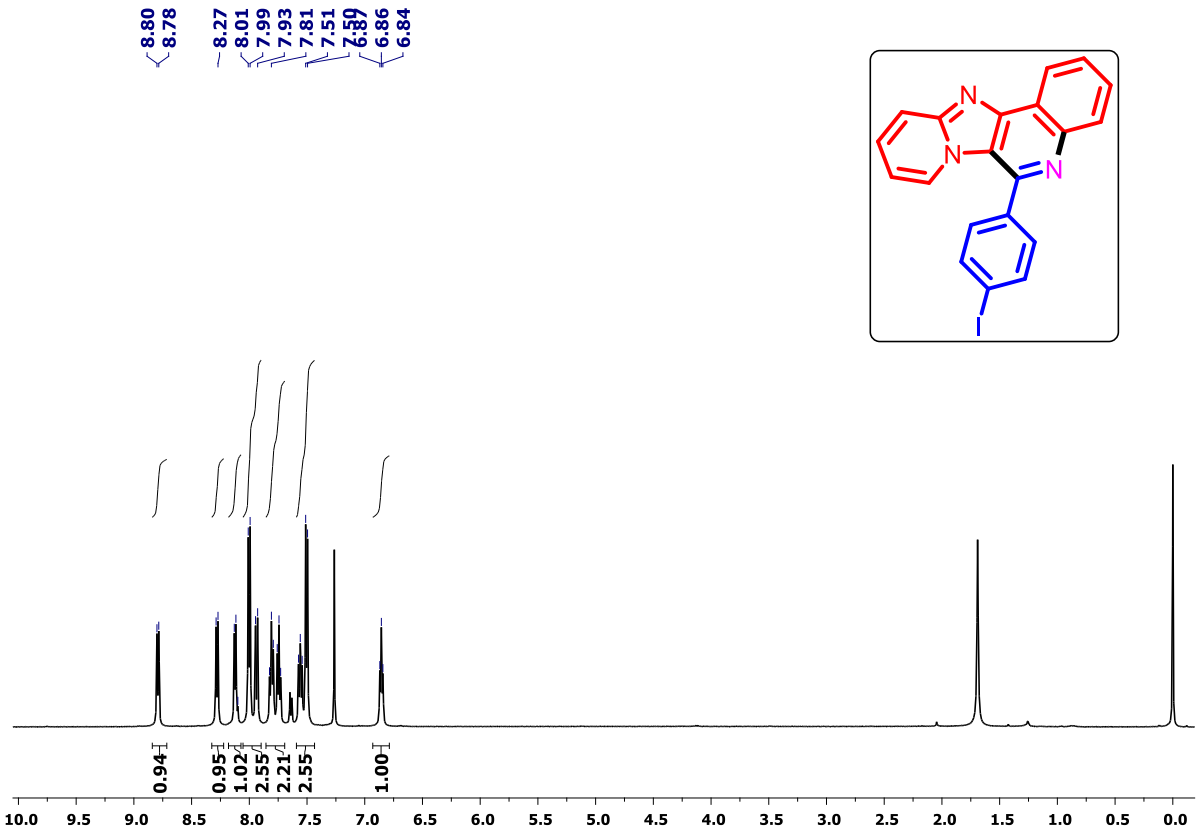
^{13}C NMR spectrum of compound **3e** ($CDCl_3$, 125 MHz)



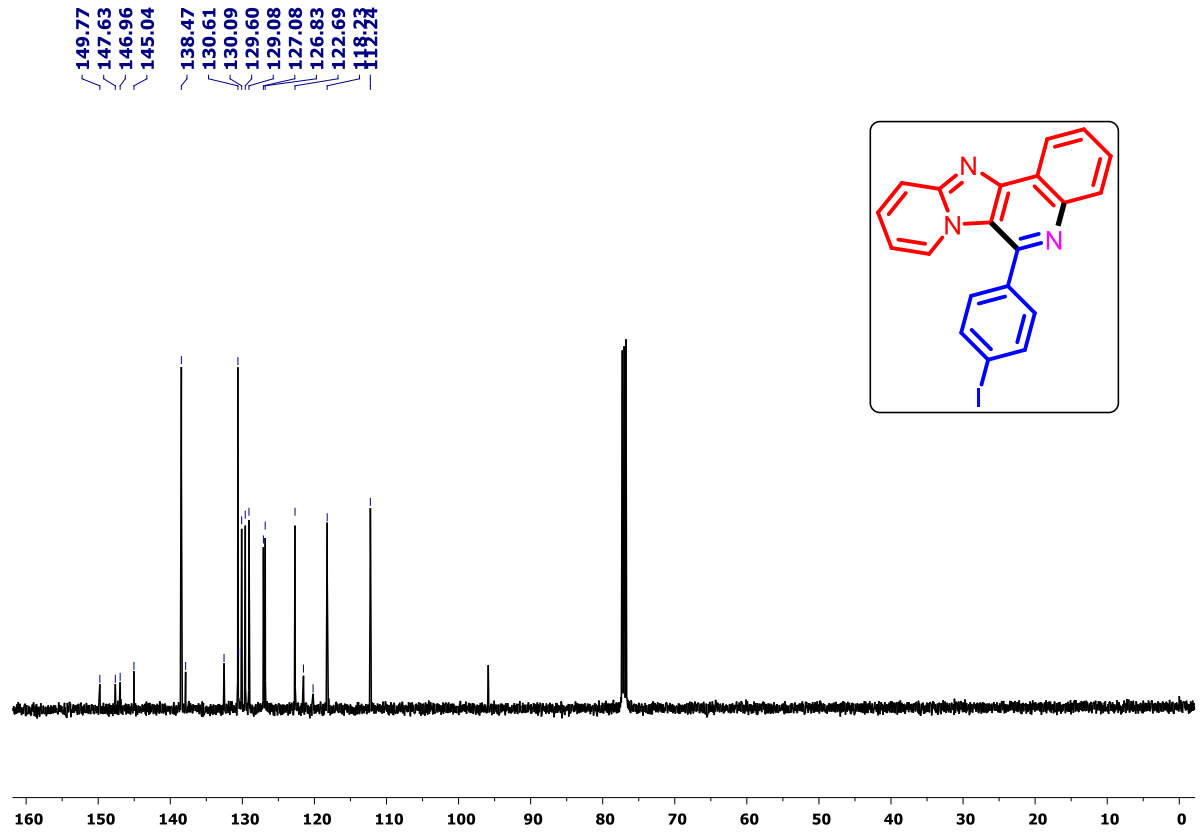
^{1}H NMR spectrum of compound **3f** ($CDCl_3$, 500 MHz)



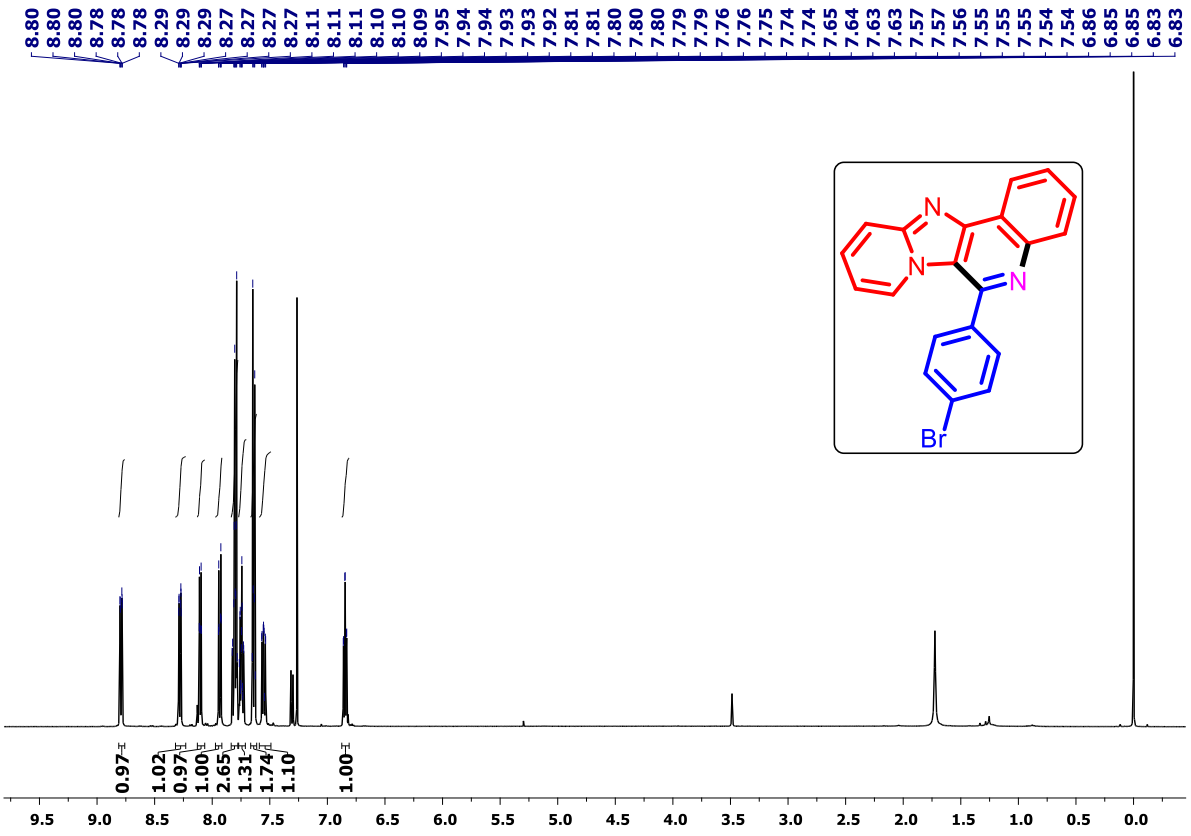
^{13}C NMR spectrum of compound **3f** ($CDCl_3$, 125 MHz)



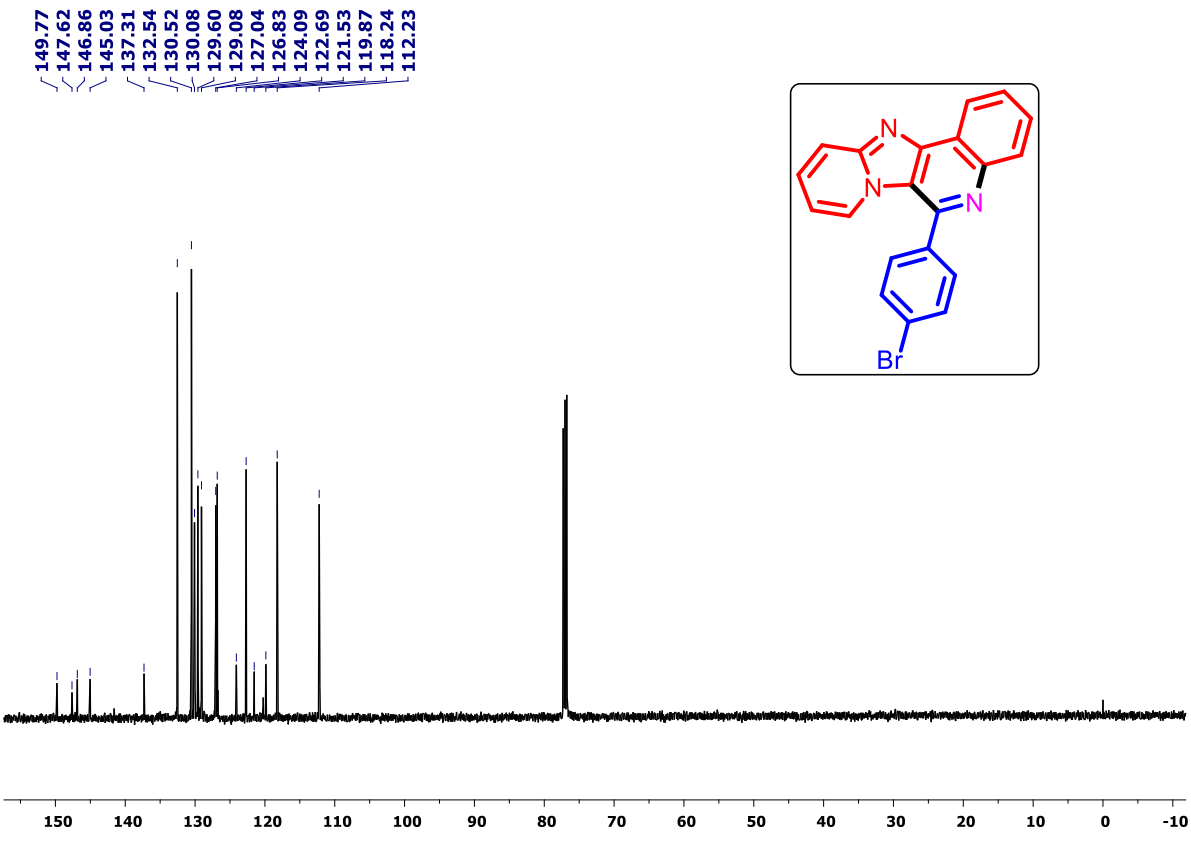
^{1}**H NMR** spectrum of compound **3g** ($CDCl_3$, 500 MHz)



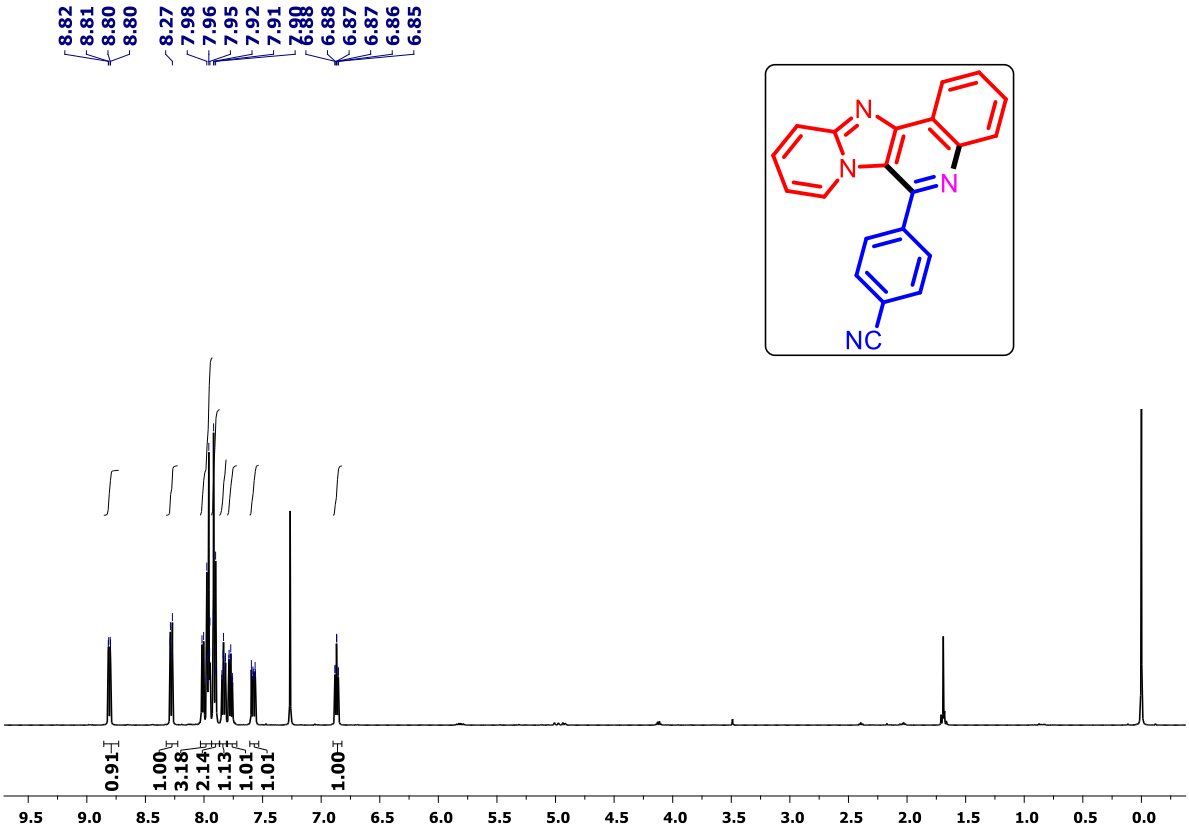
^{13}**C NMR** spectrum of compound **3g** ($CDCl_3$, 125 MHz)



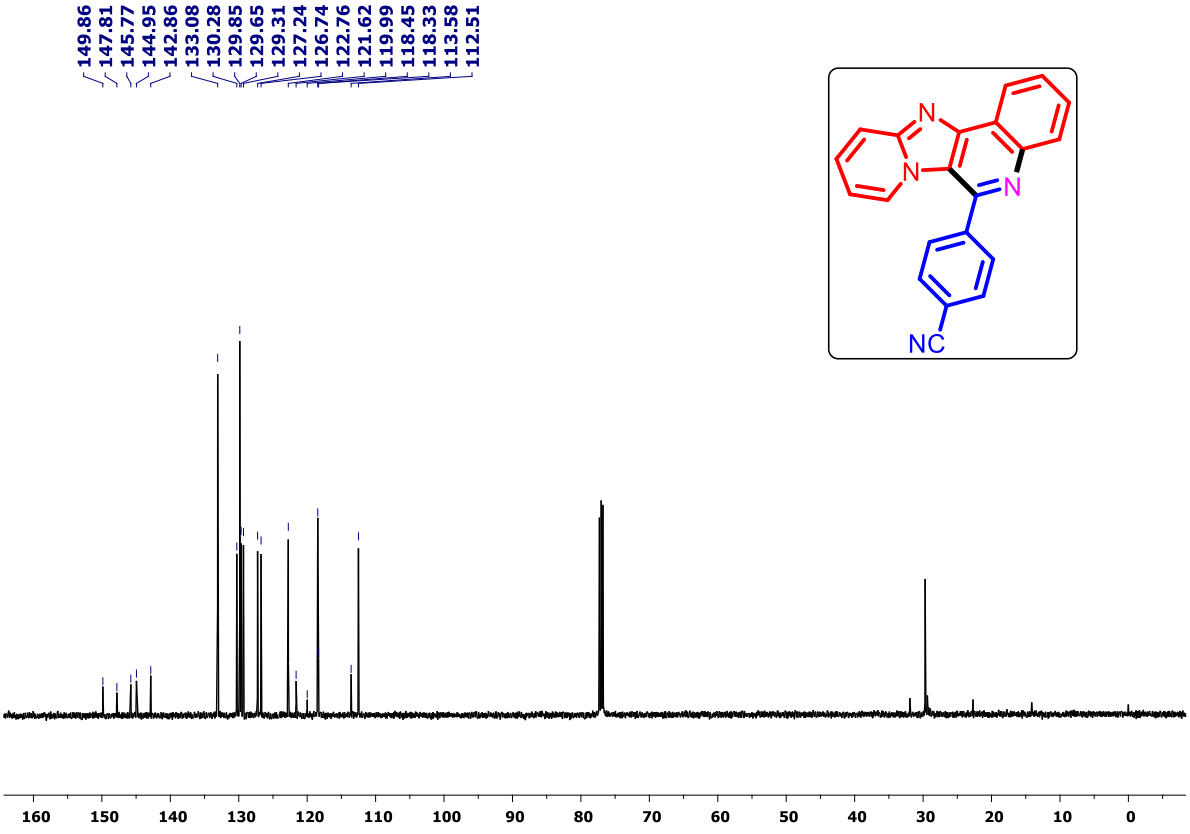
^{1}H NMR spectrum of compound **3h** ($CDCl_3$, 500 MHz)



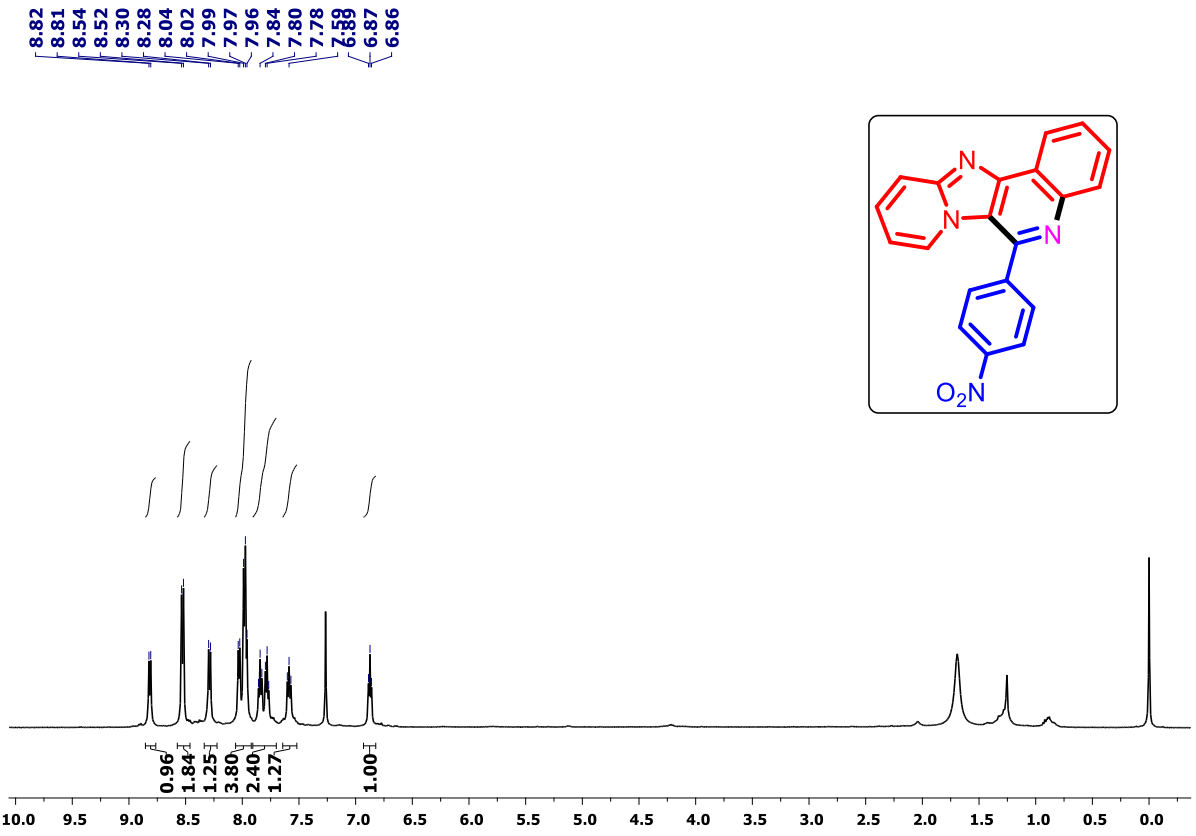
^{13}C NMR spectrum of compound **3h** ($CDCl_3$, 125 MHz)



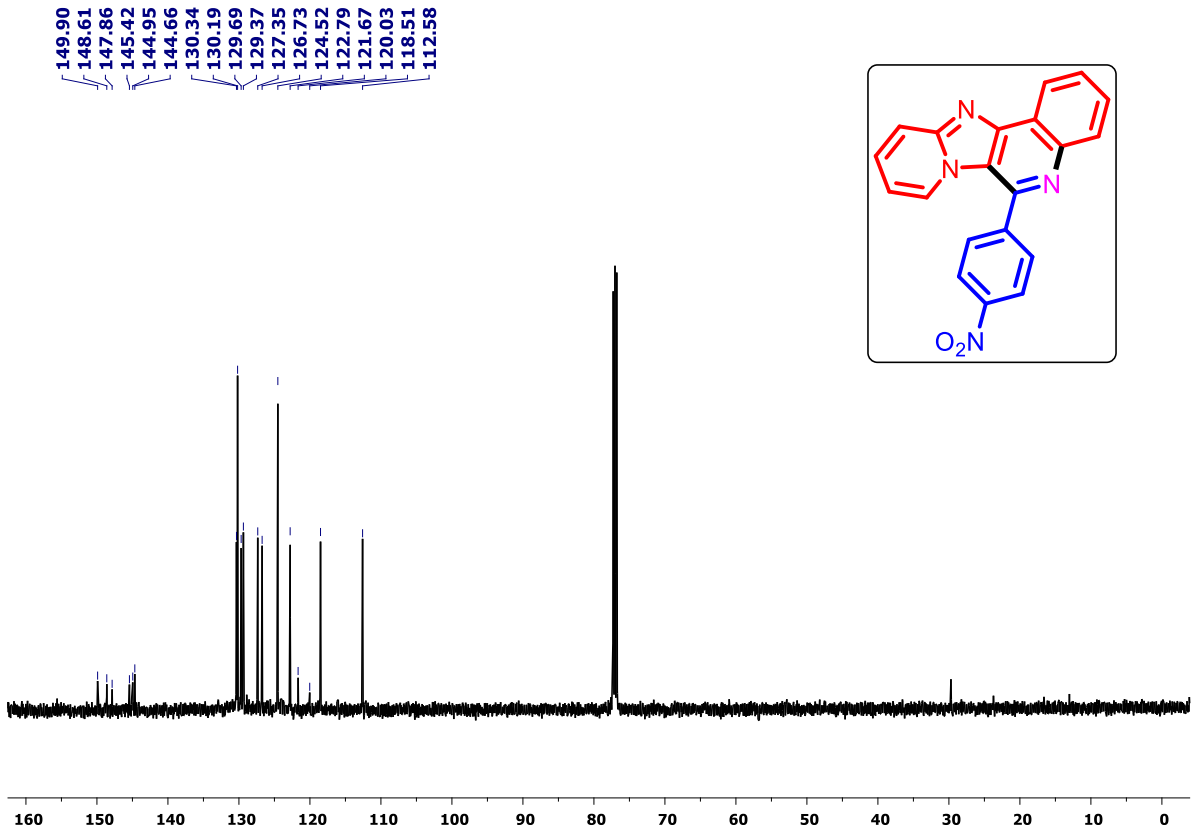
^{1}H NMR spectrum of compound **3i** ($CDCl_3$, 500 MHz)



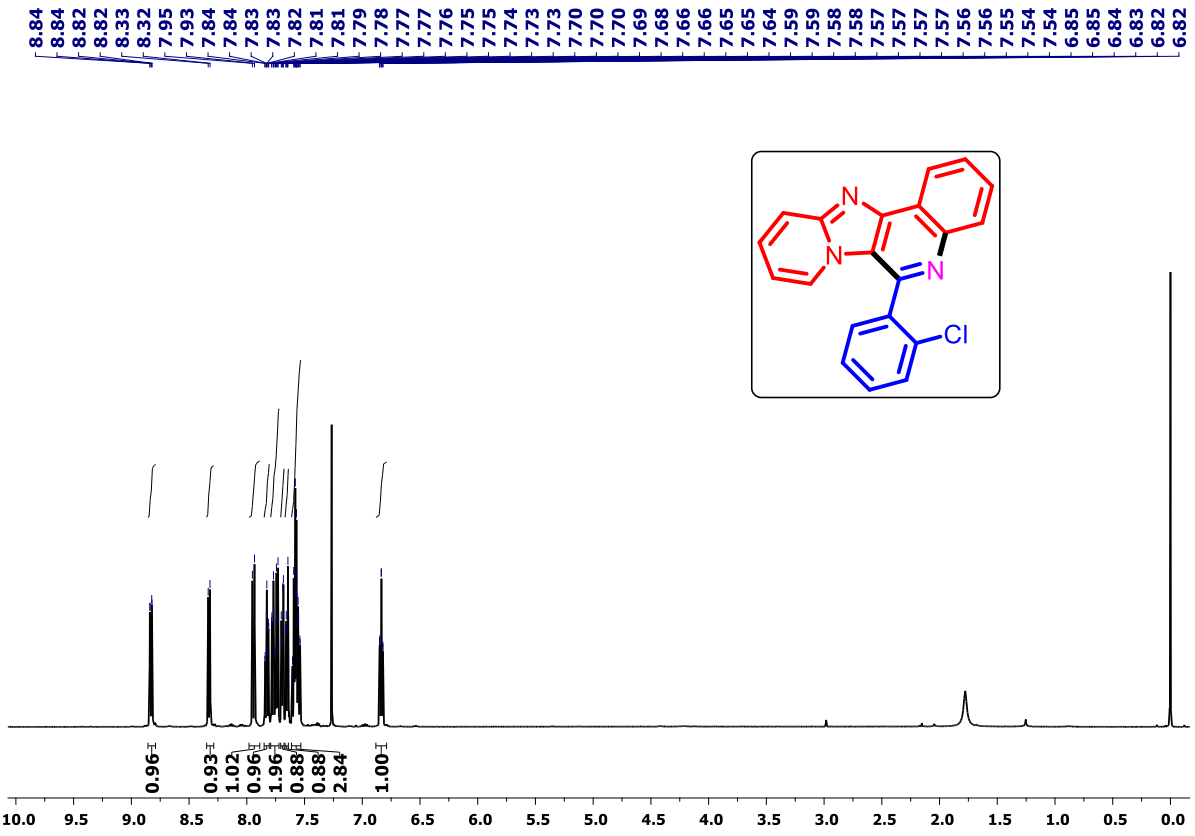
^{13}C NMR spectrum of compound **3i** ($CDCl_3$, 125 MHz)



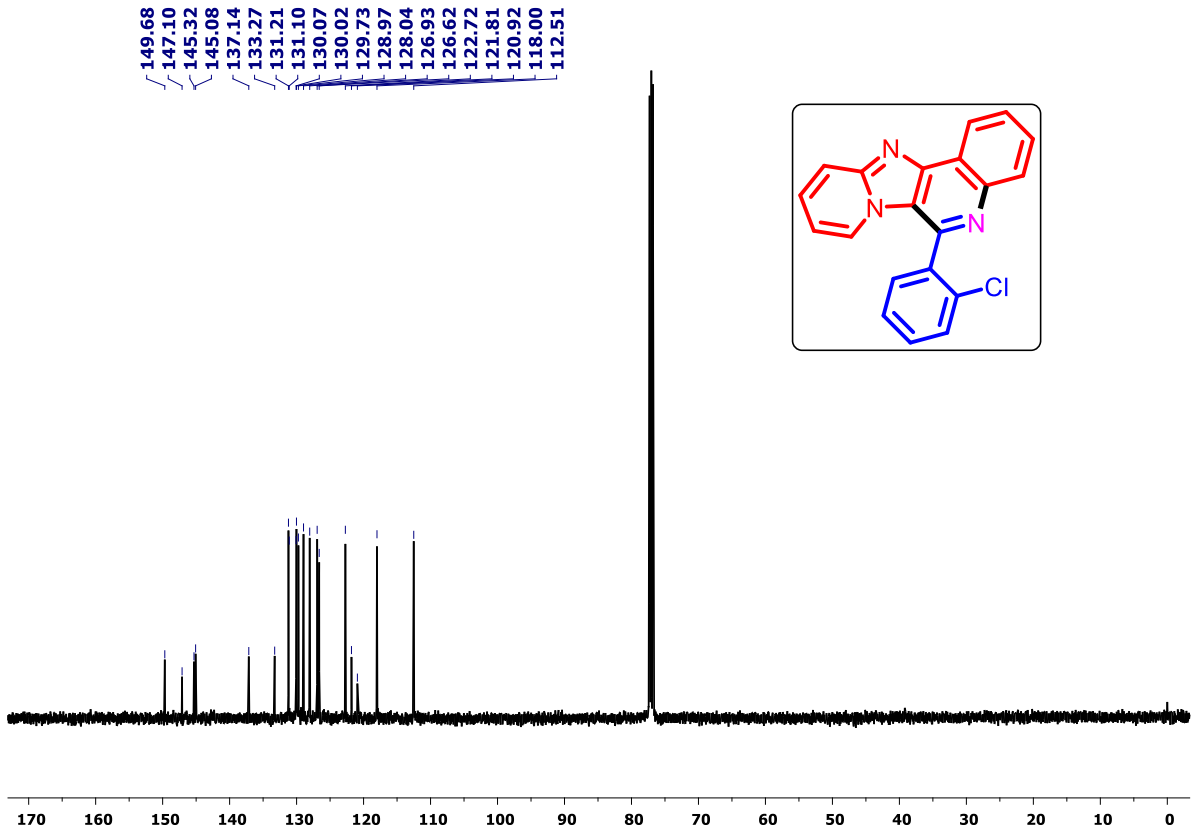
^{1}H NMR spectrum of compound **3j** ($CDCl_3$, 500 MHz)



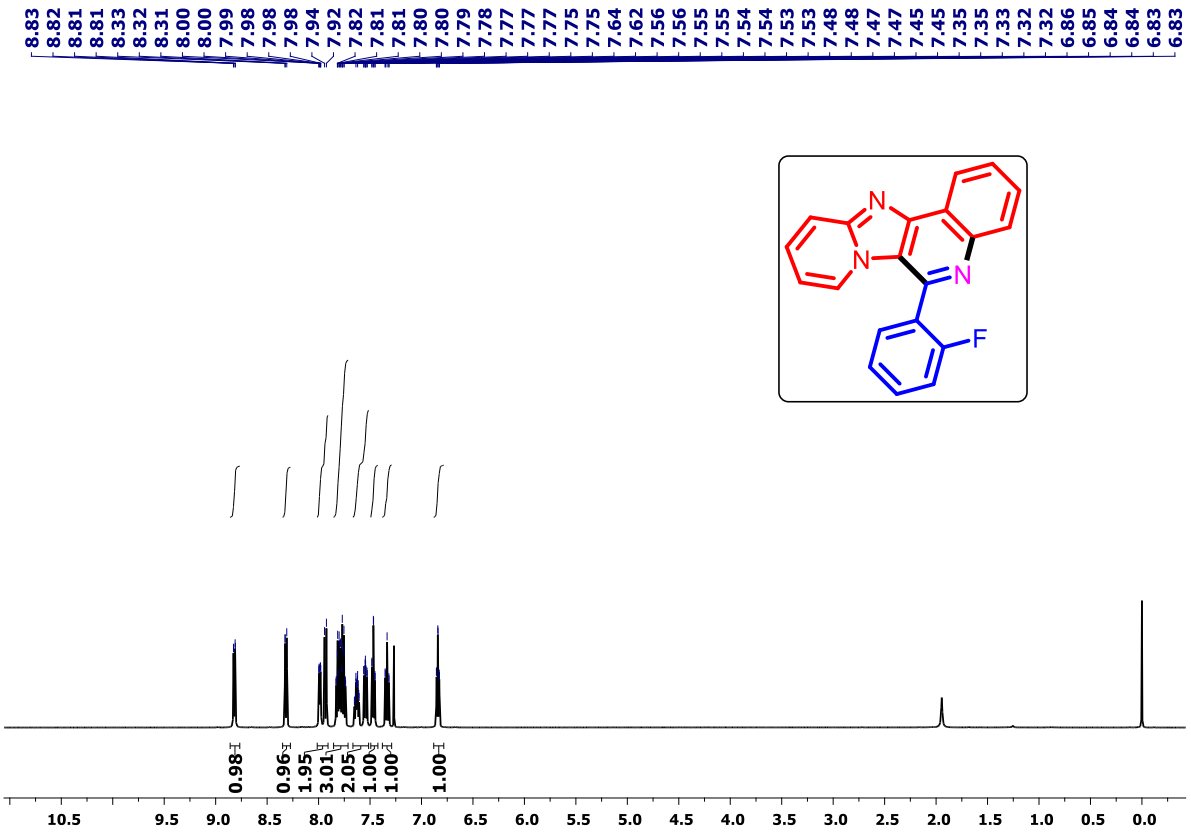
^{13}C NMR spectrum of compound **3j** ($CDCl_3$, 125 MHz)



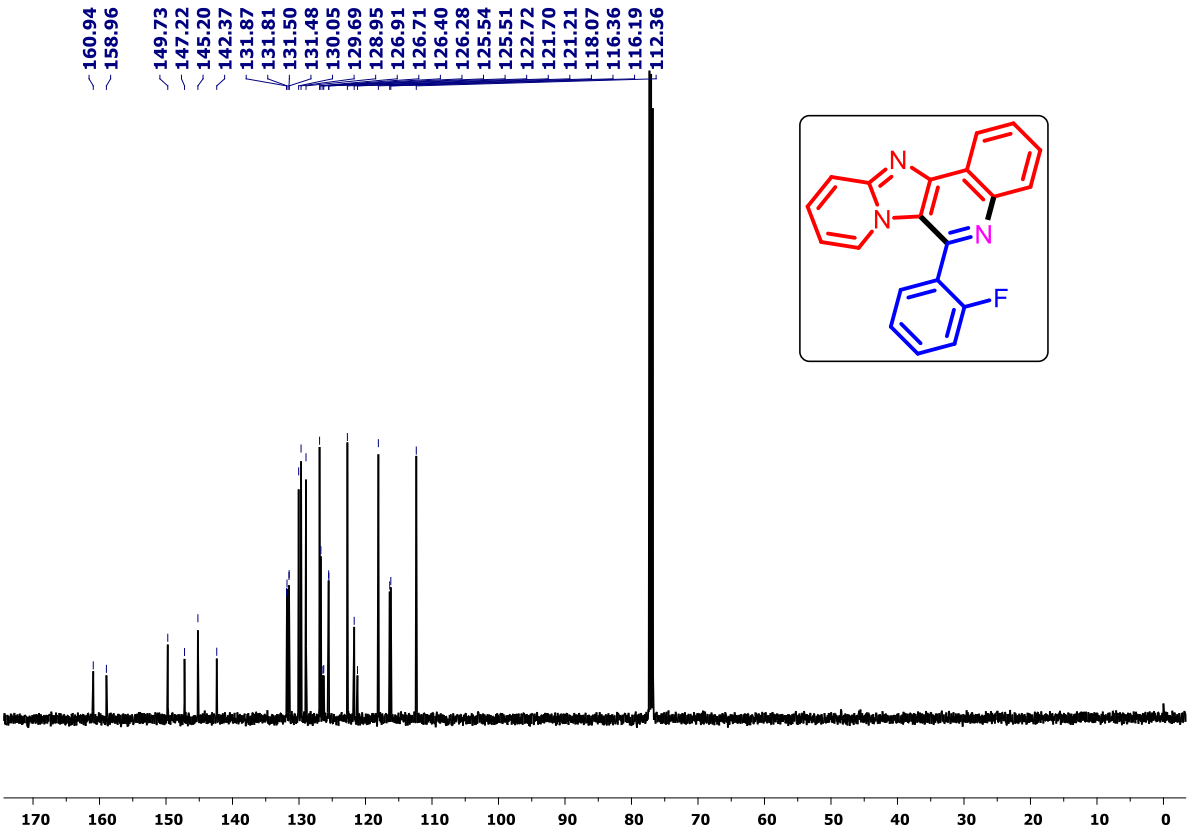
^{1}H NMR spectrum of compound **3k** ($CDCl_3$, 500 MHz)



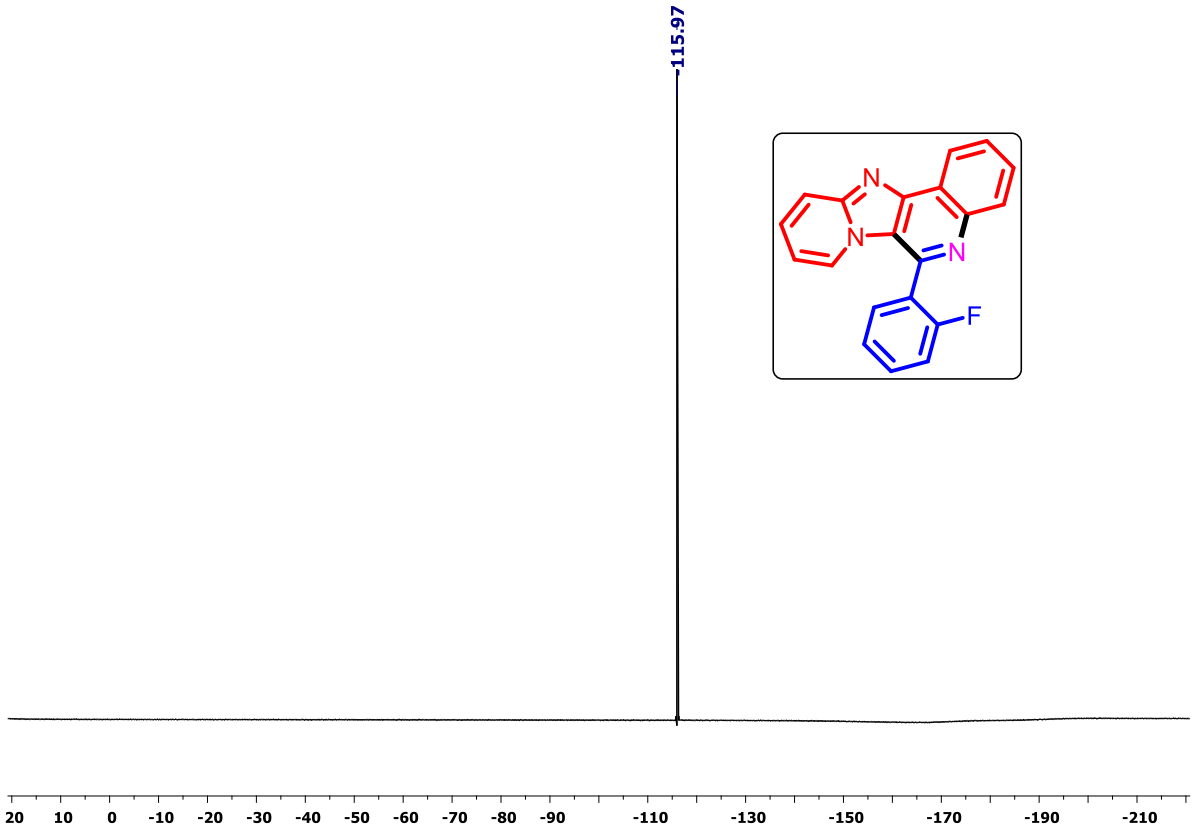
^{13}C NMR spectrum of compound **3k** ($CDCl_3$, 125 MHz)



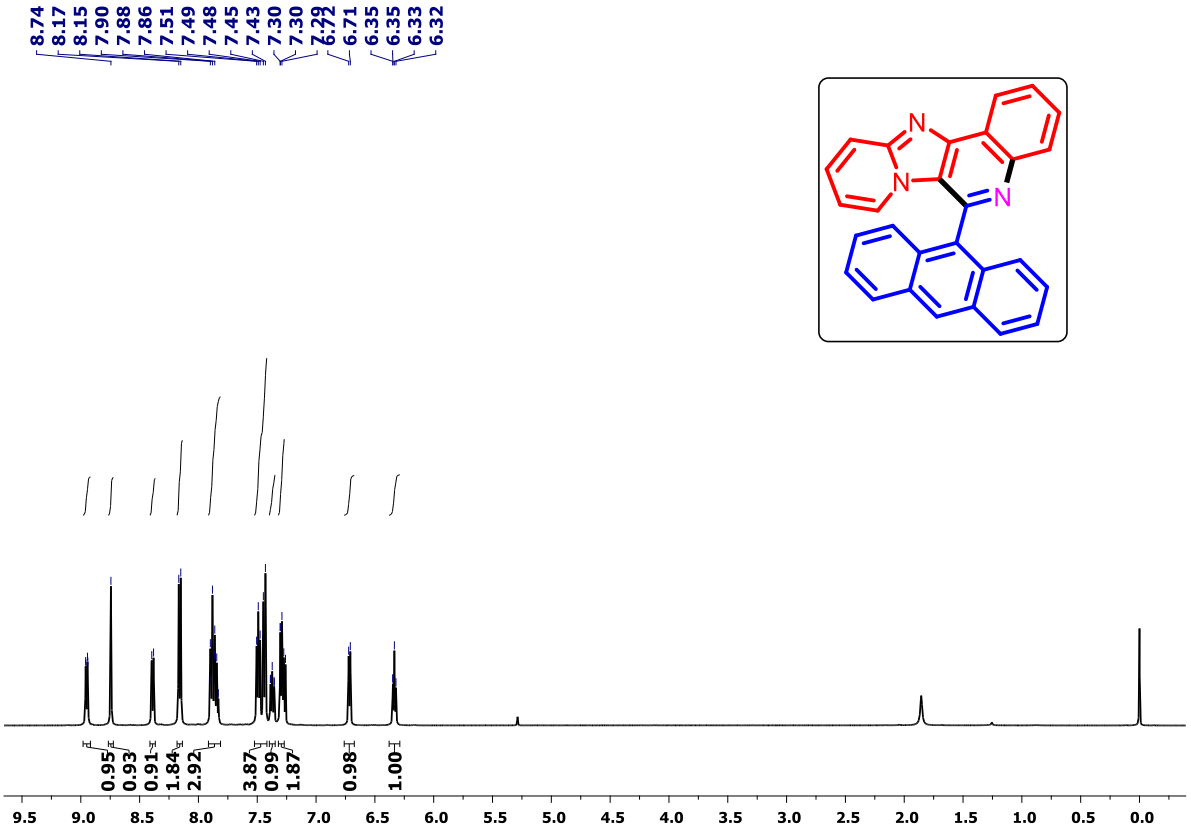
^{1}**H NMR** spectrum of compound **3l** ($CDCl_3$, 500 MHz)



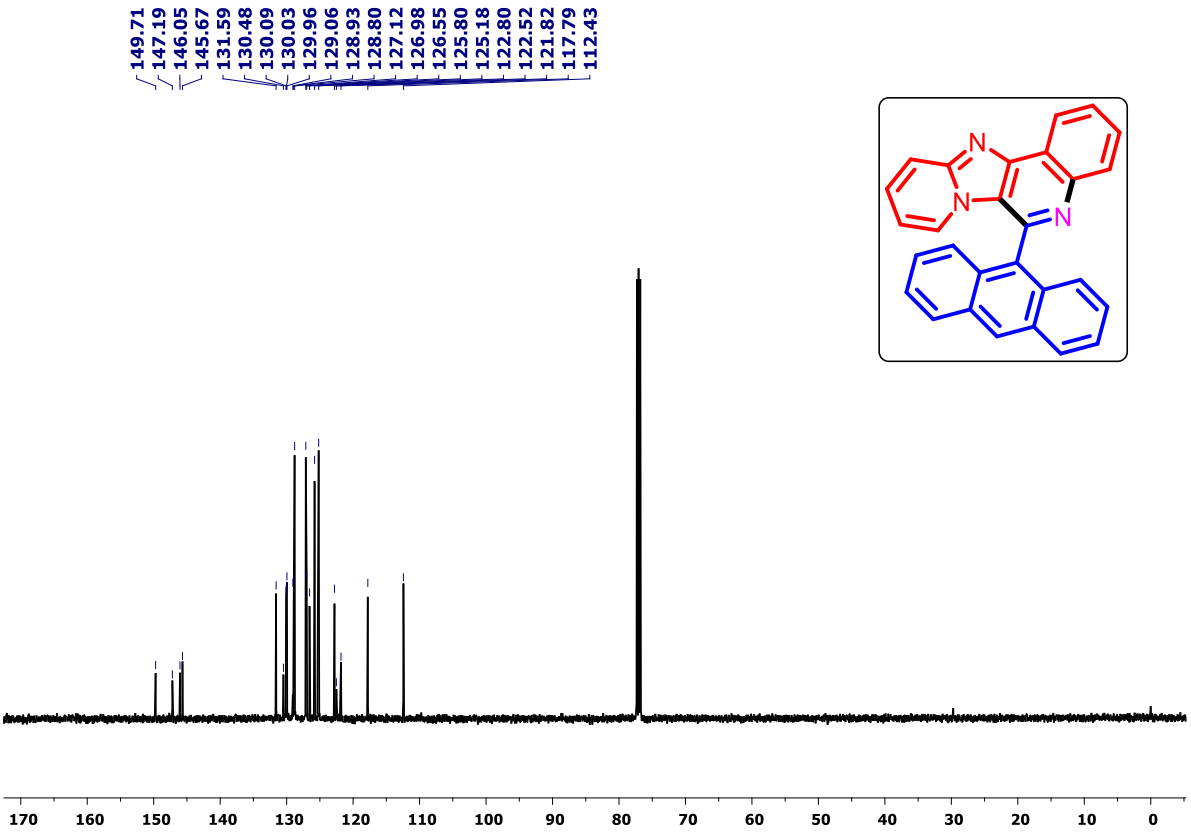
^{13}**C NMR** spectrum of compound **3l** ($CDCl_3$, 125 MHz)



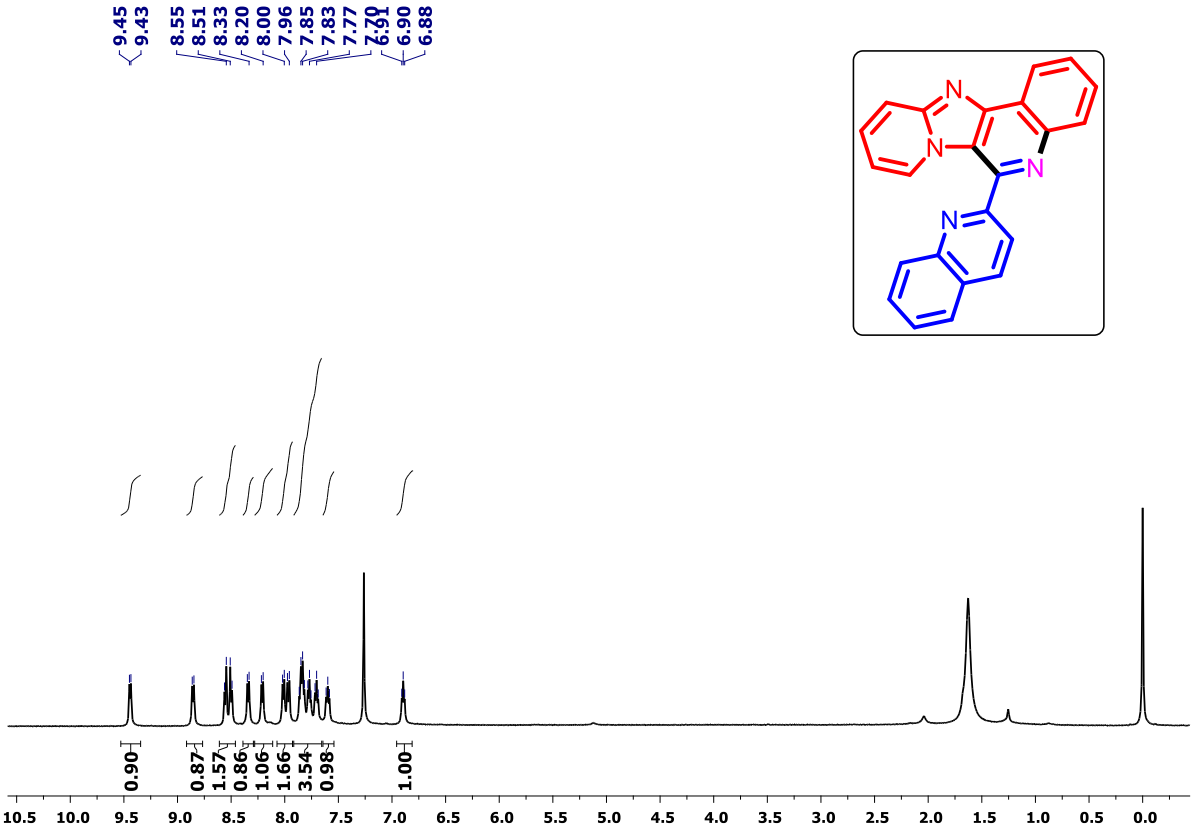
^{19}F NMR spectrum of compound **3l** ($CDCl_3$, 470 MHz)



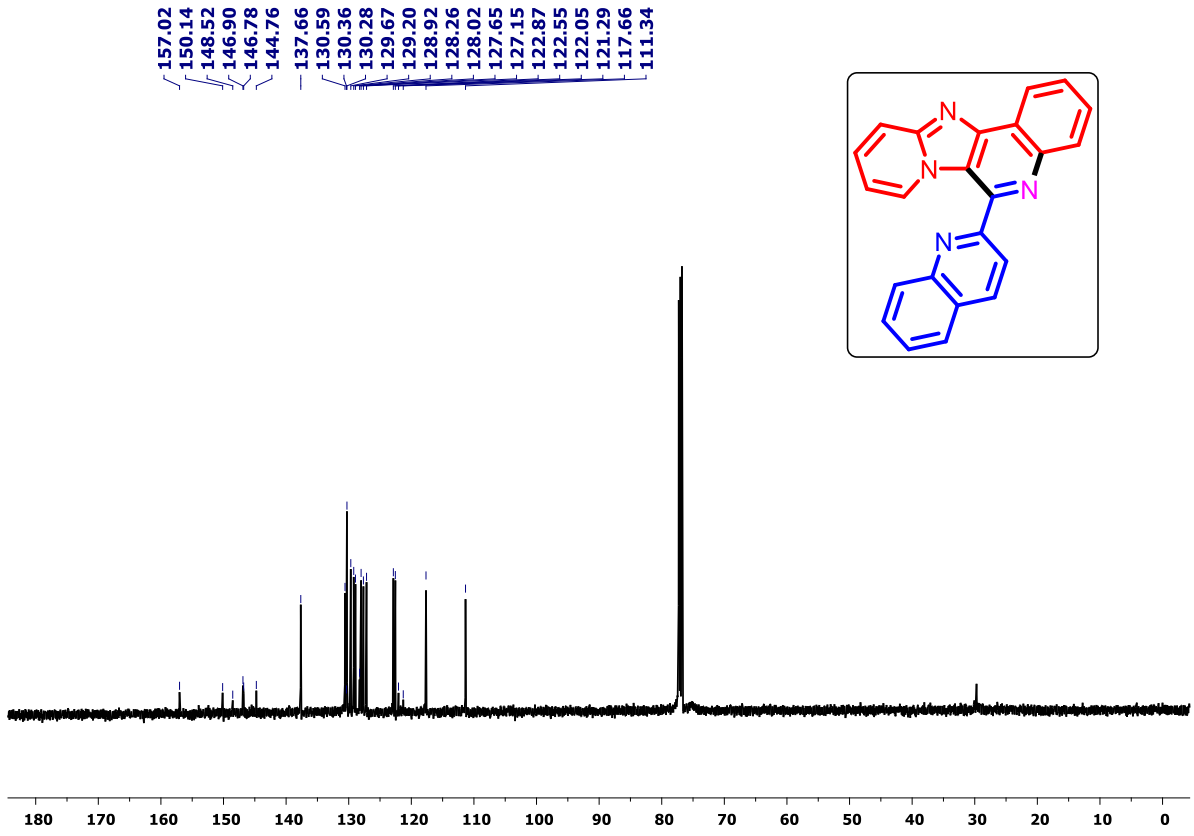
^{1}**H NMR** spectrum of compound **3m** ($CDCl_3$, 500 MHz)



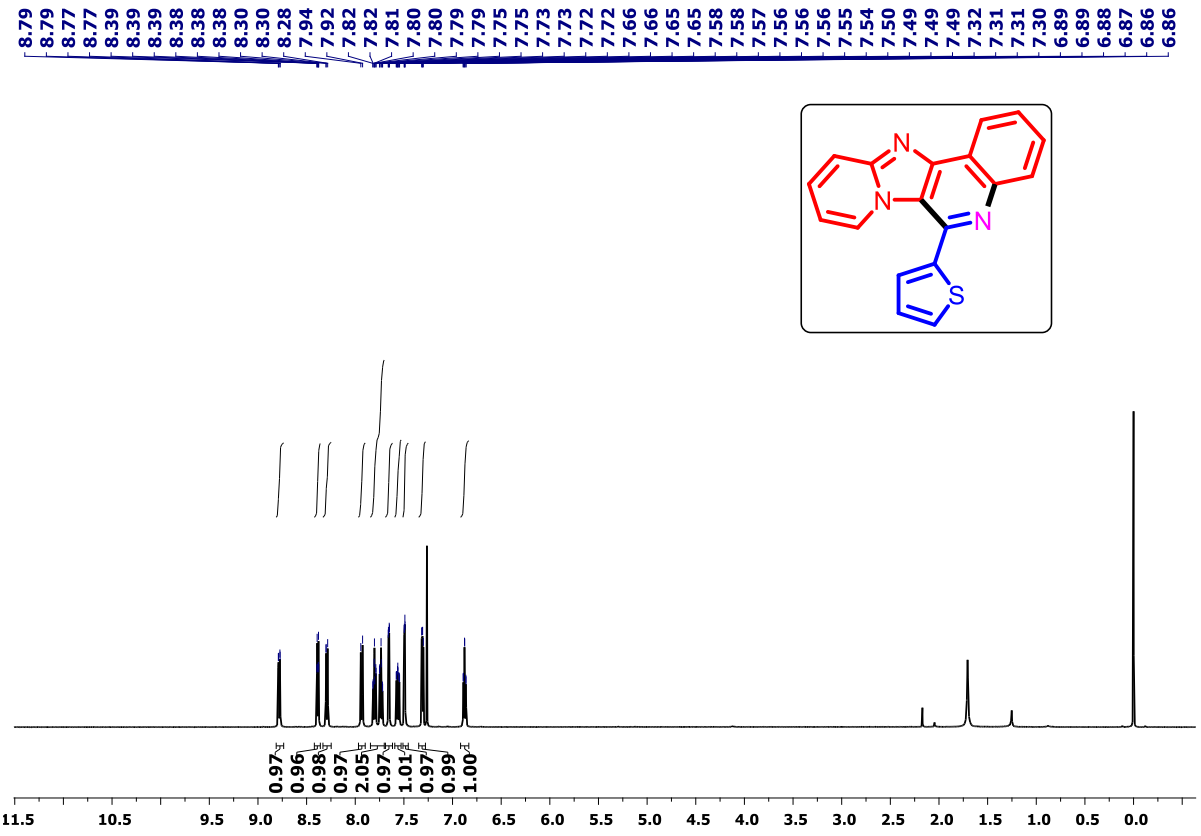
^{13}**C NMR** spectrum of compound **3m** ($CDCl_3$, 125 MHz)



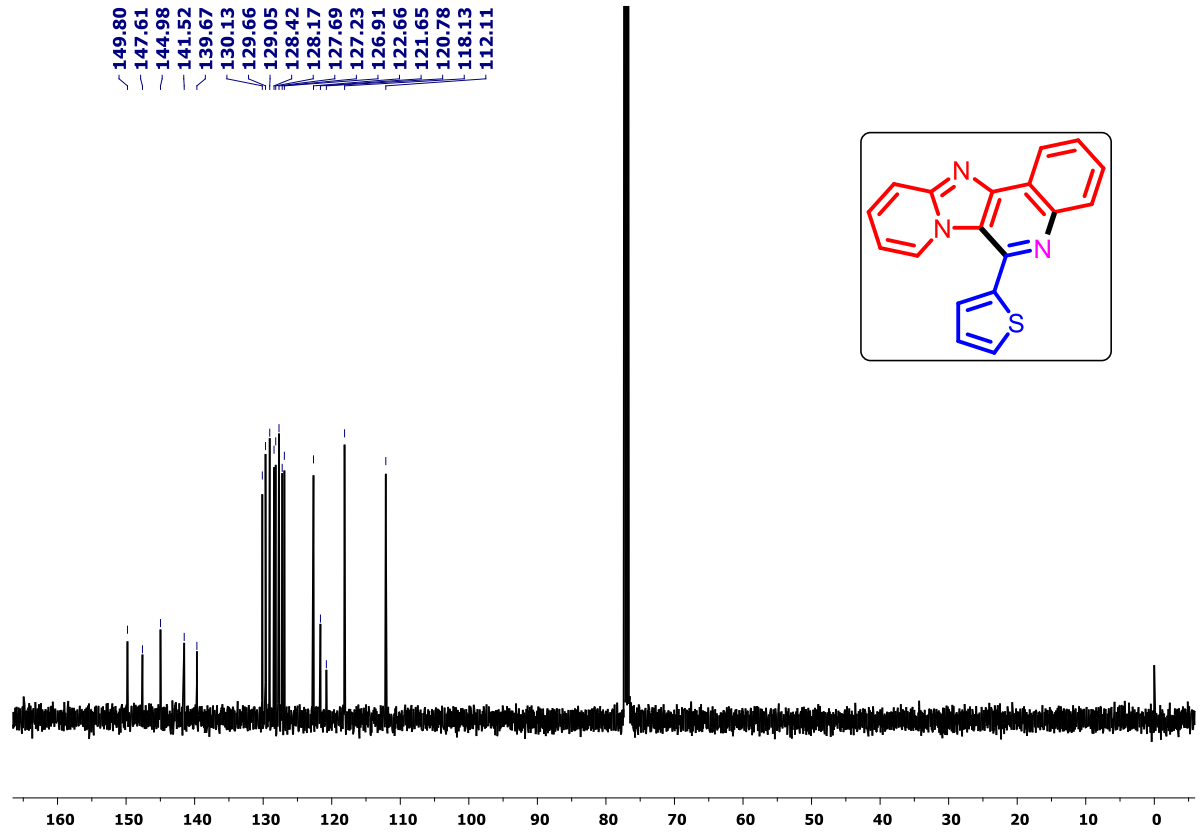
^{1}**H NMR** spectrum of compound **3n** ($CDCl_3$, 500 MHz)



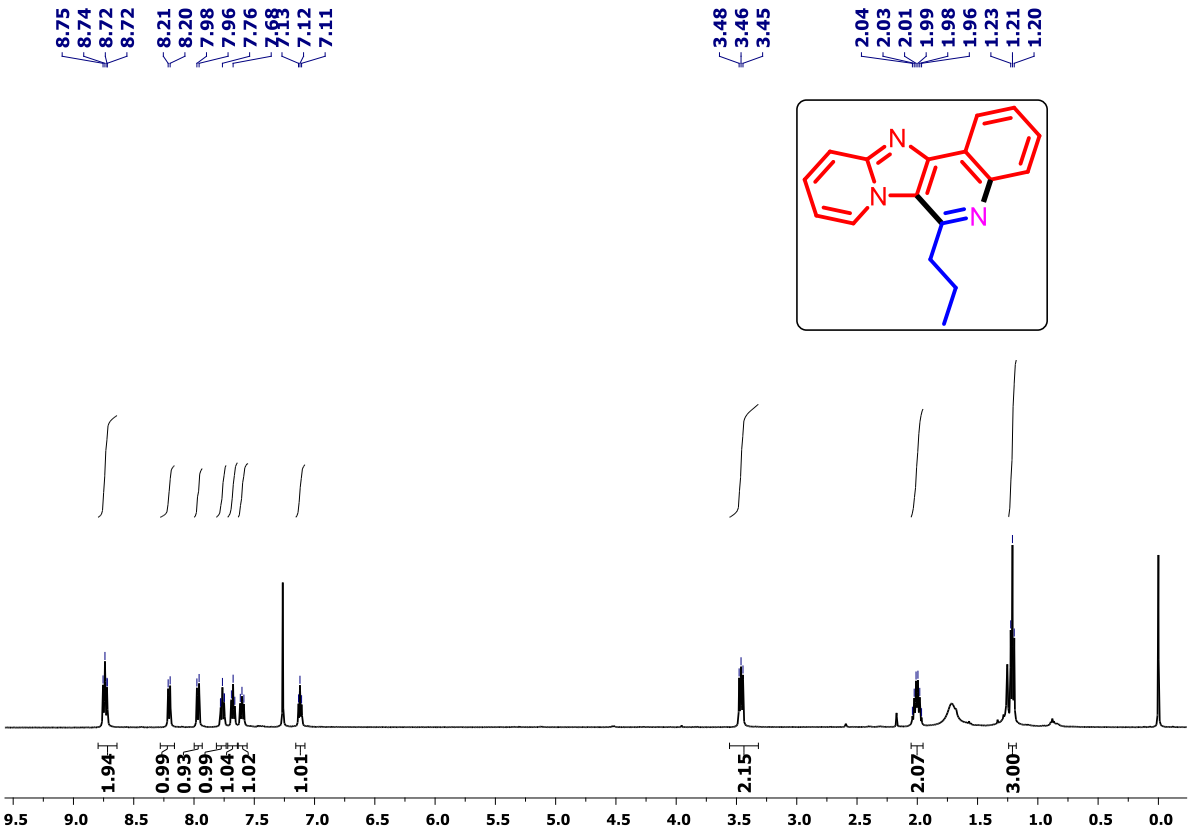
^{13}**C NMR** spectrum of compound **3n** ($CDCl_3$, 125 MHz)



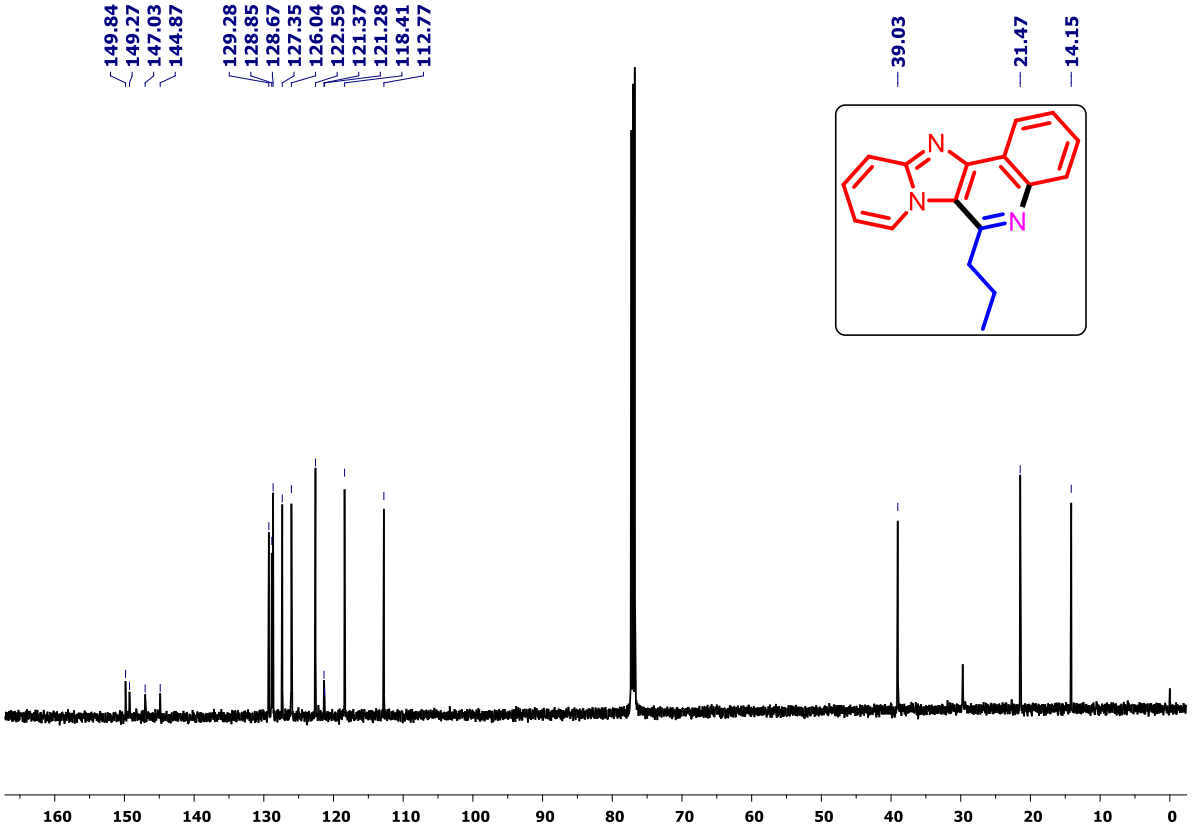
^{1}H NMR spectrum of compound **3o** ($CDCl_3$, 500 MHz)



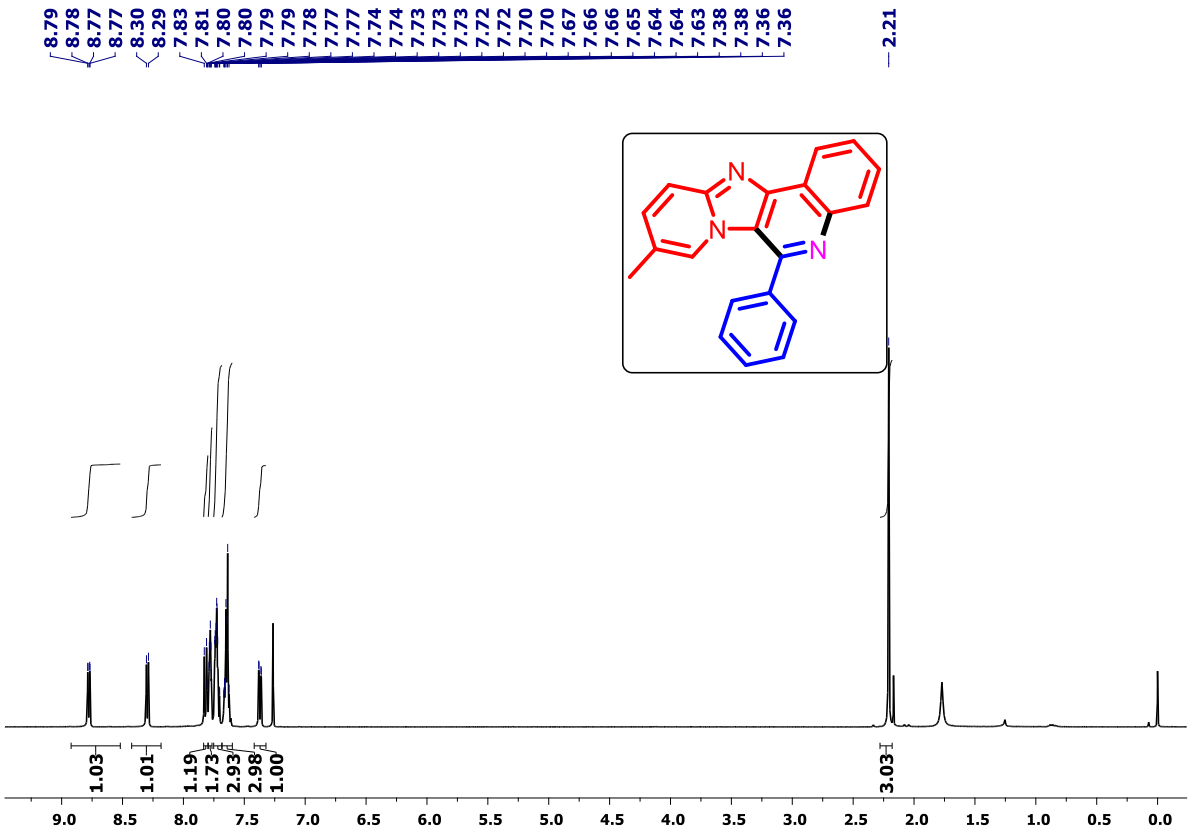
^{13}C NMR spectrum of compound **3o** ($CDCl_3$, 125 MHz)



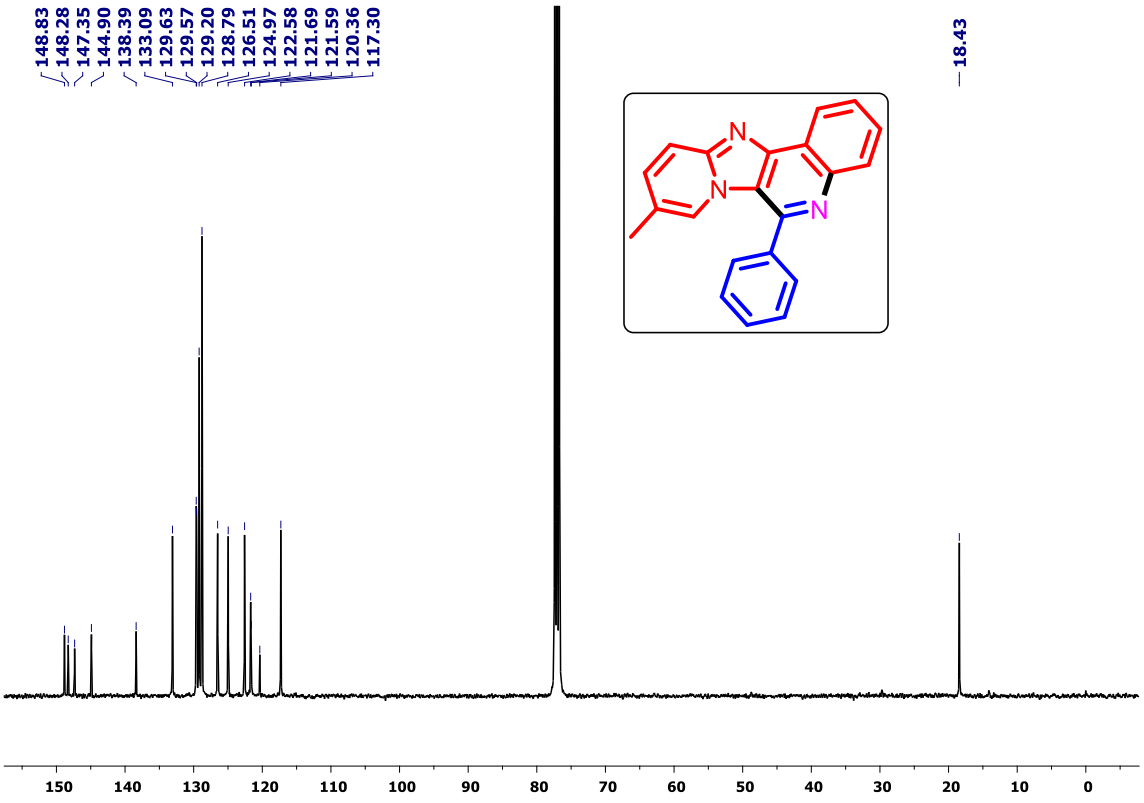
^{1}H NMR spectrum of compound **3p** ($CDCl_3$, 500 MHz)



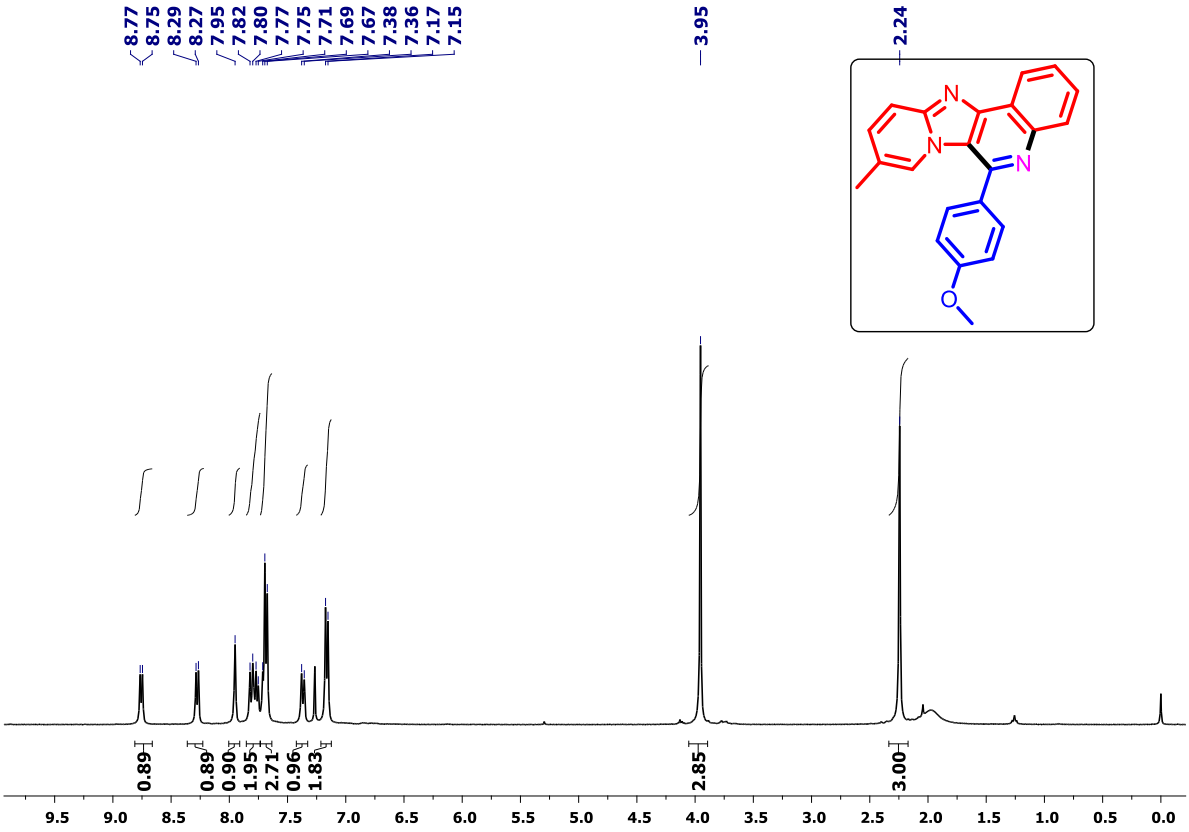
^{13}C NMR spectrum of compound **3p** ($CDCl_3$, 125 MHz)



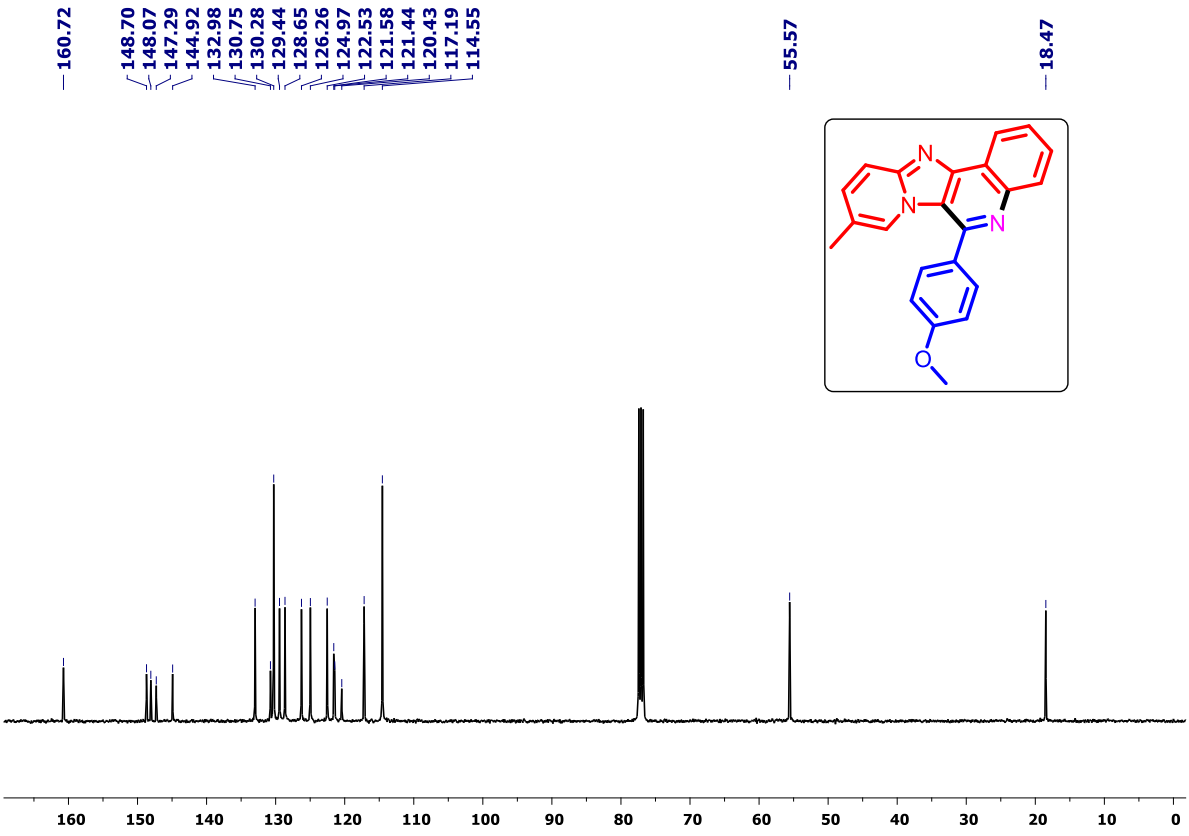
^{1}H NMR spectrum of compound **3q** ($CDCl_3$, 500 MHz)



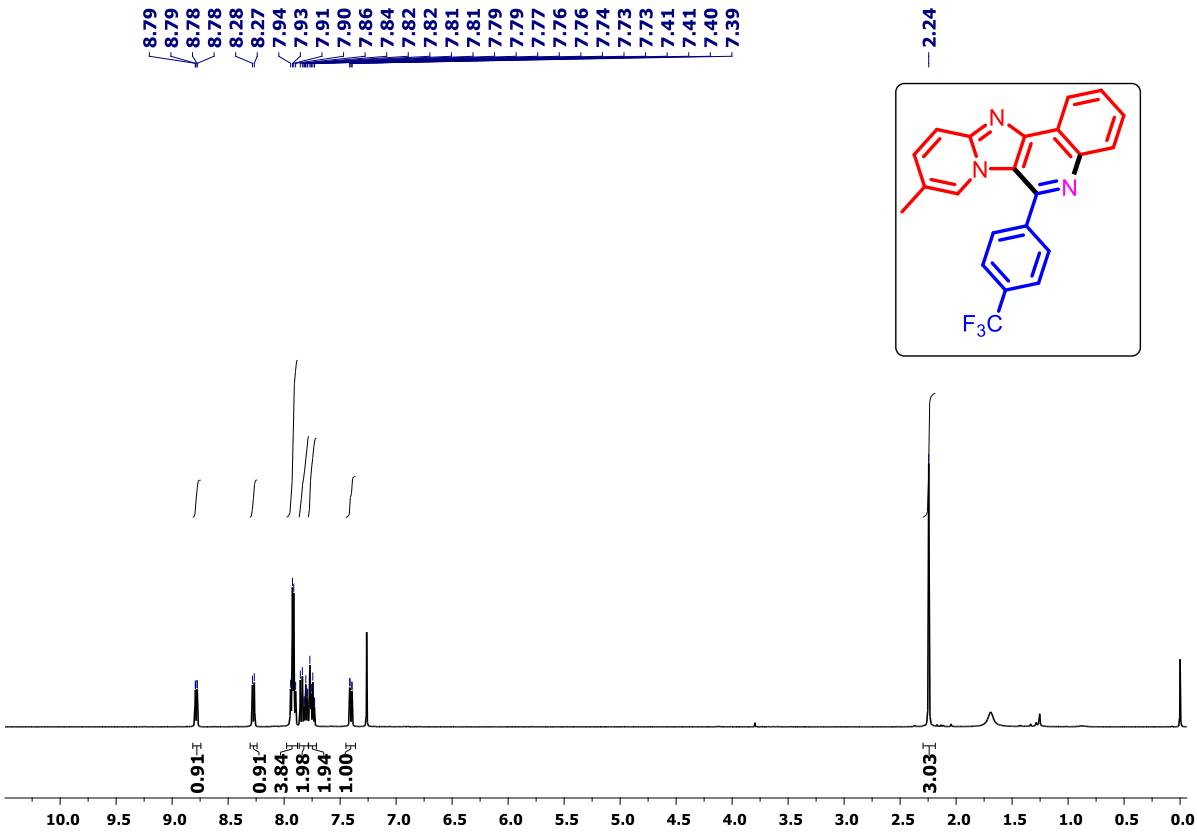
^{13}C NMR spectrum of compound **3q** ($CDCl_3$, 125 MHz)



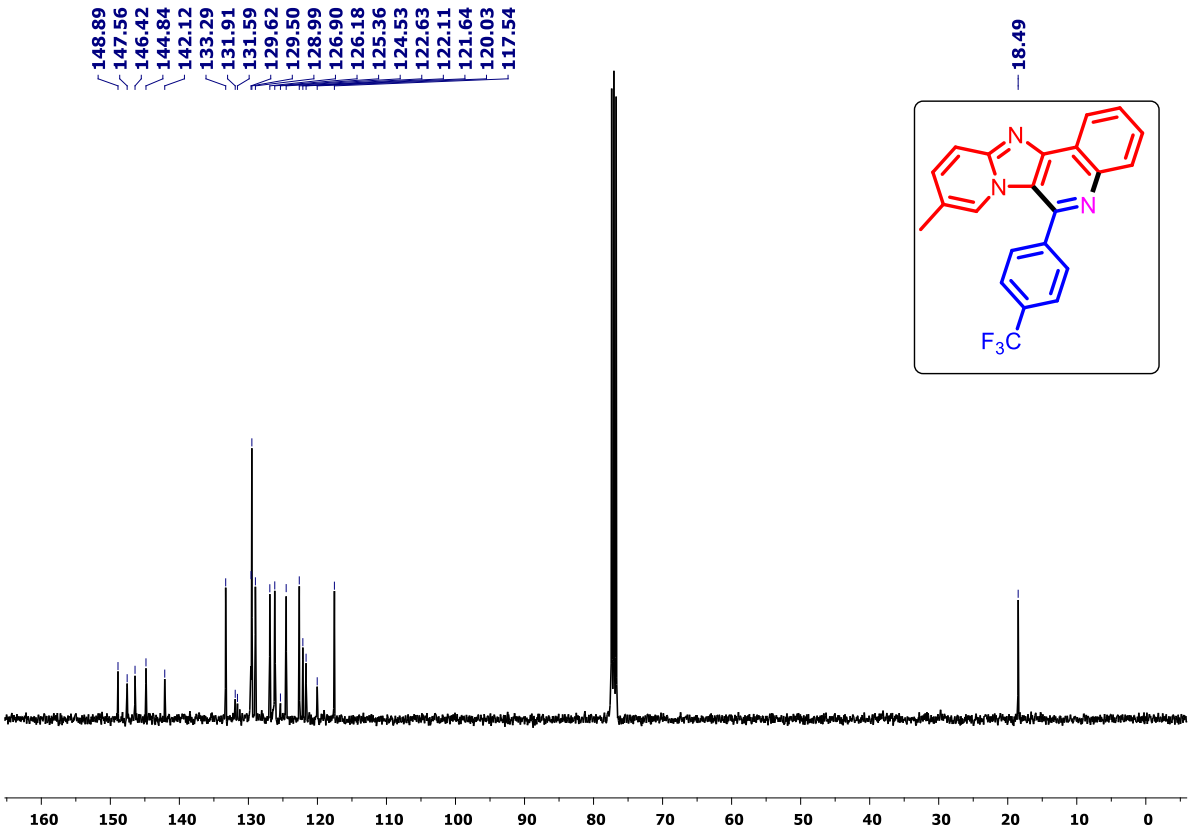
^{1}H NMR spectrum of compound **3r** ($CDCl_3$, 500 MHz)



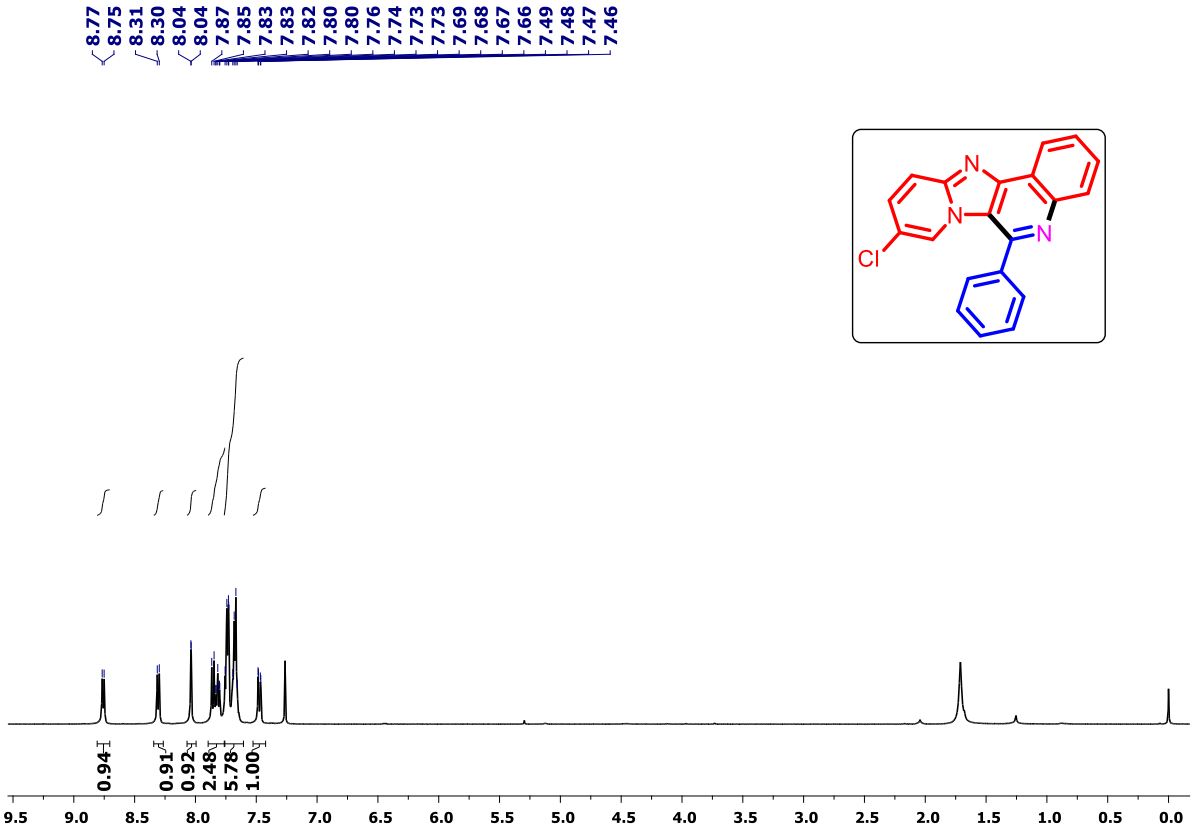
^{13}C NMR spectrum of compound **3r** ($CDCl_3$, 125 MHz)



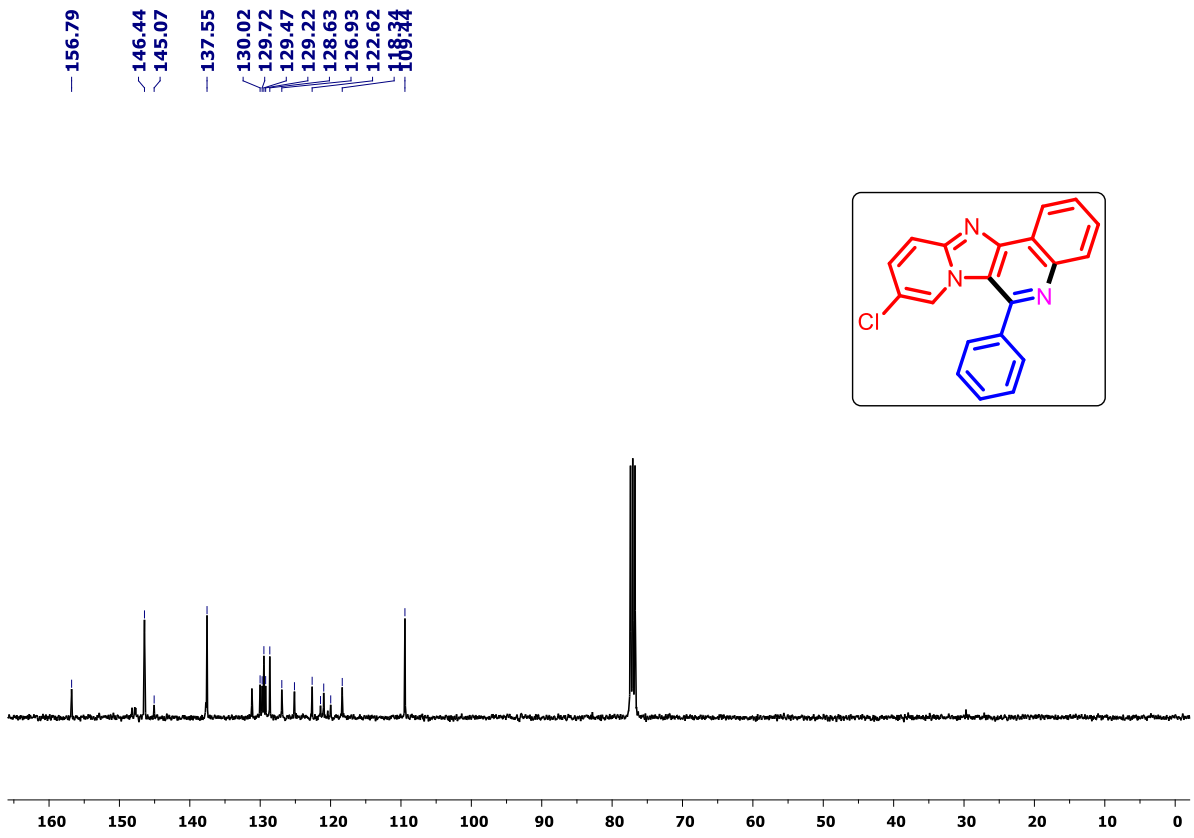
^{1}**H NMR** spectrum of compound **3s** ($CDCl_3$, 500 MHz)



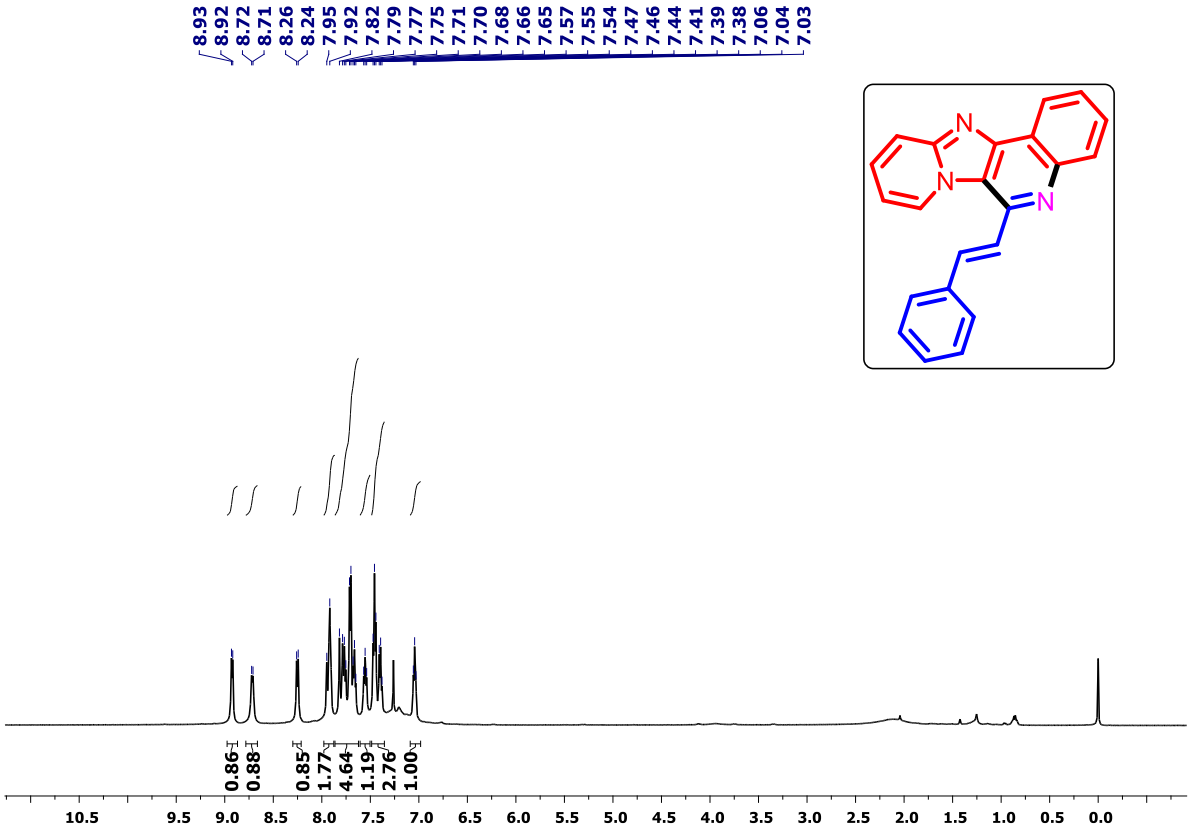
^{13}**C NMR** spectrum of compound **3s** ($CDCl_3$, 125 MHz)



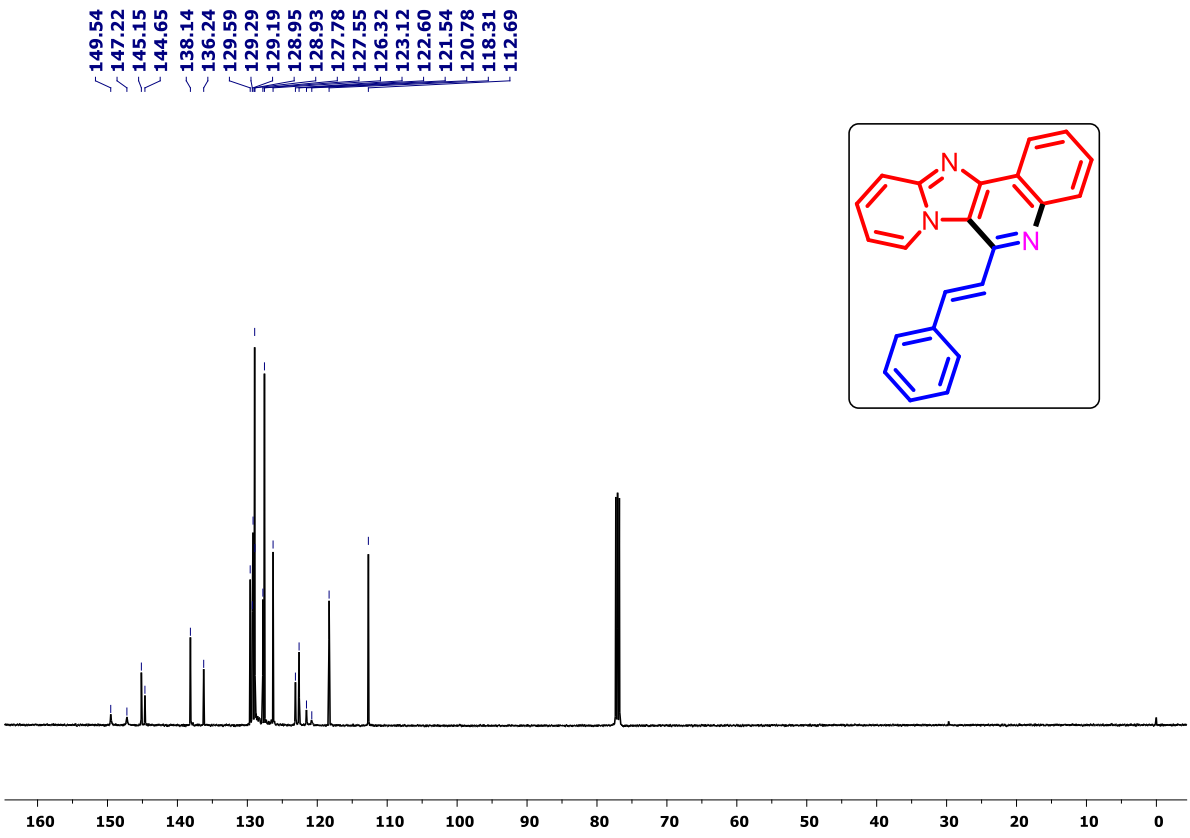
^{1}**H NMR** spectrum of compound **3t** ($CDCl_3$, 500 MHz)



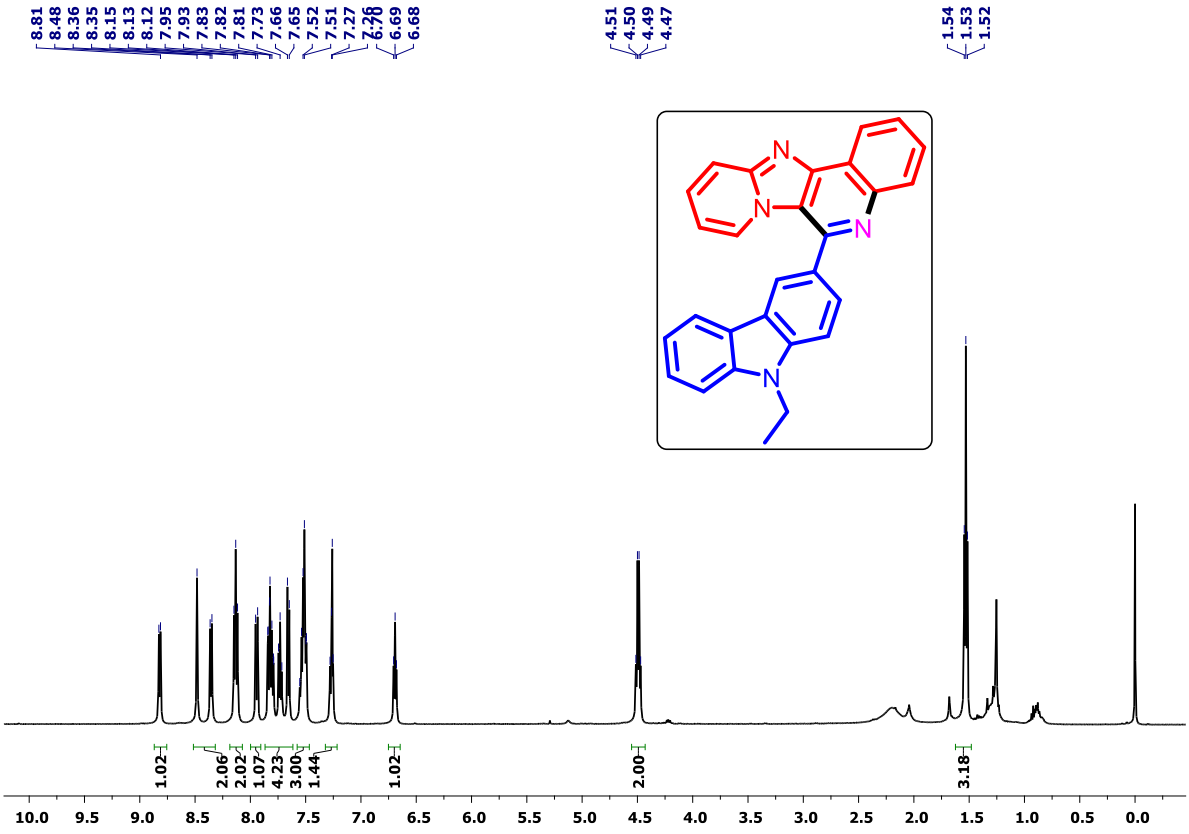
^{13}**C NMR** spectrum of compound **3t** ($CDCl_3$, 125 MHz)



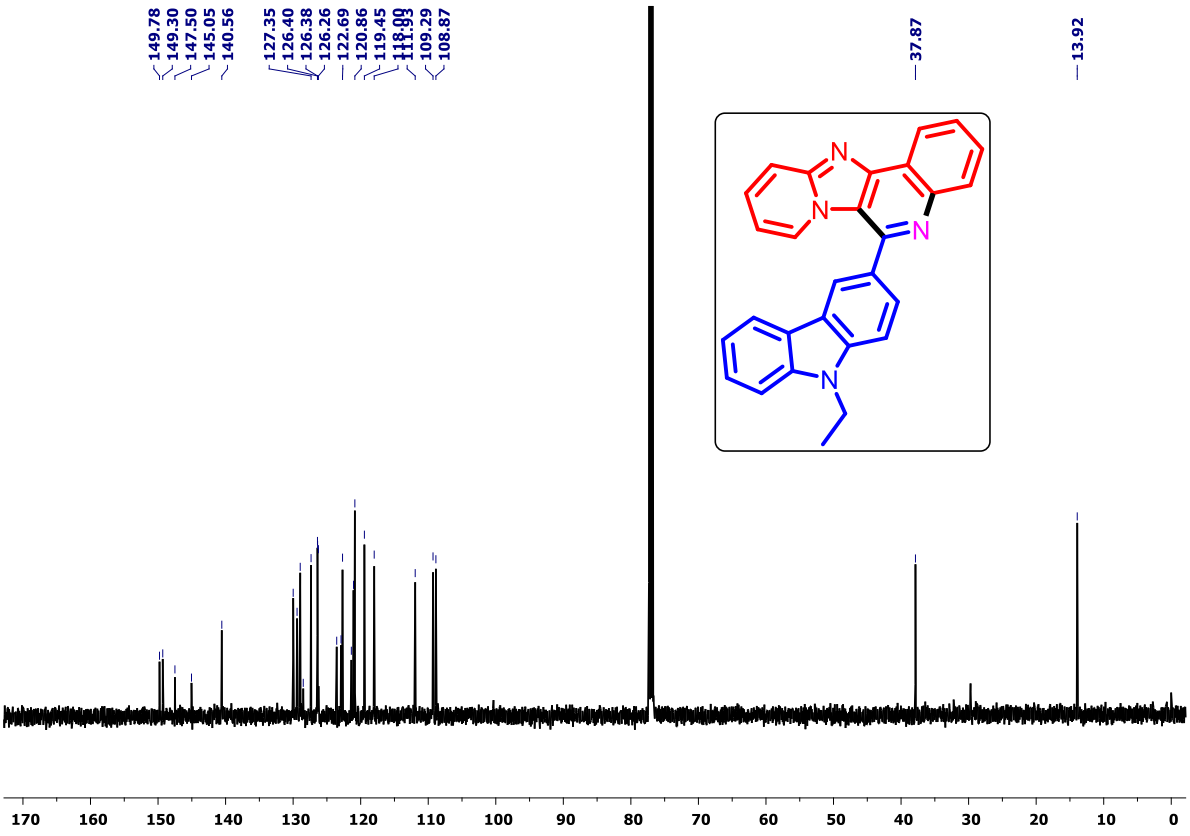
^{1}**H NMR** spectrum of compound **3u** ($CDCl_3$, 500 MHz)



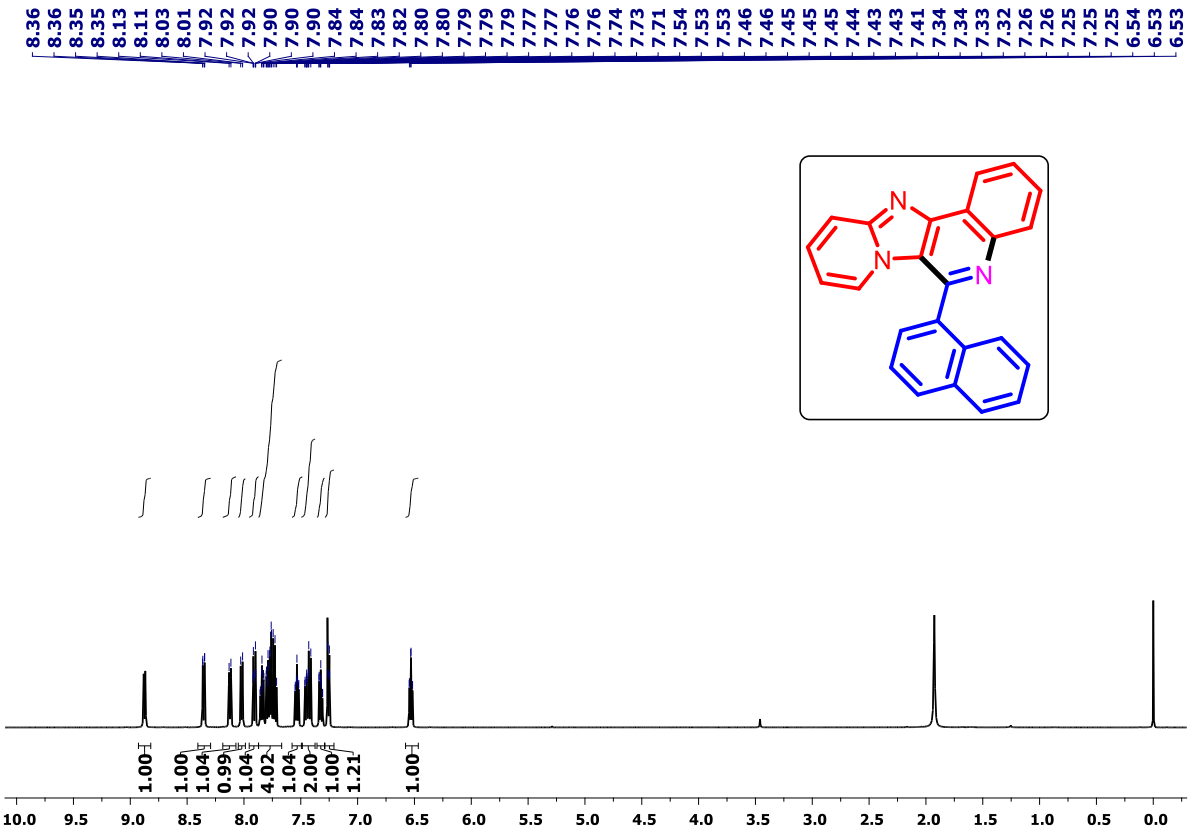
^{13}**C NMR** spectrum of compound **3u** ($CDCl_3$, 125 MHz)



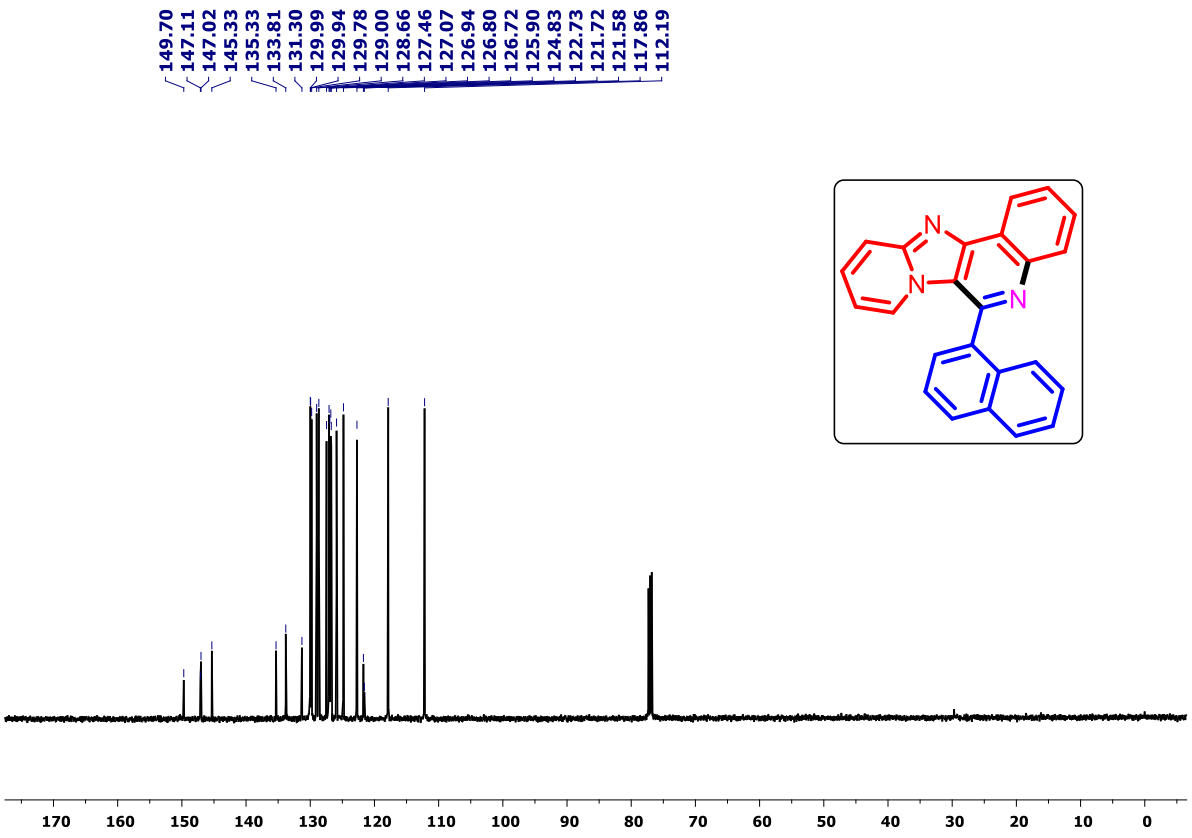
^{1}H NMR spectrum of compound **3v** ($CDCl_3$, 500 MHz)



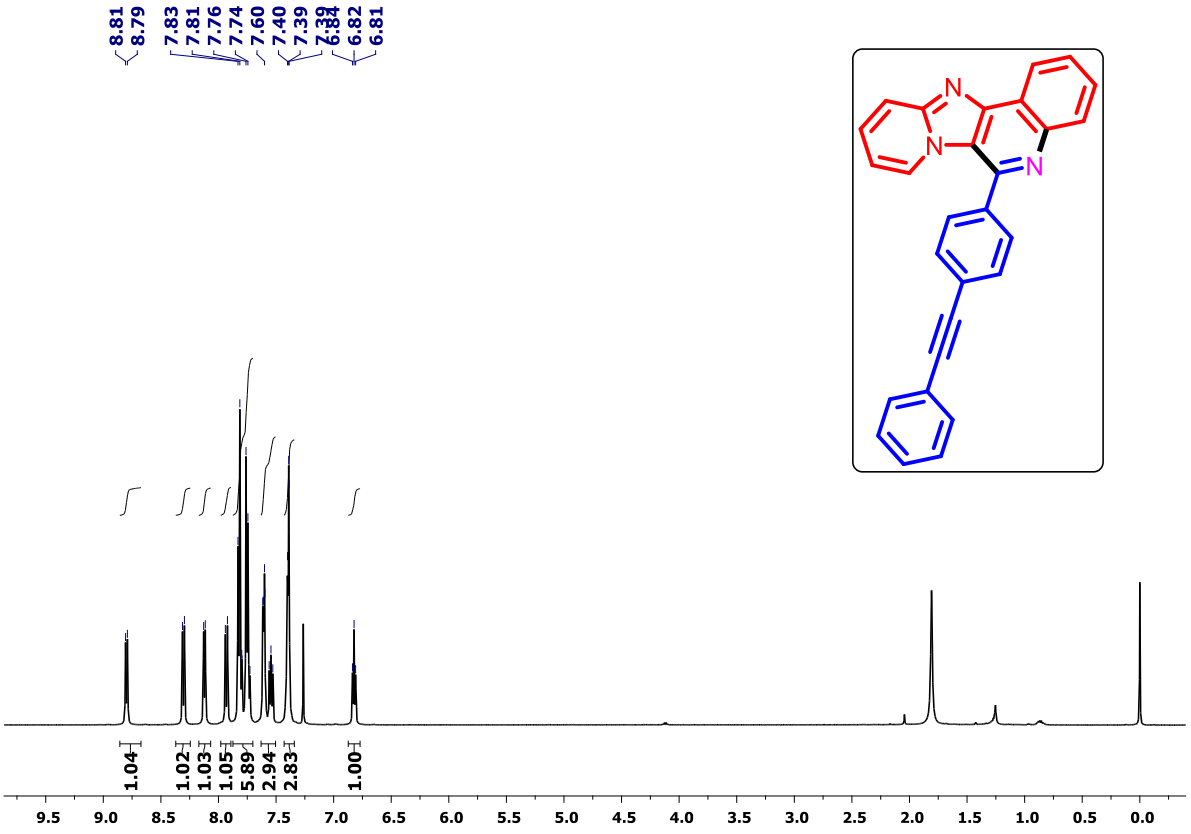
^{13}C NMR spectrum of compound **3v** ($CDCl_3$, 125 MHz)



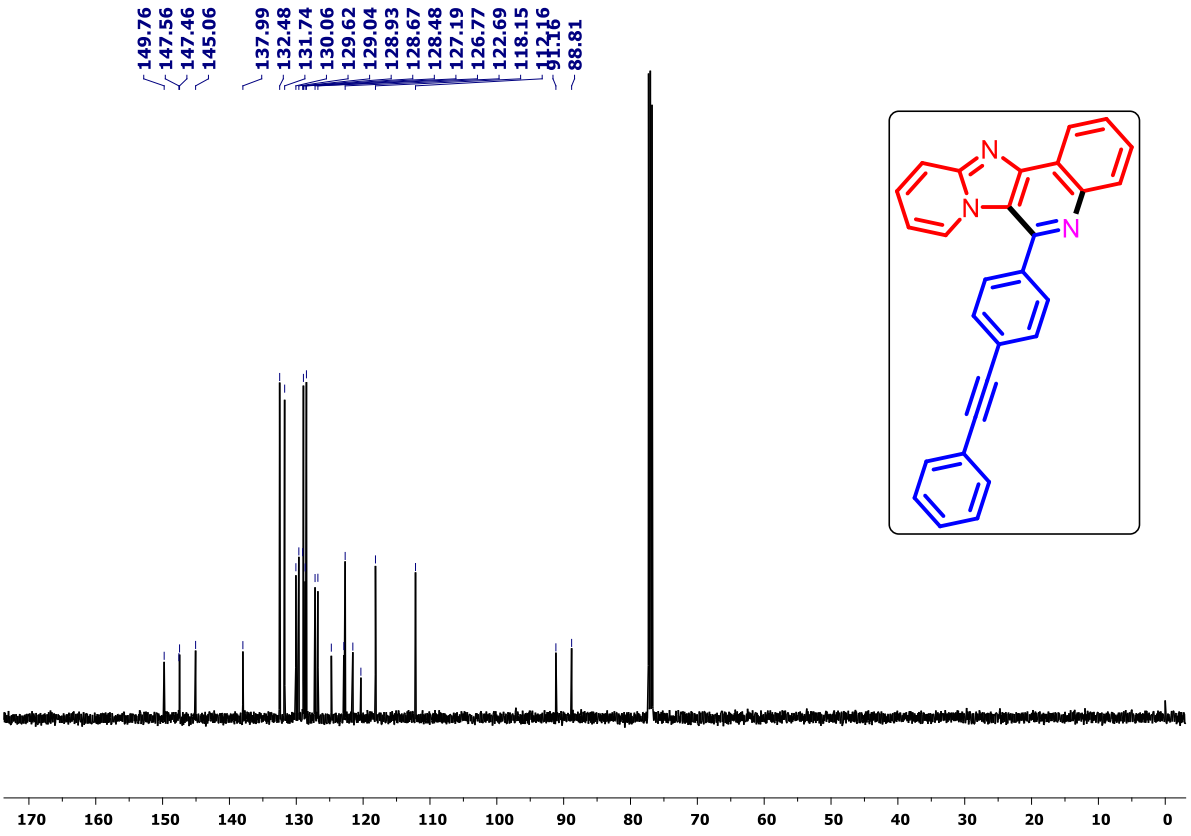
^{1}**H NMR** spectrum of compound 3w ($CDCl_3$, 500 MHz)



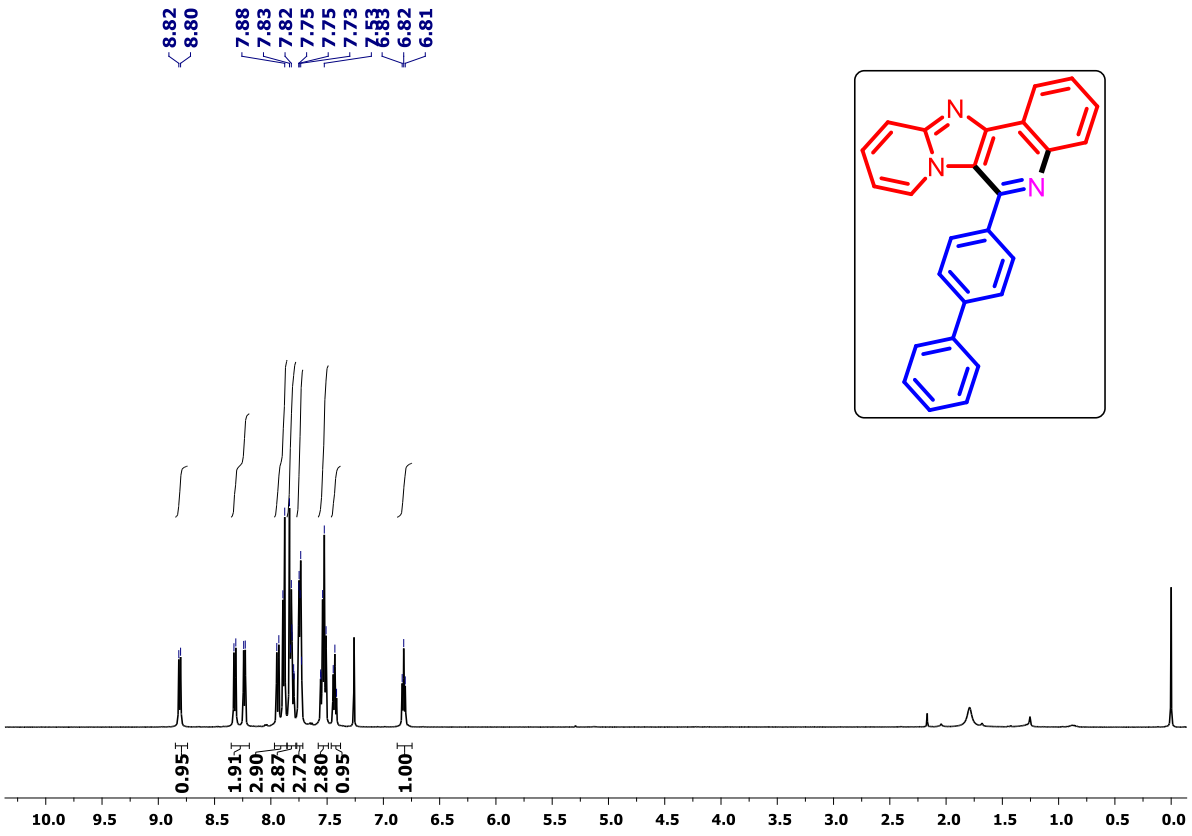
^{13}**C NMR** spectrum of compound **3w** ($CDCl_3$, 125 MHz)



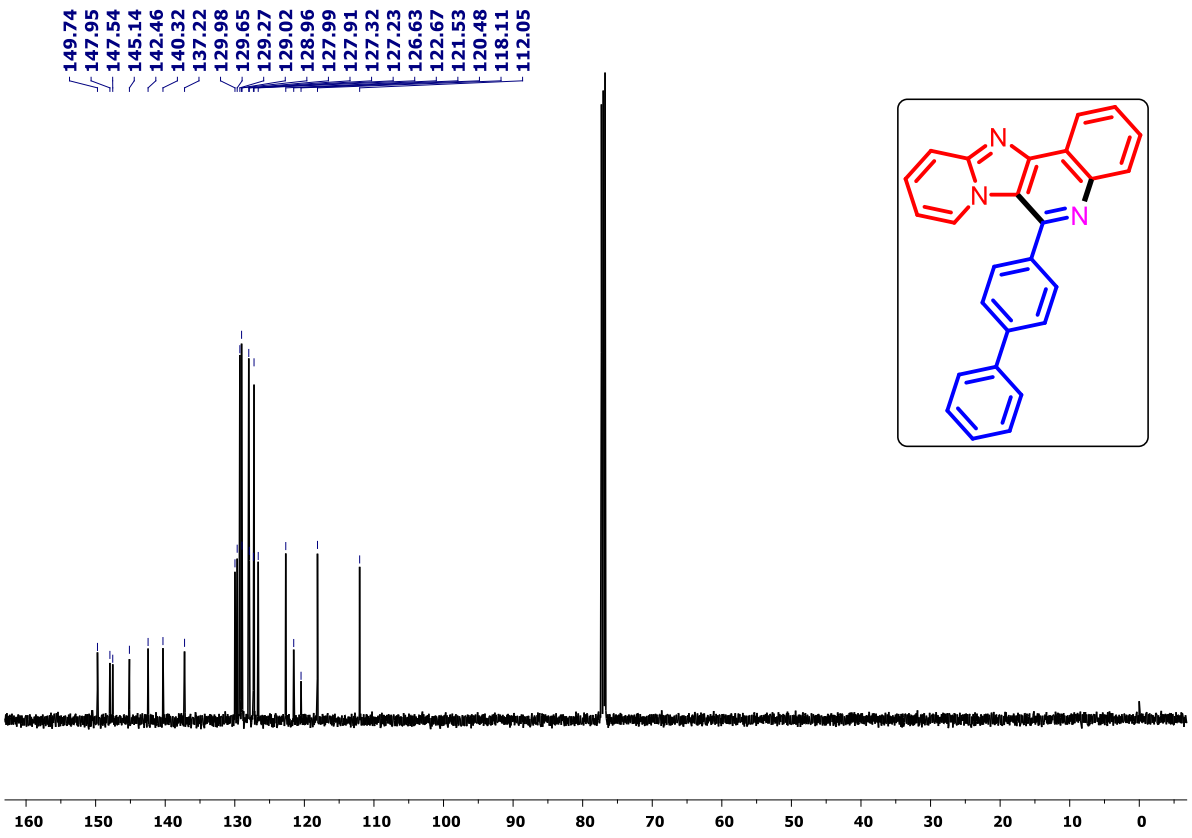
^{1}H NMR spectrum of compound **3x** ($CDCl_3$, 500 MHz)



^{13}C NMR spectrum of compound **3x** ($CDCl_3$, 125 MHz)



^{1}H NMR spectrum of compound **3y** ($CDCl_3$, 500 MHz)



^{13}C NMR spectrum of compound **3y** ($CDCl_3$, 125 MHz)