Supporting Information

Atmospheric Oxygen Mediated Oxidation Coupling of Primary and Secondary Alcohols: Synthesis of Pyrazolo[1,5-*a*]pyrimidines

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1. General

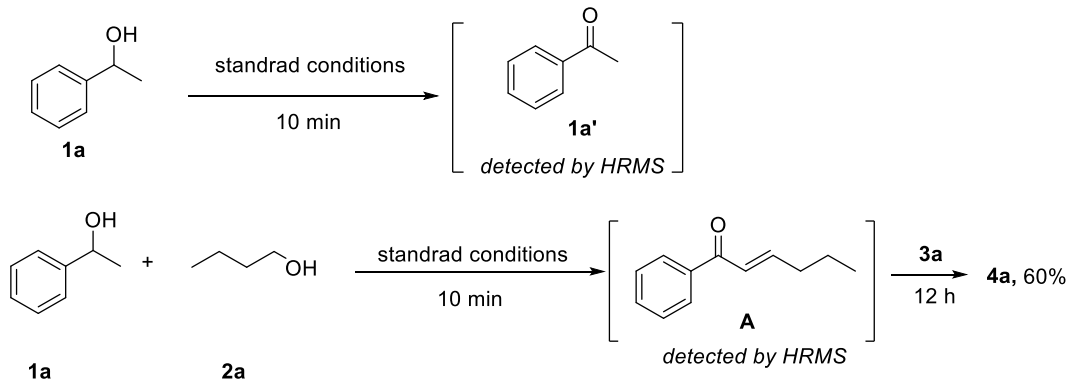
All other substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). All ^{1}H NMR, $^{13}C\{^{1}H\}$ and $^{19}F\{^{1}H\}$ NMR spectra were recorded on 400 MHz Bruker FT-NMR spectrometers (400/100/377 MHz). All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet; qd, quartet of doublets. The coupling constants, *J*, are reported in Hertz (Hz). High resolution mass spectroscopy data of the product were collected on an Agilent Technologies 6540 UHD Accurate-Mass Q-TOF LC/MS (ESI). Crystallographic data of product **4g** was collected on Bruker SMART APEX II (Mo target, voltage 50 KV, current 30 mA).

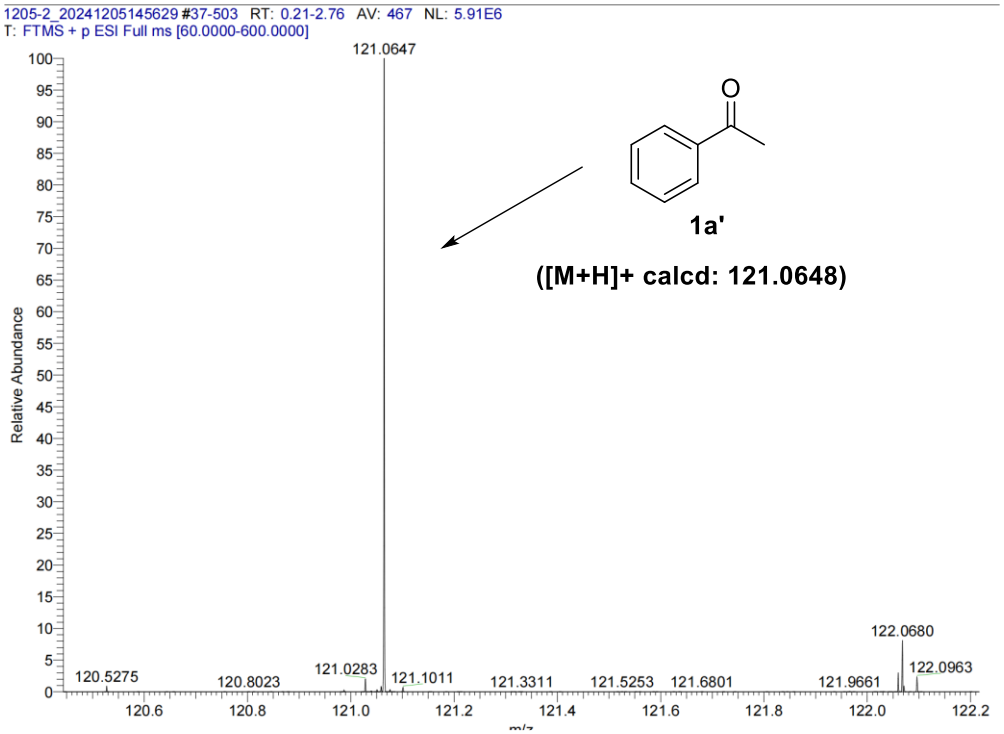
2. General procedure for the synthesis of 4 (4a as an example)

1-phenylethan-1-ol **1a** (244 mg, 2 mmol), butan-1-ol **2a** (296 mg, 4 mmol), and 1H-pyrazol-3-amine **3a** (83 mg, 1 mmol) and NaOH (80 mg, 2 mmol) were added to a tube, the reaction mixture was stirred in tube at 140 °C for 12 h. The reaction was monitored by TLC. After completion of the reaction, the mixture was diluted with water and extracted with ethyl acetate, the organic layer was combined, dried over by anhydrous Na_2SO_4, and filtered, then concentrated to yield the crude product, which was further purified by flash chromatography (petroleum ether/ethyl acetate = 15:1, V/V) to give the product **4a** (159 mg) in 67% yield.

3. Mechanistic studies

For study on the reaction mechanism, **1a** was separately exposed to the standard conditions for 10 minutes, and the corresponding oxidation products were detected HRMS. Finally, when **1a** and **2a** were reacted under standard conditions for 10 minutes, compound **A** was detected by HRMS. After adding **3a** and continuing the reaction for 12 hours, the final product **4a** was obtained in 60% yield.

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O
1a'
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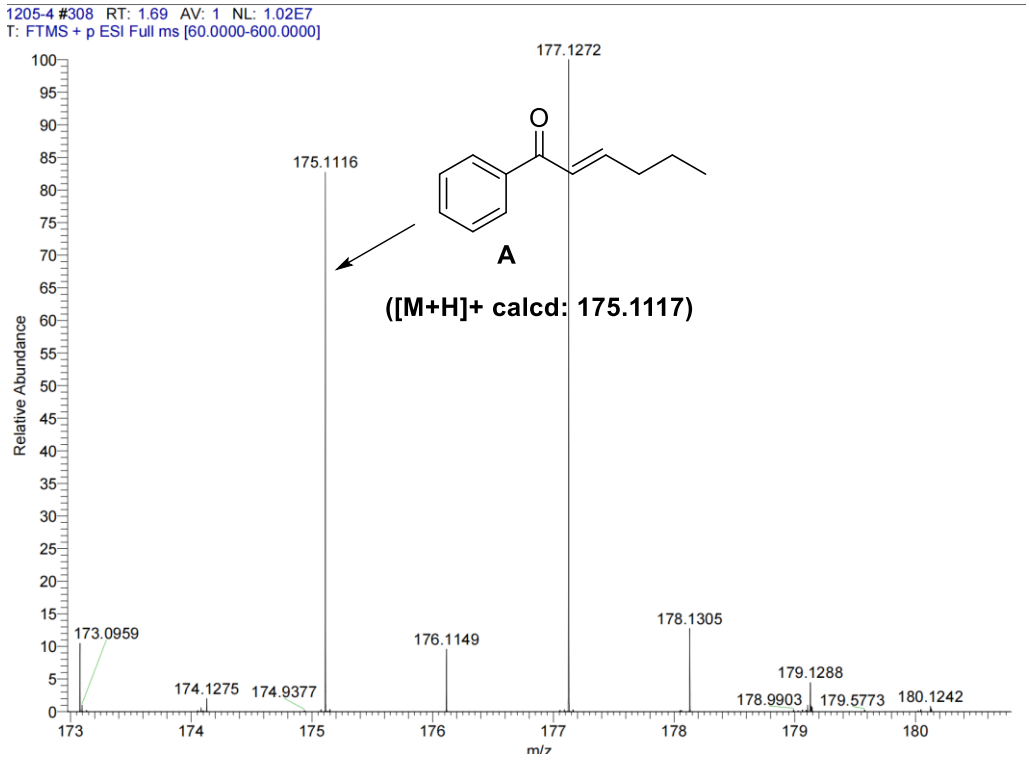
m/z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O
175.1116
A
([M+H]+ calcd: 175.1117)
Relative Abundance
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173.0959
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174.1275
174.9377
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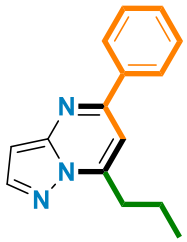
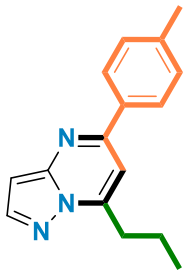
180.1242
m/z

4. Characterization data for compounds 4, 5, 6



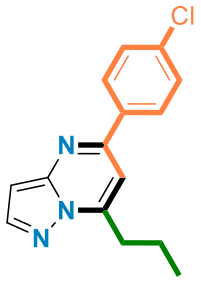
5-phenyl-7-propylpyrazolo[1,5-a]pyrimidine (4a):

Yield 67%; 159 mg; yellow solid; column chromatography, silica gel (PE/EA, 15:1); mp 66.7-66.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 2.4 Hz, 1H), 8.09–8.07 (m, 2H), 7.53–7.46 (m, 3H), 7.12 (s, 1H), 6.72 (d, J = 2.4 Hz, 1H), 3.21 (t, J = 7.6 Hz, 2H), 2.02–1.92 (m, 2H), 1.12 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 155.9, 149.5, 148.9, 144.7, 137.7, 130.1, 128.8, 127.3, 103.8, 96.9, 32.6, 19.4, 13.9; HRMS (ESI) m/z calcd for $C_{15}H_{16}N_3^+$ $(M+H)^+$: 238.1339, found: 238.1338.



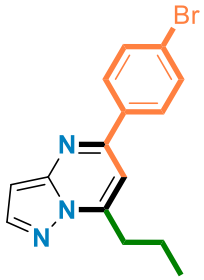
7-propyl-5-(p-tolyl)pyrazolo[1,5-a]pyrimidine (4b):

Yield 70%; 176 mg; yellow solid; column chromatography, silica gel (PE/EA, 15:1); mp 53.4-53.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 2.4 Hz, 1H), 7.98 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.10 (s, 1H), 6.70 (d, J = 2.4 Hz, 1H), 3.19 (t, J = 7.6 Hz, 2H), 2.42 (s, 3H), 2.01–1.92 (m, 2H), 1.11 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 155.9, 149.3, 148.9, 144.6, 140.4, 134.8, 129.6, 127.2, 103.6, 96.7, 32.6, 21.4, 19.4, 13.9; HRMS (ESI) m/z calcd for $C_{16}H_{18}N_3^+$ $(M+H)^+$ 252.1495, found: 252.1494.



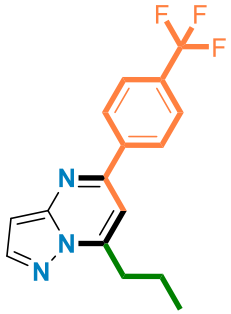
5-(4-chlorophenyl)-7-propylpyrazolo[1,5-a]pyrimidine (4c):

Yield 60%; 163 mg; white solid; column chromatography, silica gel (PE/EA, 20:1); mp 82.3-83.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 8.03 (d, J = 8.8 Hz, 2H), 7.48 (d, J = 8.8 Hz, 2H), 7.08 (s, 1H), 6.72 (s, 1H), 3.21 (t, J = 7.6 Hz, 2H), 2.01–1.92 (m, 2H), 1.12 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 154.6, 149.7, 148.8, 144.9, 136.4, 136.1, 129.1, 128.6, 103.4, 97.0, 32.7, 19.4, 13.9; HRMS (ESI) m/z calcd for $C_{15}H_{15}ClN_3^+$ $(M+H)^+$ 272.0949, found: 272.0948.



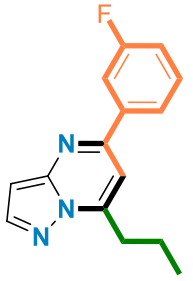
5-(4-bromophenyl)-7-propylpyrazolo[1,5-a]pyrimidine (4d):

Yield 57%; 179 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 75.9-76.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 2.4 Hz, 1H), 7.95 (d, J = 8.8 Hz, 2H), 7.63 (d, J = 8.8 Hz, 2H), 7.07 (s, 1H), 6.72 (d, J = 2.4 Hz, 1H), 3.20 (t, J = 7.6 Hz, 2H), 2.01–1.93 (m, 2H), 1.11 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 154.5, 149.7, 148.7, 144.8, 136.4, 131.9, 128.7, 127.2, 103.2, 97.0, 32.6, 19.4, 13.9; HRMS (ESI) m/z calcd for $C_{15}H_{15}BrN_3^+$ $(M+H)^+$ 316.0444, found: 316.0445.



7-propyl-5-(4-(trifluoromethyl)phenyl)pyrazolo[1,5-a]pyrimidine (4e):

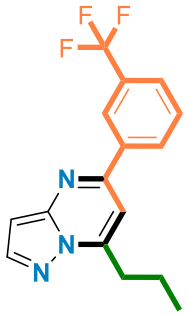
Yield 45%; 137 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 56.3-57.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21–8.17 (m, 3H), 7.76 (d, J = 8.4 Hz, 2H), 7.13 (s, 1H), 6.77 (d, J = 2.5 Hz, 1H), 3.23 (t, J = 7.7 Hz, 2H), 2.03–1.93 (m, J = 7.5 Hz, 2H), 1.13 (t, J = 7.4 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 154.1, 150.0, 148.8, 145.0, 141.0, 131.8 (q, J = 33 Hz), 127.6, 125.8 (q, J = 4 Hz), 124.0 (q, J = 270 Hz), 103.6, 97.4, 32.7, 19.4, 13.9; HRMS (ESI) m/z calcd for $C_{16}H_{15}F_3N_3^+$ $(M+H)^+$ 306.1213, found: 306.1211.



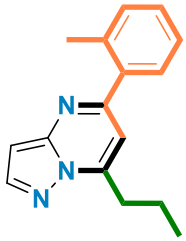
5-(3-fluorophenyl)-7-propylpyrazolo[1,5-a]pyrimidine (4f):

Yield 43%; 110 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 61.5-62.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 2.4 Hz, 1H), 7.87–7.81 (m, 2H), 7.52–7.45 (m, 1H), 7.21–7.16 (m, 1H), 7.10 (s, 1H), 6.74 (d, J = 2.4 Hz, 1H), 3.22 (d, J = 7.6 Hz, 2H), 2.03–1.93 (m, 2H), 1.13 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 163.2 (d, J = 244 Hz), 154.4, 149.8, 148.8, 144.9, 140.0, 139.9 (d, J = 7 Hz), 130.4, (d, J = 8 Hz) 122.8 (d, J = 3 Hz), 117.0 (d, J = 21 Hz), 114.2 (d,

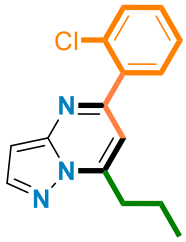
J = 22 Hz) 103.6, 97.2, 32.6, 19.4, 13.9; ^{19}F NMR (377 MHz, $CDCl_3$) δ -112.32; HRMS (ESI) m/z calcd for $C_{15}H_{15}FN_3^+$ $(M+H)^+$ 256.1245, found: 256.1243.



7-propyl-5-(3-(trifluoromethyl)phenyl)pyrazolo[1,5-a]pyrimidine (4g):
Yield 50%; 152 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 50.5-51.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.26 (d, *J* = 8.0 Hz, 1H), 8.16 (d, *J* = 2.4 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* = 8.0 Hz, 1H), 7.12 (s, 1H), 6.75 (d, *J* = 2.0 Hz, 1H), 3.22 (t, *J* = 7.6 Hz, 2H), 2.02–1.93 (m, 2H), 1.12 (t, *J* = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 154.0, 150.0, 148.8, 145.0, 138.4, 131.3 (q, *J* = 32 Hz), 130.4, 129.4, 126.6 (q, *J* = 4 Hz), 124.1(q, *J* = 4 Hz), 124.0 (q, *J* = 271 Hz), 103.36, 97.3, 32.7, 19.5, 13.9; HRMS (ESI) m/z calcd for $C_{16}H_{15}F_3N_3^+$ $(M+H)^+$ 306.1213, found: 306.1211.

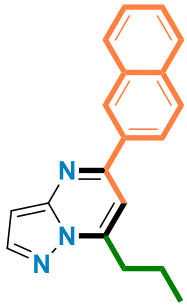


7-propyl-5-(o-tolyl)pyrazolo[1,5-a]pyrimidine (4h):
Yield 44%; 110 mg; yellow solid; column chromatography, silica gel (PE/EA, 15:1); mp 49.4-50.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 2.4 Hz, 1H), 7.49–7.47 (m, 1H), 7.37–7.28 (m, 3H), 6.82 (s, 1H), 6.71 (d, *J* = 2.4 Hz, 1H), 3.21 (t, *J* = 7.6 Hz, 2H), 2.45 (s, 3H), 2.00–1.90 (m, 2H), 1.11 (t, *J* = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.9, 148.9, 148.6, 144.5, 138.8, 135.8, 131.0, 129.3, 129.1, 126.0, 107.4, 96.8, 32.4, 20.3, 19.2, 13.9; HRMS (ESI) m/z calcd for $C_{16}H_{18}N_3^+$ $(M+H)^+$ 252.1495, found: 252.1494.



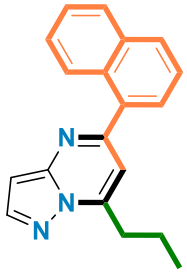
5-(2-chlorophenyl)-7-propylpyrazolo[1,5-a]pyrimidine (4i):
Yield 49%; 133 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 46.9-47.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 2.4 Hz, 1H), 7.68–7.65 (m, 1H), 7.50–7.47 (m, 1H), 7.39–7.37 (m, 2H), 7.05 (s, 1H), 6.75 (d, *J* = 2.4 Hz, 1H), 3.21 (t, *J* = 7.6 Hz, 2H), 1.99–1.90 (m, 2H), 1.10 (t, *J* = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100

MHz, $CDCl_3$) δ 155.9, 148.6, 144.5, 137.8, 132.1, 131.3, 130.4, 130.2, 127.2, 107.8, 97.2, 32.3, 19.2, 13.8; HRMS (ESI) m/z calcd for $C_{15}H_{15}ClN_3^+$ $(M+H)^+$ 272.0949, found: 272.0949.



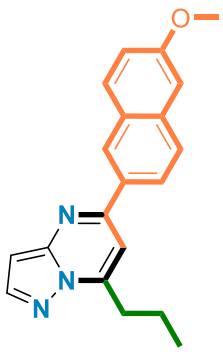
5-(naphthalen-2-yl)-7-propylpyrazolo[1,5-a]pyrimidine (4j):

Yield 61%; 175 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 79.4-80.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 8.8 Hz, 1H), 8.24 (t, J = 6.8 Hz, 1H), 8.15 (s, 1H), 7.97–7.92 (m, 2H), 7.90–7.85 (m, 1H), 7.54–7.51 (m, 2H), 7.26–7.21 (m, 1H), 6.76 (s, 1H), 3.24–3.17 (m, 2H), 2.04–1.92 (m, 2H), 1.16–1.11 (m, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 155.6, 149.4, 148.9, 144.7, 134.9, 134.1, 133.2, 128.8, 128.6, 127.7, 127.13, 127.11, 126.5, 124.3, 103.8, 96.9, 32.6, 19.4, 13.9; HRMS (ESI) m/z calcd for $C_{19}H_{18}N_3^+$ $(M+H)^+$ 288.1495, found: 288.1494.



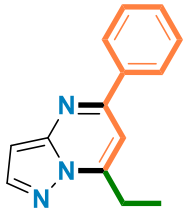
5-(naphthalen-1-yl)-7-propylpyrazolo[1,5-a]pyrimidine (4k):

Yield 53%; 152 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 62.2-62.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22–8.19 (m, 2H), 7.97–7.92 (m, 2H), 7.72–7.70 (m, 1H), 7.58 (t, J = 7.2 Hz, 1H), 7.56–7.51 (m, 2H), 7.00 (s, 1H), 6.79 (d, J = 2.4 Hz, 1H), 3.25 (t, J = 7.6 Hz, 2H), 2.02–1.93 (m, 2H), 1.13 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.0, 149.2, 148.8, 144.7, 136.8, 133.9, 130.7, 129.8, 128.5, 127.6, 126.9, 126.1, 125.22, 125.20, 108.2, 97.1, 32.5, 19.3, 13.9; HRMS (ESI) m/z calcd for $C_{19}H_{18}N_3^+$ $(M+H)^+$ 288.1495, found: 288.1494.



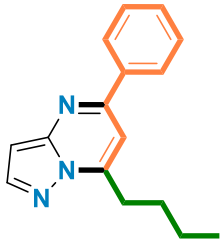
5-(6-methoxynaphthalen-2-yl)-7-propylpyrazolo[1,5-a]pyrimidine (4l):

Yield 56%; 177 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 85.4-86.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.23 (d, J = 8.8 Hz, 1H), 8.14 (d, J = 2.4 Hz, 1H), 7.89–7.85 (m, 2H), 7.22–7.18 (m, 2H), 6.74 (d, J = 2.4 Hz, 1H), 3.96 (s, 3H), 3.24 (t, J = 7.6 Hz, 2H), 2.06–1.97 (m, 2H), 1.15 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.7, 155.9, 149.4, 149.0, 144.7, 135.6, 132.8, 130.4, 128.7, 127.5, 127.0, 124.9, 119.5, 105.7, 103.7, 96.8, 55.4, 32.7, 19.5, 13.9; HRMS (ESI) m/z calcd for $C_{20}H_{20}N_3O^+$ $(M+H)^+$ 318.1601, found: 318.1599.



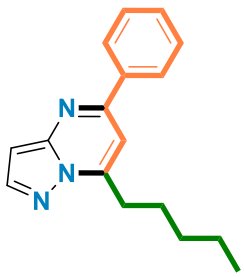
7-ethyl-5-phenylpyrazolo[1,5-a]pyrimidine (5a):

Yield 64%; 143 mg; yellow oil; column chromatography, silica gel (PE/EA, 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 2.4 Hz, 1H), 8.07 (d, J = 7.6 Hz, 2H), 7.51–7.44 (m, 3H), 7.11 (s, 1H), 6.72 (d, J = 2.4 Hz, 1H), 3.25 (q, J = 7.6 Hz, 2H), 1.49 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 155.9, 150.7, 148.8, 144.6, 137.6, 130.1, 128.8, 127.2, 102.8, 96.9, 23.8, 10.3; HRMS (ESI) m/z calcd for $C_{14}H_{14}N_3^+$ $(M+H)^+$ 224.1182, found: 224.1179.



7-butyl-5-phenylpyrazolo[1,5-a]pyrimidine (5b):

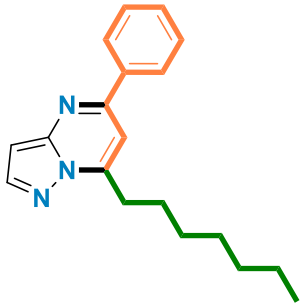
Yield 62%; 156 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 48.9-49.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 2.4 Hz, 1H), 8.11–8.04 (m, 2H), 7.54–7.45 (m, 3H), 7.12 (s, 1H), 6.73 (d, J = 2.4 Hz, 1H), 3.27–3.20 (m, 2H), 1.95–1.87 (m, 2H), 1.58–1.49 (m, 2H), 1.01 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 155.9, 149.8, 148.9, 144.7, 137.7, 130.1, 128.8, 127.3, 103.7, 96.9, 30.4, 28.1, 22.6, 13.8; HRMS (ESI) m/z calcd for $C_{16}H_{18}N_3^+$ $(M+H)^+$ 252.1495, found: 252.1493.



7-pentyl-5-phenylpyrazolo[1,5-a]pyrimidine (5c):

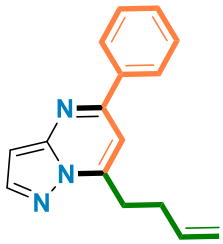
Yield 68%; 180 mg; yellow oil; column chromatography, silica gel (PE/EA, 30:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 2.4 Hz, 1H), 8.09–8.07 (m, 2H), 7.54–7.48 (m, 3H), 7.12 (s, 1H), 6.73 (d, J = 2.4 Hz, 1H), 3.24–3.20 (m, 2H), 1.97–1.89 (m, 2H), 1.53–

1.38 (m, 4H), 0.94 (t, J = 7.2 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 155.9, 149.8, 148.9, 144.7, 137.7, 130.1, 128.9, 127.3, 103.7, 96.9, 31.5, 30.7, 25.7, 22.4, 13.9; HRMS (ESI) m/z calcd for $C_{17}H_{20}N_3^+$ $(M+H)^+$ 266.1652, found: 266.1650.



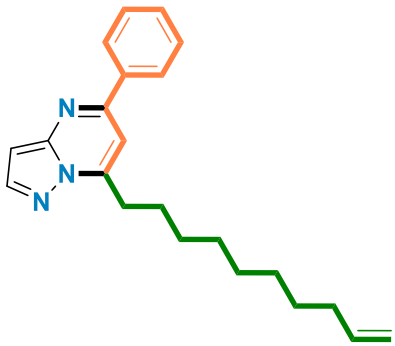
7-heptyl-5-phenylpyrazolo[1,5-a]pyrimidine (5d):

Yield 55%; 161 mg; yellow oil; column chromatography, silica gel (PE/EA, 30:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 2.4 Hz, 1H), 8.03–8.00 (m, 2H), 7.47–7.41 (m, 3H), 7.05 (s, 1H), 6.66 (d, J = 2.4 Hz, 1H), 3.17–3.13 (m, 2H), 1.89–1.82 (m, 2H), 1.47–1.40 (m, 2H), 1.37–1.32 (m, 2H), 1.26–1.23 (m, 3H), 1.21–1.82 (m, 2H), 0.85–0.81 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 155.9, 149.8, 148.9, 144.6, 137.7, 130.1, 128.8, 128.3, 127.2, 125.8, 103.6, 96.9, 31.7, 30.6, 29.3, 29.0, 26.0, 22.6, 14.0; HRMS (ESI) m/z calcd for $C_{19}H_{24}N_3^+$ $(M+H)^+$ 294.1965, found: 294.1964.



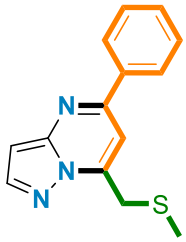
7-(but-3-en-1-yl)-5-phenylpyrazolo[1,5-a]pyrimidine (5e):

Yield 63%; 157 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 63.2-63.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 2.4 Hz, 1H), 8.08–8.05 (m, 2H), 7.53–7.46 (m, 3H), 7.12 (s, 1H), 6.73 (d, J = 2.4 Hz, 1H), 5.98–5.88 (m, 1H), 5.17–5.06 (m, 2H), 3.33 (t, J = 7.6 Hz, 2H), 2.70 (q, J = 7.2 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 155.79, 148.88, 148.64, 144.69, 137.58, 136.29, 130.13, 128.83, 127.22, 116.29, 103.99, 96.96, 30.00, 29.80; HRMS (ESI) m/z calcd for $C_{16}H_{16}N_3^+$ $(M+H)^+$ 250.1339, found: 250.1336.



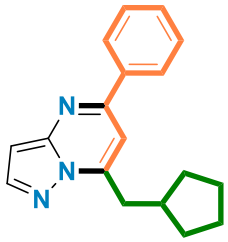
7-(dec-9-en-1-yl)-5-phenylpyrazolo[1,5-a]pyrimidine (5f):

Yield 56%; 186 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 31.9-32.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 2.4 Hz, 1H), 8.09–8.06 (m, 2H), 7.52–7.45 (m, 3H), 7.11 (s, 1H), 6.72 (d, J = 2.4 Hz, 1H), 5.85–5.75 (m, 1H), 5.01–4.91 (m, 2H), 3.21 (t, J = 8.0 Hz, 2H), 2.06–2.01 (m, 2H), 1.95–1.87 (m, 2H), 1.51–1.47 (m, 2H), 1.43–1.36 (m, 3H), 1.32–1.24 (m, 5H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 155.8, 149.7, 148.9, 144.6, 139.1, 137.6, 130.1, 128.8, 127.2, 114.1, 103.6, 96.8, 33.7, 30.6, 29.34, 29.27, 29.2, 29.0, 28.8, 25.9; HRMS (ESI) m/z calcd for $C_{22}H_{28}N_3^+$ $(M+H)^+$334.2278, found: 334.2273.



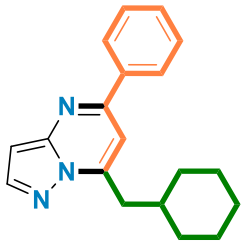
7-((methylthio)methyl)-5-phenylpyrazolo[1,5-a]pyrimidine (5g):

Yield 36%; 92 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 66.2-66.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 2.4 Hz, 1H), 8.09–8.06 (m, 2H), 7.53–7.46 (m, 3H), 7.15 (s, 1H), 6.74 (d, J = 2.4 Hz, 1H), 2.86 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 155.8, 148.8, 145.9, 144.8, 137.5, 130.2, 128.9, 127.3, 105.1, 97.1, 17.5; HRMS (ESI) m/z calcd for $C_{14}H_{14}N_3S^+$ $(M+H)^+$ 256.0903, found: 256.0899.



7-(cyclopentylmethyl)-5-phenylpyrazolo[1,5-a]pyrimidine (5h):

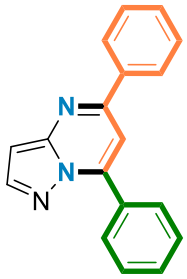
Yield 64%; 177 mg; yellow oil; column chromatography, silica gel (PE/EA, 30:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 2.4 Hz, 1H), 8.09–8.07 (m, 2H), 7.54–7.46 (m, 3H), 7.13 (s, 1H), 6.73 (d, J = 2.4 Hz, 1H), 3.23 (d, J = 7.6 Hz, 2H), 2.66–2.55 (m, 1H), 1.91–1.84 (m, 2H), 1.76–1.68 (m, 2H), 1.64–1.54 (m, 2H), 1.39–1.32 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 154.6, 149.3, 143.7, 142.5, 137. 6, 130.2, 128.9, 127.3, 103.8, 98.2, 37.0, 36.7, 32.8, 25.0; HRMS (ESI) m/z calcd for $C_{18}H_{20}N_3^+$ $(M+H)^+$ 278.1652, found: 278.1650.



7-(cyclohexylmethyl)-5-phenylpyrazolo[1,5-a]pyrimidine (5i):

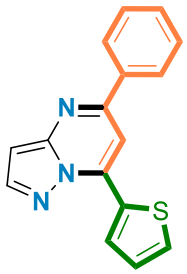
Yield 65%; 189 mg; yellow oil; column chromatography, silica gel (PE/EA, 30:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 2.4 Hz, 1H), 8.09–8.05 (m, 2H), 7.53–7.45 (m, 3H), 7.07 (s, 1H), 6.72 (d, J = 2.4 Hz, 1H), 3.10 (d, J = 7.2 Hz, 2H), 2.14–2.03 (m, 1H),

1.80–1.76 (m, 2H), 1.74–1.64 (m, 3H), 1.30–1.19 (m, 3H), 1.17–1.06 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 155.6, 149.0, 148.4, 144.7, 137.6, 130.1, 128.8, 127.2, 105.0, 96.8, 38.7, 35.0, 33.3, 26.2, 26.0; HRMS (ESI) m/z calcd for $C_{19}H_{22}N_3^+$ $(M+H)^+$ 292.1808, found: 292.1806.



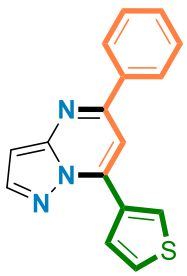
5,7-diphenylpyrazolo[1,5-a]pyrimidine (5j):

Yield 41%; 111 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 49.6-50.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 2.4 Hz, 1H), 8.14–8.12 (m, 2H), 8.07–8.05 (m, 2H), 7.59–7.54 (m, 3H), 7.54–7.49 (m, 3H), 7.33 (s, 1H), 6.81 (d, J = 2.4 Hz, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 156.1, 149.8, 146.7, 145.1, 137.4, 131.4, 130.9, 130.2, 129.2, 128.8, 128.6, 127.2, 105.1, 97.1; HRMS (ESI) m/z calcd for $C_{18}H_{14}N_3^+$ $(M+H)^+$ 272.1182, found: 272.1179.



5-phenyl-7-(thiophen-2-yl)pyrazolo[1,5-a]pyrimidine (5k):

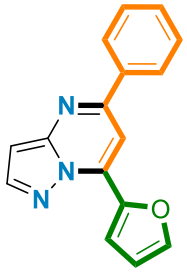
Yield 50%; 138 mg; yellow oil; column chromatography, silica gel (PE/EA, 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34–8.31 (m, 1H), 8.24–8.23 (m, 1H), 8.11–8.08 (m, 2H), 7.68–7,64 (m, 1H), 7.61–7.58 (m, 1H), 7.52–7.46 (m, 3H), 7.24–7.19 (m, 1H), 6.79–6.78 (m, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 155.5, 149.7, 144.67, 144.65, 139.8, 137.49, 137.47, 131.8, 131.64, 131.62, 131.1, 130.0, 128.8, 128.7, 127.44, 127.42, 127.1, 101.49, 101.46, 97.0; HRMS (ESI) m/z calcd for $C_{16}H_{12}N_3S^+$ $(M+H)^+$ 278.0746, found: 278.0744.



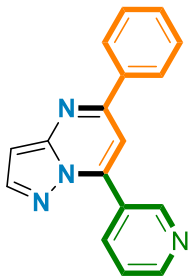
5-phenyl-7-(thiophen-3-yl)pyrazolo[1,5-a]pyrimidine (5l):

Yield 41%; 113 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 88.3-89.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04–9.03 (m, 1H), 8.23 (d, J = 2.4 Hz, 1H), 8.14–8.12 (m, 2H), 7.87 (d, J = 5.2 Hz, 1H), 7.55–7.48 (m, 5H), 6.81 (d, J = 2.4

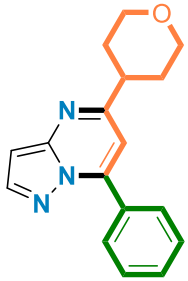
Hz, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 155.9, 150.1, 145.0, 140.9, 137.7, 131.3, 131.2, 130.2, 128.9, 127.2, 127.0, 126.1, 103.4, 97.1; HRMS (ESI) m/z calcd for $C_{16}H_{12}N_3S^+$ $(M+H)^+$ 278.0746, found: 278.0745.



7-(furan-2-yl)-5-phenylpyrazolo[1,5-a]pyrimidine (5m):
Yield 37%; 96 mg; yellow oil; column chromatography, silica gel (PE/EA, 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24–8.23 (m, 2H), 8.18–8.15 (m, 2H), 7.82 (s, 1H), 7.73–7.72 (m, 1H), 7.56–7.48 (m, 3H), 6.80 (d, J = 2.4, 1H), 6.74–6.72 (m, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 149.7, 145.4, 145.1, 144.4, 137.7, 135.8, 130.2, 128.9, 127.3, 119.2, 113.0, 100.2, 97.0; HRMS (ESI) m/z calcd for $C_{16}H_{12}N_3O^+$ $(M+H)^+$ 262.0975, found: 262.0973.

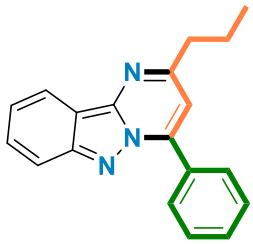


5-phenyl-7-(pyridin-3-yl)pyrazolo[1,5-a]pyrimidine (5n):
Yield 32%; 87 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 162.9-163.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 2.4 Hz, 1H), 8.14–8.11 (m, 2H), 8.07–8.04 (m, 2H), 7.61–7.56 (m, 3H), 7.54–7.49 (m, 3H), 7.33 (s, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 156.1, 149.8, 146.7, 145.1, 137.4, 131.4, 130.9, 130.2, 129.2, 128.8, 128.6, 127.2, 105.1, 97.1; HRMS (ESI) m/z calcd for $C_{17}H_{13}N_4^+$ $(M+H)^+$ 273.1135, found: 273.1133.



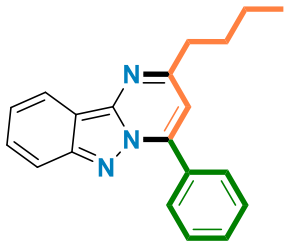
7-phenyl-5-(tetrahydro-2H-pyran-4-yl)pyrazolo[1,5-a]pyrimidine (6a):
Yield 46%; 128 mg; yellow oil; column chromatography, silica gel (PE/EA, 30:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 2.4 Hz, 1H), 8.01–7.98 (m, 2H), 7.57–7.55 (m, 3H), 6.79 (s, 1H), 6.68 (d, J = 2.4 Hz, 1H), 4.14–4.10 (m, 2H), 3.60–3.54 (m, 2H), 3.07–3.02 (m, 1H), 2.06–1.91 (m, 4H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 164.0, 149.5,

146.8, 144.8, 131.3, 130.9, 129.1, 128.7, 106.0, 96.2, 67.8, 43.5, 31.6; HRMS (ESI) m/z calcd for $C_{17}H_{18}N_3O^+$ $(M+H)^+$ 280.1444, found: 280.1441.



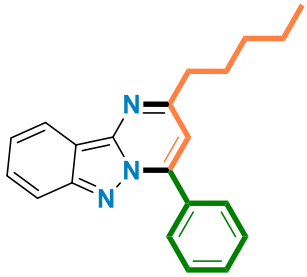
4-phenyl-2-propylpyrimido[1,2-b]indazole (6b):

Yield 53%; 152 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 132.5-132.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 8.4 Hz, 1H), 8.17–8.15 (m, 2H), 7.82 (d, J = 8.8 Hz, 1H), 7.63–7.56 (m, 4H), 7.26 (t, J = 7.6 Hz, 1H), 7.17 (s, 1H), 3.01 (t, J = 7.6 Hz, 2H), 1.98–1.89 (m, 2H), 1.08 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.3, 151.1, 144.9, 144.7, 131.5, 130.9, 129.6, 129.3, 128.7, 120.9, 120.2, 116.3, 112.9, 111.5, 40.2, 22.8, 13.9; HRMS (ESI) m/z calcd for $C_{19}H_{18}N_3^+$ $(M+H)^+$ 288.1495, found: 288.1493.



2-butyl-4-phenylpyrimido[1,2-b]indazole (6c):

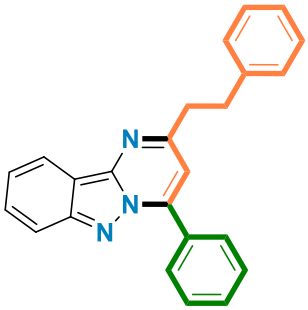
Yield 32%; 96 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 129.3-129.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 8.4 Hz, 1H), 8.20–8.14 (m, 2H), 7.82 (d, J = 8.8 Hz, 1H), 7.64–7.56 (m, 4H), 7.28–7.24 (m, 2H), 7.17 (s, 1H), 3.04 (t, J = 8.0 Hz, 2H), 1.93–1.85 (m, 2H), 1.55–1,46 (m, 2H), 1.01 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.5, 151.2, 144.9, 144.7, 131.6, 130.9, 129.6, 129.4, 128.8, 121.0, 120.2, 116.3, 113.0, 111.5, 38.0, 31.7, 22.6, 13.9; HRMS (ESI) m/z calcd for $C_{20}H_{20}N_3^+$ $(M+H)^+$ 302.1652, found: 302.1650.



2-pentyl-4-phenylpyrimido[1,2-b]indazole (6d):

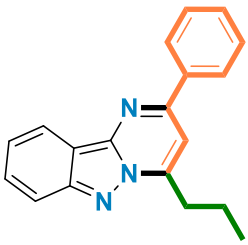
Yield 22%; 69 mg; yellow oil; column chromatography, silica gel (PE/EA, 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 8.4 Hz, 1H), 8.20–8.14 (m, 2H), 7.82 (d, J = 8.8 Hz, 1H), 7.64–7.56 (m, 3H), 7.28–7.24 (m, 2H), 7.17 (s, 1H), 3.03 (t, J = 8.0 Hz, 2H), 1.94–1.85 (m, 2H), 1.55–1.46 (m, 4H), 0.94 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.5, 151.2, 144.9, 144.7, 131.6, 130.9, 129.6, 129.4, 128.8,

121.0, 120.2, 116.3, 112.9, 111.5, 38.3, 31.6, 29.2, 22.5, 14.0; HRMS (ESI) m/z calcd for $C_{21}H_{22}N_3^+$ $(M+H)^+$ 316.1808, found: 316.1805.



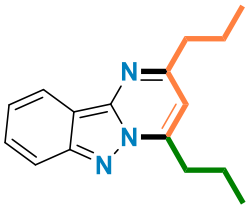
2-phenethyl-4-phenylpyrimido[1,2-b]indazole (6e):

Yield 44%; 154 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 160.1-160.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, J = 8.4, 1H), 8.10–8.07 (m, 2H), 7.84 (d, J = 8.8, 1H), 7.63–7.56 (m, 4H), 7.34–7.21 (m, 6H), 7.02 (s, 1H), 3.38–3.34 (m, 2H), 3.27–3.23 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.0, 151.2, 144.8, 140.9, 131.5, 130.9, 129.6, 129.4, 128.7, 128.6, 128.5, 126.2, 121.0, 120.4, 116.3, 113.0, 111.8, 39.8, 35.3; HRMS (ESI) m/z calcd for $C_{24}H_{20}N_3^+$ $(M+H)^+$ 350.1652, found: 350.1650.



2-phenyl-4-propylpyrimido[1,2-b]indazole (6f):

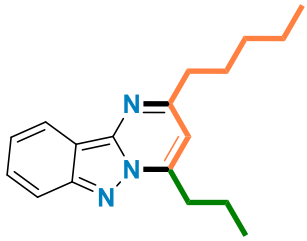
Yield 64%; 184 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 138.6-139.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, J = 8.4 Hz, 1H), 8.21 (d, J = 7.6 Hz, 2H), 7.86 (d, J = 8.8 Hz, 1H), 7.61 (t, J = 7.6 Hz, 1H), 7.56–7.46 (m, 4H), 7.27 (t, J = 7.6 Hz, 1H), 3.36 (t, J = 7.6 Hz, 2H), 2.09–2.00 (m, 2H), 1.15 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 152.3, 151.2, 148.2, 143.9, 137.4, 130.0, 129.8, 128.9, 127.2, 121.2, 120.4, 116.2, 114.0, 106.9, 32.9, 19.0, 13.9; HRMS (ESI) m/z calcd for $C_{19}H_{18}N_3^+$ $(M+H)^+$ 288.1495, found: 288.1494.



2,4-dipropylpyrimido[1,2-b]indazole (6g):

Yield 33%; 83 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 46.3-47.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 8.4 Hz, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.61–7.57 (m, 1H), 7.26–7.22 (m, 2H), 6.96 (s, 1H), 3.33 (t, J = 7.6 Hz, 2H), 2.96 (t, J = 7.6 Hz, 2H), 2.06–1.96 (m, 2H), 1.94–1.85 (m, 2H), 1.13 (t, J = 7.6 Hz, 3H), 1.05 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.1, 151.0, 147.9, 143.8,

129.5, 121.0, 120.0, 116.0, 113.1, 110.0, 40.2, 32.7, 22.9, 19.0, 13.89, 13.87; HRMS (ESI) m/z calcd for $C_{16}H_{20}N_3^+$ $(M+H)^+$ 254.1652, found: 254.1650.



2-pentyl-4-propylpyrimido[1,2-b]indazole (6h):

Yield 32%; 90 mg; yellow oil; column chromatography, silica gel (PE/EA, 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 8.4 Hz, 1H), 7.83 (d, J = 8.8 Hz, 1H), 7.57 (t, J = 7.6 Hz, 1H), 7.22 (t, J = 6.4 Hz, 1H), 6.91 (s, 1H), 3.29 (t, J = 7.6 Hz, 2H), 2.94 (t, J = 6.8 Hz, 2H), 2.03–1.93 (m, 2H), 1.88–1.80 (m, 2H), 1.43–1.38 (m, 2H), 1.29–1.25 (m, 2H), 0.94–0.89 (m, 3H), 0.93–0.86 (m, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.3, 150.9, 147.8, 143.6, 129.4, 121.0, 119.9, 115.9, 113.1, 109.9, 38.2, 32.6, 31.5, 29.2, 22.4, 18.9, 13.9, 13.8; HRMS (ESI) m/z calcd for $C_{18}H_{24}N_3^+$ $(M+H)^+$ 282.1965, found: 282.1959.

5. Crystallographic data and molecular structure of 4g

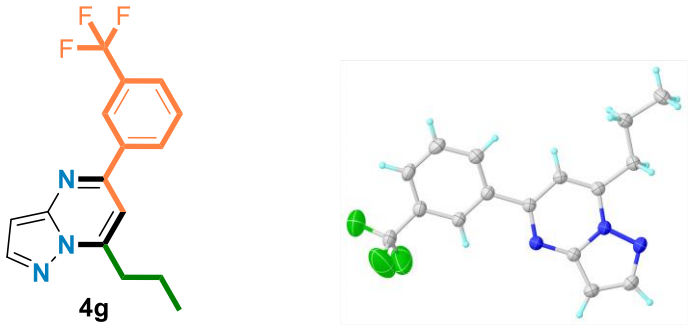


Figure S1. X-ray crystal structure of **4g** thermal ellipsoids shown at 50% probability level. Sample preparation: 20 mg of **4g** was dissolved in 5 ml DCM at room temperature for slow evaporation about a week. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX II diffractometer with Mo Kα radiation (0.71073 Å) at room temperature. Crystal Data for Compound **4g**: CCDC 2407478 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Datablock: mo230825a

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell: a=26.52(5) b=17.03(3) c=15.65(4)
alpha=90 beta=124.81(5) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	5803(21)	5803(21)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C16 H14 F3 N3	C16 H14 F3 N3
Sum formula	C16 H14 F3 N3	C16 H14 F3 N3
Mr	305.30	305.30
Dx,g cm-3	1.398	1.398
Z	16	16
Mu (mm-1)	0.112	0.112
F000	2528.0	2528.0
F000'	2529.45	
h,k,lmax	37,24,22	37,23,22
Nref	8782	8229
Tmin,Tmax	0.983,0.987	0.866,1.000
Tmin'	0.983	

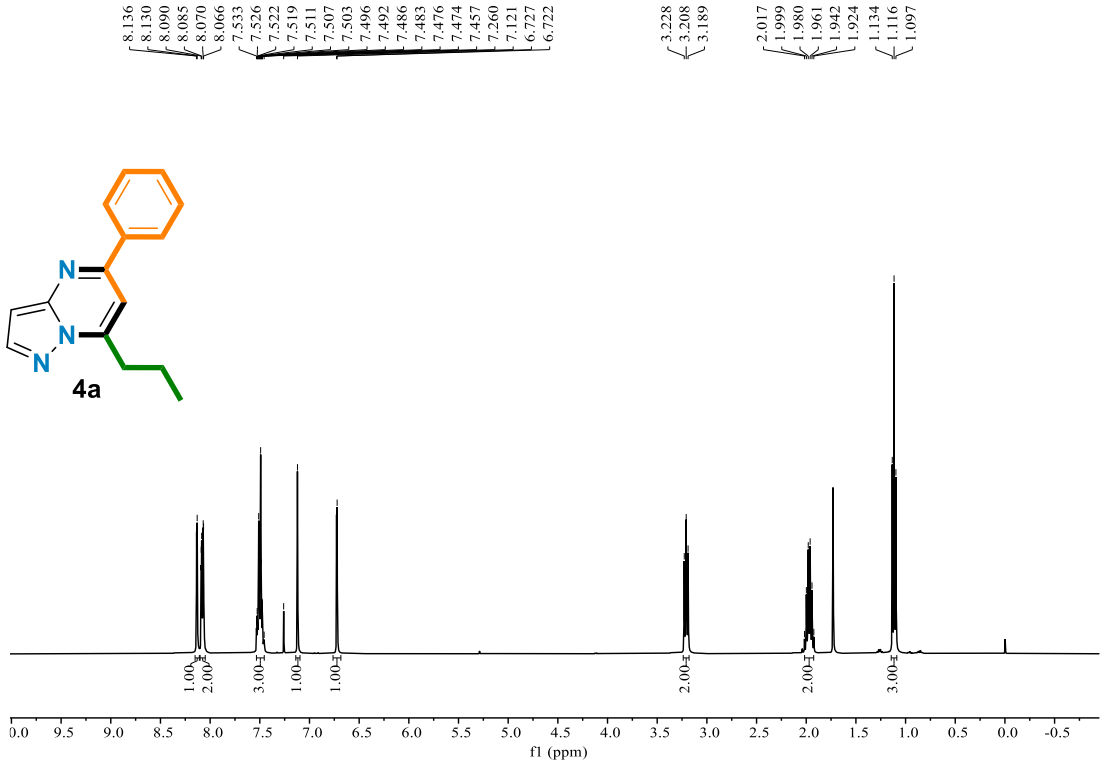
Correction method= # Reported T Limits: Tmin=0.866 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.937 Theta(max)= 30.398

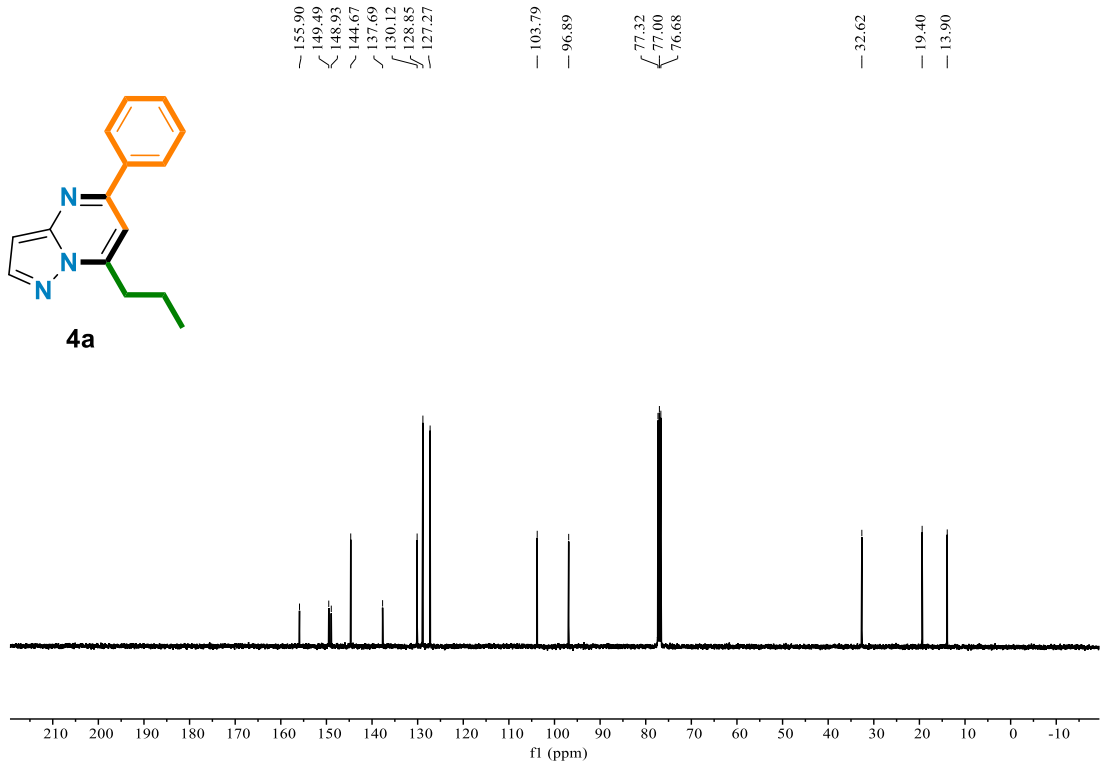
R(reflections)= 0.0513(4743) wR2(reflections)= 0.1485(8229)

S = 1.016 Npar= 427

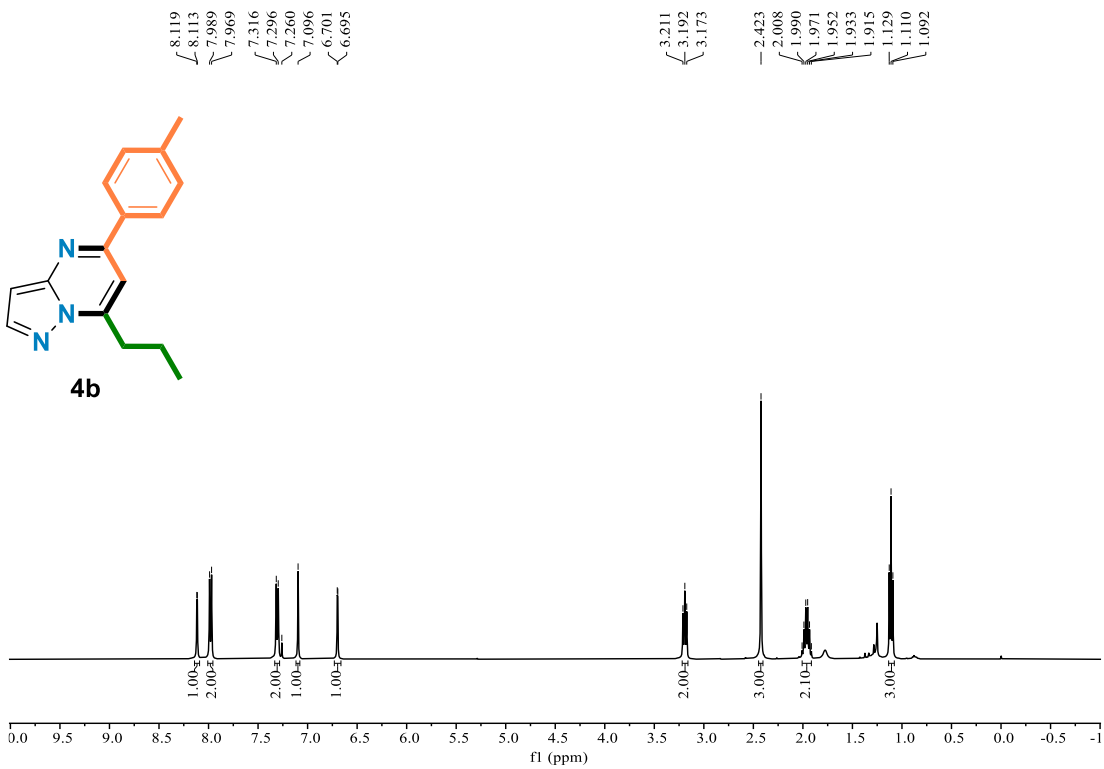
6. ^{1}H and $^{13}C\{^{1}H\}$, $^{19}F\{^{1}H\}$ NMR spectra of compounds 4, 5, 6



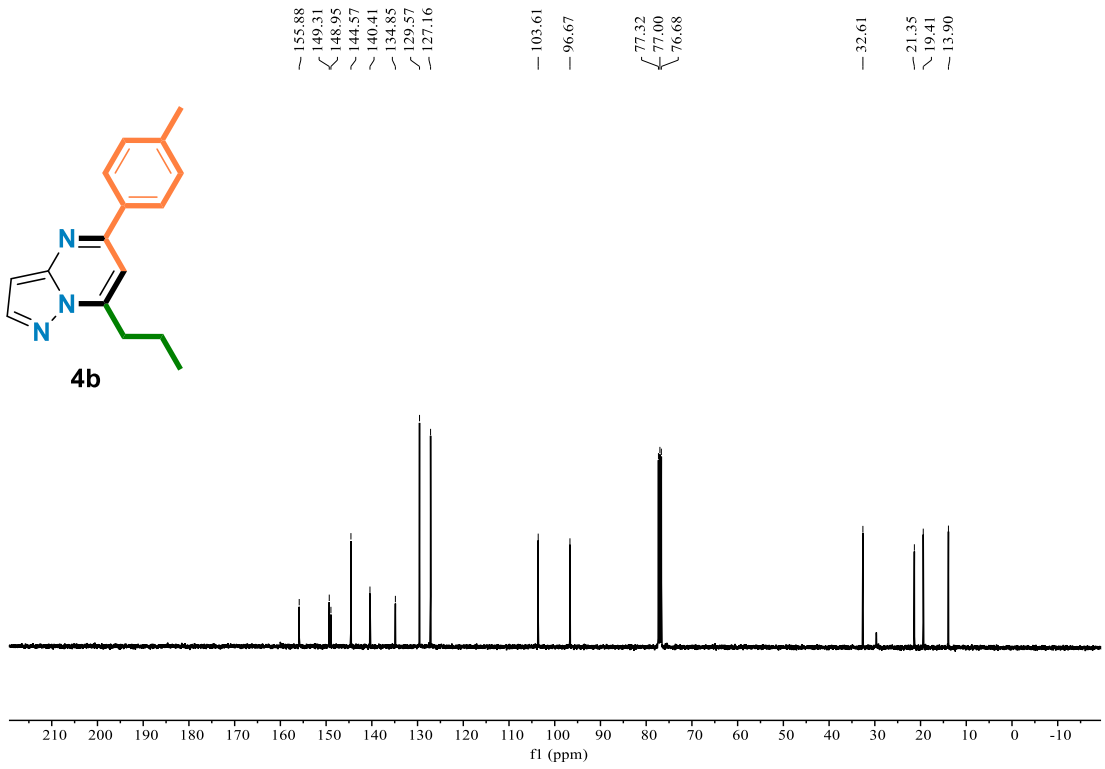
^{1}H NMR Spectrum of Compound **4a** (400 MHz, $CDCl_3$)



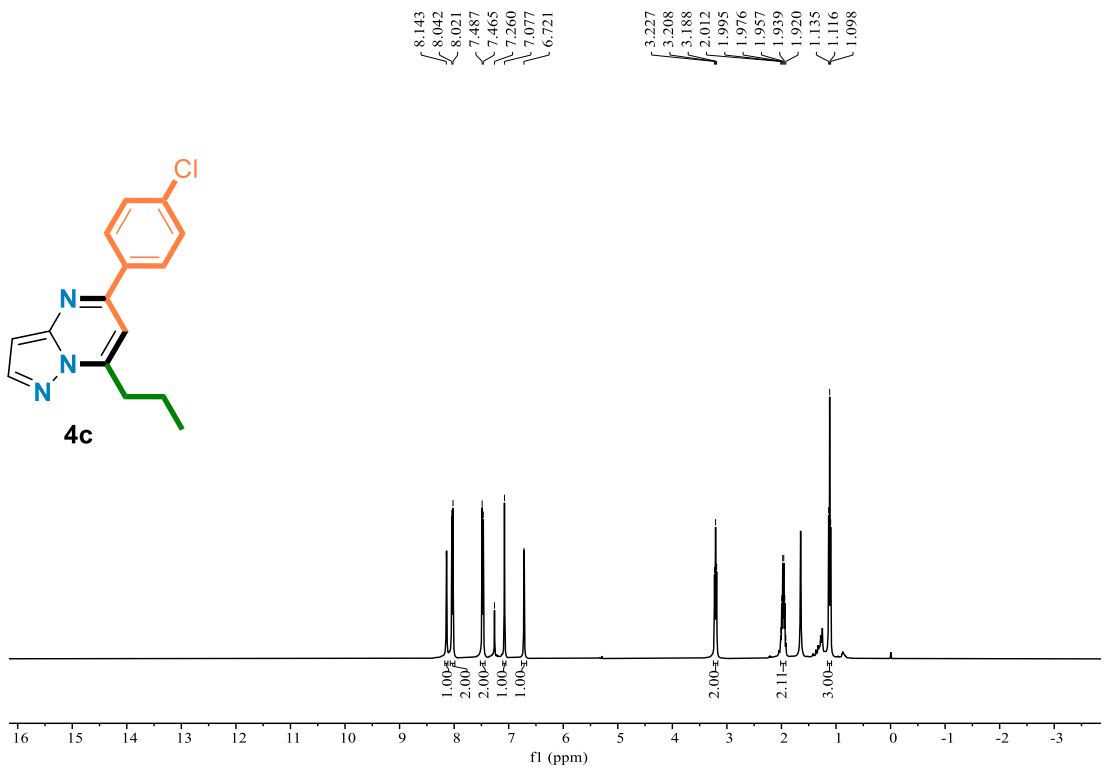
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **4a** (100 MHz, $CDCl_3$)



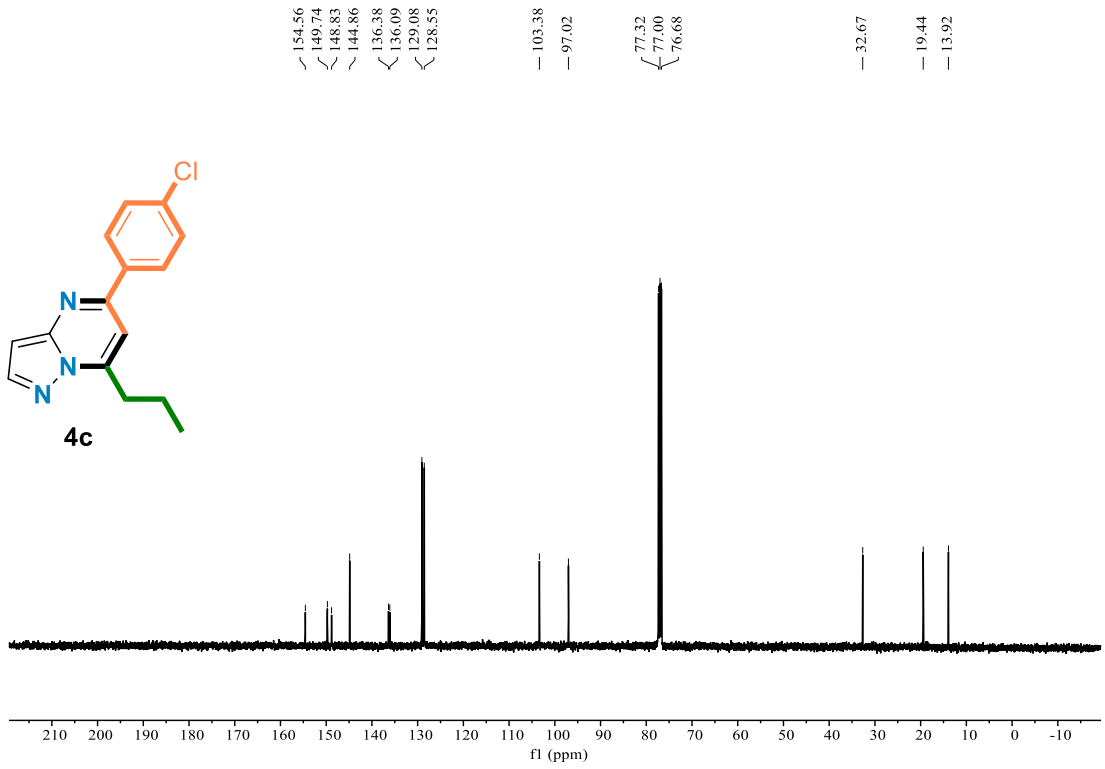
^{1}H NMR Spectrum of Compound **4b** (400 MHz, $CDCl_3$)



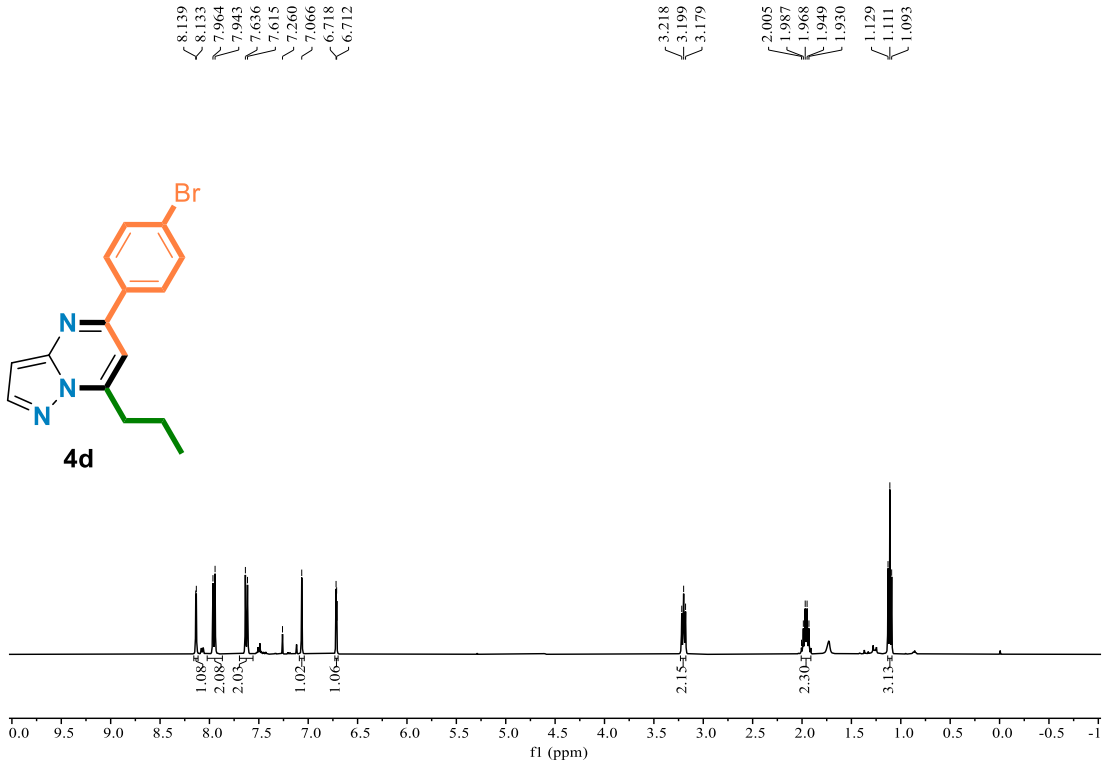
^{13}C{^{1}H} NMR Spectrum of Compound **4b** (100 MHz, $CDCl_3$)



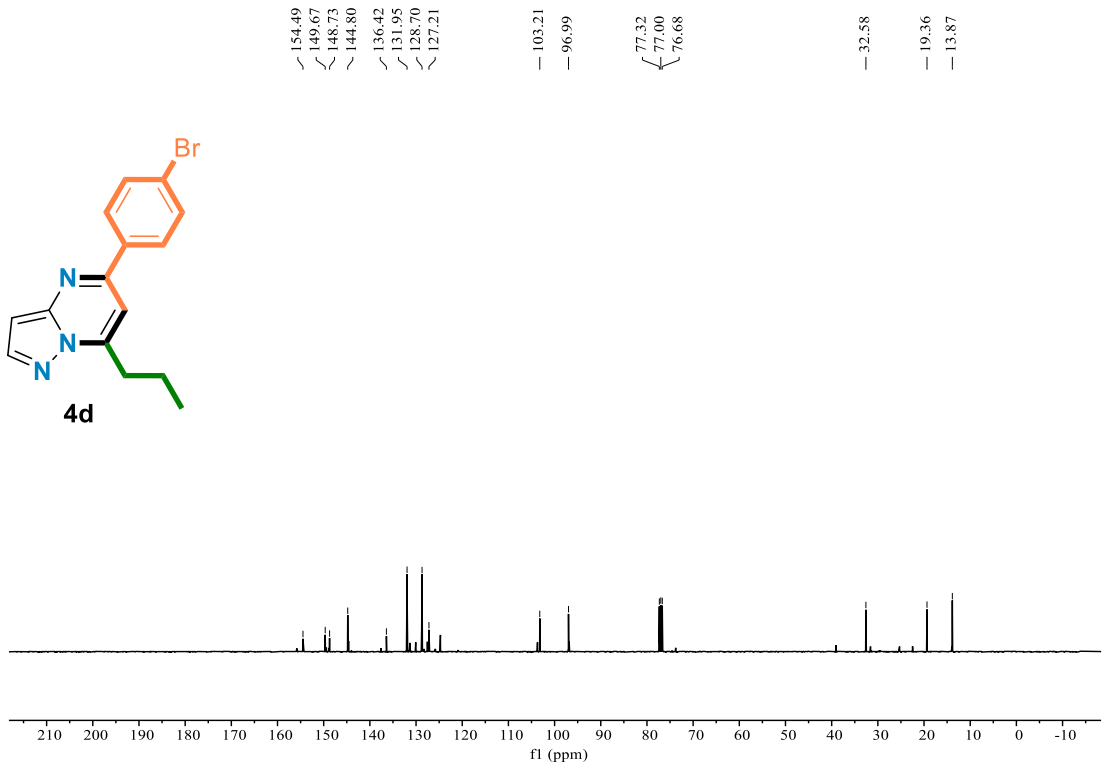
^{1}H NMR Spectrum of Compound **4c** (400 MHz, $CDCl_3$)



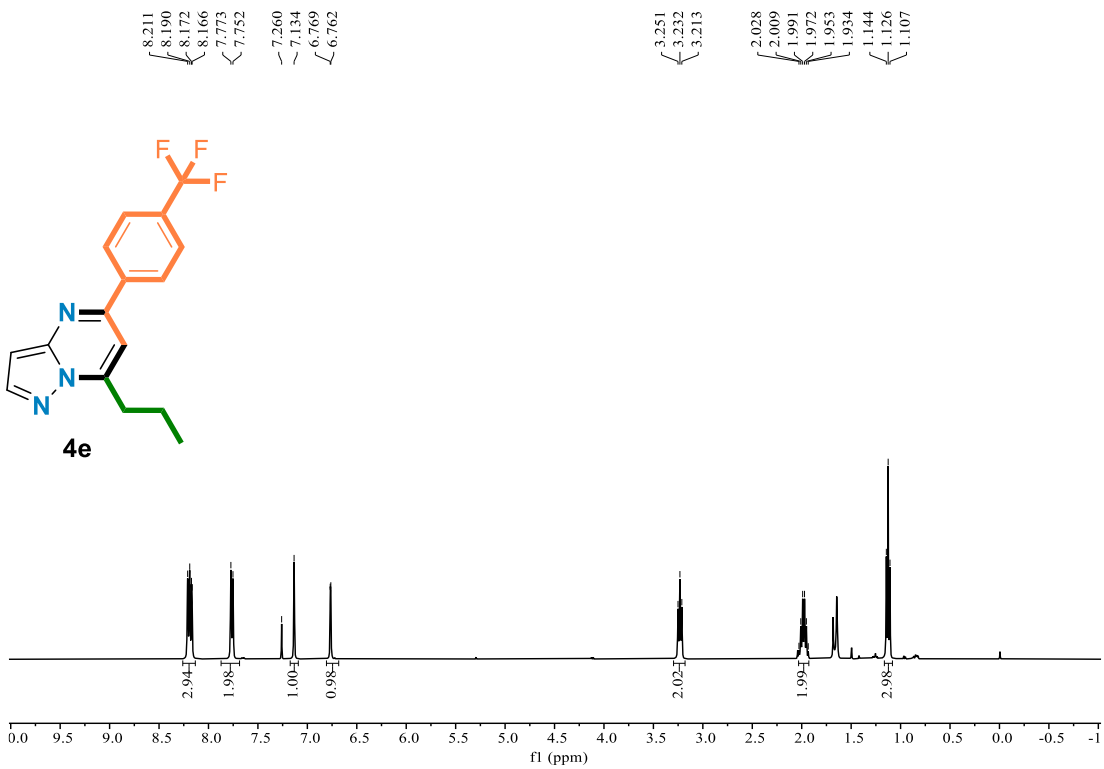
^{13}C{^{1}H} NMR Spectrum of Compound **4c** (100 MHz, $CDCl_3$)



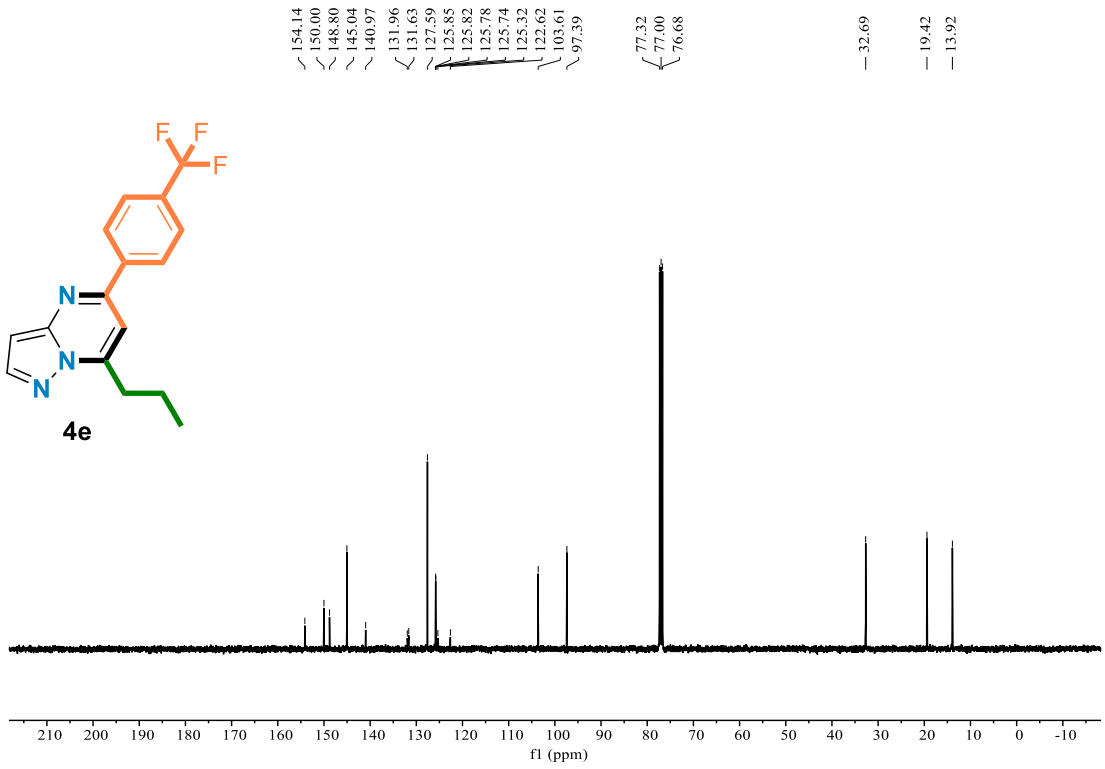
^{1}H NMR Spectrum of Compound **4d** (400 MHz, $CDCl_3$)



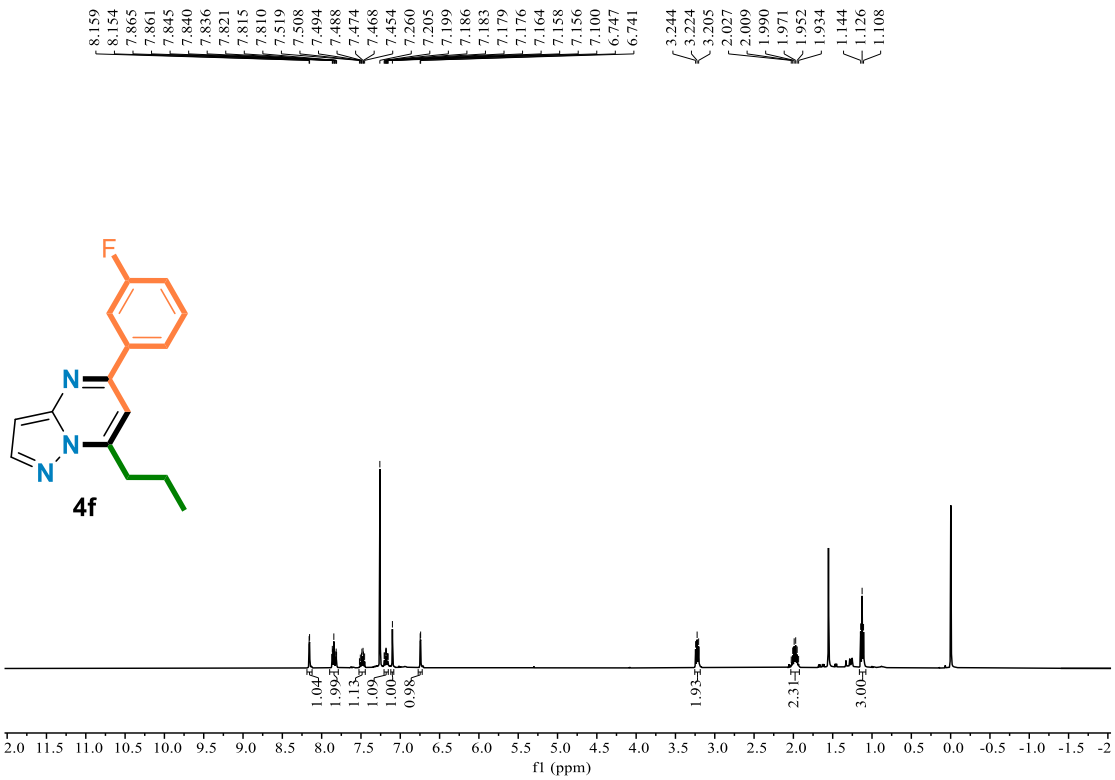
^{13}C{^{1}H} NMR Spectrum of Compound **4d** (100 MHz, $CDCl_3$)



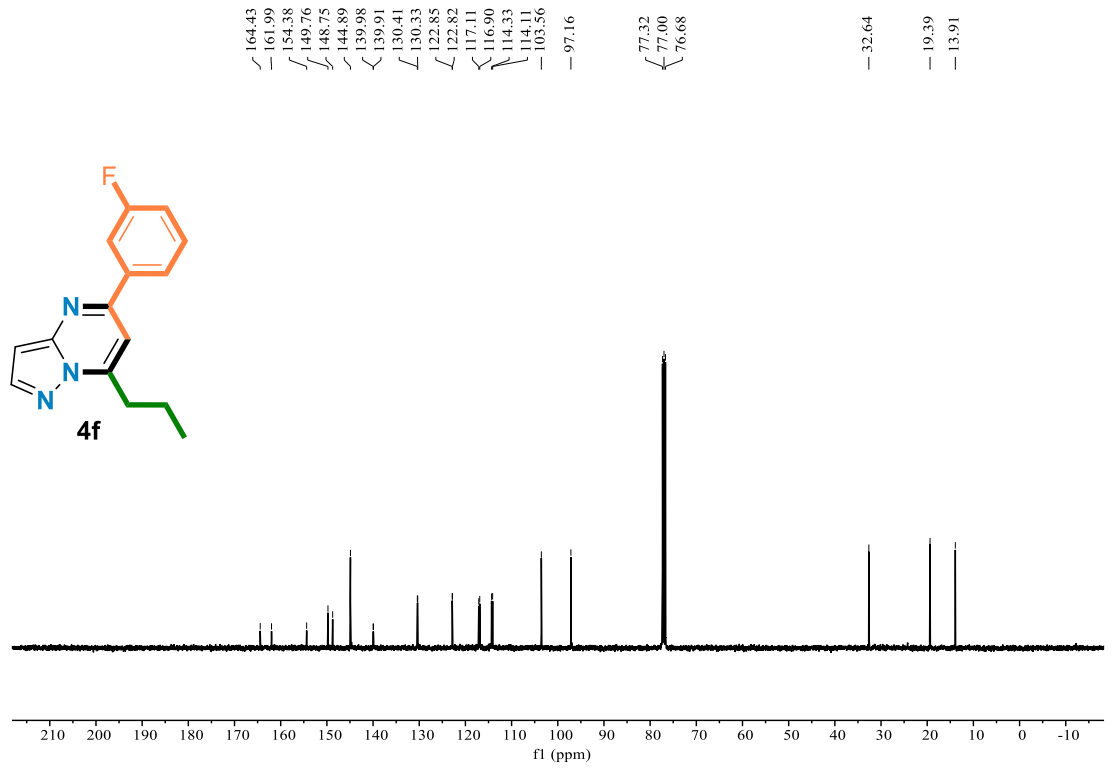
^{1}H NMR Spectrum of Compound **4e** (400 MHz, $CDCl_3$)



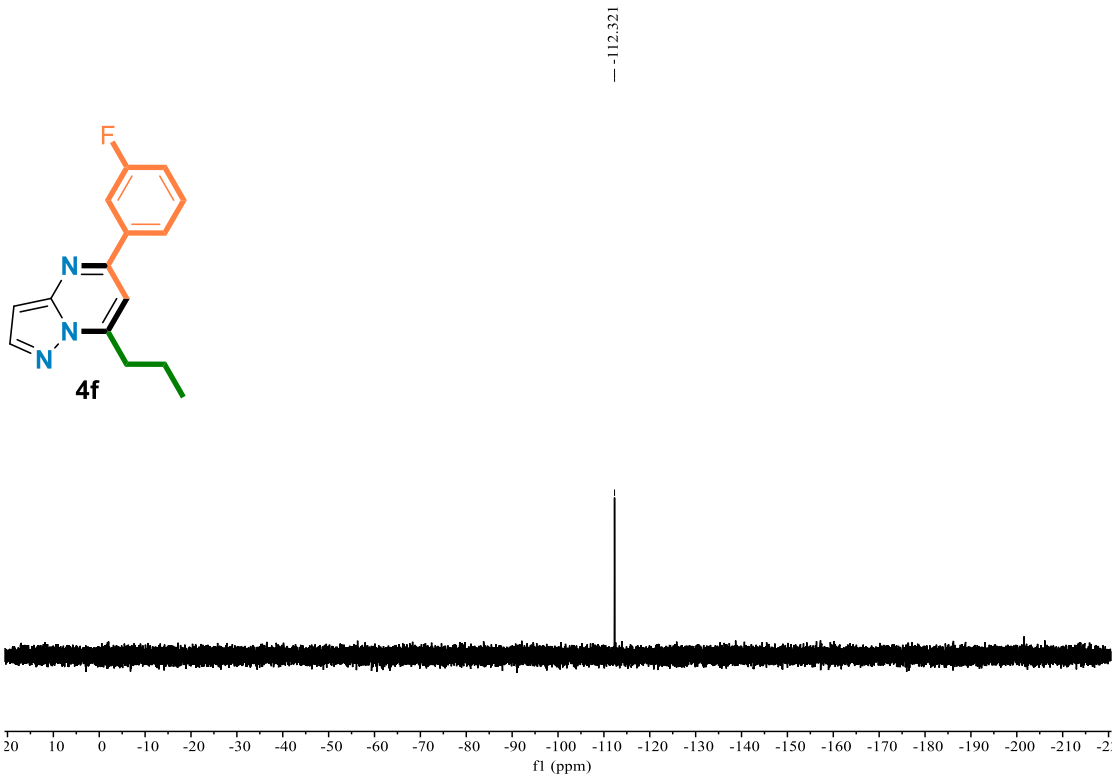
^{13}C{^{1}H} NMR Spectrum of Compound **4e** (100 MHz, $CDCl_3$)



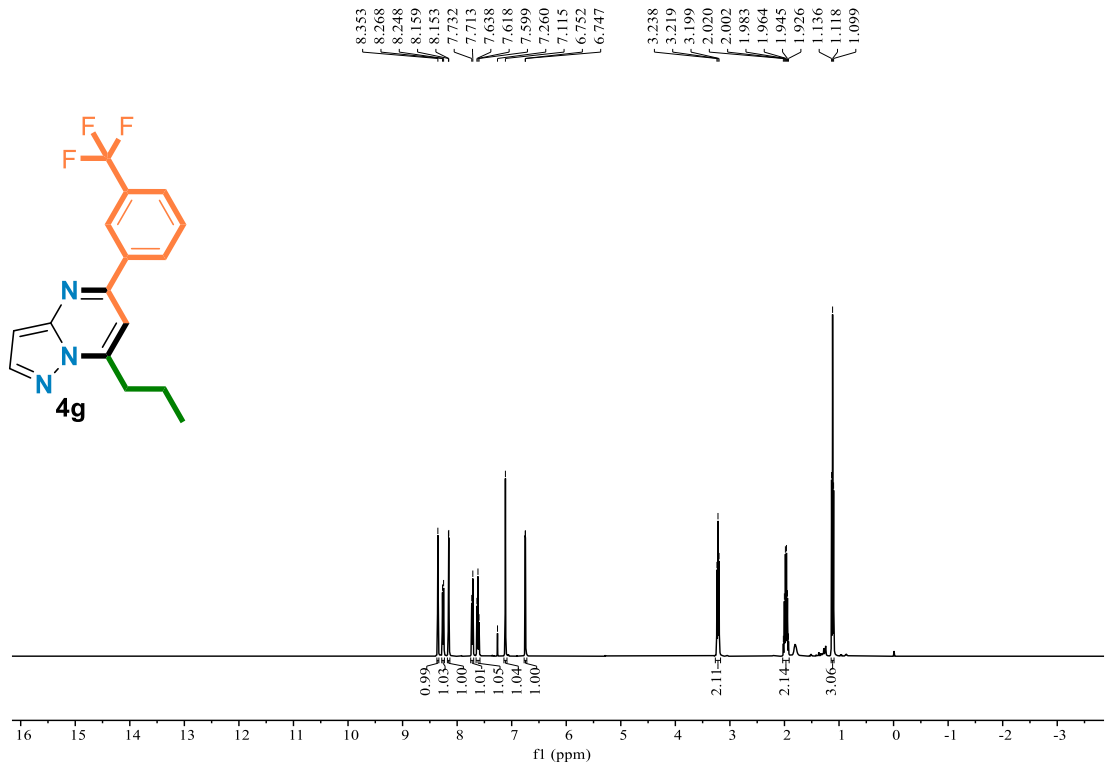
^{1}H NMR Spectrum of Compound **4f** (400 MHz, $CDCl_3$)



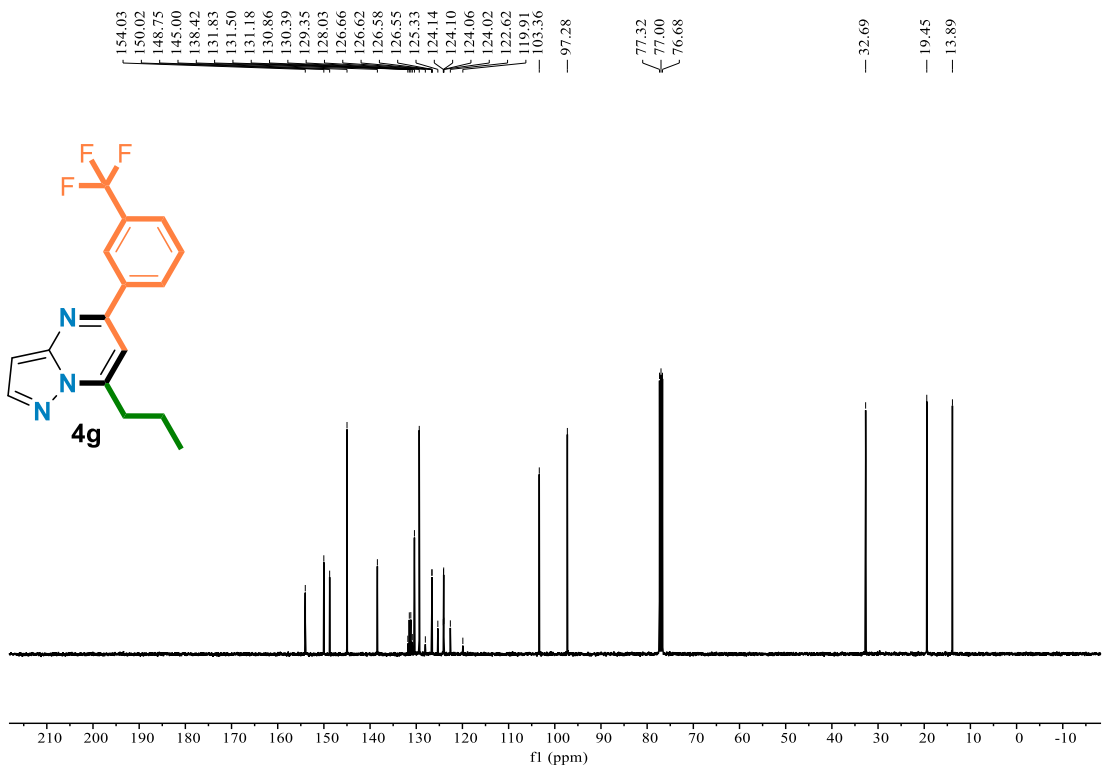
^{13}C{^{1}H} NMR Spectrum of Compound **4f** (100 MHz, $CDCl_3$)



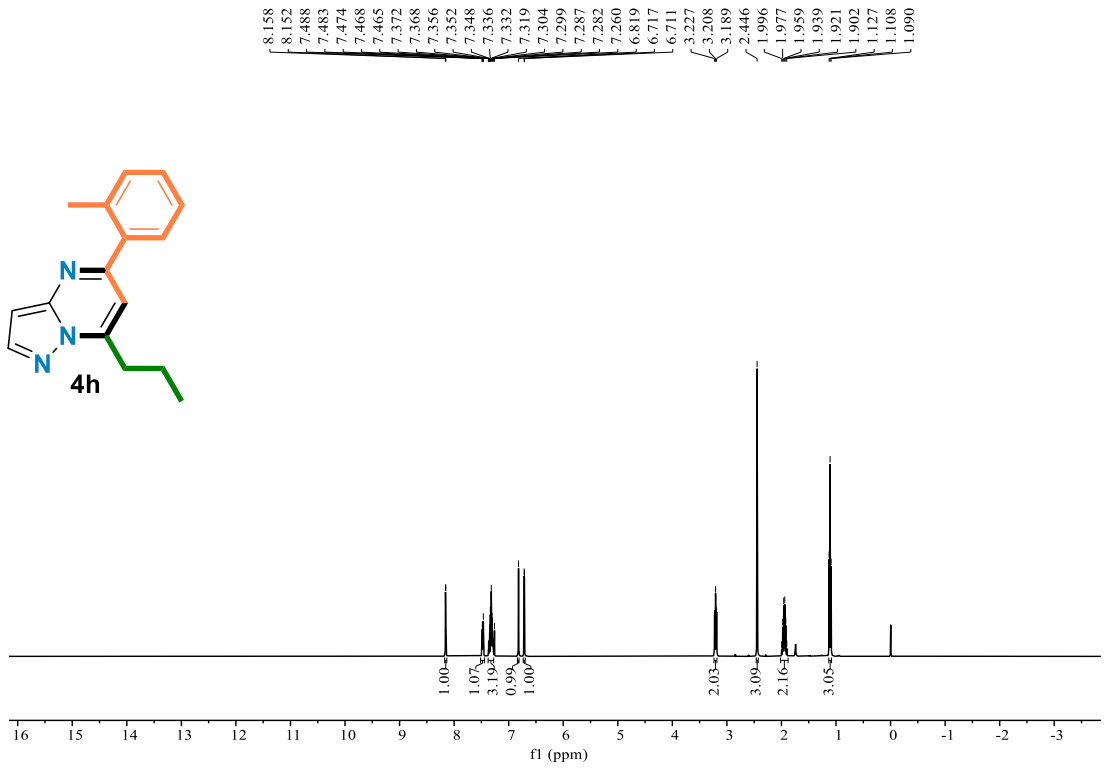
^{19}F NMR Spectrum of Compound **4f** (377 MHz, $CDCl_3$)



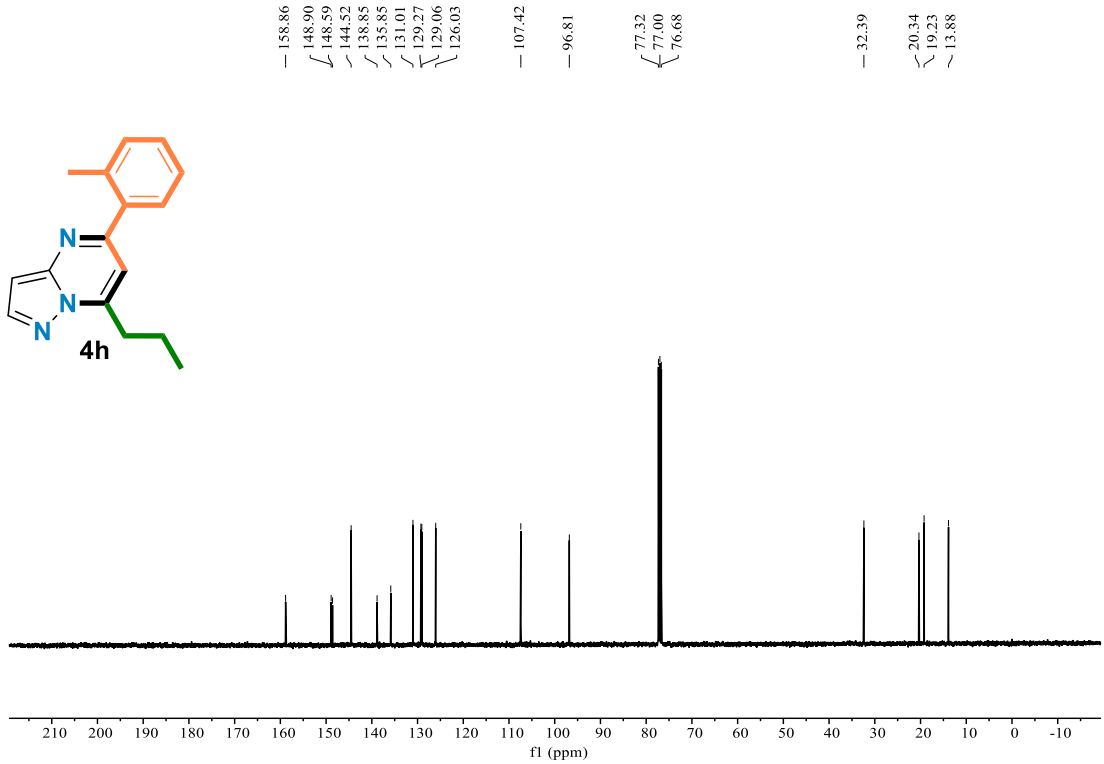
^{1}H NMR Spectrum of Compound **4g** (400 MHz, $CDCl_3$)



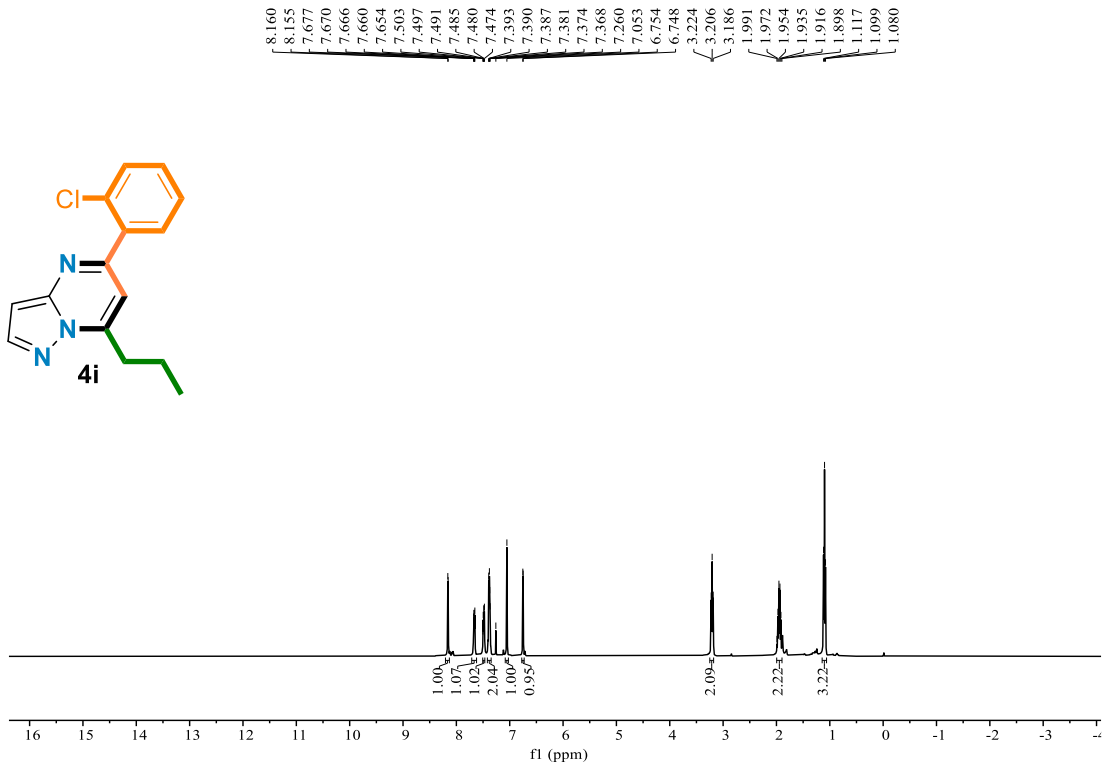
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **4g** (100 MHz, $CDCl_3$)



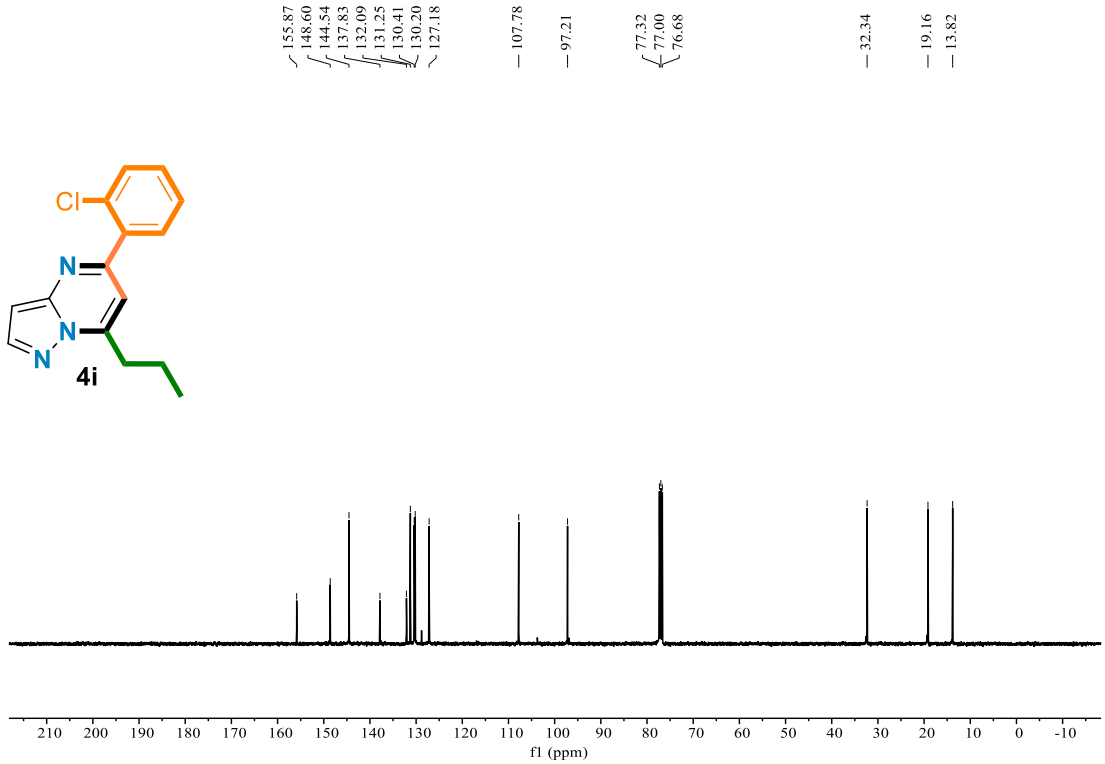
^{1}H NMR Spectrum of Compound **4h** (400 MHz, $CDCl_3$)



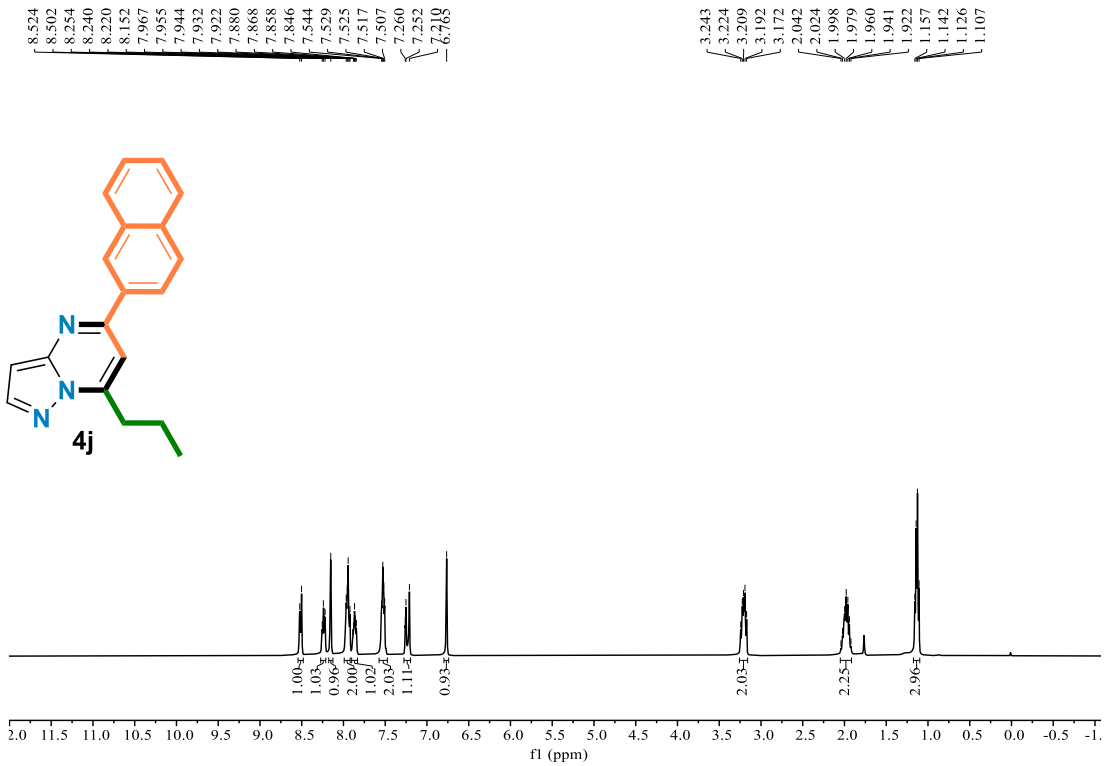
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **4h** (100 MHz, $CDCl_3$)



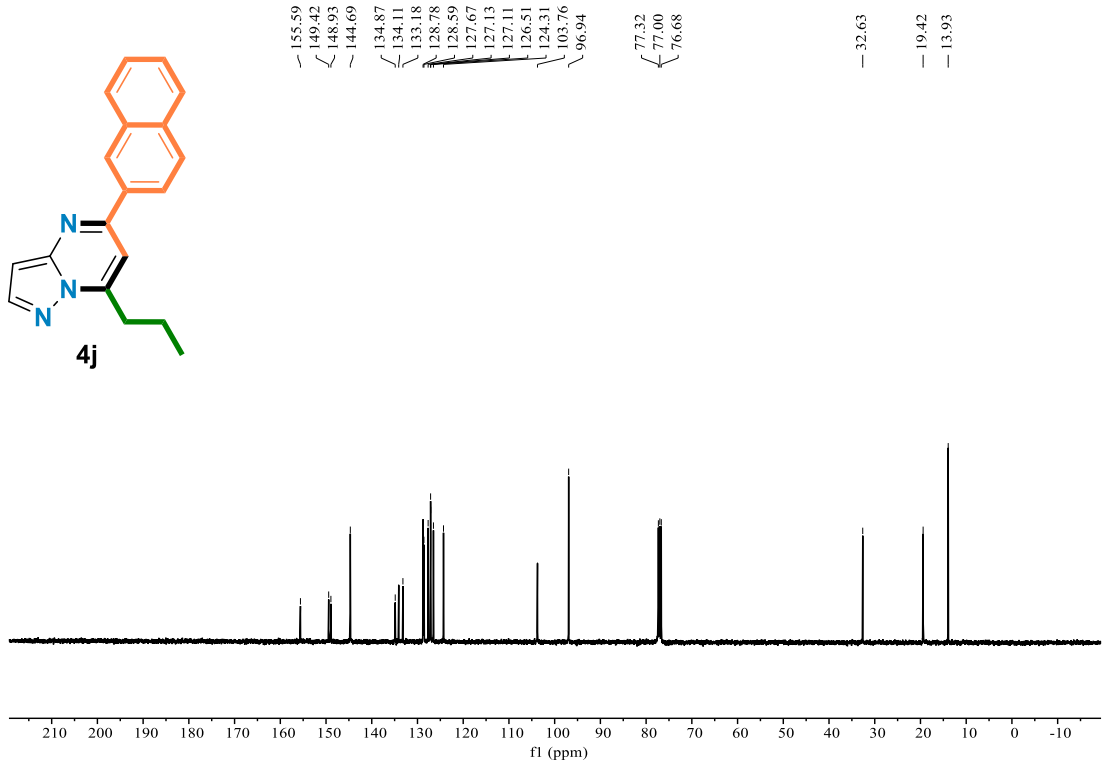
^{1}H NMR Spectrum of Compound **4i** (400 MHz, $CDCl_3$)



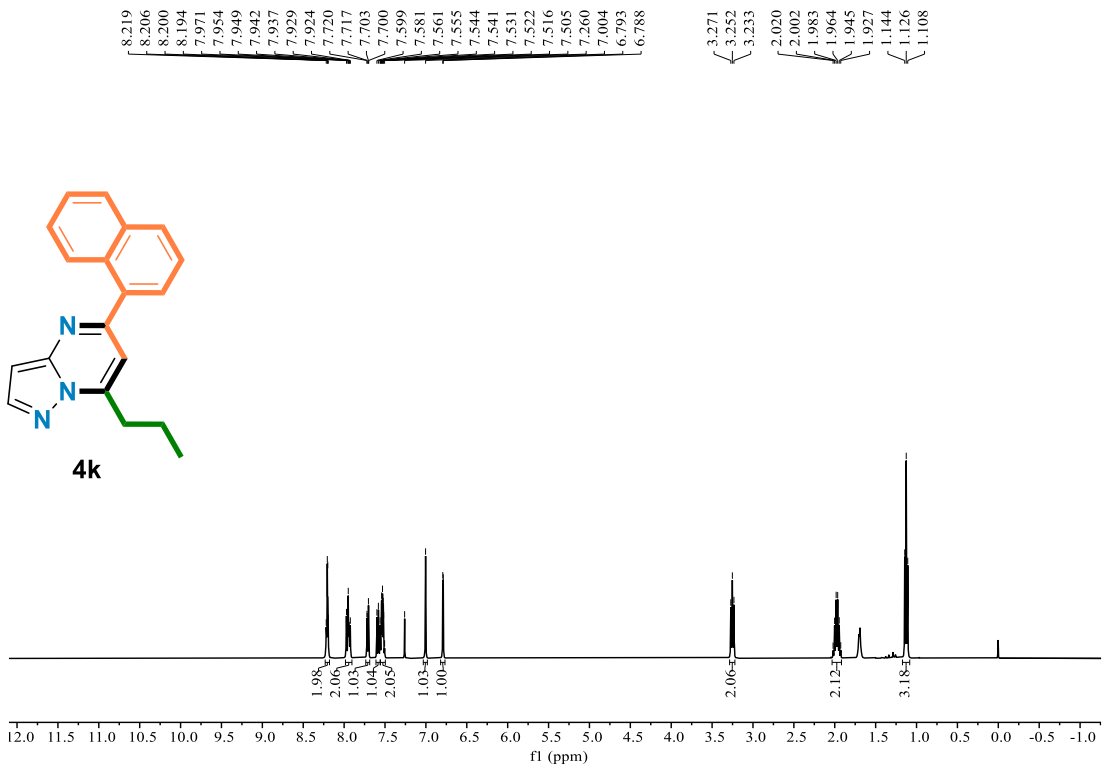
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **4i** (100 MHz, $CDCl_3$)



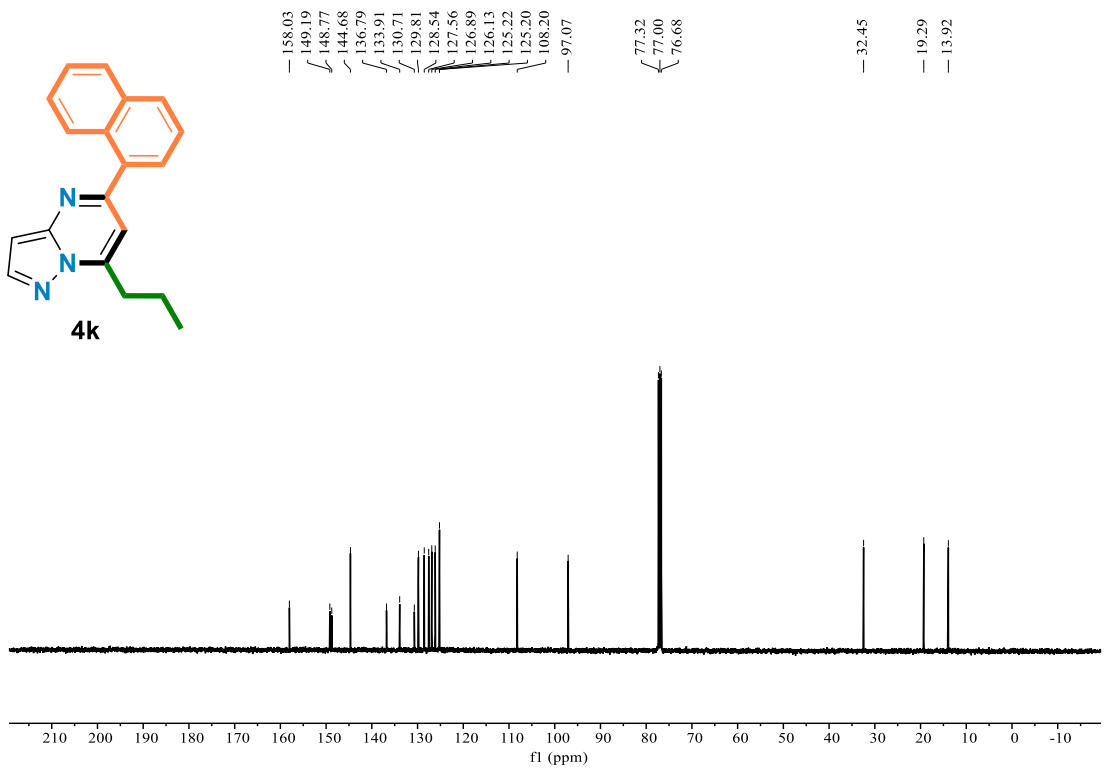
^{1}H NMR Spectrum of Compound **4j** (400 MHz, $CDCl_3$)



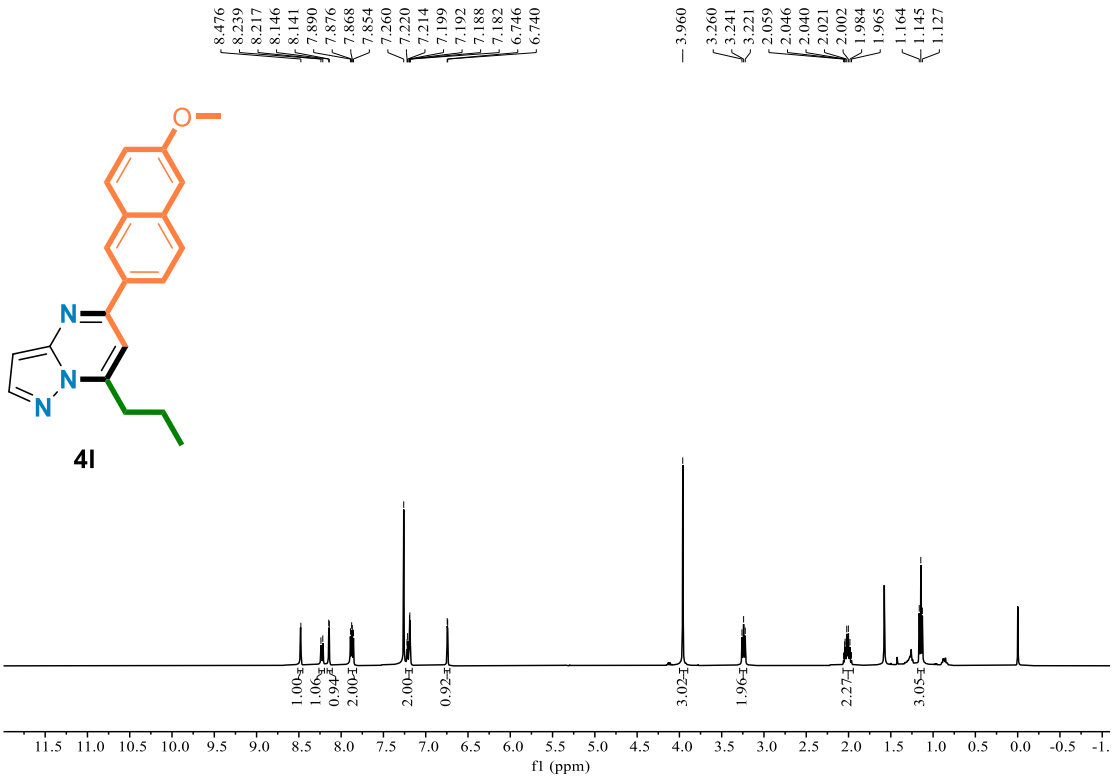
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **4j** (100 MHz, $CDCl_3$)



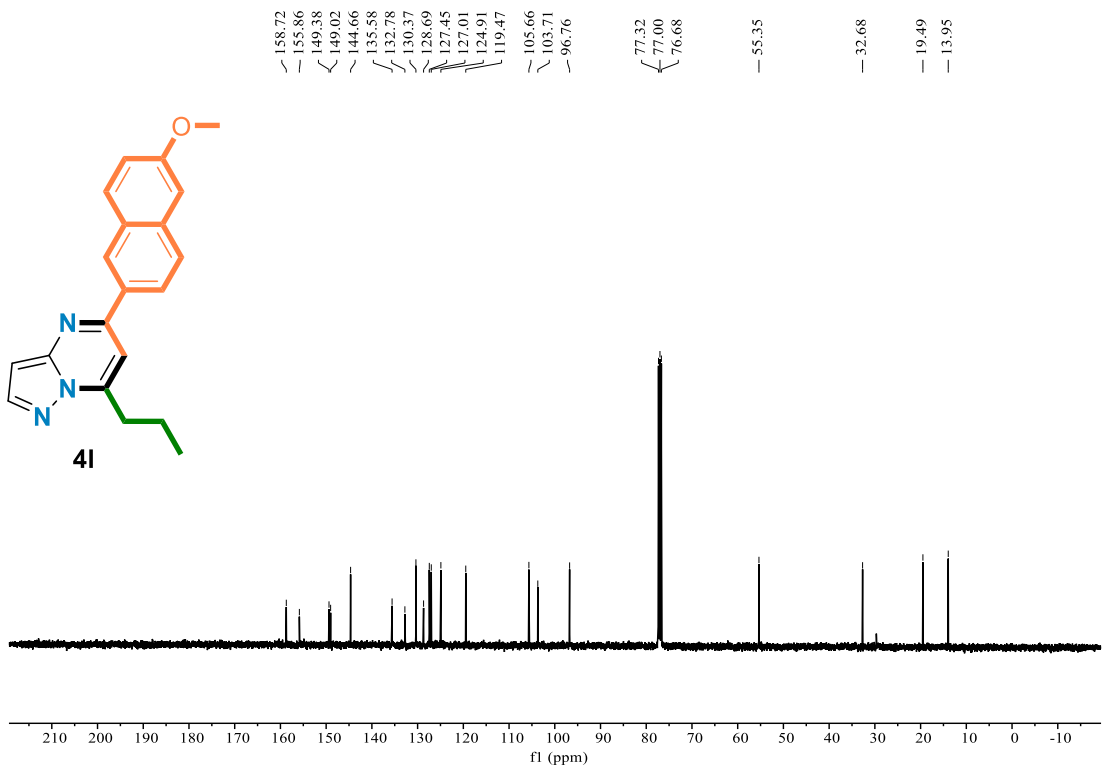
^{1}H NMR Spectrum of Compound **4k** (400 MHz, $CDCl_3$)



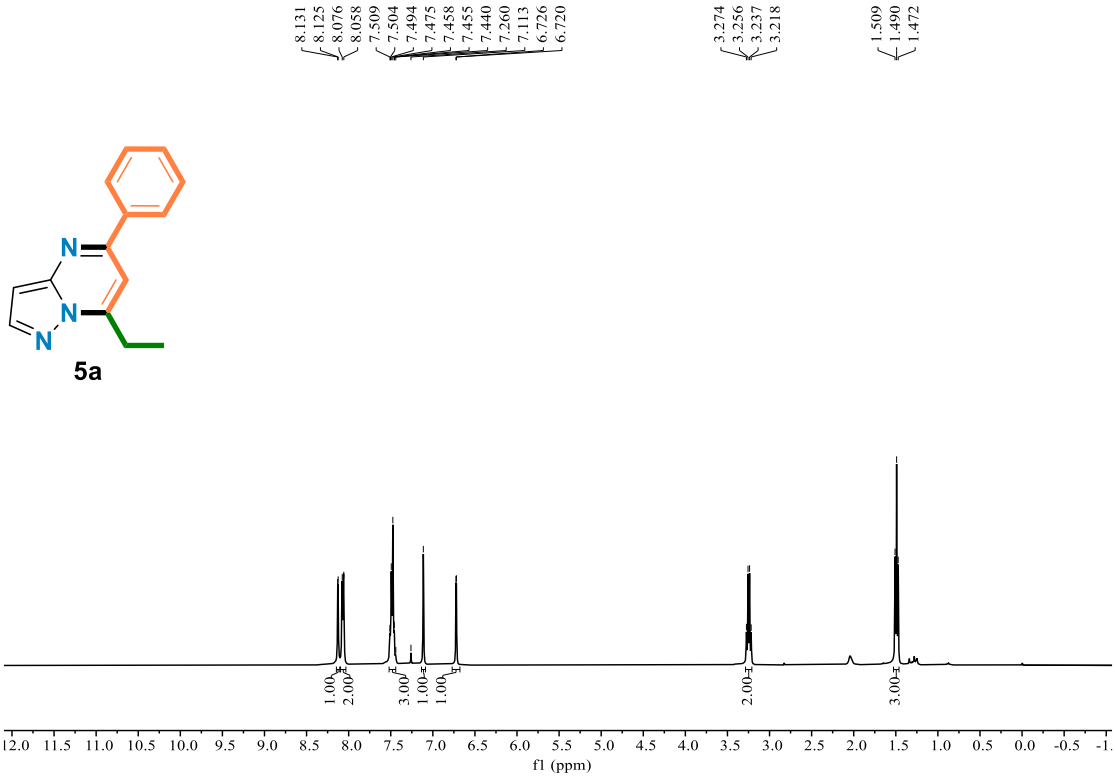
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **4k** (100 MHz, $CDCl_3$)



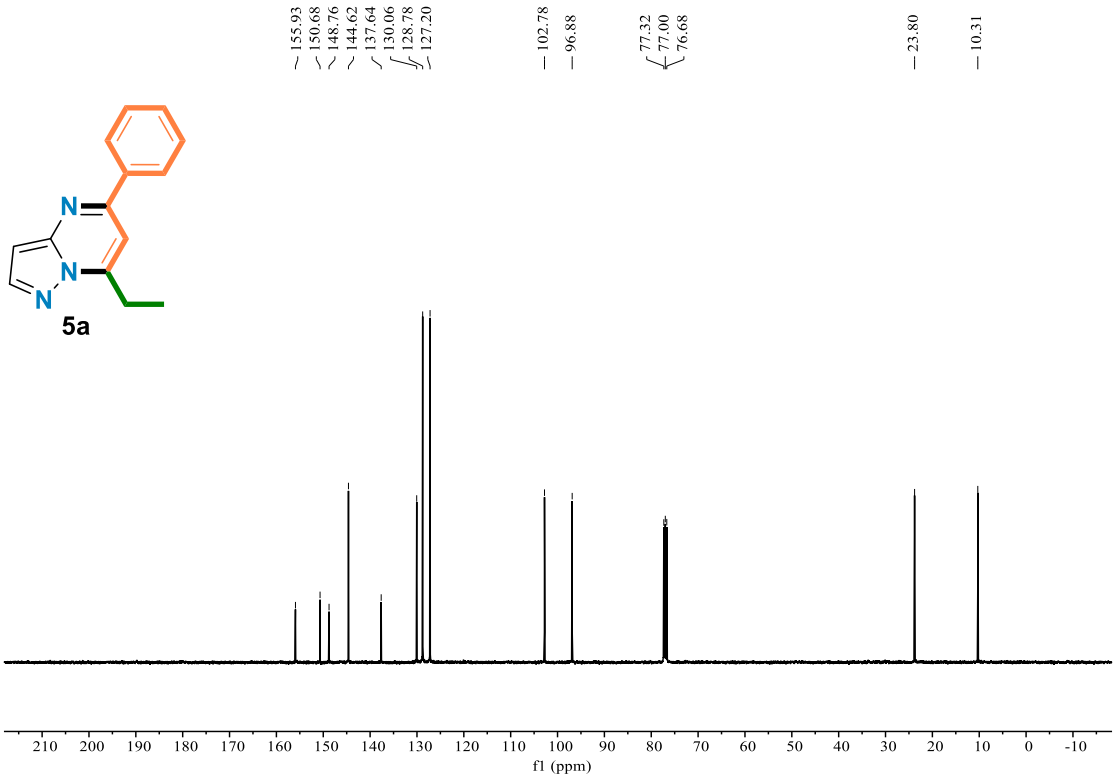
^{1}H NMR Spectrum of Compound **4l** (400 MHz, $CDCl_3$)



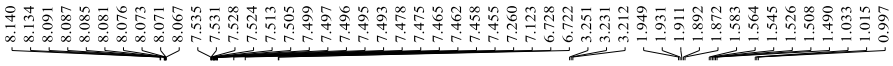
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **4l** (100 MHz, $CDCl_3$)

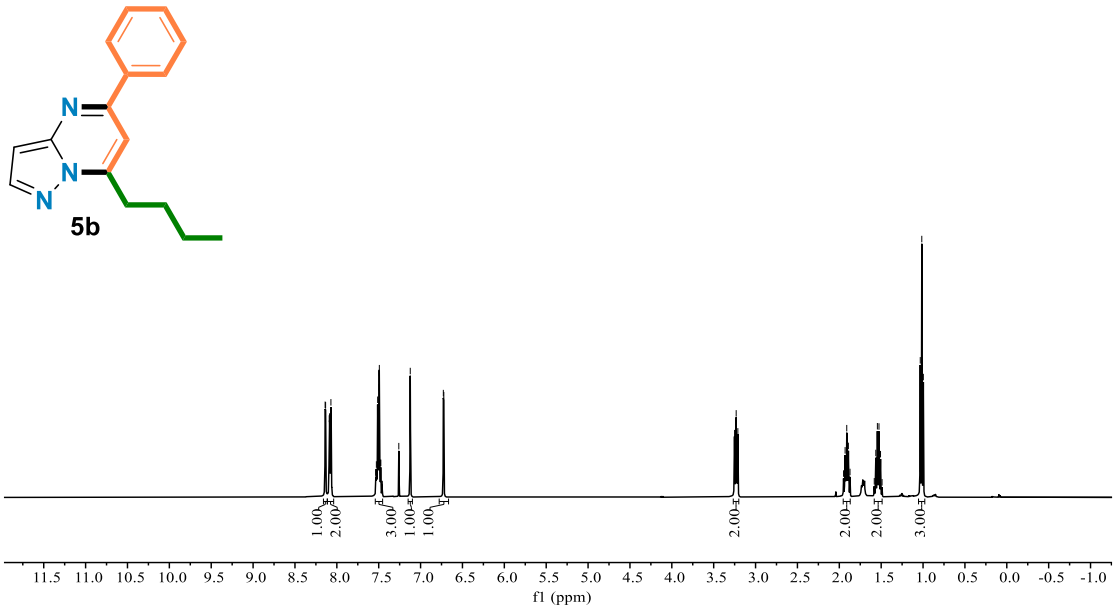


^{1}H NMR Spectrum of Compound **5a** (400 MHz, $CDCl_3$)

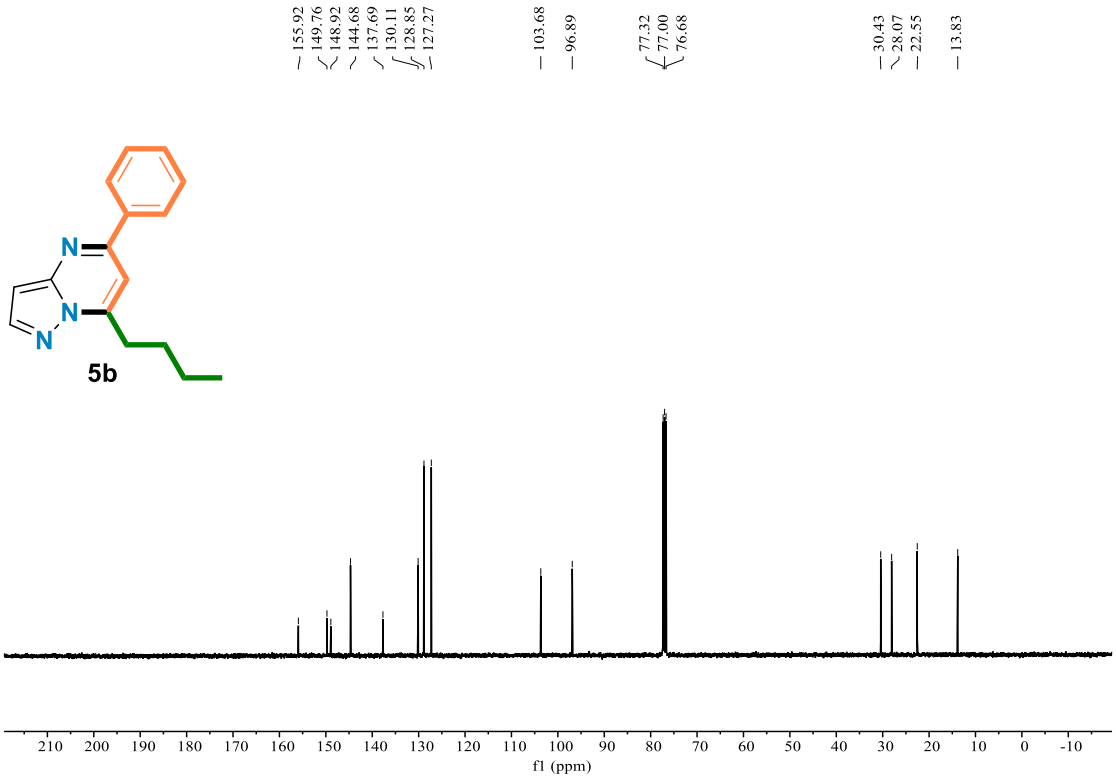


$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5a** (100 MHz, $CDCl_3$)

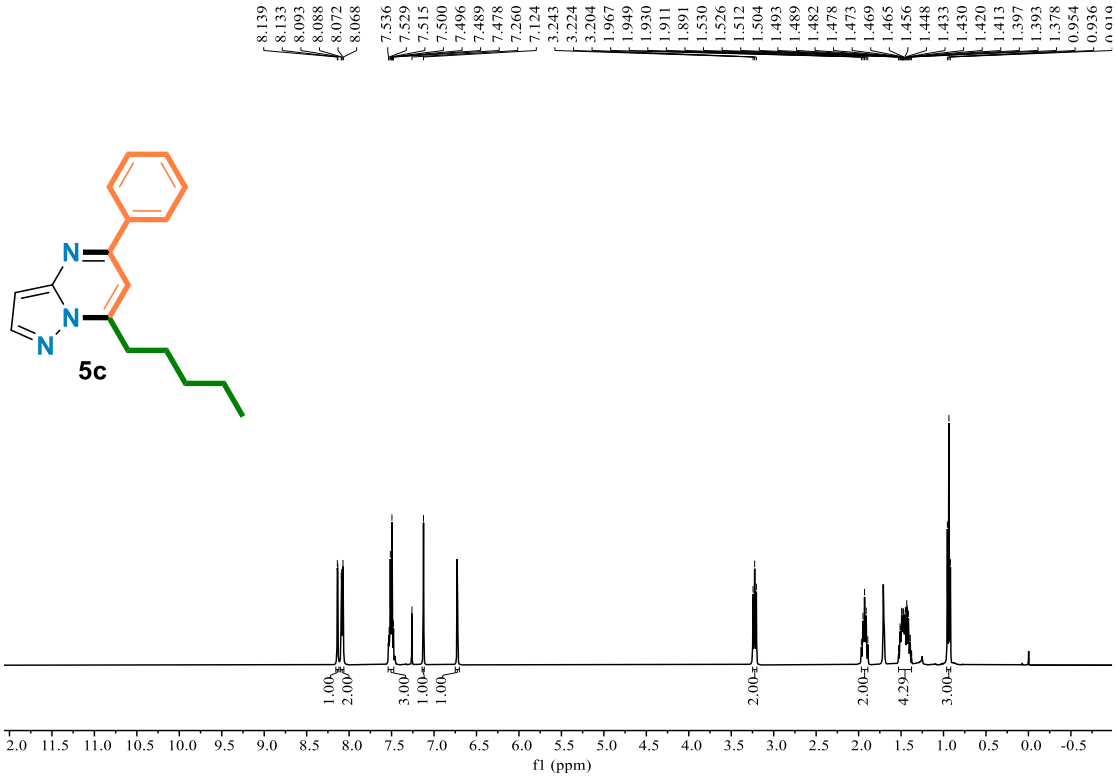




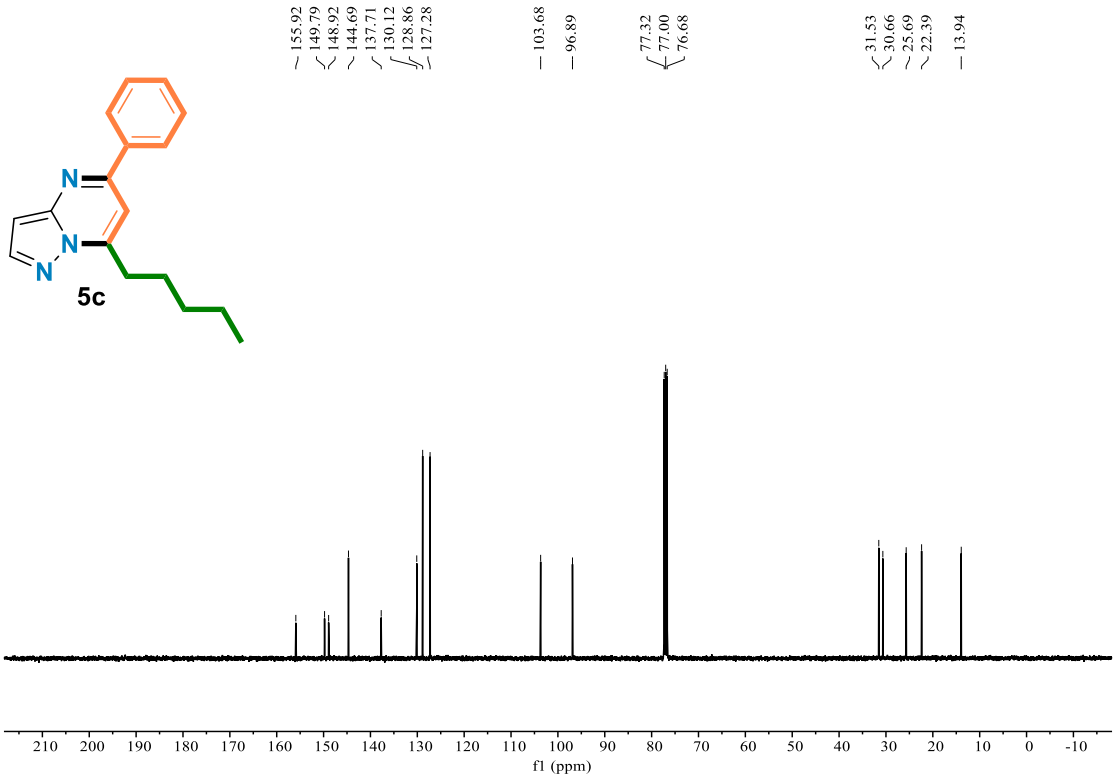
^{1}H NMR Spectrum of Compound **5b** (400 MHz, $CDCl_3$)



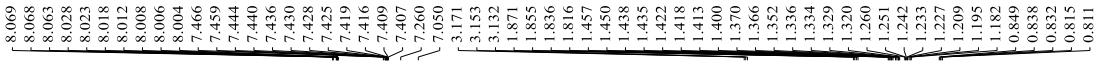
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5b** (100 MHz, $CDCl_3$)

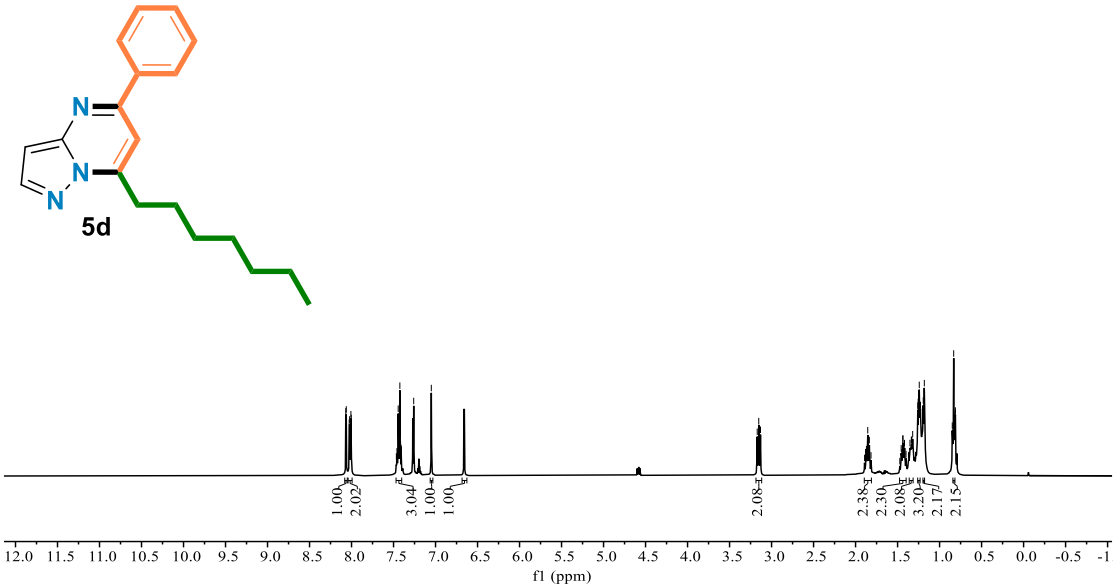


^{1}H NMR Spectrum of Compound **5c** (400 MHz, $CDCl_3$)

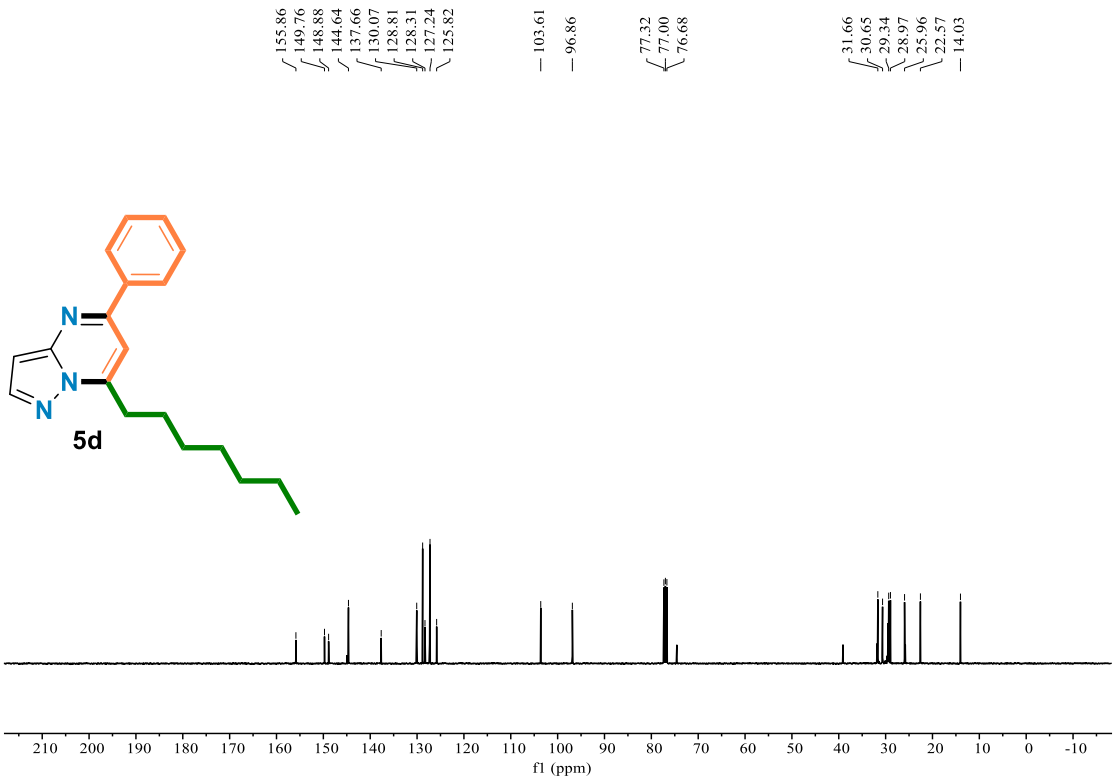


$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5c** (100 MHz, $CDCl_3$)

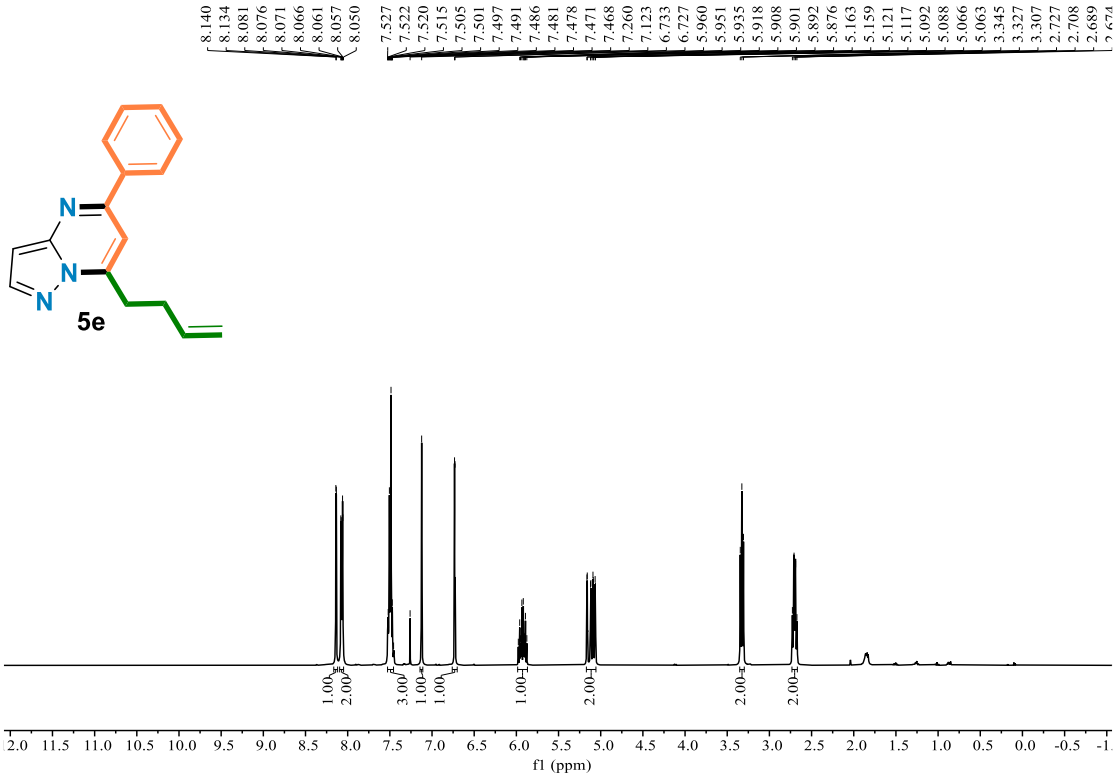




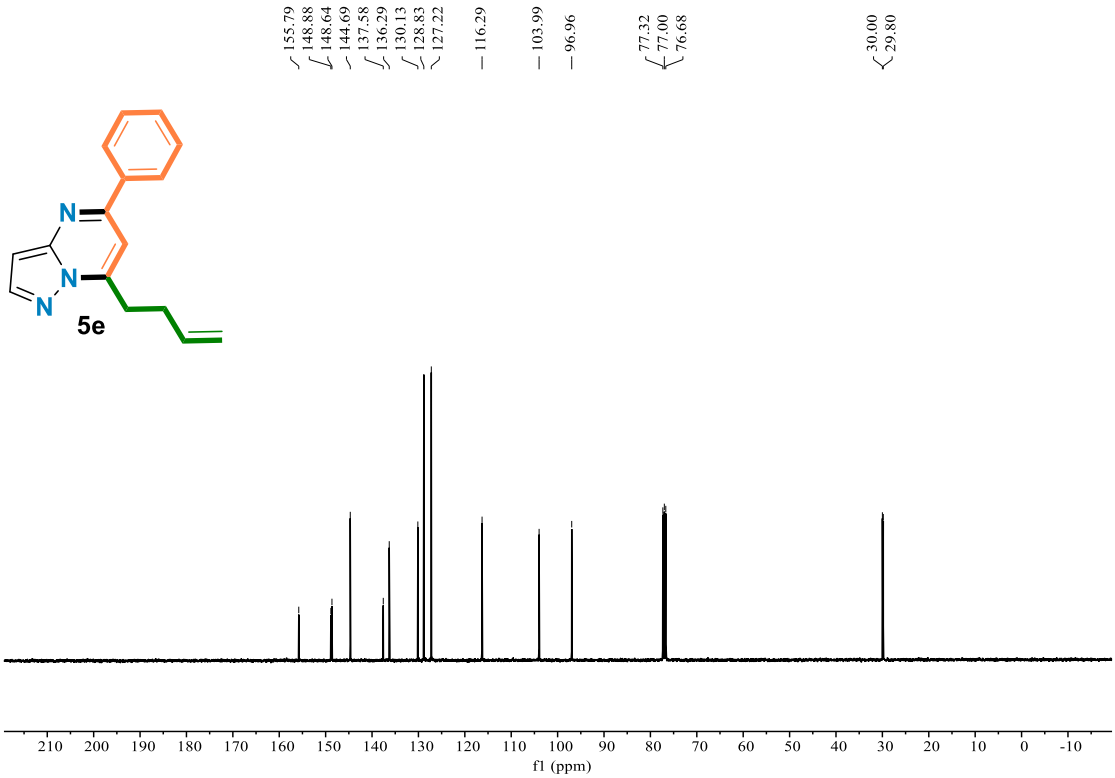
^{1}H NMR Spectrum of Compound **5d** (400 MHz, $CDCl_3$)



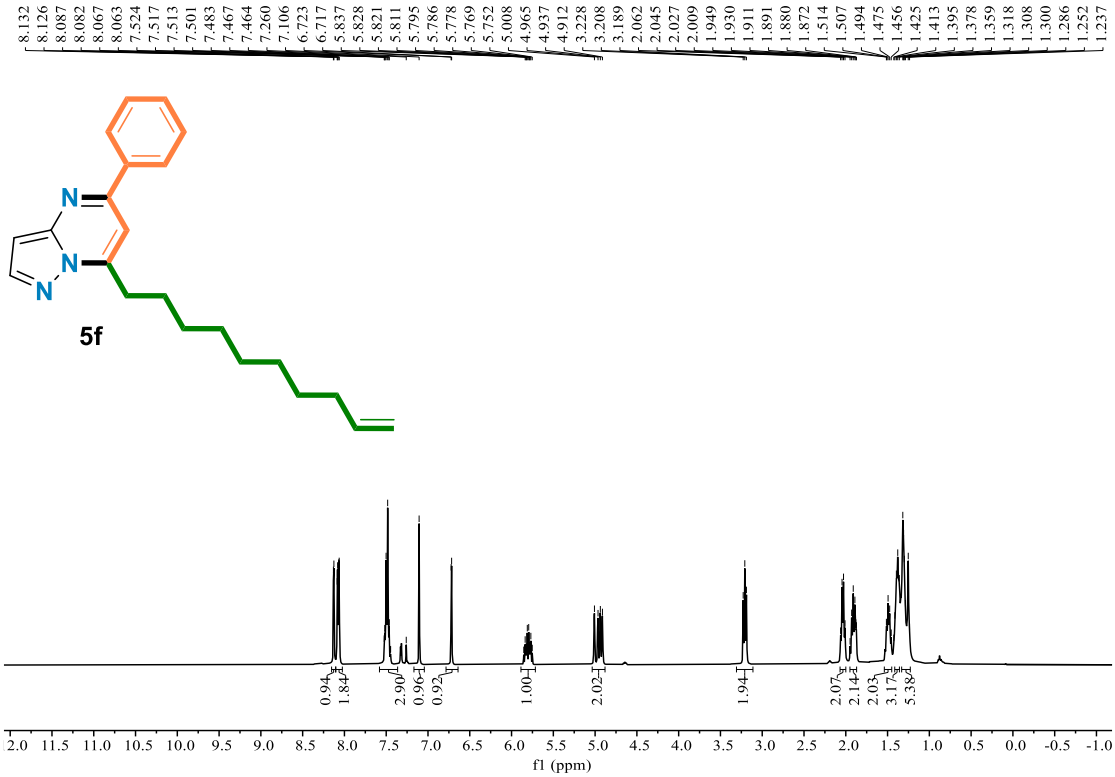
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5d** (100 MHz, $CDCl_3$)



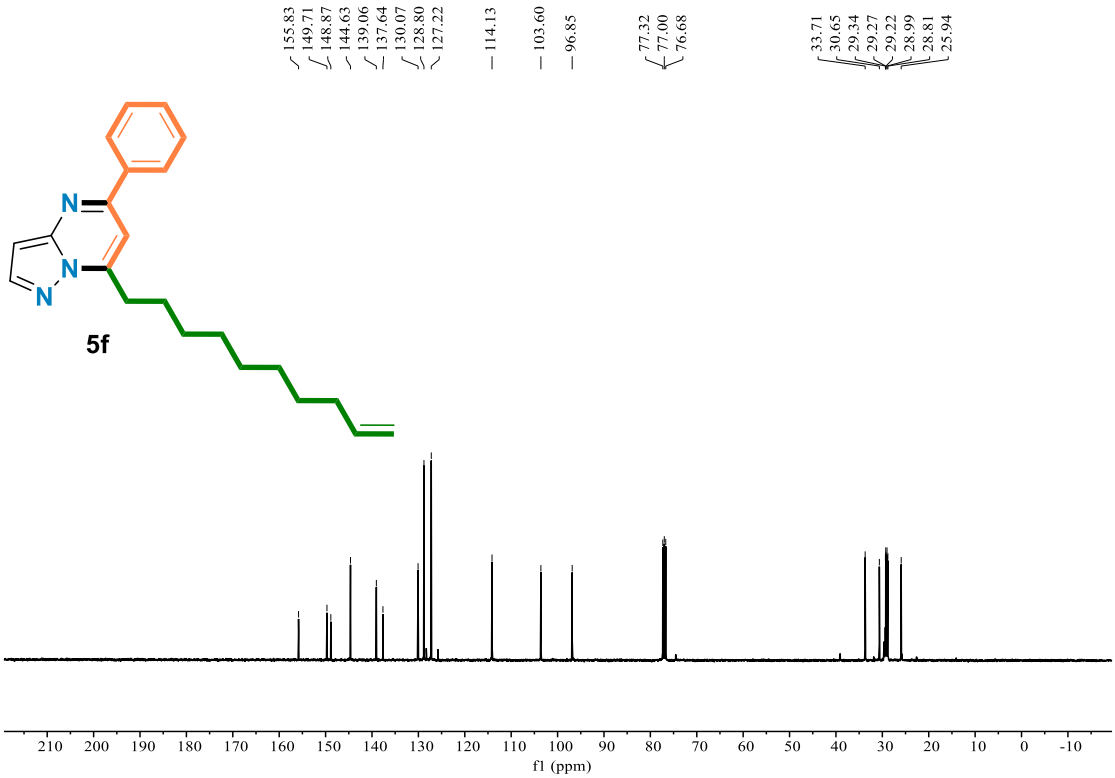
^{1}H NMR Spectrum of Compound **5e** (400 MHz, $CDCl_3$)



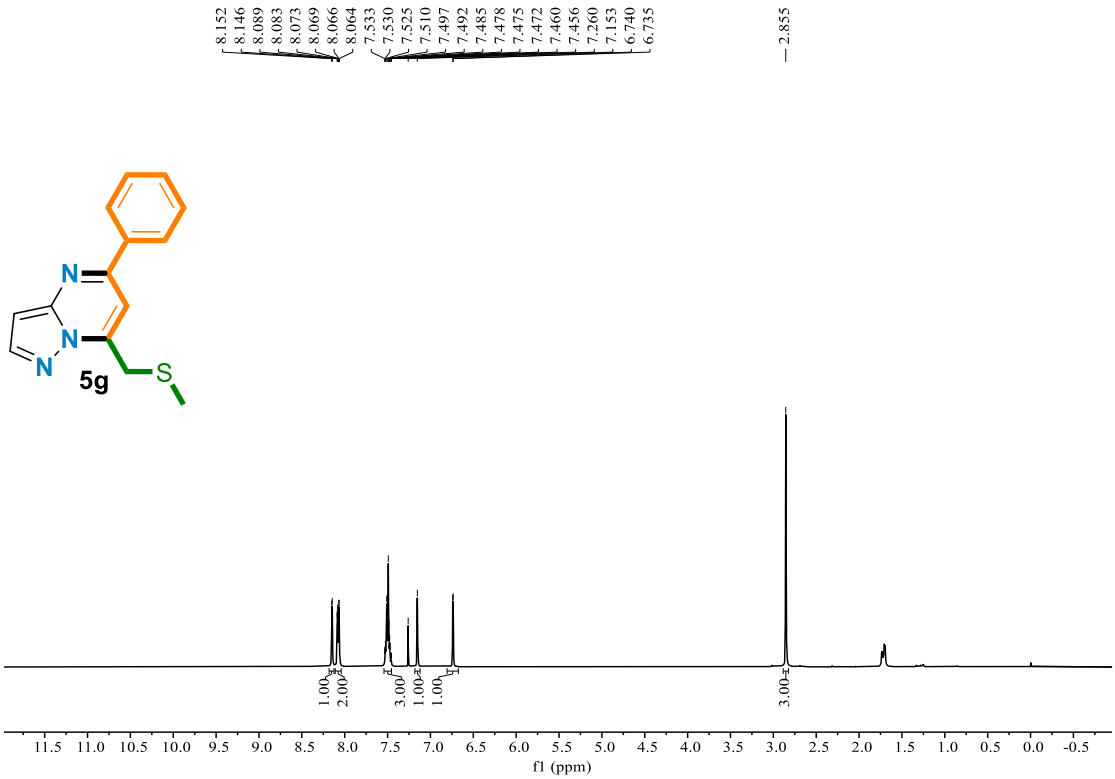
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5e** (100 MHz, $CDCl_3$)



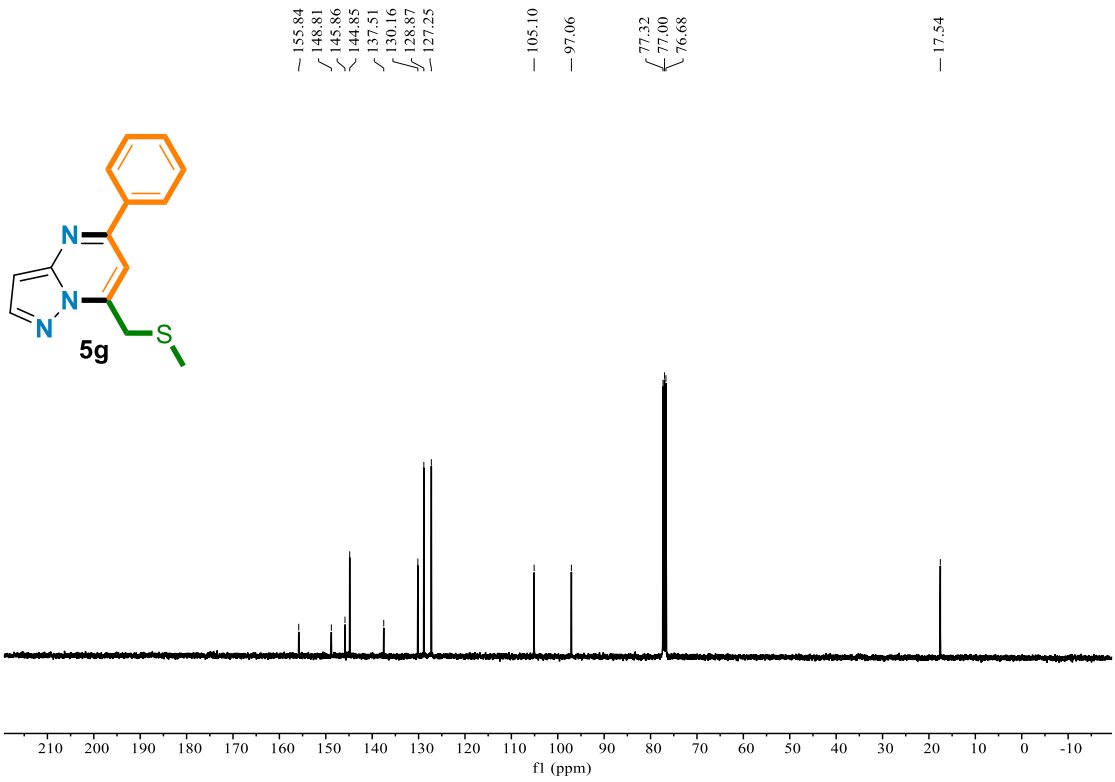
^{1}H NMR Spectrum of Compound **5f** (400 MHz, $CDCl_3$)



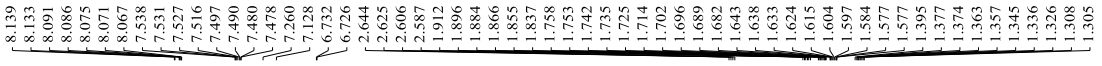
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5f** (100 MHz, $CDCl_3$)



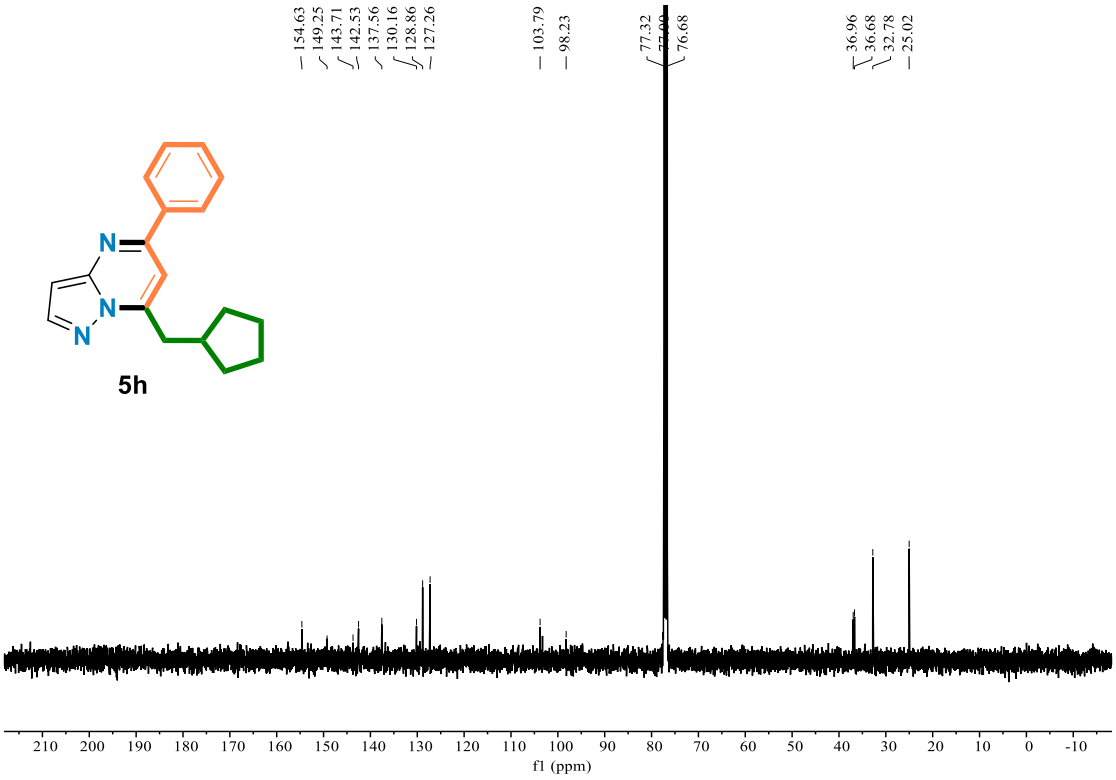
^{1}H NMR Spectrum of Compound **5g** (400 MHz, $CDCl_3$)



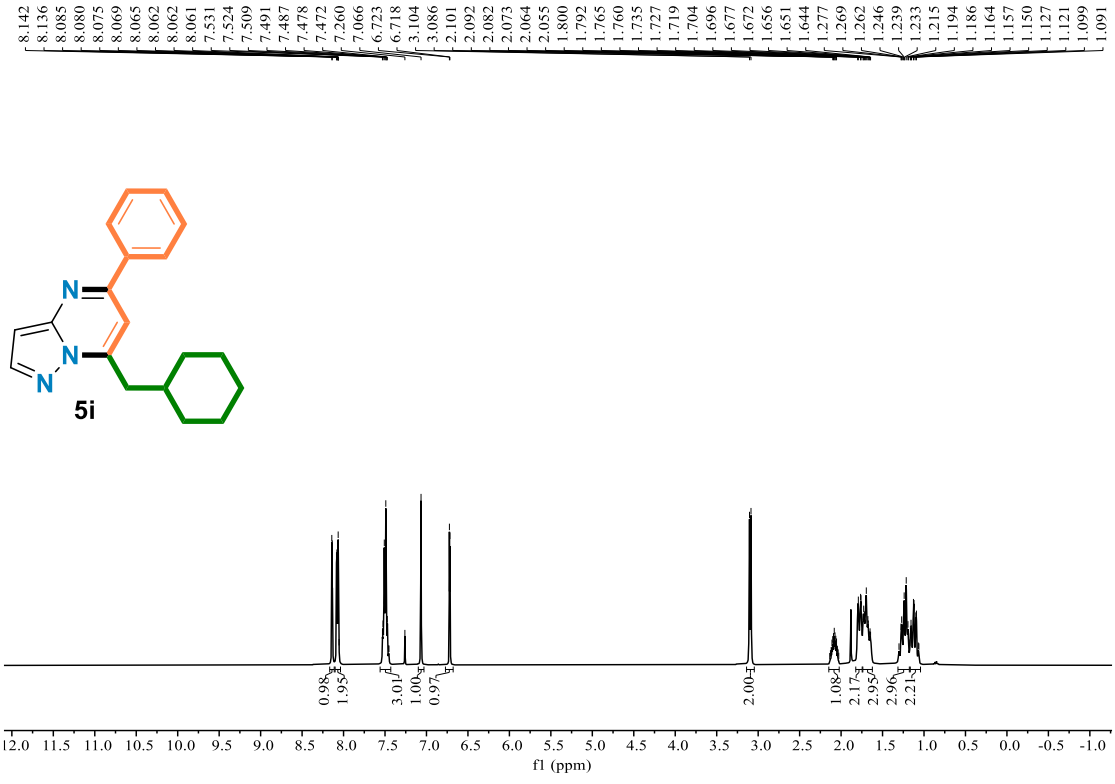
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5g** (100 MHz, $CDCl_3$)



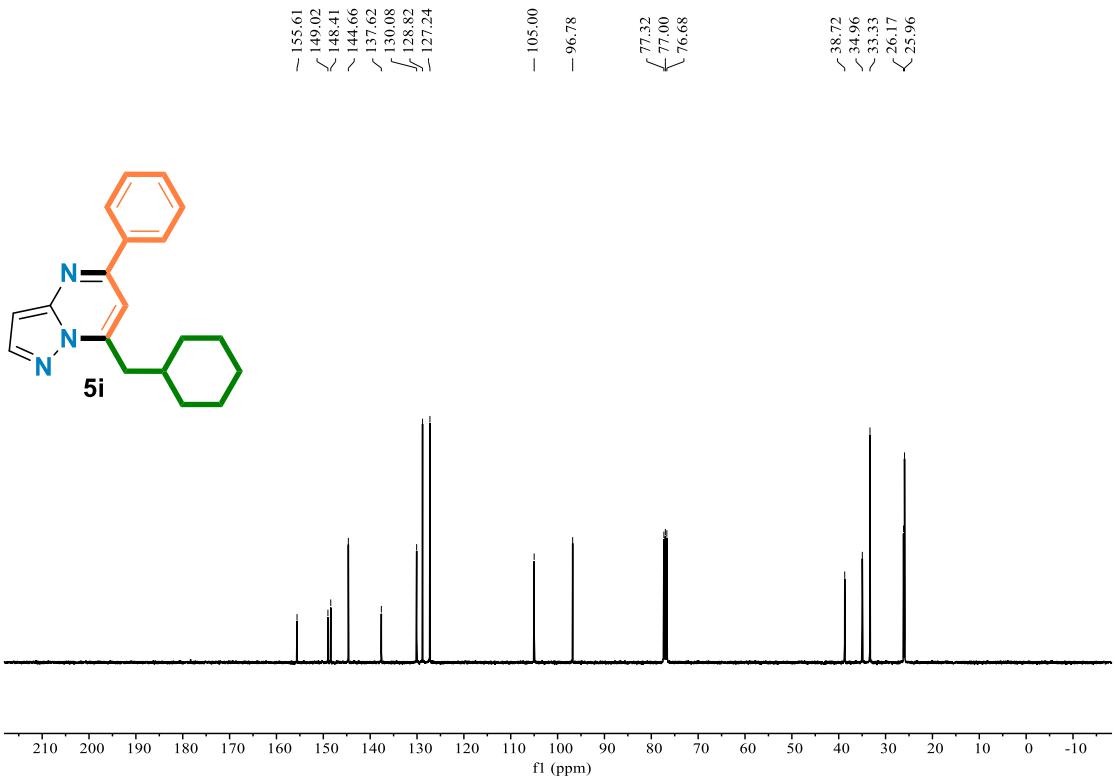
^{1}H NMR Spectrum of Compound **5h** (400 MHz, $CDCl_3$)



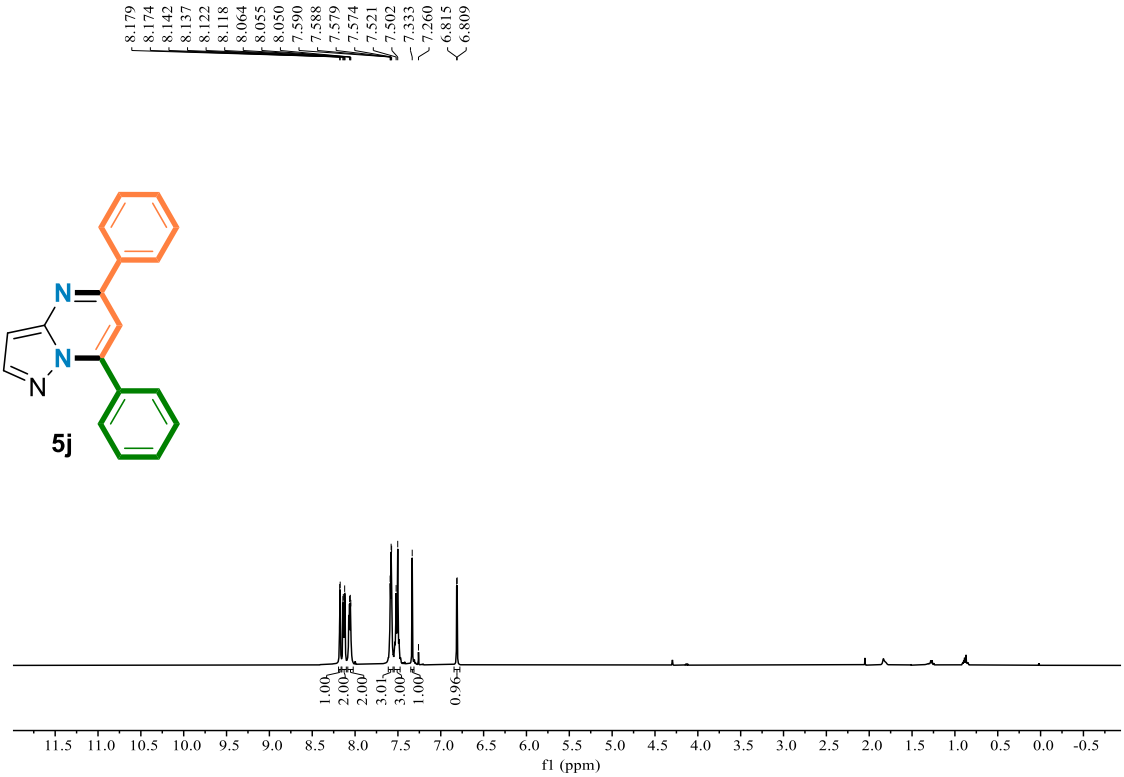
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5h** (100 MHz, $CDCl_3$)



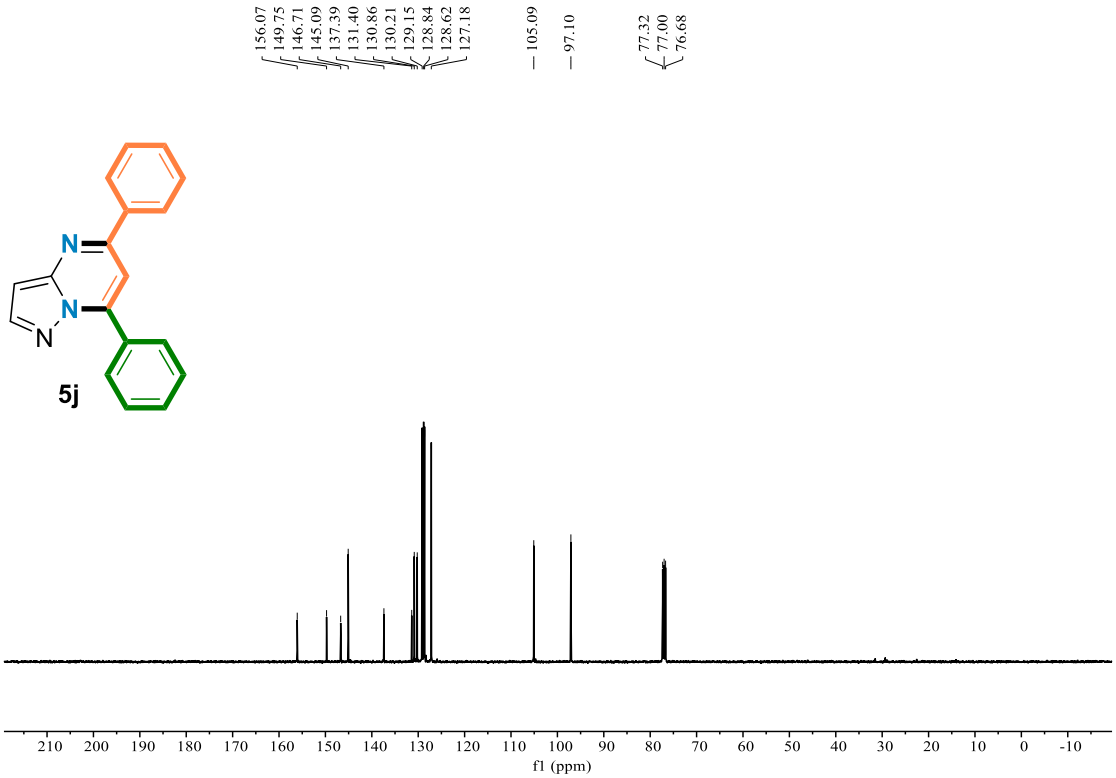
^{1}H NMR Spectrum of Compound **5i** (400 MHz, $CDCl_3$)



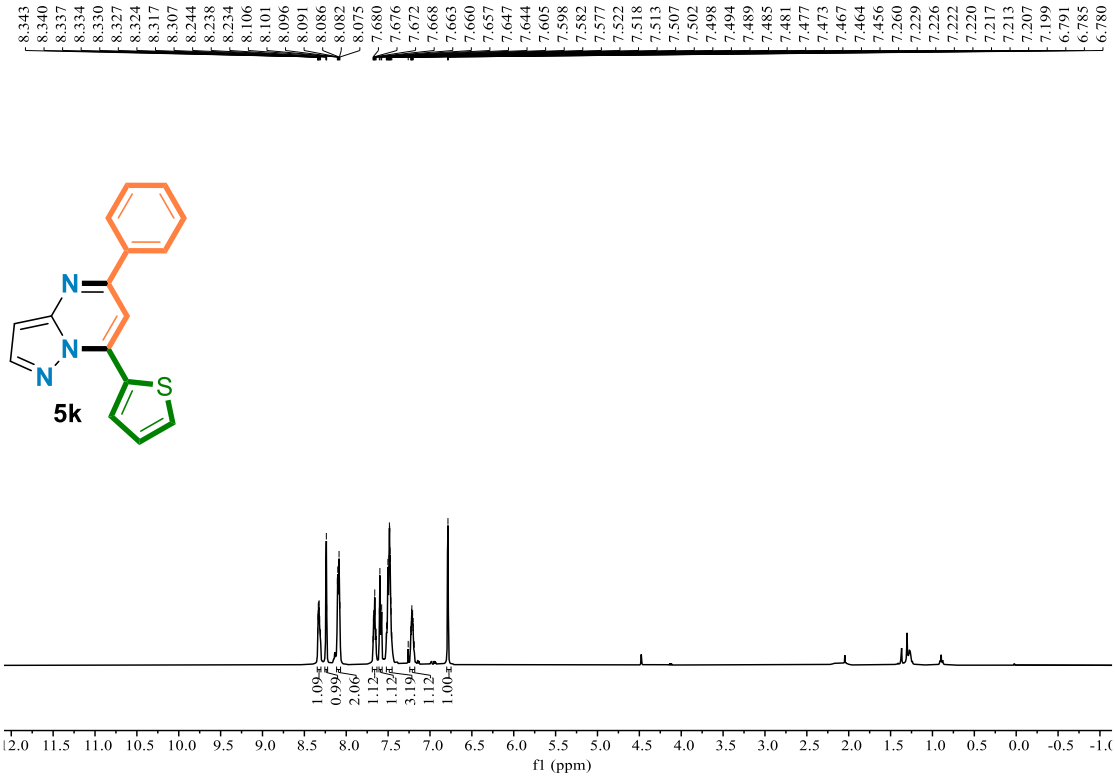
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5i** (100 MHz, $CDCl_3$)



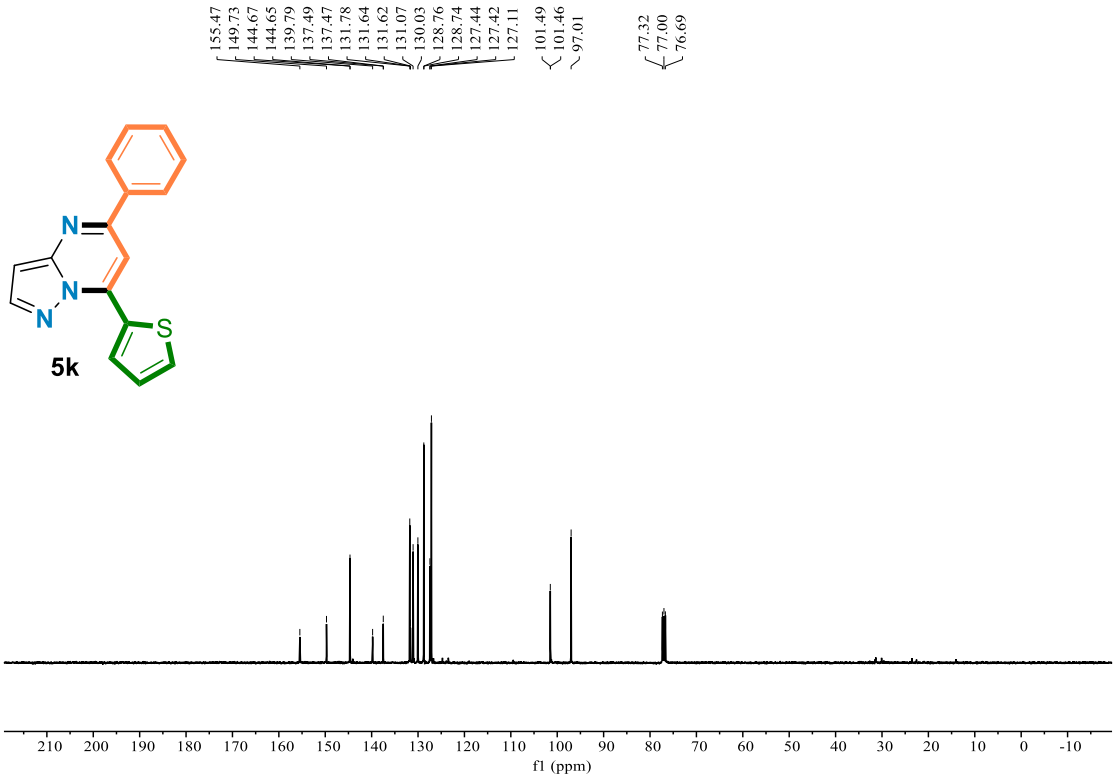
^{1}H NMR Spectrum of Compound **5j** (400 MHz, $CDCl_3$)



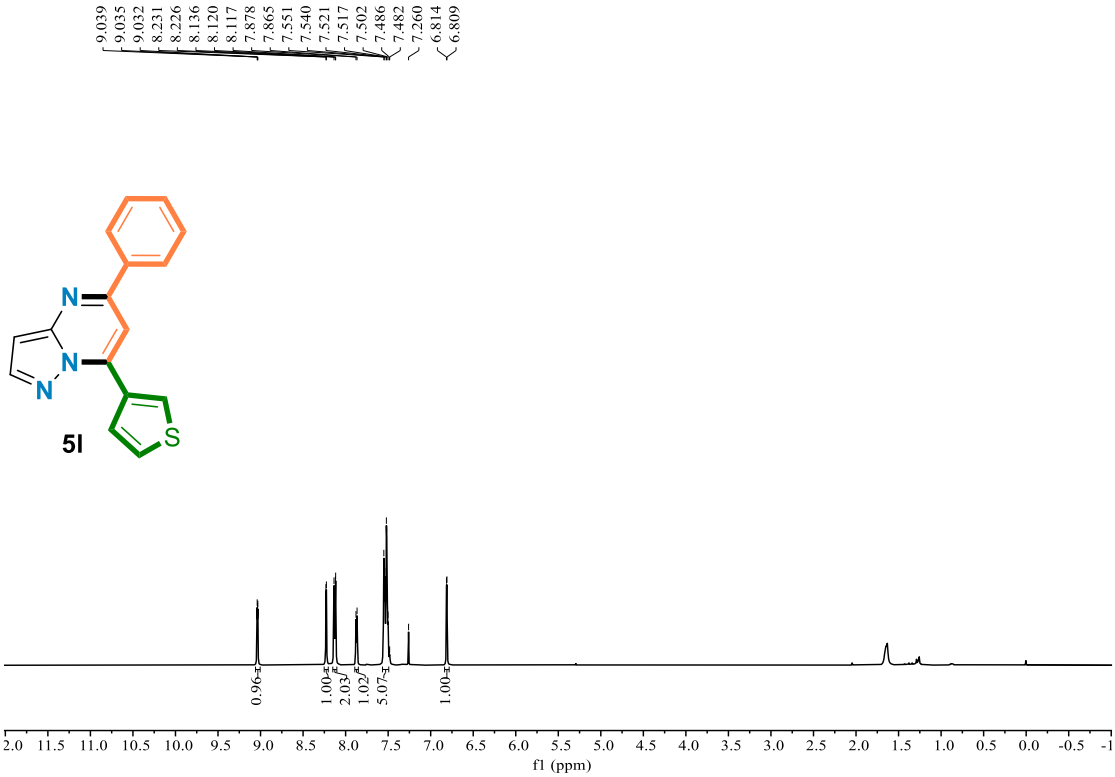
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5j** (100 MHz, $CDCl_3$)



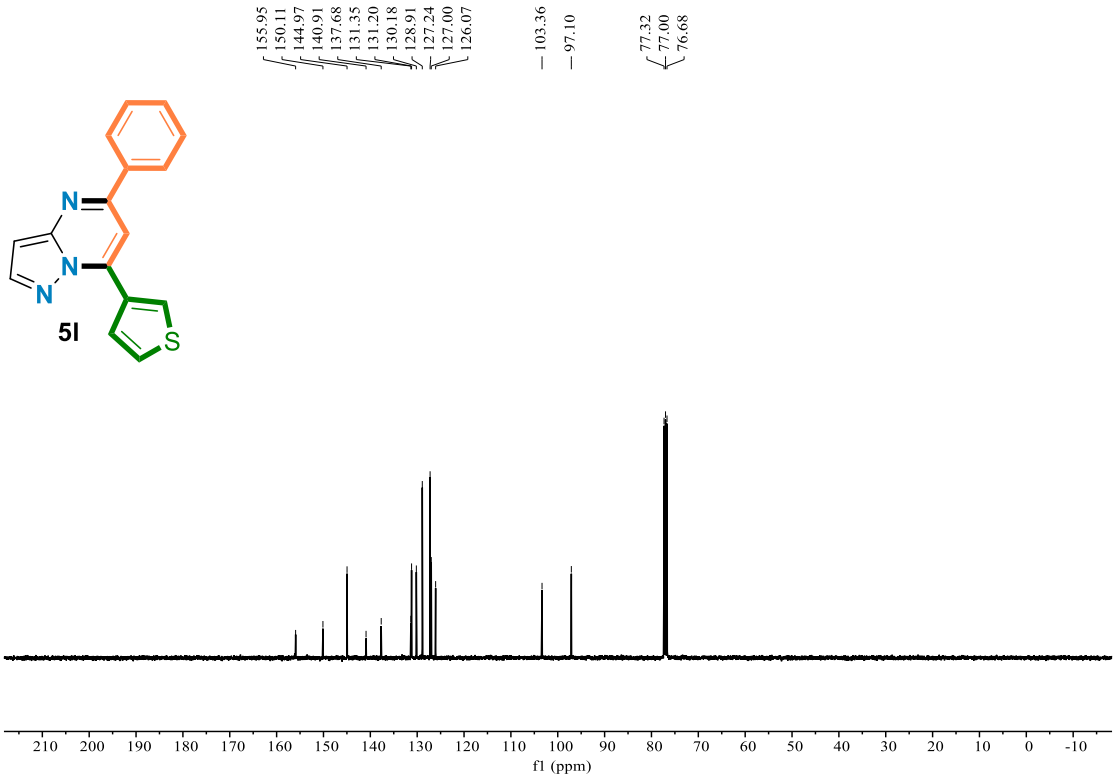
^{1}H NMR Spectrum of Compound **5k** (400 MHz, $CDCl_3$)



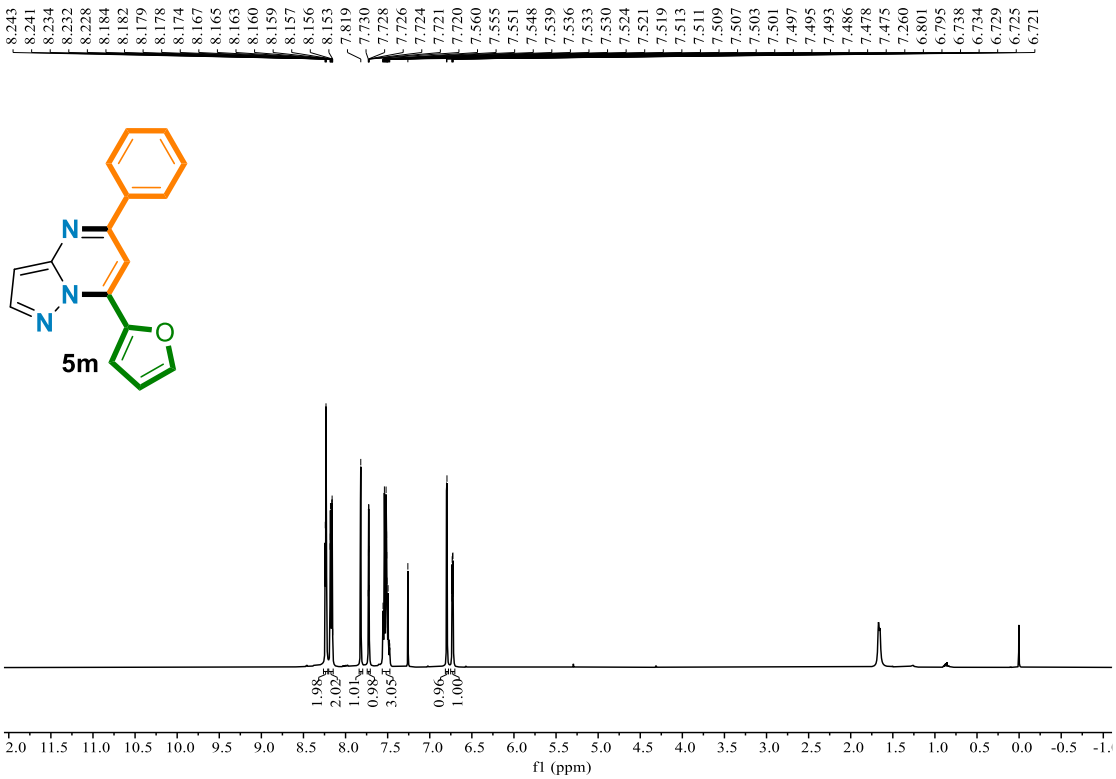
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5k** (100 MHz, $CDCl_3$)



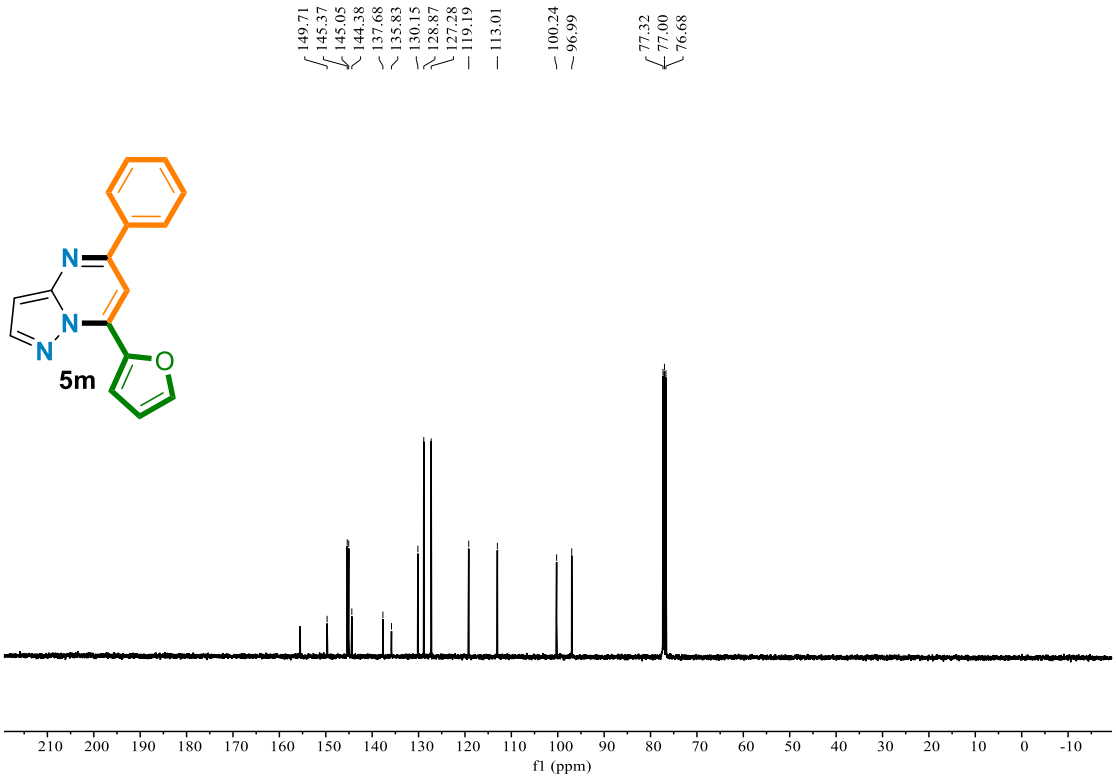
^{1}H NMR Spectrum of Compound **5l** (400 MHz, $CDCl_3$)



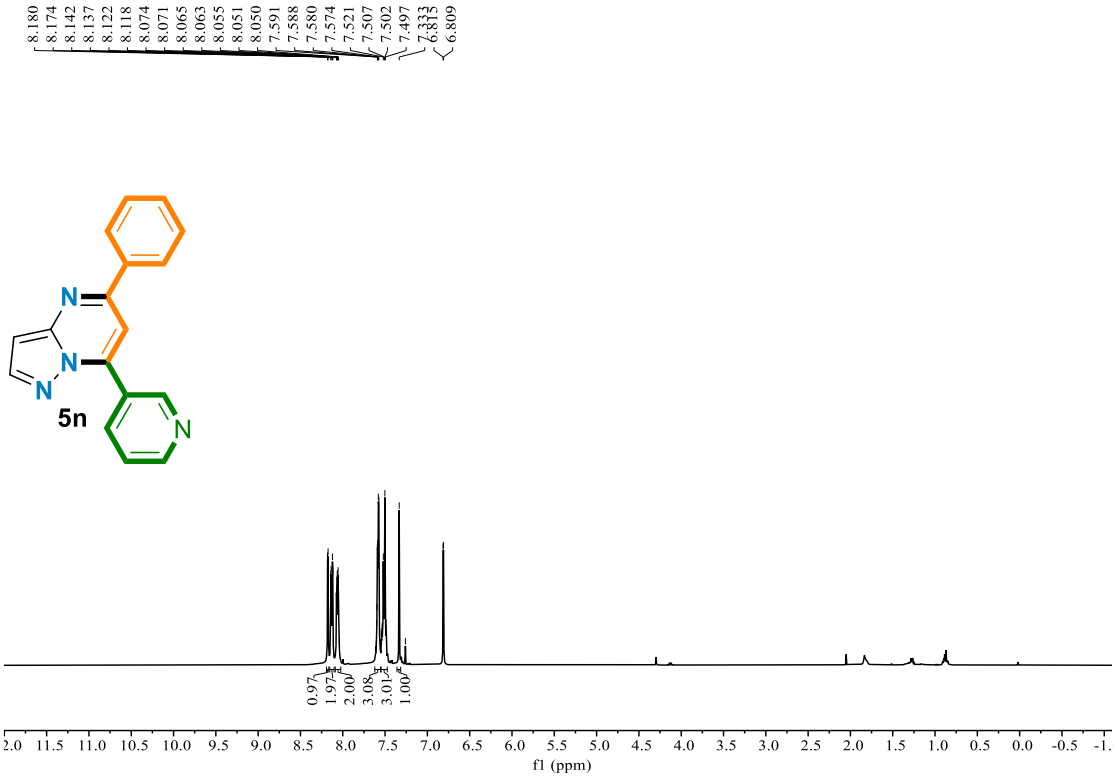
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5l** (100 MHz, $CDCl_3$)



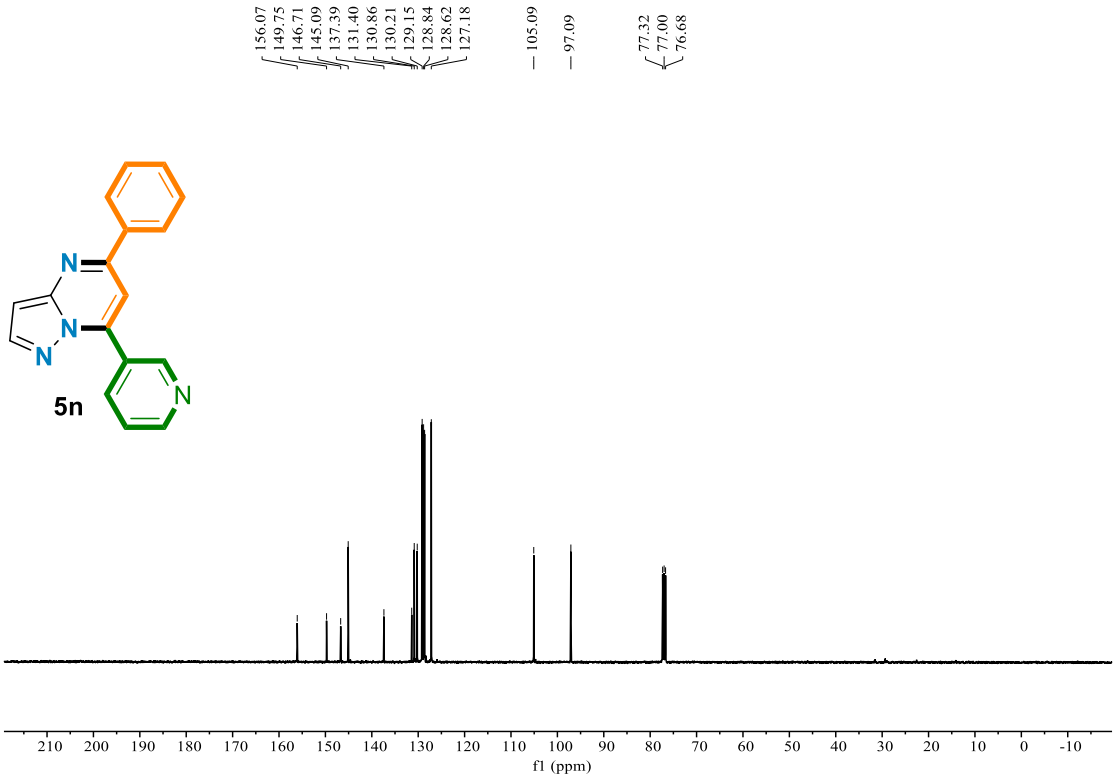
^{1}H NMR Spectrum of Compound **5m** (400 MHz, $CDCl_3$)



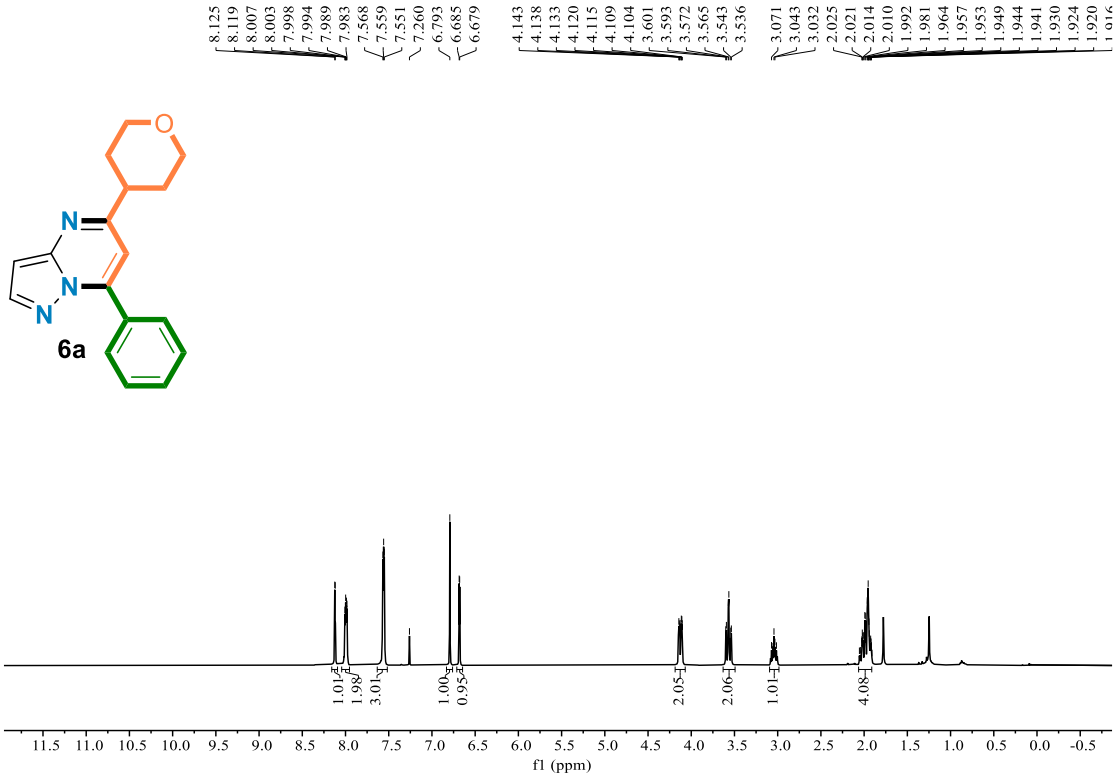
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5m** (100 MHz, $CDCl_3$)



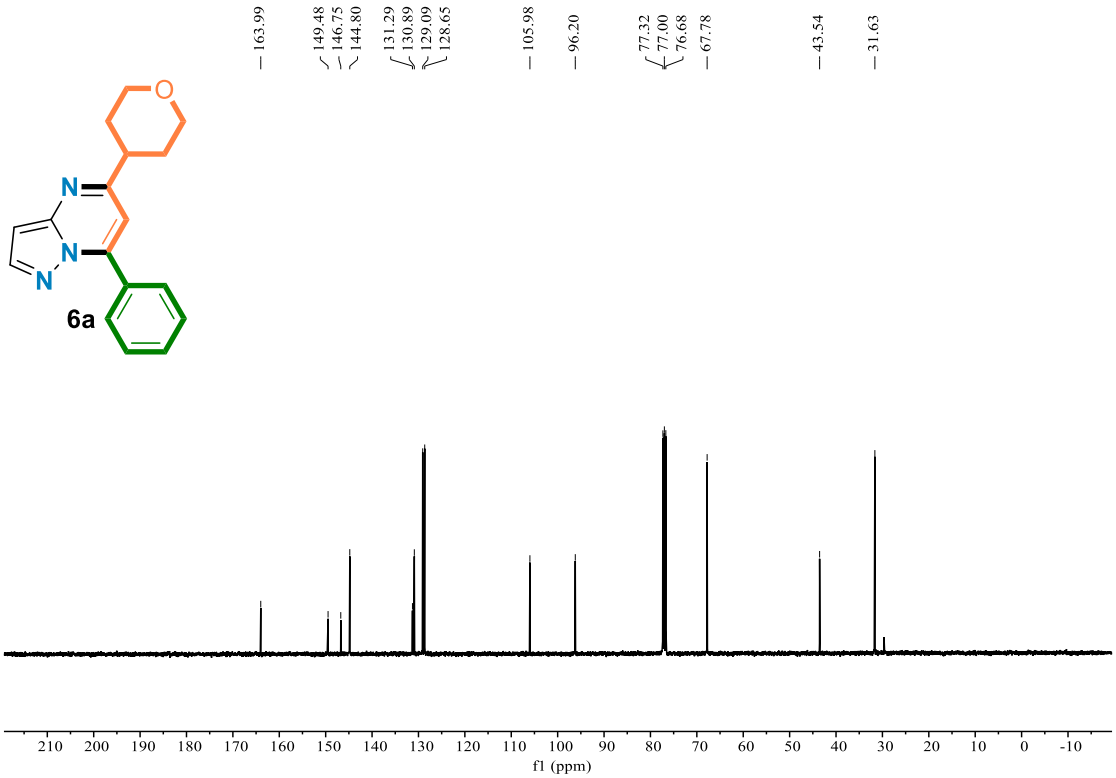
^{1}H NMR Spectrum of Compound **5n** (400 MHz, $CDCl_3$)



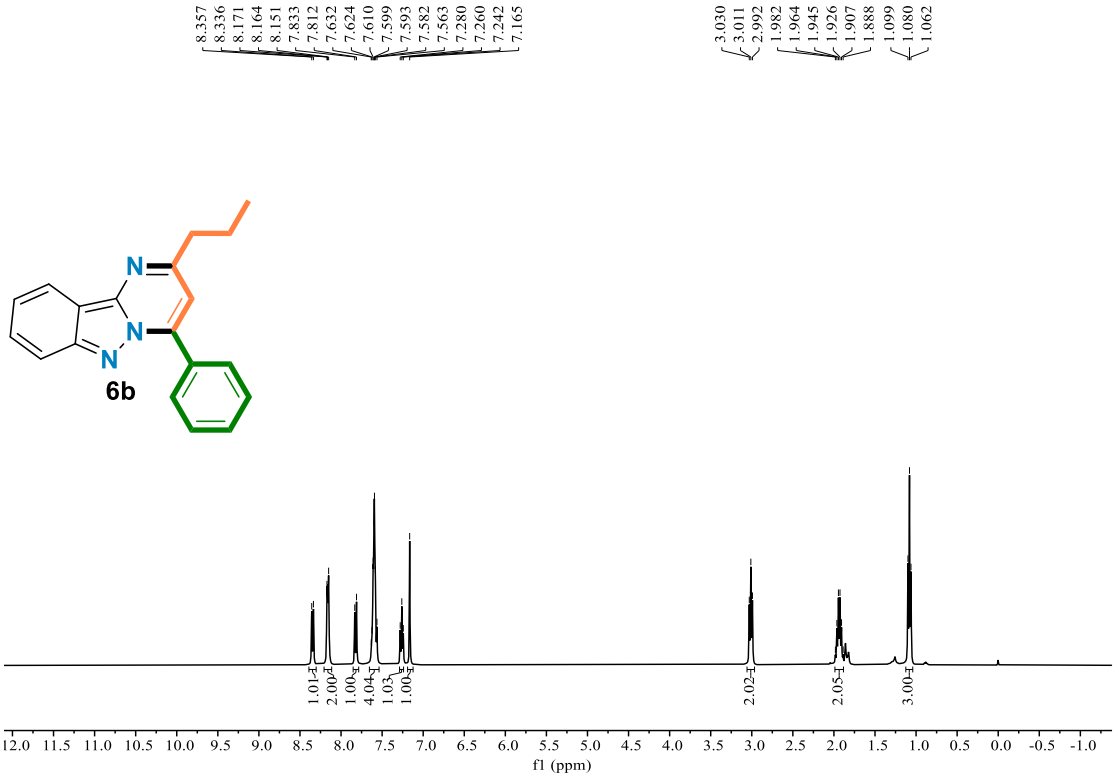
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **5n** (100 MHz, $CDCl_3$)



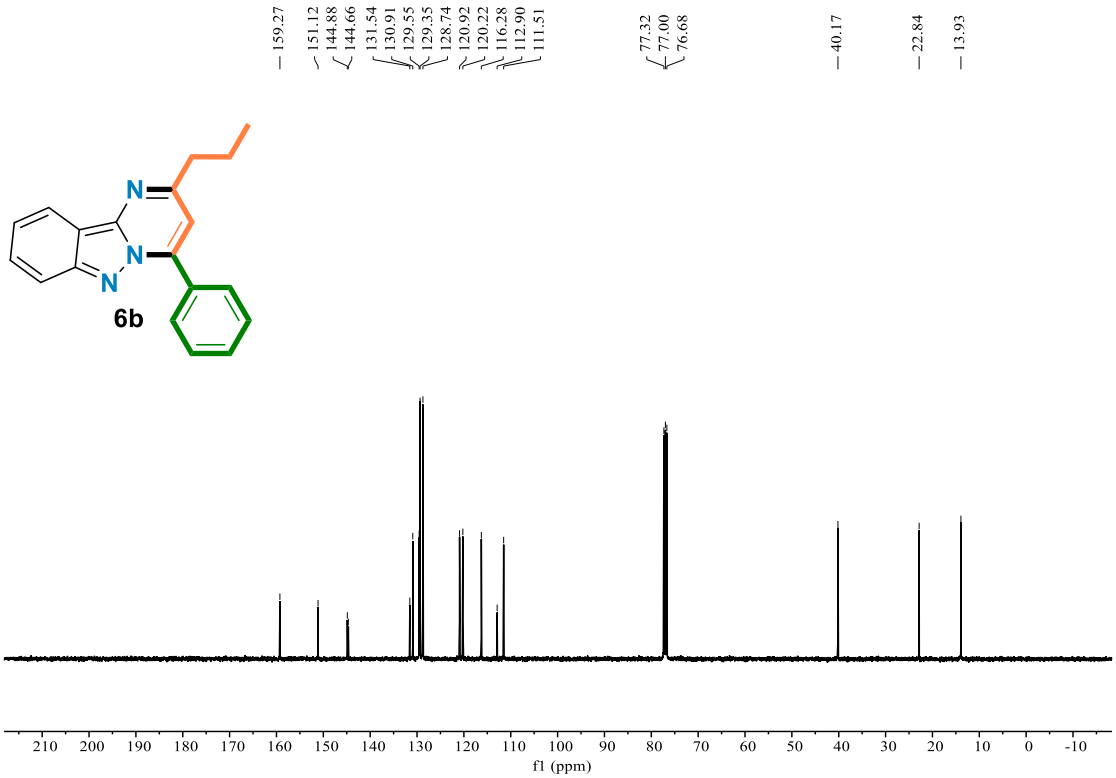
^{1}H NMR Spectrum of Compound **6a** (400 MHz, $CDCl_3$)



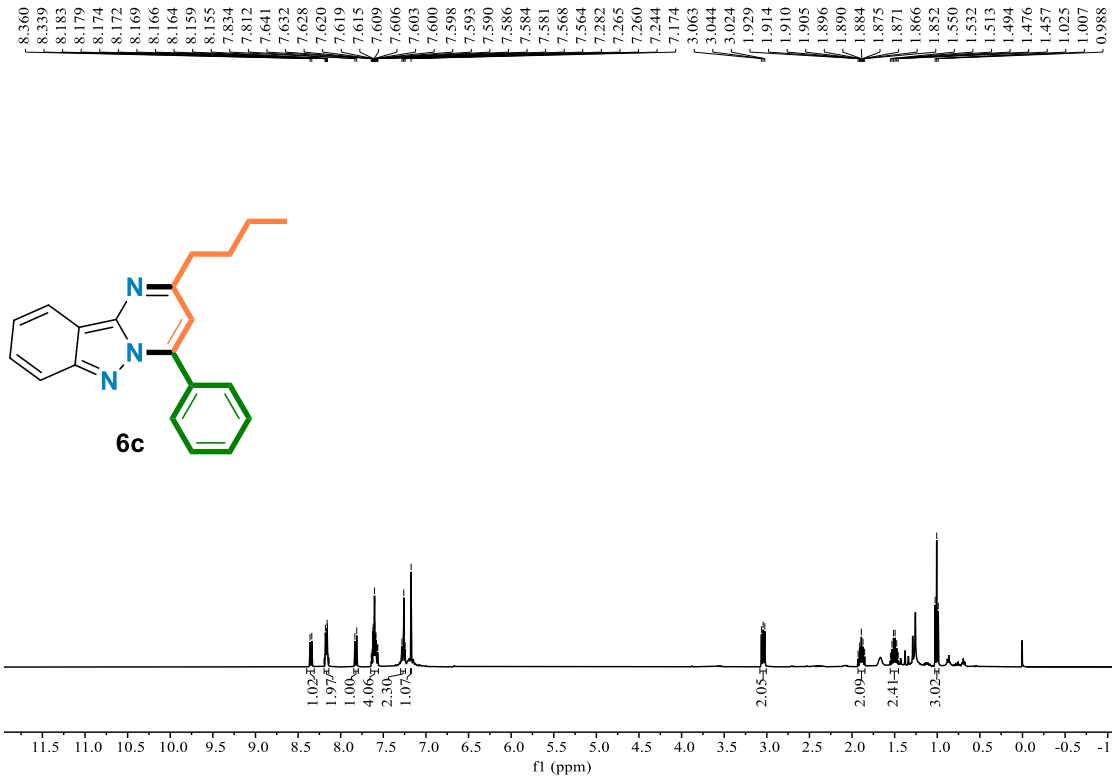
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **6a** (100 MHz, $CDCl_3$)



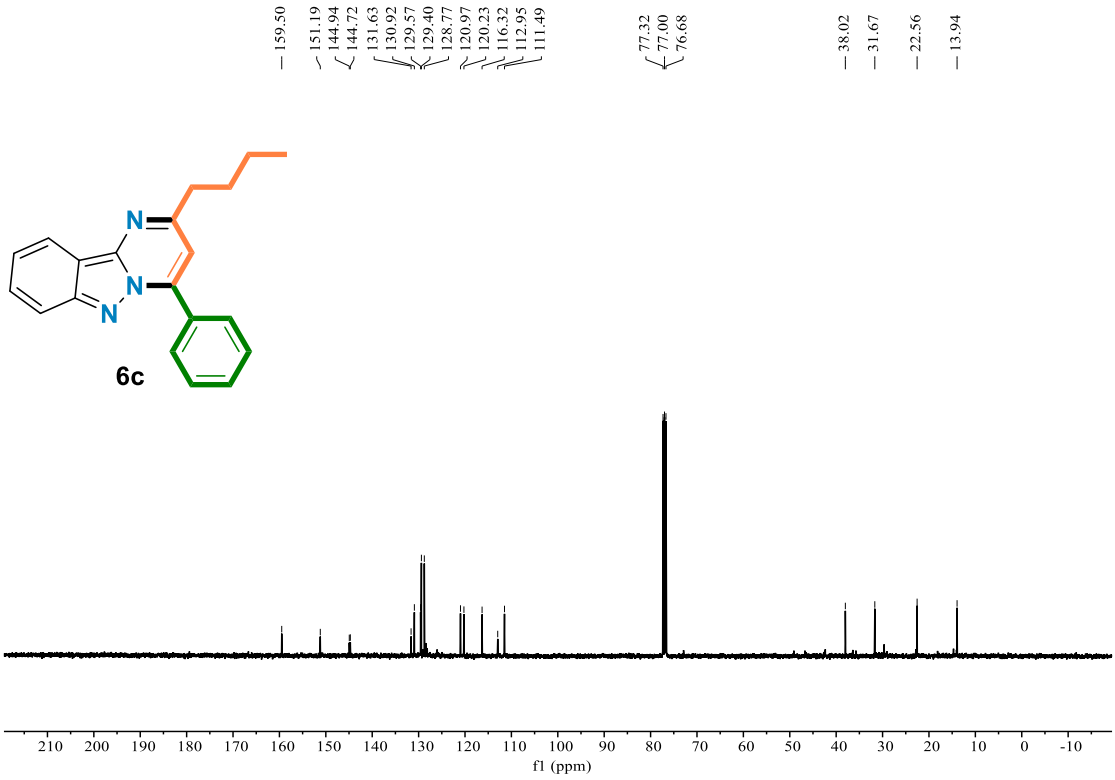
^{1}H NMR Spectrum of Compound **6b** (400 MHz, $CDCl_3$)



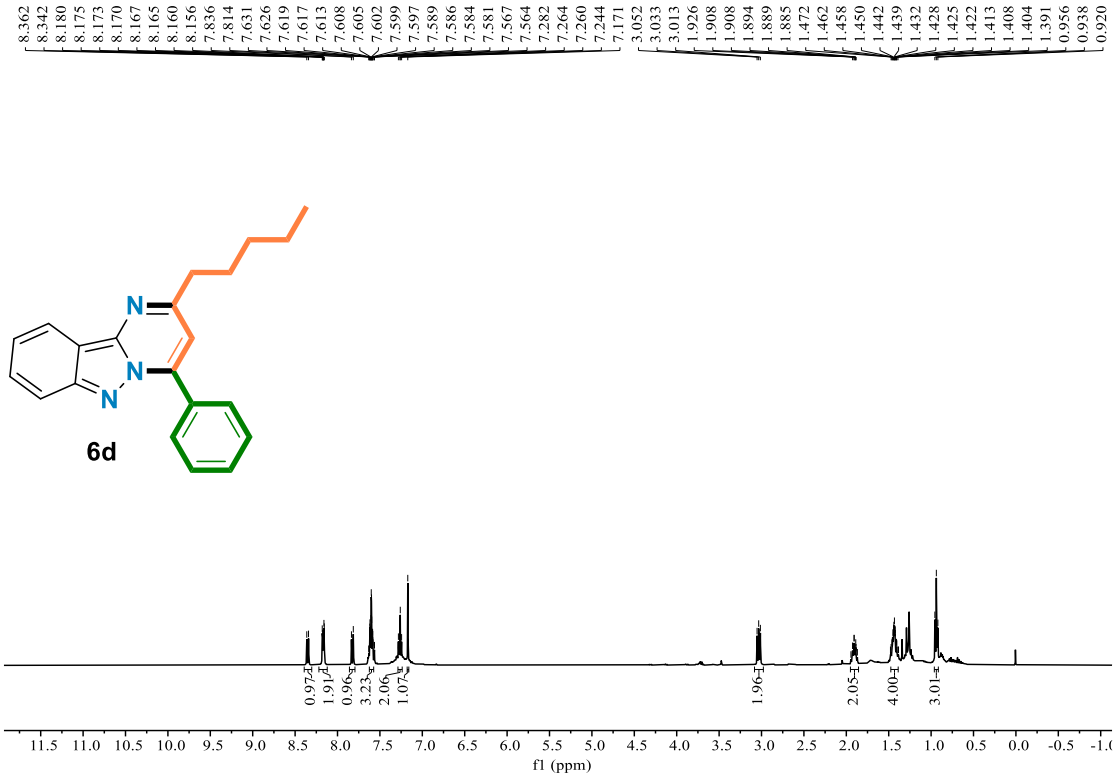
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **6b** (100 MHz, $CDCl_3$)



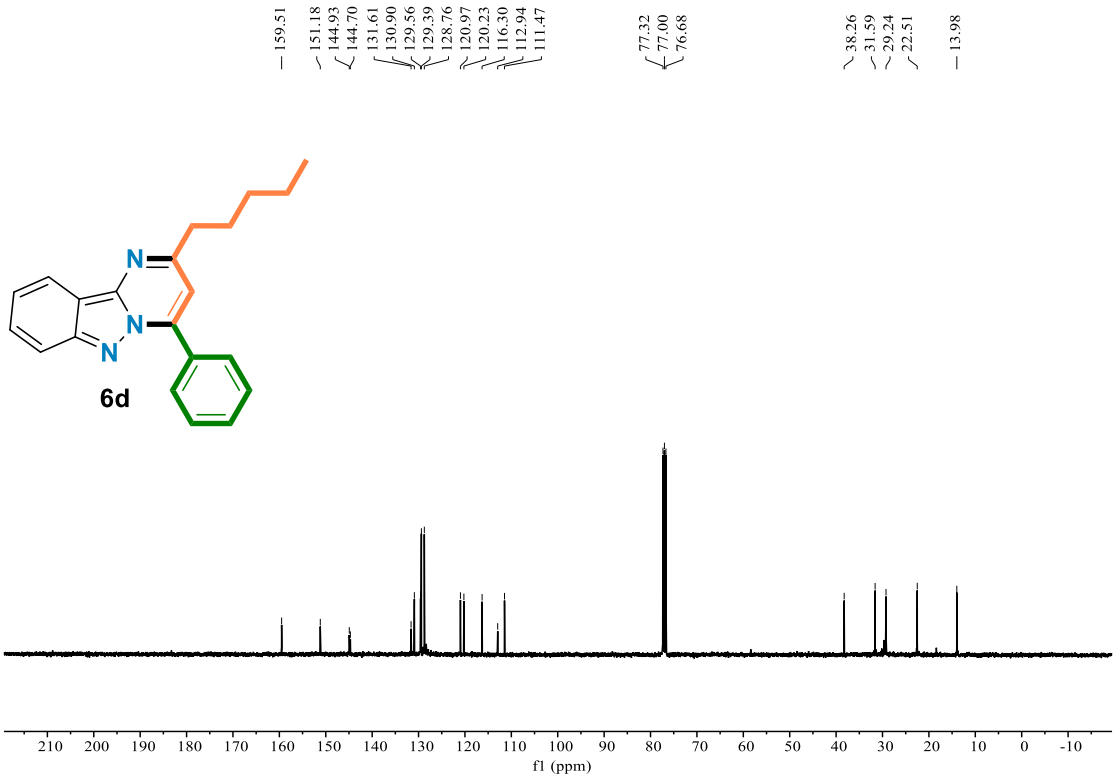
^{1}H NMR Spectrum of Compound **6c** (400 MHz, $CDCl_3$)



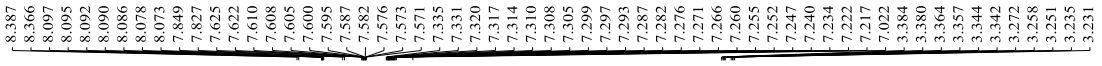
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **6c** (100 MHz, $CDCl_3$)

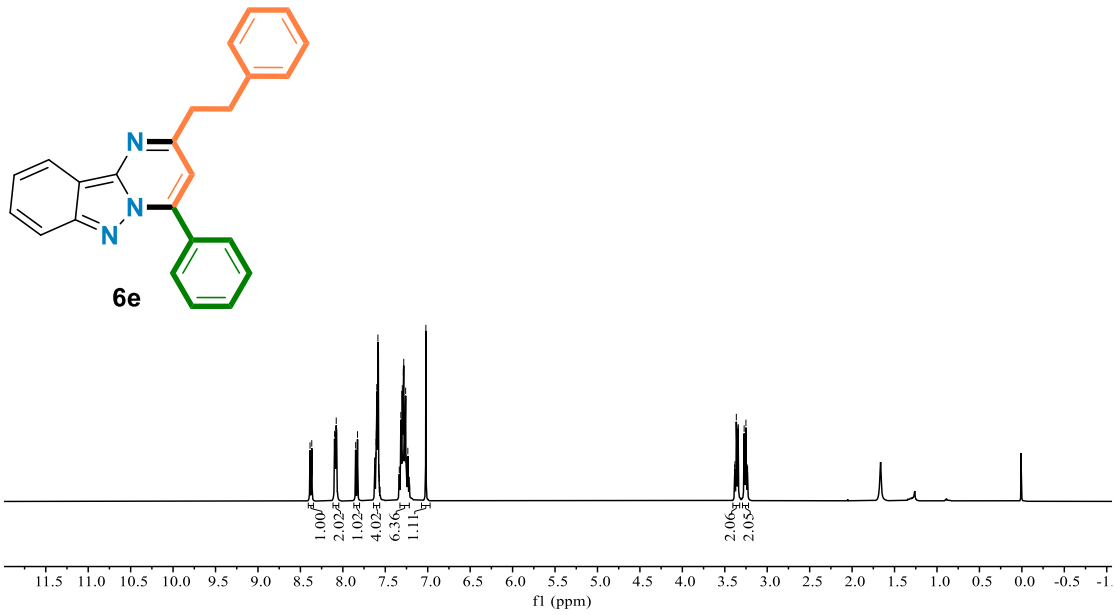


^{1}H NMR Spectrum of Compound **6d** (400 MHz, $CDCl_3$)

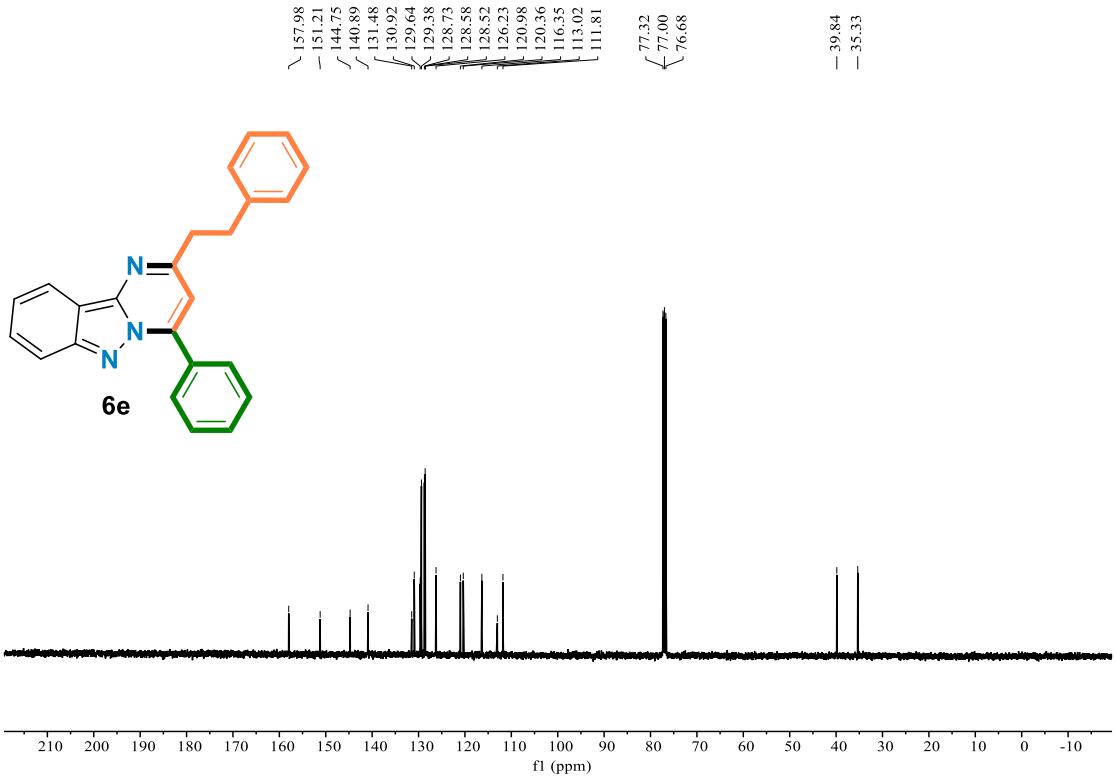


$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **6d** (100 MHz, $CDCl_3$)

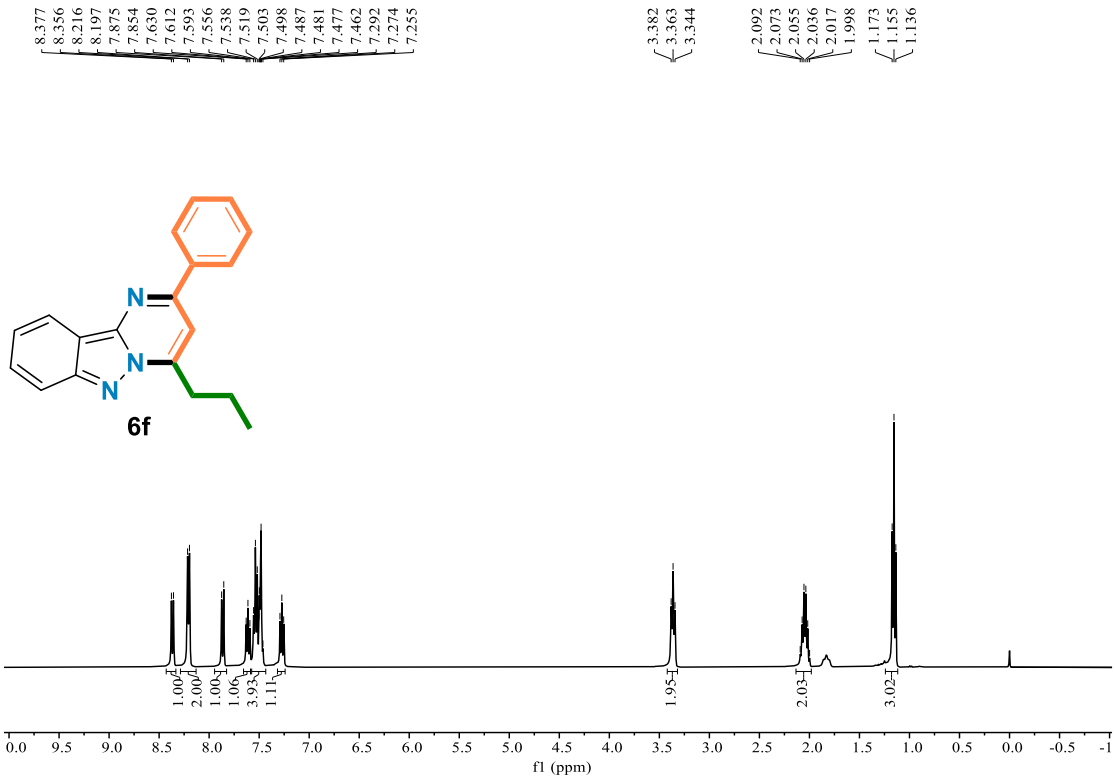




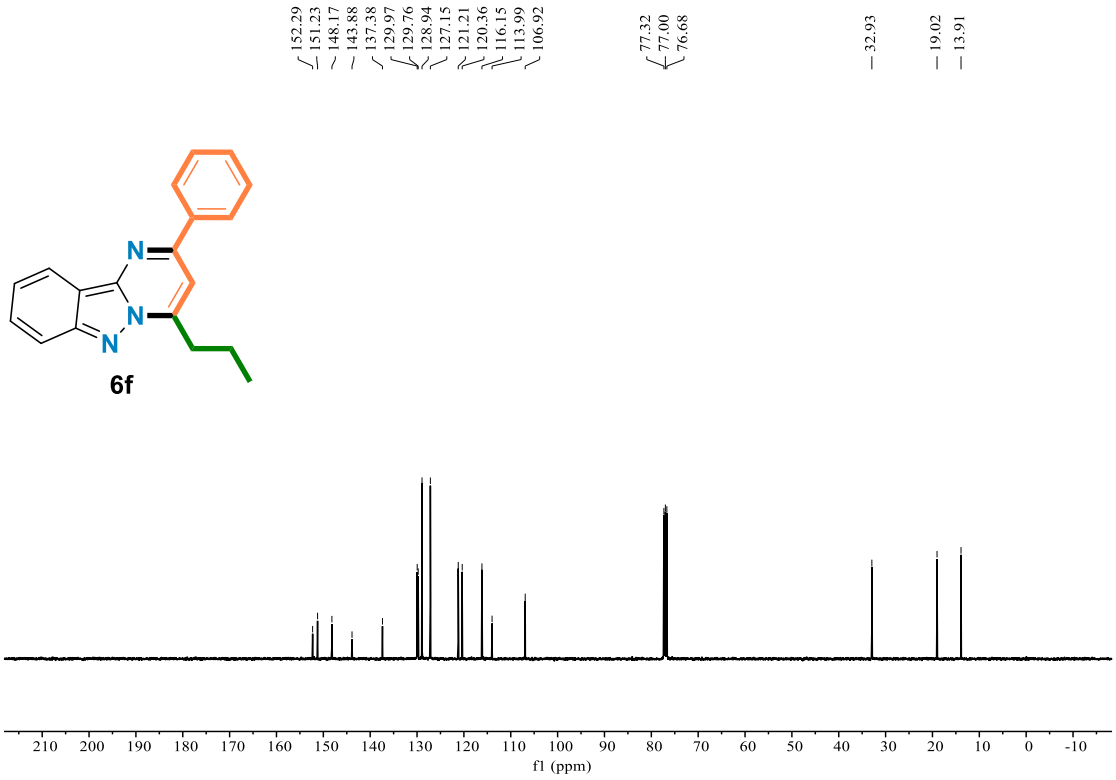
^{1}H NMR Spectrum of Compound **6e** (400 MHz, $CDCl_3$)



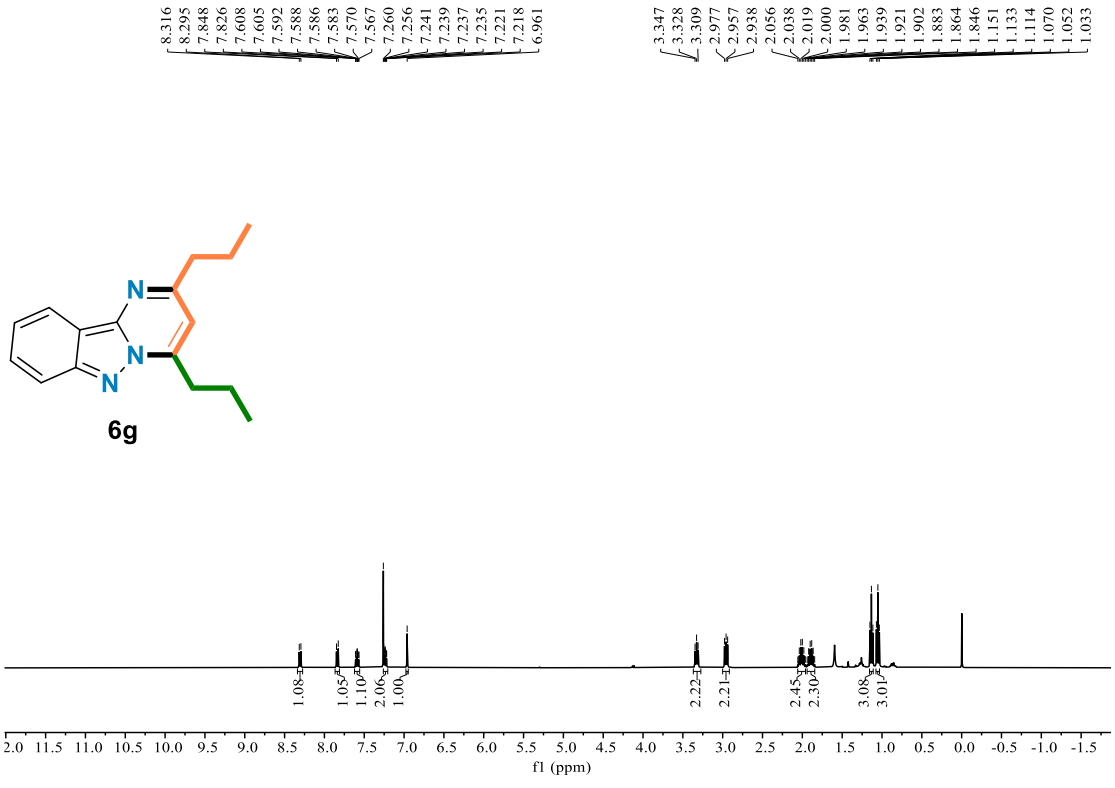
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **6e** (100 MHz, $CDCl_3$)



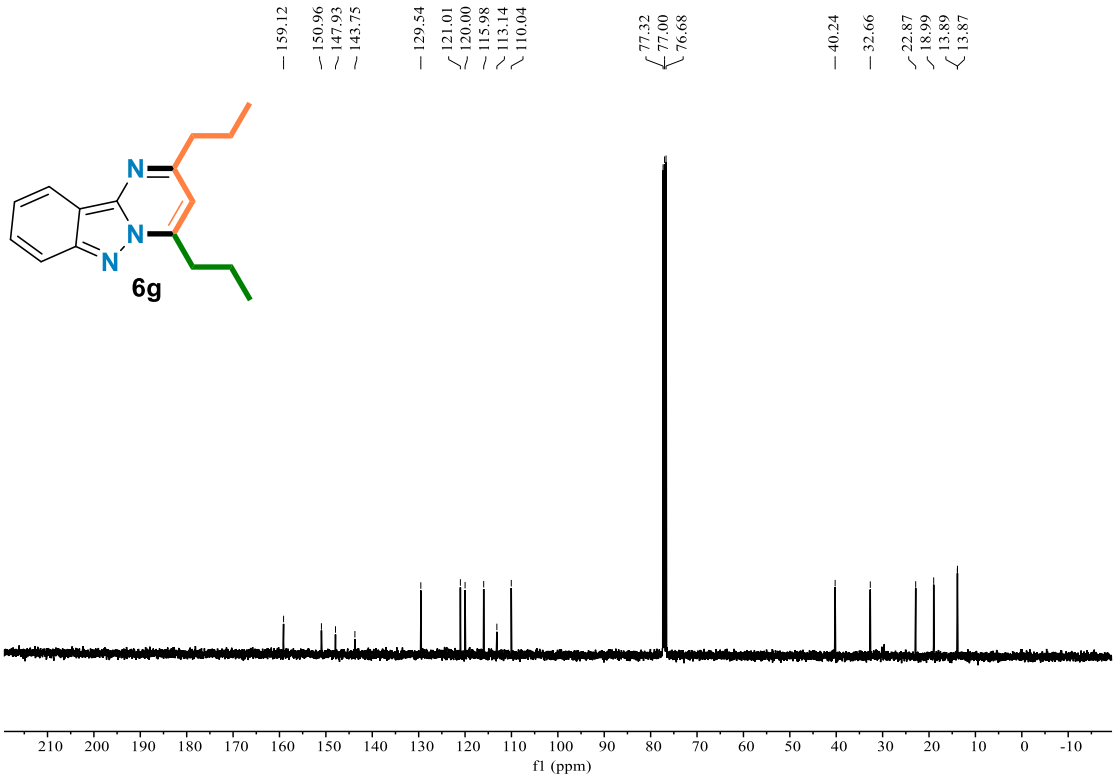
^{1}H NMR Spectrum of Compound **6f** (400 MHz, $CDCl_3$)



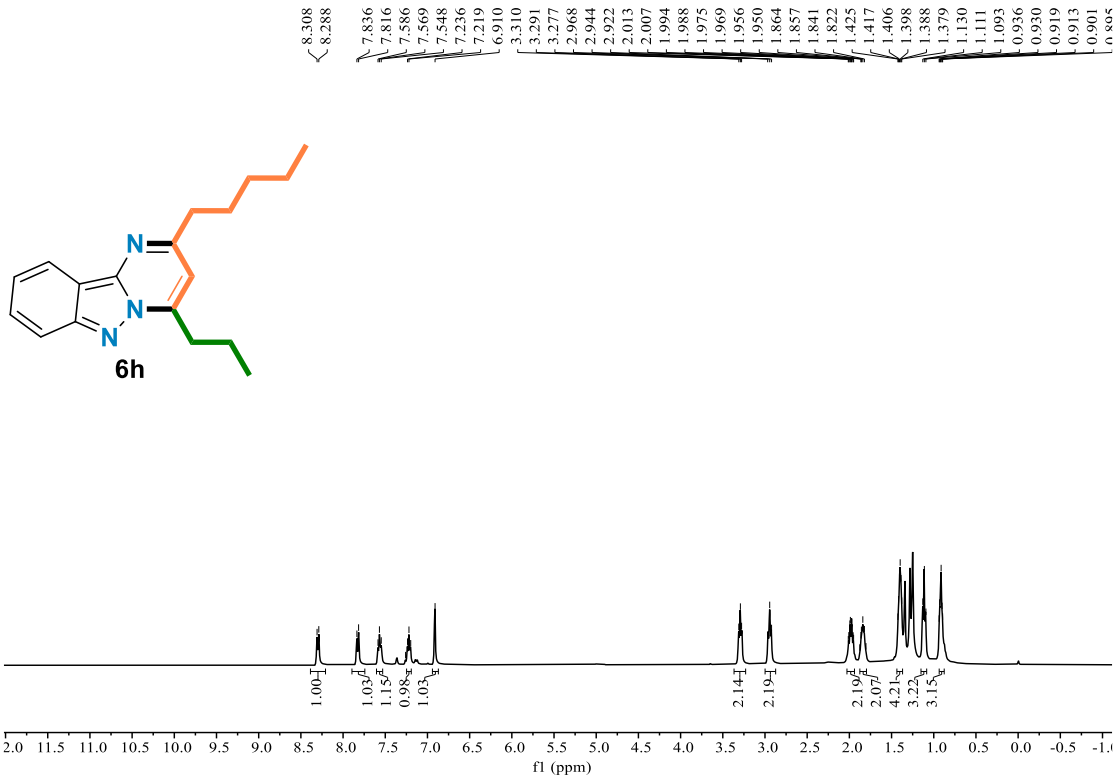
$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **6f** (100 MHz, $CDCl_3$)



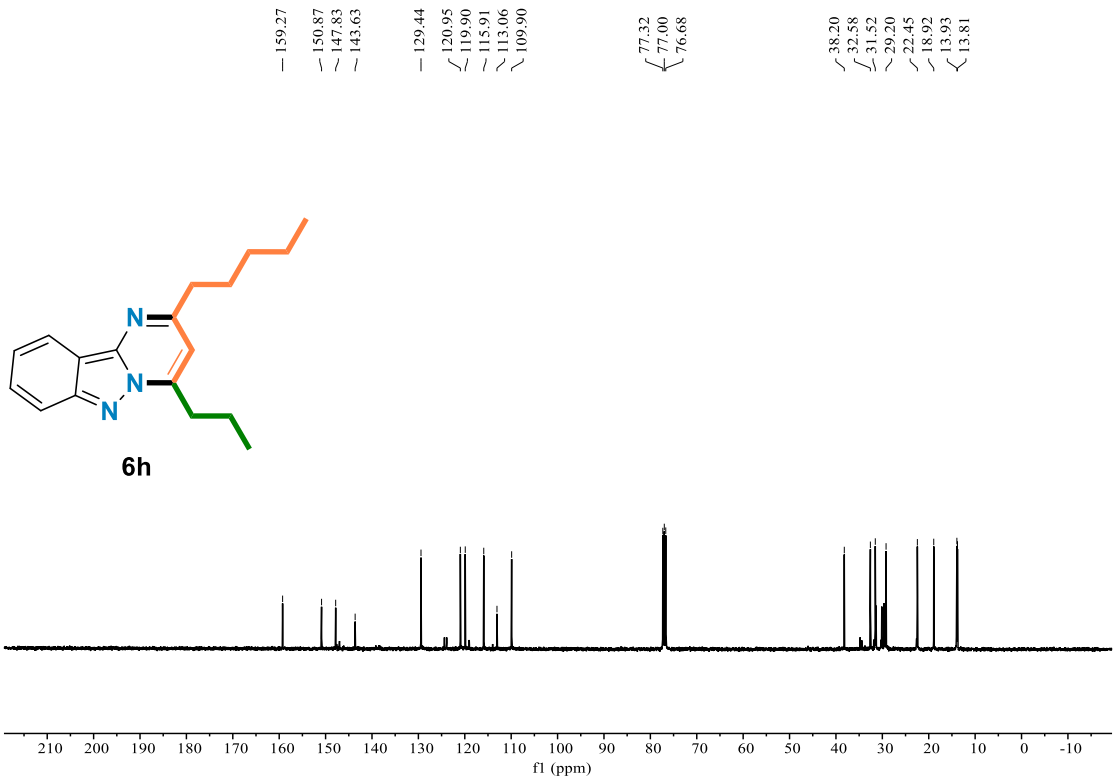
^{1}H NMR Spectrum of Compound **6g** (400 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **6g** (100 MHz, $CDCl_3$)



^{1}H NMR Spectrum of Compound **6h** (400 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR Spectrum of Compound **6h** (100 MHz, $CDCl_3$)