

# **A transition-metal-free azide-alkyne cycloaddition / hydroamination cascade reaction for the construction of triazole-fused piperazin-2-ones**

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## **Supporting Information**

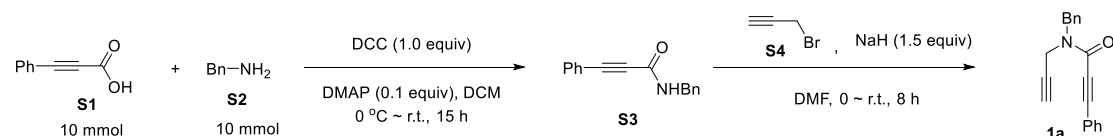
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## I. General Remarks

$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker AV-400 or 500 MHz spectrometer. Chemical shifts ( $\delta$ ) are given in relative to tetramethylsilane ( $\delta$  0.00 ppm) in  $\text{CDCl}_3$ . Coupling constants,  $J$ , were reported in hertz unit (Hz). High resolution mass spectra (HRMS) were obtained on a Q-STAR Elite ESI-LC-MS/MS Spectrometer. Chemical names were generated using Cambridge Soft. ChemDraw Ultra 16.0. Commercially obtained reagents were used without further purification.

## II. Synthesis of Substrates



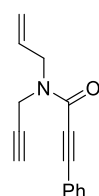
Stir a solution of **S-1** (1.46 g, 10 mmol, 1.0 equiv.), DCC (2.0 g, 10.0 mmol, 1.0 equiv.), DMAP (0.122g, 0.1 equiv) in  $\text{CH}_2\text{Cl}_2$  (20mL) at 0 °C. Benzylamine (1.07 g, 10 mmol, 1.0 equiv.) was added dropwise to the solution. Stir the reaction mixture at room temperature until full consumption of the starting material as monitored by thin layer chromatography. After completion, the reaction mixture was diluted in  $\text{CH}_2\text{Cl}_2$  and following organic content was washed 3 times by 0.5 M aq. HCl, dried over  $\text{Na}_2\text{SO}_4$ , and concentrated under reduced pressure. The crude residue was purified by a silica gel column chromatography to give the corresponding desired **S3** as white solid.

NaH (560 mg, 60% in mineral oil, 14.0 mmol, 2.0 equiv) was added to a solution of **S-3** (2.09 g, 7.0 mmol, 1.0 equiv) in DMF (20.0 mL) at 0 °C in portions. The above solution was stirred for 20 mins at 0 °C then 3-bromopropyne **S-3**(0.99 g, 8.4 mmol, 1.2 equiv) was added dropwise into the flask. The reaction mixture was allowed to stirred at room temperature for another 8 h. After completion, the reaction was quenched with water and extract with ethyl acetate three times. The organic phase was dried over  $\text{Na}_2\text{SO}_4$ , and concentrated under reduced pressure. The crude residue was purified by a silica gel column chromatography to give the corresponding desired **1a** as yellow oil.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.57 (d,  $J$  = 7.6 Hz, 1H), 7.51 (d,  $J$  = 7.6 Hz, 1H), 7.48-7.14 (m, 8H), 5.00&4.80 (s, 2H), 4.34&4.19 (s, 2H), 2.41&2.31 (s, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.3, 154.2, 135.8, 135.6, 132.6, 132.5, 130.4, 129.0, 128.8, 128.64, 128.59, 128.2, 127.93, 127.89, 120.2, 120.1, 91.4, 91.1, 81.4, 81.0, 77.82, 77.78, 73.5, 72.8, 51.6, 46.8, 37.7, 32.6. HRMS calcd for  $\text{C}_{19}\text{H}_{16}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 274.1226, found 274.1224.

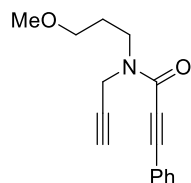
The propiolamides **1b~1ka** were prepared according to similar procedure of **1a**.

N-allyl-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1b**)



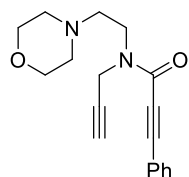
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.56-7.41 (m, 2H), 7.40 – 7.26 (m, 3H), 5.90-5.62 (m, 1H), 5.36 – 5.08 (m, 2H), 4.36&4.21 (d,  $J = 2.0$  Hz, 2H), 4.32&4.13 (d,  $J = 6.0$  Hz, 2H), 2.35&2.24 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.1, 153.9, 132.5, 132.4, 132.1, 131.6, 130.31, 130.28, 128.6, 120.14, 120.11, 118.78, 118.75, 90.9, 90.5, 81.1, 81.0, 78.0, 77.9, 73.1, 72.4, 50.6, 46.3, 37.8, 32.9. HRMS calcd for  $\text{C}_{15}\text{H}_{14}\text{NO}^+(\text{M}+\text{H})^+$ , 224.1070, found 224.1072

N-(4-methoxybutyl)-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1c**)



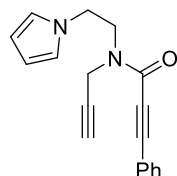
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.62-7.54 (m, 2H), 7.47-7.40 (m, 1H), 7.40-7.32 (m, 2H), 4.45&4.30 (d,  $J = 2.4$  Hz, 2H), 3.90-3.64 (t,  $J = 7.2$  Hz, 2H), 3.52-3.39 (m, 2H), 3.35&3.32 (s, 3H), 2.35&2.26 (t,  $J = 2.4$  Hz, 1H), 2.07 – 1.85 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.4, 154.3, 132.54, 132.51, 130.2, 128.5, 120.4, 120.3, 90.7, 90.4, 81.2, 78.3, 78.2, 72.9, 72.2, 70.1, 69.4, 58.7, 58.6, 46.0, 42.6, 39.2, 33.7, 28.6, 27.5. HRMS calcd for  $\text{C}_{16}\text{H}_{18}\text{NO}_2^+(\text{M}+\text{H})^+$ , 256.1332, found 256.1331

N-(2-morpholinoethyl)-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1d**)



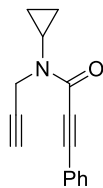
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.60 – 7.56 (m, 1H), 7.55 – 7.51 (m, 1H), 7.49-7.40 (m, 1H), 7.41-7.34 (m, 2H), 4.61&4.41 (d,  $J = 2.4$  Hz, 2H), 3.90 (t,  $J = 6.4$  Hz, 1H), 3.77-3.57 (m, 5H), 2.67&2.61 (t,  $J = 6.4$  Hz, 2H), 2.59-2.46 (m, 4H), 2.32 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.4, 154.2, 132.5, 132.3, 130.3, 128.7, 128.6, 120.3, 91.0, 90.3, 81.4, 81.1, 78.3, 78.2, 73.1, 72.5, 67.03, 66.96, 57.1, 56.2, 53.9, 53.7, 45.1, 40.7, 39.5, 34.1. HRMS calcd for  $\text{C}_{18}\text{H}_{21}\text{N}_2\text{O}_2^+(\text{M}+\text{H})^+$ , 297.1598, found 297.1595

N-(2-(1H-pyrrol-1-yl)ethyl)-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1e**)



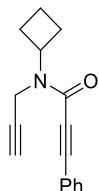
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.63 – 7.54 (m, 2H), 7.51 – 7.36 (m, 3H), 6.74 – 6.63 (m, 2H), 6.25 – 6.14 (m, 2H), 4.25&4.18 (t,  $J = 6.4$  Hz, 2H), 4.13 – 4.04 (m, 2H), 3.91 (d,  $J = 2.4$  Hz, 1H), 3.83 (t,  $J = 6.0$  Hz, 1H), 2.34 – 2.28 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.3, 154.2, 132.6, 132.5, 130.5, 130.4, 128.7, 128.6, 120.74, 120.72, 120.0, 109.3, 109.1, 91.3, 90.7, 80.8, 80.7, 78.03, 77.98, 73.1, 72.9, 49.7, 48.3, 47.2, 46.6, 39.6, 34.2. HRMS calcd for  $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}^+(\text{M}+\text{H})^+$ , 277.1335, found 277.1336

N-cyclopropyl-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1f**)



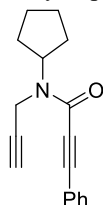
yellow solid, melt point (78-81 °C)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.60 – 7.53 (m, 2H), 7.48 – 7.34 (m, 3H), 4.39&4.23 (d,  $J = 2.4$  Hz, 2H), 3.02 – 2.77 (m, 1H), 2.33&2.22 (t,  $J = 2.4$  Hz, 1H), 1.05 – 0.83 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  156.5, 132.53, 132.46, 130.24, 130.16, 128.6, 120.7, 91.5, 82.7, 78.8, 72.4, 71.4, 39.9, 35.7, 30.3, 28.5, 8.9, 7.1. HRMS calcd for  $\text{C}_{15}\text{H}_{14}\text{NO}^+(\text{M}+\text{H})^+$ , 224.1070, found 224.1072

N-cyclobutyl-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1g**)



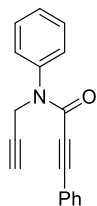
yellow solid, melt point (80-83 °C)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.55 (d,  $J = 6.8$  Hz, 2H), 7.45 – 7.31 (m, 3H), 4.99 – 4.75 (m, 1H), 4.41&4.27 (d,  $J = 2.4$  Hz, 2H), 2.55-2.09(m, 5H), 1.84 – 1.62 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.3, 153.8, 132.5, 132.4, 130.18, 130.15, 128.6, 128.5, 120.5, 120.4, 90.9, 90.3, 81.8, 81.6, 79.81, 79.78, 72.2, 71.0, 53.0, 49.3, 35.4, 30.5, 29.0, 28.5, 15.3, 14.8. HRMS calcd for  $\text{C}_{16}\text{H}_{16}\text{NO}^+(\text{M}+\text{H})^+$ , 238.1226, found 238.1228

N-cyclopentyl-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1h**)



yellow solid, melt point (83-85 °C)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.61 – 7.18 (m, 5H), 4.91-4.59 (m,  $J = 24.9, 8.3$  Hz, 1H), 4.28&4.08 (d,  $J = 2.4$  Hz, 2H), 2.31&2.17 (t,  $J = 2.0$  Hz, 1H), 2.04 – 1.85 (m, 2H), 1.81 – 1.49 (m, 6H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.7, 154.3, 132.5, 132.3, 130.13, 130.09, 128.6, 128.5, 120.5, 120.4, 90.7, 90.3, 81.9, 81.5, 80.1, 79.9, 72.1, 70.9, 60.3, 55.5, 35.2, 30.4, 29.8, 28.9, 24.0, 23.8. HRMS calcd for  $\text{C}_{17}\text{H}_{18}\text{NO}^+(\text{M}+\text{H})^+$ , 252.1383, found 252.1382

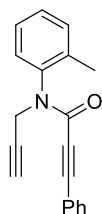
N,3-diphenyl-N-(prop-2-yn-1-yl)propiolamide (**1i**)



yellow solid, melt point (80-83 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.55 – 7.38 (m, 5H),

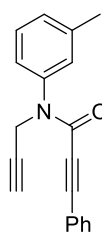
7.36 – 7.30 (m, 1H), 7.28-7.18 (m, 2H), 7.18 – 7.05 (m, 2H), 4.60 (d,  $J = 2.8$  Hz, 2H), 2.27 (t,  $J = 2.4$  Hz, 1H).<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  153.9, 141.1, 132.5, 130.2, 129.2, 128.7, 128.5, 128.4, 120.1, 91.8, 82.1, 78.3, 72.7, 37.8. HRMS calcd for C<sub>18</sub>H<sub>14</sub>NO<sup>+</sup>(M+H)<sup>+</sup>, 260.1070, found 260.1073

3-phenyl-N-(prop-2-yn-1-yl)-N-(o-tolyl)propiolamide (**1j**)



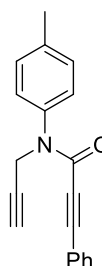
yellow oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  7.41 – 7.26 (m, 5H), 7.21 (t,  $J = 7.6$  Hz, 2H), 7.10 – 7.02 (m, 2H), 4.76&4.73 (d,  $J = 2.4$  Hz, 1H), 4.37&4.33 (d,  $J = 2.4$  Hz, 1H), 2.36 (s, 3H), 2.24 (t,  $J = 2.4$  Hz, 1H).<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  154.3, 139.8, 137.2, 132.7, 132.6, 131.0, 130.2, 129.7, 129.1, 128.7, 128.4, 126.9, 120.1, 90.6, 82.0, 77.9, 77.6, 77.2, 76.9, 72.8, 37.0, 17.8. HRMS calcd for C<sub>19</sub>H<sub>16</sub>NO<sup>+</sup>(M+H)<sup>+</sup>, 274.1226, found 274.1225

3-phenyl-N-(prop-2-yn-1-yl)-N-(m-tolyl)propiolamide (**1k**)



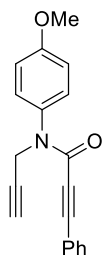
yellow oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  7.40 – 7.21 (m, 7H), 7.19-7.11 (m, 2H), 4.60 (d,  $J = 2.4$  Hz, 2H), 2.43 (s, 3H), 2.40&2.27 (t,  $J = 2.4$  Hz, 1H).<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  153.9, 141.0, 139.2, 132.5, 130.1, 129.3, 128.9, 128.8, 128.6, 128.4, 125.5, 120.3, 91.6, 82.2, 78.4, 72.5, 37.8, 21.3. HRMS calcd for C<sub>19</sub>H<sub>16</sub>NO<sup>+</sup>(M+H)<sup>+</sup>, 274.1226, found 274.1227

3-phenyl-N-(prop-2-yn-1-yl)-N-(p-tolyl)propiolamide (**1l**)



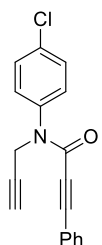
yellow oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  7.49 – 7.20 (m, 7H), 7.19-7.03 (m,  $J = 7.5$  Hz, 2H), 4.56 (d,  $J = 1.6$  Hz, 2H), 2.54 – 2.18 (m, 4H).<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  154.0, 138.6, 138.5, 132.5, 130.1, 129.8, 128.4, 128.2, 120.3, 91.6, 82.3, 78.4, 72.6, 37.8, 21.3. HRMS calcd for C<sub>19</sub>H<sub>16</sub>NO<sup>+</sup>(M+H)<sup>+</sup>, 274.1226, found 274.1227

N-(4-methoxyphenyl)-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1m**)



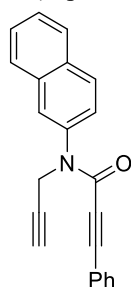
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.42-7.31 (m, 3H), 7.29 – 7.22 (m, 2H), 7.22-7.13 (m, 2H), 6.99 (d,  $J = 8.8$  Hz, 2H), 4.57 (d,  $J = 2.4$  Hz, 2H), 3.88 (s, 3H), 2.27 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  159.6, 154.2, 133.9, 132.5, 130.1, 129.8, 128.4, 120.3, 114.3, 91.8, 82.2, 78.4, 72.6, 55.6, 37.9. HRMS calcd for  $\text{C}_{19}\text{H}_{16}\text{NO}_2^+(\text{M}+\text{H})^+$ , 290.1176, found 290.1175

N-(4-chlorophenyl)-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1n**)



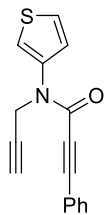
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.66 – 7.34 (m, 6H), 7.36-7.24 (m,  $J = 7.2$  Hz, 1H), 7.18 (d,  $J = 7.6$  Hz, 2H), 4.59 (s, 2H), 2.28 (s, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  153.6, 139.6, 134.5, 132.5, 130.4, 129.9, 129.4, 128.5, 119.9, 92.2, 81.9, 78.0, 73.0, 37.7. HRMS calcd for  $\text{C}_{18}\text{H}_{13}\text{ClNO}^+(\text{M}+\text{H})^+$ , 294.0680, found 294.0680

N-(naphthalen-2-yl)-3-phenyl-N-(prop-2-yn-1-yl)propiolamide (**1o**)



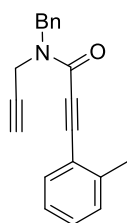
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  8.02 – 7.88 (m, 4H), 7.67 – 7.51 (m, 3H), 7.26 (t,  $J = 7.6$  Hz, 1H), 7.14 (t,  $J = 7.6$  Hz, 2H), 7.01 (d,  $J = 7.6$  Hz, 2H), 4.71 (d,  $J = 2.4$  Hz, 2H), 2.30 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.0, 138.4, 133.3, 132.9, 132.4, 130.1, 129.1, 128.3, 128.1, 127.8, 127.1, 127.0, 126.9, 126.0, 120.0, 92.0, 82.3, 78.3, 77.5, 72.8, 38.0. HRMS calcd for  $\text{C}_{22}\text{H}_{16}\text{NO}^+(\text{M}+\text{H})^+$ , 310.1226, found 310.1222

3-phenyl-N-(prop-2-yn-1-yl)-N-(thiophen-3-yl)propiolamide (**1p**)



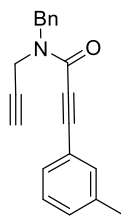
yellow oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.61 – 7.30 (m, 4H), 7.29-7.21 (m, 2H), 7.20 (d,  $J = 4.8$  Hz, 1H), 4.84&4.55 (d,  $J = 2.4$  Hz, 2H), 2.43&2.29 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  153.9, 139.2, 132.7, 130.6, 130.3, 128.7, 128.5, 126.6, 125.2, 124.6, 123.6, 122.4, 120.1, 116.2, 91.6, 81.9, 78.4, 73.6, 72.7, 41.8, 37.6. HRMS calcd for  $\text{C}_{16}\text{H}_{12}\text{NOS}^+(\text{M}+\text{H})^+$ , 266.0634, found 266.0635

N-benzyl-N-(prop-2-yn-1-yl)-3-(o-tolyl)propionamide (**1q**)



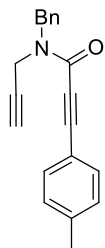
yellow oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.63-7.46 (m, 1H), 7.46 – 7.30 (m, 6H), 7.29 – 7.10 (m, 2H), 5.06&4.83 (s, 2H), 4.38&4.23 (s, 2H), 2.53&2.42(s, 3H), 2.38&2.30 (s, 1H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.4, 141.6, 141.5, 135.9, 135.6, 133.2, 133.1, 130.37, 130.35, 129.8, 128.9, 128.8, 128.7, 128.2, 127.9, 127.8, 125.9, 120.1, 90.5, 90.2, 85.0, 84.7, 77.85, 77.81, 73.3, 72.6, 51.5, 46.8, 37.6, 32.6, 20.8, 20.7. HRMS calcd for  $\text{C}_{20}\text{H}_{18}\text{NO}^+(\text{M}+\text{H})^+$ , 288.1383, found 288.1386.

N-benzyl-N-(prop-2-yn-1-yl)-3-(m-tolyl)propionamide (**1r**)



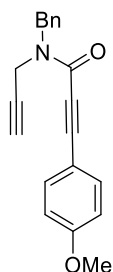
yellow oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.51 – 7.05 (m, 9H), 5.03&4.83(s, 2H), 4.36&4.21 (s, 2H), 2.48 – 2.12 (m, 4H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.4, 154.3, 138.4, 135.8, 135.6, 133.0, 131.3, 129.7, 129.0, 128.8, 128.6, 128.5, 128.2, 127.94, 127.90, 120.0, 91.7, 91.4, 81.0, 80.7, 77.82, 77.79, 73.3, 72.6, 51.6, 46.74, 37.66, 32.5, 21.22, 21.20. HRMS calcd for  $\text{C}_{20}\text{H}_{18}\text{NO}^+(\text{M}+\text{H})^+$ , 288.1383, found 288.1385.

N-benzyl-N-(prop-2-yn-1-yl)-3-(p-tolyl)propionamide (**1s**)



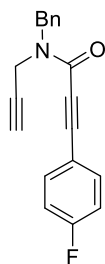
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.49 (d,  $J = 8.0$  Hz, 1H), 7.43 (d,  $J = 8.0$  Hz, 1H), 7.45 – 7.28 (m, 5H), 7.19 (t,  $J = 8.8$  Hz, 2H), 5.03&4.82(s, 2H), 4.36&4.21 (d,  $J = 2.4$ &2.8 Hz, 2H), 2.34 (s, 3H), 2.40-2.25(m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.5, 154.4, 140.9, 135.9, 135.7, 132.6, 132.5, 129.4, 128.0, 128.8, 128.6, 128.2, 127.9, 127.8, 117.08, 117.06, 91.9, 91.6, 81.0, 80.6, 77.9, 77.8, 73.4, 72.7, 51.6, 46.7, 37.7, 32.5, 21.7. HRMS calcd for  $\text{C}_{20}\text{H}_{18}\text{NO}^+(\text{M}+\text{H})^+$ , 288.1383, found 288.1382.

N-benzyl-3-(4-methoxyphenyl)-N-(prop-2-yn-1-yl)propiolamide (**1t**)



yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.53(d,  $J = 8.8$  Hz, 1H), 7.47 (d,  $J = 8.4$  Hz, 1H), 7.42-7.25 (m, 5H), 6.88 (t,  $J = 9.2$  Hz, 2H), 5.00&4.80(s, 2H), 4.27&4.19 (d,  $J = 2.0$  Hz, 2H), 3.87-3.77 (m, 3H), 2.44-2.16 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  161.3, 154.6, 154.5, 135.9, 135.7, 134.4, 134.3, 128.9, 128.8, 128.6, 128.1, 127.9, 127.8, 114.3, 112.0, 111.9, 92.1, 91.8, 80.7, 80.3, 77.92, 77.88, 73.3, 72.6, 55.4, 51.6, 46.7, 37.7, 32.5. HRMS calcd for  $\text{C}_{20}\text{H}_{18}\text{NO}_2^+(\text{M}+\text{H})^+$ , 304.1332, found 304.1331.

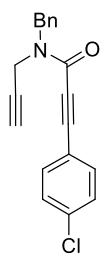
N-benzyl-3-(4-fluorophenyl)-N-(prop-2-yn-1-yl)propiolamide (**1u**)



yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.61 – 7.45 (m, 2H), 7.42 – 7.26 (m, 5H), 7.12 – 7.00 (m, 2H), 5.00&4.80 (s,  $J = 78.9$  Hz, 2H), 4.27& 4.20(d,  $J = 2.4$  Hz, 2H), 2.39&2.29 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  163.7 (d,  $J = 251.3$  Hz), 154.2, 154.1, 135.7, 135.5, 134.77&134.73(d,  $J = 8.8$  Hz), 129.0, 128.8, 128.6, 128.2, 127.9, 127.8, 116.33, 116.30, 116.26, 116.1 (d,  $J = 22.2$  Hz), 90.4, 90.1, 81.2, 80.8, 77.74, 77.69, 73.4, 72.4, 51.6, 46.8, 37.7, 32.6. HRMS calcd for  $\text{C}_{19}\text{H}_{15}\text{FNO}^+(\text{M}+\text{H})^+$ , 292.1132, found 292.1133.

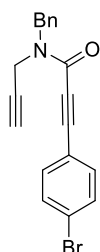


N-benzyl-3-(4-chlorophenyl)-N-(prop-2-yn-1-yl)propiolamide (**1v**)



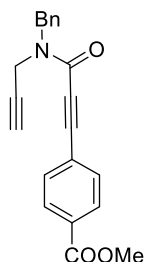
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.57 – 7.43 (m, 2H), 7.43 – 7.30 (m, 7H), 5.00&4.81 (s, 2H), 4.33&4.21 (d,  $J = 2.4$  Hz, 2H), 2.38&2.28 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.1, 154.0, 136.67, 135.65, 135.5, 133.8, 133.7, 129.1, 129.0, 128.8, 128.6, 128.2, 128.0, 127.8, 118.7, 118.6, 90.1, 89.8, 82.1, 81.7, 77.7, 77.6, 73.3, 72.6, 51.6, 46.8, 37.63, 32.61. HRMS calcd for  $\text{C}_{19}\text{H}_{15}\text{ClNO}^+(\text{M}+\text{H})^+$ , 308.0837, found 308.0838.

N-benzyl-3-(4-bromophenyl)-N-(prop-2-yn-1-yl)propiolamide (**1w**)



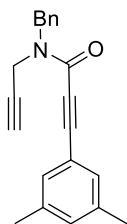
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.58 – 7.47 (m, 2H), 7.47 – 7.30 (m, 7H), 5.00&4.81 (s, 2H), 4.33&4.20 (d,  $J = 2.4$  Hz, 2H), 2.38&2.28 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.1, 154.0, 135.6, 135.4, 133.9, 133.8, 132.0, 129.0, 128.8, 128.6, 128.3, 128.0, 127.8, 125.0, 119.12, 119.07, 90.2, 89.9, 82.2, 81.9, 77.7, 77.6, 73.4, 72.7, 51.6, 46.8, 37.7, 32.6. HRMS calcd for  $\text{C}_{19}\text{H}_{15}\text{BrNO}^+(\text{M}+\text{H})^+$ , 354.0311, found 354.0314.

methyl 4-(3-(benzyl(prop-2-yn-1-yl)amino)-3-oxoprop-1-yn-1-yl)benzoate (**1x**)



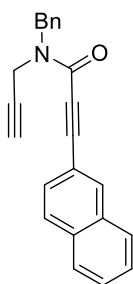
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  8.02 (t,  $J = 8.4$  Hz, 2H), 7.62 (d,  $J = 8.4$  Hz, 1H), 7.57 (d,  $J = 8.4$  Hz, 1H), 7.41 – 7.27 (m, 5H), 4.99&7.80 (s, 2H), 4.33&4.19 (d,  $J = 2.4$  Hz, 2H), 3.96-3.80 (m, 3H), 2.40&2.30 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  166.05, 166.03, 153.9, 153.8, 135.6, 135.4, 132.40, 132.37, 131.4, 129.6, 129.0, 128.8, 128.6, 128.3, 128.0, 127.8, 124.7, 124.6, 90.0, 89.7, 83.4, 83.0, 77.60, 77.55, 73.5, 72.8, 52.4, 51.6, 46.9, 37.7, 32.7. HRMS calcd for  $\text{C}_{21}\text{H}_{18}\text{NO}_3^+(\text{M}+\text{H})^+$ , 332.1281, found 332.1281.

N-benzyl-3-(3,5-dimethylphenyl)-N-(prop-2-yn-1-yl)propiolamide (**1y**)



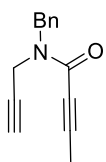
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.45 – 7.29 (m, 5H), 7.22 (s, 1H), 7.17 (s, 1H), 7.11-7.03 (m, 1H), 5.03&4.83 (s, 2H), 4.36&4.21 (d,  $J = 2.4$  Hz, 2H), 2.51 – 2.19 (m, 7H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.5, 154.4, 138.3, 135.9, 135.7, 132.3, 130.2, 128.9, 128.8, 128.6, 128.2, 128.0, 127.9, 119.80, 119.77, 92.0, 91.7, 80.7, 80.4, 77.84, 77.82, 73.3, 72.6, 51.6, 46.7, 37.7, 32.5, 21.09, 21.07. HRMS calcd for  $\text{C}_{21}\text{H}_{20}\text{NO}^+(\text{M}+\text{H})^+$ , 302.1539, found 302.1538.

N-benzyl-3-(naphthalen-2-yl)-N-(prop-2-yn-1-yl)propiolamide (**1z**)



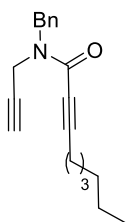
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  8.22-8.04 (m, 1H), 7.91-6.76 (m, 3H), 7.64 – 7.46 (m, 3H), 7.48 – 7.32 (m, 5H), 5.08&4.85 (s, 2H), 4.41&4.24 (d,  $J = 2.4$  Hz, 2H), 2.40&2.30 (t,  $J = 2.4$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.4, 154.3, 135.8, 135.7, 133.7, 133.6, 132.7, 129.0, 128.8, 128.7, 128.4, 128.3, 128.13, 128.11, 128.09, 128.0, 127.94, 127.90, 127.8, 127.0, 117.39, 117.35, 91.9, 91.6, 81.5, 81.2, 77.9, 77.8, 73.4, 72.6, 51.8, 46.8, 37.7, 32.6. HRMS calcd for  $\text{C}_{23}\text{H}_{18}\text{NO}^+(\text{M}+\text{H})^+$ , 324.1383, found 324.1384

N-benzyl-N-(prop-2-yn-1-yl)but-2-ynamide (**1aa**)



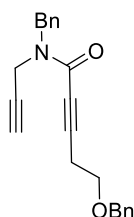
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.69 – 7.02 (m, 5H), 4.92&4.74 (s, 2H), 4.26&4.12 (s, 2H), 2.34&2.23 (s, 1H), 2.05&2.02 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.3, 135.9, 135.7, 128.9, 128.7, 128.5, 128.1, 127.8, 90.4, 90.1, 77.9, 77.8, 73.1, 72.8, 72.4, 51.4, 46.4, 37.5, 32.3, 4.1. HRMS calcd for  $\text{C}_{14}\text{H}_{14}\text{NO}^+(\text{M}+\text{H})^+$ , 212.1070, found 212.1070

N-benzyl-N-(prop-2-yn-1-yl)oct-2-ynamide (**1ba**)



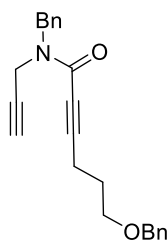
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.44 – 7.25 (m, 5H), 4.91&4.73 (s, 2H), 4.25&4.12(d,  $J = 2.4$  Hz, 2H), 2.43 – 2.33 (m, 2H), 2.33&2.23 (t,  $J = 2.4$  Hz, 1H), 1.67 – 1.49 (m, 2H), 1.47 – 1.20 (m, 4H), 0.96-0.76 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.4, 135.9, 135.7, 128.8, 128.7, 128.5, 128.0, 127.8, 94.6, 94.3, 77.9, 73.8, 73.7, 73.0, 72.4, 51.4, 46.5, 37.5, 32.3, 31.01, 30.99, 27.39, 27.36, 22.11, 22.07, 18.94, 18.92, 13.90, 13.86. HRMS calcd for  $\text{C}_{18}\text{H}_{22}\text{NO}^+(\text{M}+\text{H})^+$ , 268.1696, found 268.1696

N-benzyl-5-(benzyloxy)-N-(prop-2-yn-1-yl)pent-2-ynamide (**1ca**)



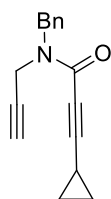
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.43 – 7.18 (m, 10H), 4.93&4.76 (s, 2H), 4.58&4.52 (s, 2H), 4.26&4.14(d,  $J = 2.4$  Hz, 2H), 3.75-3.59 (m, 2H), 2.71 (q,  $J = 2.8$  Hz, 2H), 2.33&2.25 (t,  $J = 2.0$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.1, 137.8, 137.7, 135.8, 135.7, 128.9, 128.7, 128.6, 128.50, 128.46, 128.1, 127.9, 127.83, 127.80, 127.77, 127.7, 91.1, 90.9, 77.9, 77.8, 74.5, 74.22, 73.16, 73.1, 72.4, 67.3, 51.4, 46.5, 37.5, 32.3, 20.6. HRMS calcd for  $\text{C}_{22}\text{H}_{22}\text{NO}_2^+(\text{M}+\text{H})^+$ , 332.1645, found 332.1645

N-benzyl-6-(benzyloxy)-N-(prop-2-yn-1-yl)hex-2-ynamide (**1da**)



yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.47 – 7.13 (m, 10H), 4.90&4.75 (s, 2H), 4.54&4.46 (s, 2H), 4.15&4.14 (d,  $J = 2.4$  Hz, 2H), 3.61&3.54 (t,  $J = 2.4$  Hz, 2H), 2.60-2.46 (m, 2H), 2.32&2.25 (t,  $J = 2.4$  Hz, 1H), 2.01 – 1.80 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.3, 138.2, 135.7, 128.9, 128.7, 128.6, 128.4, 128.1, 127.82, 127.75, 127.7, 127.6, 93.8, 93.5, 77.92, 77.86, 73.9, 73.7, 73.1, 73.0, 72.4, 68.44, 68.39, 51.4, 46.5, 37.5, 32.4, 28.03, 28.01, 16.00, 15.97. HRMS calcd for  $\text{C}_{23}\text{H}_{24}\text{NO}_2^+(\text{M}+\text{H})^+$ , 346.1802, found 346.1805

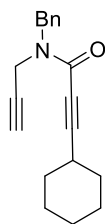
N-benzyl-3-cyclopropyl-N-(prop-2-yn-1-yl)propiolamide (**1ea**)



yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.40 – 7.16 (m, 5H), 4.84&4.68 (s, 2H), 4.18&4.06(d,  $J = 2.4$  Hz, 2H), 2.33&2.22 (t,  $J = 2.4$  Hz, 1H), 1.43 – 1.30 (m, 1H), 0.99 – 0.71 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.3, 154.2, 135.9, 135.8, 128.8, 128.7, 128.4,

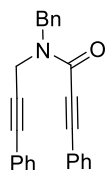
128.0, 127.7, 97.9, 97.6, 77.9, 73.2, 72.5, 69.0, 68.7, 51.3, 46.5, 37.5, 32.3, 9.18, 9.15. HRMS calcd for  $C_{16}H_{16}NO^+(M+H)^+$ , 238.1226, found 238.1227

N-benzyl-3-cyclohexyl-N-(prop-2-yn-1-yl)propiolamide (**1fa**)



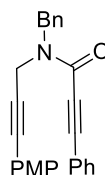
yellow oil;  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  7.41– 7.20 (m, 5H), 4.90&4.72 (s, 2H), 4.24&4.11 (d,  $J = 2.4$  Hz, 2H), 2.62 – 2.50 (m, 1H), 2.33&2.23 (t,  $J = 2.4$  Hz, 1H), 1.88 – 1.75 (m, 2H), 1.74 – 1.59 (m, 2H), 1.59 – 1.23 (m, 6H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  154.5, 154.4, 134.0, 135.8, 128.8, 128.7, 128.5, 128.0, 127.80, 127.75, 97.9, 97.5, 77.9, 73.8, 73.4, 73.0, 72.4, 51.4, 46.5, 37.6, 32.3, 31.6, 31.5, 29.1, 25.7, 25.6, 24.60, 24.56. HRMS calcd for  $C_{19}H_{22}NO^+(M+H)^+$ , 280.1696, found 280.1695

N-benzyl-3-phenyl-N-(3-phenylprop-2-yn-1-yl)propiolamide (**1ga**)



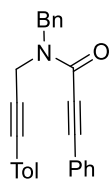
yellow oil;  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  7.63 – 7.31 (m, 15H), 5.10&4.90 (s, 2H), 4.61-4.47 (s, 2H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  154.4, 154.3, 136.0, 135.8, 132.6, 132.5, 131.9, 131.8, 130.3, 129.0, 128.8, 128.7, 128.64, 128.60, 128.5, 128.4, 128.3, 128.2, 127.93, 127.86, 122.5, 122.3, 120.32, 120.25, 91.5, 91.0, 85.1, 84.4, 83.13, 83.08, 81.4, 81.2, 51.8, 47.1, 38.7, 33.5. HRMS calcd for  $C_{25}H_{20}NO^+(M+H)^+$ , 350.1539, found 350.1537

N-benzyl-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-3-phenylpropiolamide (**1ha**)



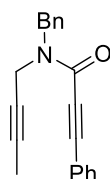
yellow oil;  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  7.68-5.59 (m, 1H), 7.57 – 7.53 (m, 1H), 7.47 – 7.33 (m, 9H), 6.93-6.82 (m, 2H), 5.10&4.90 (s, 2H), 4.60&4.46 (s, 2H), 3.82(s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  159.9, 159.8, 154.3, 136.0, 135.9, 133.30, 133.25, 132.54, 132.51, 130.2, 128.9, 128.7, 128.62, 128.56, 128.1, 127.9, 127.8, 120.3, 114.6, 114.4, 114.0, 113.9, 91.4, 90.9, 85.0, 84.3, 81.62, 81.60, 81.5, 81.2, 55.3, 51.7, 47.0 38.8, 33.6. HRMS calcd for  $C_{26}H_{22}NO_2^+(M+H)^+$ , 380.1645, found 380.1649

N-benzyl-3-phenyl-N-(3-(p-tolyl)prop-2-yn-1-yl)propiolamide (**1ia**)



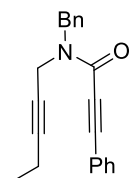
yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.68-7.49 (m, 2H), 7.49 – 7.31 (m, 10H), 7.20 – 7.11 (m, 2H), 5.11&4.91 (s, 2H), 4.62&4.48 (s, 2H), 2.37 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.4, 154.3, 138.9, 138.7, 136.1, 135.9, 132.6, 132.5, 131.8, 131.7, 130.3, 129.2, 129.1, 129.0, 128.8, 128.6, 128.4, 128.1, 127.93, 127.86, 120.33, 120.25, 119.5, 119.3, 91.4, 91.0, 85.3, 84.6, 82.5, 82.4, 81.5, 81.3, 60.4, 51.8, 47.1, 38.8, 33.6, 21.5, 21.1, 14.3. HRMS calcd for  $\text{C}_{26}\text{H}_{22}\text{NO}^+(\text{M}+\text{H})^+$ , 364.1696, found 364.1694

N-benzyl-N-(but-2-yn-1-yl)-3-phenylpropiolamide (**1ja**)



yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.59 – 7.49 (m, 2H), 7.46 – 7.23 (m, 8H), 5.00&4.80 (s, 2H), 4.34 – 4.11 (m, 2H), 1.85&1.83 (t,  $J = 2.4$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.3, 154.2, 136.1, 136.0, 132.51, 132.48, 130.3, 130.2, 128.9, 128.7, 128.58, 128.56, 128.0, 127.83, 127.75, 120.4, 120.3, 91.1, 90.7, 81.6, 81.23, 81.17, 80.3, 73.1, 73.0, 51.6, 46.7, 38.2, 33.1, 3.6. HRMS calcd for  $\text{C}_{20}\text{H}_{18}\text{NO}^+(\text{M}+\text{H})^+$ , 288.1383, found 288.1382

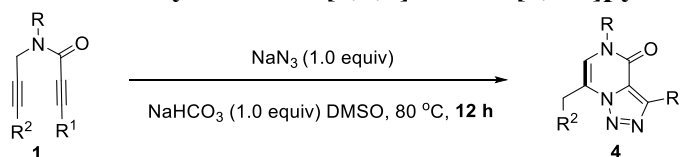
N-benzyl-N-(pent-2-yn-1-yl)-3-phenylpropiolamide (**1ka**)



yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.61 – 7.56 (m, 1H), 7.55 – 7.51 (m, 1H), 7.48 – 7.27 (m, 8H), 5.01&4.81 (s, 2H), 4.27 (t,  $J = 2.0$  Hz, 2H), 2.30-2.14 (m, 2H), 1.22-1.06 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  154.3, 154.2, 136.2, 136.0, 132.51, 132.49, 130.22, 130.20, 128.8, 128.7, 128.6, 128.0, 127.9, 127.7, 120.4, 120.3, 91.1, 90.7, 87.1, 86.3, 81.6, 81.2, 73.2, 73.1, 51.5, 46.7, 38.3, 33.1, 13.82, 13.81, 12.4. HRMS calcd for  $\text{C}_{21}\text{H}_{20}\text{NO}^+(\text{M}+\text{H})^+$ , 302.1539, found 302.1537

### III. Procedure for the Tandem Azide-alkyne Cycloaddition/hydroamination Reactions

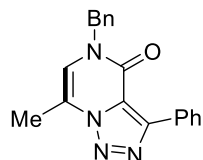
#### General procedure for the synthesis of [1,2,3]triazolo[1,5-a]pyrazin-4(5H)-ones



A mixture of **1** (0.2 mmol, 1.0 equiv),  $\text{NaN}_3$  (0.2 mmol, 13.6 mg, 1.0 equiv),  $\text{NaHCO}_3$  (0.2 mmol,

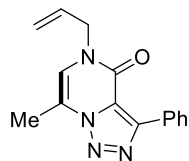
16.8 mg, 1.0 equiv) in DMSO (2 mL) was stirred in 80 °C for 12 hours under the atmosphere of argon. After the reaction was complete (monitored by TLC), H<sub>2</sub>O (15.0 mL) and ethyl acetate (50.0 mL) were added. The organic phase was separated, and the aqueous phase was extracted with ethyl acetate (10.0 mL × 3). The combined organic phase was washed with H<sub>2</sub>O (10.0 mL × 5) and brine, dried over Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure, The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/4) to afford the desired products **4**.

5-benzyl-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4a**)



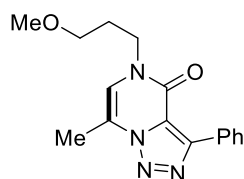
58.2 mg, 92%, white solid, melt point (120-125 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.39 (d, *J* = 7.2 Hz, 2H), 7.52 (t, *J* = 7.2 Hz, 2H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.41 – 7.29 (m, 5H), 6.52 (s, 1H), 5.12 (s, 2H), 2.56 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.8, 147.8, 135.7, 129.6, 129.3, 129.2, 129.1, 128.4, 128.3, 128.2, 123.2, 118.3, 117.0, 50.4, 13.6. HRMS calcd for C<sub>19</sub>H<sub>17</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 317.1397, found 317.1394.

5-allyl-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4b**)



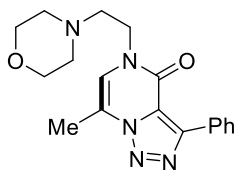
43.0 mg, 81%, white solid, melt point (145-148 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.38 (t, *J* = 7.6 Hz, 2H), 7.51 (t, *J* = 7.2 Hz, 2H), 7.44 (t, *J* = 7.2 Hz, 1H), 6.53 (s, 1H), 6.12 – 5.84 (m, 1H), 5.40-5.24 (m, 2H), 4.58 (d, *J* = 5.6 Hz, 2H), 2.65 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.5, 147.8, 131.8, 129.5, 129.2, 129.1, 128.3, 123.2, 119.4, 118.2, 116.9, 49.5, 13.6. HRMS calcd for C<sub>15</sub>H<sub>15</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 267.1240, found 267.1242.

5-(3-methoxypropyl)-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4c**)



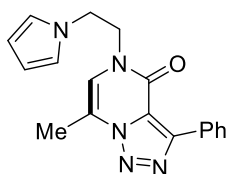
56.0 mg, 94%, white solid, melt point (150-153 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.37 (d, *J* = 7.2 Hz, 2H), 7.50 (t, *J* = 7.2 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 1H), 6.60 (s, 1H), 4.05 (t, *J* = 7.2 Hz, 2H), 3.44 (t, *J* = 5.6 Hz, 2H), 3.37 (s, 3H), 2.63 (s, 3H), 2.12 – 1.96 (m, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.7, 147.6, 129.6, 129.2, 129.1, 128.3, 123.3, 119.5, 116.4, 68.9, 58.7, 45.9, 28.6, 13.6. HRMS calcd for C<sub>16</sub>H<sub>19</sub>N<sub>4</sub>O<sub>2</sub><sup>+</sup>(M+H)<sup>+</sup>, 299.1503, found 299.1504.

7-methyl-5-(2-morpholinoethyl)-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4d**)



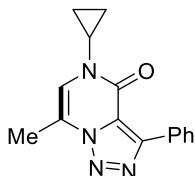
59.4 mg, 89%, yellow solid, melt point (150-152 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.35 (d, *J* = 7.6 Hz, 2H), 7.50 (t, *J* = 7.2 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 1H), 6.60 (s, 1H), 4.04 (t, *J* = 6.4 Hz, 2H), 3.70 (t, *J* = 4.4 Hz, 4H), 2.70 (t, *J* = 6.4 Hz, 2H), 2.62 (s, 3H), 2.53 (m, *J* = 4 Hz, 4H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.7, 147.6, 129.6, 129.2, 129.1, 128.4, 123.1, 119.4, 116.2, 67.0, 57.0, 53.7, 44.9, 13.6. HRMS calcd for C<sub>18</sub>H<sub>22</sub>N<sub>5</sub>O<sub>2</sub><sup>+</sup>(M+H)<sup>+</sup>, 340.1768, found 340.1763.

5-(2-(1H-pyrrol-1-yl)ethyl)-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4e**)



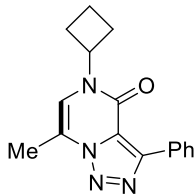
55.0 mg, 86%, yellow solid, melt point (158-160 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.36 (d, *J* = 7.2 Hz, 2H), 7.53 (t, *J* = 7.2 Hz, 2H), 7.46 (t, *J* = 7.2 Hz, 1H), 6.59 (t, *J* = 1.6 Hz, 2H), 6.19 (t, *J* = 2.0 Hz, 2H), 5.71 (s, 1H), 4.36-4.14 (m, 4H), 2.45 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.6, 147.9, 129.4, 129.2, 129.2, 128.4, 122.8, 120.7, 118.7, 116.5, 109.6, 50.3, 47.8, 13.3. HRMS calcd for C<sub>18</sub>H<sub>18</sub>N<sub>5</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 320.1506, found 320.1500.

5-cyclopropyl-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4f**)



52.0 mg, 99%, yellow solid, melt point (155-158 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.39 (d, *J* = 7.2 Hz, 2H), 7.61 – 7.45 (t, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 7.2 Hz, 1H), 6.60 (s, 1H), 3.27 – 3.14 (m, 1H), 2.59 (s, 3H), 1.23 – 1.09 (m, 2H), 1.02 – 0.82 (m, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 156.0, 147.5, 129.6, 129.2, 129.1, 128.3, 123.2, 119.0, 116.2, 31.1, 13.6, 7.3. HRMS calcd for C<sub>15</sub>H<sub>15</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 267.1240, found 267.1242.

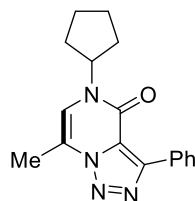
5-cyclobutyl-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4g**)



55.0 mg, 98%, white solid, melt point (160-163 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.35 (d, *J* = 7.2 Hz, 2H), 7.50 (t, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 7.2 Hz, 1H), 6.72 (s, 1H), 5.26 – 5.07 (m, 1H), 2.66 (s, 3H), 2.56-2.41 (m, 2H), 2.36 – 2.19 (m, 2H), 1.97 – 1.82 (m, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.6,

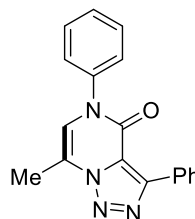
147.6, 129.7, 129.2, 129.0, 128.3, 123.1, 116.4, 114.9, 50.0, 29.7, 14.9, 13.8. HRMS calcd for  $C_{16}H_{17}N_4O^+(M+H)^+$ , 281.1397, found 281.1395.

5-cyclopentyl-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4h**)



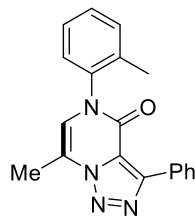
56.2 mg, 96%, white solid, melt point (150-153 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.41 – 8.30 (m, 2H), 7.50 (t,  $J = 7.6$  Hz, 2H), 7.42 (t,  $J = 7.2$  Hz, 1H), 6.56 (s, 1H), 5.34 (p,  $J = 8.4$  Hz, 1H), 2.65 (s, 3H), 2.26-2.10 (m, 2H), 1.96 – 1.85 (m, 2H), 1.81 – 1.66 (m, 4H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  154.9, 147.6, 129.7, 129.3, 129.0, 128.3, 123.0, 117.0, 114.9, 55.1, 31.6, 24.5, 13.9. HRMS calcd for  $C_{17}H_{19}N_4O^+(M+H)^+$ , 295.1553, found 295.1550.

7-methyl-3,5-diphenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4i**)



51.2 mg, 85%, white solid, melt point (125-130 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.39 (d,  $J = 7.2$  Hz, 2H), 7.54 (t,  $J = 7.2$  Hz, 2H), 7.50-7.35 (m, 6H), 6.73 (s, 1H), 2.67 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  154.5, 148.4, 139.1, 129.7, 129.4, 129.3, 129.2, 128.9, 128.3, 126.7, 123.2, 119.6, 116.8, 13.6. HRMS calcd for  $C_{18}H_{15}N_4O^+(M+H)^+$ , 303.1240, found 303.1247

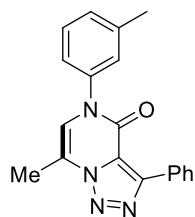
7-methyl-3-phenyl-5-(o-tolyl)-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4j**)



50.1 mg, 79%, white solid, melt point (145-148 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.47 – 8.40 (m, 2H), 7.51 – 7.33 (m, 6H), 7.30-7.22 (m, 1H), 6.58 (d,  $J = 1.2$  Hz, 1H), 2.67 (d,  $J = 0.8$  Hz, 3H), 2.24 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  154.2, 148.3, 138.2, 135.5, 131.4, 129.6, 129.4, 129.3, 129.2, 128.3, 127.5, 123.3, 119.5, 116.7, 17.8, 13.6. HRMS calcd for  $C_{19}H_{17}N_4O^+(M+H)^+$ , 317.1397, found 317.1395.

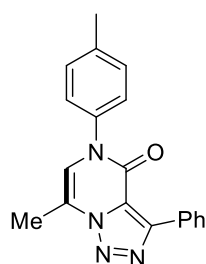
7-methyl-3-phenyl-5-(m-tolyl)-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4k**)





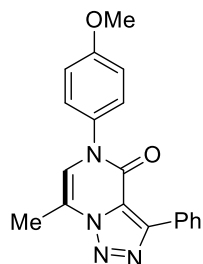
50.0 mg, 79%, yellow solid, melt point (135-138 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.72 (d, *J* = 7.6Hz, 2H), 7.84-7.66 (m, 4H), 7.64 – 7.47 (m, 3H), 7.04 (s, 1H), 2.99 (s, 3H), 2.76 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.8, 148.6, 140.0, 139.2, 129.8, 129.6, 129.5, 129.4, 128.6, 128.5, 127.5, 123.9, 123.5, 119.9, 116.8, 21.5, 13.7. HRMS calcd for C<sub>19</sub>H<sub>17</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 317.1397, found 317.1398.

7-methyl-3-phenyl-5-(p-tolyl)-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4l**)



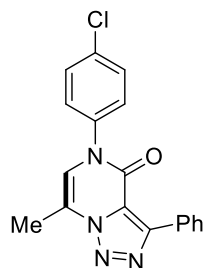
50.2 mg, 79%, white solid, melt point (146-149 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.44 – 8.26 (m, 2H), 7.50 – 7.37 (m, 3H), 7.35 – 7.25 (m, 4H), 6.71 (s, 1H), 2.64 (s, 3H), 2.42 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.6, 148.4, 139.0, 136.5, 130.2, 129.4, 129.3, 129.2, 128.3, 126.4, 123.3, 119.8, 116.7, 21.2, 13.6. HRMS calcd for C<sub>19</sub>H<sub>17</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 317.1397, found 317.1398

5-(4-methoxyphenyl)-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4m**)



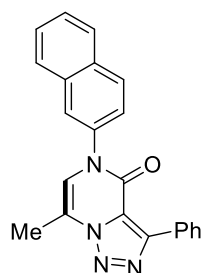
53.2mg, 80%, white solid, melt point (132-135 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.40 (d, *J* = 7.2 Hz, 2H), 7.51-7.37 (m, 3H), 7.33 (d, *J* = 8.8 Hz, 2H), 7.03 (t, *J* = 8.8 Hz, 2H), 6.69 (s, 1H), 3.86 (d, *J* = 9.8 Hz, 3H), 2.66 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.8, 154.9, 148.4, 131.9, 129.5, 129.4, 129.2, 128.4, 127.9, 123.4, 120.0, 116.9, 114.9, 55.8, 13.6. HRMS calcd for C<sub>19</sub>H<sub>17</sub>N<sub>4</sub>O<sub>2</sub><sup>+</sup>(M+H)<sup>+</sup>, 333.1346, found 333.1347.

5-(4-chlorophenyl)-7-methyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4n**)



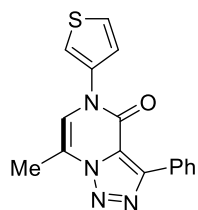
56.1 mg, 83%, white solid, melt point (131-134 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.36 (d, *J* = 7.6 Hz, 2H), 7.64-7.31 (m, 7H), 6.67 (s, 1H), 2.67 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.4, 148.6, 137.5, 134.8, 129.8, 129.3, 129.3, 128.4, 128.1, 123.0, 119.0, 117.2, 100.0, 13.5. HRMS calcd for C<sub>18</sub>H<sub>14</sub>ClN<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 337.0851, found 337.0856.

7-methyl-5-(naphthalen-2-yl)-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4o**)



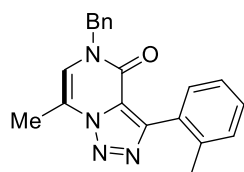
62.1 mg, 88%, white solid, melt point (140-143 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.44 – 8.35 (m, 2H), 7.99 (d, *J* = 8.8 Hz, 1H), 7.95 – 7.84 (m, 3H), 7.63 – 7.41 (m, 6H), 6.81 (s, 1H), 2.68 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.7, 148.5, 136.6, 133.3, 132.8, 129.6, 129.4, 129.3, 129.2, 128.4, 128.1, 127.9, 127.2, 127.1, 125.3, 124.3, 123.2, 119.7, 116.9, 13.6. HRMS calcd for C<sub>22</sub>H<sub>17</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 353.1397, found 353.1393.

7-methyl-3-phenyl-5-(thiophen-3-yl)-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4p**)



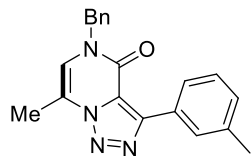
60.2 mg, 99%, yellow solid, melt point (160-163 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.37 (d, *J* = 7.2 Hz, 2H), 7.55-7.31 (m, 5H), 7.27 (d, *J* = 5.2 Hz, 1H), 6.77 (s, 1H), 2.66 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.1, 148.6, 136.7, 129.3, 128.4, 126.1, 124.7, 123.1, 120.1, 119.3, 117.0, 13.6. HRMS calcd for C<sub>16</sub>H<sub>13</sub>N<sub>4</sub>OS<sup>+</sup>(M+H)<sup>+</sup>, 309.0805, found 309.0807.

5-benzyl-7-methyl-3-(o-tolyl)-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4q**)



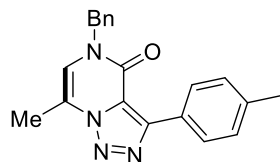
58.2 mg, 88%, white solid, melt point (128-131 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.53 (d, *J* = 7.2 Hz, 1H), 7.42 – 7.29 (m, 8H), 6.54 (s, 1H), 5.10 (s, 2H), 2.62 (s, 3H), 2.40 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.4, 147.7, 137.8, 135.7, 131.3, 130.4, 129.2, 129.1, 128.8, 128.5, 128.3, 125.4, 124.1, 118.3, 116.9, 50.1, 20.4, 13.6. HRMS calcd for C<sub>20</sub>H<sub>19</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 331.1553, found 331.1551.

5-benzyl-7-methyl-3-(*m*-tolyl)-[1,2,3]triazolo[1,5-*a*]pyrazin-4(5H)-one (**4r**)



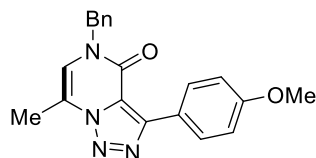
60.2 mg, 91%, white solid, melt point (128-131 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.23-8.13 (m, 2H), 7.46 – 7.31 (m, 6H), 7.29 – 7.24 (m, 1H), 6.52 (s, 1H), 5.15 (s, 2H), 2.58 (s, 3H), 2.48 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.8, 148.1, 138.0, 135.7, 130.0, 129.7, 129.4, 129.1, 128.4, 128.3, 128.2, 126.6, 123.1, 118.2, 117.0, 50.3, 21.6, 13.7. HRMS calcd for C<sub>20</sub>H<sub>19</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 331.1553, found 331.1551.

5-benzyl-7-methylene-3-(*p*-tolyl)-6,7-dihydro-[1,2,3]triazolo[1,5-*a*]pyrazin-4(5H)-one (**4s**)



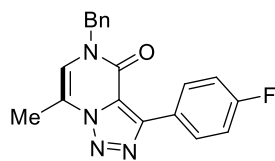
60.1 mg, 91%, white solid, melt point (128-130 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.29 (d, *J* = 8.0 Hz, 2H), 7.46 – 7.28 (m, 7H), 6.51 (s, 1H), 5.11 (s, 2H), 2.55 (s, 3H), 2.43 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.8, 147.8, 139.1, 135.8, 129.2, 129.10, 129.07, 128.4, 128.2, 126.7, 122.9, 118.3, 117.0, 50.3, 21.5, 13.6. HRMS calcd for C<sub>20</sub>H<sub>19</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 331.1553, found 331.1555.

5-benzyl-3-(4-methoxyphenyl)-7-methyl-[1,2,3]triazolo[1,5-*a*]pyrazin-4(5H)-one (**4t**)



62.2 mg, 90%, white solid, melt point (128-131 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.37 (d, *J* = 8.4 Hz, 2H), 7.36 (m, 5H), 7.04 (d, *J* = 8.4 Hz, 2H), 6.50 (s, 1H), 5.13 (s, 2H), 3.88 (s, 3H), 2.56 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 160.4, 155.0, 147.8, 135.8, 130.7, 129.1, 128.4, 128.2, 122.6, 122.1, 118.1, 117.0, 113.8, 55.3, 50.3, 13.6. HRMS calcd for C<sub>20</sub>H<sub>19</sub>N<sub>4</sub>O<sub>2</sub><sup>+</sup>(M+H)<sup>+</sup>, 347.1503, found 347.1506.

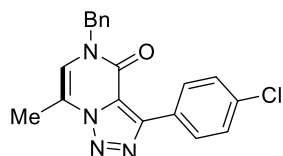
5-benzyl-3-(4-fluorophenyl)-7-methyl-[1,2,3]triazolo[1,5-*a*]pyrazin-4(5H)-one (**4u**)



60.1 mg, 90%, white solid, melt point (128-131 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.50-8.35 (m, 2H), 7.49 – 7.31 (m, 5H), 7.19 (t, *J* = 8.4 Hz, 2H), 6.54 (s, 1H), 5.14 (s, 2H), 2.58 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 164.4(d, *J* = 247.3 Hz), 154.8, 147.0, 135.6, 131.2(d, *J* = 8.8 Hz), 129.2, 128.5, 128.2,

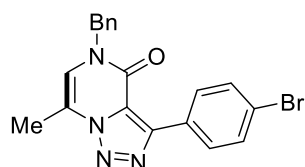
125.74, 125.71, 123.0, 118.3, 117.1, 115.4(d,  $J = 21.5$  Hz), 50.4, 13.6. HRMS calcd for  $C_{19}H_{16}FN_4O^+(M+H)^+$ , 335.1303, found 335.1303.

5-benzyl-3-(4-chlorophenyl)-7-methyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4v**)



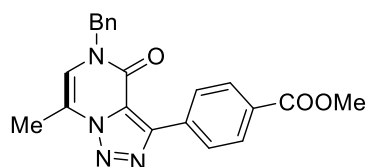
64.2 mg, 91%, yellow solid, melt point (121-124 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.42 – 8.36 (m, 2H), 7.49 – 7.44 (m, 2H), 7.42 – 7.31 (m, 5H), 6.54 (d,  $J = 1.2$  Hz, 1H), 5.13 (s, 2H), 2.57 (d,  $J = 1.2$  Hz, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  154.7, 146.7, 135.6, 135.2, 130.5, 129.2, 128.6, 128.5, 128.2, 128.1, 123.2, 118.4, 117.1, 50.5, 13.6. HRMS calcd for  $C_{19}H_{16}ClN_4O^+(M+H)^+$ , 351.1007, found 351.1009.

5-benzyl-3-(4-bromophenyl)-7-methyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4w**)



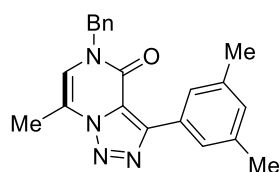
70.1 mg, 89%, white solid, melt point (123-126 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.33 (d,  $J = 8.4$  Hz, 2H), 7.63 (d,  $J = 8.4$  Hz, 2H), 7.43 – 7.33 (m, 5H), 6.55 (s, 1H), 5.14 (s, 2H), 2.58 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  154.7, 146.8, 135.5, 131.6, 130.8, 129.2, 128.5, 128.2, 125.9, 123.6, 123.3, 118.4, 117.1, 50.5, 13.6. HRMS calcd for  $C_{19}H_{16}BrN_4O^+(M+H)^+$ , 397.0482, found 397.0481.

methyl 4-(5-benzyl-7-methyl-4-oxo-4,5-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-3-yl)benzoate (**4x**)



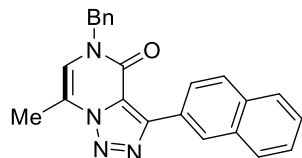
64.1 mg, 86%, yellow solid, melt point (128-131 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.53 (d,  $J = 8.4$  Hz, 2H), 8.18 (d,  $J = 8.4$  Hz, 2H), 7.43 – 7.31 (m, 5H), 6.57 (d,  $J = 1.2$  Hz, 1H), 5.16 (s, 2H), 3.97 (s, 3H), 2.61 (d,  $J = 1.2$  Hz, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  166.9, 154.6, 146.7, 135.5, 133.9, 130.3, 129.6, 129.2, 129.1, 128.5, 128.2, 123.7, 118.5, 117.1, 52.2, 50.5, 13.6. HRMS calcd for  $C_{21}H_{19}N_4O_3^+(M+H)^+$ , 375.1452, found 375.1459.

5-benzyl-3-(3,5-dimethylphenyl)-7-methyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4y**)



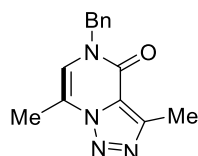
60.0 mg, 87%, white solid, melt point (127-130 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.99 (s, 2H), 7.43 – 7.32 (m, 5H), 7.10 (s, 1H), 6.50 (s, 1H), 5.16 (s, 2H), 2.58 (s, 3H), 2.44 (s, 6H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.8, 148.2, 137.8, 135.8, 130.9, 129.3, 129.1, 128.4, 128.2, 127.0, 123.0, 118.1, 117.0, 50.2, 21.5, 13.7. HRMS calcd for C<sub>21</sub>H<sub>21</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 345.1710, found 345.1715.

5-benzyl-7-methyl-3-(naphthalen-2-yl)-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4z**)



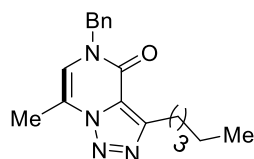
70.1 mg, 96%, white solid, melt point (129-132 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.01 (s, 1H), 8.52 (d, *J* = 8.8 Hz, 1H), 8.06 – 8.00 (m, 1H), 7.98 (d, *J* = 8.8 Hz, 1H), 7.92 – 7.87 (m, 1H), 7.59 – 7.49 (m, 2H), 7.42 – 7.31 (m, 5H), 6.51 (s, 1H), 5.15 (s, 2H), 2.58 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.8, 147.9, 135.7, 133.6, 133.3, 129.13, 129.05, 128.9, 128.4, 128.2, 127.9, 127.6, 127.0, 126.7, 126.5, 126.1, 123.4, 118.3, 117.1, 50.4, 13.7. HRMS calcd for C<sub>23</sub>H<sub>19</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 367.1553, found 367.1554.

5-benzyl-3,7-dimethyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4aa**)



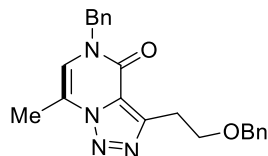
42.3 mg, 83%, colourless oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.43 – 7.23 (m, 5H), 6.45 (s, 1H), 5.11 (s, 2H), 2.78 (s, 3H), 2.54 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.4, 145.4, 135.7, 129.1, 128.4, 128.1, 124.1, 118.0, 117.1, 49.9, 13.4, 11.4. HRMS calcd for C<sub>14</sub>H<sub>15</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 255.1240, found 255.1241.

5-benzyl-7-methyl-3-pentyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4ba**)



52.2 mg, 84%, colourless oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.44 – 7.31 (m, 5H), 6.44 (d, *J* = 0.8 Hz, 1H), 5.10 (s, 2H), 3.18 (t, *J* = 7.6 Hz, 2H), 2.53 (d, *J* = 0.8 Hz, 3H), 1.90 – 1.79 (m, 2H), 1.46 – 1.27 (m, 6H), 0.92 (t, *J* = 7.2 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.2, 149.9, 135.8, 129.1, 128.4, 128.2, 123.7, 117.9, 117.0, 49.8, 31.5, 29.2, 25.7, 22.5, 14.0, 13.4. HRMS calcd for C<sub>18</sub>H<sub>23</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 311.1866, found 311.1869.

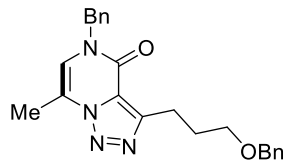
5-benzyl-3-(2-(benzyloxy)ethyl)-7-methyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4ca**)



60.1 mg, 80%, colourless oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.44 – 7.26 (m, 10H), 6.45 (s, 1H), 5.08 (s,

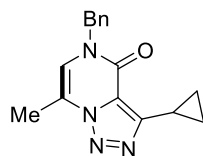
2H), 4.60 (s, 2H), 3.99 (t,  $J = 6.8$  Hz, 2H), 3.53 (t,  $J = 6.8$  Hz, 2H), 2.51 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.0, 146.4, 138.4, 135.7, 129.1, 128.4, 128.3, 128.2, 127.7, 127.4, 124.4, 118.0, 117.0, 72.6, 68.9, 49.9, 26.4, 13.4. HRMS calcd for  $\text{C}_{22}\text{H}_{23}\text{N}_4\text{O}_2^+(\text{M}+\text{H})^+$ , 375.1816, found 375.1819.

5-benzyl-3,7-dimethyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4da**)



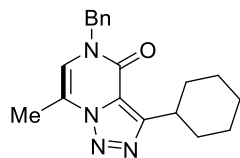
63.2 mg, 81%, colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41 – 7.25 (m, 10H), 6.44 (s, 1H), 5.08 (s, 2H), 4.53 (s, 2H), 3.64 (t,  $J = 6.4$  Hz, 2H), 3.30 (t,  $J = 7.6$  Hz, 2H), 2.51 (s, 3H), 2.24 – 2.15 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.1, 149.2, 138.7, 135.8, 129.1, 128.4, 128.3, 128.2, 127.6, 127.4, 123.9, 118.0, 117.0, 72.8, 69.8, 49.9, 29.3, 22.7, 13.4. HRMS calcd for  $\text{C}_{23}\text{H}_{25}\text{N}_4\text{O}_2^+(\text{M}+\text{H})^+$ , 389.1972, found 389.1977.

5-benzyl-3-cyclopropyl-7-methyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4ea**)



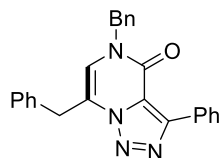
45.1 mg, 80%, colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44 – 7.29 (m, 5H), 6.42 (s, 1H), 5.10 (s, 2H), 2.83 – 2.67 (m, 1H), 2.49 (s, 3H), 1.34 – 1.19 (m, 2H), 1.17-1.05 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.4, 151.5, 135.8, 129.1, 128.4, 128.1, 123.9, 117.8, 117.1, 49.8, 13.4, 9.6, 6.9. HRMS calcd for  $\text{C}_{16}\text{H}_{17}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 281.1397, found 281.1399.

5-benzyl-3-cyclohexyl-7-methyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4fa**)



52.0 mg, 81%, colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41 – 7.27 (m, 5H), 6.46 (s, 1H), 5.09 (s, 2H), 3.58-3.36 (m, 1H), 2.51 (s, 3H), 2.09-1.93(m, 3H), 1.87 – 1.72 (m, 4H), 1.52 – 1.31 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.2, 154.3, 135.8, 129.1, 128.4, 128.1, 122.9, 117.8, 117.0, 49.9, 35.4, 32.3, 26.4, 25.9, 13.5. HRMS calcd for  $\text{C}_{19}\text{H}_{23}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 323.1866, found 323.1864.

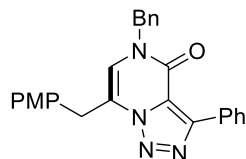
5,7-dibenzyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4ga**)



65.1 mg, 82%, yellow solid, melt point (153-156 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.38 (d,  $J = 7.2$  Hz, 2H), 7.51 (t,  $J = 7.2$  Hz, 2H), 7.48 – 7.28 (m, 11H), 6.53 (s, 1H), 4.89 (s, 2H), 4.28 (s, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  164.0, 162.3, 156.7, 148.3, 147.5, 135.6, 132.3, 129.4,

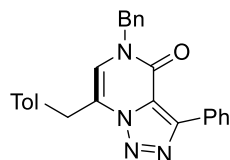
129.1, 129.0, 128.36, 128.35, 128.22, 128.20, 127.1, 123.5, 122.8, 51.4, 49.4. HRMS calcd for  $C_{25}H_{21}N_4O^+(M+H)^+$ , 393.1710, found 393.1710.

5-benzyl-7-(4-methoxybenzyl)-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4ha**)



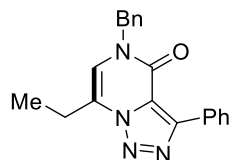
70.1 mg, 83%, yellow solid, melt point (156-158 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.38 (d,  $J = 7.2$  Hz, 2H), 7.55 – 7.36 (m, 10H), 6.88 (d,  $J = 8.8$  Hz, 2H), 6.45 (s, 1H), 4.88 (s, 2H), 4.25 (s, 2H), 3.84 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  160.3, 156.8, 148.2, 135.6, 131.3, 129.4, 129.2, 129.08, 129.05, 128.3, 128.2, 124.5, 123.8, 122.8, 122.7, 121.5, 113.8, 55.3, 51.8, 49.4. HRMS calcd for  $C_{26}H_{23}N_4O_2^+(M+H)^+$ , 423.1816, found 423.1812.

5-benzyl-7-(4-methylbenzyl)-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4ia**)



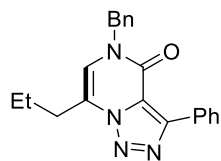
66.2 mg, 81%, yellow solid, melt point (150-152 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.39 (d,  $J = 7.2$  Hz, 2H), 7.51 (t,  $J = 7.2$  Hz, 2H), 7.48 – 7.27 (m, 8H), 7.16 (d,  $J = 7.6$  Hz, 2H), 6.48 (s, 1H), 4.88 (s, 2H), 4.25 (s, 2H), 2.37 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  156.8, 148.2, 139.3, 135.6, 129.54, 129.45, 129.4, 129.3, 129.2, 129.09, 129.08, 129.06, 128.3, 128.2, 123.8, 122.9, 122.7, 51.5, 49.4, 21.4. HRMS calcd for  $C_{26}H_{23}N_4O^+(M+H)^+$ , 407.1866, found 407.1866.

5-benzyl-7-ethyl-3-phenyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4ja**)



35.1 mg, 53%, yellow solid, melt point (140-143 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.38 (d,  $J = 7.6$  Hz, 2H), 7.52 (t,  $J = 7.2$  Hz, 2H), 7.44 (t,  $J = 7.2$  Hz, 1H), 7.42 – 7.32 (m, 5H), 6.51 (s, 1H), 5.16 (s, 2H), 3.04 (q,  $J = 7.2$  Hz, 2H), 1.39 (t,  $J = 7.6$  Hz, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  154.8, 147.7, 135.7, 129.5, 129.2, 129.1, 128.40, 128.35, 128.1, 123.1, 122.5, 117.2, 50.5, 21.1, 11.3. HRMS calcd for  $C_{20}H_{19}N_4O^+(M+H)^+$ , 331.1553, found 331.1550.

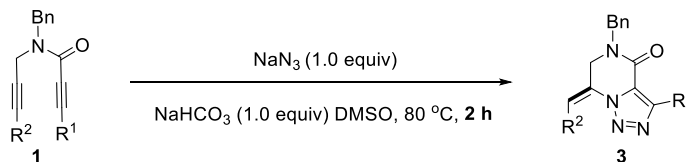
5-benzyl-3-phenyl-7-propyl-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**4ka**)



38.1 mg, 55%, yellow solid, melt point (145-148 °C);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.38 (d,  $J = 7.6$  Hz, 2H), 7.52 (t,  $J = 7.2$  Hz, 2H), 7.44 (t,  $J = 7.2$  Hz, 1H), 7.41 – 7.30 (m, 5H), 6.51 (s, 1H), 5.16 (s, 2H), 2.96 (t,  $J = 7.6$  Hz, 2H), 1.93 – 1.78 (m, 2H), 1.04 (t,  $J = 7.2$  Hz, 3H).  $^{13}C$  NMR (100 MHz,

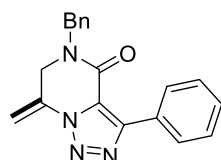
CDCl<sub>3</sub>)  $\delta$  154.8, 140.4, 135.7, 129.6, 129.3, 129.1, 128.41, 128.36, 128.1, 125.1, 123.2, 120.9, 117.9, 50.5, 29.6, 20.1, 13.6. HRMS calcd for C<sub>21</sub>H<sub>21</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 345.1710, found 345.1716.

### General procedure for the synthesis of 6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one



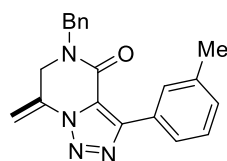
A mixture of **1** (0.2 mmol, 1.0 equiv), NaN<sub>3</sub> (0.2 mmol, 13.6 mg, 1.0 equiv), NaHCO<sub>3</sub> (0.2 mmol, 16.8 mg, 1.0 equiv) in DMSO (2 mL) was stirred in 80 °C for 2 hours under the atmosphere of argon. After the reaction was complete (monitored by TLC), H<sub>2</sub>O (15.0 mL) and ethyl acetate (50.0 mL) were added. The organic phase was separated, and the aqueous phase was extracted with ethyl acetate (10.0 mL  $\times$  3). The combined organic phase was washed with H<sub>2</sub>O (10.0 mL  $\times$  5) and brine, dried over Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/4) to afford the desired products **3**.

5-benzyl-7-methylene-3-phenyl-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3a**)



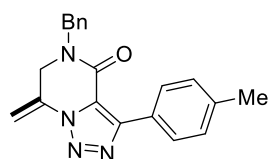
40.1 mg, 63%, white solid, melt point (110-113 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.32 (d, *J* = 7.6 Hz, 2H), 7.57 – 7.15 (m, 8H), 6.12 (s, 1H), 5.15 (s, 1H), 4.82 (s, 2H), 4.31 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  156.1, 149.5, 135.4, 131.9, 129.5, 129.2, 129.1, 129.0, 128.3, 128.2, 128.2, 122.5, 103.0, 100.0, 49.3, 48.4. HRMS calcd for C<sub>19</sub>H<sub>17</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 317.1397, found 317.1396.

5-benzyl-7-methylene-3-(*m*-tolyl)-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3b**)



45.1 mg, 68%, white solid, melt point (108-110 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.27 – 8.07 (m, 2H), 7.35 (d, *J* = 7.4 Hz, 7H), 6.09 (s, 1H), 5.13 (s, 1H), 4.81 (s, 2H), 4.29 (s, 2H), 2.47 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  156.1, 149.6, 137.9, 135.5, 131.9, 130.2, 129.6, 129.0, 128.2, 126.4, 122.5, 103.9, 49.2, 48.4, 21.6. HRMS calcd for C<sub>20</sub>H<sub>19</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 331.1553, found 331.1554.

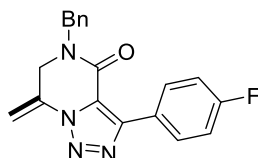
5-benzyl-7-methylene-3-phenyl-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3c**)





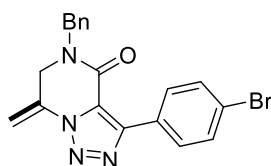
43.1 mg, 65%, white solid, melt point (108-110 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.22 (d, *J* = 8.0 Hz, 2H), 7.55-7.24 (m, 7H), 6.11 (s, 1H), 5.14 (s, 1H), 4.83 (s, 2H), 4.31 (s, 2H), 2.44 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 156.2, 149.7, 139.5, 135.5, 132.0, 129.0, 128.24, 128.20, 126.2, 122.2, 103.8, 49.3, 48.4, 21.5. HRMS calcd for C<sub>20</sub>H<sub>19</sub>N<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 331.1553, found 331.1550.

5-benzyl-3-(4-fluorophenyl)-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3d**)



42.2 mg, 63%, white solid, melt point (108-110 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.47-8.25 (m, 2H), 7.48-7.28 (m, 5H), 7.19 (t, *J* = 8.4 Hz, 2H), 6.11 (s, 1H), 5.16 (s, 1H), 4.82 (s, 2H), 4.32 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 163.5(d, *J* = 248 Hz), 156.2, 148.6, 135.3, 131.8, 131.2, 131.1, 129.2, 128.3, 128.2, 125.3 (d, *J* = 3.2 Hz), 122.4, 115.3(d, *J* = 21.5 Hz), 104.1, 49.3, 48.4. HRMS calcd for C<sub>19</sub>H<sub>16</sub>FN<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 335.1303, found 335.1309.

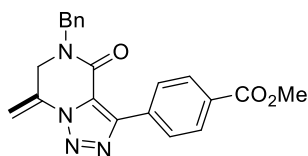
5-benzyl-3-(4-bromophenyl)-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3e**)



51.1 mg, 65%, white solid, melt point (108-113 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.26 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.44-7.31 (m, 5H), 6.11 (s, 1H), 5.17 (s, 1H), 4.81 (s, 2H), 4.31 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 156.0, 148.4, 135.3, 131.8, 131.5, 130.7, 129.1, 128.3, 128.2, 128.1, 123.9, 122.7, 104.3, 49.4, 48.4. HRMS calcd for C<sub>19</sub>H<sub>16</sub>BrN<sub>4</sub>O<sup>+</sup>(M+H)<sup>+</sup>, 397.0482, found 397.0483.

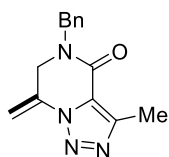
5-benzyl-3-methyl-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**6**)

methyl 4-(5-benzyl-7-methylene-4-oxo-4,5,6,7-tetrahydro-[1,2,3]triazolo[1,5-a]pyrazin-3-yl)benzoate (**3f**)



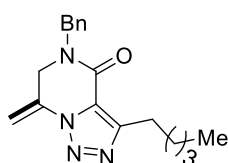
48.2 mg, 64%, white solid, melt point (106-108 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.45 (d, *J* = 8.8 Hz, 2H), 8.17 (d, *J* = 8.8 Hz, 2H), 7.49-7.31 (m, 5H), 6.14 (d, *J* = 1.6 Hz, 1H), 5.19 (d, *J* = 1.6 Hz, 1H), 4.83 (s, 2H), 4.33 (s, 2H), 3.97 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 166.9, 155.9, 148.4, 135.2, 133.5, 131.7, 130.6, 129.6, 129.10, 129.06, 128.31, 128.25, 123.2, 104.5, 52.2, 49.4, 48.4. HRMS calcd for C<sub>21</sub>H<sub>19</sub>N<sub>4</sub>O<sub>3</sub><sup>+</sup>(M+H)<sup>+</sup>, 375.1452, found 375.1459.

5-benzyl-3-methyl-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3g**)



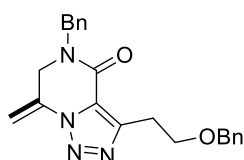
32.1 mg, 63%, colourless oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.48 – 7.30 (m, 5H), 6.02 (d,  $J = 1.6$  Hz, 1H), 5.08 (d,  $J = 1.6$  Hz, 1H), 4.77 (s, 2H), 4.26 (s, 2H), 2.68 (s, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.7, 147.3, 135.4, 131.8, 129.0, 128.23, 128.20, 123.3, 103.2, 48.8, 48.9, 11.2. HRMS calcd for  $\text{C}_{14}\text{H}_{15}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 255.1240, found 255.1240.

5-benzyl-7-methylene-3-pentyl-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3h**)



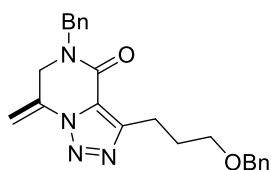
40.2 mg, 65%, colourless oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44-7.25 (m, 5H), 6.02 (s, 1H), 5.08 (d,  $J = 1.2$  Hz, 1H), 4.77 (s, 2H), 4.26 (s, 2H), 3.08 (t,  $J = 7.6$  Hz, 2H), 1.89 – 1.63 (m, 3H), 1.45 – 1.37 (m, 4H), 0.97 – 0.86 (m, 4H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.6, 151.8, 135.5, 131.9, 129.0, 128.24, 128.19, 122.9, 103.1, 48.8, 48.6, 31.5, 28.8, 25.4, 22.4, 14.0. HRMS calcd for  $\text{C}_{18}\text{H}_{23}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 311.1866, found 311.1867.

5-benzyl-3-(2-(benzyloxy)ethyl)-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3i**)



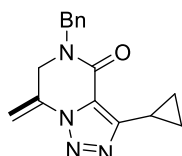
49.1 mg, 65%, colourless oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41 – 7.24 (m, 10H), 6.03 (s, 1H), 5.09 (s, 1H), 4.76 (s, 2H), 4.58 (s, 2H), 4.25 (s, 2H), 3.96 (t,  $J = 6.8$  Hz, 2H), 3.44 (t,  $J = 6.8$  Hz, 2H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.4, 148.3, 138.4, 135.4, 131.8, 130.6, 129.0, 128.3, 128.2, 127.7, 127.5, 123.7, 103.3, 72.6, 68.5, 48.8, 48.6, 26.1. HRMS calcd for  $\text{C}_{22}\text{H}_{23}\text{N}_4\text{O}_2^+(\text{M}+\text{H})^+$ , 375.1816, found 375.1810.

5-benzyl-3-(3-(benzyloxy)propyl)-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3j**)



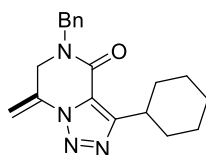
54.1 mg, 70%, colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.48 – 7.18 (m, 10H), 6.03 (d,  $J = 1.2$  Hz, 1H), 5.08 (d,  $J = 1.6$  Hz, 1H), 4.76 (s, 2H), 4.54 (s, 2H), 4.22 (s, 2H), 3.64 (t,  $J = 6.4$  Hz, 2H), 3.20 (t,  $J = 7.6$  Hz, 2H), 2.33 – 2.11 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.5, 151.1, 138.7, 135.4, 131.8, 129.0, 128.3, 128.3, 128.2, 127.6, 127.4, 123.1, 103.2, 72.8, 69.8, 48.8, 48.6, 28.8, 22.4. HRMS calcd for  $\text{C}_{23}\text{H}_{25}\text{N}_4\text{O}_2^+(\text{M}+\text{H})^+$ , 389.1972, found 389.1971.

5-benzyl-3-cyclopropyl-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3k**)



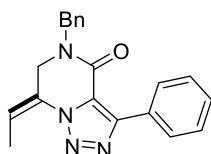
38.1 mg, 68%, colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45-7.28 (m, 5H), 5.98 (s, 1H), 5.07 (s, 1H), 4.78 (s, 2H), 4.24 (s, 2H), 2.76 – 2.61 (m, 1H), 1.33 – 1.16 (m, 2H), 1.16 – 1.04 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.9, 153.3, 135.5, 131.8, 129.0, 128.24, 128.17, 123.1, 102.9, 48.8, 48.6, 9.3, 6.6. HRMS calcd for  $\text{C}_{16}\text{H}_{17}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 281.1397, found 281.1393.

5-benzyl-3-cyclohexyl-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3l**)



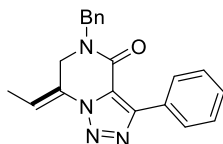
45.2 mg, 70%, colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.43 – 7.27 (m, 5H), 6.01 (d,  $J = 1.2$  Hz, 1H), 5.06 (d,  $J = 1.6$  Hz, 1H), 4.77 (s, 2H), 4.25 (s, 2H), 3.47-3.33 (m, 1H), 2.03-1.92 (m, 2H), 1.91 – 1.84 (m, 2H), 1.82-1.75 (m, 2H), 1.53 – 1.31 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.6, 156.1, 135.5, 131.9, 129.0, 128.20, 128.17, 122.0, 103.1, 48.8, 48.5, 34.9, 31.9, 26.4, 25.9. HRMS calcd for  $\text{C}_{19}\text{H}_{23}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 323.1866, found 323.1867.

(Z)-5-benzyl-7-ethylidene-3-phenyl-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3m**)



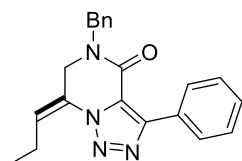
24.1 mg, 36%, colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.41 – 8.27 (m, 2H), 7.57 – 7.32 (m, 8H), 5.69 (q,  $J = 7.6$  Hz, 1H), 4.80 (s, 2H), 4.15 (s, 2H), 2.22 (d,  $J = 7.2$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.6, 148.1, 135.7, 129.3, 129.13, 129.11, 129.0, 128.4, 128.3, 128.2, 128.1, 125.1, 119.7, 50.3, 49.2, 14.1. HRMS calcd for  $\text{C}_{20}\text{H}_{19}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 331.1553, found 331.1551.

(E)-5-benzyl-7-ethylidene-3-phenyl-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3n**)



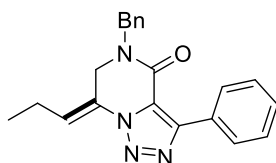
18.1 mg, 27%, colourless oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02 (d,  $J = 7.2$  Hz, 2H), 7.53 – 7.45 (m, 2H), 7.45 – 7.32 (m, 6H), 5.66 (q,  $J = 7.2$  Hz, 1H), 4.81 (s, 2H), 3.71 (d,  $J = 7.6$  Hz, 2H), 2.46 (s, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.6, 149.4, 139.7, 136.6, 129.8, 129.0, 128.9, 128.6, 128.5, 128.3, 128.1, 128.0, 116.7, 50.9, 42.0, 19.4. HRMS calcd for  $\text{C}_{20}\text{H}_{19}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 331.1553, found 331.1558.

(Z)-5-benzyl-7-ethylidene-3-phenyl-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3n**)



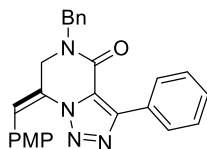
30.1 mg, 43%, colourless oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (d,  $J = 7.2$  Hz, 2H), 7.55 – 7.32 (m, 8H), 5.61 (t,  $J = 7.2$  Hz, 1H), 4.86 (s, 2H), 3.73 (d,  $J = 7.6$  Hz, 2H), 2.90 (q,  $J = 7.2$  Hz, 2H), 1.13 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.6, 145.1, 136.4, 129.7, 129.03, 128.96, 128.9, 128.6, 128.5, 128.4, 128.3, 128.2, 115.5, 100.0, 50.9, 42.0, 26.0, 11.4. HRMS calcd for  $\text{C}_{21}\text{H}_{21}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 345.1710, found 345.1716.

(E)-5-benzyl-3-phenyl-7-propylidene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3n**)



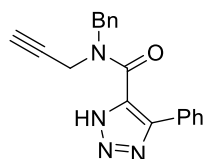
12.1 mg, 17%, colourless oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (d,  $J = 7.6$  Hz, 2H), 7.56 – 7.31 (m, 8H), 5.60 (t,  $J = 7.6$  Hz, 1H), 4.82 (s, 2H), 4.15 (s, 2H), 2.73 (p,  $J = 7.6$  Hz, 2H), 1.15 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.7, 149.1, 135.7, 129.31, 129.28, 129.2, 129.1, 129.0, 128.3, 128.2, 128.1, 126.8, 123.7, 100.5, 50.4, 49.3, 21.6, 13.7. HRMS calcd for  $\text{C}_{21}\text{H}_{21}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 345.1710, found 345.1716.

(Z)-5-benzyl-7-(4-methoxybenzylidene)-3-phenyl-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**3o**)



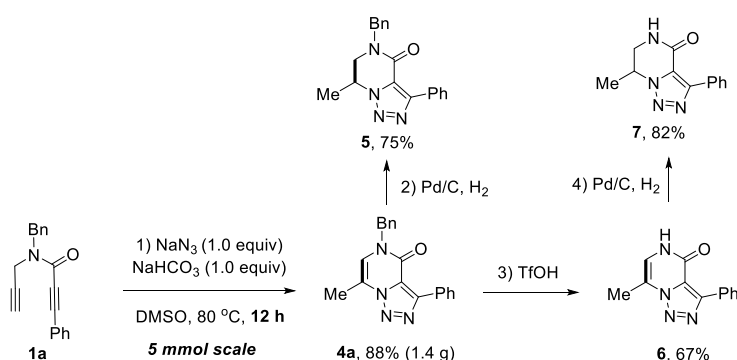
42.1 mg, 50%, colourless oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.37 (d,  $J = 7.6$  Hz, 2H), 7.58 – 7.28 (m, 10H), 6.89 (d,  $J = 8.4$  Hz, 2H), 6.29 (s, 1H), 5.09 (s, 2H), 4.26 (s, 2H), 3.83 (s, 3H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.9, 152.4, 139.2, 130.52, 130.46, 129.23, 129.21, 129.15, 129.13, 129.06, 128.4, 128.1, 128.0, 126.9, 121.1, 119.0, 114.3, 55.3, 50.7, 32.8. HRMS calcd for  $\text{C}_{26}\text{H}_{23}\text{N}_4\text{O}_2^+(\text{M}+\text{H})^+$ , 423.1816, found 423.1812.

## 5-benzyl-3-cyclohexyl-7-methylene-6,7-dihydro-[1,2,3]triazolo[1,5-a]pyrazin-4(5H)-one (**2a**)



58.3 mg, 92%, colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  13.95 (s, 1H), 7.83 – 7.57 (m, 2H), 7.50 – 7.11 (m, 8H), 4.98&4.58(s, 2H), 4.32&4.02 (s, 2H), 2.31&2.20 (s, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  164.8, 164.6, 143.2, 137.0, 136.9, 135.6, 135.0, 129.2, 128.9, 128.82, 128.77, 128.2, 128.1, 128.02, 127.96, 127.6, 127.5, 73.6, 72.7, 51.6, 47.8, 37.9, 33.6. HRMS calcd for  $\text{C}_{19}\text{H}_{17}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 317.1397, found 317.1395.

## IV. Synthetic Transformations



**Gram synthesis of 4a:** A mixture of **1a** (5 mmol, 1.37 g),  $\text{NaN}_3$  (5 mmol, 340 mg),  $\text{NaHCO}_3$  (5 mmol, 420 mg) in DMSO (10 mL) was stirred in 80 °C for 12 hours under the atmosphere of argon. After the reaction was complete (monitored by TLC),  $\text{H}_2\text{O}$  (15.0 mL) and ethyl acetate (50.0 mL) were added. The organic phase was separated, and the aqueous phase was extracted with ethyl acetate (10.0 mL  $\times$  3). The combined organic phase was washed with  $\text{H}_2\text{O}$  and brine, dried over  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/4) to afford the desired products **4a** in 88% yield. Notably, the above resulting crude product was able to be recrystallized from petroleum ether and DCM to afford pure compound **4a** as white solid (77% yield).

**Synthesis of 5:** A mixture of **4a** (0.2 mmol, 63.2 mg), Pd/C (0.02 mmol, 2.1 mg, 10 mol%) in EtOH (2 mL) was stirred in 70 °C for 12 hours under the hydrogen. After the reaction was completed, the mixture was concentrated in vacuum and then loaded on silica column (ethyl acetate/petroleum ether = 1:4) to afford the title compound **5** in 75% yield. Colourless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.32 (d,  $J = 7.6$  Hz, 2H), 7.53 – 7.46 (m, 2H), 7.47 – 7.32 (m, 6H), 4.94 – 4.69 (m, 3H), 3.78-3.69 (m, 1H), 3.57 – 3.38 (m, 1H), 1.63 (d,  $J = 6.4$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.1, 149.2, 136.0, 129.6, 129.2, 129.02, 128.96, 128.5, 128.3, 128.2, 123.6, 52.1, 50.6, 49.5, 17.1. HRMS calcd for  $\text{C}_{19}\text{H}_{19}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 319.1553, found 319.1557.

**Synthesis of 6:** A mixture of **4a** (0.2 mmol, 63.2 mg) in TfOH (2 mL) was stirred at 70 °C for 12 hours. After the reaction was completed, the mixture was concentrated in vacuum and then loaded on silica column (ethyl acetate/petroleum ether = 1:2) to afford the title compound **6** in 67% yield. Yellow solid, melt point (252-255 °C);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  11.49 (s, 1H), 8.32 (d,  $J = 7.2$  Hz, 2H),

7.50 (t,  $J = 7.2$  Hz, 2H), 7.43 (t,  $J = 7.2$  Hz, 1H), 6.98 (s, 1H), 2.51 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz, DMSO)  $\delta$  155.6, 146.2, 130.2, 129.3, 129.1, 128.8, 124.1, 117.1, 116.0, 100.0, 97.5, 13.4. HRMS calcd for  $\text{C}_{12}\text{H}_{11}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 227.0927, found 227.0923.

**Synthesis of 7:** A mixture of **6** (0.2 mmol, 45.2 mg), Pd/C (0.02 mmol, 2.1 mg, 10 mol%) in EtOH (2 mL) was stirred at 70 °C for 12 hours under the hydrogen. After the reaction was completed, the mixture was concentrated in vacuum and then loaded on silica column (ethyl acetate/petroleum ether = 1:2) to afford the title compound **7** in 82% yield. White solid, melt point (253-258 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.31 (d,  $J = 7.6$  Hz, 2H), 7.54 – 7.39 (m, 3H), 6.56 (s, 1H), 4.96 – 4.81 (m, 1H), 3.90-3.79 (m,  $J = 12.8$  Hz, 1H), 3.60 – 3.51 (m, 1H), 1.81 (d,  $J = 6.4$  Hz, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 149.3, 129.4, 129.3, 128.8, 128.3, 123.3, 52.7, 45.9, 17.1. HRMS calcd for  $\text{C}_{12}\text{H}_{13}\text{N}_4\text{O}^+(\text{M}+\text{H})^+$ , 229.1089, found 229.1087

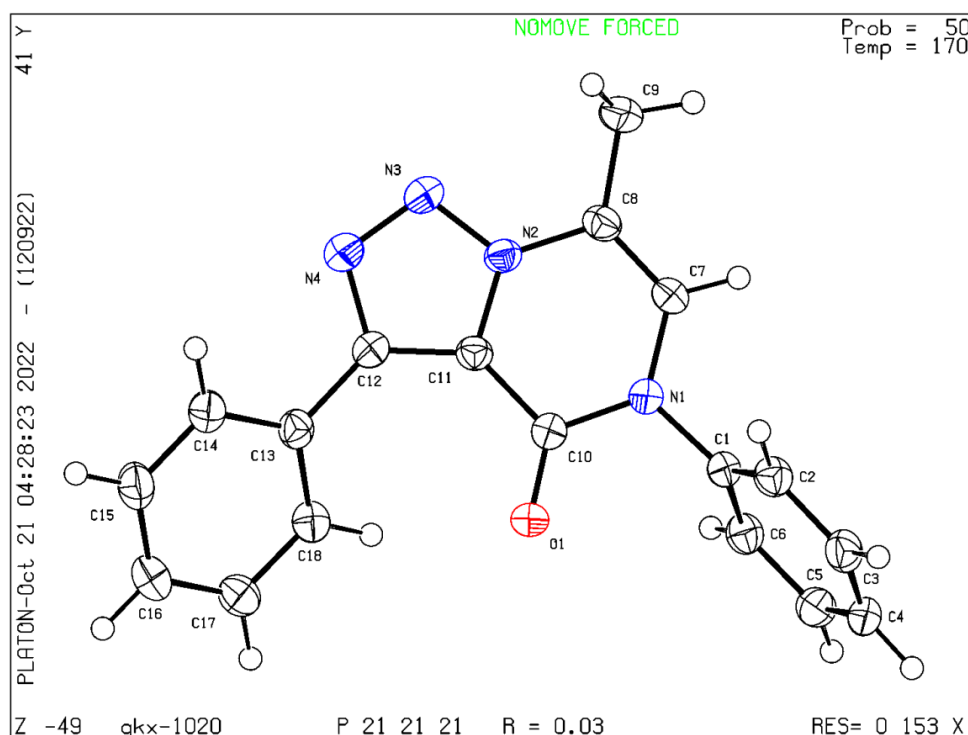
## V. X-Ray Crystallographic Data 4i

### X-Ray Crystallographic Data of 4i

Compounds **4i** were collected at 100 K on a Rigaku Oxford Diffraction Supernova Dual Source, Cu at Zero equipped with an AtlasS2 CCD using Cu  $K\alpha$  radiation. The data were collected and processed using CrysAlisPro22.

Compound **4i** was completely dissolved in ethyl acetate (0.3 mL). Hexanes (1.0 mL) was added slowly to the solution at room temperature. The solvent diffused slowly, and the single crystal was obtained after two days. The structure in Figure S1 showed the absolute configuration of **4i**. The CCDC number is 2299580. These details can be obtained free of charge via [www.ccdc.com.ac.uk/data\\_request/cif](http://www.ccdc.com.ac.uk/data_request/cif) from the Cambridge Crystallographic Data Centre.

**Figure S1. Thermal Ellipsoid Plot for 4i (30% probability level)**



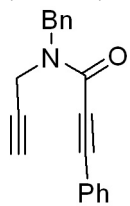
## Crystal Data for 4i

**Table 1 Crystal data and structure refinement for QKX-1020.**

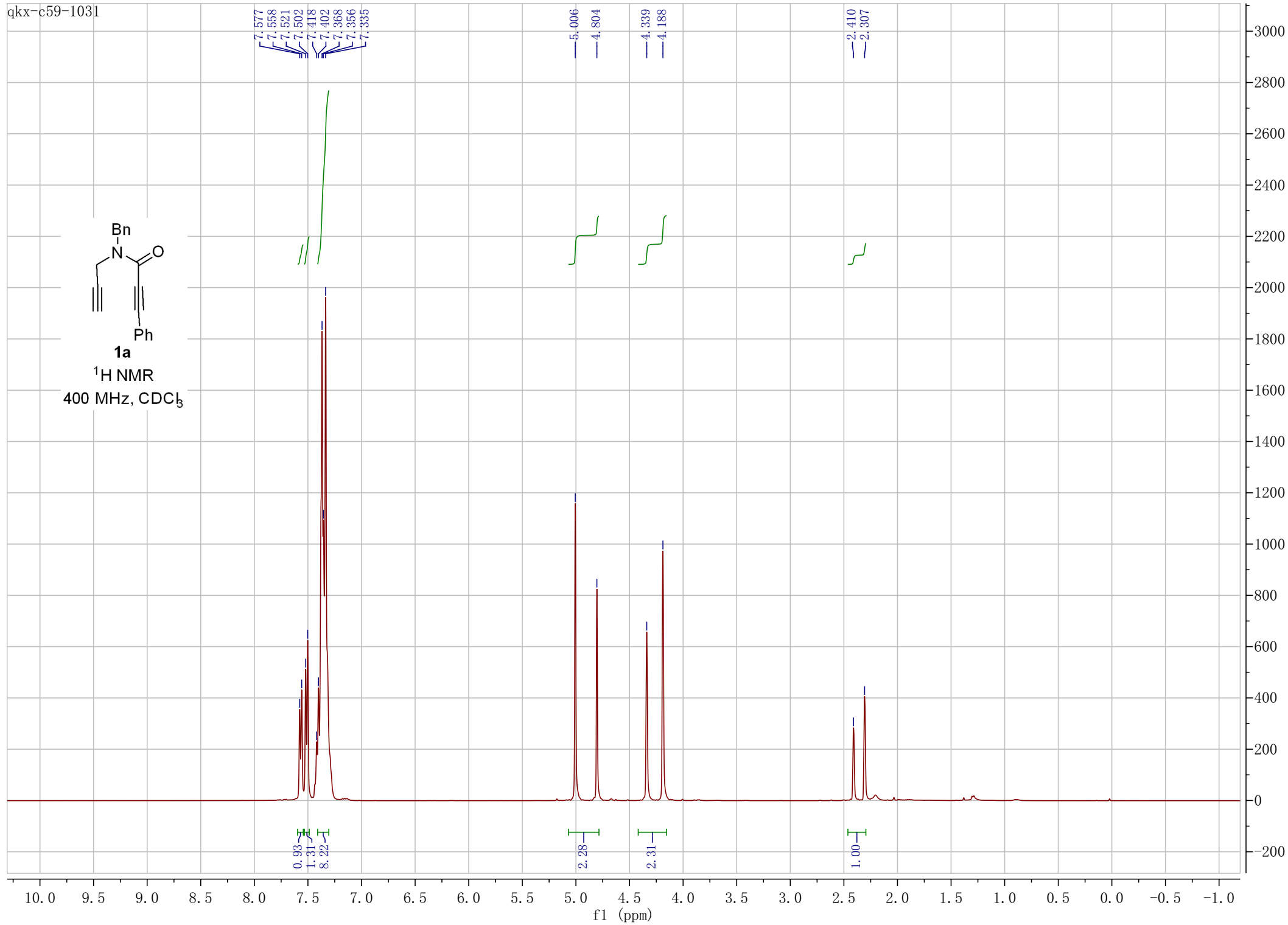
Identification code	QKX-1020
Empirical formula	C <sub>18</sub> H <sub>14</sub> N <sub>4</sub> O
Formula weight	302.33
Temperature/K	169.99(10)
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	5.52660(10)
b/Å	12.2496(3)
c/Å	21.7057(5)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	1469.45(6)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.367
μ/mm <sup>-1</sup>	0.714
F(000)	632.0
Crystal size/mm <sup>3</sup>	0.14 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	8.146 to 147.544
Index ranges	-3 ≤ h ≤ 6, -15 ≤ k ≤ 10, -22 ≤ l ≤ 26
Reflections collected	5181
Independent reflections	2873 [R <sub>int</sub> = 0.0273, R <sub>sigma</sub> = 0.0373]
Data/restraints/parameters	2873/0/210
Goodness-of-fit on F <sup>2</sup>	1.032
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0318, wR <sub>2</sub> = 0.0810
Final R indexes [all data]	R <sub>1</sub> = 0.0341, wR <sub>2</sub> = 0.0828
Largest diff. peak/hole / e Å <sup>-3</sup>	0.14/-0.14
Flack parameter	0.26(19)

## VI. NMR Spectra

qkx-c59-1031

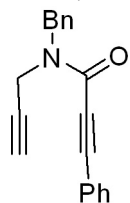


<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>





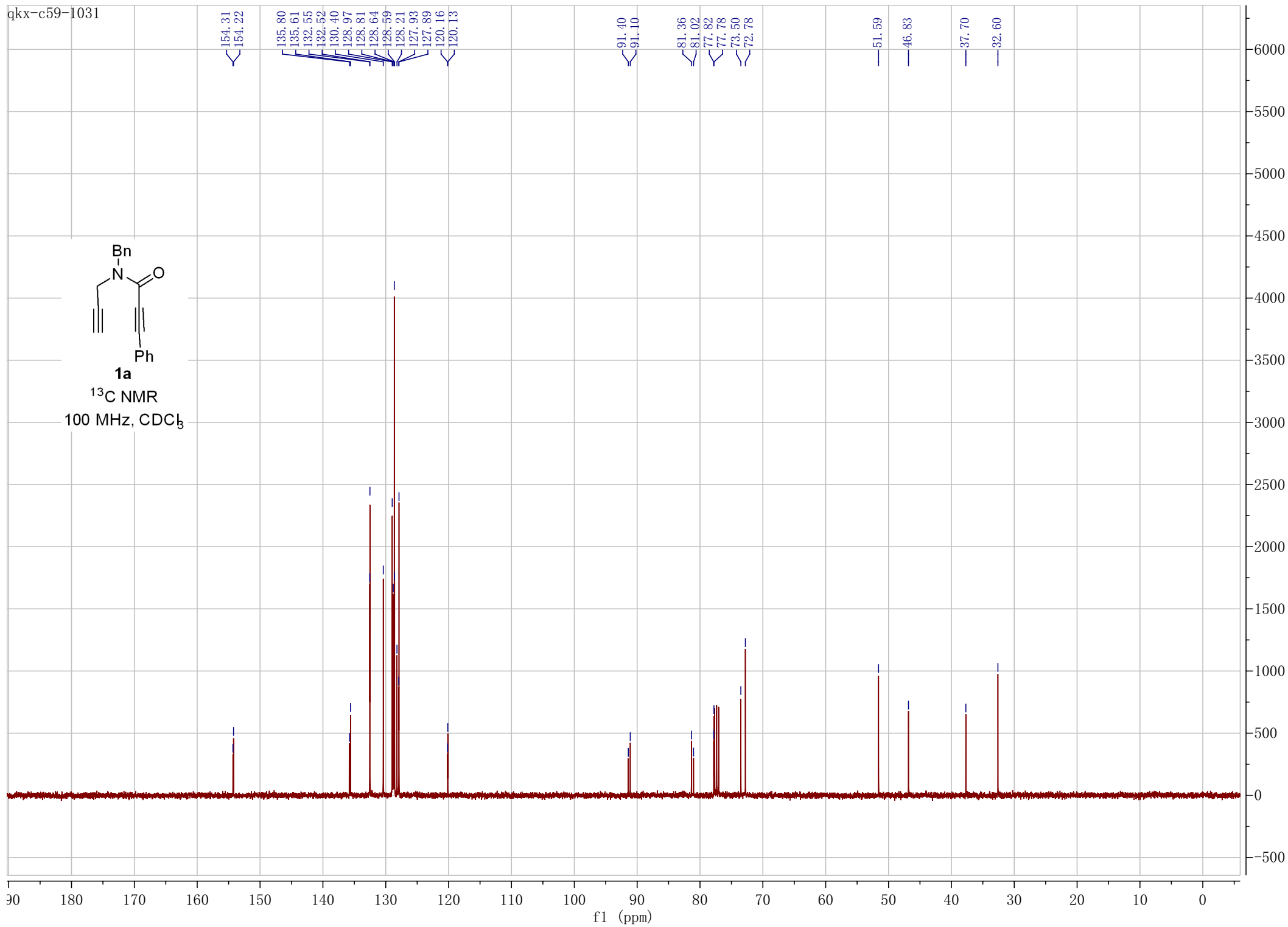
qkx-c59-1031

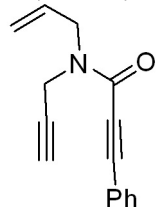


**1a**

<sup>13</sup>C NMR

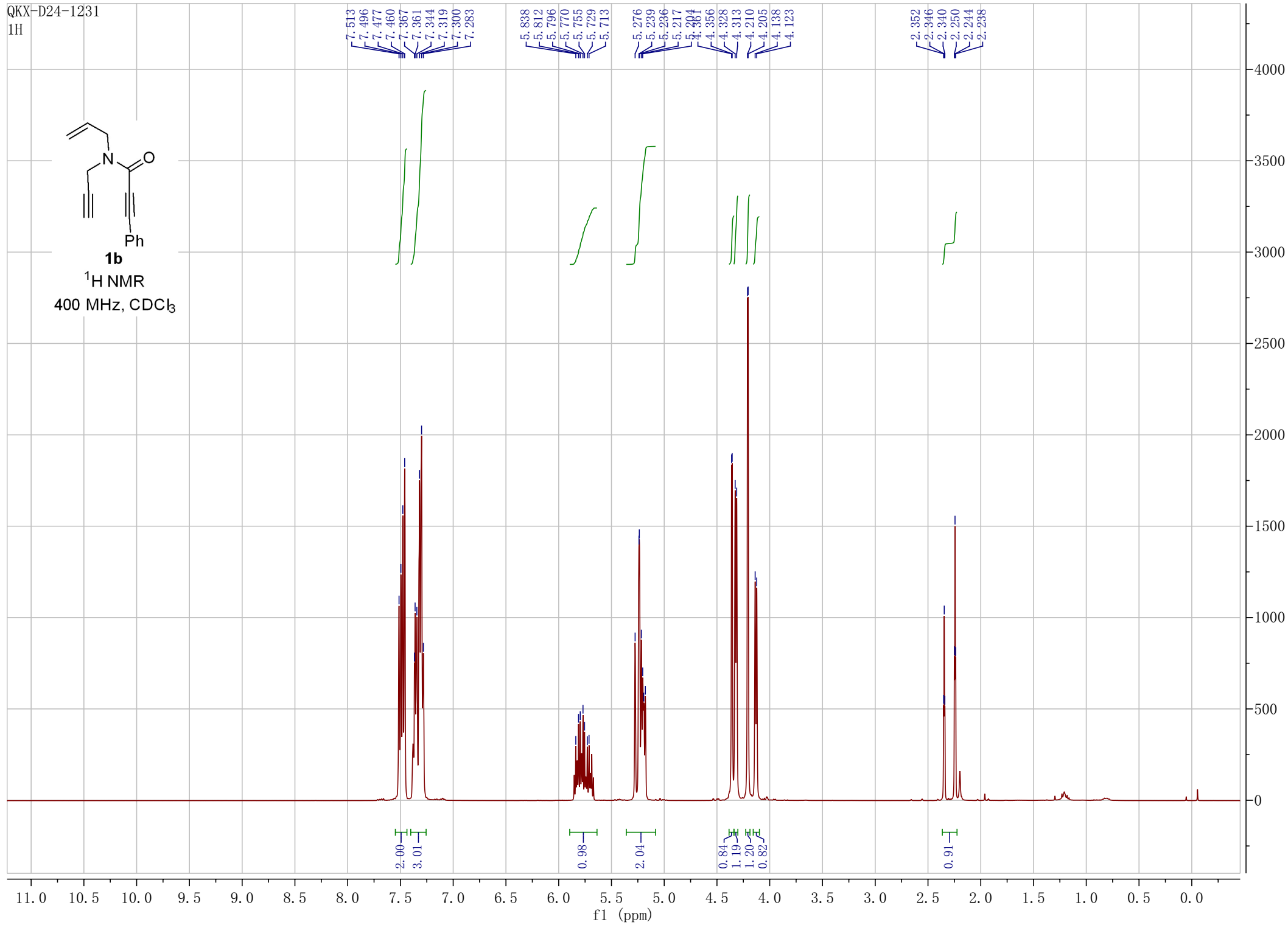
100 MHz, CDCl<sub>3</sub>





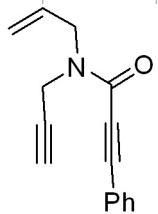
**1b**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



QKX-D24-1231

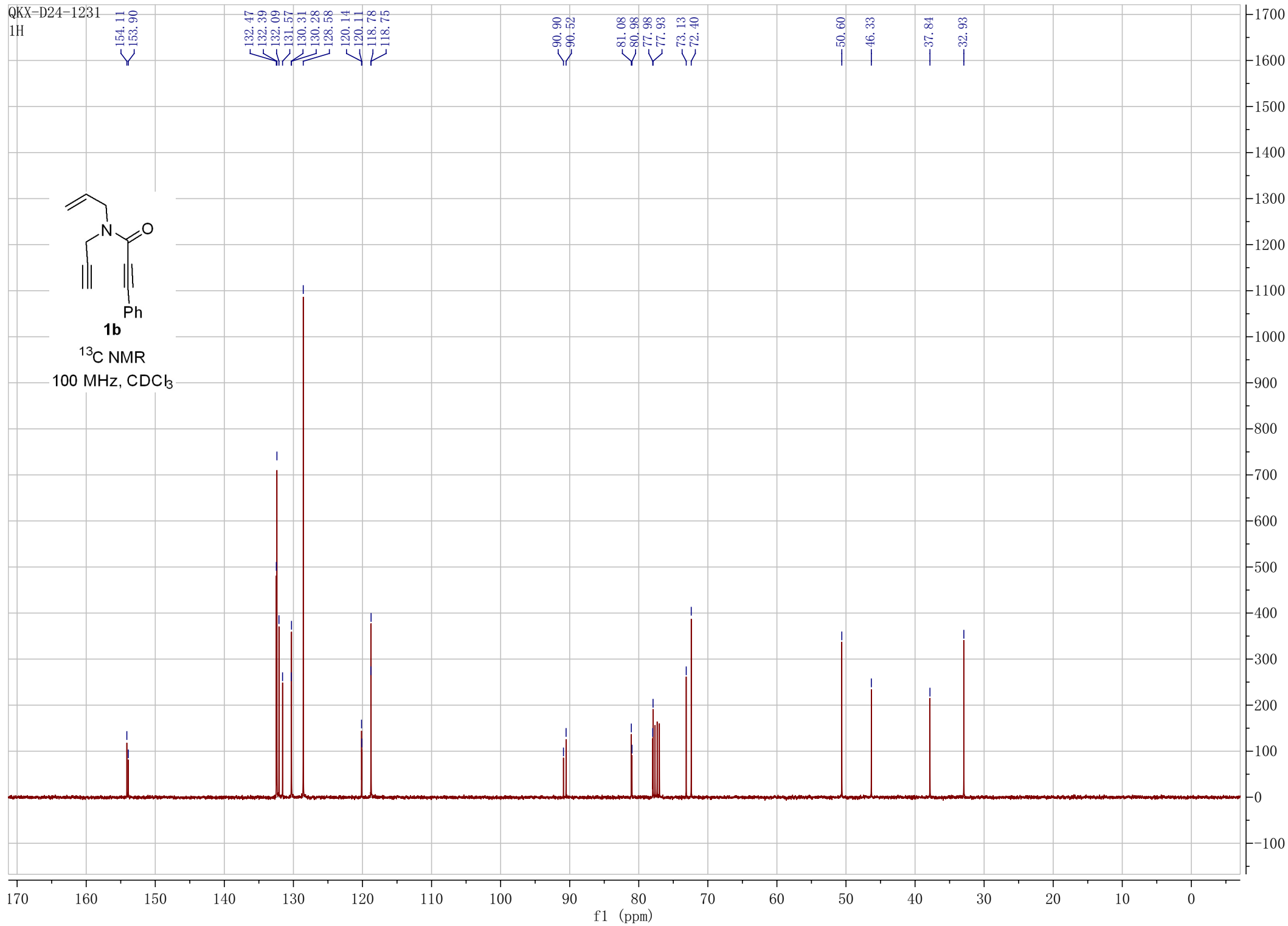
1H



**1b**

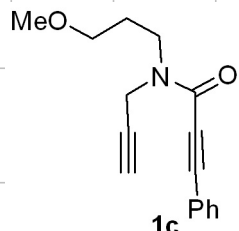
<sup>13</sup>C NMR

100 MHz, CDCl<sub>3</sub>



qkx-d17-1227

1



<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.585  
7.563  
7.453  
7.442  
7.434  
7.416  
7.392  
7.374  
7.355

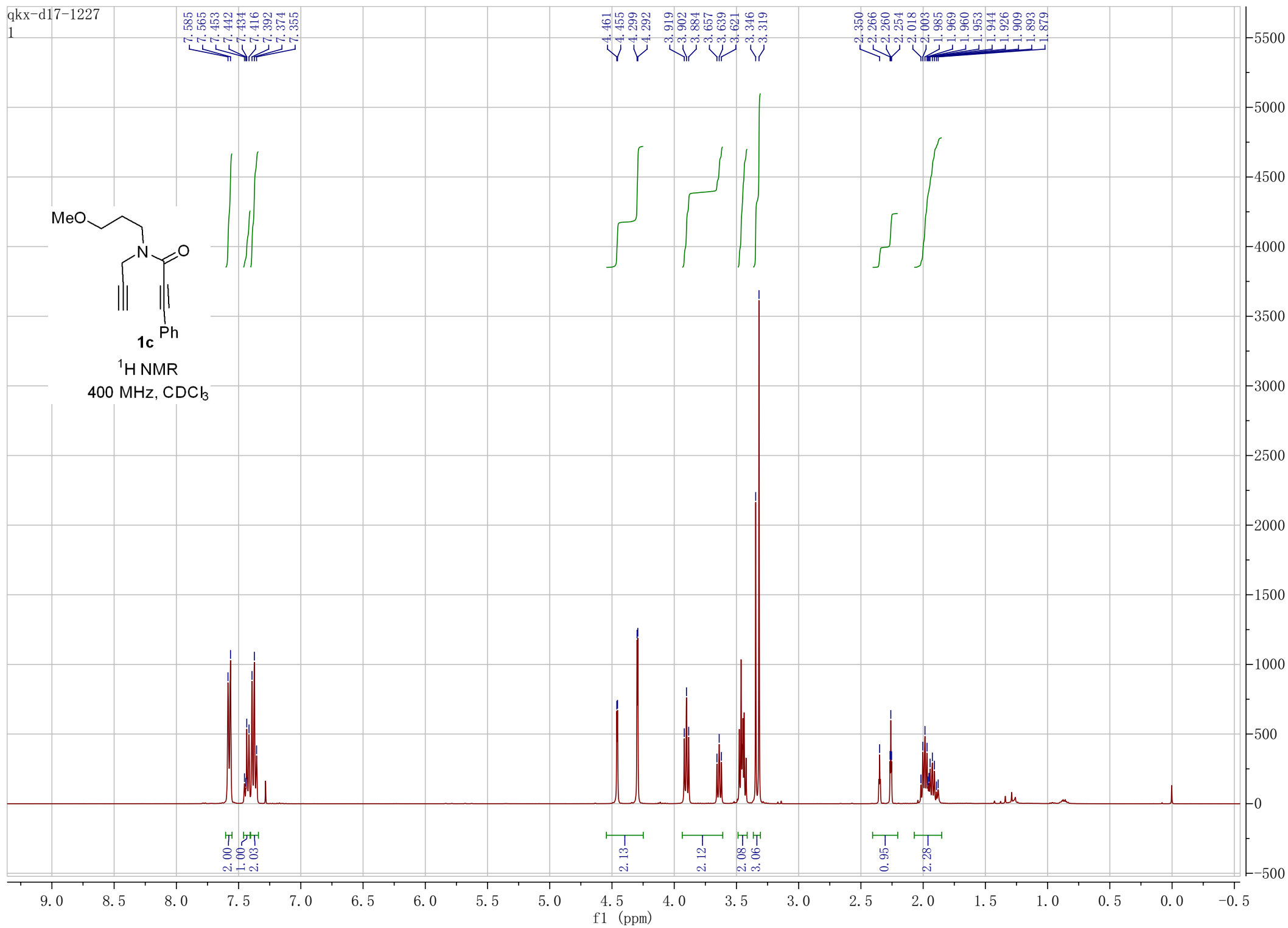
4.461  
4.455  
4.299  
4.292  
3.919  
3.902  
3.884  
3.657  
3.639  
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3.346  
3.319

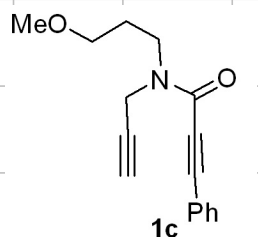
2.350  
2.266  
2.260  
2.254  
2.018  
2.003  
1.985  
1.969  
1.960  
1.953  
1.944  
1.926  
1.909  
1.893  
1.879

2.00  
1.00  
2.03

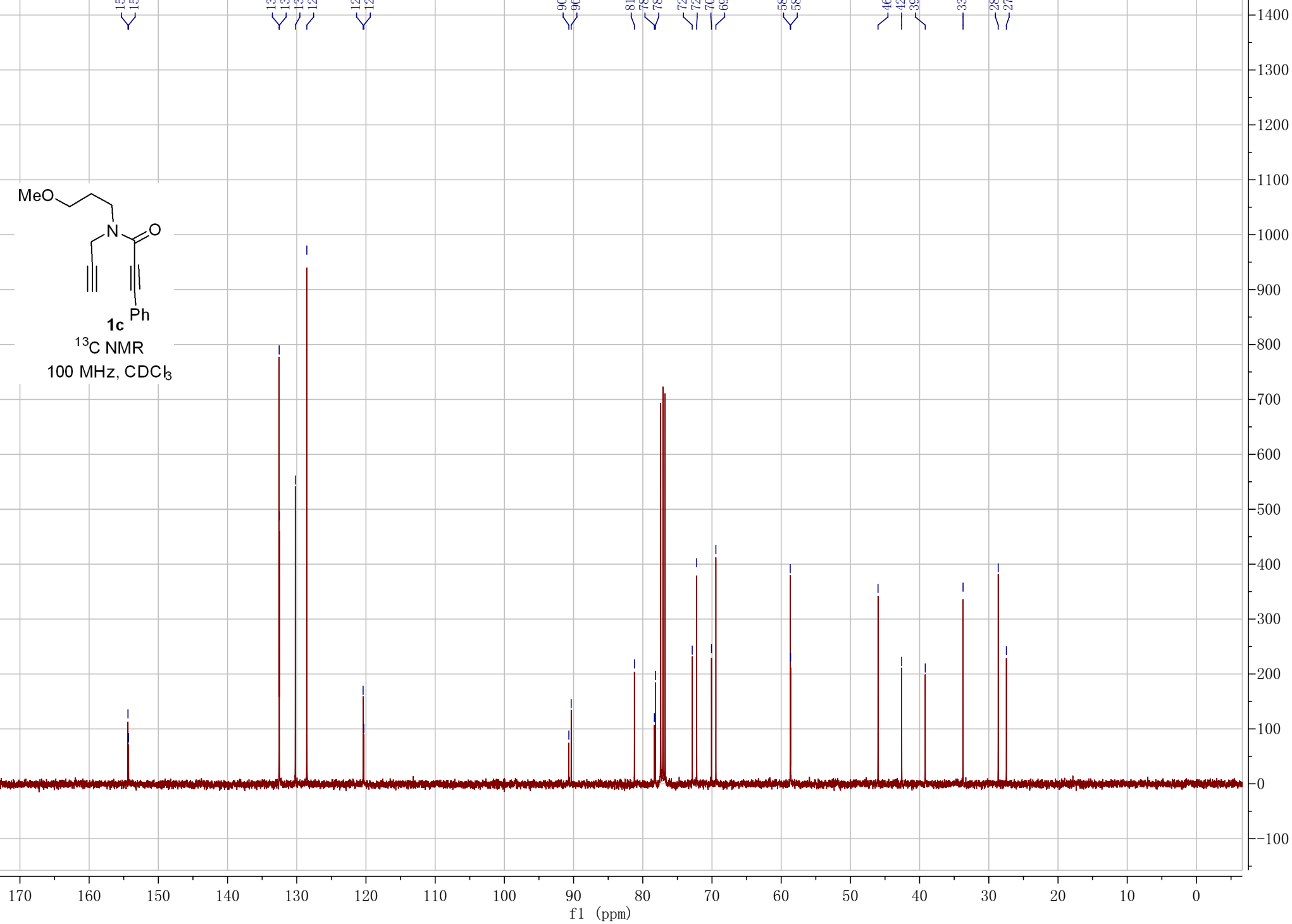
2.13  
2.12  
2.08  
3.06

0.95  
2.28



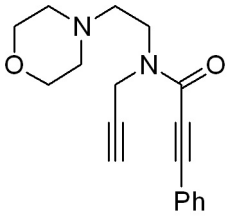


**1c**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



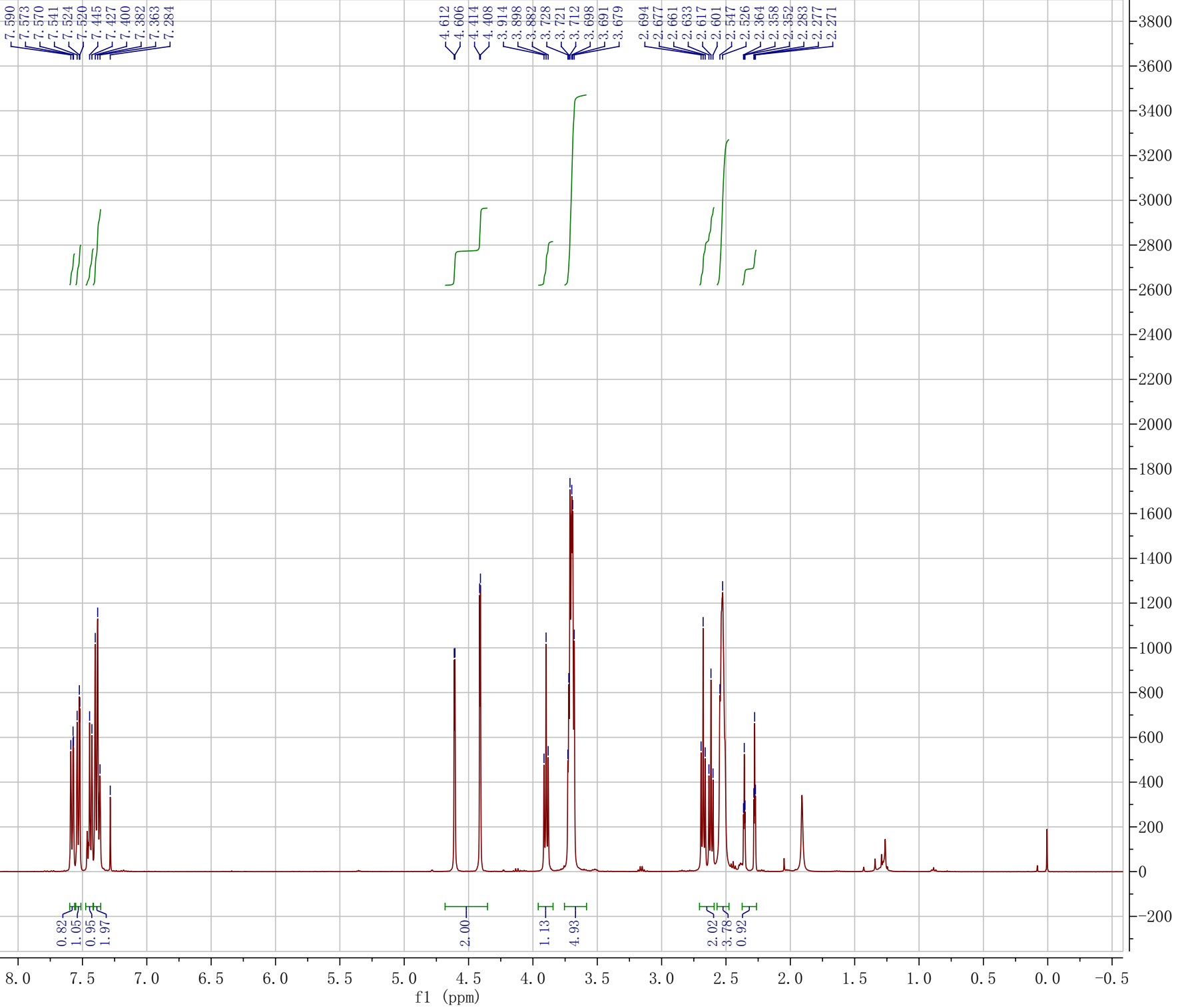
qkx-037-0204

13c



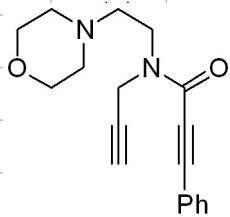
1d

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



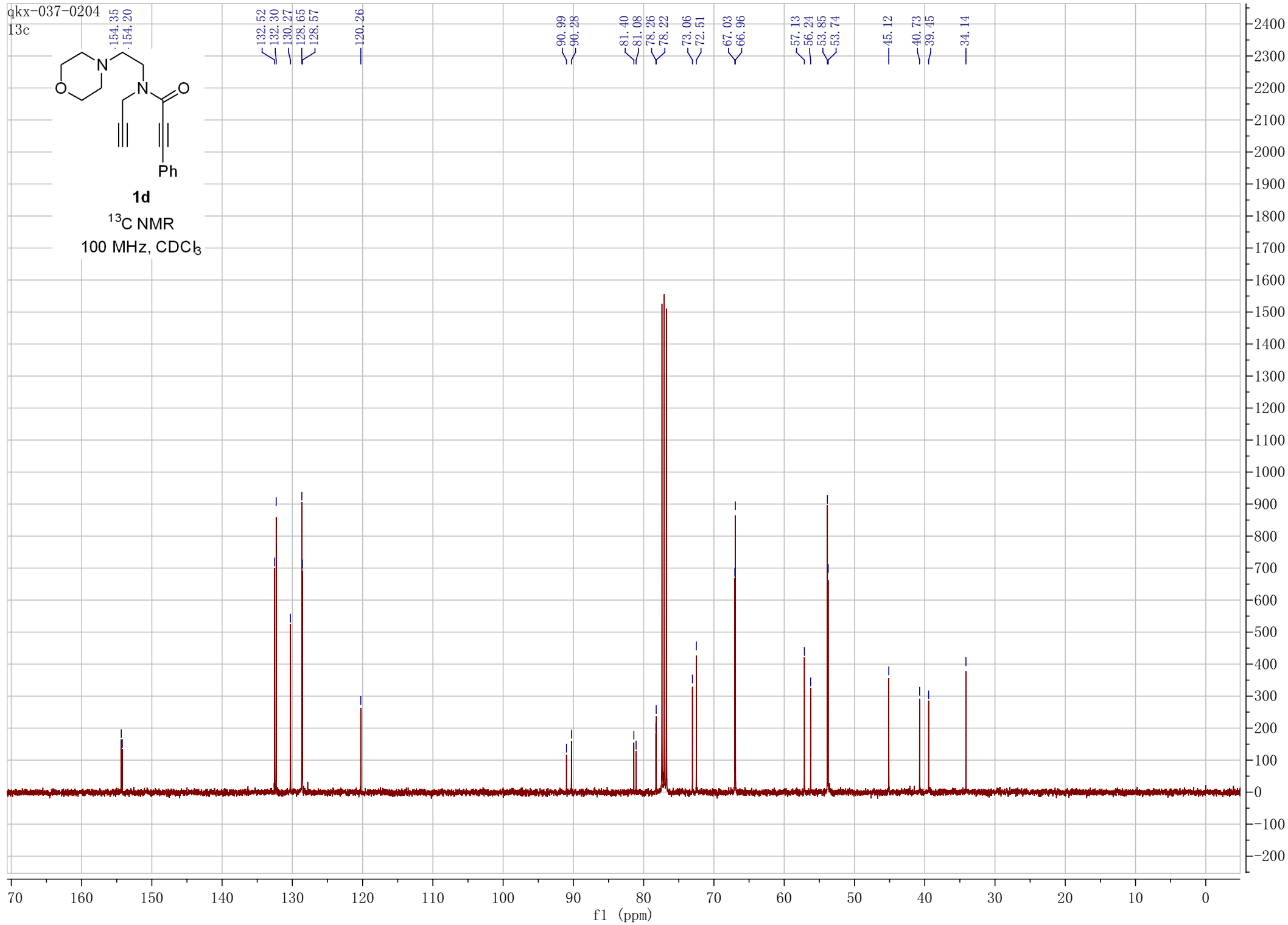
qkx-037-0204

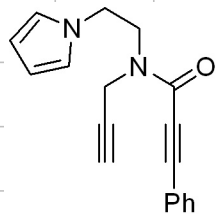
<sup>13</sup>C



**1d**

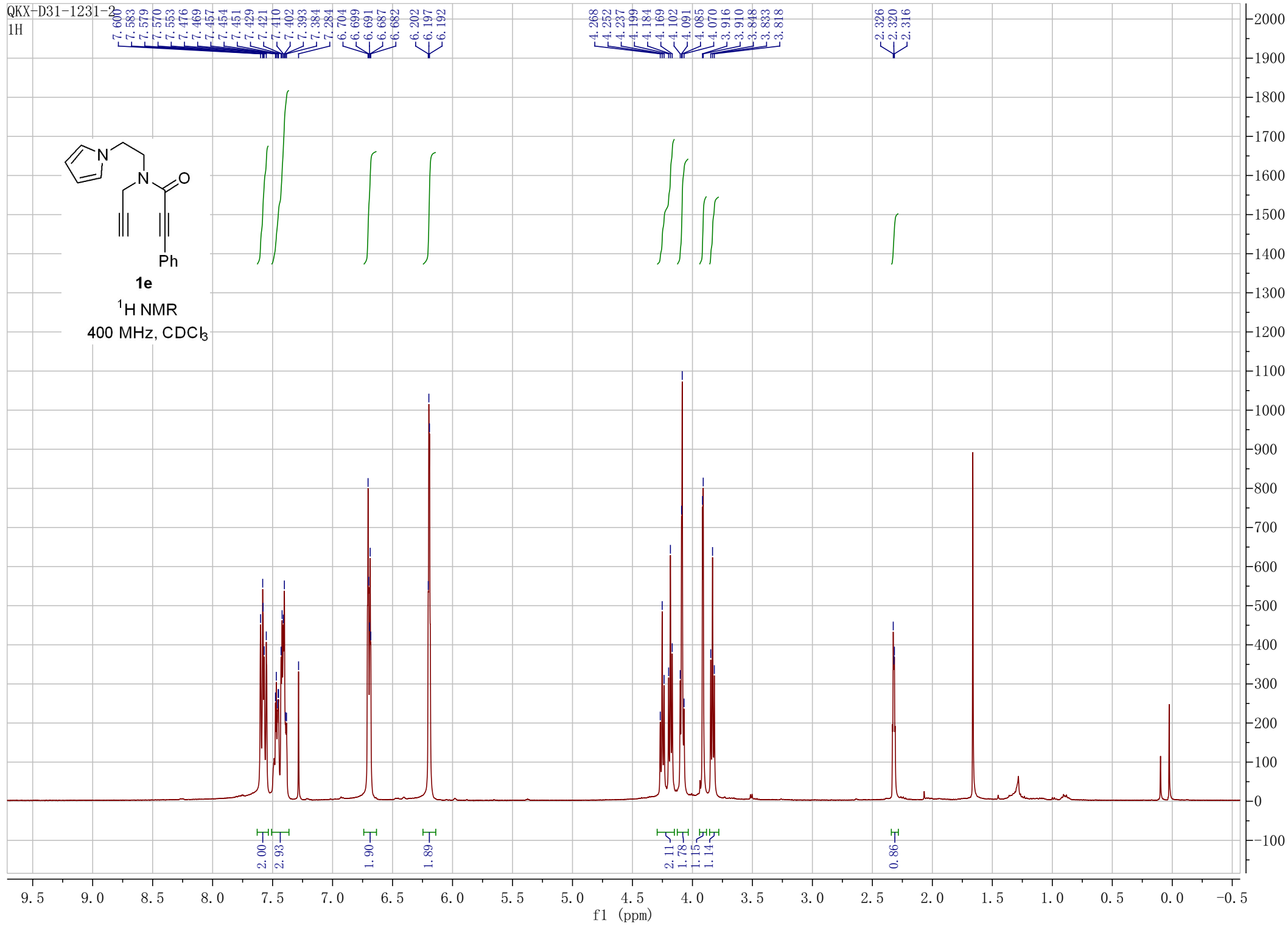
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>





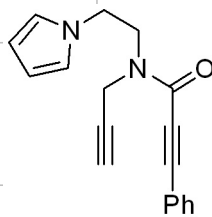
**1e**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>





QKX-d31-1231



**1e**

$^{13}\text{C}$  NMR  
100 MHz,  $\text{CDCl}_3$

154.31  
154.23

132.62  
132.52  
130.46  
130.42  
128.66  
128.63

120.74  
120.72  
120.03

109.33  
109.11

91.31  
90.62

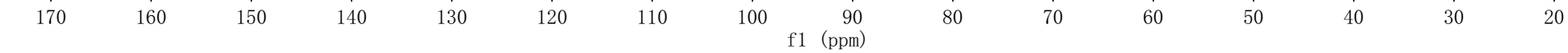
80.77  
80.72  
78.03  
77.98

73.15  
72.91

49.72  
48.31  
47.17  
46.61

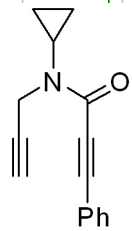
39.55

34.22



QKX-D32-1231

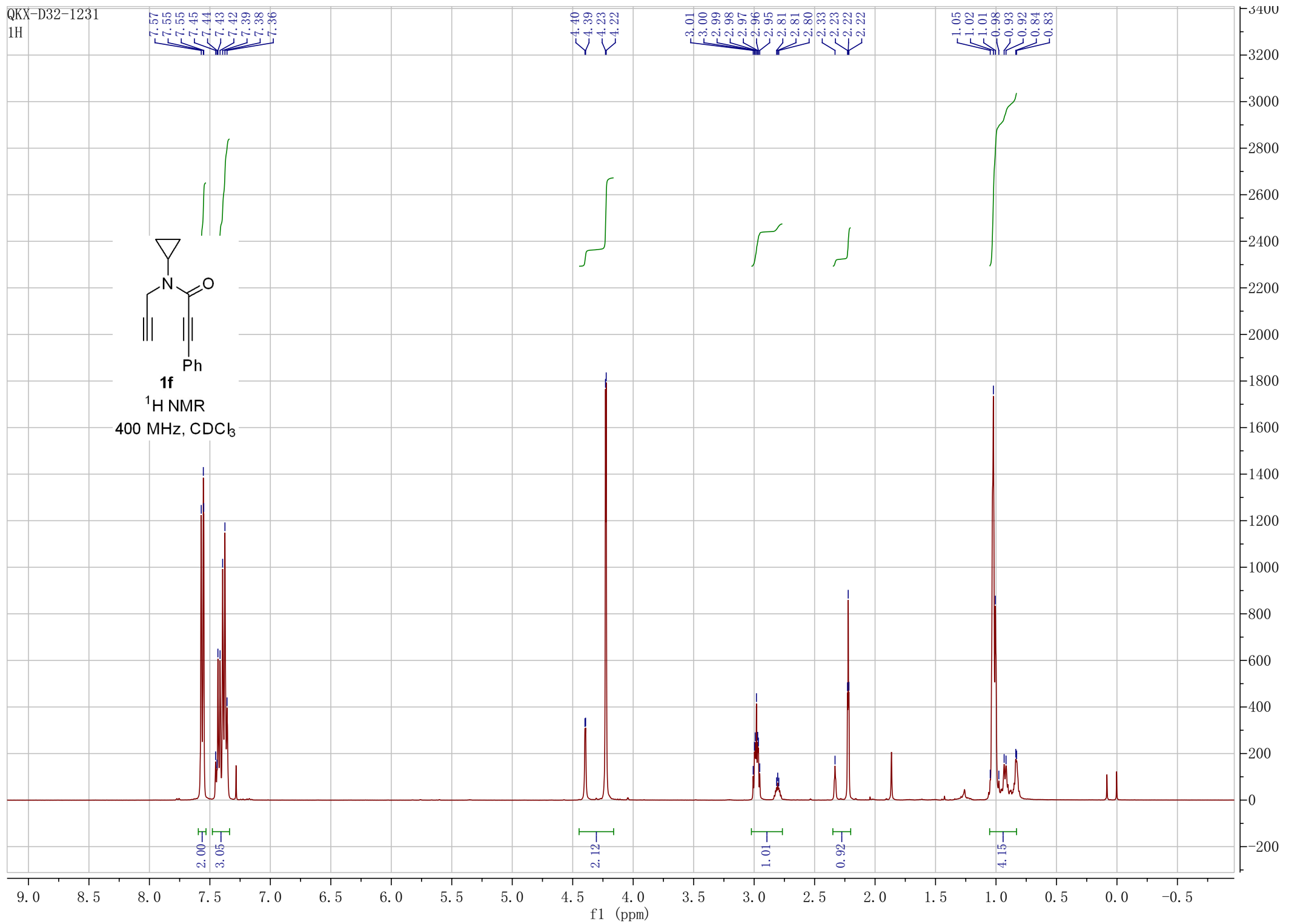
<sup>1</sup>H



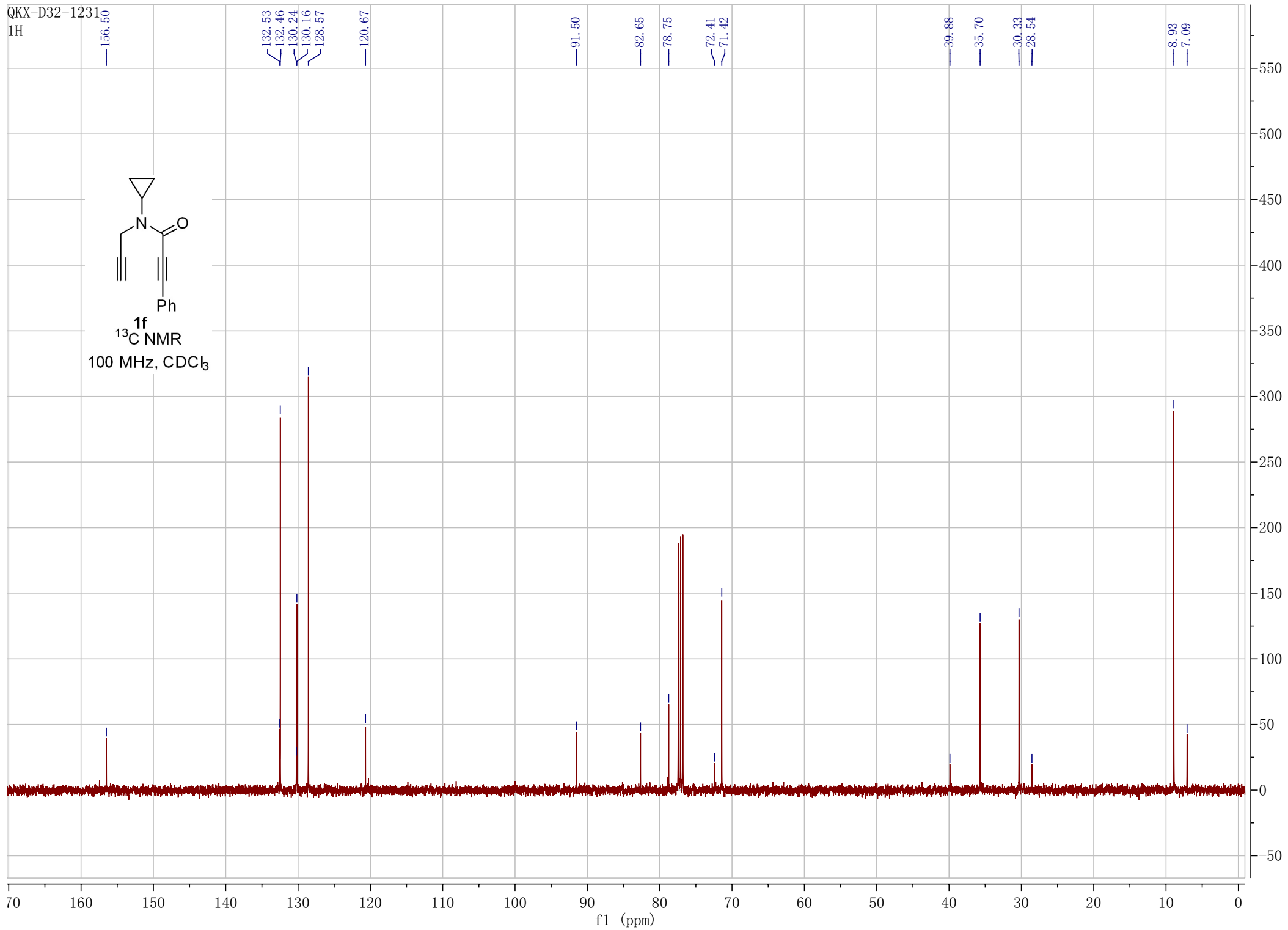
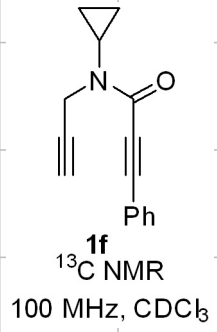
**1f**

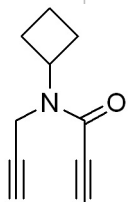
<sup>1</sup>H NMR

400 MHz, CDCl<sub>3</sub>



QKX-D32-1231  
1H





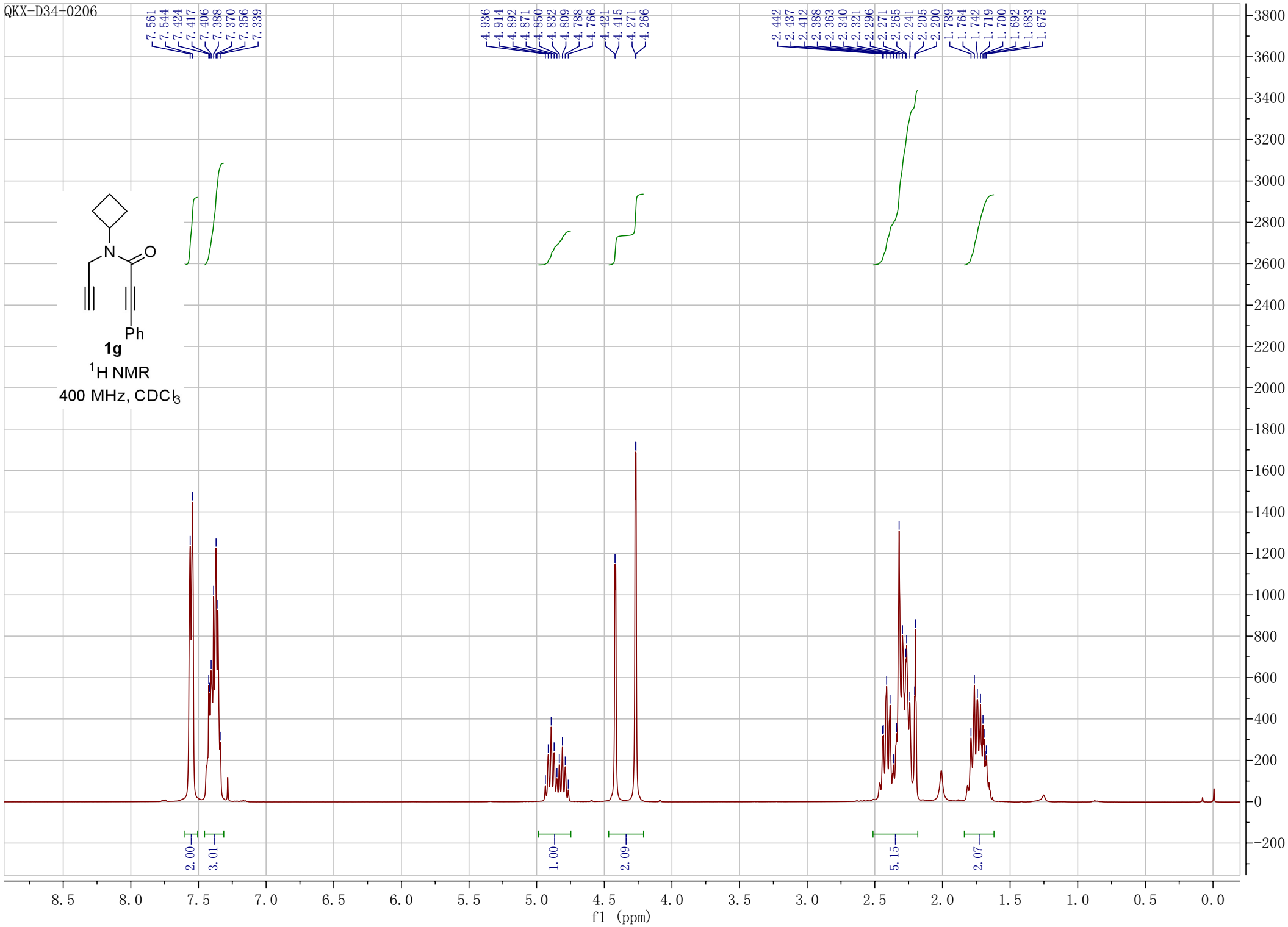
**1g**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

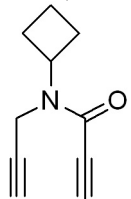
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7.424  
7.417  
7.406  
7.388  
7.370  
7.356  
7.339

4.936  
4.914  
4.892  
4.871  
4.850  
4.832  
4.809  
4.788  
4.766  
4.421  
4.415  
4.271  
4.266

2.442  
2.437  
2.412  
2.388  
2.363  
2.340  
2.321  
2.296  
2.271  
2.265  
2.241  
2.205  
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1.764  
1.742  
1.719  
1.700  
1.692  
1.683  
1.675



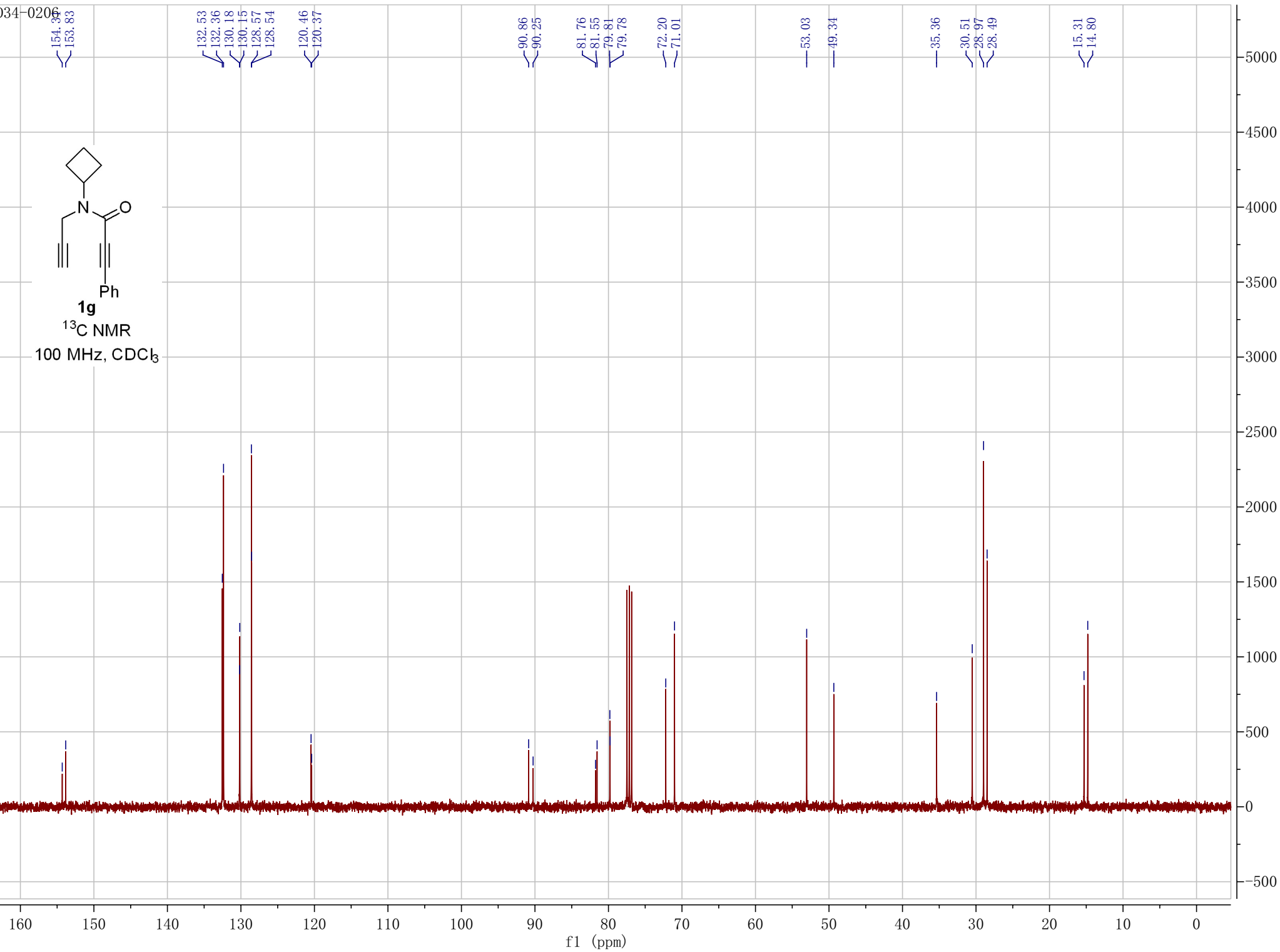
QKX-D34-0206



**1g**

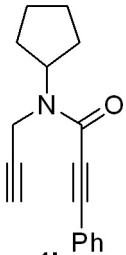
<sup>13</sup>C NMR

100 MHz, CDCl<sub>3</sub>



qkx-022-0204

13c



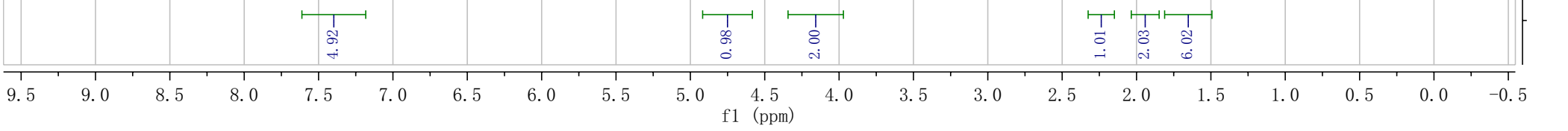
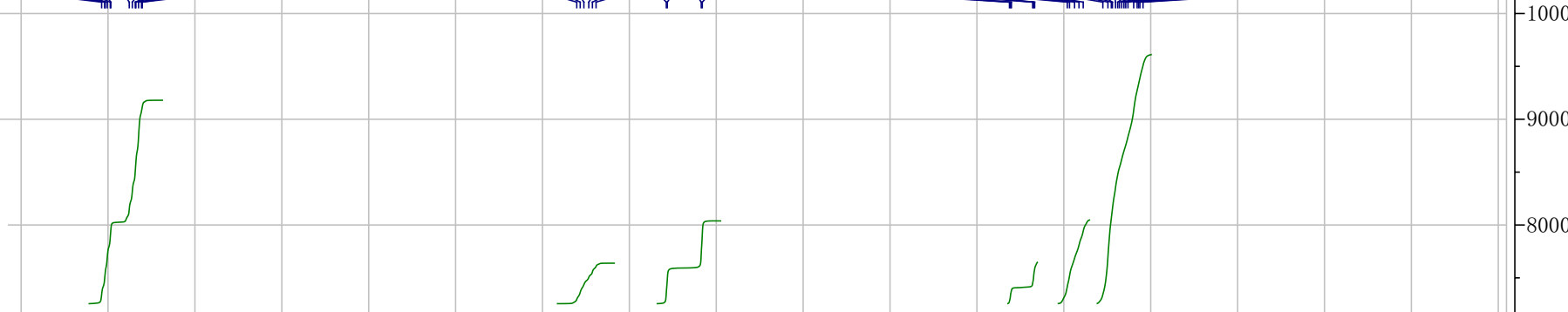
**1h**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.537  
7.519  
7.516  
7.504  
7.487  
7.484  
7.378  
7.360  
7.343  
7.340  
7.324  
7.307  
7.303

4.803  
4.783  
4.762  
4.733  
4.713  
4.692  
4.287  
4.282  
4.086  
4.080

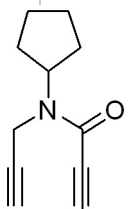
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2.302  
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1.938  
1.913  
1.888  
1.775  
1.746  
1.727  
1.720  
1.702  
1.690  
1.680  
1.667  
1.654  
1.644  
1.631  
1.598  
1.578  
1.570  
1.562  
1.544



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

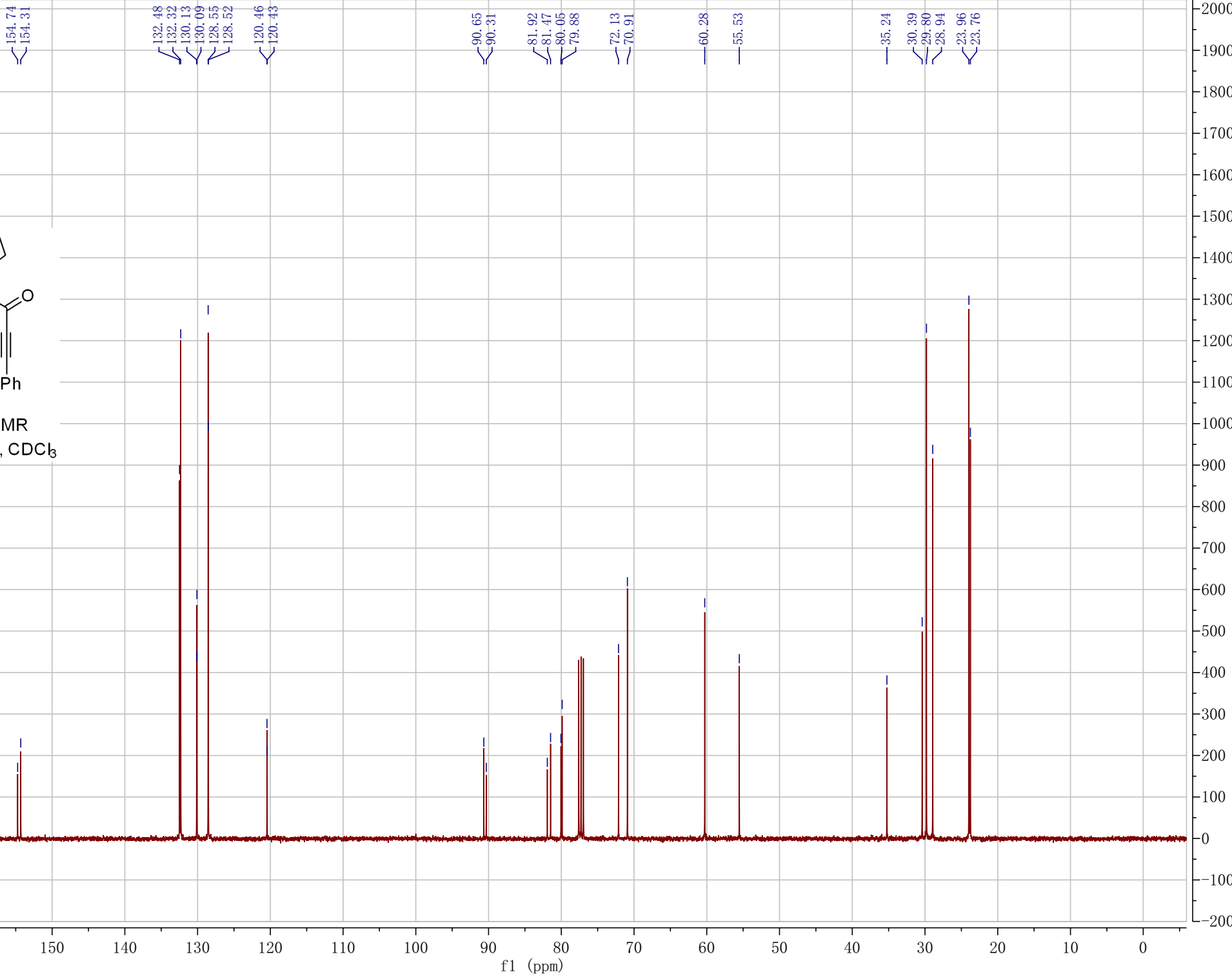
f1 (ppm)

qkx-022-0204  
13c

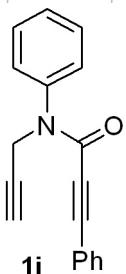


**1h**

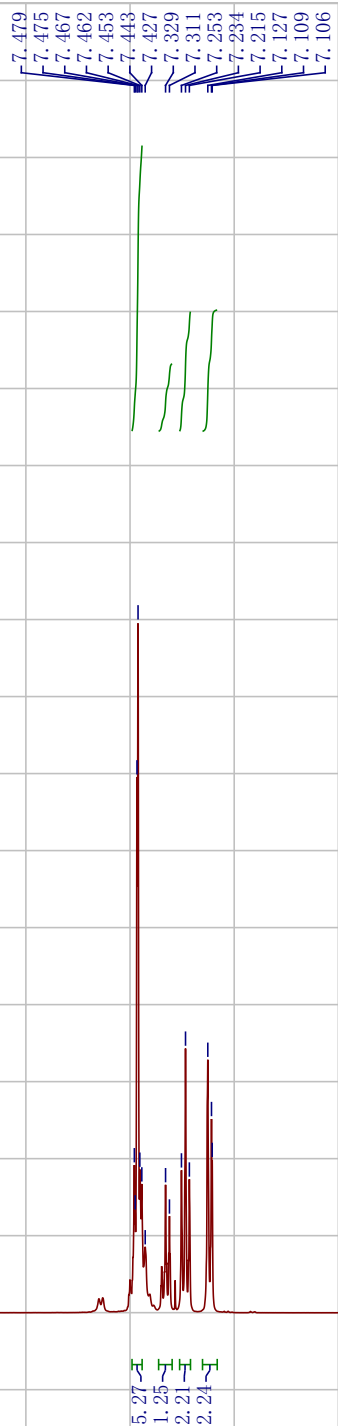
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



qkx-c1109-ph



<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

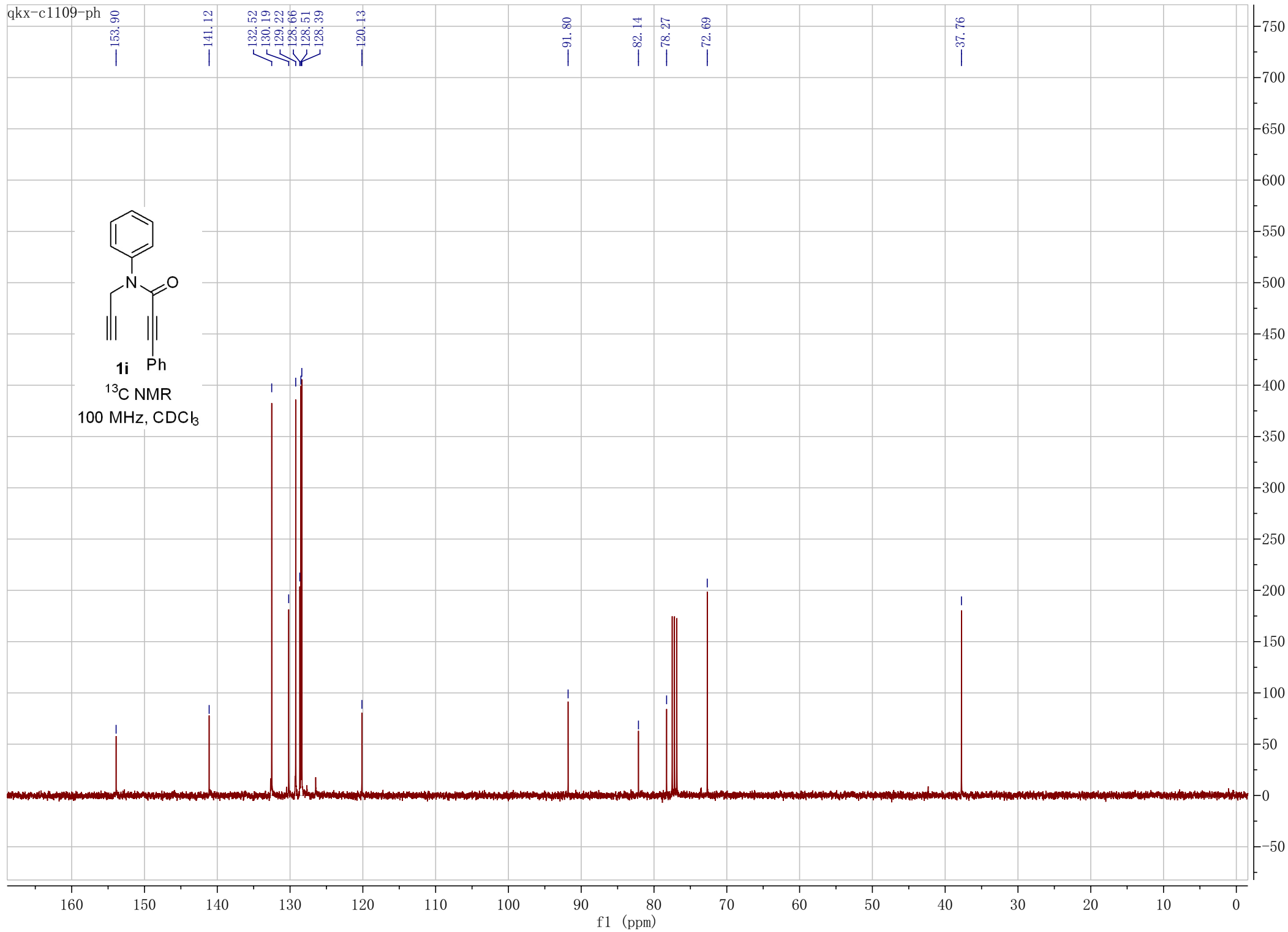
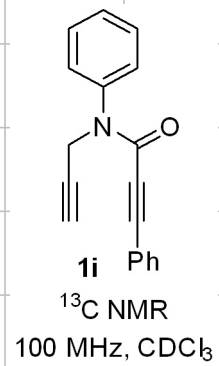


9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)

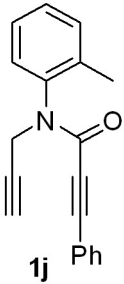


qkx-c1109-ph



qkx-c127-1214

1

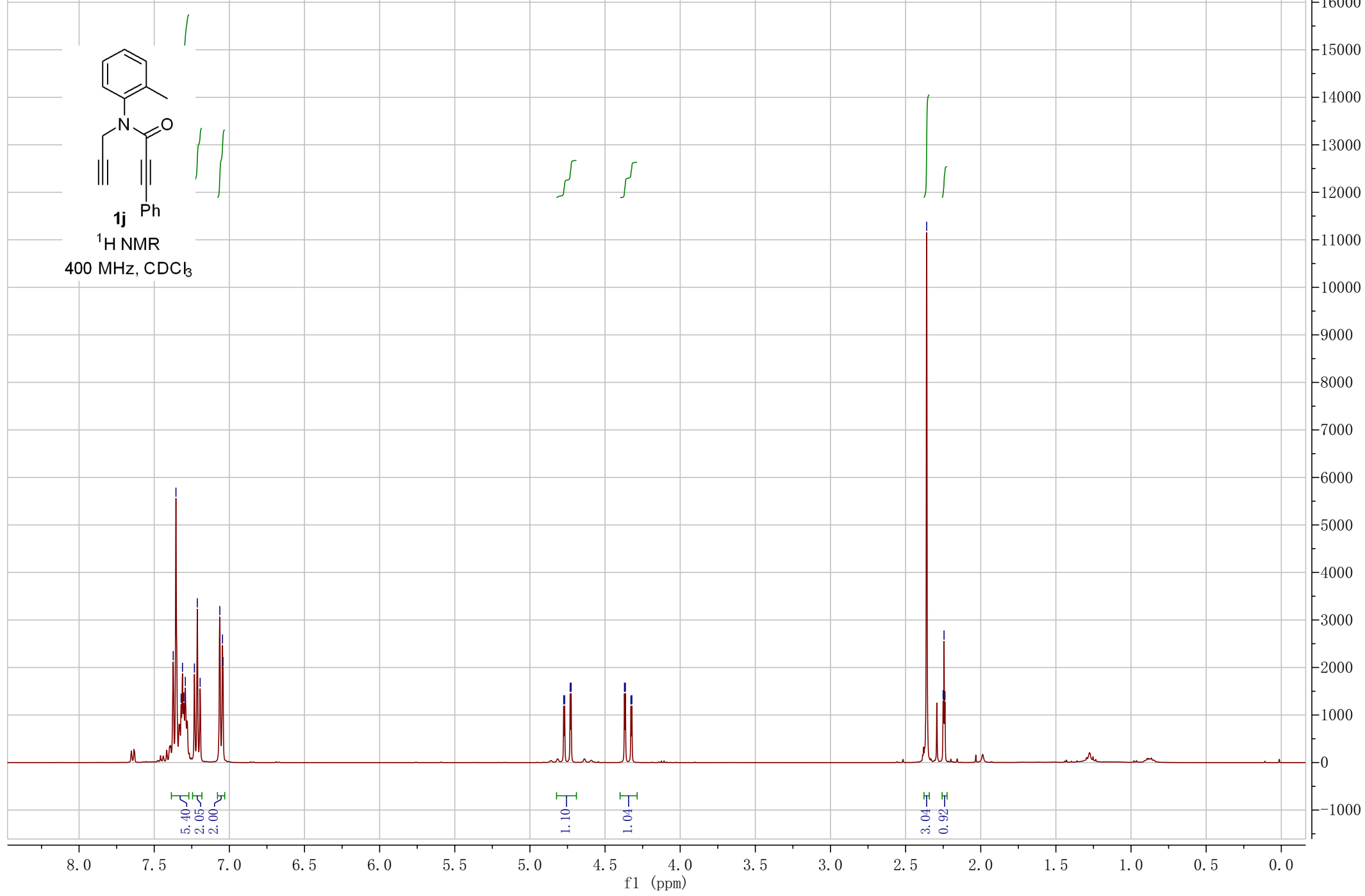


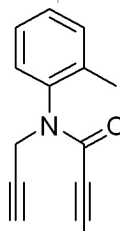
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.374  
7.355  
7.321  
7.312  
7.303  
7.293  
7.233  
7.213  
7.194  
7.064  
7.046  
7.043

4.775  
4.769  
4.732  
4.726  
4.371  
4.365  
4.328  
4.322

2.360  
2.250  
2.244  
2.238

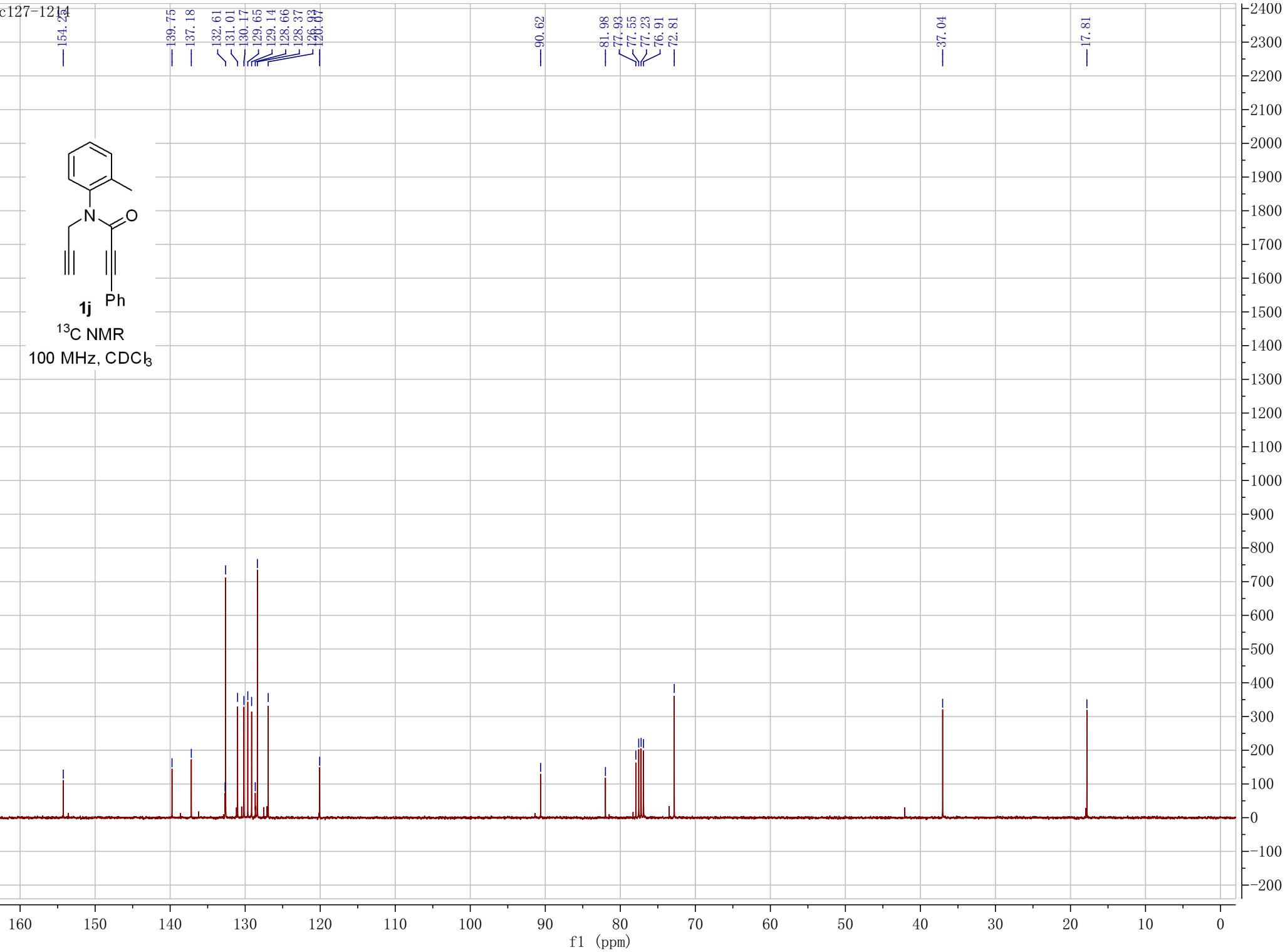




1j

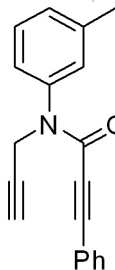
Ph

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



qkx-c135-0309

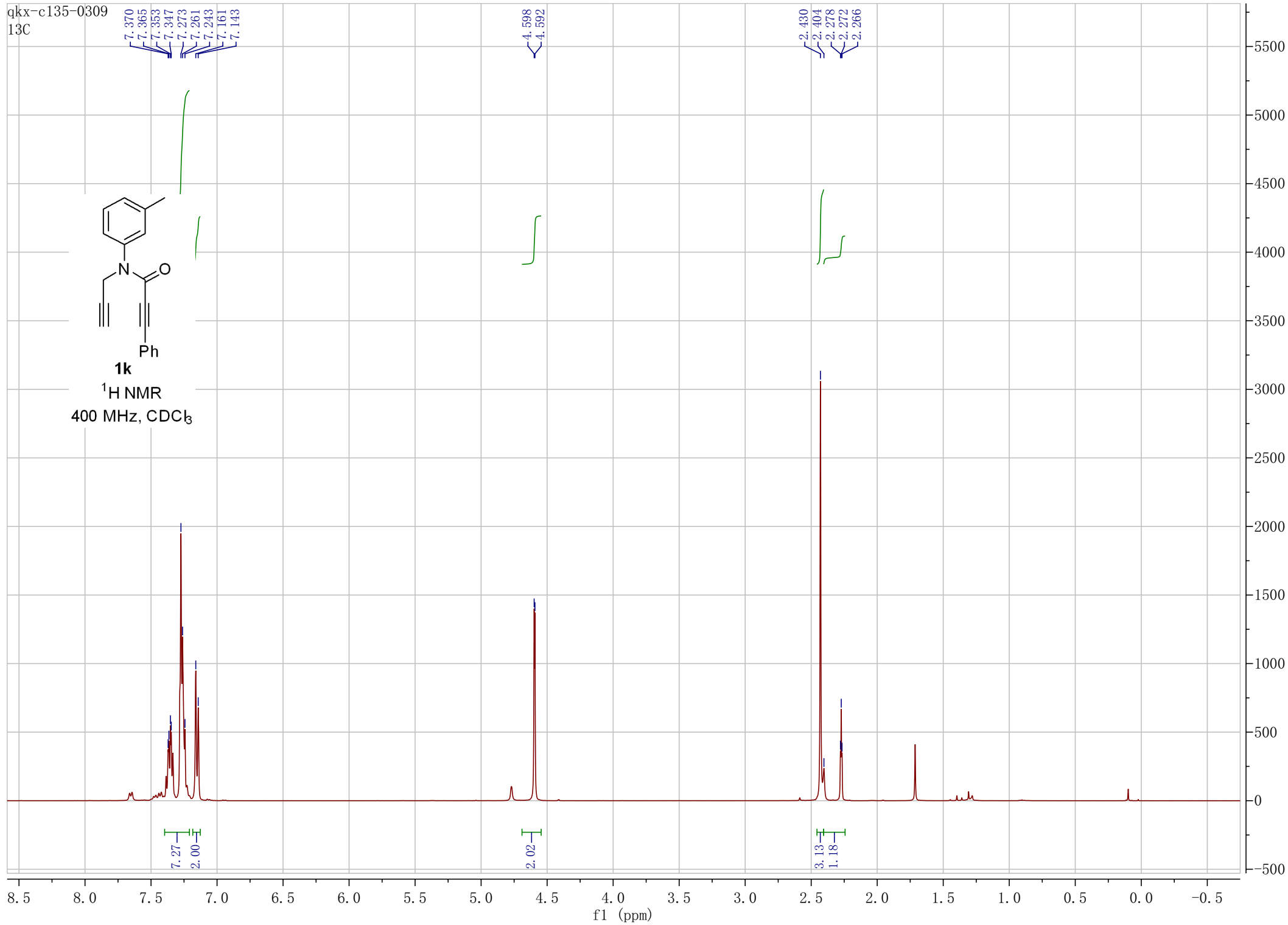
<sup>13</sup>C



**1k**

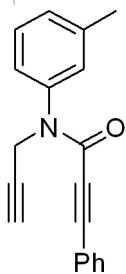
<sup>1</sup>H NMR

400 MHz, CDCl<sub>3</sub>



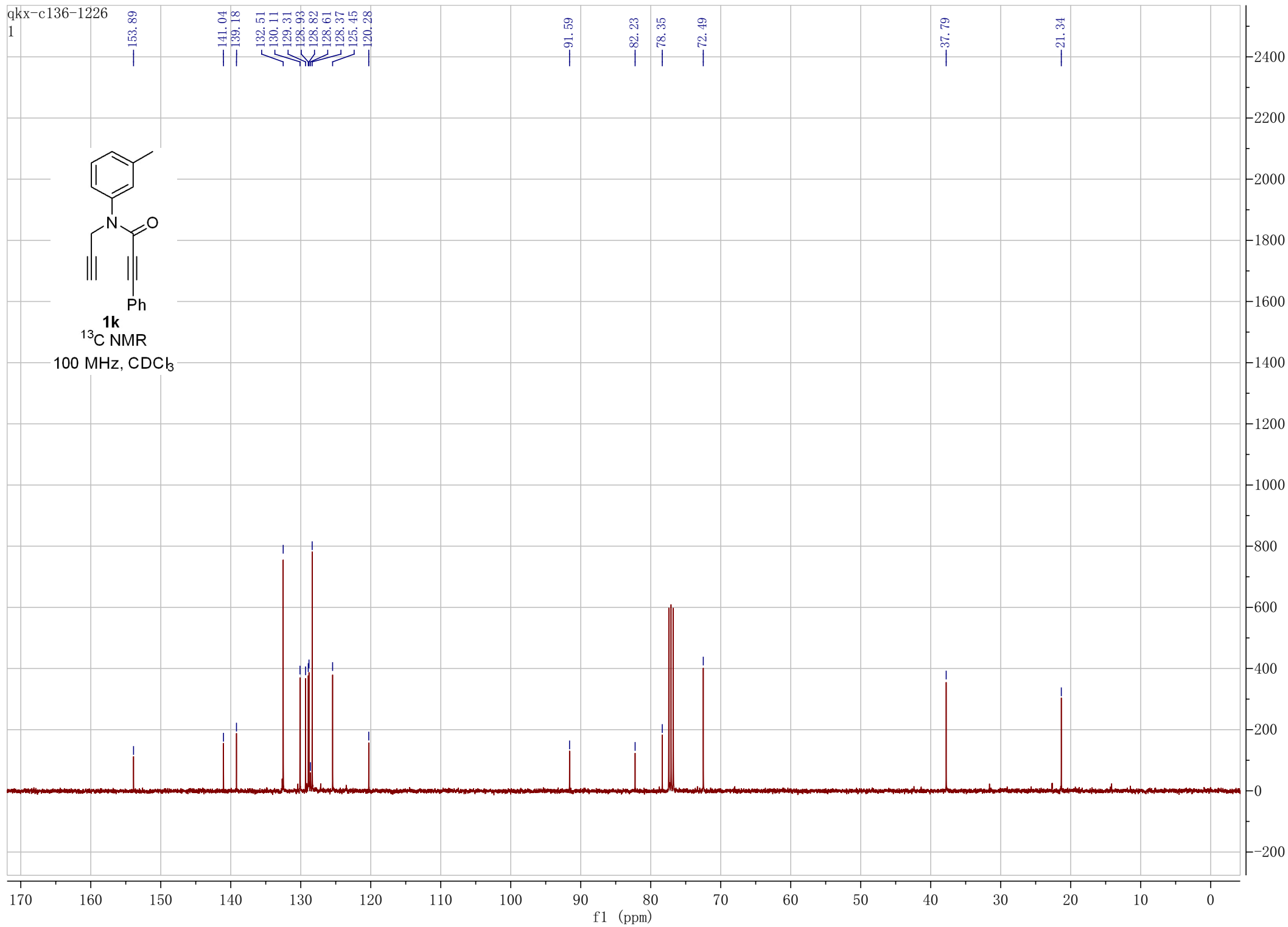
qkx-c136-1226

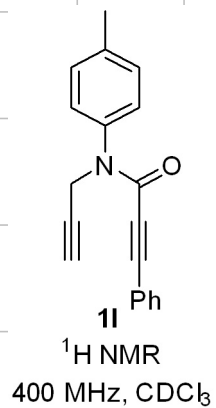
1



**1k**  
<sup>13</sup>C NMR

100 MHz, CDCl<sub>3</sub>

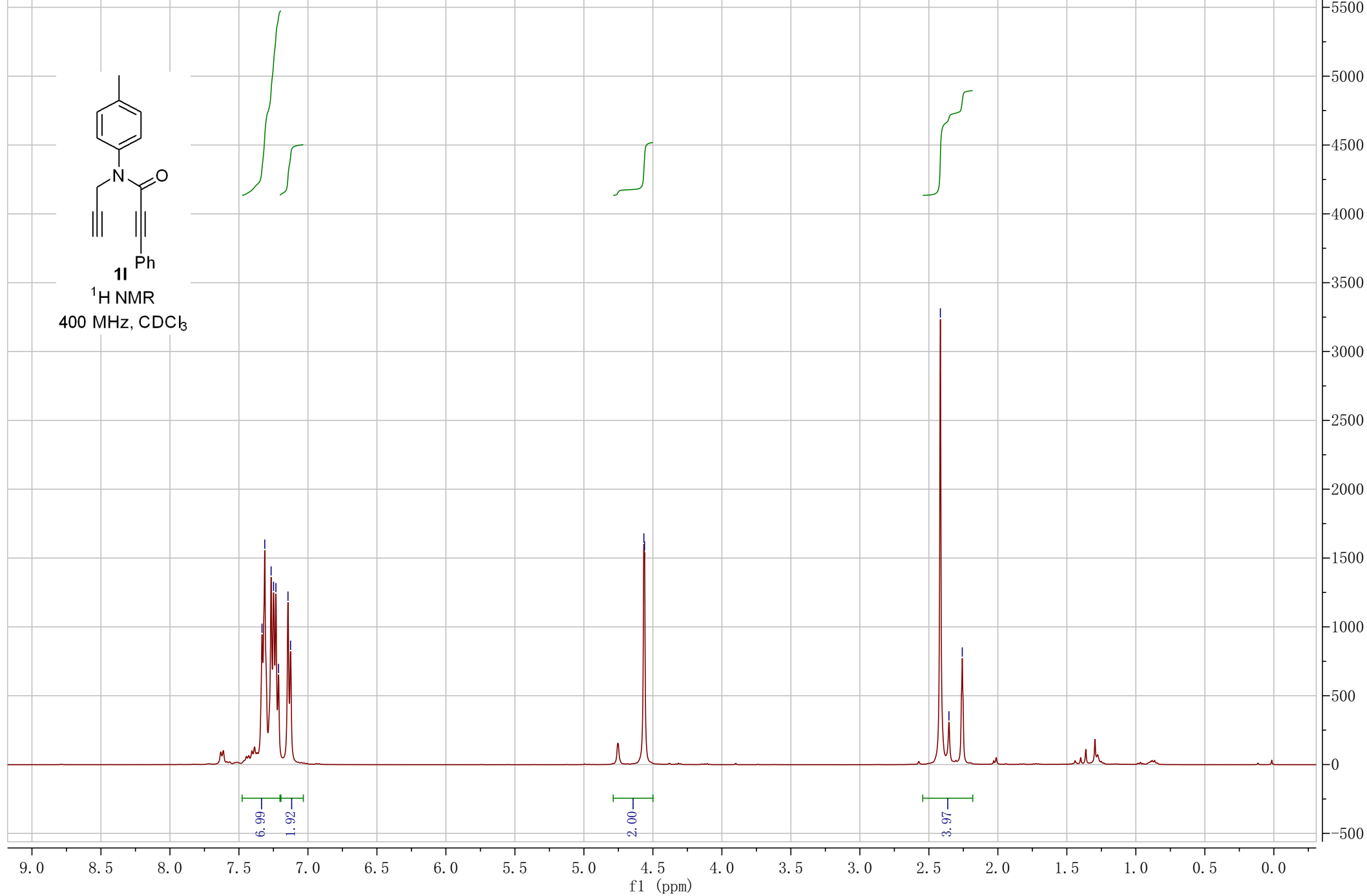


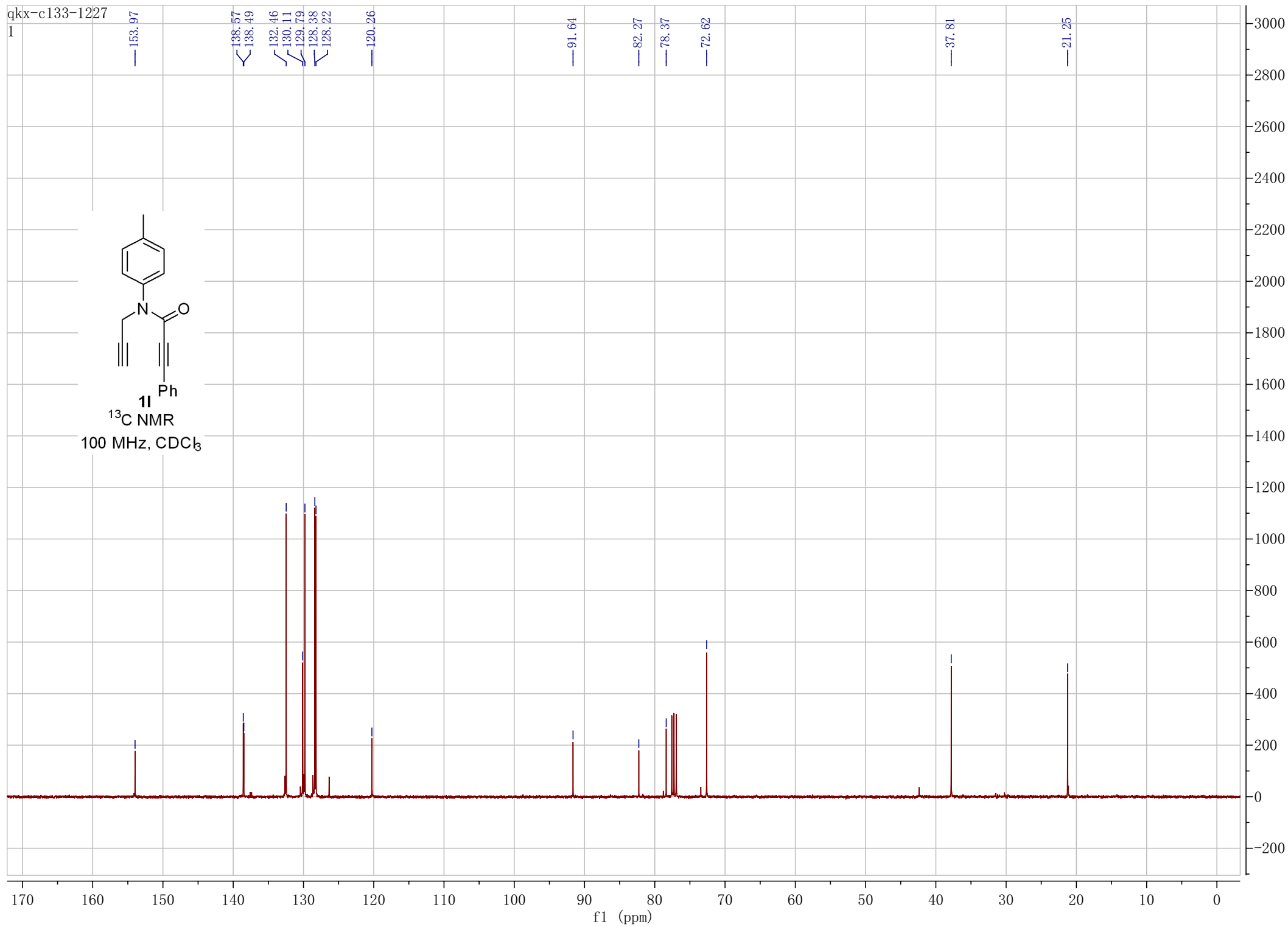
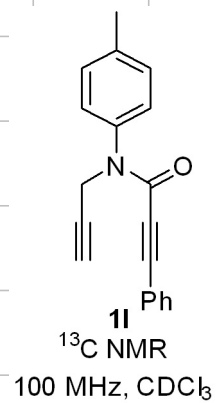


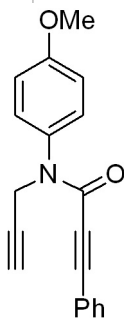
7.333  
 7.313  
 7.267  
 7.249  
 7.232  
 7.213  
 7.145  
 7.126

4.565  
4.561

2.417  
2.354  
2.258





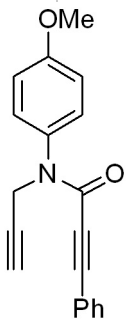


**1m**  
<sup>1</sup>H NMR  
 400 MHz, CDCl<sub>3</sub>



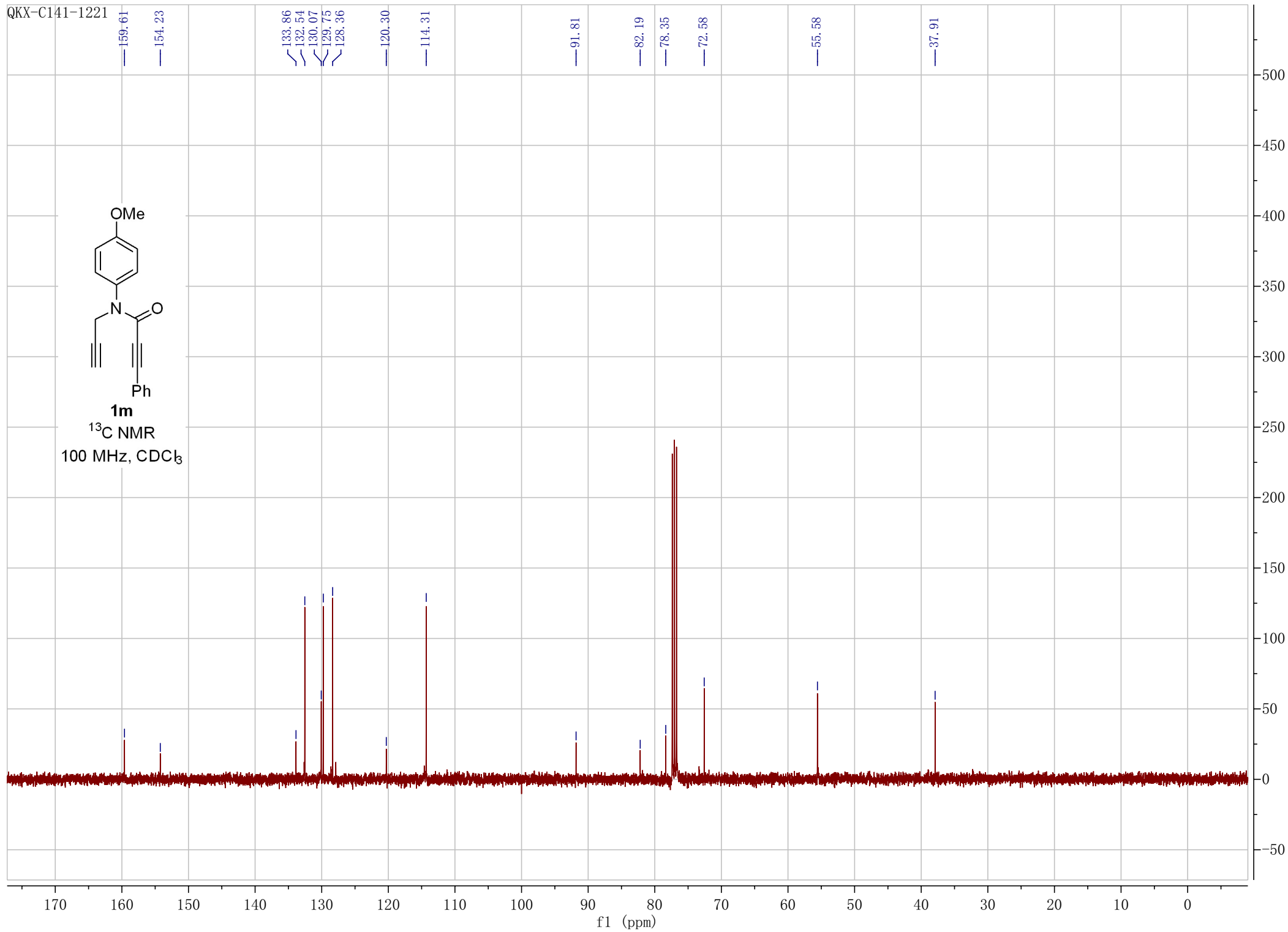


QKX-C141-1221

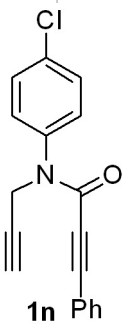


**1m**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



qkx-c143-0417

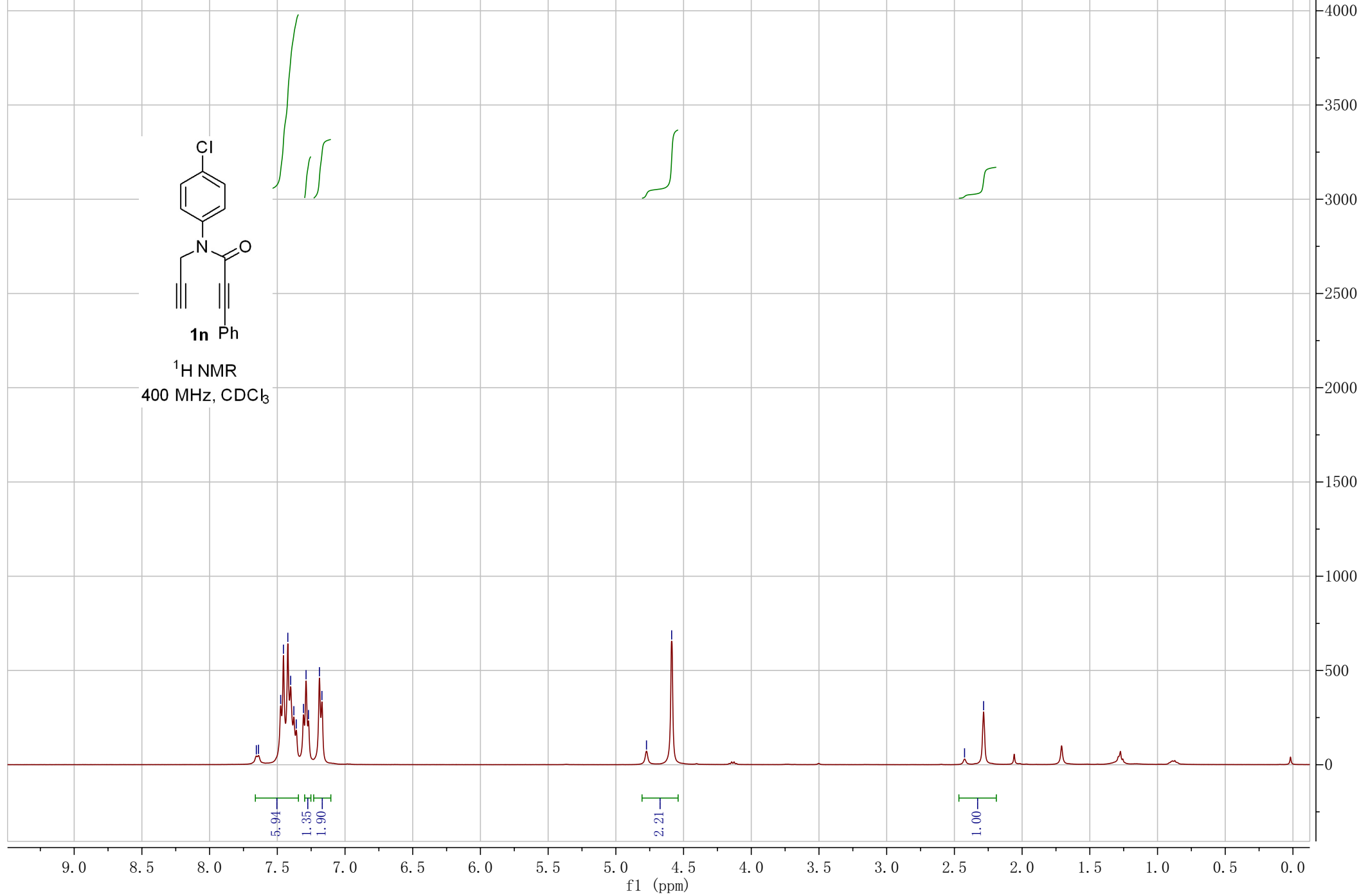


<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.655  
7.638  
7.475  
7.455  
7.422  
7.401  
7.378  
7.360  
7.307  
7.288  
7.270  
7.189  
7.170

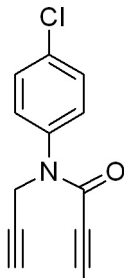
4.774  
4.588

2.425  
2.284



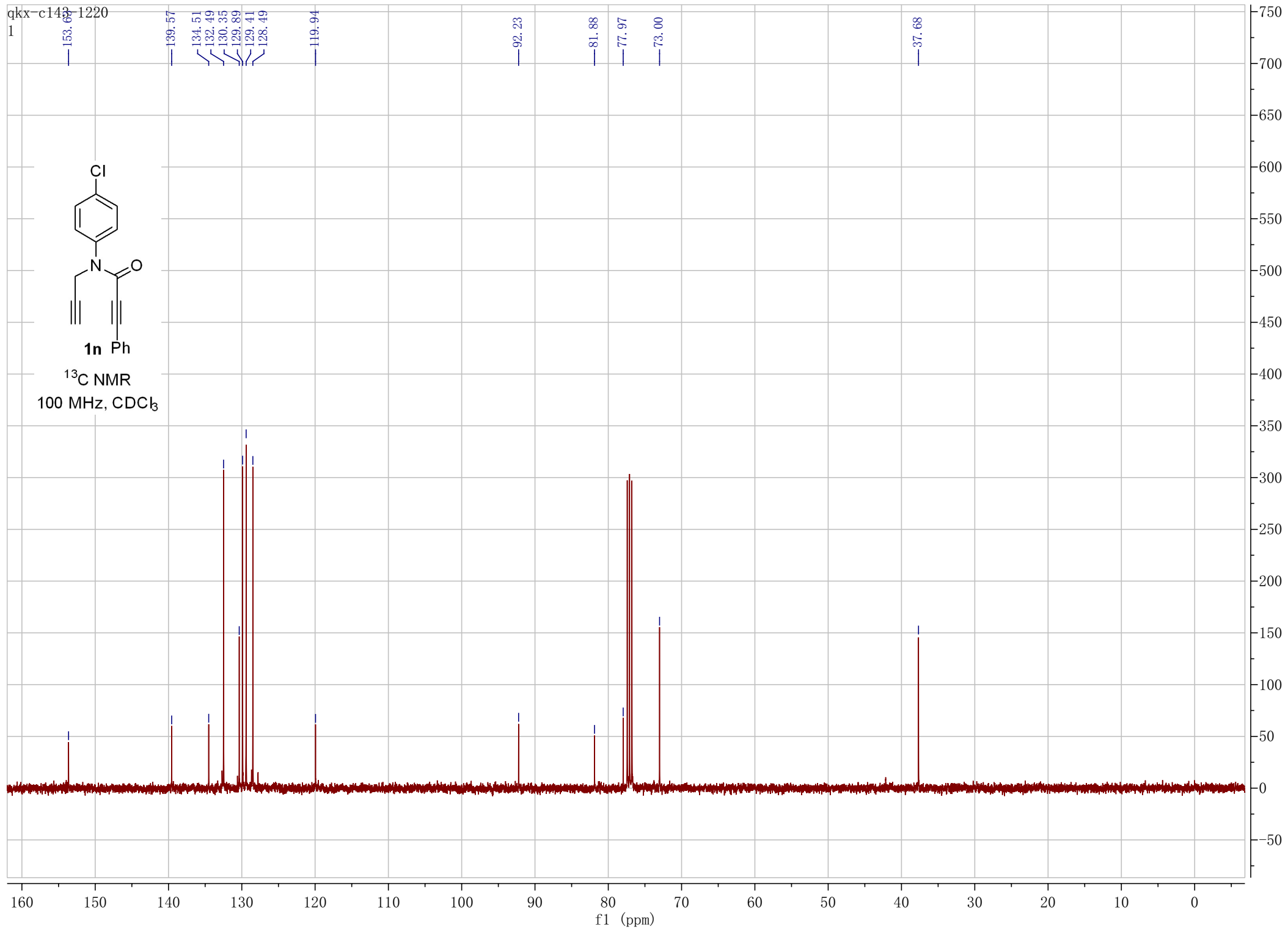
qkx-c143-1220

1

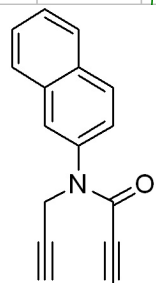


**1n** Ph

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

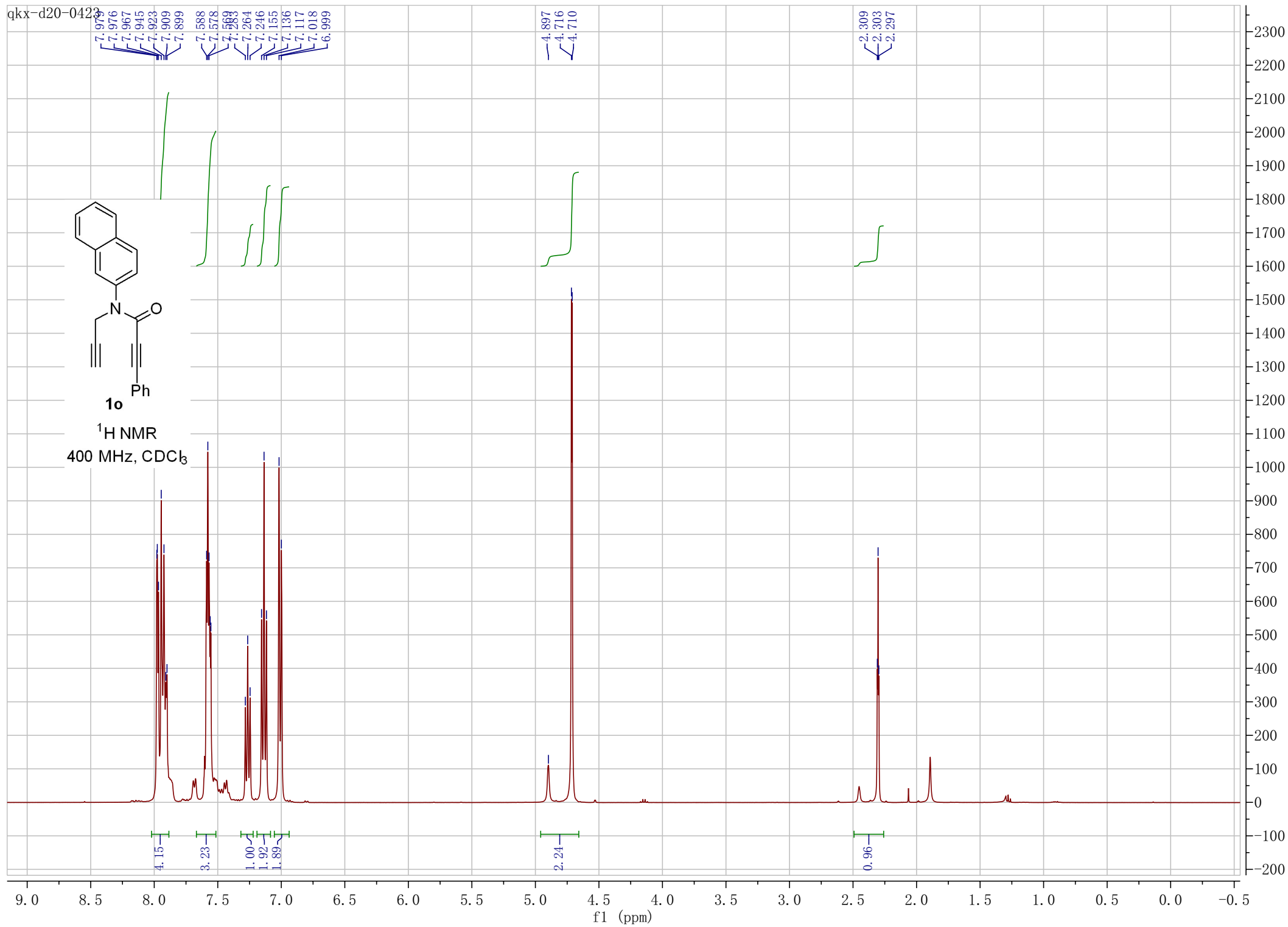


qkx-d20-0423

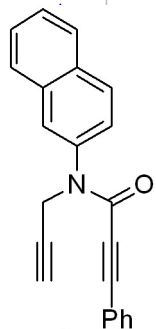


**1o**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



qkx-d20-0423



**1o**

<sup>13</sup>C NMR

100 MHz, CDCl<sub>3</sub>

154.01  
138.44  
132.44  
129.10  
128.32  
128.15  
127.84  
127.10  
126.85  
126.64

91.97

82.32

78.34

77.50

72.84

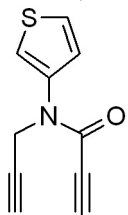
37.99

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

700  
650  
600  
550  
500  
450  
400  
350  
300  
250  
200  
150  
100  
50  
0  
-50

qkx-d27-1230



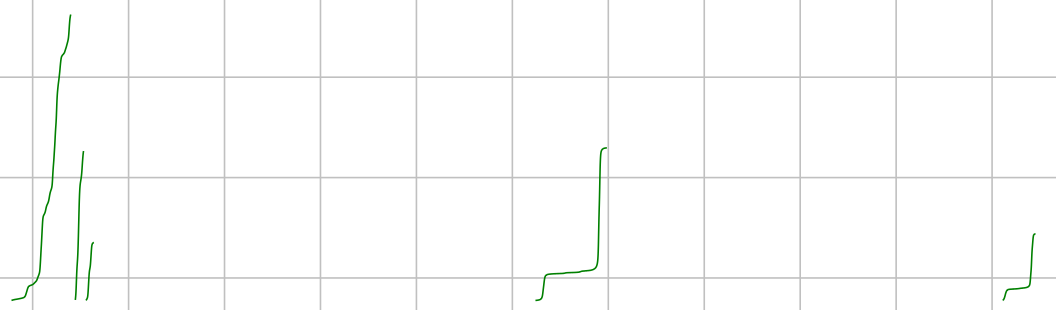
**1p**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.645  
7.627  
7.529  
7.458  
7.451  
7.431  
7.412  
7.395  
7.388  
7.383  
7.375  
7.357  
7.331  
7.323  
7.310  
7.290  
7.272  
7.259  
7.242  
7.208  
7.196

4.840  
4.835  
4.550  
4.544

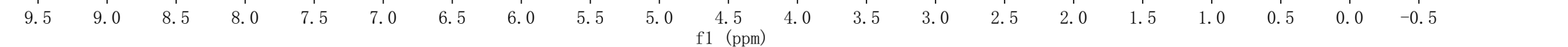
2.432  
2.300  
2.294  
2.288



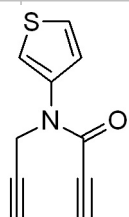
4.29  
2.24  
0.87

2.29

1.00



qkx-d27-1231



**1p**

<sup>13</sup>C NMR

100 MHz, CDCl<sub>3</sub>

153.85  
139.21  
132.69  
130.56  
130.29  
128.67  
128.47  
126.60  
125.24  
123.63  
122.41  
118.15

91.60

81.90

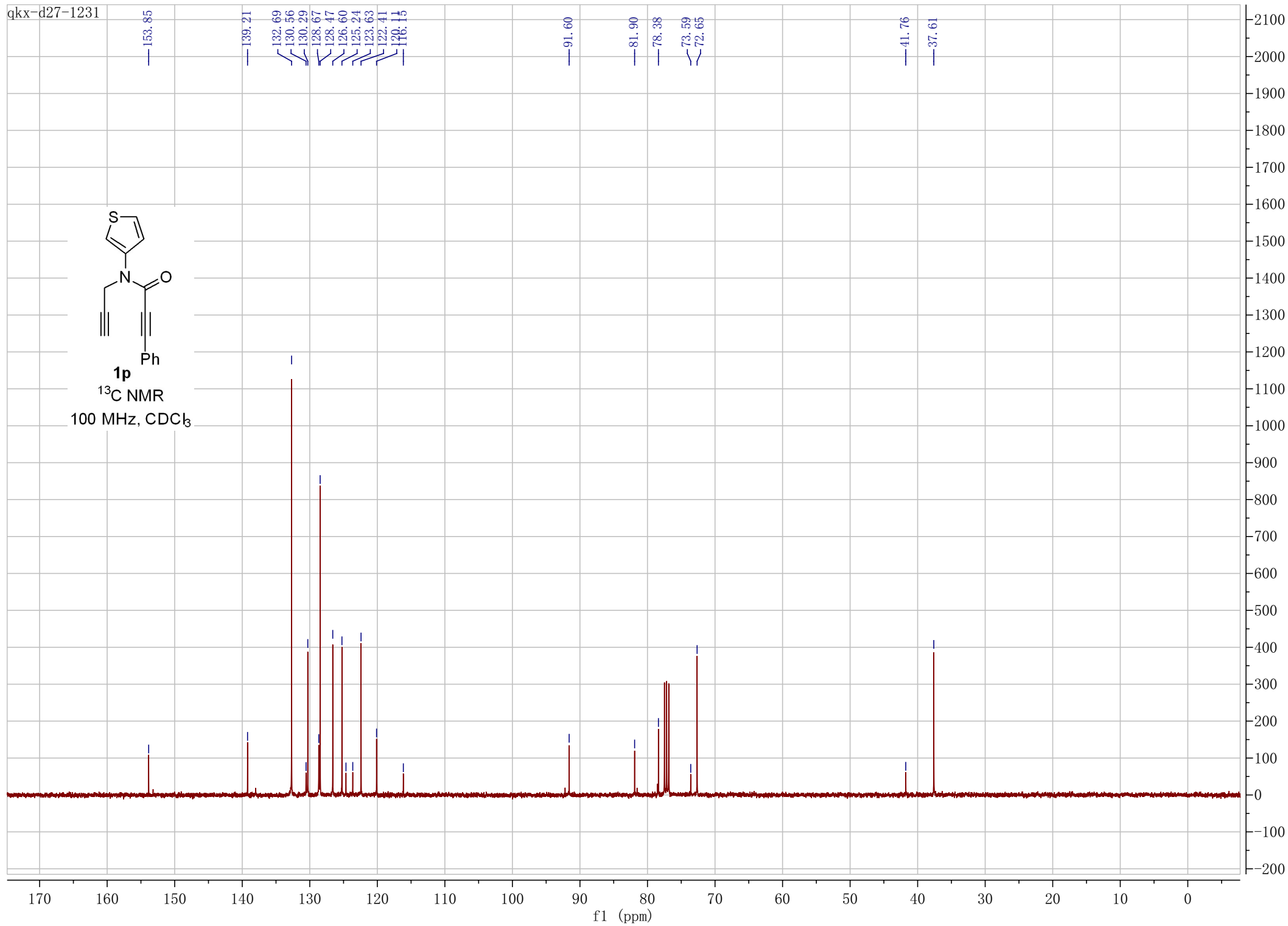
78.38

73.59

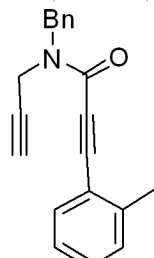
72.65

41.76

37.61



qkx-c72-1018



**1q**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.586  
7.567  
7.537  
7.518  
7.387  
7.366  
7.348  
7.328  
7.309  
7.272  
7.253  
7.236  
7.213  
7.190  
7.171

5.057

4.831

4.376

4.226

2.533

2.422

2.380

2.295

1.00

5.92

2.26

2.12

2.05

2.97

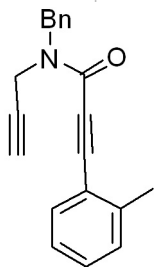
1.03

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0  
f1 (ppm)

4000  
3800  
3600  
3400  
3200  
3000  
2800  
2600  
2400  
2200  
2000  
1800  
1600  
1400  
1200  
1000  
800  
600  
400  
200  
0  
-200

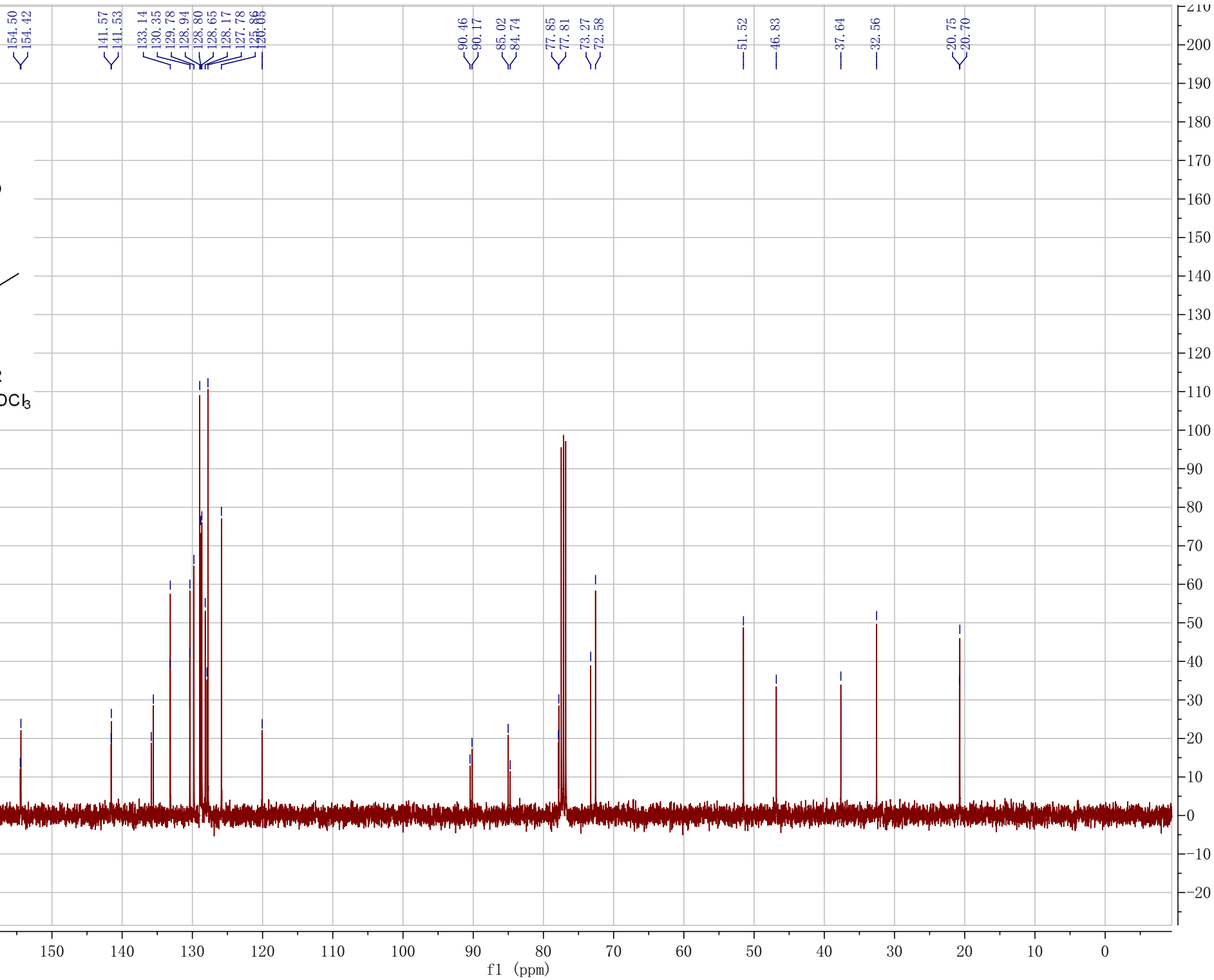


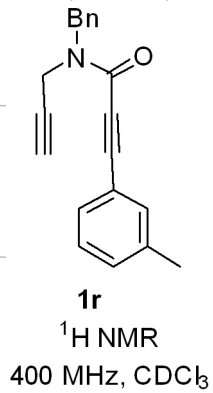
qkx-c72-1018



**1q**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



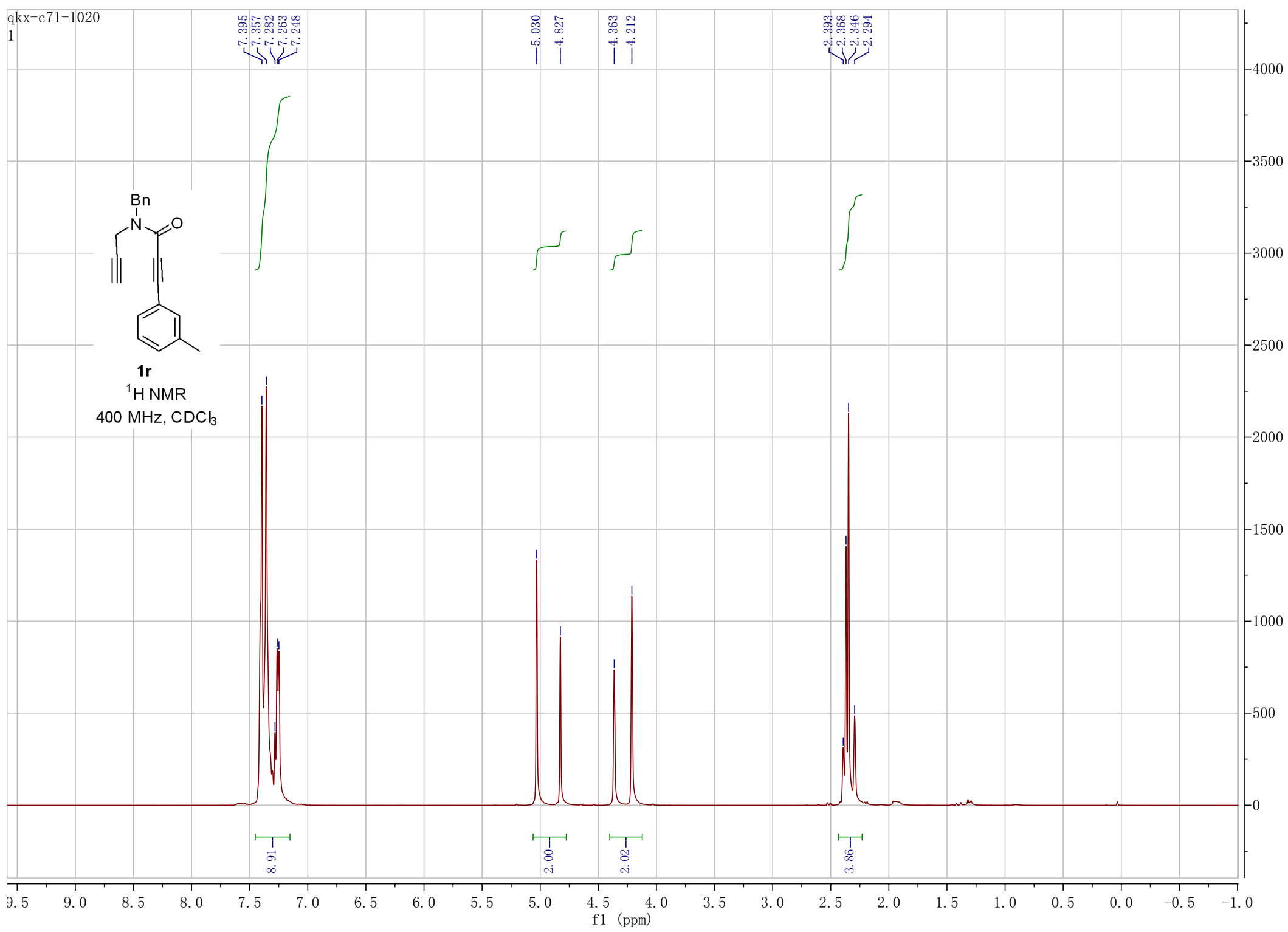


7.395  
7.357  
7.282  
7.263  
7.248

5.030  
4.827

4.363  
4.212

2.393  
2.368  
2.346  
2.294



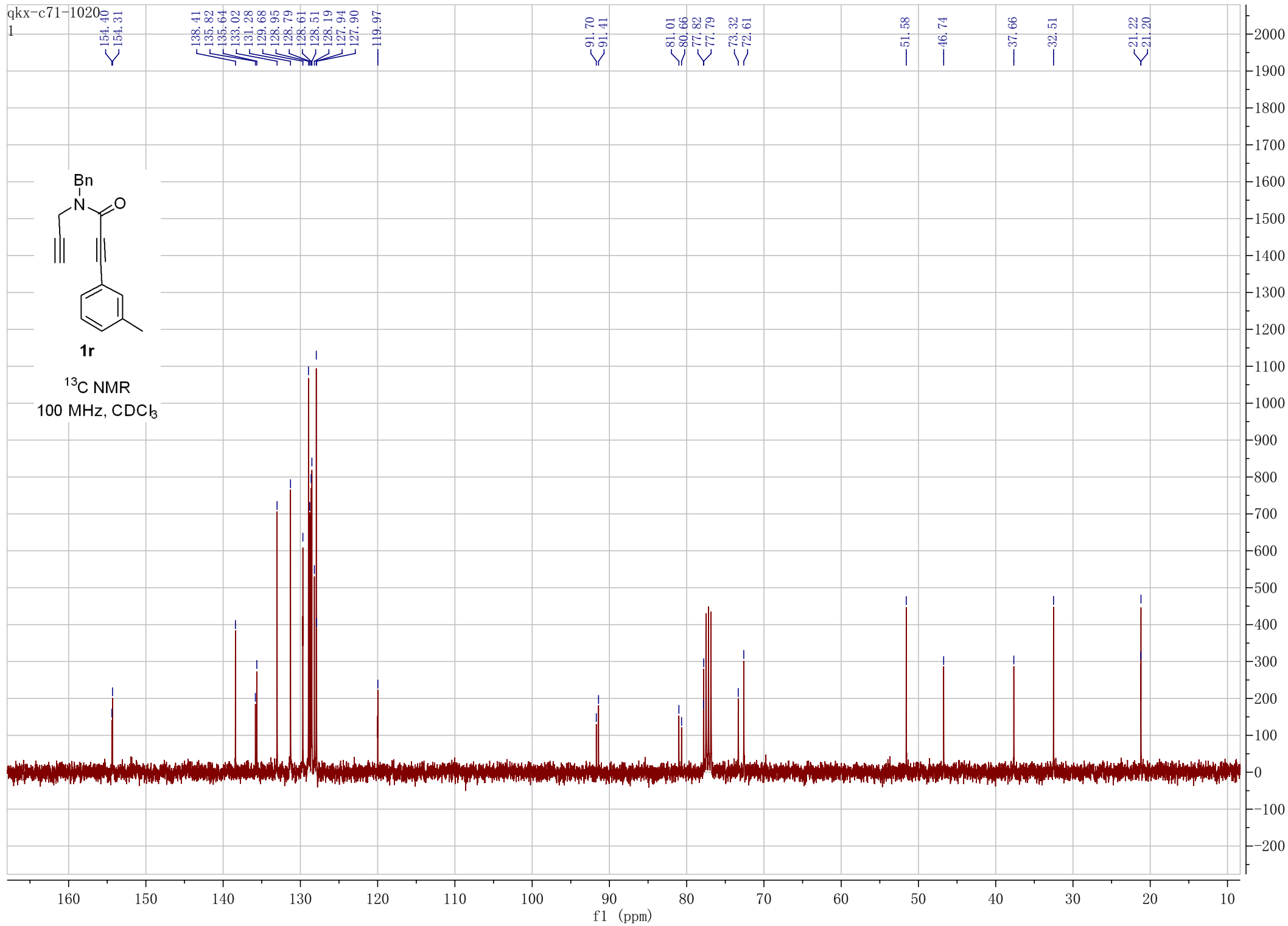
8.91

2.00

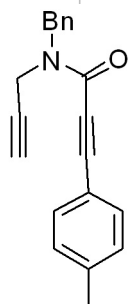
2.02

3.86

f1 (ppm)



qkx-c79-0306



**1s**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.501  
7.481  
7.448  
7.428  
7.399  
7.389  
7.380  
7.369  
7.354  
7.343  
7.337  
7.209  
7.187  
7.166

5.025

4.823

4.362

4.356

4.213

4.206

2.384

2.290

2.284

2.277



0.83

1.20

4.90

1.97

2.00

2.00

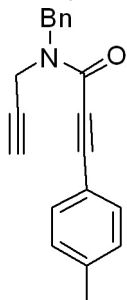
3.00

0.93

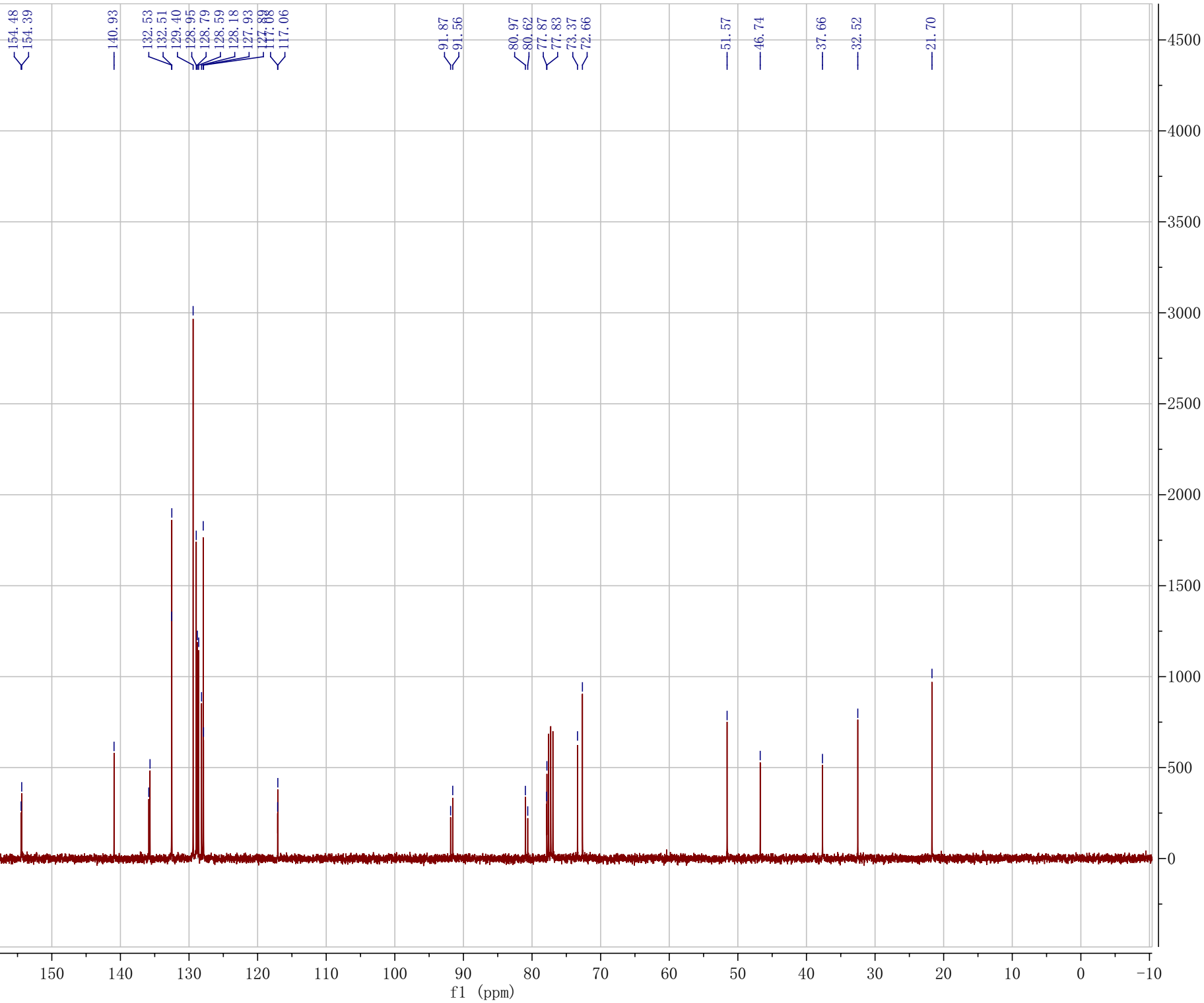
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)

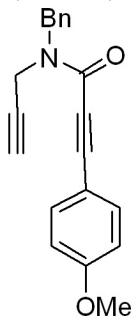
6500  
6000  
5500  
5000  
4500  
4000  
3500  
3000  
2500  
2000  
1500  
1000  
500  
0  
-500

**1s**

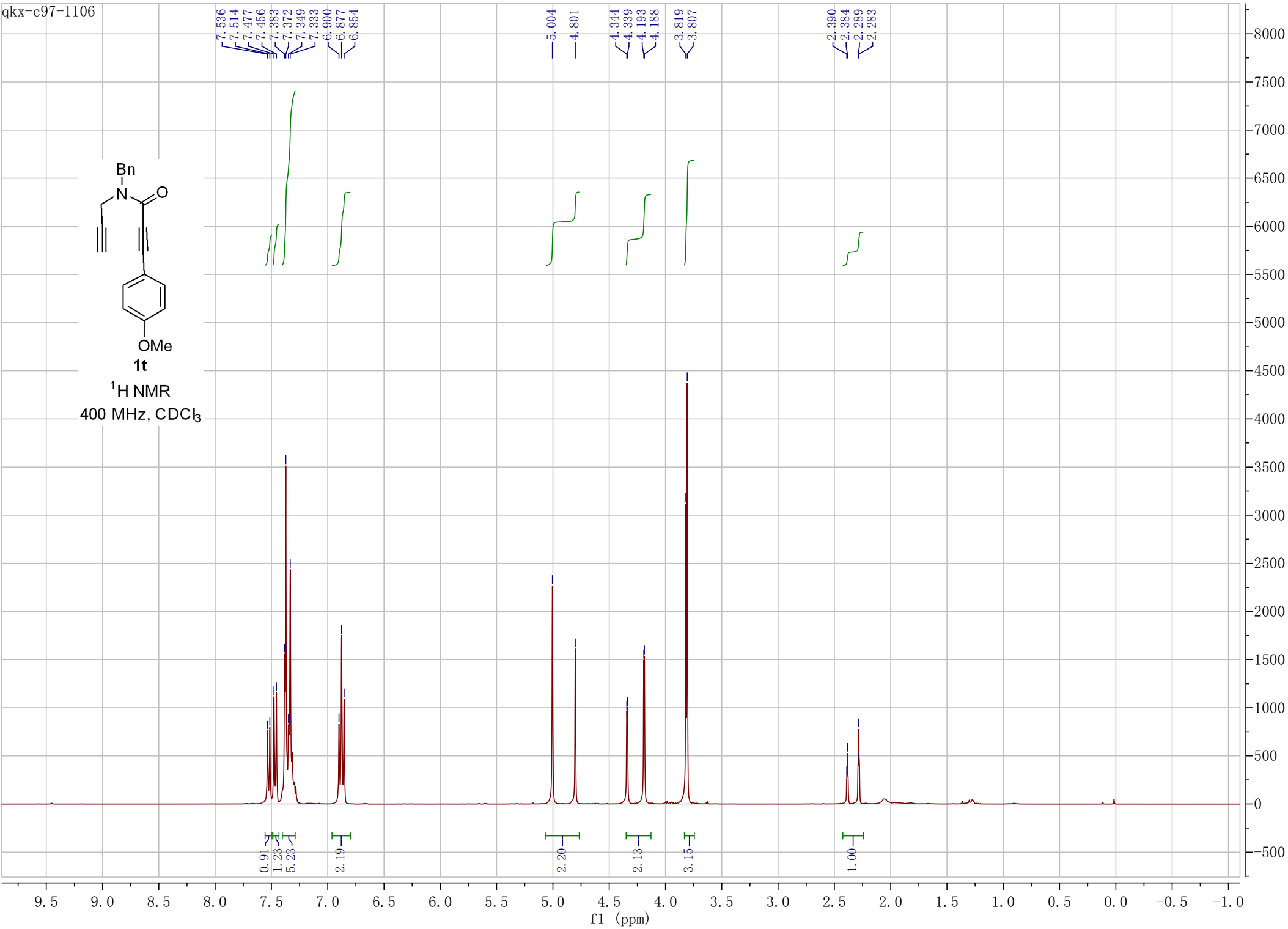
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



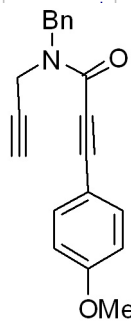
qkx-c97-1106



<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

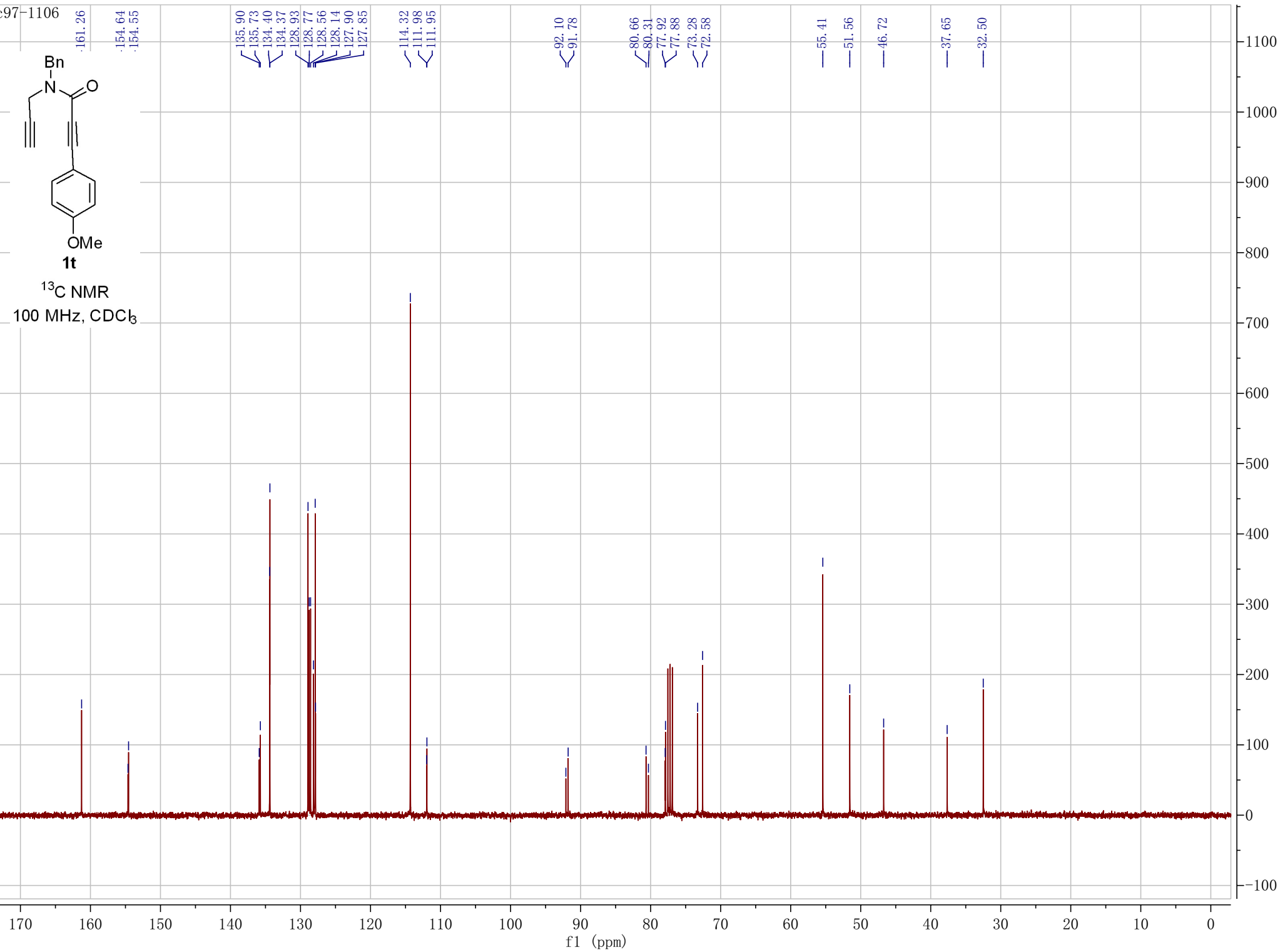


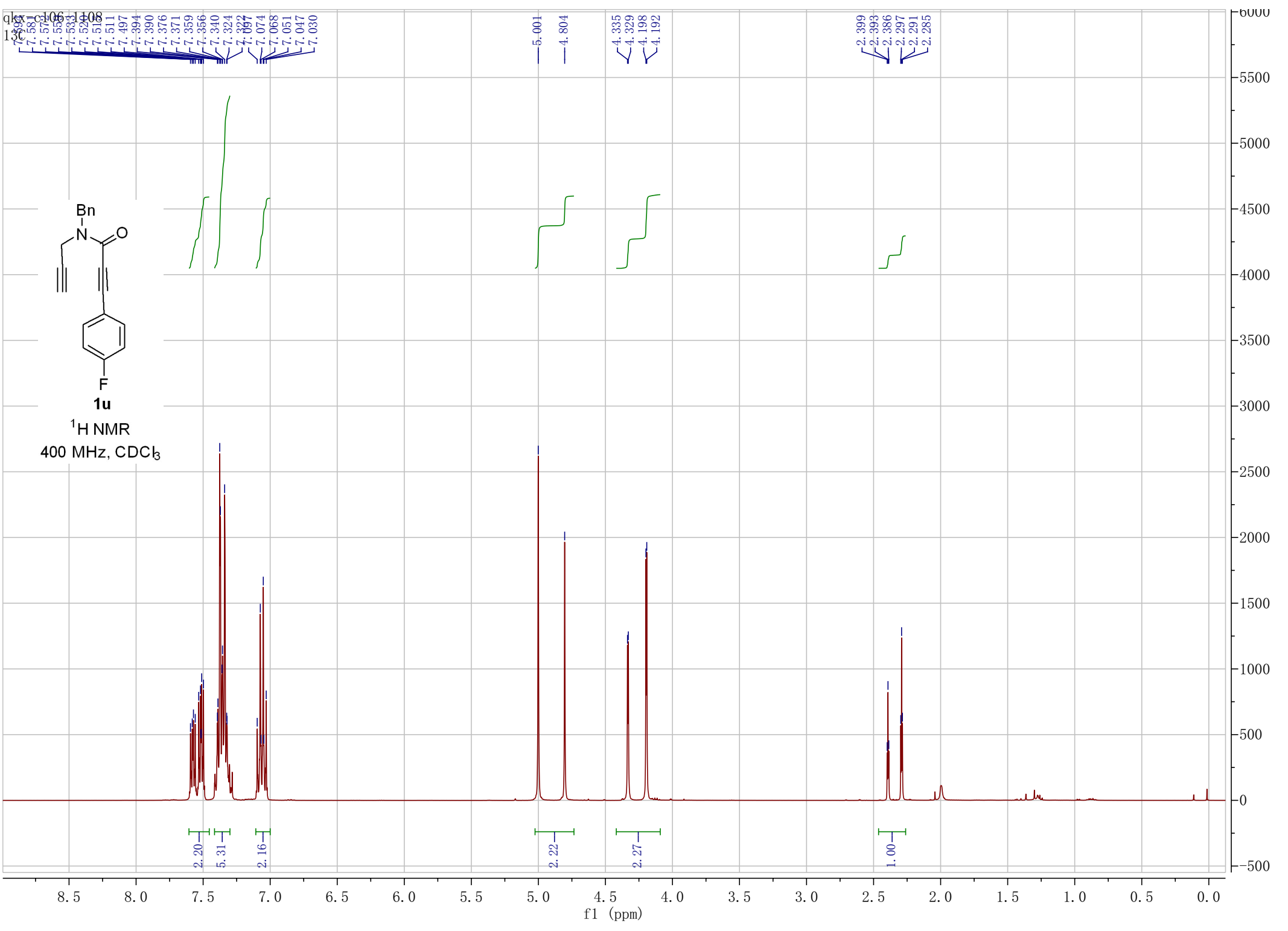
qkx-c97-1106



**1t**

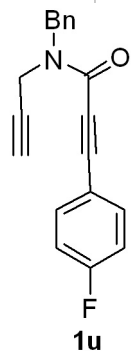
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



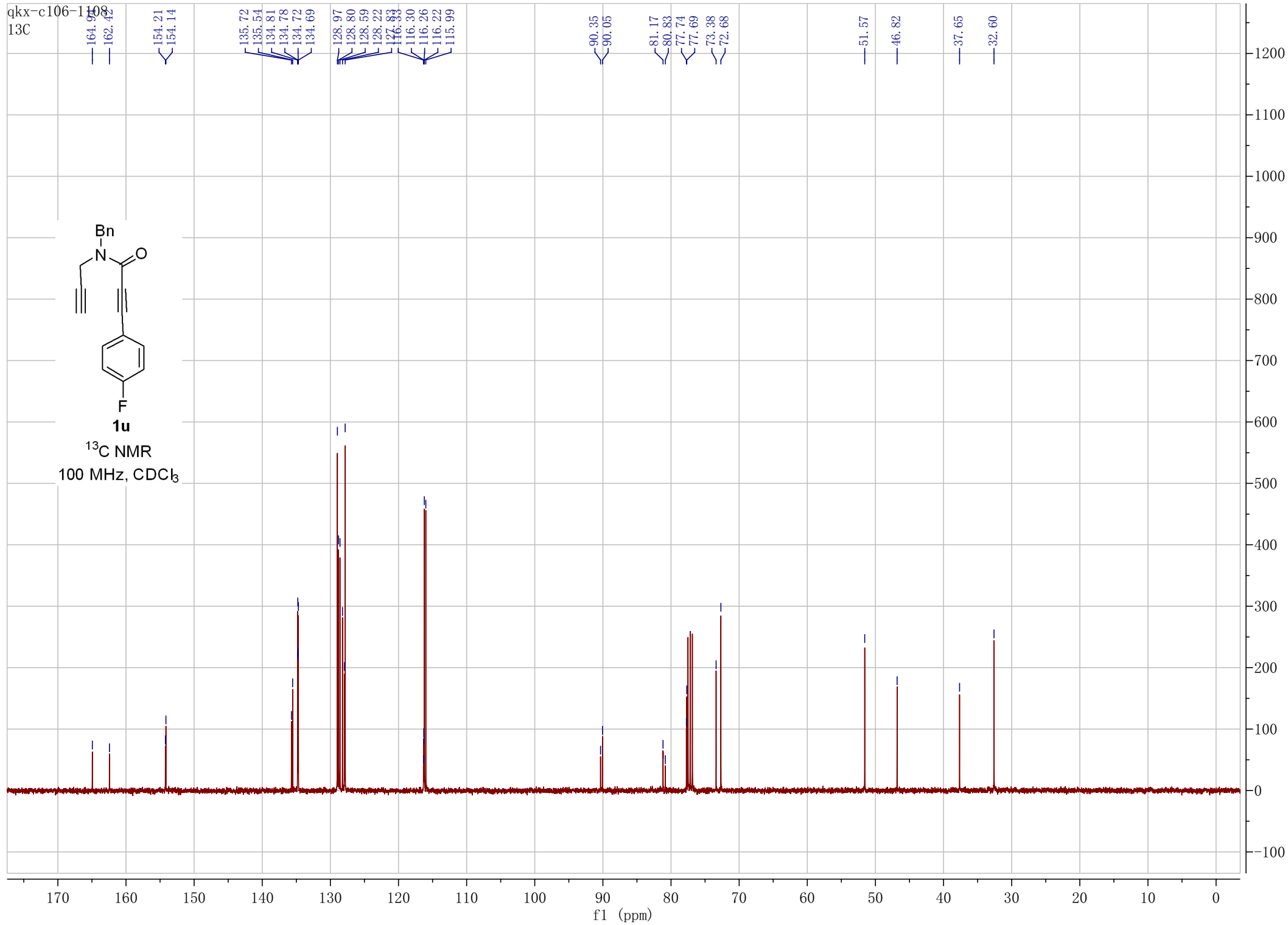




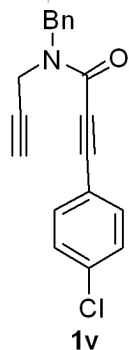
qkx-c106-1108  
13C



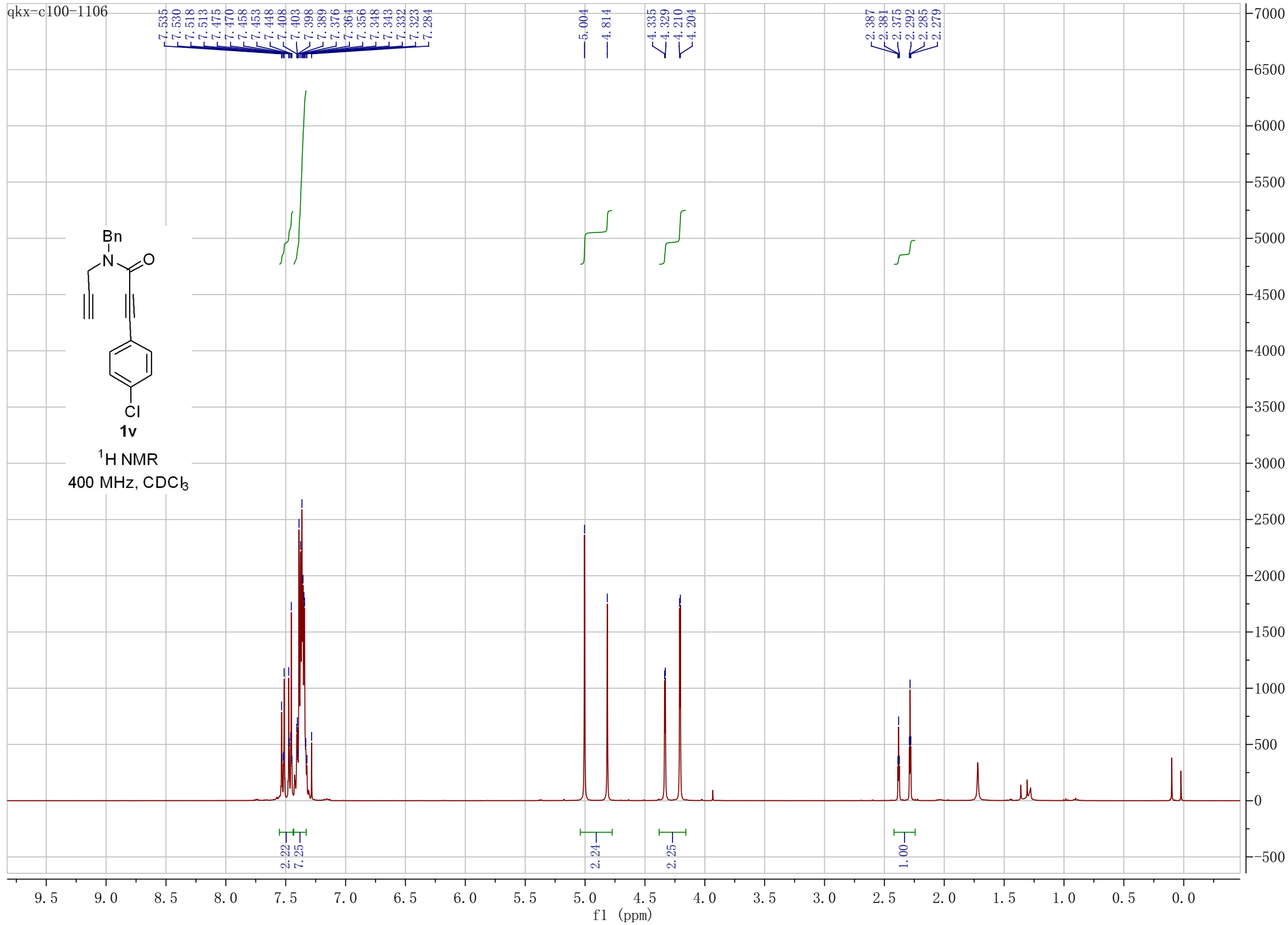
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



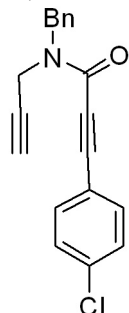
qkx-c100-1106



<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

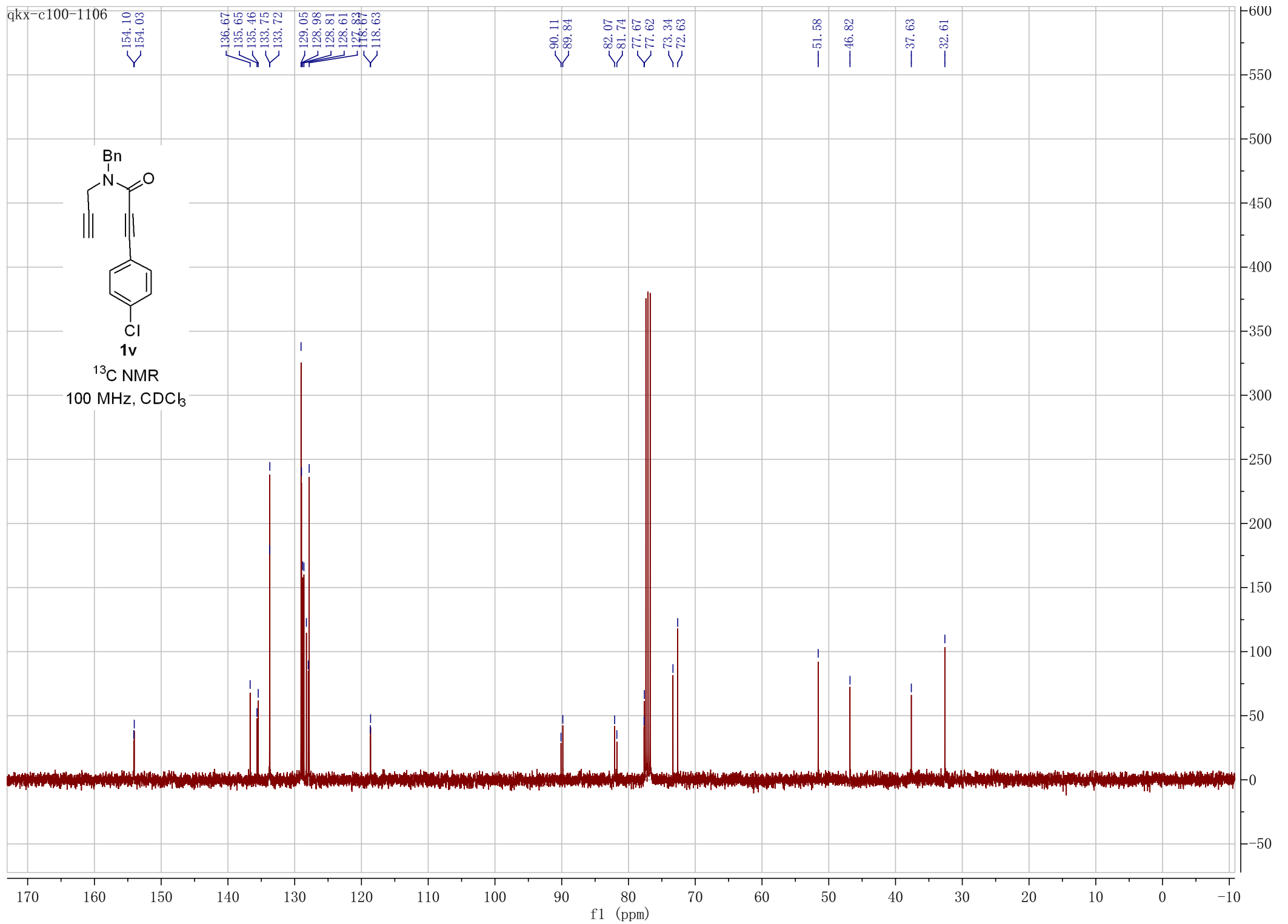


qkx-c100-1106

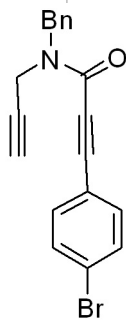


**1v**

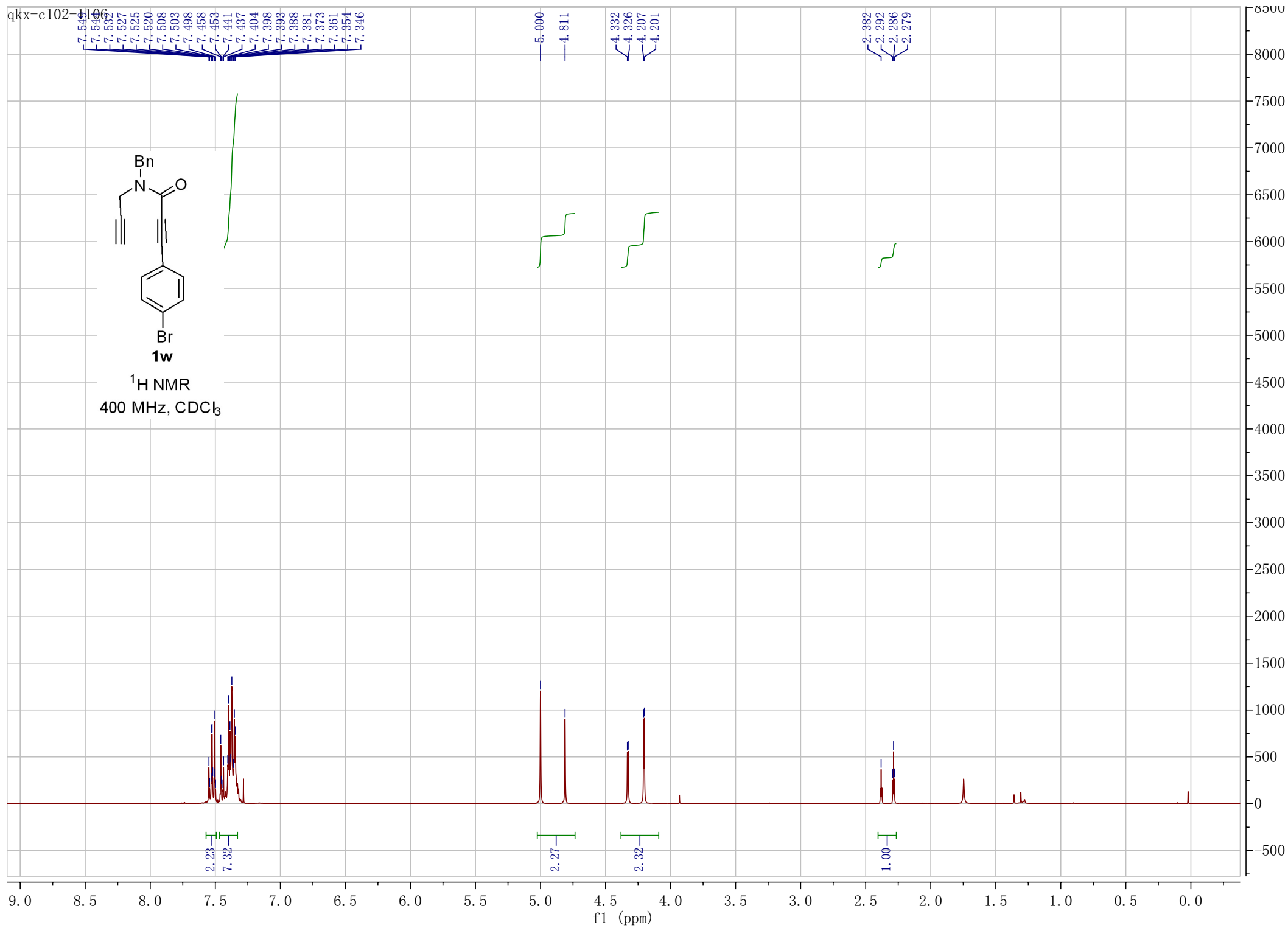
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



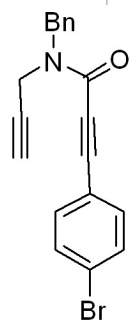
qkx-c102-1106



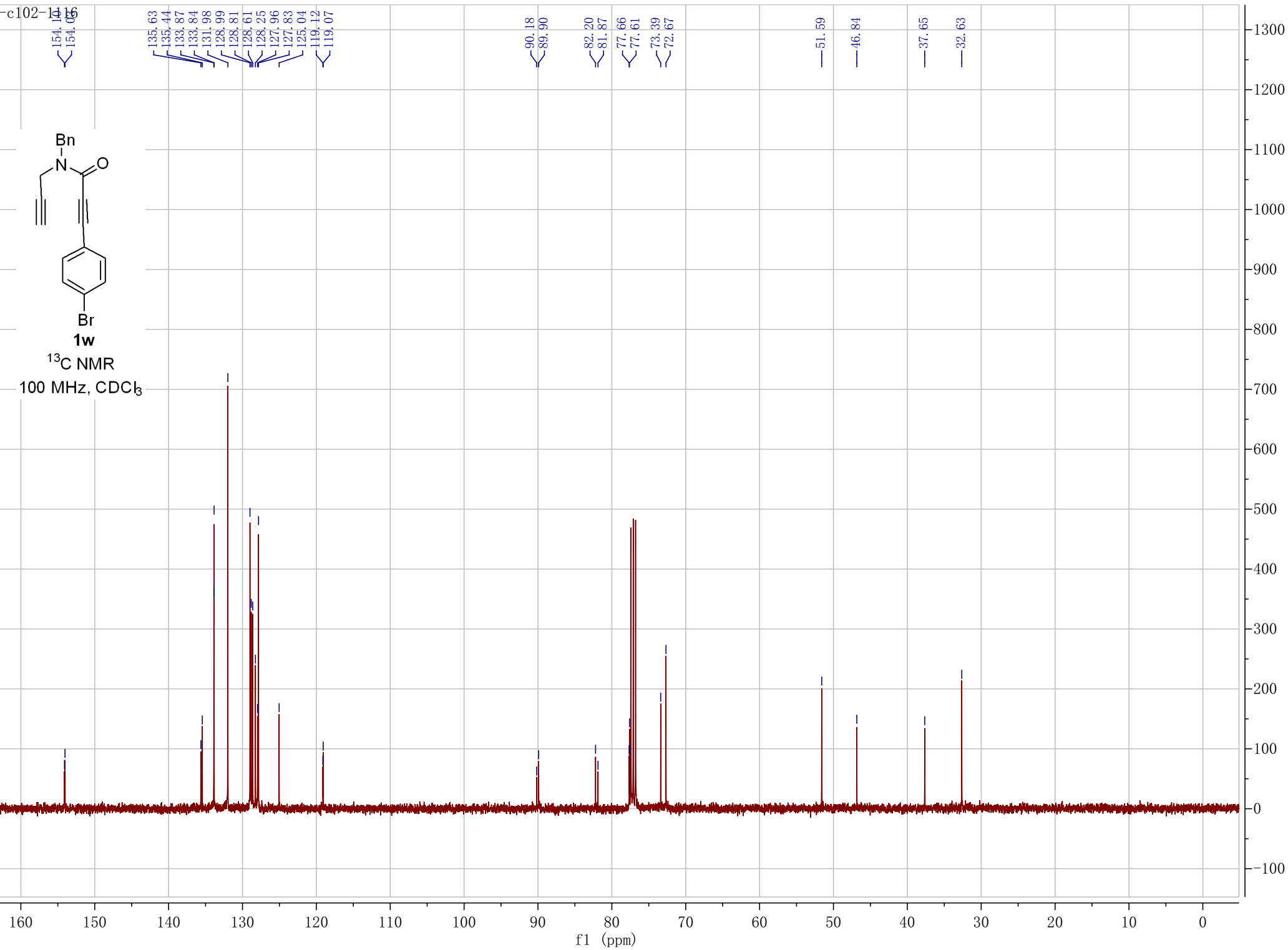
**1w**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



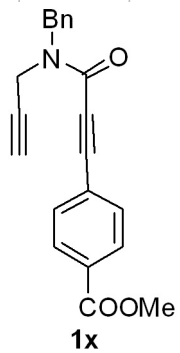
qkx-c102-1416



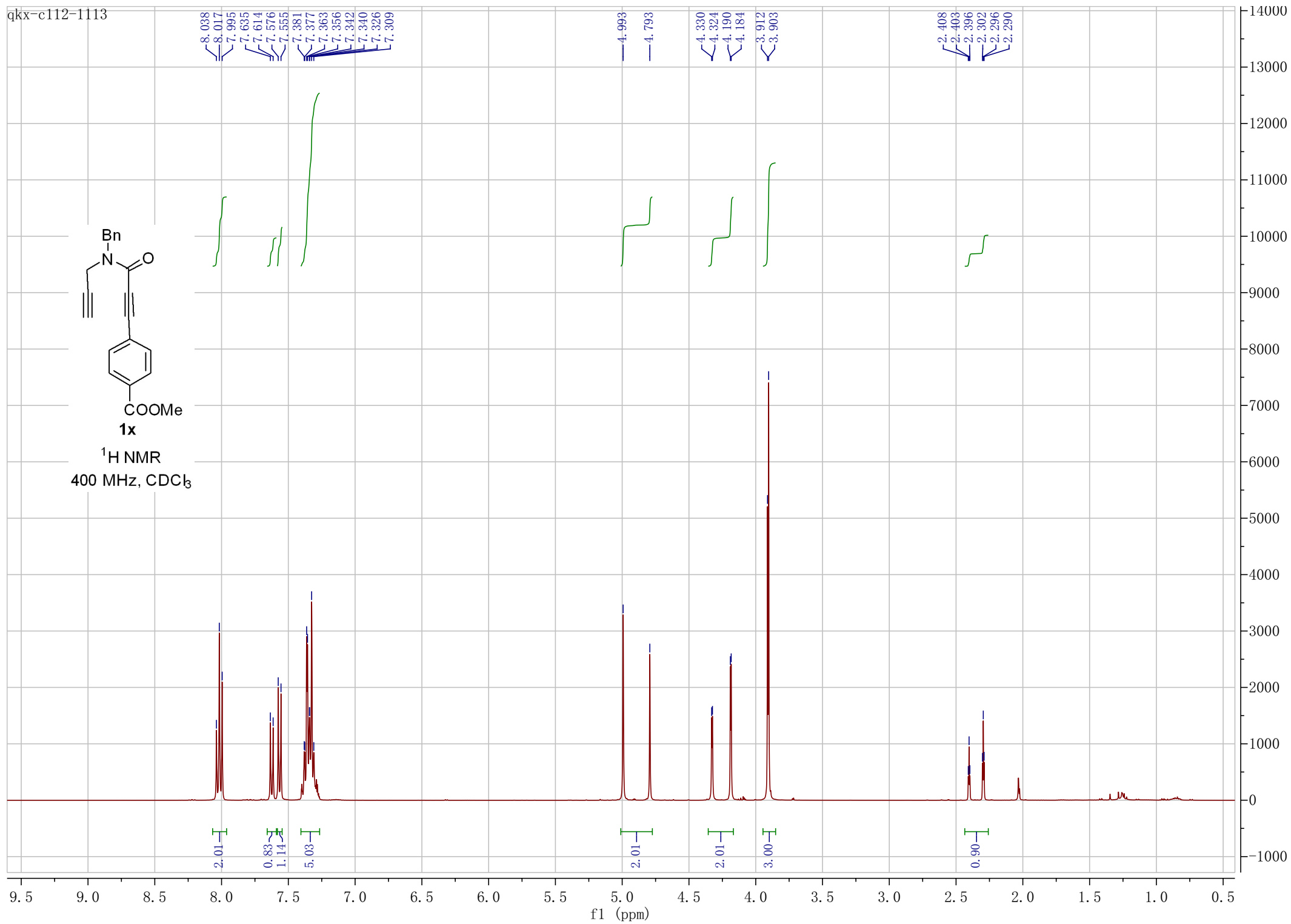
**1w**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



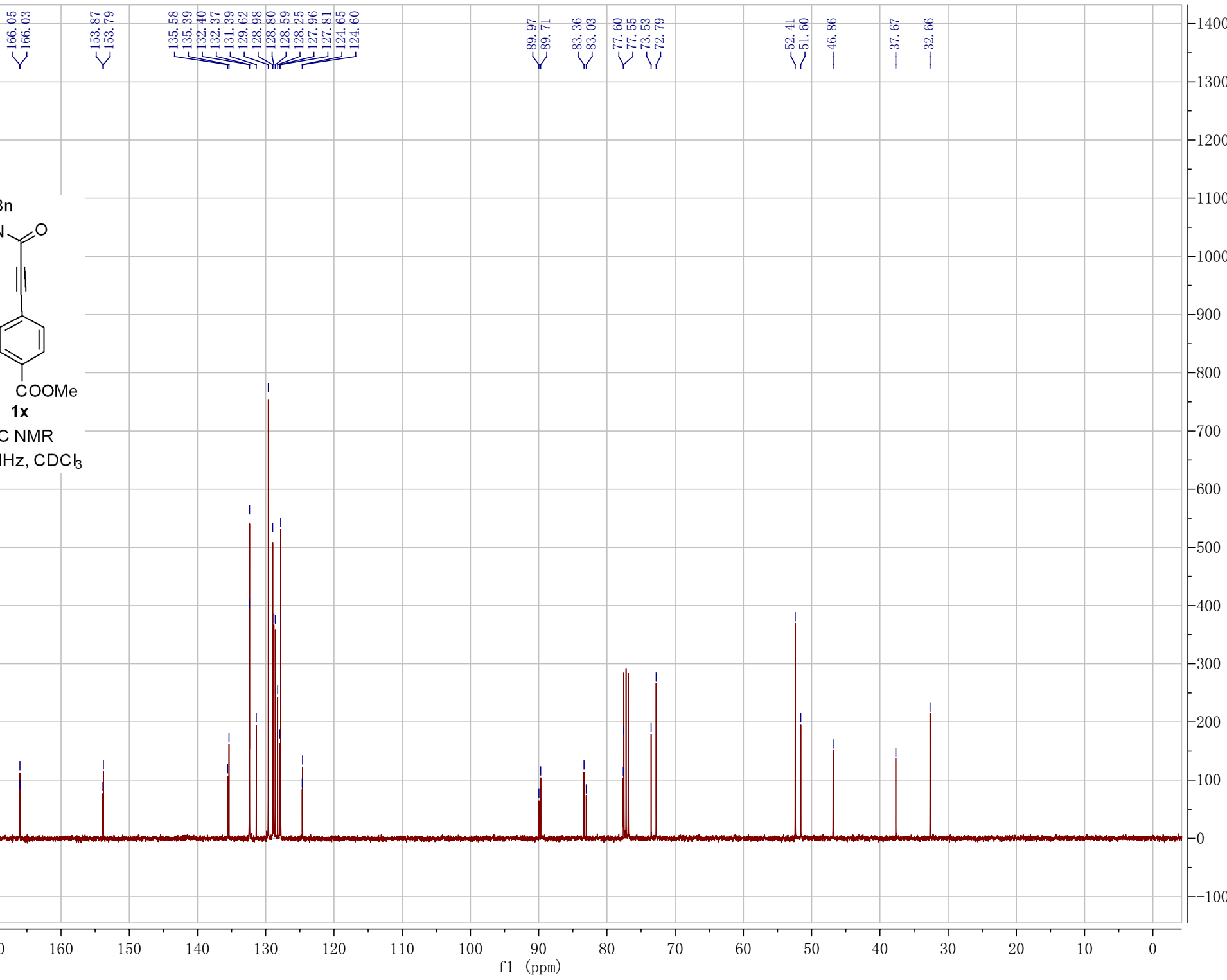
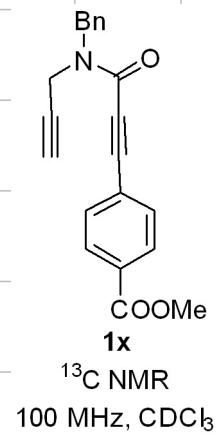
qkx-c112-1113



<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

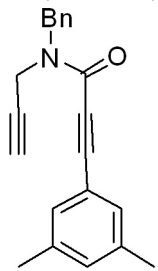


qkx-c112-1113



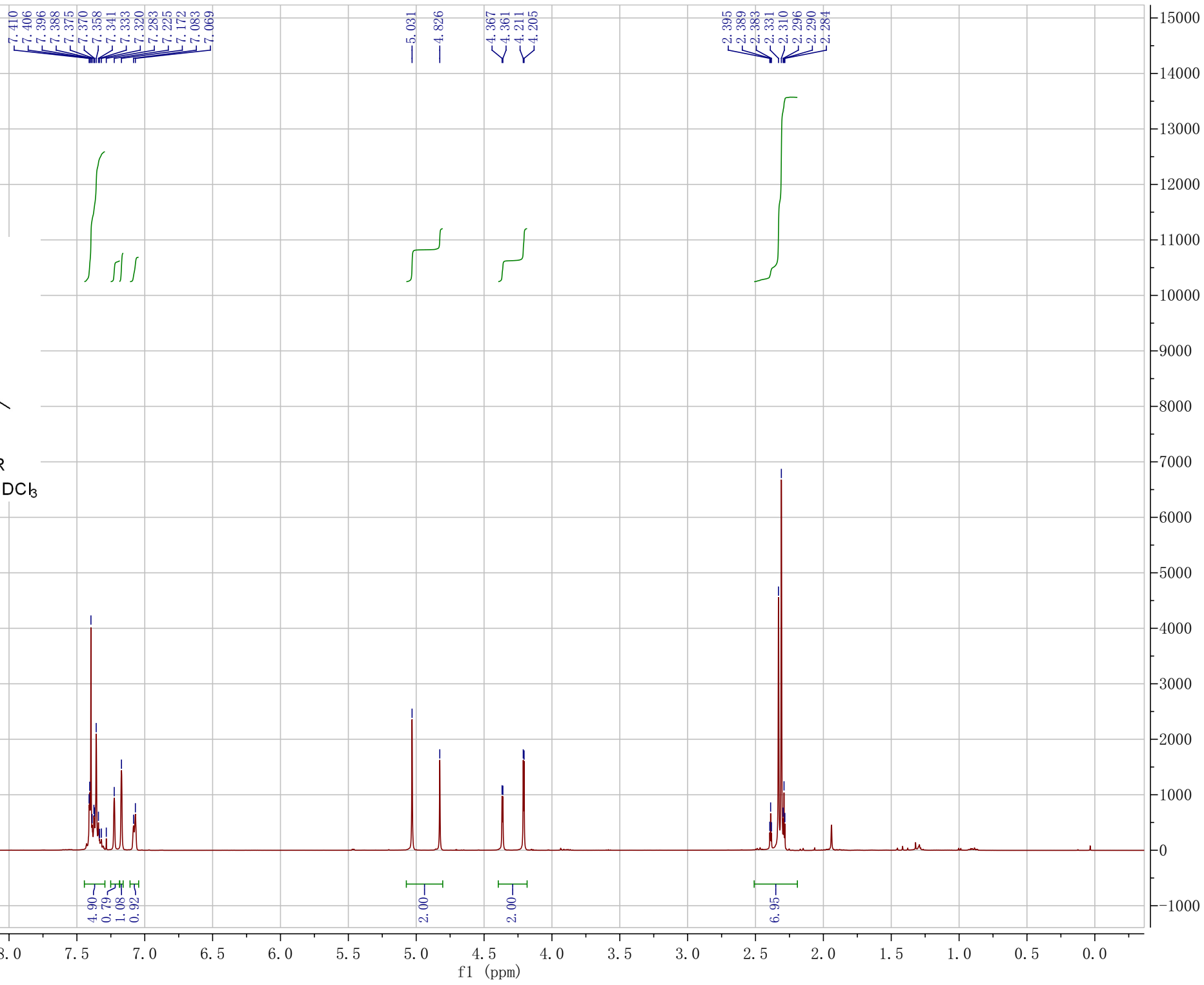
qkx-c11112

1



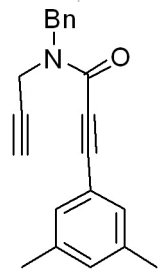
**1y**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



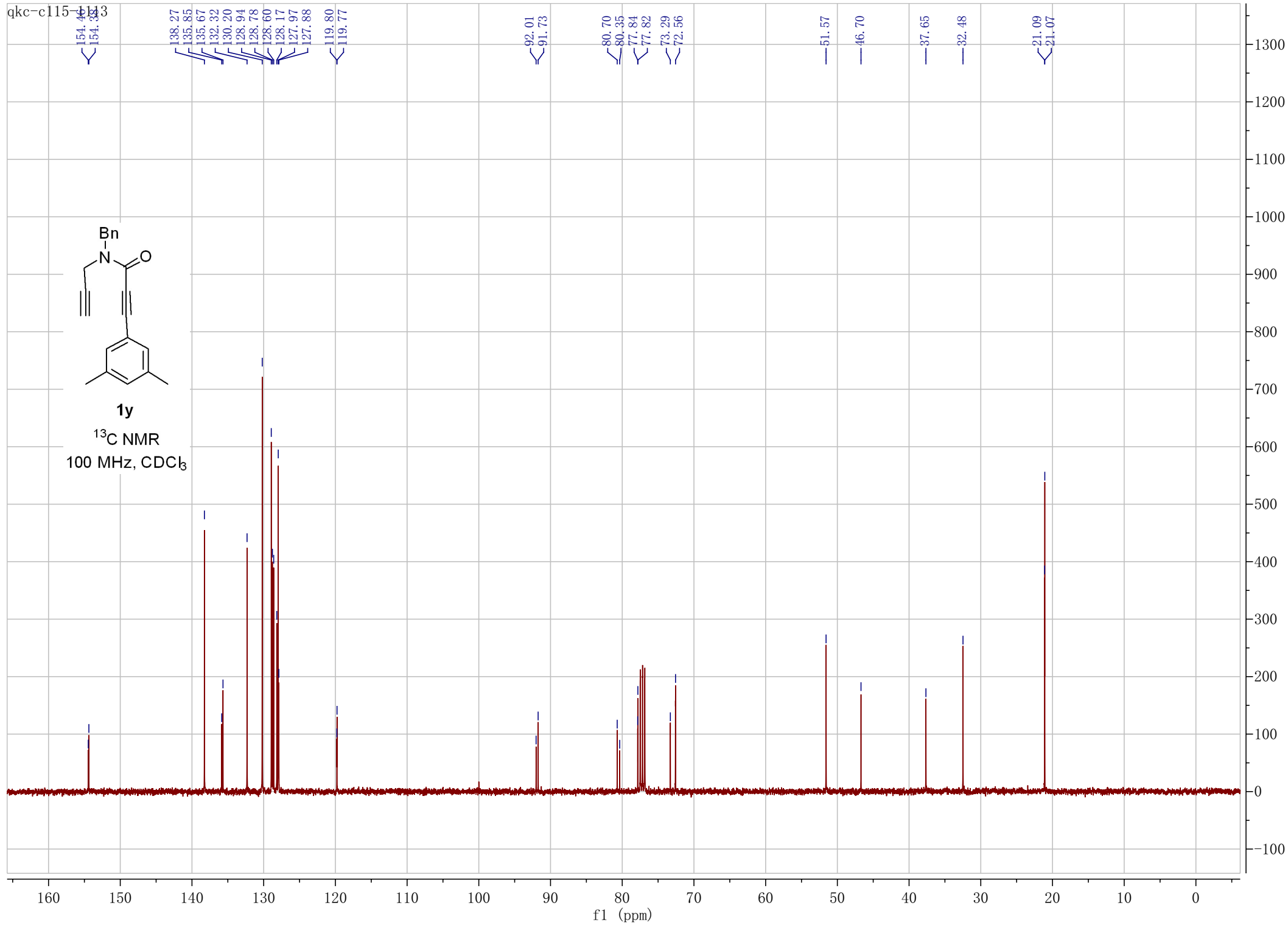


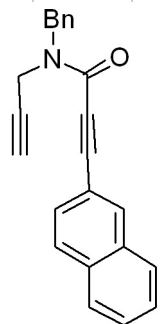
qkc-c115-113



1y

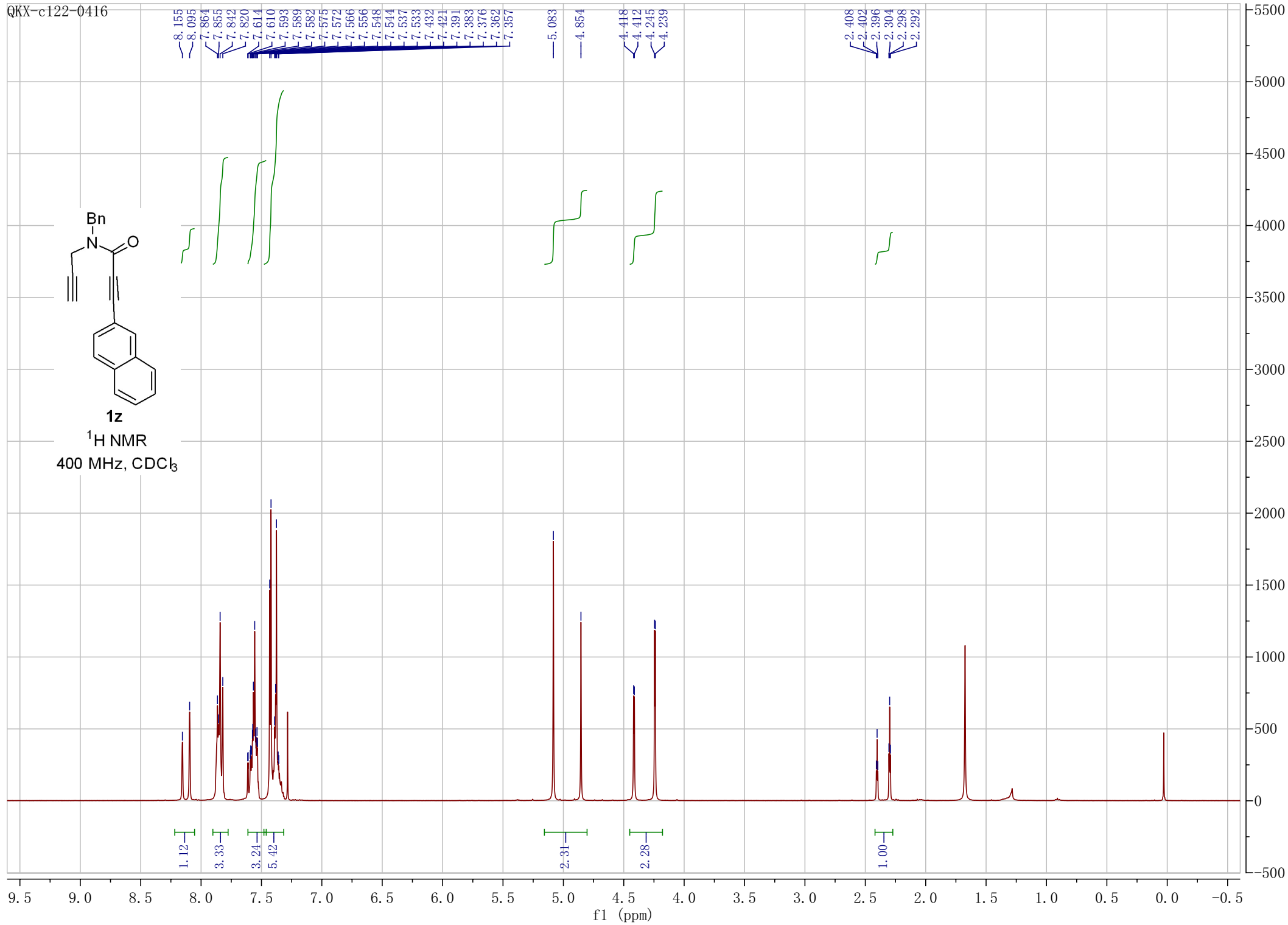
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



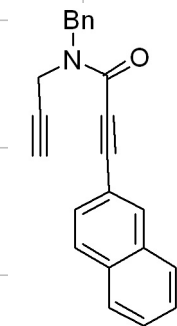


**1z**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

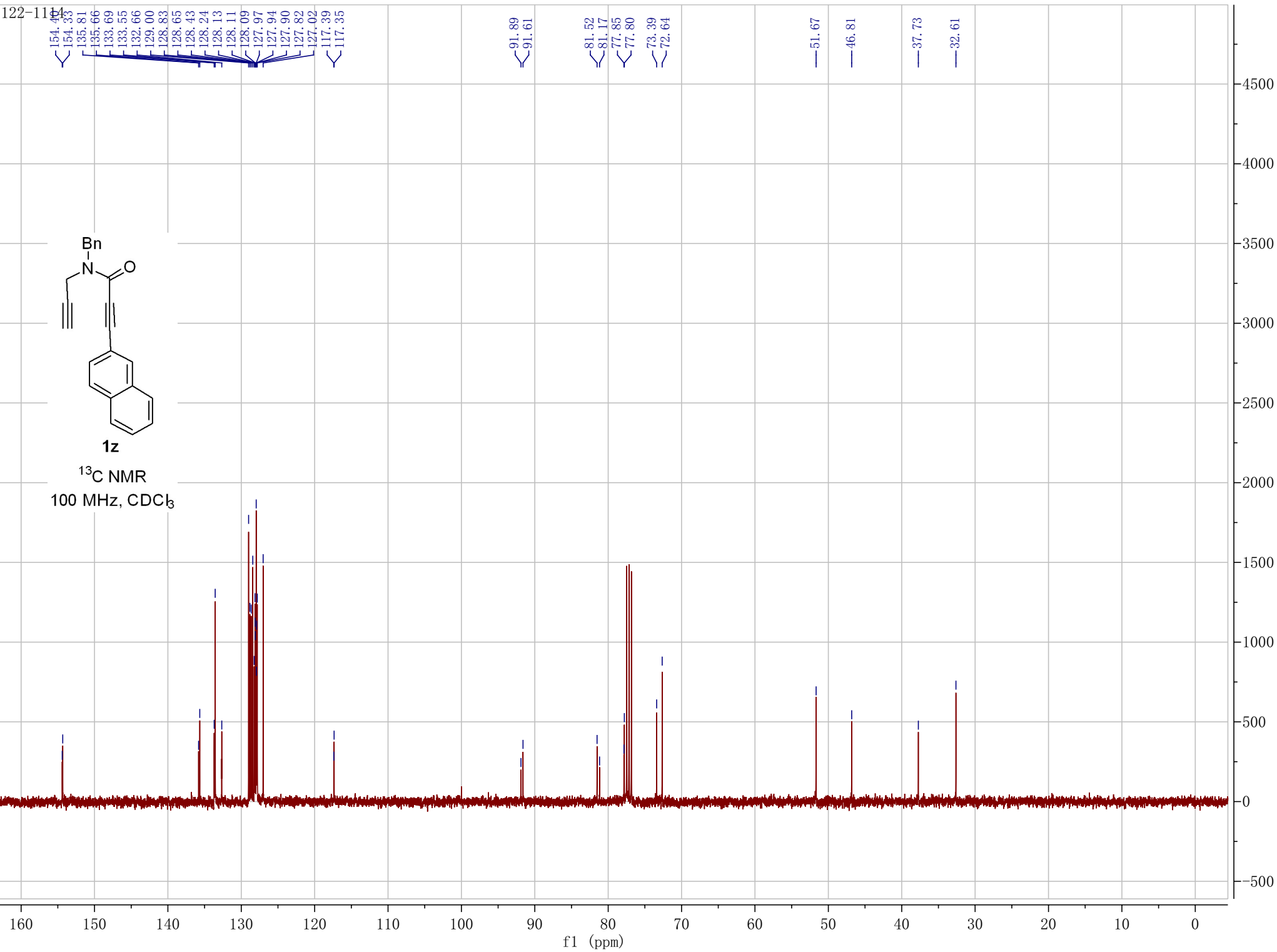


qkx-c122-1114

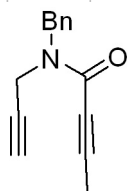


**1z**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

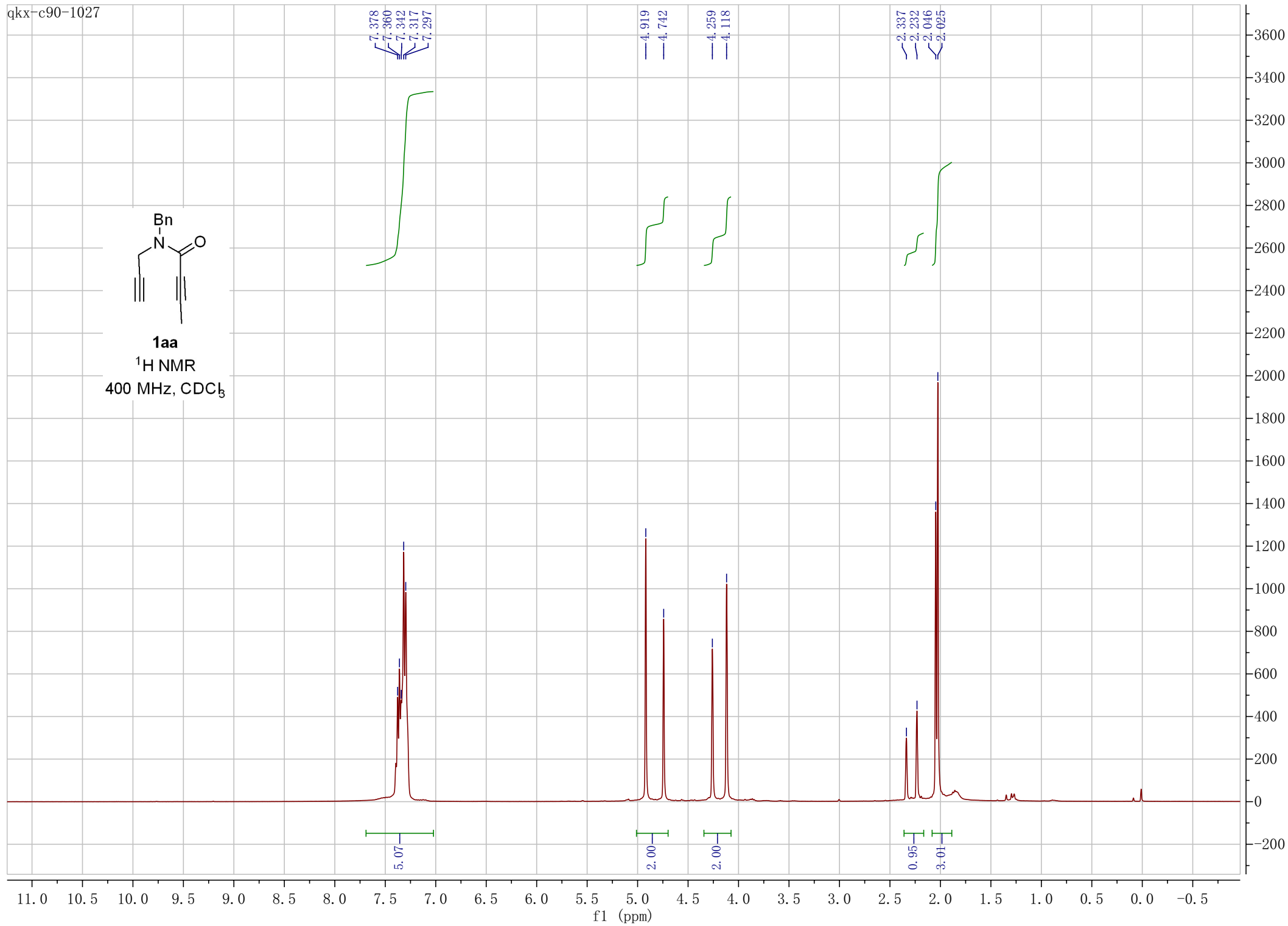


qkx-c90-1027

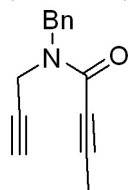


**1aa**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

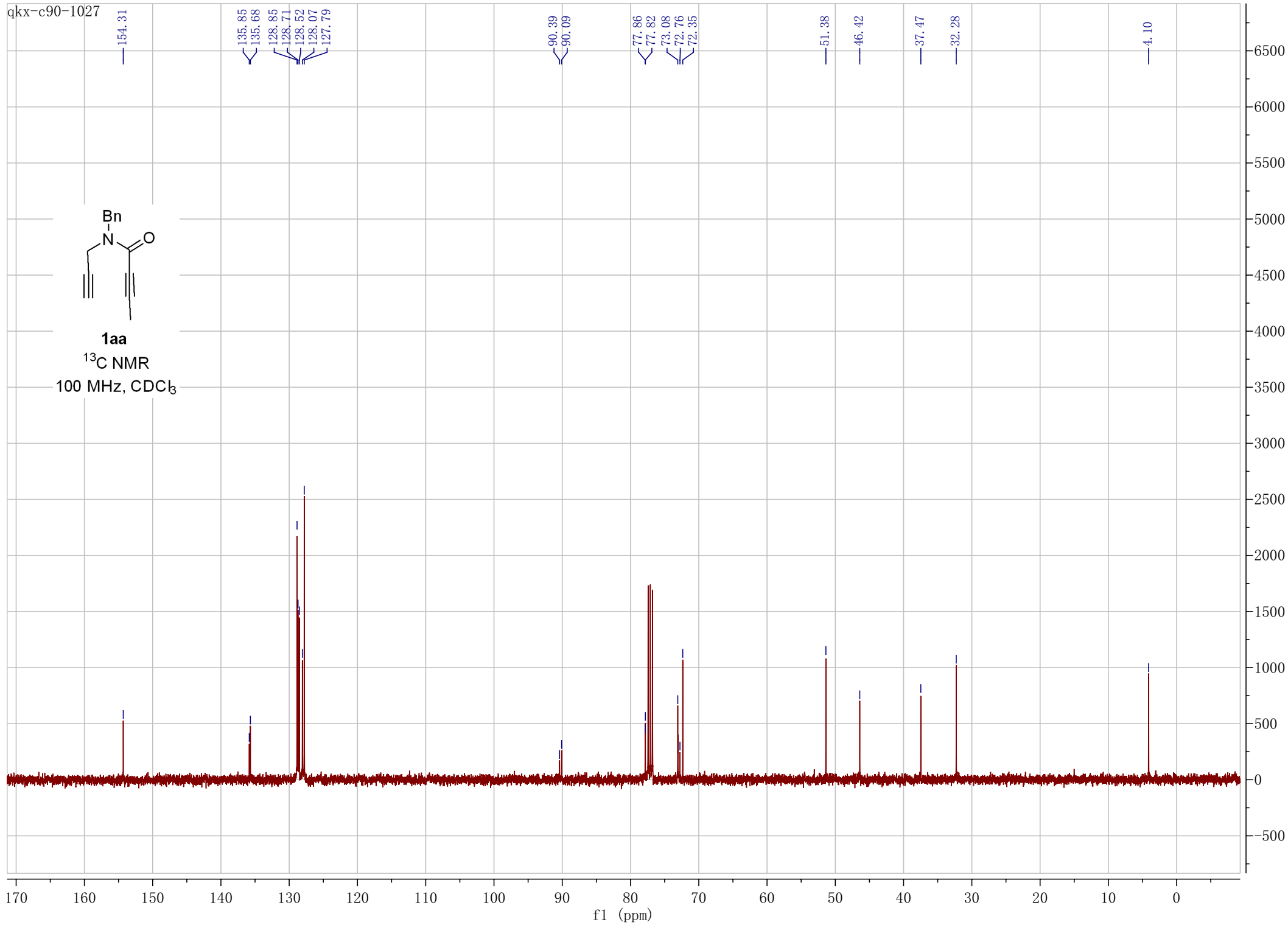


qkx-c90-1027

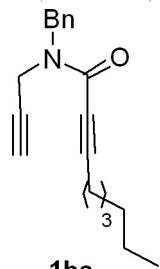


**1aa**

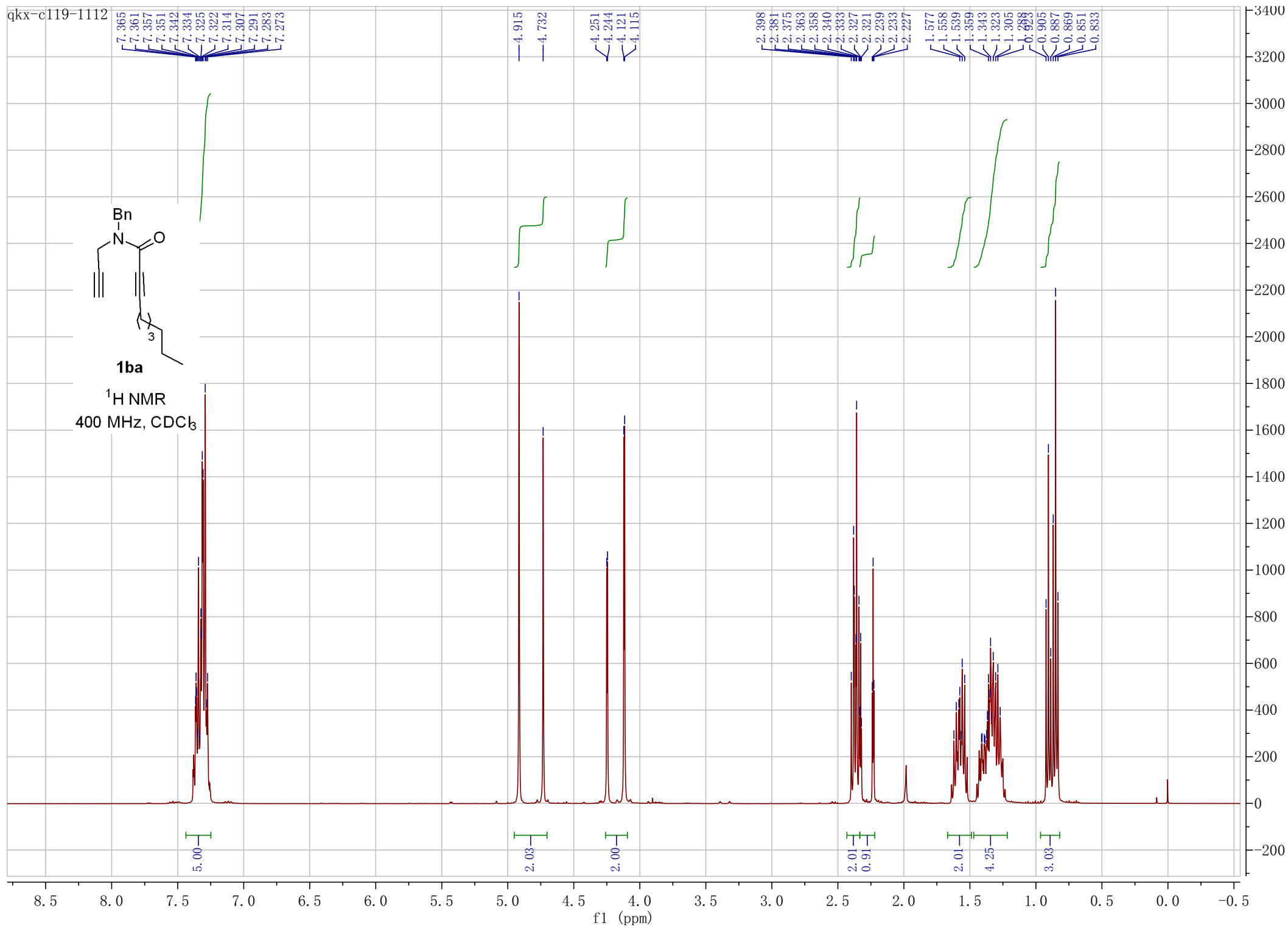
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



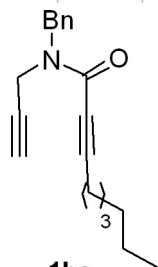
qkx-c119-1112



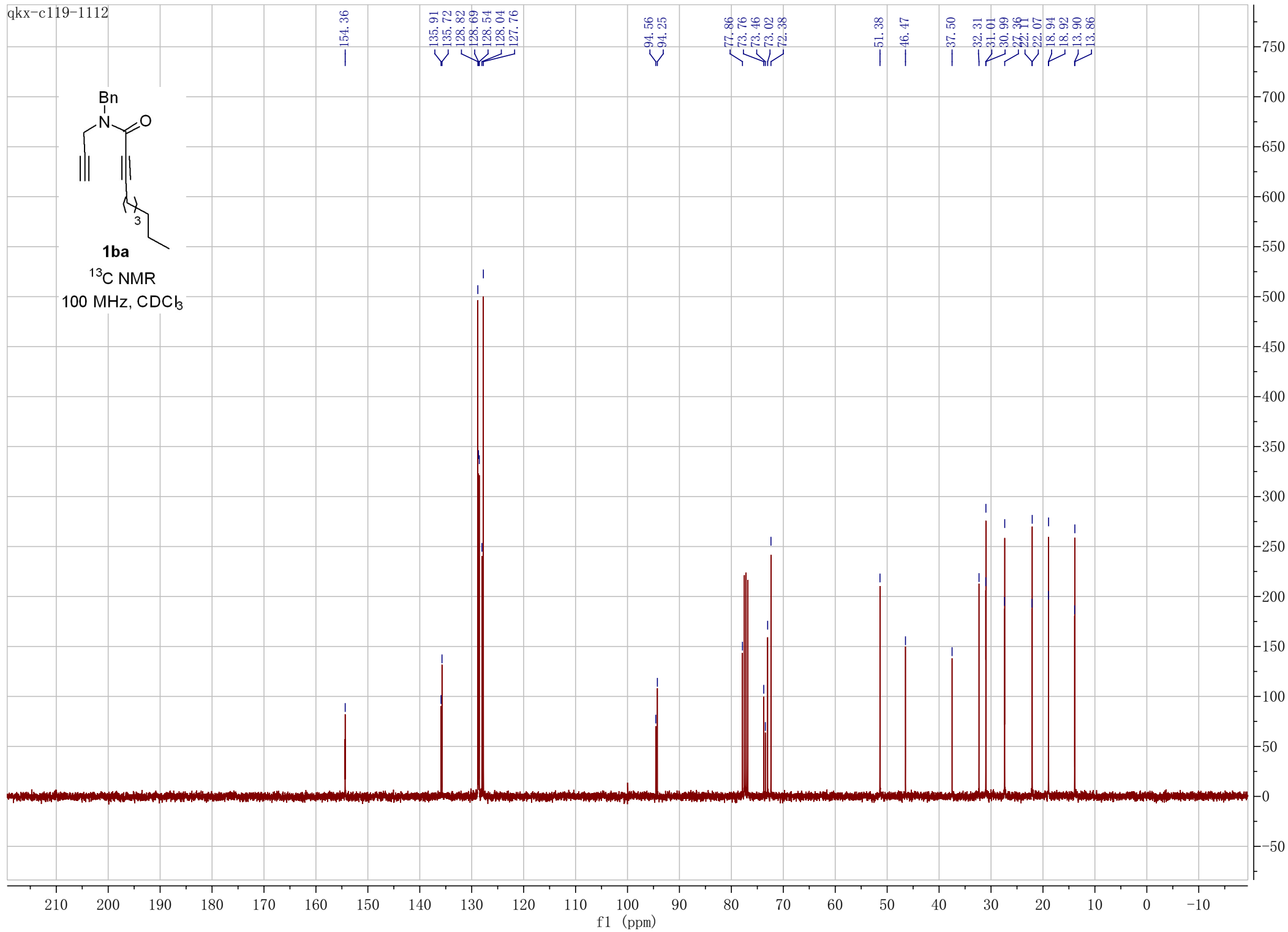
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

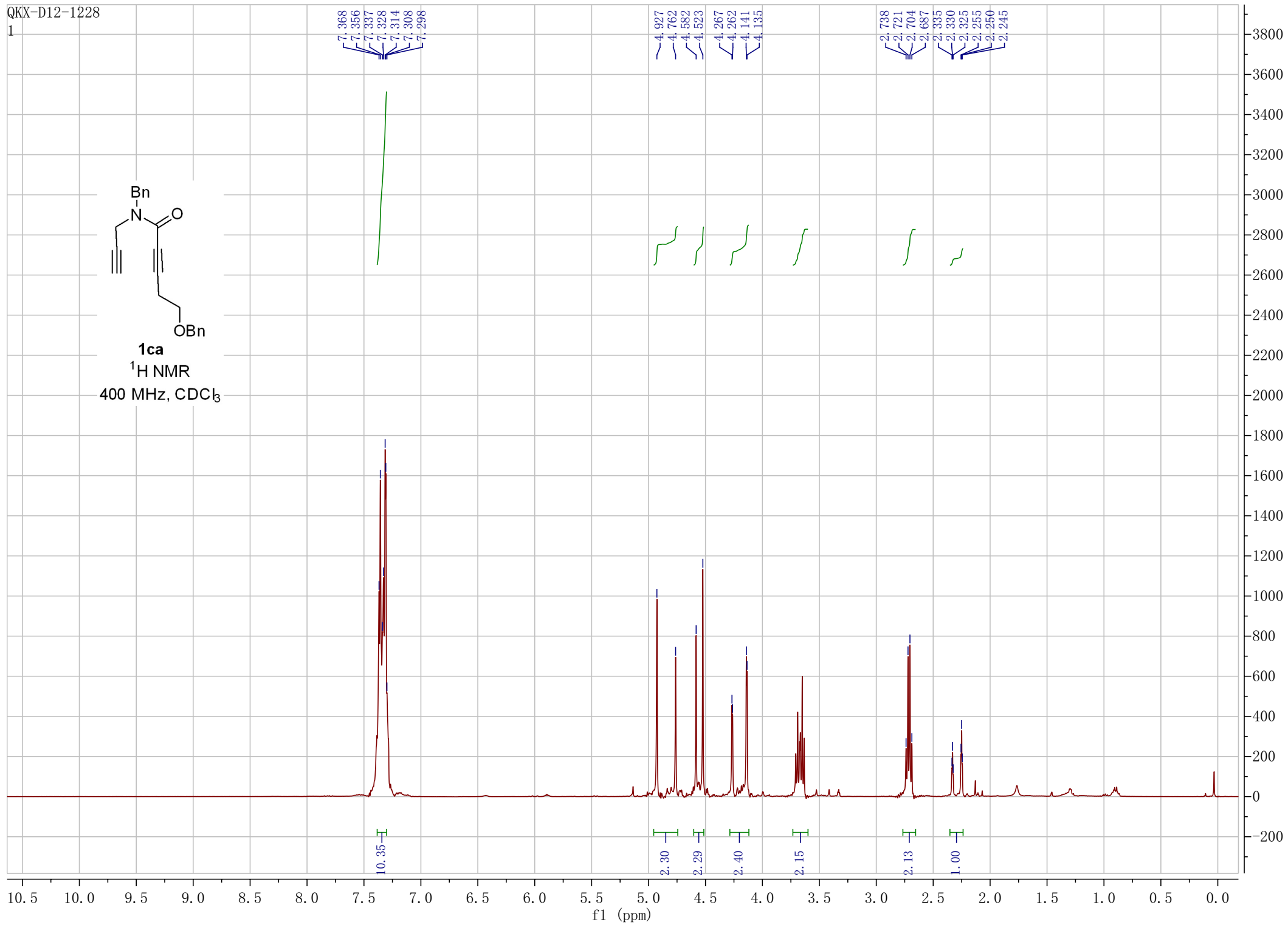
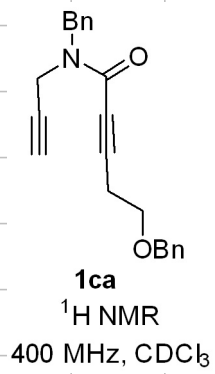


qkx-c119-1112

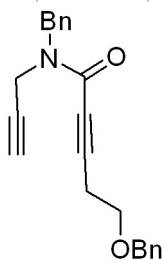


<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

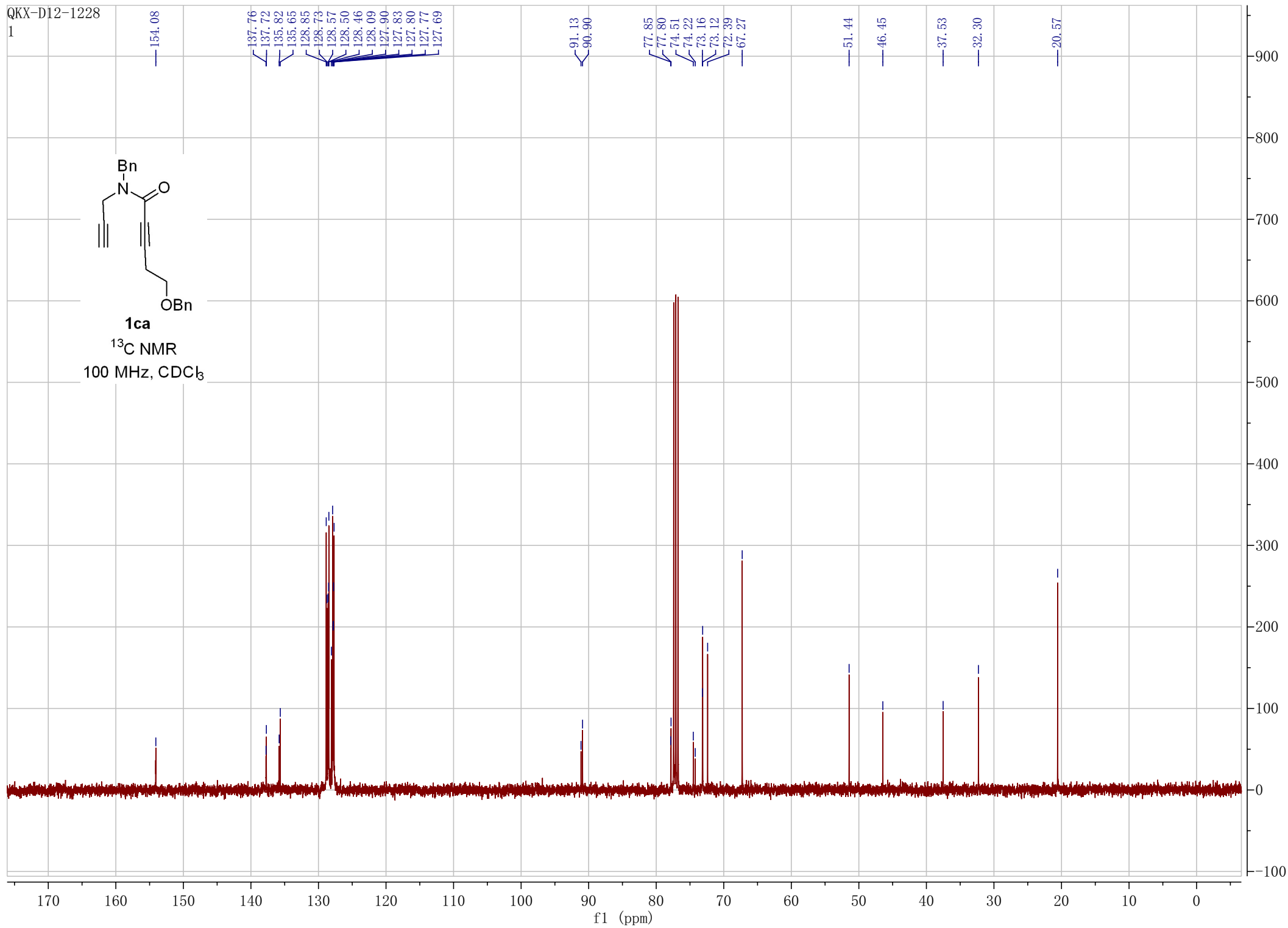






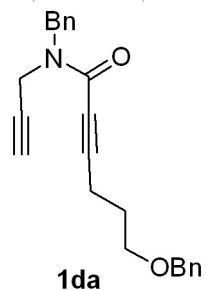
**1ca**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

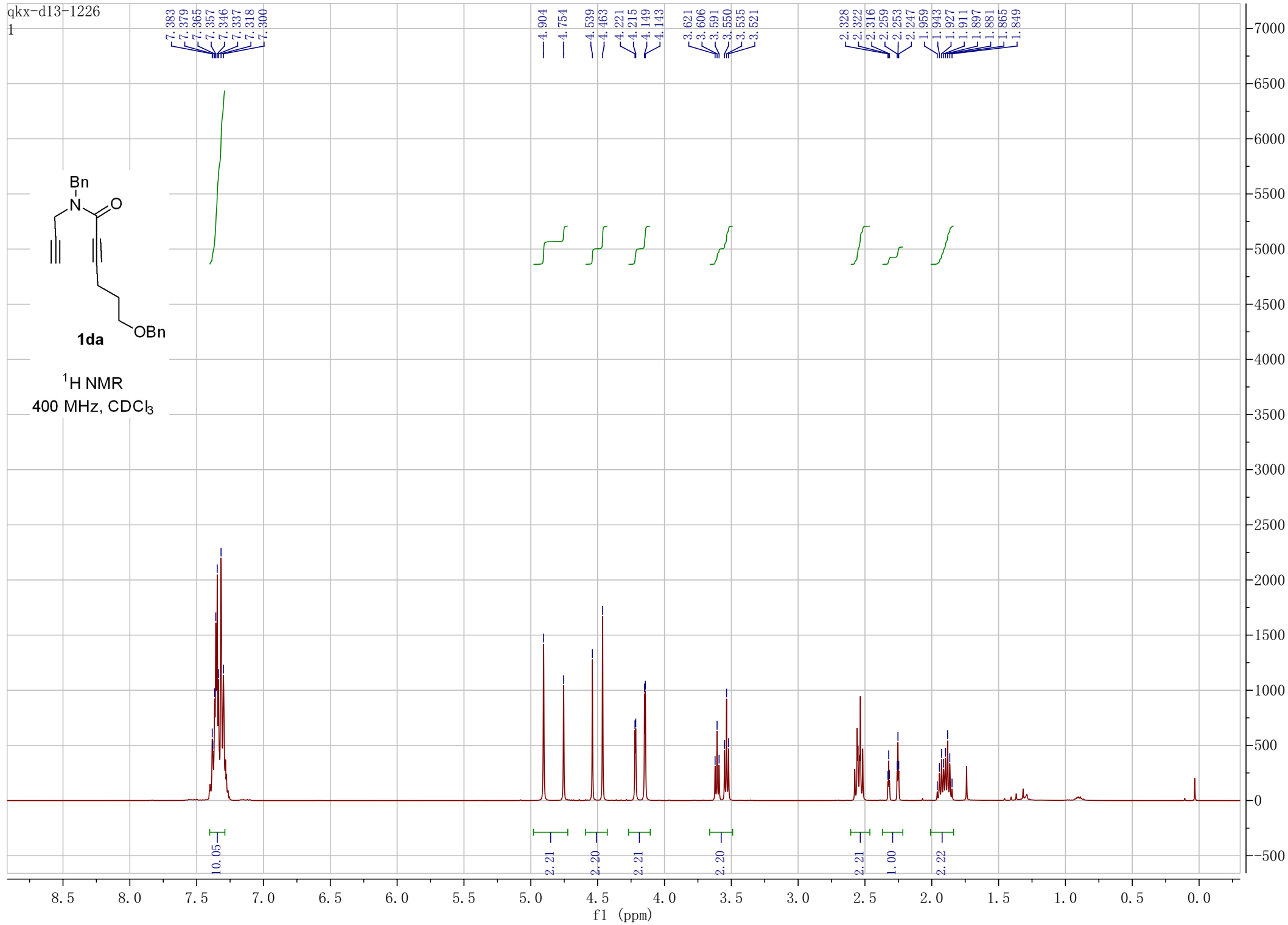


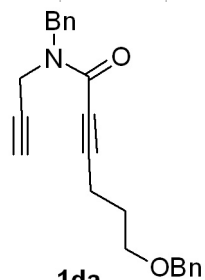
qkx-d13-1226

1

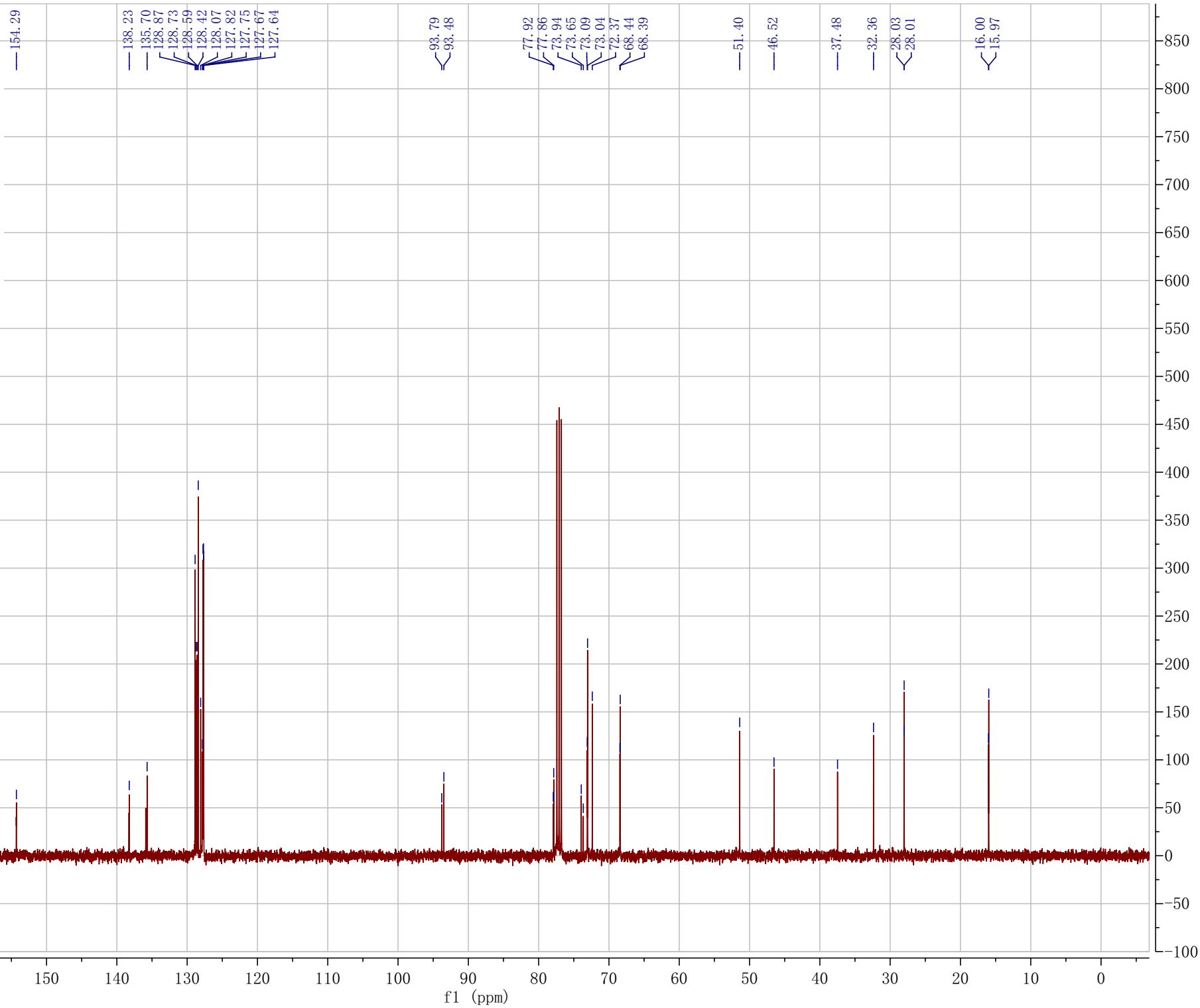


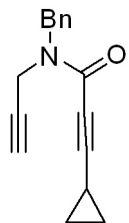
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



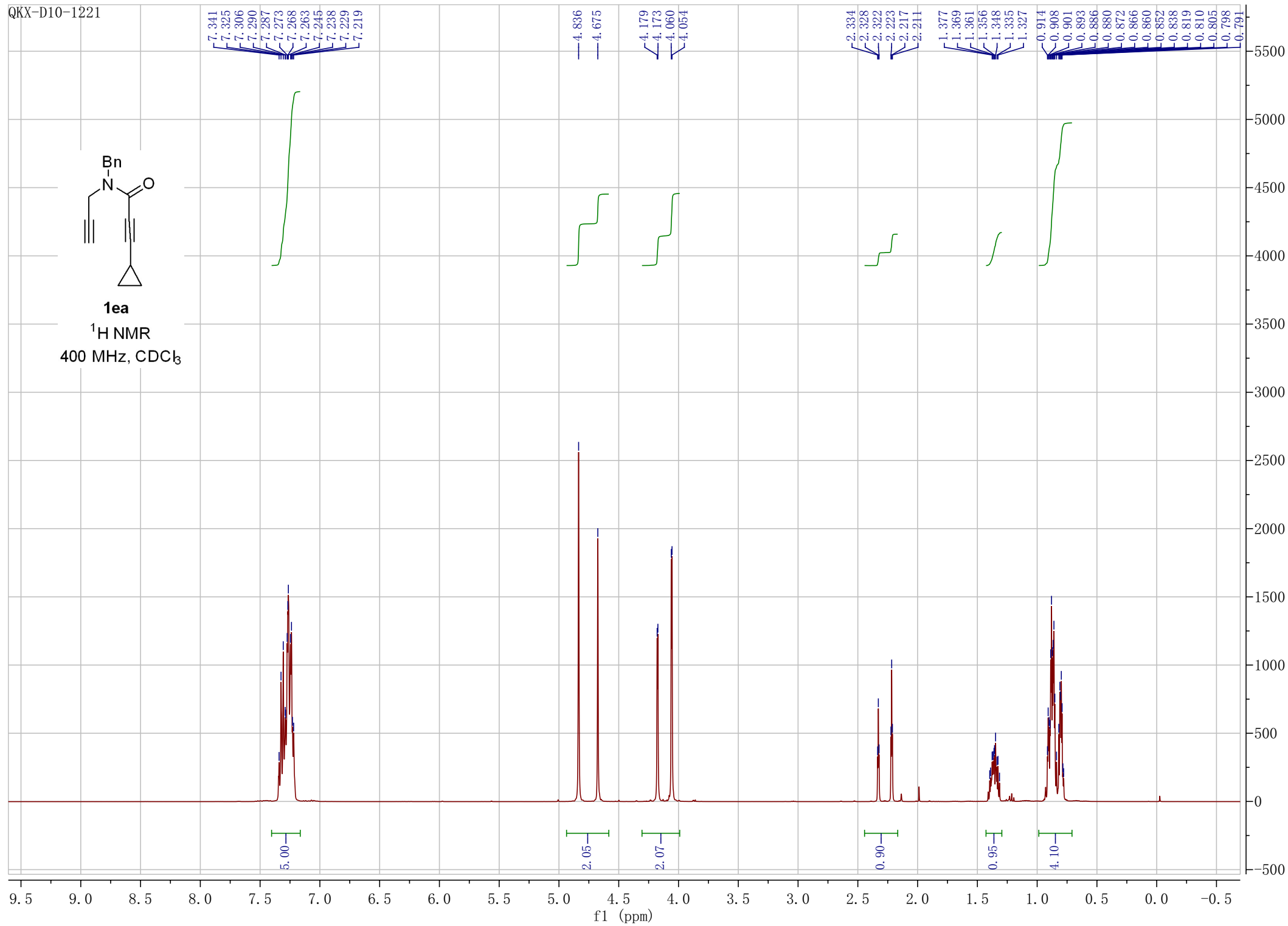


**1da**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

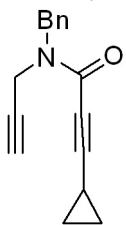


**1ea**

$^1\text{H NMR}$   
400 MHz,  $\text{CDCl}_3$

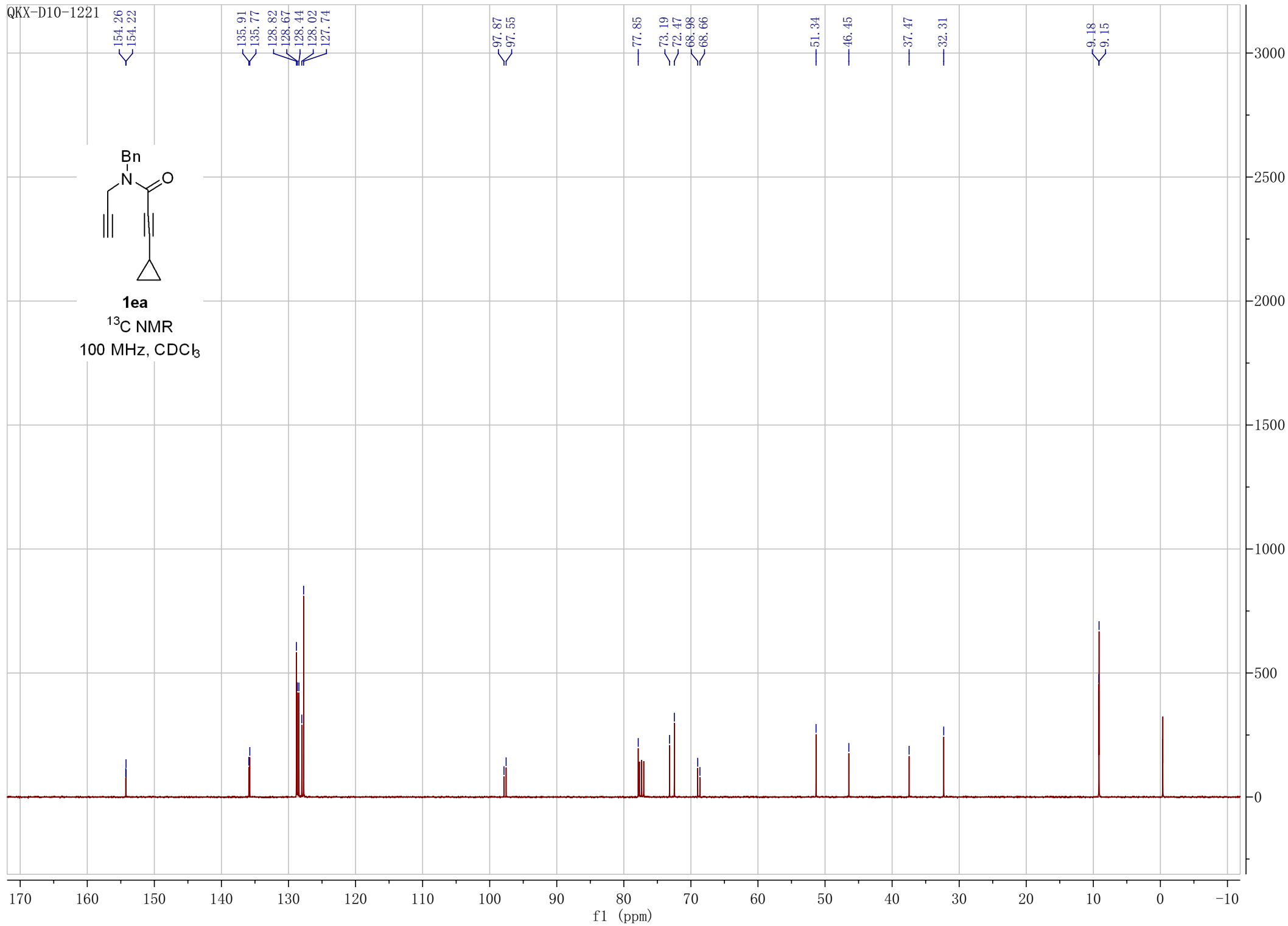


QKX-D10-1221

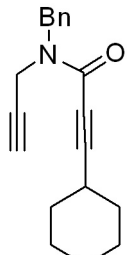


**1ea**

$^{13}\text{C}$  NMR  
100 MHz,  $\text{CDCl}_3$

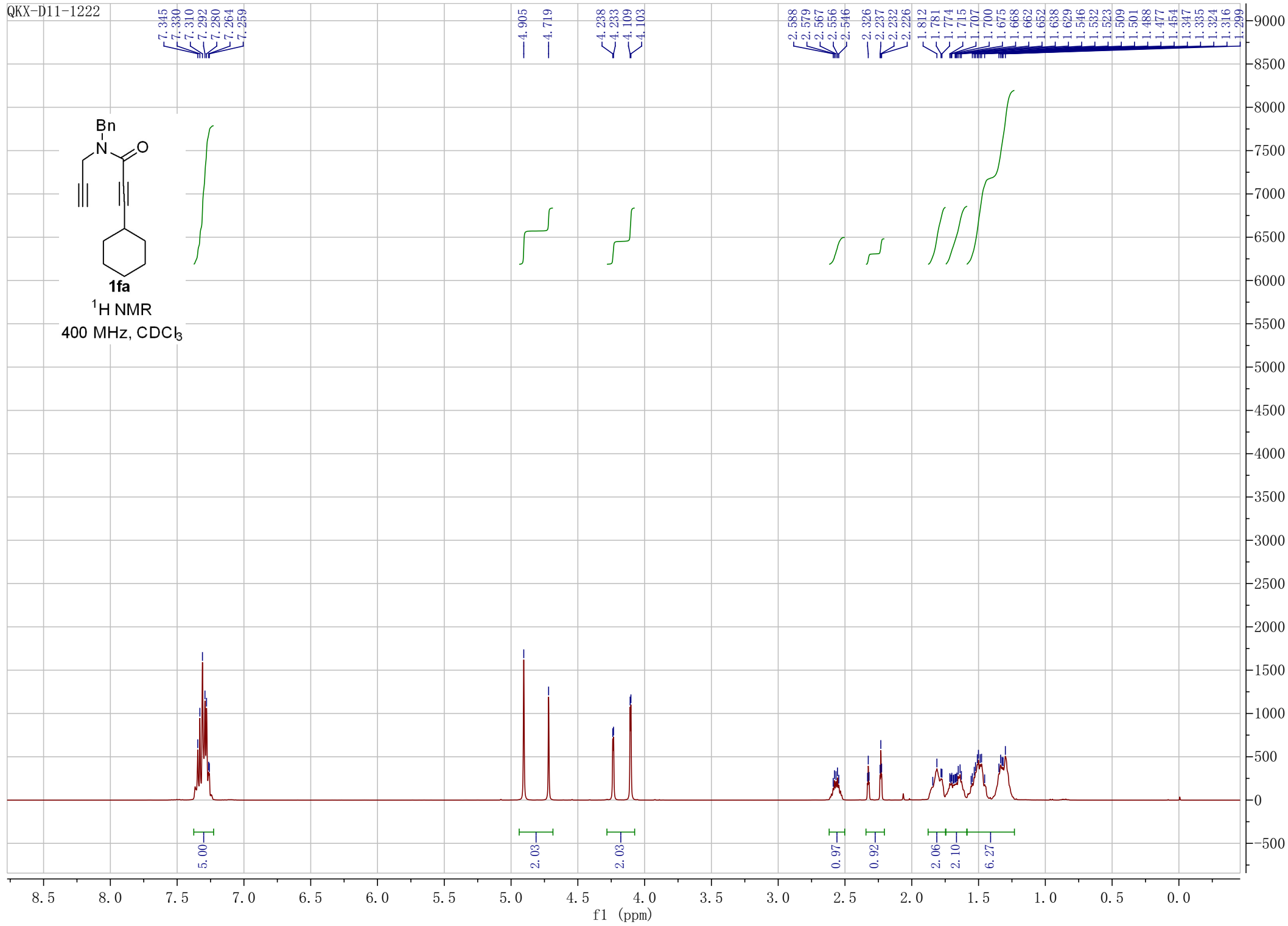


QKX-D11-1222

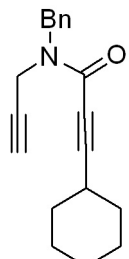


**1fa**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



QKX-D11-1222



**1fa**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

154.49  
154.39

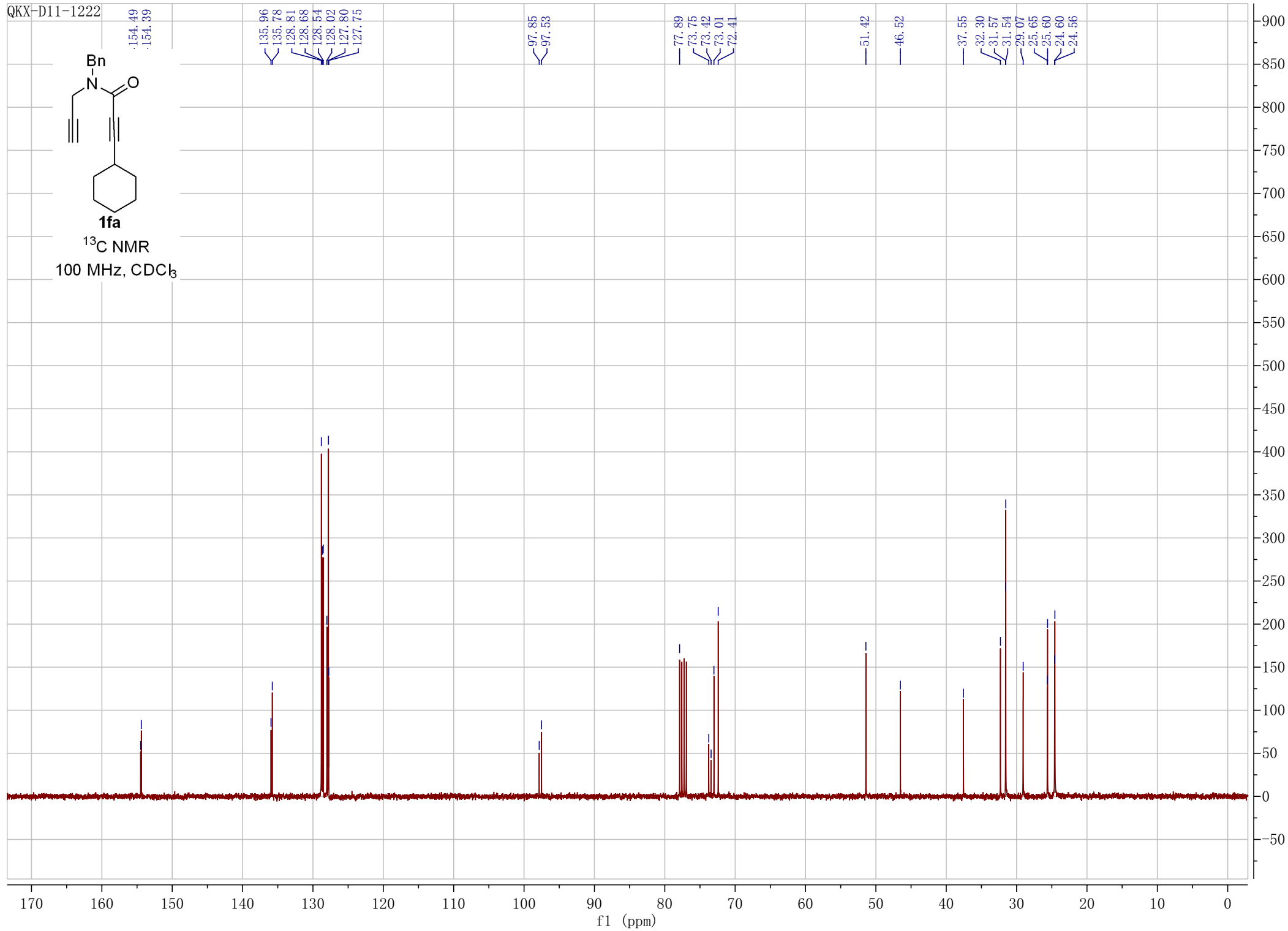
135.96  
135.78  
128.81  
128.68  
128.54  
128.02  
127.80  
127.75

97.85  
97.53

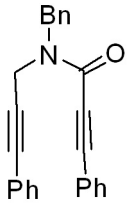
77.89  
73.75  
73.42  
73.01  
72.41

51.42  
46.52

37.55  
32.30  
31.57  
31.54  
29.07  
25.65  
25.60  
24.60  
24.56



qkx-d41-0510  
1H

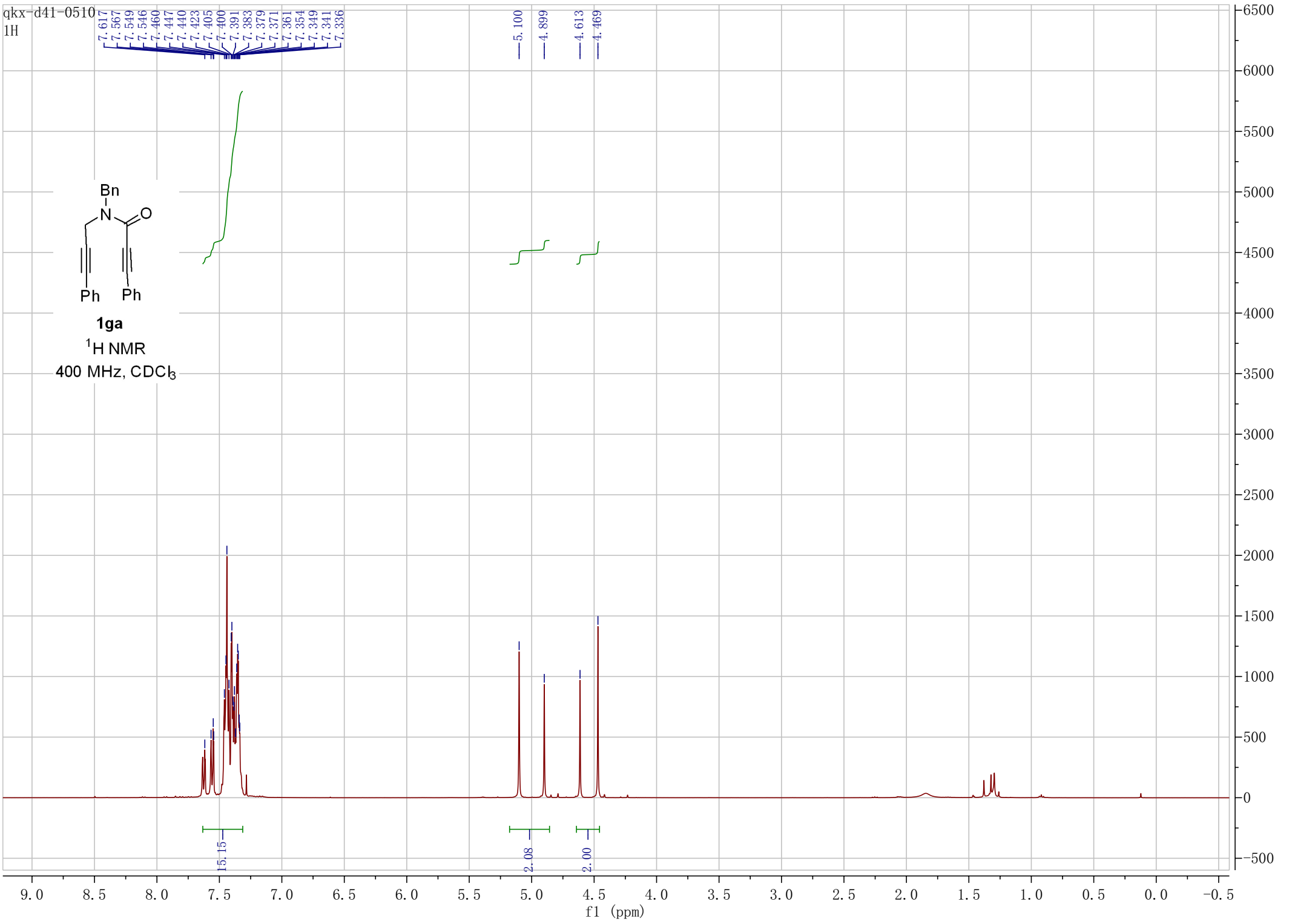


**1ga**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.617  
7.567  
7.549  
7.546  
7.460  
7.447  
7.440  
7.423  
7.405  
7.400  
7.391  
7.383  
7.379  
7.371  
7.361  
7.354  
7.349  
7.341  
7.336

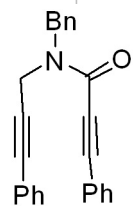
5.100  
4.899  
4.613  
4.469





qkx-d41-0510

1H



**1ga**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

154.44  
154.34  
132.57  
132.54  
131.86  
131.80  
130.30  
128.95  
128.79  
128.64  
128.60  
128.53  
128.40  
128.33  
127.93  
122.31  
120.32  
120.25

91.45  
91.04  
85.09  
84.41  
83.13  
83.08  
81.43  
81.18

51.81

47.08

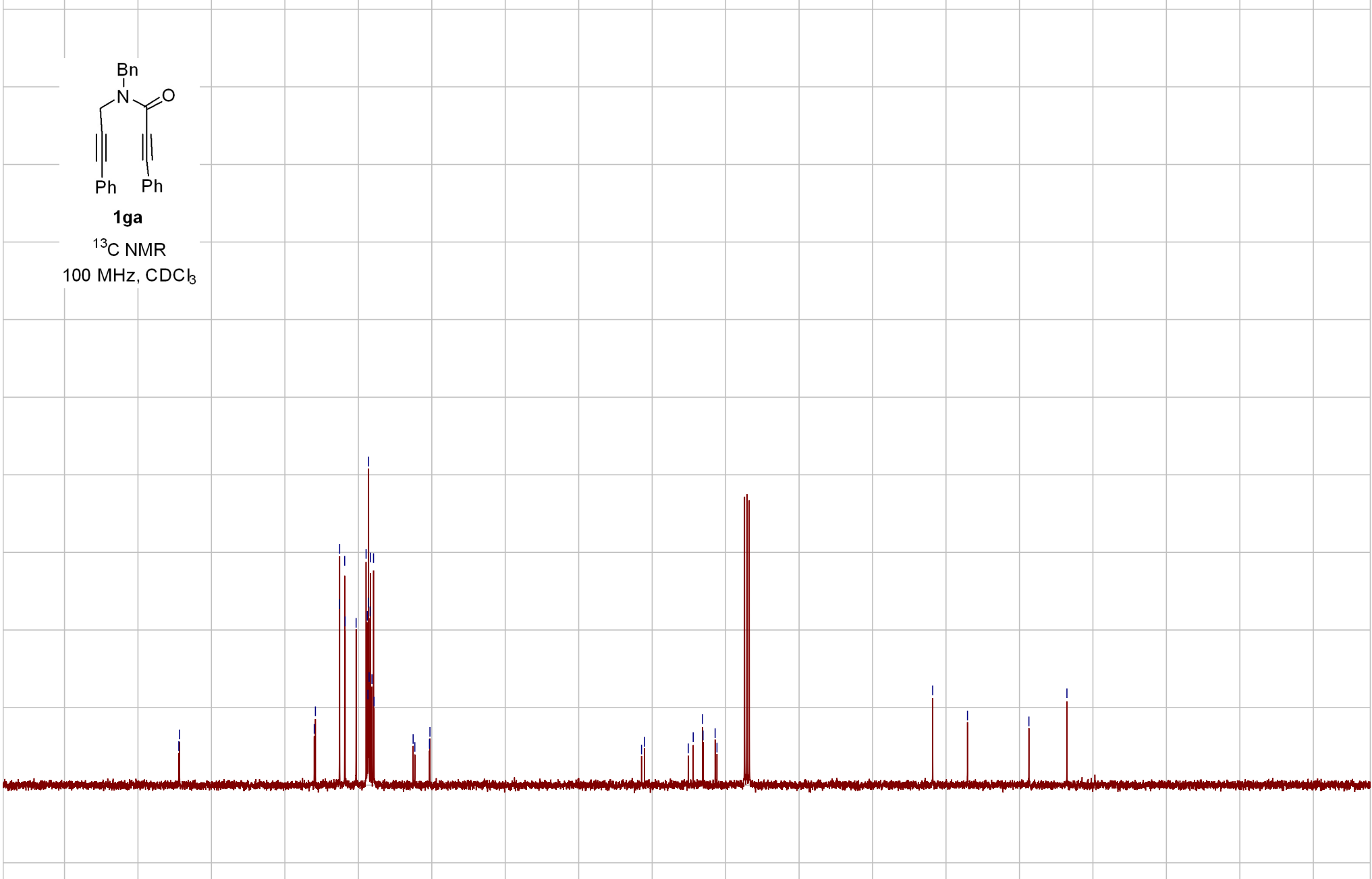
38.71

33.54

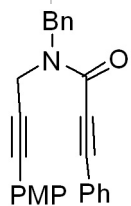
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

1100  
1000  
900  
800  
700  
600  
500  
400  
300  
200  
100  
0  
-100

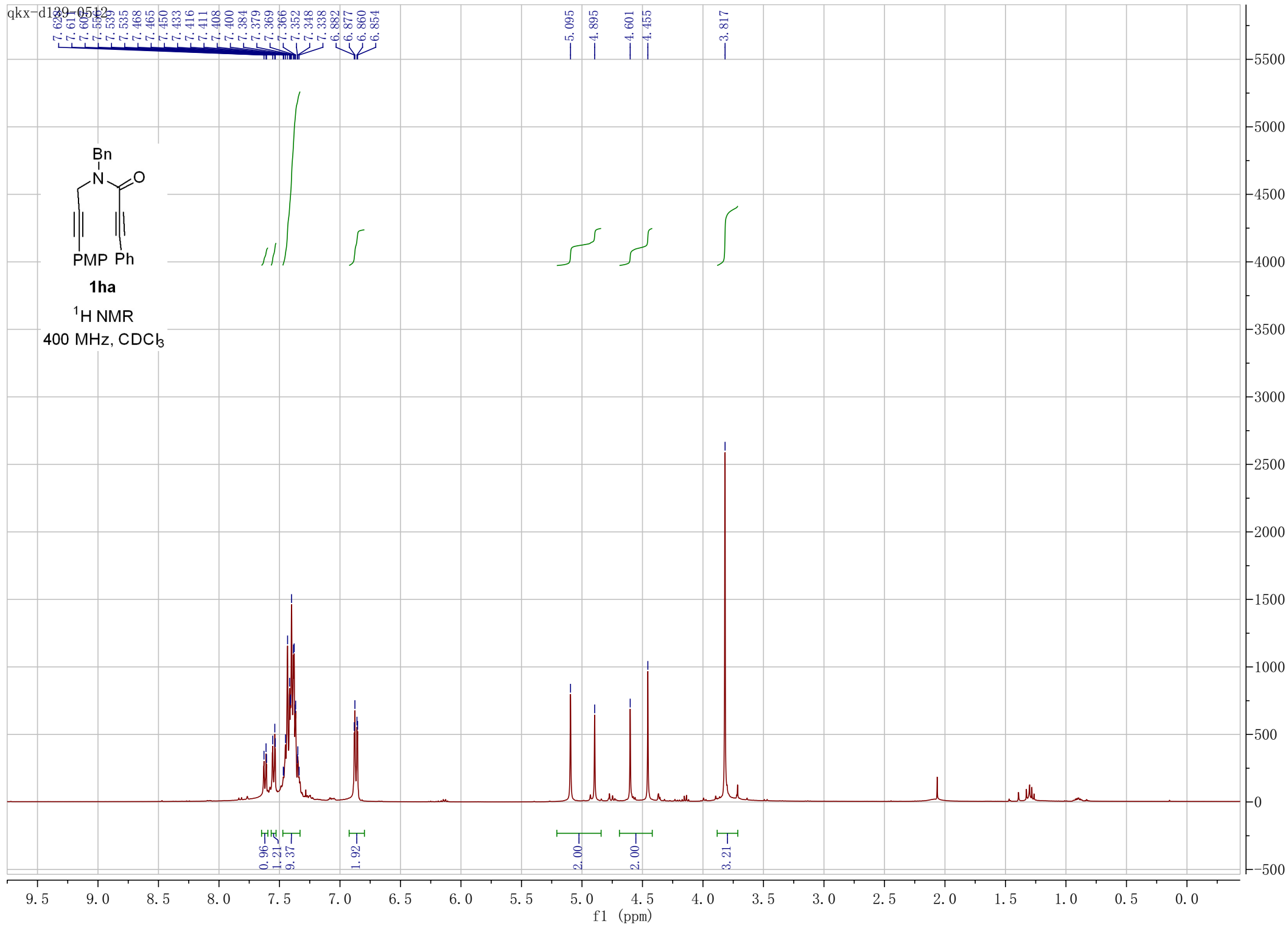


qkx-d139-0512

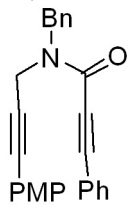


**1ha**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

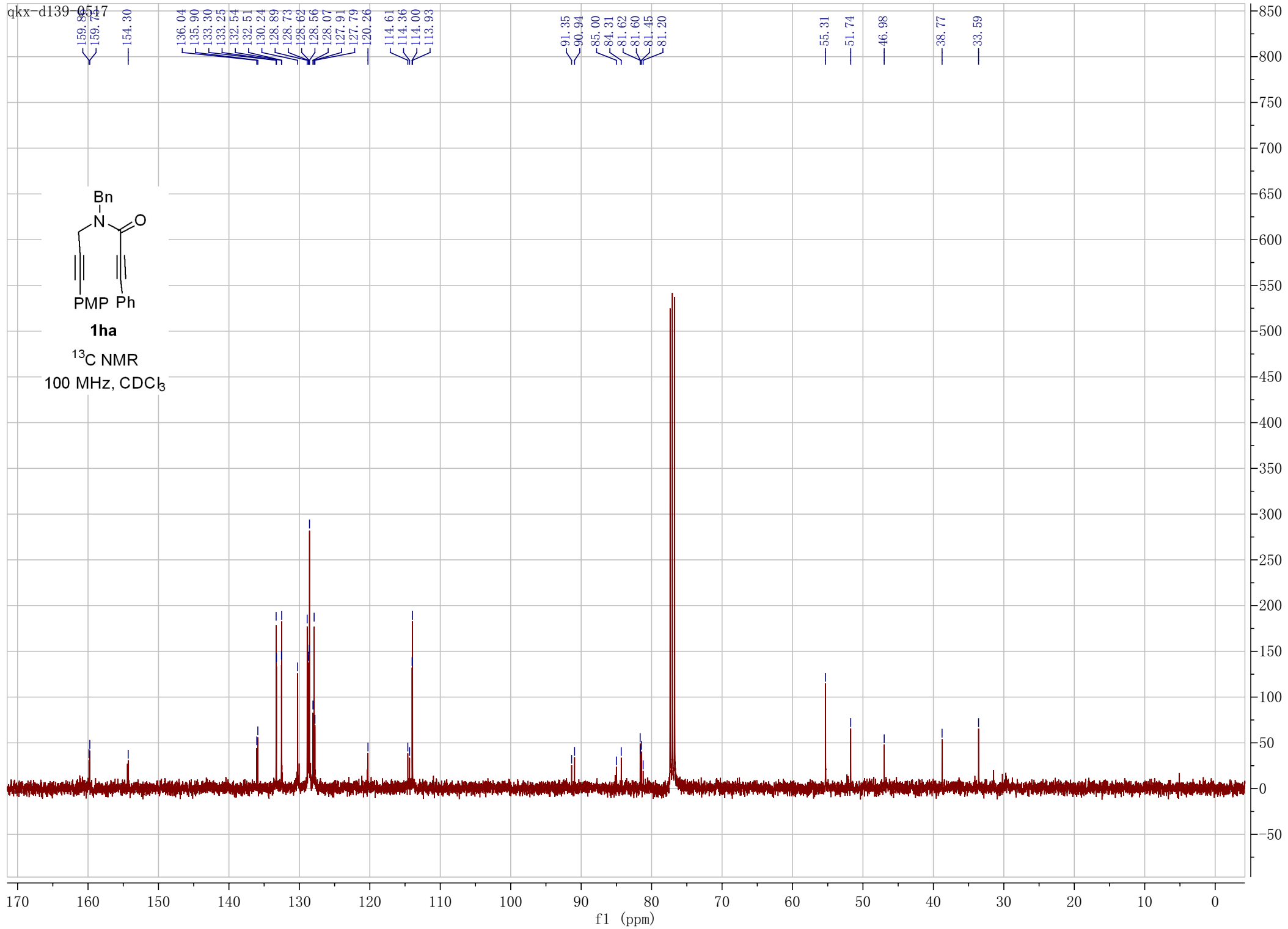


qkx-d139-0517



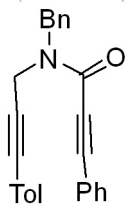
**1ha**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



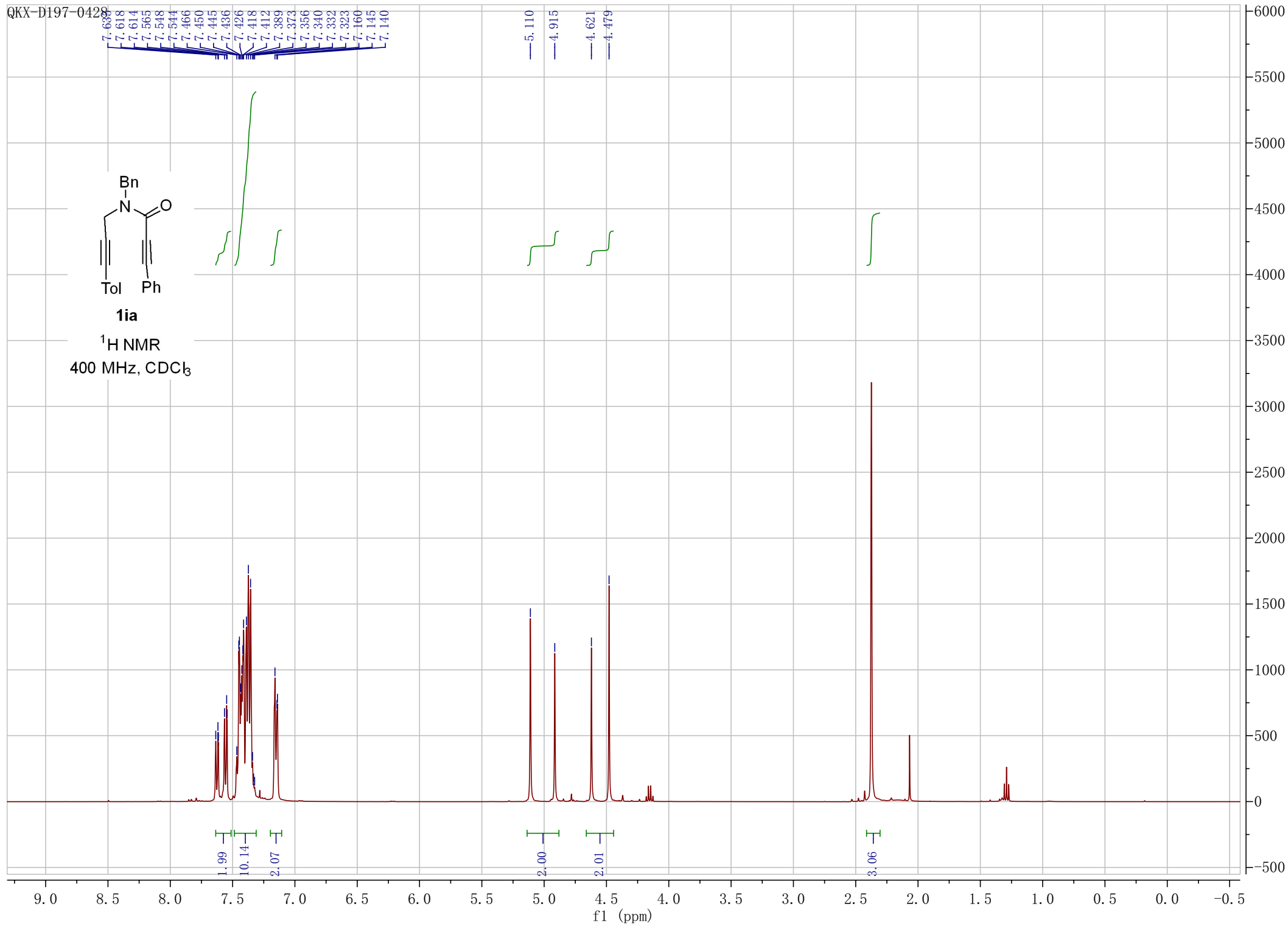
7.639  
7.618  
7.614  
7.565  
7.548  
7.544  
7.466  
7.450  
7.445  
7.436  
7.426  
7.418  
7.412  
7.389  
7.373  
7.356  
7.340  
7.332  
7.323  
7.323  
7.160  
7.145  
7.140

5.110  
4.915  
4.621  
4.479

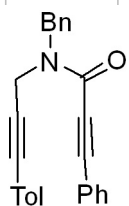


**1ia**

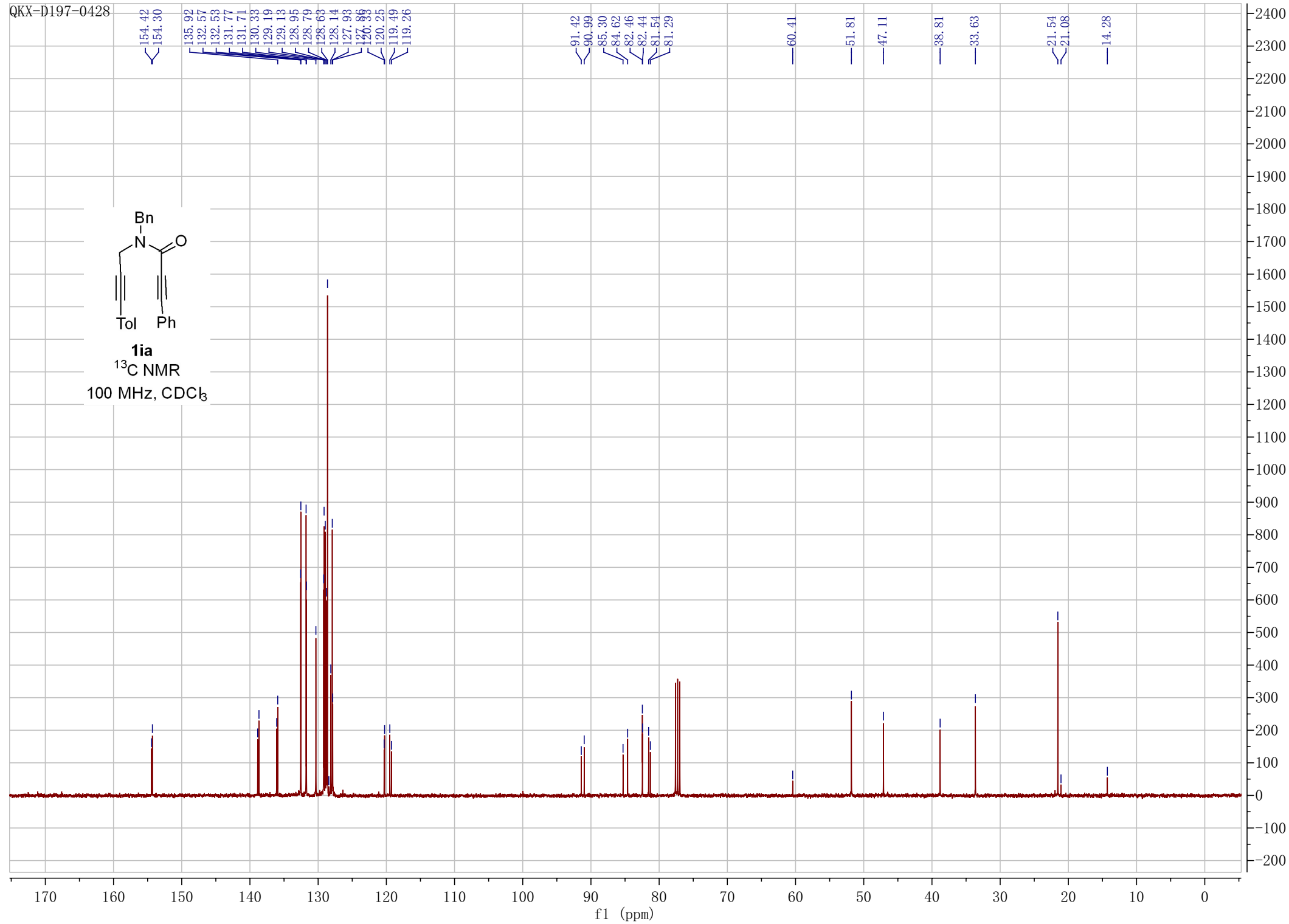
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



QKX-D197-0428

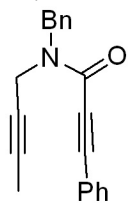


**1ia**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



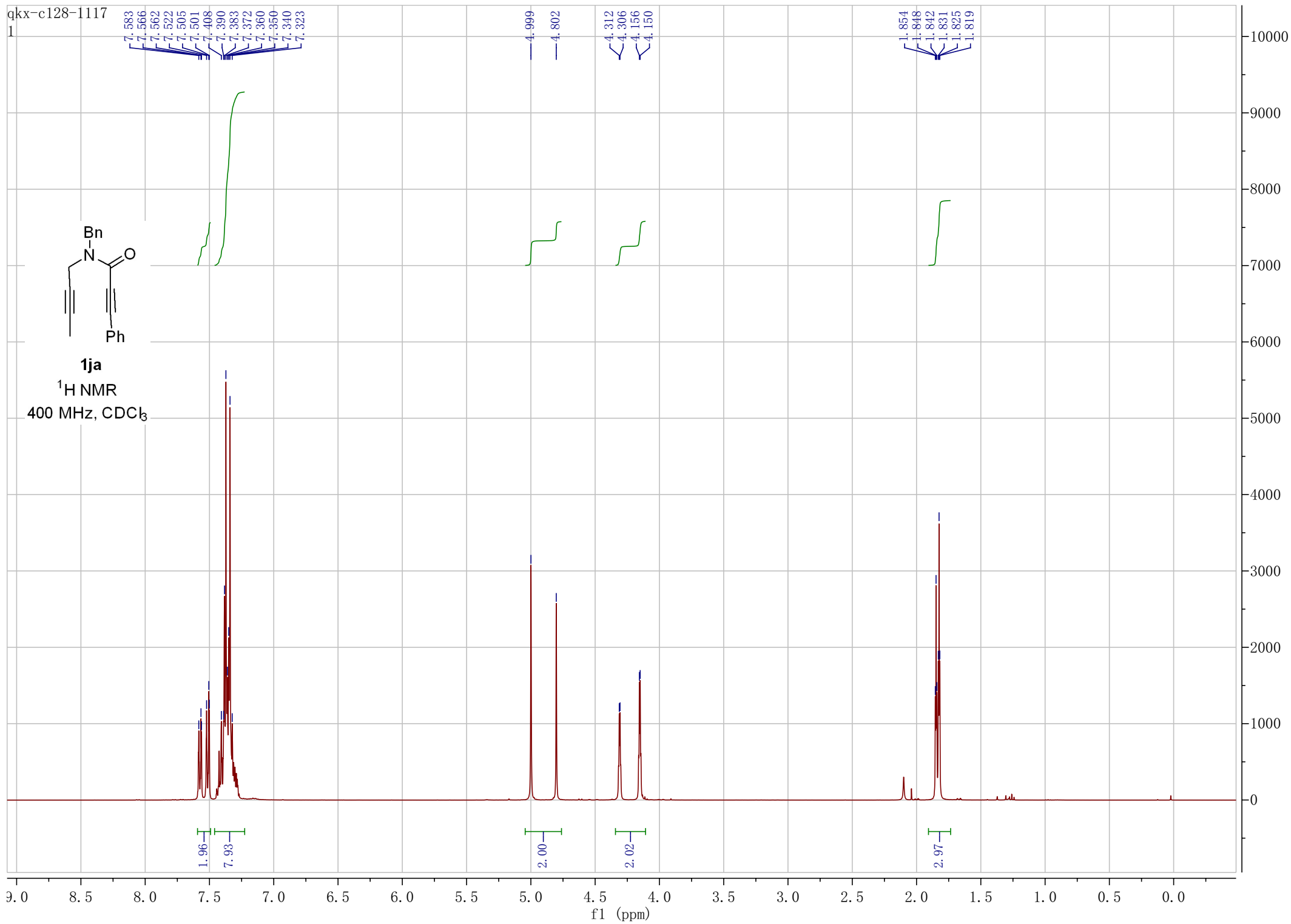
qkx-c128-1117

1

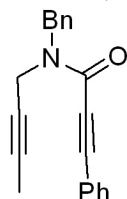


**1ja**

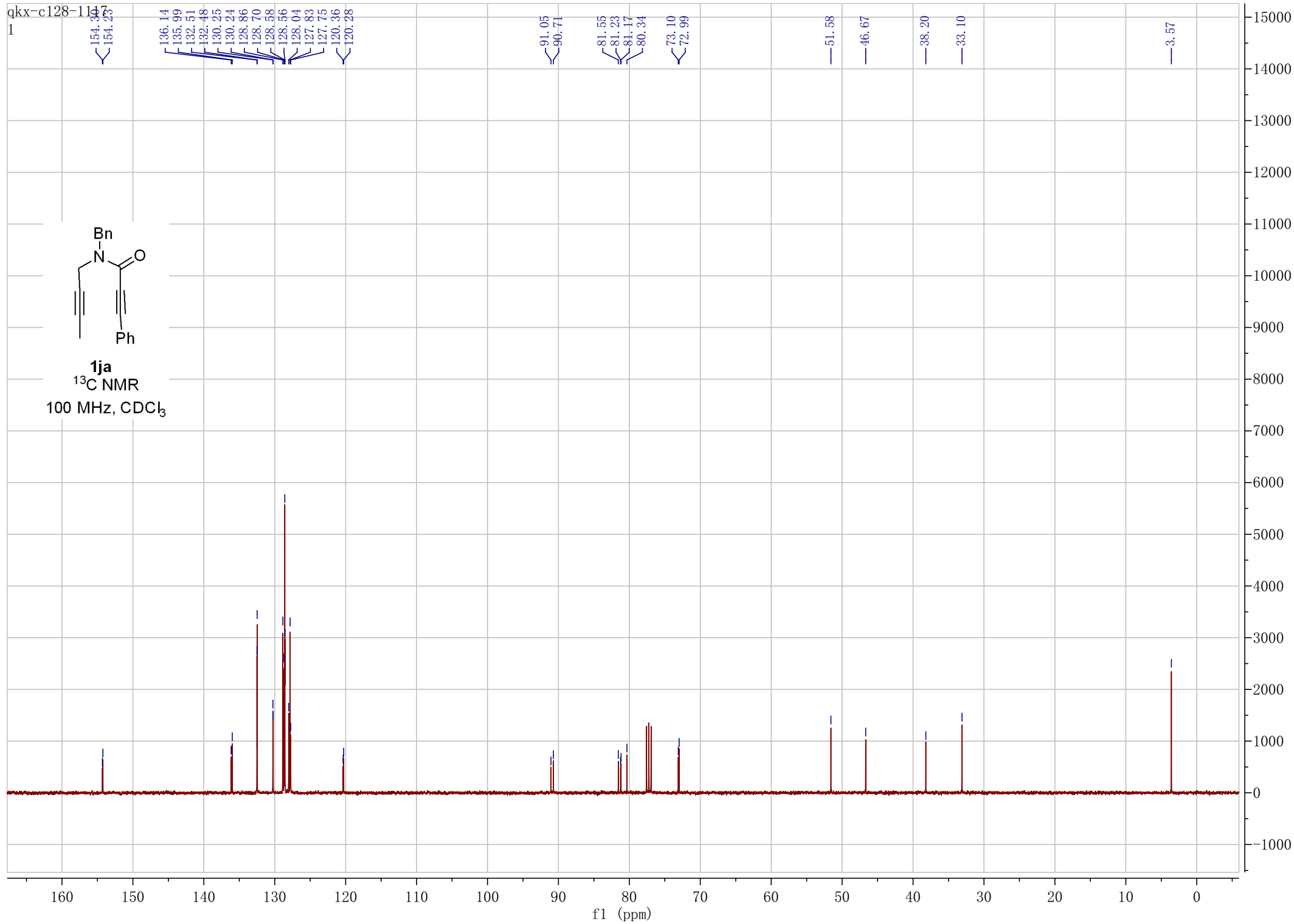
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



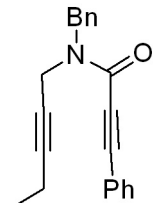
qkx-c128-1117-1



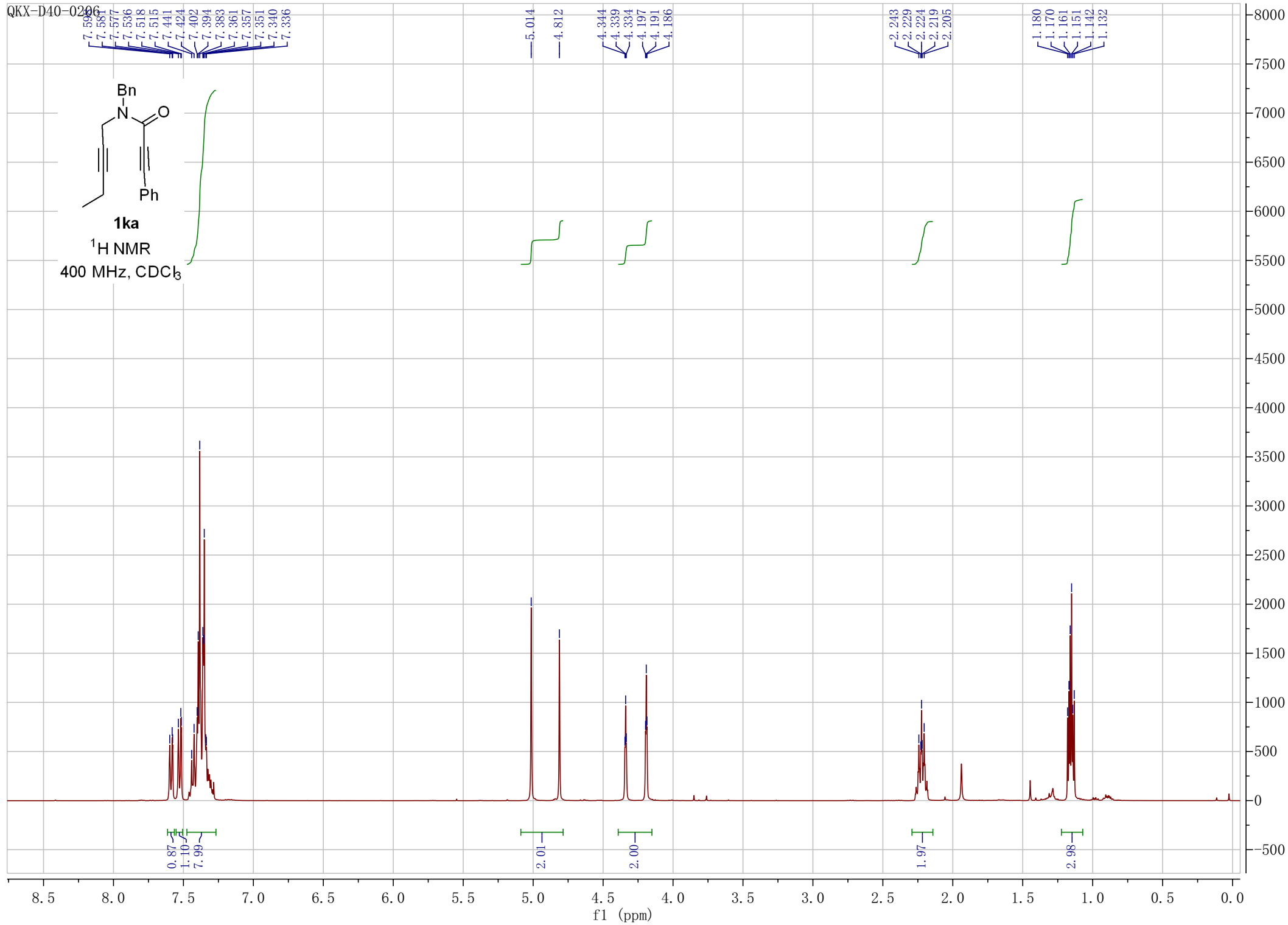
**1ja**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



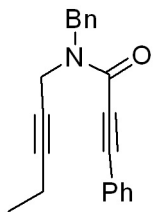
QKX-D40-0206



**1ka**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>





**1ka**

$^{13}\text{C}$  NMR  
100 MHz,  $\text{CDCl}_3$

154.34  
154.22

136.15  
136.01  
132.51  
132.49  
130.22  
130.20  
128.84  
128.68  
128.57  
128.01  
127.85  
127.72  
120.41  
120.32

91.06  
90.70  
87.09  
86.32  
81.57  
81.24  
73.19  
73.06

51.52

46.69

38.26

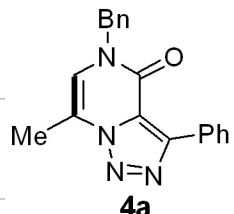
33.12

13.82  
13.81  
12.41

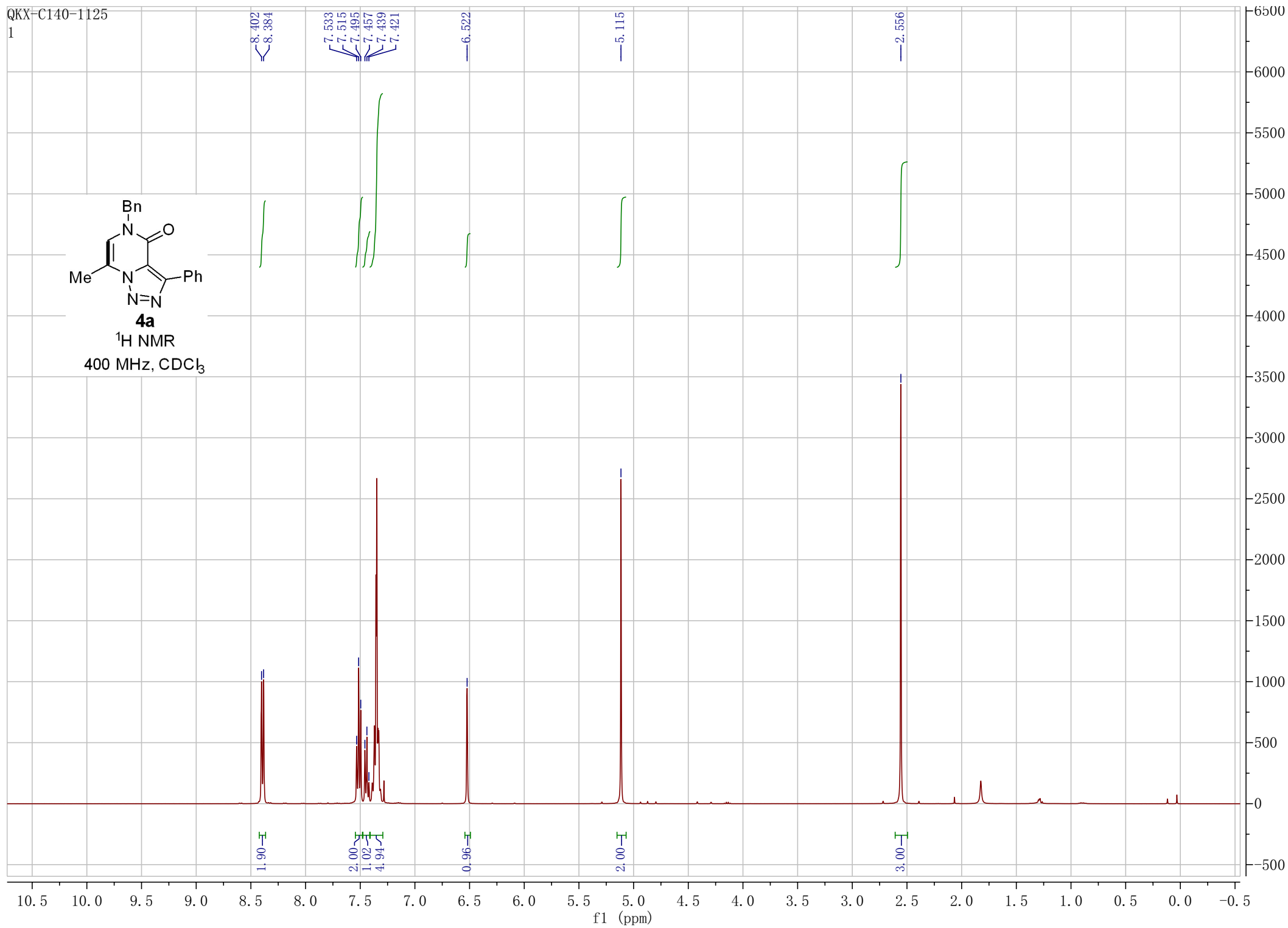
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

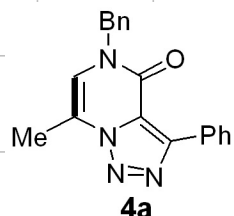
f1 (ppm)

15000  
14000  
13000  
12000  
11000  
10000  
9000  
8000  
7000  
6000  
5000  
4000  
3000  
2000  
1000  
0  
-1000

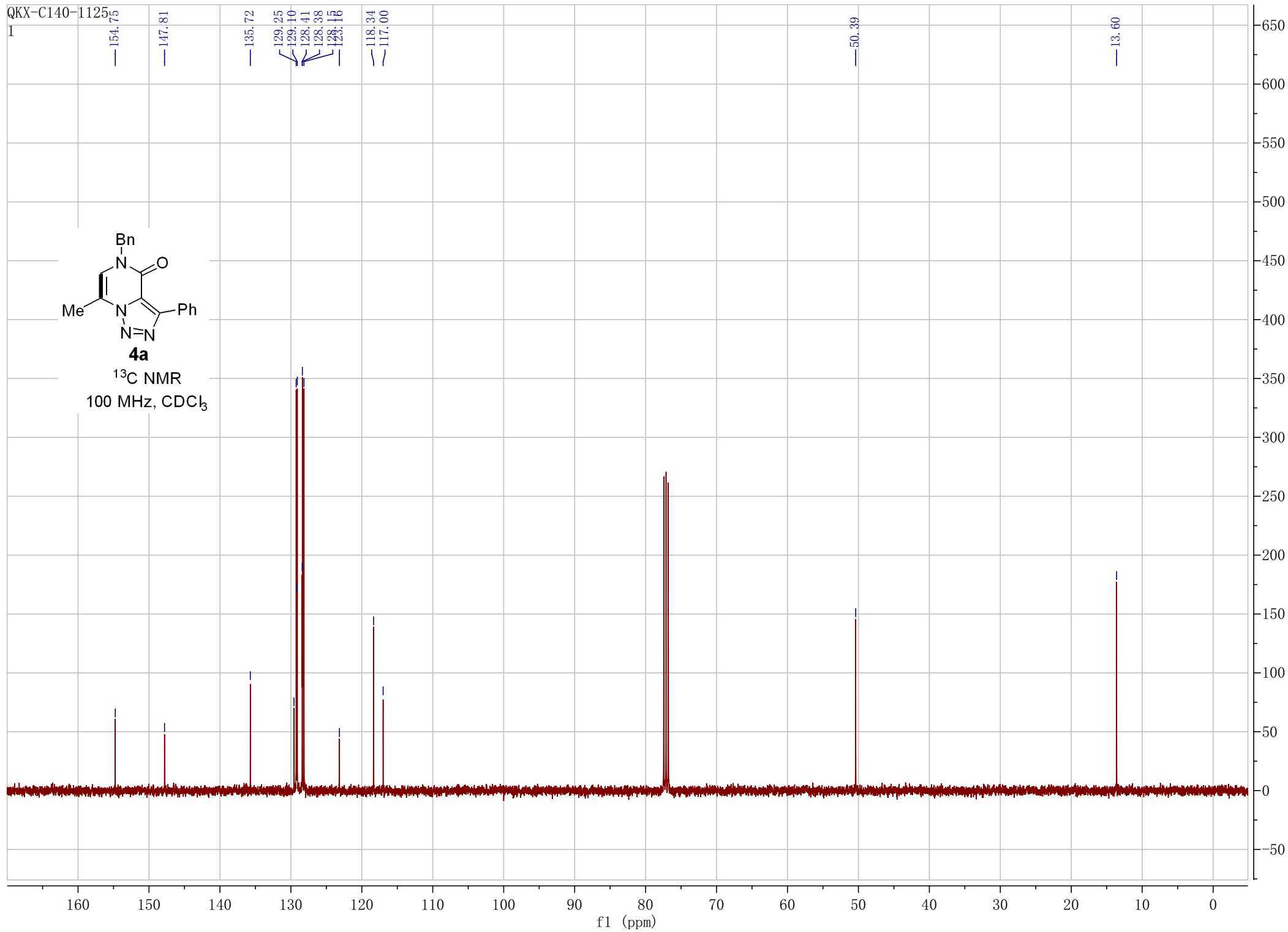


<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

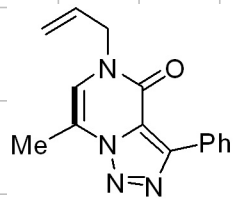




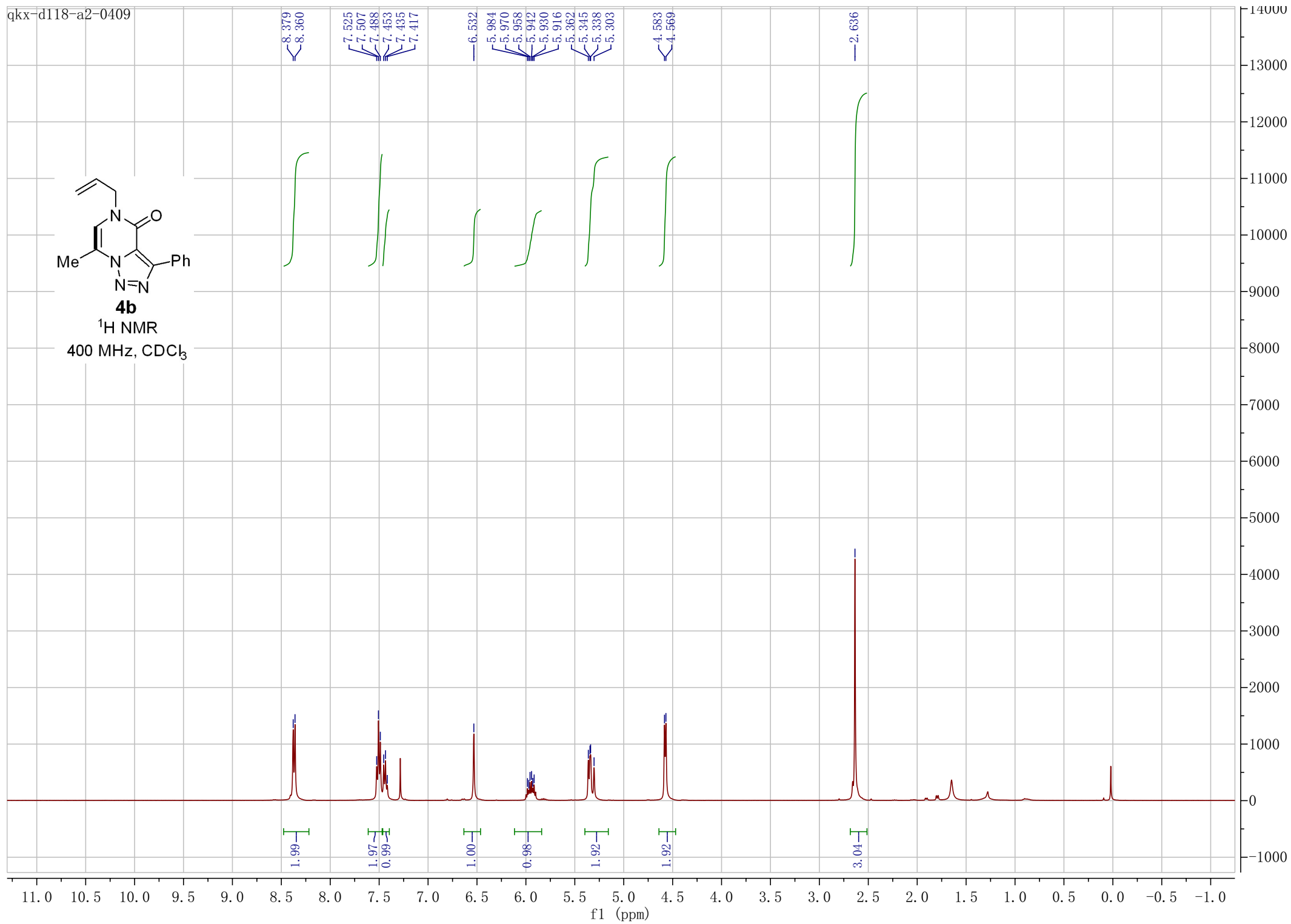
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



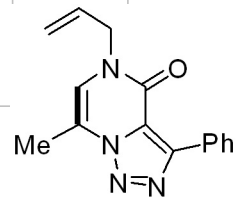
qkx-d118-a2-0409



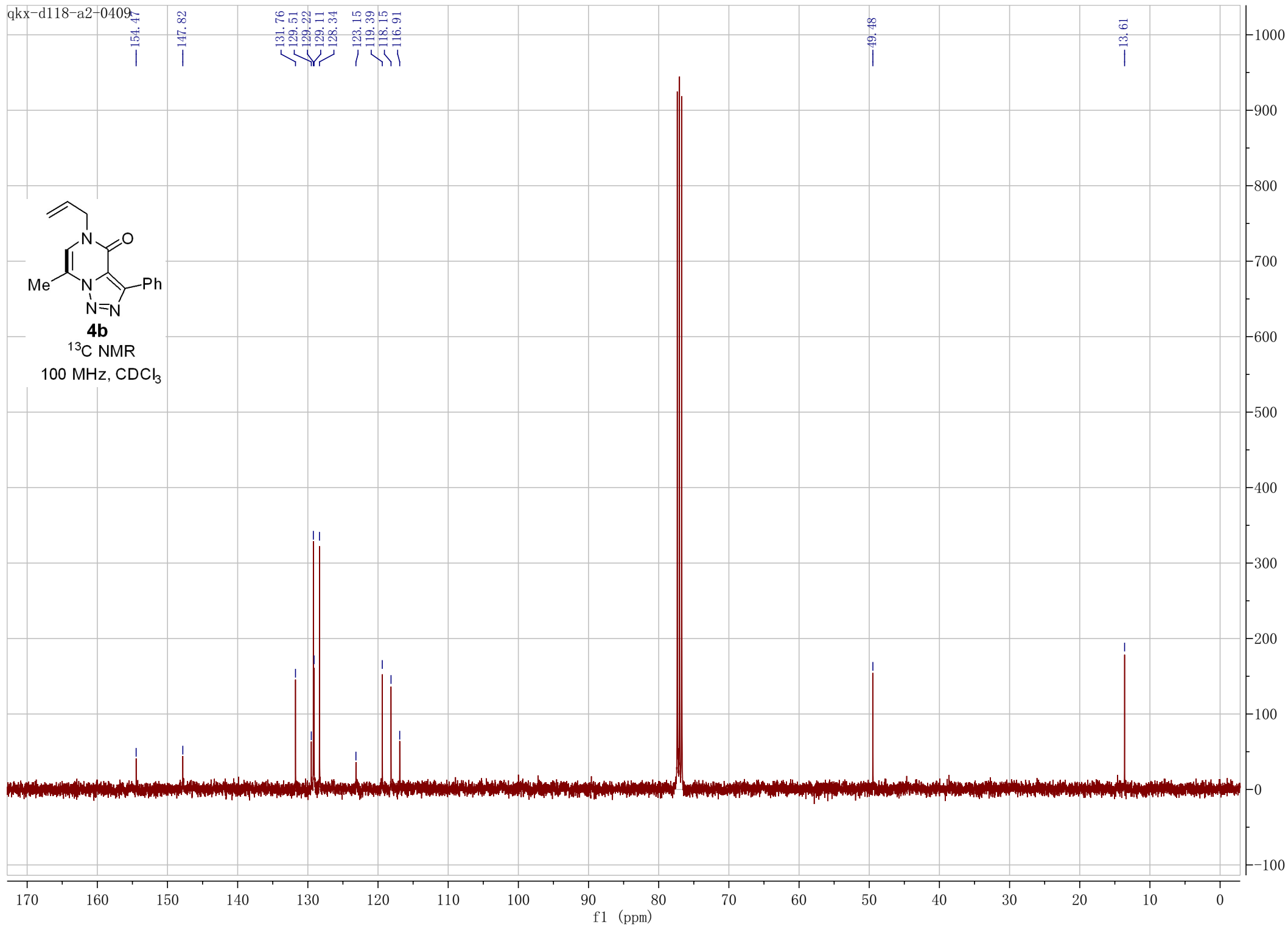
**4b**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



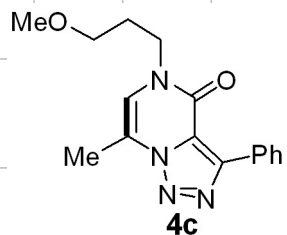
qkx-d118-a2-0409



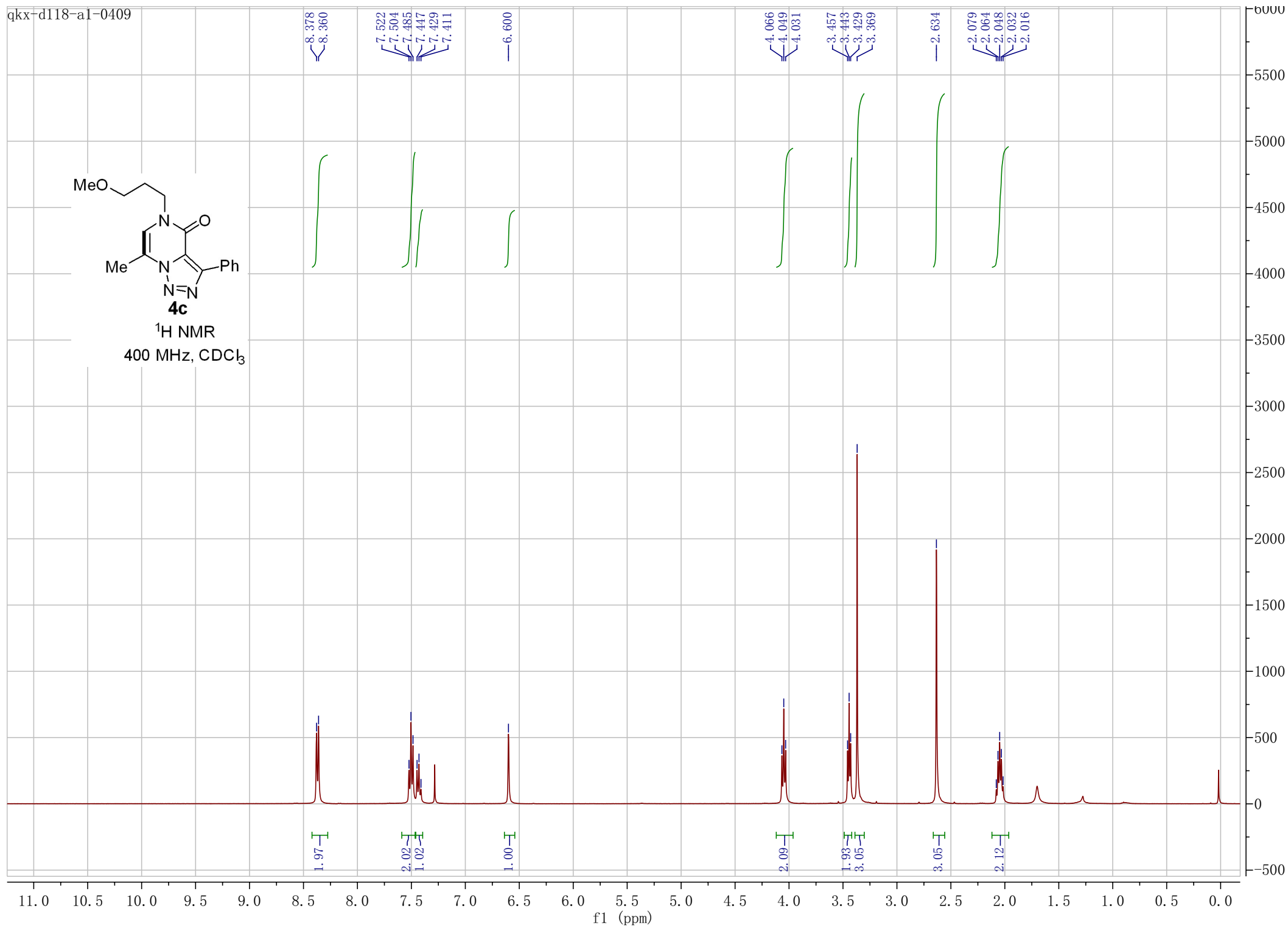
**4b**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



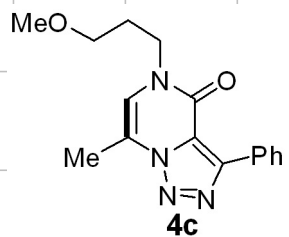
qkx-d118-a1-0409



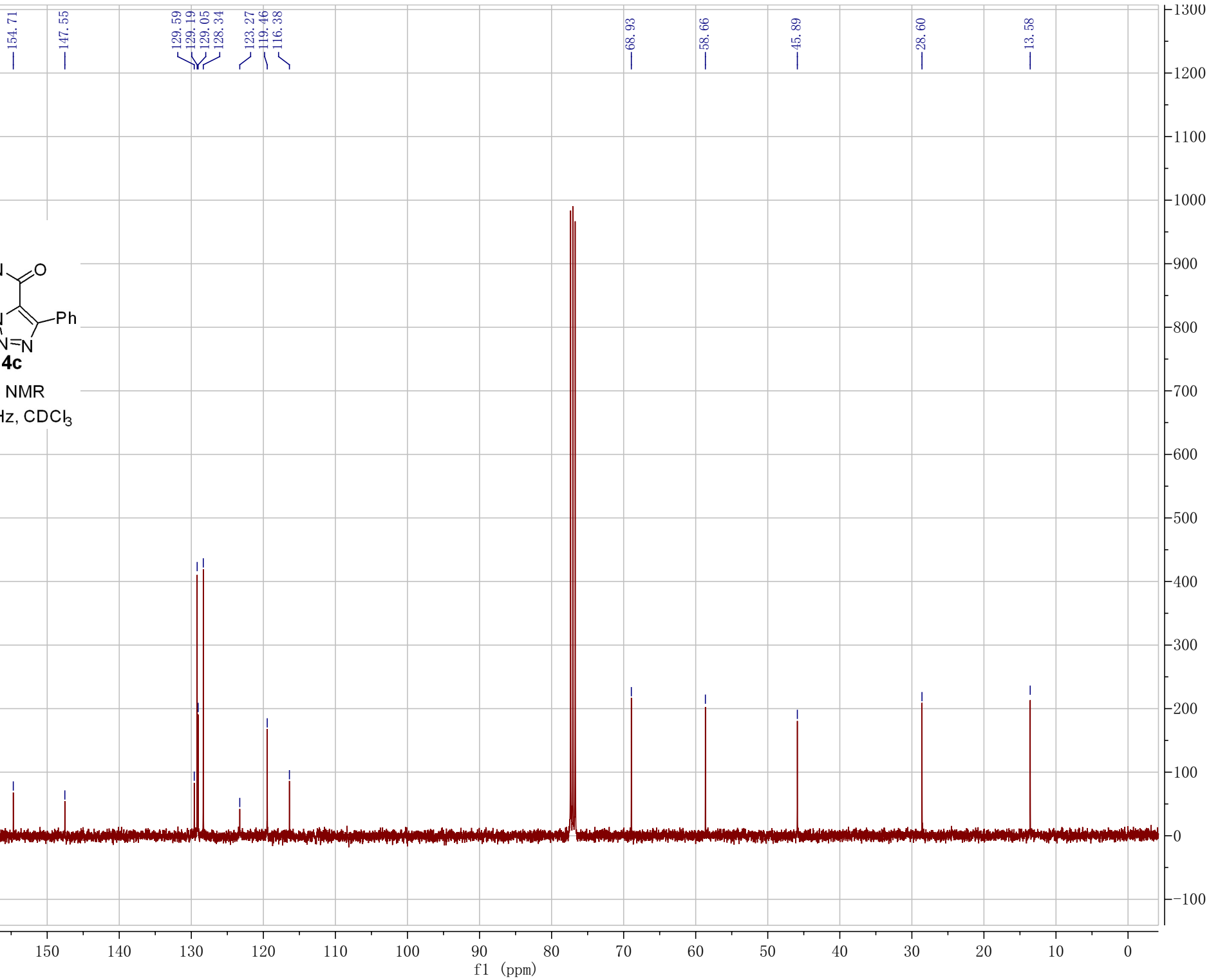
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

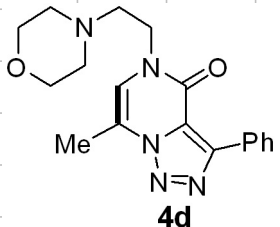


qkx-d118-a1-0409

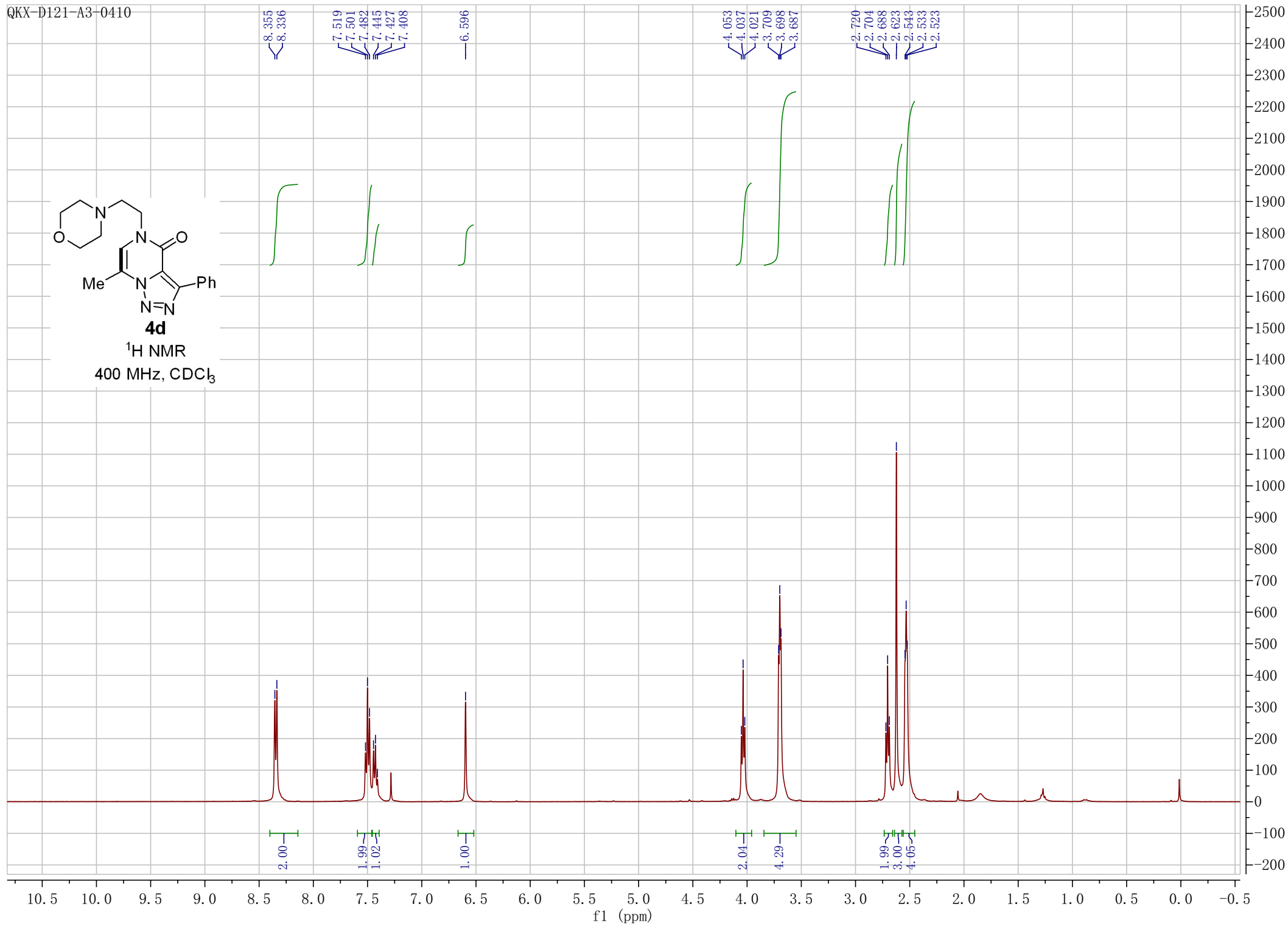


<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

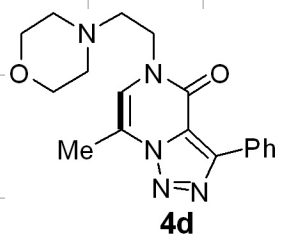




<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>







<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

154.65

147.62

129.58

129.17

129.08

128.35

123.13

119.40

116.23

66.96

57.00

53.74

44.90

13.61

170

160

150

140

130

120

110

100

90

80

70

60

50

40

30

20

170

160

150

140

130

120

110

100

90

80

70

60

50

40

30

20

f1 (ppm)

5000

4500

4000

3500

3000

2500

2000

1500

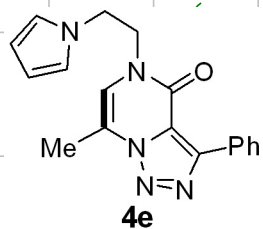
1000

500

0

-500

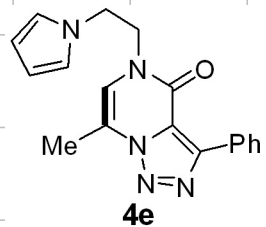
qkx-d121-a2-0424



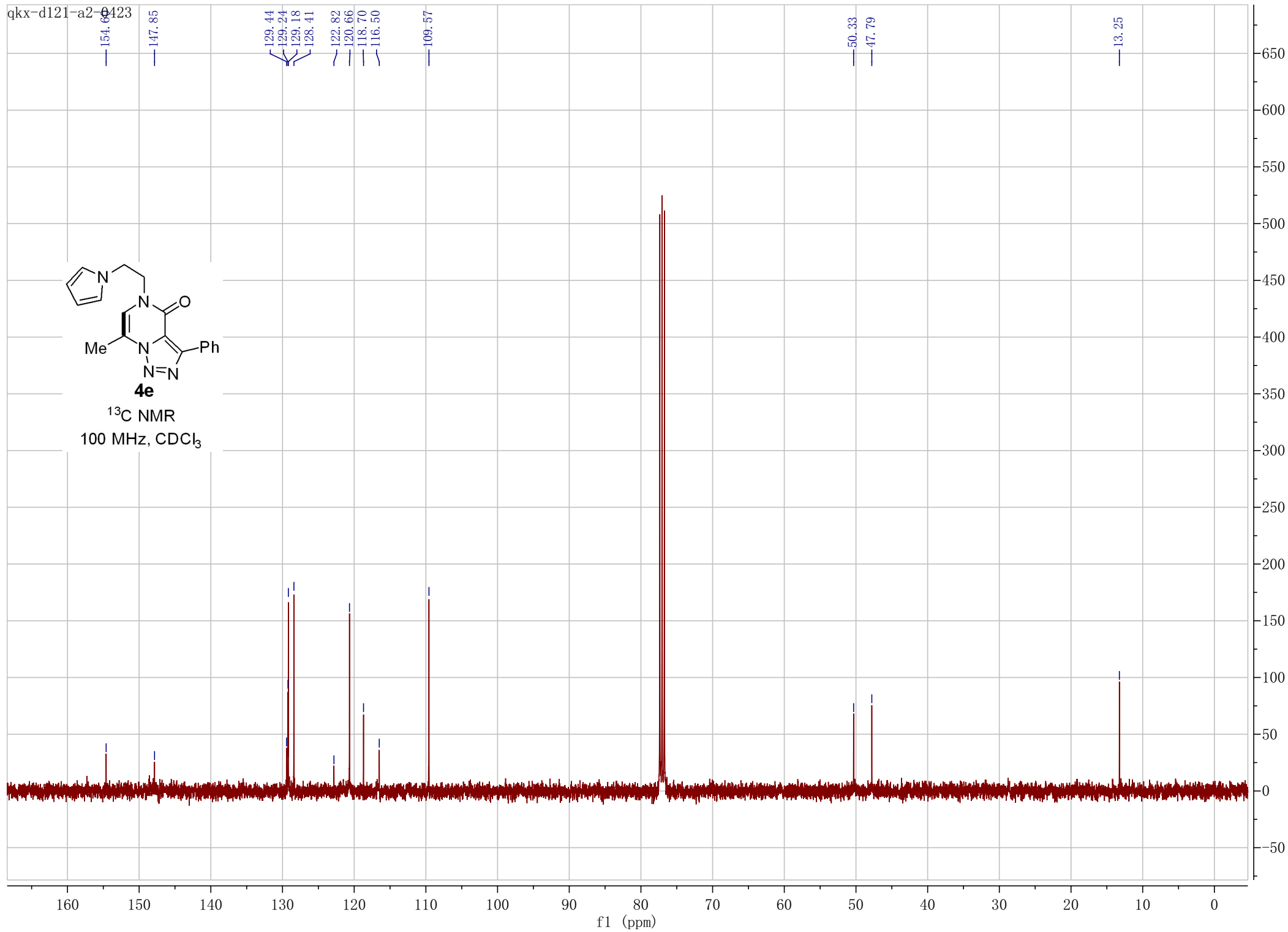
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



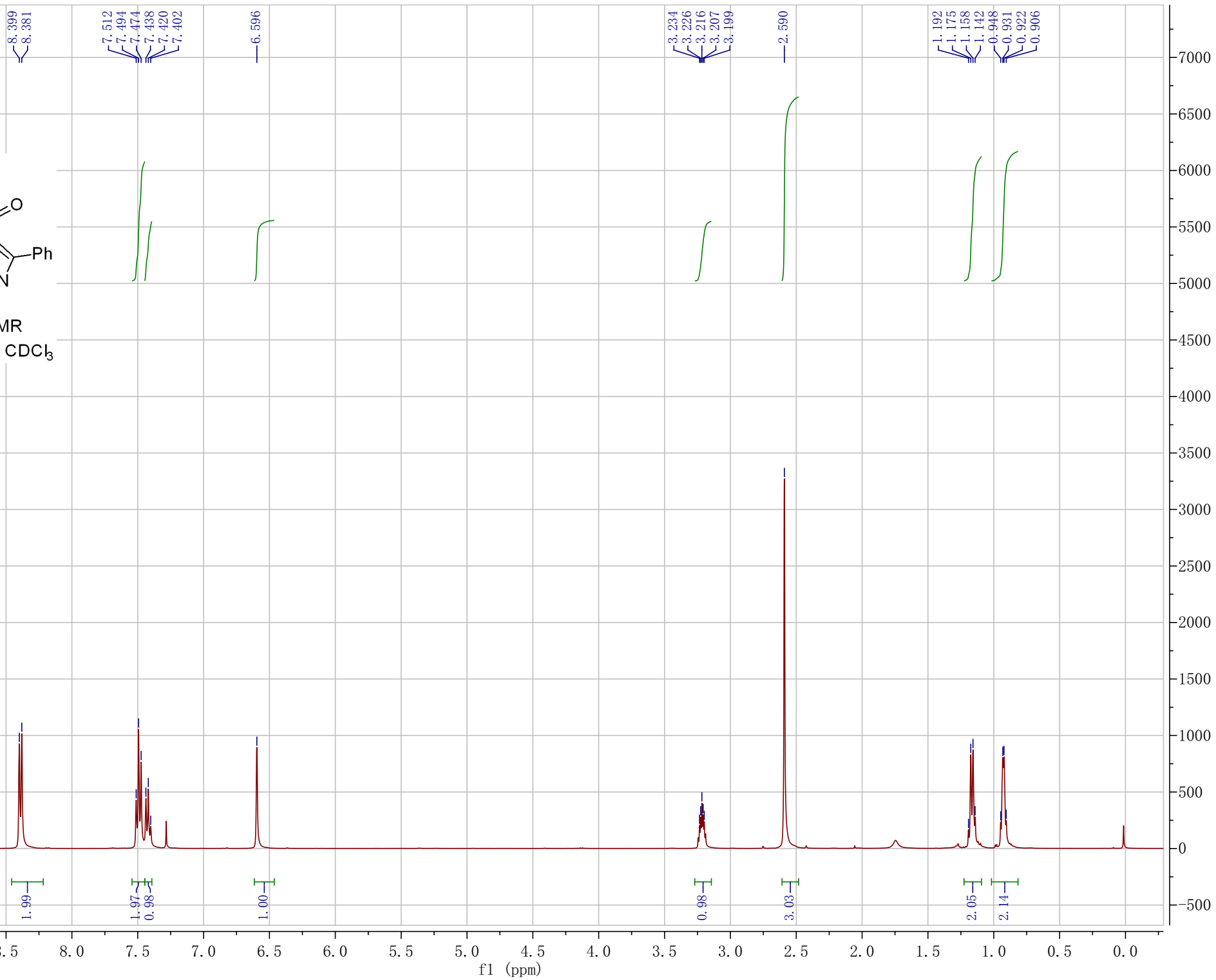
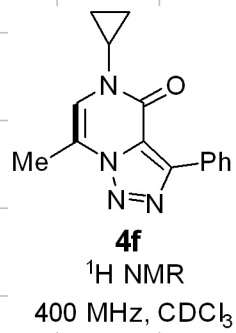
qkx-d121-a2-0423



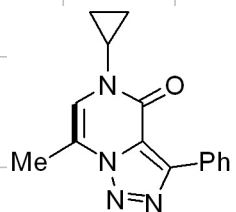
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



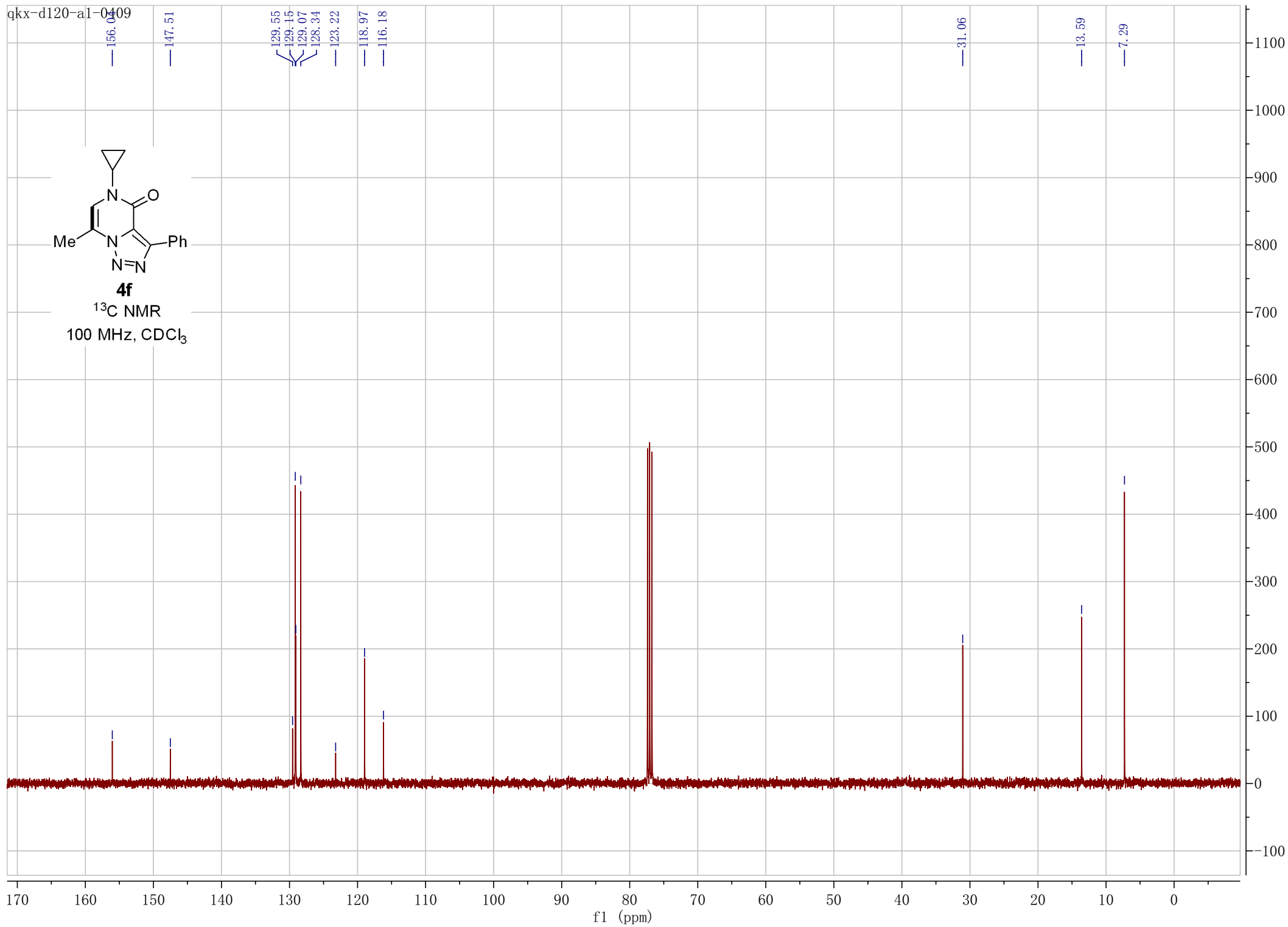
qkx-d120-a1-0409

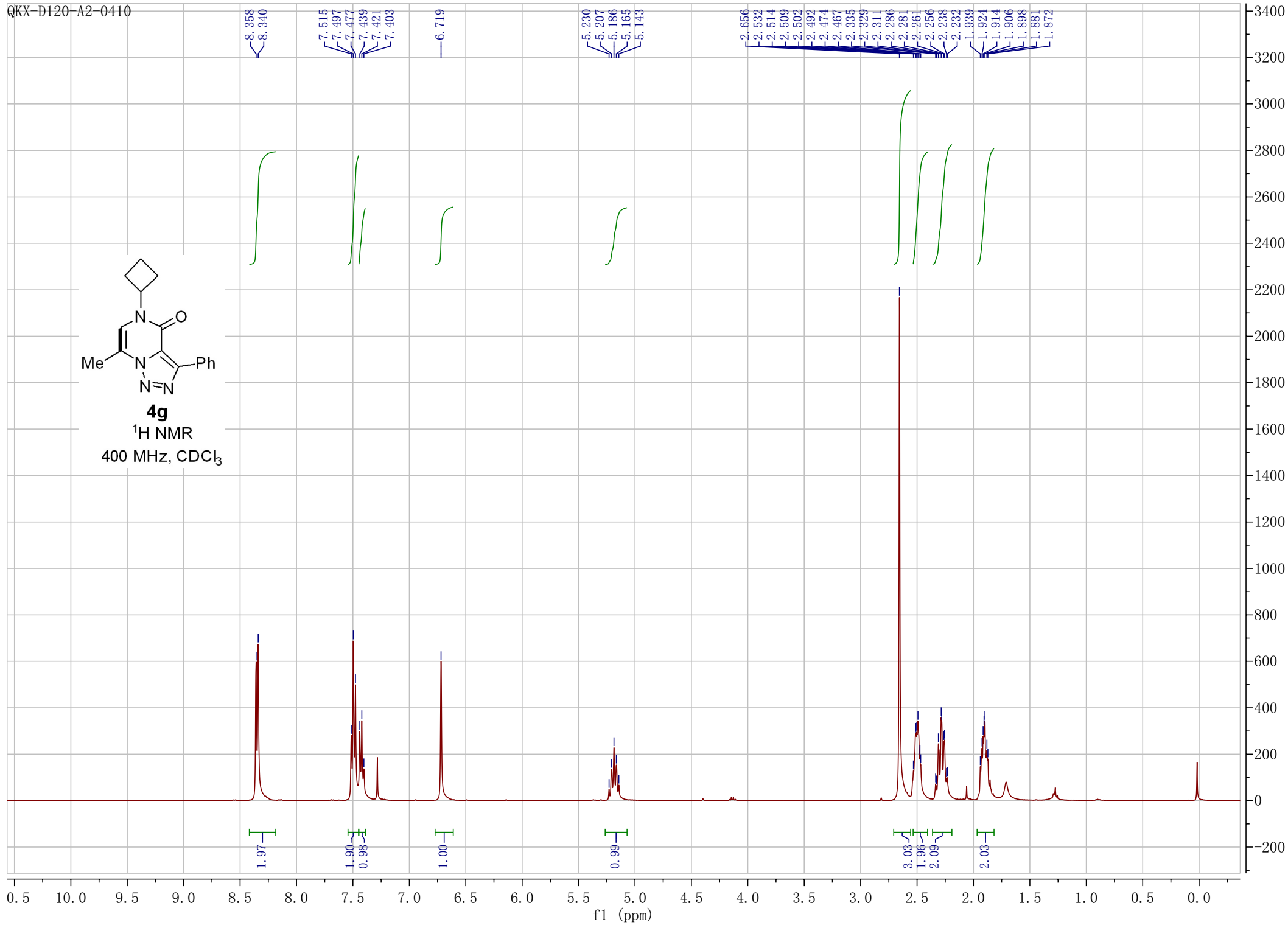
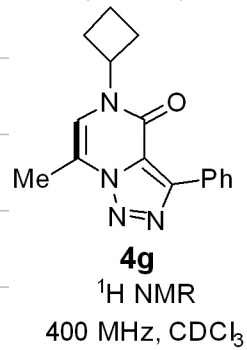


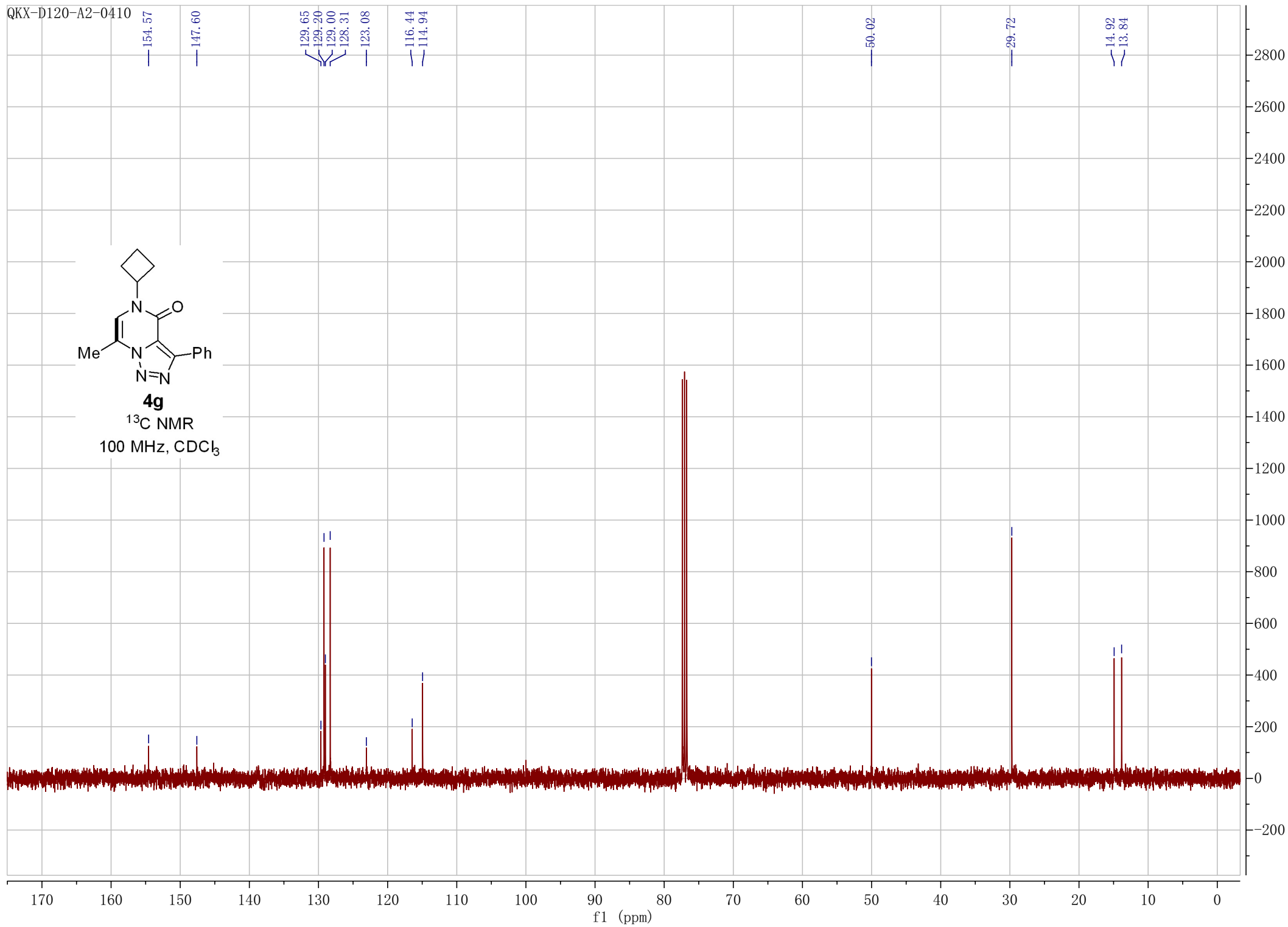
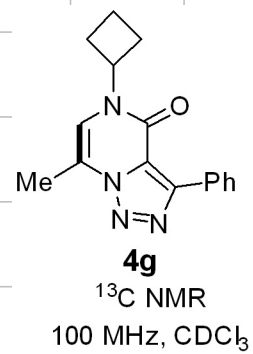
qkx-d120-a1-0409

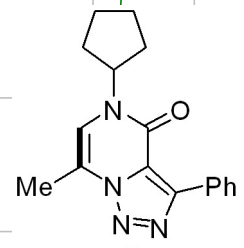


**4f**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

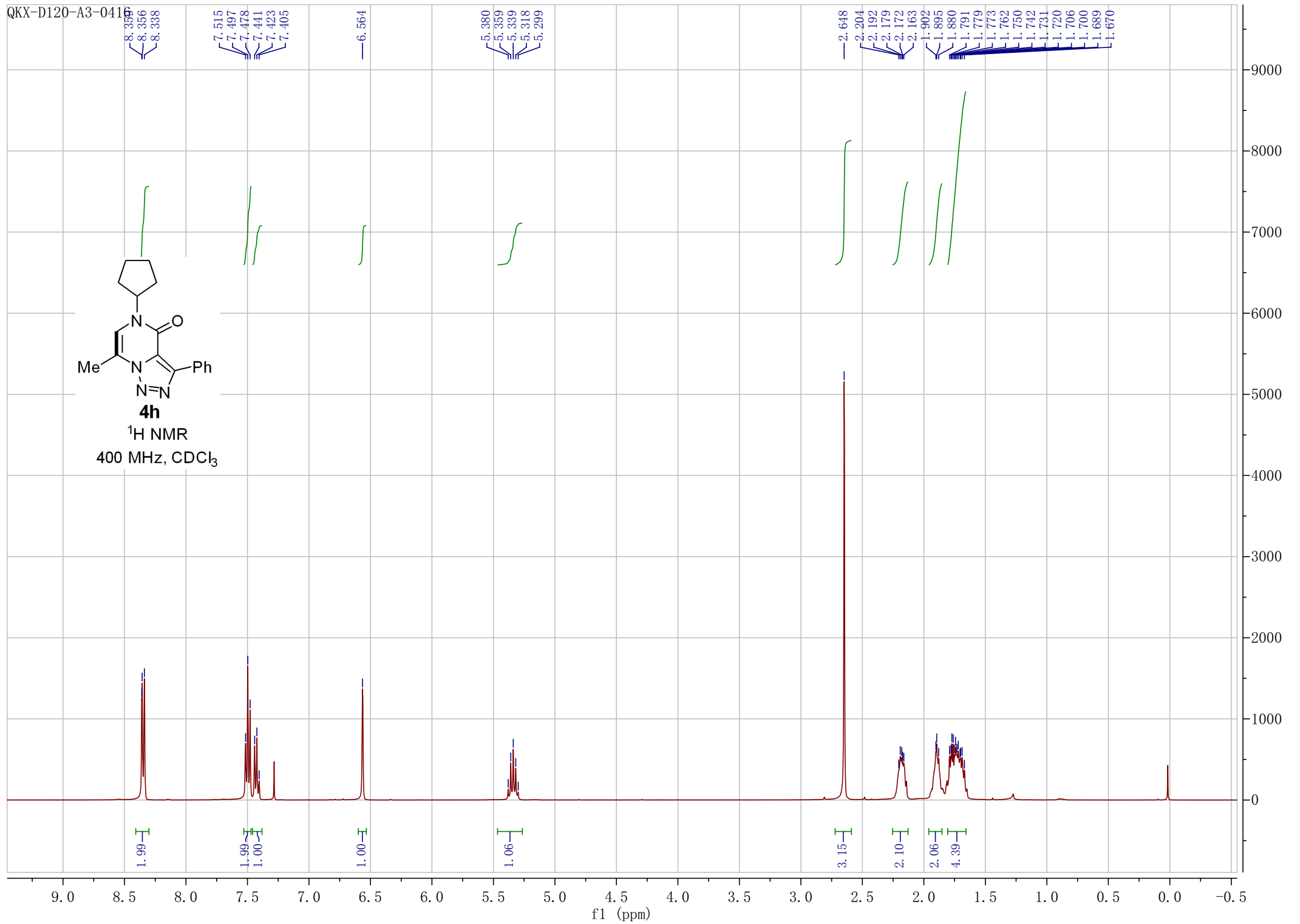




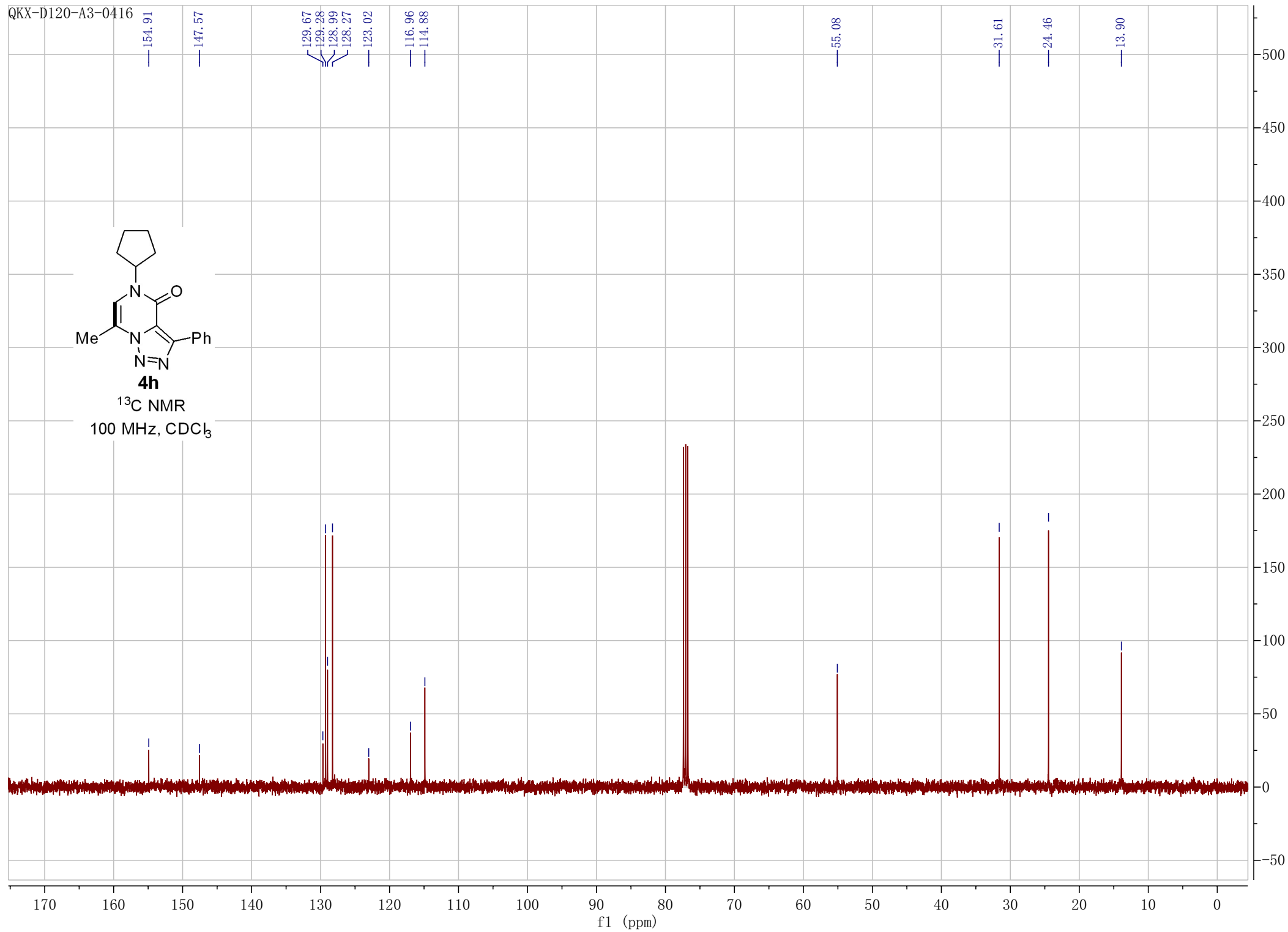
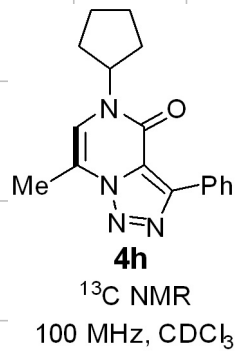


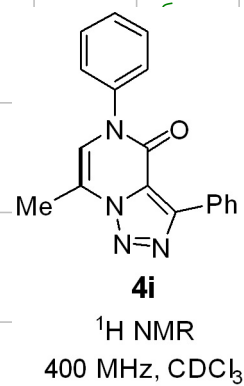


**4h**  
<sup>1</sup>H NMR  
 400 MHz, CDCl<sub>3</sub>

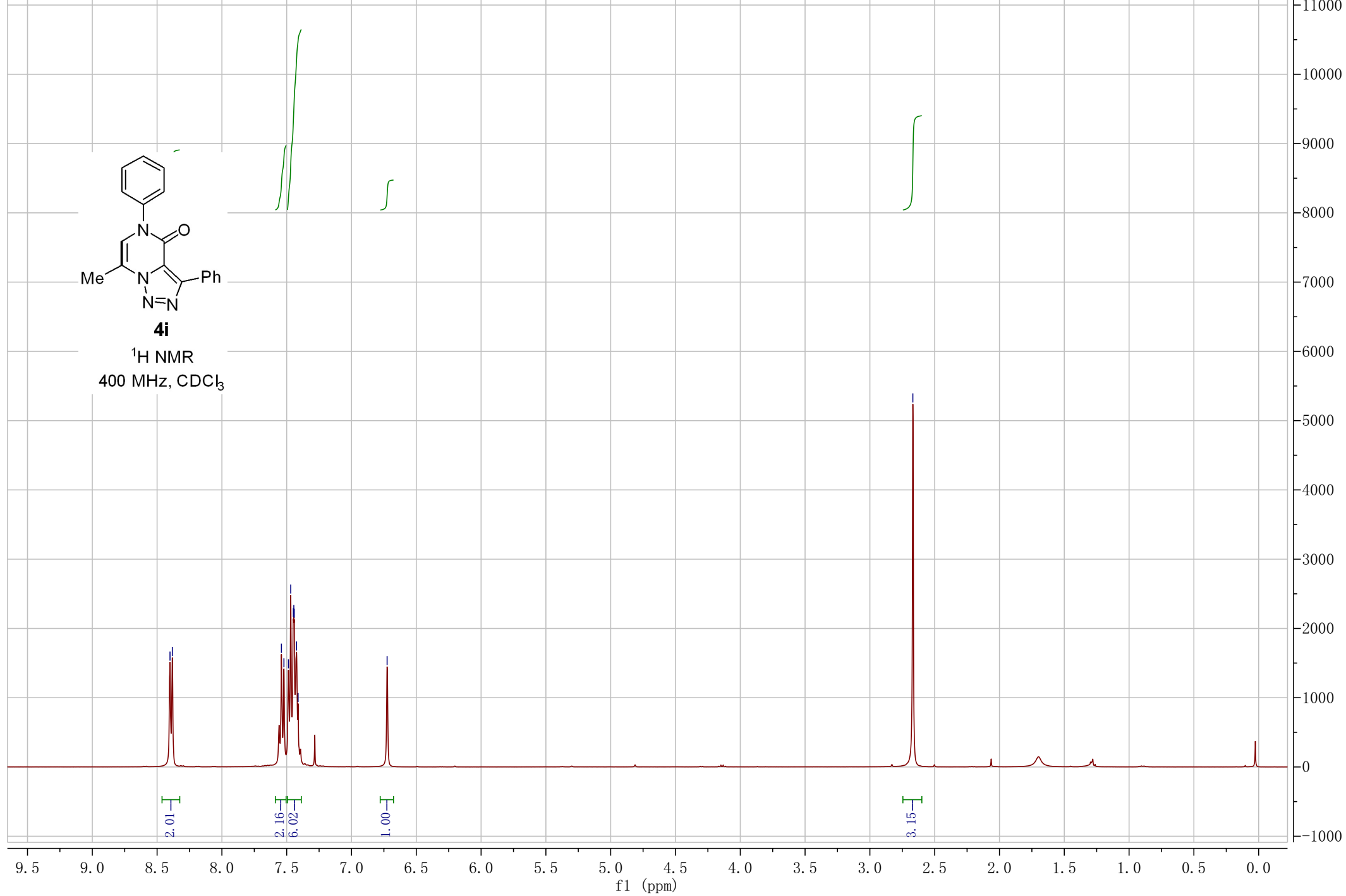




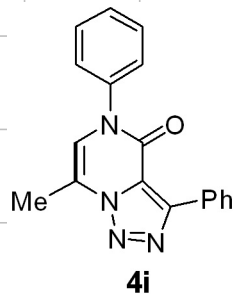




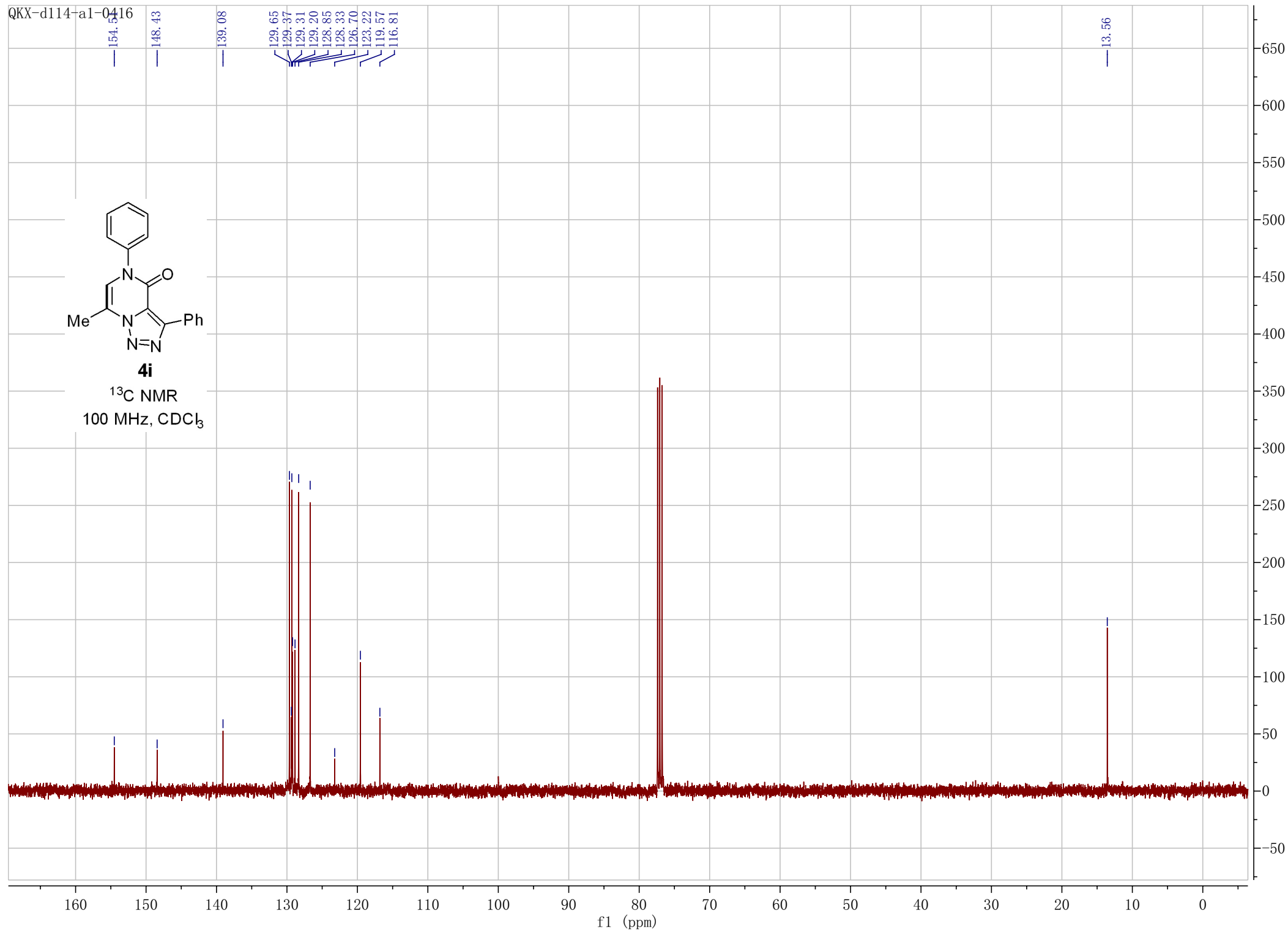
8.400  
8.382  
7.541  
7.521  
7.486  
7.469  
7.449  
7.445  
7.442  
7.424  
7.412  
6.725  
2.668



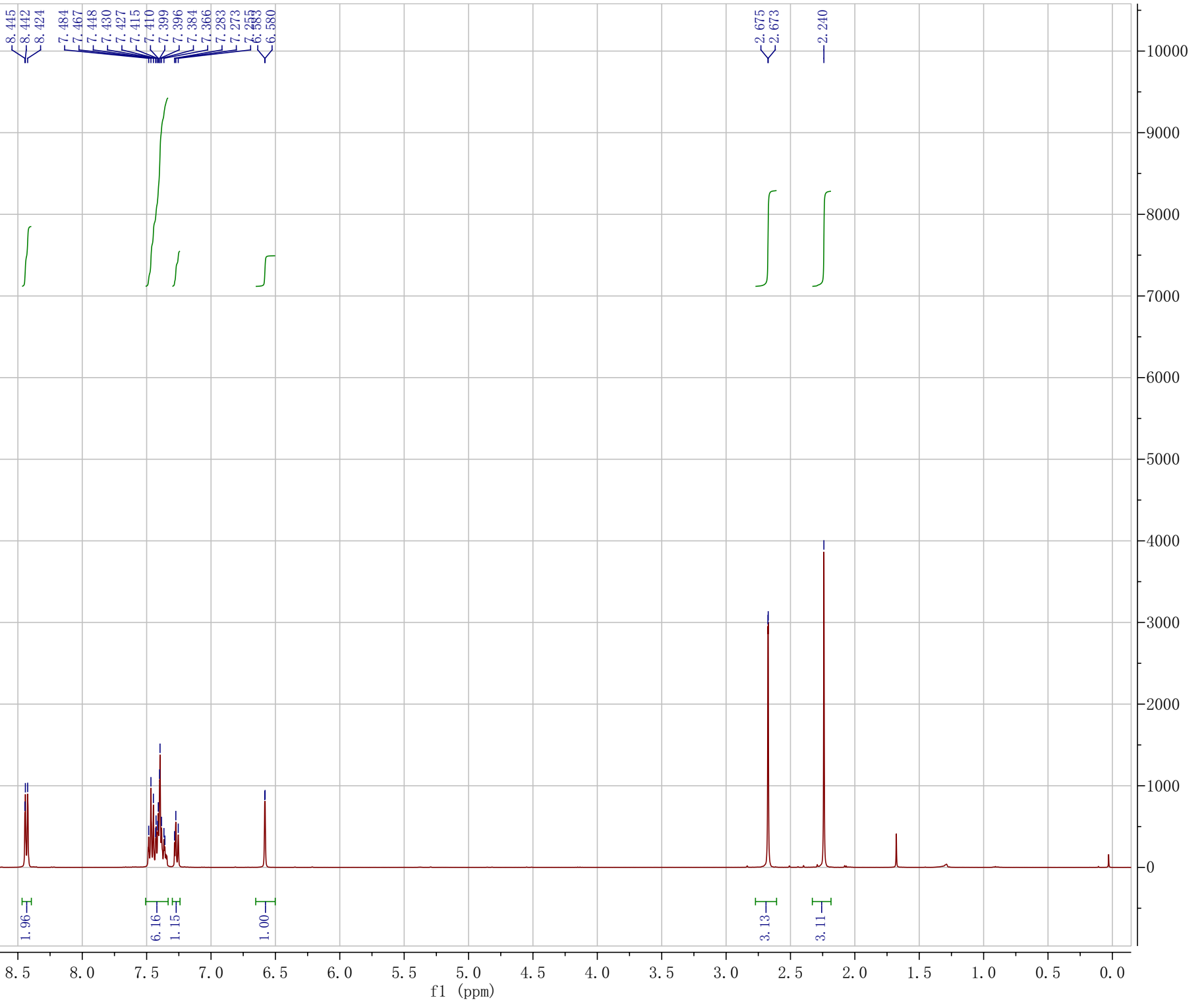
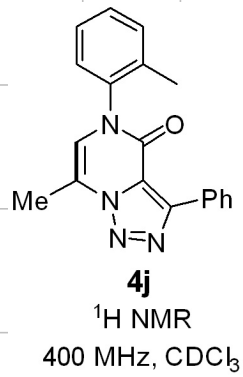
QKX-d114-a1-0416



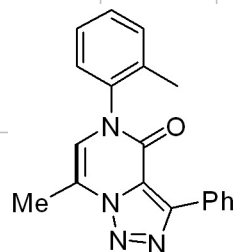
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



qkx-d50-a2

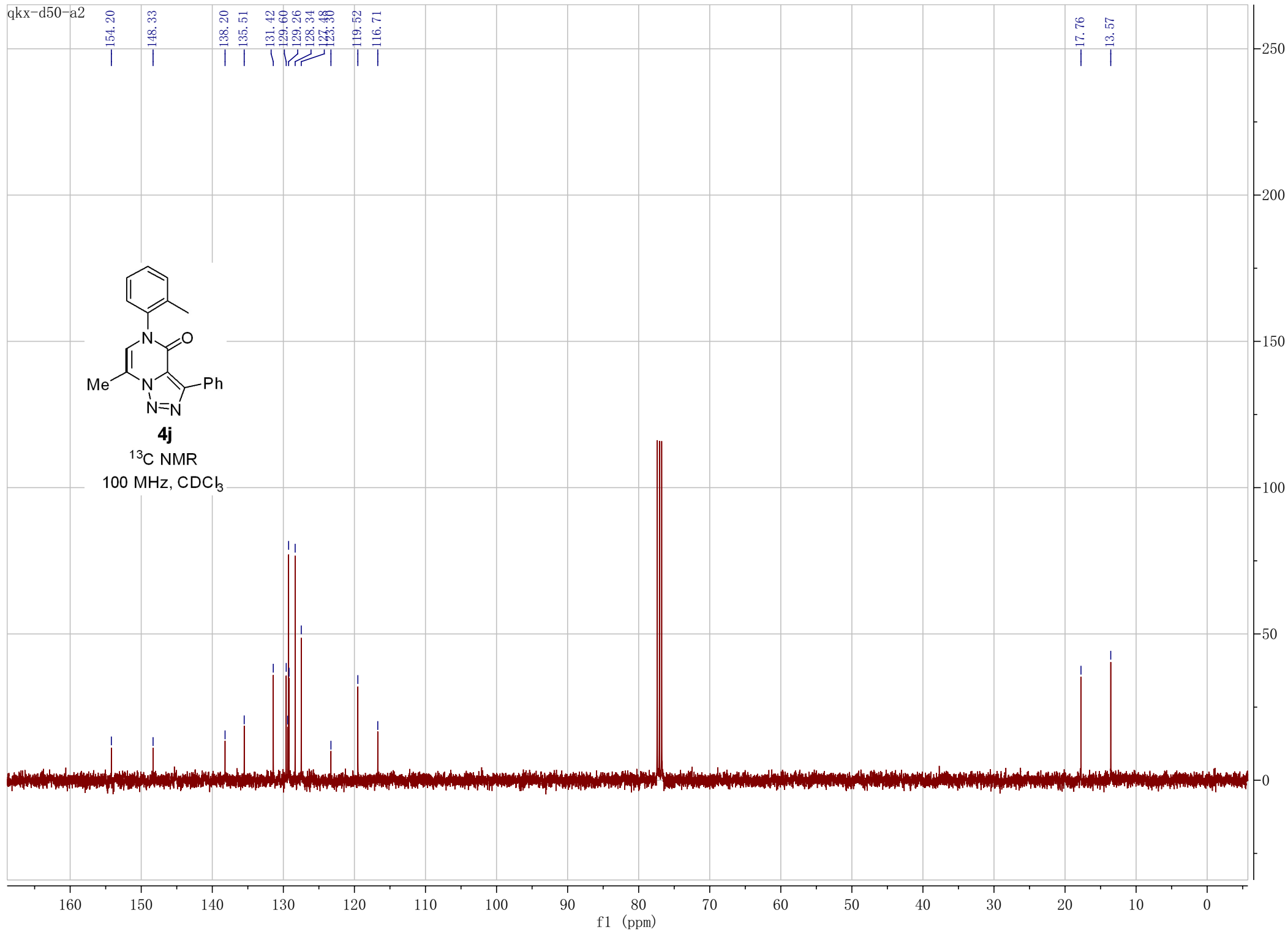


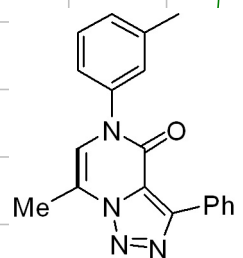
qkx-d50-a2



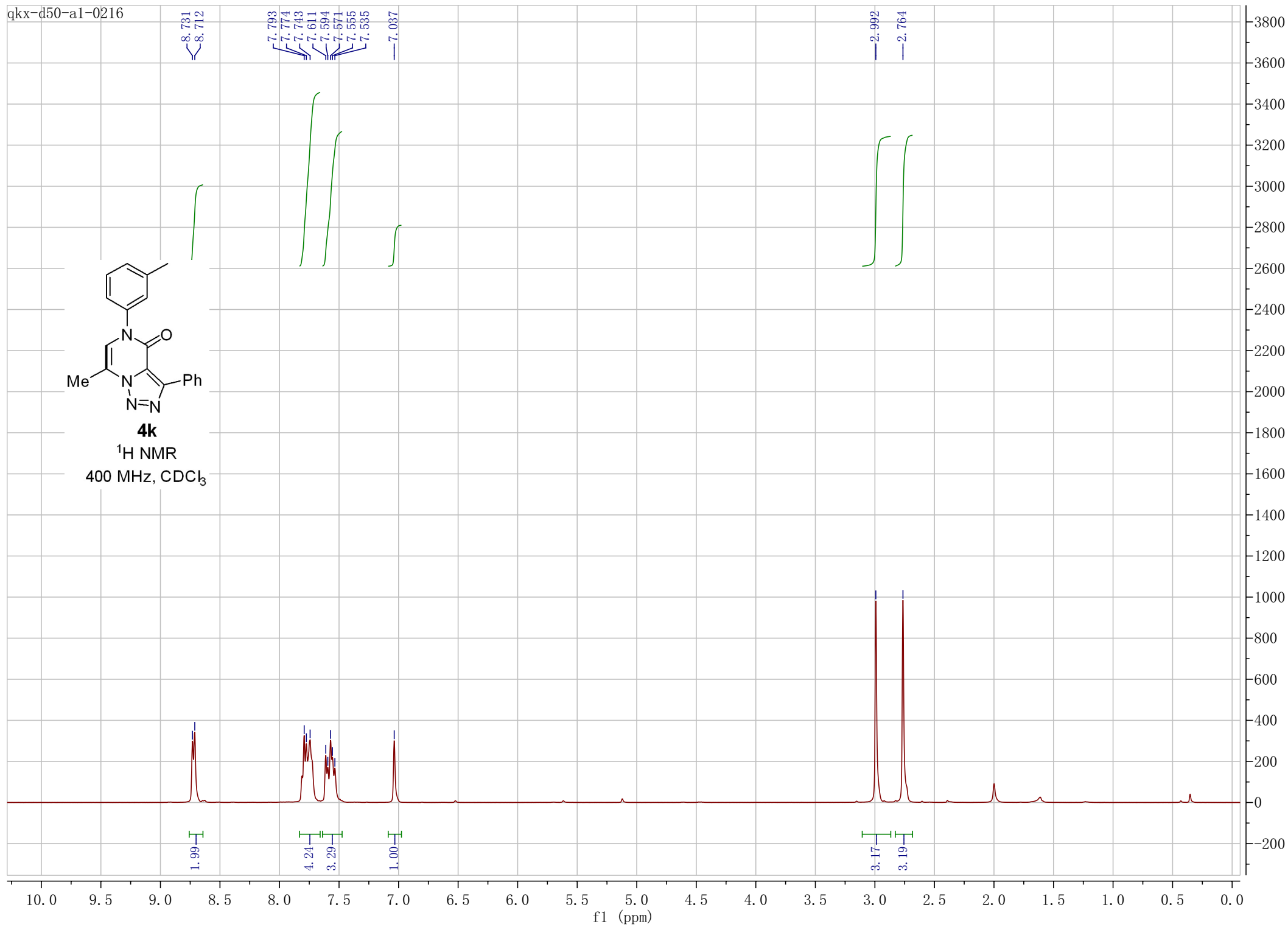
**4j**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

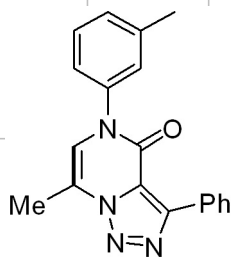


**4k**

$^1\text{H}$  NMR  
400 MHz,  $\text{CDCl}_3$

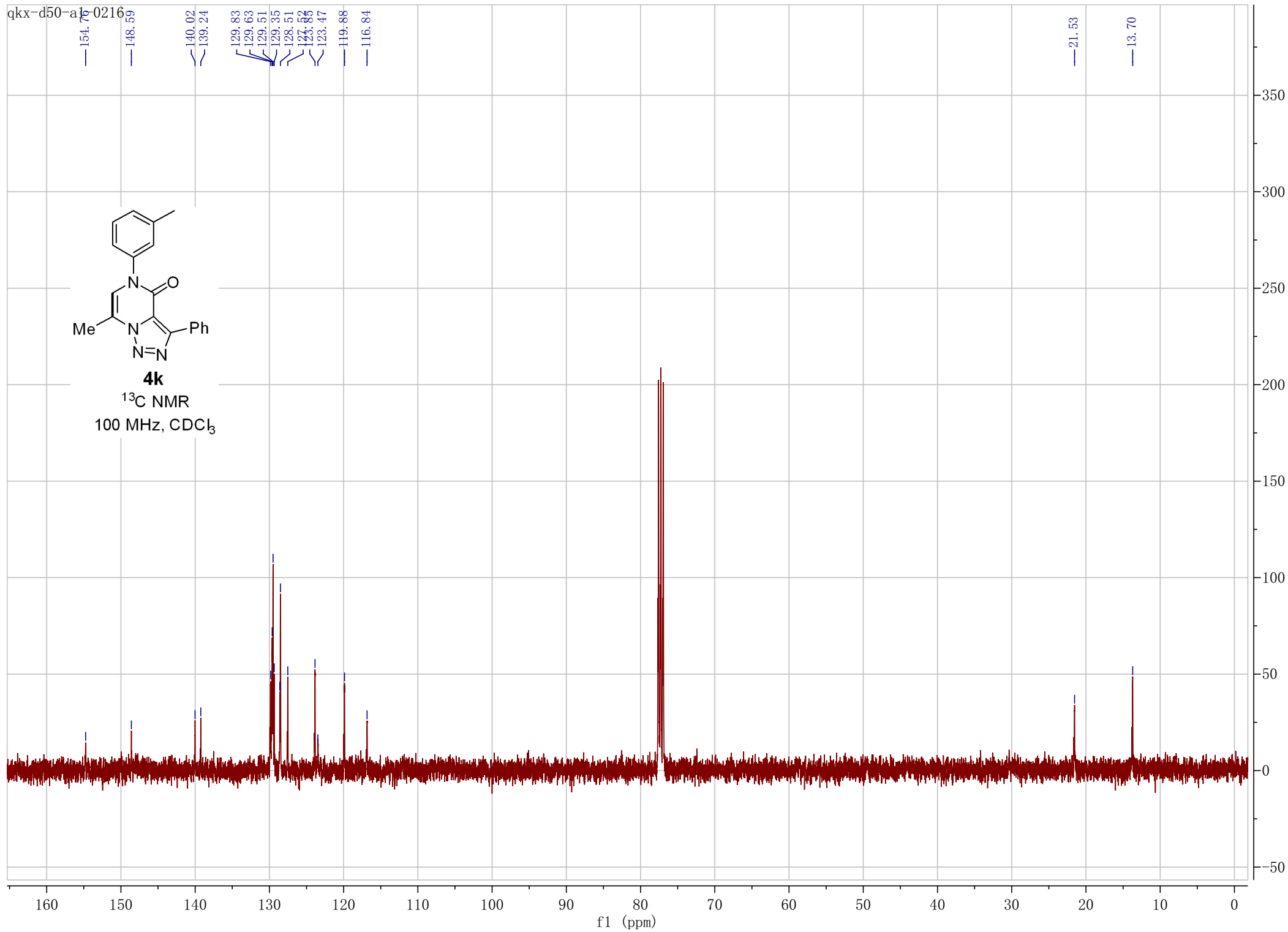


qkx-d50-a1-0216

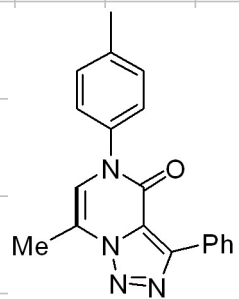


**4k**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

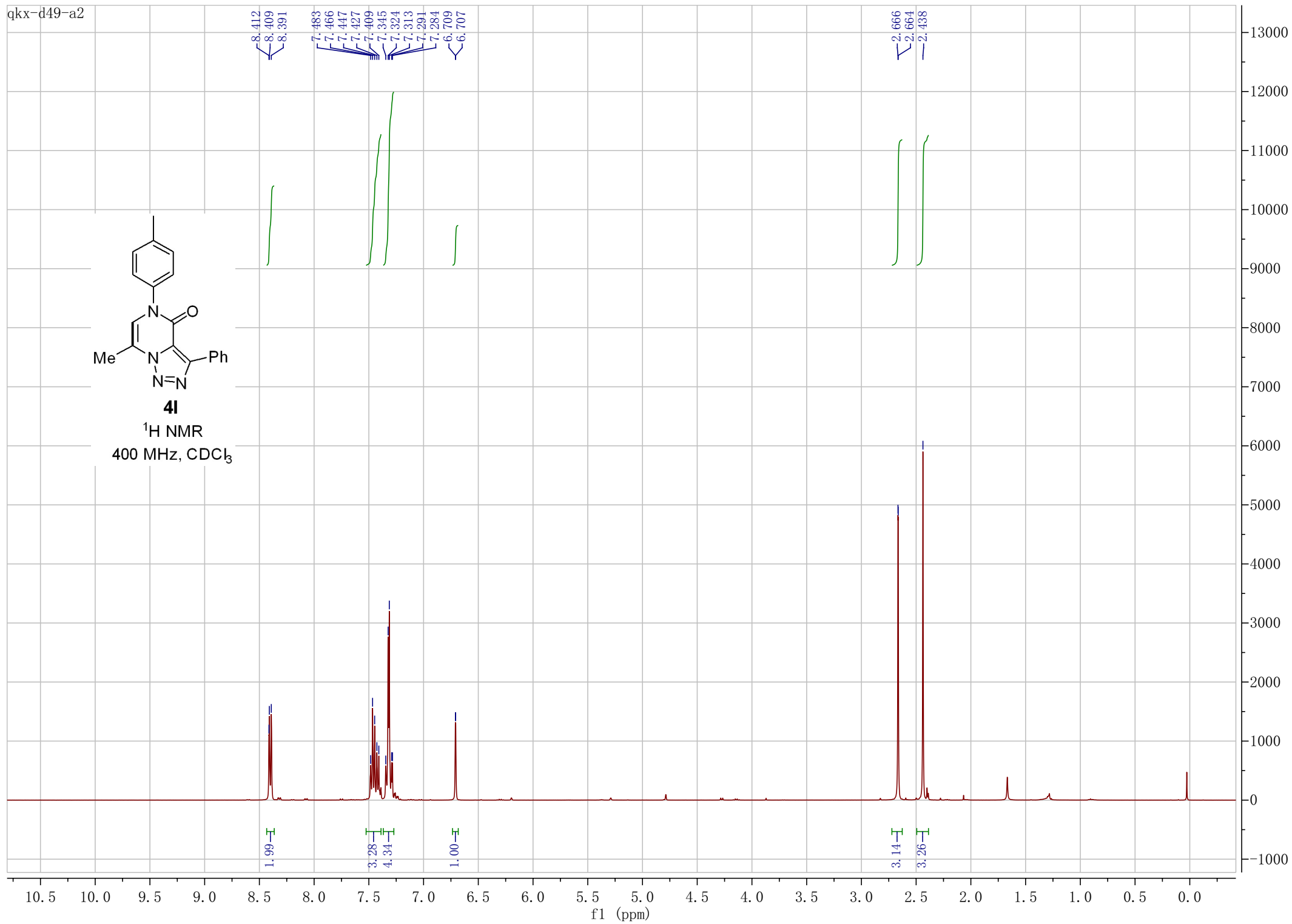


qkx-d49-a2



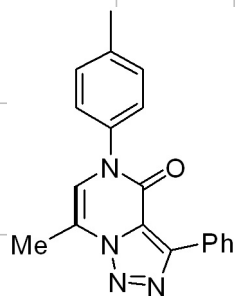
**4I**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



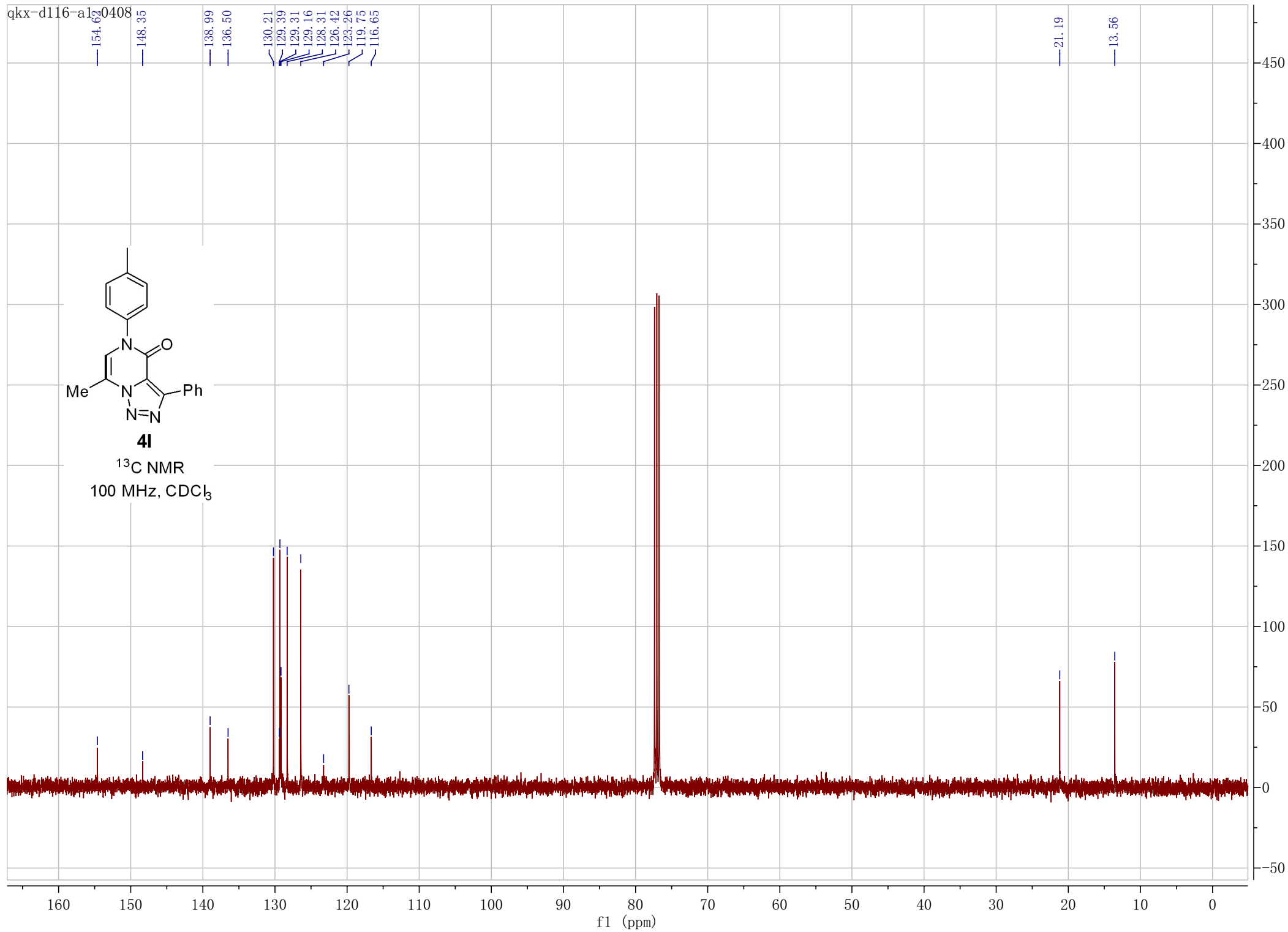


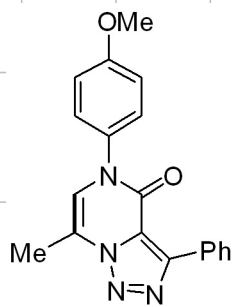
qkx-d116-a10408



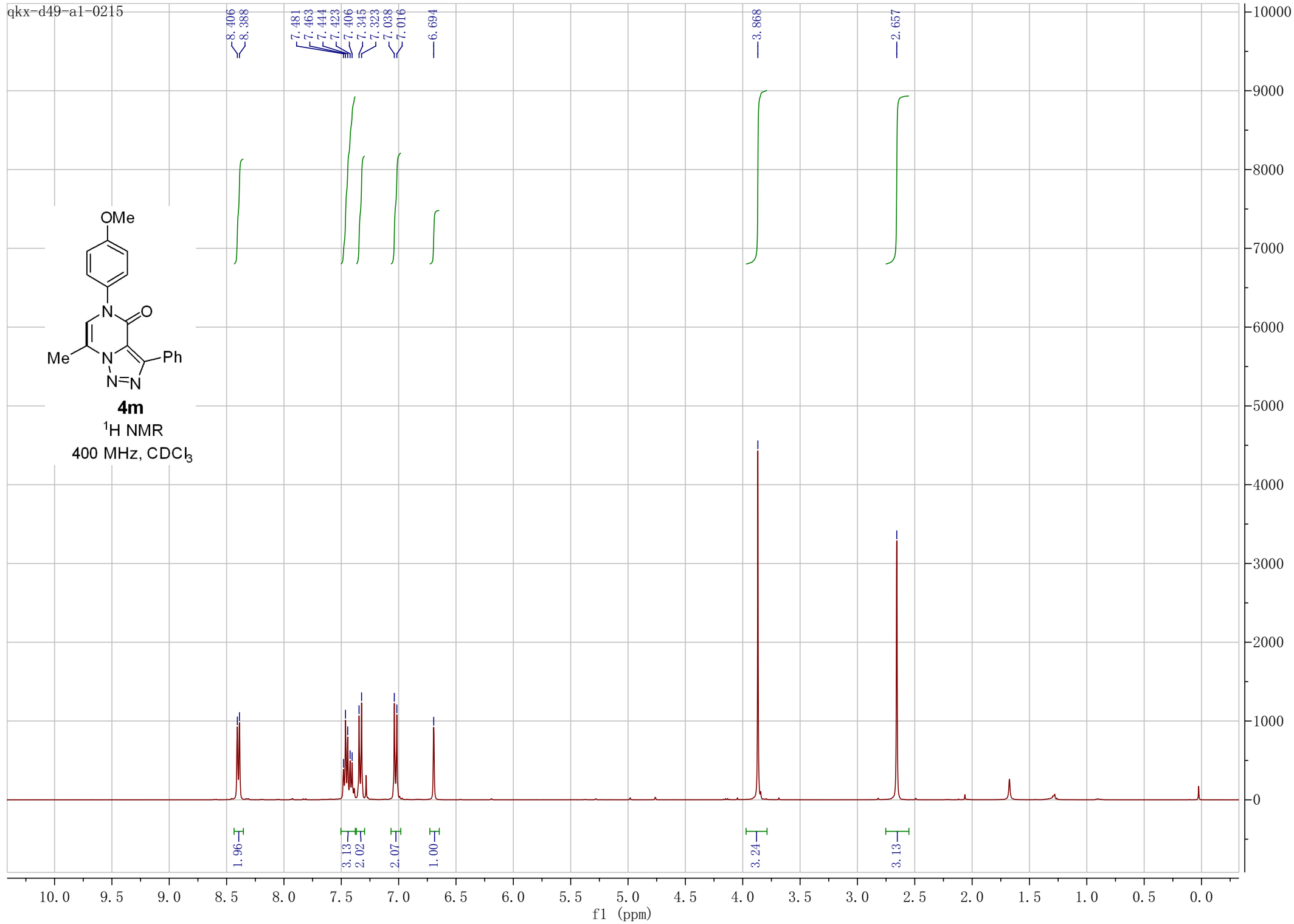
**4I**

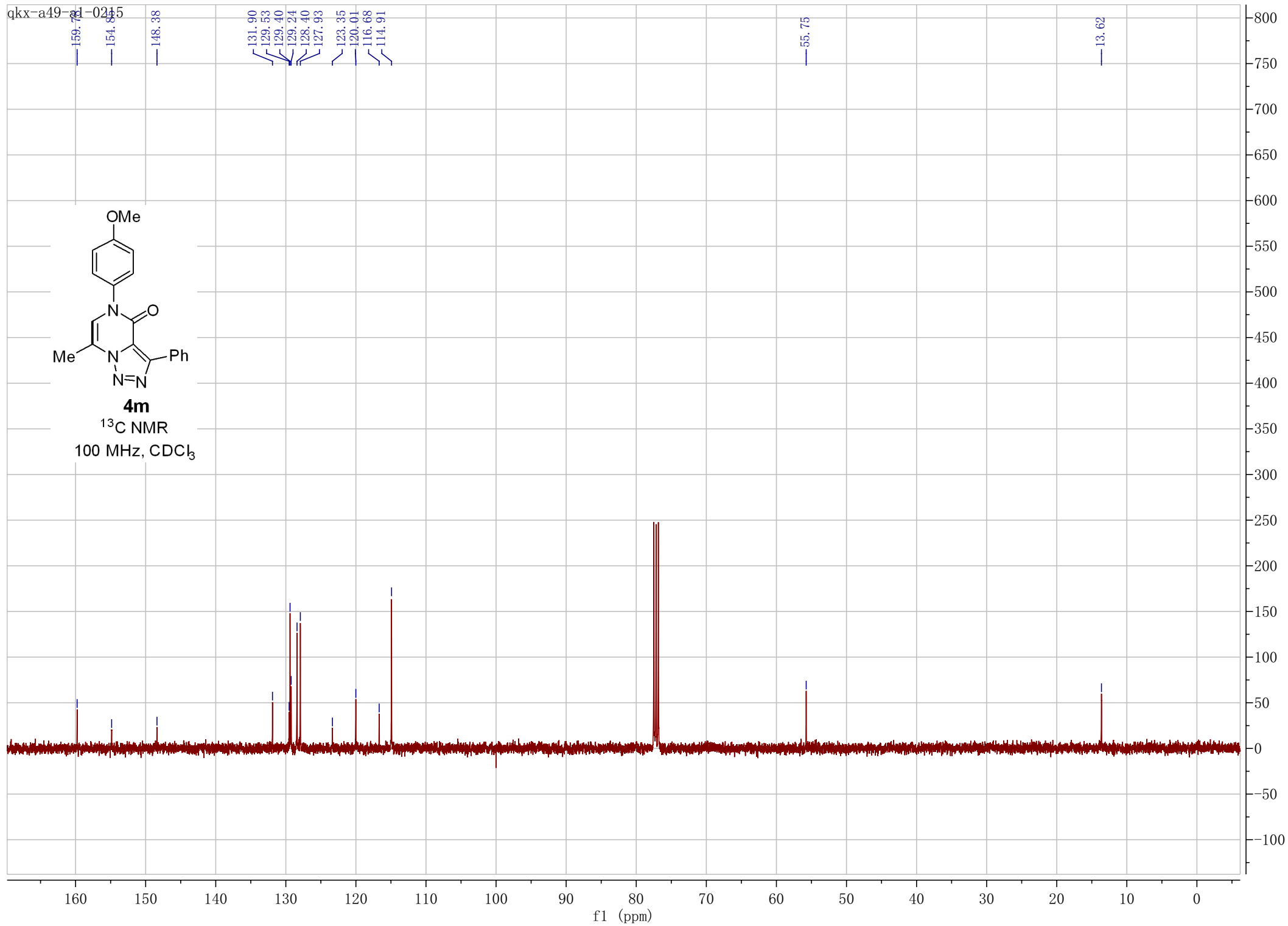
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



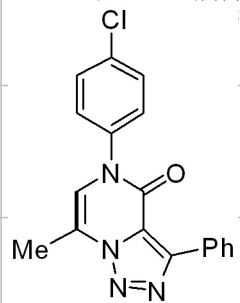


**4m**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>





qkx-d49-a30-0215



**4n**

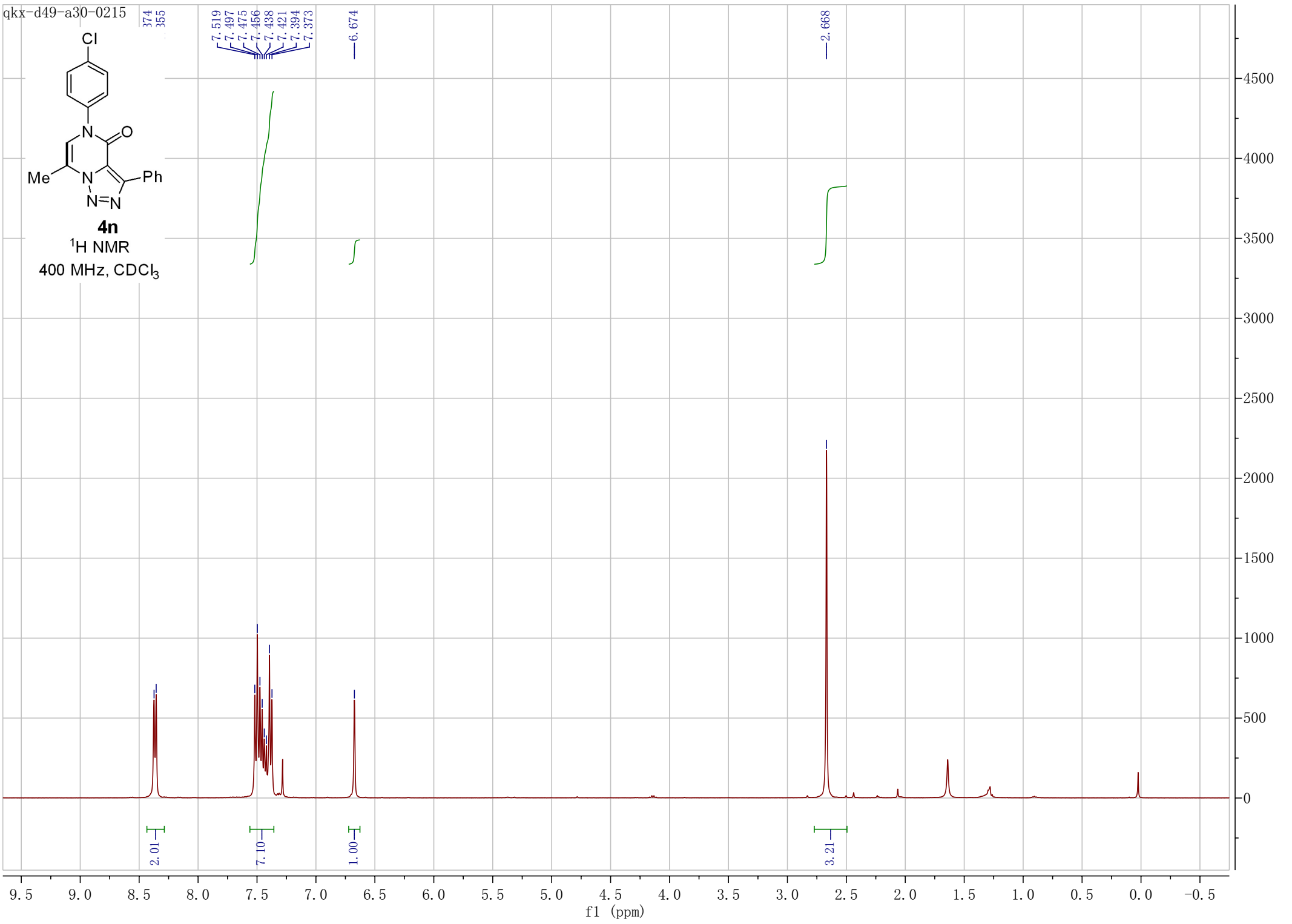
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

374  
355

7.519  
7.497  
7.475  
7.456  
7.438  
7.421  
7.394  
7.373

6.674

2.668



2.01

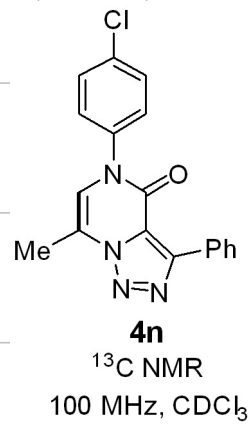
7.10

1.00

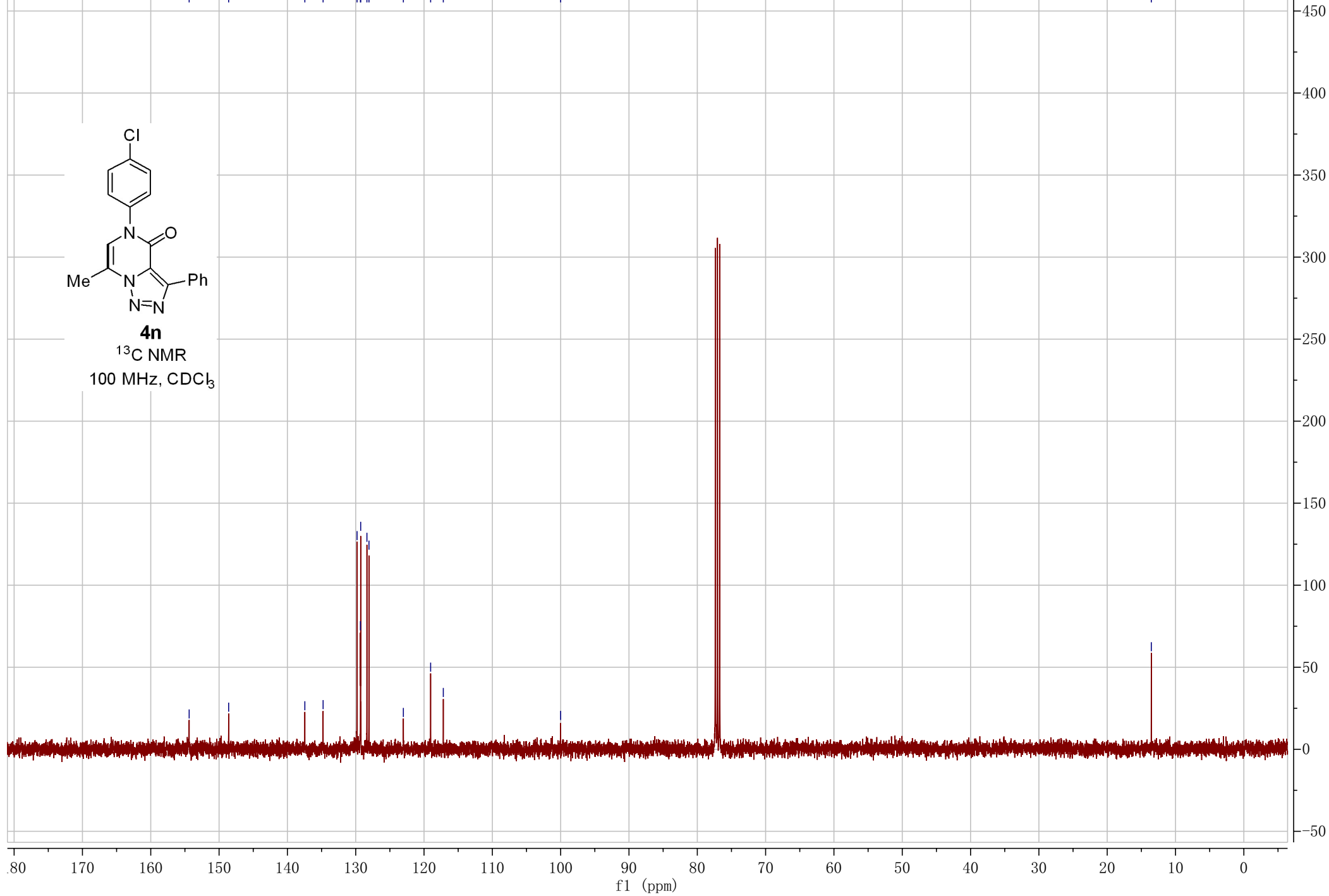
3.21

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5  
f1 (ppm)

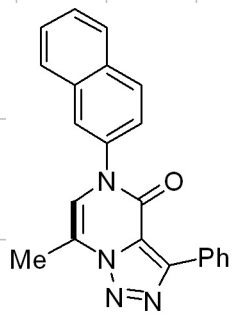
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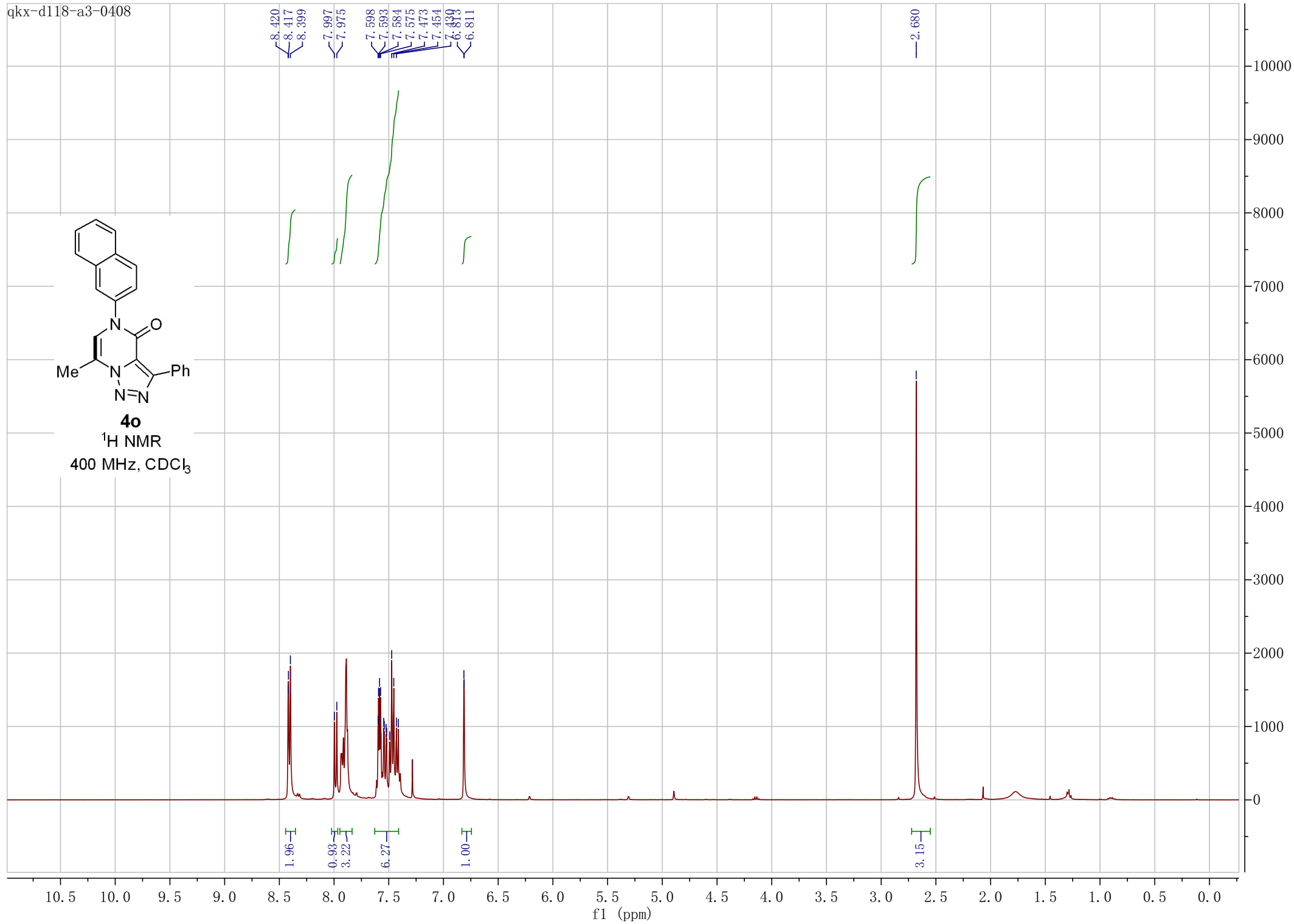
154.38  
148.60  
137.45  
134.77  
129.80  
129.31  
129.27  
128.36  
128.06  
123.03  
119.03  
117.18  
100.00  
13.54



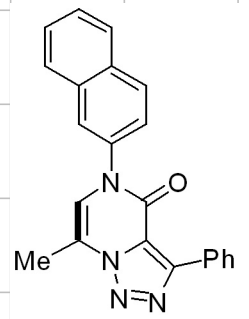
qkx-d118-a3-0408



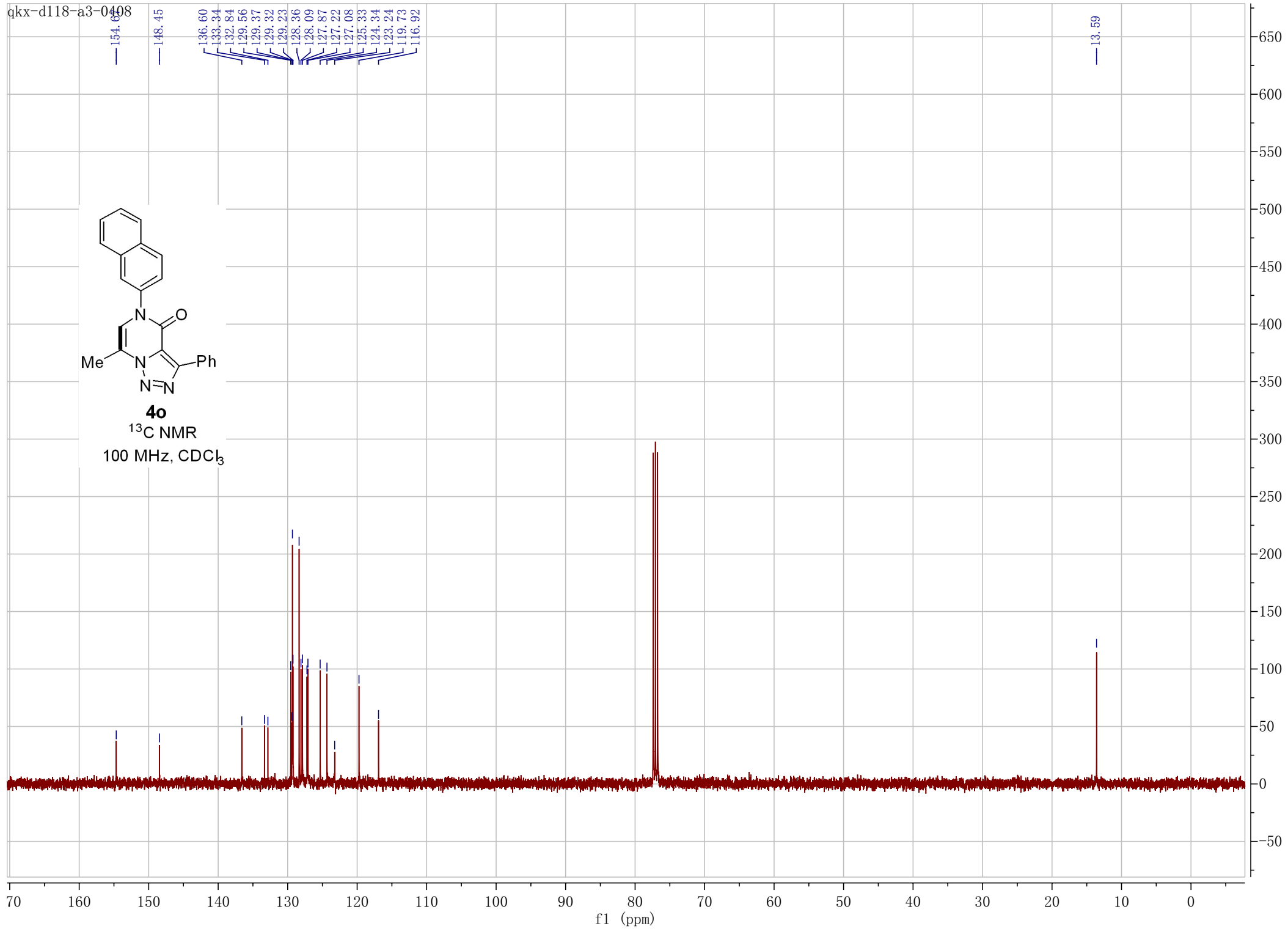
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



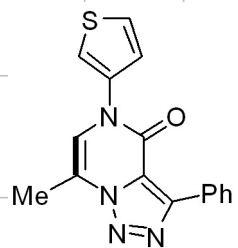
qkx-d118-a3-0408



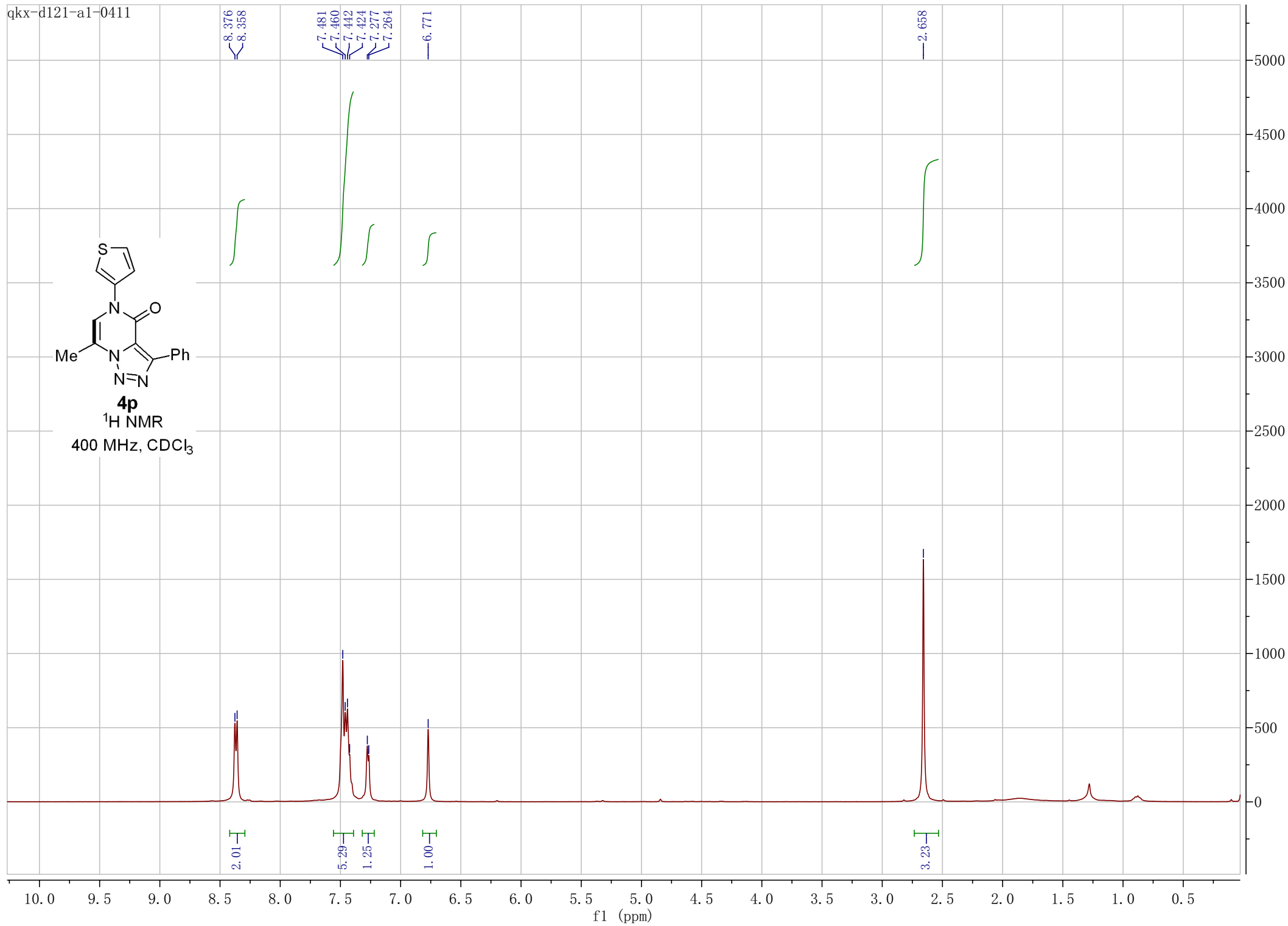
**4o**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



qkx-d121-a1-0411

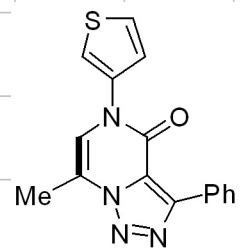


<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



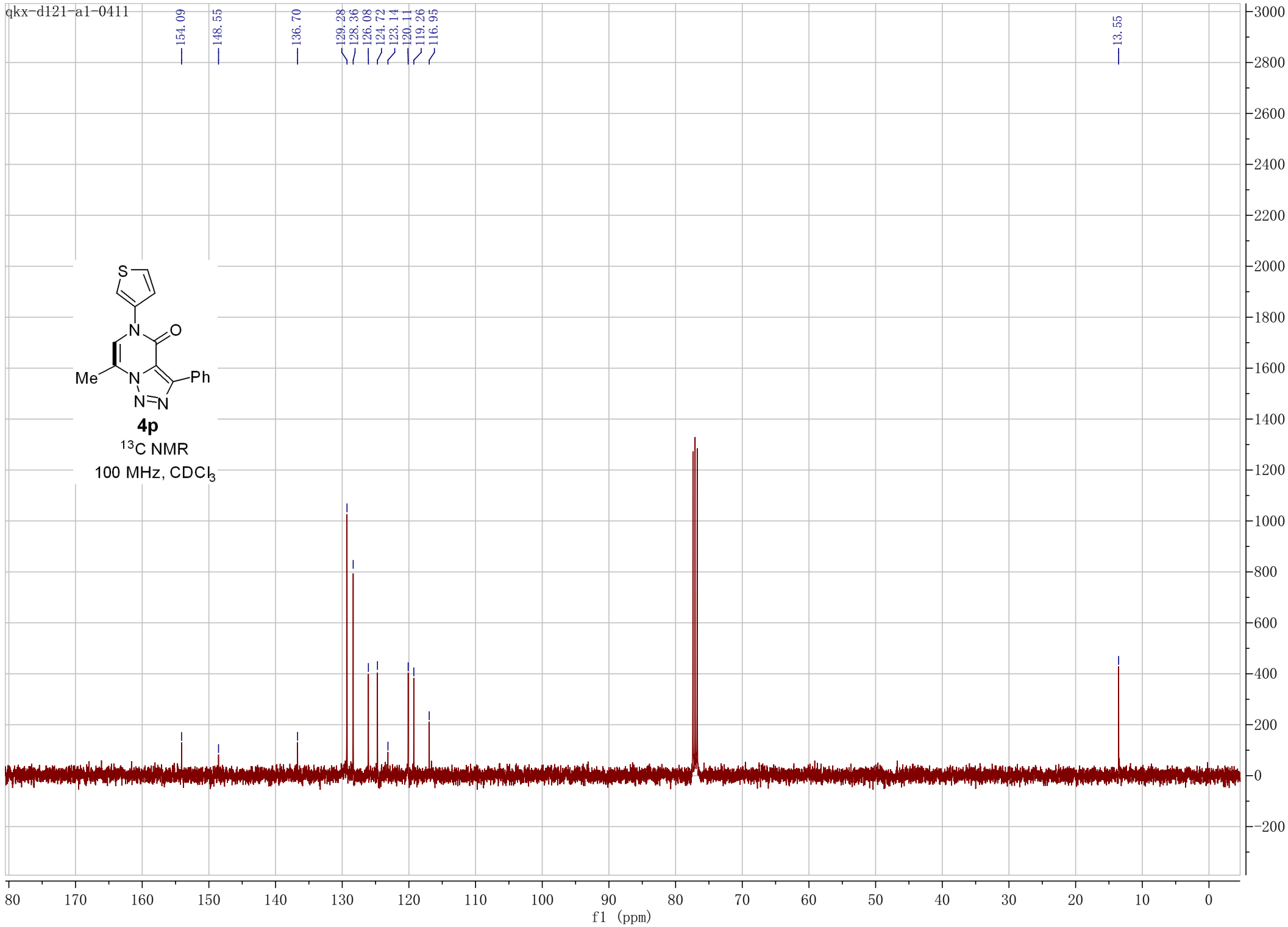


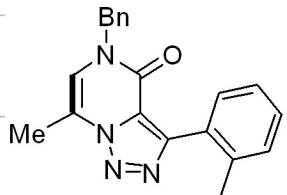
qkx-d121-a1-0411



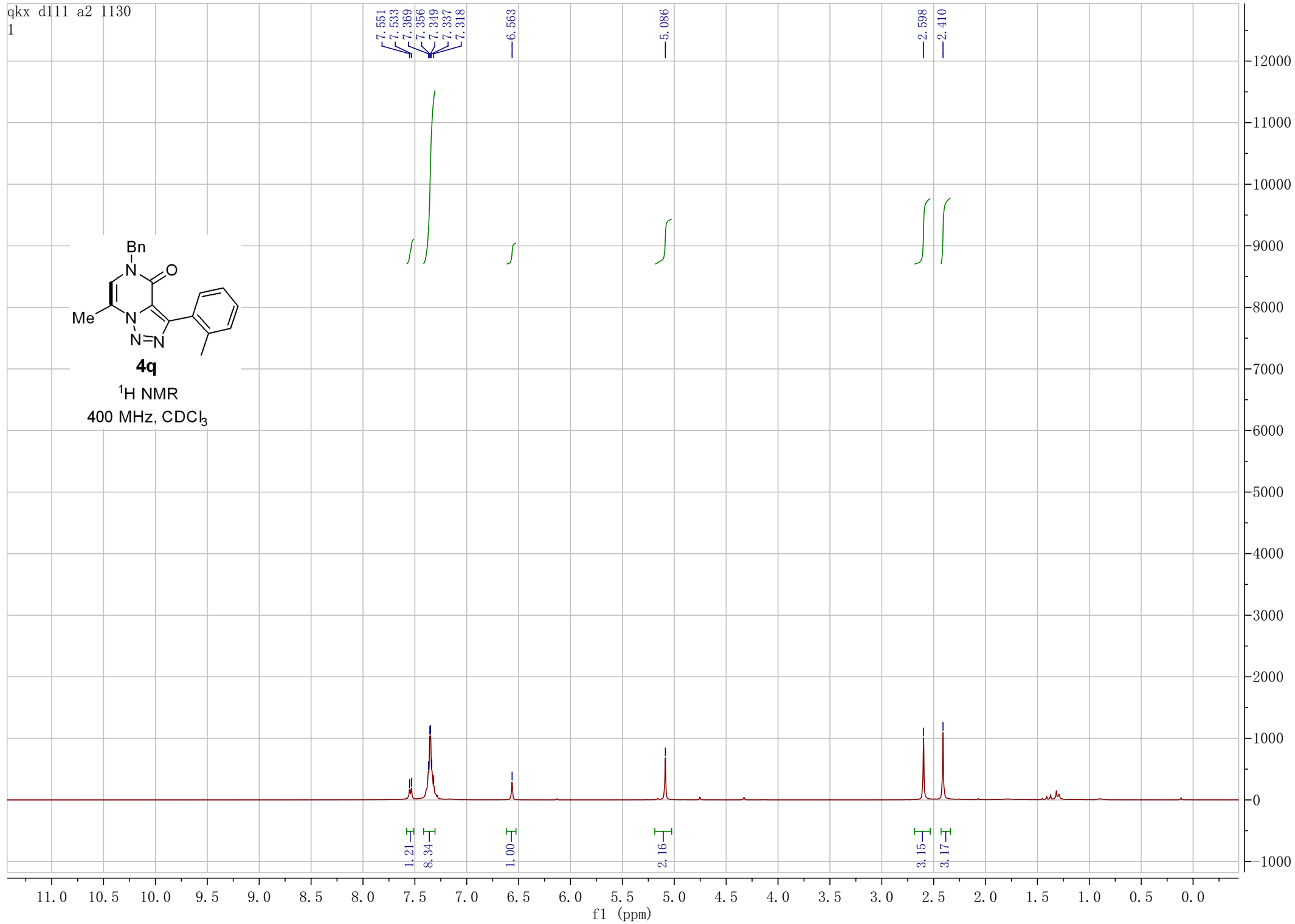
**4p**

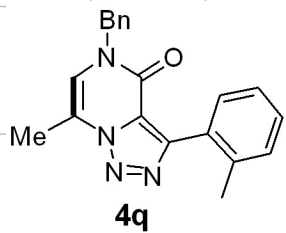
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



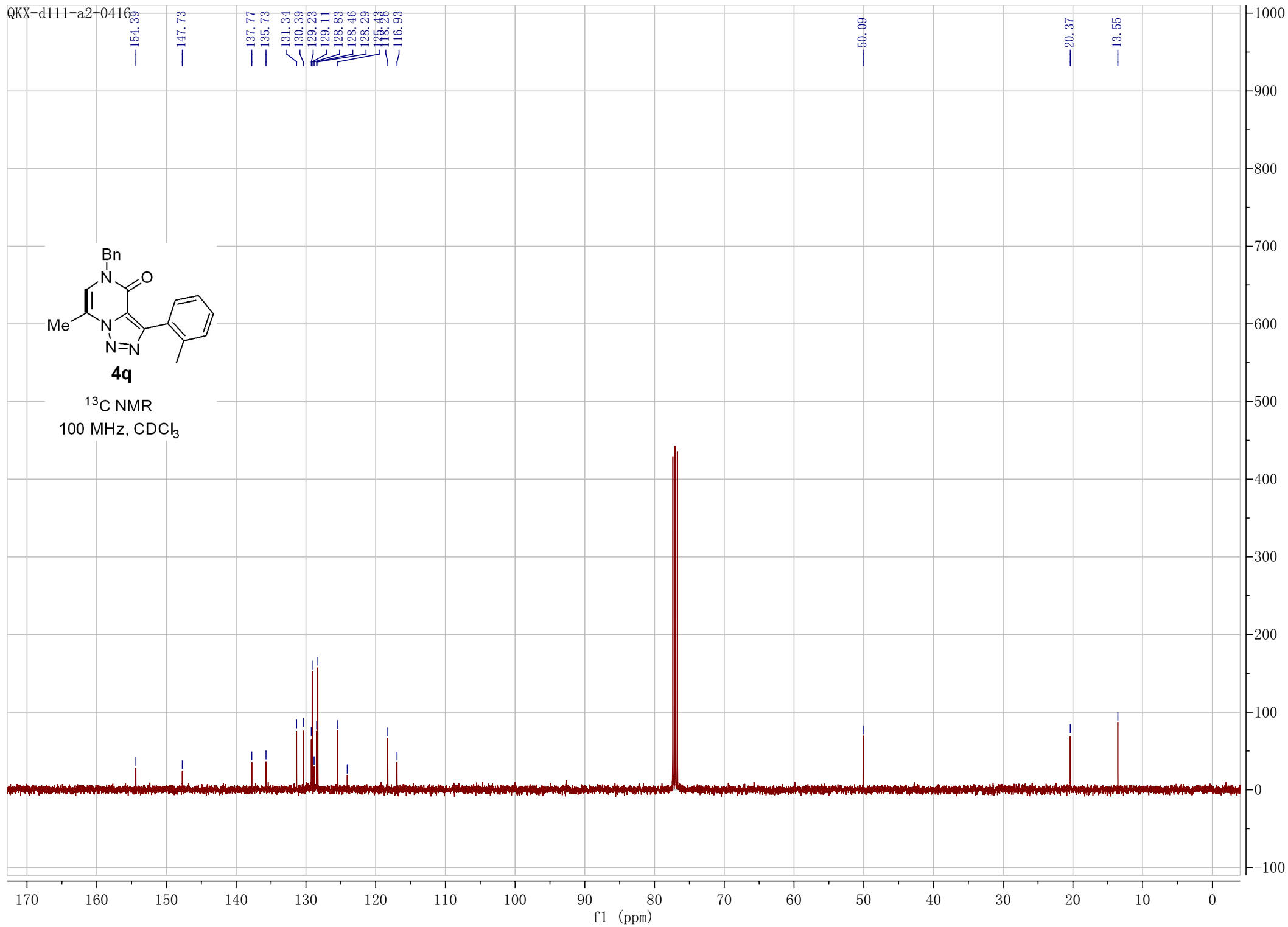


<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

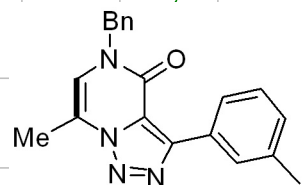




$^{13}\text{C}$  NMR  
100 MHz,  $\text{CDCl}_3$

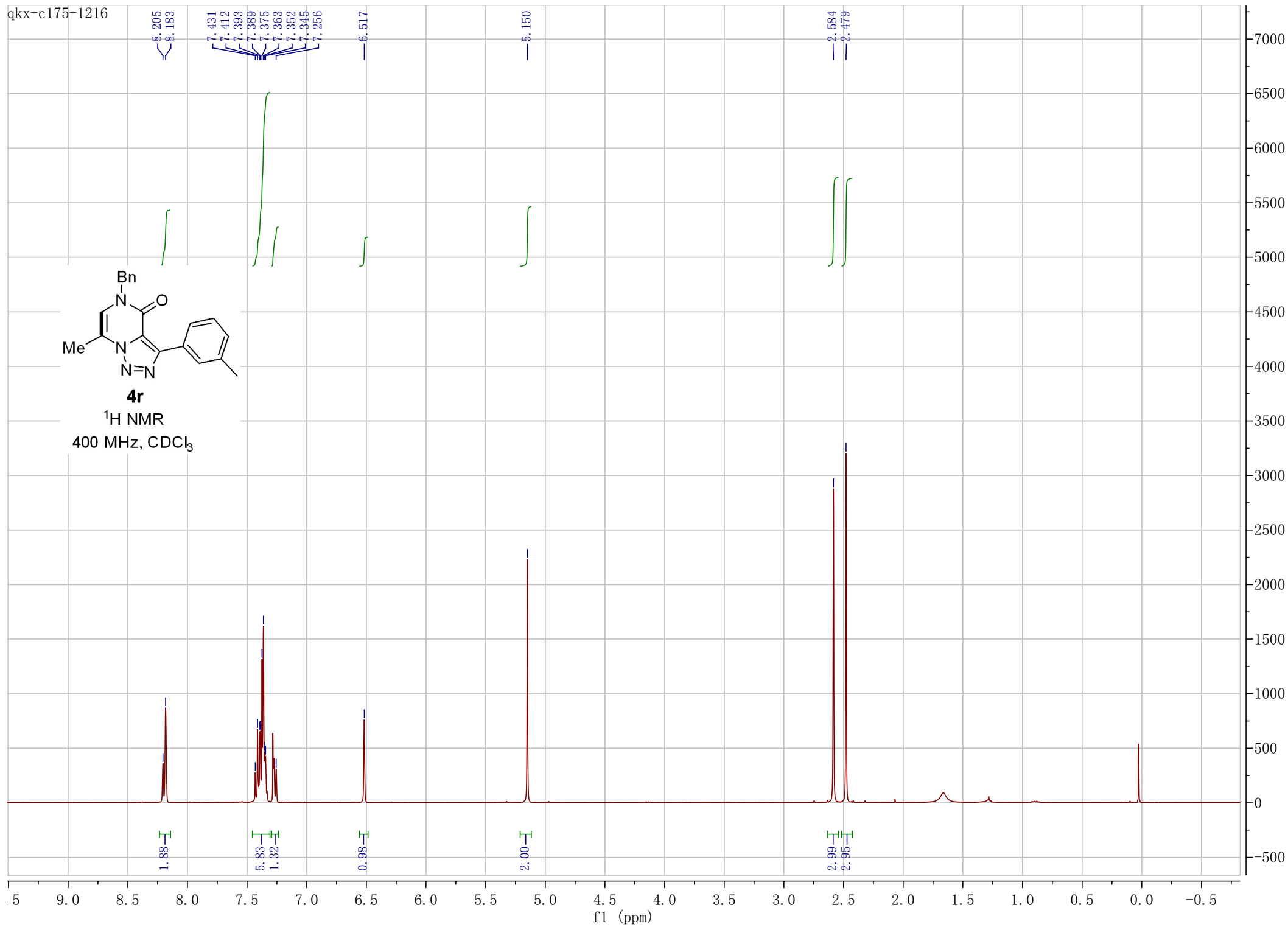


qkx-c175-1216

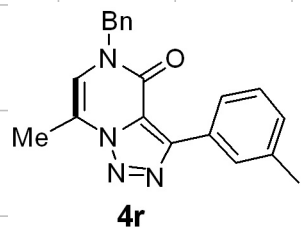


**4r**

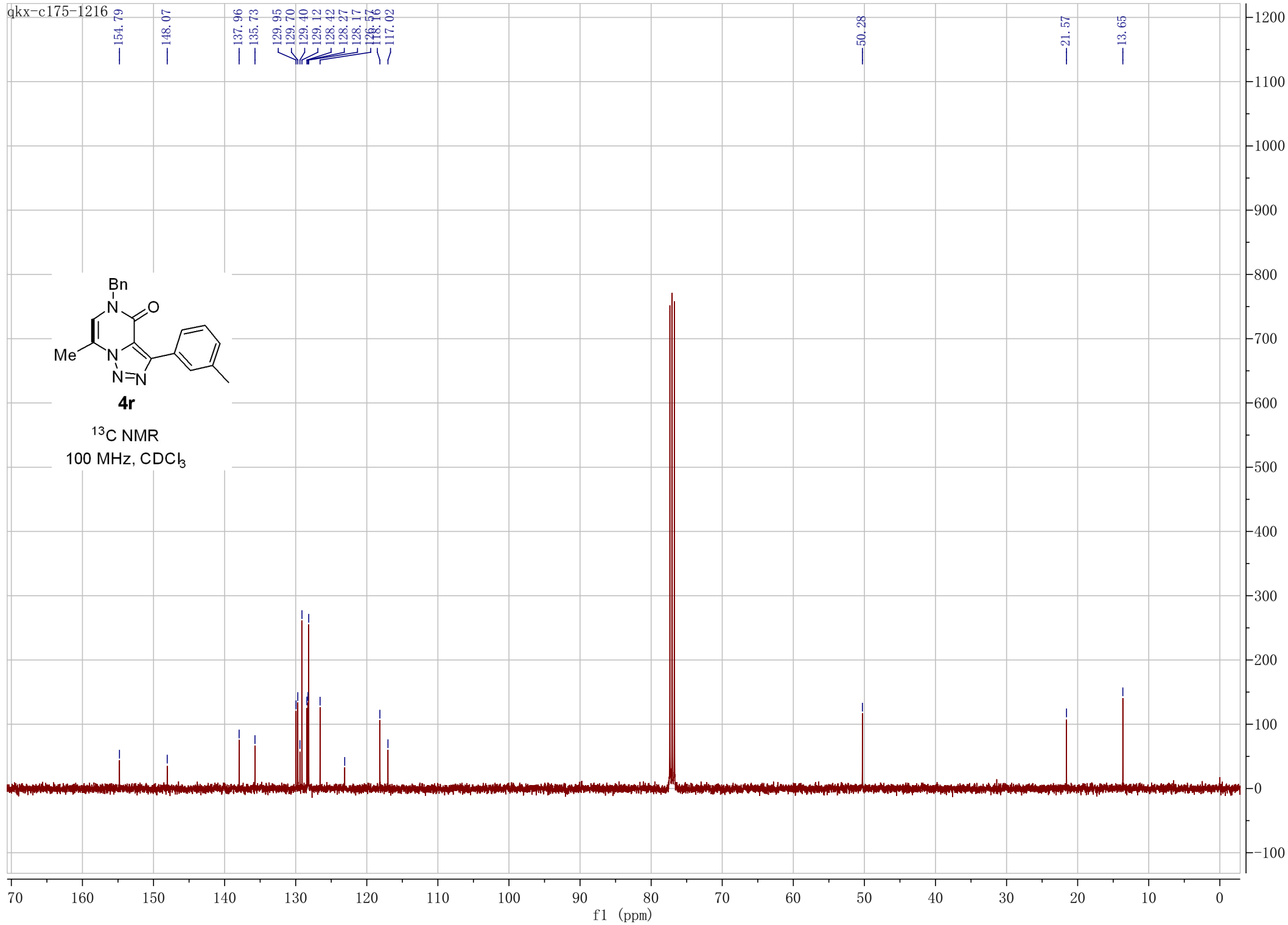
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



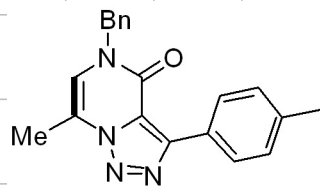
qkx-c175-1216



<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

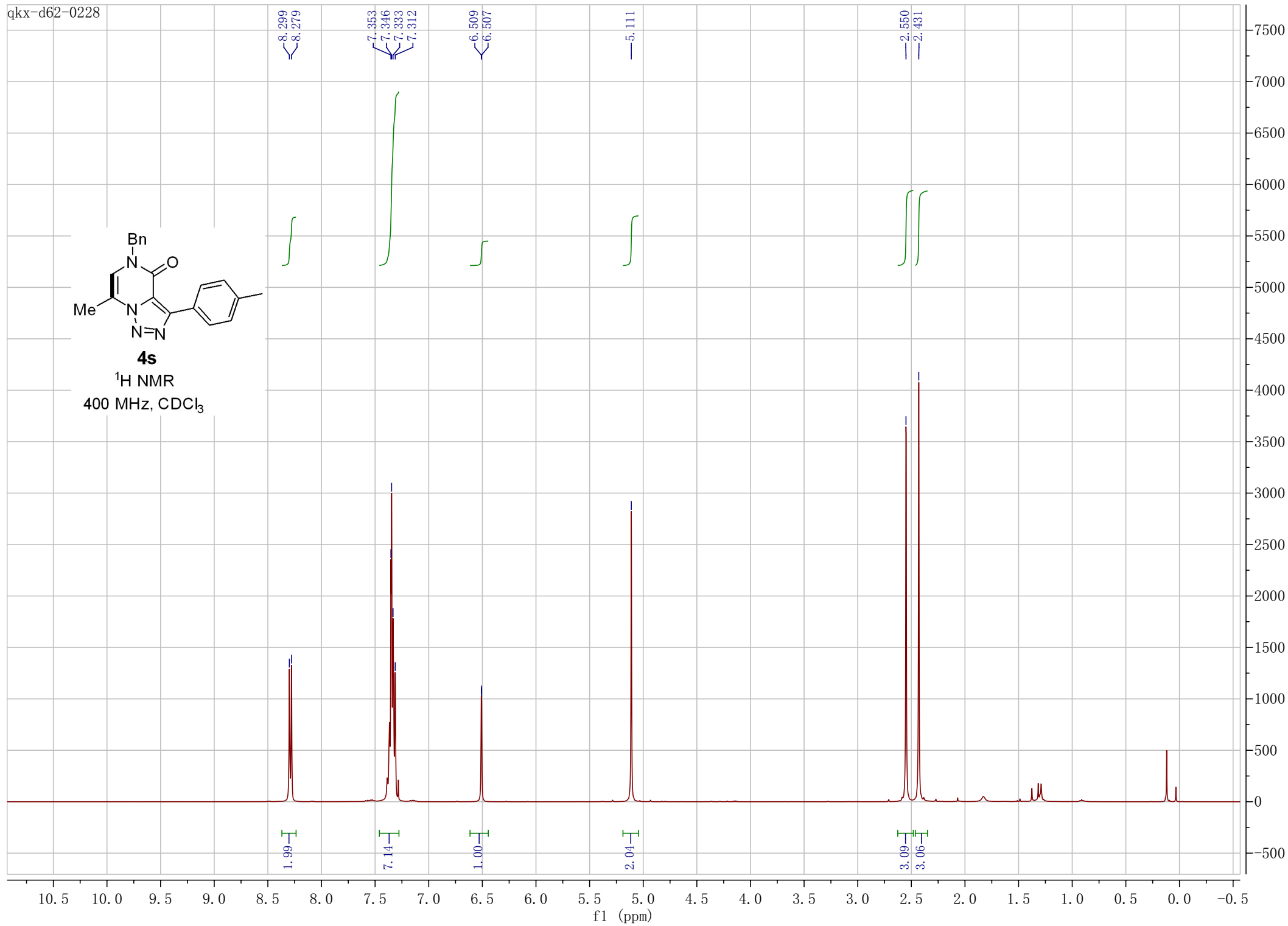


qkx-d62-0228

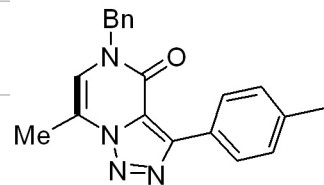


**4s**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

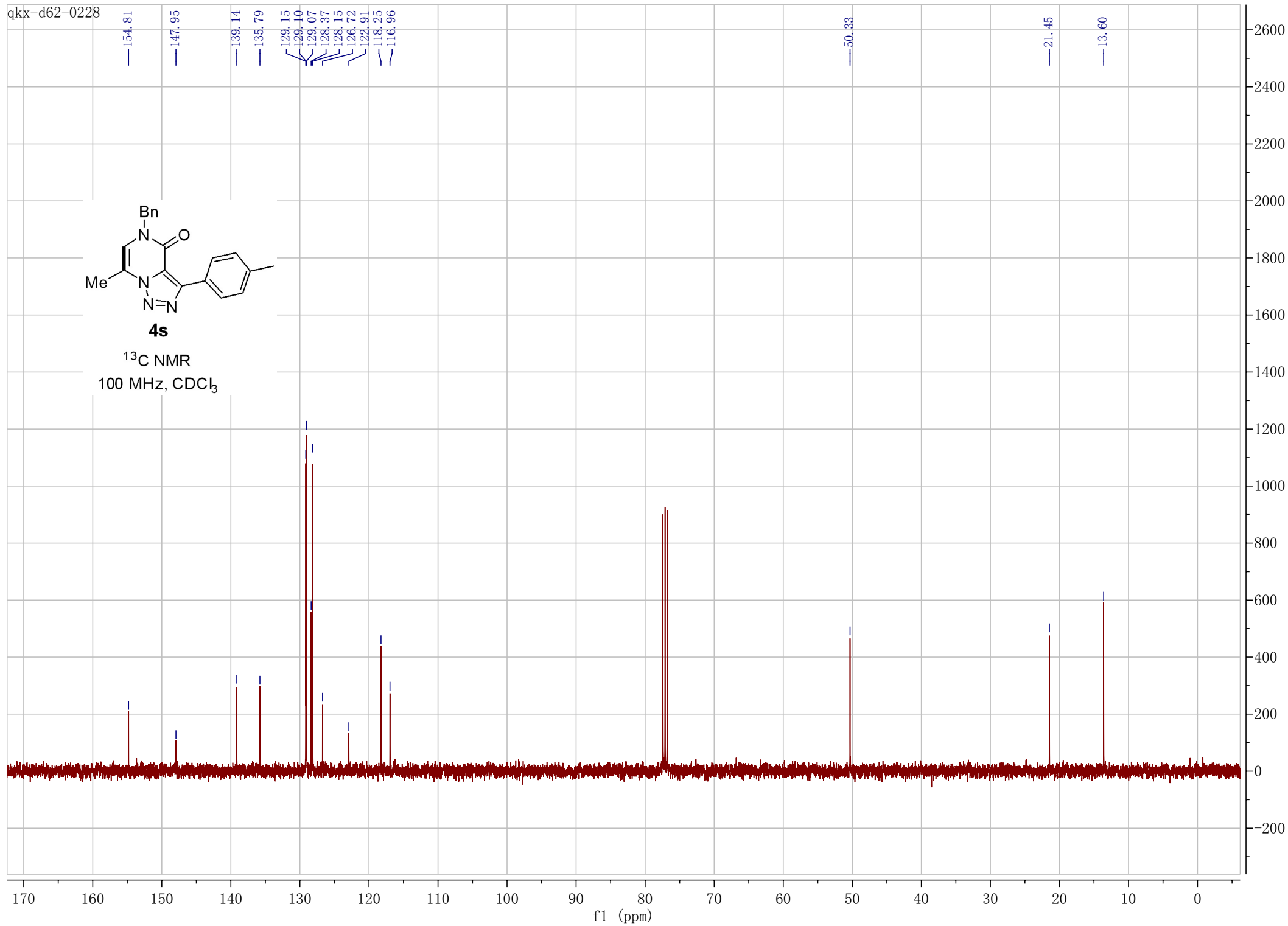


qkx-d62-0228

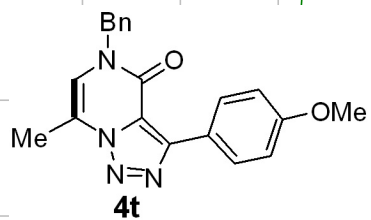


**4s**

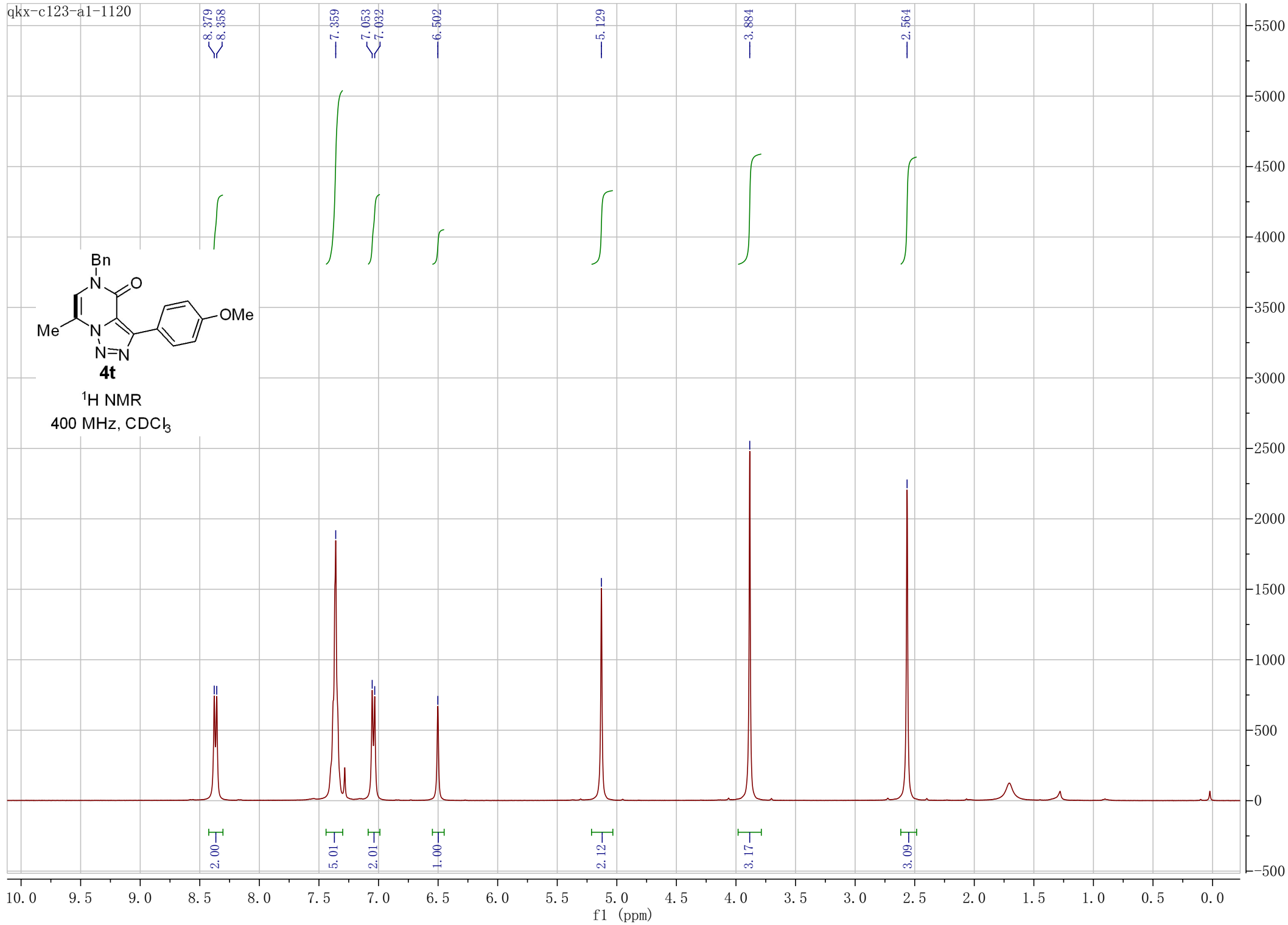
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



qkx-c123-a1-1120

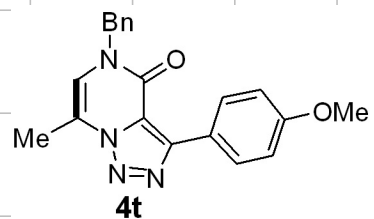


<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

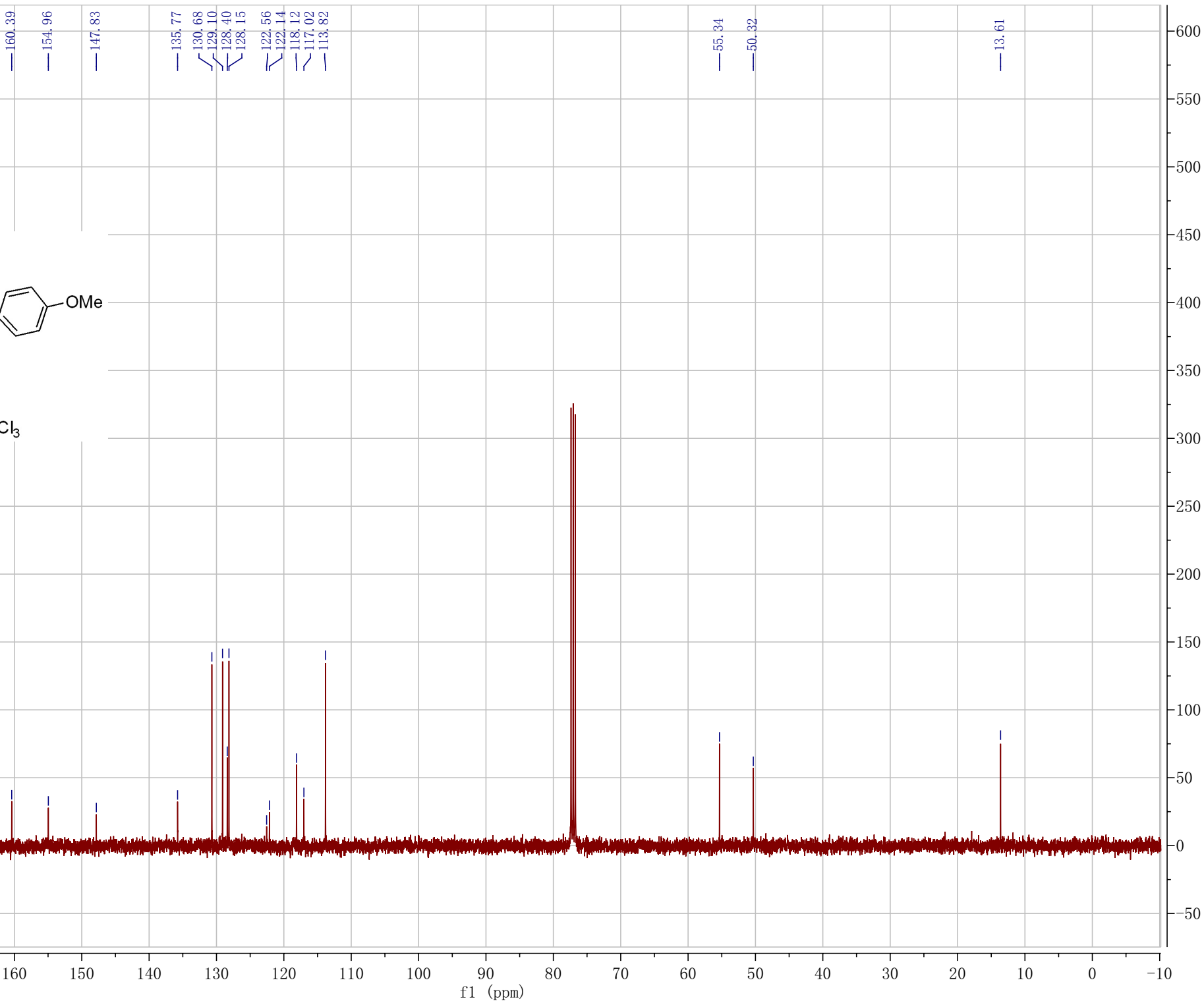




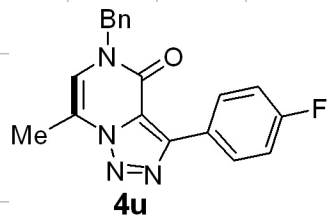
qkx-c123-a1-1120



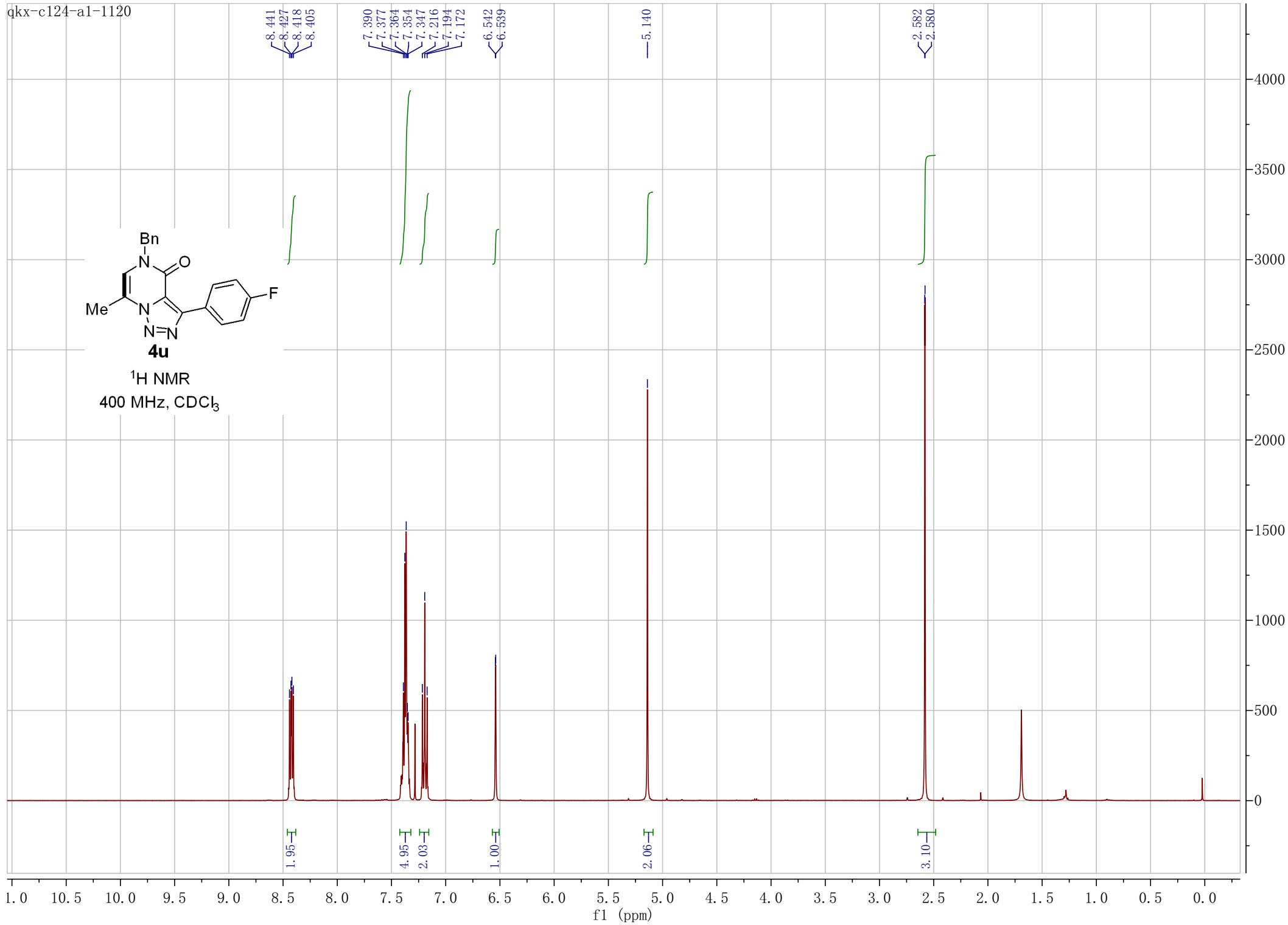
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



qkx-c124-a1-1120

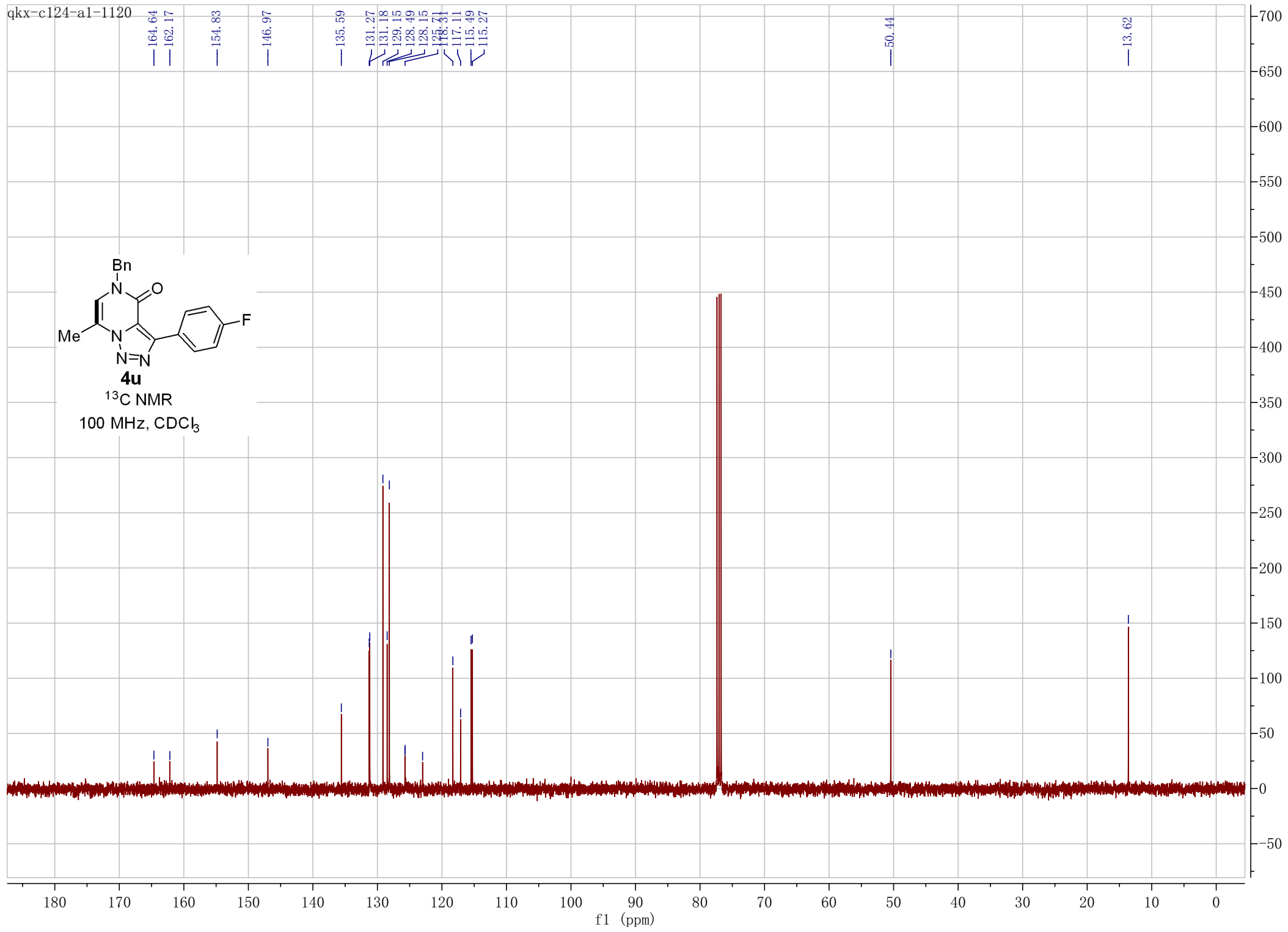
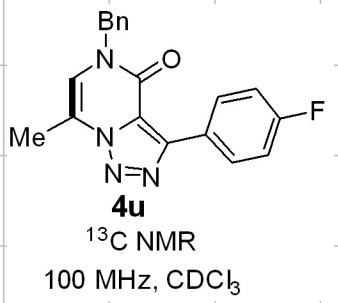


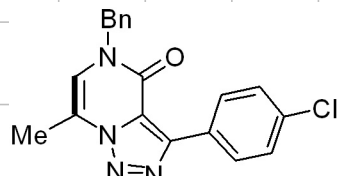
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



qkx-c124-a1-1120

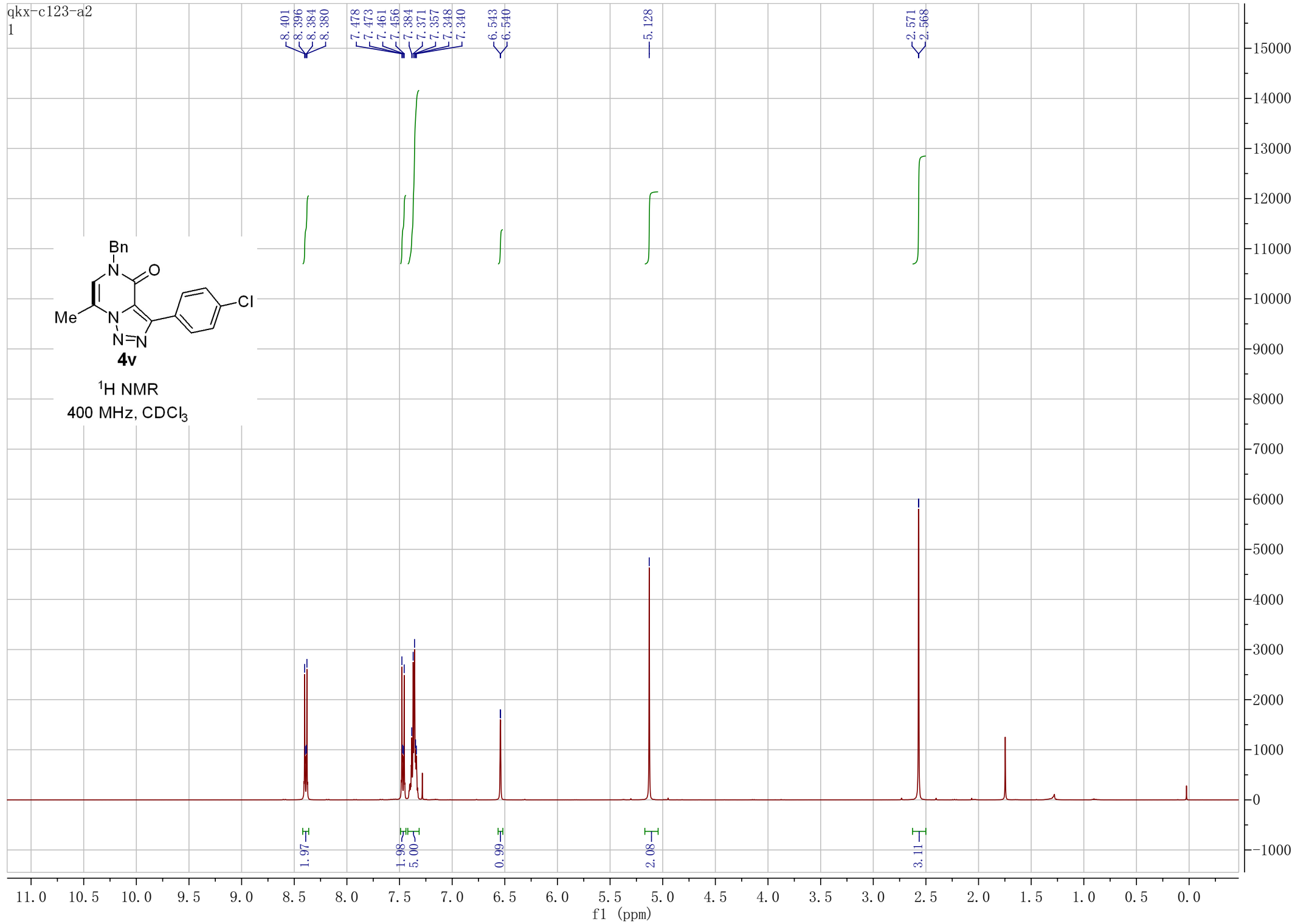
164.64  
162.17  
154.83  
146.97  
135.59  
131.27  
131.18  
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128.49  
128.15  
118.31  
117.11  
115.49  
115.27  
50.44  
13.62

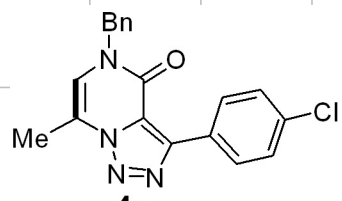
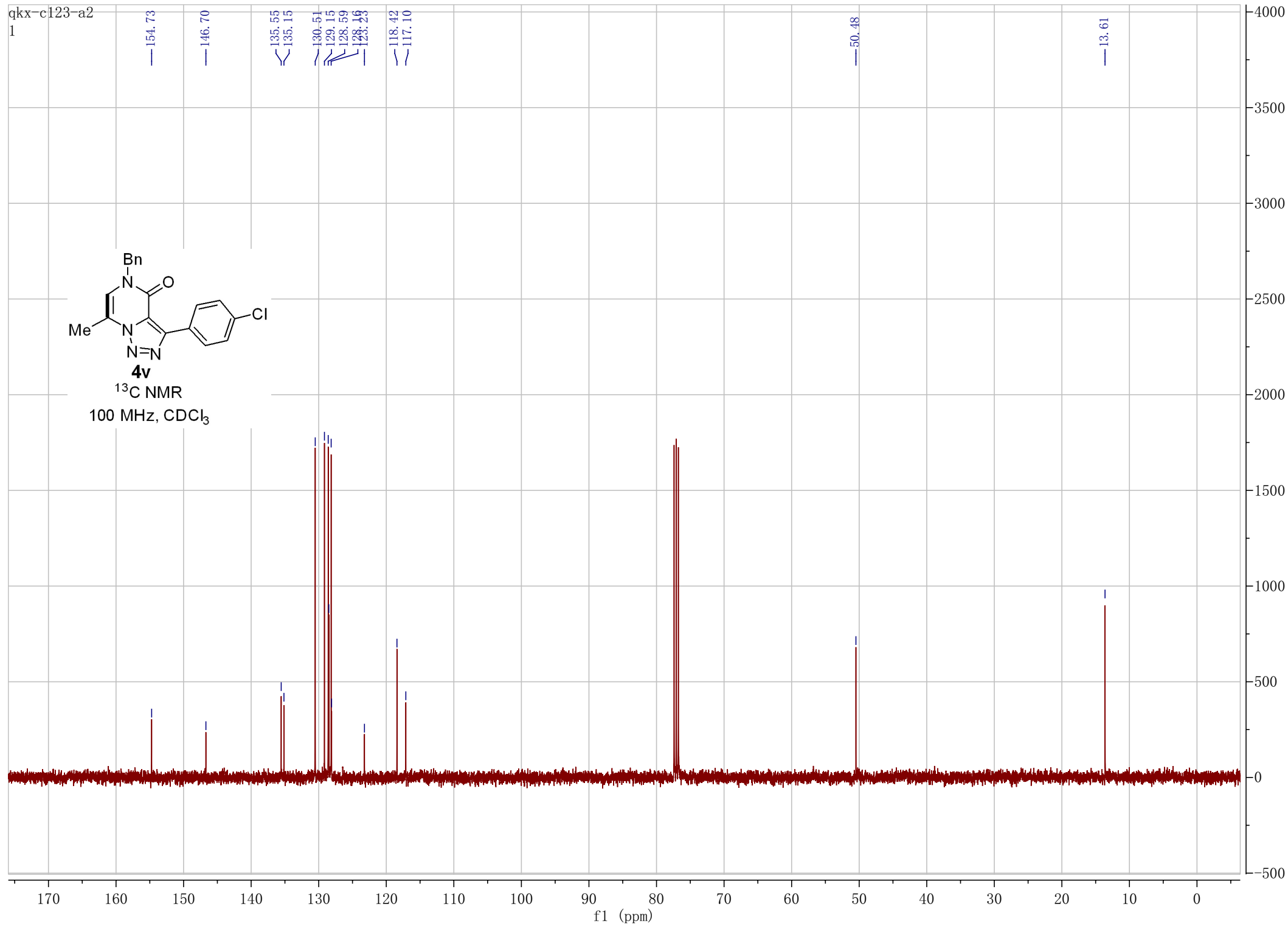


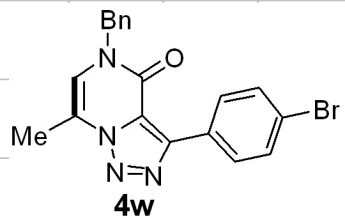


4v

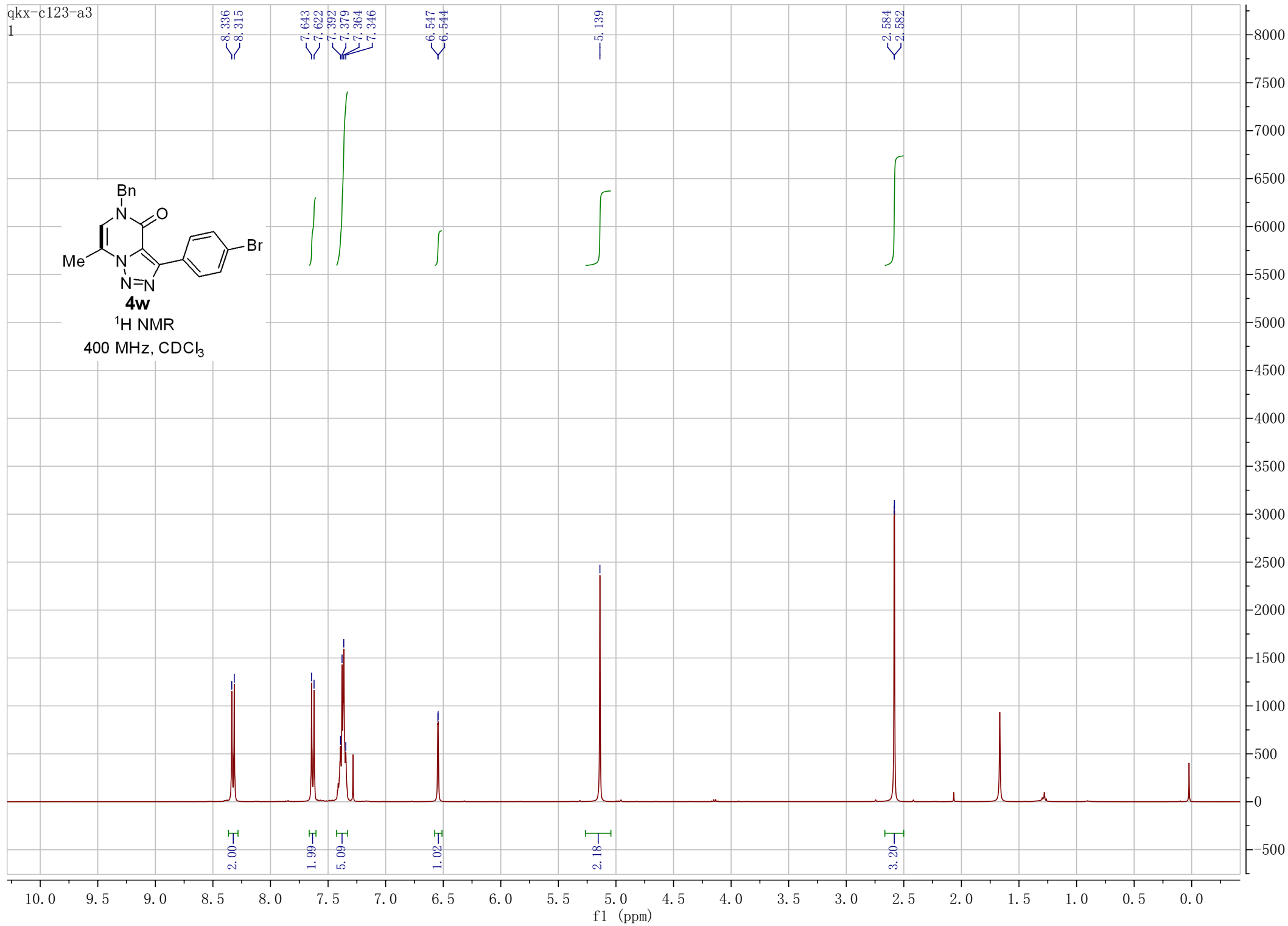
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



**4v**<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

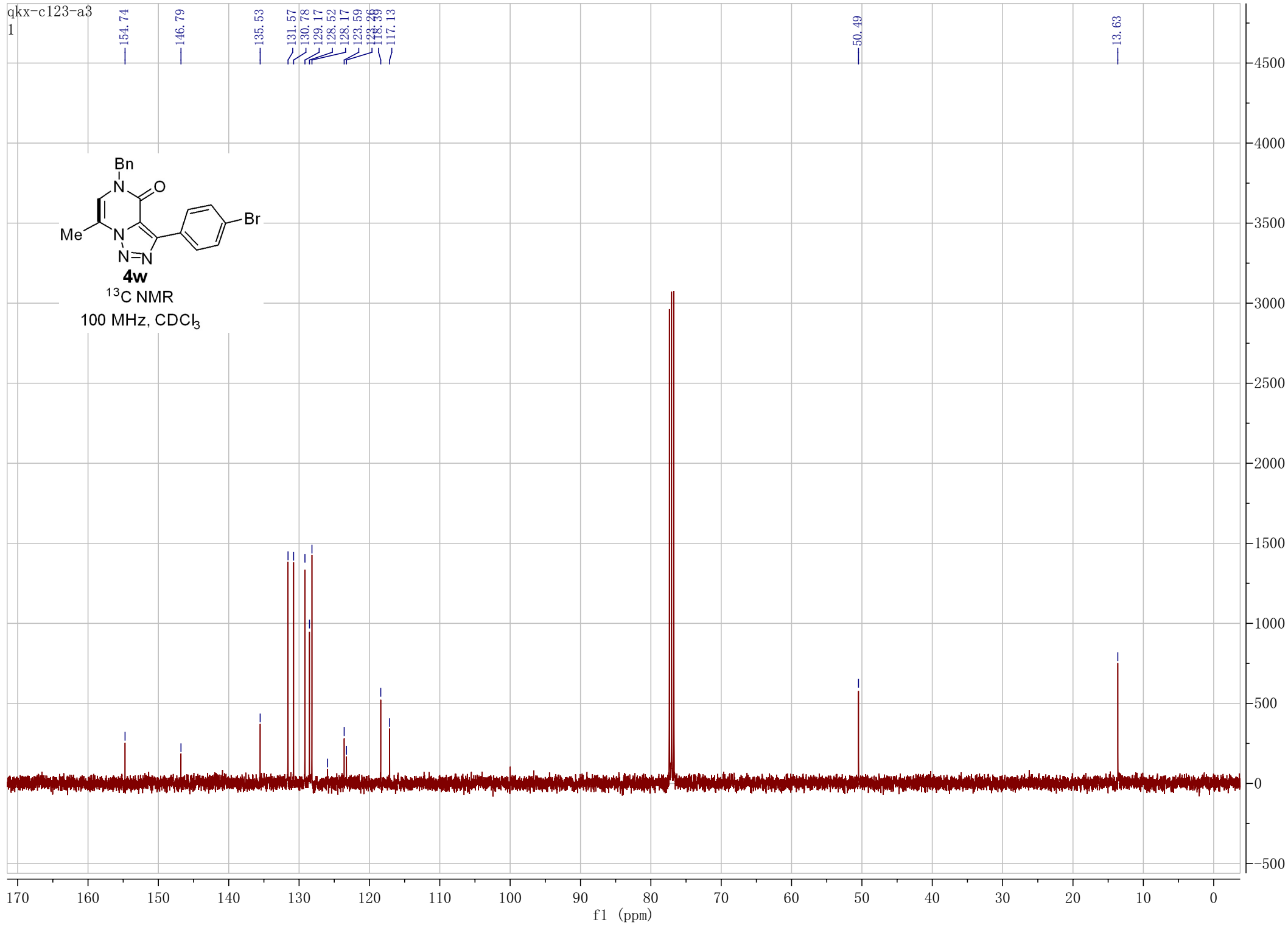
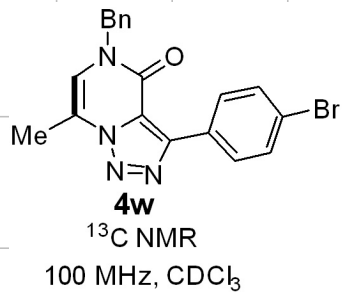


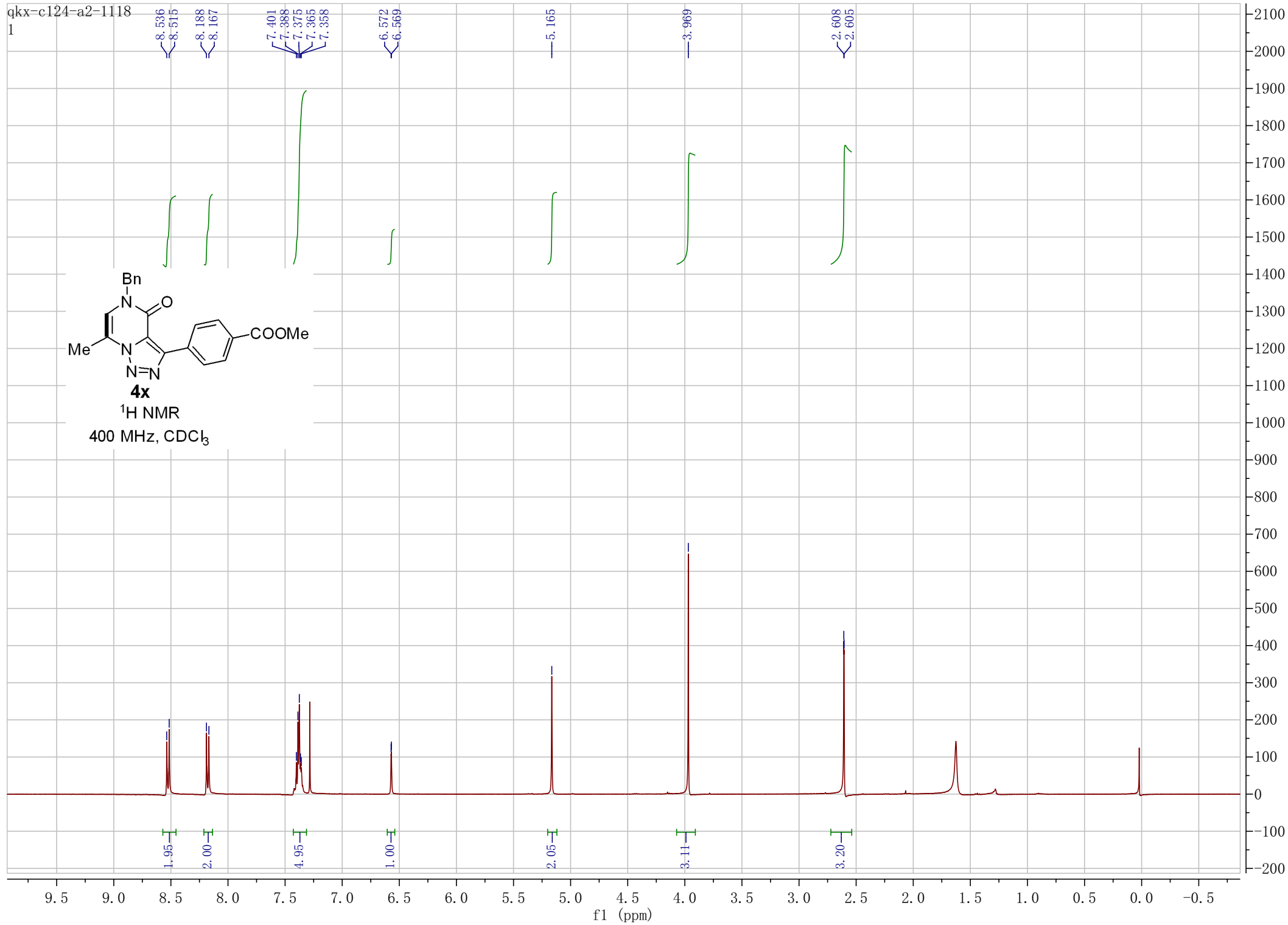
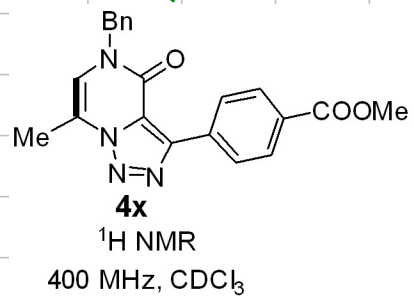
**4w**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



qkx-c123-a3

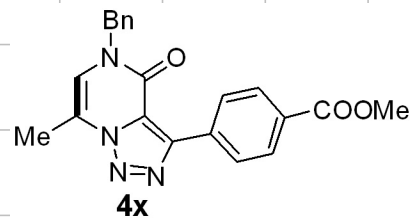
1



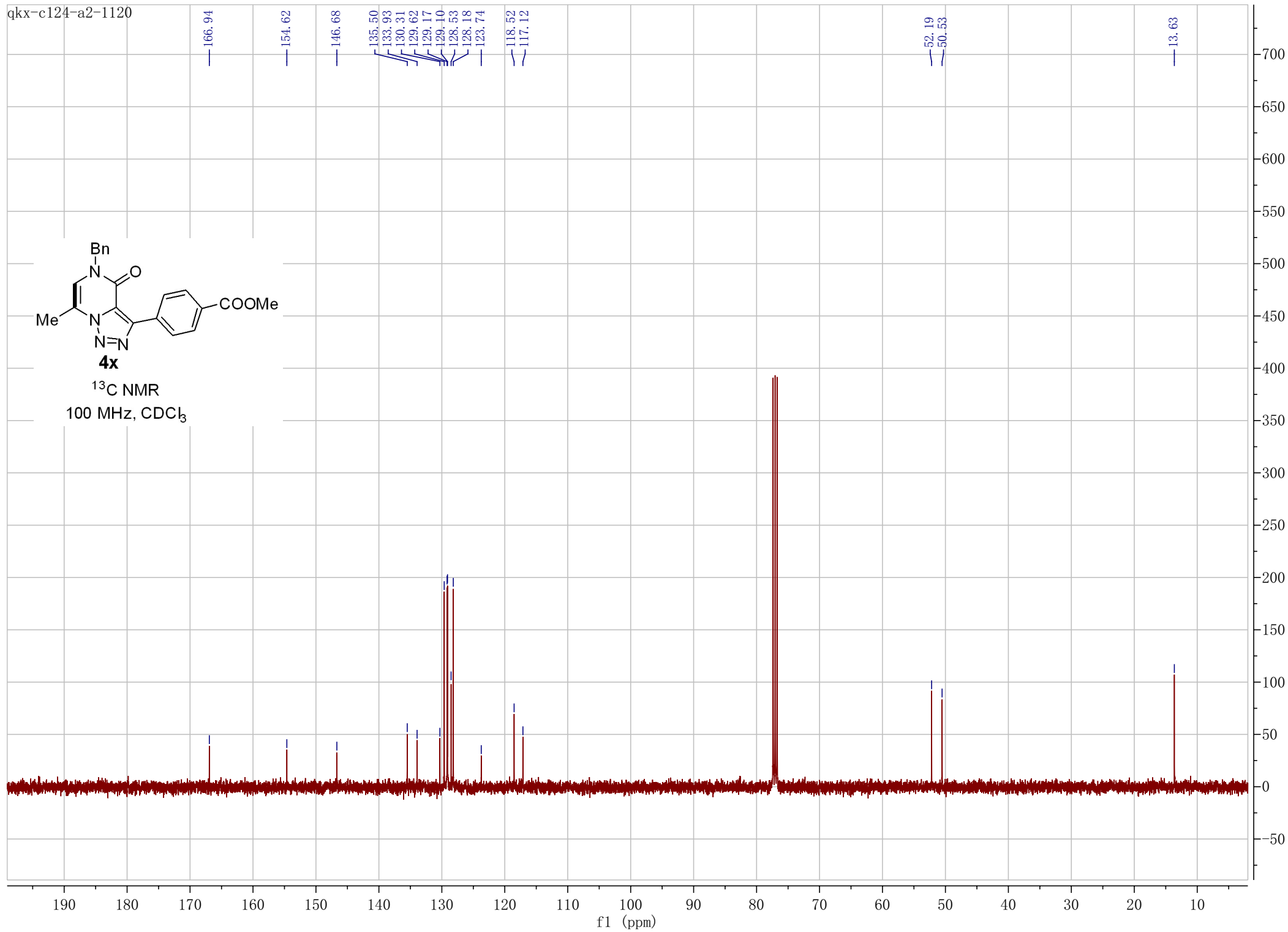


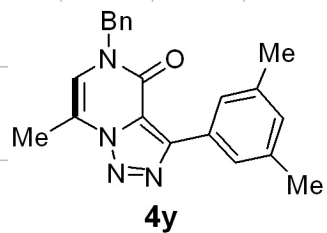


qkx-c124-a2-1120

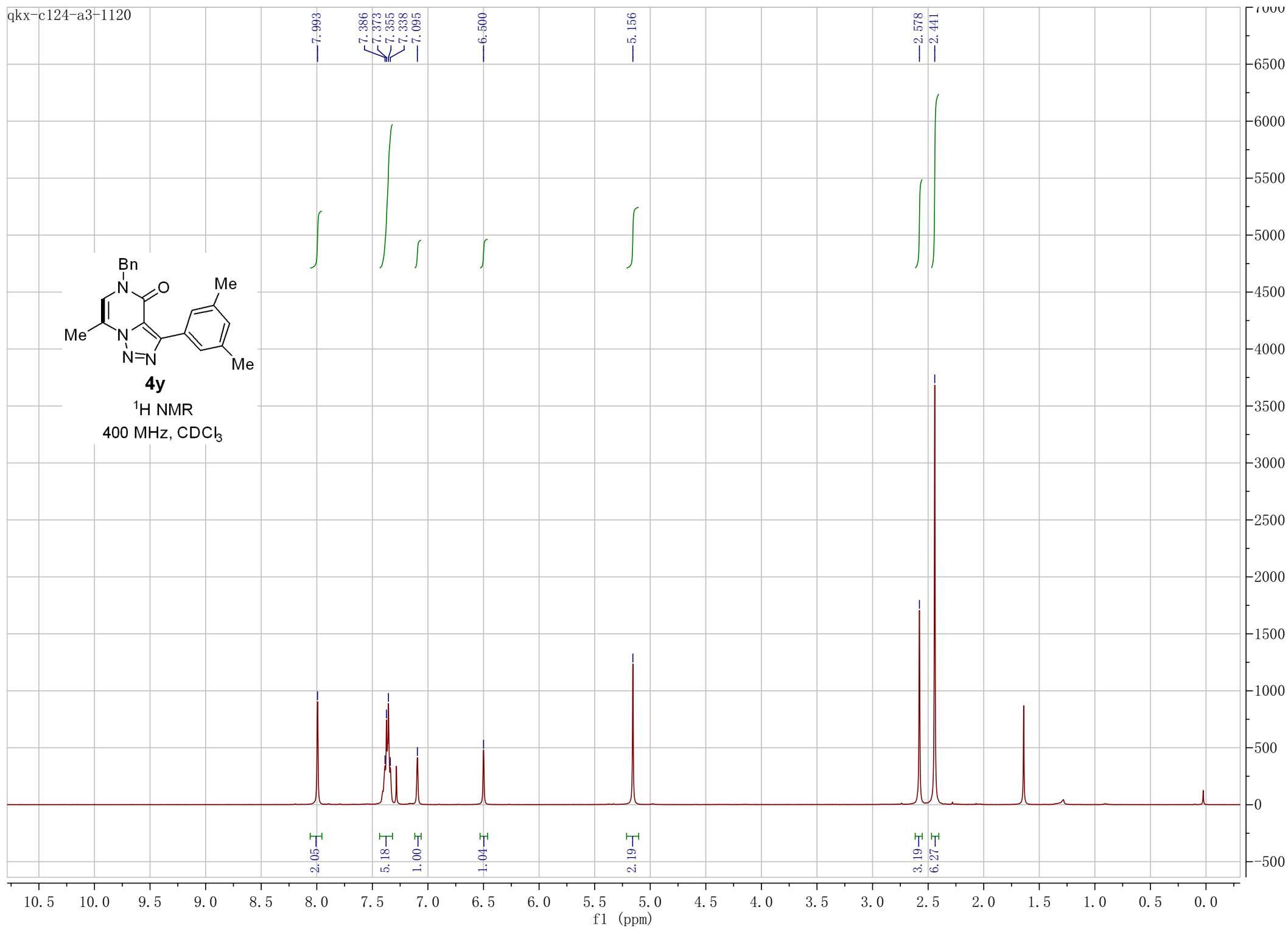


<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

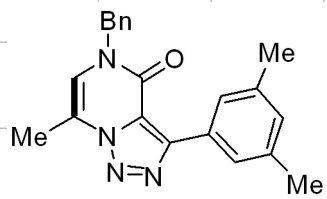


**4y**

$^1\text{H NMR}$   
400 MHz,  $\text{CDCl}_3$



qkx-c124-a3-1120



**4y**

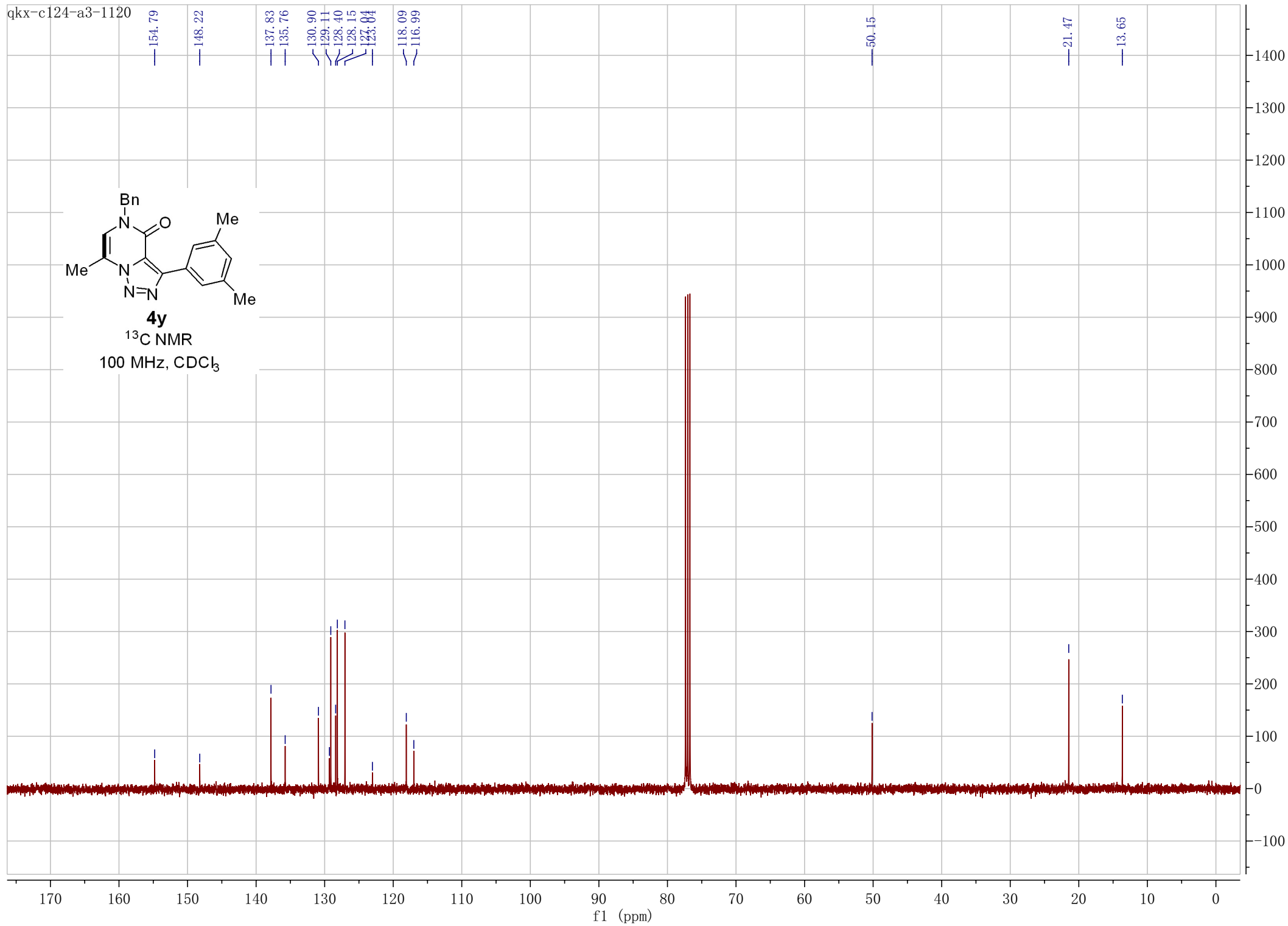
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

154.79  
148.22  
137.83  
135.76  
130.90  
129.11  
128.40  
128.15  
127.84  
118.09  
116.99

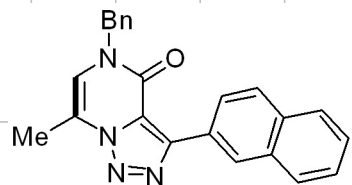
50.15

21.47

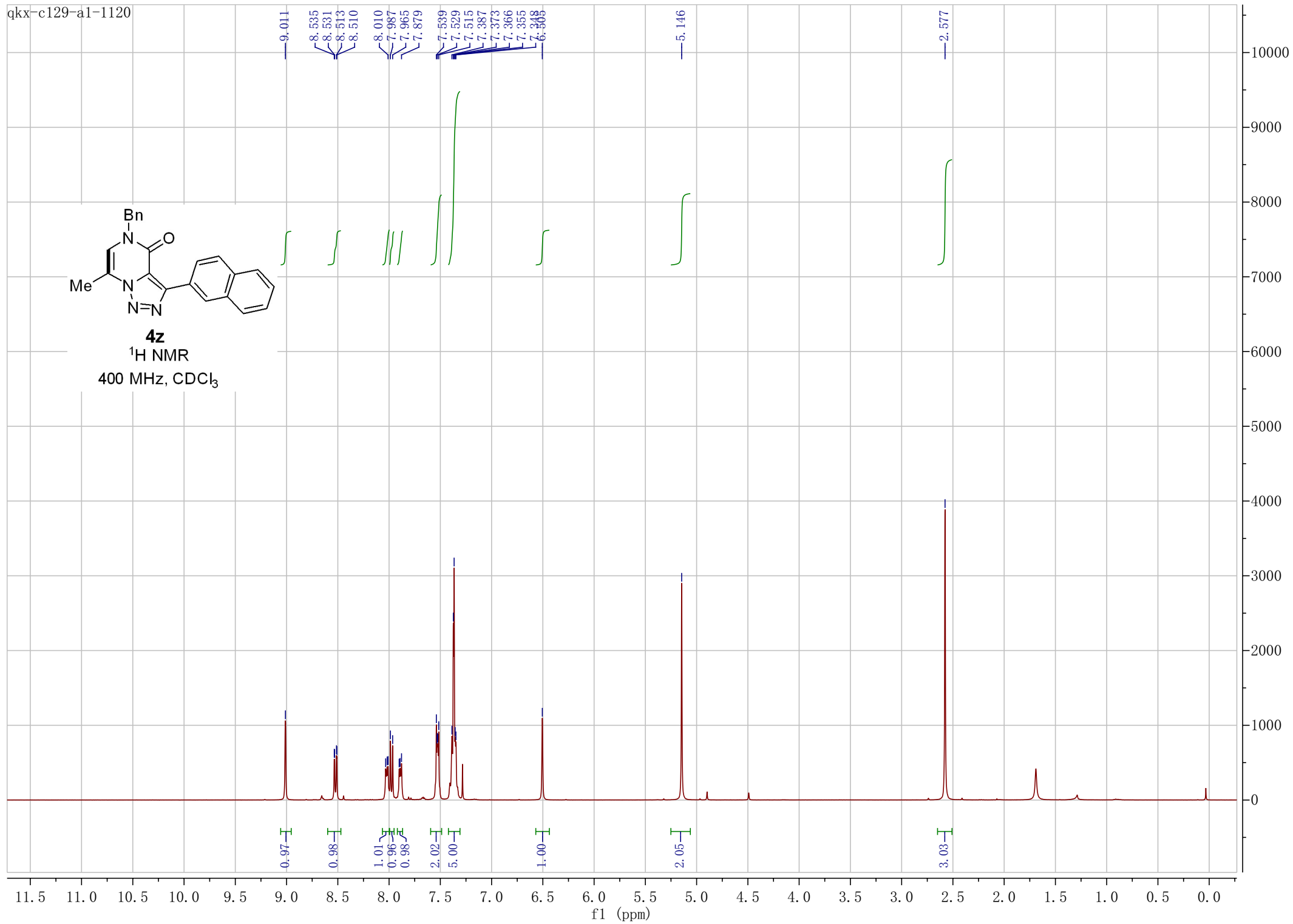
13.65



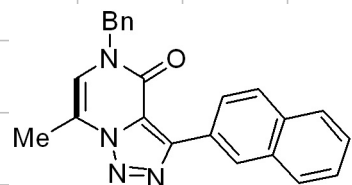
qkx-c129-a1-1120



**4z**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

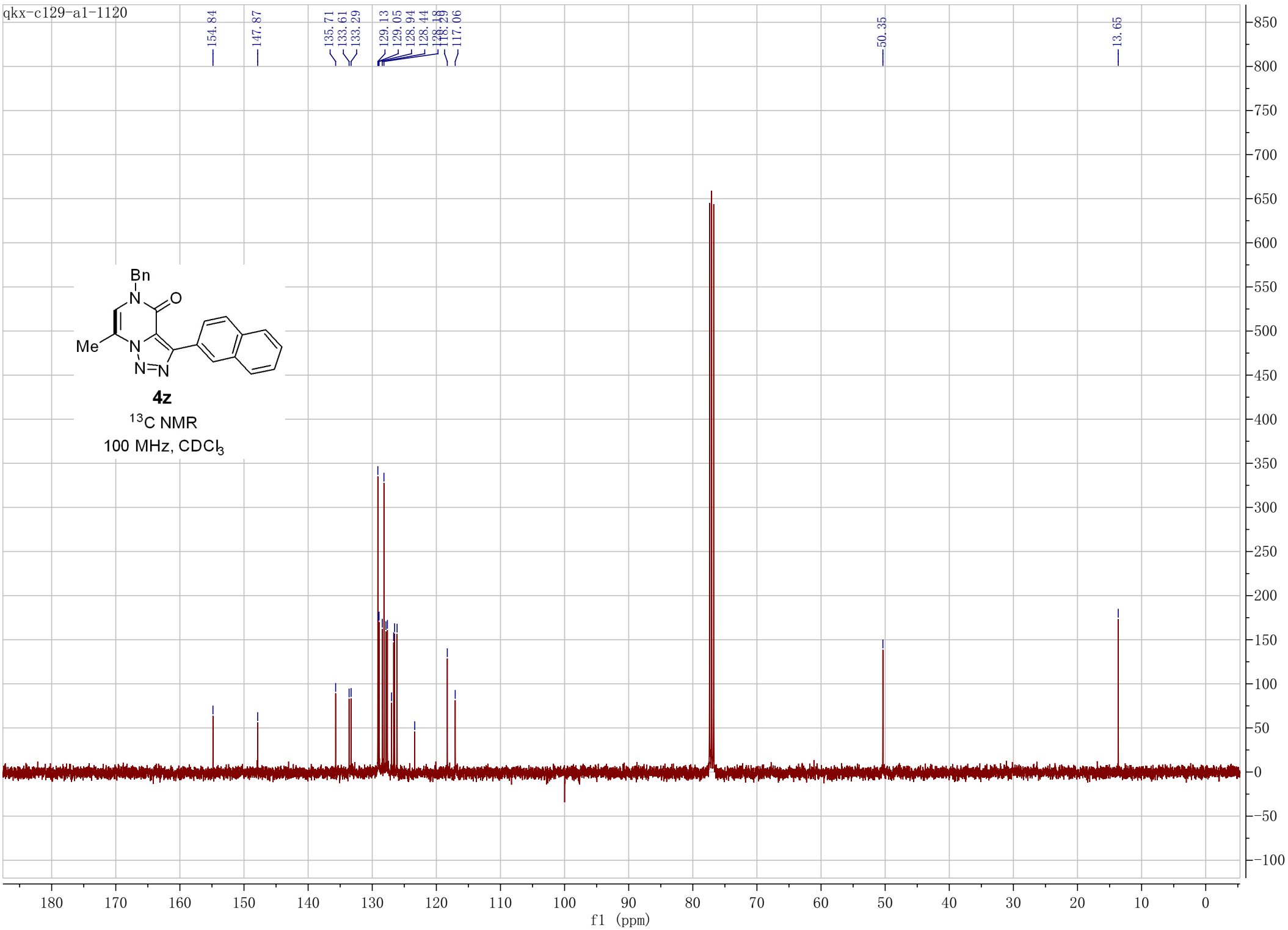


qkx-c129-a1-1120

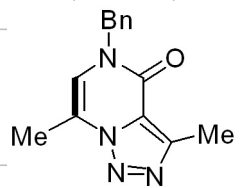


**4z**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

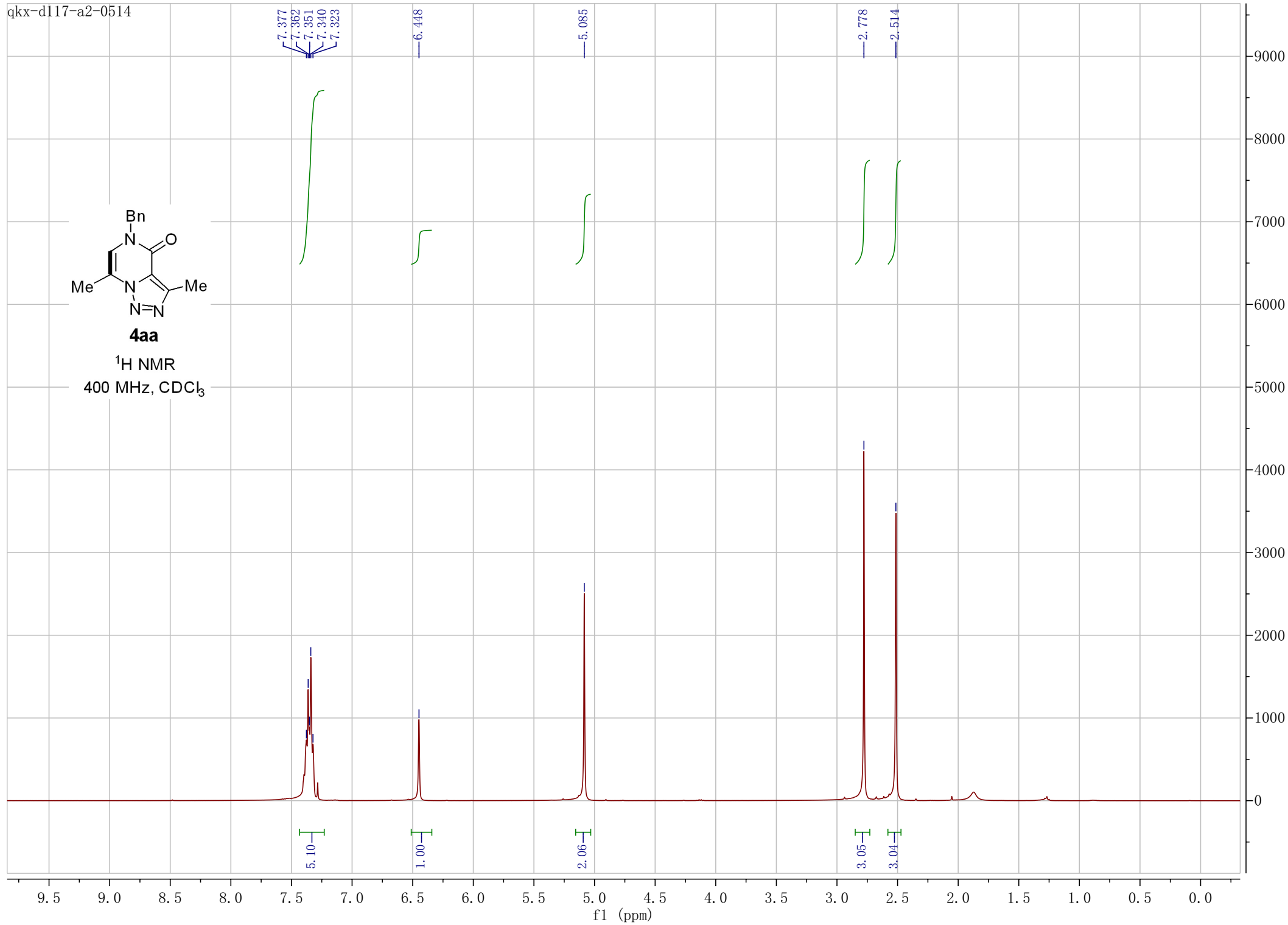


qkx-d117-a2-0514

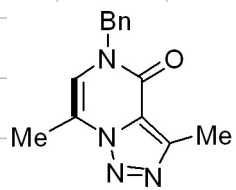


**4aa**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

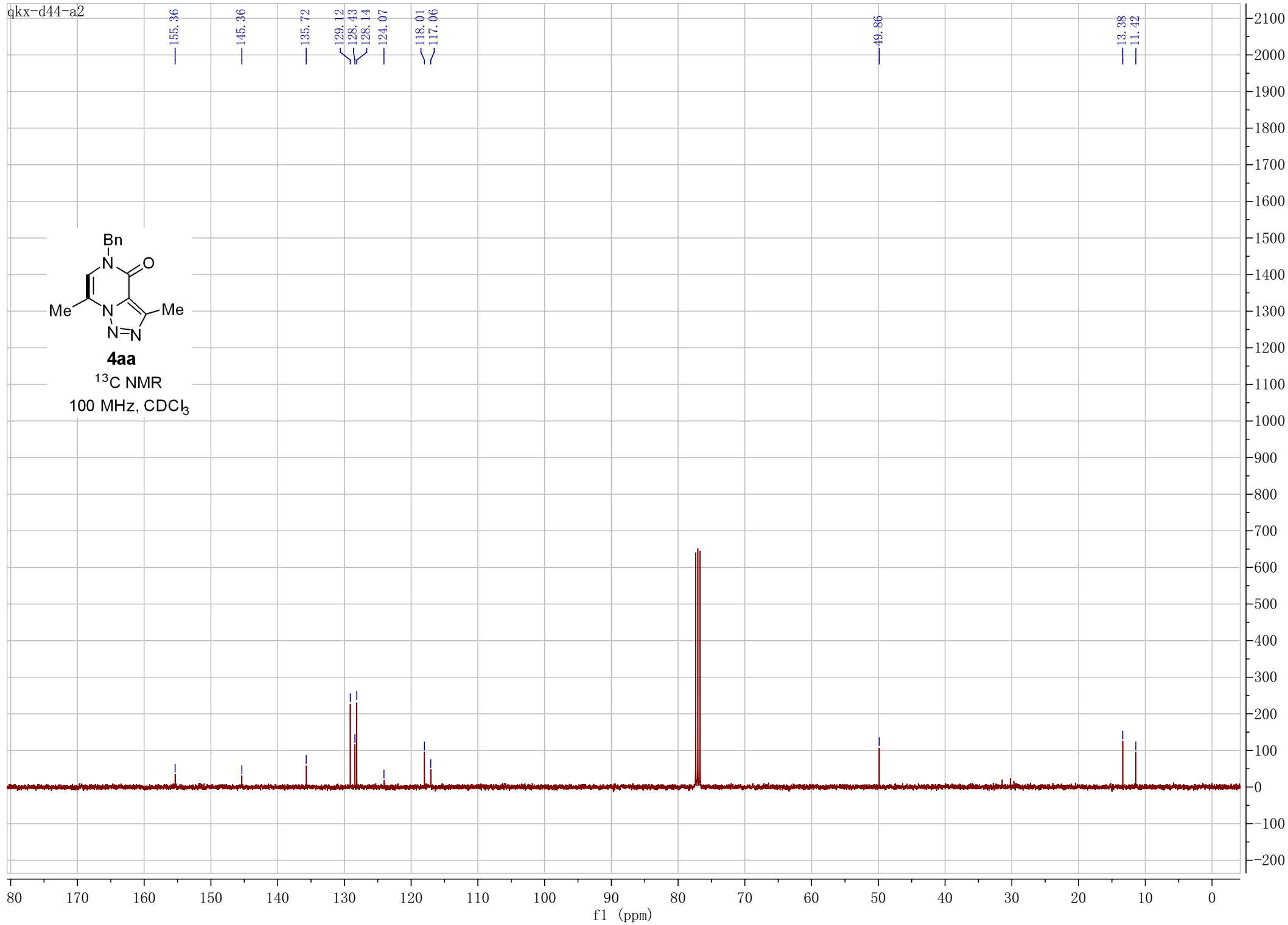


qkx-d44-a2

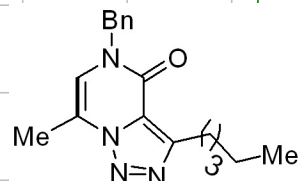


**4aa**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

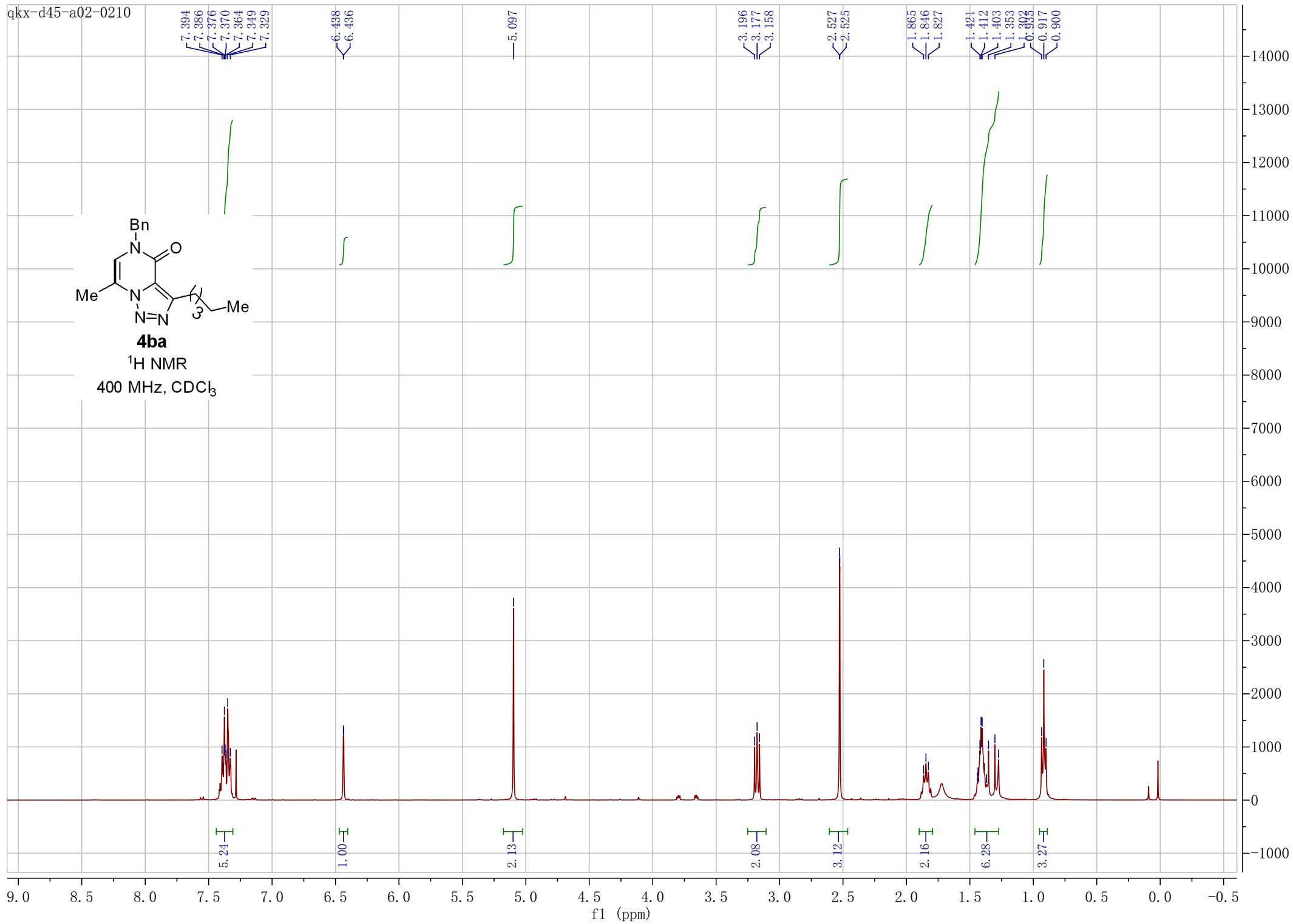


qkx-d45-a02-0210



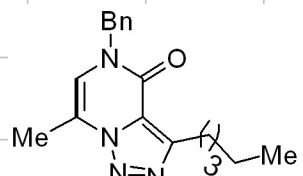
**4ba**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



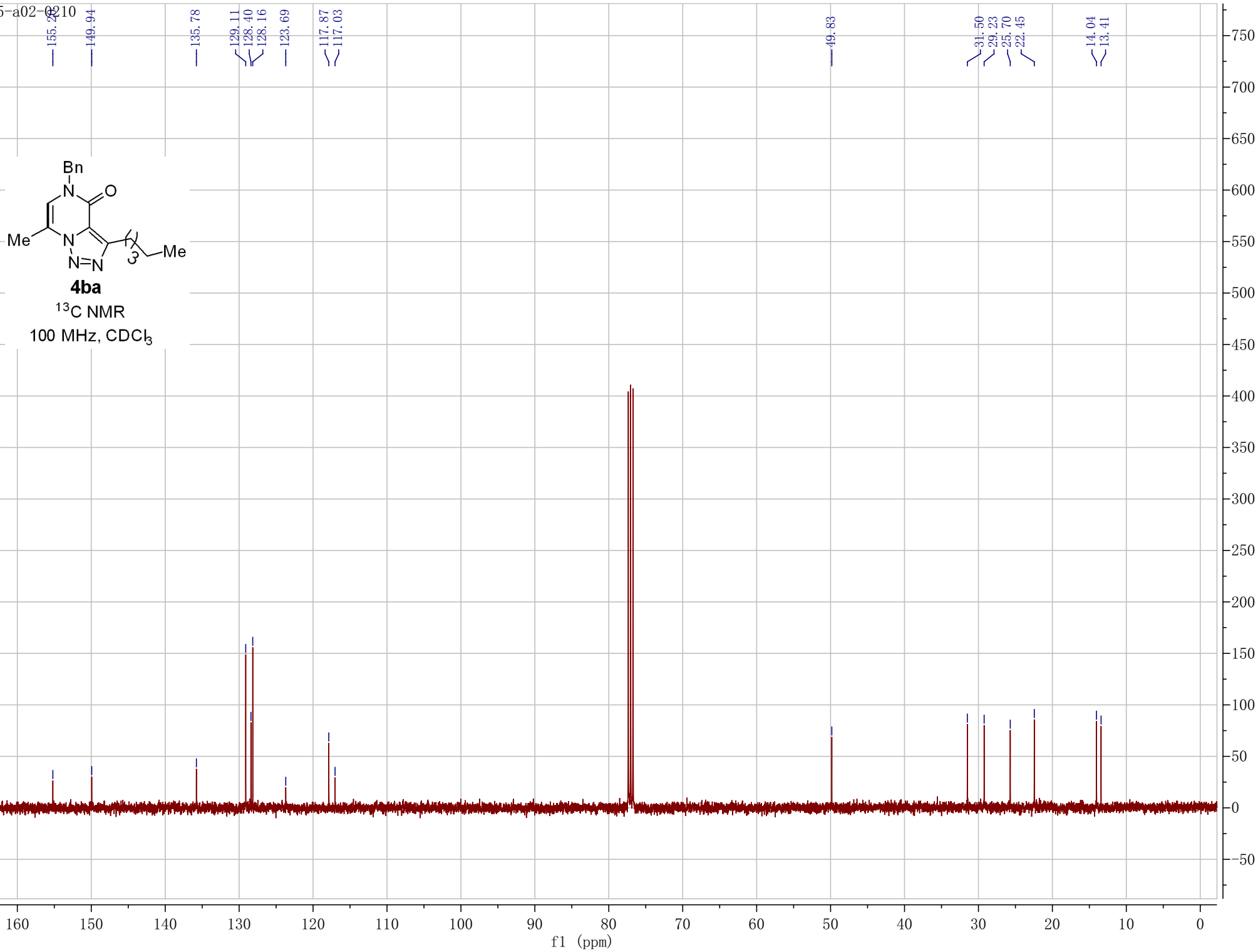


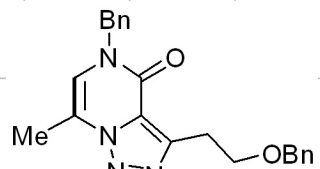
qkx-d45-a02-0210



**4ba**

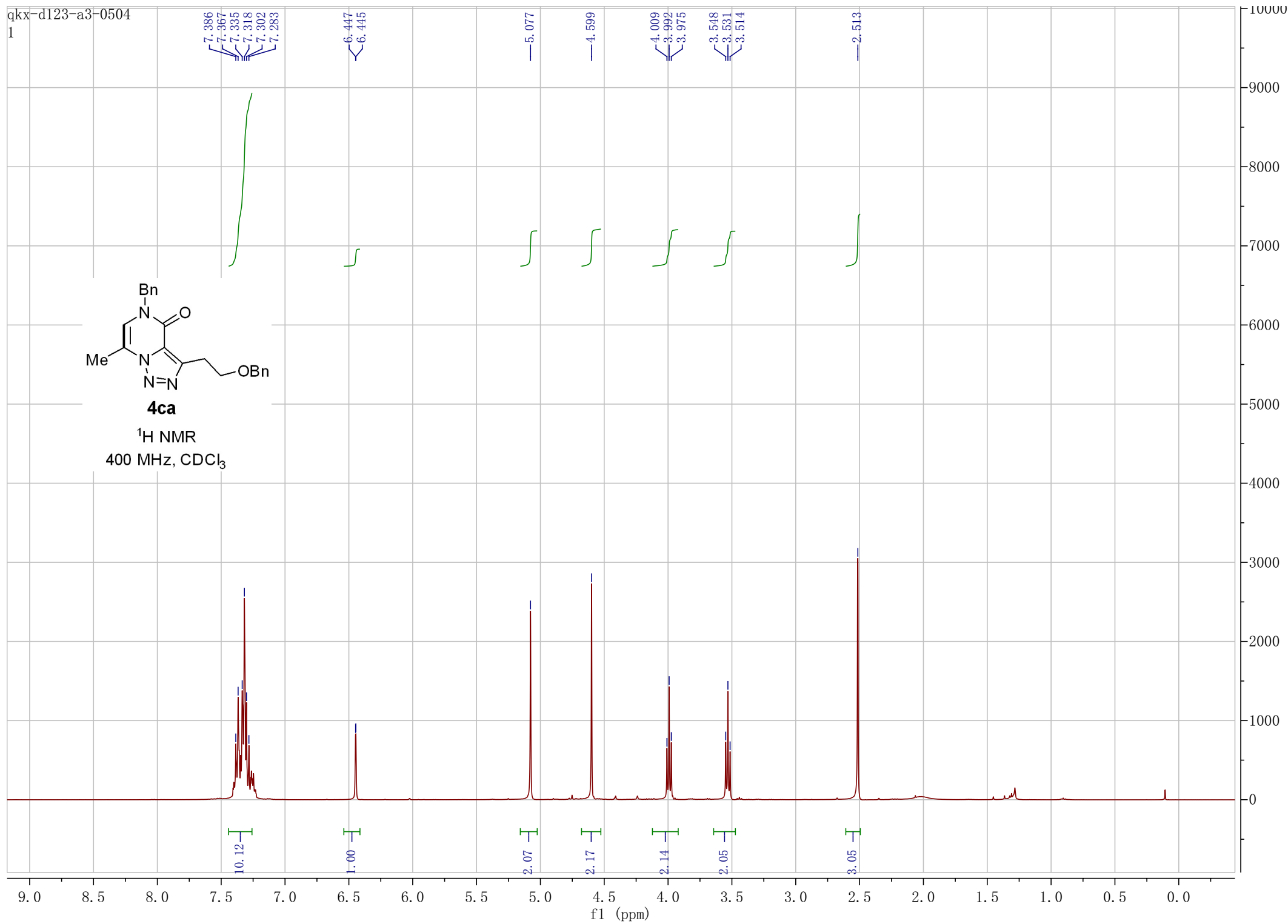
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



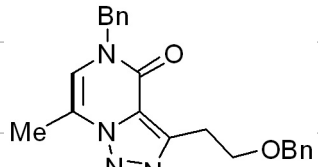


**4ca**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

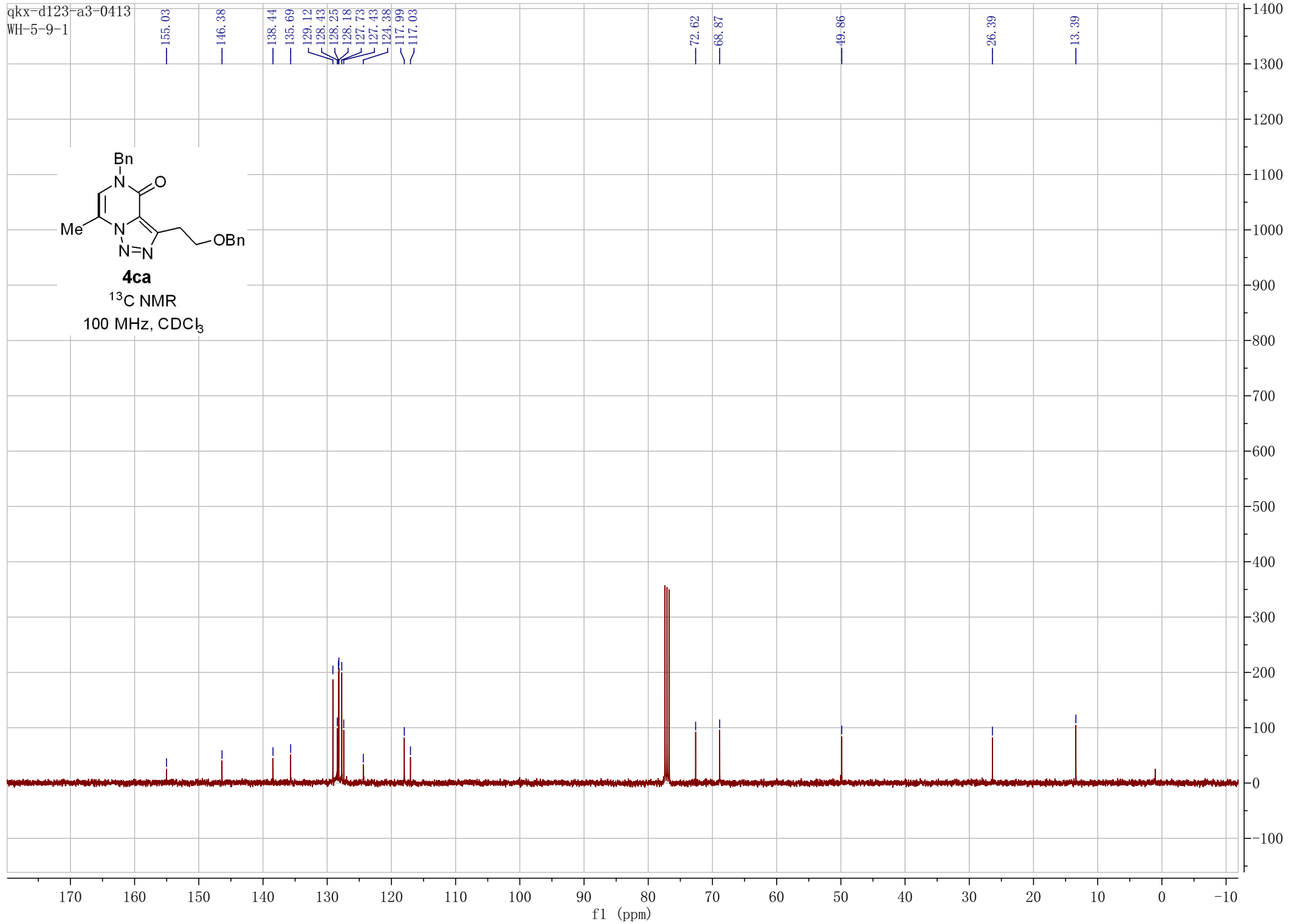


qkx-d123-a3-0413  
WH-5-9-1

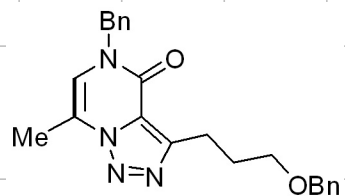


**4ca**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

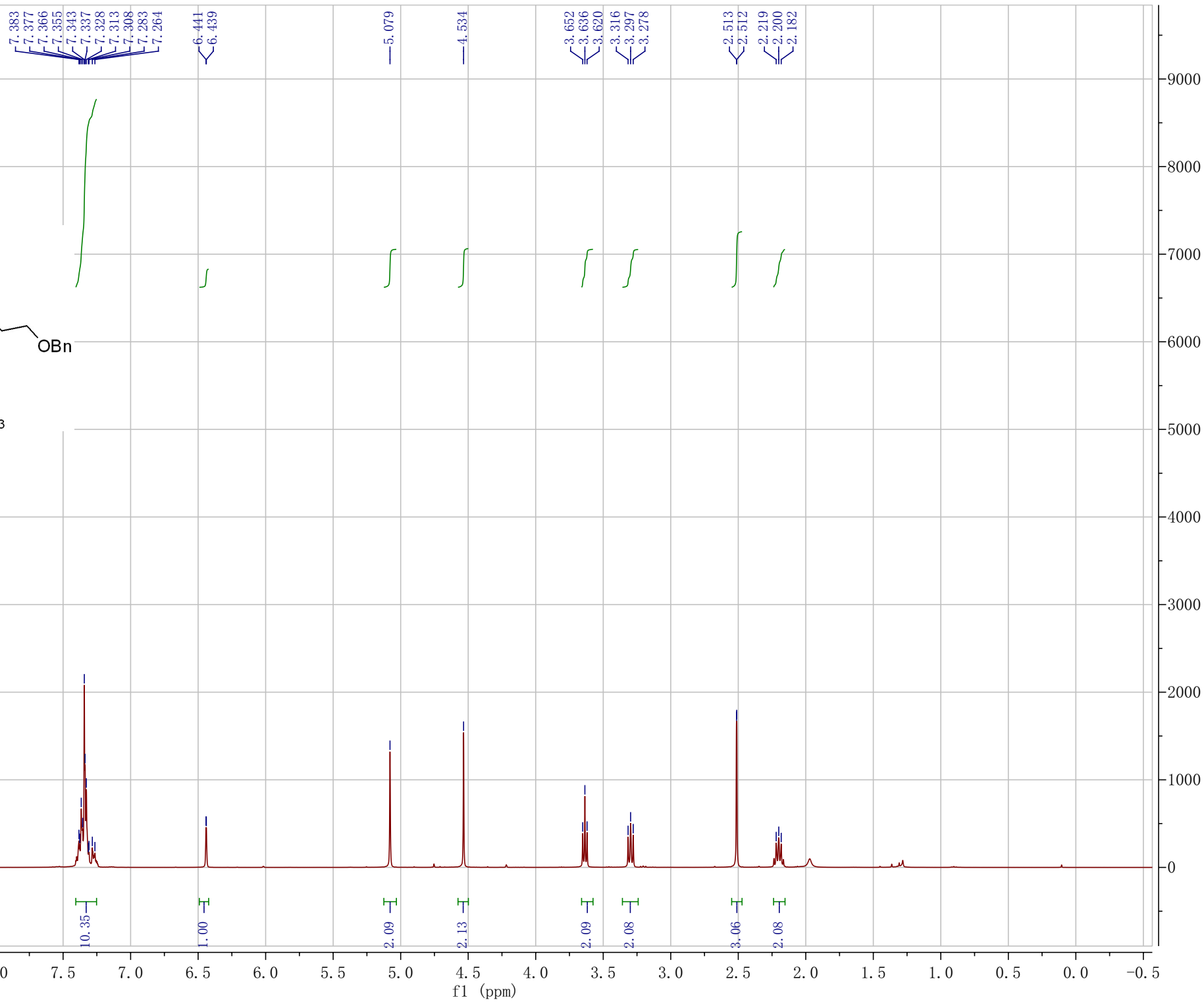


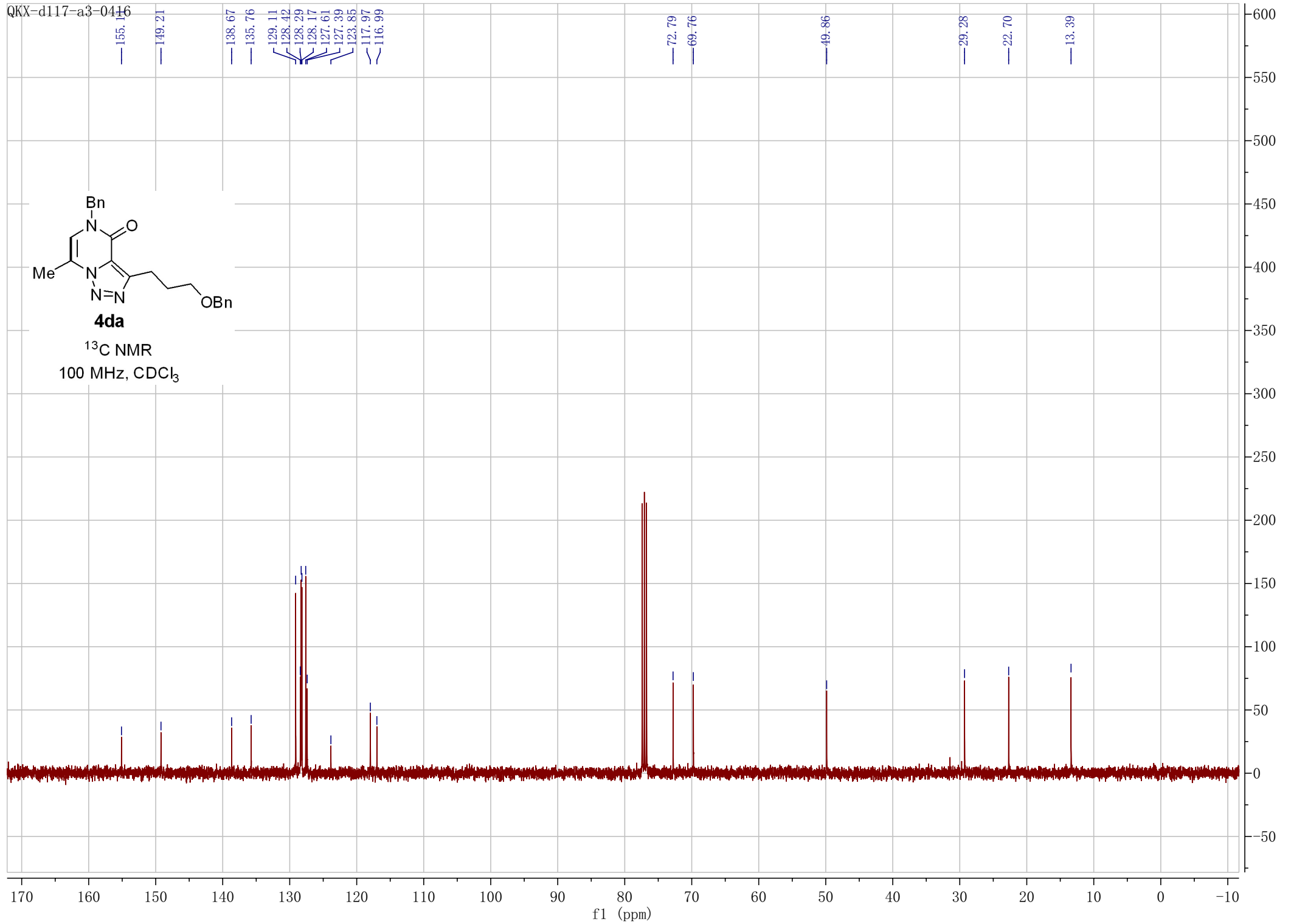
qkx-d117-a3-0514

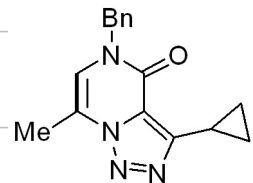


**4da**

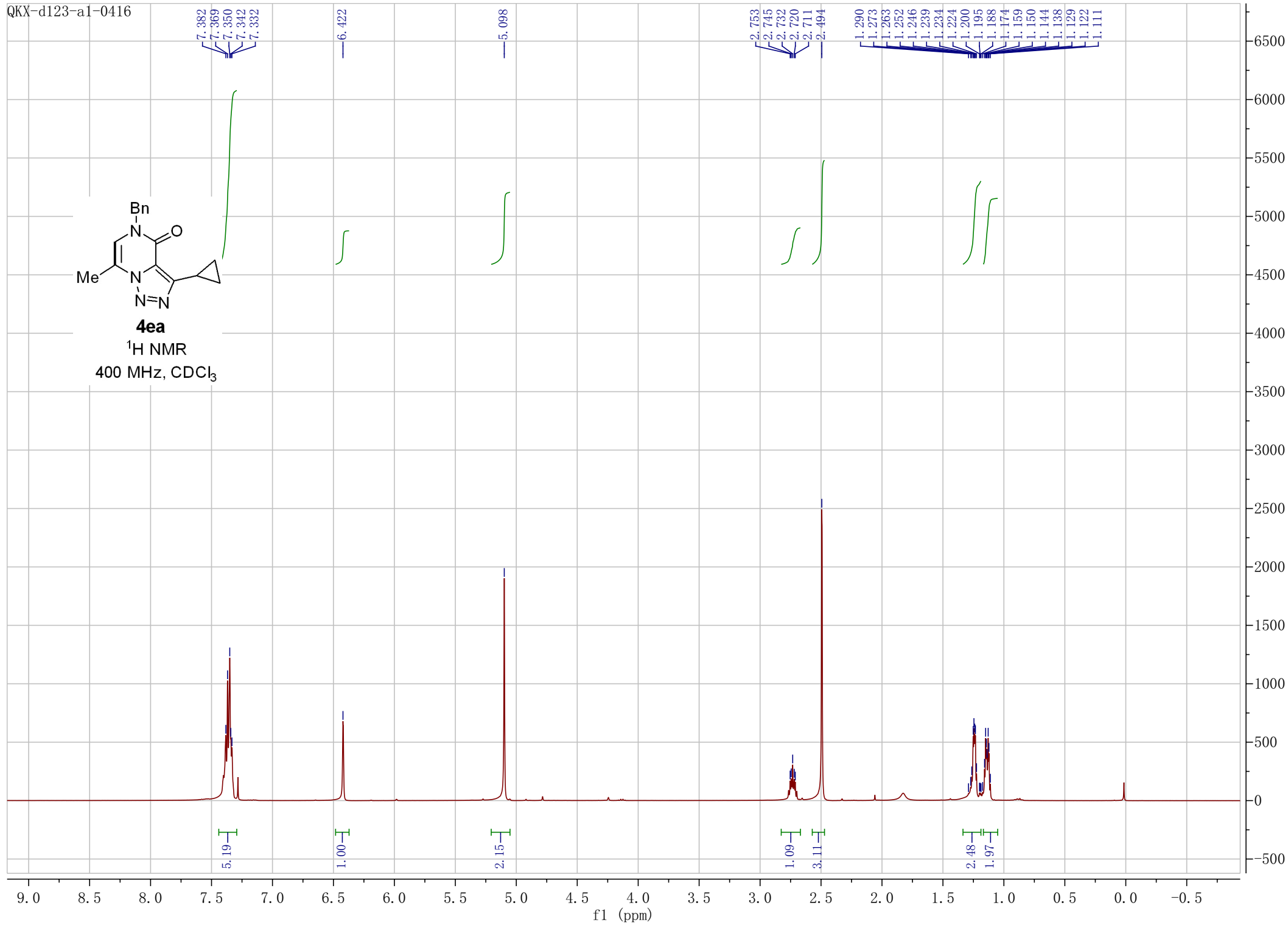
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

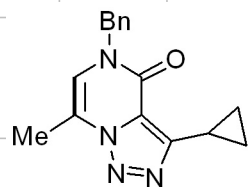




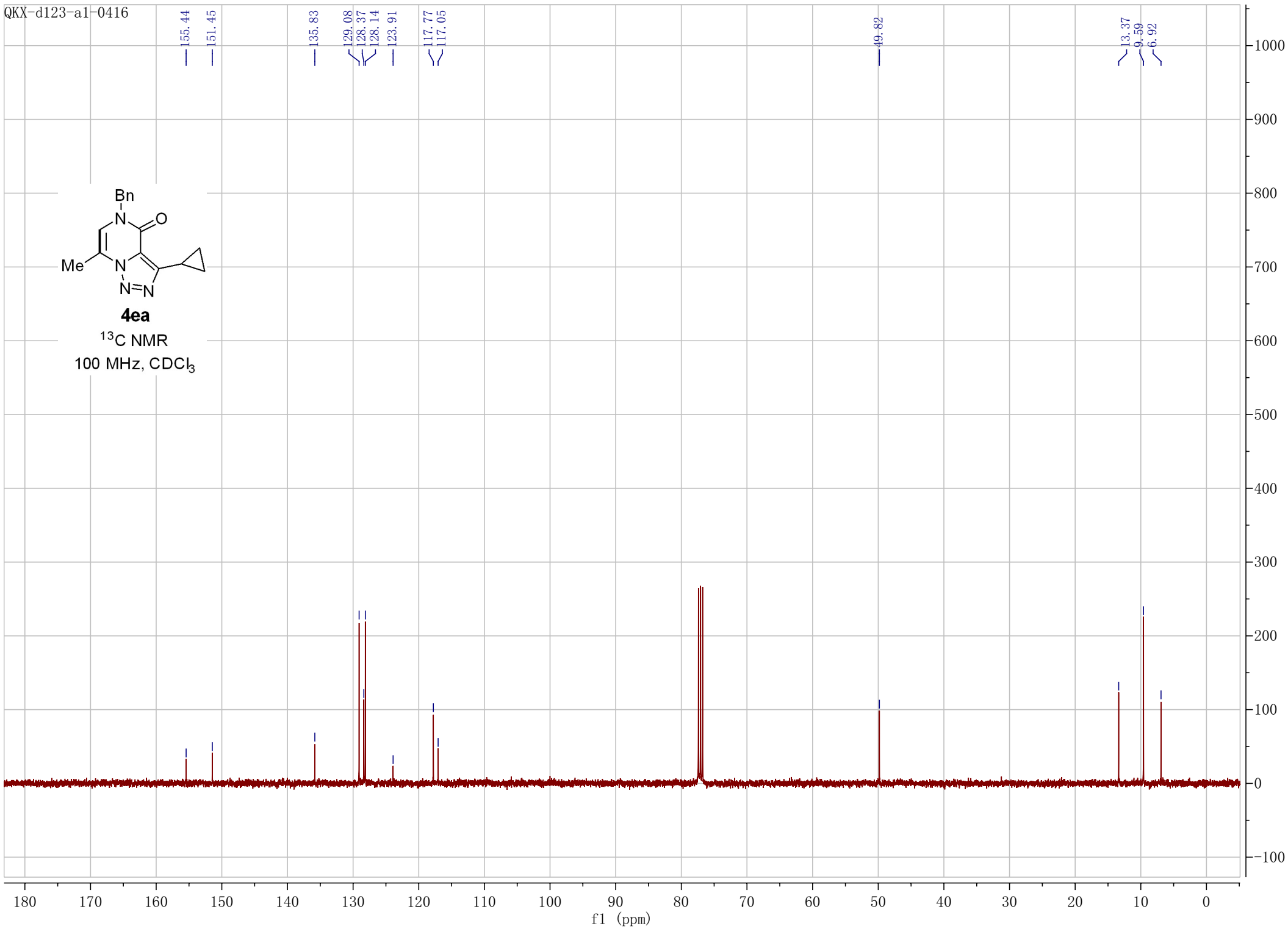


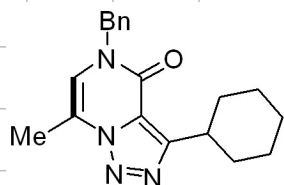
**4a**  
<sup>1</sup>H NMR  
 400 MHz, CDCl<sub>3</sub>



**4a**

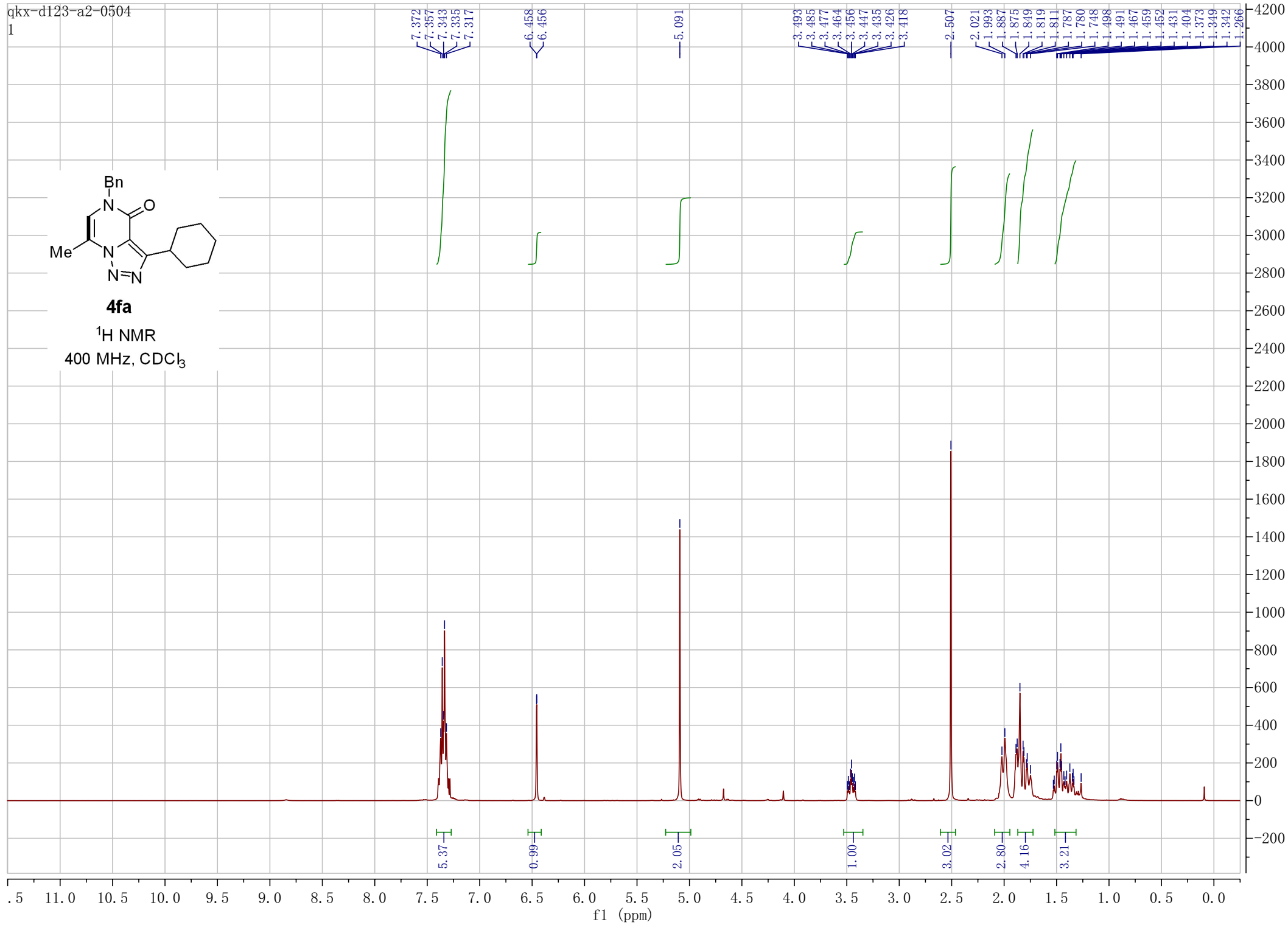
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>





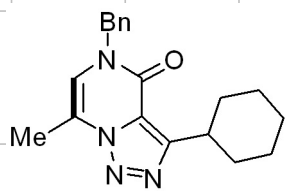
**4fa**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



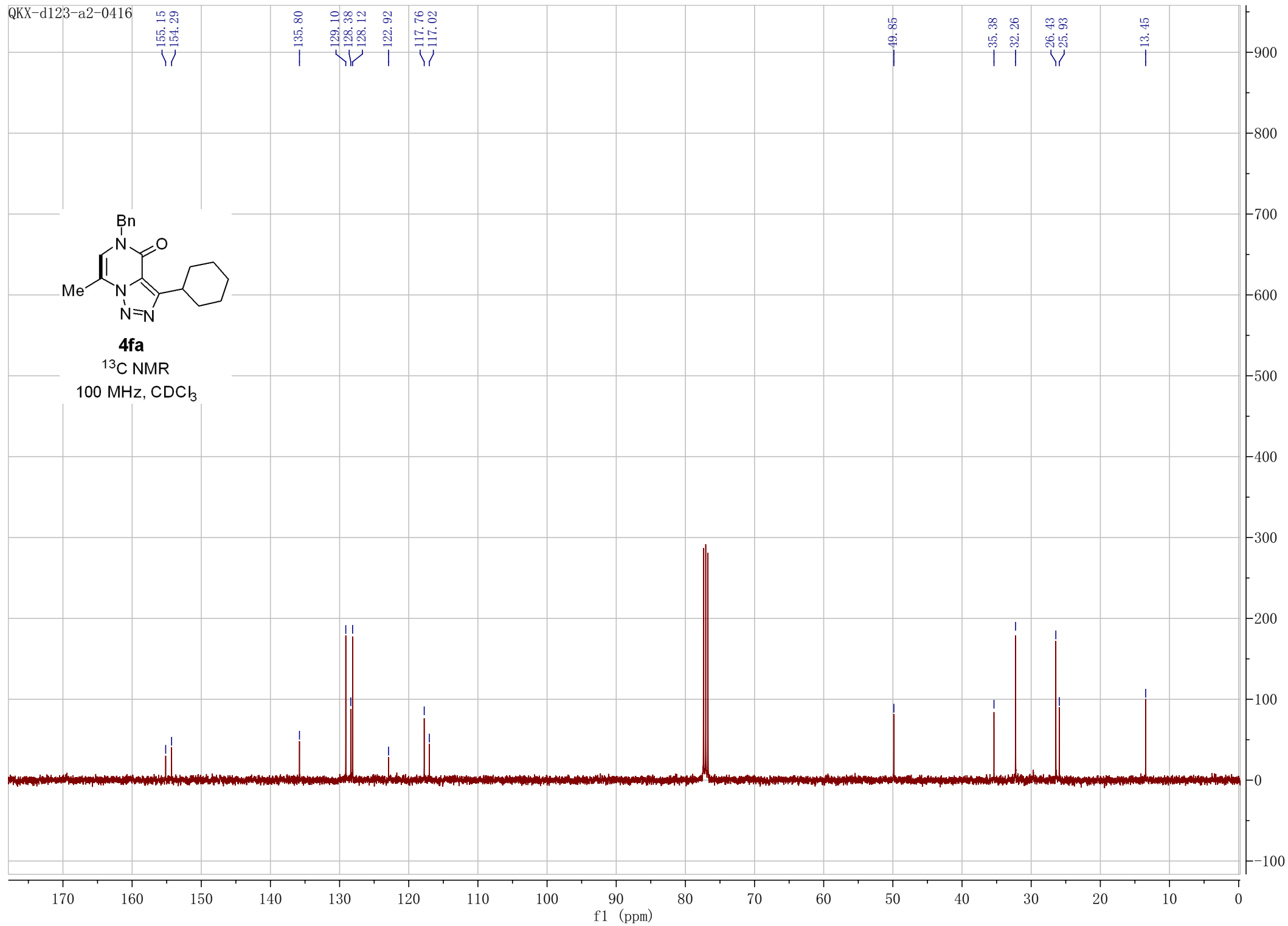


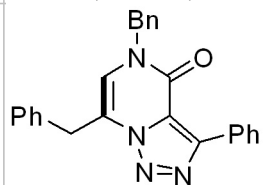
QKX-d123-a2-0416



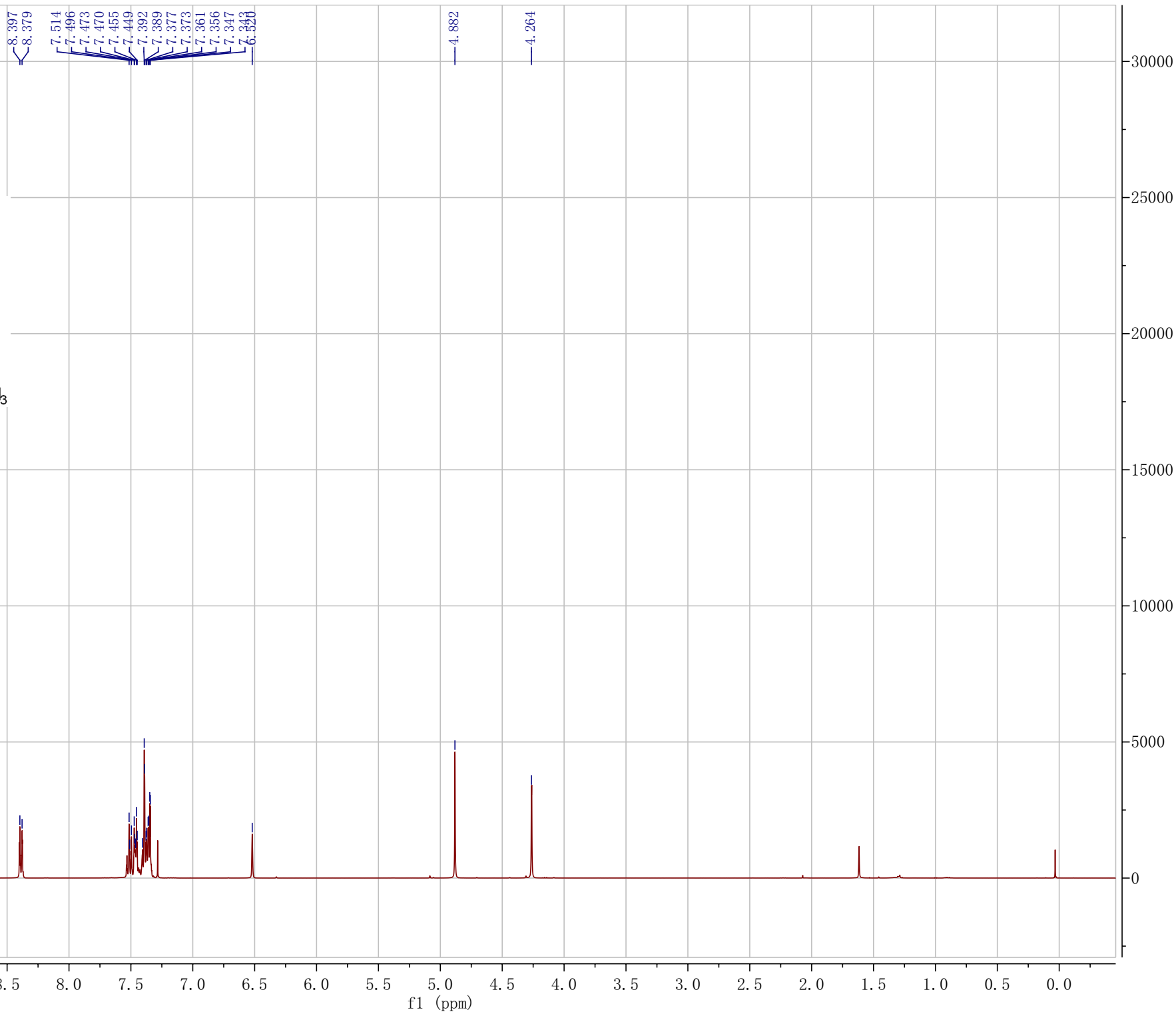
**4fa**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

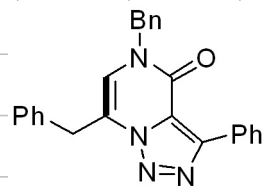


**4ga**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



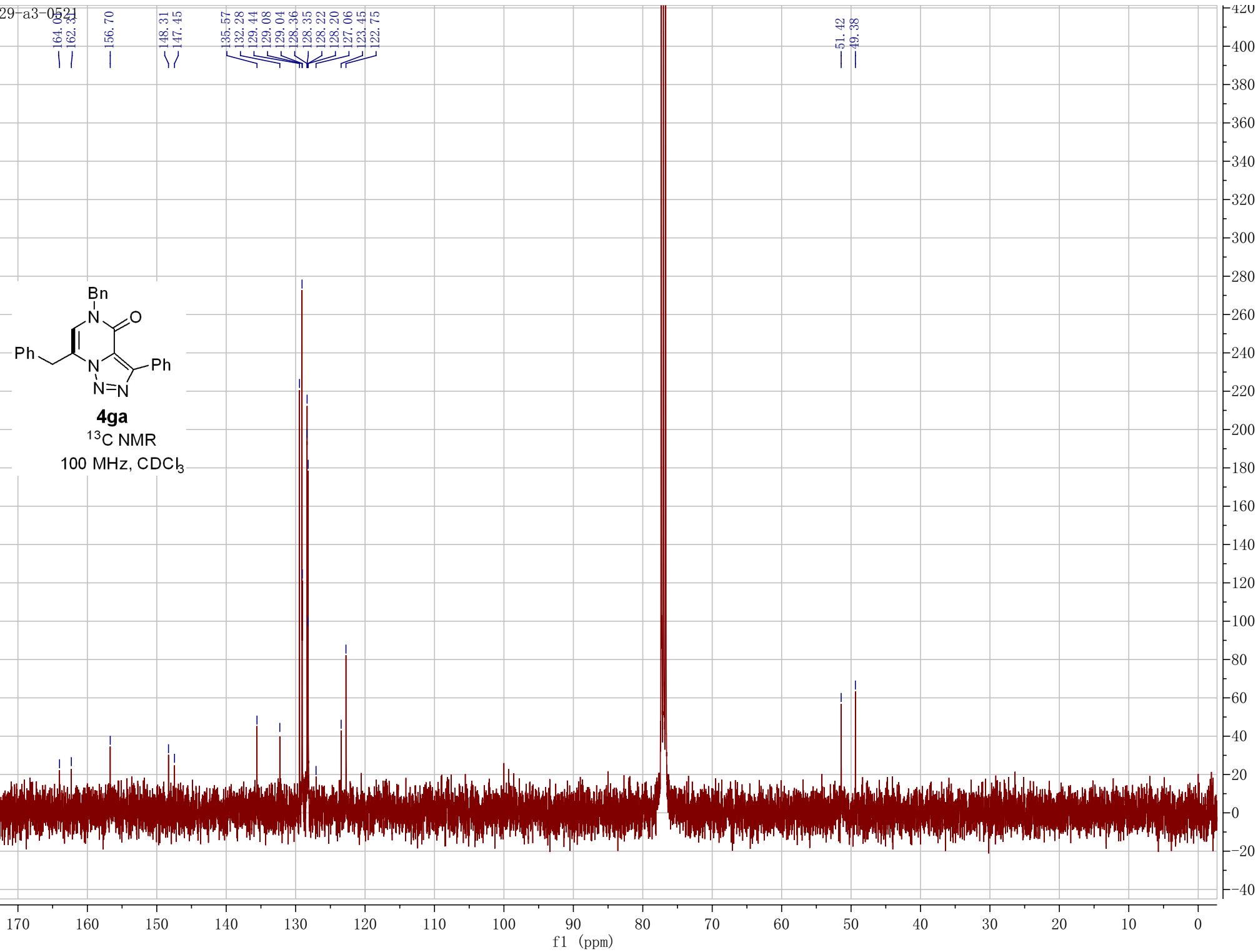
qkx-d129-a3-0521



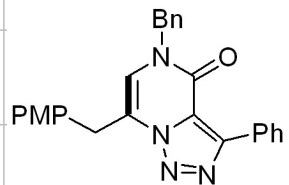
**4ga**

<sup>13</sup>C NMR

100 MHz, CDCl<sub>3</sub>

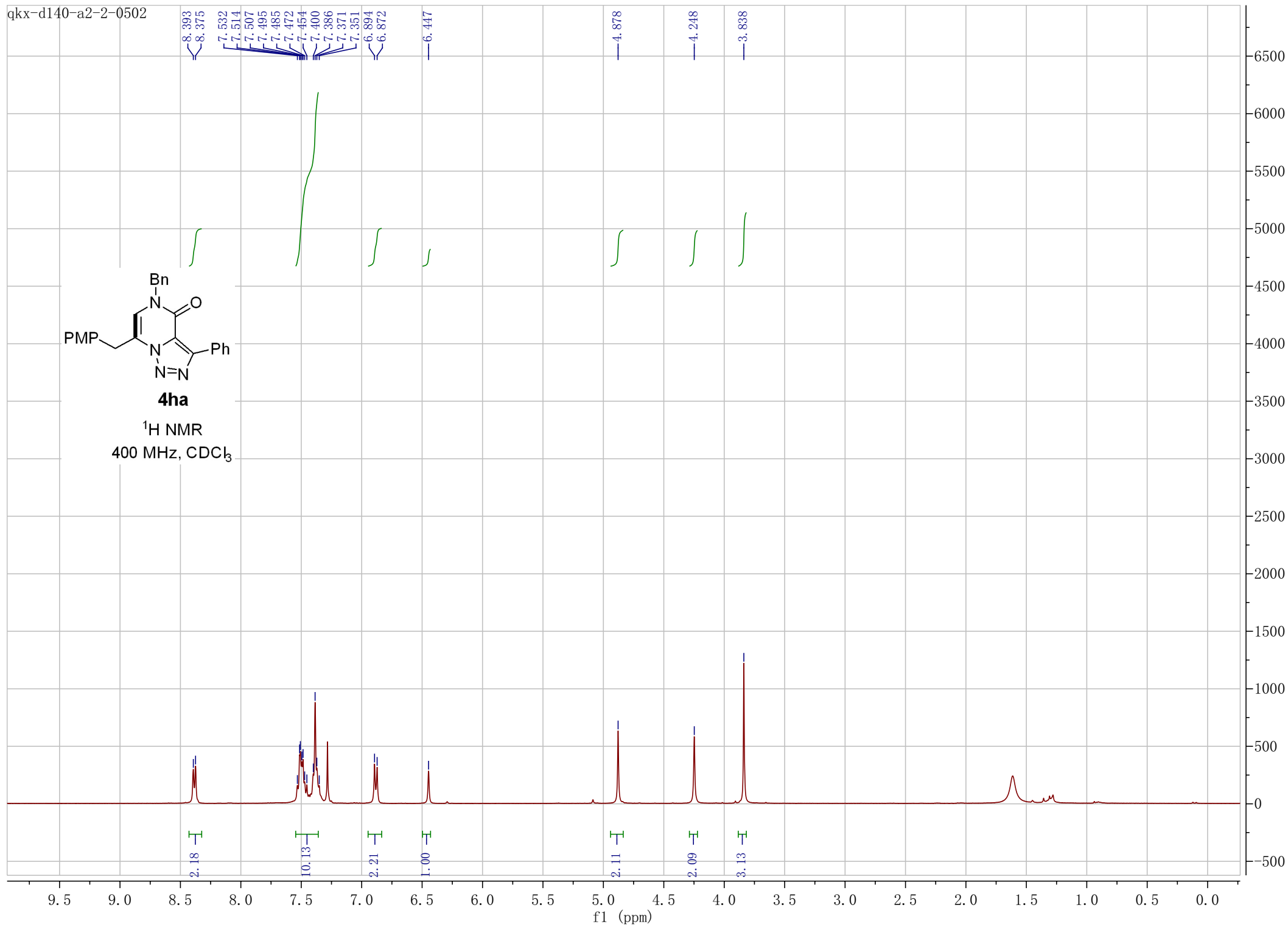


qkx-d140-a2-2-0502

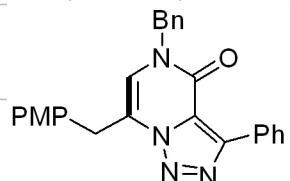


**4ha**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

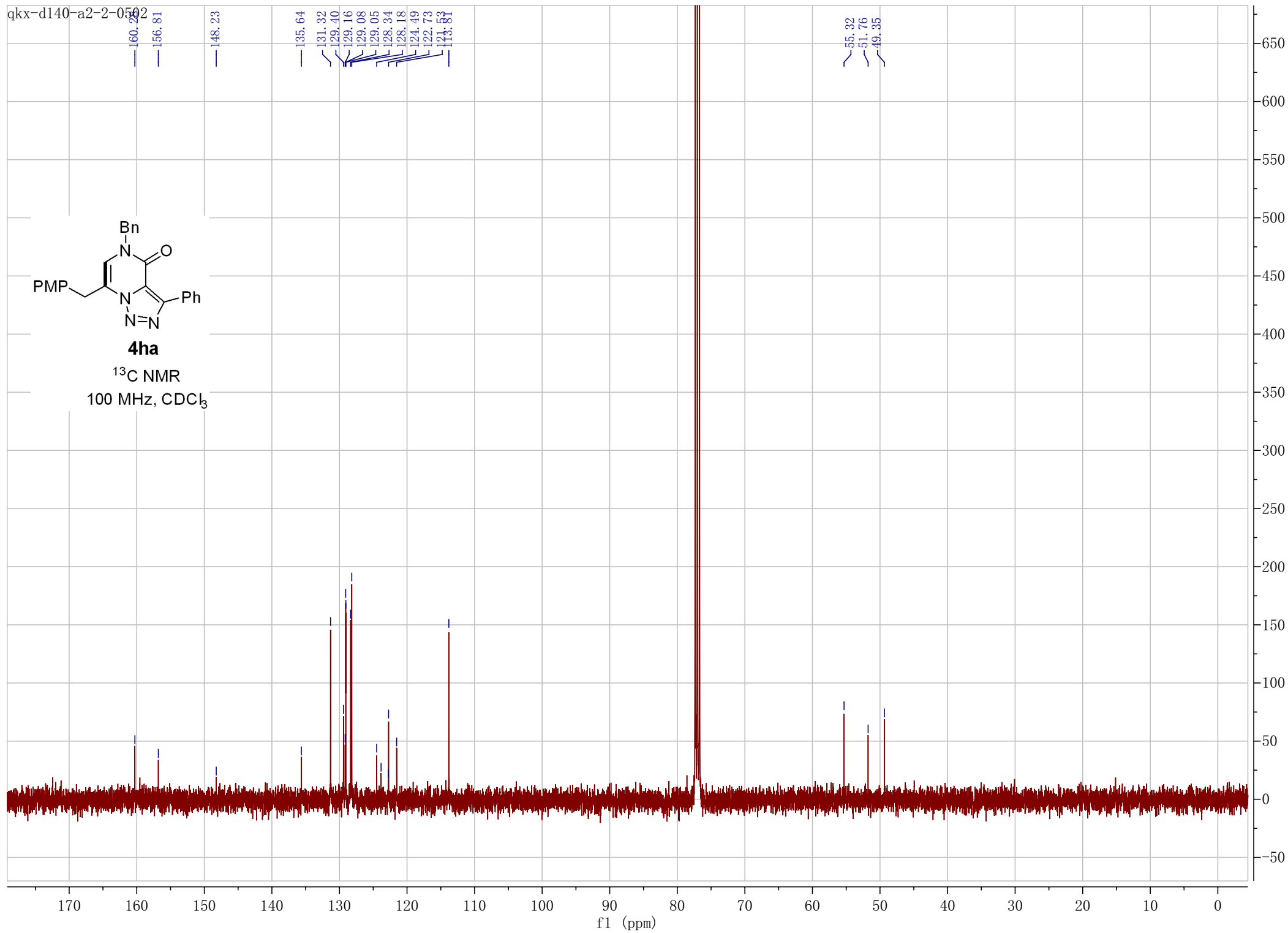


qkx-d140-a2-2-0502

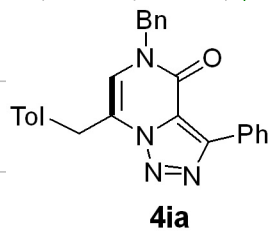


**4ha**

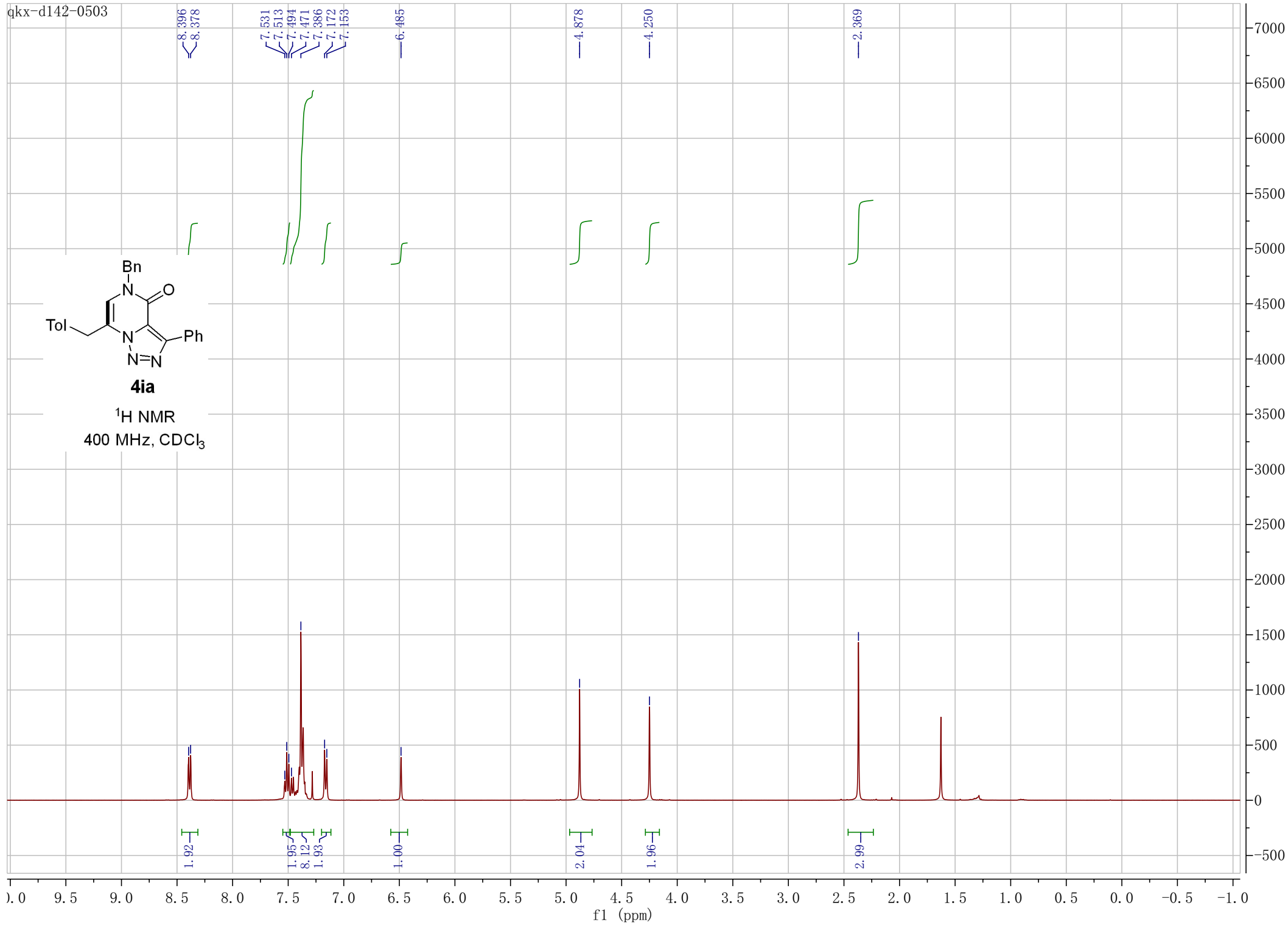
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



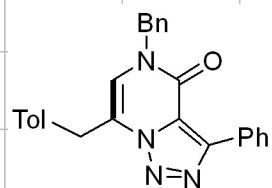
qkx-d142-0503



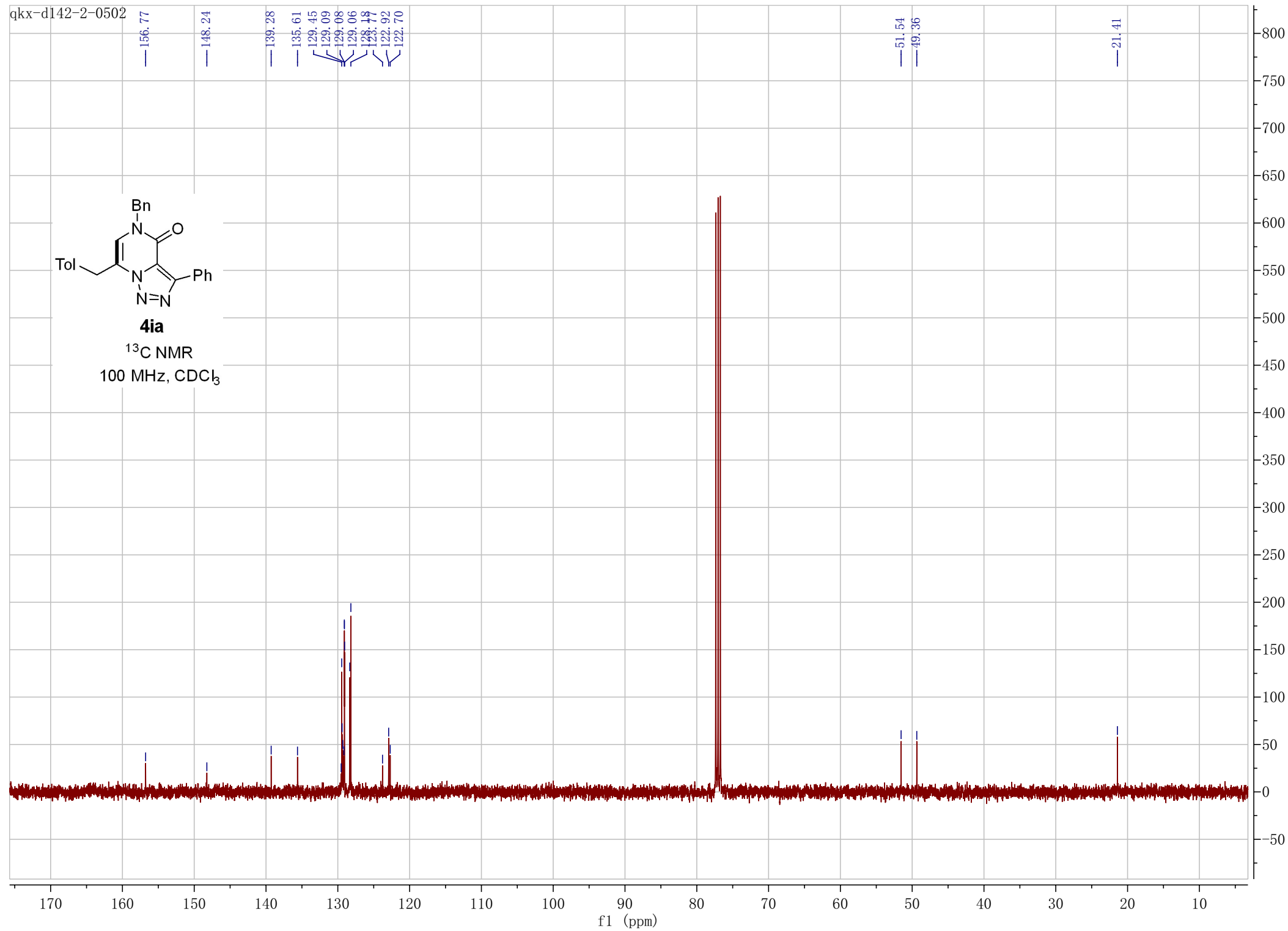
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



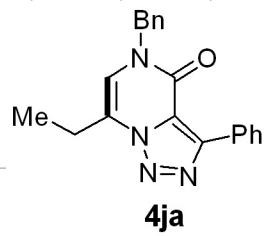
qkx-d142-2-0502



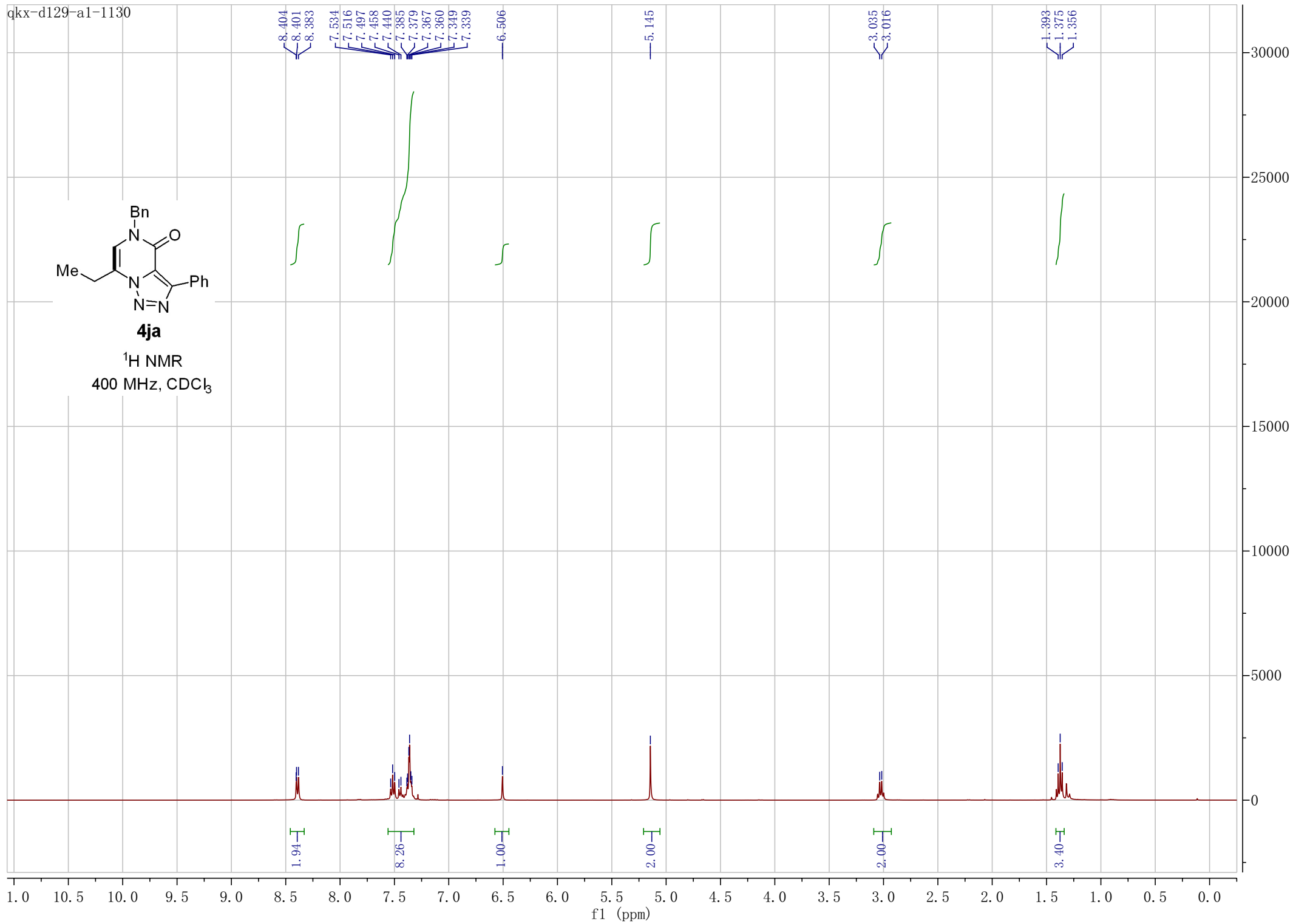
**4ia**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



qkx-d129-a1-1130

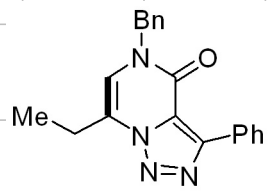


<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



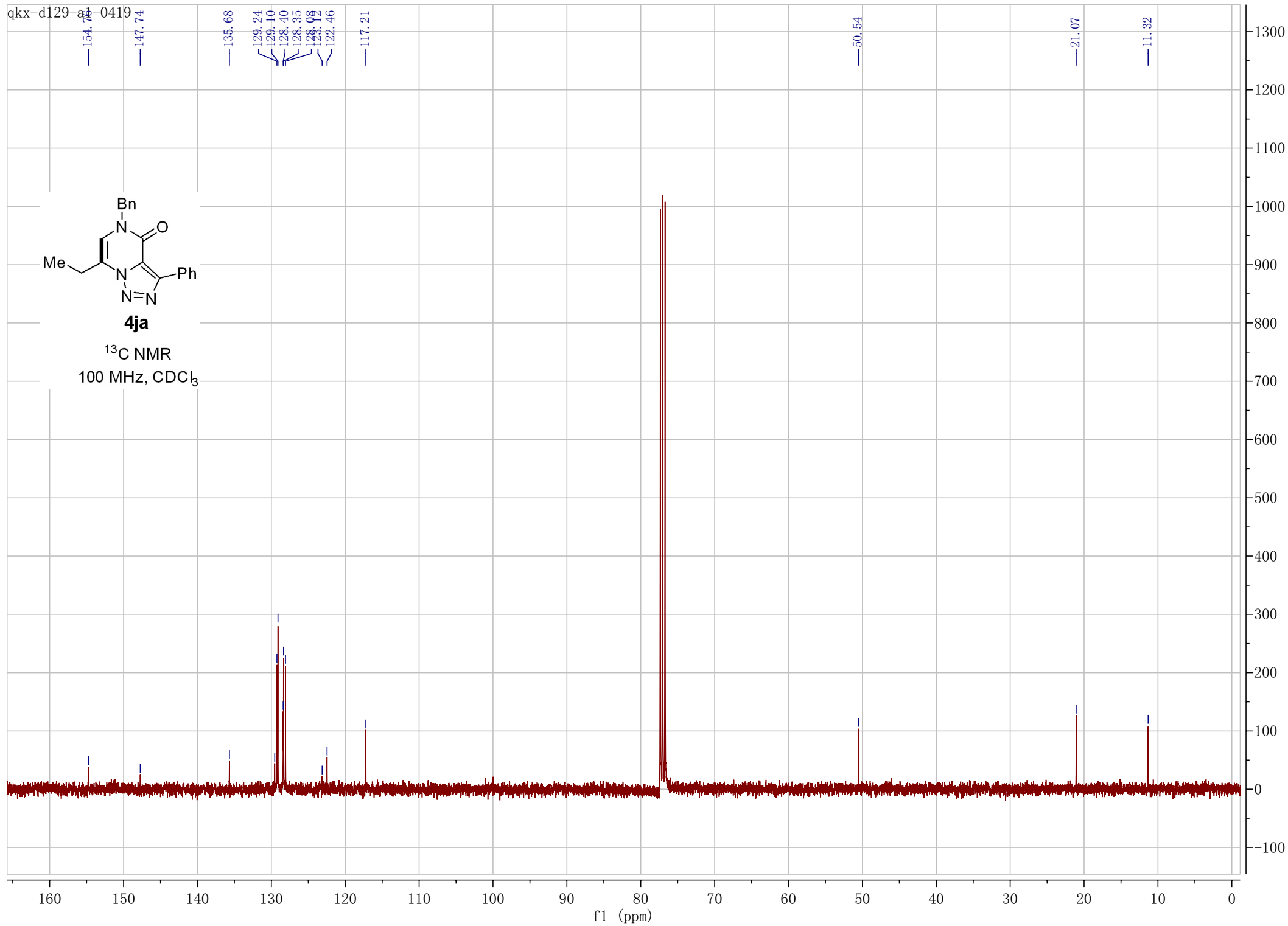


qkx-d129-a1-0419

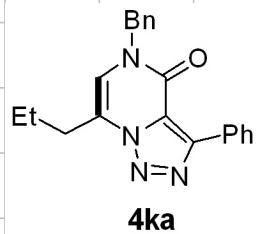


**4ja**

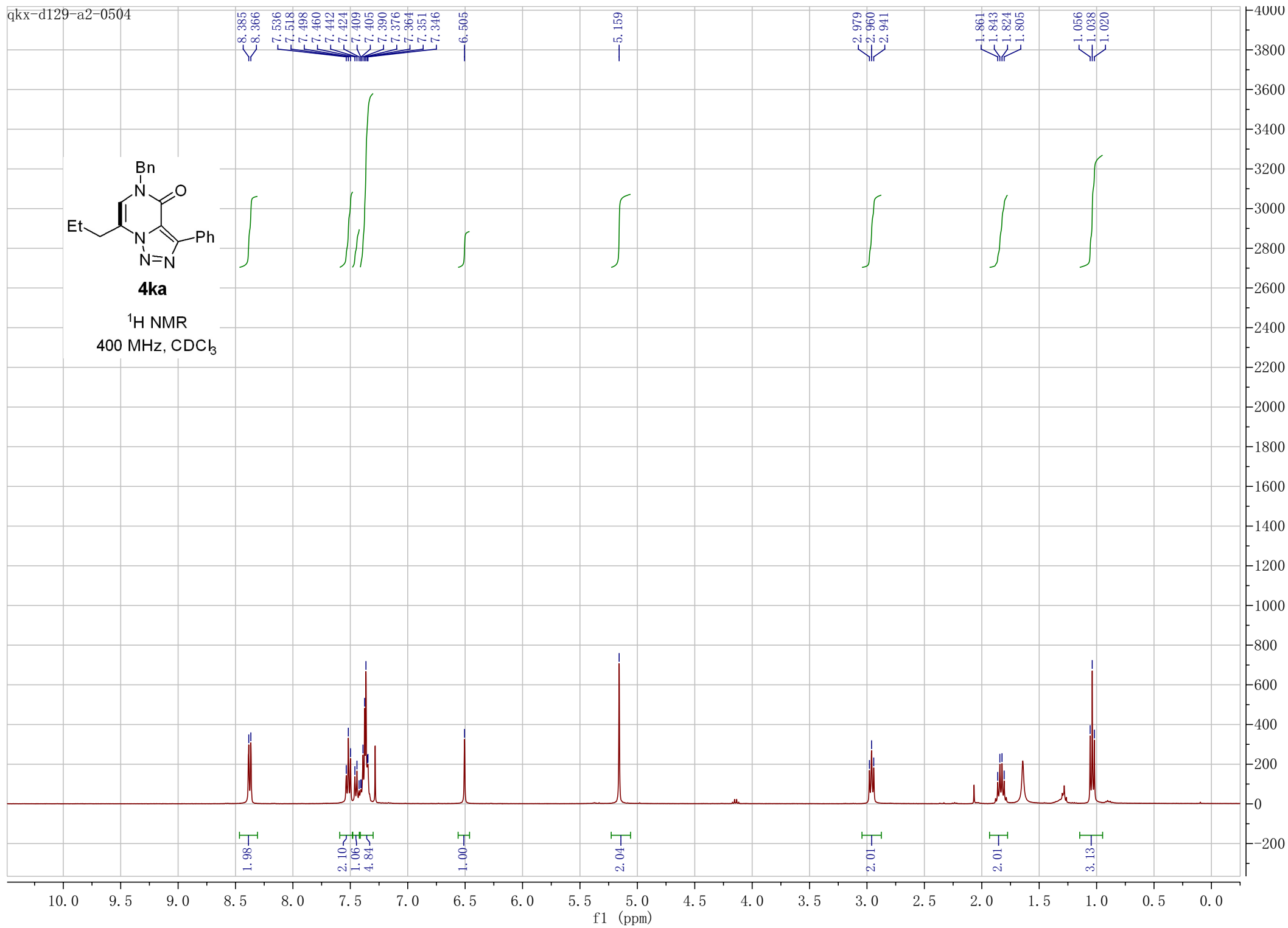
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



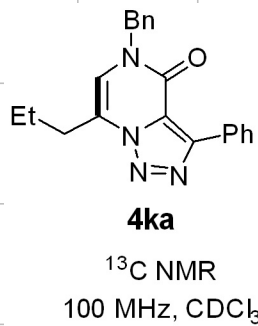
qkx-d129-a2-0504



<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

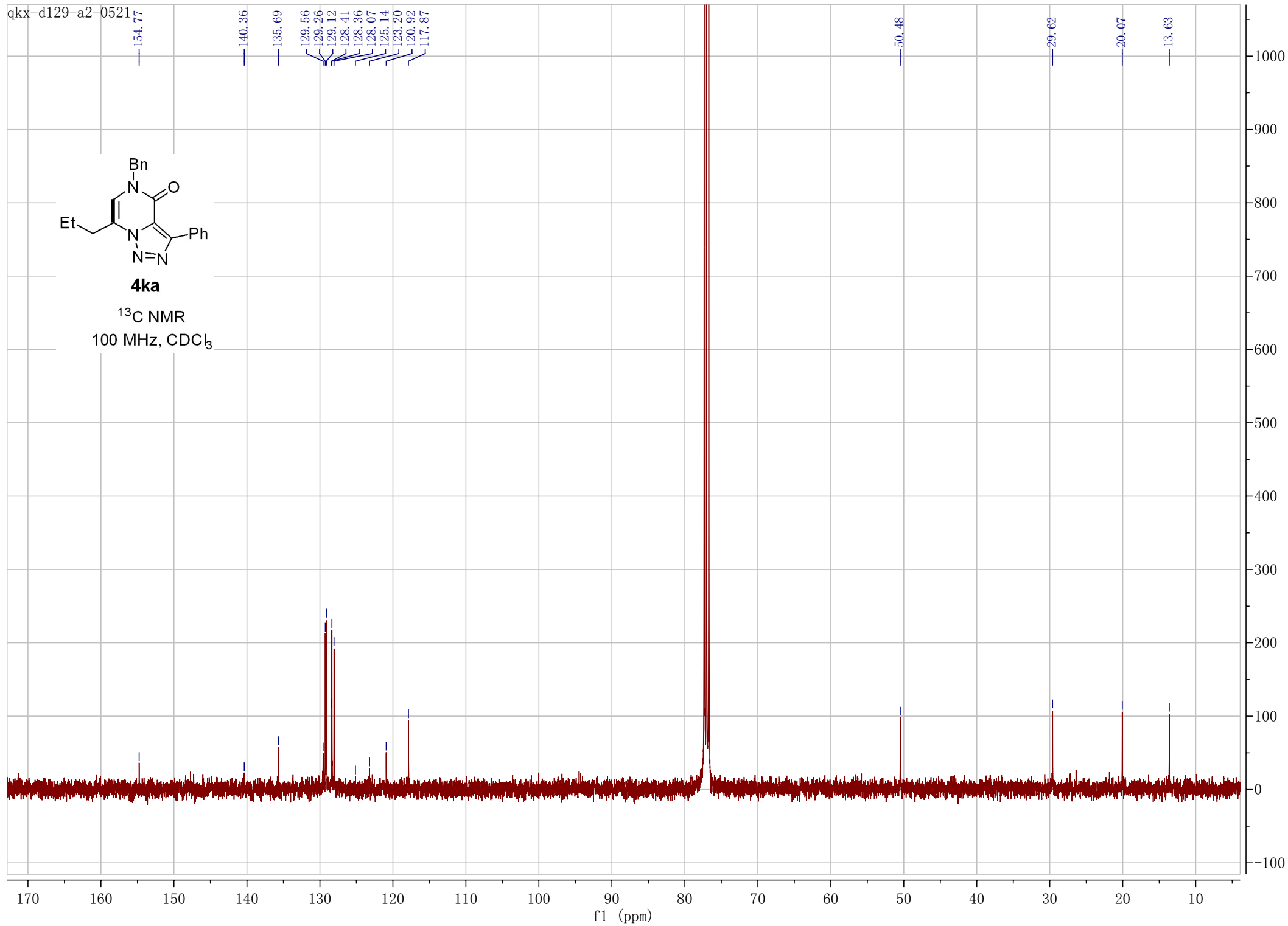


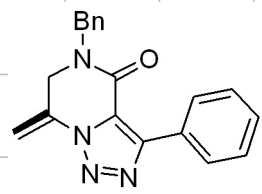
qkx-d129-a2-0521



154.77  
140.36  
135.69  
129.56  
129.26  
129.12  
128.41  
128.36  
128.07  
125.14  
123.20  
120.92  
117.87

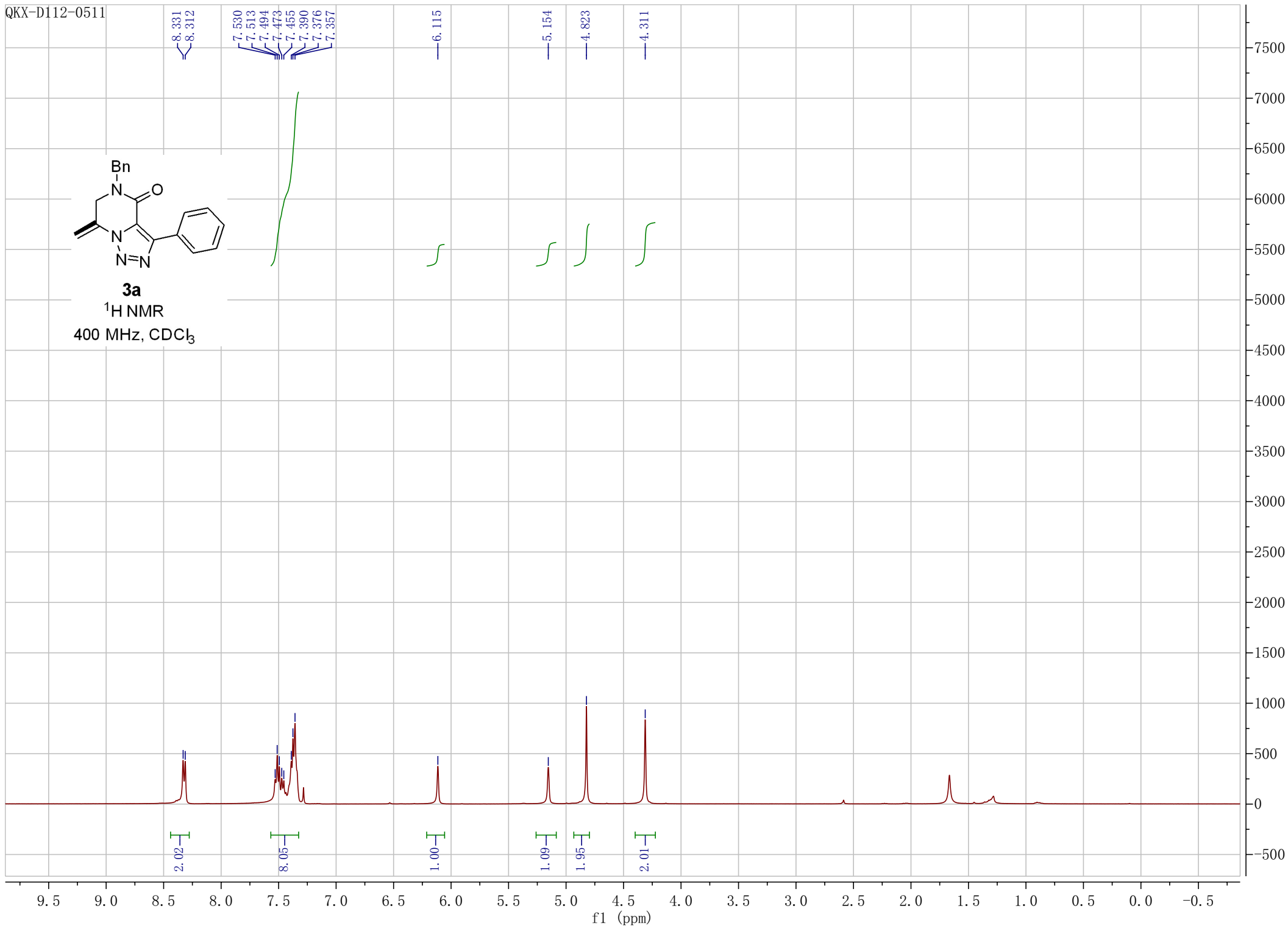
50.48  
29.62  
20.07  
13.63



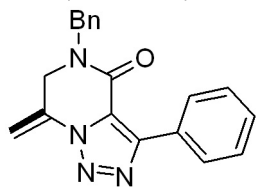


**3a**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

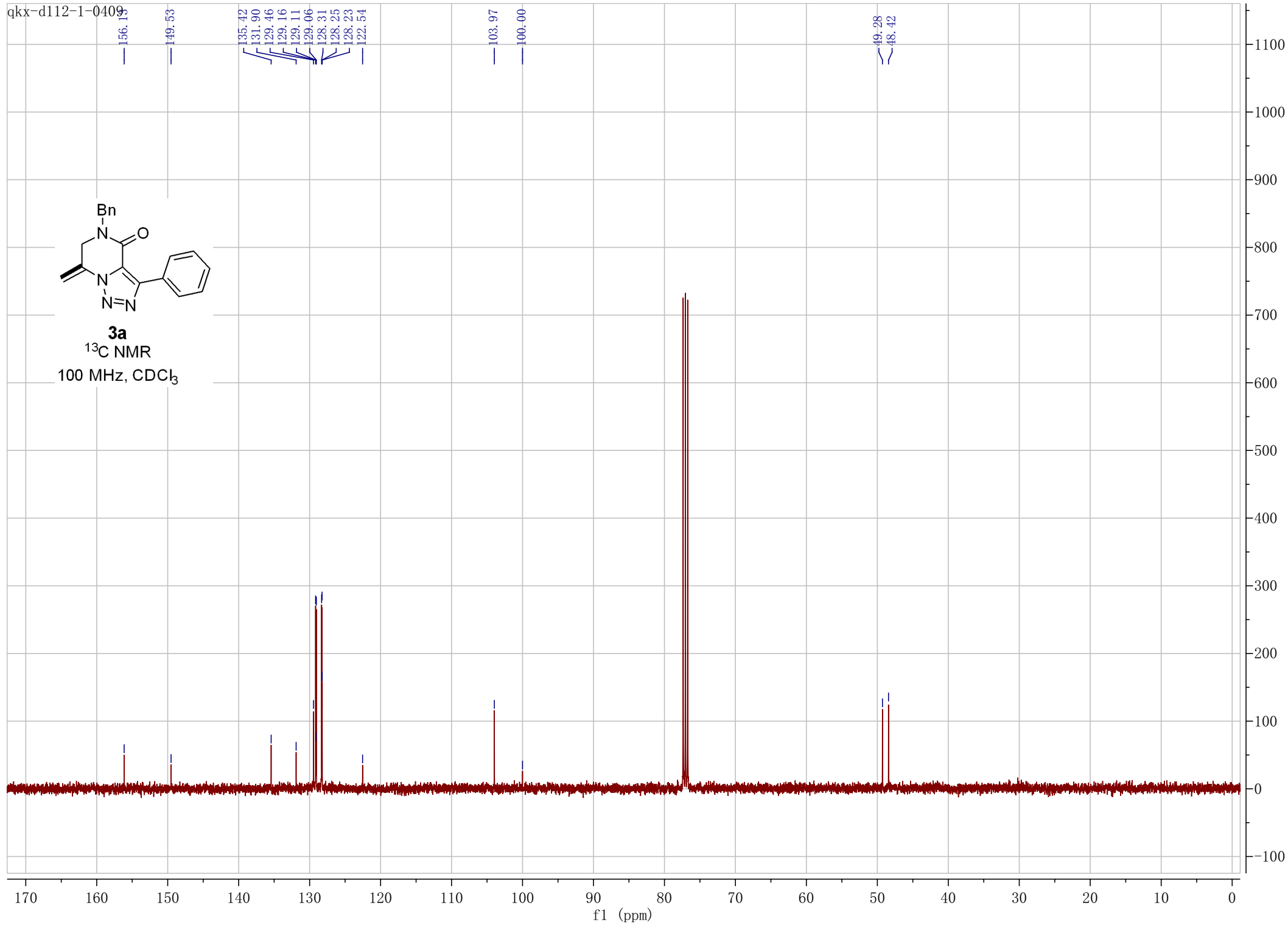


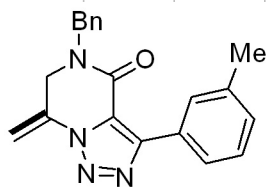
qkx-d112-1-0409



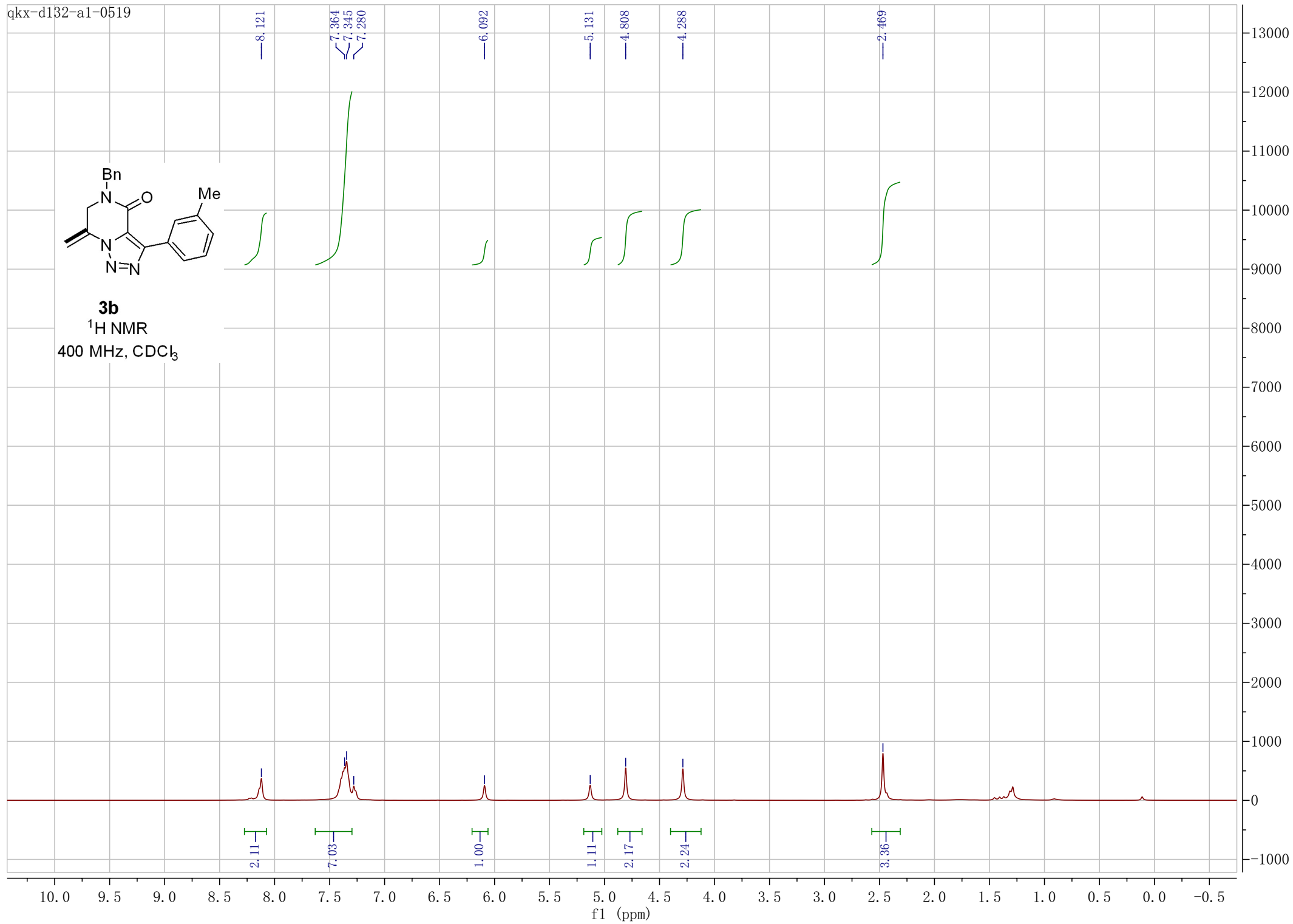
**3a**

$^{13}\text{C}$  NMR  
100 MHz,  $\text{CDCl}_3$

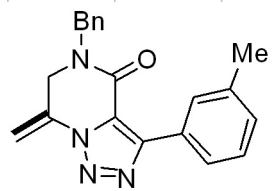




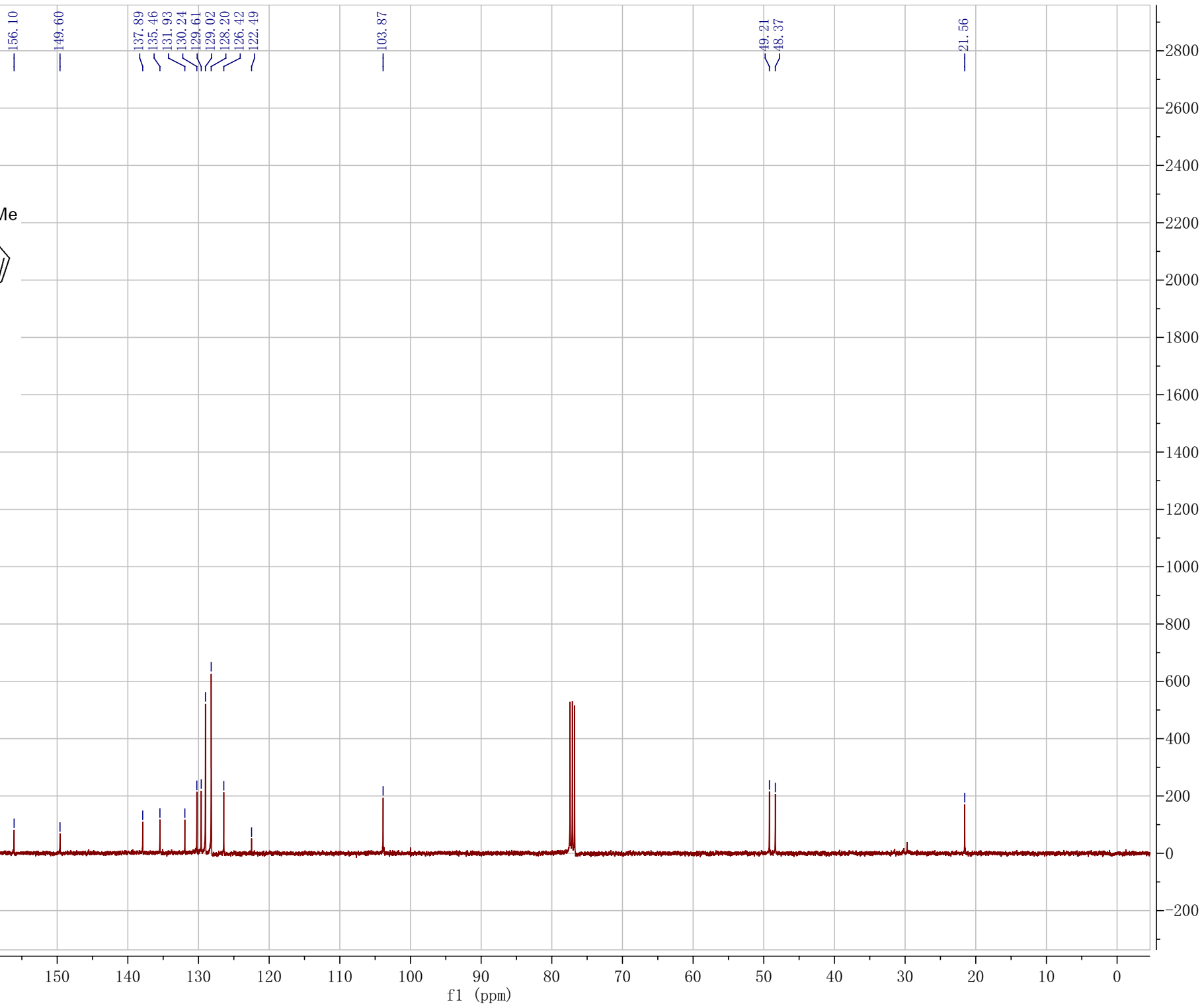
**3b**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

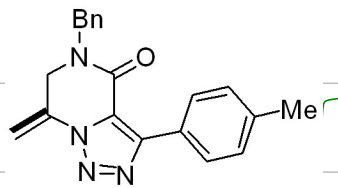


qkx-d132-a1-0519



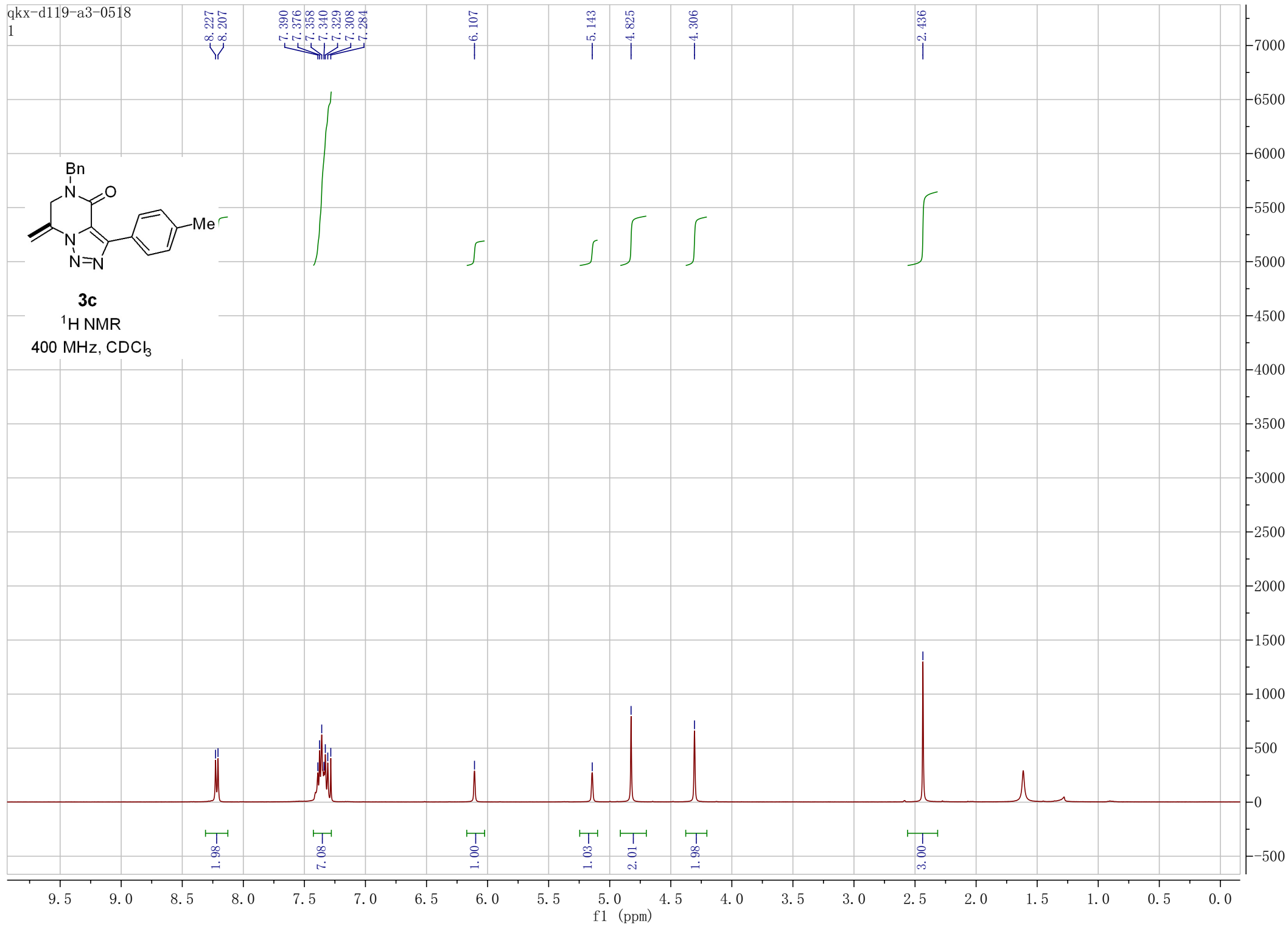
**3b**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



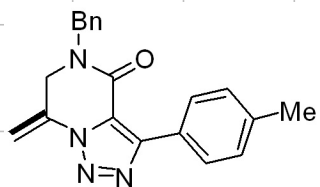


**3c**

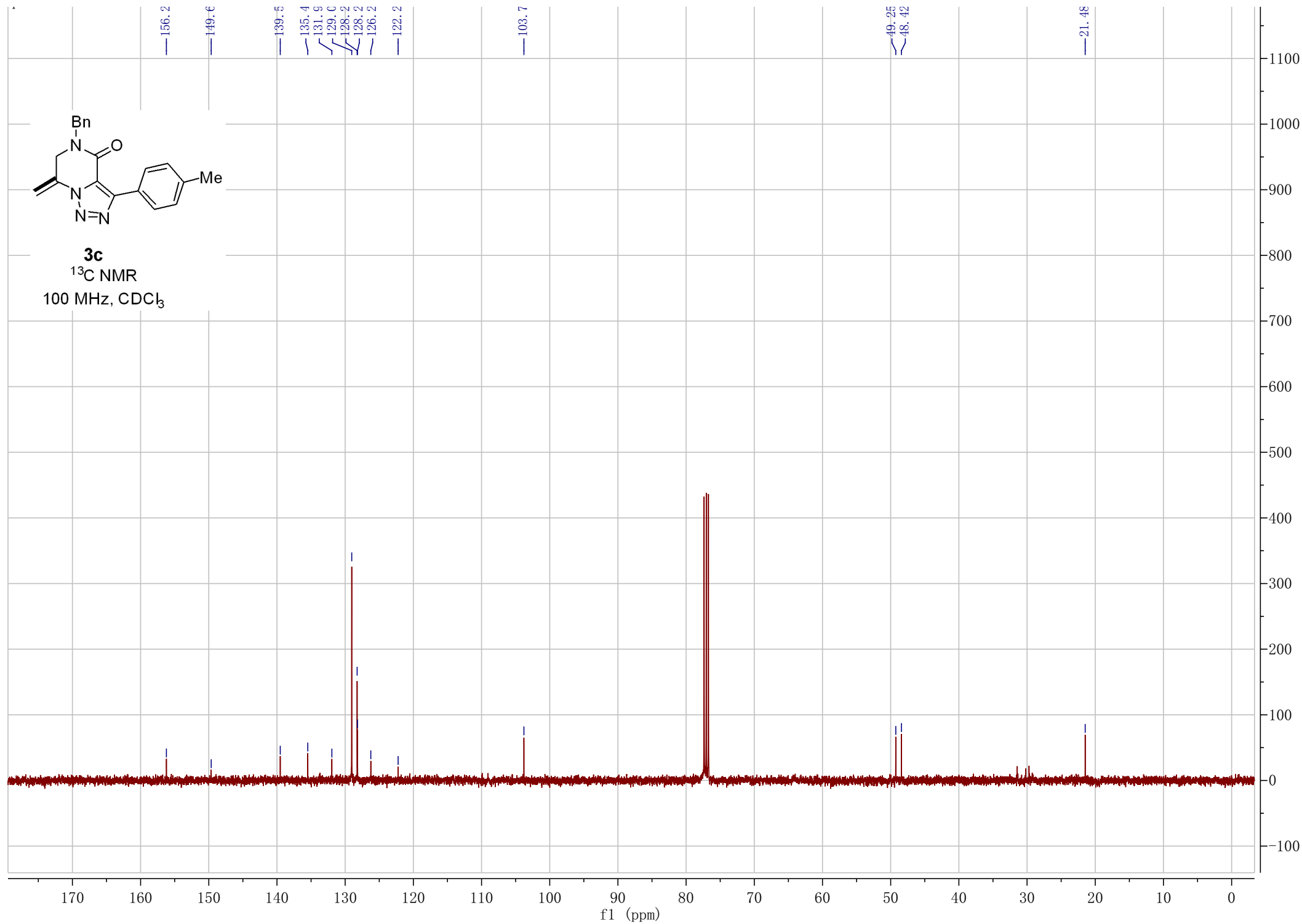
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



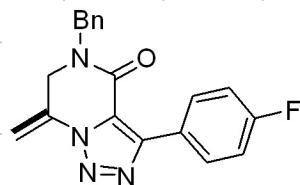




**3c**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

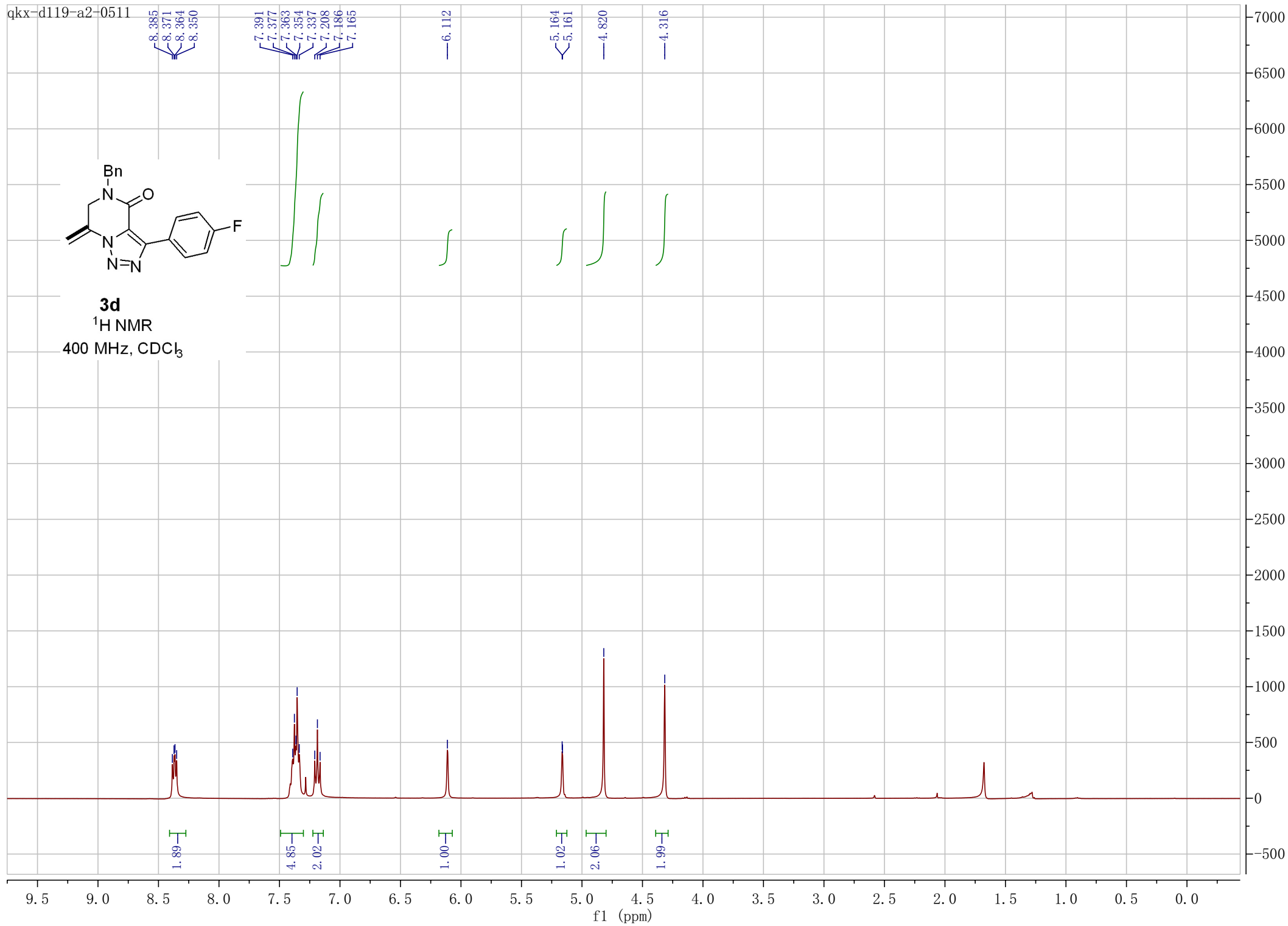


qkx-d119-a2-0511

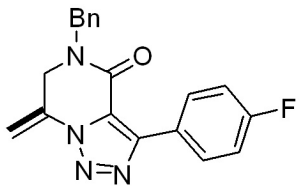


**3d**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

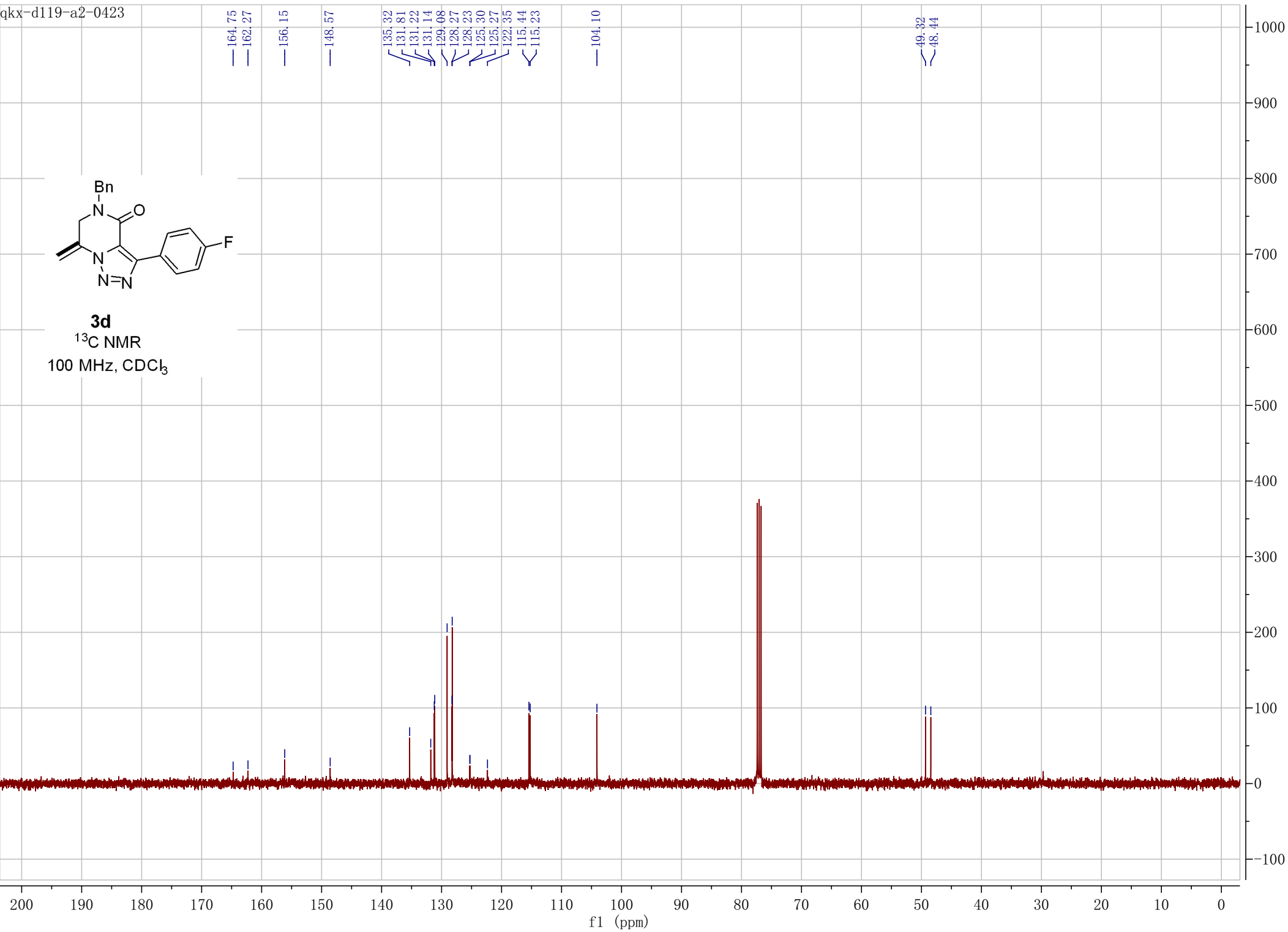
8.385  
8.371  
8.364  
8.350  
7.391  
7.377  
7.363  
7.354  
7.337  
7.208  
7.186  
7.165  
6.112  
5.164  
5.161  
4.820  
4.316



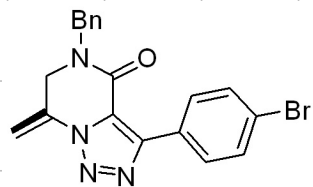
qkx-d119-a2-0423



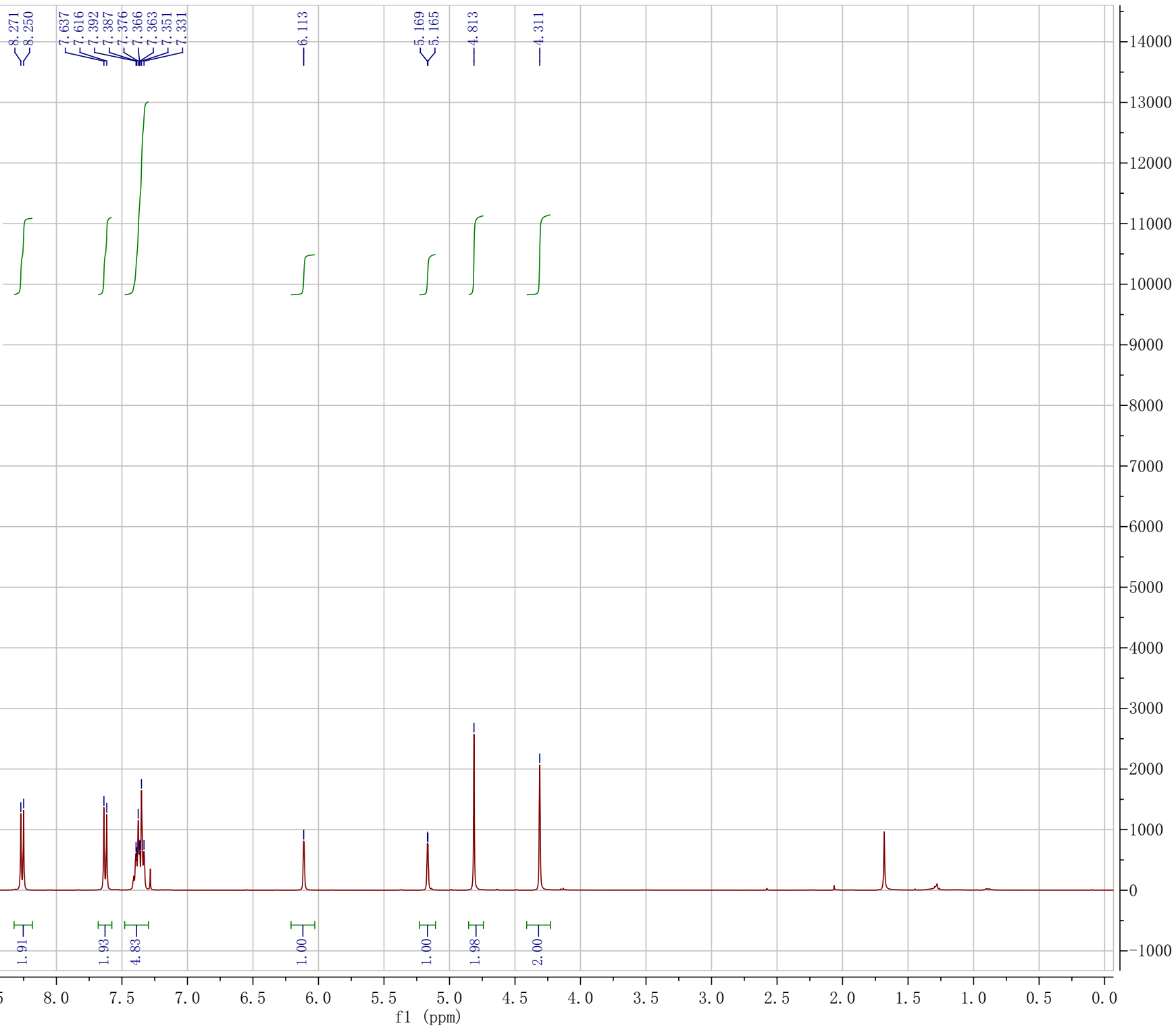
**3d**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



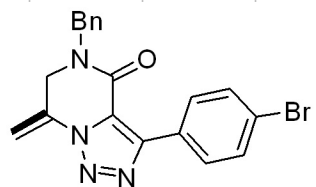
qkx-d137-0605



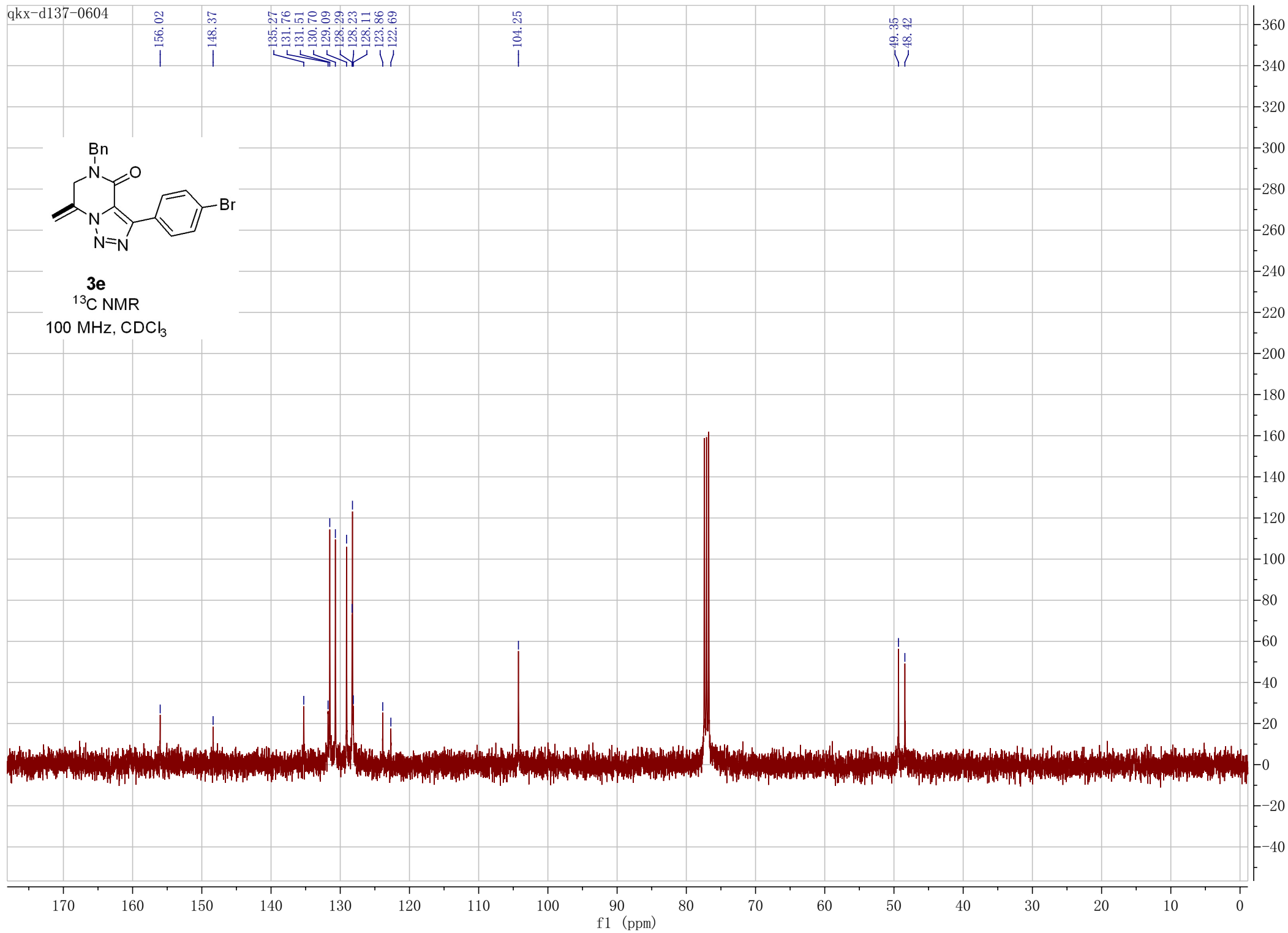
**3e**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



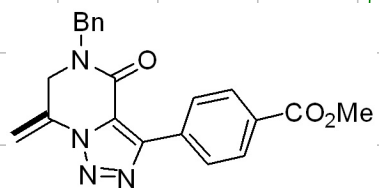
qkx-d137-0604



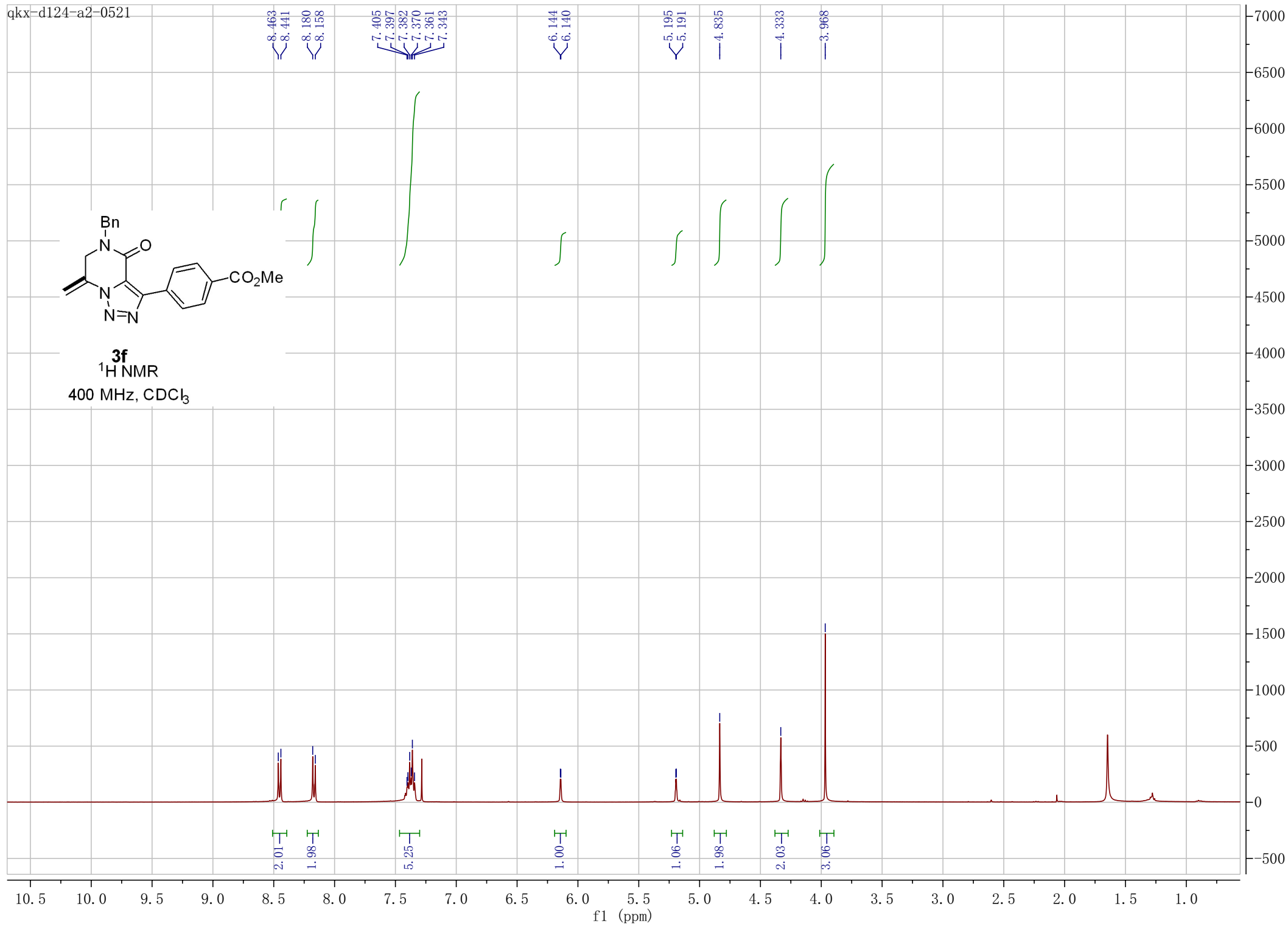
**3e**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



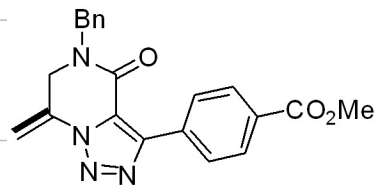
qkx-d124-a2-0521



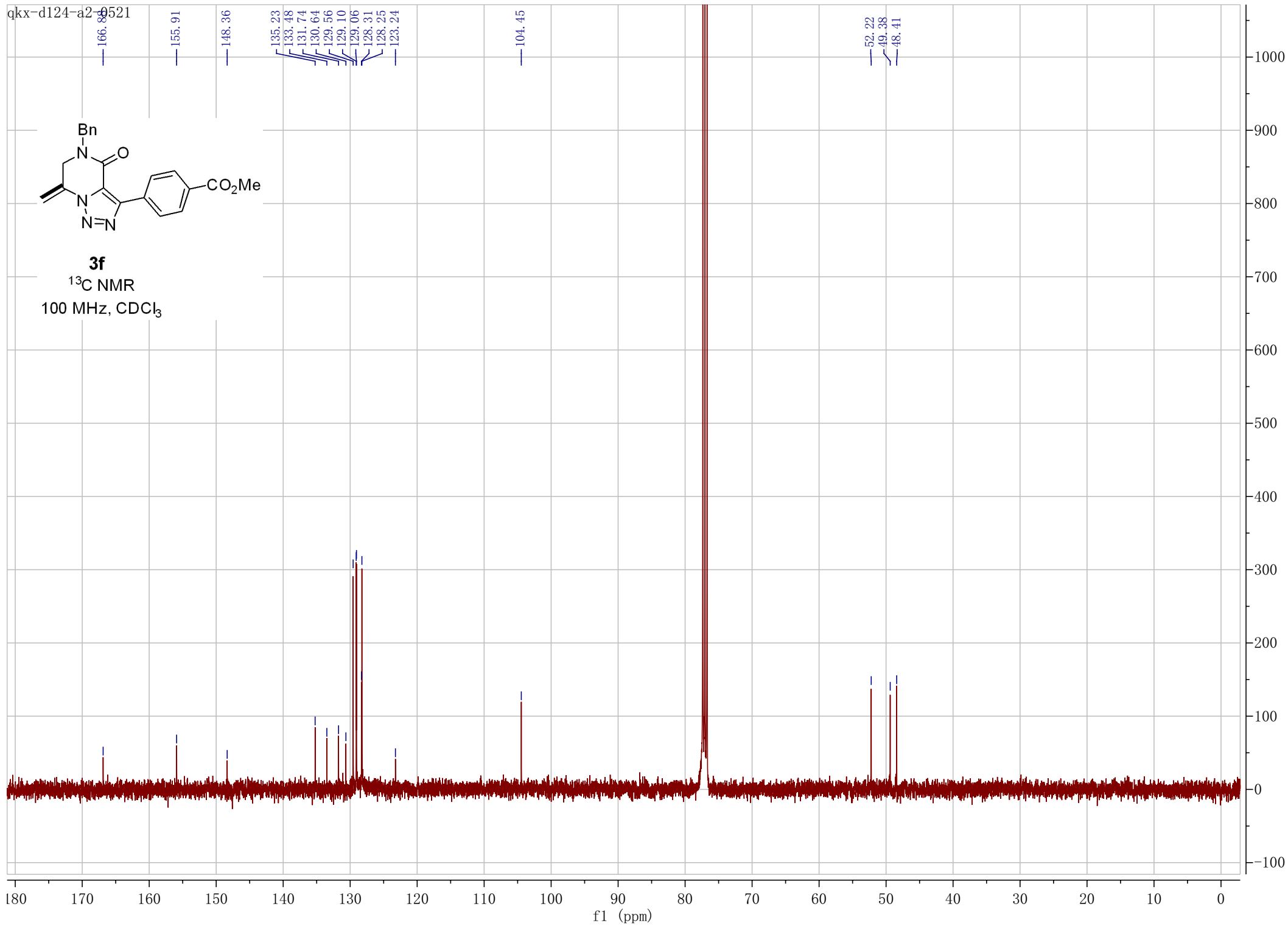
**3f**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



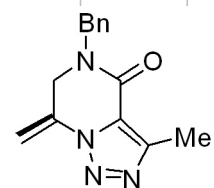
qkx-d124-a2-0521



**3f**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

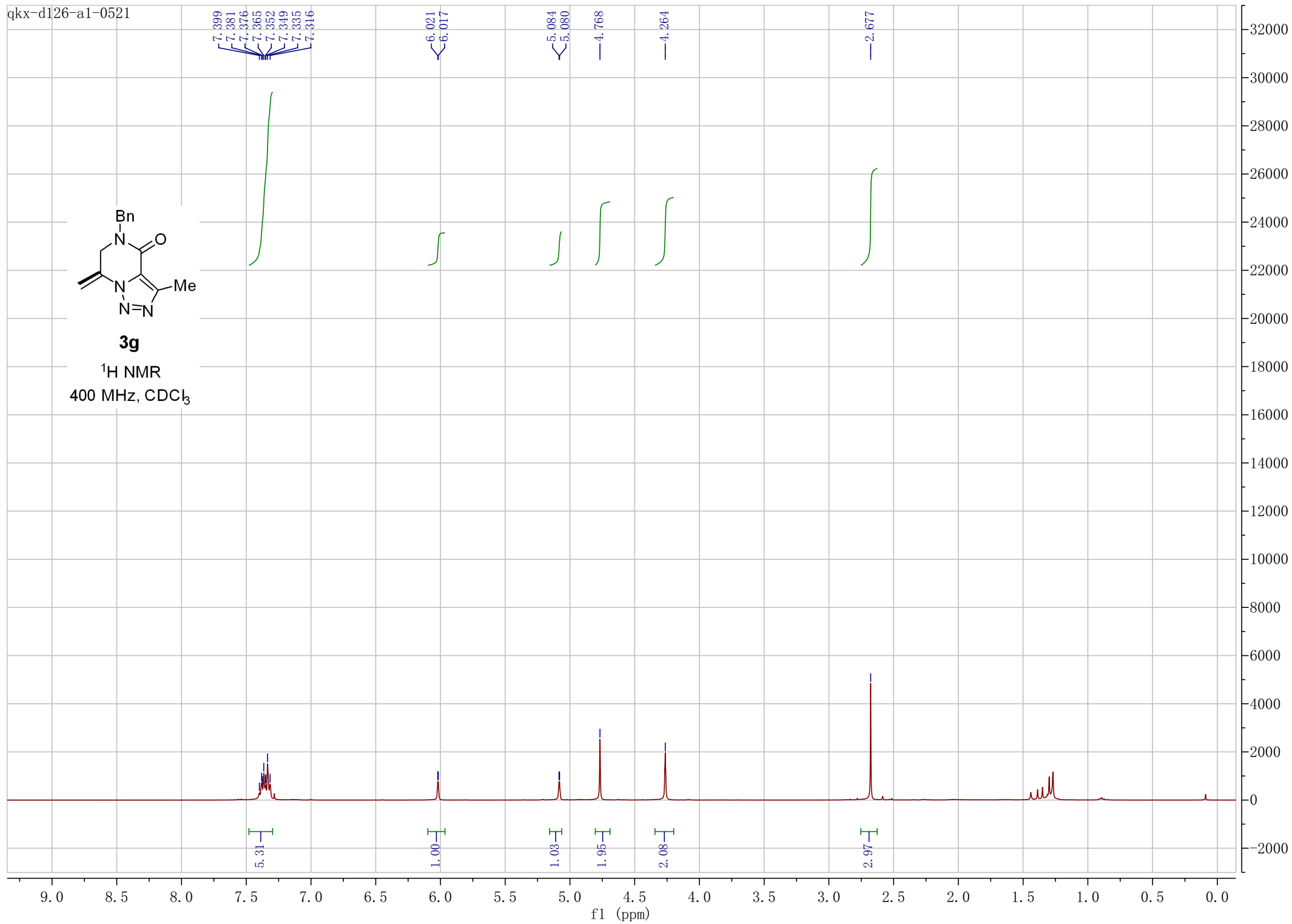


qkx-d126-a1-0521



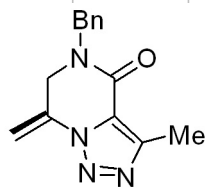
**3g**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



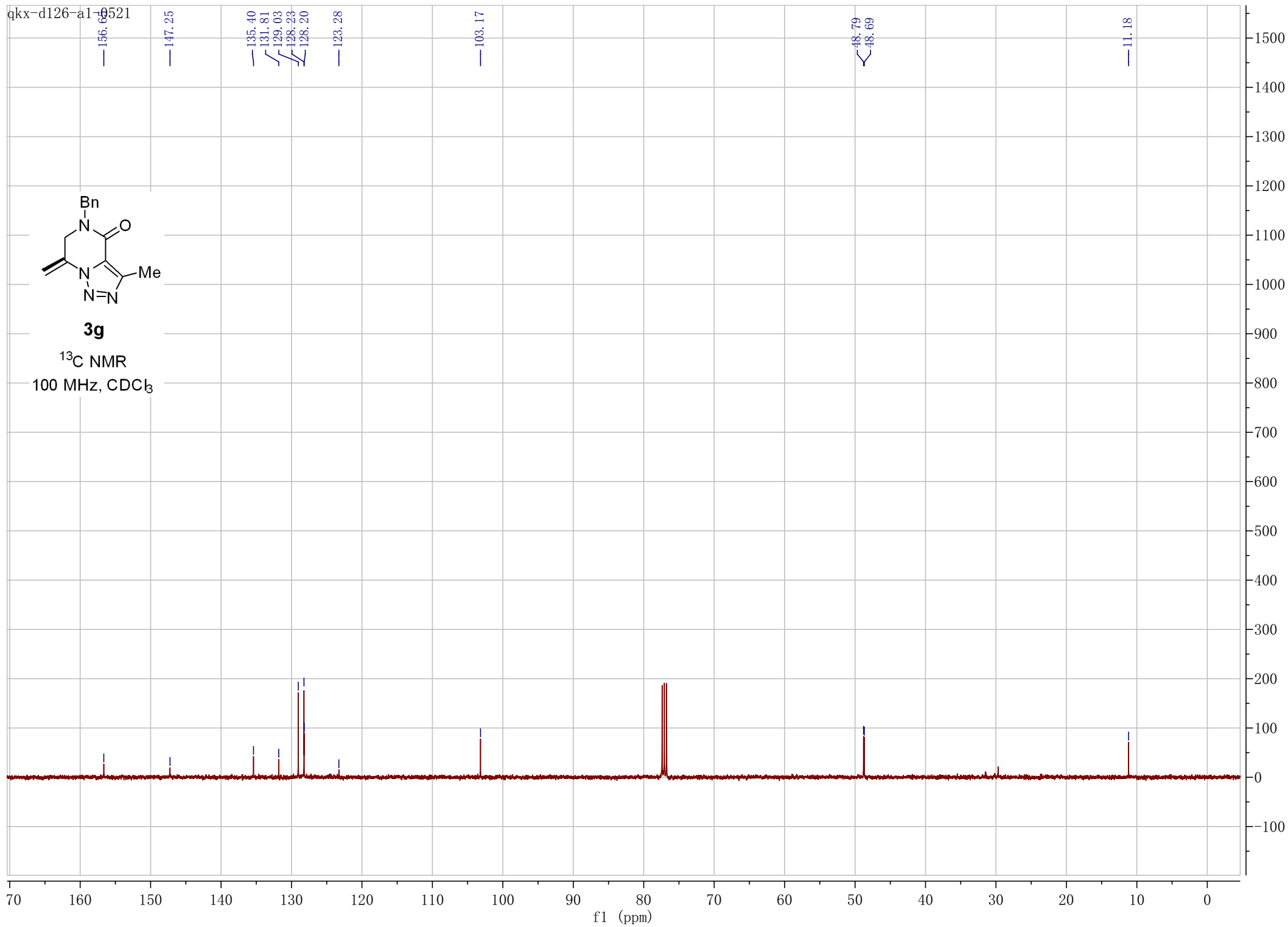


qkx-d126-a1-0521

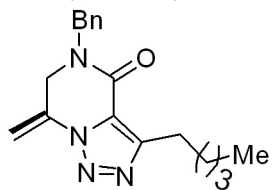


**3g**

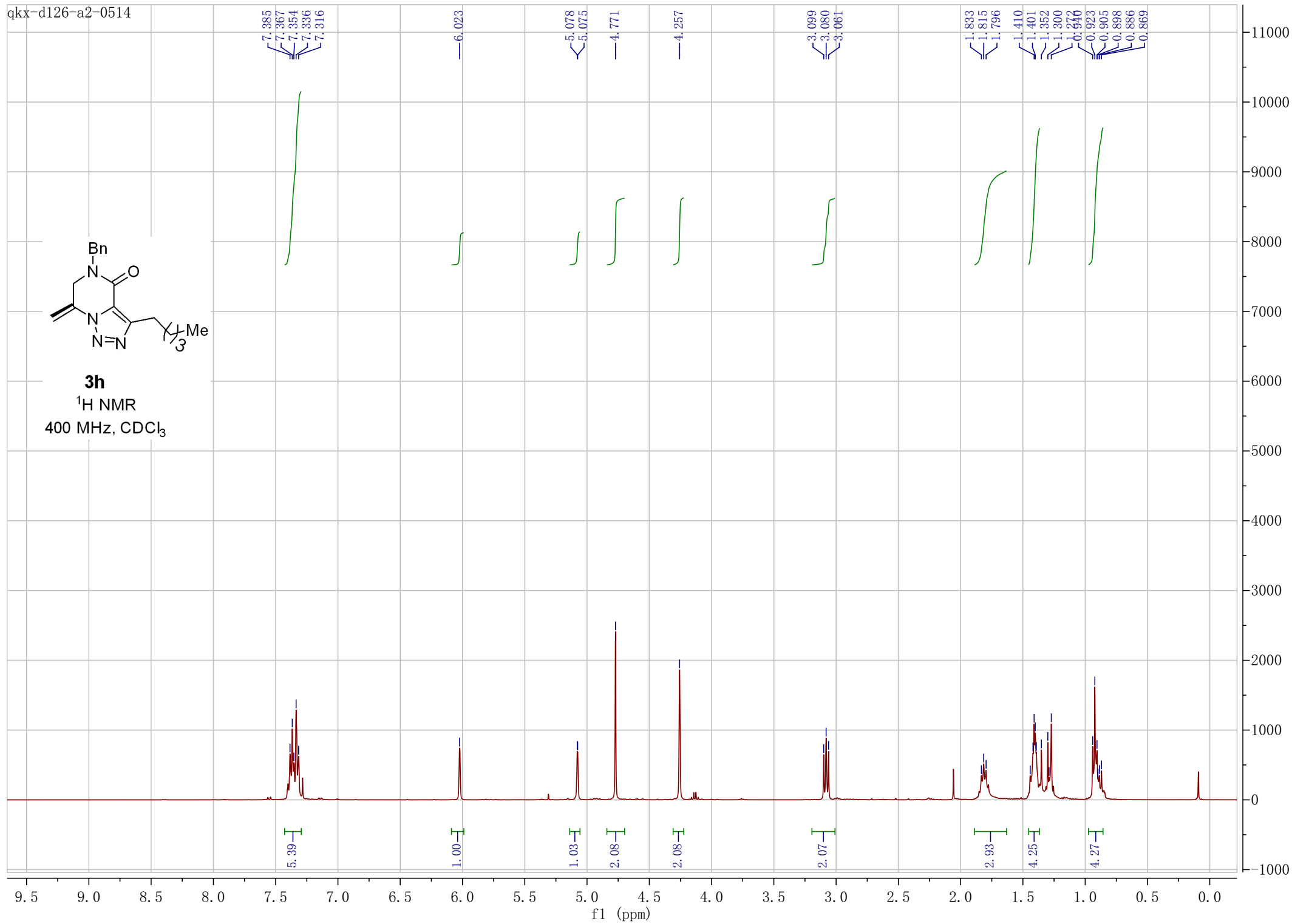
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



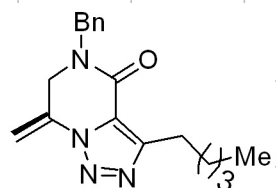
qkx-d126-a2-0514



**3h**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

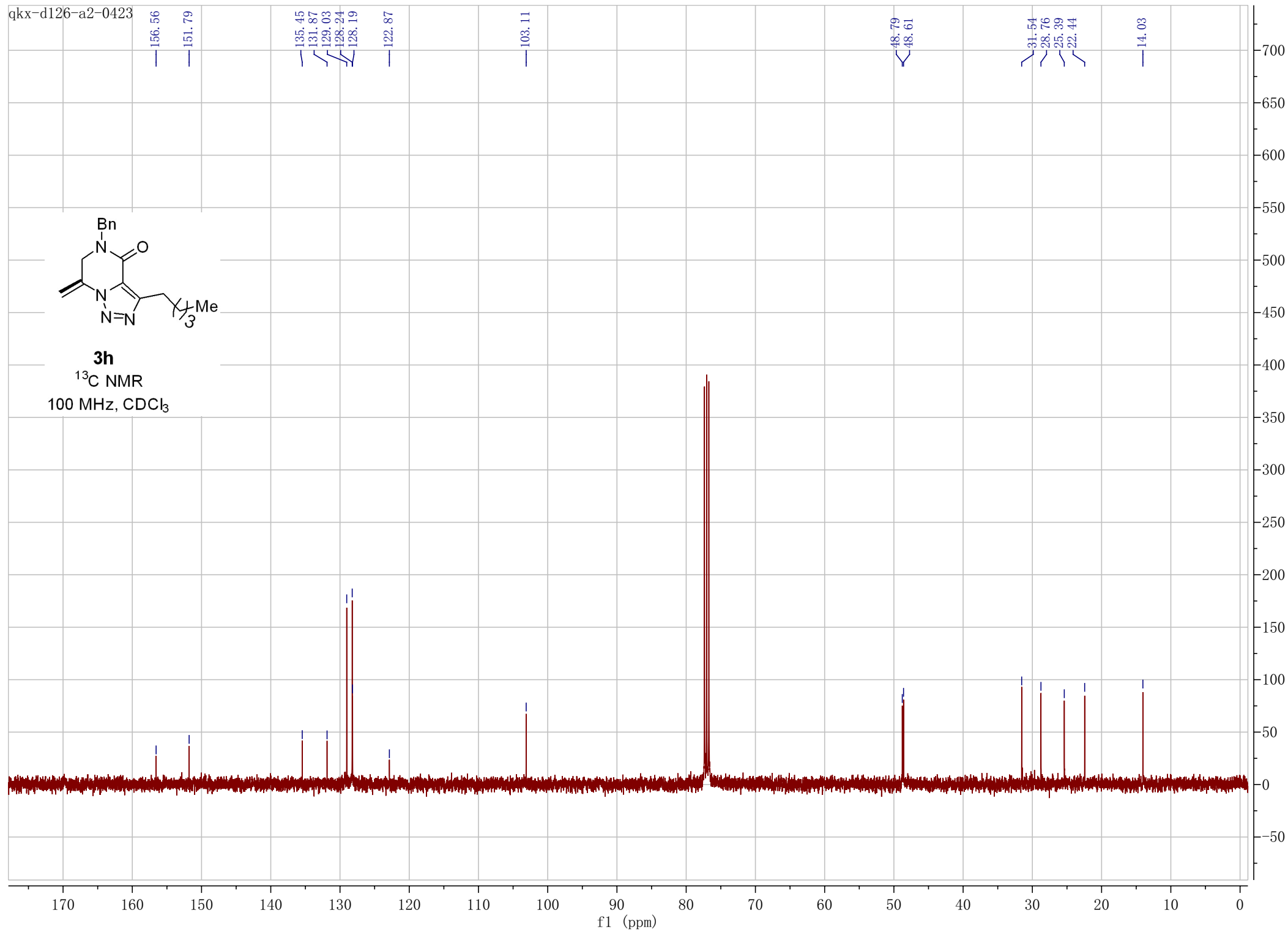


qkx-d126-a2-0423

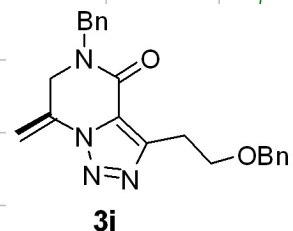


**3h**

$^{13}\text{C}$  NMR  
100 MHz,  $\text{CDCl}_3$



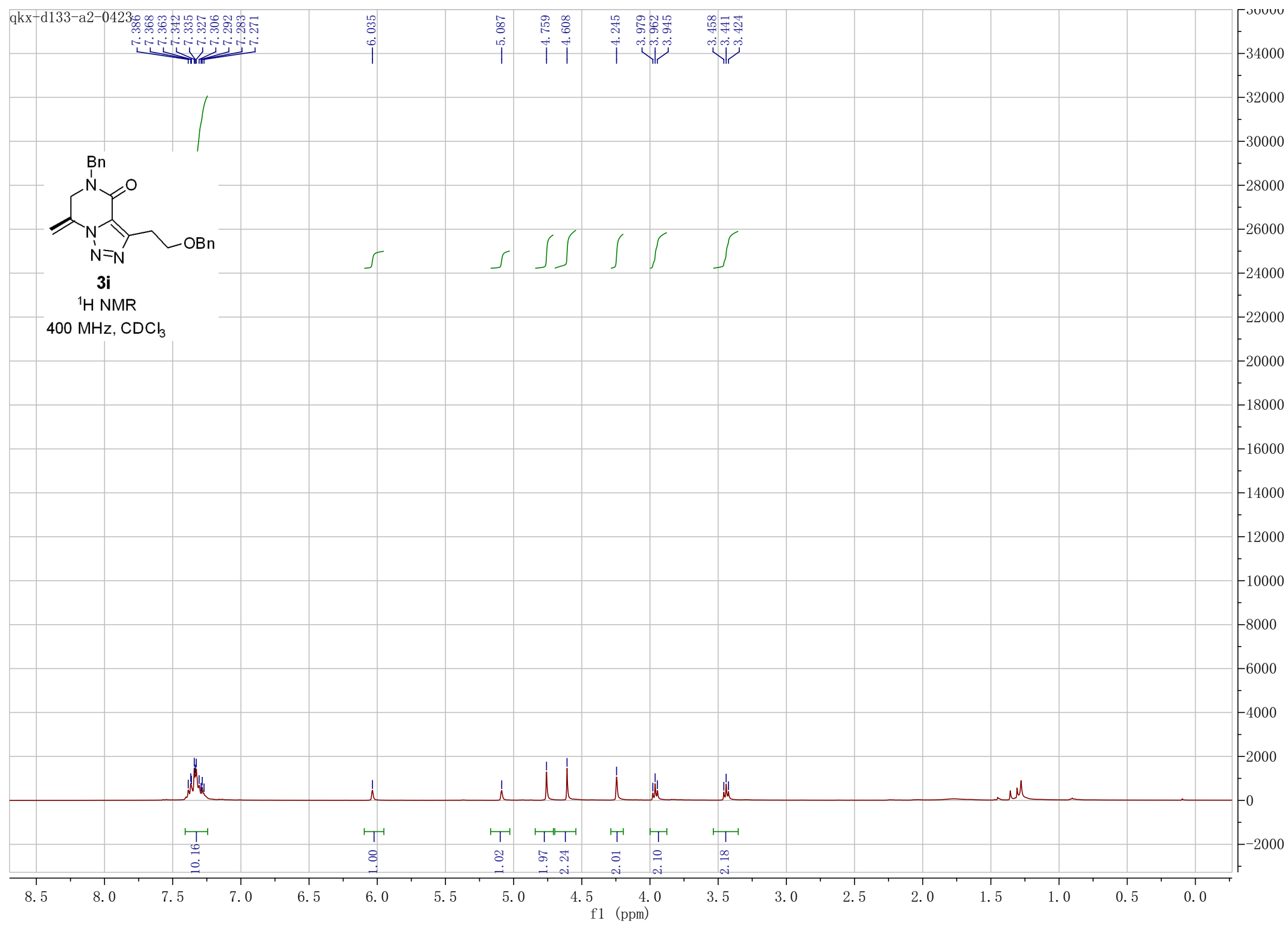
qkx-d133-a2-0423



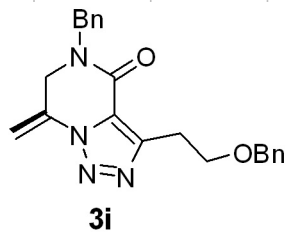
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

7.386  
7.368  
7.363  
7.342  
7.335  
7.327  
7.306  
7.292  
7.283  
7.271

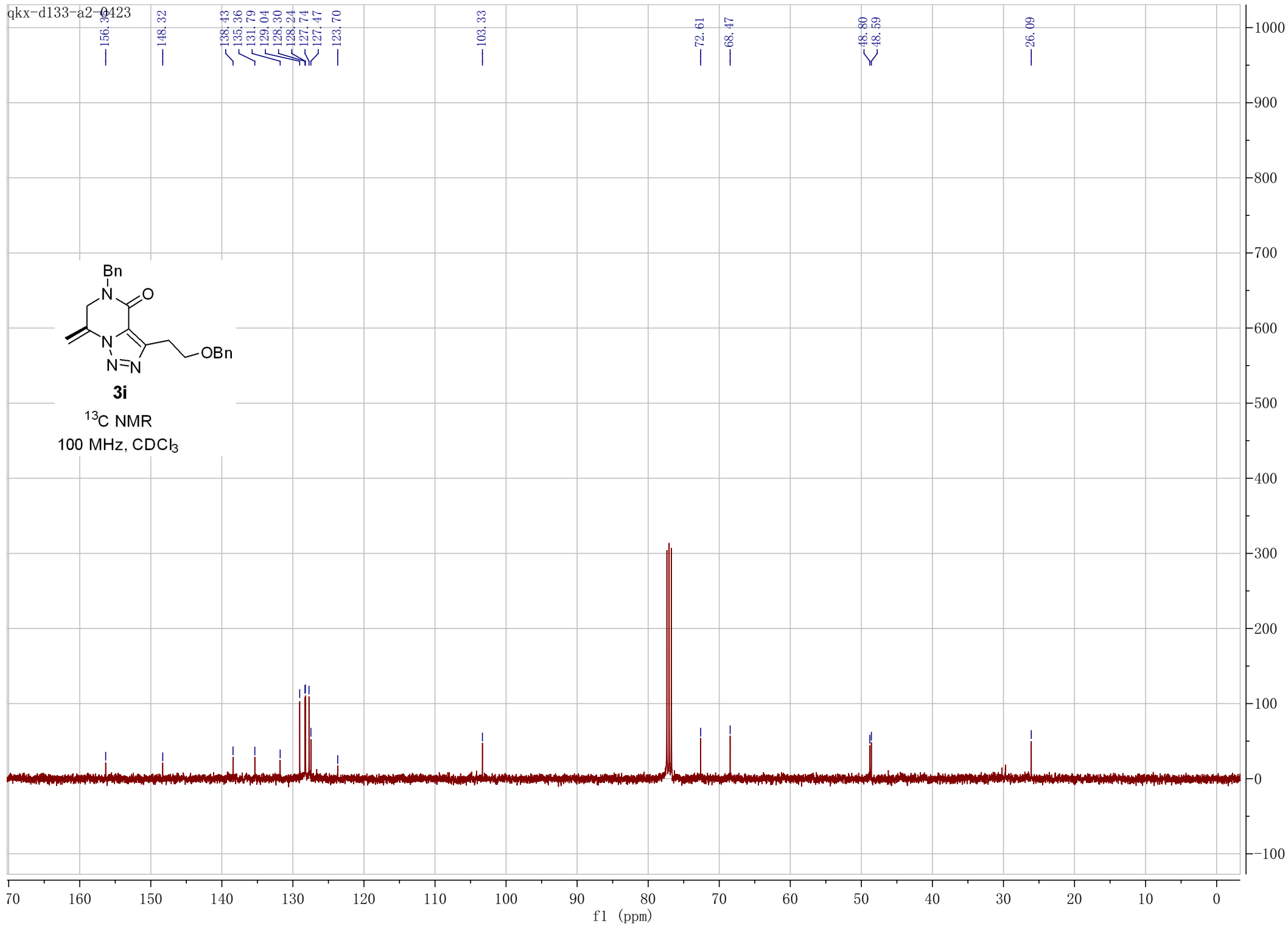
6.035  
5.087  
4.759  
4.608  
4.245  
3.979  
3.962  
3.945  
3.458  
3.441  
3.424



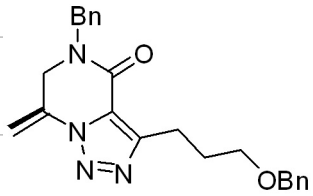
qkx-d133-a2-0423



<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

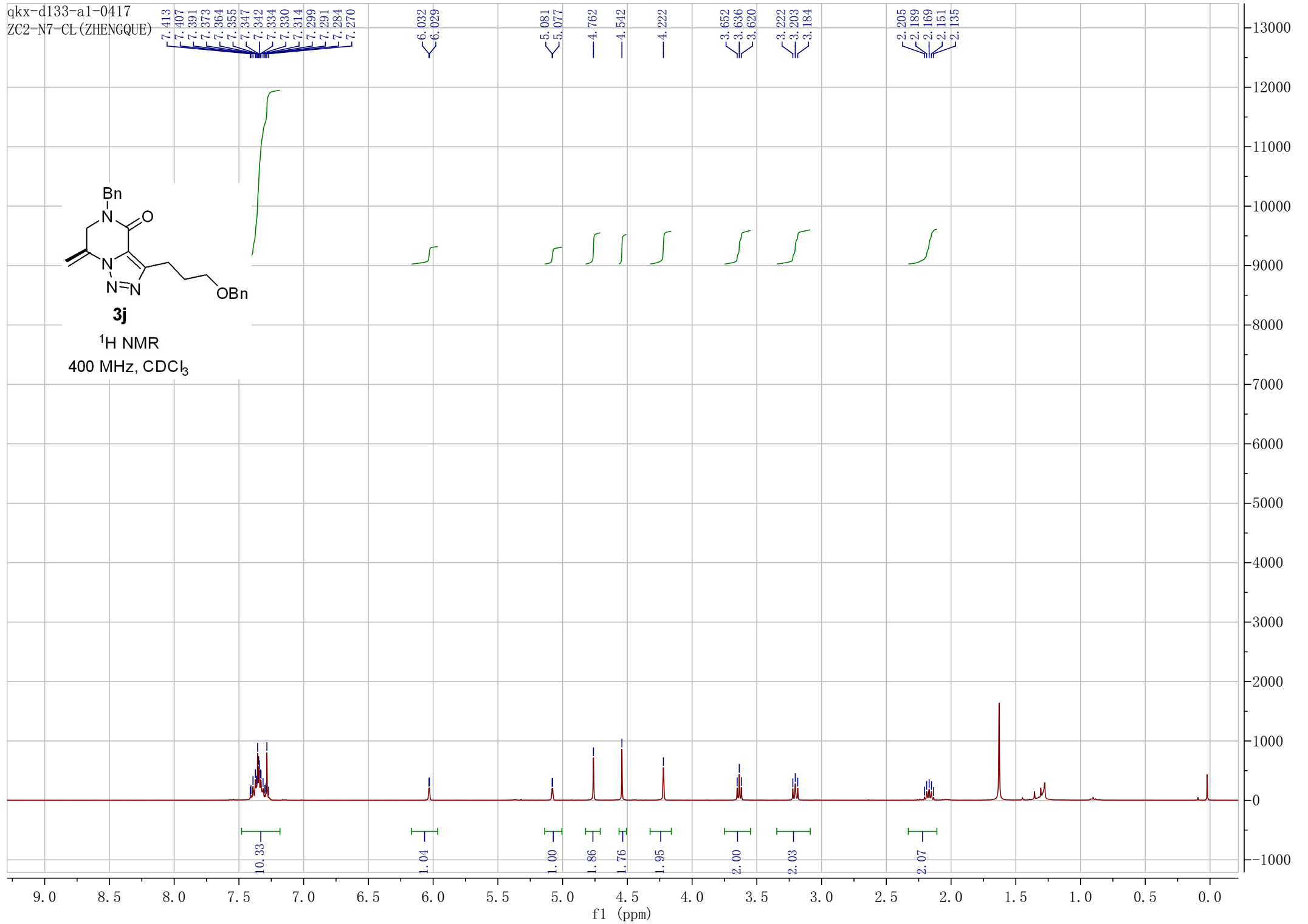


qkx-d133-a1-0417  
ZC2-N7-CL (ZHENGQUE)

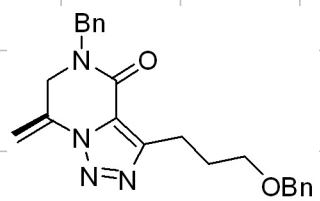


**3j**

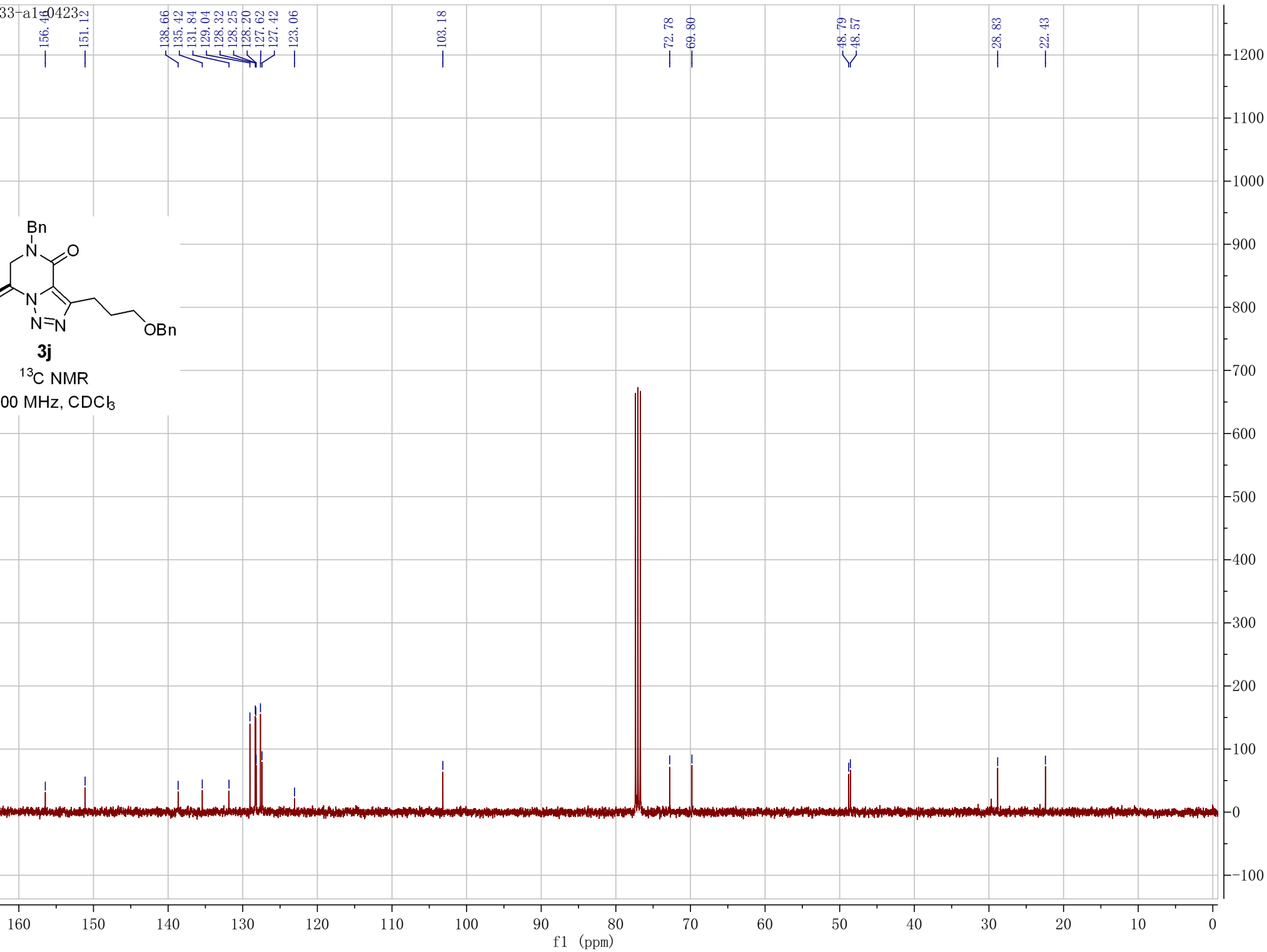
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

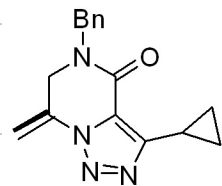


qkx-d133-a1-0423



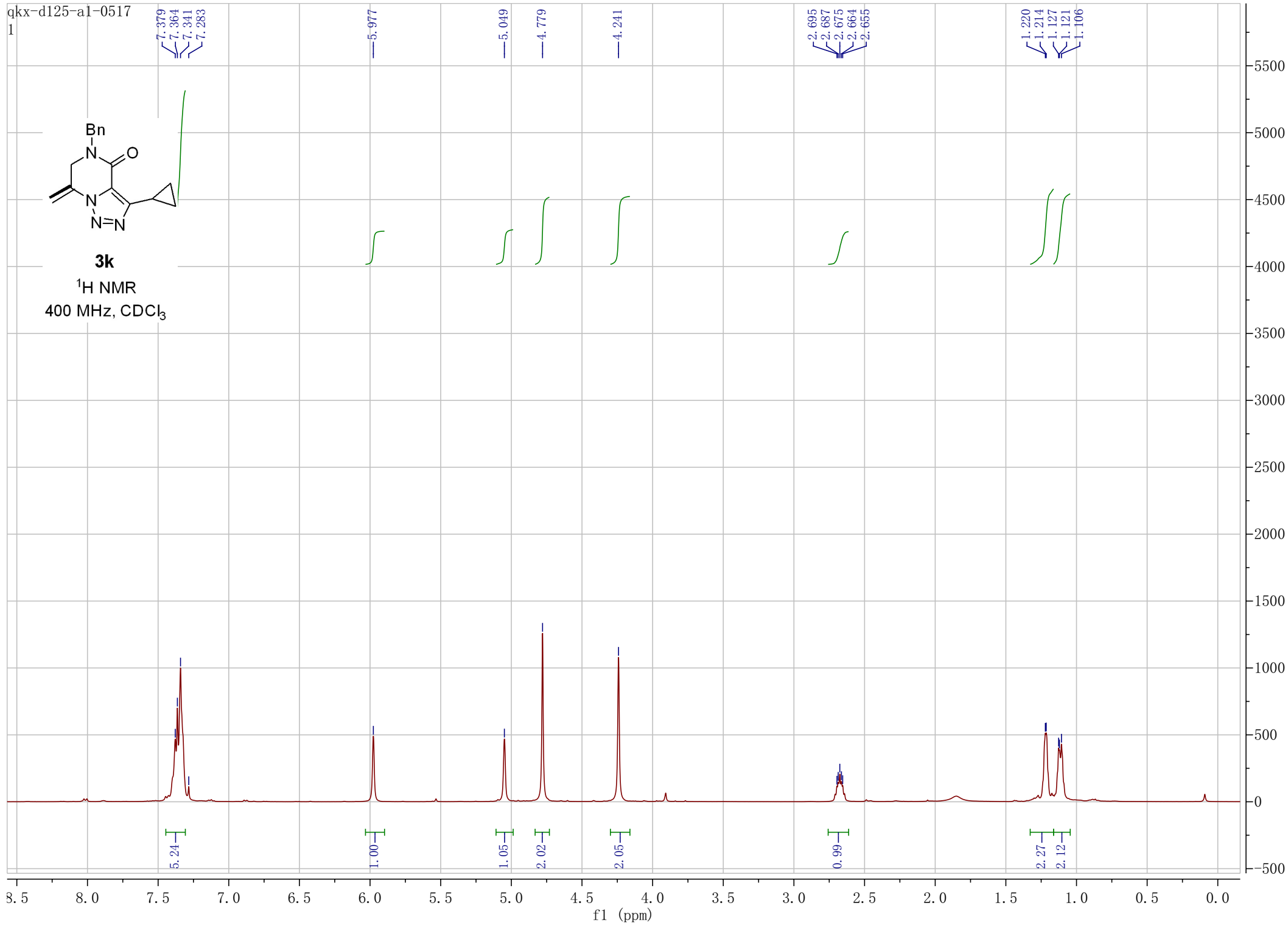
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>





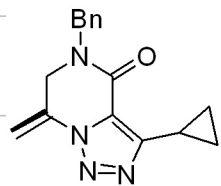
**3k**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



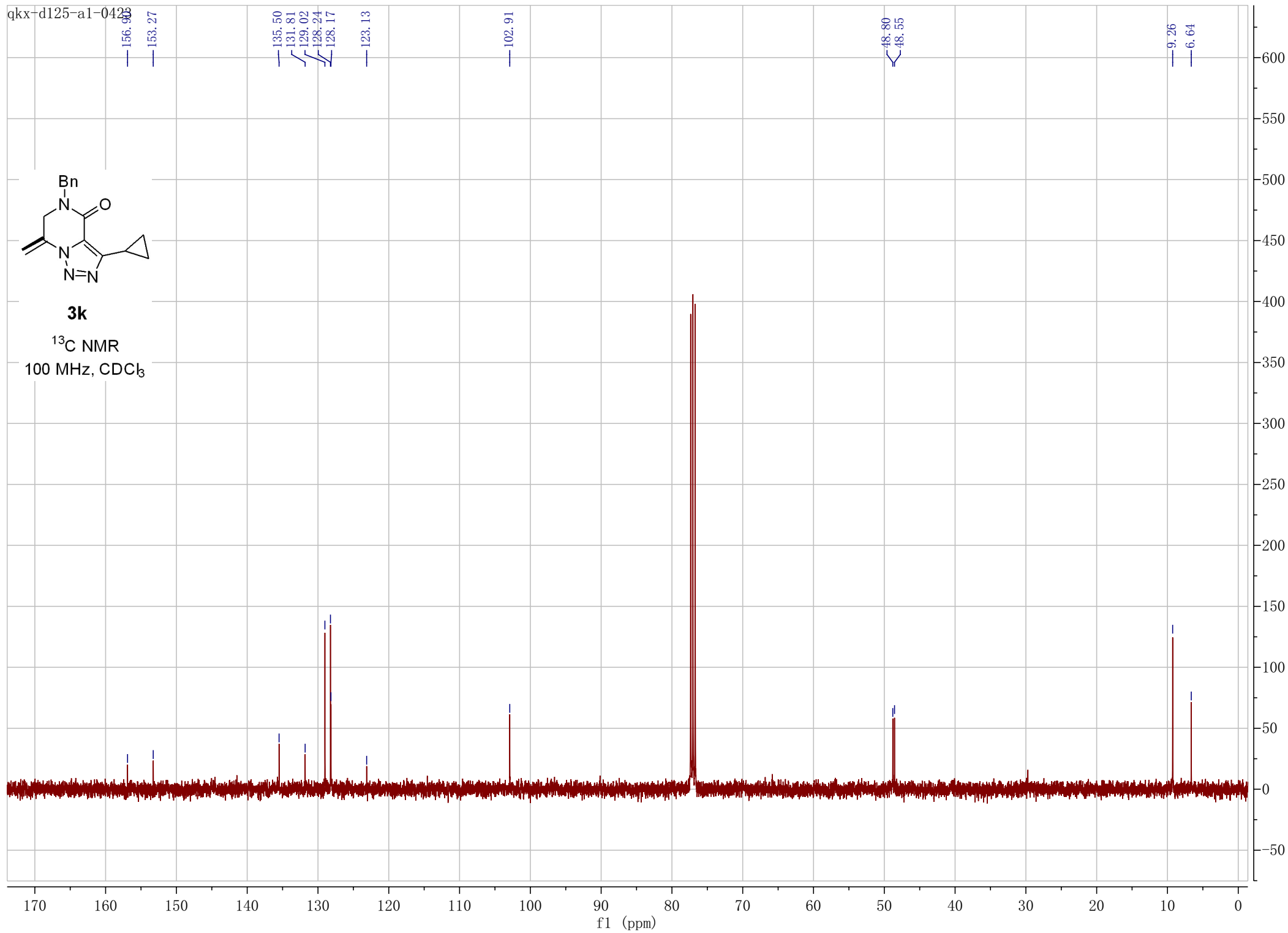


qkx-d125-a1-0428

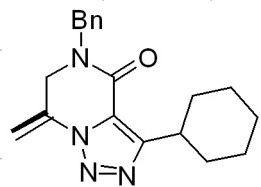


**3k**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

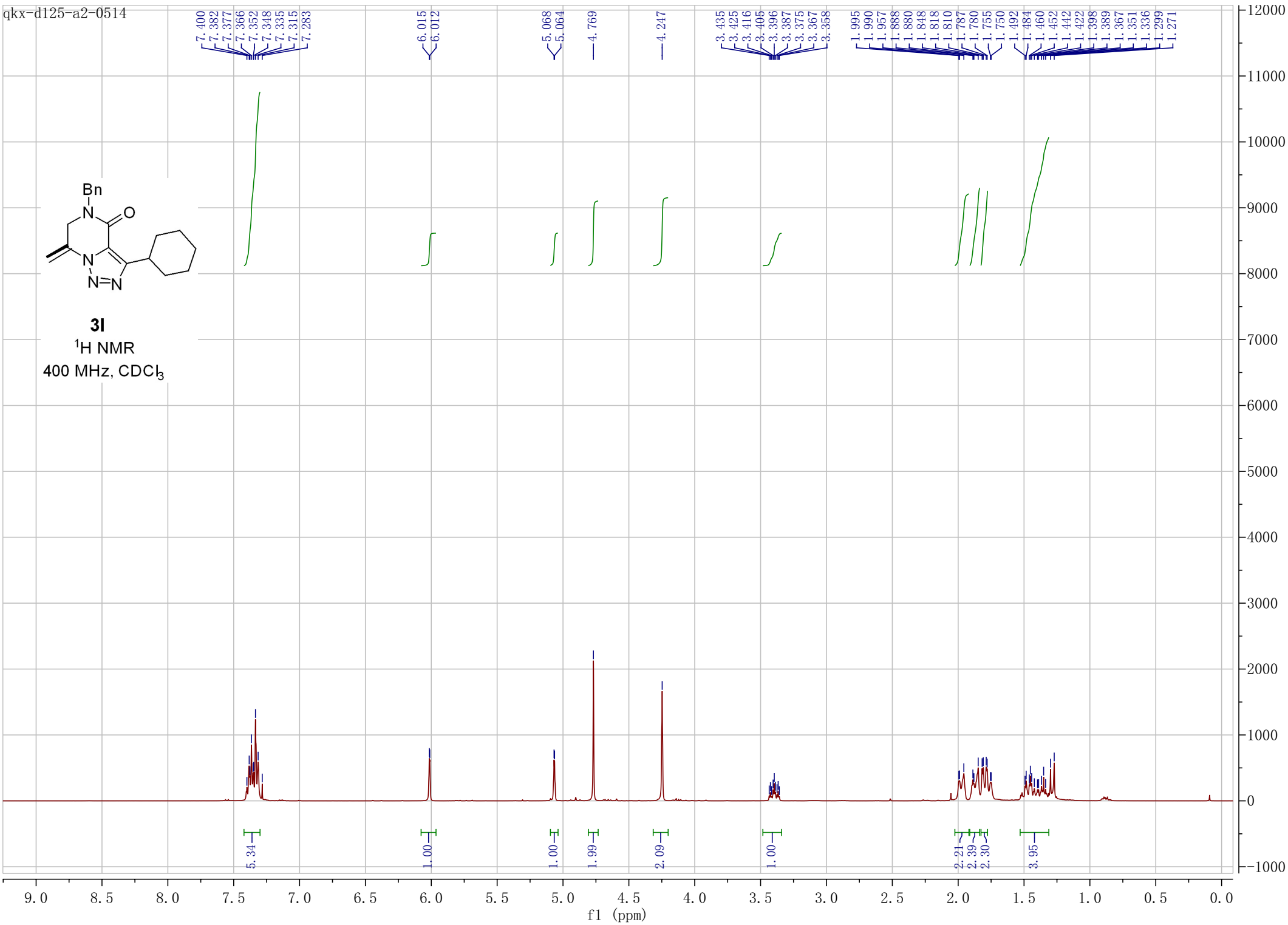


qkx-d125-a2-0514

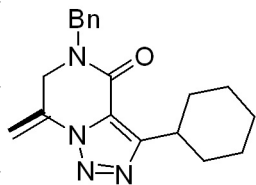


**3I**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

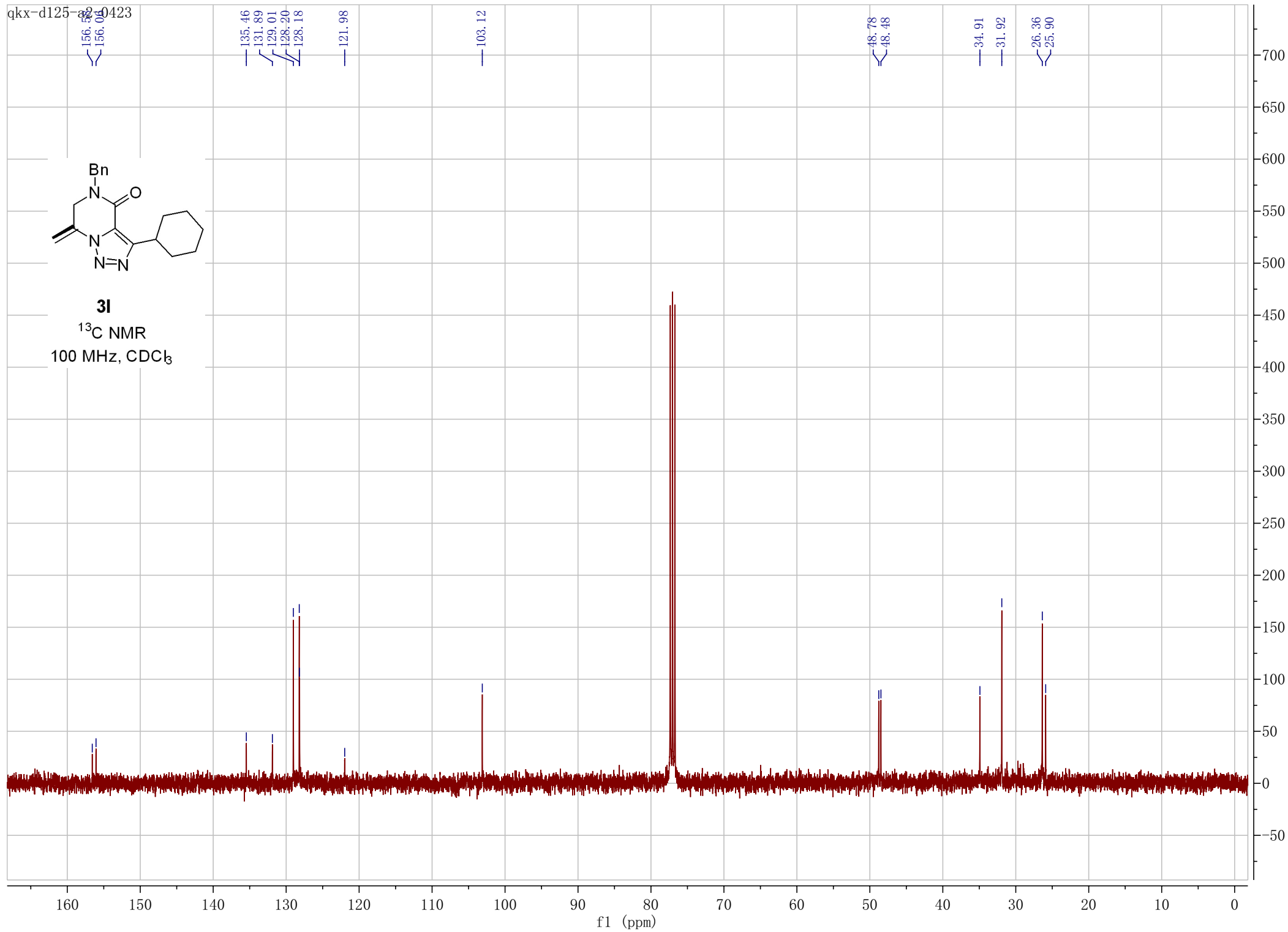


qkx-d125-a2-0423



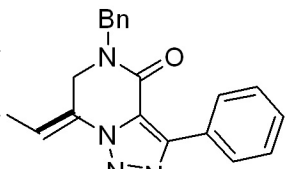
**3I**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



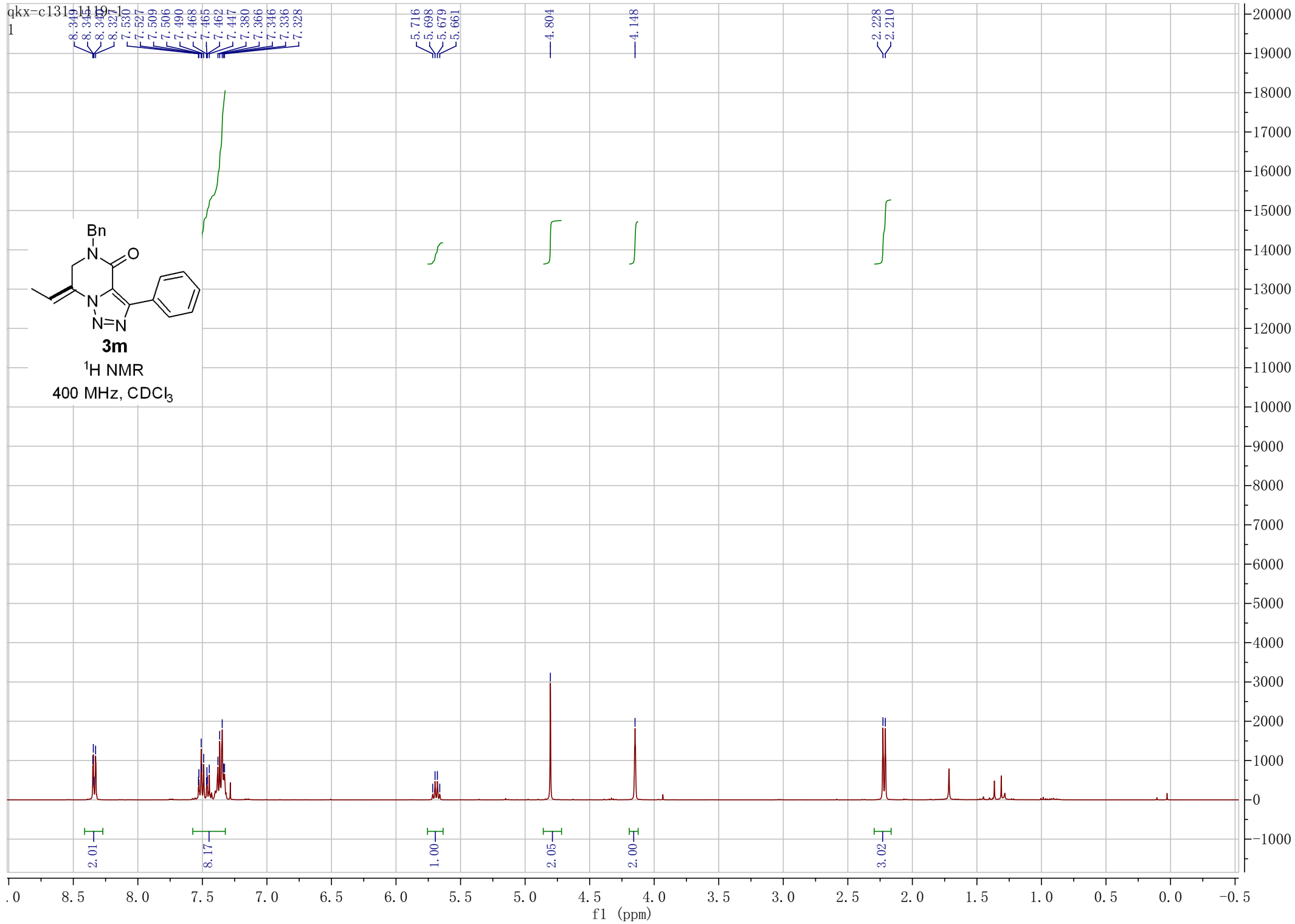
qkx-c131-1119

1

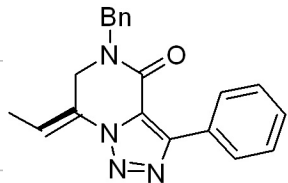


**3m**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

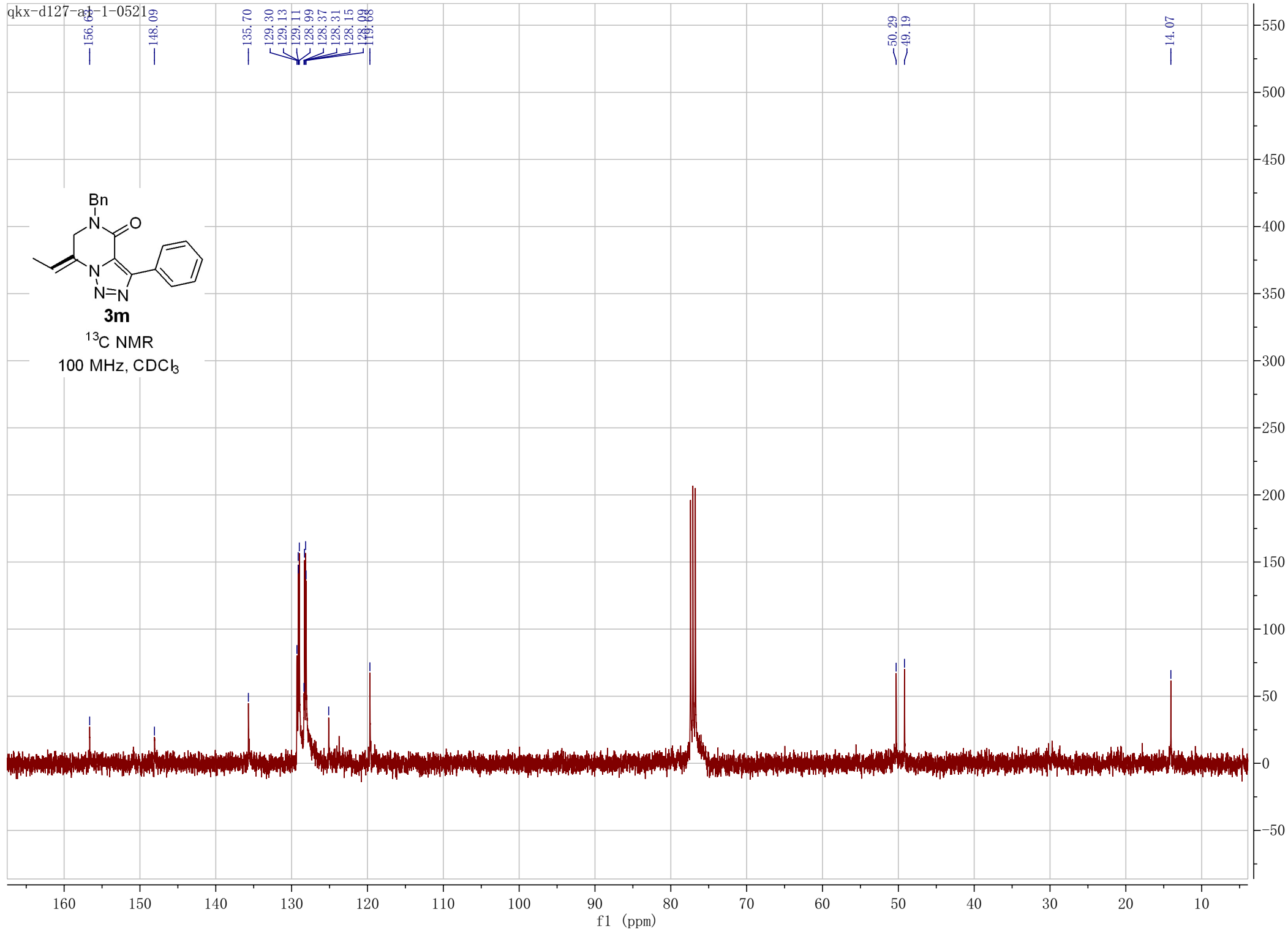


qkx-d127-a1-1-0521

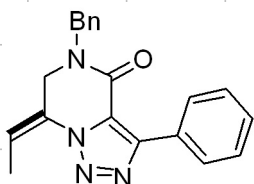


**3m**

<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



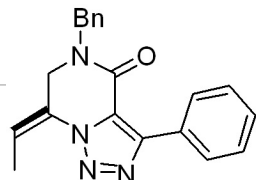
QKX-D129-A1-2-0511



**3m**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



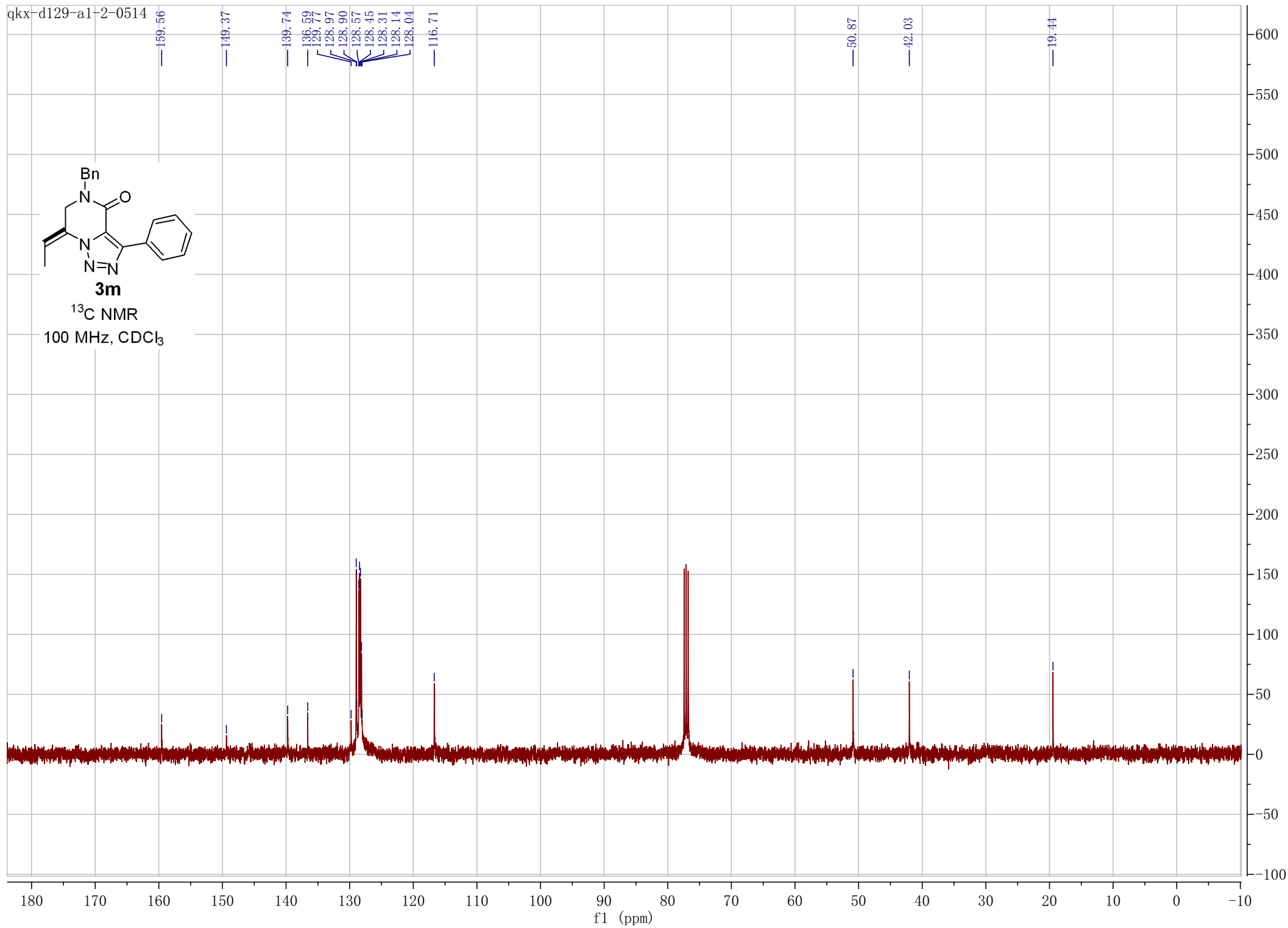
qkx-d129-a1-2-0514

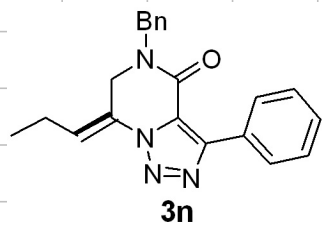


**3m**

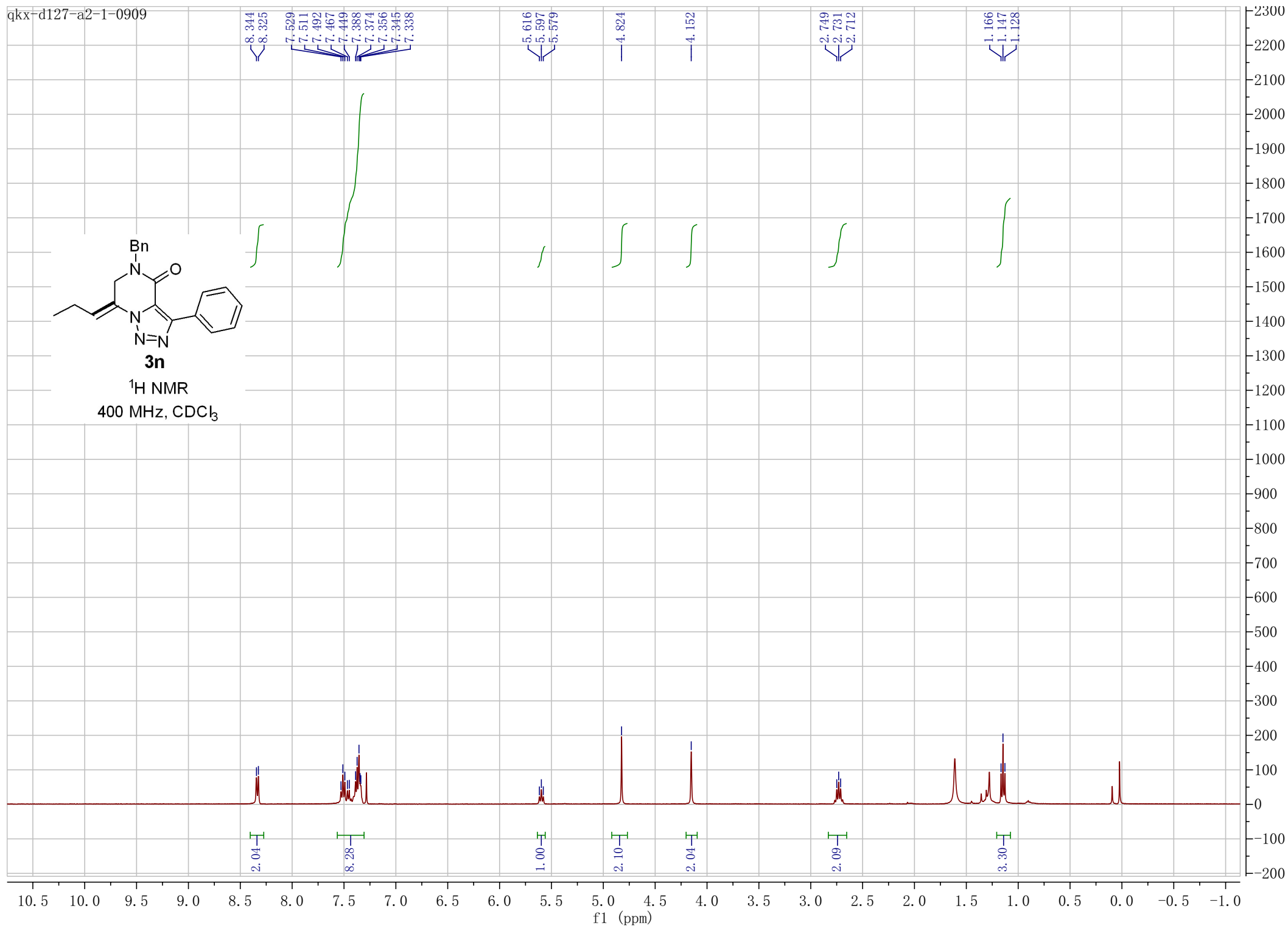
<sup>13</sup>C NMR

100 MHz, CDCl<sub>3</sub>



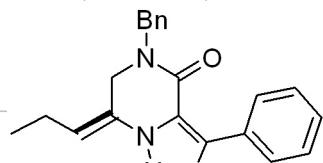


**3n**  
 $^1\text{H NMR}$   
400 MHz,  $\text{CDCl}_3$

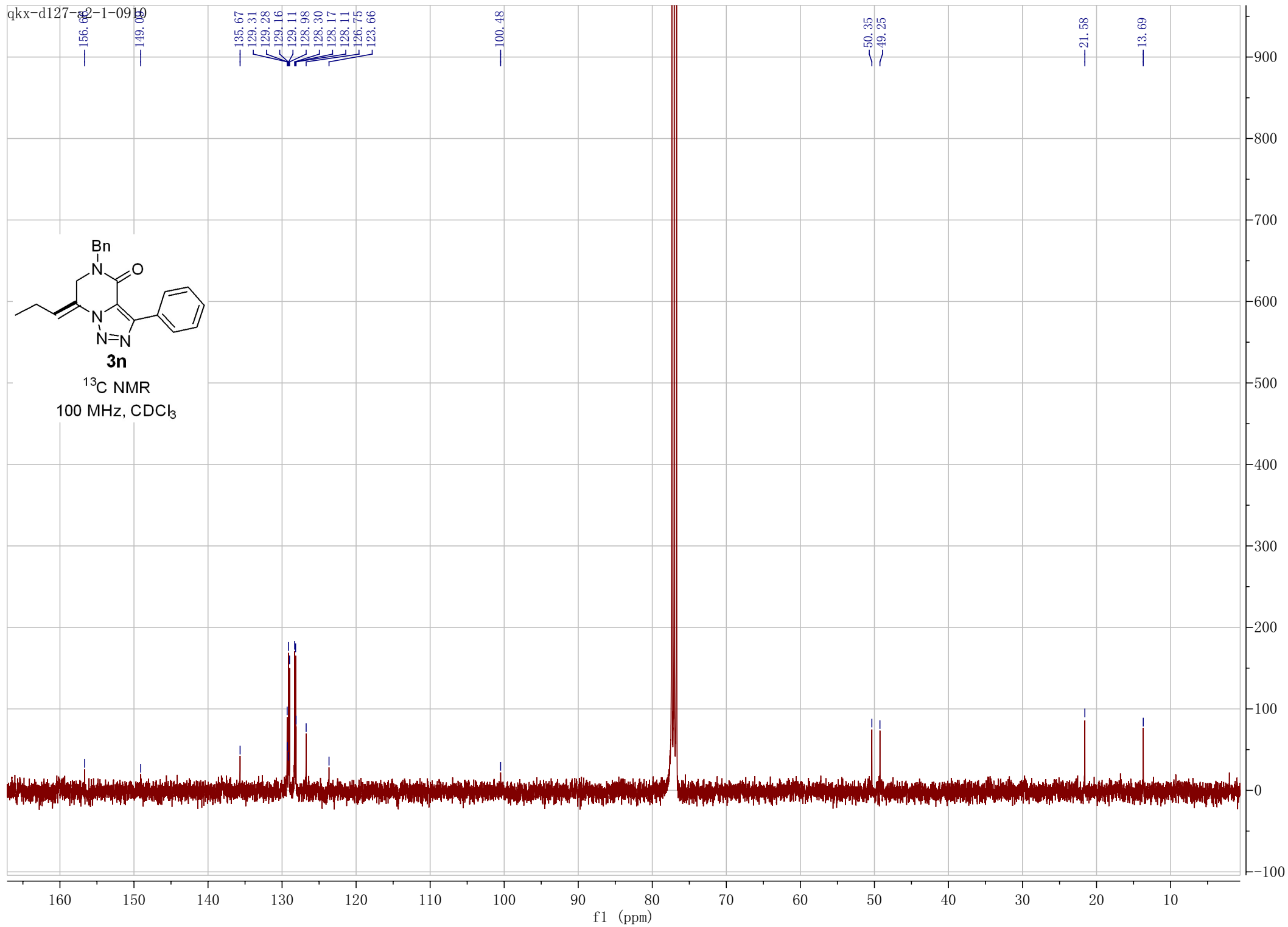




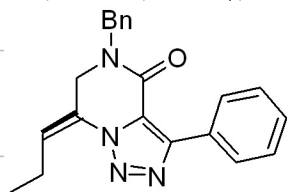
qkx-d127-2-1-0910



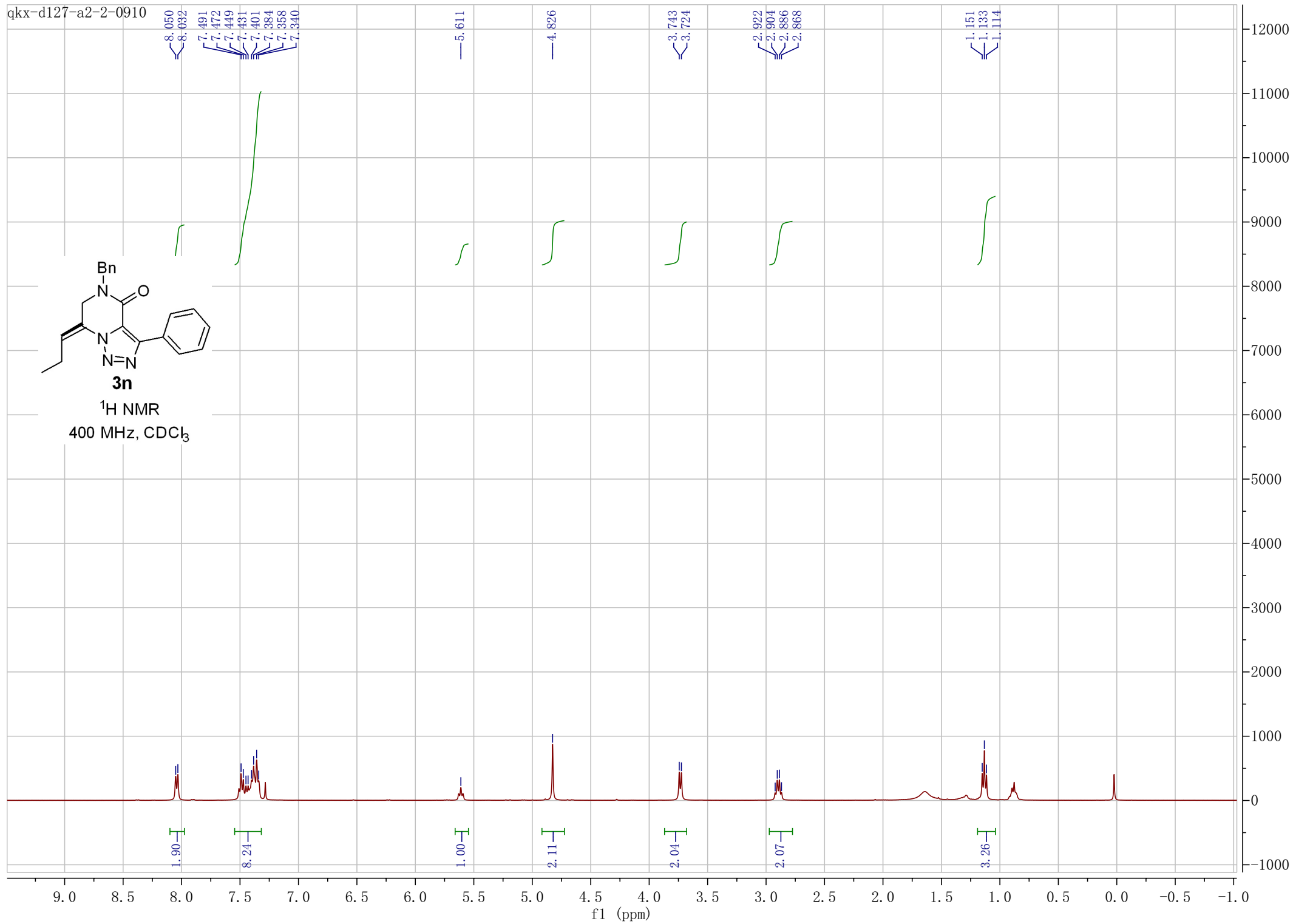
**3n**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>



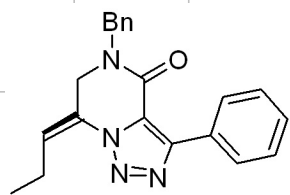
qkx-d127-a2-2-0910



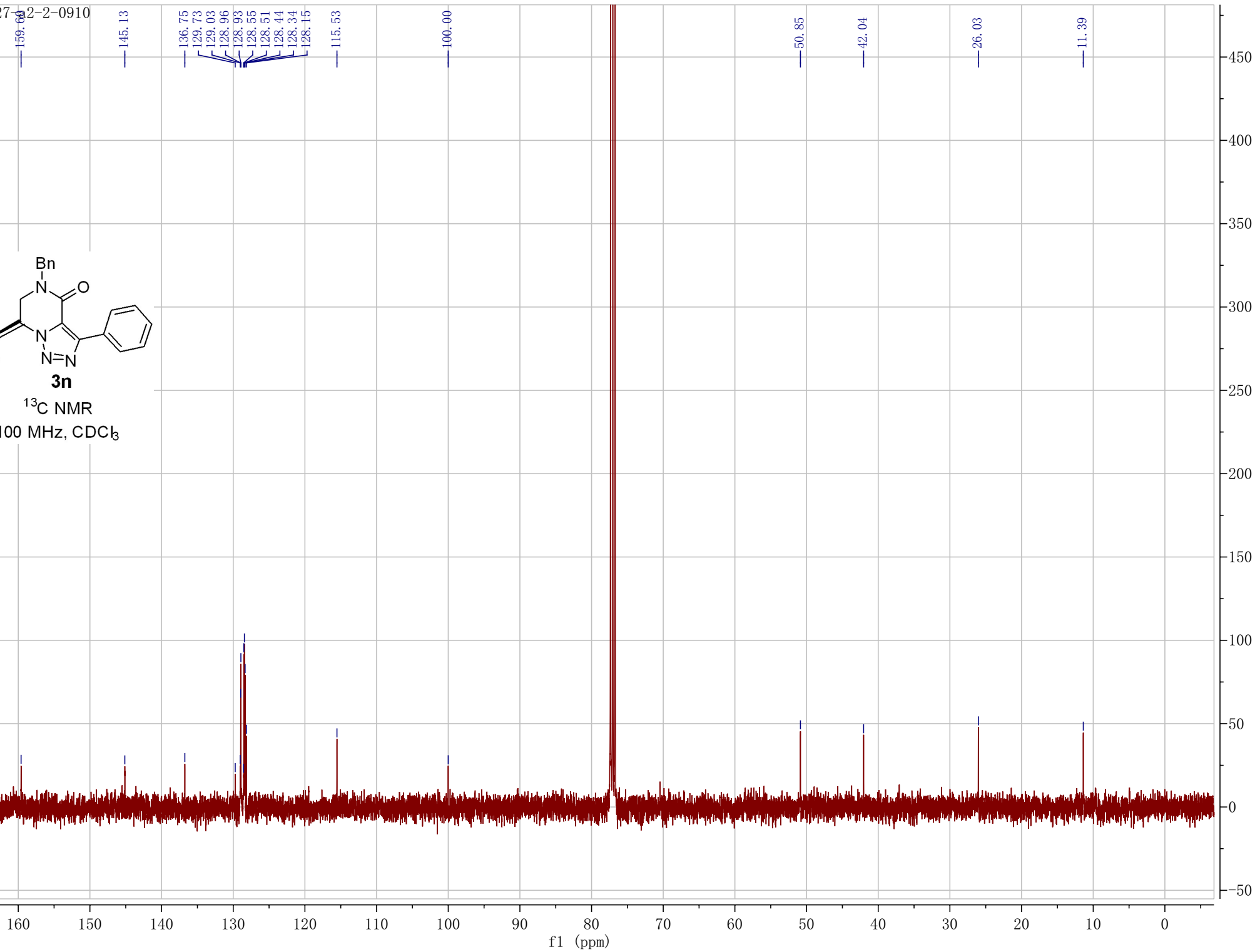
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



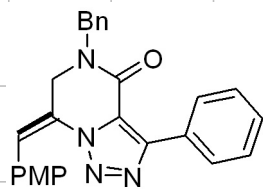
qkx-d127-2-2-0910



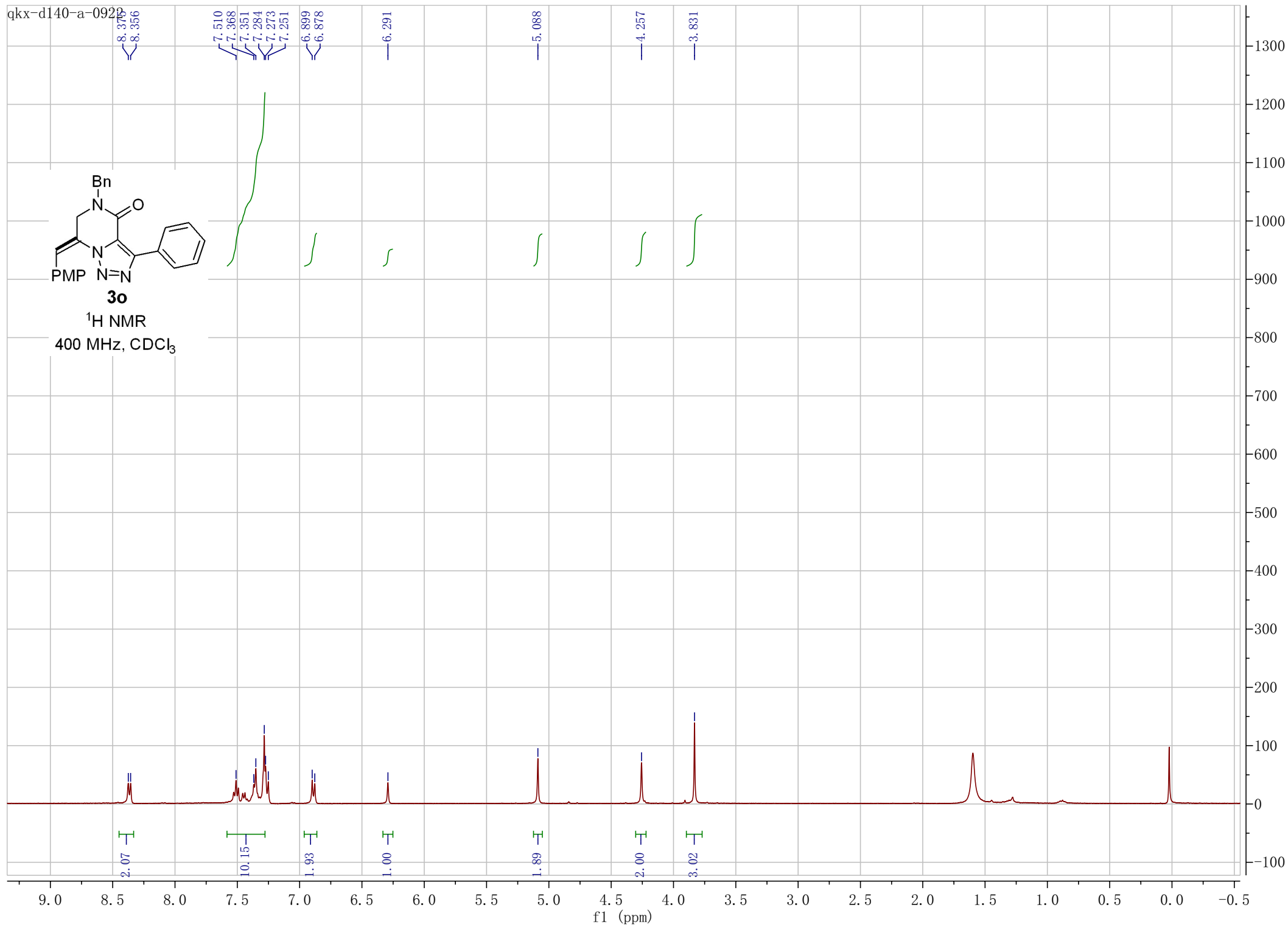
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

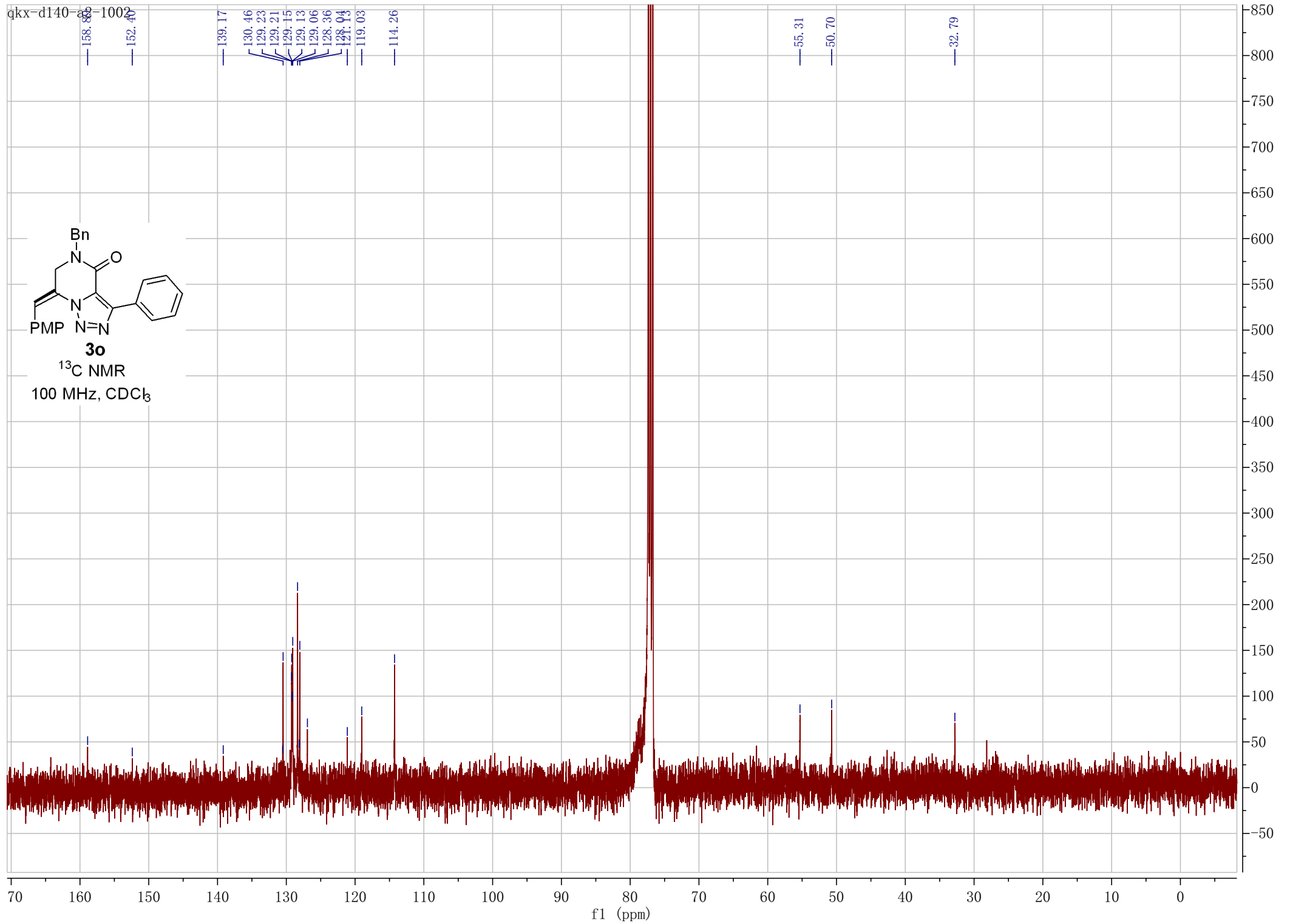


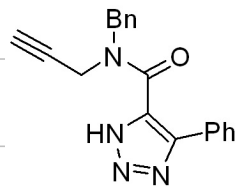
qkx-d140-a-0922



**3o**  
<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

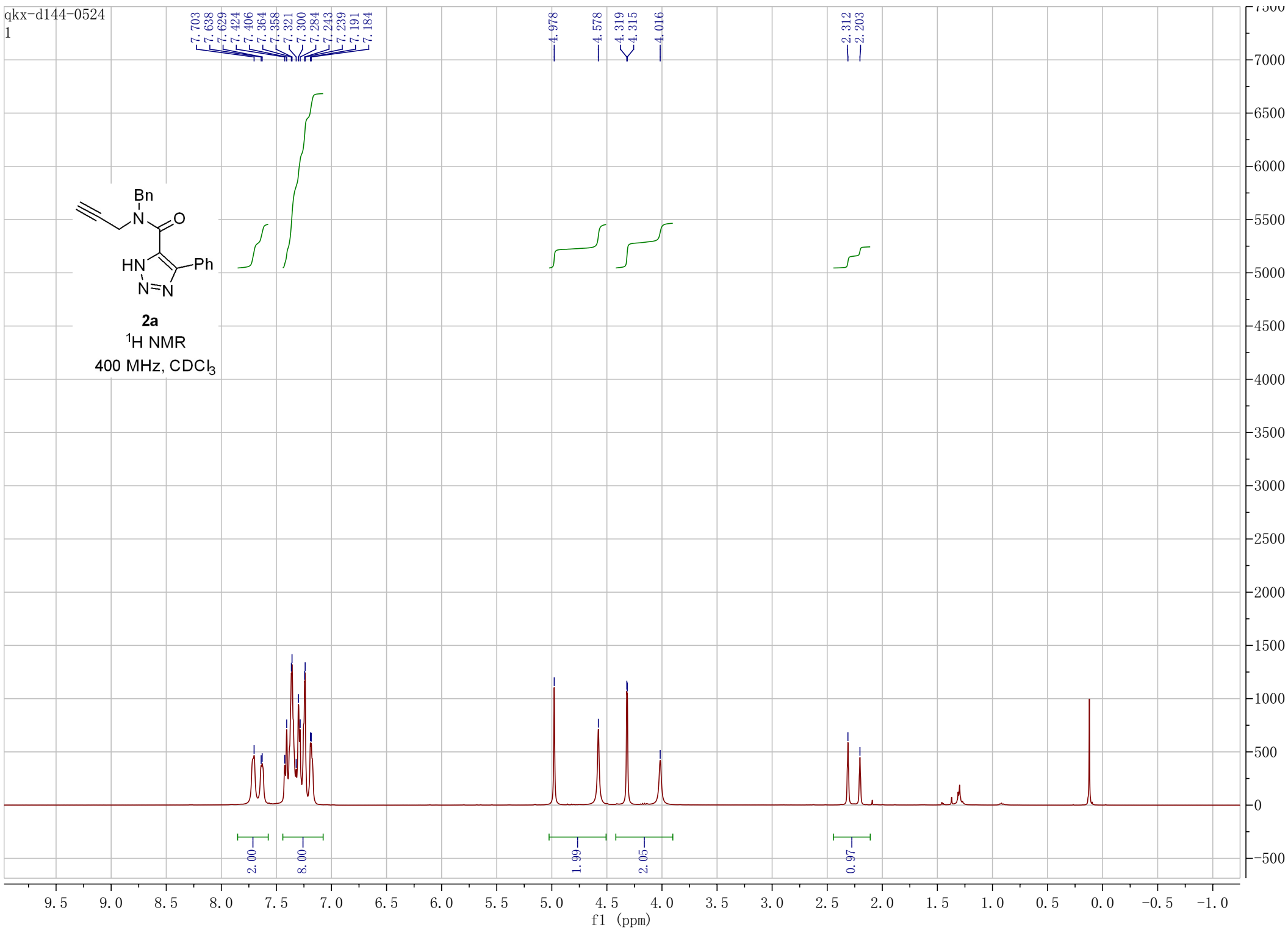




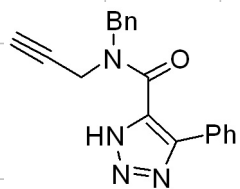


**2a**

<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>

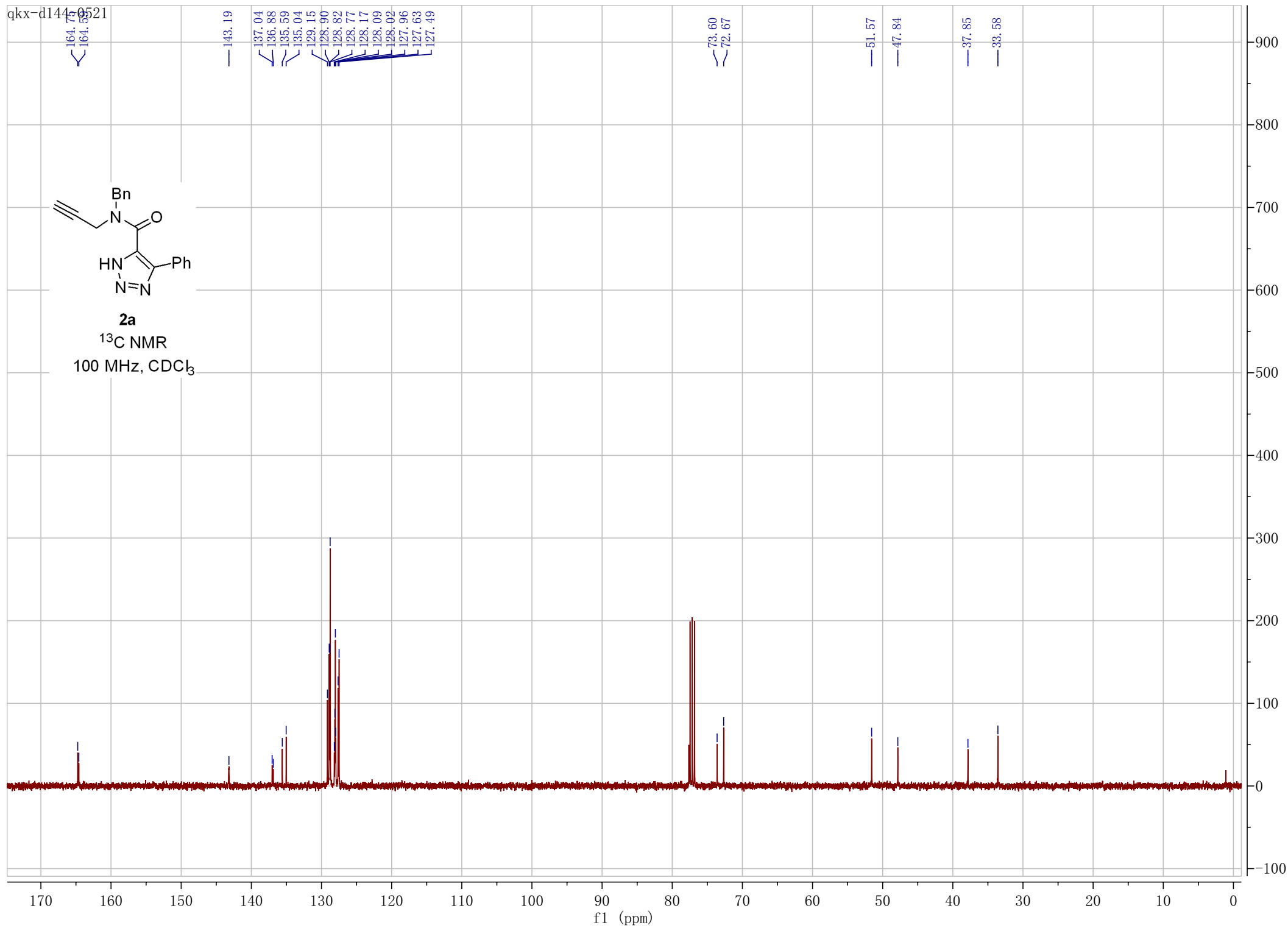


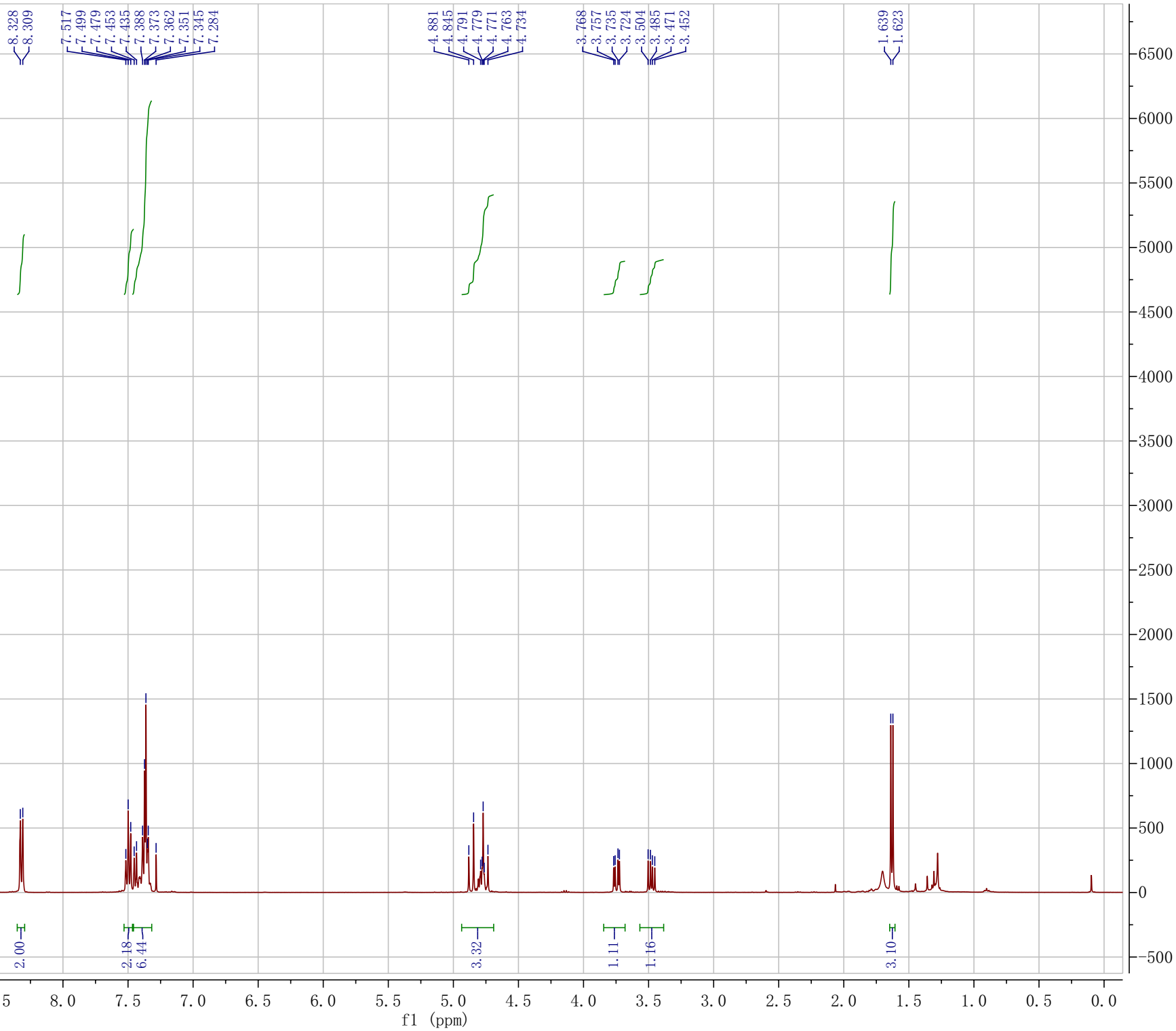
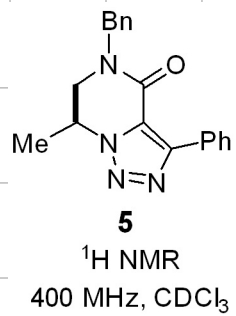
qkx-d144-0521



**2a**

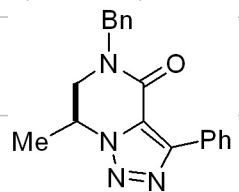
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>







qkx-d1460509



**5**  
<sup>13</sup>C NMR  
100 MHz, CDCl<sub>3</sub>

157.08

149.21

135.95

129.19

129.02

128.96

128.48

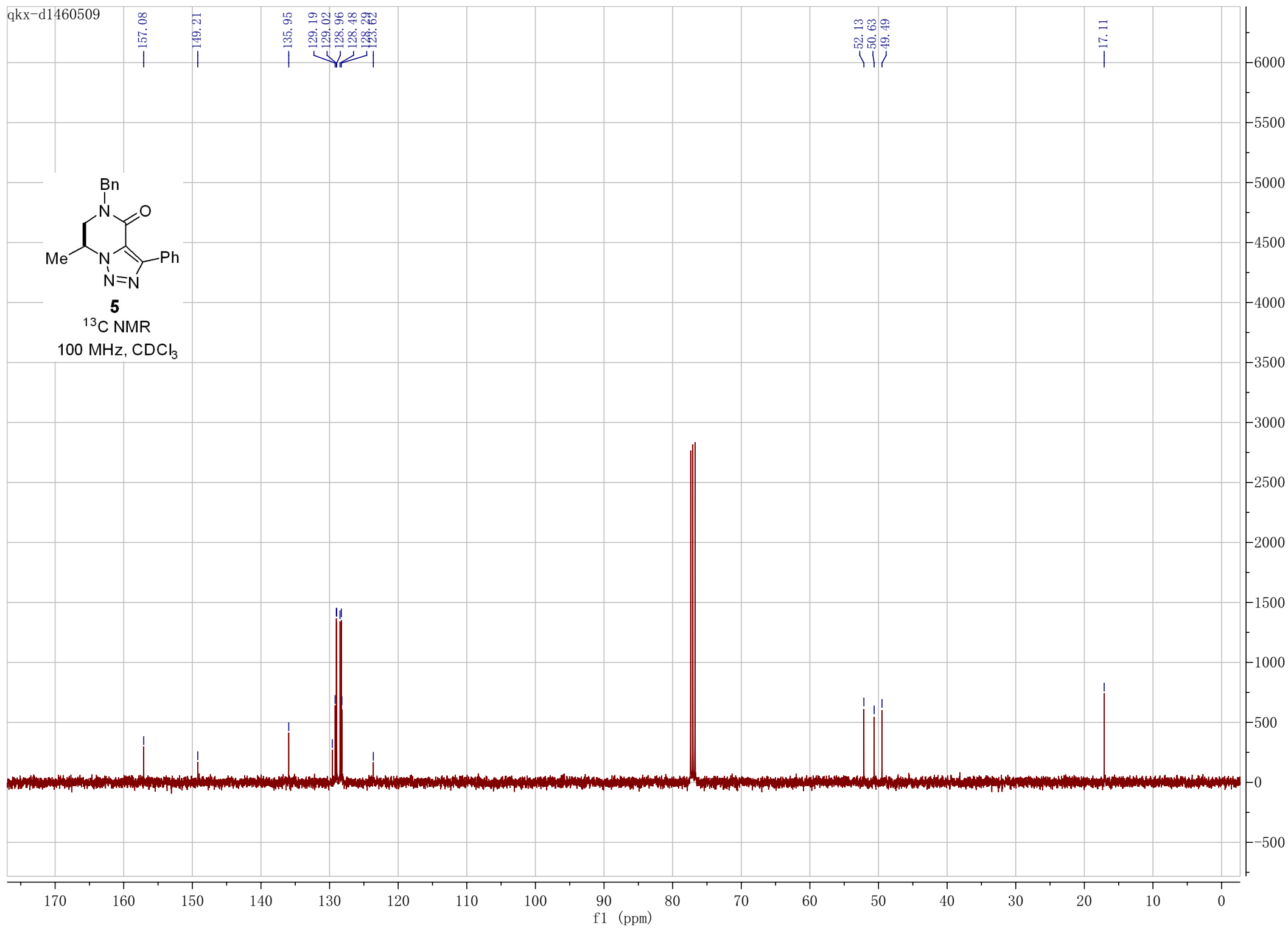
128.62

52.13

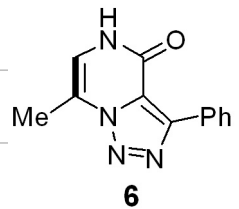
50.63

49.49

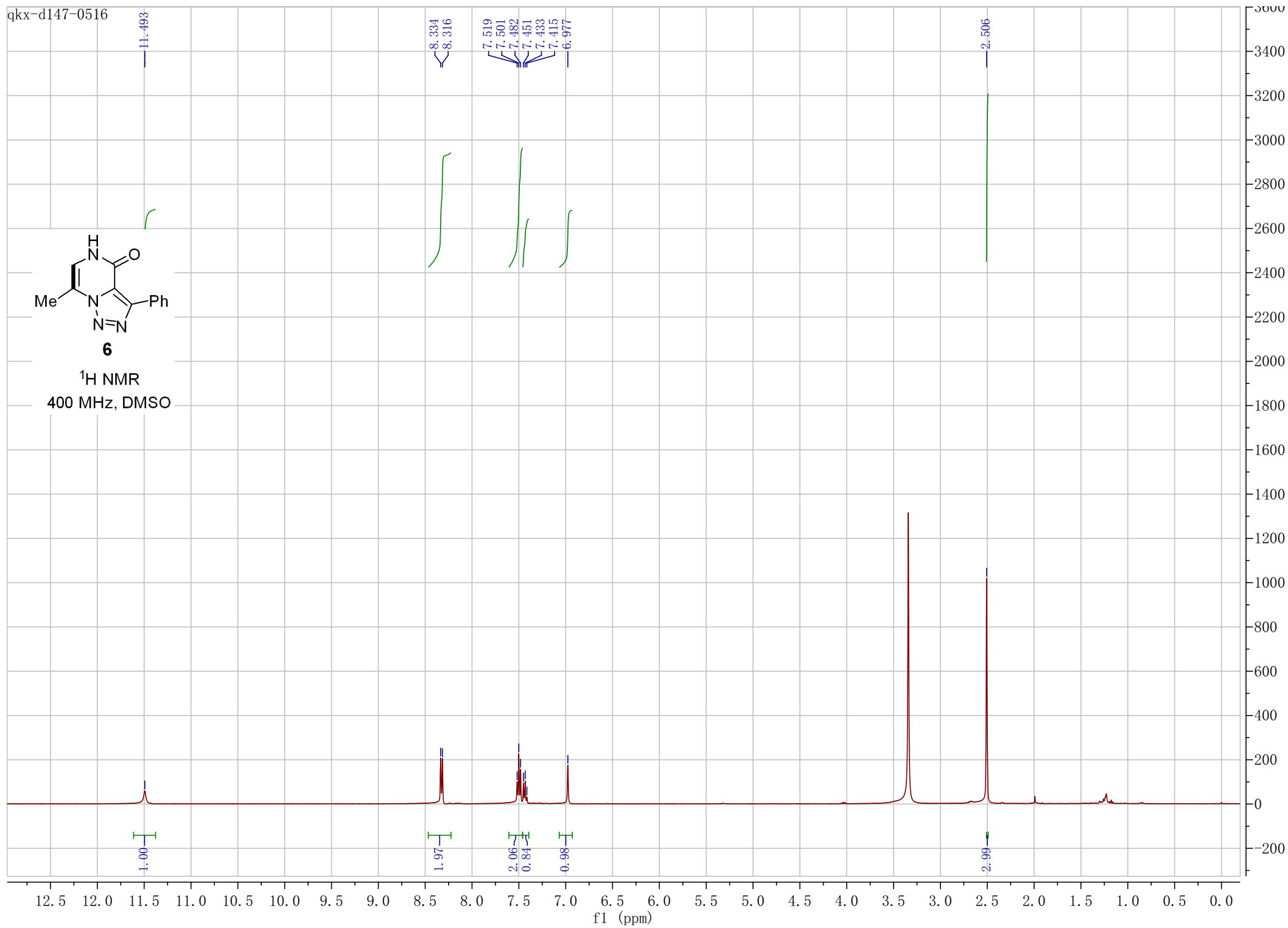
17.11



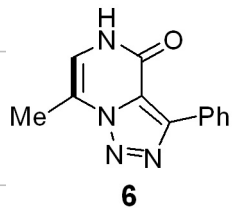
qkx-d147-0516



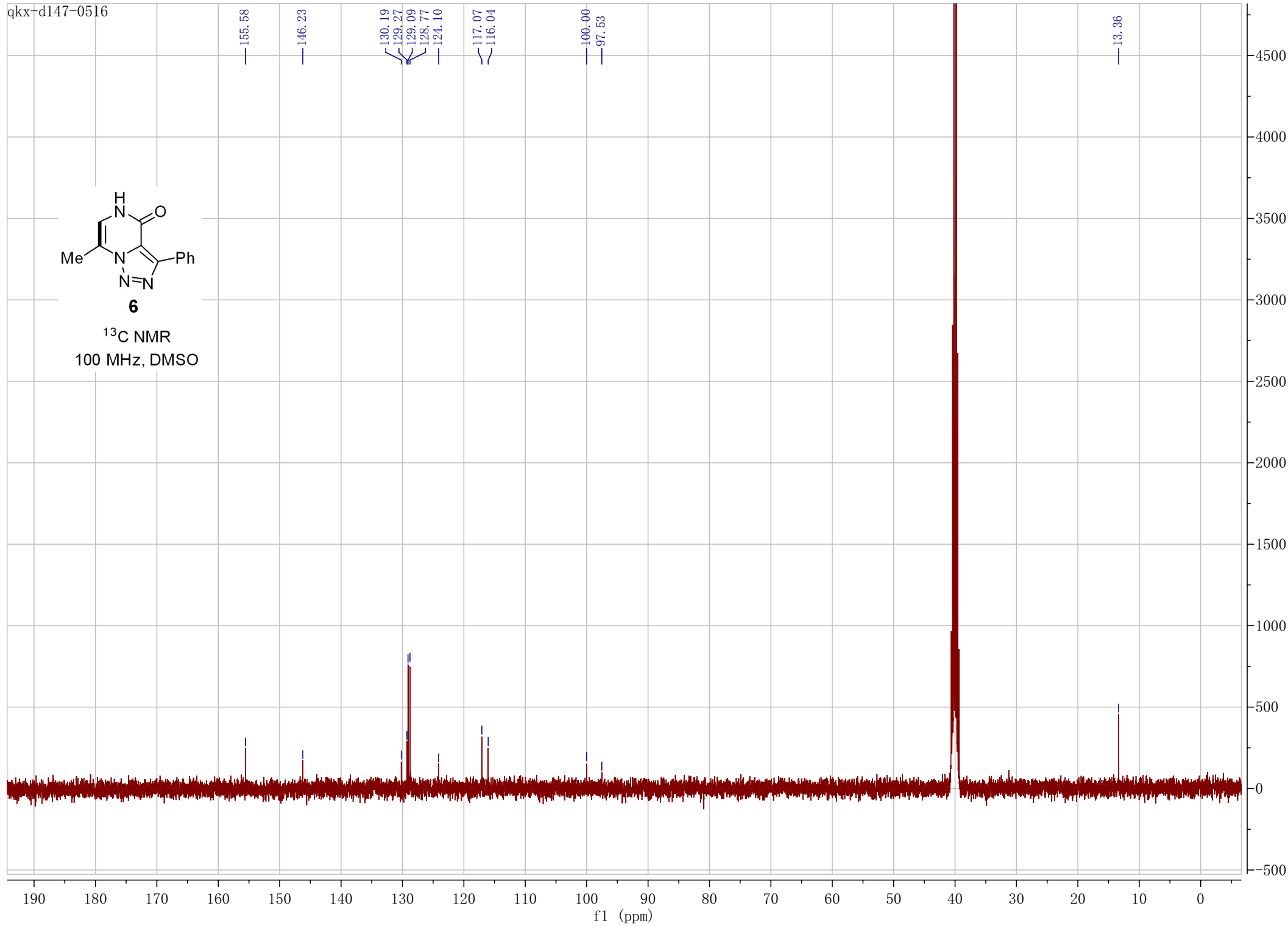
<sup>1</sup>H NMR  
400 MHz, DMSO



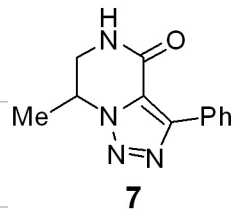
qkx-d147-0516



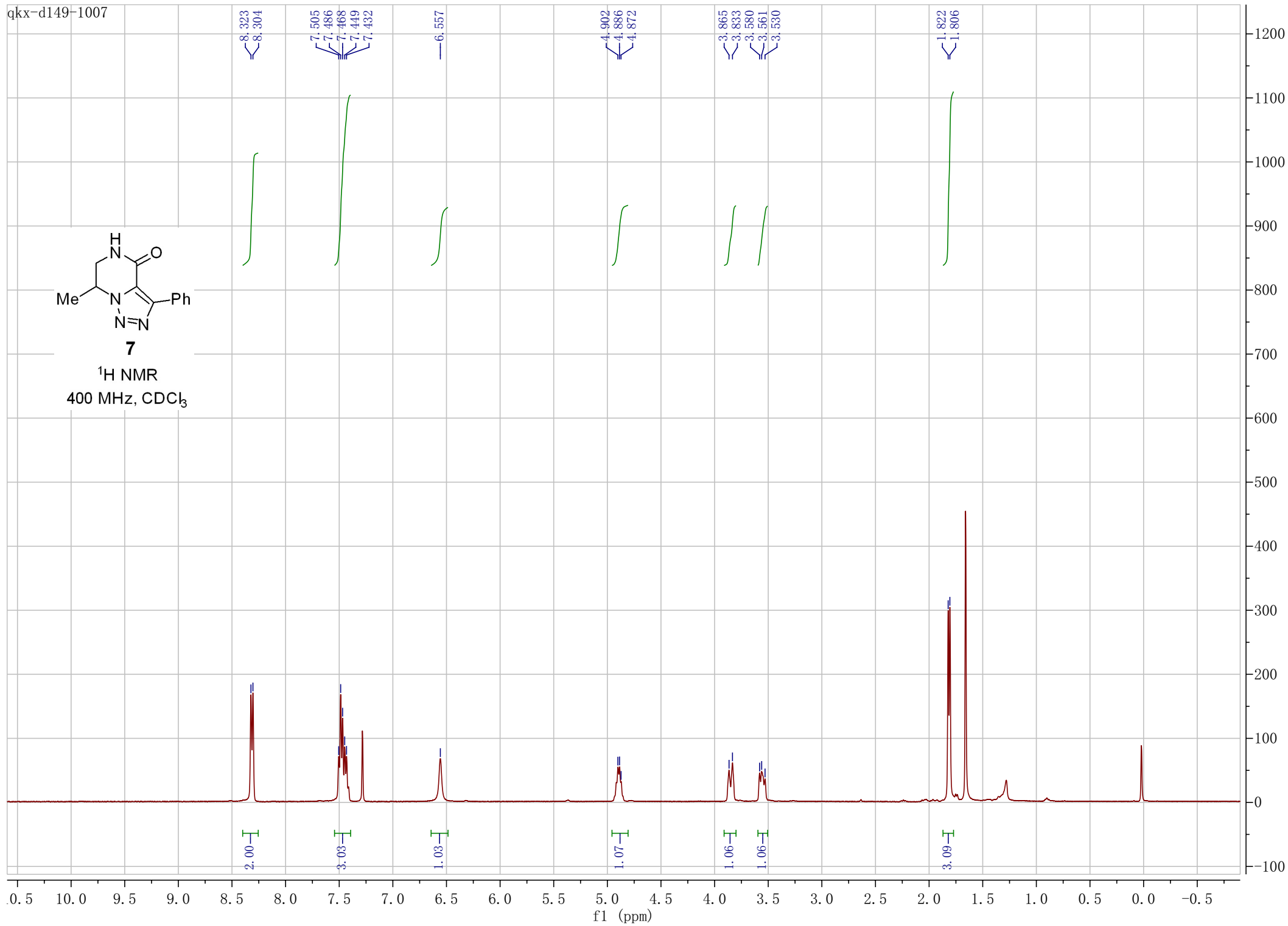
<sup>13</sup>C NMR  
100 MHz, DMSO

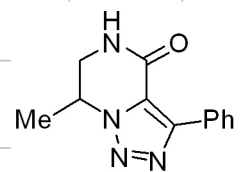


qkx-d149-1007



<sup>1</sup>H NMR  
400 MHz, CDCl<sub>3</sub>



**7**

<sup>13</sup>C NMR  
150 MHz, CDCl<sub>3</sub>

