

Supporting Information

Ligand-free Pd-catalysed decarboxylative arylation of Imidazo[1,2-a]pyridine-3-carboxylic acids with Aryl bromides†

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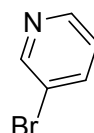
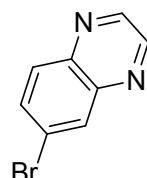
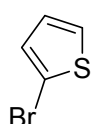
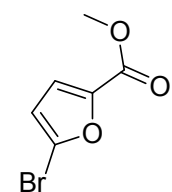
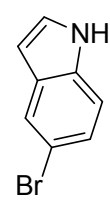
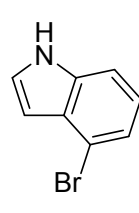
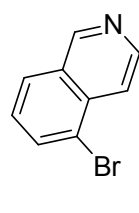
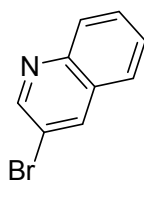
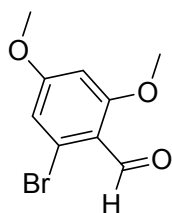
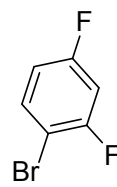
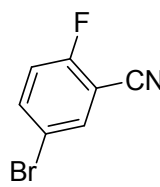
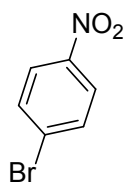
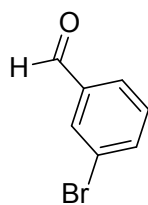
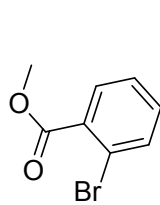
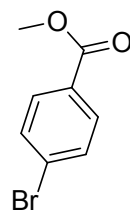
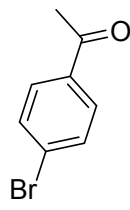
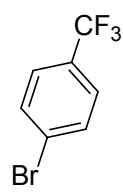
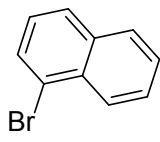
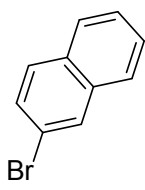
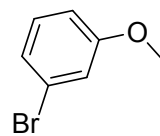
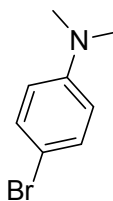
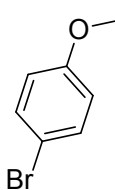
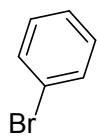
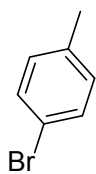
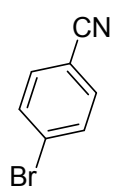
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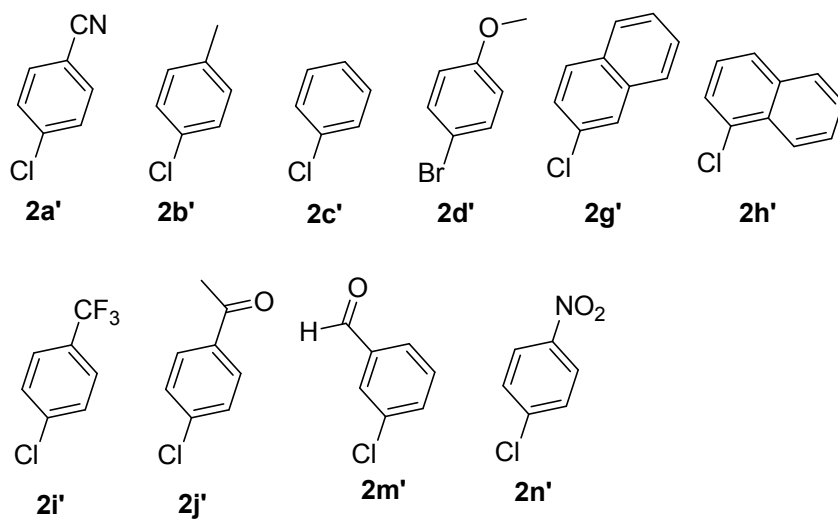
Materials and Methods

^1H and ^{13}C NMR spectra were recorded on a Bruker Avance 300 or 400 or 500 spectrometer and are referred to the residual solvent signal: dimethylsulfoxide- d_6 (2.50) for ^1H and (39.52) for ^{13}C ; CDCl_3 : (7.26) for ^1H and (77.16) for ^{13}C . Chemical shifts (δ) are given in ppm and coupling constants (J) were measured in Hz. The following abbreviations are used; s-singlet, d-doublet, dd-doublet of doublet, t-triplet, td-triplet of doublet, dt-doublet of triplet, q-quartet, qd-quartet of doublet, qn-quintet, br-broad. ESI- and HR ESI-MS were recorded using Finnigan MAT 1020B and Thermo Scientific Q Exactive hybrid quadrupole-Orbitrap mass; values are given in m/z. Column chromatography was carried out using silica gel (60–120 mesh) packed in glass columns. Analytical TLC was carried out on Macherey-Nagel 60 F245 aluminium-backed silica gel plates. Melting point of compound was measured on Stuart melting point apparatus SMP3. Anhydrous solvents and chemical materials were purchased from commercial sources.

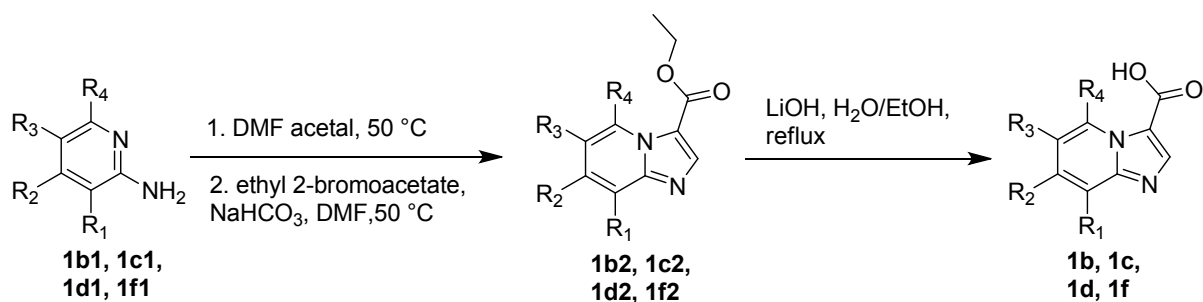
Bromides used in the study



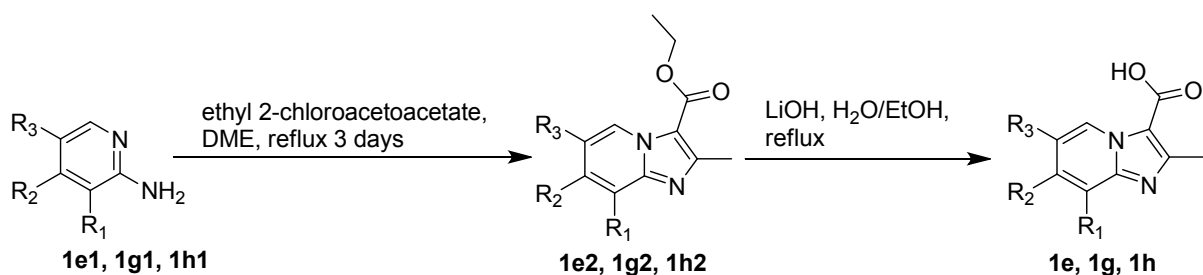
Chlorides used in the study



Synthesis of starting materials



No.	R ₁	R ₂	R ₃	R ₄	ester synthesis reaction time (h)		ester hydrolysis reaction time (h)
					stage 1	stage 2	
1b1/1b2/1b	H	H	CH ₃	H	4	12	12
1c1/1c2/1c	H	CH ₃	H	H	24	12	12
1d1/1d2/1d	CH ₃	H	H	H	7	15	24
1f1/1f2/1f	H	H	Cl	H	8	12	72



No.	R ₁	R ₂	R ₃	ester hydrolysis reaction time (h)
1e1/1e2/1e	H	CH ₃	H	24
1g1/1g2/1g	H	H	Cl	48
1h1/1h2/1h	CF ₃	H	H	36

Imidazo[1,2-*a*]pyridine-3-carboxylic acids **1b-1h** were synthesized using reporting procedure or modification thereof.¹ Below is the brief description of their preparation and analysis.

Synthesis of **1b**, **1c**, **1d**, **1f**

6-methylimidazo[1,2-*a*]pyridine-3-carboxylic acid (**1b**)

5-Methylpyridin-2-amine **1b1** (5g, 46.23 mmol) and *N,N*-dimethyl formamide dimethyl acetal (30 mL) were stirred at 50 °C for 4 hrs. Upon completion, reaction mixture was evaporated on rotary evaporator and dried. The dried residue, ethyl 2-bromoacetate (11.50 g, 69.29 mmol) and NaHCO₃ (5.8 gm, 69.04 mmol) in DMF (30 mL) were stirred at 50 °C. The progress of reaction was monitored by TLC. After 15 hrs the reaction mixture was added in water (200 mL) and extracted with ethyl acetate (2x150 mL). The combined organic phase was separated, washed with water (100 mL), brine (100 mL) and dried with sodium sulphate. The organic solvent was evaporated on rotary evaporator and crude material obtained was purified using silica gel column chromatography with 20% ethyl acetate in hexane. **1b2** was obtained as green liquid (5g, 53% yield). ¹H NMR (400 MHz, CDCl₃): δ 9.11 (s, 1H), 8.25 (s, 1H), 7.66 (d, *J* = 9.1 Hz, 1H), 7.27 (dd, *J* = 9.1, 1.7 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 2.41 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 160.6, 147.1, 140.8, 130.5, 125.4, 124.2, 116.8, 115.4, 60.3, 18.3, 14.4; HRMS (ESI-MS): Calc. for C₁₁H₁₃N₂O₂ [(M+H)⁺]: 205.0972, Found: 205.0976.

1b2(2g, 9.8 mmol) was dissolved in ethanol (24 mL) and 20 mL of LiOH (1 N aq. solution, 19.6 mmol) was added drop wise. The resulting reaction mixture was refluxed for 12 hrs. Ethanol was then removed on rotary evaporator and resulting mixture was cooled at ice bath temperature. The 4N HCl was added drop wise till the P^H of reaction mixture became ≈ 4. The precipitated solid was filtered off and dried to furnish **1b²** as white solid (1.2 gm, 91 % yield). mp= 188-190°C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 9.07 (s, 1H), 8.18 (s, 1H), 7.68 (d, *J* = 9.1 Hz, 1H), 7.40 (dd, *J* = 9.1, 1.7 Hz, 1H), 2.37 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 161.4, 146.8, 140.8, 130.7, 125.0, 124.1, 116.8, 115.6, 17.9; HRMS (ESI-MS): Calc. for C₉H₉N₂O₂ [(M+H)⁺]: 177.0659, Found: 177.0667.

In an analogous way **1c**, **1d**, **1f** were synthesized.

1c²: Obtained 6.19 g (65%) **1c2** as white solid from 5.0g of **1c1**. mp= 72-74°C; ¹H NMR (400 MHz, CDCl₃): δ 9.15-9.09 (m, 1H), 8.24-8.17 (m, 1H), 7.46 (s, 1H), 6.84 (d, *J* = 6.8 Hz, 1H), 4.42-4.33 (m, 2H), 2.43 (s, 3H), 1.40-1.32 (m, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 160.6, 148.8, 141.4, 138.7, 126.6, 116.6, 116.3, 115.3, 60.2, 21.3, 14.4; HRMS (ESI-MS): Calc. for C₁₁H₁₃N₂O₂ [(M+H)⁺]: 205.09715, Found: 205.09837.

1c²: Obtained 0.64 g (74%) **1c** as white solid from 1.0g of **1c2**. mp= 189-192°C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 9.16 (d, *J* = 7.0 Hz, 1H), 8.13 (s, 1H), 7.55 (s, 1H), 7.04 (dd, *J* = 7.0, 1.5 Hz, 1H), 2.42 (s, 3H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 161.4, 148.1, 140.9, 138.6, 126.6, 116.8, 115.9, 115.6, 20.7; HRMS (ESI-MS): Calc. for C₉H₉N₂O₂ [(M+H)⁺]: 177.0659, Found: 177.0667.

1d²: Obtained 3.25 g (34%) **1d2** as red solid from 5.0g of **1d1**. mp= 72-74°C; ¹H NMR (400 MHz, CDCl₃) δ 9.13 (d, *J* = 7.0 Hz, 1H), 8.25 (s, 1H), 7.19-7.15 (m, 1H), 6.91 (t, *J* = 7.0 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.63 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (125 MHz,

CDCl₃): δ 160.8, 148.7, 140.8, 127.7, 126.5, 125.5, 116.3, 114.3, 60.5, 17.0, 14.6; HRMS (ESI-MS):Calc. for C₁₁H₁₃N₂O₂ [(M+H)⁺]: 205.0972, Found: 205.0977.

1d: Obtained 0.65 g (49%) **1d** as violet solid from 1.5 g of **1d2**. mp= 184-185°C; ¹H NMR (400 MHz, DMSO-d₆): δ 9.20 (d, *J* = 7.0 Hz, 1H), 8.44 (s, 1H), 7.54 (d, *J* = 7.1 Hz, 1H), 7.27 (t, *J* = 7.0 Hz, 1H), 2.59 (s, 3H); ¹³C NMR (75 MHz, DMSO-d₆): δ 160.8, 144.9, 135.5, 129.9, 125.8, 125.5, 117.0, 116.4, 16.5; HRMS (ESI-MS):Calc. for C₉H₉N₂O₂ [(M+H)⁺]: 177.06585, Found: 177.06720.

1f2^{1c}: Obtained 5.5 g (63%) **1f2** as yellow semisolid from 5.0g of **1f1**. ¹H NMR (400 MHz, CDCl₃) δ 9.39 (dd, *J* = 2.0, 0.8 Hz, 1H), 8.29 (s, 1H), 7.68 (dd, *J* = 9.5, 0.8 Hz, 1H), 7.39 (dd, *J* = 9.5, 2.0 Hz, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 160.5, 146.8, 141.9, 129.0, 125.9, 122.9, 118.2, 116.4, 60.9, 14.6; HRMS (ESI-MS):Calc. for C₁₀H₁₀ClN₂O₂ [(M+H)⁺]: 225.0425, Found: 225.0428.

1f1^{1c}: Obtained 0.72 g (54%) **1f1** as violet solid from 1.5 g of **1f2**. mp= 206°C; ¹H NMR (400 MHz, DMSO-d₆): δ 9.31 (dd, *J* = 2.0, 0.6 Hz, 1H), 8.27 (s, 1H), 7.84 (dd, *J* = 9.5, 0.6 Hz, 1H), 7.62 (dd, *J* = 9.5, 2.0 Hz, 1H); ¹³C NMR (100 MHz, DMSO-d₆): 160.1, 140.2, 127.4, 126.8, 124.0, 120.3, 117.8, 117.2; HRMS (ESI-MS):Calc. for C₈H₆ClN₂O₂ [(M+H)⁺]: 197.01123, Found: 197.01253.

Synthesis of **1e**, **1g**, **1h**

Ethyl-2-chloroacetoacetate (7.93 g, 45.8 mmol) and 2-Amino-4-picoline (10.0 g, 91.5 mmol) were dissolved in 95 mL of 1,2-dimethoxyethane (DME) and heated for 48 hrs at reflux. The reaction mixture was cooled and solid (2-amino-4-picoline hydrochloride salt) was collected and washed with hexane. The filtrate was concentrated in vacuo and resulting residue was dissolved in dichloromethane (200 mL) and washed with 5% acetic acid solution (2x 50 mL) and brine. The organic phase was dried with sodium sulfate, filtered and concentrated in vacuo. Crude product was purified by silica gel with 22% ethyl acetate in hexane to furnish 7.0 g (34%) of ethyl 2,7-dimethylimidazo[1,2-*a*]pyridine-3-carboxylate (**1e2**)^{1a} as a yellowish solid. mp= 66°C; ¹H NMR (500 MHz, CDCl₃): δ 9.12 (d, *J* = 7.1 Hz, 1H), 7.35 (s, 1H), 6.76 (dd, *J* = 7.1, 1.2 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.66 (s, 3H), 2.40 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 161.4, 152.6, 147.2, 139.1, 127.1, 116.1, 115.3, 112.1, 60.2, 21.3, 16.5, 14.5; HRMS (ESI-MS):Calc. for C₁₂H₁₅N₂O₂ [(M+H)⁺]: 219.11280, Found: 219.11397.

1e2 (4.0 g, 18.34 mmol) was dissolved in 55 mL ethanol and 37 mL of 1 N LiOH solution (36.58 mmol) was added. The reaction mixture was refluxed for 48 hrs. Once complete, ethanol was removed on rotary evaporator and resulting mixture was cooled at ice bath temperature. The 4N HCl was added drop wise till the pH of reaction mixture became \approx 4. The precipitated solid was filtered off and dried under vacuum to furnish **1e**^{1a} as white solid (2.6 gm, 78 % yield). mp= 216-218°C; ¹H NMR (400 MHz, DMSO-d₆): δ 9.33 (d, *J* = 7.1 Hz, 1H), 7.79 (s, 1H), 7.45 (dd, *J* = 7.1, 1.5 Hz, 1H), 2.71 (s, 3H), 2.55 (s, 3H); ¹³C NMR (75 MHz, DMSO-d₆): δ 160.9, 146.4, 141.9, 140.0, 128.4, 120.1, 113.3, 110.8, 21.0, 12.3; HRMS (ESI-MS):Calc. for C₁₀H₁₁N₂O₂ [(M+H)⁺]: 191.08150, Found: 191.08264.

In an analogous way **1g** and **1h** were synthesized.

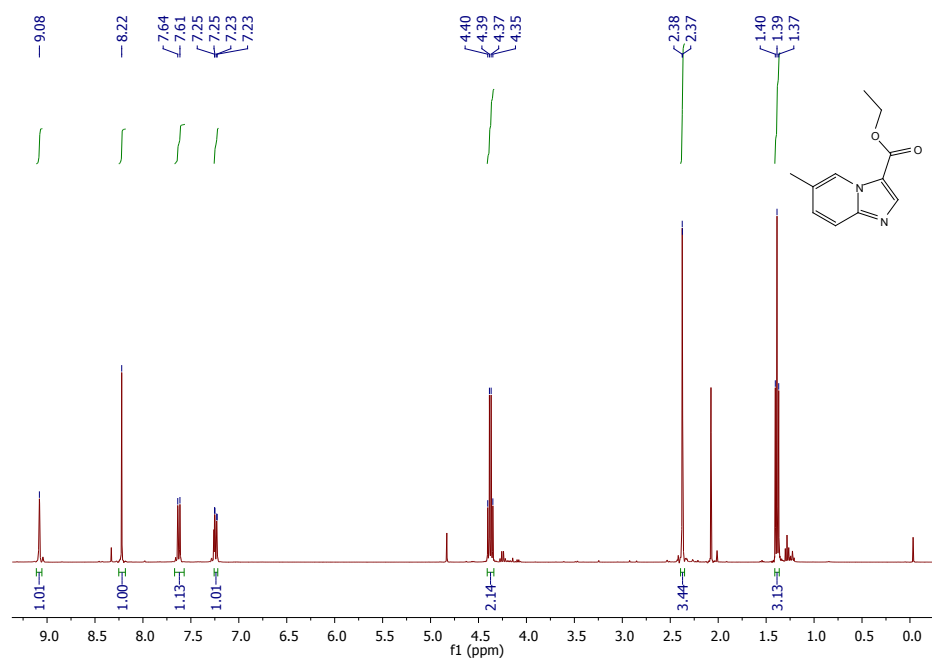
1g2^{1c}: Obtained 4.0 g (43%) **1g2** as yellow solid from 10.0 g of **1g1**. mp= 102-104°C; ¹H NMR (500 MHz, CDCl₃): δ 9.40 (dd, *J* = 2.0, 0.7 Hz, 1H), 7.56 (d, *J* = 9.3 Hz, 1H), 7.35 (dd, *J* = 9.3, 2.0 Hz, 1H), 4.44 (q, *J* = 7.1 Hz, 2H), 2.71 (s, 3H), 1.44 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 161.3, 153.3, 145.2, 128.9, 126.1, 122.1, 117.0, 113.2, 60.7, 16.7, 14.6; HRMS (ESI-MS): Calc. for C₁₁H₁₂ClN₂O₂ [(M+H)⁺]: 239.05818, Found: 239.05941.

1g1^c: Obtained 1.5g (68%) **1g** as white solid from 1.0 g of **1g2**. mp= 158-160°C; ¹H NMR (400 MHz, DMSO-d₆): δ 9.31 (dd, *J* = 2.1, 0.6 Hz, 1H), 7.71 (dd, *J* = 9.5, 0.6 Hz, 1H), 7.59 (dd, *J* = 9.5, 2.1 Hz, 1H), 2.59 (s, 3H); ¹³C NMR (75 MHz, DMSO-d₆) δ 161.9, 151.7, 144.2, 128.7, 125.4, 120.8, 117.0, 113.1, 15.9; HRMS (ESI-MS): Calc. for C₉H₈ClN₂O₂ [(M+H)⁺]: 211.02688, Found: 211.02825.

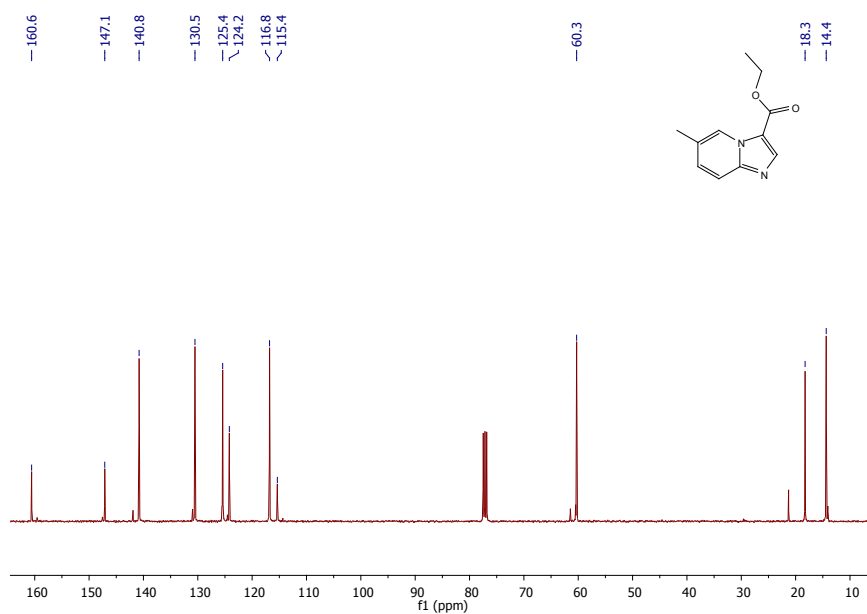
1h2: Obtained 0.72 g (45%) **1h2** as yellow solid from 1.0 g of **1h1**. mp= 88-90°C; ¹H NMR (500 MHz, CDCl₃): δ 9.51 (d, *J* = 7.0 Hz, 1H), 7.70 (d, *J* = 7.1 Hz, 1H), 7.04 (t, *J* = 7.1 Hz, 1H), 4.45 (q, *J* = 7.1 Hz, 2H), 2.78 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H), ¹³C NMR (100 MHz, DMSO-d₆): δ 161.3, 153.7, 142.5, 131.1, 125.7, 125.6, 122.2 (q, *J* = 272.2 Hz), 113.5, 112.0, 60.8, 16.9, 14.4; HRMS (ESI-MS): Calc. for C₁₂H₁₂F₃N₂O₂ [(M+H)⁺]: 273.08454, Found: 273.08563.

1h: Obtained 0.29 g (52%) **1h** as pale yellow solid from 0.62 g of **1h2**. mp= 171-173°C; ¹H NMR (400 MHz, DMSO-d₆): δ 9.49 (d, *J* = 7.0 Hz, 1H), 7.94 (d, *J* = 7.3 Hz, 1H), 7.26 (t, *J* = 7.1 Hz, 1H), 2.65 (s, 3H); ¹³C NMR (75 MHz, DMSO-d₆): δ 162.0, 152.1, 141.3, 131.7, 126.3 (X2), 119.2 (q, *J* = 272.1 Hz), 112.5, 16.1; HRMS (ESI-MS): Calc. for C₁₀H₈F₃N₂O₂ [(M+H)⁺]: 245.05324, Found: 245.05448.

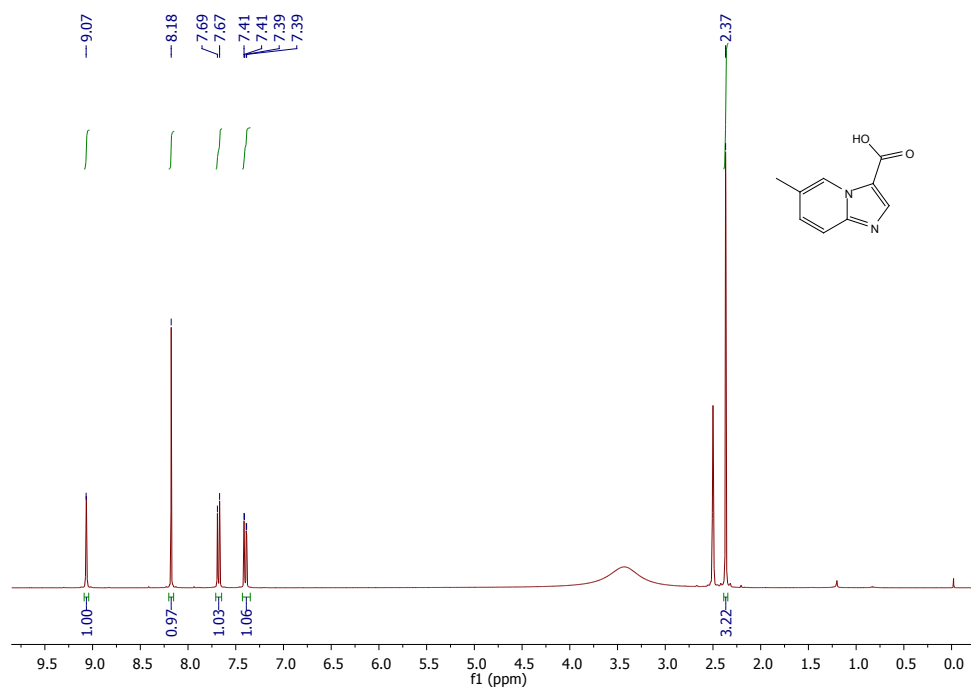
^1H and ^{13}C NMR spectra of the compounds



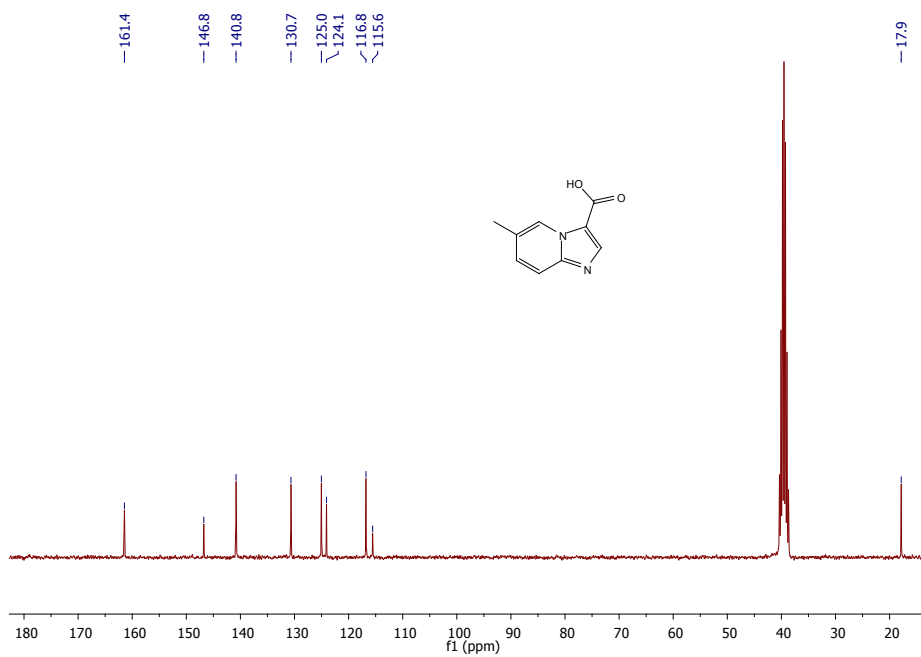
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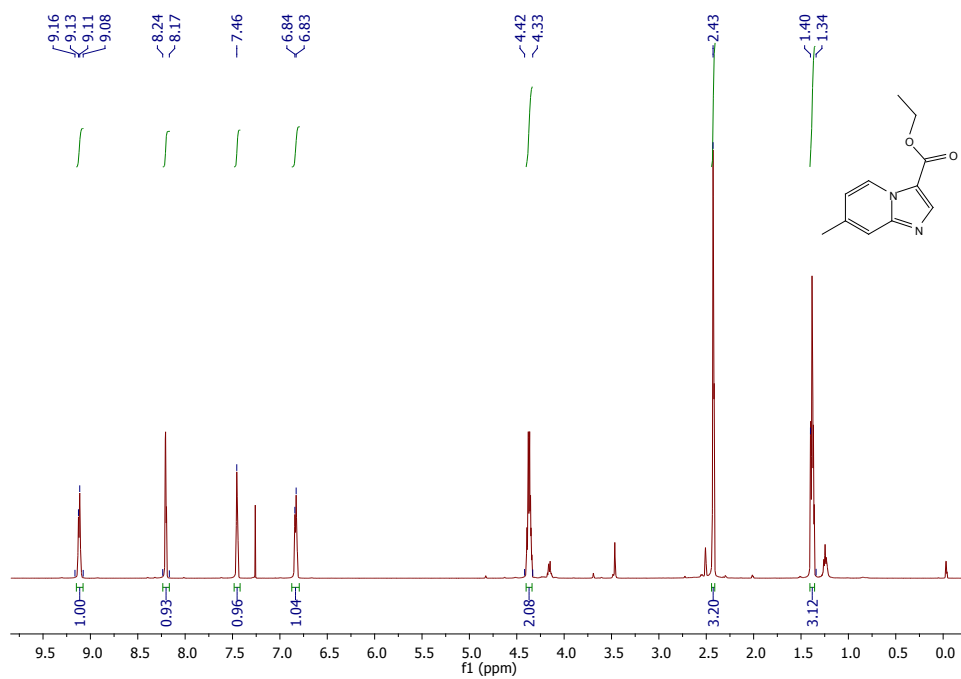
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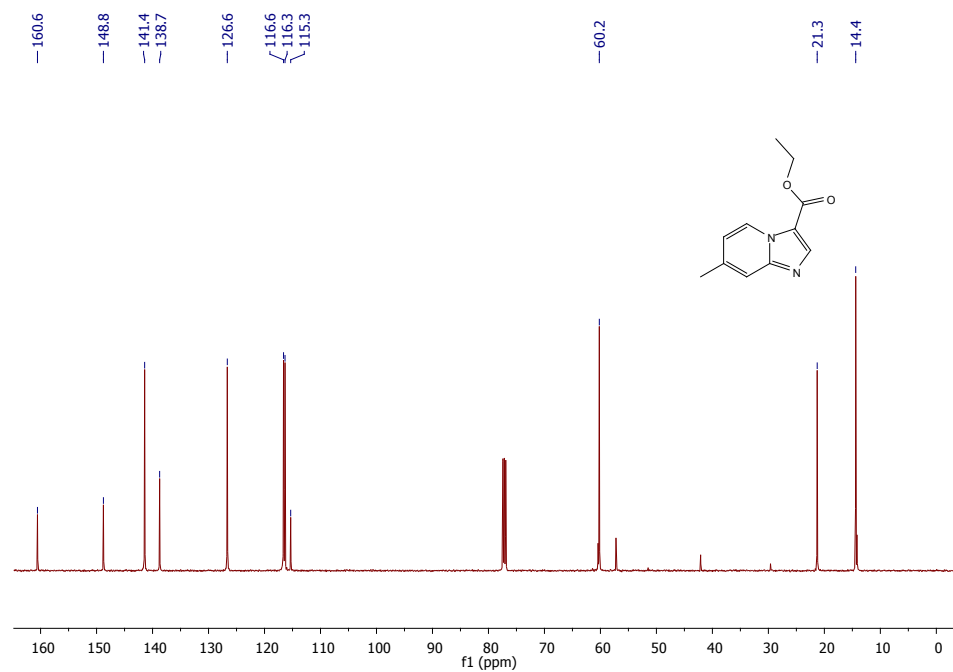
^1H NMR spectrum of **1b**



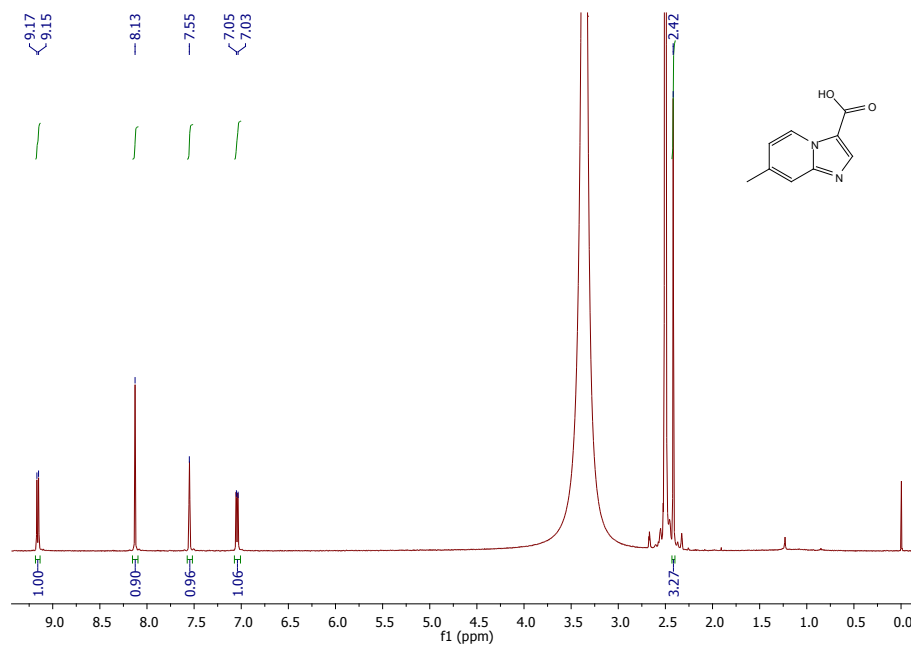
^{13}C NMR spectrum of **1b**



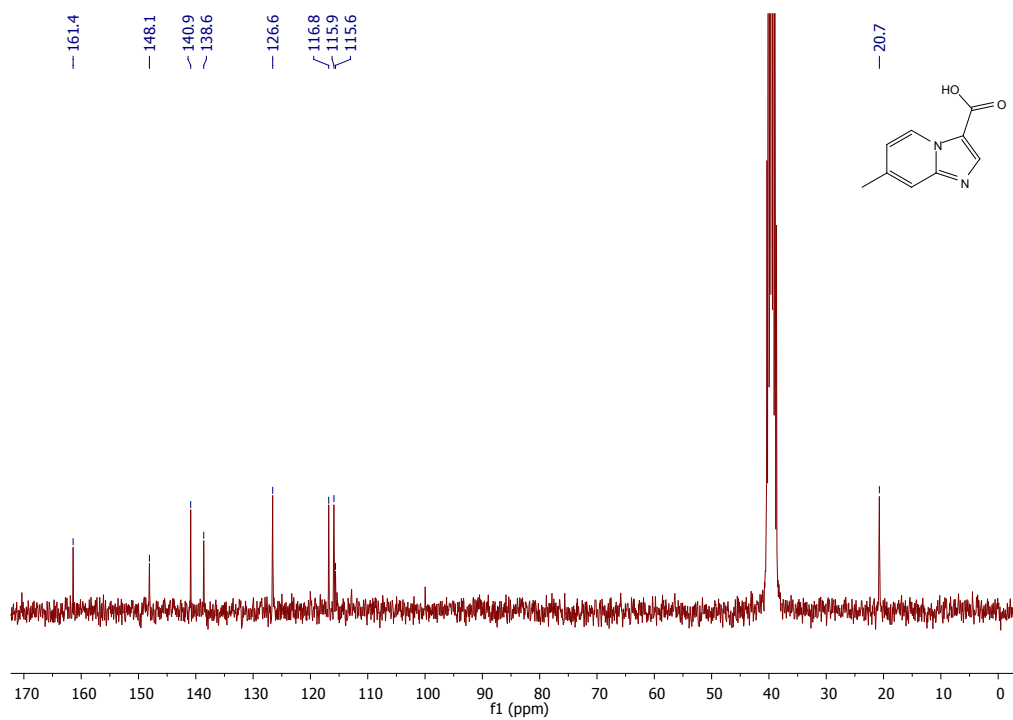
^1H NMR spectrum of **1c2**



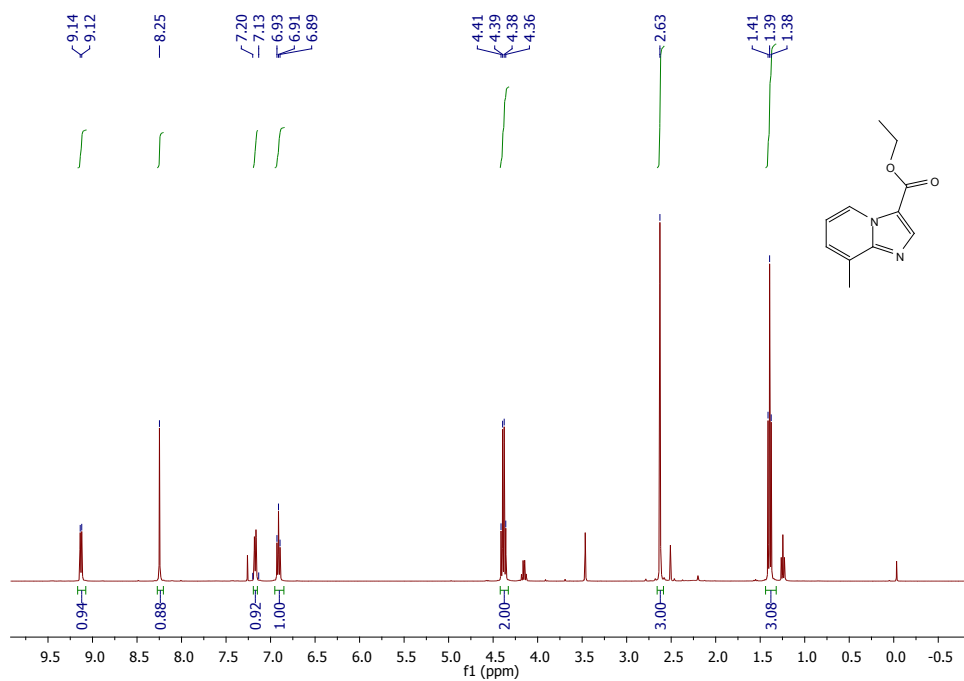
^{13}C NMR spectrum of **1c2**



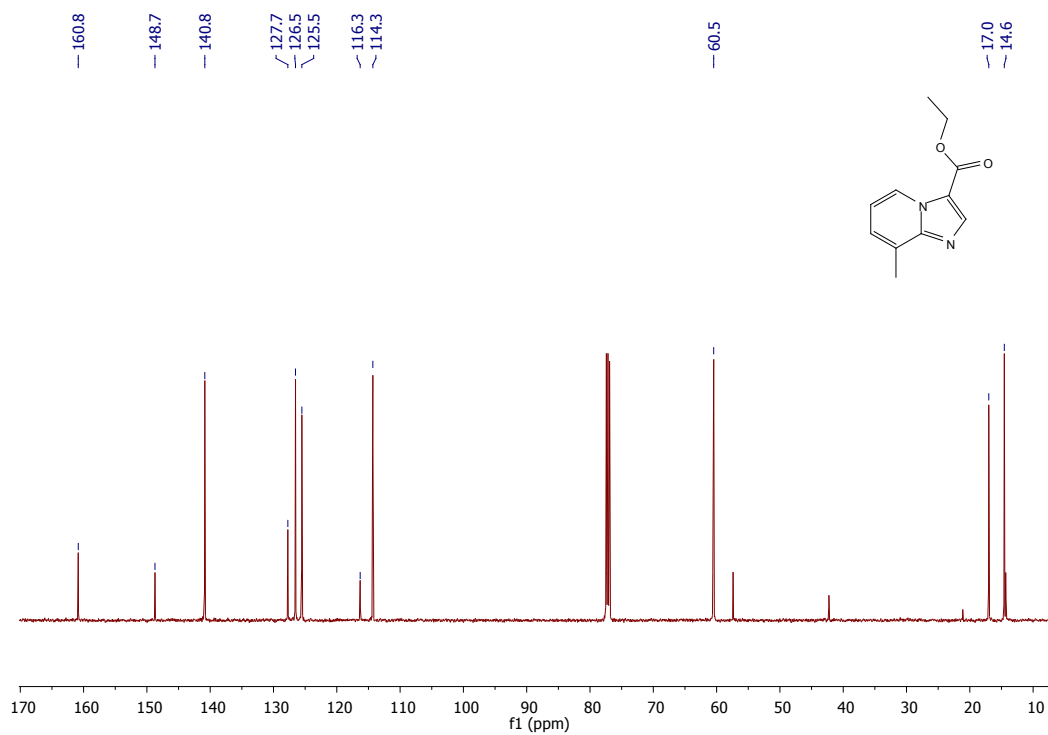
^1H NMR spectrum of **1c**



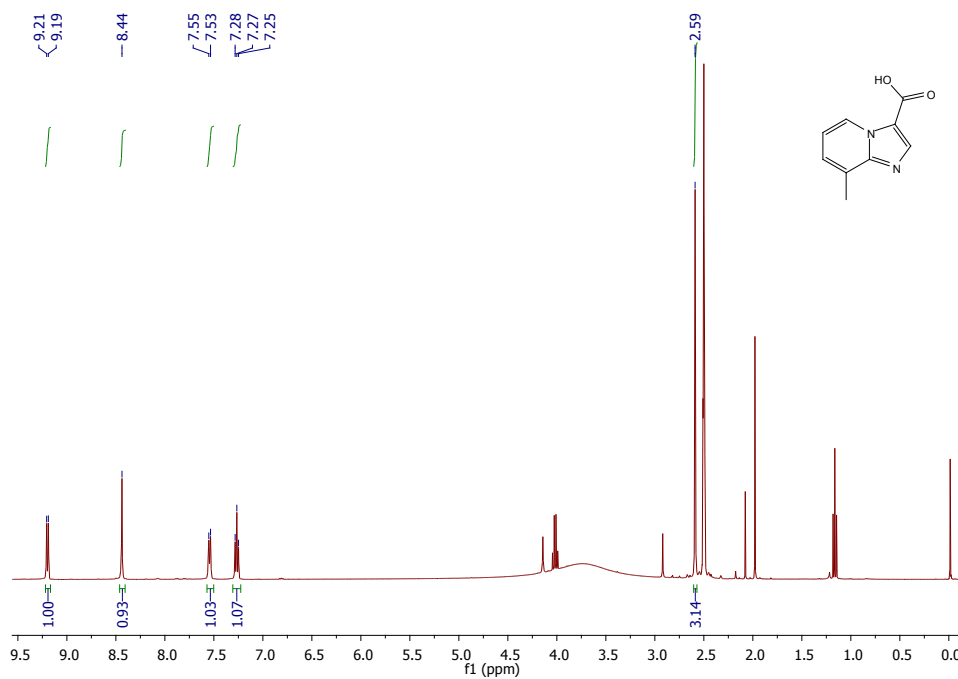
^{13}C NMR spectrum of **1c**



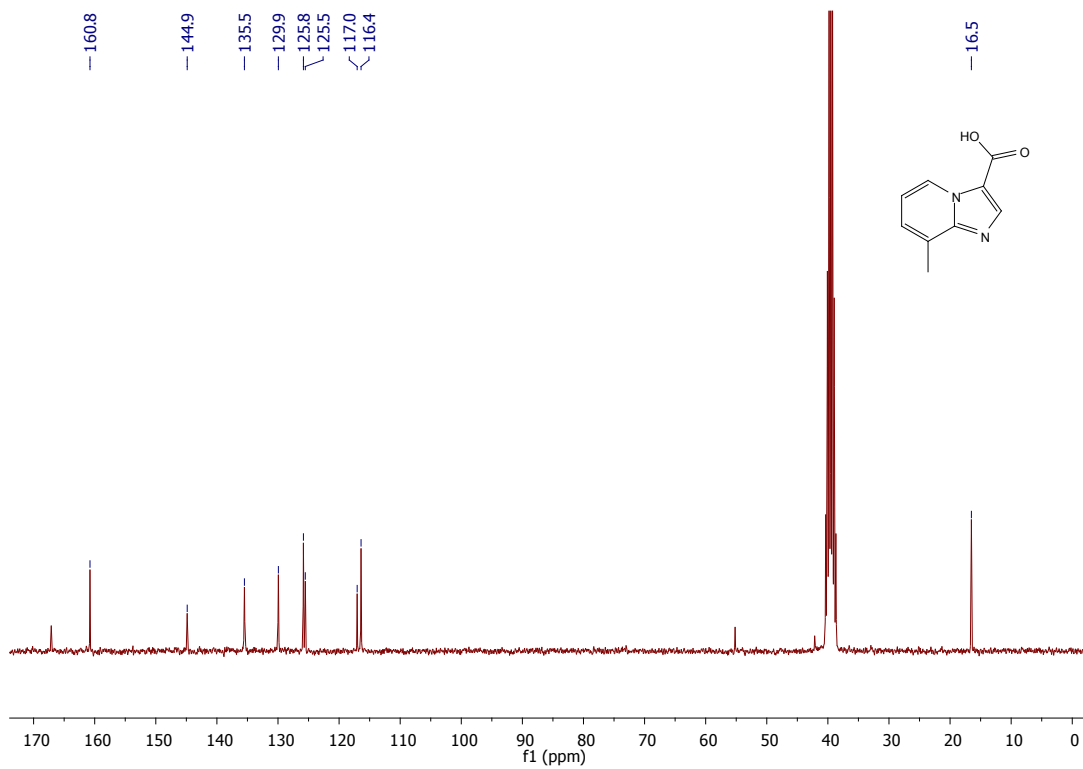
^1H NMR spectrum of **1d2**



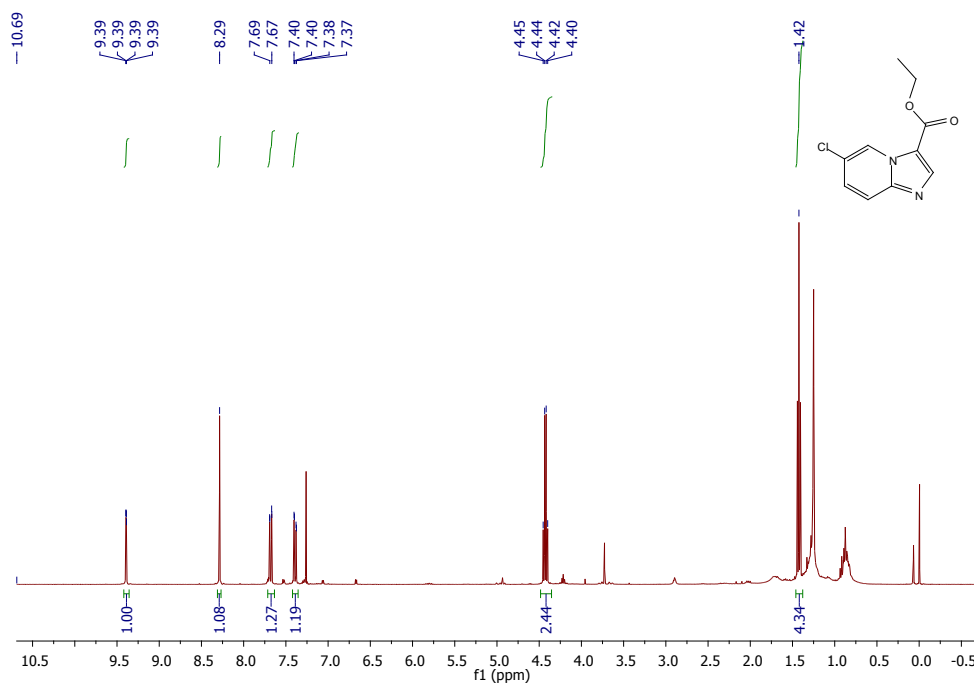
^{13}C NMR spectrum of **1d2**



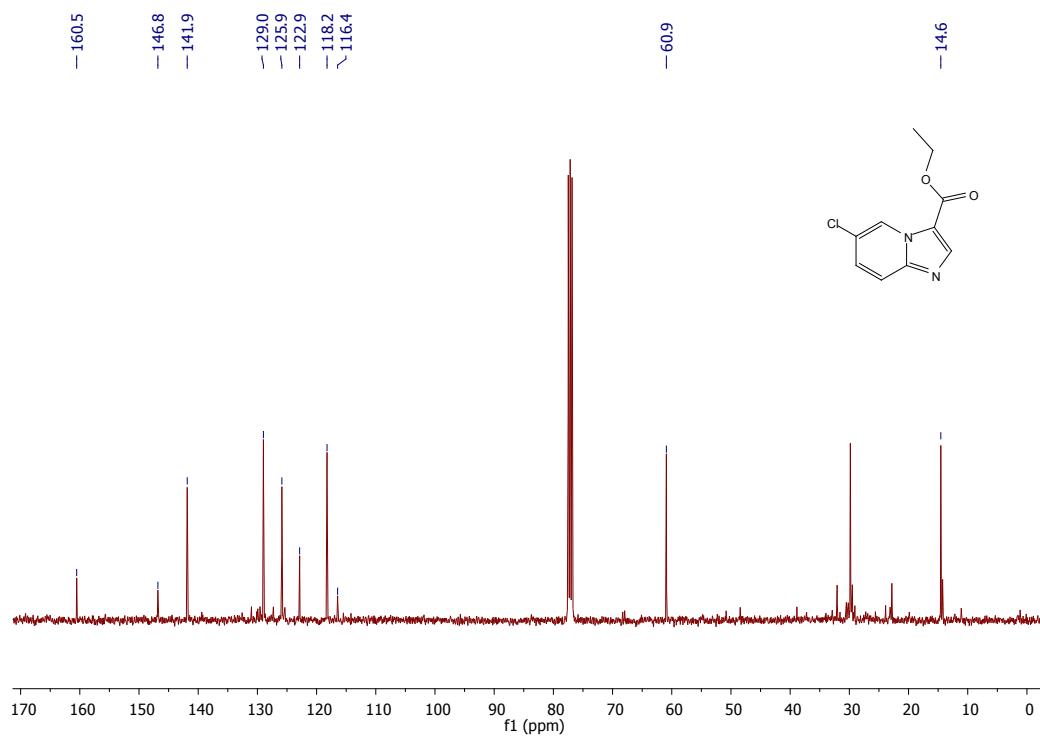
^1H NMR spectrum of **1d**



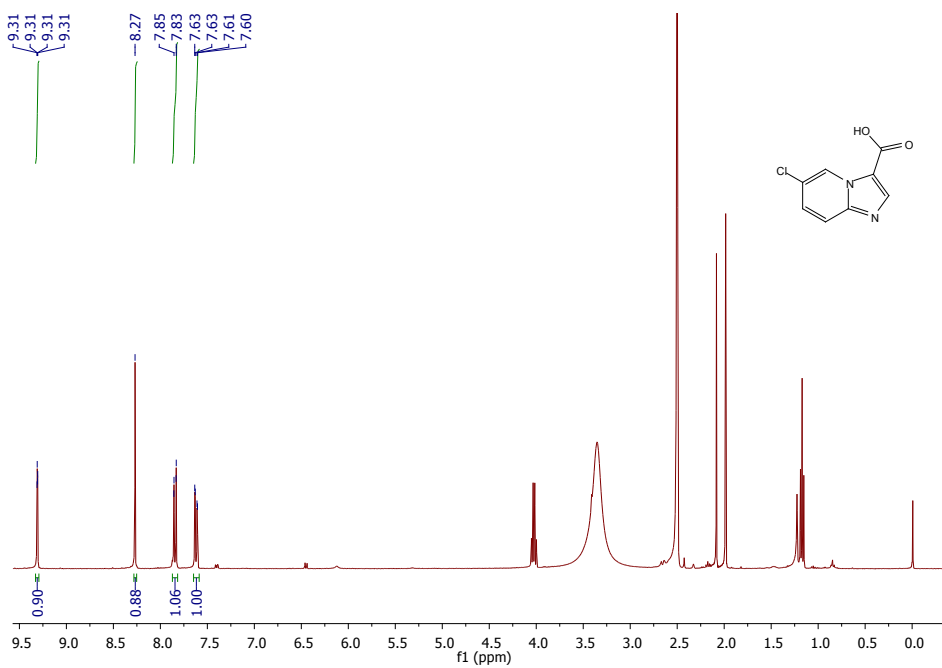
^{13}C NMR spectrum of **1d**



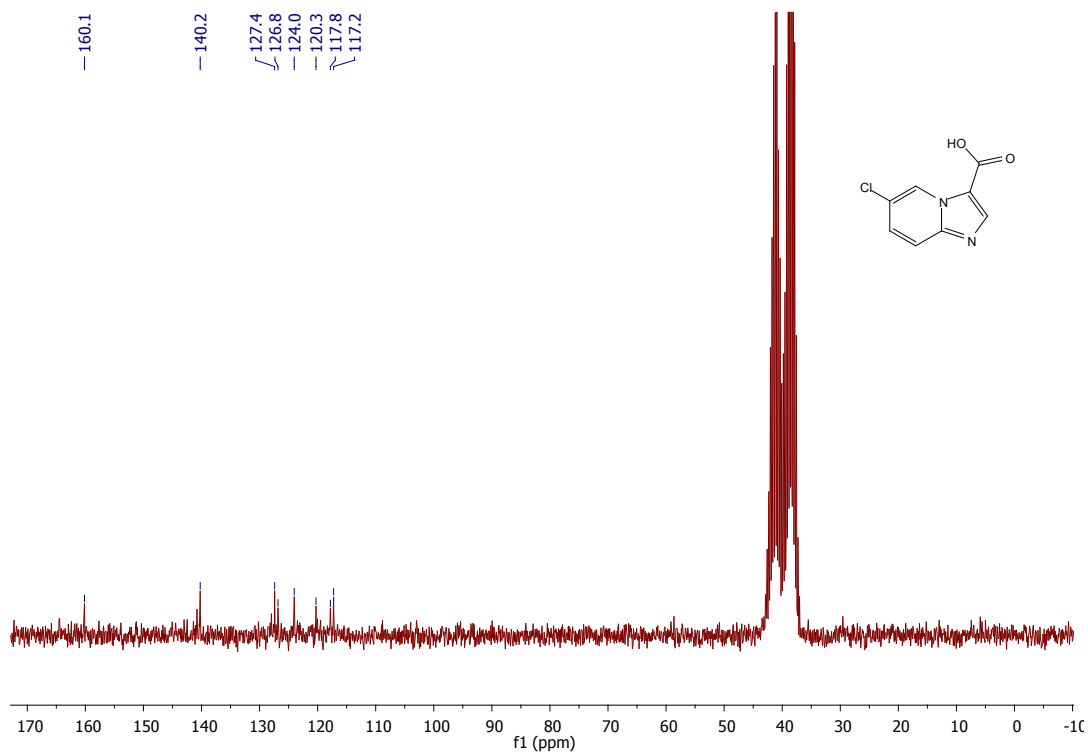
^1H NMR spectrum of **1f2**



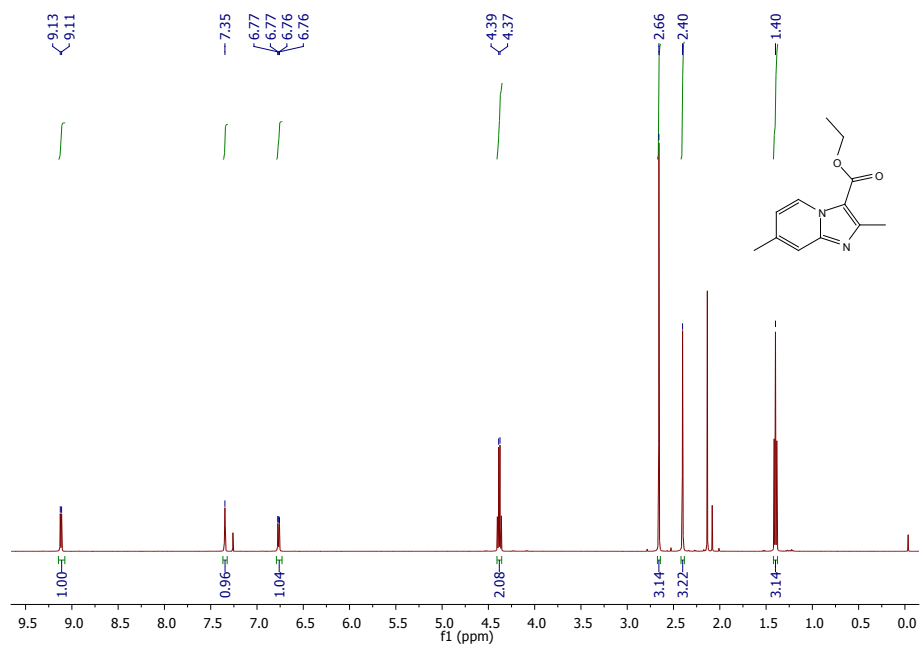
^{13}C NMR spectrum of **1f2**



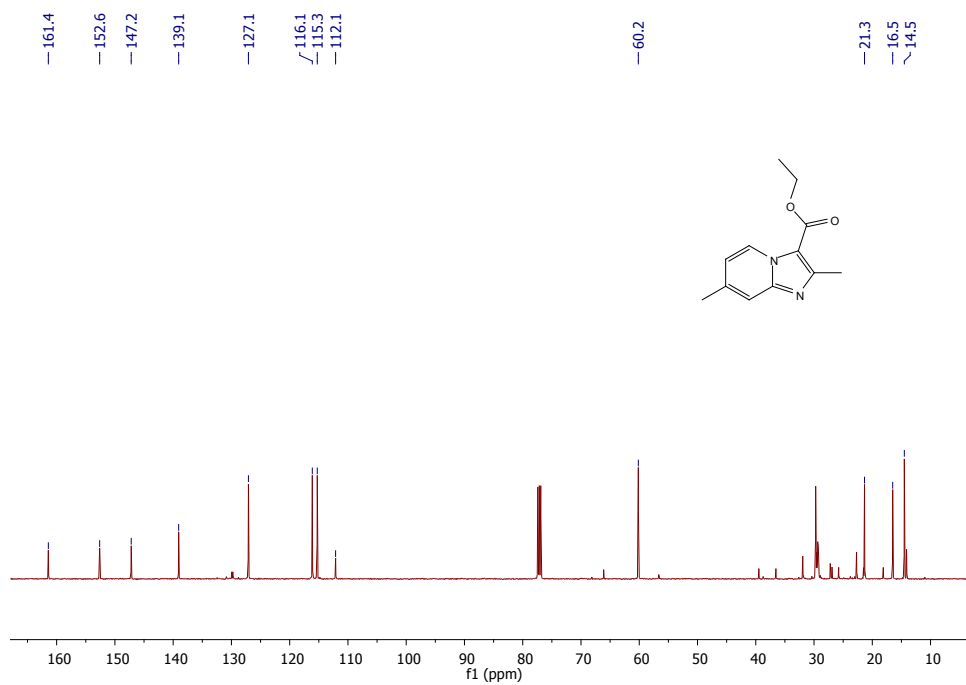
¹H NMR spectrum of **1f**



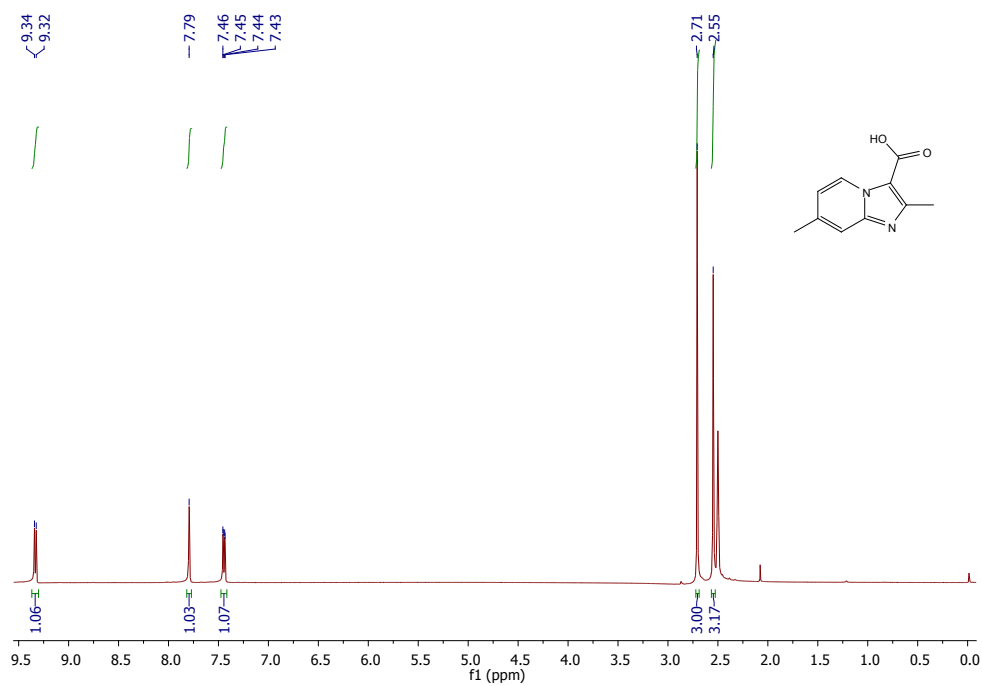
¹³C NMR spectrum of **1f**



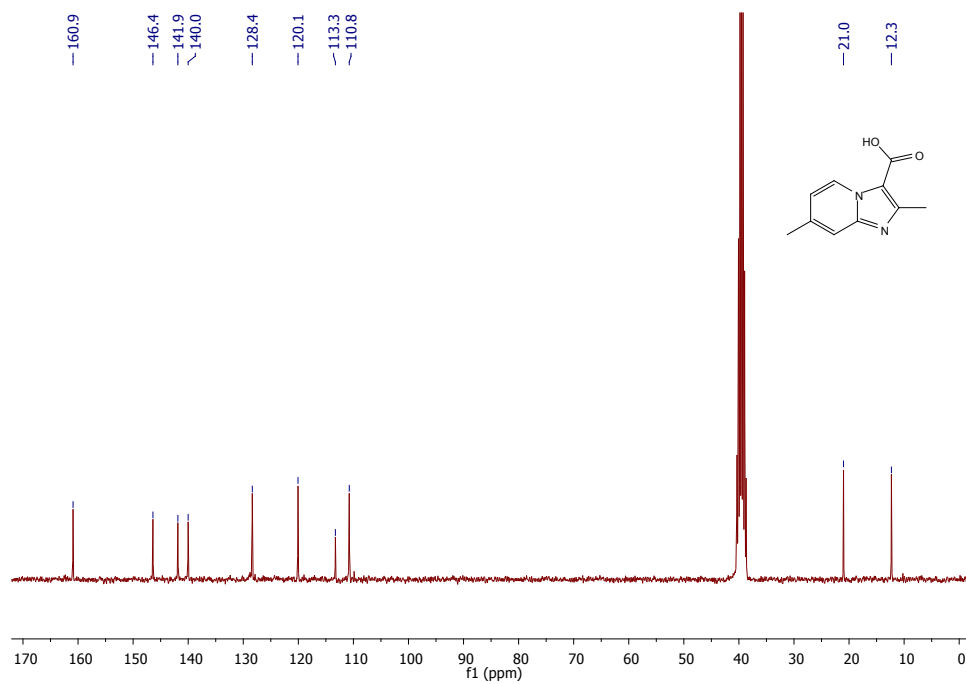
^1H NMR spectrum of **1e2**



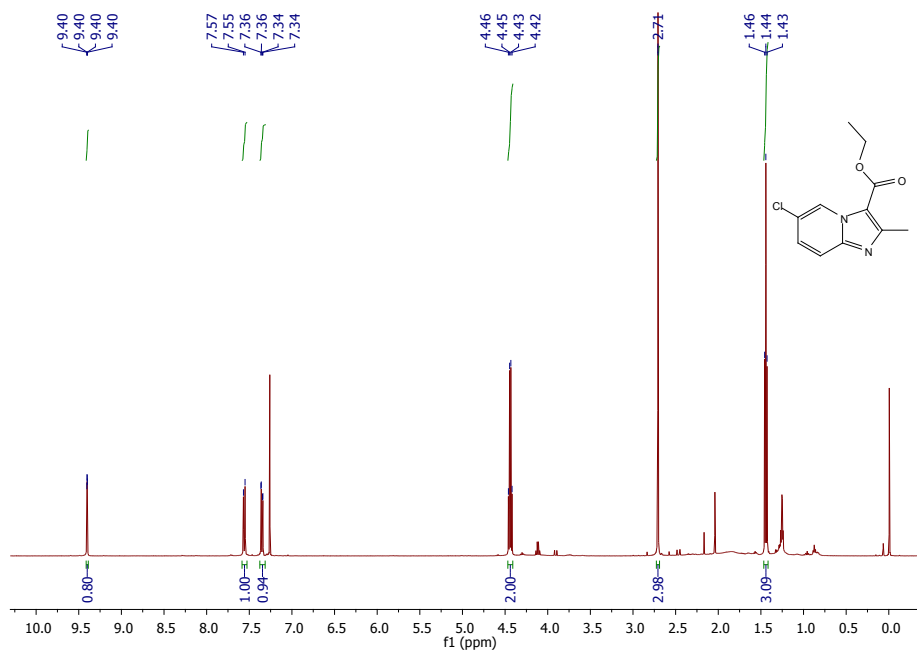
^{13}C NMR spectrum of **1e2**



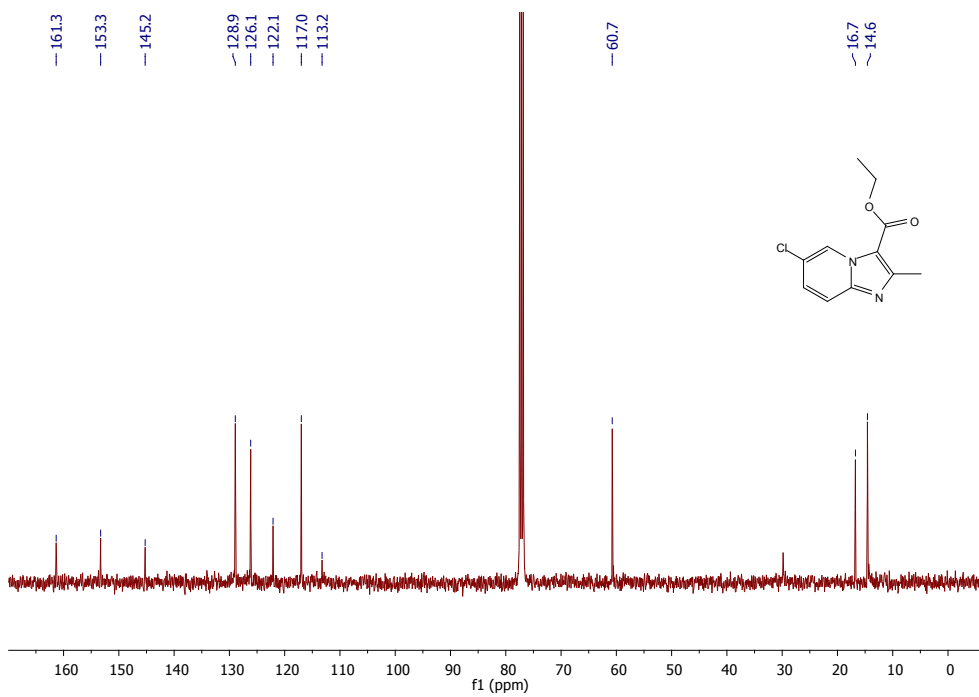
^1H NMR spectrum of **1e**



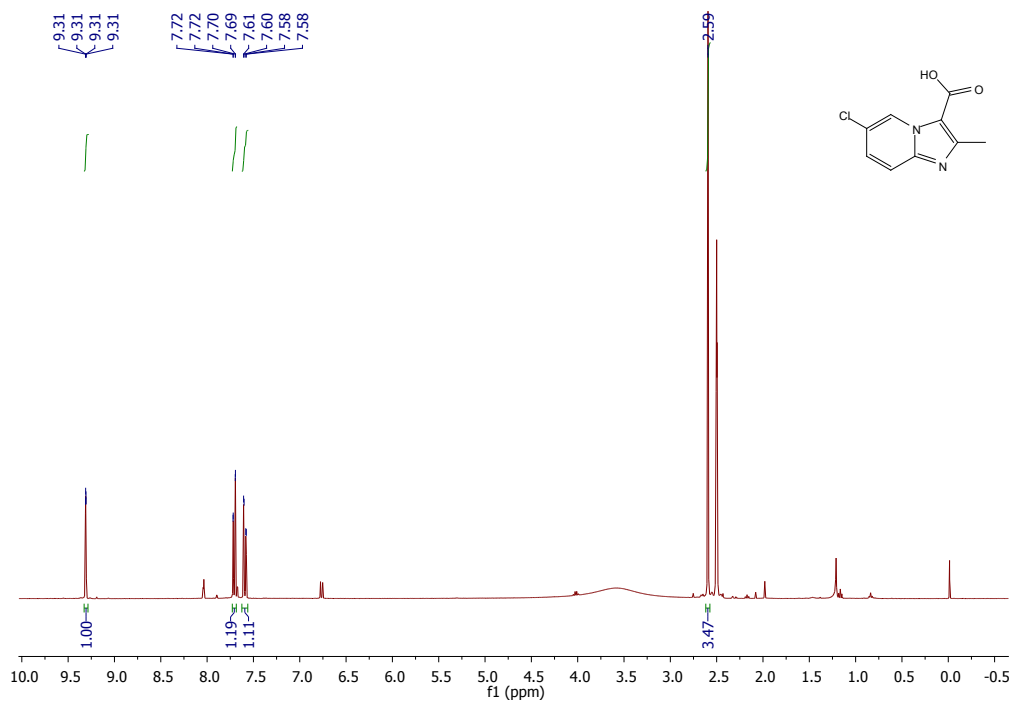
^{13}C NMR spectrum of **1e**



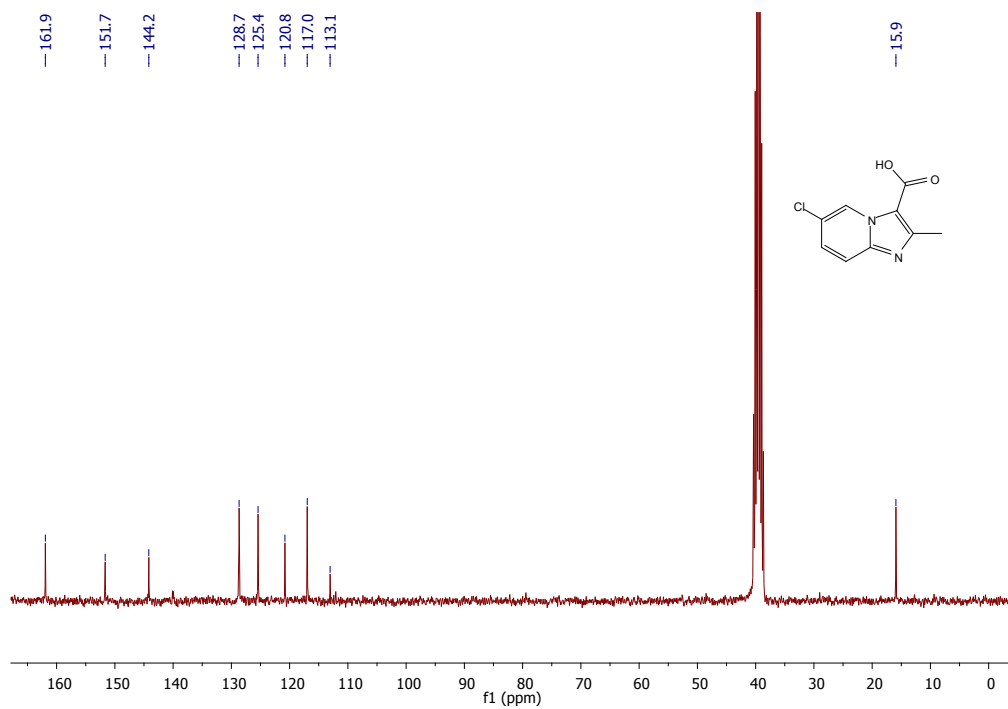
^1H NMR spectrum of **1g2**



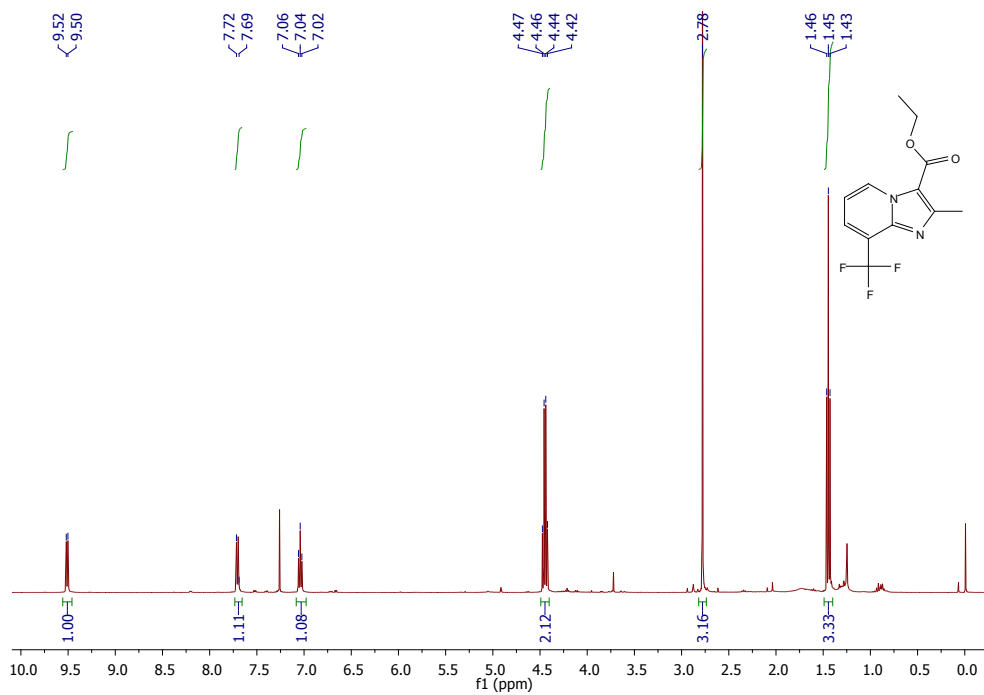
^{13}C NMR spectrum of **1g2**



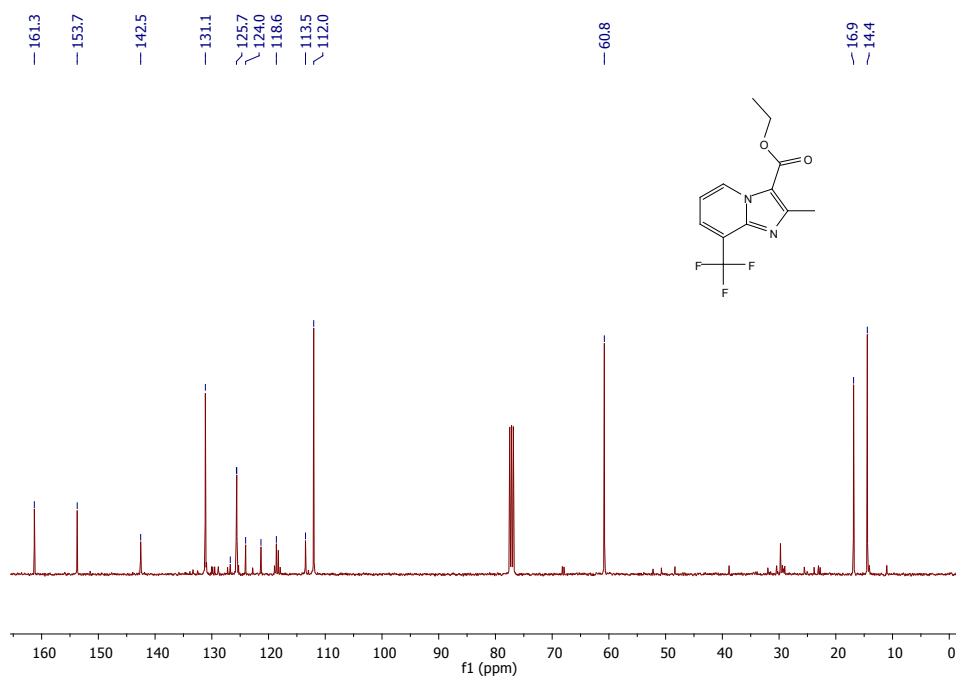
^1H NMR spectrum of **1g**



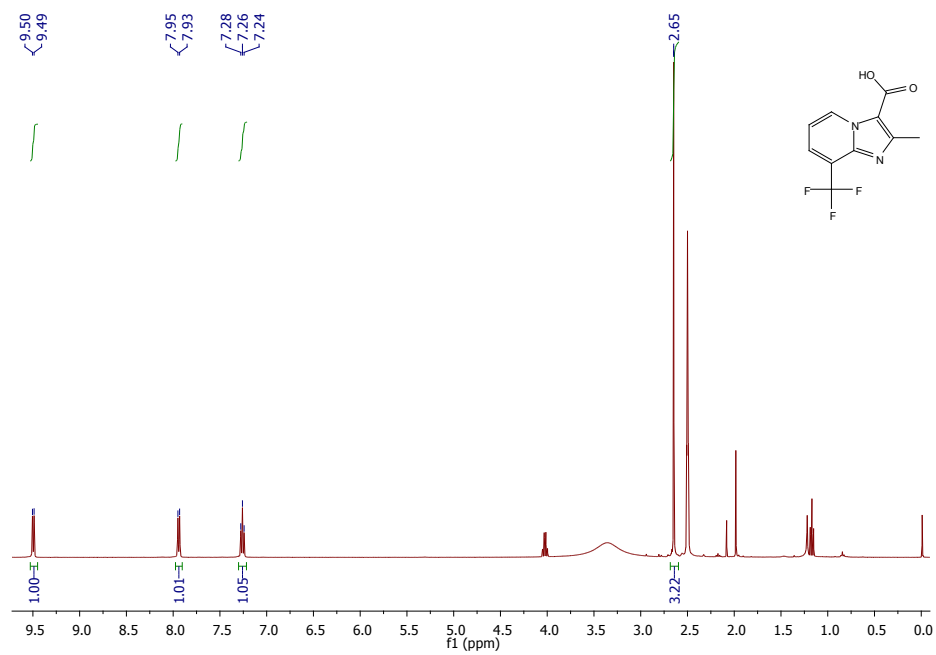
^{13}C NMR spectrum of **1g**



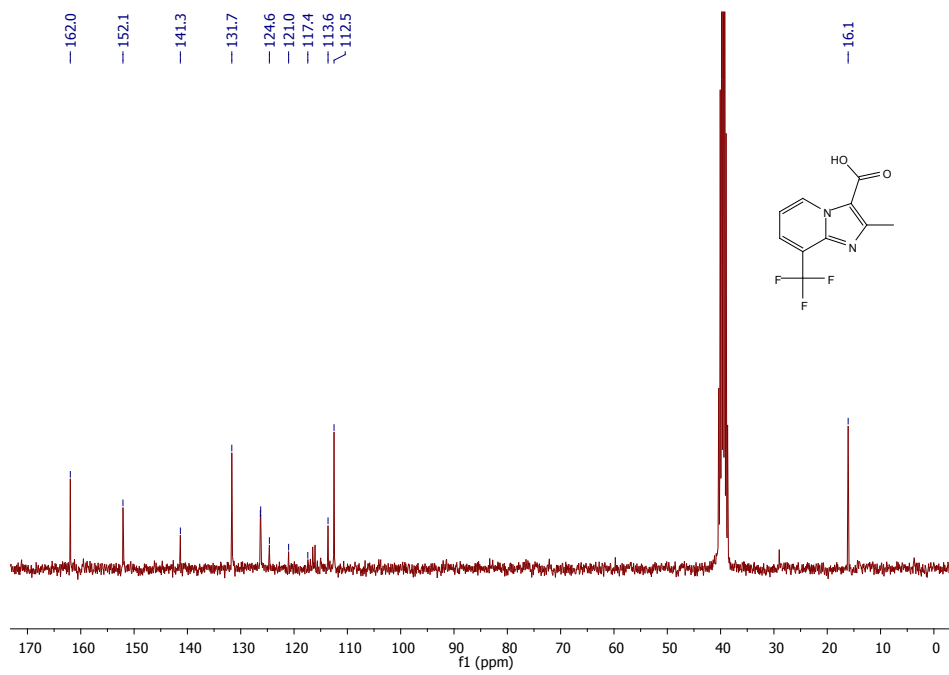
^1H NMR spectrum of **1h2**



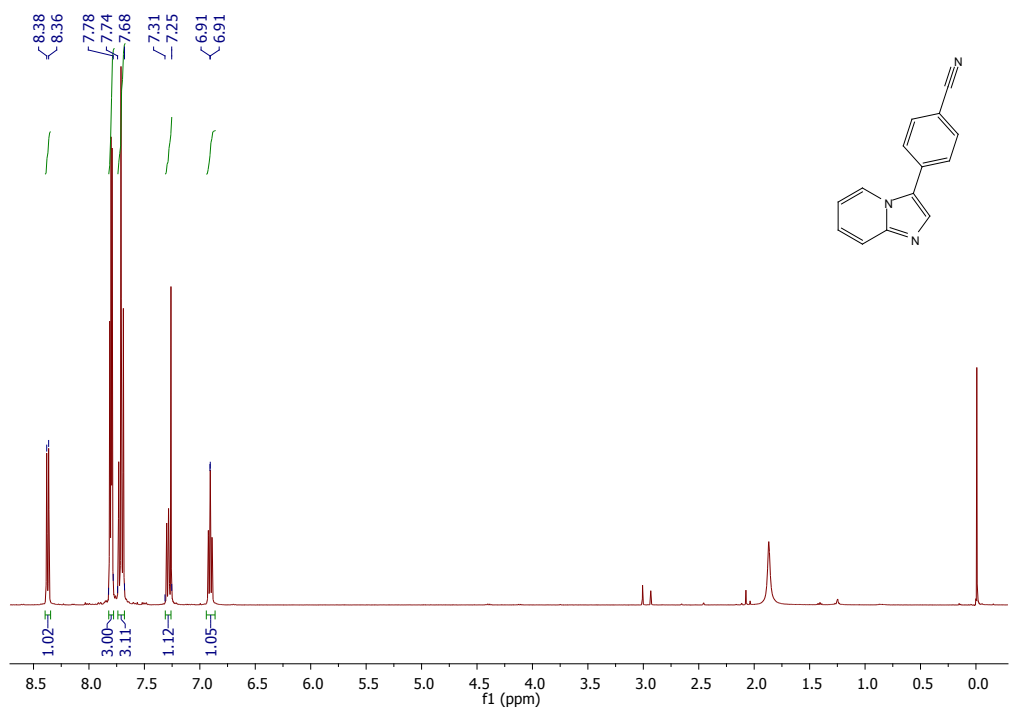
^{13}C NMR spectrum of **1h2**



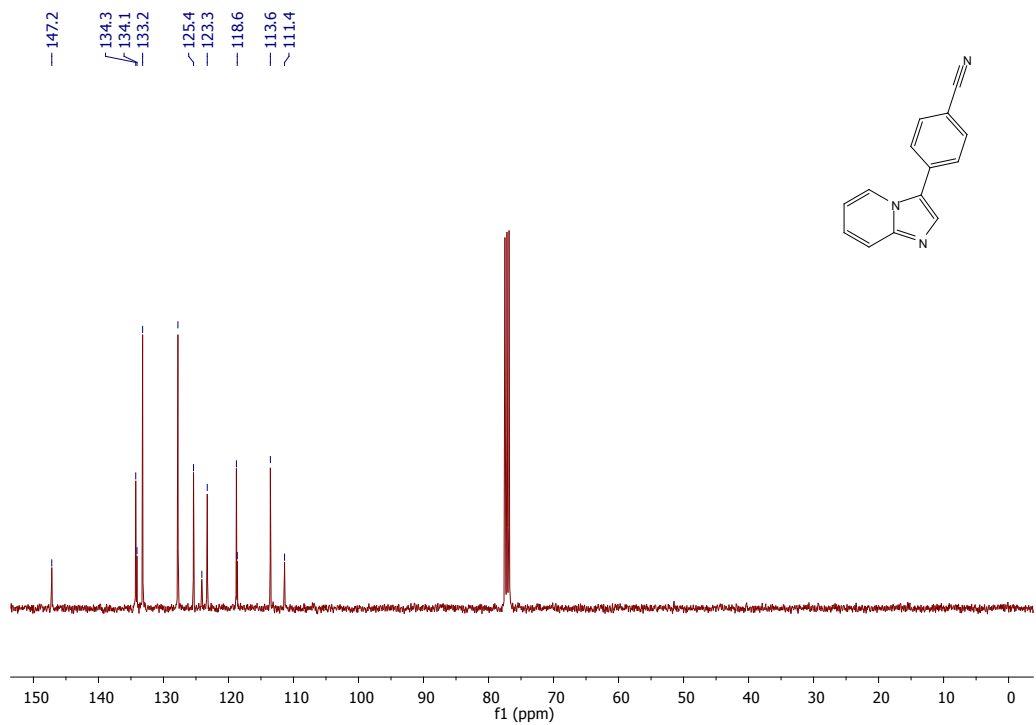
^1H NMR spectrum of **1h**



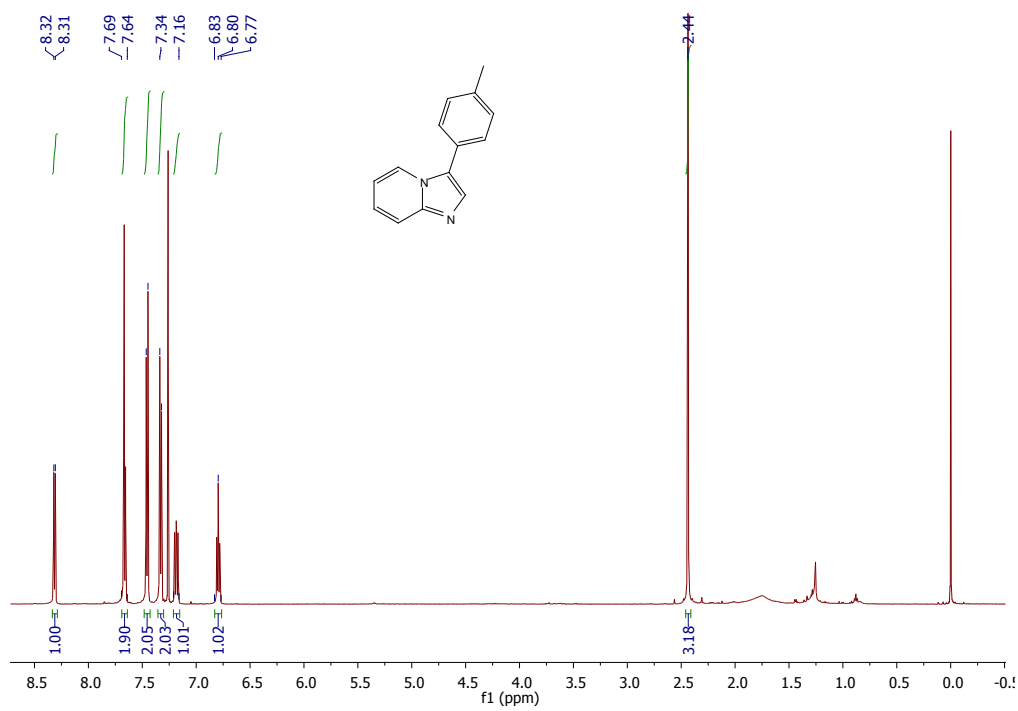
^{13}C NMR spectrum of **1h**



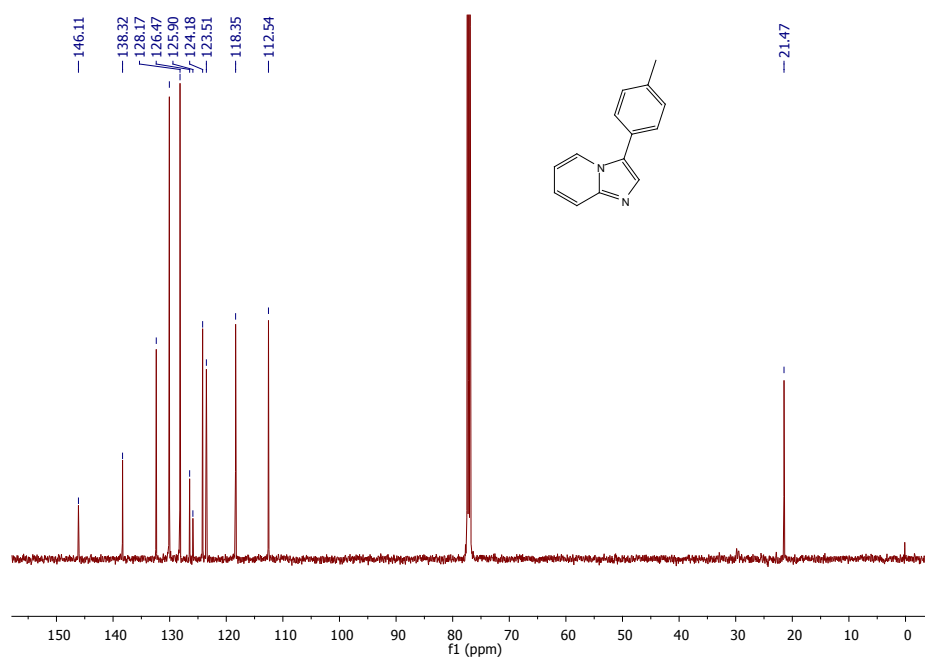
¹H NMR spectrum of **3a**



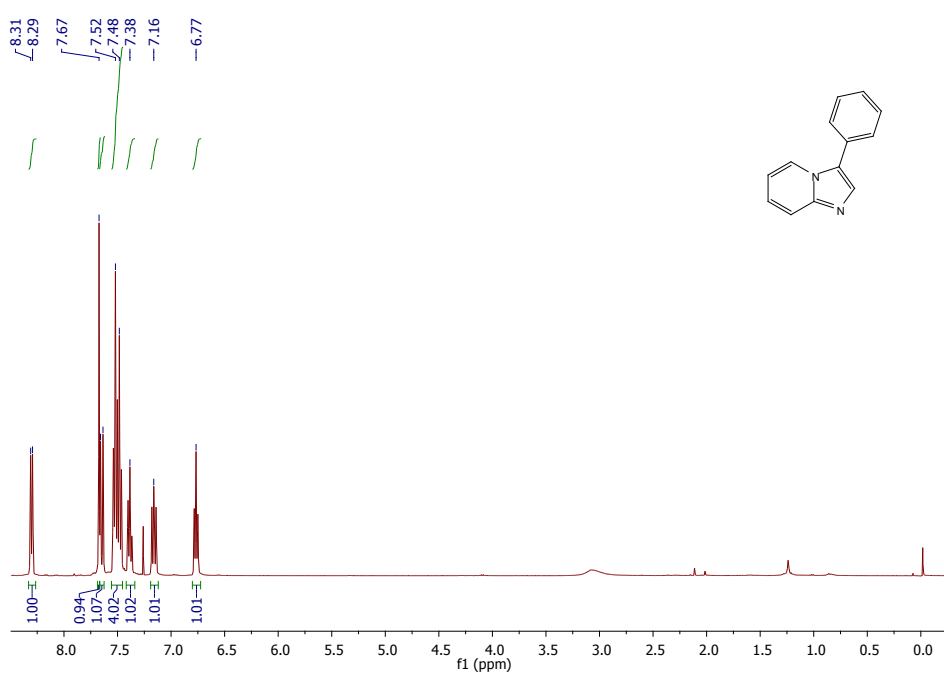
¹³C NMR spectrum of **3a**



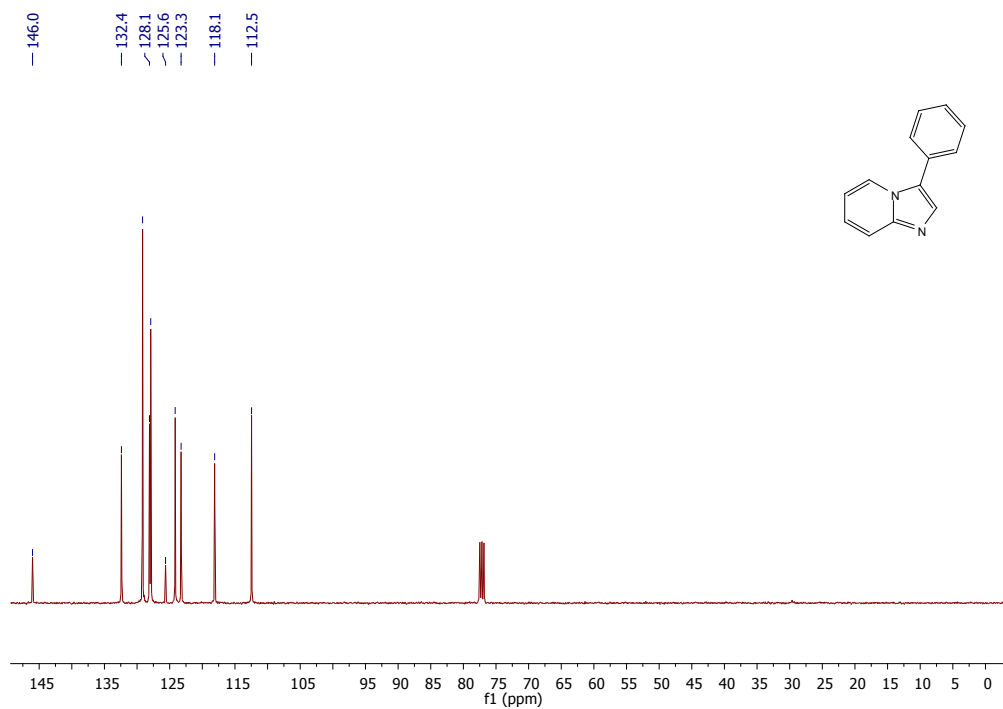
^1H NMR spectrum of **3b**



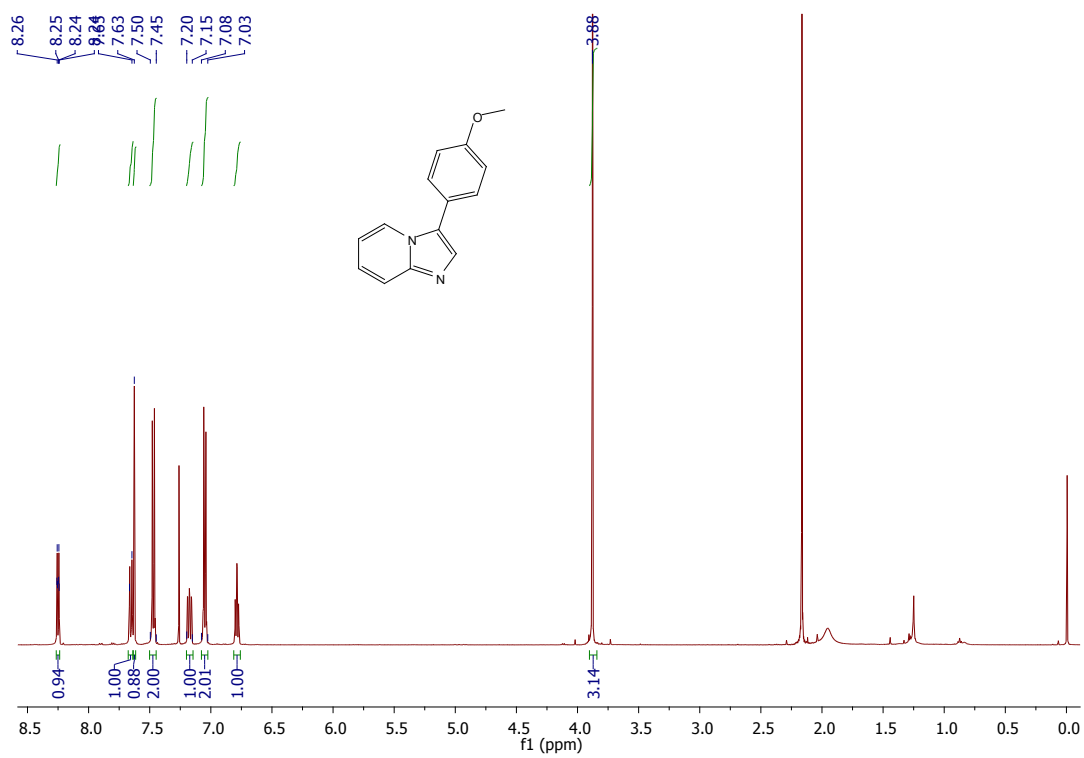
^{13}C NMR spectrum of **3b**



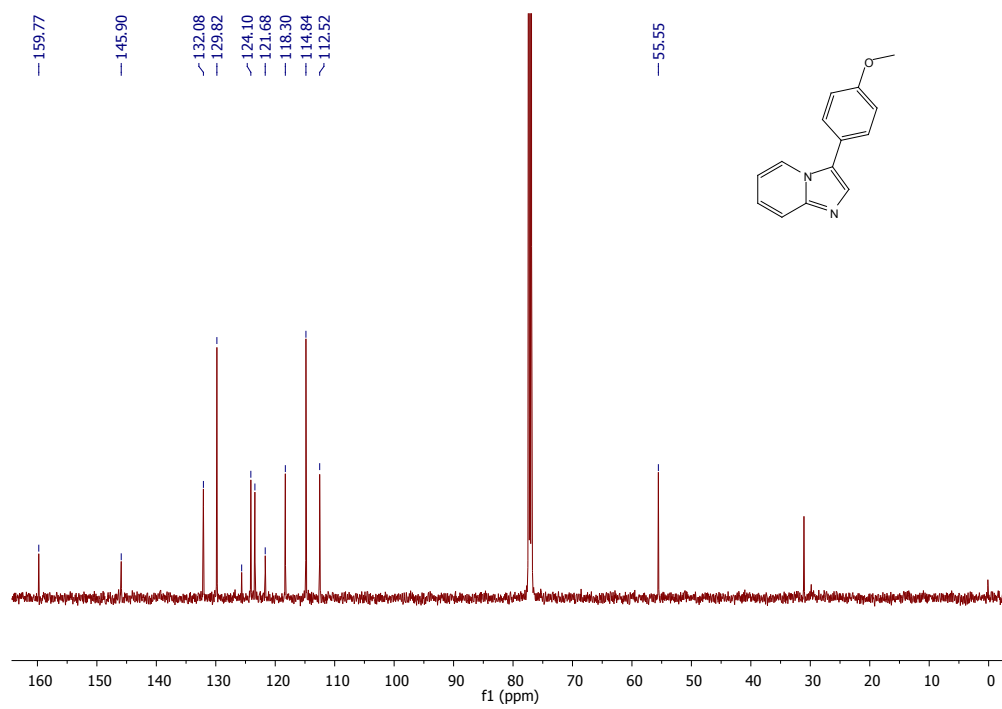
^1H NMR spectrum of **3c**



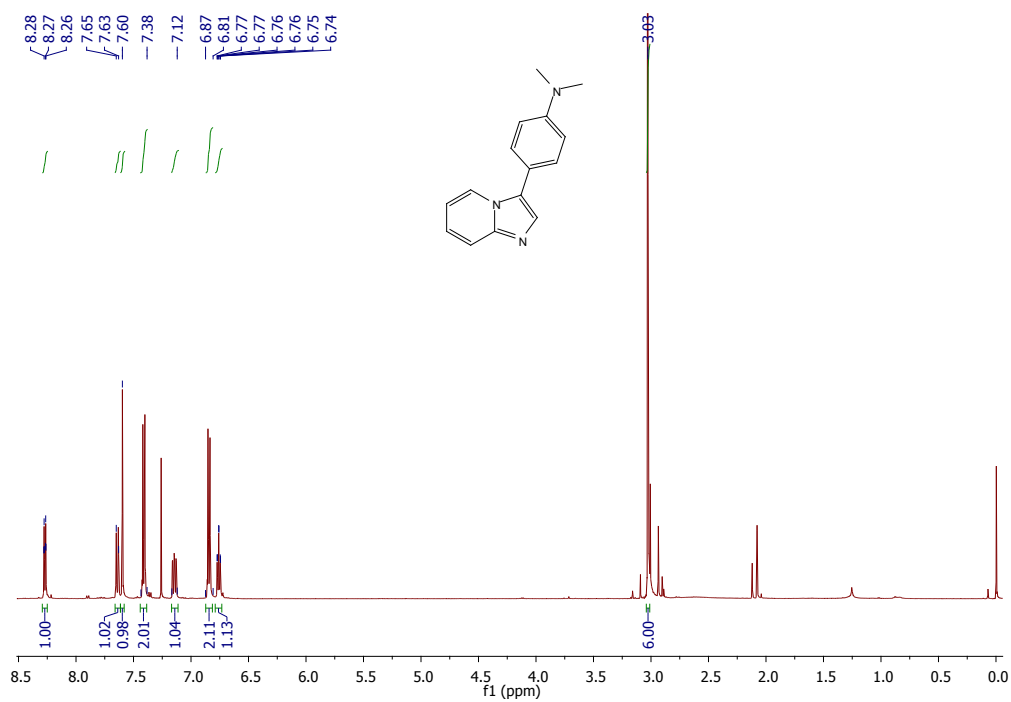
^{13}C NMR spectrum of **3c**



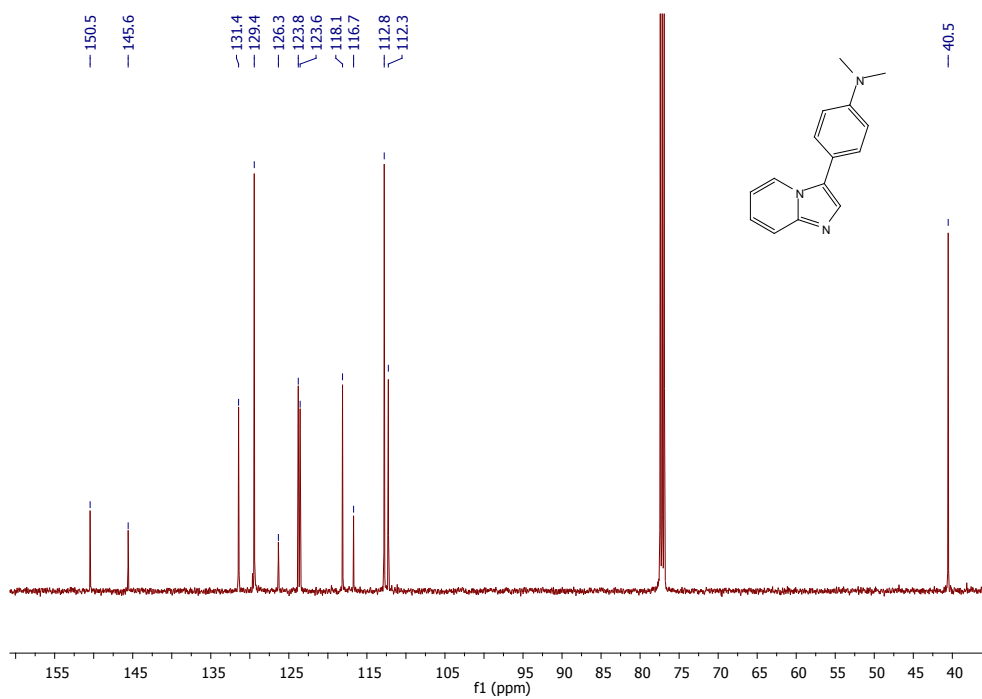
^1H NMR spectrum of **3d**



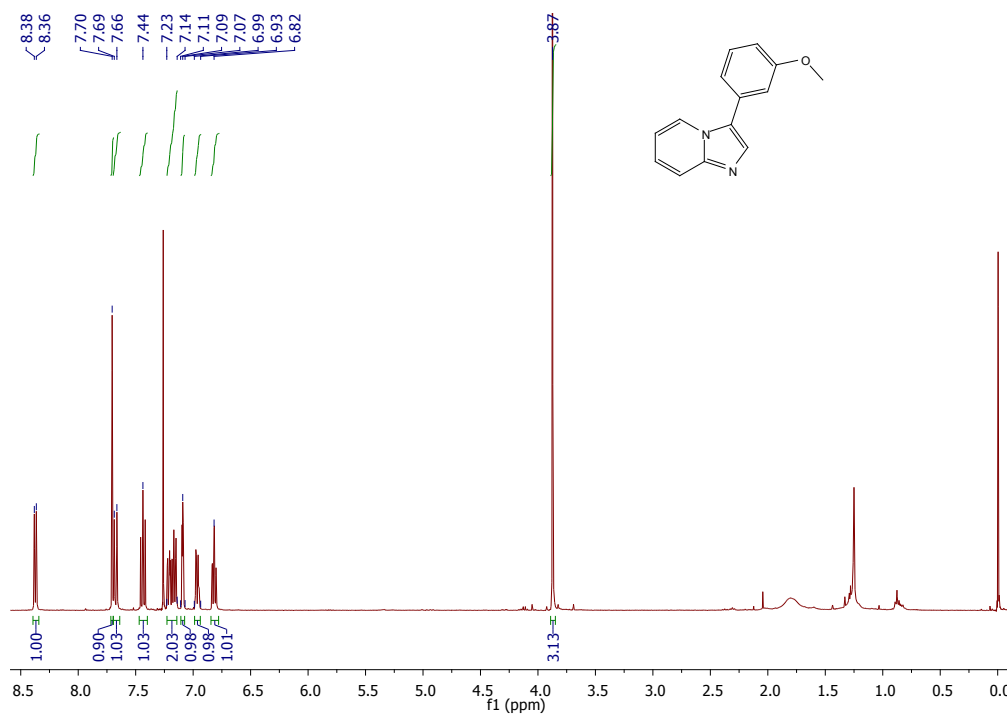
^{13}C NMR spectrum of **3d**



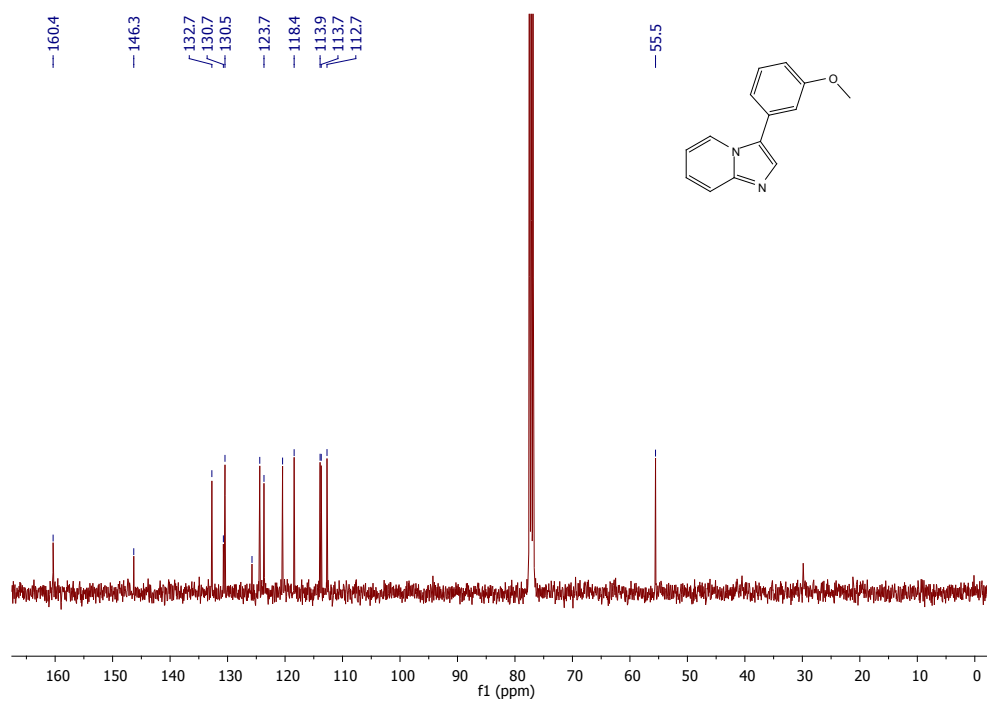
^1H NMR spectrum of **3e**



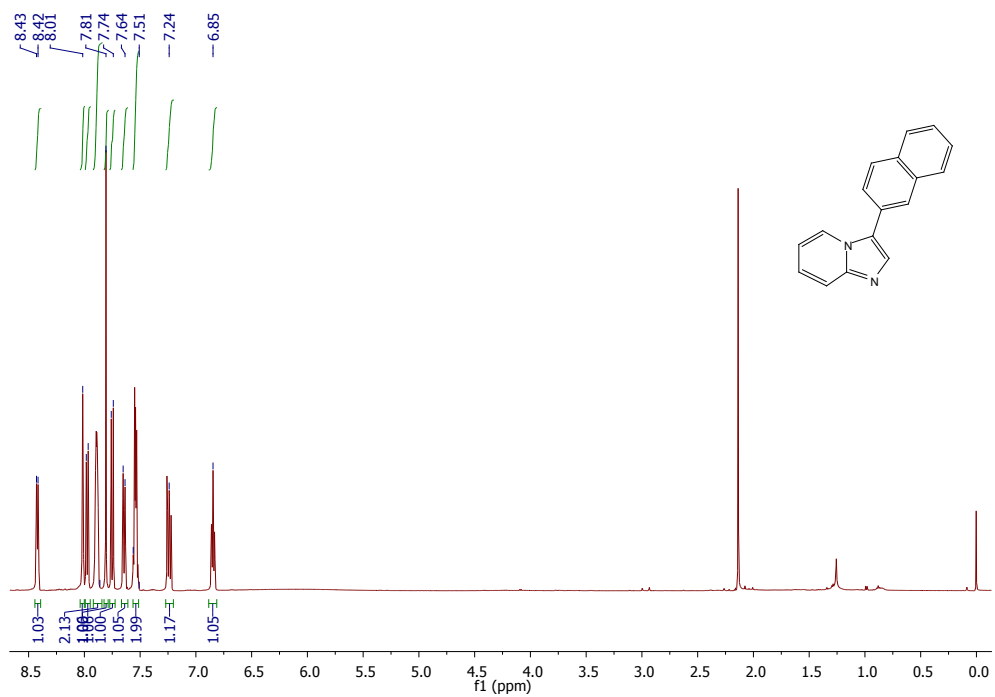
^{13}C NMR spectrum of **3e**



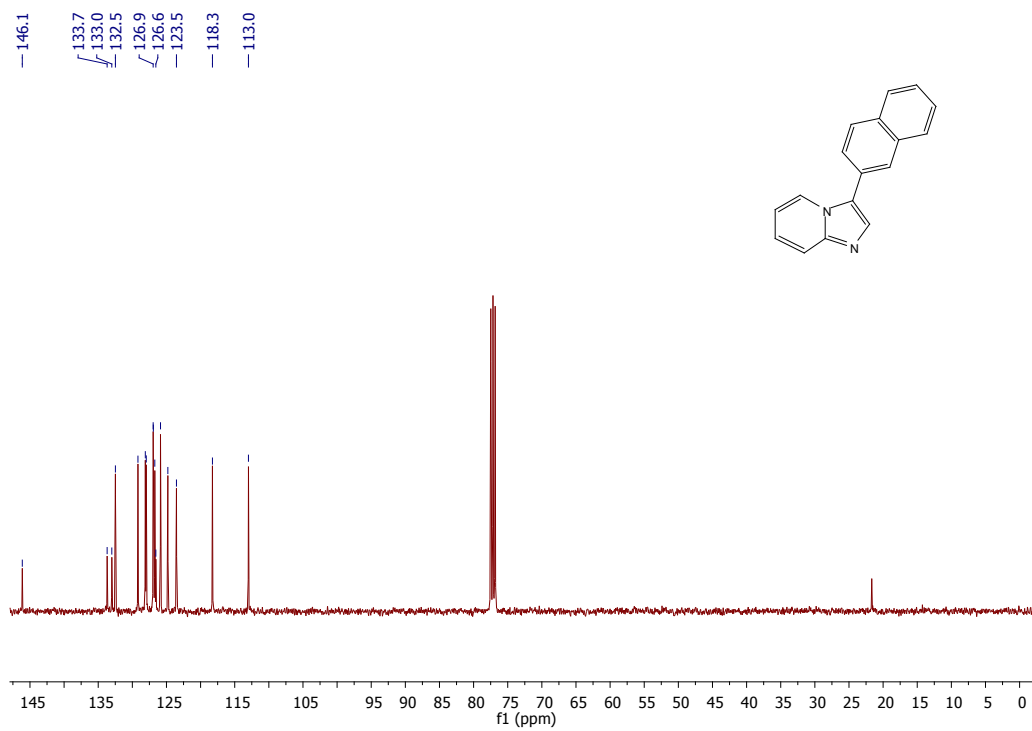
^1H NMR spectrum of **3f**



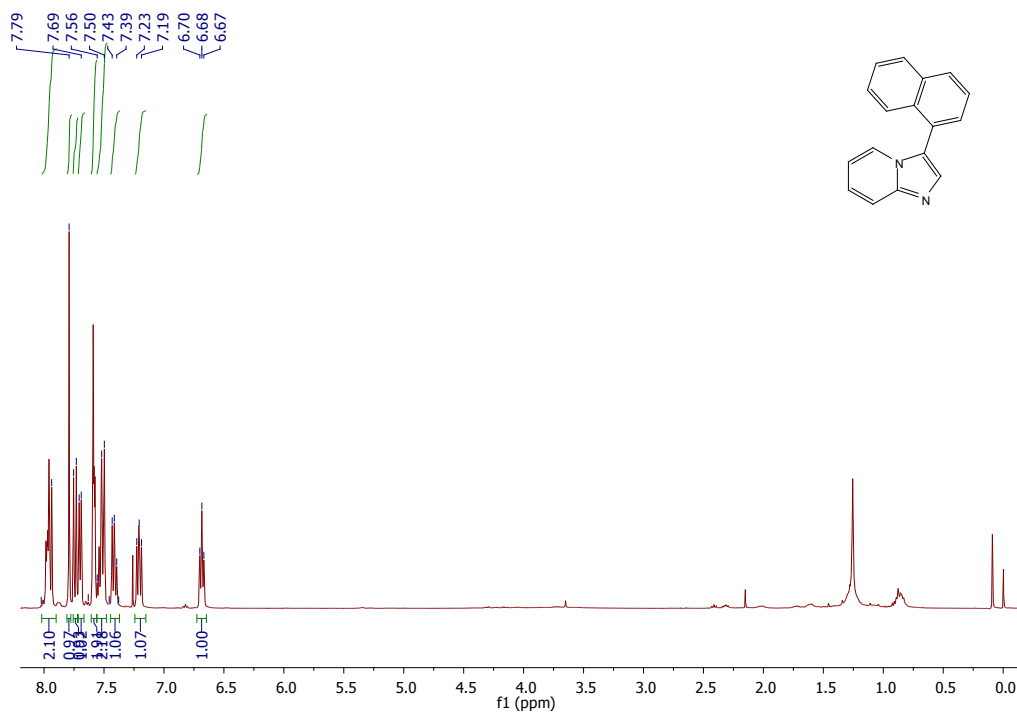
^{13}C NMR spectrum of **3f**



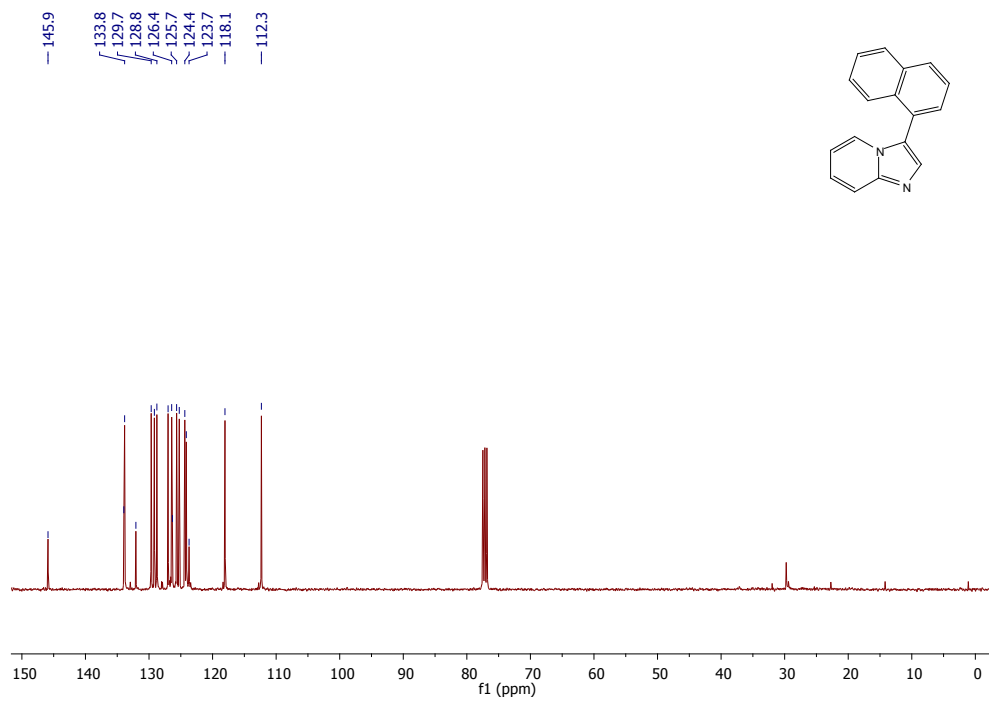
^1H NMR spectrum of **3g**



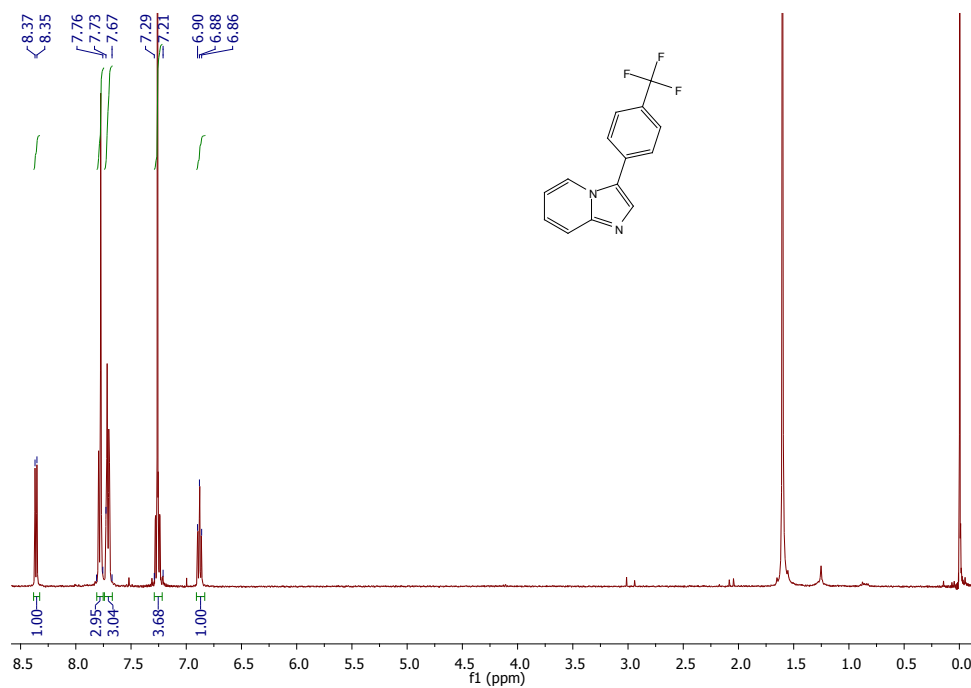
^{13}C NMR spectrum of **3g**



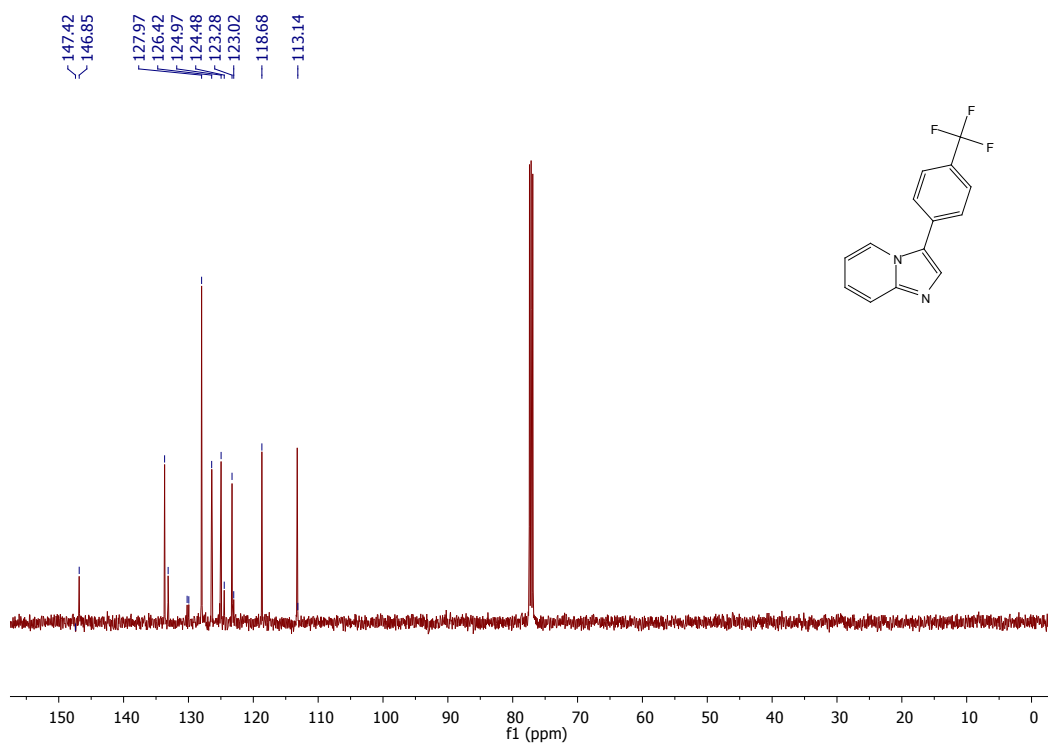
¹H NMR spectrum of **3h**



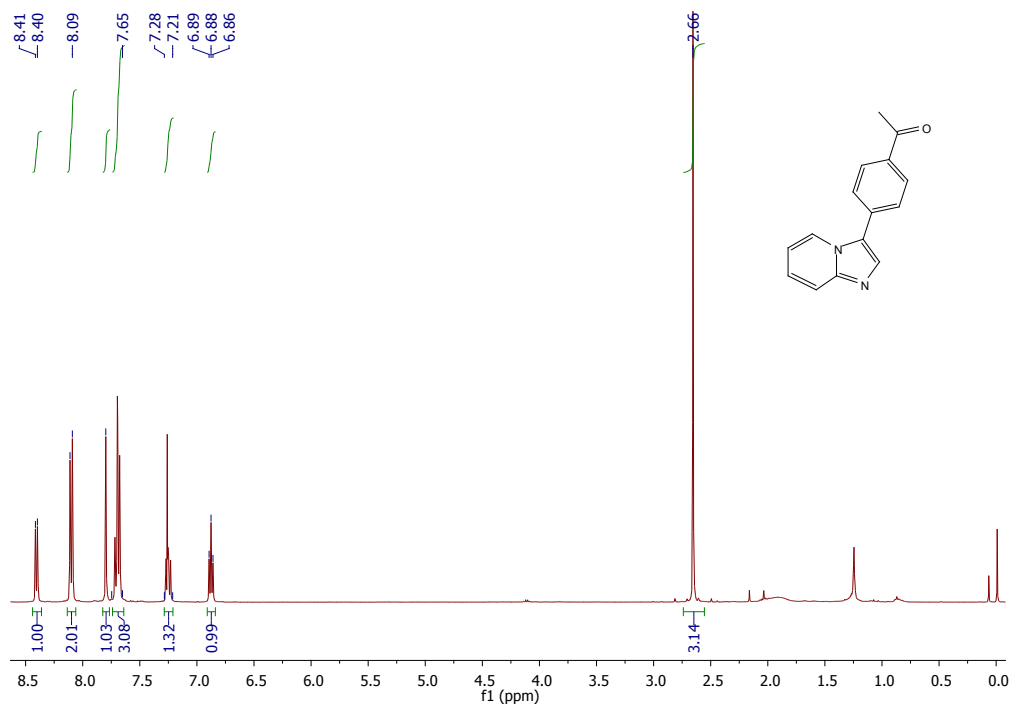
¹³C NMR spectrum of **3h**



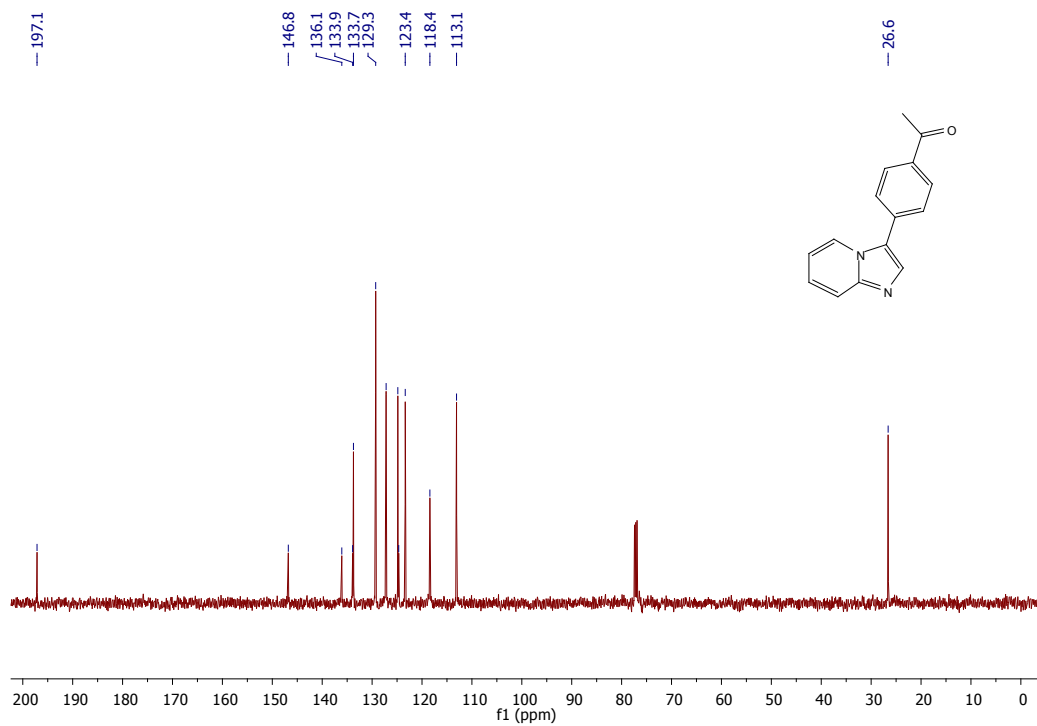
^1H NMR spectrum of **3i**



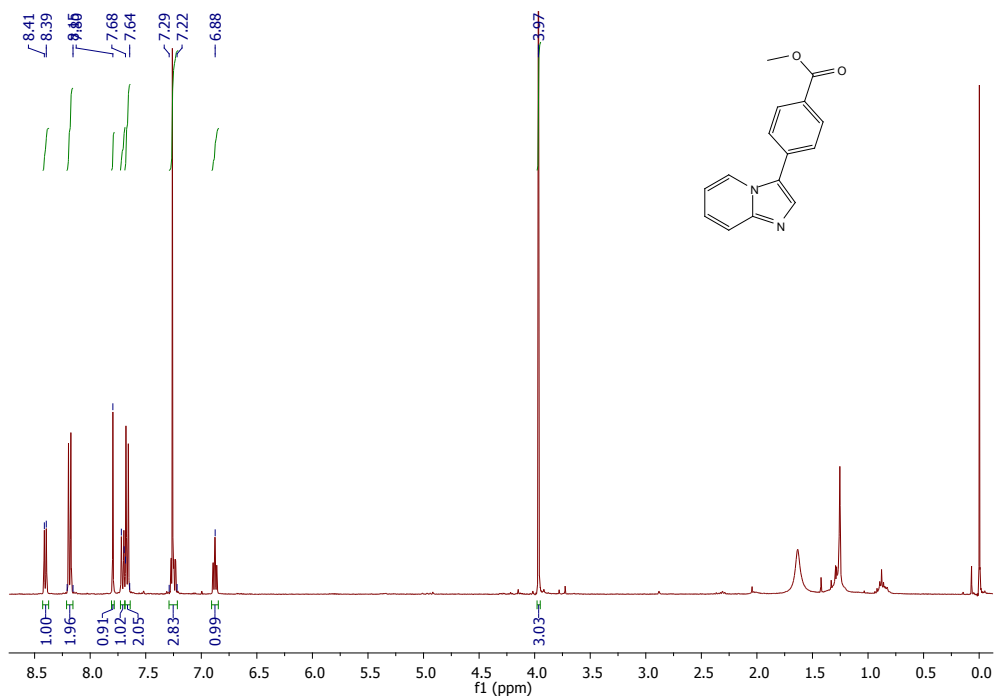
^{13}C NMR spectrum of **3i**



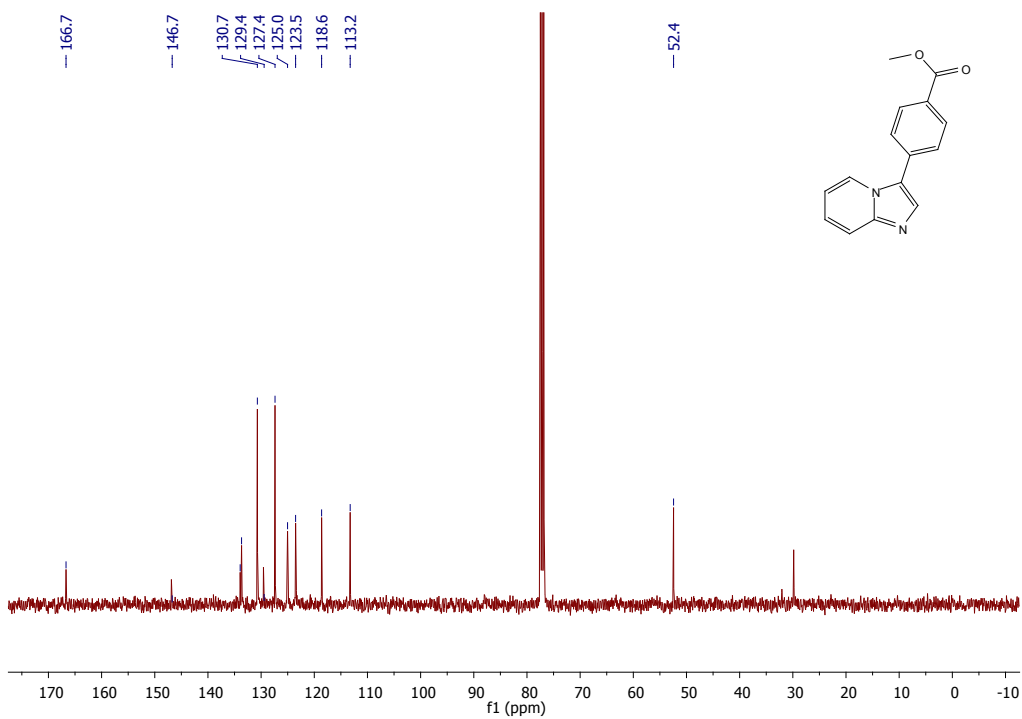
^1H NMR spectrum of **3j**



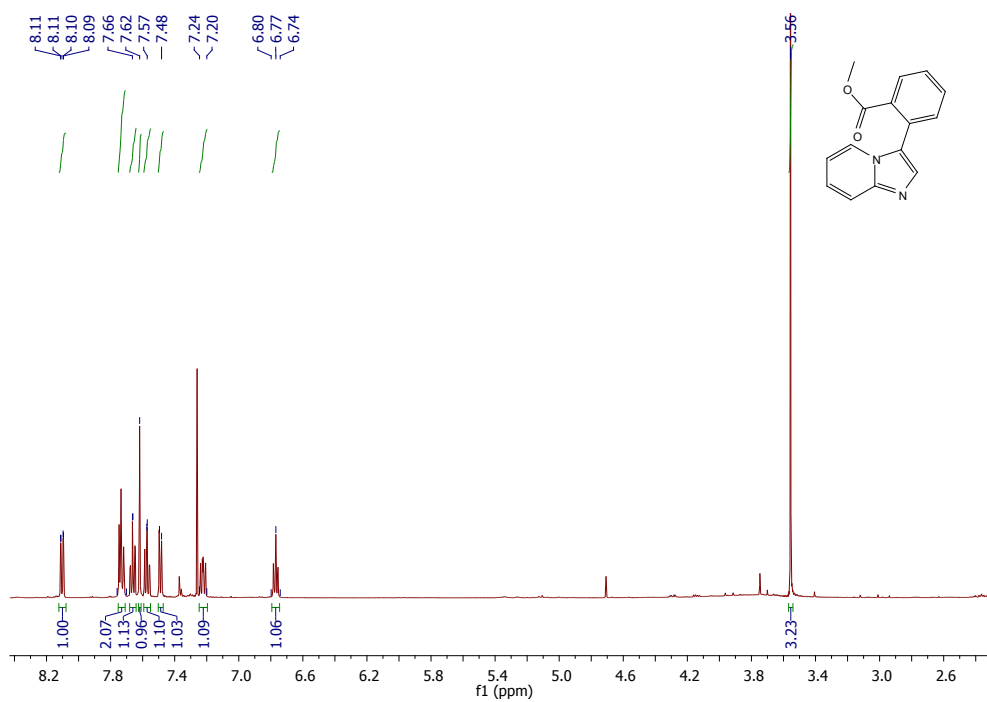
^{13}C NMR spectrum of **3j**



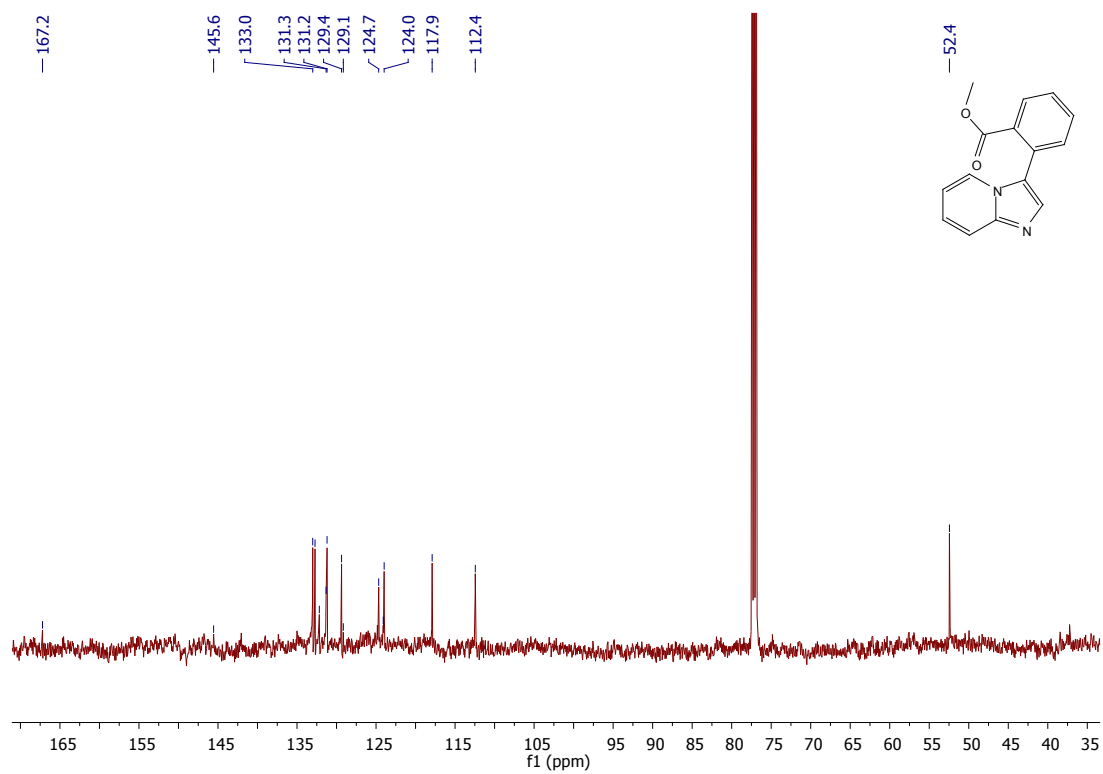
^1H NMR spectrum of **3k**



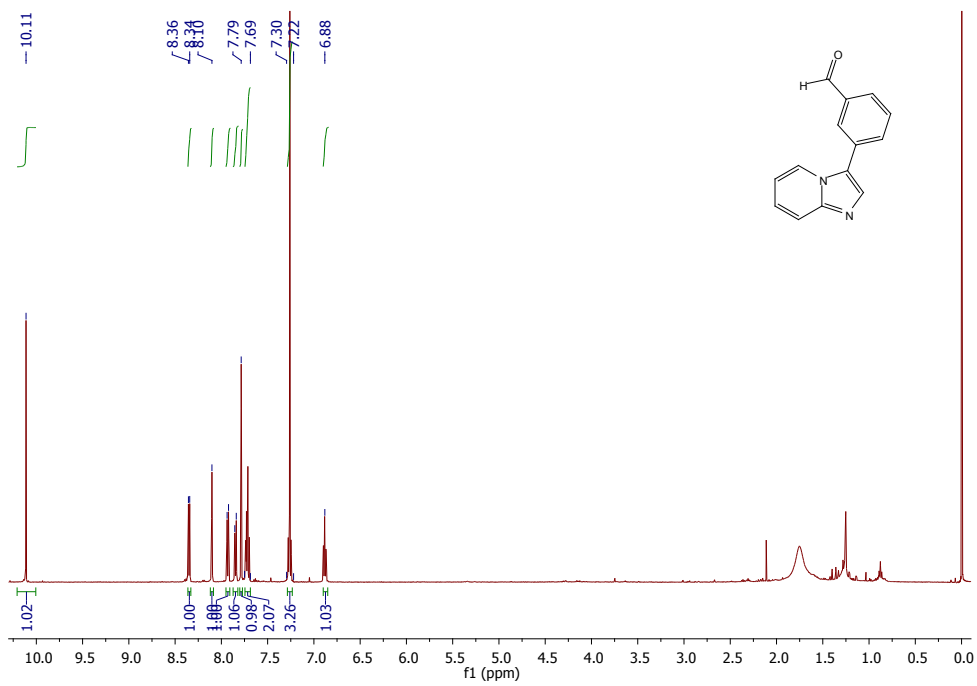
^{13}C NMR spectrum of **3k**



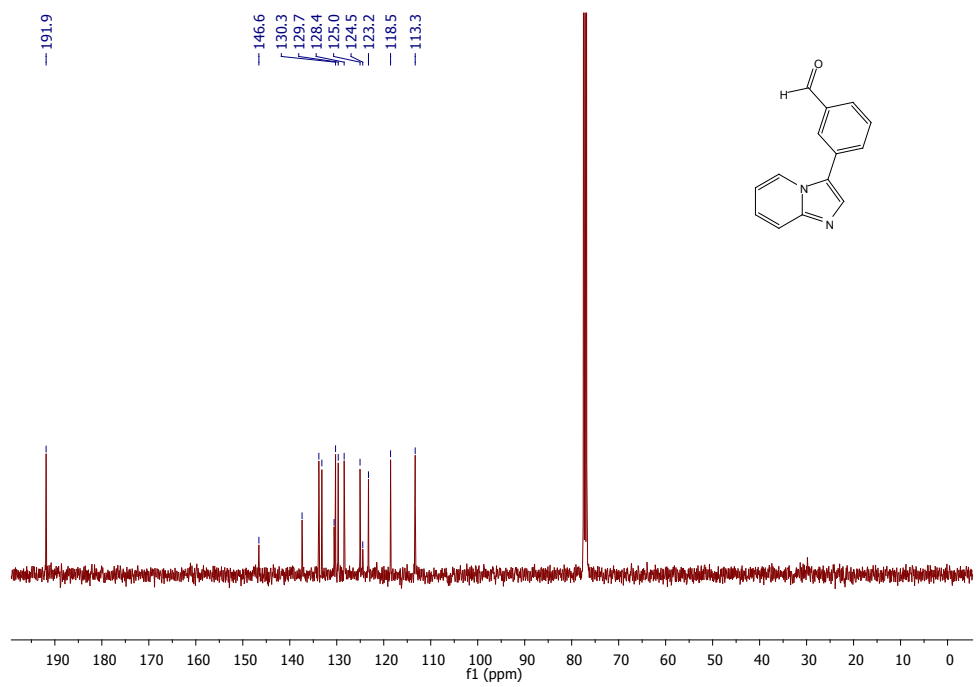
^1H NMR spectrum of **31**



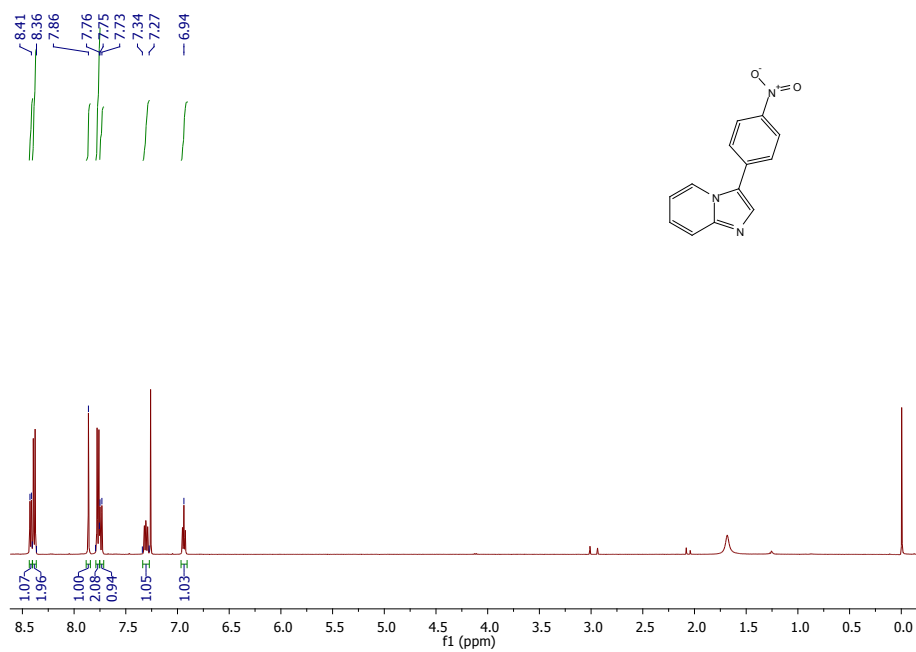
^{13}C NMR spectrum of **31**



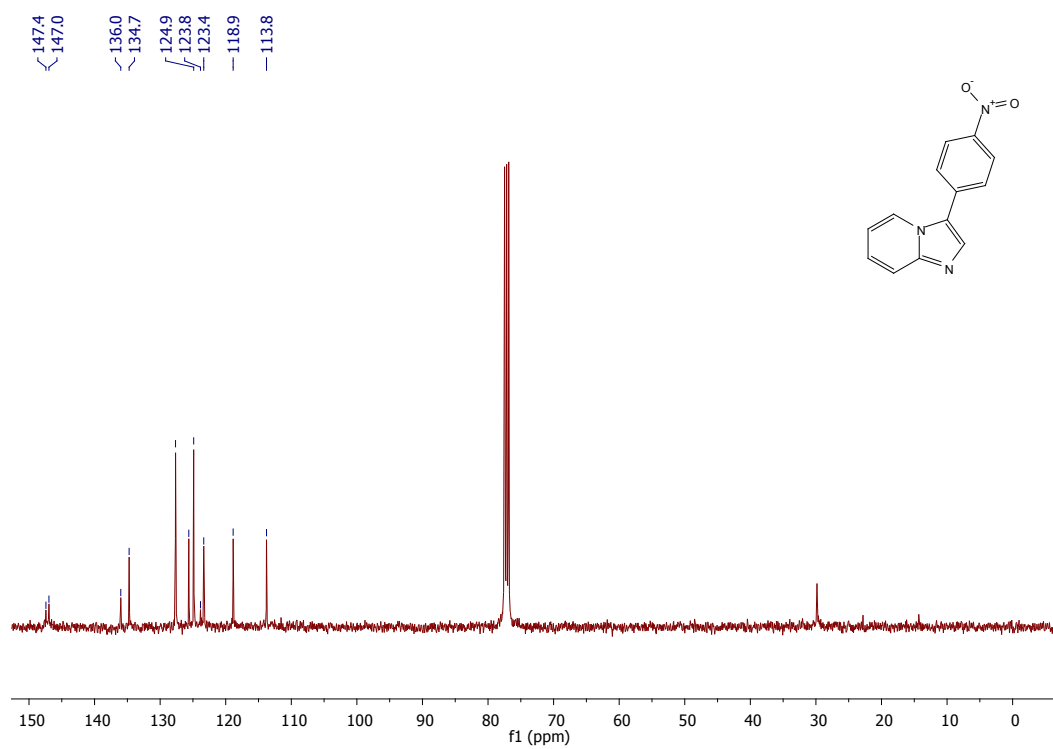
^1H NMR spectrum of **3m**



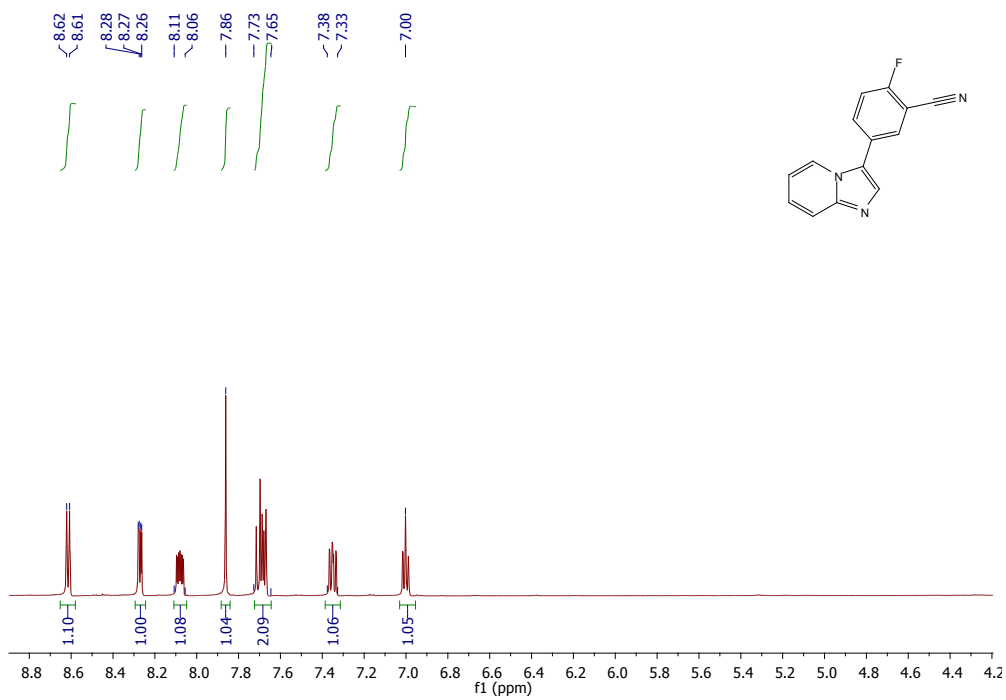
^{13}C NMR spectrum of **3m**



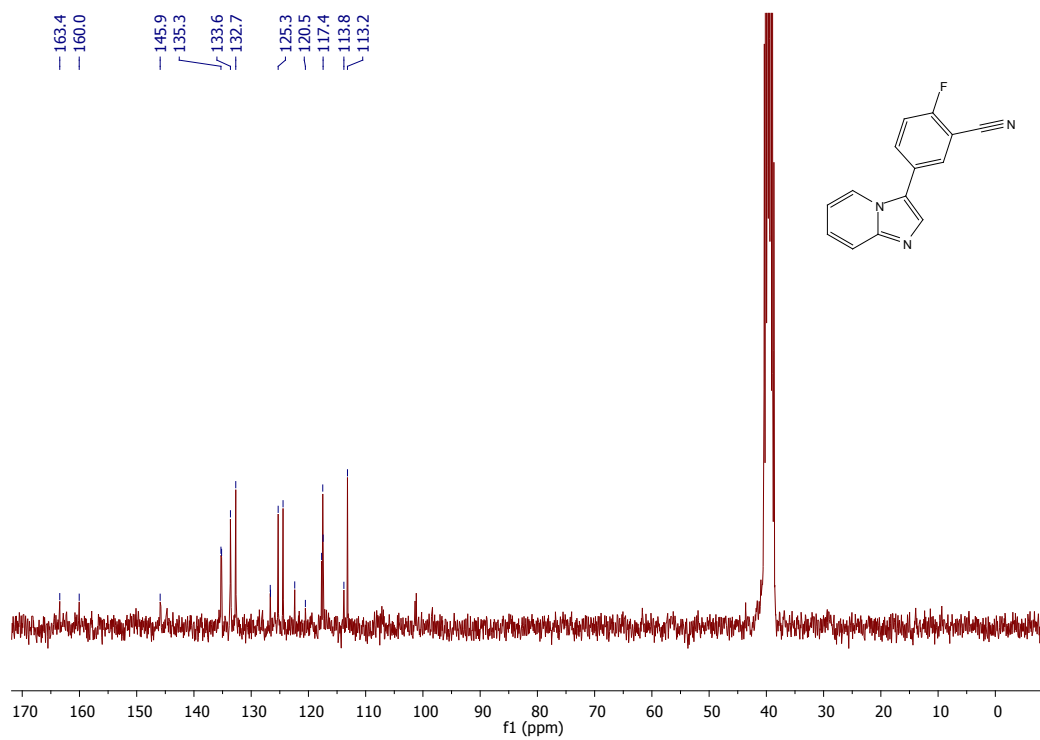
¹H NMR spectrum of **3n**



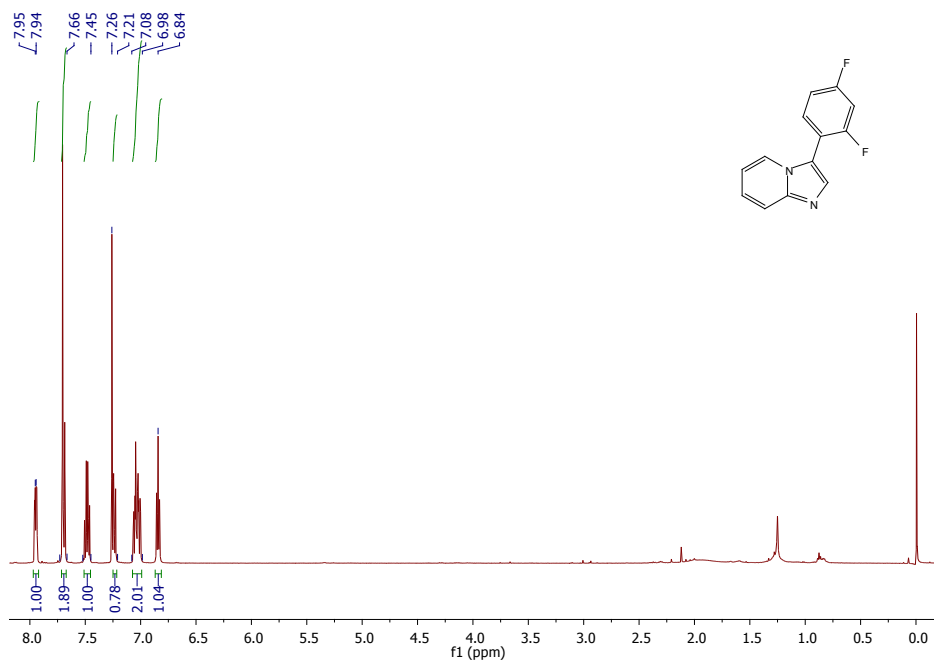
¹³C NMR spectrum of **3n**



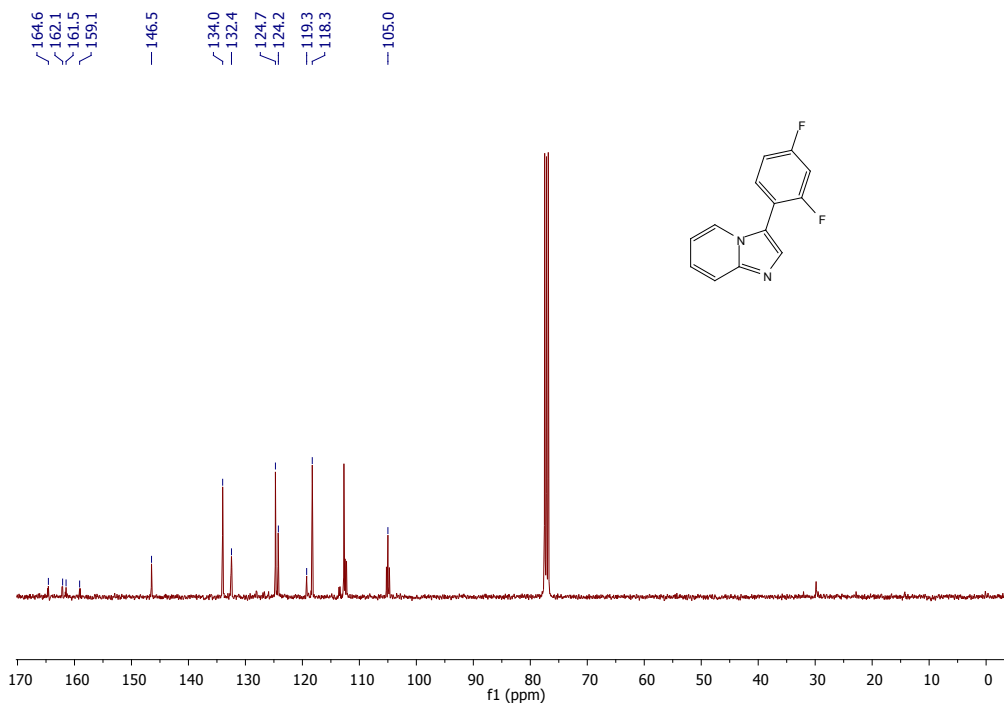
^1H NMR spectrum of **3o**



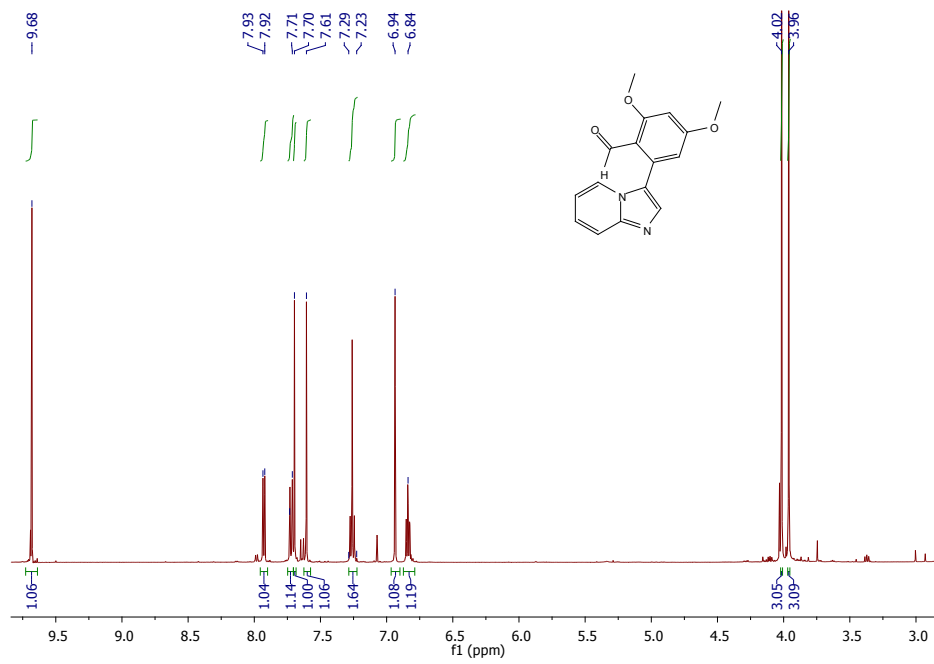
^{13}C NMR spectrum of **3o**



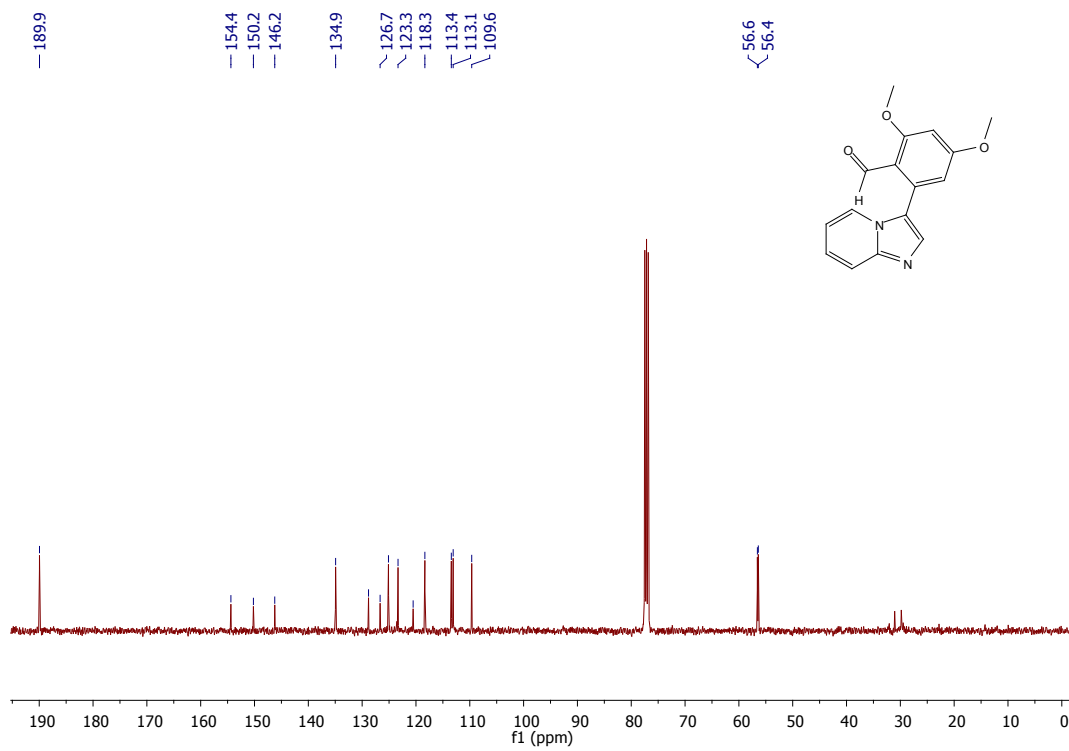
^1H NMR spectrum of **3p**



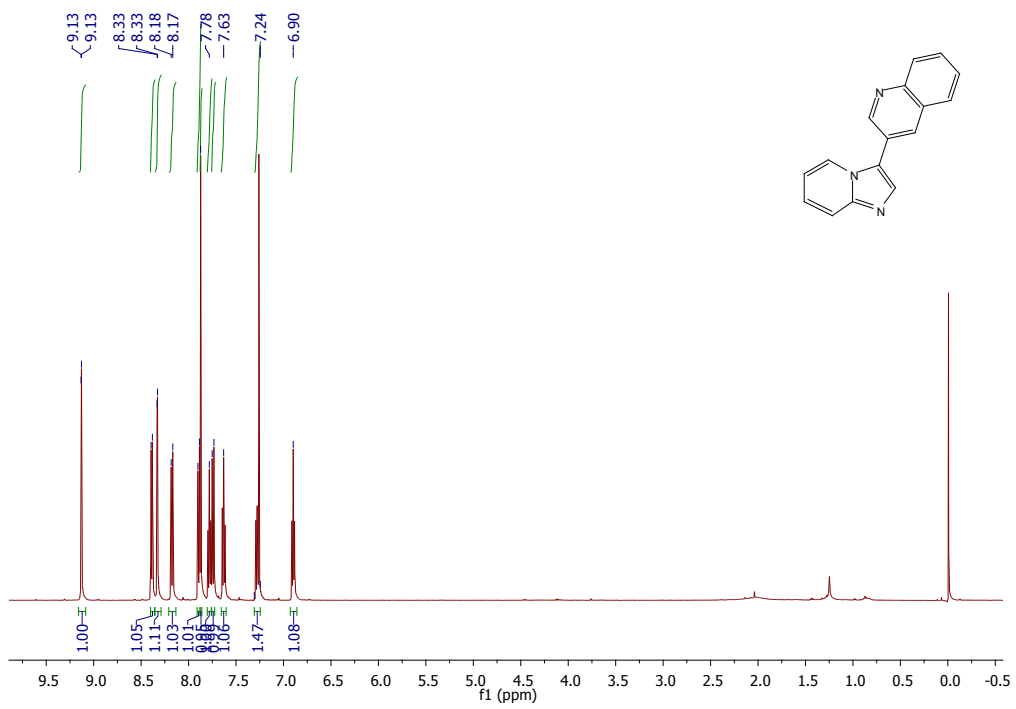
^{13}C NMR spectrum of **3p**



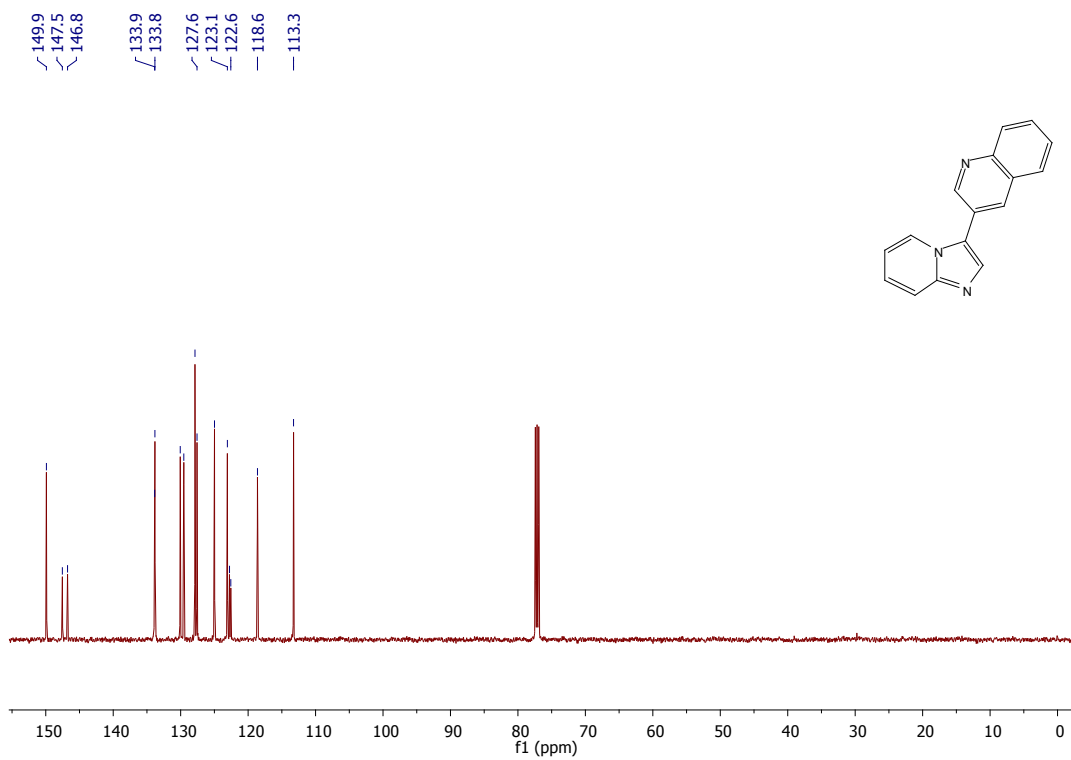
^1H NMR spectrum of **3q**



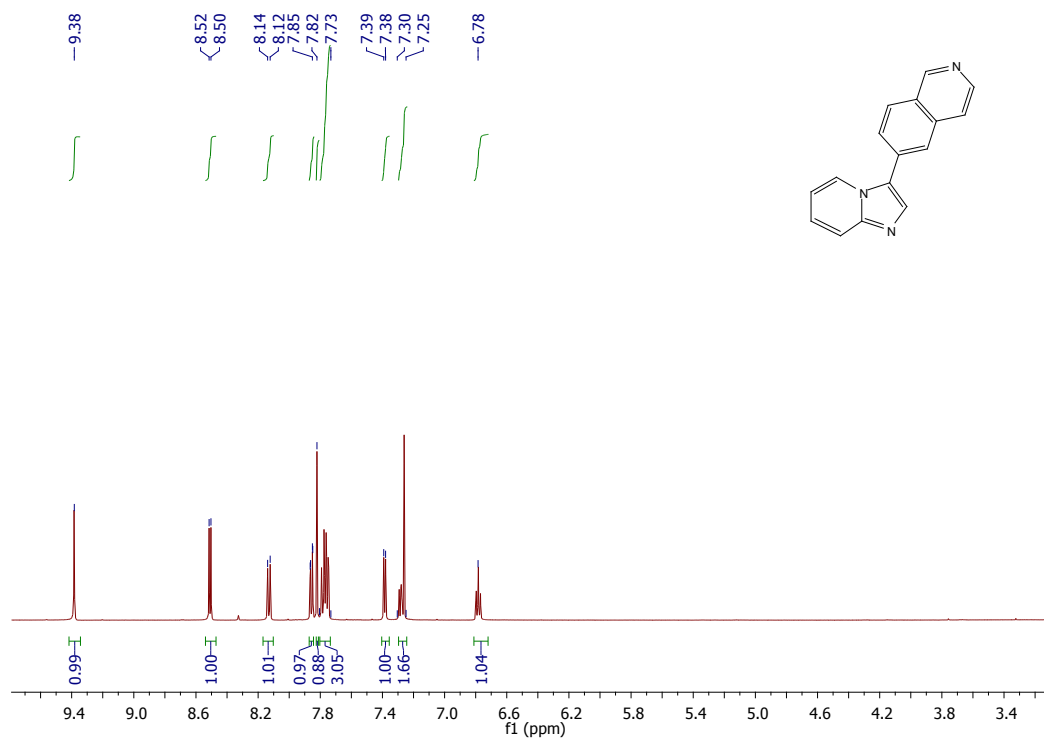
^{13}C NMR spectrum of **3q**



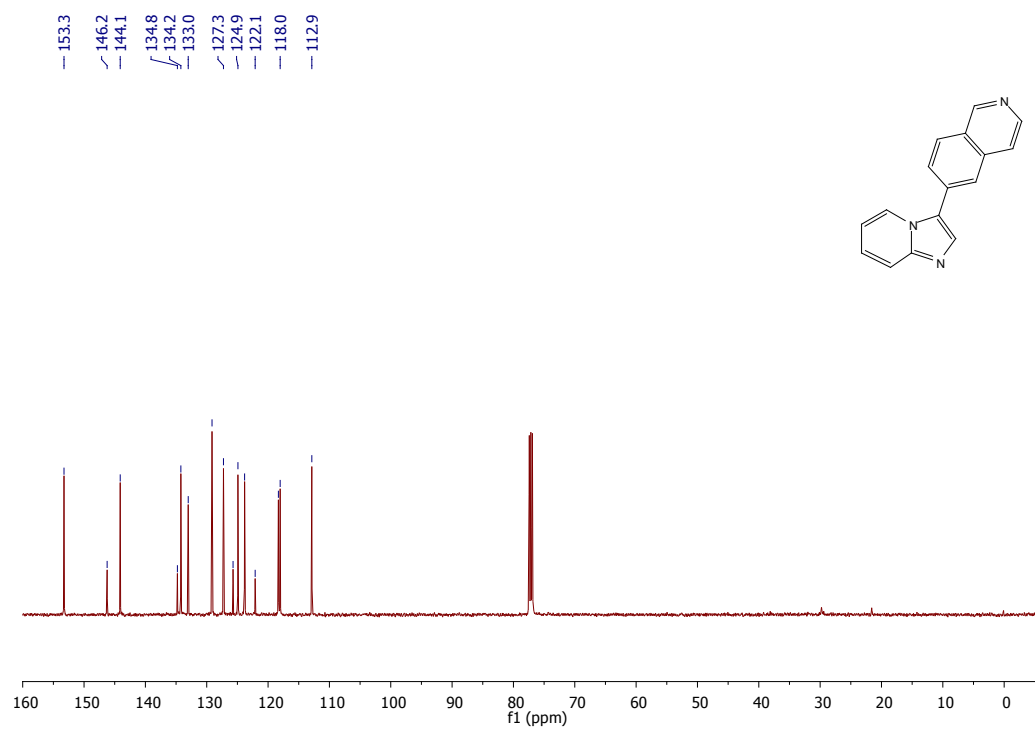
¹H NMR spectrum of **3r**



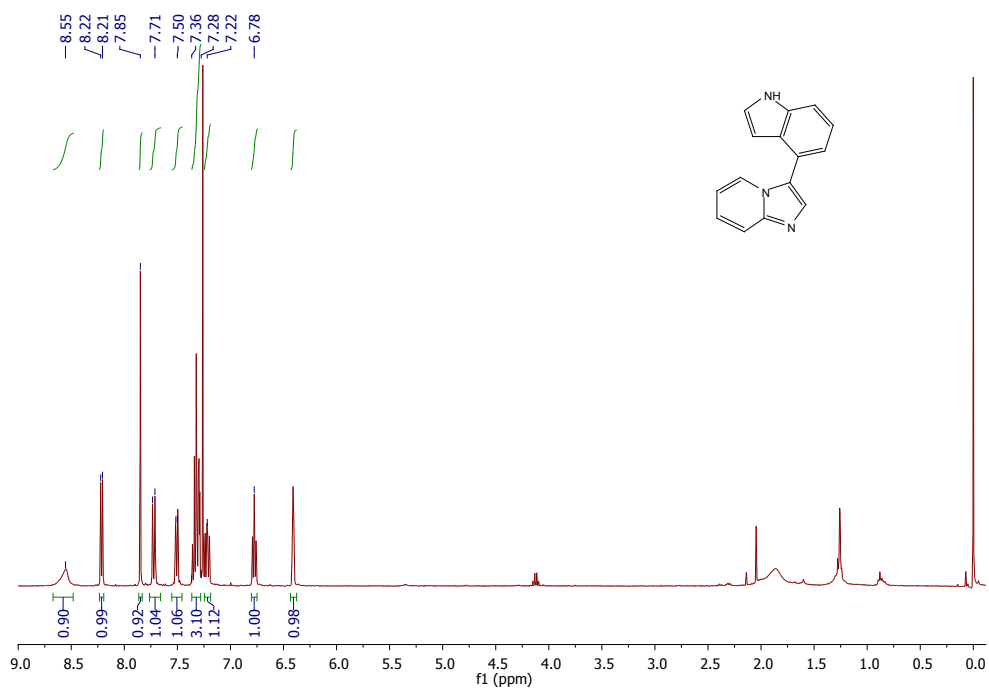
¹³C NMR spectrum of **3r**



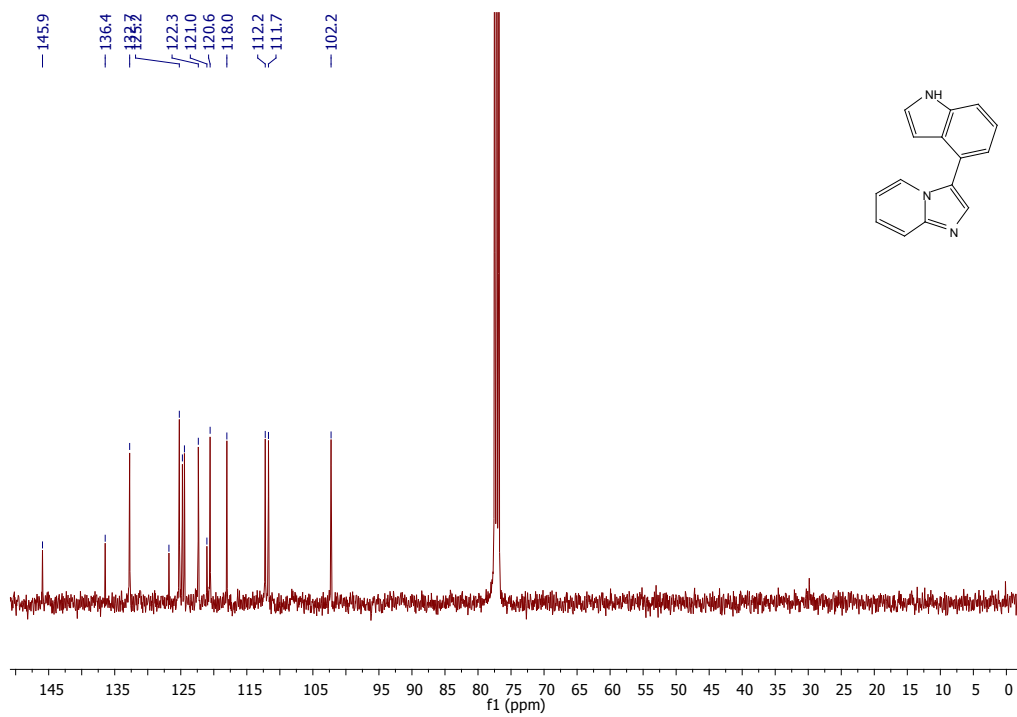
^1H NMR spectrum of **3s**



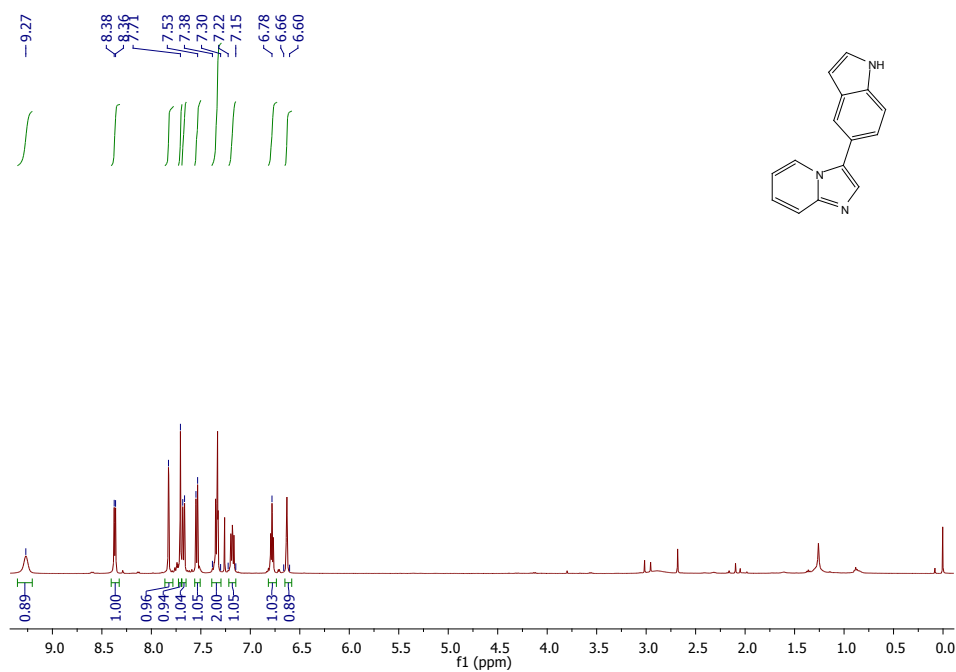
^{13}C NMR spectrum of **3s**



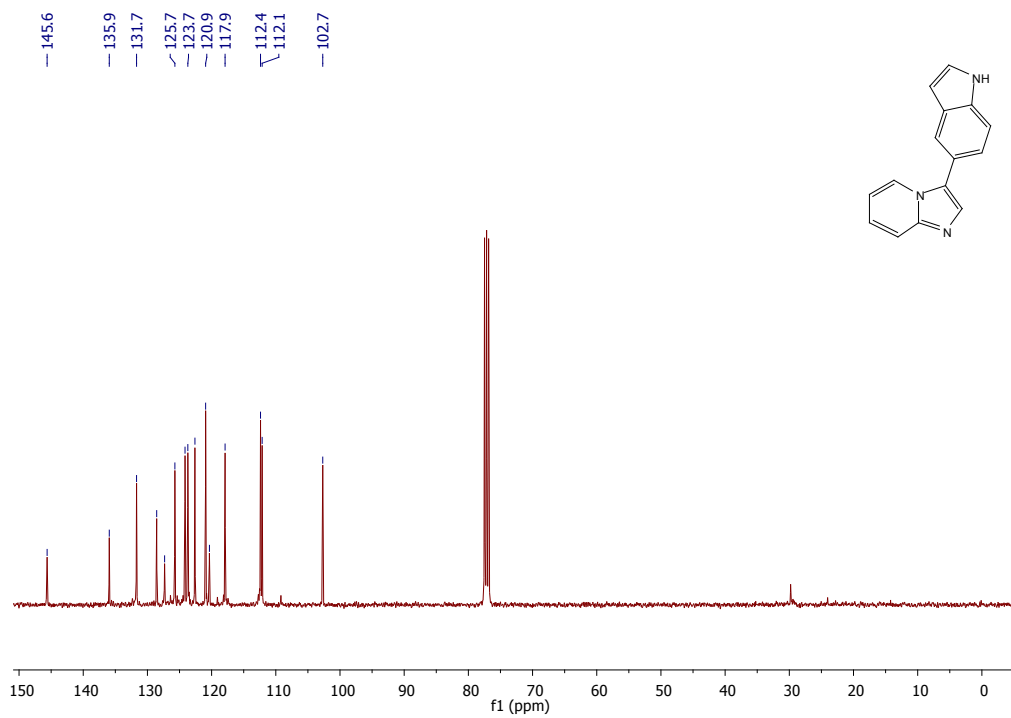
^1H NMR spectrum of **3t**



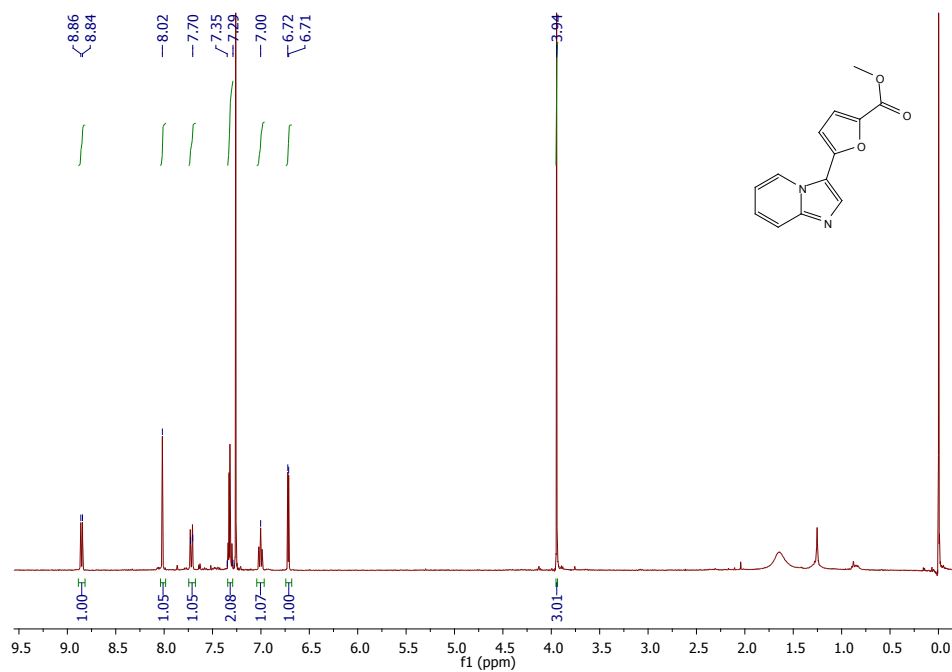
^{13}C NMR spectrum of **3t**



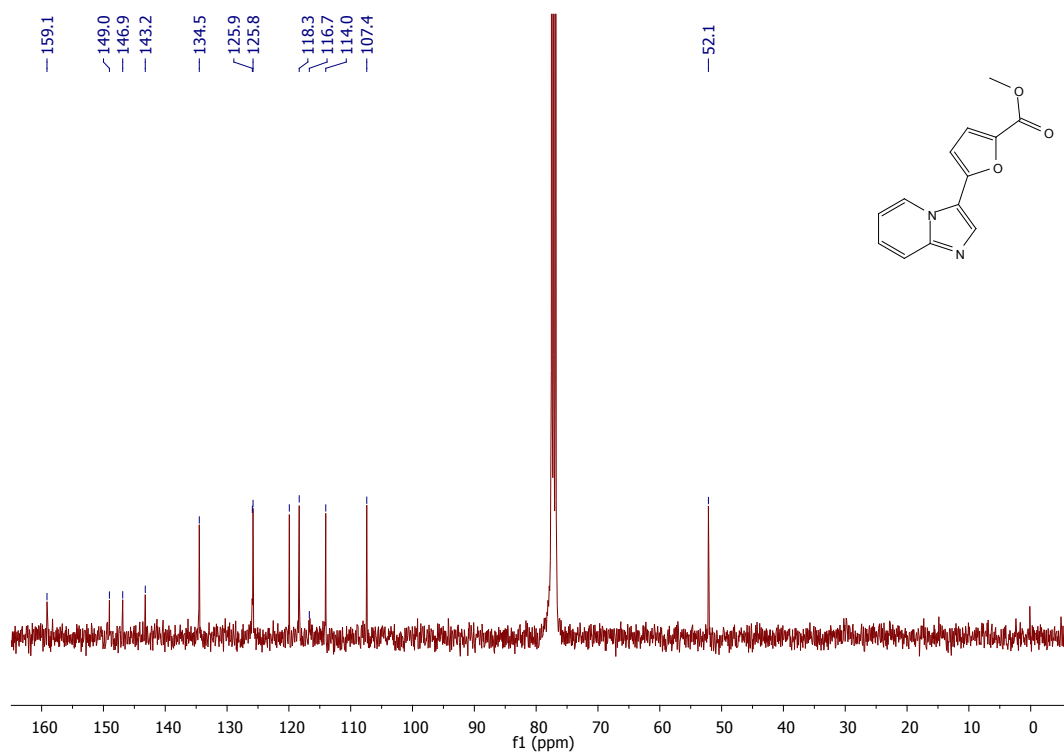
^1H NMR spectrum of **3u**



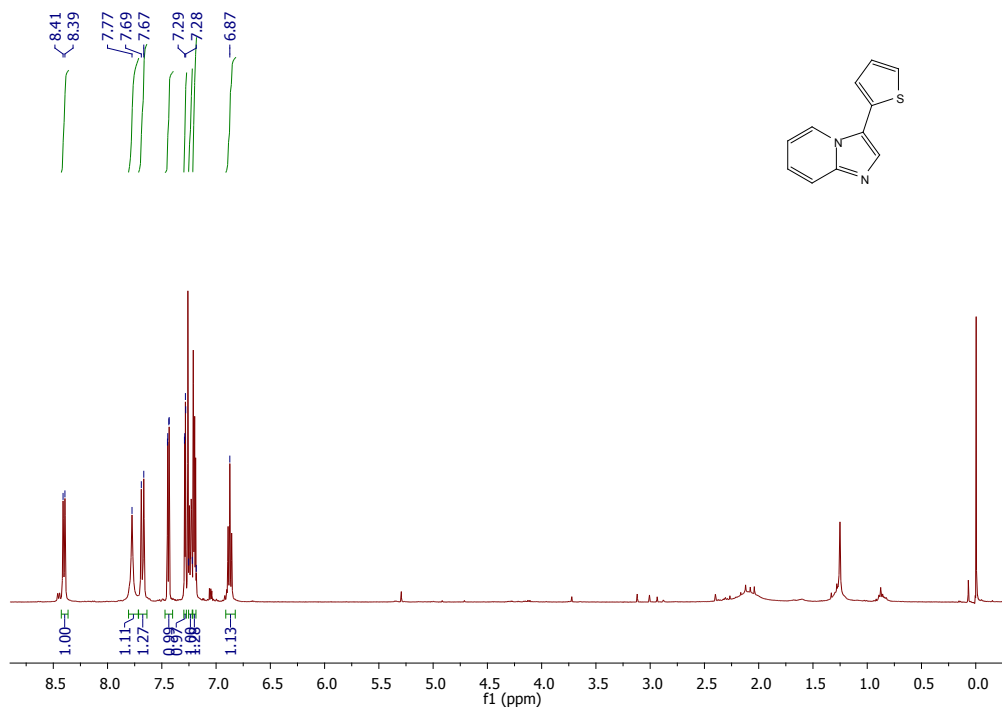
^{13}C NMR spectrum of **3u**



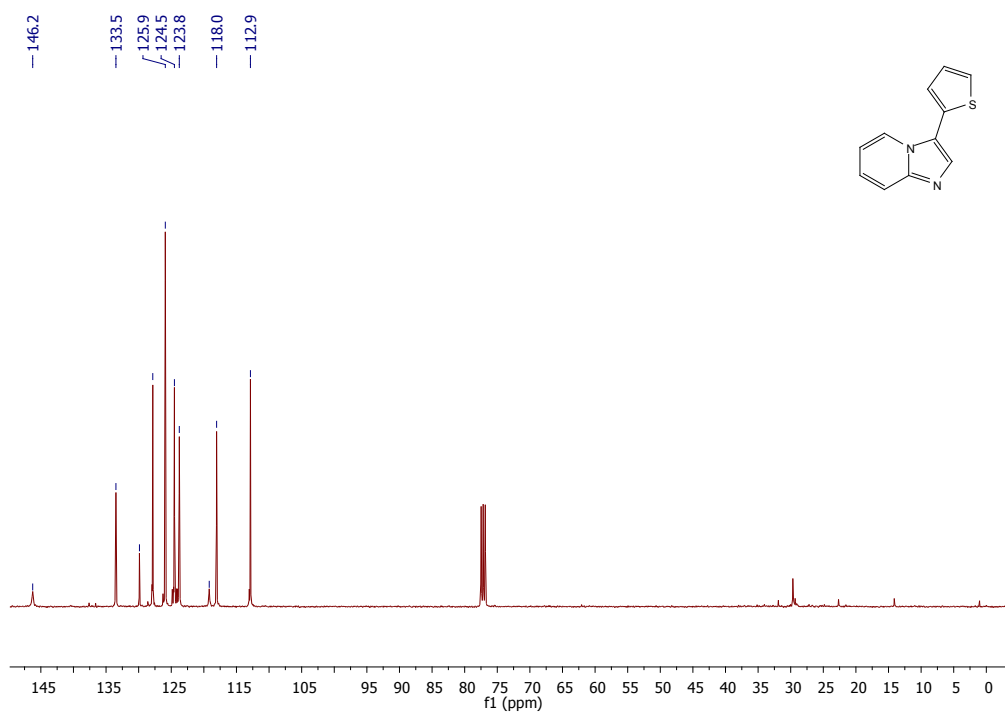
^1H NMR spectrum of **3v**



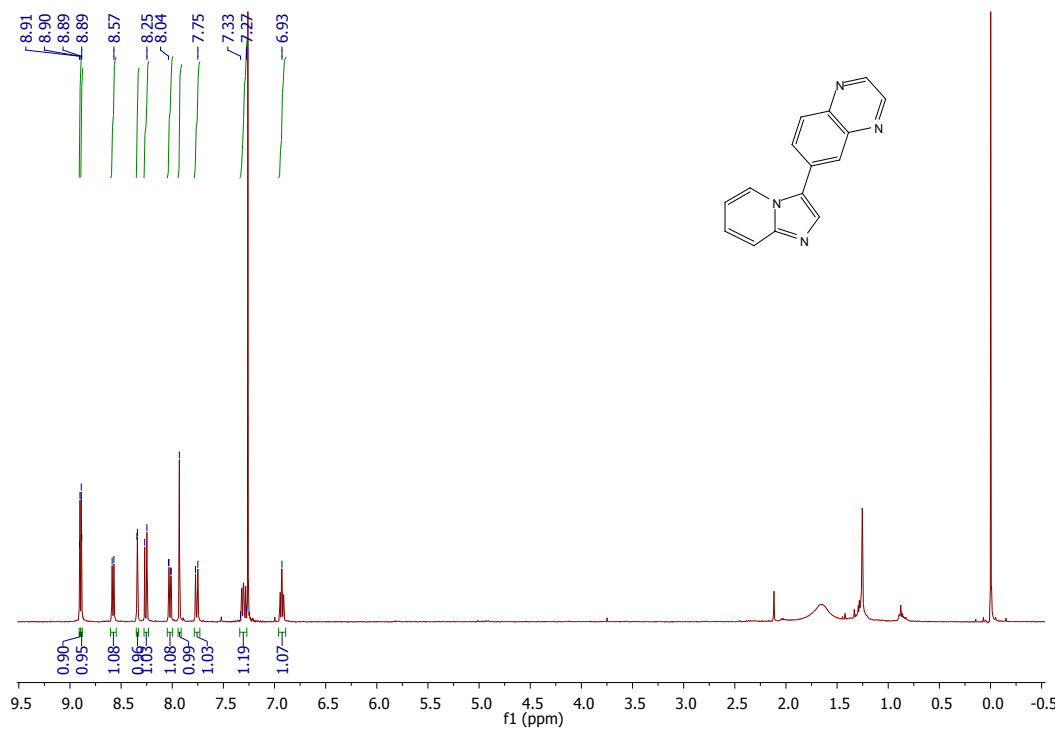
^{13}C NMR spectrum of **3v**



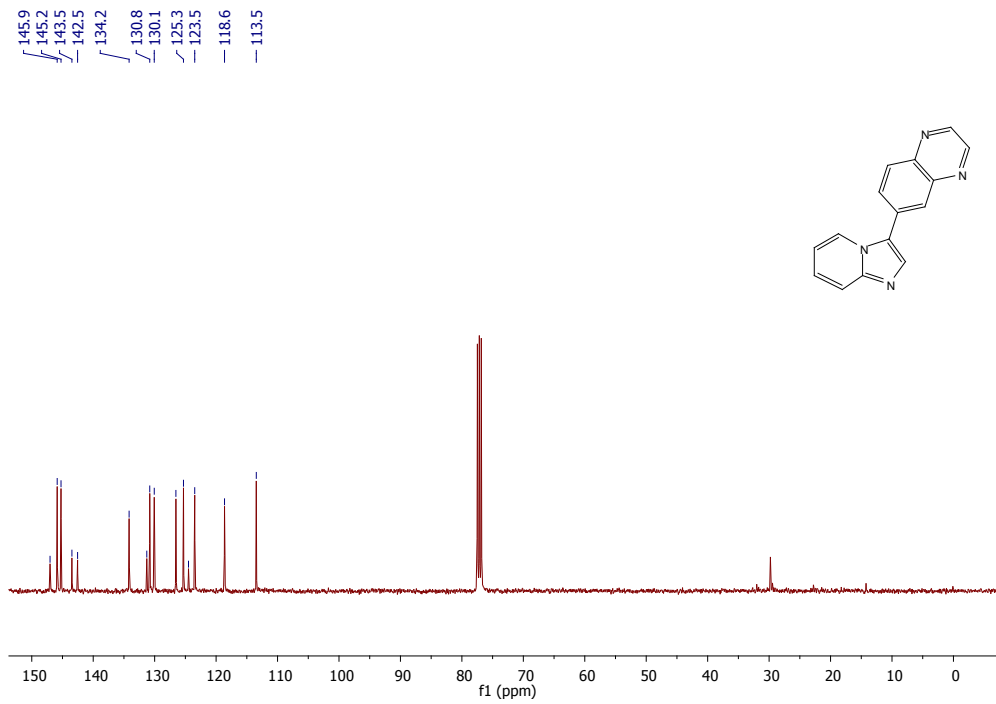
¹H NMR spectrum of **3w**



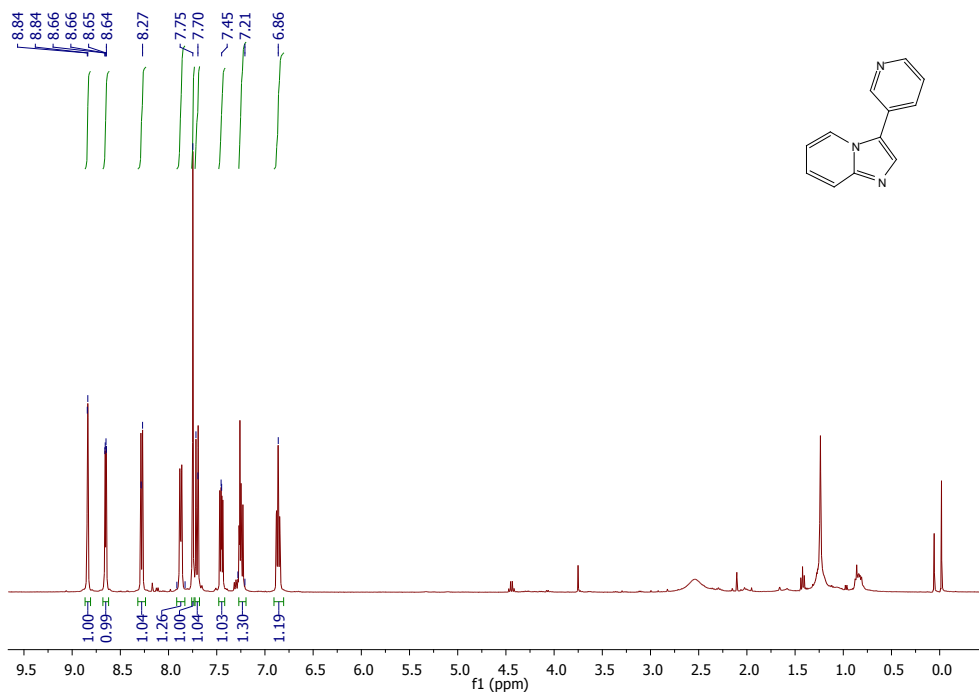
¹³C NMR spectrum of **3w**



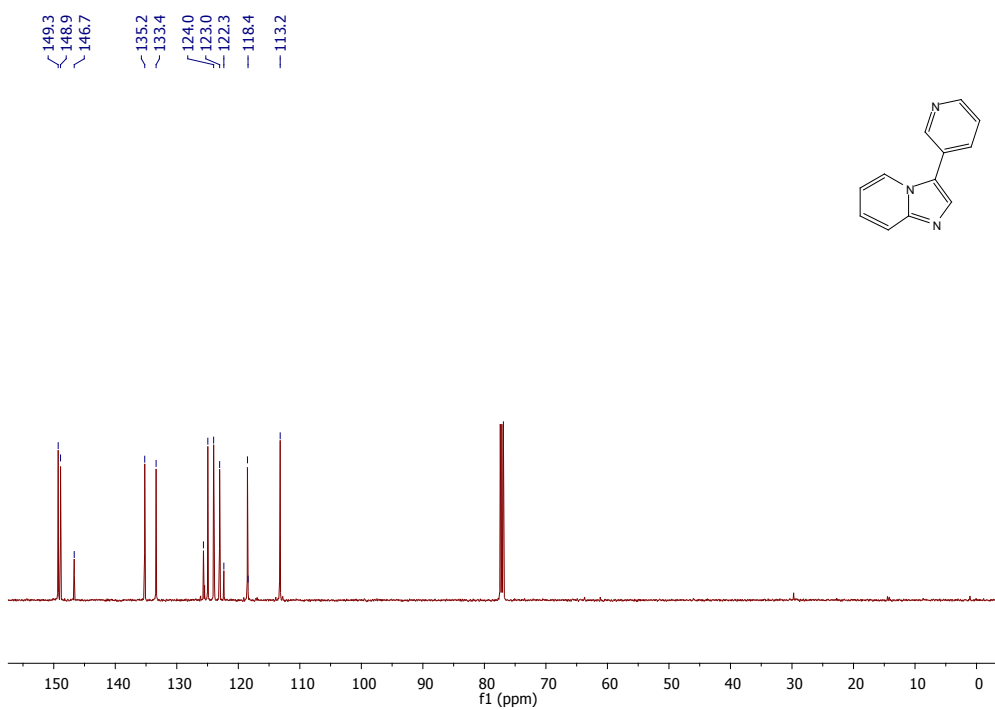
^1H NMR spectrum of **3x**



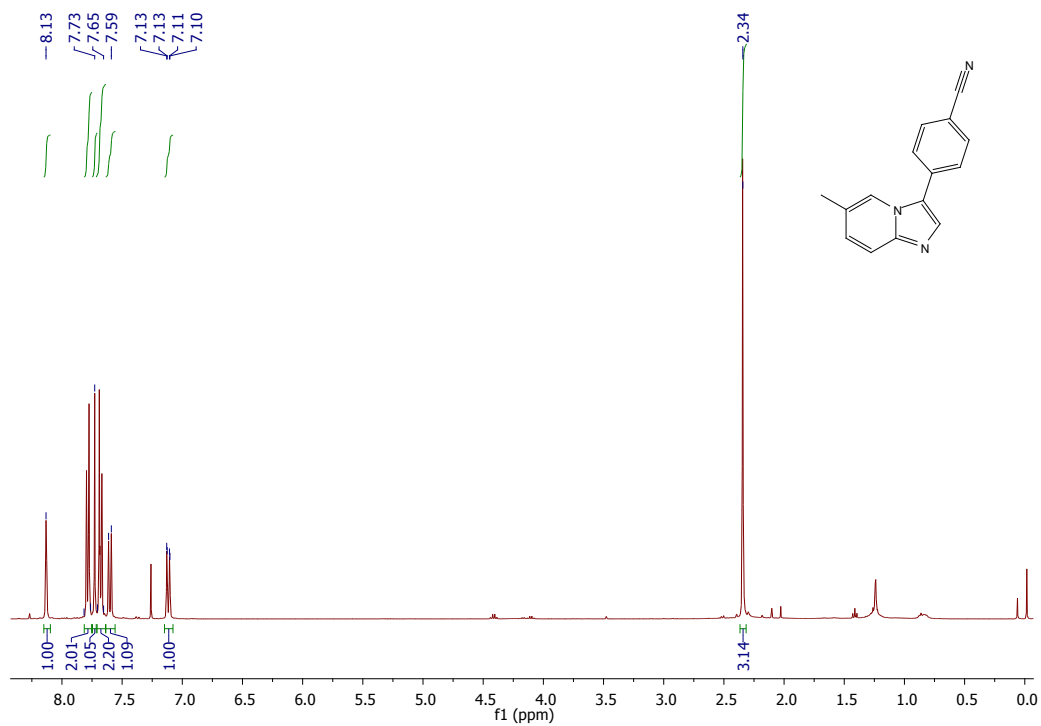
^{13}C NMR spectrum of **3x**



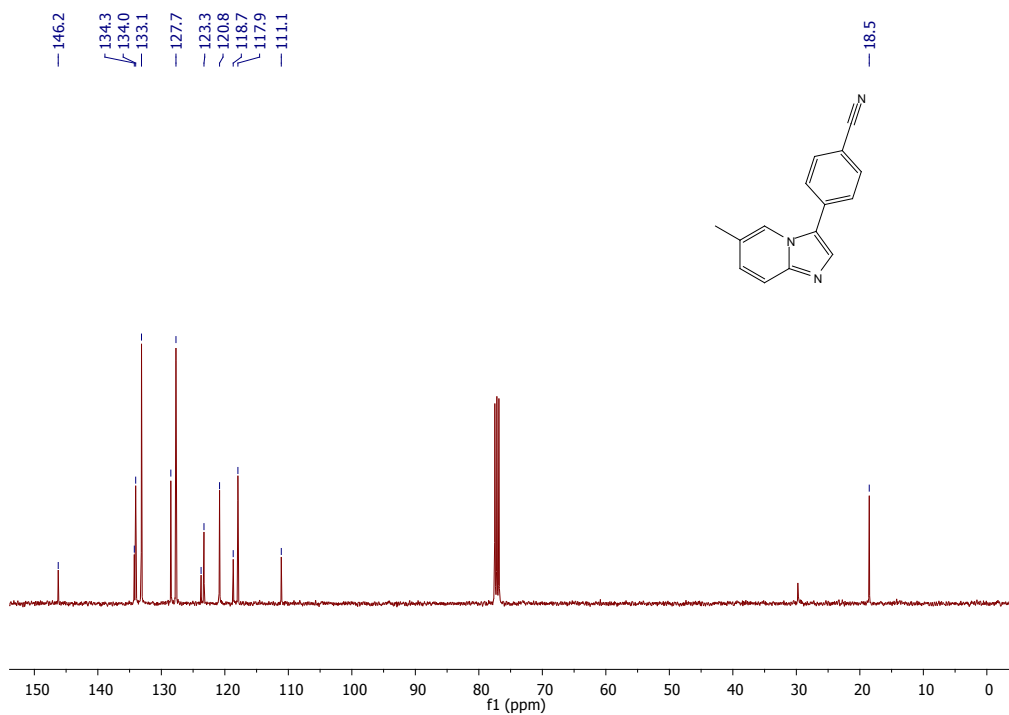
^1H NMR spectrum of **3y**



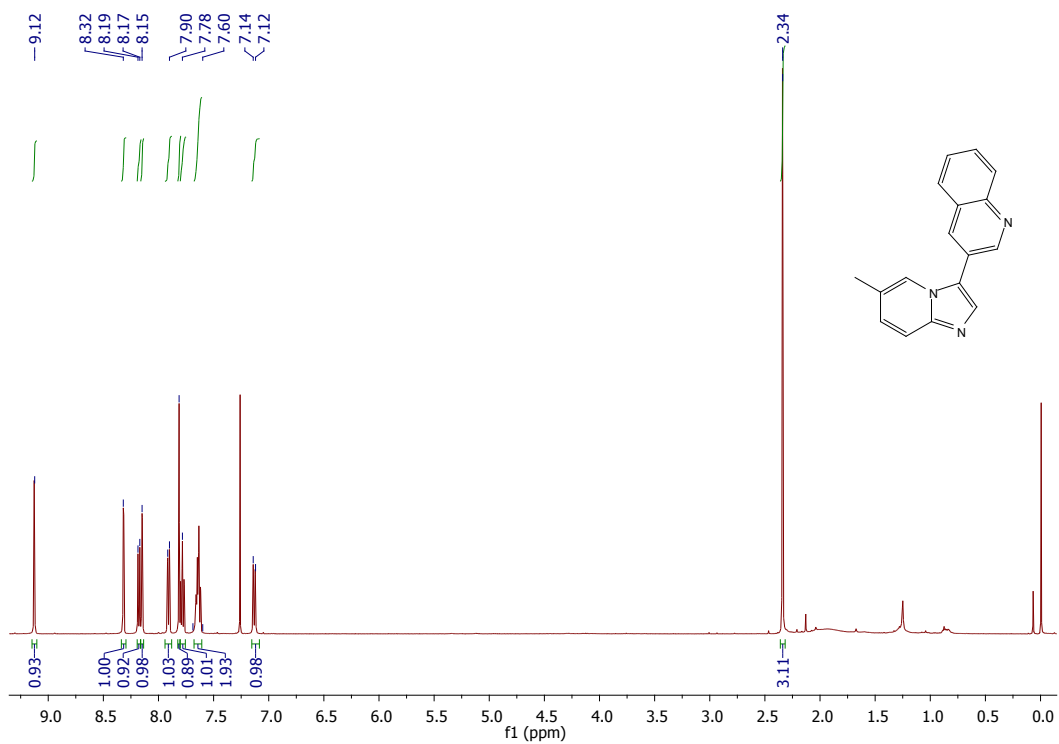
^{13}C NMR spectrum of **3y**



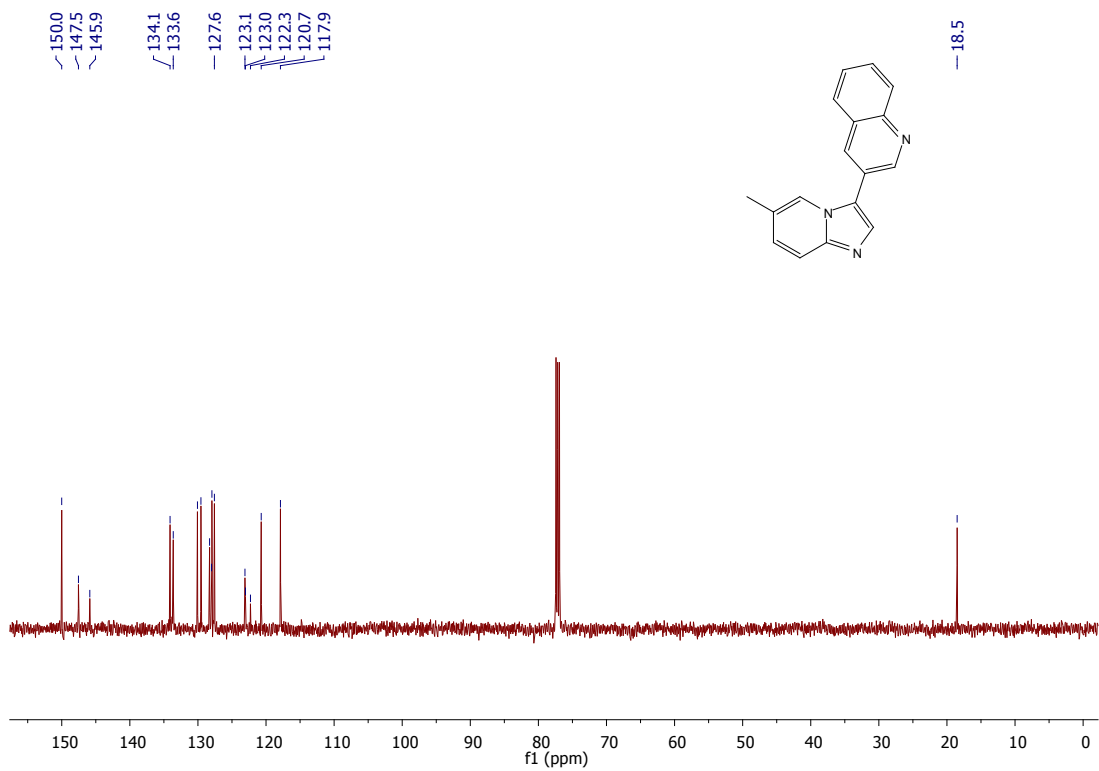
^1H NMR spectrum of **4a**



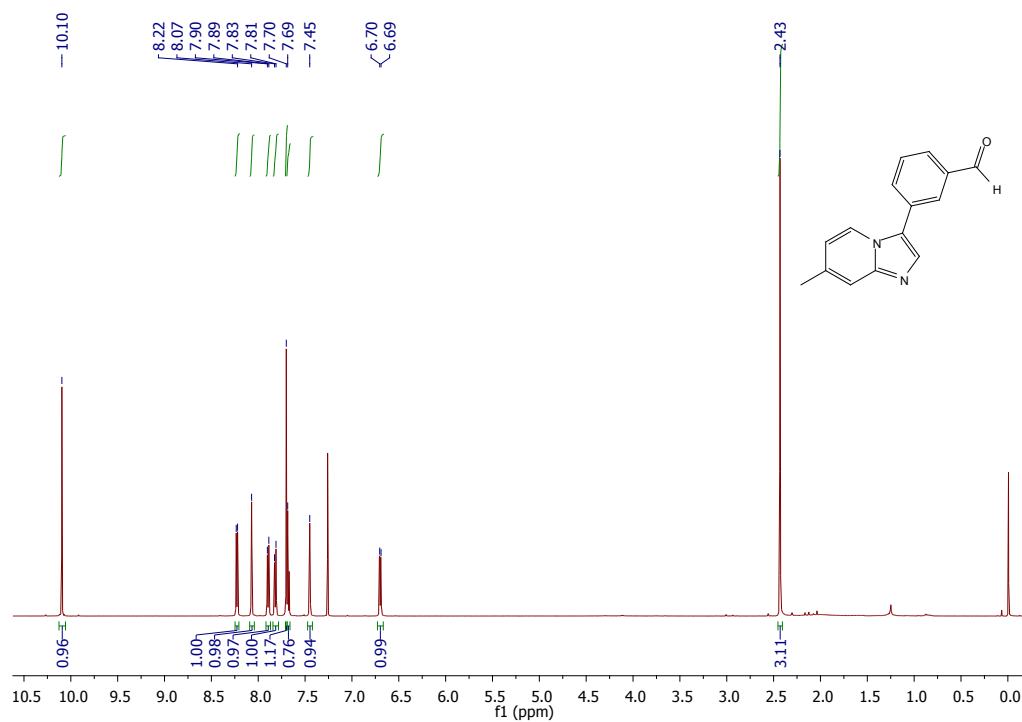
^{13}C NMR spectrum of **4a**



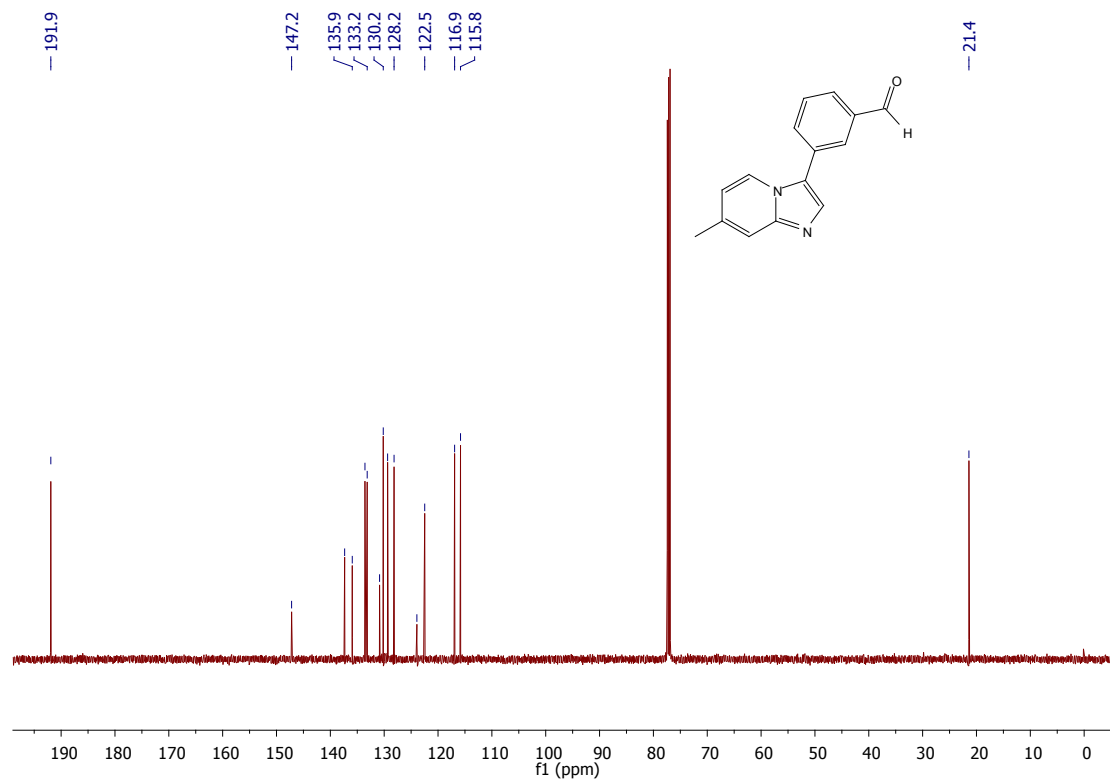
^1H NMR spectrum of **4b**



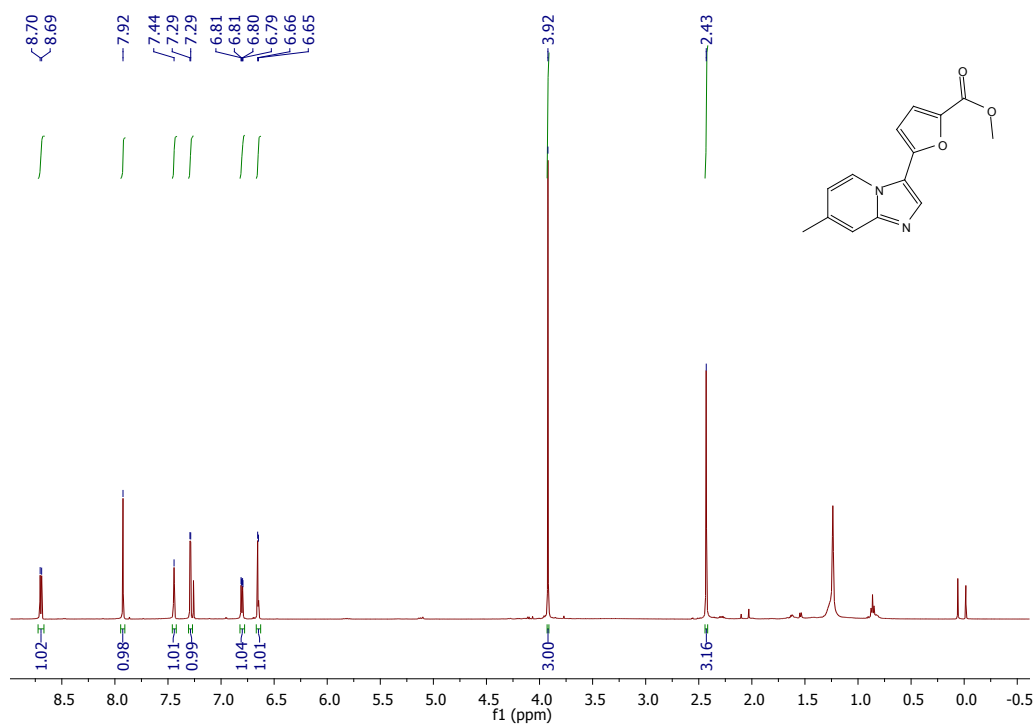
^{13}C NMR spectrum of **4b**



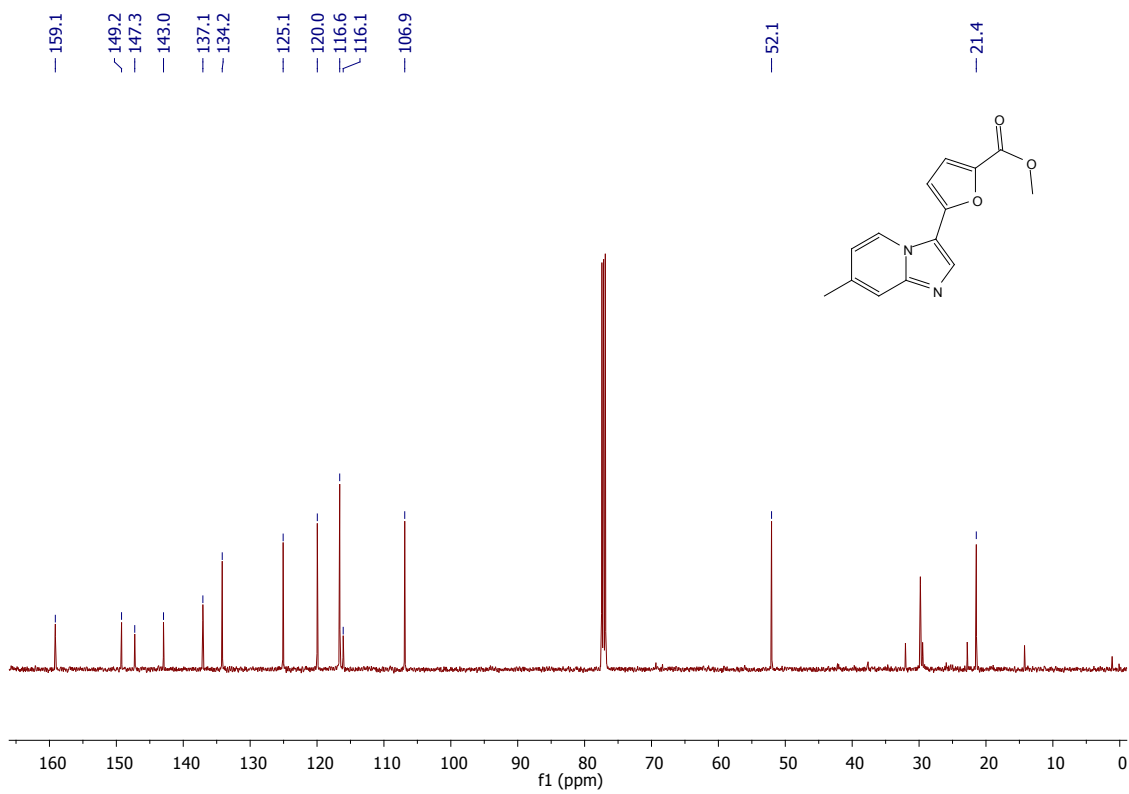
^1H NMR spectrum of **4c**



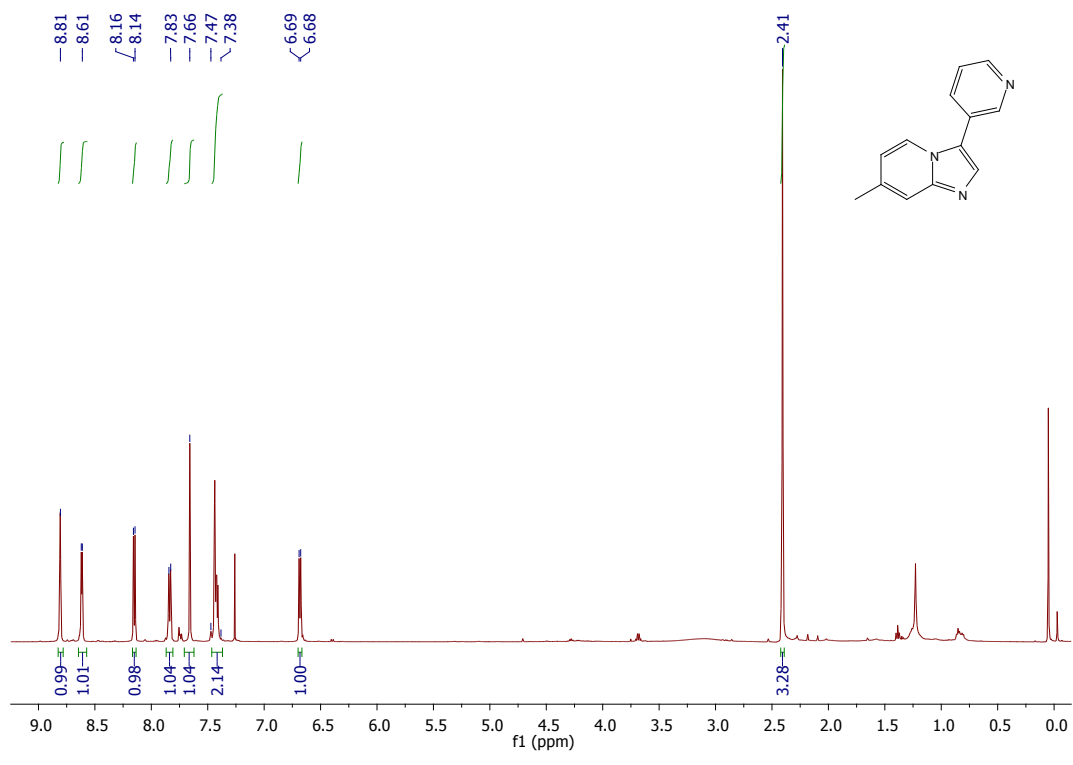
^{13}C NMR spectrum of **4c**



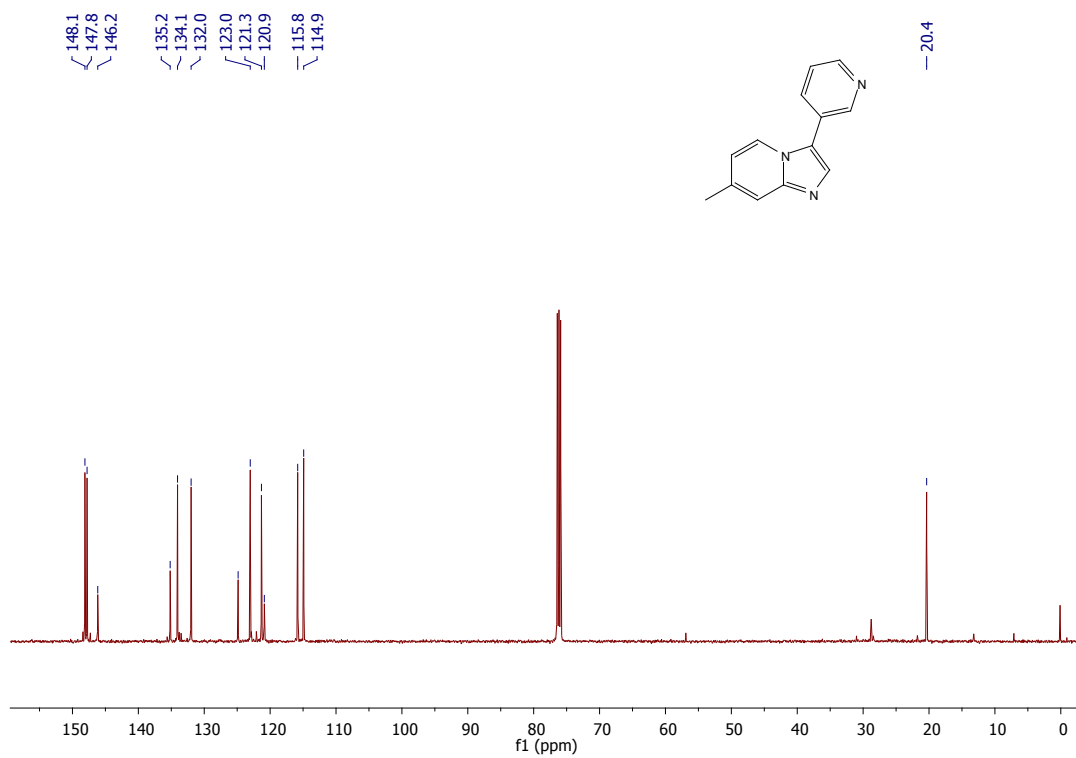
^1H NMR spectrum of **4d**



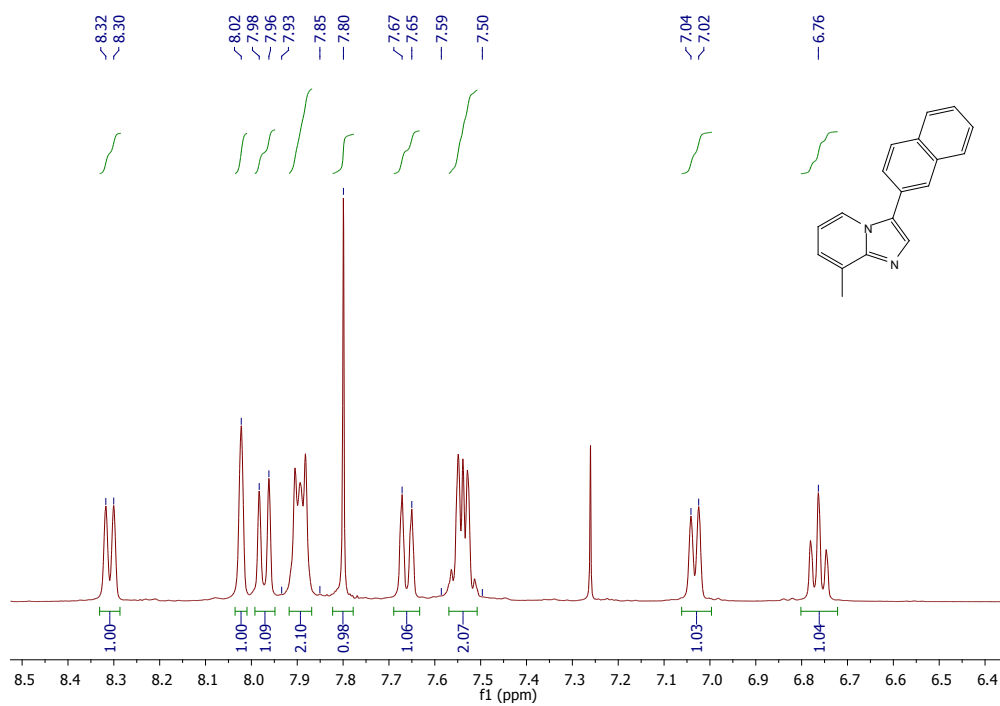
^{13}C NMR spectrum of **4d**



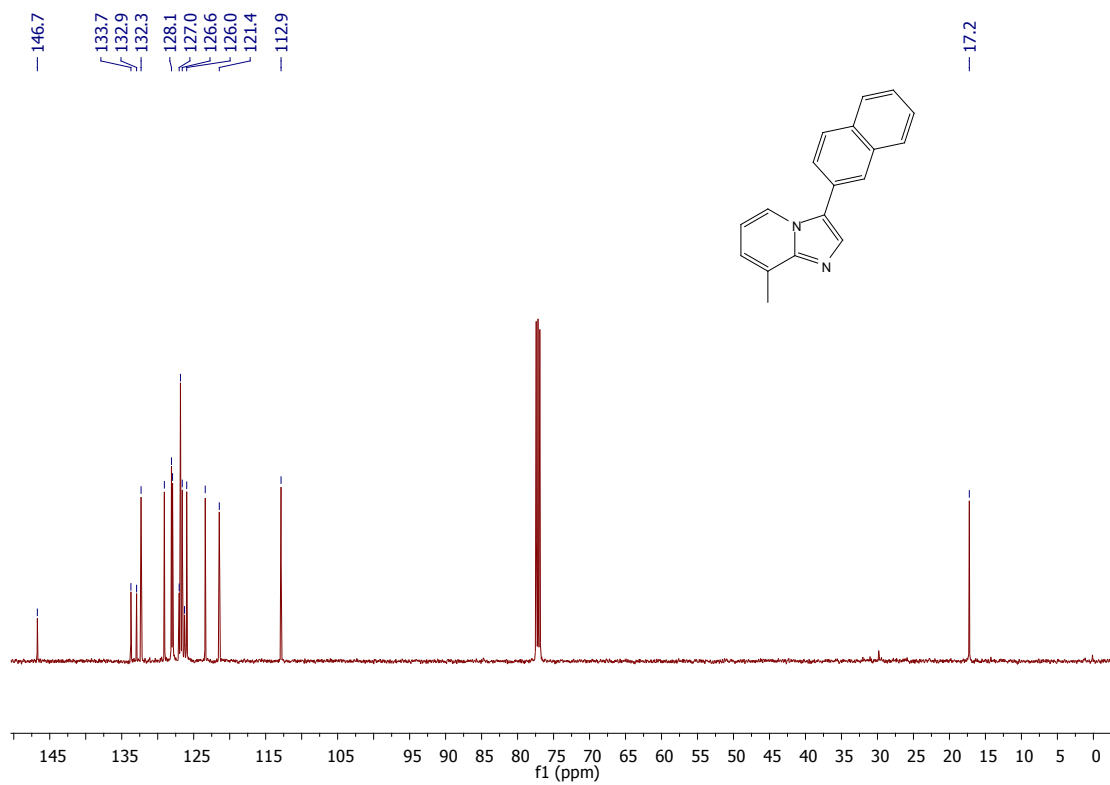
¹H NMR spectrum of 4e



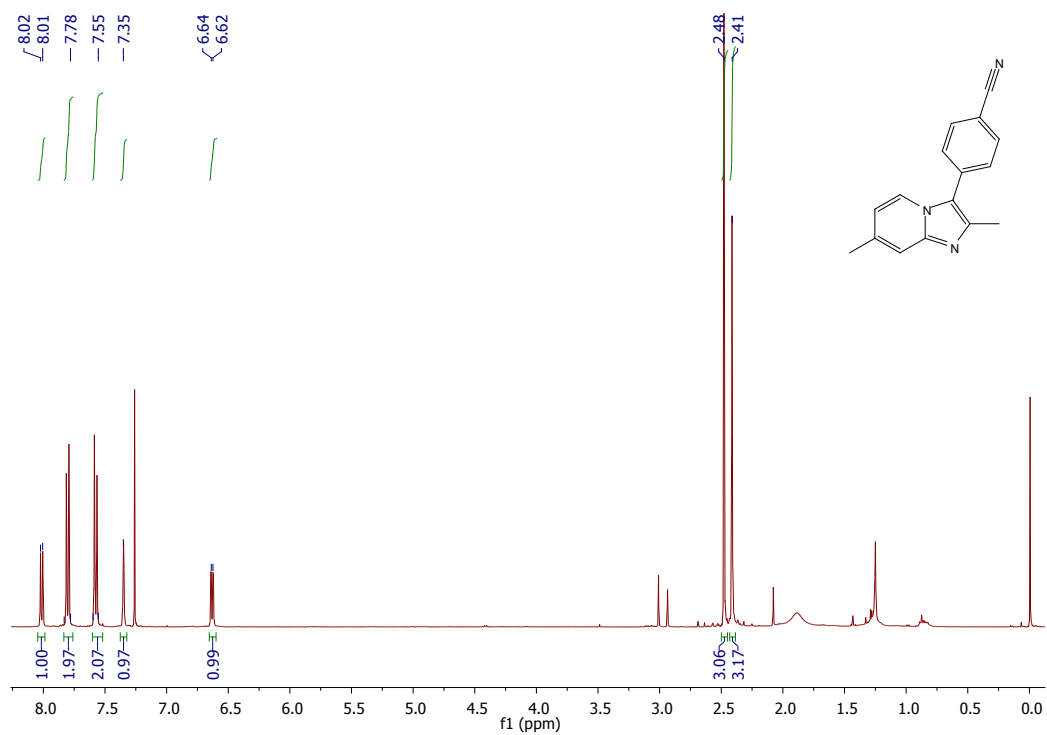
¹³C NMR spectrum of 4e



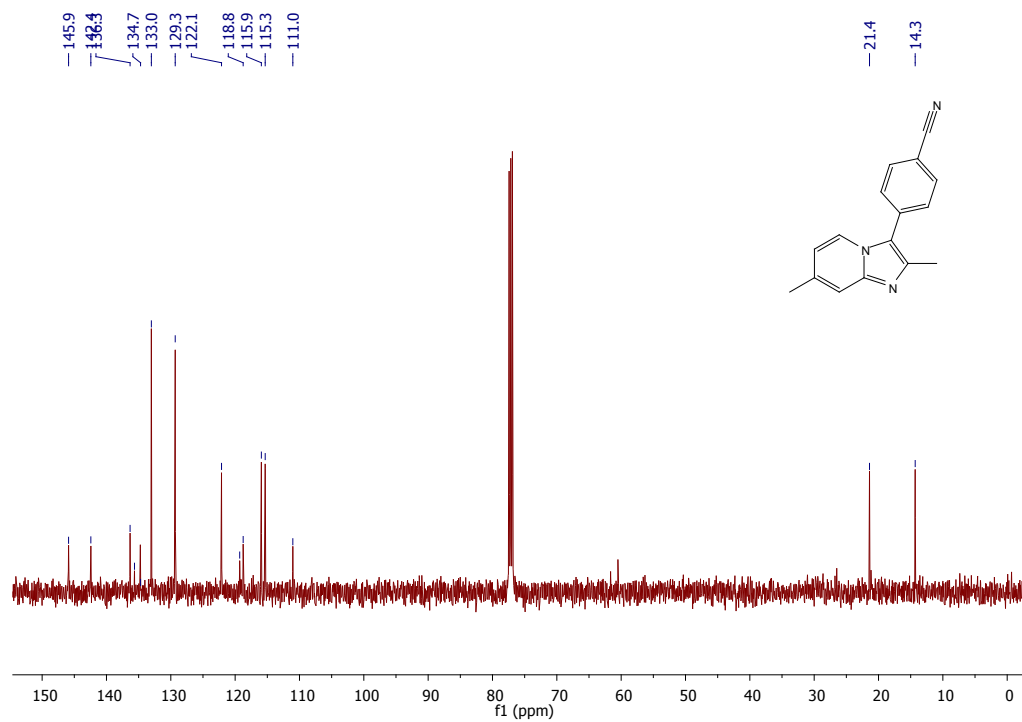
^1H NMR spectrum of **4f**



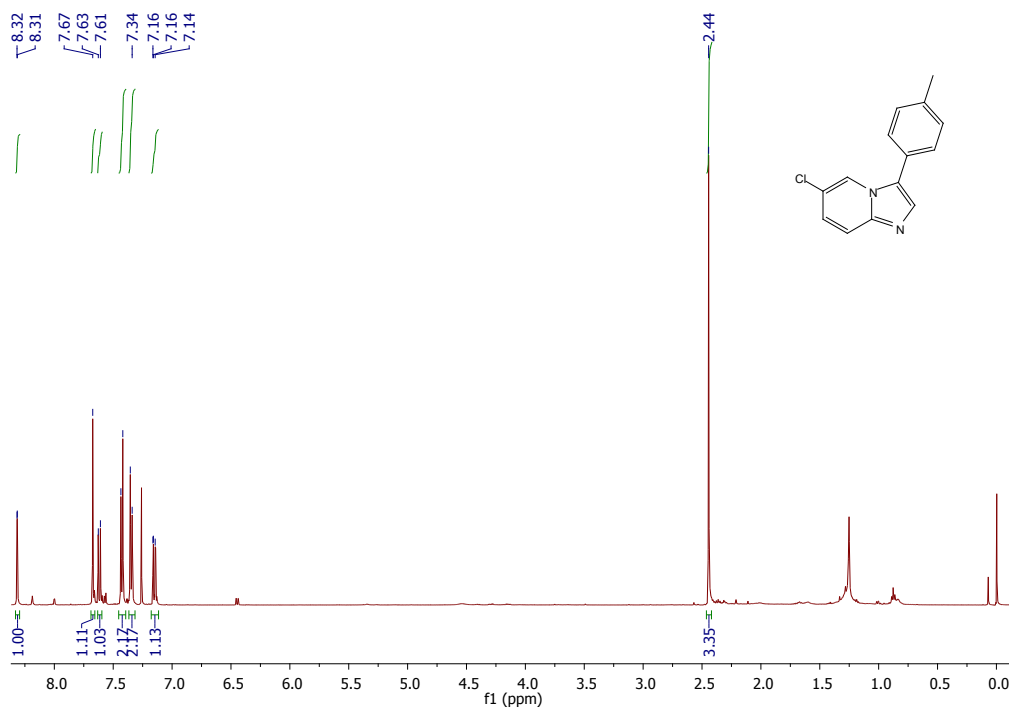
^{13}C NMR spectrum of **4f**



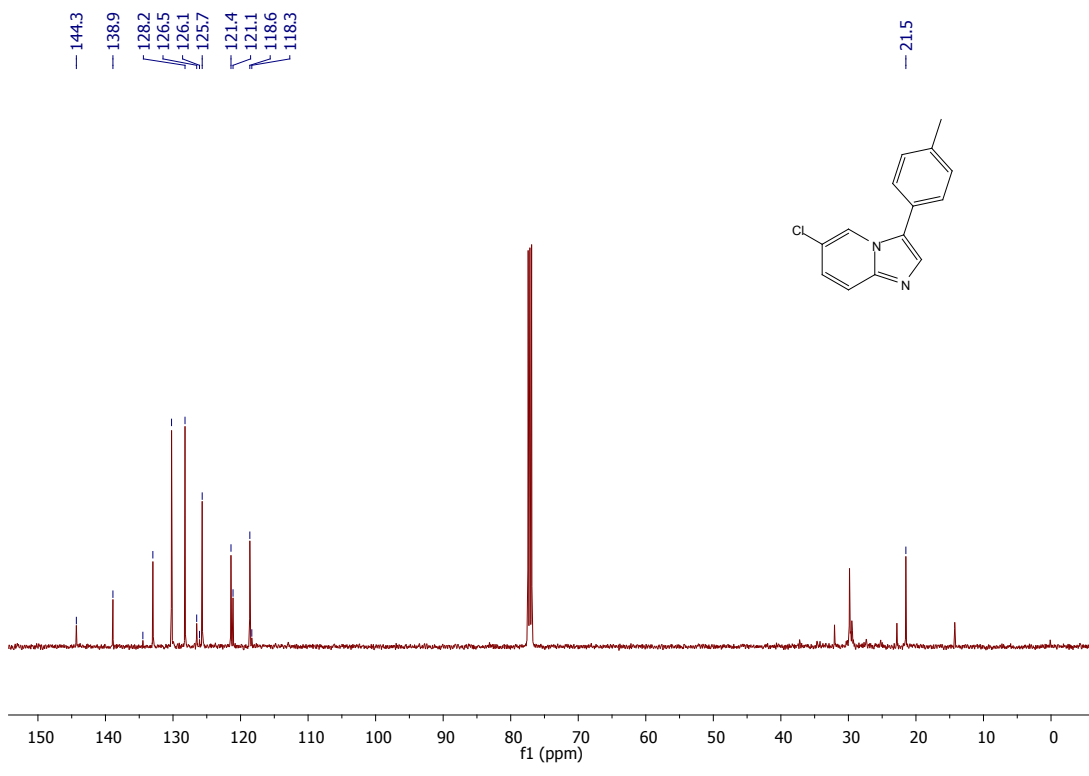
^1H NMR spectrum of **4g**



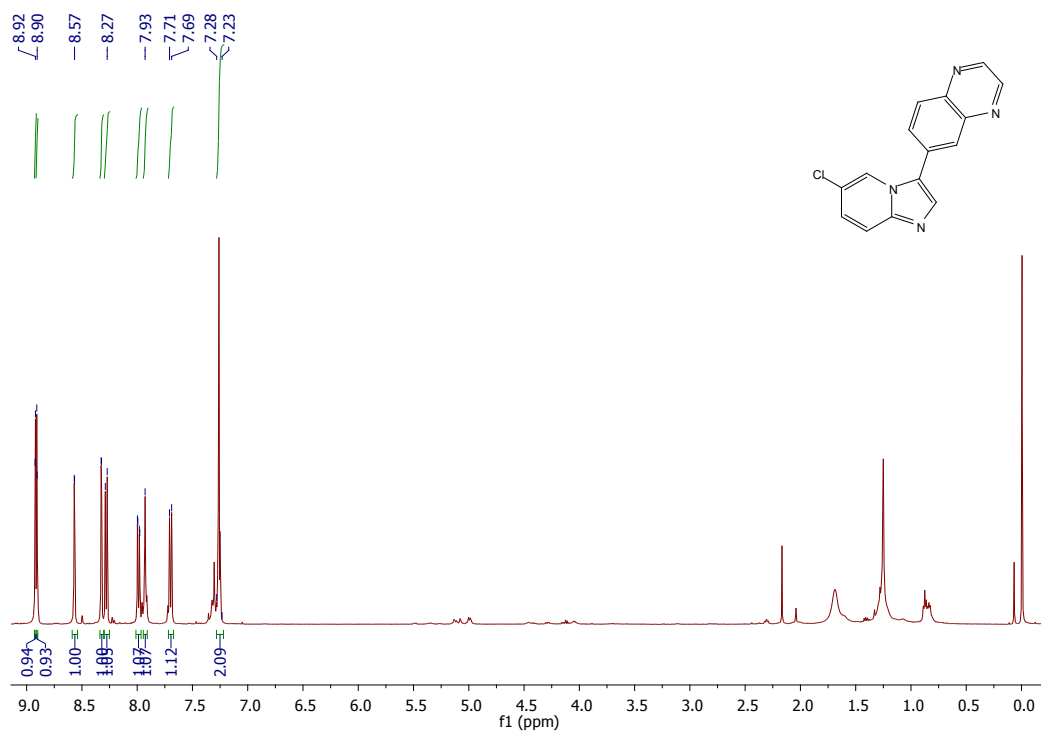
^{13}C NMR spectrum of **4g**



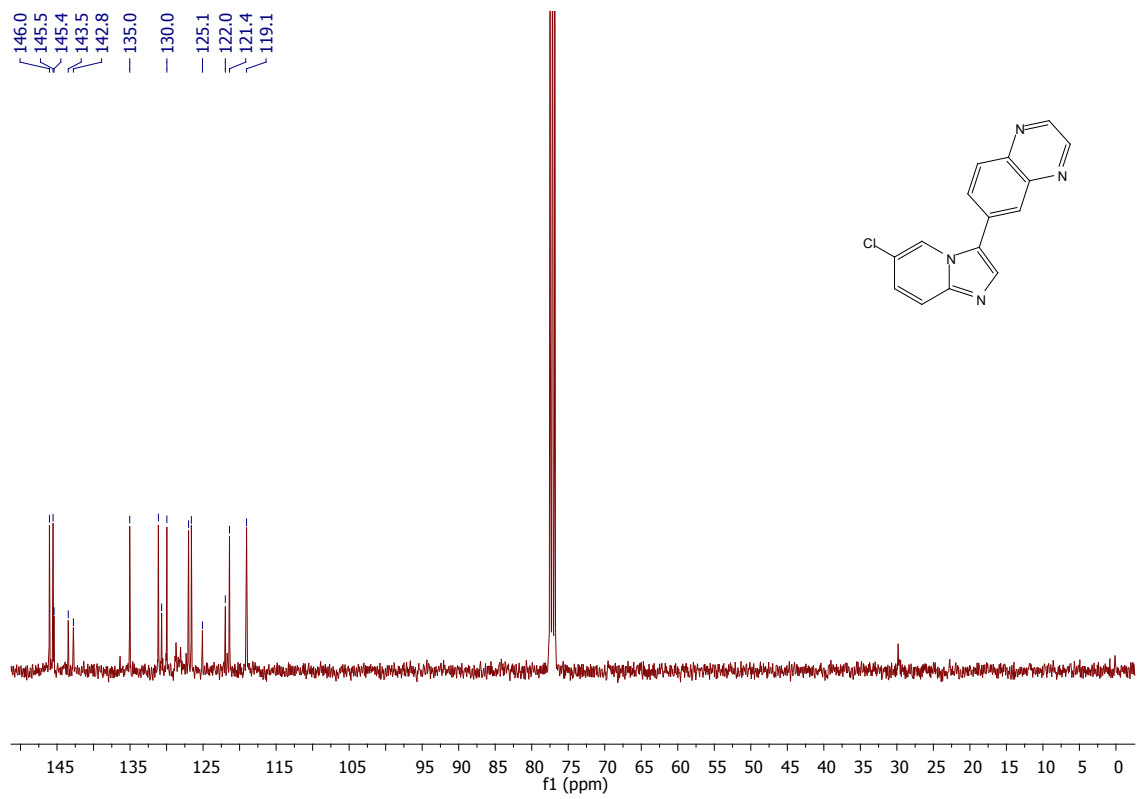
¹H NMR spectrum of **4h**



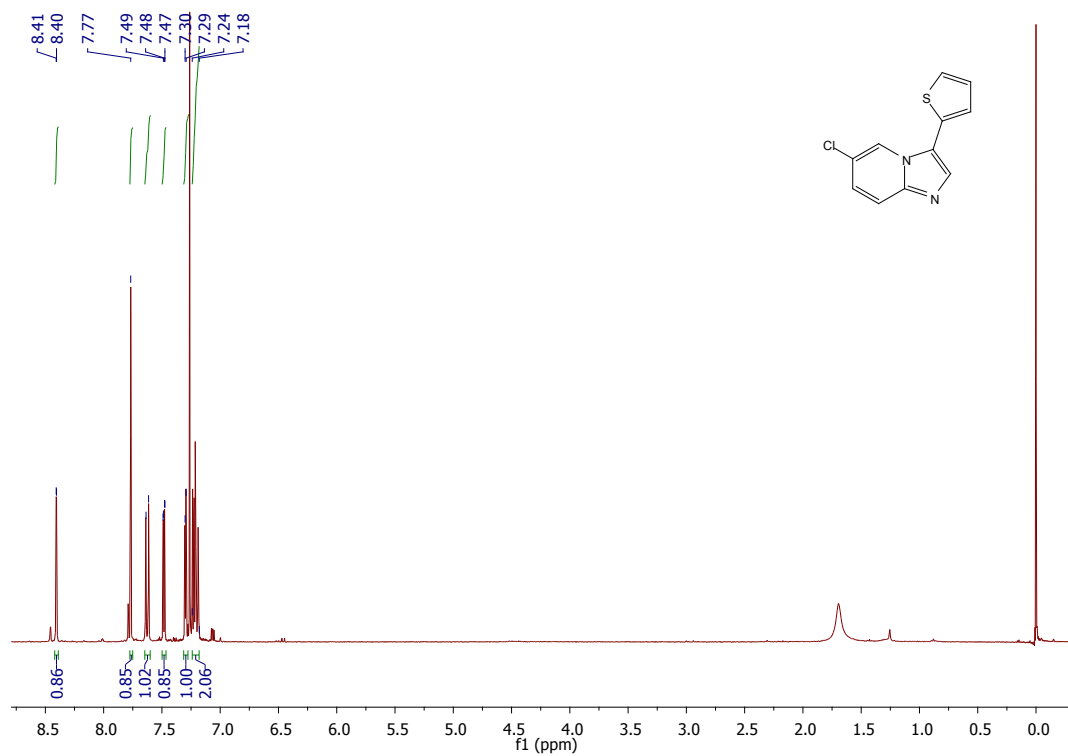
¹³C NMR spectrum of **4h**



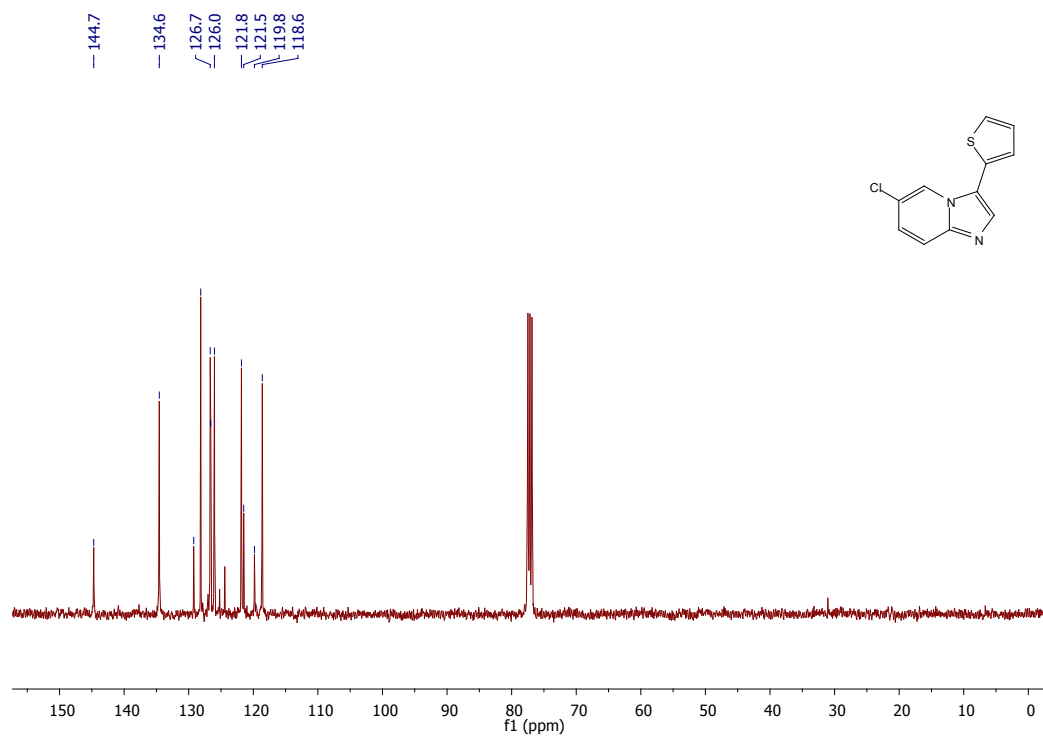
¹H NMR spectrum of **4i**



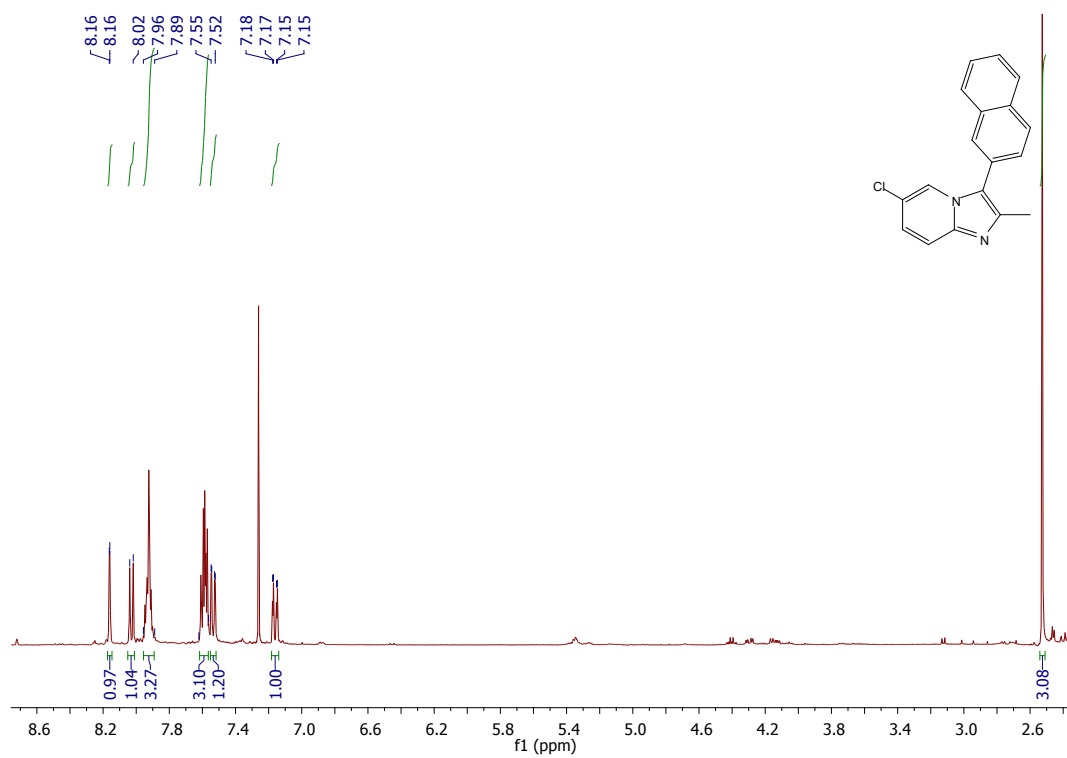
¹³C NMR spectrum of **4i**



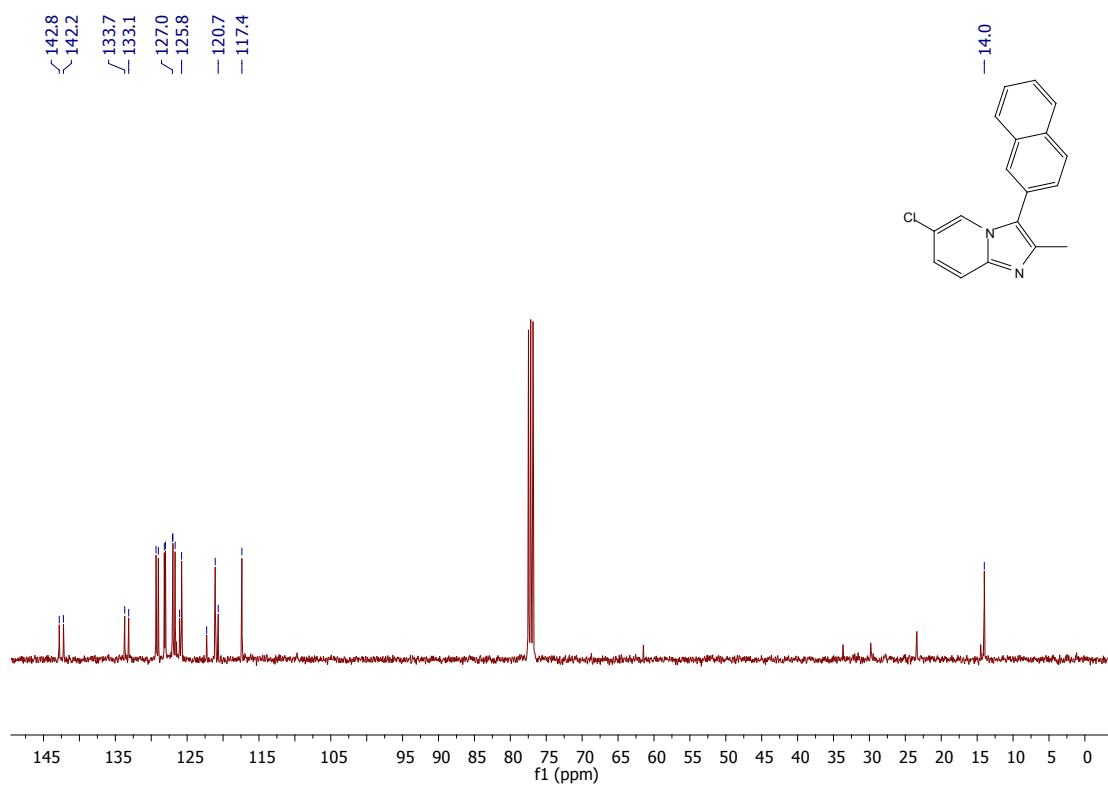
^1H NMR spectrum of **4j**



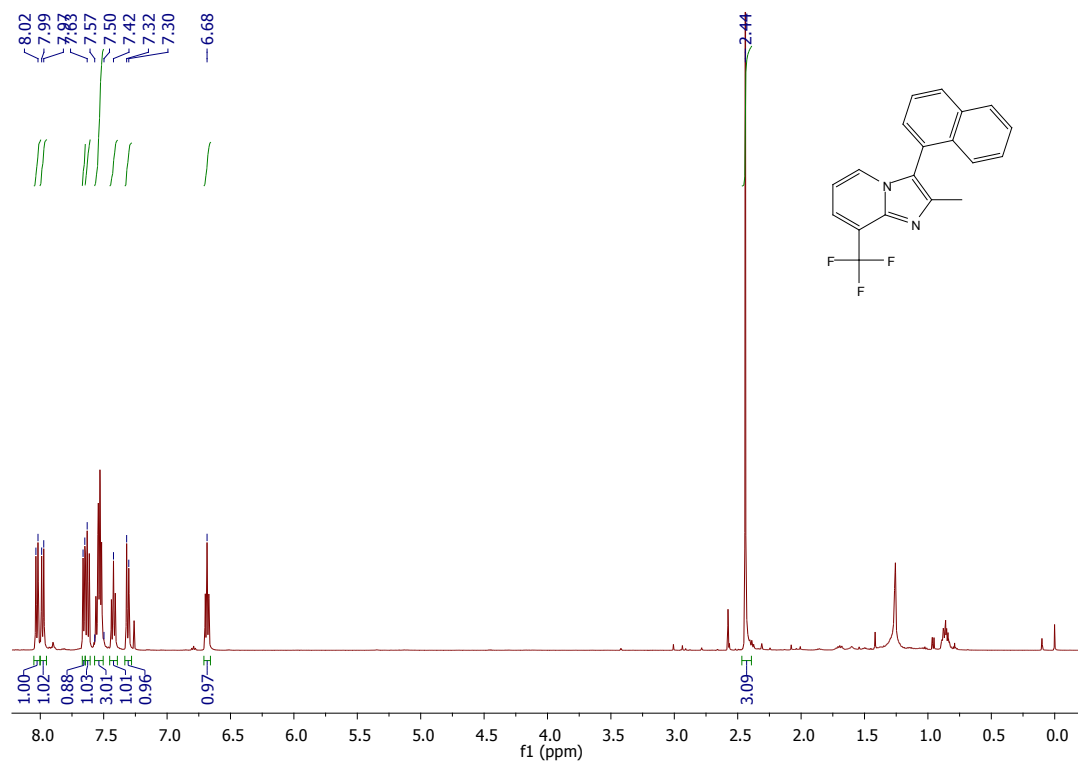
^{13}C NMR spectrum of **4j**



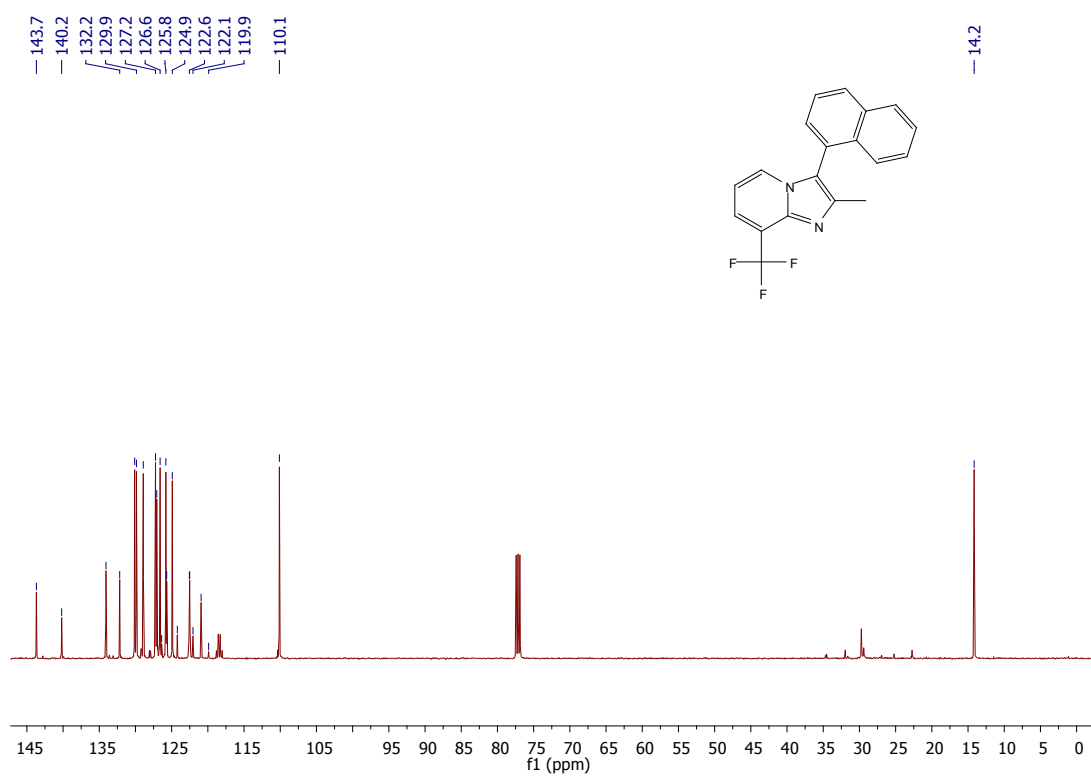
^1H NMR spectrum of **4k**



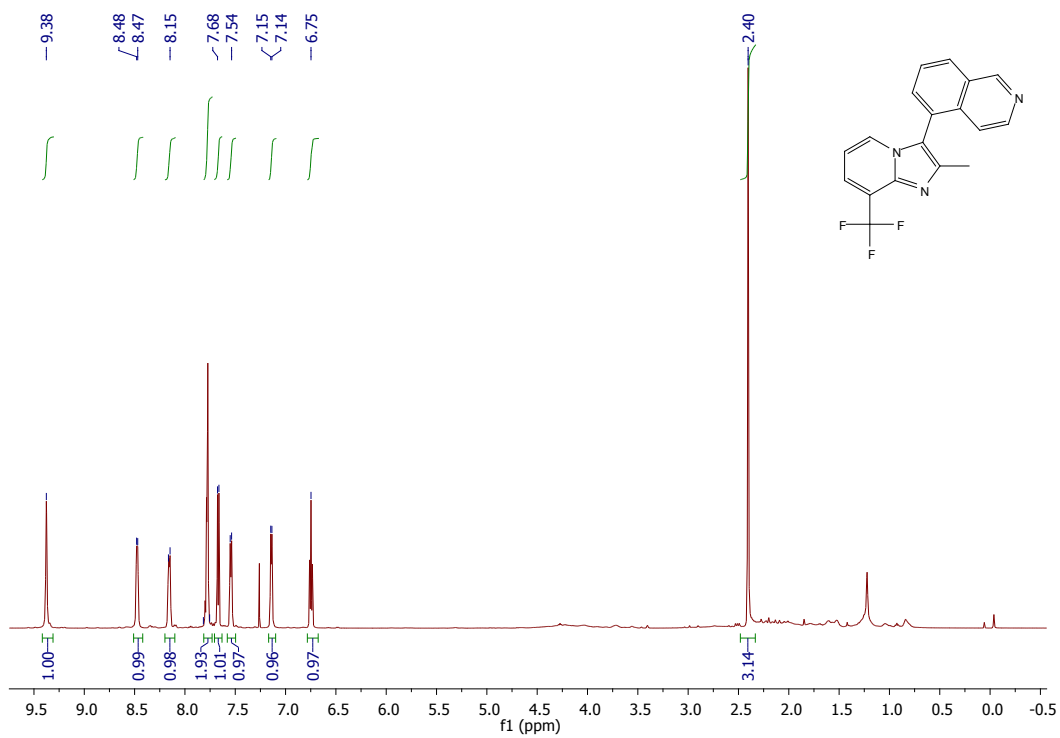
^{13}C NMR spectrum of **4k**



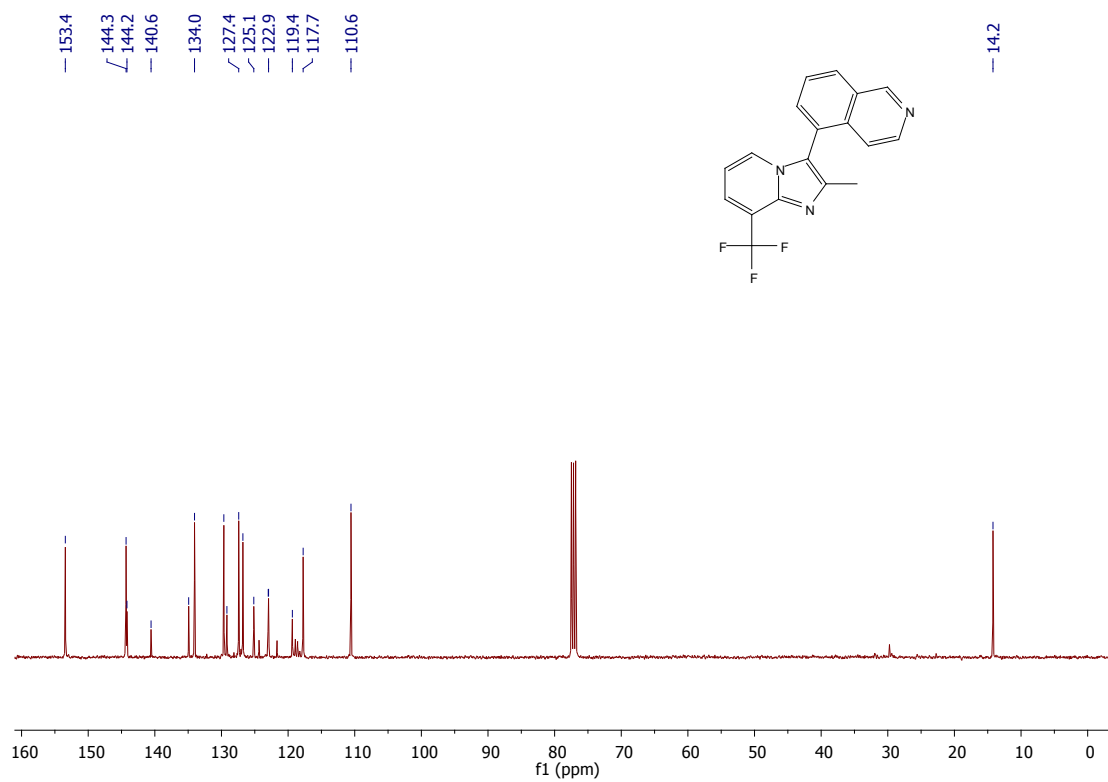
¹H NMR spectrum of **41**



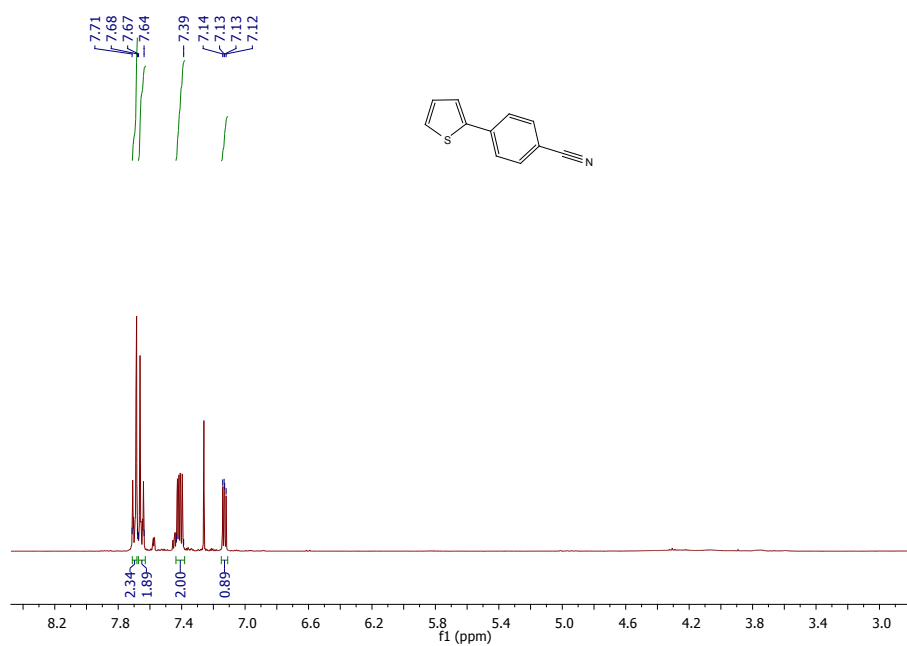
¹³C NMR spectrum of **41**



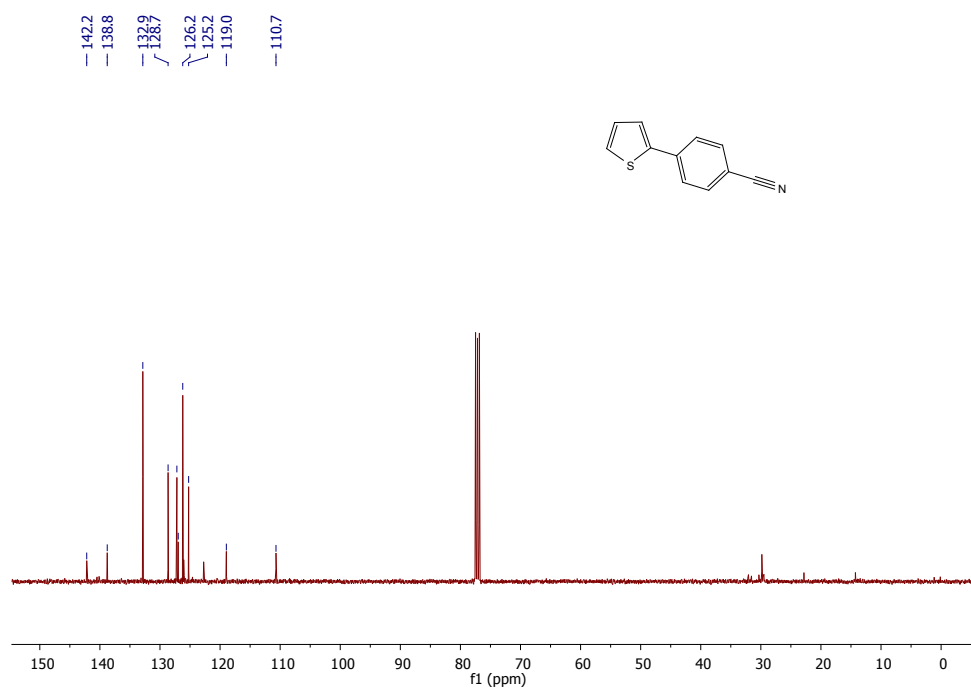
^1H NMR spectrum of **4m**



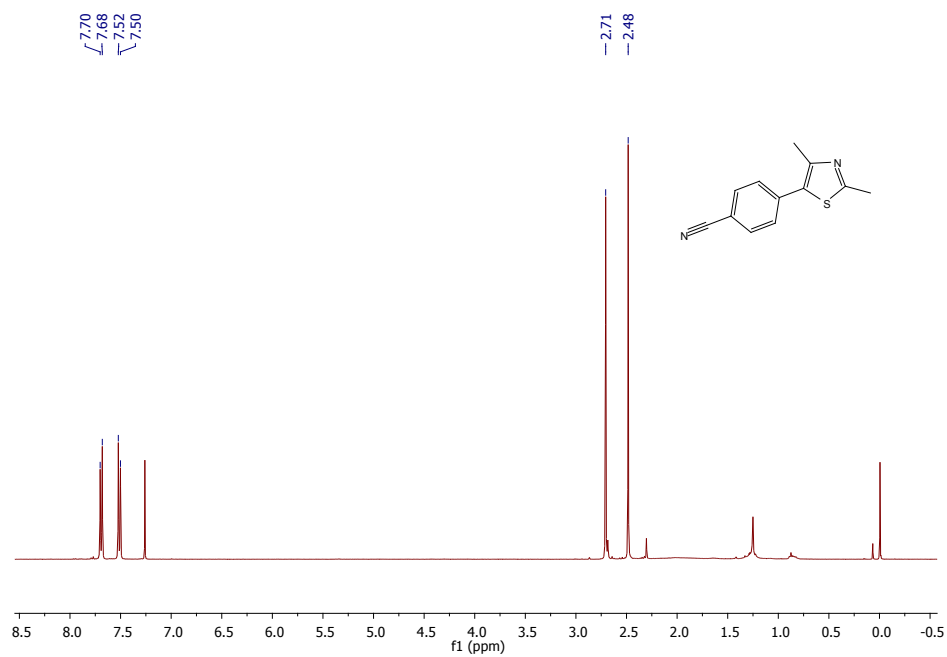
^{13}C NMR spectrum of **4m**



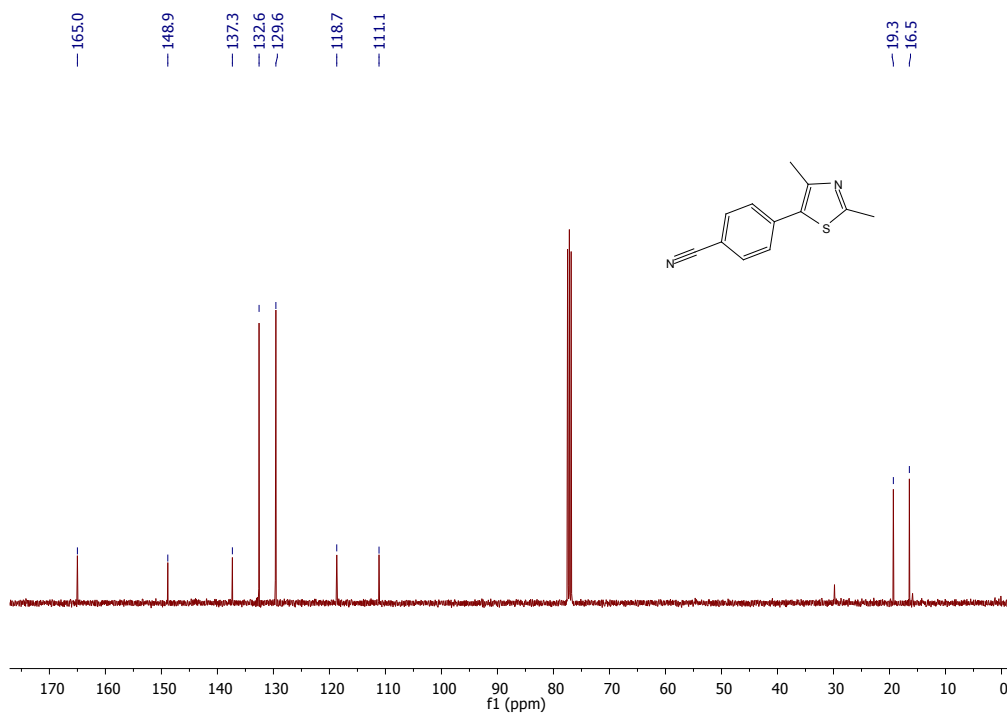
^1H NMR spectrum of **5a**



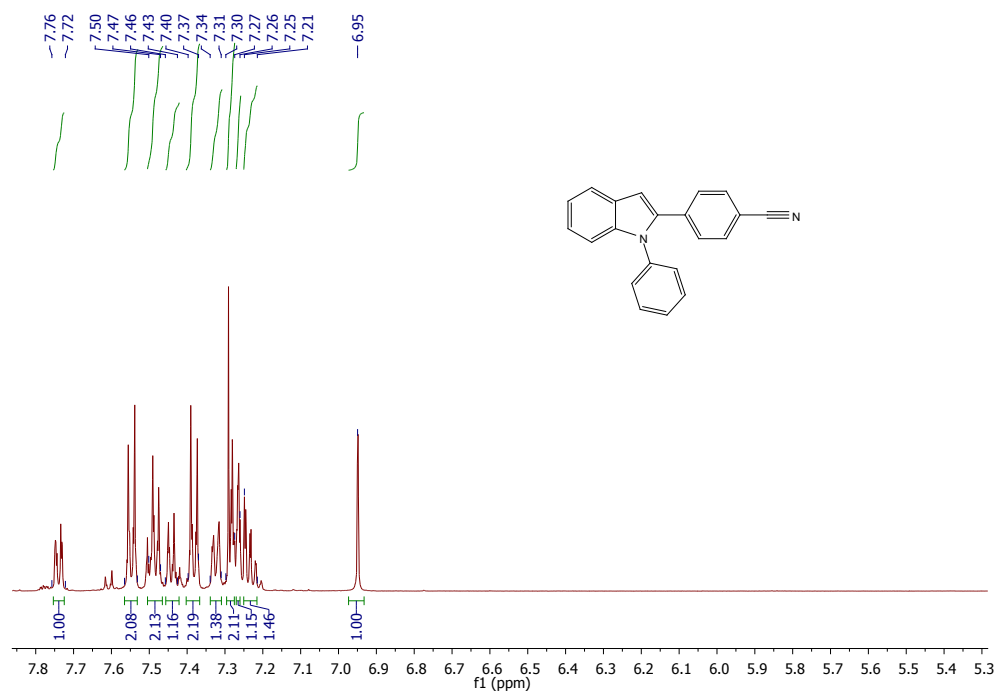
^{13}C NMR spectrum of **5a**



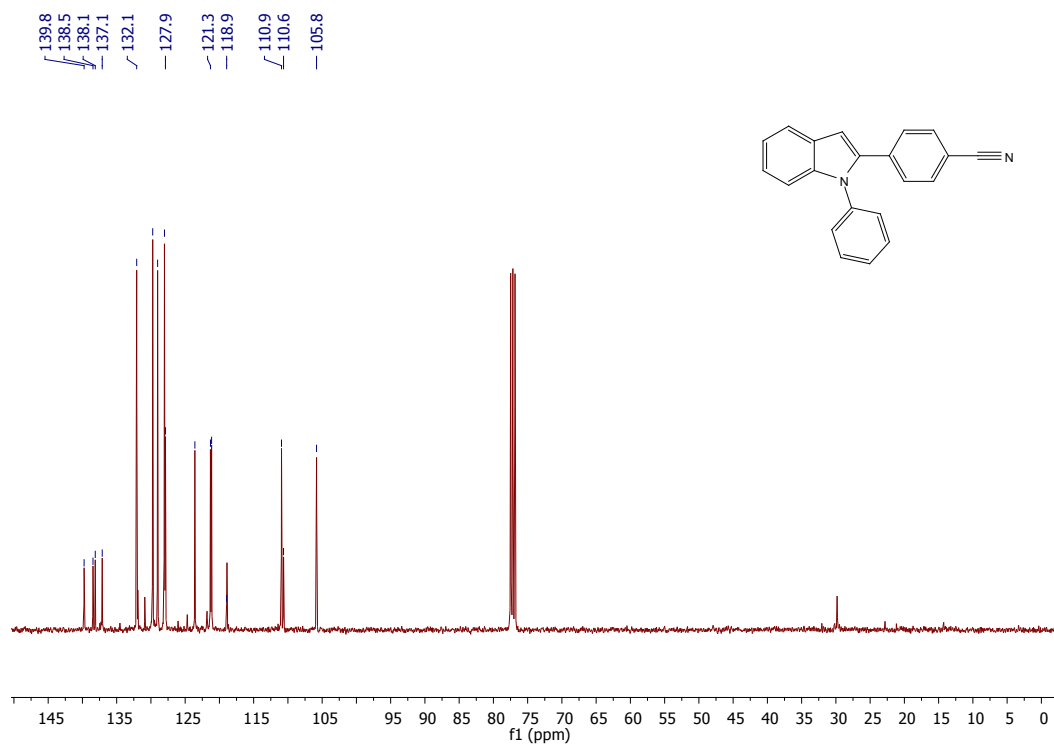
^1H NMR spectrum of **5b**



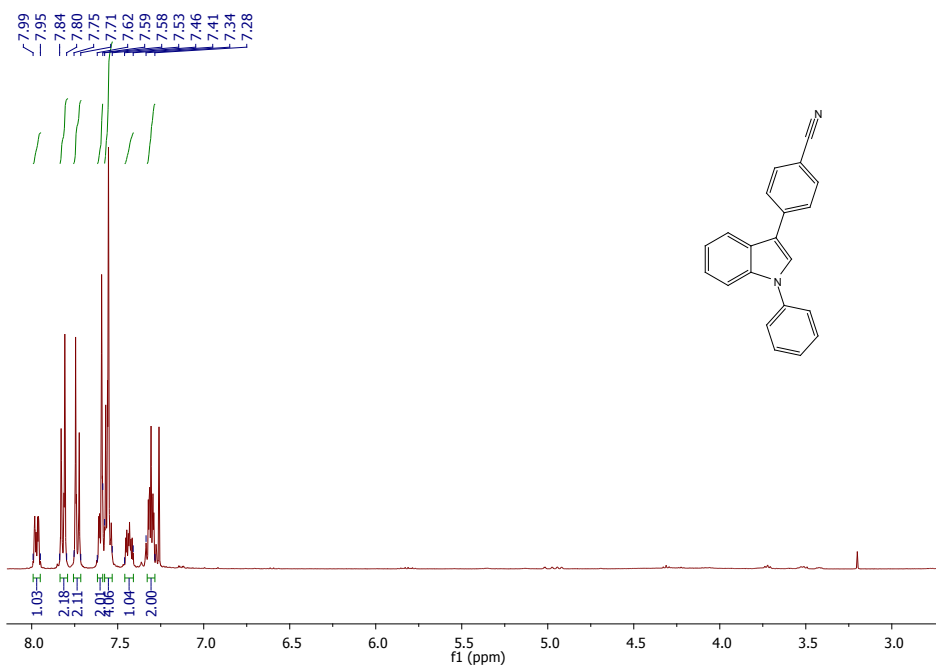
^{13}C NMR spectrum of **5b**



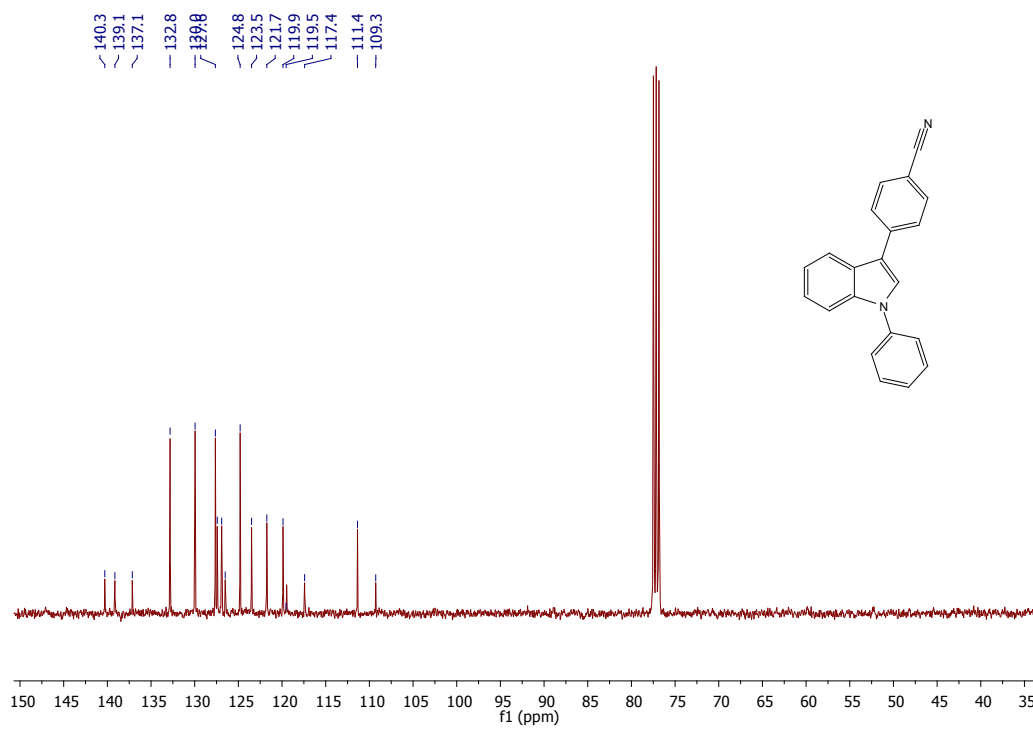
¹H NMR spectrum of **5c**



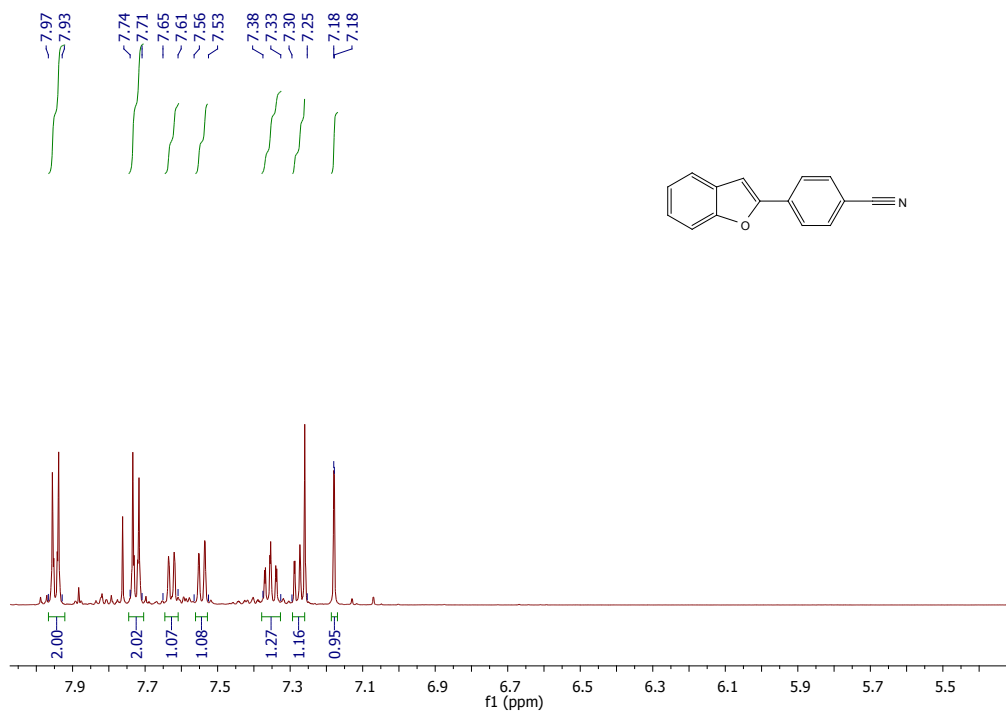
¹³C NMR spectrum of **5c**



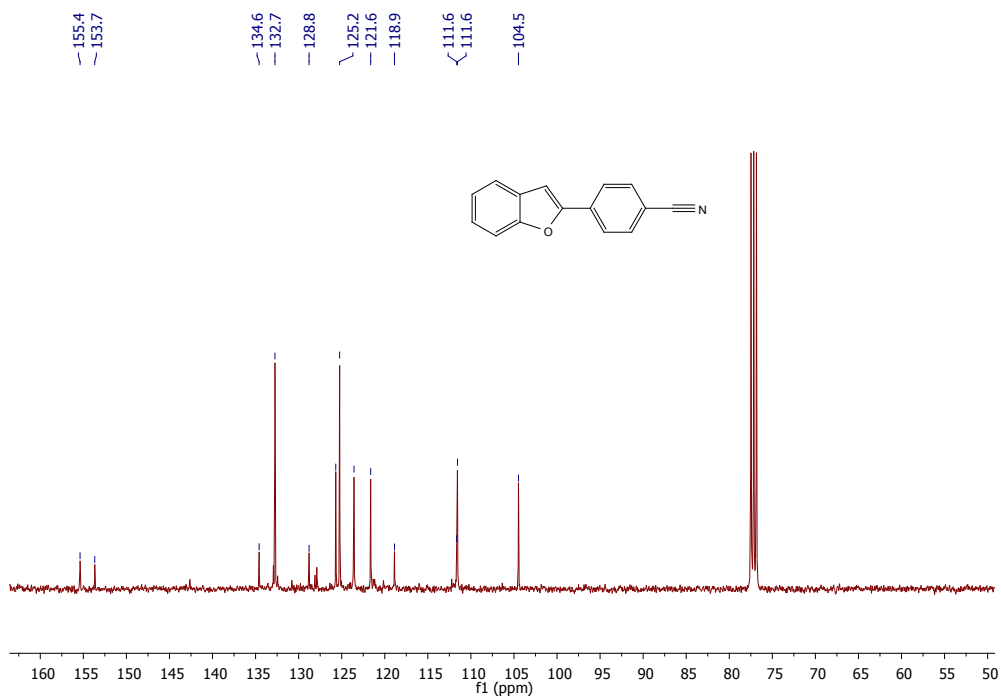
¹H NMR spectrum of 5c'



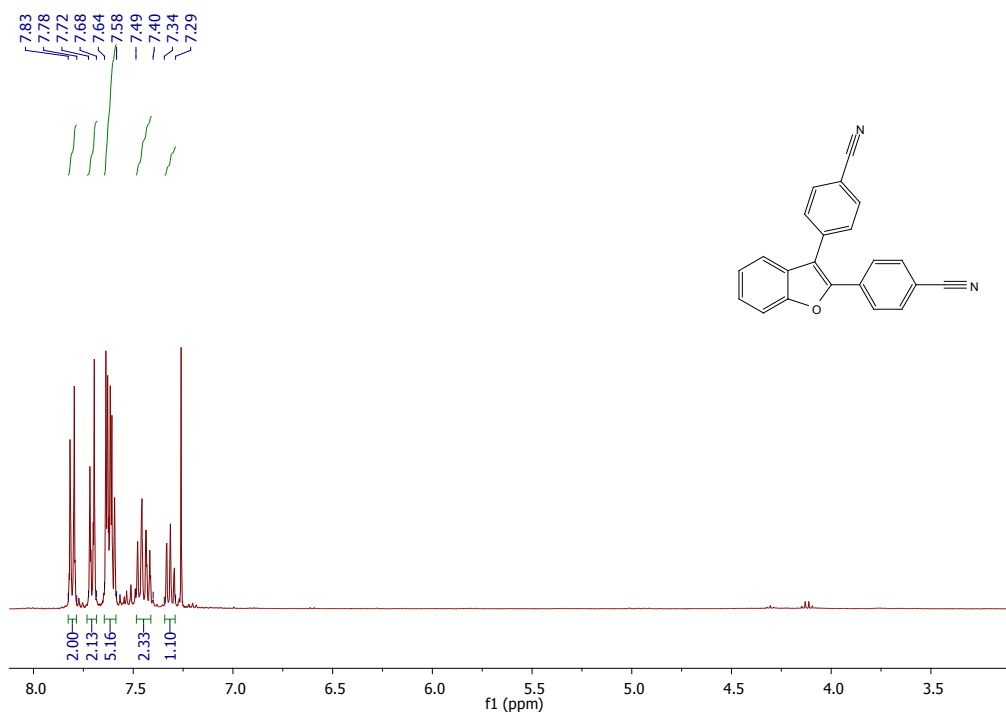
¹³C NMR spectrum of 5c'



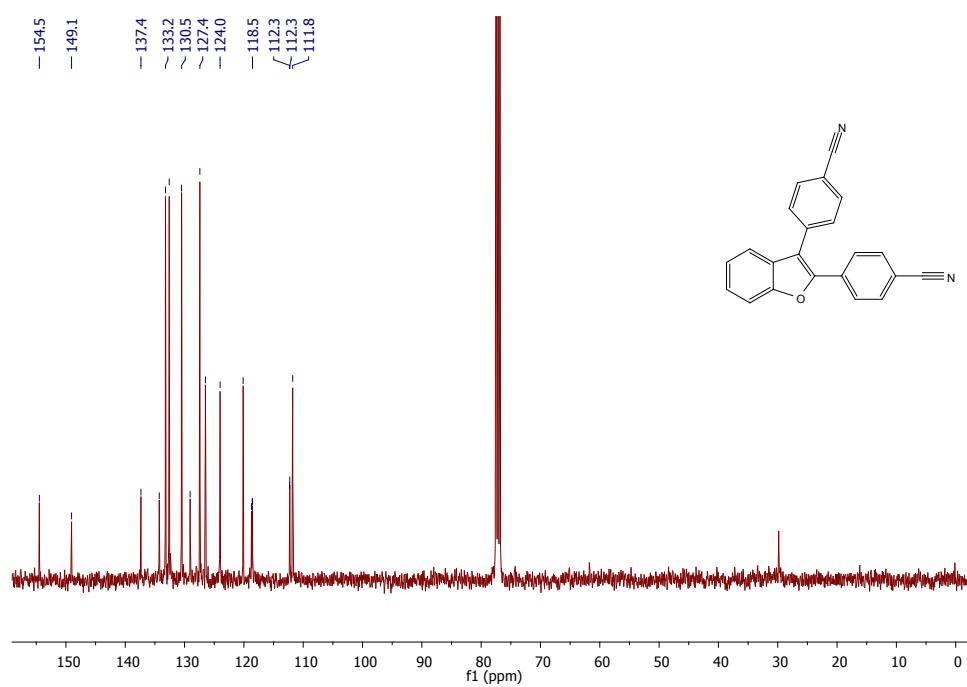
^1H NMR spectrum of **5d**



^{13}C NMR spectrum of **5d**



¹H NMR spectrum of **5d'**



¹³C NMR spectrum of **5d'**

Antibacterial assay

The screening panel consist of *E. coli* ATCC 25922, *S. aureus* ATCC 29213, *P. aeruginosa* ATCC 27853, *K. pneumoniae* BAA-1705 and *A. baumannii* BAA-1605. The bacterial strains were procured from ATCC (ATCC, Manassas, VA, USA) and Mueller Hinton broth II (MHB II) (Becton Dickinson) was used to propagate the bacteria. The compounds were serially diluted utilizing 2-fold dilutions and bacteria were subsequently added to a final count of 10⁴-10⁵ cfu/ml. The 96-well plates were incubated at 37°C for 24 hrs and the antimicrobial activity was determined by visual inspection. The MIC of the active compounds was determined and was defined as the lowest concentration of the compound that inhibited visible growth after 24 hrs.

References

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