



## Supporting Information

for

### **A one-pot electrochemical synthesis of 2-aminothiazoles from active methylene ketones and thioureas mediated by $\text{NH}_4\text{I}$**

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**Experimental procedures, characterization data and copies of spectra of the all synthesized compounds ( $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS)**

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### 1. General information

Starting materials and solvents were obtained from commercial sources and used without further purification. Chromatographic purification of products was accomplished by flash chromatography on silica gel (petroleum ether/EtOAc). The product spots on the thin layer chromatography (TLC) were identified/visualized by fluorescence quenching or by potassium permanganate. NMR spectra were recorded with a 300 MHz spectrometer (300 MHz  $^1\text{H}$  frequency, 75 MHz  $^{13}\text{C}$  frequency). Chemical shifts were referenced to residual undeuterated solvent peaks (note: DMSO- $d_6$ : 2.50 ppm  $^1\text{H}$  NMR, 40 ppm  $^{13}\text{C}$  NMR). Coupling constants are reported in Hz. High resolution mass spectra (HRMS) were obtained on a Solarix mass spectrometer.

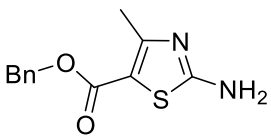
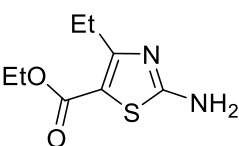
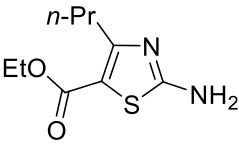
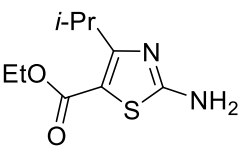
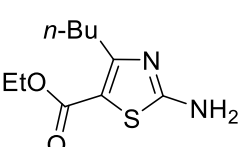
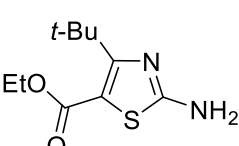
### 2. General procedure for the one-pot electrochemically synthesis of 2-aminothiazoles from active methylene ketones and thioureas

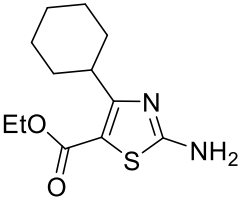
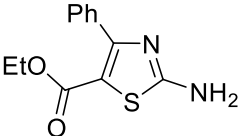
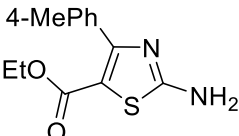
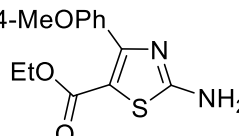
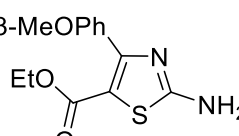
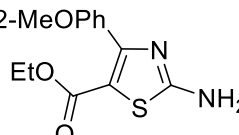
A 50 mL undivided cell was equipped with a graphite plate cathode and a graphite plate anode (each about  $2 \times 2 \text{ cm}^2$ ) which were connected to a DC regulated power supply. To the cell was added active methylene ketone **1** (2 mmol), thiourea **2** (1 mmol),  $\text{NH}_4\text{I}$  (0.1 mmol), DL-alanine (1 mmol) and  $\text{LiClO}_4$  (0.5 mmol) dissolved in a mixed solvent of DMSO (1 mL) and  $\text{H}_2\text{O}$  (14 mL). The mixture was electrolyzed under constant current conditions at  $5 \text{ mA/cm}^2$  at  $30^\circ\text{C}$  while stirring. The electrolysis was terminated when 6 F/mol of charge had been consumed. After the electrolysis, the reaction mixture was washed with a saturated aqueous  $\text{Na}_2\text{S}_2\text{O}_3$  and the product was then extracted with DCM ( $3 \times 10 \text{ mL}$ ), dried over  $\text{MgSO}_4$ , and concentrated in vacuum. The residue was purified by column chromatography on silica gel using a mixture of petroleum ether/EtOAc as eluent.

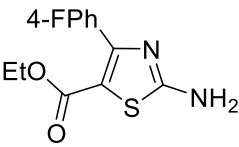
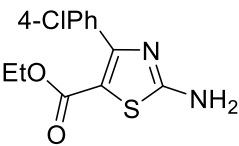
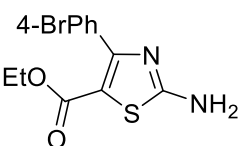
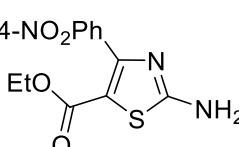
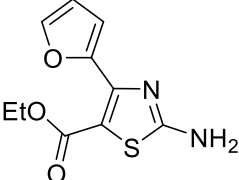
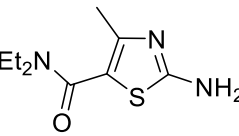
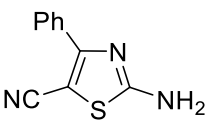
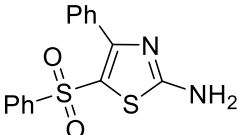


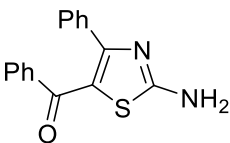
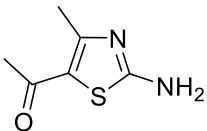
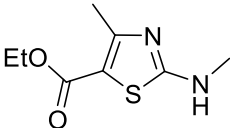
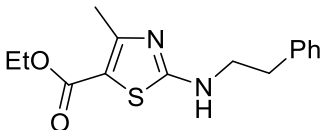
### 3. Compounds characterization

|                                                                                        |                                                                                                                                                                                                                                                                                                                                                                                         |
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| ethyl 2-amino-4-methylthiazole-5-carboxylate ( <b>3a</b> ) <sup>[1]</sup>              |                                                                                                                                                                                                                                                                                                                                                                                         |
|                                                                                        | Yield: 140 mg, 75%; white solid; M.P.: 173-174 °C<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.22 (t, <i>J</i> = 7.2 Hz, 3H), 2.37 (s, 3H), 4.14 (q, <i>J</i> = 7.2 Hz, 2H), 7.72(br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.8, 17.6, 60.2, 107.9, 159.8, 162.5, 170.7.                                             |
| methyl 2-amino-4-methylthiazole-5-carboxylate ( <b>3b</b> ) <sup>[2]</sup>             |                                                                                                                                                                                                                                                                                                                                                                                         |
|                                                                                        | Yield: 138 mg, 80%; light yellow solid; M.P.: 218-220 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 2.37 (s, 3H), 3.67 (s, 3H), 7.74 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 17.6, 51.7, 107.3, 160.1, 162.8, 170.8.                                                                                              |
| <i>tert</i> -butyl 2-amino-4-methylthiazole-5-carboxylate ( <b>3c</b> ) <sup>[1]</sup> |                                                                                                                                                                                                                                                                                                                                                                                         |
|                                                                                        | Yield: 109 mg, 51%; yellow solid; M.P.: 162-163 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.45(s, 9H), 2.33(s, 3H), 7.62(br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 17.6, 28.5, 80.6, 109.7, 158.8, 162.0, 170.3.                                                                                                 |
| pentyl 2-amino-4-methylthiazole-5-carboxylate ( <b>3d</b> ) <sup>[2]</sup>             |                                                                                                                                                                                                                                                                                                                                                                                         |
|                                                                                        | Yield: 52 mg, 30%; yellow waxy solid.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 0.87 (t, <i>J</i> = 6.6 Hz, 3H), 1.23-1.32 (m, 4H), 1.54-1.64 (m, 2H), 2.37(s, 3H), 4.09 (t, <i>J</i> = 6.6 Hz, 2H), 7.74 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.4, 17.7, 22.3, 28.3, 28.5, 64.3, 107.9, 159.8, 162.5, 170.8. |
| allyl 2-amino-4-methylthiazole-5-carboxylate ( <b>3e</b> ) <sup>[2]</sup>              |                                                                                                                                                                                                                                                                                                                                                                                         |
|                                                                                        | Yield: 155 mg, 78%; white solid; M.P.: 151-154 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 2.38 (s, 3H), 4.63-4.64 (m, 2H), 5.2-5.33 (m, 2H), 5.91-6.01 (m, 1H), 7.79 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 17.7, 64.6, 107.3,                                                                                |

|                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
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|                                                                                     | 117.9, 133.5, 160.5, 162.0, 170.9.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| benzyl 2-amino-4-methylthiazole-5-carboxylate ( <b>3f</b> )                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|    | Yield: 130 mg, 52%; light yellow solid; M.P.: 135-138 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 2.38 (s, 3H), 5.19 (s, 2H), 7.31-7.39 (m, 5H), 7.78 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 17.7, 65.6, 107.3, 128.2, 128.4, 129.0, 137.0, 160.5, 162.2, 171.0;<br>HRMS (ESI) calcd for C <sub>12</sub> H <sub>13</sub> N <sub>2</sub> O <sub>2</sub> S (M+H) <sup>+</sup> 249.06914, found 249.06923.                                                                                                                |
| ethyl 2-amino-4-ethylthiazole-5-carboxylate ( <b>3g</b> )                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|    | Yield: 127 mg, 65%; yellow solid; M.P.: 174-178 °C<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.11 (t, <i>J</i> = 7.5 Hz, 3H), 1.21 (t, <i>J</i> = 7.2 Hz, 3H), 2.82 (q, <i>J</i> = 6.3 Hz, 2H), 4.13 (q, <i>J</i> = 7.2 Hz, 2H), 7.75 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 13.9, 14.9, 24.2, 60.3, 107.2, 162.3, 165.5, 171.1;<br>HRMS (ESI) calcd for C <sub>8</sub> H <sub>13</sub> N <sub>2</sub> O <sub>2</sub> S (M+H) <sup>+</sup> 201.06921, found 201.06923.                                                   |
| ethyl 2-amino-4-propylthiazole-5-carboxylate ( <b>3h</b> ) <sup>[1]</sup>           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|    | Yield: 130 mg, 61%; yellow solid; M.P.: 134-135 °C<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 0.87 (t, <i>J</i> = 7.5 Hz, 3H), 1.22 (t, <i>J</i> = 7.2 Hz, 3H), 1.52-1.62 (m, 2H), 2.80 (t, <i>J</i> = 7.5 Hz, 2H), 4.13 (q, <i>J</i> = 7.2 Hz, 2H), 7.73 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.3, 14.8, 22.4, 32.6, 60.3, 108.0, 162.3, 164.1, 170.9.                                                                                                                                                                |
| ethyl 2-amino-4-isopropylthiazole-5-carboxylate ( <b>3i</b> ) <sup>[3]</sup>        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|  | Yield: 114 mg, 58%; yellow solid; M.P.: 171-173 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.120 (d, <i>J</i> = 6.6 Hz, 6H), 1.213 (t, <i>J</i> = 6.9 Hz, 3H), 3.745-3.900 (m, 1H), 4.136 (q, <i>J</i> = 6.9 Hz, 2H), 7.776 (br s, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.8, 22.4, 28.7, 60.2, 106.5, 162.2, 169.4, 171.2.                                                                                                                                                                                              |
| ethyl 2-amino-4-butylthiazole-5-carboxylate ( <b>3j</b> )                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|  | Yield: 95 mg, 41%; yellow solid; M.P.: 118-119 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 0.87 (t, <i>J</i> = 7.5 Hz, 3H), 1.22 (t, <i>J</i> = 7.2 Hz, 3H), 1.24-1.34 (m, 2H), 1.49-1.59 (m, 2H), 2.82 (t, <i>J</i> = 7.2 Hz, 2H), 4.13 (q, <i>J</i> = 7.2 Hz, 2H), 7.73 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.3, 14.8, 22.4, 30.2, 31.2, 60.2, 107.8, 162., 164.3, 170.9;<br>HRMS (ESI) calcd for C <sub>10</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub> S (M+H) <sup>+</sup> 229.10046, found 229.10053. |
| ethyl 2-amino-4-(tert-butyl)thiazole-5-carboxylate ( <b>3k</b> )                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|  | Yield: 51 mg, 24%; yellow waxy solid.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.21 (t, <i>J</i> = 6.9 Hz, 3H), 1.34 (s, 9H), 4.12 (q, <i>J</i> = 6.9 Hz, 2H), 7.67 (br, 2H).<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.8, 29.6, 36.4, 60.4, 107.0, 161.6, 169.4, 170.7.<br>HRMS (ESI) calcd for C <sub>10</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub> S (M+H) <sup>+</sup> 229.10036, found 229.10053.                                                                                                                   |
| ethyl 2-amino-4-cyclohexylthiazole-5-carboxylate ( <b>3l</b> )                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|                                                                                     | Yield: 84 mg, 33%; yellow solid; M.P.: 179-182 °C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |

|                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
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|    | <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.22 (t, <i>J</i> = 7.2 Hz, 3H), 1.29-1.76 (m, 10H), 3.40-3.50 (m, 1H), 4.13 (q, <i>J</i> = 6.9 Hz, 2H), 7.74 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.8, 26.2, 26.6, 32.2, 38.9, 60.2, 106.6, 162.2, 168.7, 171.1;<br>HRMS (ESI) calcd for C <sub>12</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub> S (M+H) <sup>+</sup> 255.11599, found 255.11618.                                                                                                                                                                             |
| ethyl 2-amino-4-phenylthiazole-5-carboxylate ( <b>3m</b> ) <sup>[3]</sup>           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|    | Yield: 130 mg, 52%; yellow solid; M.P.: 147-149 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.14 (t, <i>J</i> = 6.9 Hz, 3H), 4.08 (q, <i>J</i> = 6.9 Hz, 2H), 7.36-7.38 (m, 3H), 7.61-7.62 (m, 2H), 7.85 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.6, 60.6, 108.8, 127.8, 129.2, 130.2, 135.1, 159.3, 161.7, 170.4.                                                                                                                                                                                                                                                          |
| ethyl 2-amino-4-(p-tolyl) thiazole-5-carboxylate ( <b>3n</b> )                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|    | Yield: 107 mg, 41%; yellow solid; M.P.: 178-181 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.15 (t, <i>J</i> = 7.2 Hz, 3H), 2.33 (s, 3H), 4.08 (q, <i>J</i> = 7.2 Hz, 2H), 7.17 (d, <i>J</i> = 7.8 Hz, 2H), 7.55 (d, <i>J</i> = 7.8 Hz, 2H), 7.84 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.6, 21.4, 60.4, 108.3, 128.3, 130.1, 132.2, 138.6, 159.3, 161.7, 170.2;<br>HRMS (ESI) calcd for C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub> S (M+H) <sup>+</sup> 263.08464, found 263.08488.                                                                   |
| ethyl 2-amino-4-(4-methoxyphenyl) thiazole-5-carboxylate ( <b>3o</b> )              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|  | Yield: 51 mg, 18%; yellow solid; M.P.: 241-244 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.16 (t, <i>J</i> = 6.9 Hz, 3H), 3.79 (s, 3H), 4.09 (q, <i>J</i> = 6.0 Hz, 2H), 6.92 (d, <i>J</i> = 8.7 Hz, 2H), 7.65 (d, <i>J</i> = 8.4 Hz, 2H), 7.81 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.7, 55.6, 60.4, 107.6, 113.2, 127.3, 131.7, 159.1, 160.1, 161.8, 170.1;<br>HRMS (ESI) calcd for C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O <sub>3</sub> S (M+H) <sup>+</sup> 279.07957, found 279.07979.                                                                    |
| ethyl 2-amino-4-(3-methoxyphenyl) thiazole-5-carboxylate ( <b>3p</b> )              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|  | Yield: 147 mg, 53 %; yellow solid; M.P.: 286-304 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.14 (t, <i>J</i> = 6.9 Hz, 3H), 3.76 (s, 3H), 4.09 (q, <i>J</i> = 6.9 Hz, 2H), 6.94 (d, <i>J</i> = 6.9 Hz, 1H), 7.21-7.30 (m, 3H), 7.88 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.6, 55.6, 60.6, 109.1, 115.0, 115.5, 122.7, 128.9, 136.4, 158.9, 159.0, 161.7, 170.4;<br>HRMS (ESI) calcd for C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O <sub>3</sub> S (M+H) <sup>+</sup> 279.07970, found 279.07979.                                                                  |
| ethyl 2-amino-4-(2-methoxyphenyl) thiazole-5-carboxylate ( <b>3q</b> )              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|  | Yield: 50 mg, 17%; yellow waxy solid.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.02 (t, <i>J</i> = 7.2 Hz, 3H), 3.68 (s, 3H), 3.97 (q, <i>J</i> = 7.2 Hz, 2H), 6.93 (t, <i>J</i> = 7.2 Hz, 1H), 7.01 (d, <i>J</i> = 8.4 Hz, 1H), 7.20 (d, <i>J</i> = 7.2 Hz, 1H), 7.32 (t, <i>J</i> = 7.2 Hz, 1H), 7.76 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.5, 55.7, 60.2, 110.8, 111.4, 120.1, 125.4, 130.1, 130.6, 155.8, 157.3, 161.6, 170.3;<br>HRMS (ESI) calcd for C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O <sub>3</sub> S (M+H) <sup>+</sup> 279.07962, found 279.07979. |
| ethyl 2-amino-4-(4-fluorophenyl) thiazole-5-carboxylate ( <b>3r</b> )               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|                                                                                     | Yield: 79 mg, 30%; yellow solid; M.P.: 187-190 °C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |

|                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|-------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|    | <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.149 (t, <i>J</i> = 7.0 Hz, 3H), 4.089 (q, <i>J</i> = 7.1 Hz, 2H), 7.198 (t, <i>J</i> = 8.9 Hz, 2H), 7.671-7.719 (m, 2H), 7.881 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.6, 60.6, 108.7, 114.6 and 114.9(d, <i>J</i> (C,F) = 22.5 Hz), 131.42 and 131.46(d, <i>J</i> (C,F) = 3.0 Hz), 132.4 and 132.5(d, <i>J</i> (C,F) = 7.5 Hz), 158.1, 161.1 and 164.4 (d, <i>J</i> (C,F) = 247.5 Hz), 161.6, 170.4;<br>HRMS (ESI) calcd for C <sub>12</sub> H <sub>12</sub> FN <sub>2</sub> O <sub>2</sub> S (M+H) <sup>+</sup> 267.05958, found 267.05980. |
| ethyl 2-amino-4-(4-chlorophenyl)thiazole-5-carboxylate ( <b>3s</b> ) <sup>[3]</sup> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|    | Yield: 112 mg, 40%; light yellow solid; M.P.: 188-193 °C<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.15 (t, <i>J</i> = 6.9 Hz, 3H), 4.09 (q, <i>J</i> = 6.9 Hz, 2H), 7.44 (d, <i>J</i> = 8.4 Hz, 2H), 7.67 (d, <i>J</i> = 8.7 Hz, 2H), 7.90 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.6, 60.7, 109.1, 127.9, 132.0, 133.8, 133.8, 157.8, 161.6, 170.5.                                                                                                                                                                                                                                   |
| ethyl 2-amino-4-(4-bromophenyl)thiazole-5-carboxylate ( <b>3t</b> ) <sup>[4]</sup>  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|    | Yield: 62 mg, 19%; light yellow solid; M.P.: 187-202 °C<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.15 (t, <i>J</i> = 6.9 Hz, 3H), 4.09 (q, <i>J</i> = 6.9 Hz, 2H), 7.55-7.62 (m, 4H), 7.90 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.6, 60.7, 109.1, 122.5, 130.8, 132.2, 134.2, 157.8, 161.5, 170.5.                                                                                                                                                                                                                                                                                   |
| ethyl 2-amino-4-(4-nitrophenyl)thiazole-5-carboxylate ( <b>3u</b> ) <sup>[4]</sup>  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|  | Yield: 155 mg, 53%; yellow waxy solid.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.15 (t, <i>J</i> = 6.9 Hz, 3H), 4.11 (q, <i>J</i> = 6.9 Hz, 2H), 7.90 (d, <i>J</i> = 8.7 Hz, 2H), 7.99 (br, 2H), 8.25 (d, <i>J</i> = 8.4 Hz, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.5, 60.9, 113.0, 123.1, 131.5, 141.4, 147.7, 156.4, 161.4, 170.7.                                                                                                                                                                                                                                                     |
| ethyl 2-amino-4-(furan-2-yl)thiazole-5-carboxylate ( <b>3v</b> ) <sup>[4]</sup>     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|  | Yield: 55 mg, 23%; yellow waxy solid.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.23 (t, <i>J</i> = 6.9 Hz, 3H), 4.18 (q, <i>J</i> = 6.9 Hz, 2H), 6.60-6.62 (m, 1H), 7.48 (d, <i>J</i> = 3.3 Hz, 1H), 7.75 (s, 1H), 7.90 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.7, 60.8, 107.6, 112.2, 114.6, 144.0, 147.8, 148.5, 161.3, 170.2.                                                                                                                                                                                                                                                      |
| 2-amino-N,N-diethyl-4-methylthiazole-5-carboxamide ( <b>3w</b> ) <sup>[2]</sup>     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|  | Yield: 51 mg, 24%; light yellow solid; M.P.: 148-154 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.07 (t, <i>J</i> = 7.2 Hz, 6H), 2.05 (s, 3H), 3.31-3.38 (m, 4H), 7.19 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.1, 16.9, 41.4, 111.4, 149.5, 163.7, 167.8.                                                                                                                                                                                                                                                                                                                           |
| 2-amino-4-phenylthiazole-5-carbonitrile ( <b>3x</b> ) <sup>[5]</sup>                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|  | Yield: 95 mg, 48%; light yellow waxy solid.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 7.50-7.52 (m, 3H), 7.92 (d, <i>J</i> = 6.9 Hz, 2H), 8.26 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 84.1, 115.8, 127.9, 129.3, 130.5, 133.0, 161.5, 171.1.                                                                                                                                                                                                                                                                                                                                             |
| 4-phenyl-5-(phenylsulfonyl)thiazol-2-amine ( <b>3y</b> )                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|  | Yield: 67 mg, 22%; white solid; M.P.: 169-175 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 7.37-7.56 (m, 10H), 8.05 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 117.8, 127.0, 128.6, 130.2, 130.4, 133.7, 134.2, 143.0, 158.3, 171.6.                                                                                                                                                                                                                                                                                                                                                        |

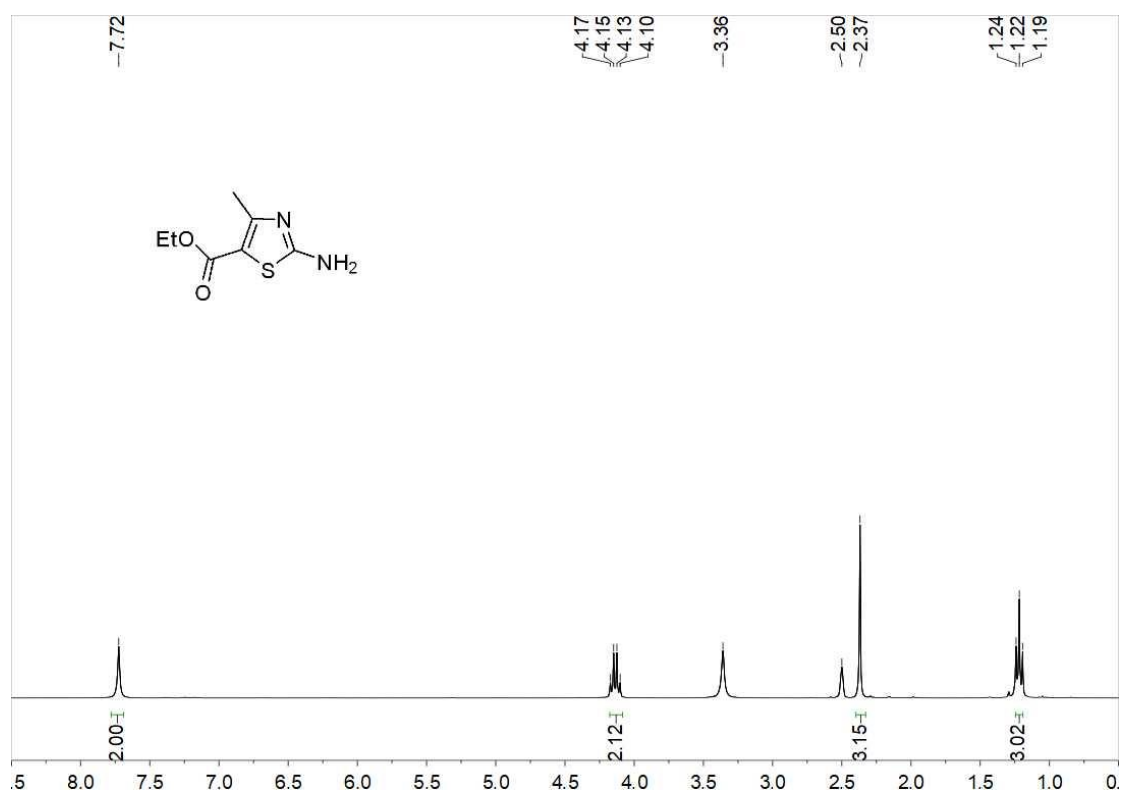
|                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                                                                     | HRMS (ESI) calcd for C <sub>15</sub> H <sub>13</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub> (M+H) <sup>+</sup> 317.04087, found 317.04130.                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| (2-amino-4-phenylthiazol-5-yl) (phenyl)methanone ( <b>3z</b> ) <sup>[6]</sup>       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|    | Yield: 12 mg, 4 %; light yellow solid; M.P.: 157-161 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 7.04-7.14 (m, 5H), 7.22-7.29 (m, 3H), 7.35-7.37 (m, 2H), 8.06 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 121.0, 127.8, 128.1, 128.8, 129.0, 130.0, 131.6, 135.3, 139.0, 159.4, 171.4, 188.0.                                                                                                                                                                                                                                                 |
| 1-(2-amino-4-methylthiazol-5-yl)ethan-1-one ( <b>3aa</b> ) <sup>[5]</sup>           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|    | Yield: 39 mg, 25%; light yellow waxy solid.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 2.32 (s, 3H), 2.40 (s, 3H), 7.84 (br, 2H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 18.8, 30.0, 121.8, 158.1, 171.0, 188.8.                                                                                                                                                                                                                                                                                                                                       |
| Ethyl 4-methyl-2-(methylamino)thiazole-5-carboxylate ( <b>3bb</b> ) <sup>[1]</sup>  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|    | Yield: 154 mg, 77%; light yellow solid; M.P.: 149-151 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.22 (t, <i>J</i> = 6.9 Hz, 3H), 2.41 (s, 3H), 2.82 (d, <i>J</i> = 4.8 Hz, 3H), 4.14 (q, <i>J</i> = 6.9 Hz, 2H), 8.28 (d, <i>J</i> = 4.2 Hz, 1H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.9, 17.8, 31.3, 60.3, 107.5, 160.2, 162.5, 171.2.                                                                                                                                                                                                      |
| ethyl 4-methyl-2-(phenethylamino) thiazole-5-carboxylate ( <b>3cc</b> )             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|  | Yield: 128 mg, 44%; yellow solid; M.P.: 100-102 °C.<br><sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 1.22 (t, <i>J</i> = 6.9 Hz, 3H), 2.40 (s, 3H), 2.85 (t, <i>J</i> = 6.9 Hz, 2H), 3.45 (q, <i>J</i> = 6.6 Hz, 2H), 4.14 (q, <i>J</i> = 6.9 Hz, 2H), 7.23-7.30 (m, 5H), 8.44 (br, 1H);<br><sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ (ppm): 14.9, 17.9, 34.9, 46.2, 60.3, 107.4, 126.8, 128.9, 129.2, 139.5, 160.0, 162.5, 170.1;<br>HRMS (ESI) calcd for C <sub>15</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub> S (M+H) <sup>+</sup> 291.11602, found 291.11618. |

#### 4. References

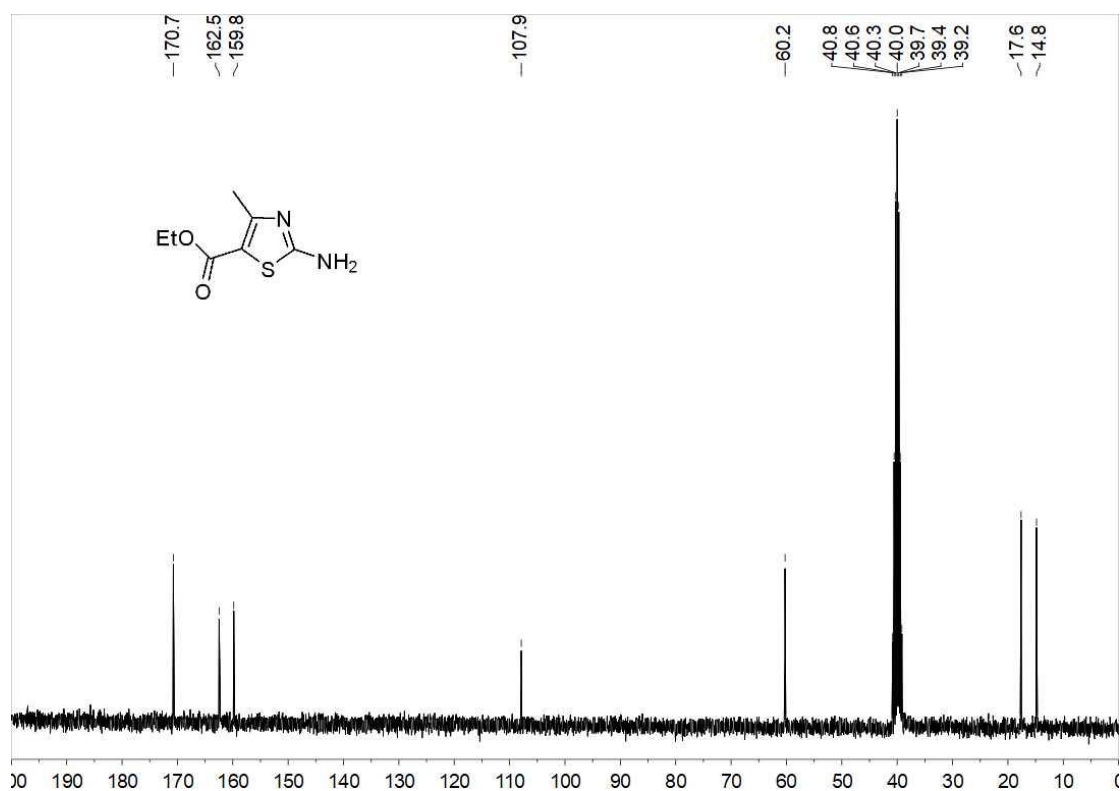
- [1] de Andrade, V. S. C.; de Mattos, M. C. S. d. *Synthesis* **2018**, 50, 4867-4874. doi:org/10.1055/s-00037-1610243.
- [2] Roslan, I. I.; Ng, K. H.; Gondal, M. A.; Basheer, C.; Dastageer, M. A.; Jaenicke, S.; Chuah, G. K. *Adv. Synth. Catal.* **2018**, 360, 1584-1589. doi:org/10.1002/adsc.201701565.
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- [6] Zhao, J. W.; Xu, J. X.; Chen, J. X.; He, M. H.; Wang, X. Q. *Tetrahedron* **2015**, 71, 539-543. doi:org/10.1016/j.tet.2014.12.044

## 5. Spectra of prepared compounds

### $^1\text{H}$ NMR of ethyl 2-amino-4-methylthiazole-5-carboxylate (3a)

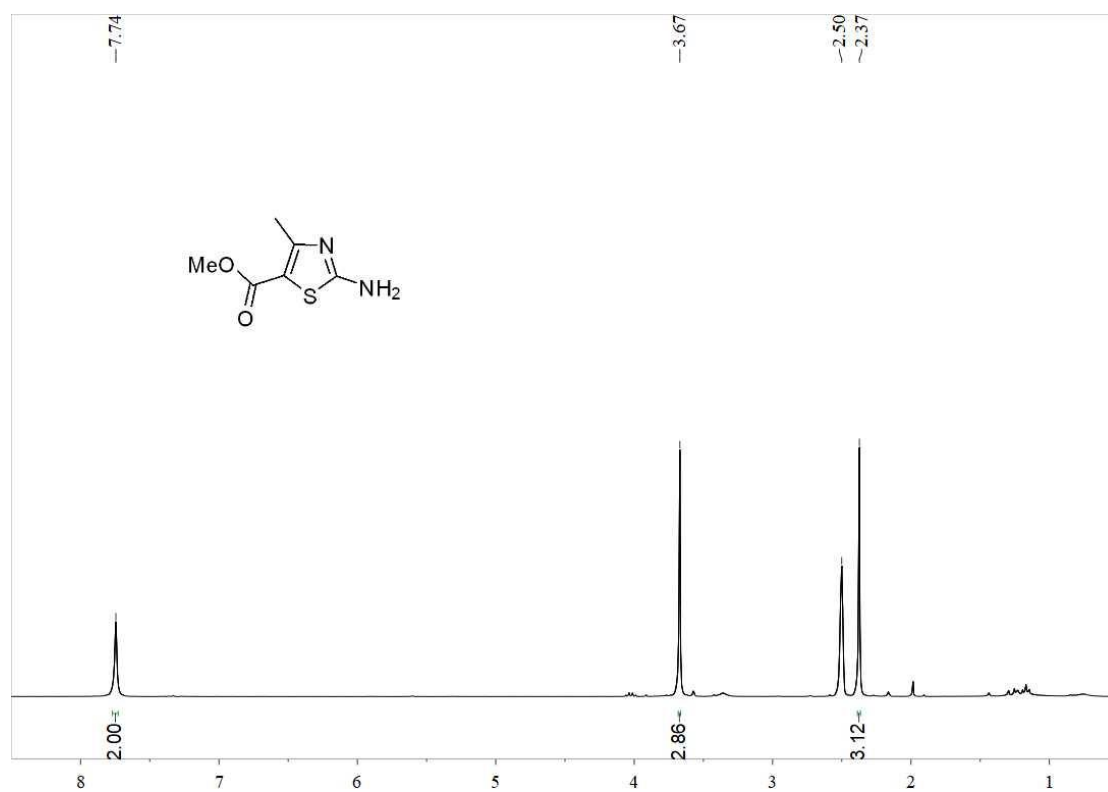


### $^{13}\text{C}$ NMR of ethyl 2-amino-4-methylthiazole-5-carboxylate (3a)

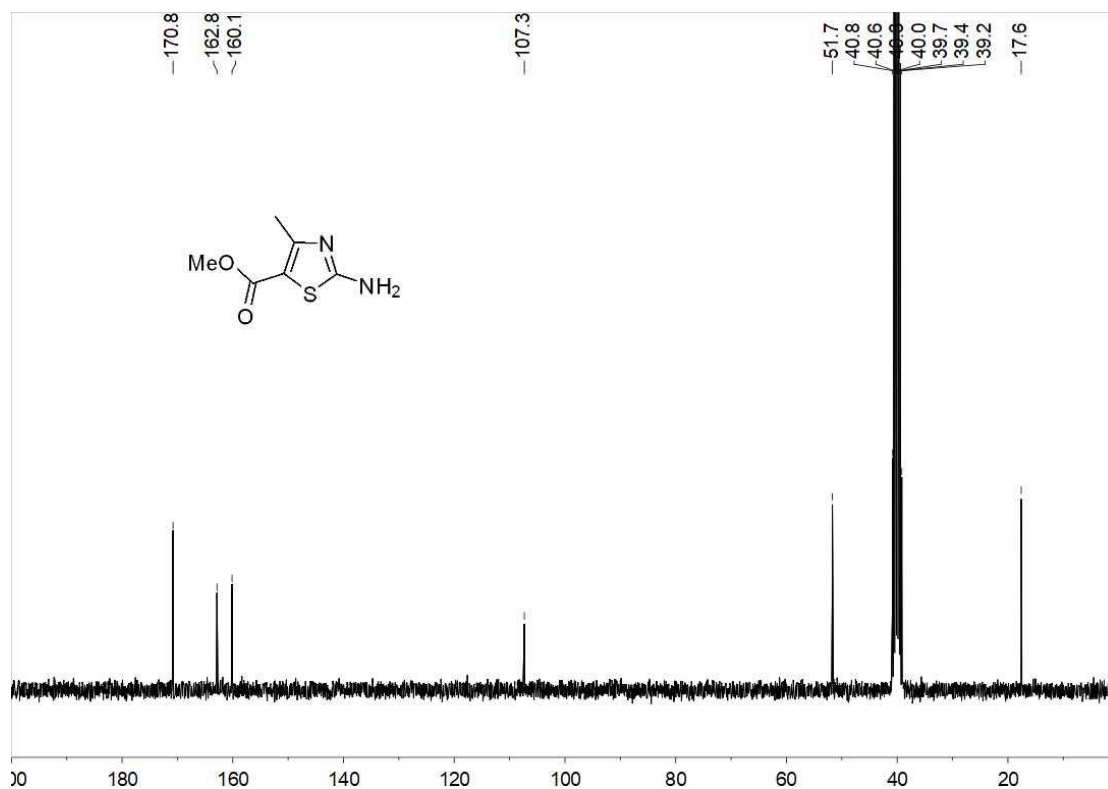




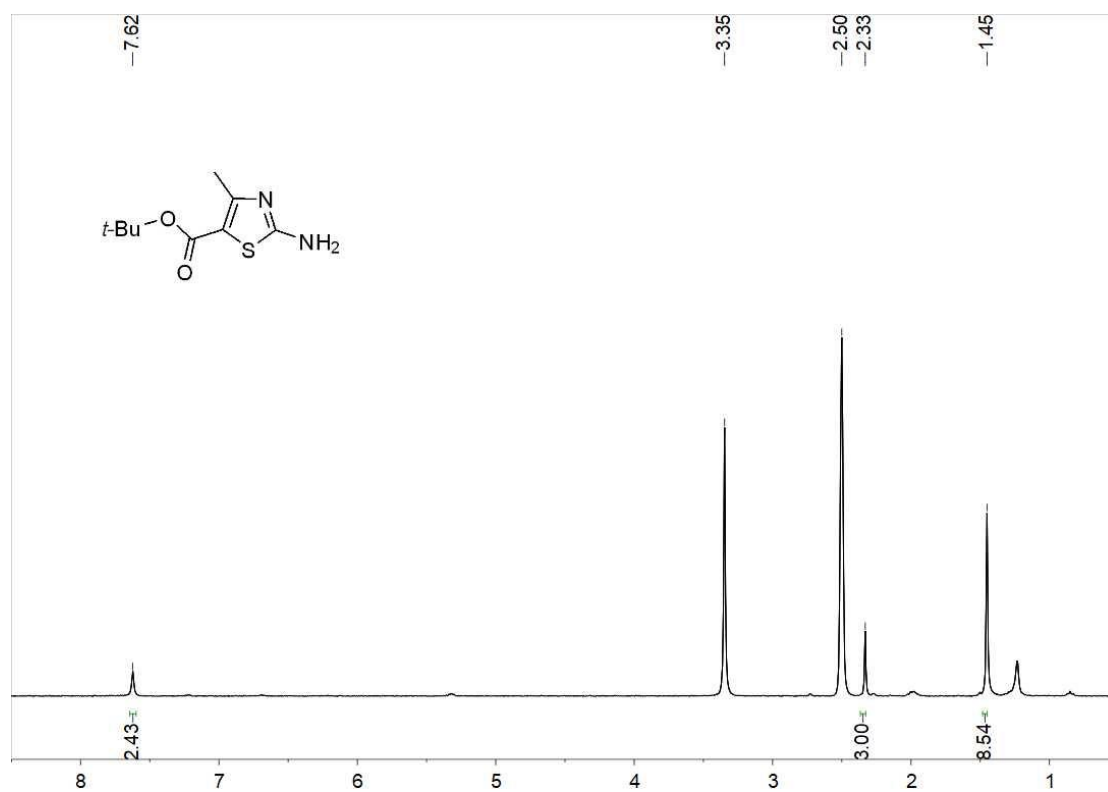
**<sup>1</sup>H NMR of methyl 2-amino-4-methylthiazole-5-carboxylate (3b)**



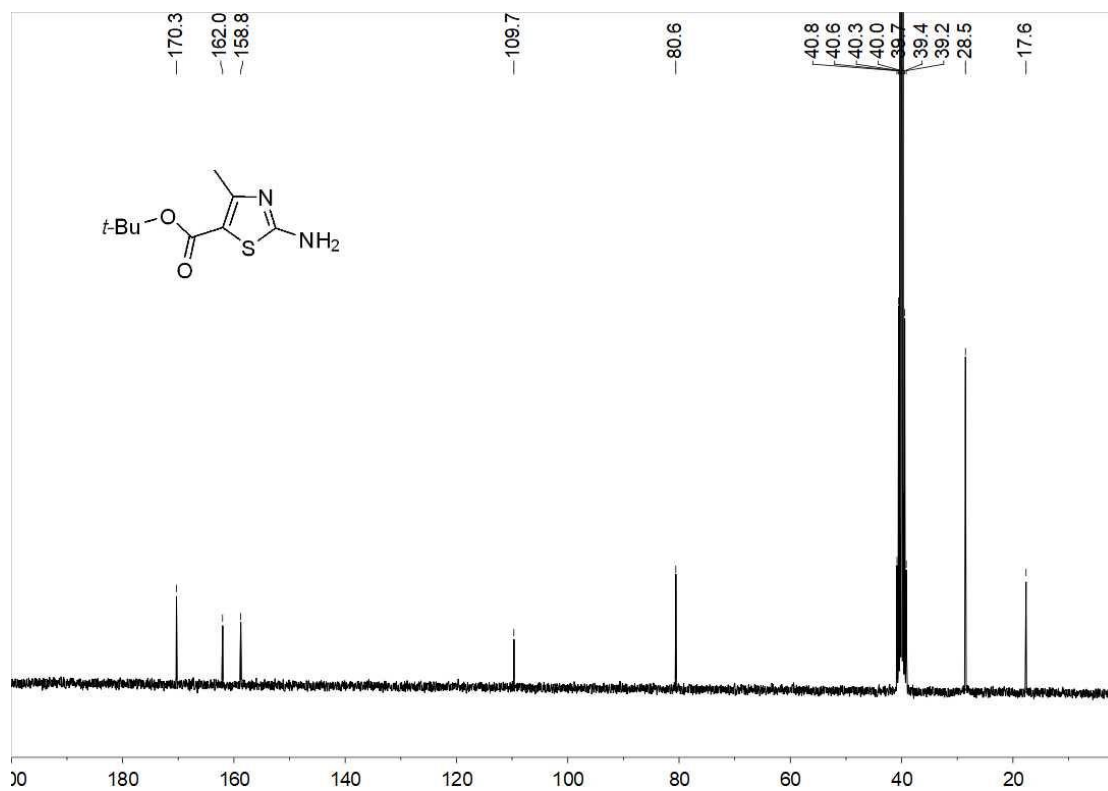
**<sup>13</sup>C NMR of methyl 2-amino-4-methylthiazole-5-carboxylate (3b)**



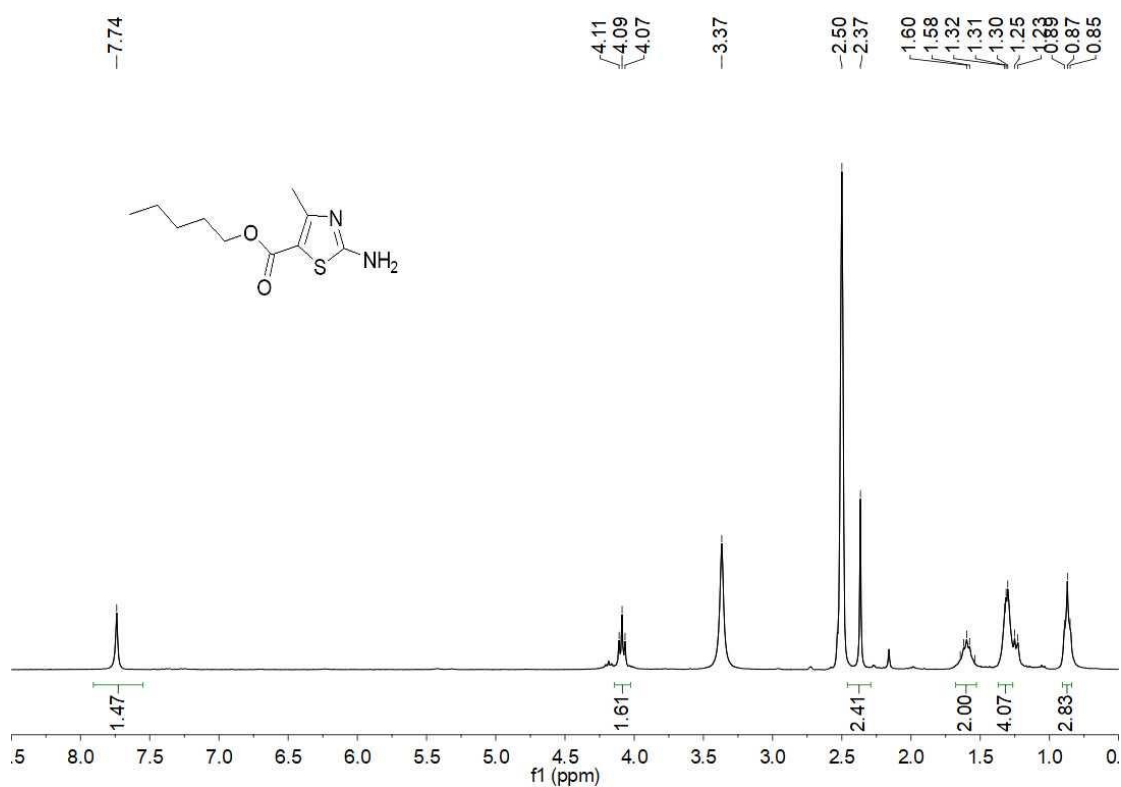
**<sup>1</sup>H NMR of *tert*-butyl 2-amino-4-methylthiazole-5-carboxylate (3c)**



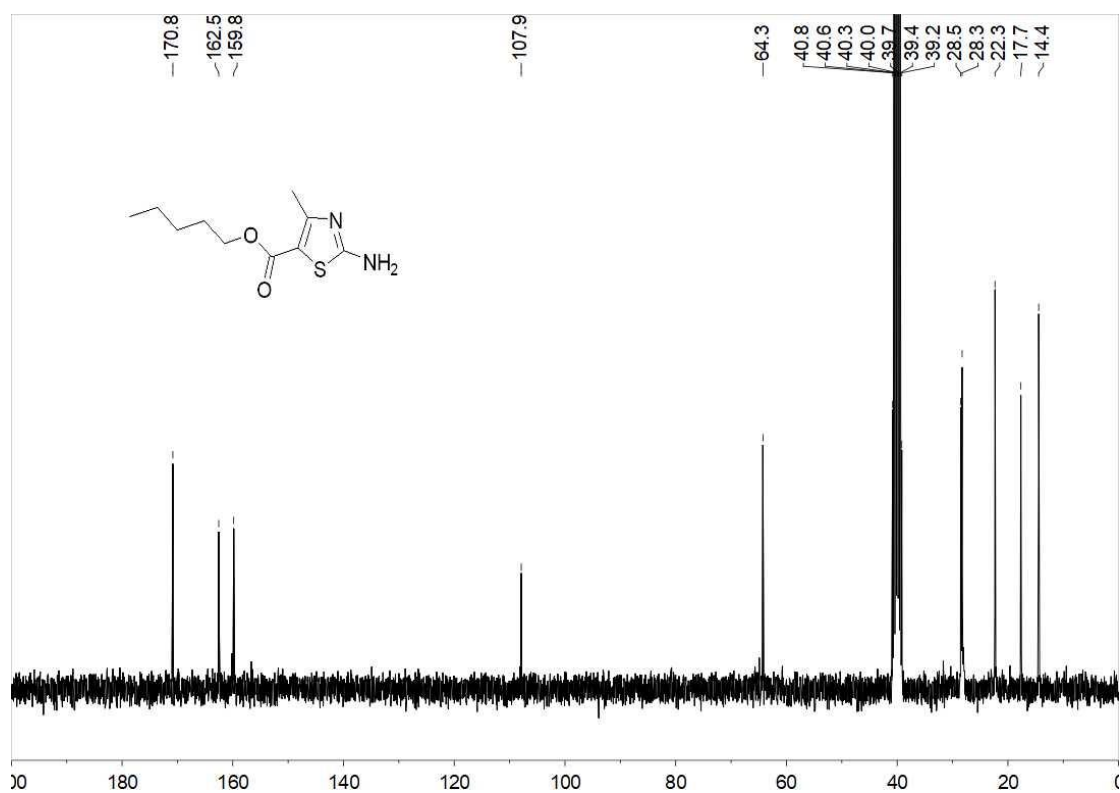
**<sup>13</sup>C NMR of *tert*-butyl 2-amino-4-methylthiazole-5-carboxylate (3c)**



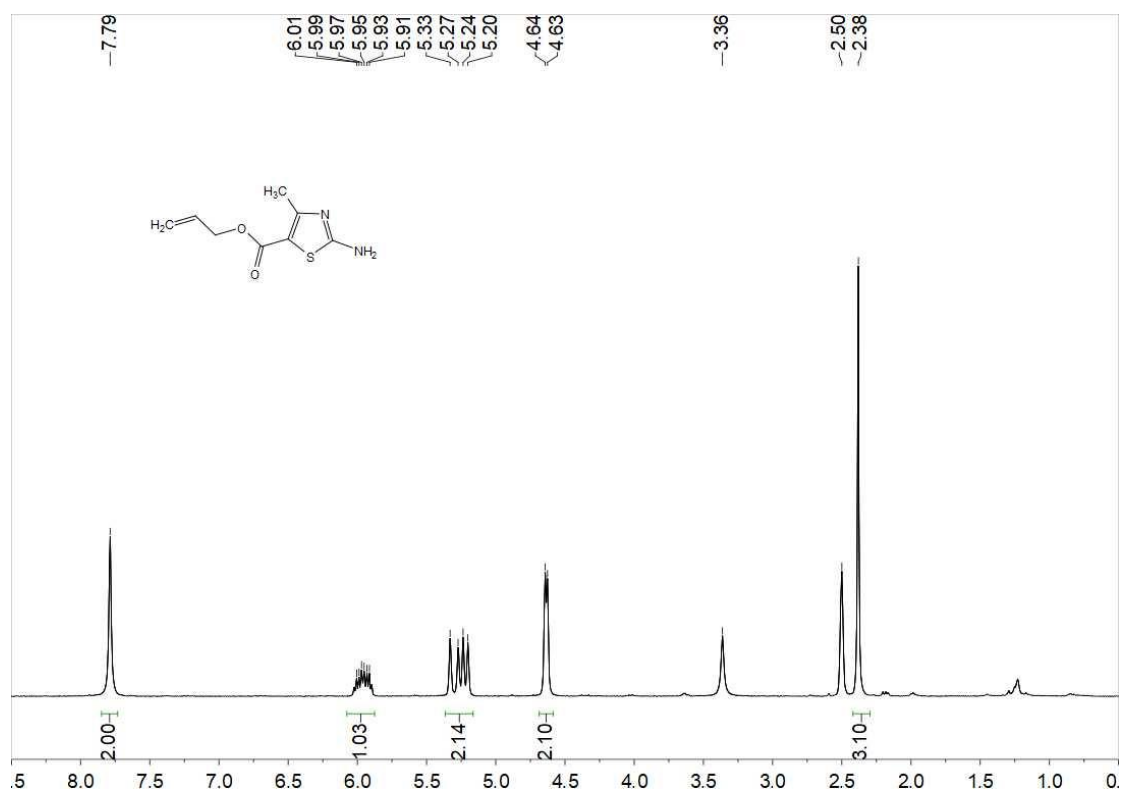
**$^1\text{H}$  NMR of pentyl 2-amino-4-methylthiazole-5-carboxylate (3d)**



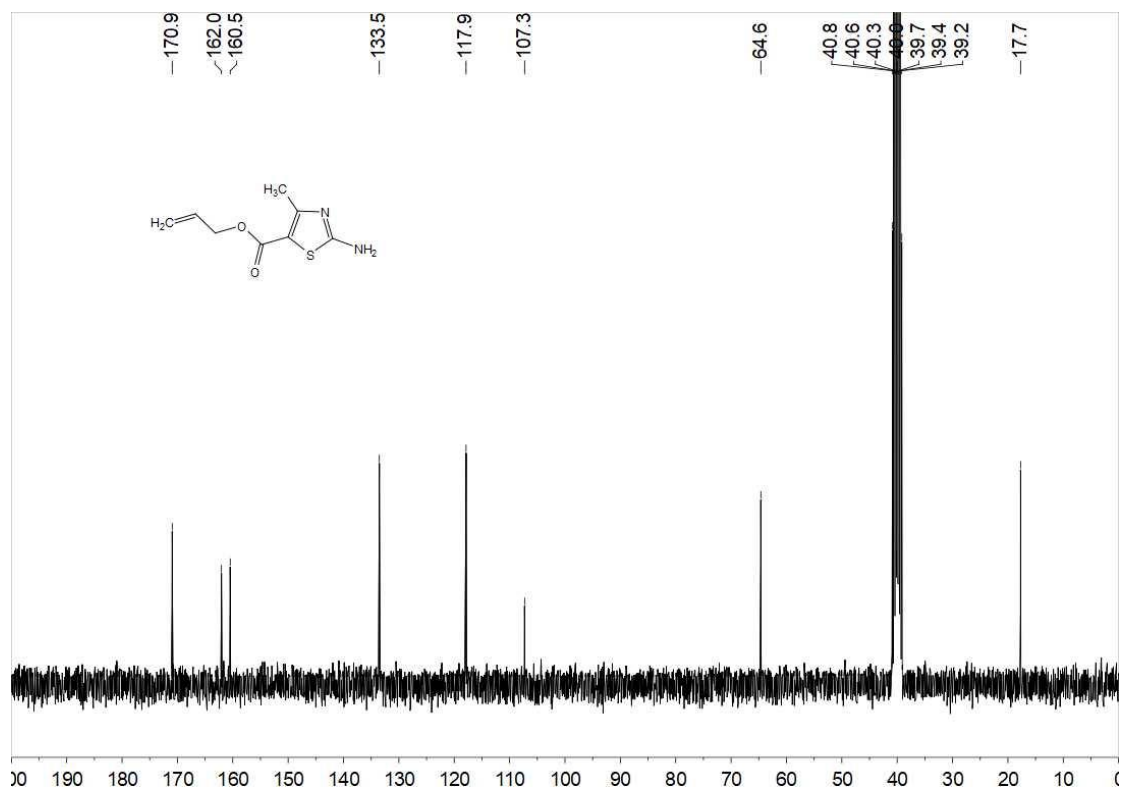
**$^{13}\text{C}$  NMR of pentyl 2-amino-4-methylthiazole-5-carboxylate (3d)**



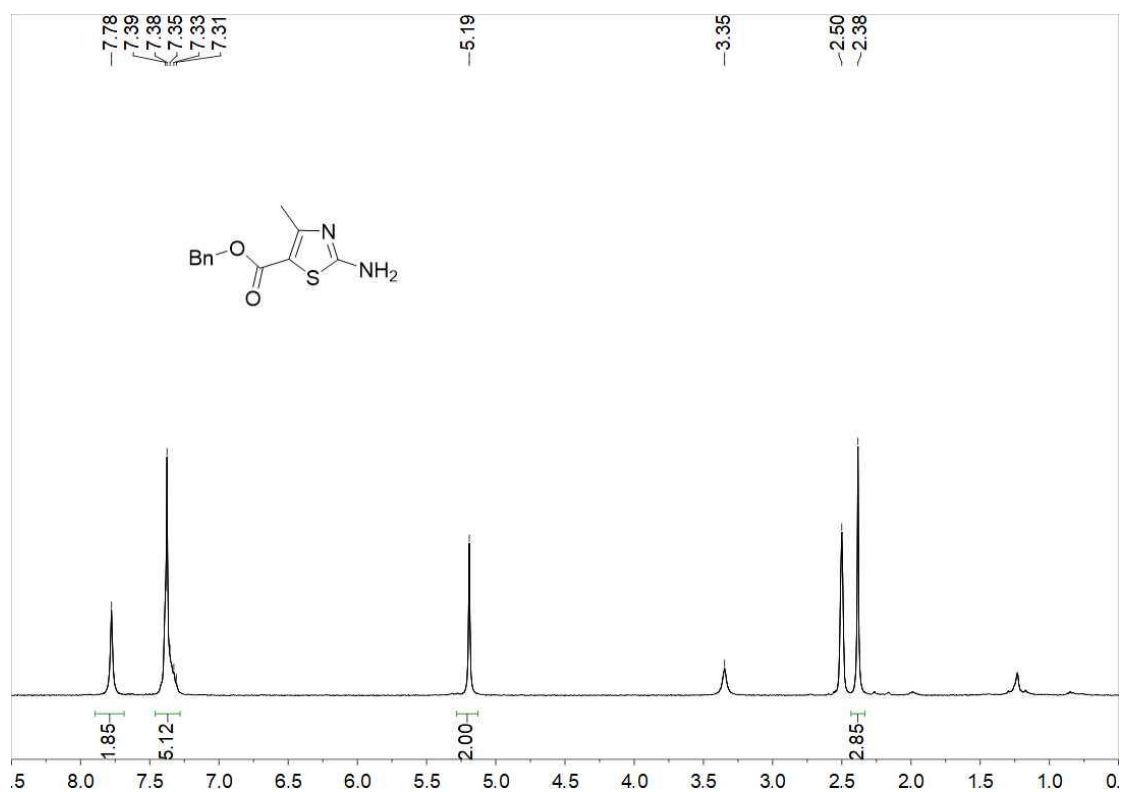
**<sup>1</sup>H NMR of allyl 2-amino-4-methylthiazole-5-carboxylate (3e)**



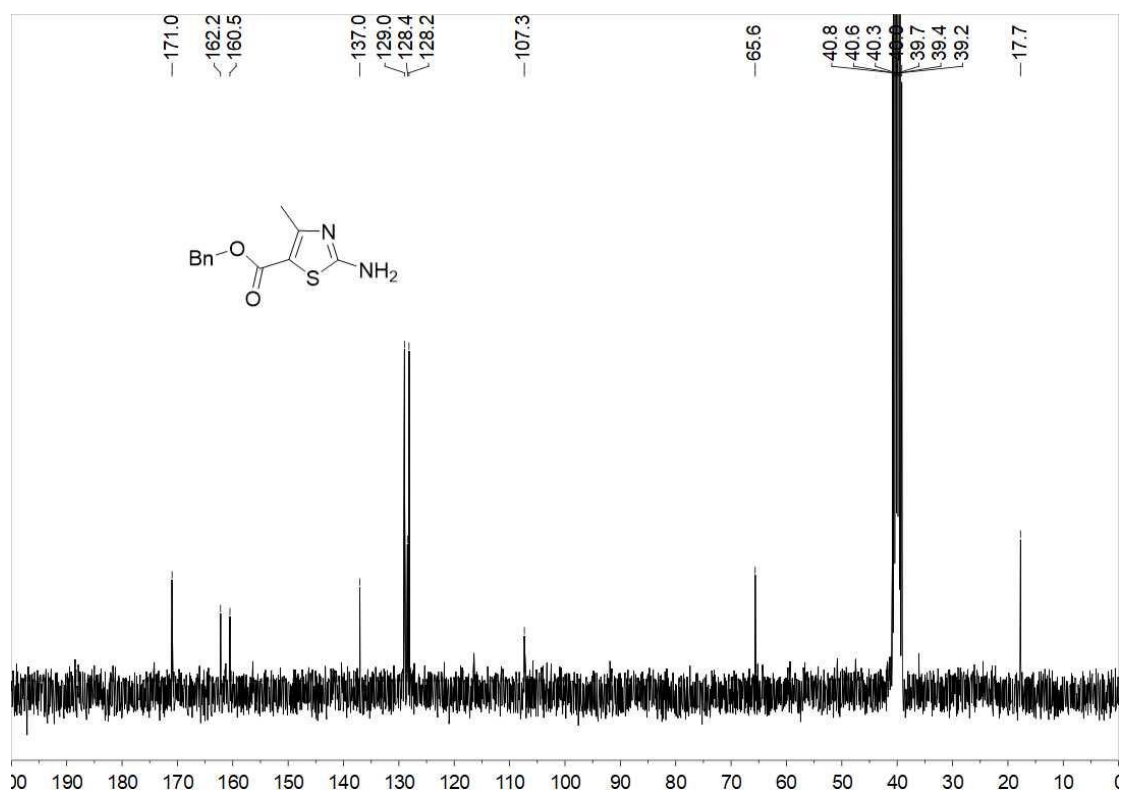
**<sup>13</sup>C NMR of allyl 2-amino-4-methylthiazole-5-carboxylate (3e)**



**<sup>1</sup>H NMR of benzyl 2-amino-4-methylthiazole-5-carboxylate (3f)**



**<sup>13</sup>C NMR of benzyl 2-amino-4-methylthiazole-5-carboxylate (3f)**



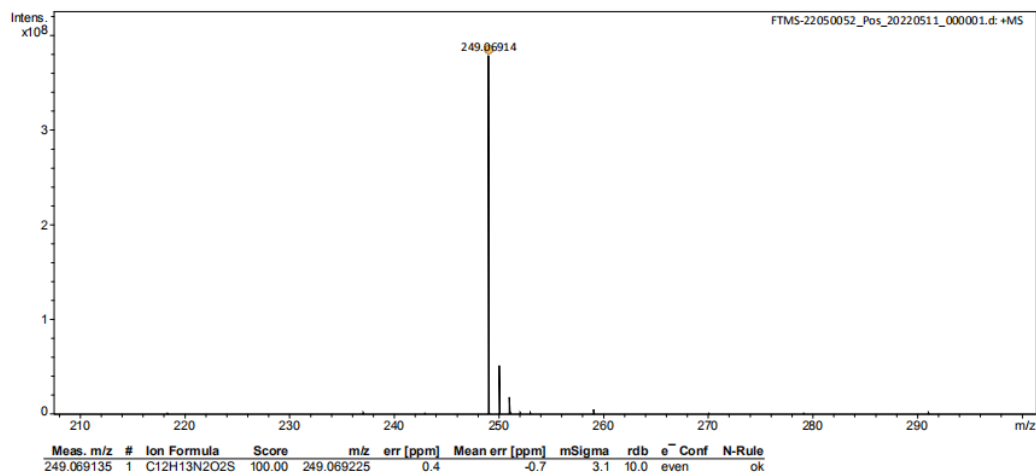
## HRMS of benzyl 2-amino-4-methylthiazole-5-carboxylate (3f)

### Peking University Mass Spectrometry Sample Analysis Report

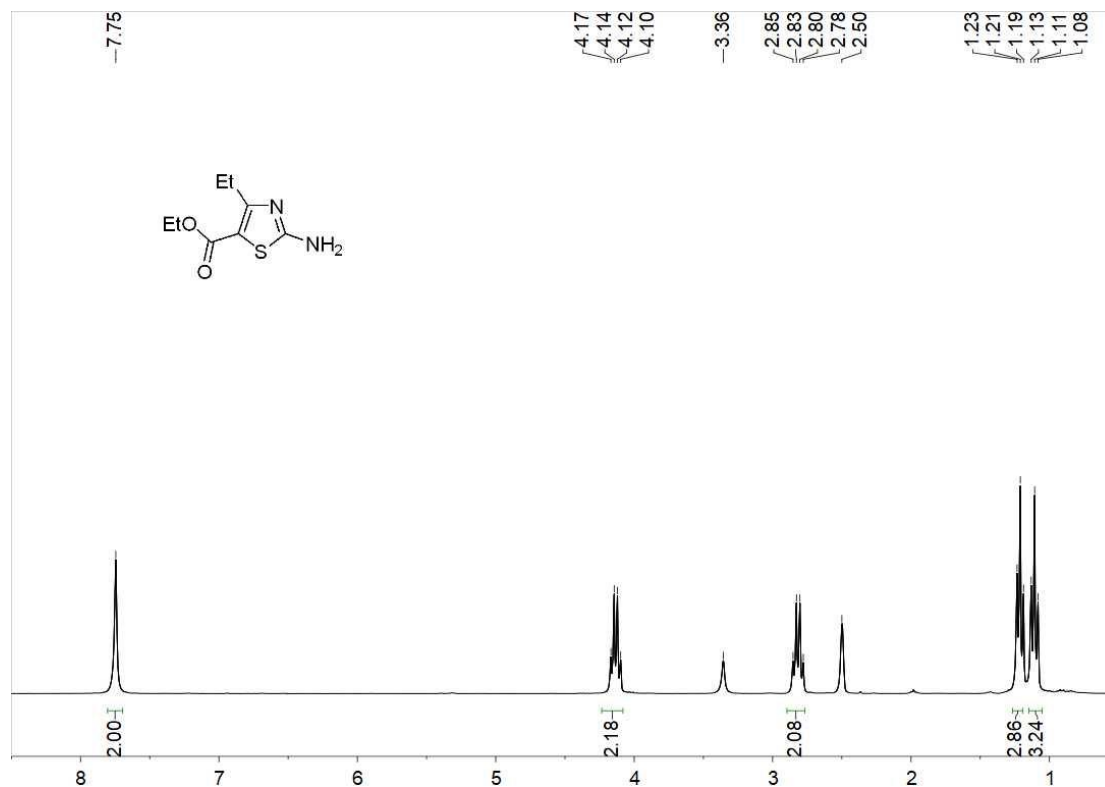
#### Analysis Info

Analysis Name FTMS-22050052\_Pos\_20220511\_000001.d  
Sample 0509-01  
Comment

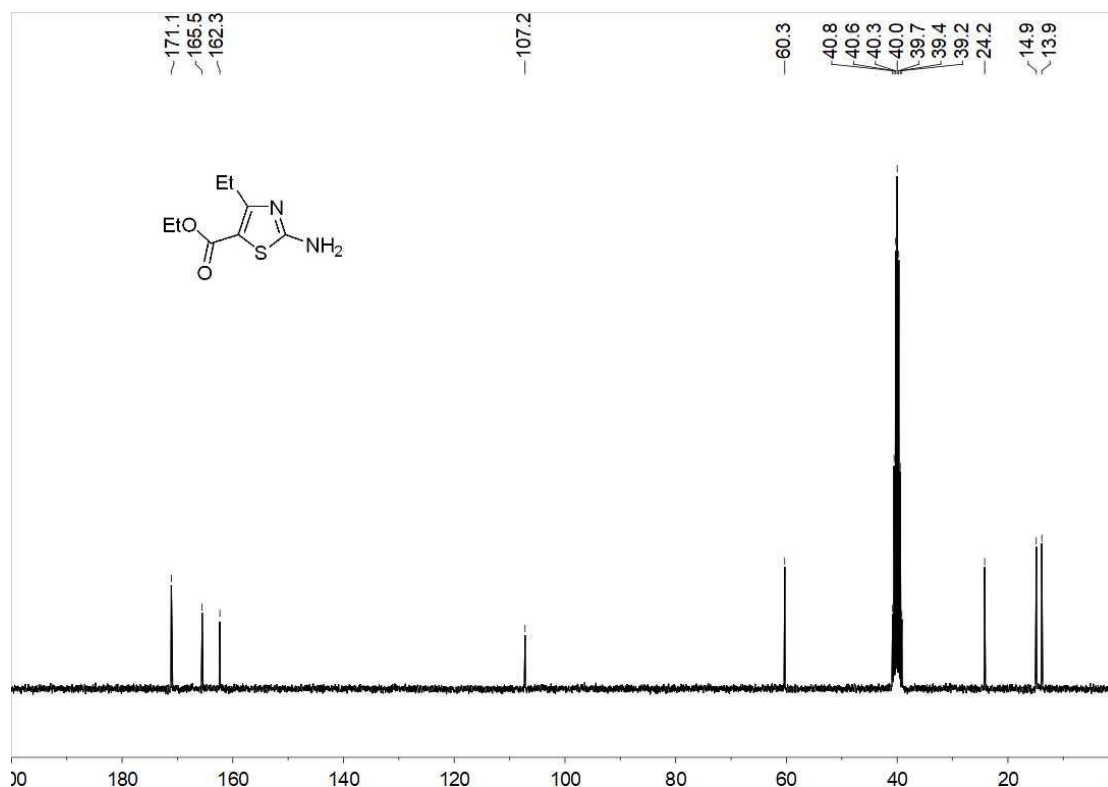
Acquisition Date 5/11/2022 2:43:57 PM  
Instrument Bruker Solarix XR FTMS  
Operator Peking University



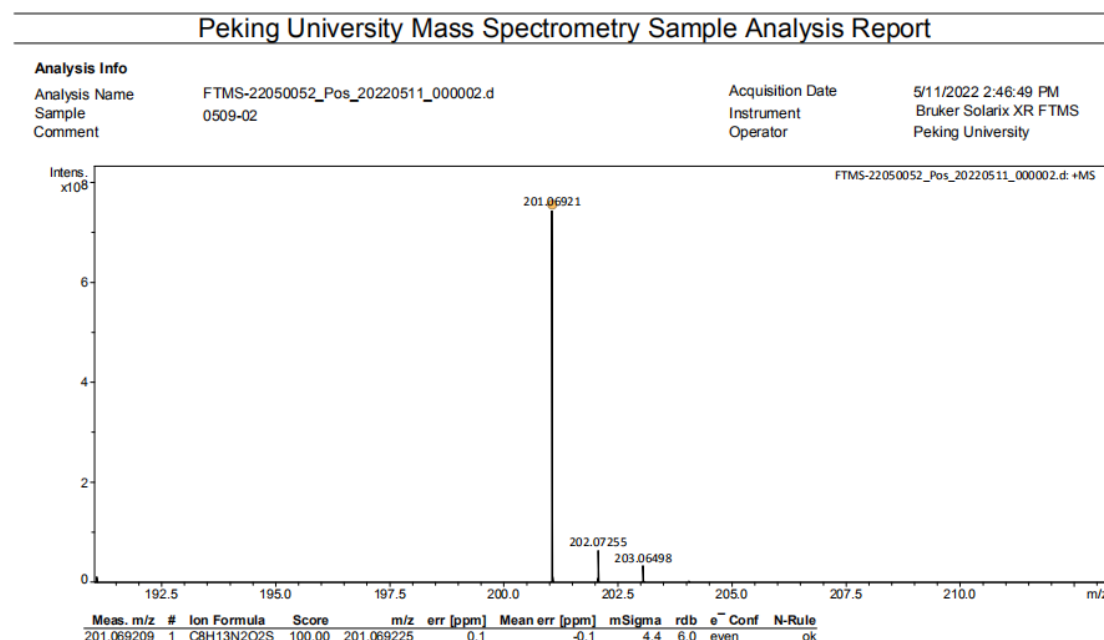
## <sup>1</sup>H NMR of ethyl 2-amino-4-ethylthiazole-5-carboxylate (3g)



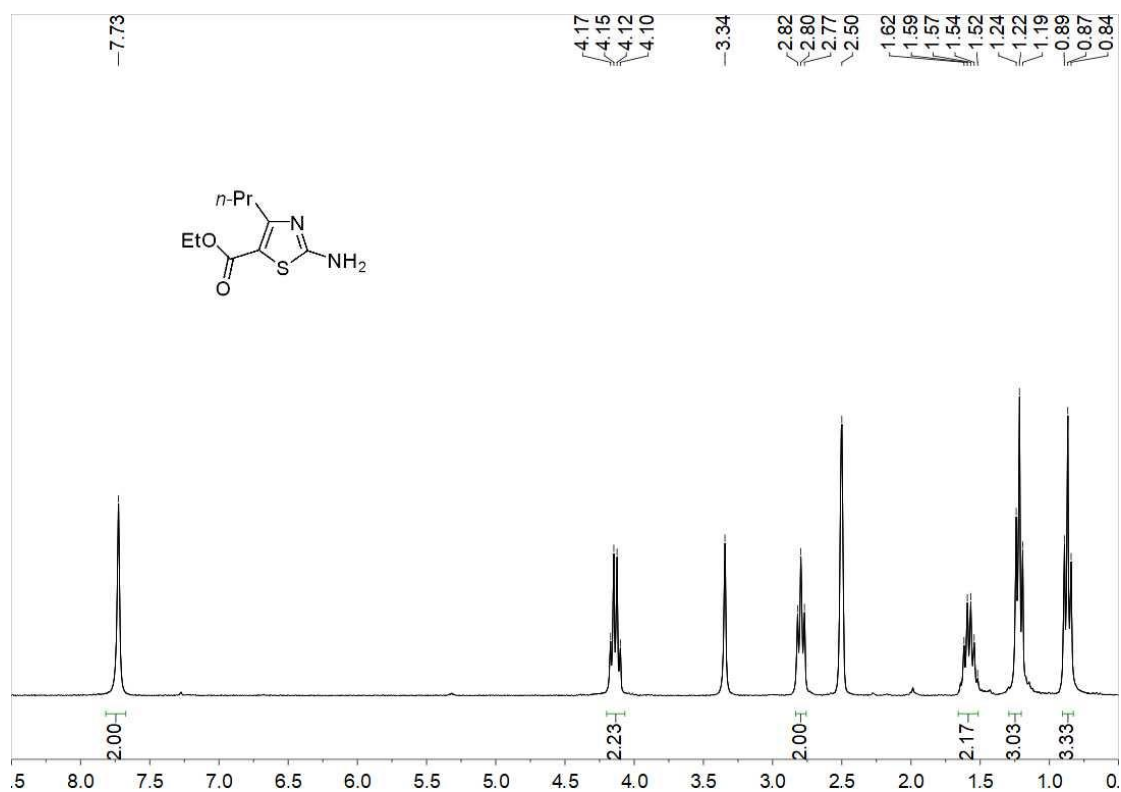
### <sup>13</sup>C NMR of ethyl 2-amino-4-ethylthiazole-5-carboxylate (3g)



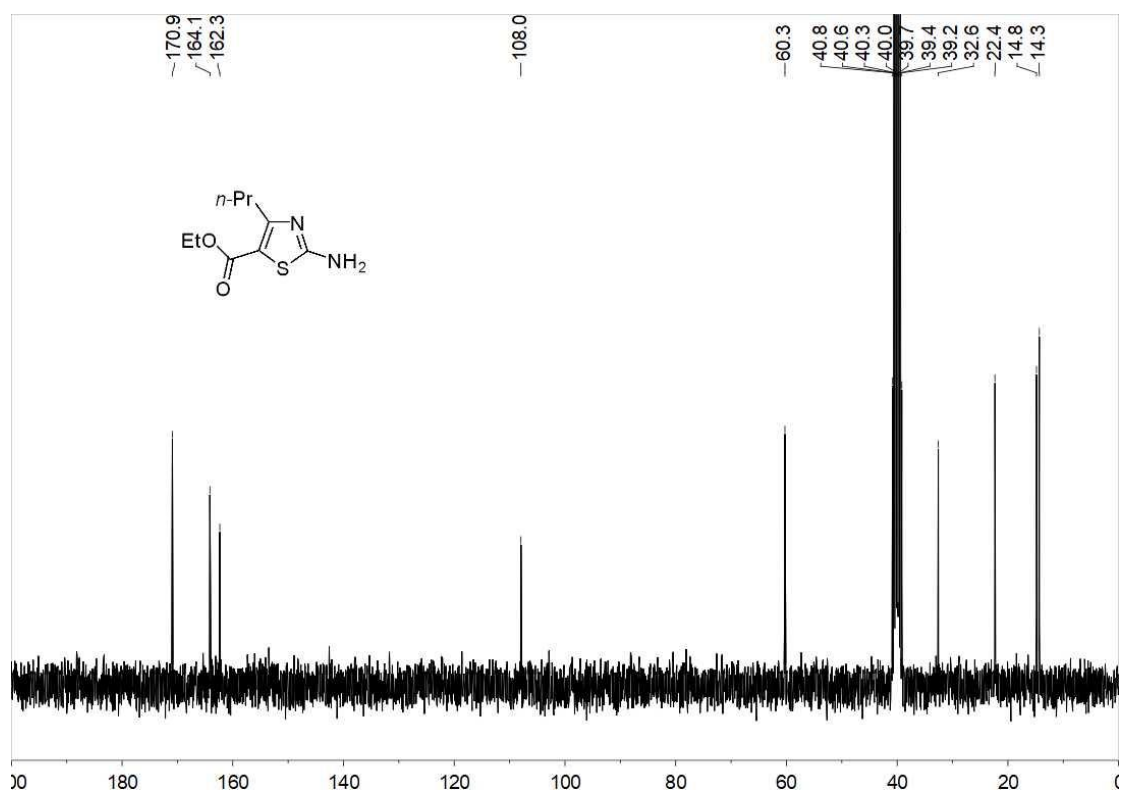
### HRMS of ethyl 2-amino-4-ethylthiazole-5-carboxylate (3g)



**$^1\text{H}$  NMR of ethyl 2-amino-4-propylthiazole-5-carboxylate (3h)**

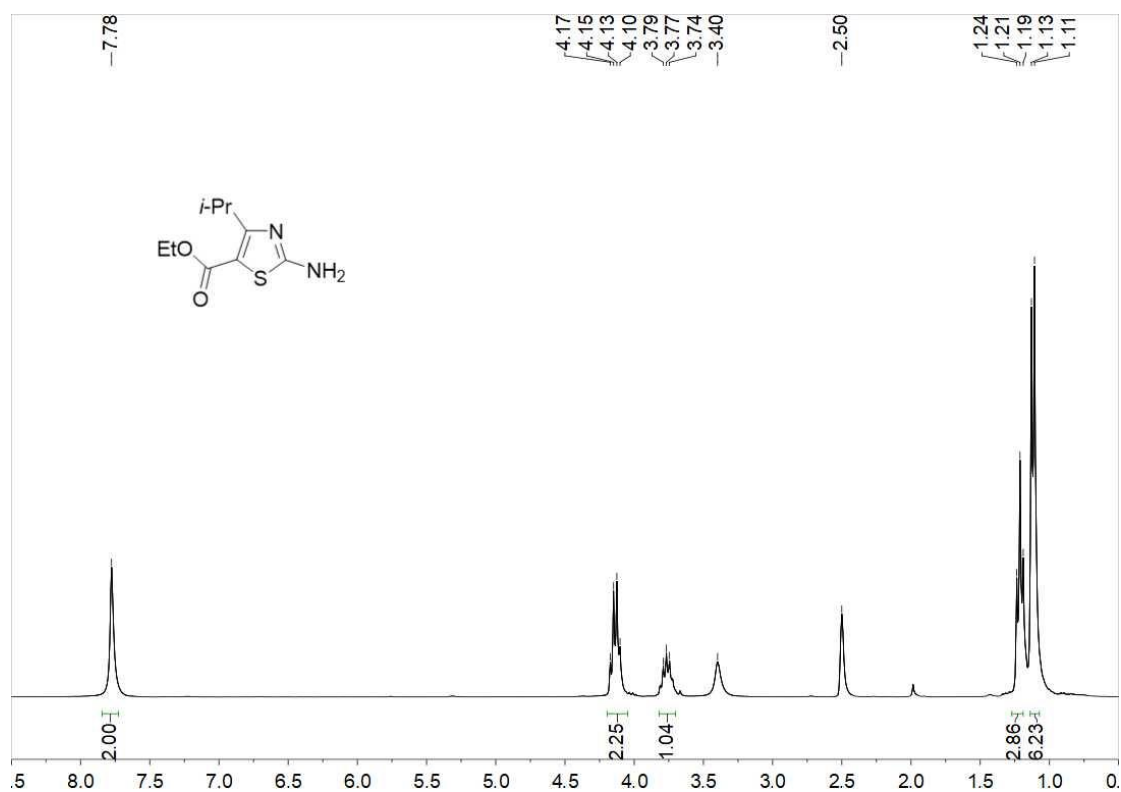


**$^{13}\text{C}$  NMR of ethyl 2-amino-4-propylthiazole-5-carboxylate (3h)**

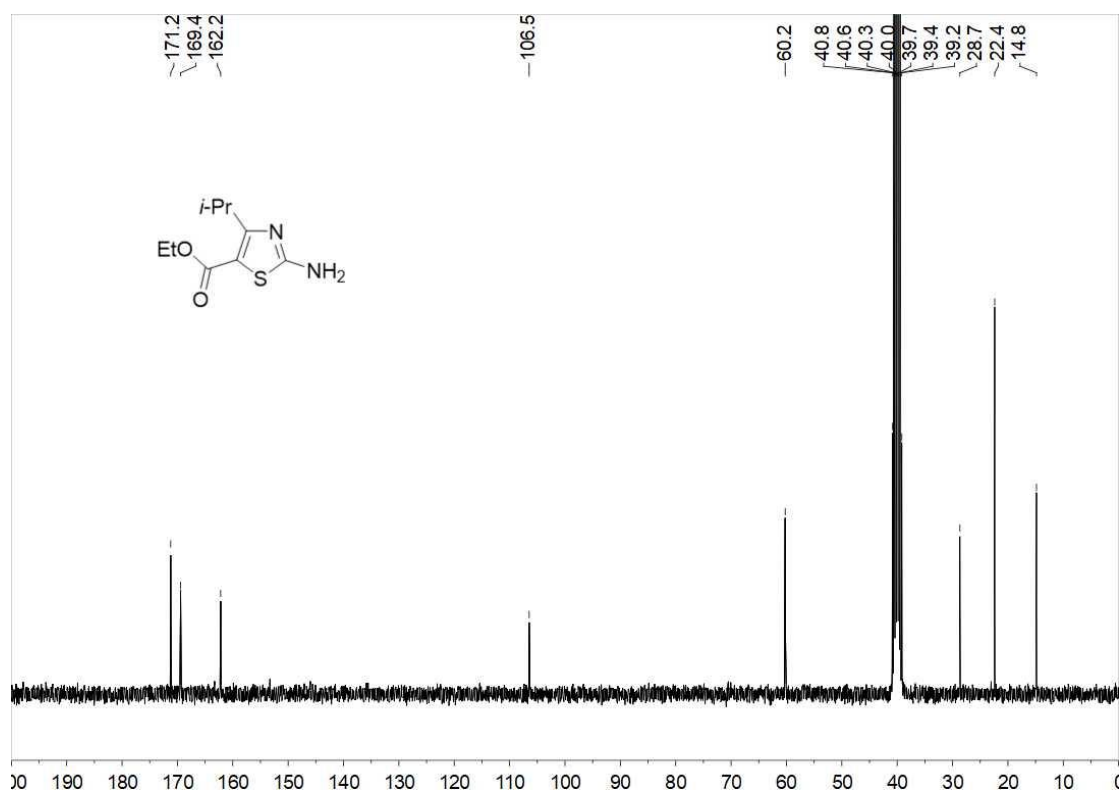




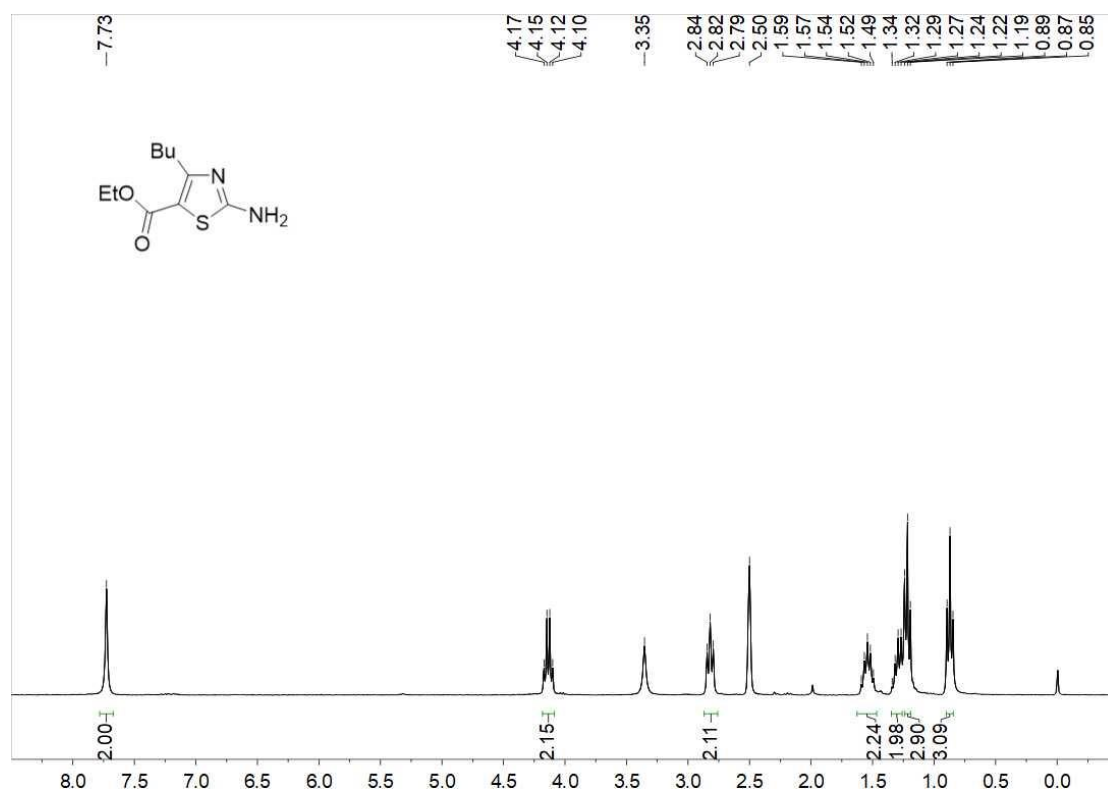
**<sup>1</sup>H NMR of ethyl 2-amino-4-isopropylthiazole-5-carboxylate (3i)**



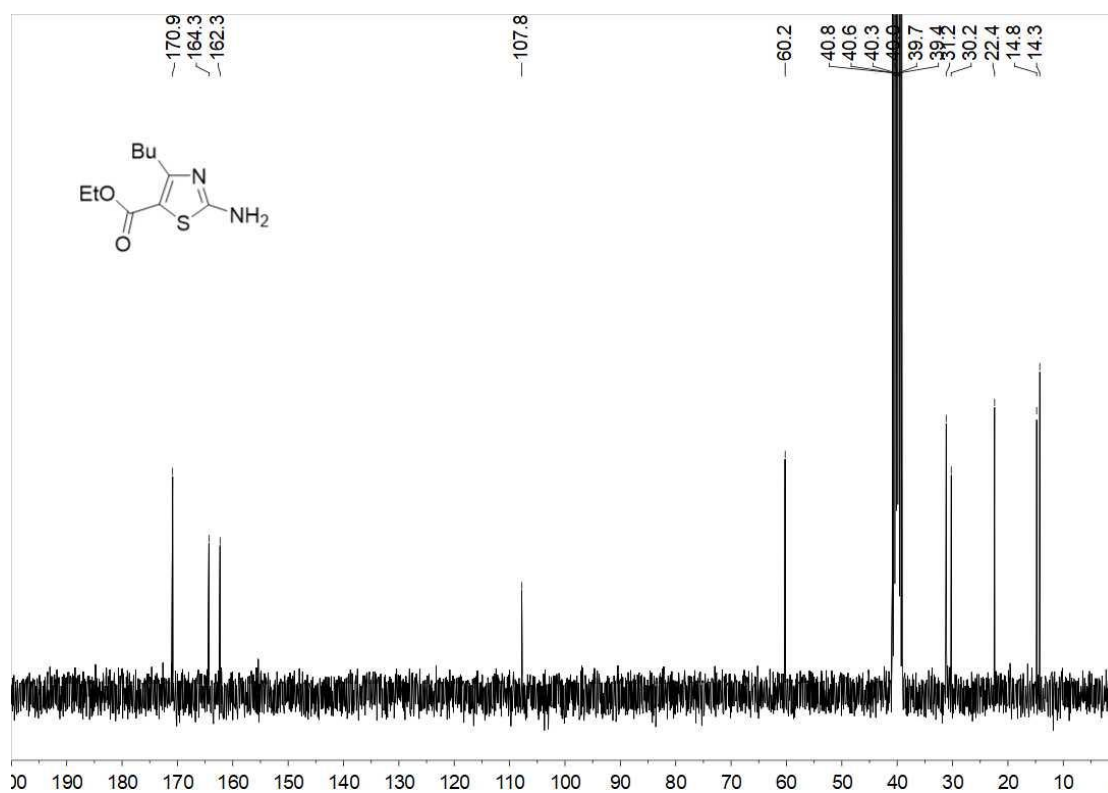
**<sup>13</sup>C NMR of ethyl 2-amino-4-isopropylthiazole-5-carboxylate (3i)**



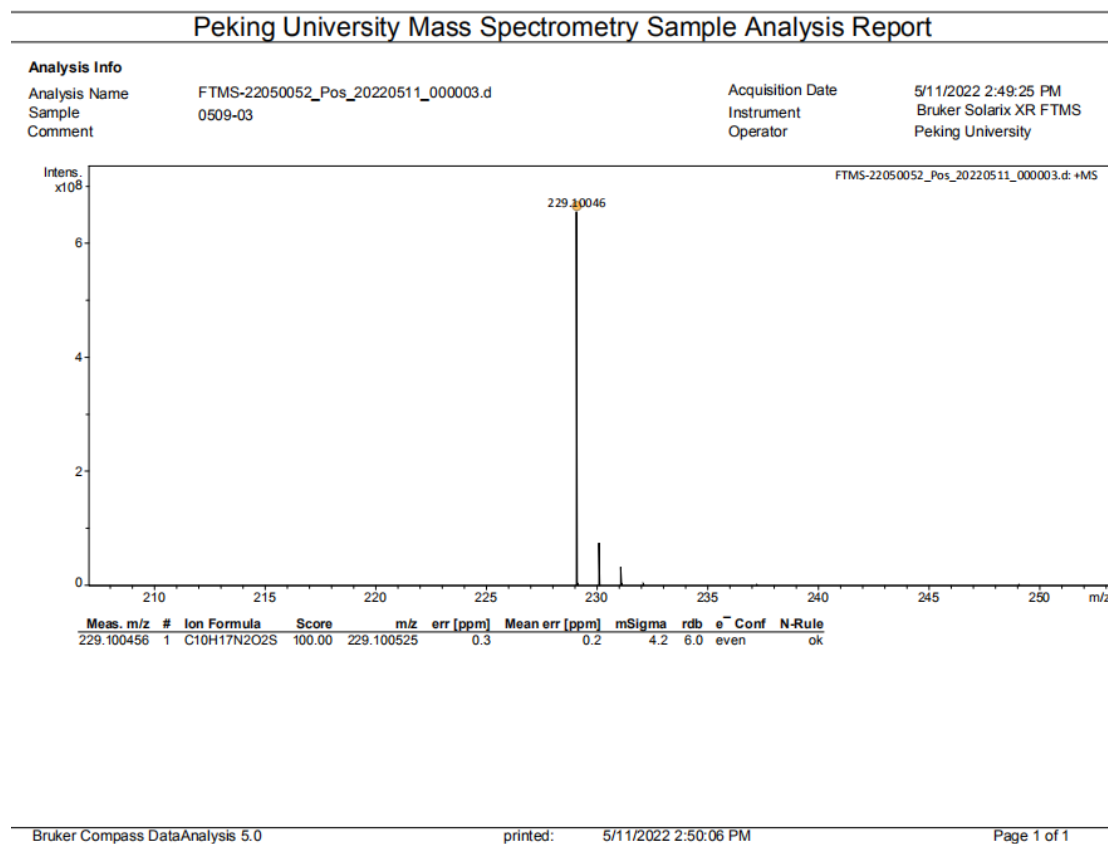
**<sup>1</sup>H NMR of ethyl 2-amino-4-butylthiazole-5-carboxylate (3j)**



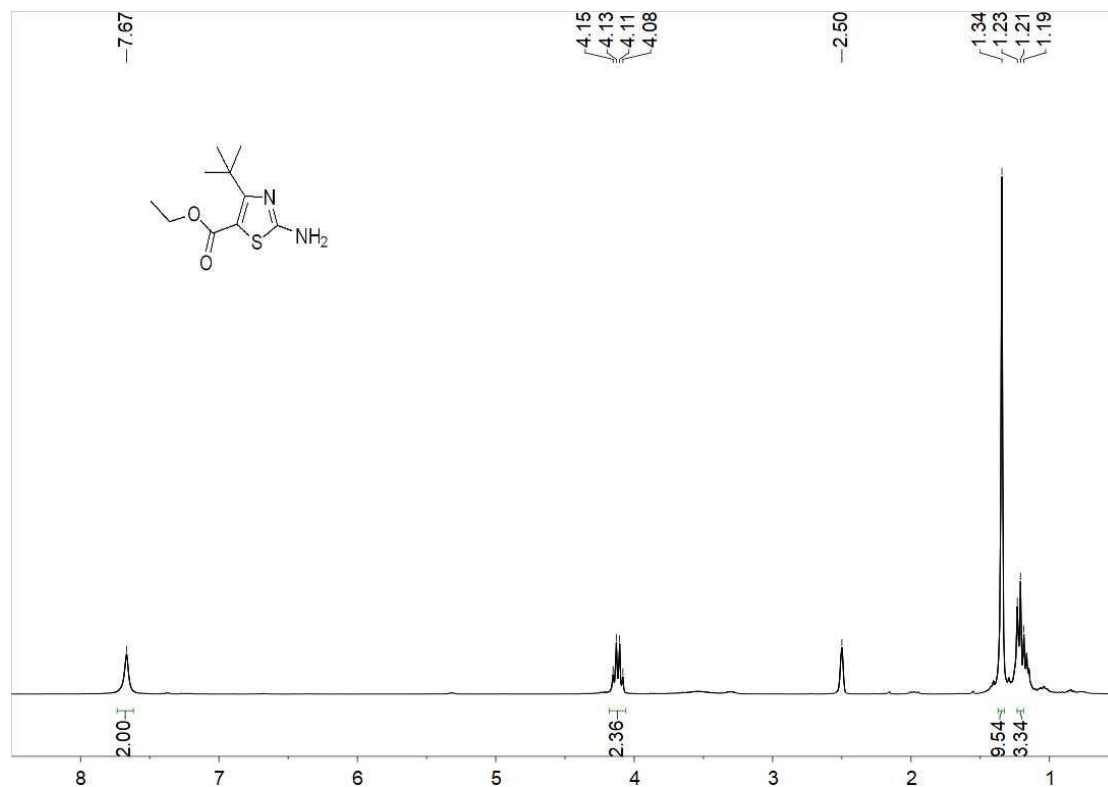
**<sup>13</sup>C NMR of ethyl 2-amino-4-butylthiazole-5-carboxylate (3j)**



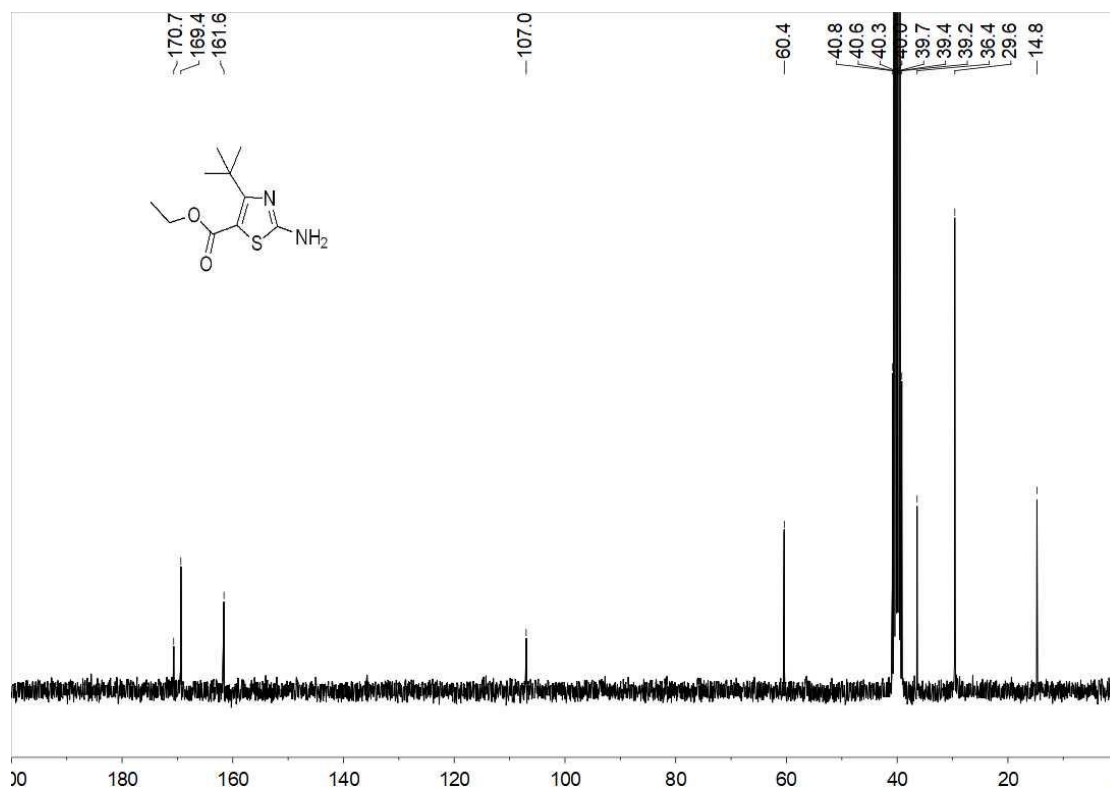
## HRMS of ethyl 2-amino-4-butylthiazole-5-carboxylate (3j)



## <sup>1</sup>H NMR of ethyl 2-amino-4-(*tert*-butyl) thiazole-5-carboxylate (3k)



### <sup>13</sup>C NMR of ethyl 2-amino-4-(*tert*-butyl) thiazole-5-carboxylate (3k)



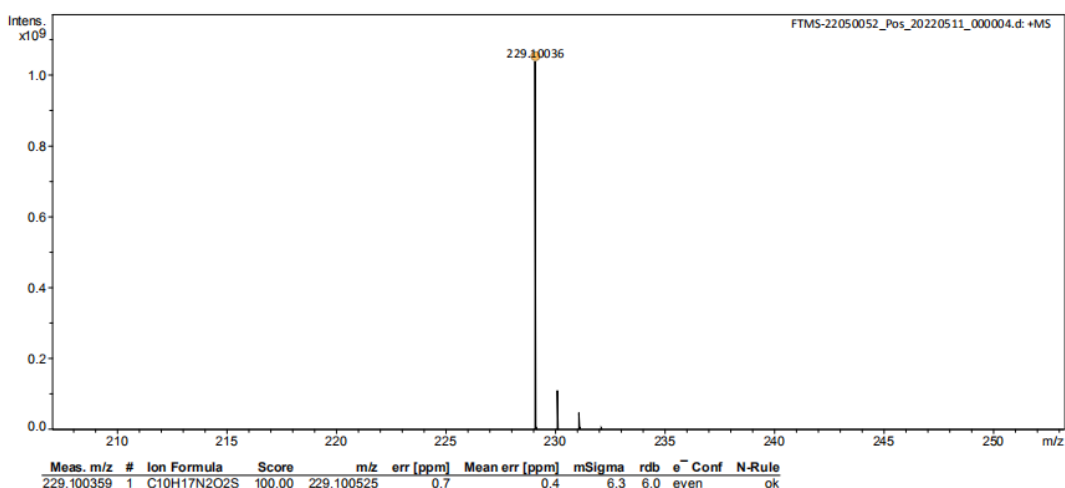
### HRMS of ethyl 2-amino-4-(*tert*-butyl) thiazole-5-carboxylate (3k)

#### Peking University Mass Spectrometry Sample Analysis Report

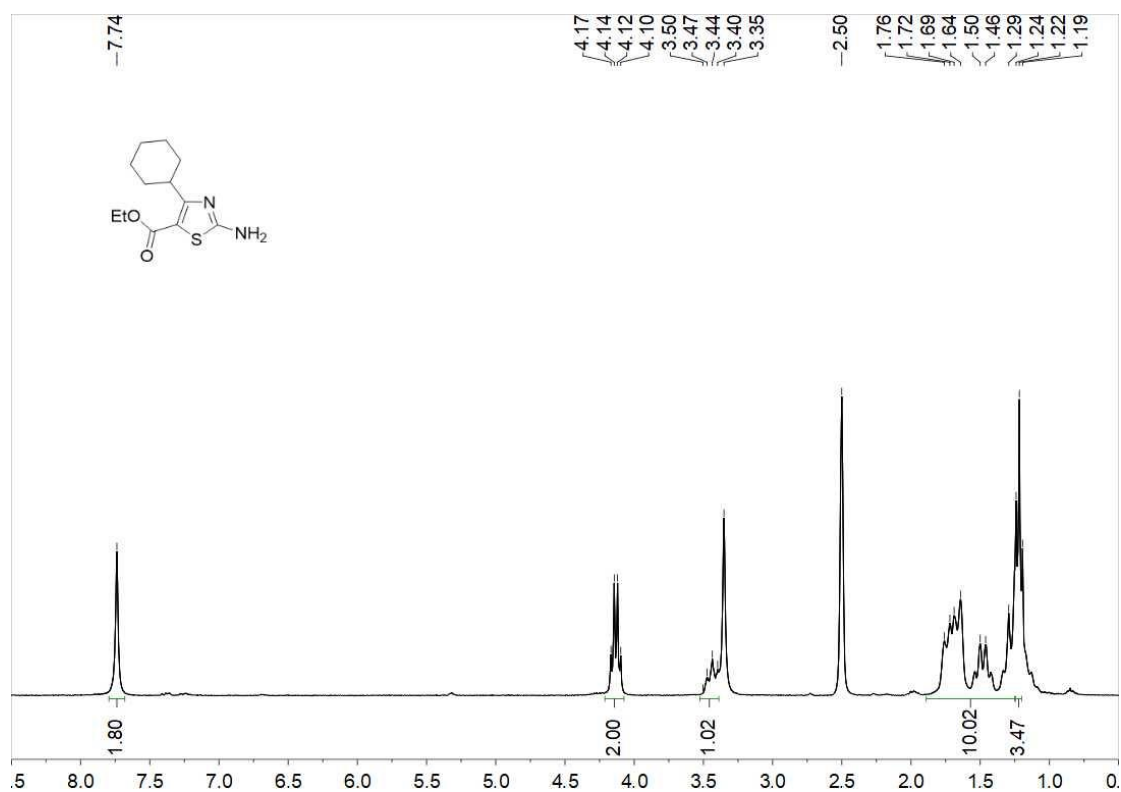
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 Sample: 0509-04  
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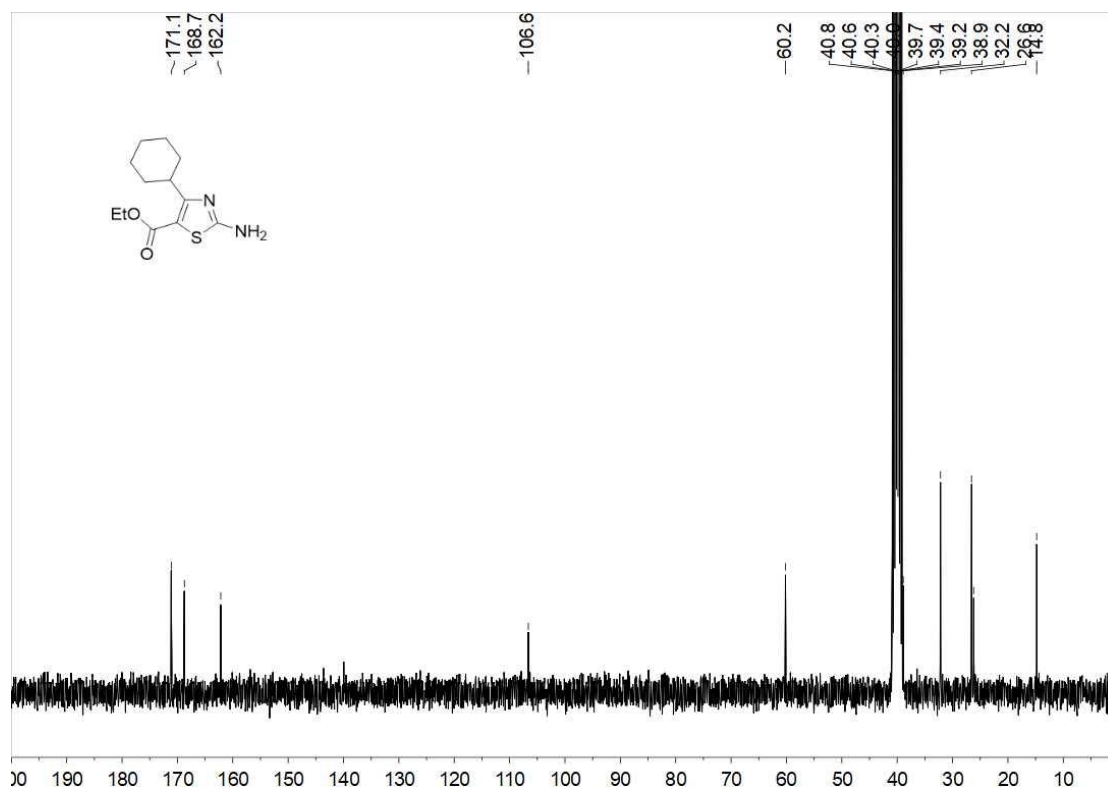
Acquisition Date: 5/11/2022 2:51:57 PM  
 Instrument: Bruker Solarix XR FTMS  
 Operator: Peking University



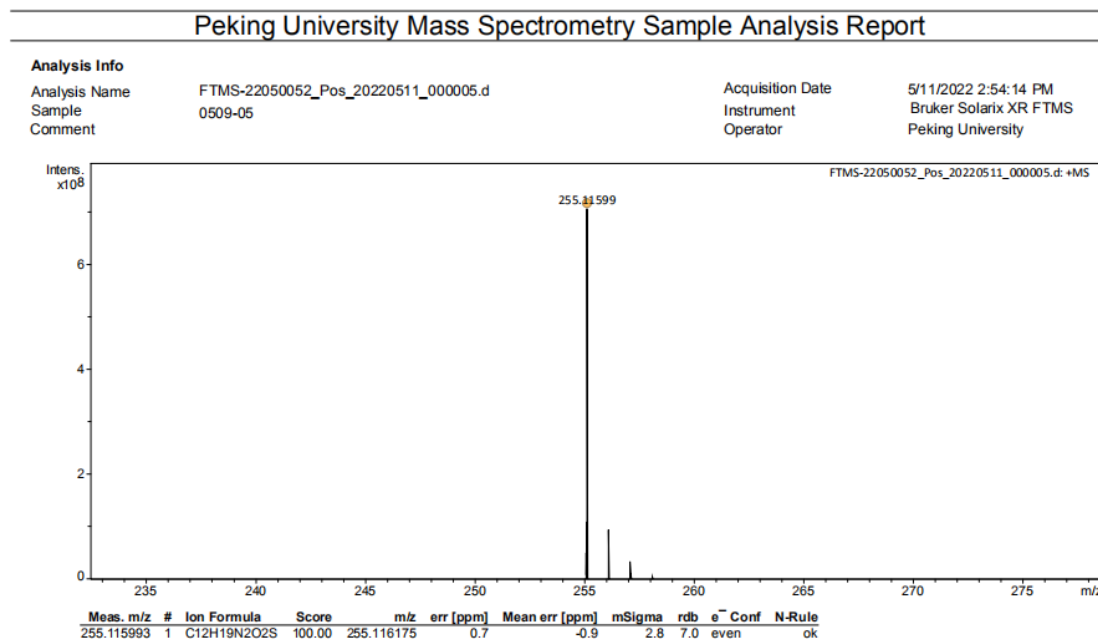
**$^1\text{H}$  NMR of ethyl 2-amino-4-cyclohexylthiazole-5-carboxylate (3l)**



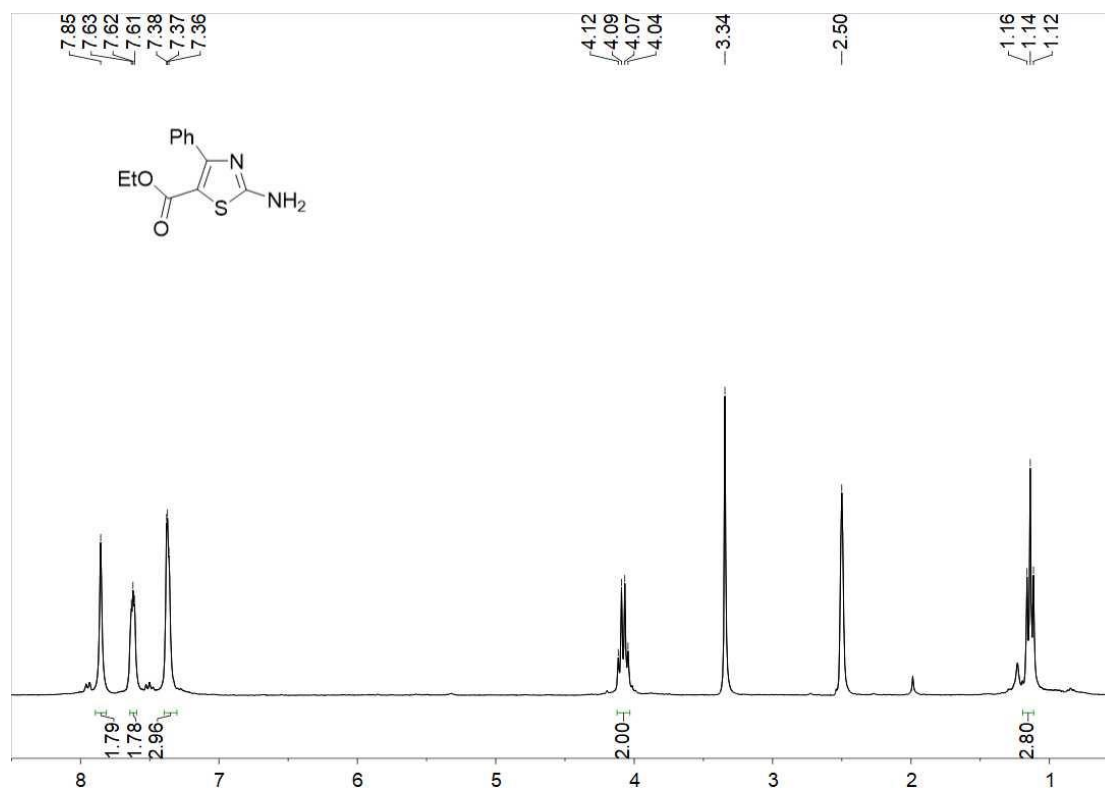
**$^{13}\text{C}$  NMR of ethyl 2-amino-4-cyclohexylthiazole-5-carboxylate (3l)**



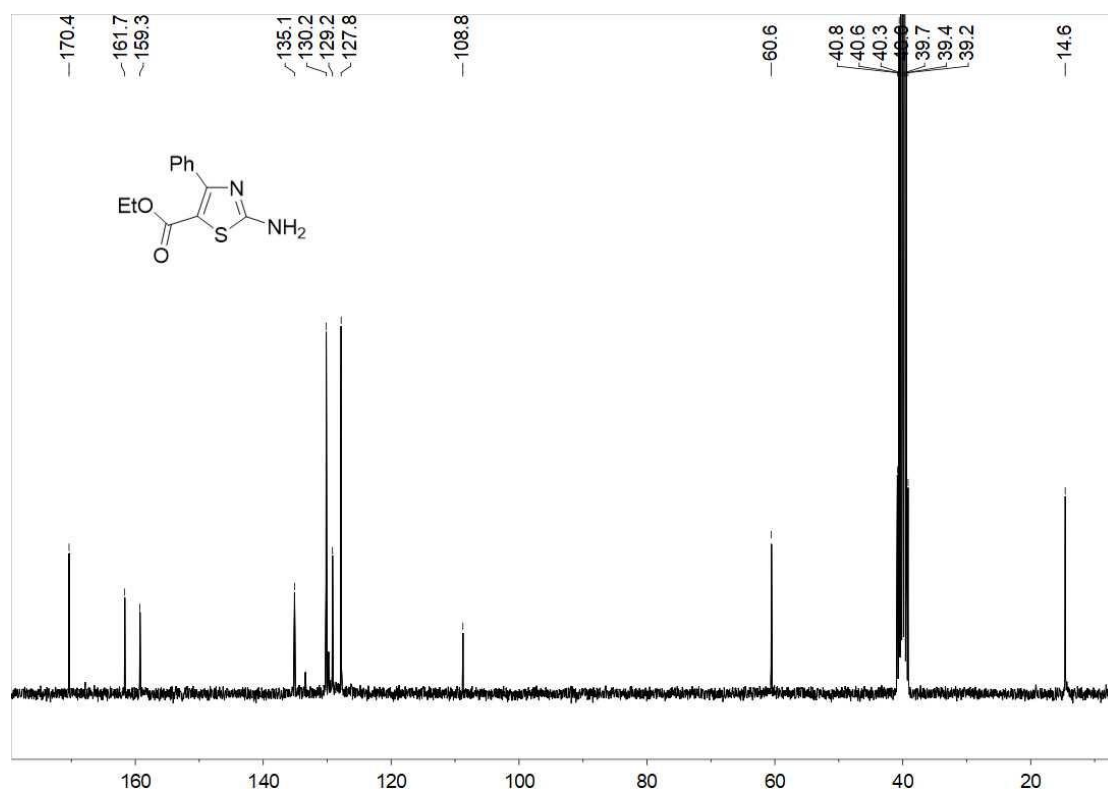
## HRMS of ethyl 2-amino-4-cyclohexylthiazole-5-carboxylate (3l)



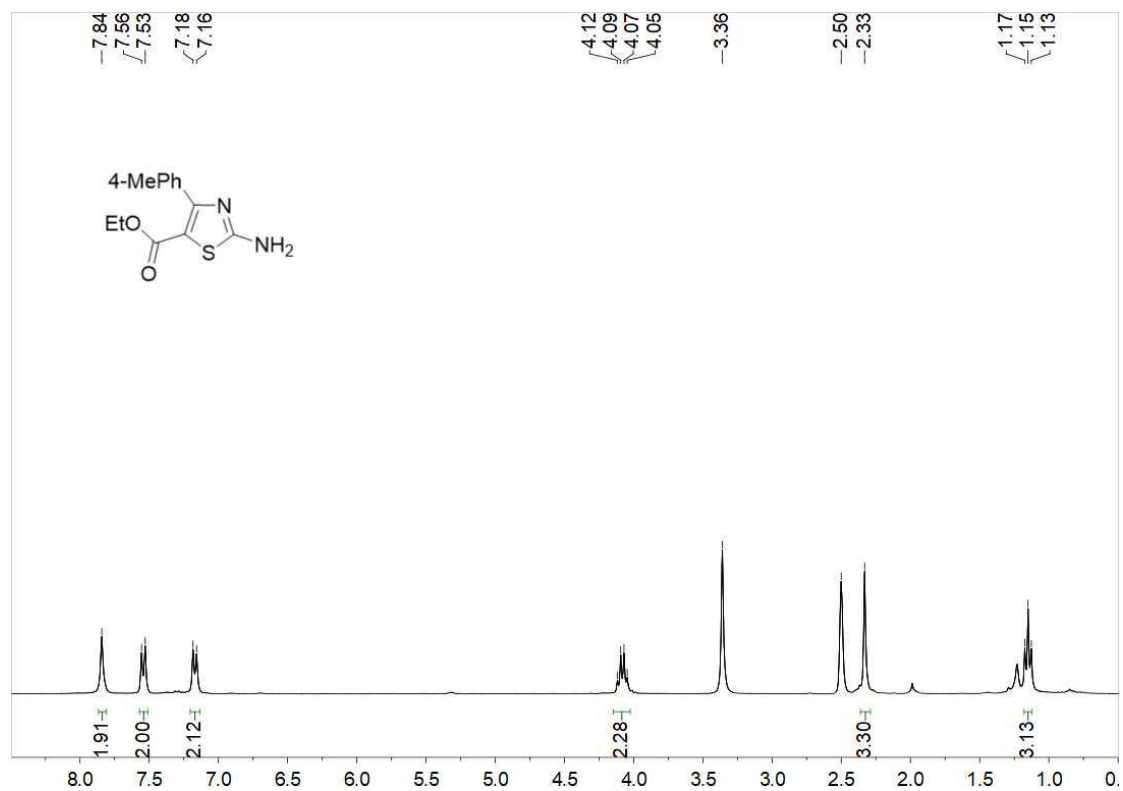
## <sup>1</sup>H NMR of ethyl 2-amino-4-phenylthiazole-5-carboxylate (3m)



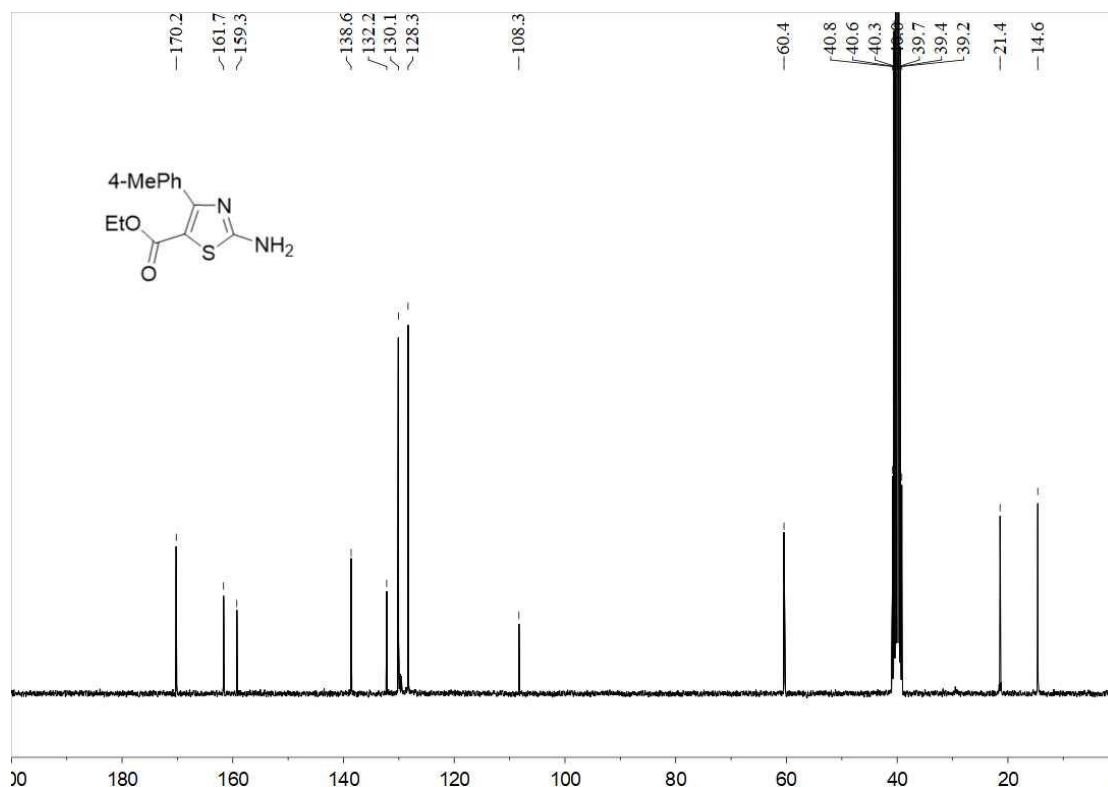
**$^{13}\text{C}$  NMR of ethyl 2-amino-4-phenylthiazole-5-carboxylate (3m)**



**$^1\text{H}$  NMR of ethyl 2-amino-4-(*p*-tolyl) thiazole-5-carboxylate (3n)**



### <sup>13</sup>C NMR of ethyl 2-amino-4-(*p*-tolyl) thiazole-5-carboxylate (3n)



### HRMS of ethyl 2-amino-4-(*p*-tolyl) thiazole-5-carboxylate (3n)

#### Peking University Mass Spectrometry Sample Analysis Report

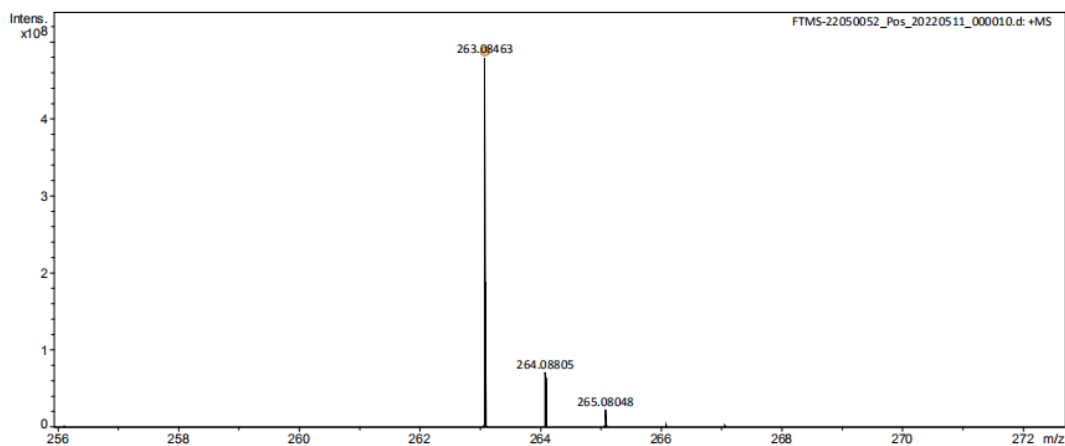
##### Analysis Info

Analysis Name  
Sample  
Comment

FTMS-22050052\_Pos\_20220511\_000010.d  
0509-10

Acquisition Date  
Instrument  
Operator

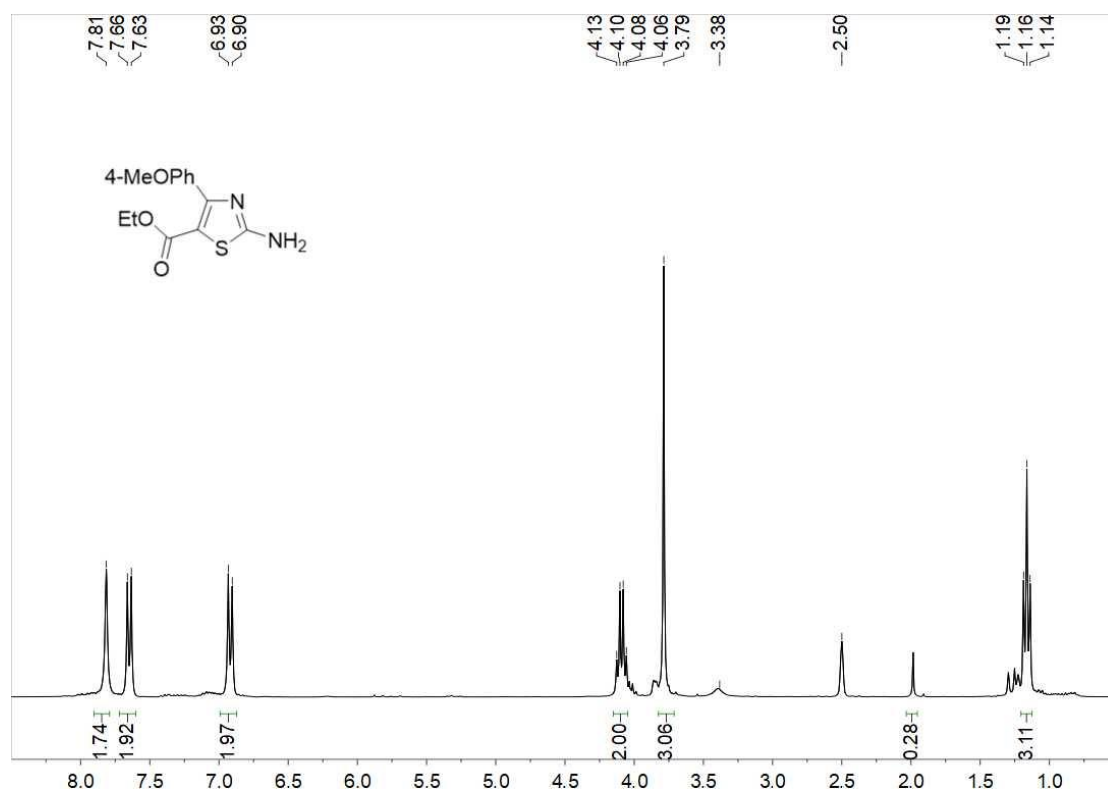
5/11/2022 3:05:30 PM  
Bruker Solarix XR FTMS  
Peking University



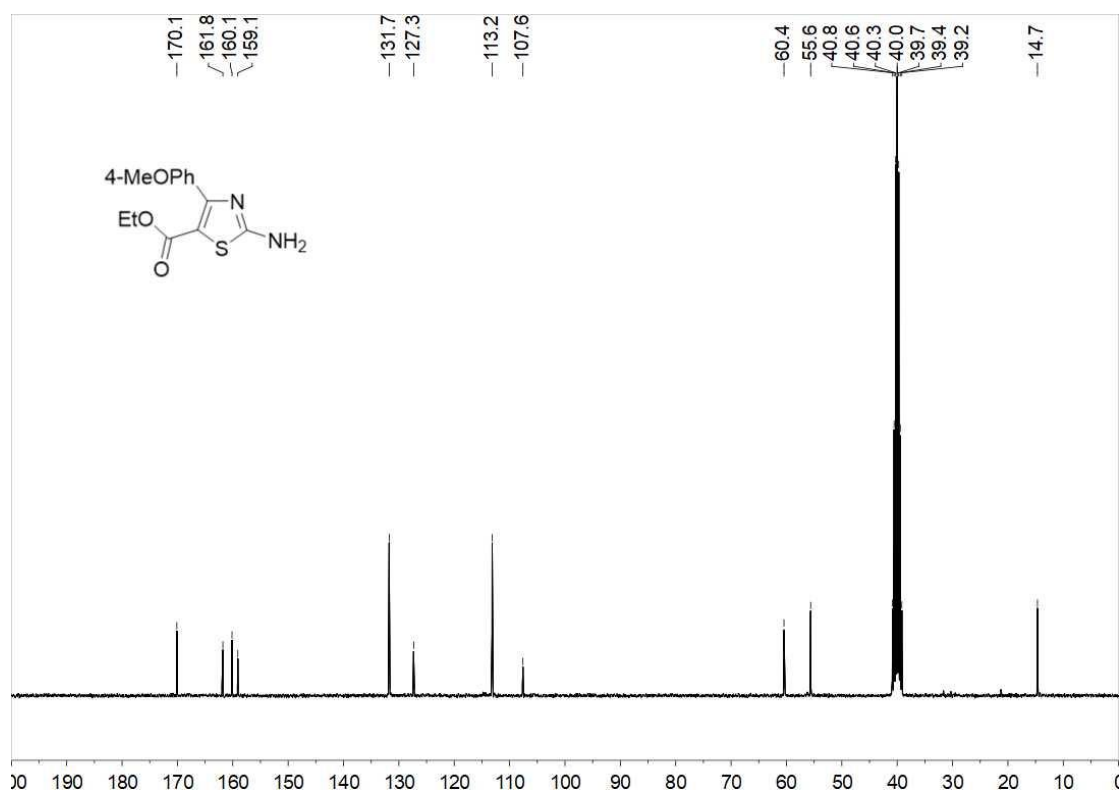
| Meas. m/z  | # | Ion Formula | Score  | m/z        | err [ppm] | Mean err [ppm] | mSigma | rdb  | e <sup>-</sup> | Conf | N-Rule |
|------------|---|-------------|--------|------------|-----------|----------------|--------|------|----------------|------|--------|
| 263.084635 | 1 | C13H15N2O2S | 100.00 | 263.084875 | 0.9       | -0.5           | 3.6    | 10.0 | even           | ok   |        |



**$^1\text{H}$  NMR of ethyl 2-amino-4-(4-methoxyphenyl) thiazole-5-carboxylate (3o)**



**$^{13}\text{C}$  NMR of ethyl 2-amino-4-(4-methoxyphenyl) thiazole-5-carboxylate (3o)**



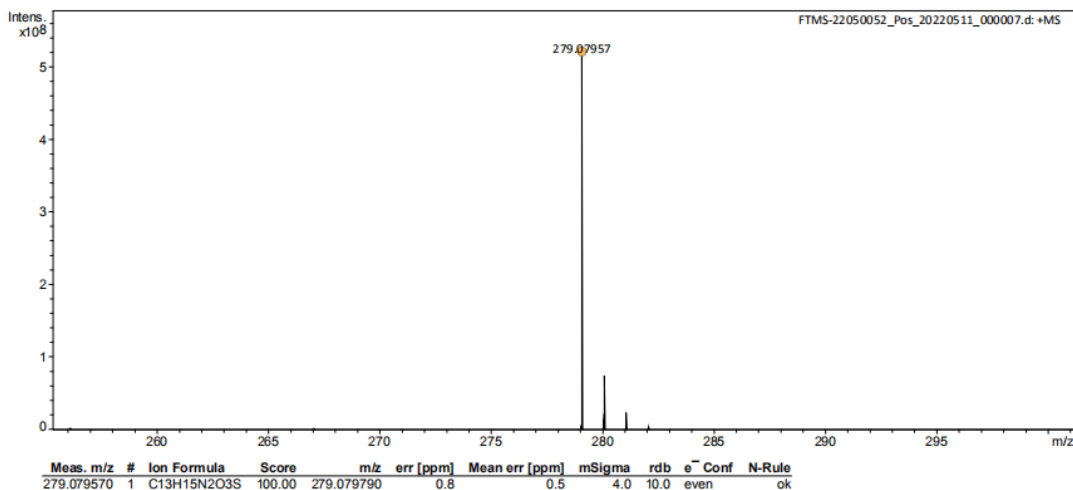
## HRMS of ethyl 2-amino-4-(4-methoxyphenyl) thiazole-5-carboxylate (3o)

### Peking University Mass Spectrometry Sample Analysis Report

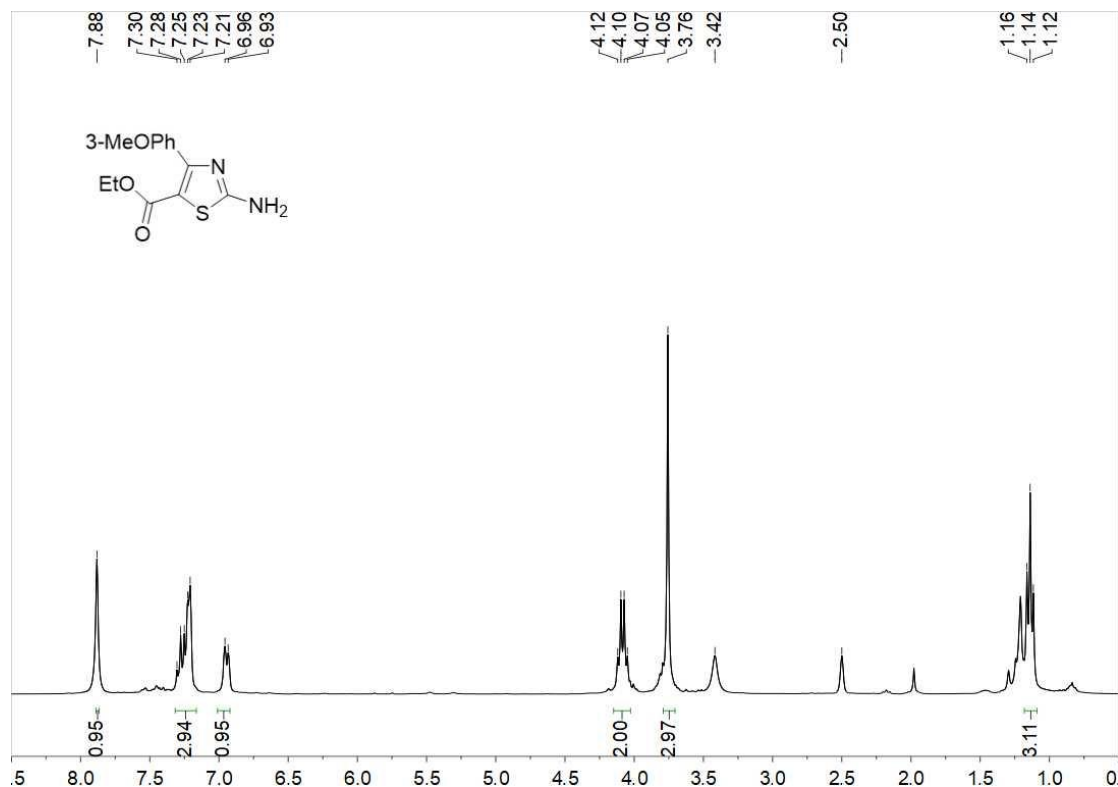
#### Analysis Info

Analysis Name FTMS-22050052\_Pos\_20220511\_000007.d  
Sample 0509-07  
Comment

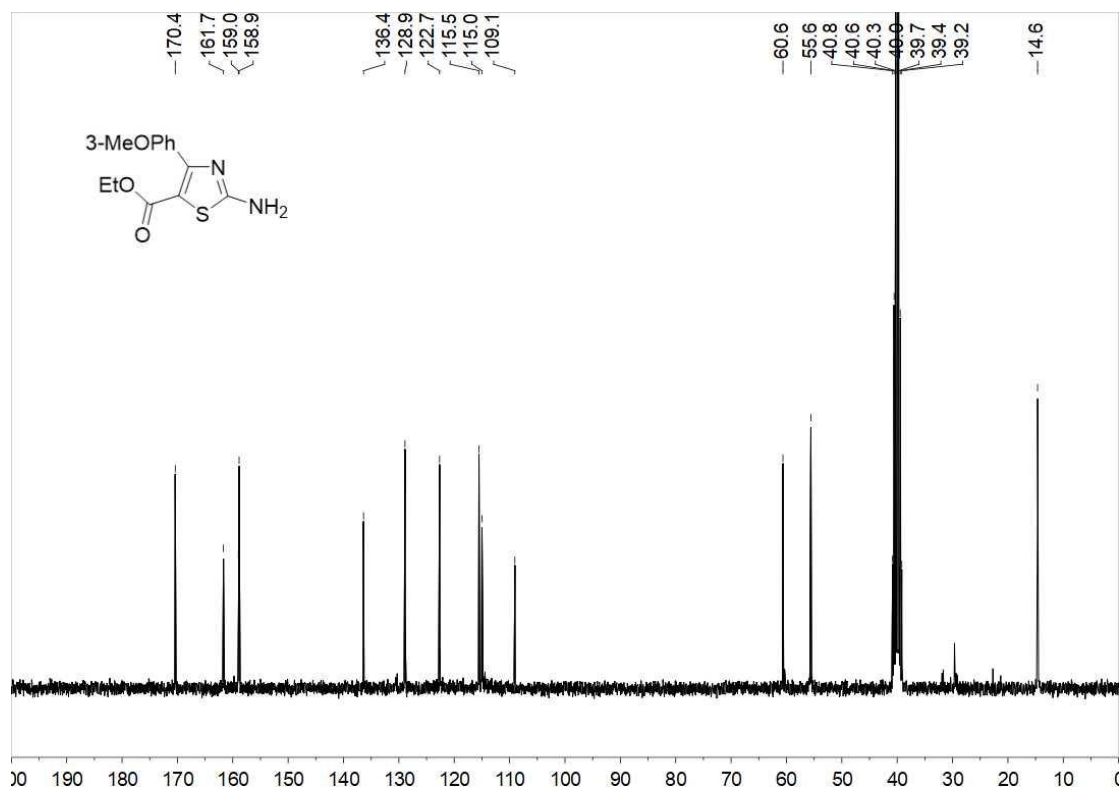
Acquisition Date 5/11/2022 2:59:08 PM  
Instrument Bruker Solarix XR FTMS  
Operator Peking University



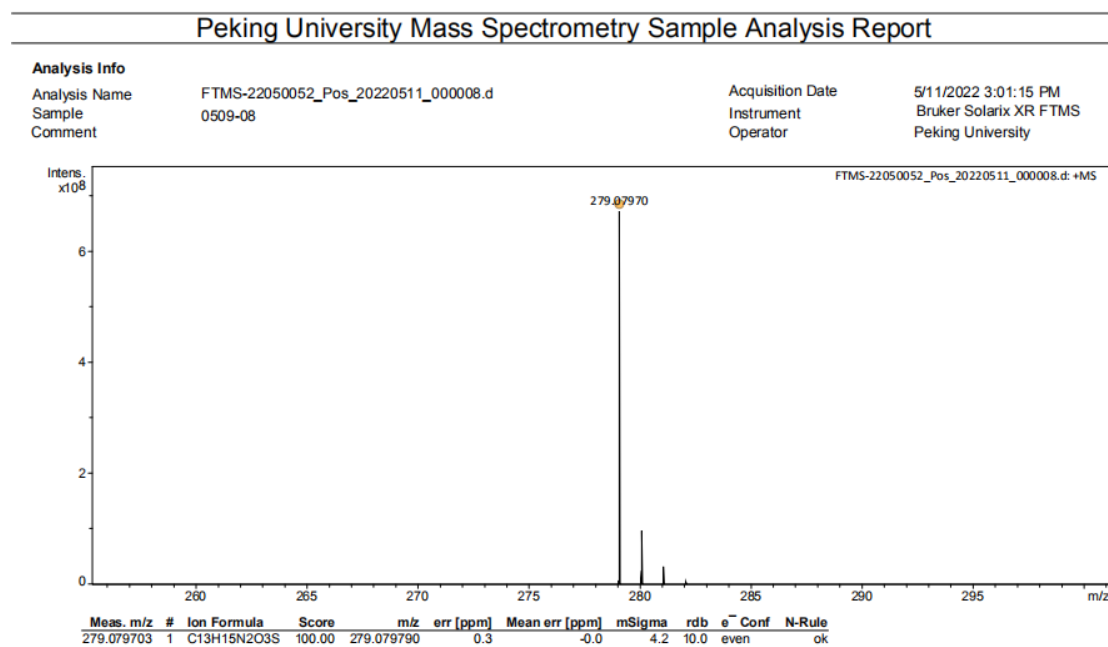
## <sup>1</sup>H NMR of ethyl 2-amino-4-(3-methoxyphenyl) thiazole-5-carboxylate (3p)



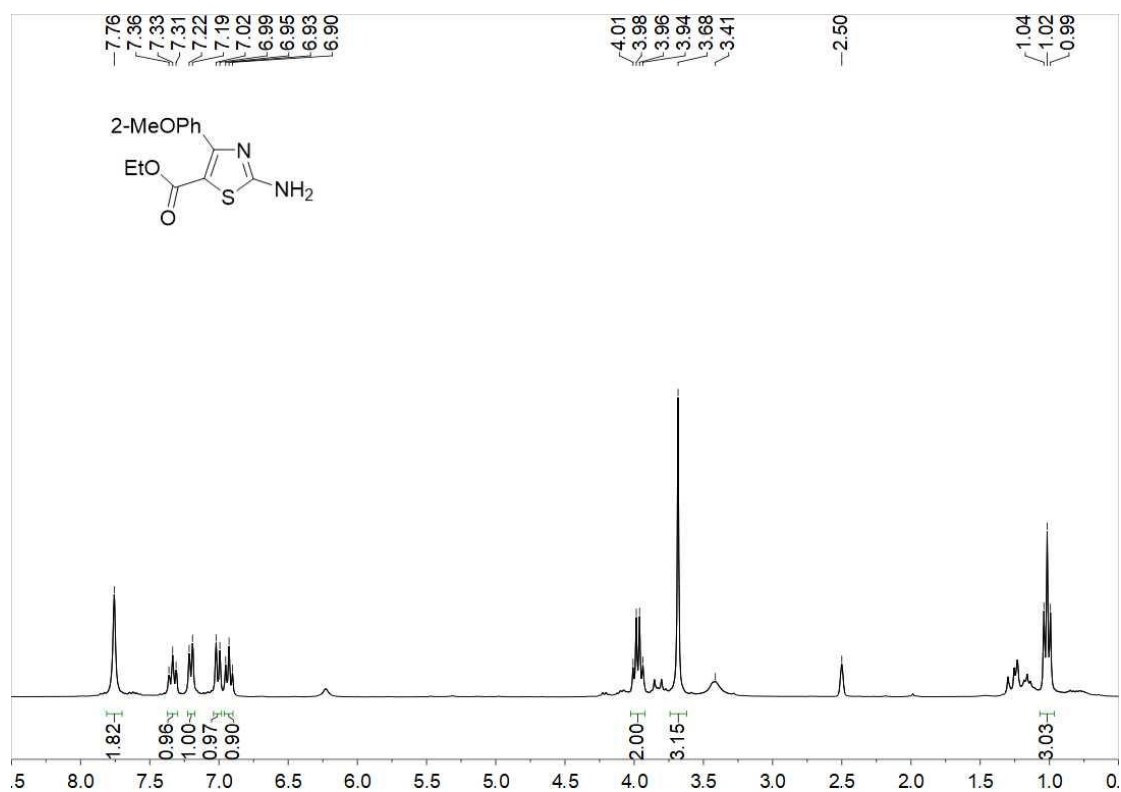
### <sup>13</sup>C NMR of ethyl 2-amino-4-(3-methoxyphenyl) thiazole-5-carboxylate (3p)



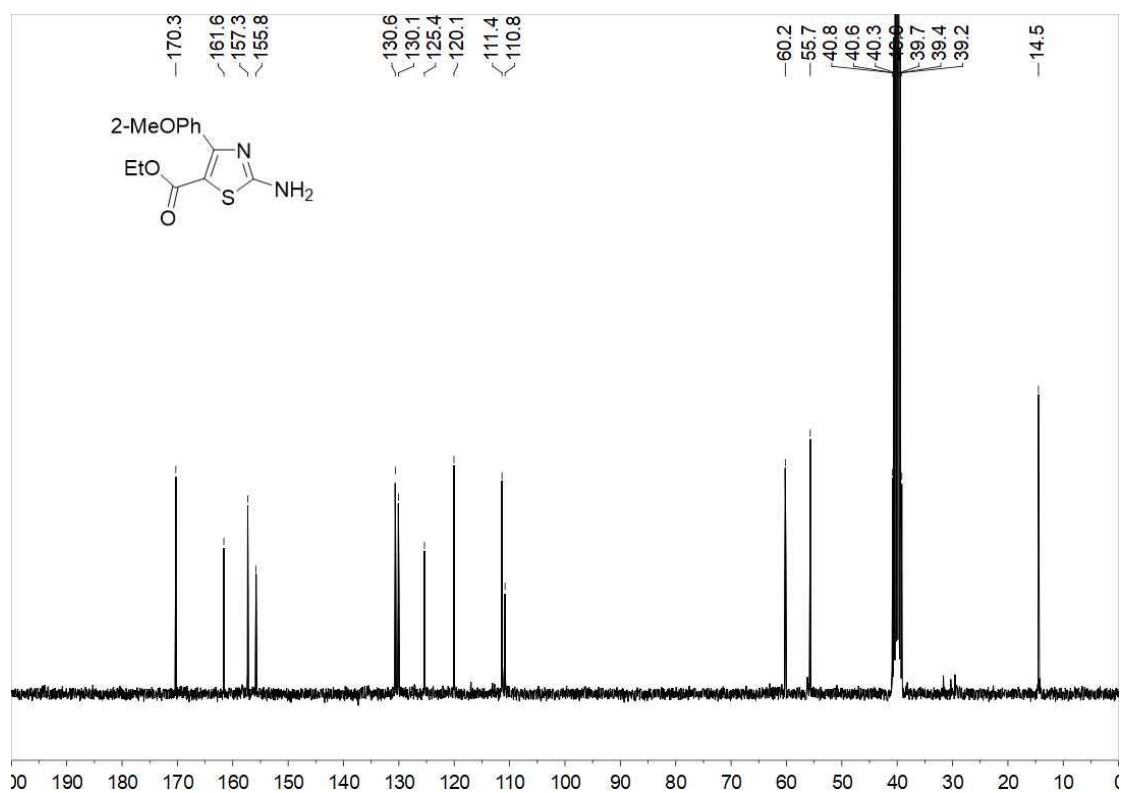
### HRMS of ethyl 2-amino-4-(3-methoxyphenyl) thiazole-5-carboxylate (3p)



**$^1\text{H}$  NMR of ethyl 2-amino-4-(2-methoxyphenyl) thiazole-5-carboxylate (3q)**



**$^{13}\text{C}$  NMR of ethyl 2-amino-4-(2-methoxyphenyl) thiazole-5-carboxylate (3q)**



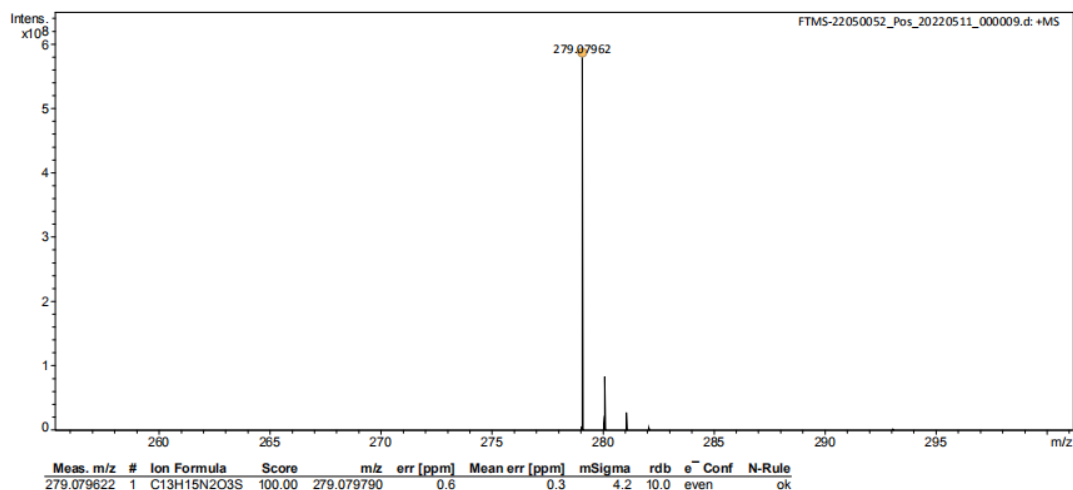
## HRMS of ethyl 2-amino-4-(2-methoxyphenyl) thiazole-5-carboxylate (3q)

### Peking University Mass Spectrometry Sample Analysis Report

#### Analysis Info

Analysis Name FTMS-22050052\_Pos\_20220511\_000009.d  
Sample 0509-09  
Comment

Acquisition Date 5/11/2022 3:03:04 PM  
Instrument Bruker Solarix XR FTMS  
Operator Peking University

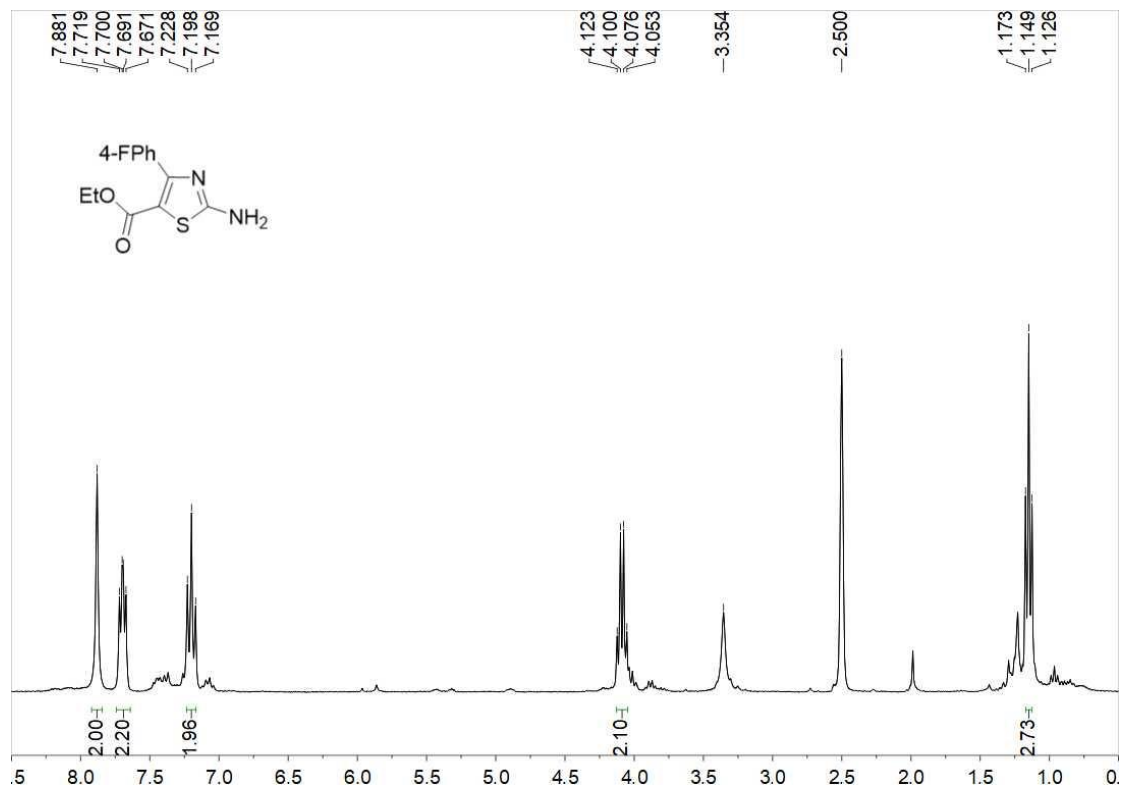


Bruker Compass DataAnalysis 5.0

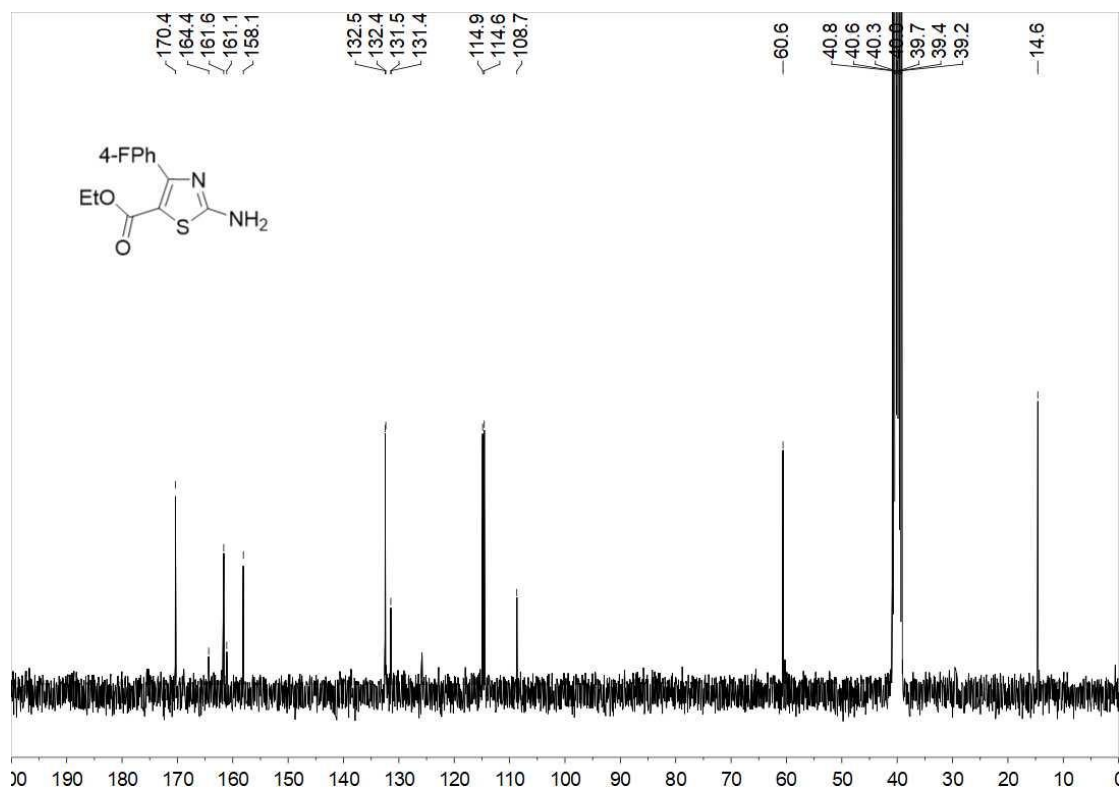
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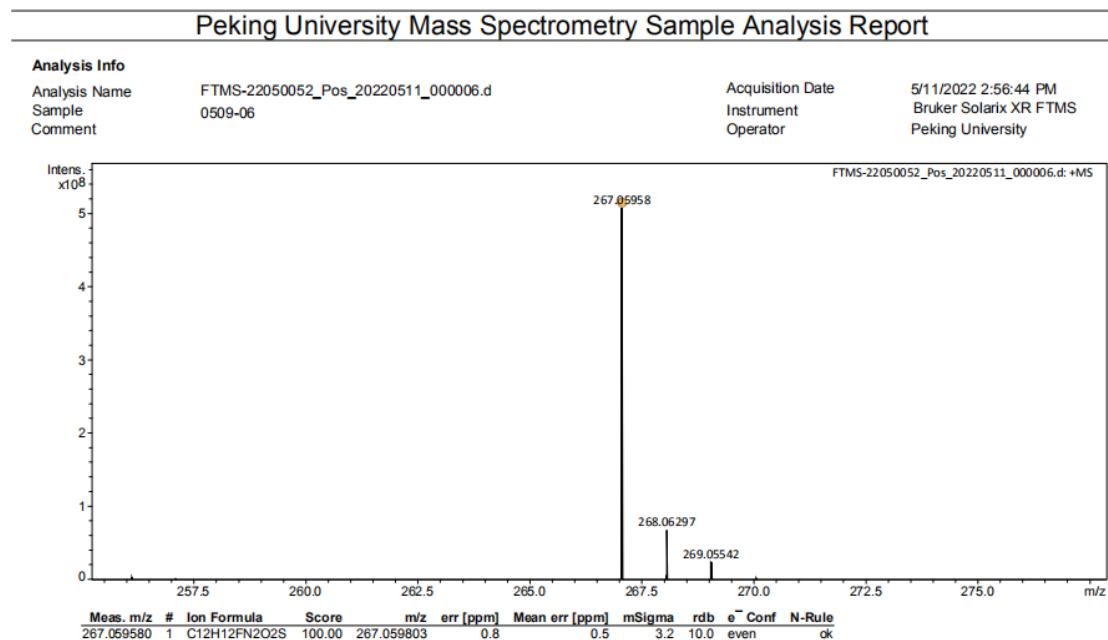
## <sup>1</sup>H NMR of ethyl 2-amino-4-(4-fluorophenyl) thiazole-5-carboxylate (3r)



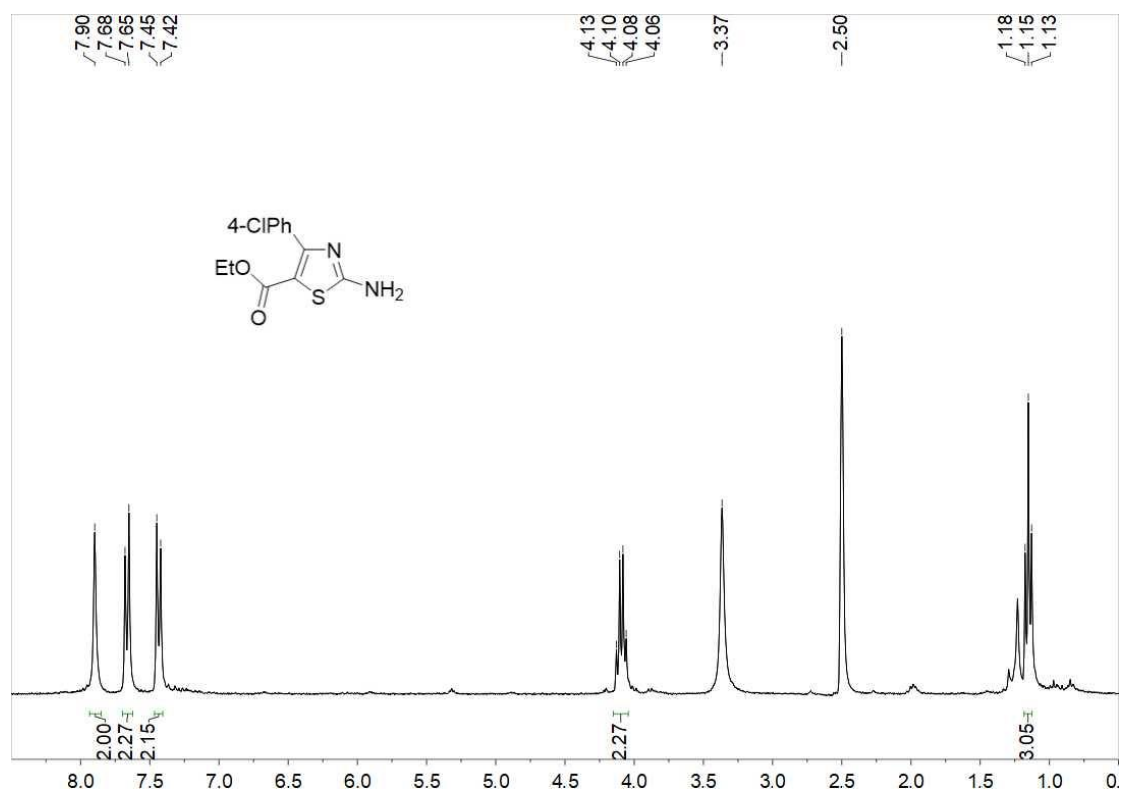
### <sup>13</sup>C NMR of ethyl 2-amino-4-(4-fluorophenyl) thiazole-5-carboxylate (3r)



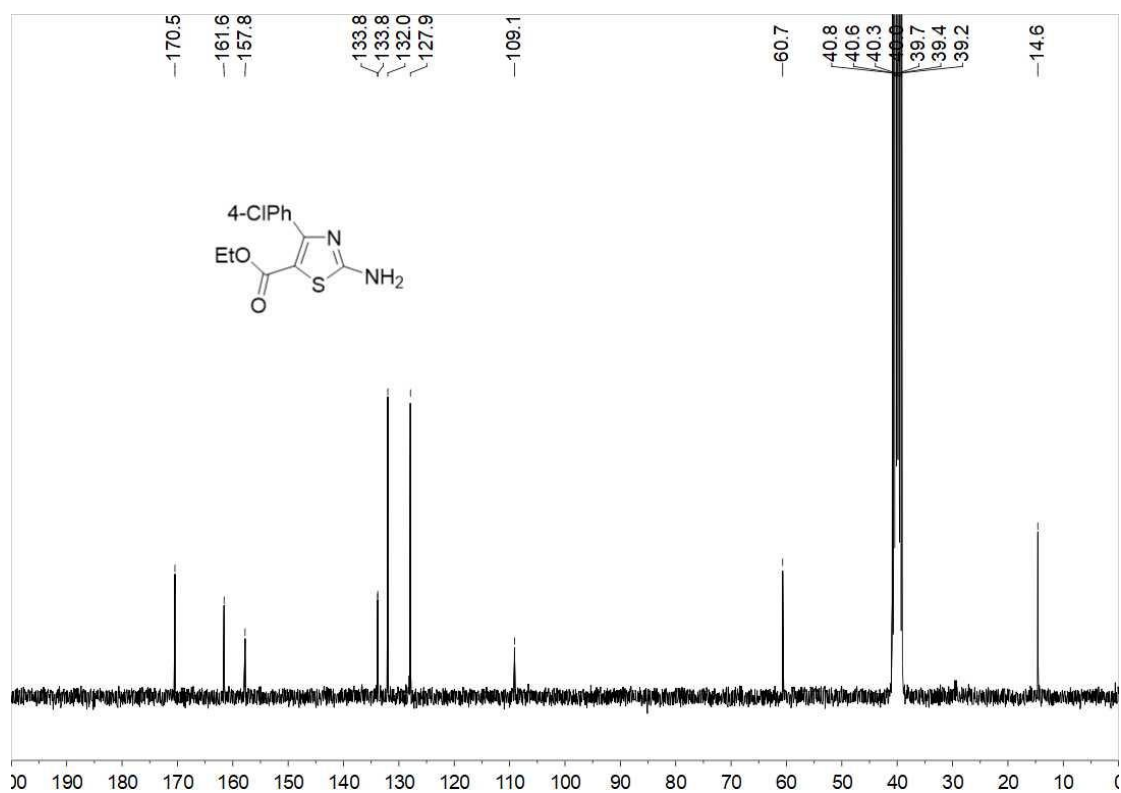
### HRMS of ethyl 2-amino-4-(4-fluorophenyl) thiazole-5-carboxylate (3r)



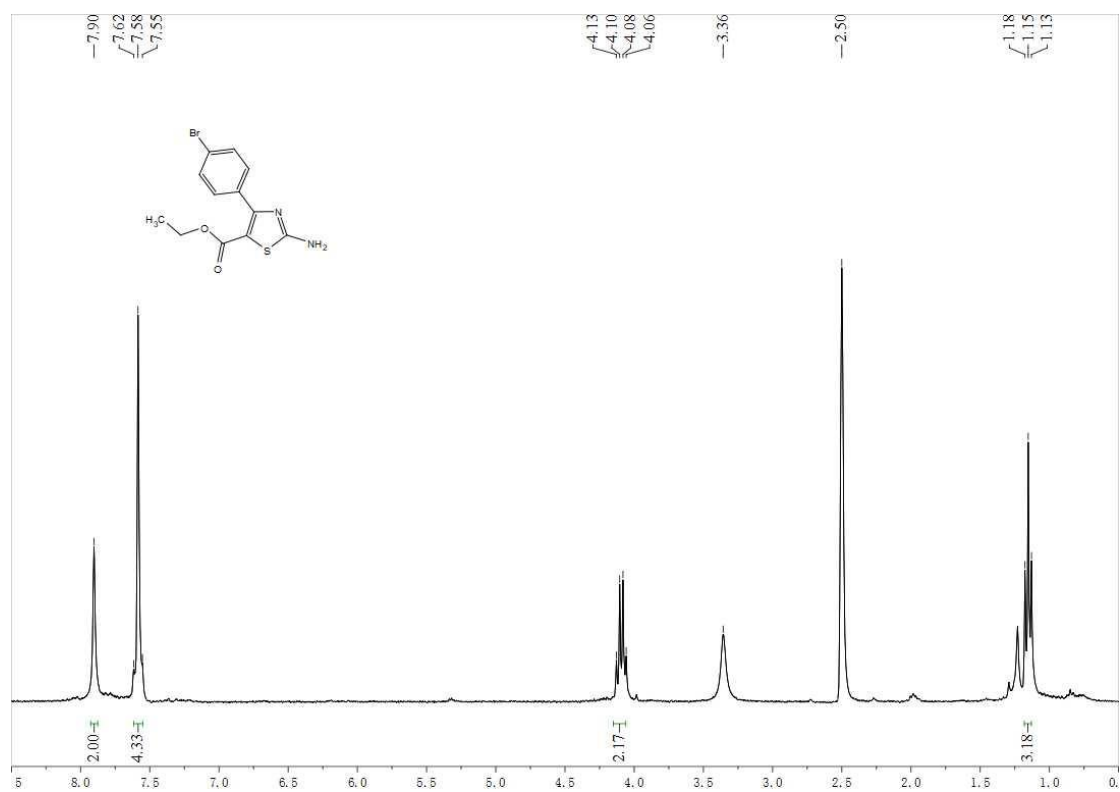
**$^1\text{H}$  NMR of ethyl 2-amino-4-(4-chlorophenyl) thiazole-5-carboxylate (3s)**



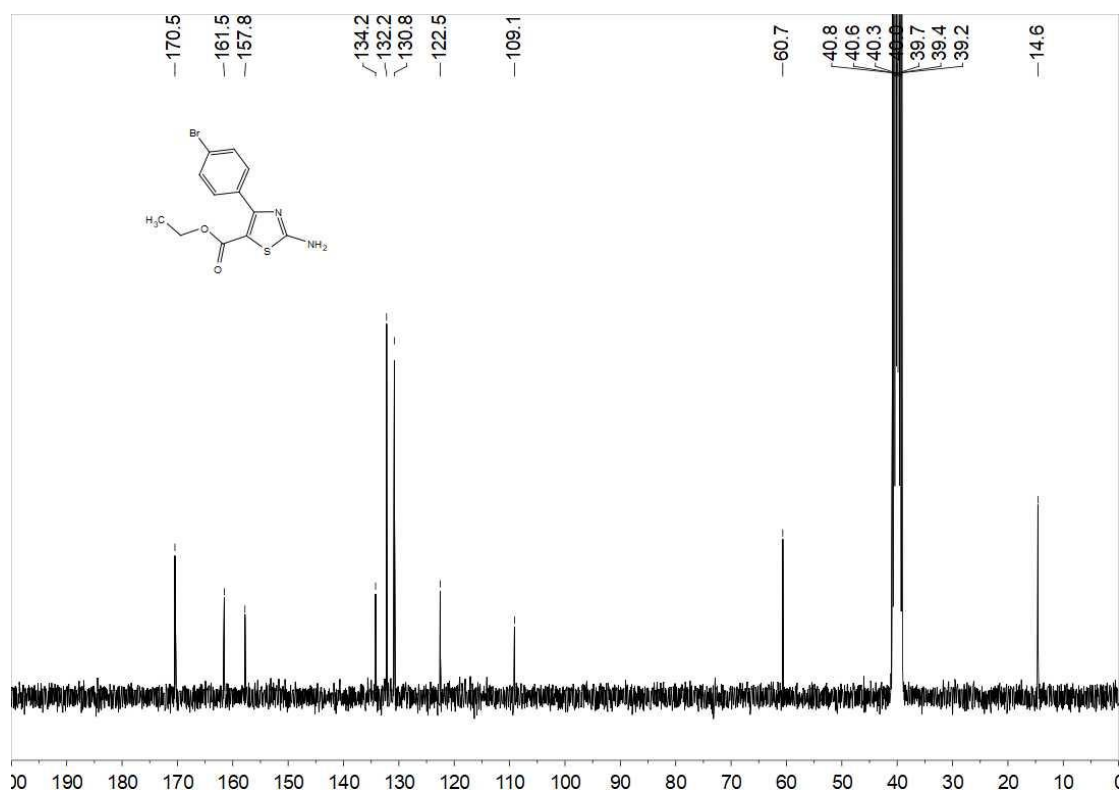
**$^{13}\text{C}$  NMR of ethyl 2-amino-4-(4-chlorophenyl) thiazole-5-carboxylate (3s)**



**<sup>1</sup>H NMR of ethyl 2-amino-4-(4-bromophenyl) thiazole-5-carboxylate (3t)**

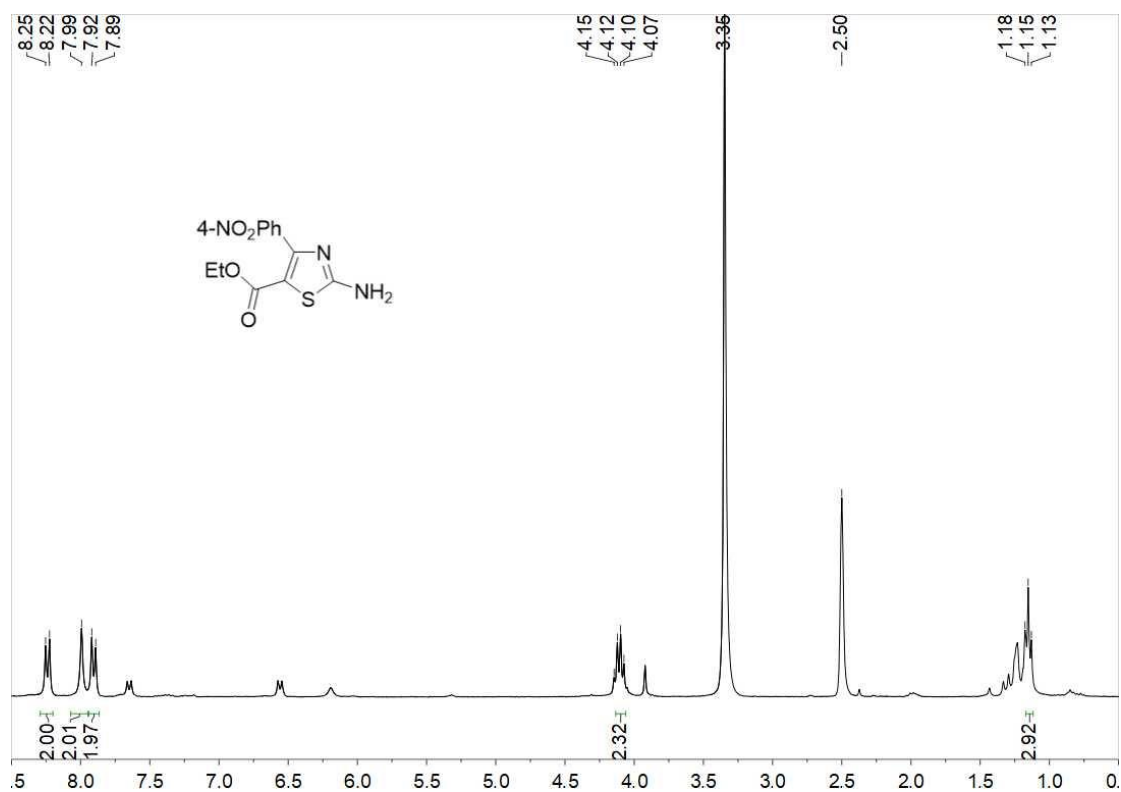


**<sup>13</sup>C NMR of ethyl 2-amino-4-(4-bromophenyl) thiazole-5-carboxylate (3t)**

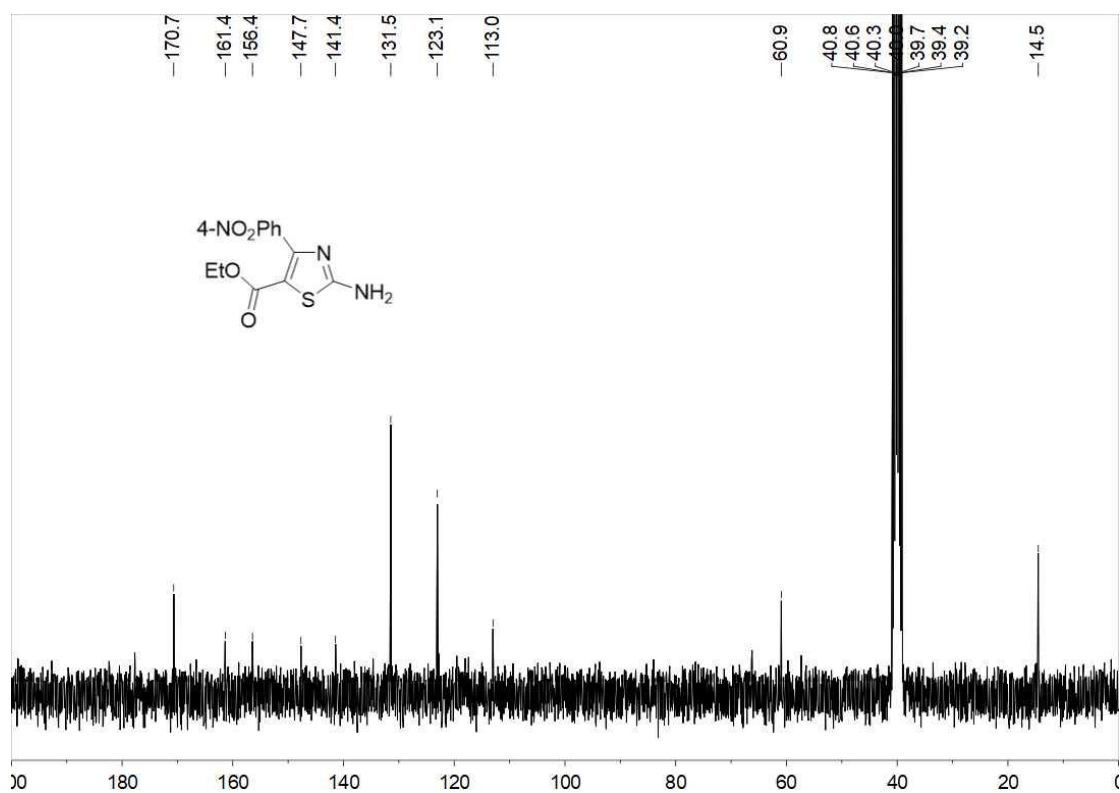




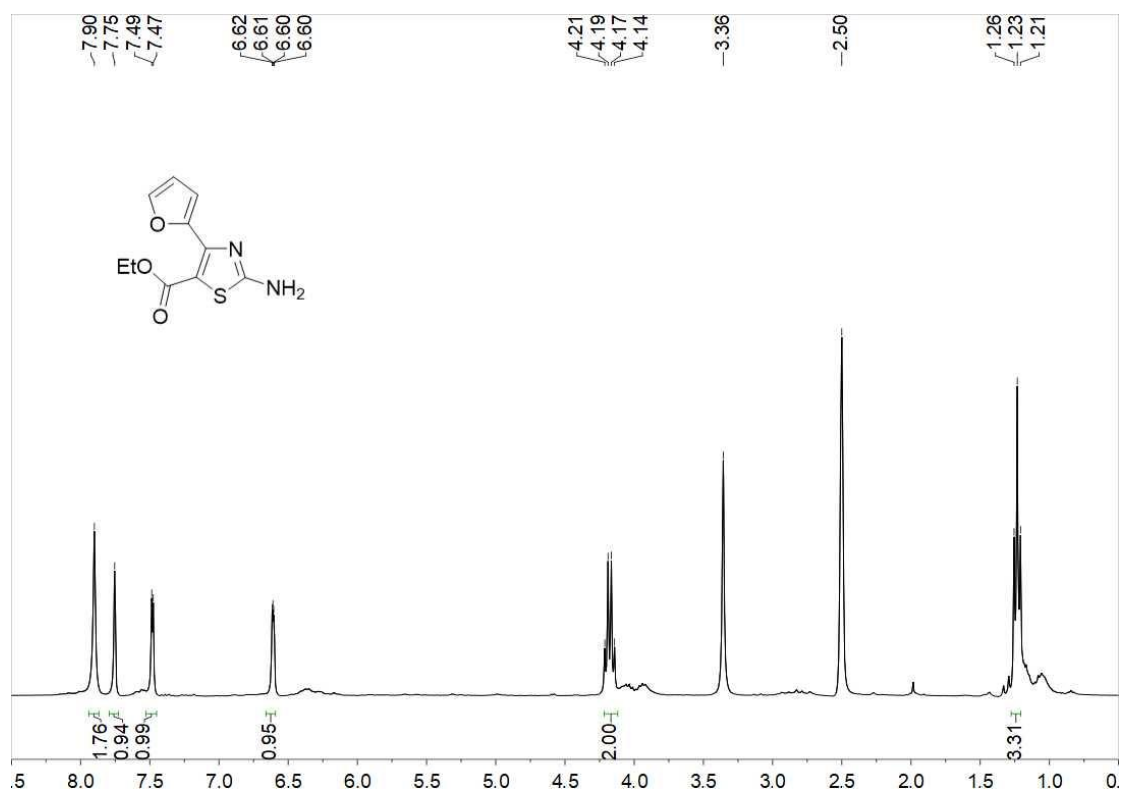
**<sup>1</sup>H NMR of ethyl 2-amino-4-(4-nitrophenyl) thiazole-5-carboxylate (3u)**



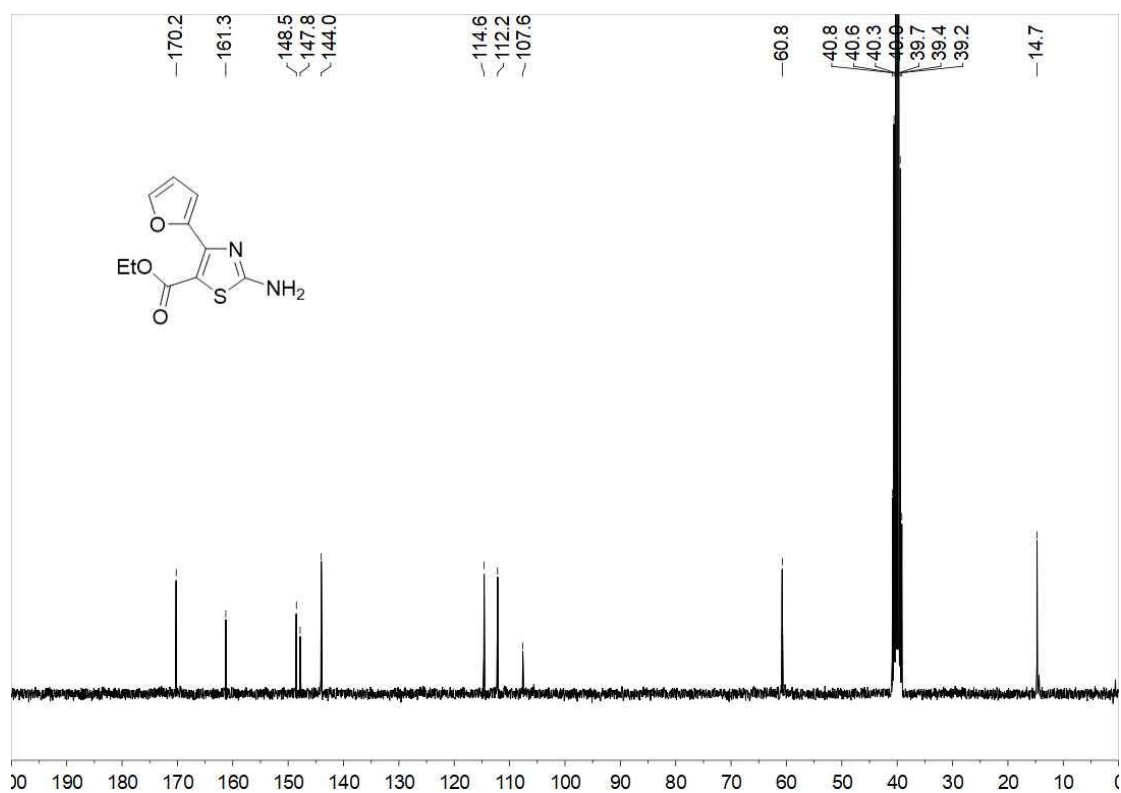
**<sup>13</sup>C NMR of ethyl 2-amino-4-(4-nitrophenyl) thiazole-5-carboxylate (3u)**



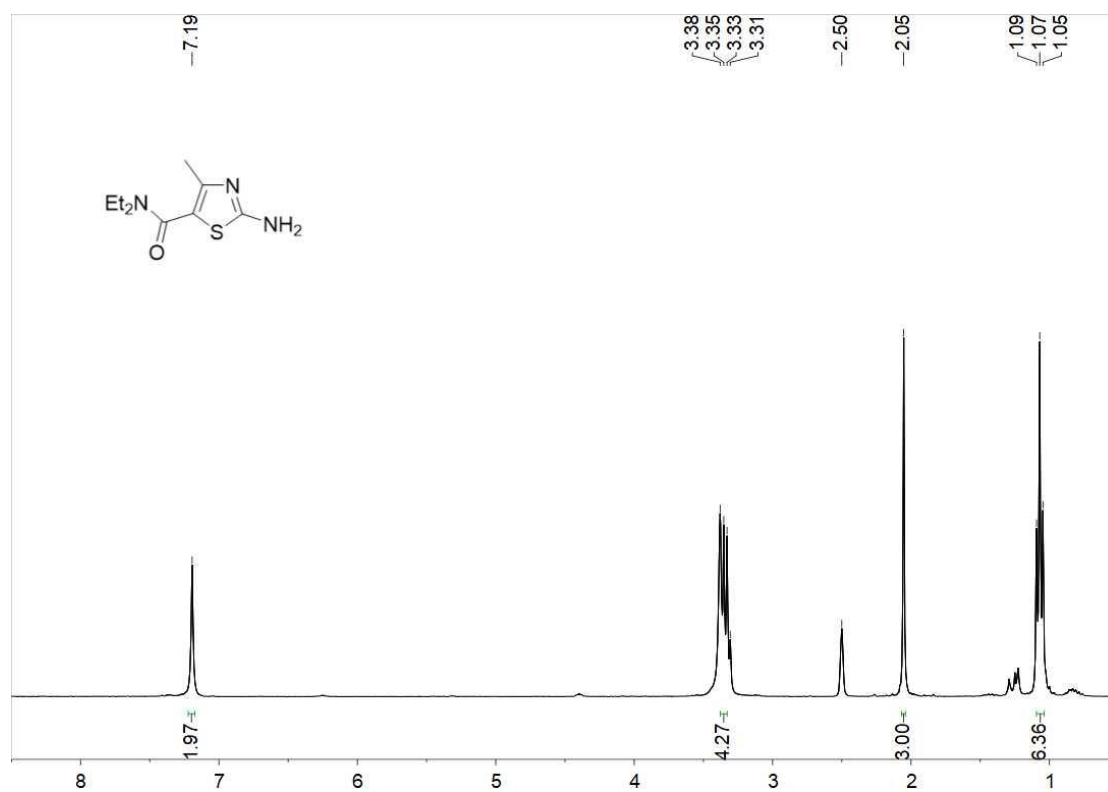
**<sup>1</sup>H NMR of ethyl 2-amino-4-(furan-2-yl) thiazole-5-carboxylate (3v)**



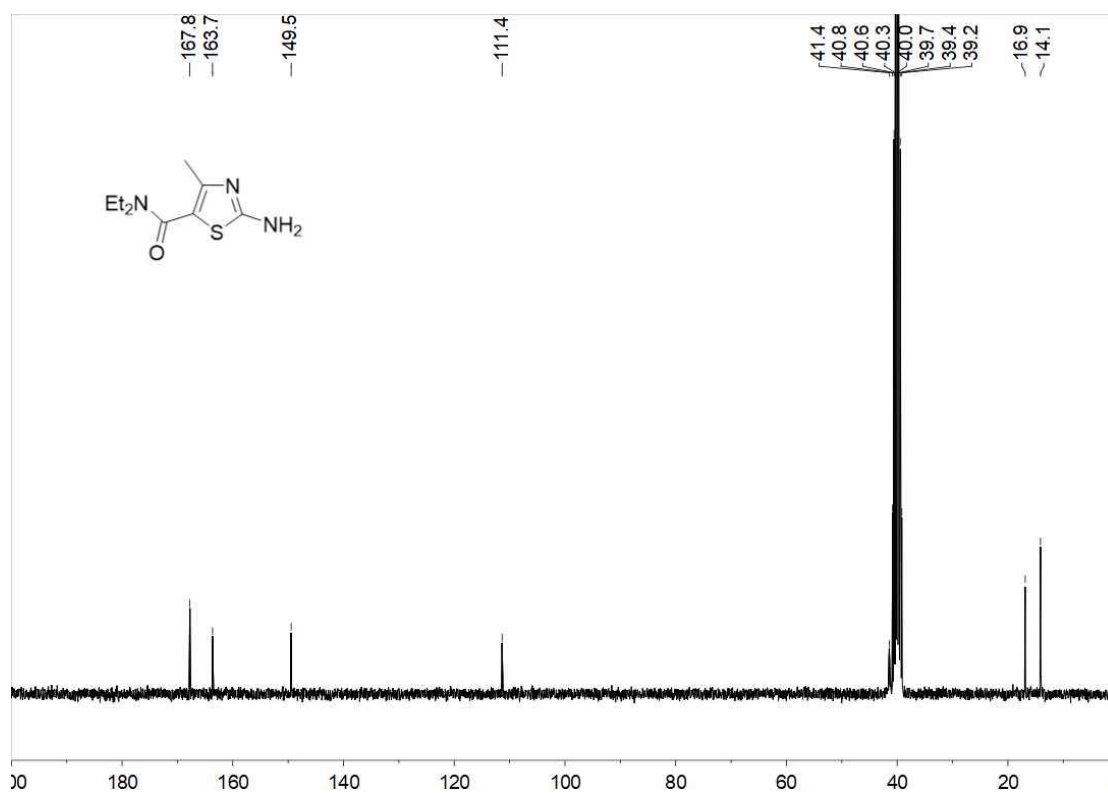
**<sup>13</sup>C NMR of ethyl 2-amino-4-(furan-2-yl) thiazole-5-carboxylate (3v)**



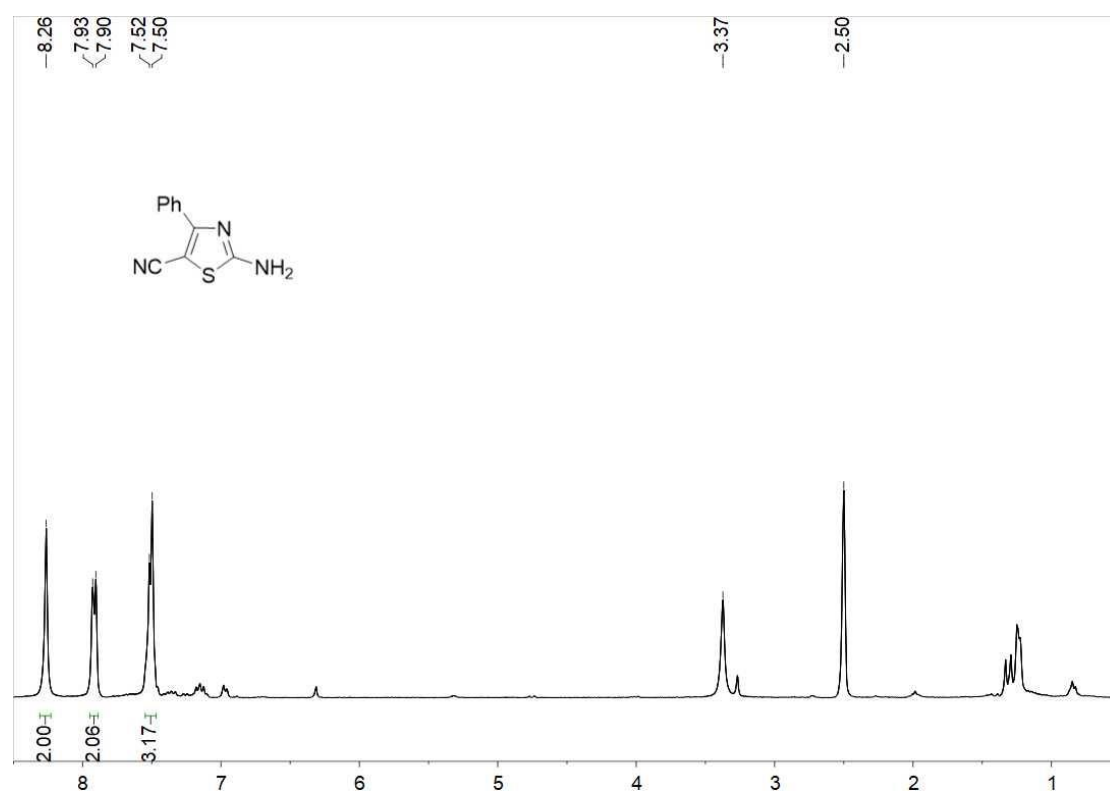
**$^1\text{H}$  NMR of 2-amino-N, N-diethyl-4-methylthiazole-5-carboxamide (3w)**



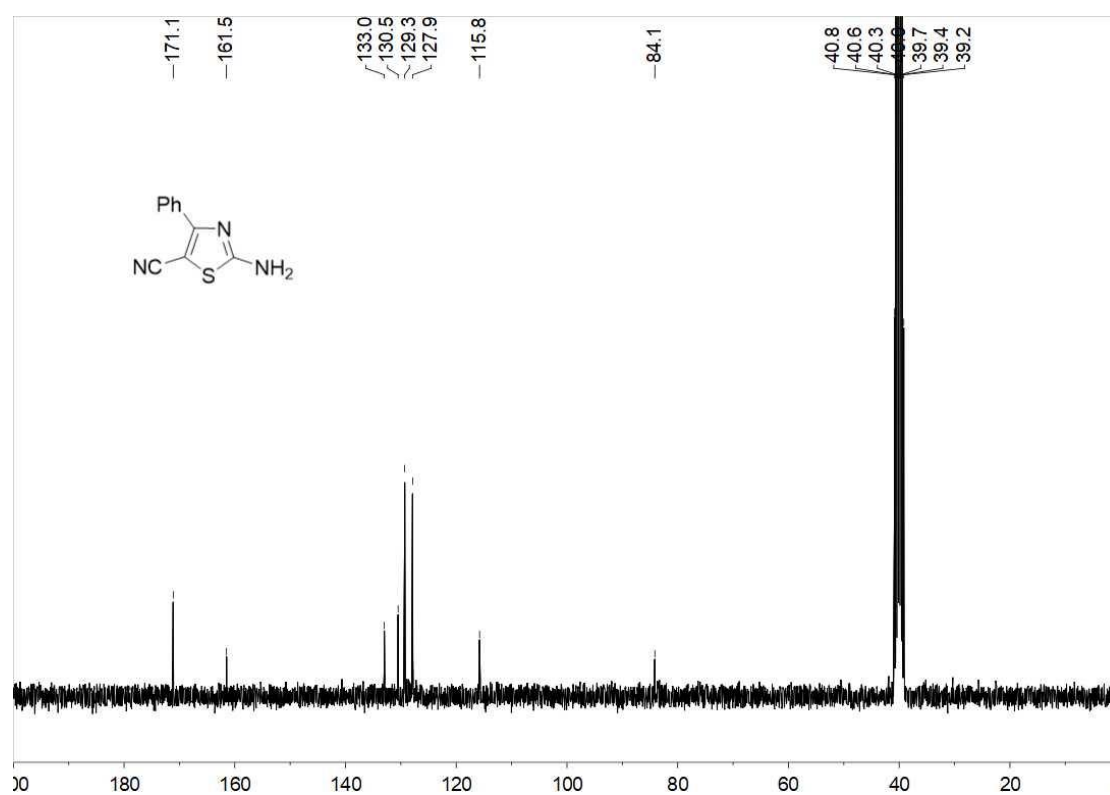
**$^{13}\text{C}$  NMR of 2-amino-N, N-diethyl-4-methylthiazole-5-carboxamide (3w)**



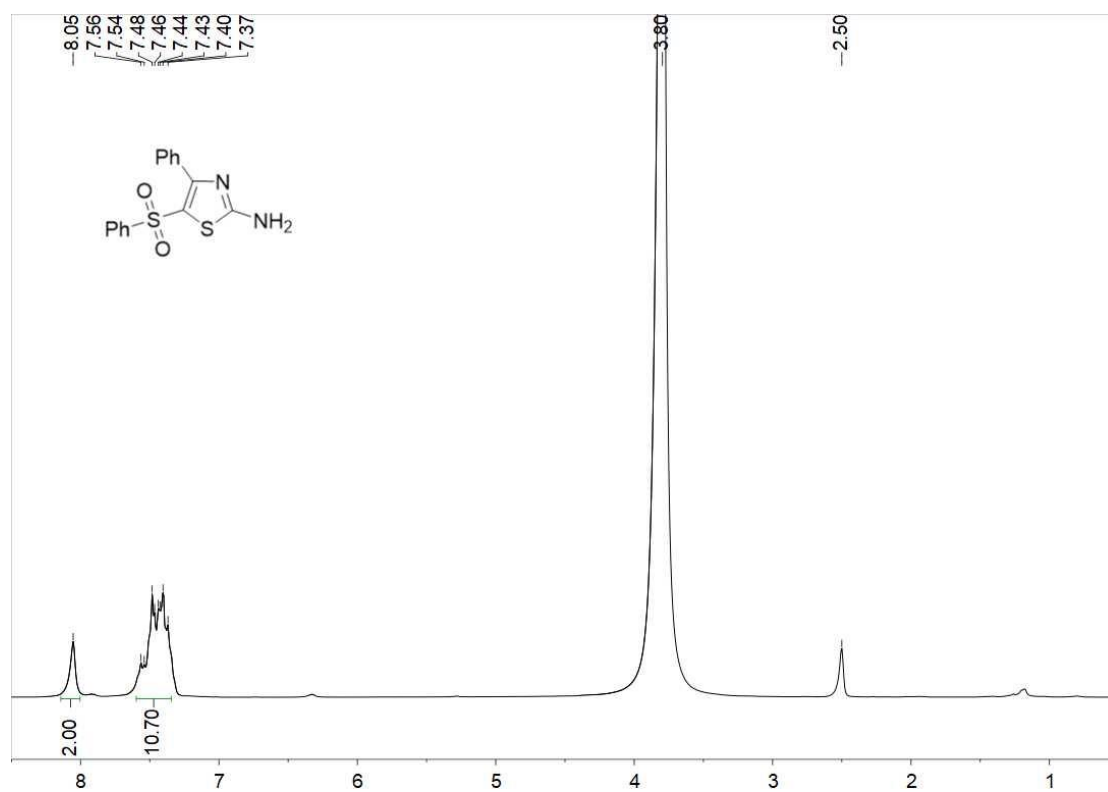
**<sup>1</sup>H NMR of 2-amino-4-phenylthiazole-5-carbonitrile (3x)**



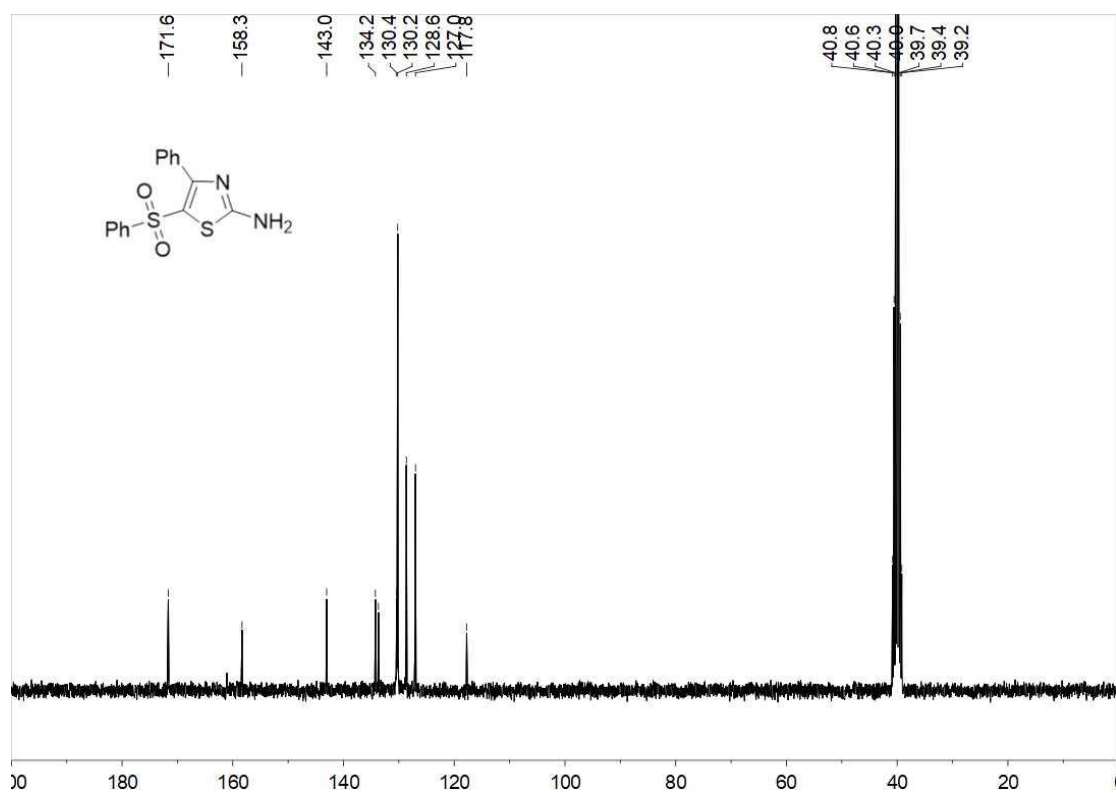
**<sup>13</sup>C NMR of 2-amino-4-phenylthiazole-5-carbonitrile (3x)**



**<sup>1</sup>H NMR of 4-phenyl-5-(phenylsulfonyl) thiazol-2-amine (3y)**



**<sup>13</sup>C NMR of 4-phenyl-5-(phenylsulfonyl) thiazol-2-amine (3y)**



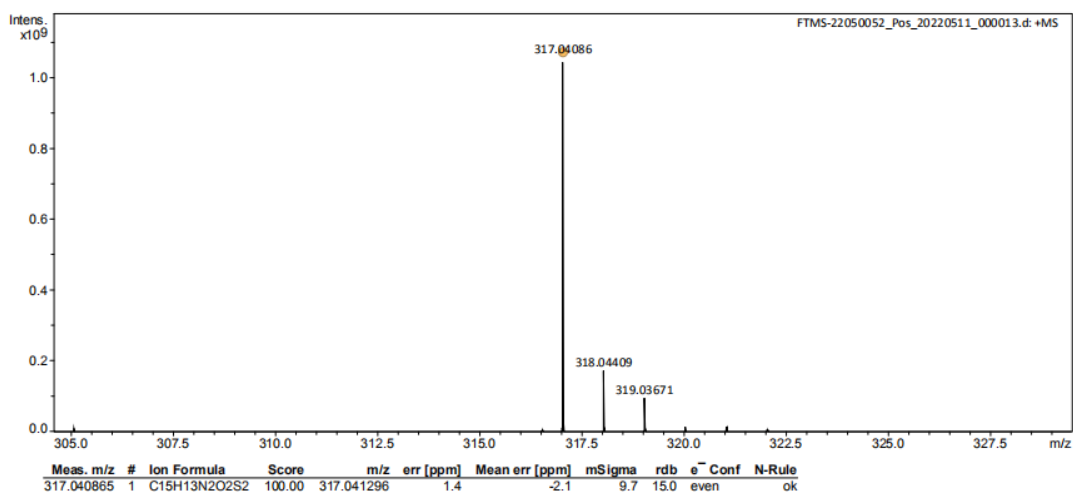
## HRMS of 4-phenyl-5-(phenylsulfonyl) thiazol-2-amine (3y)

### Peking University Mass Spectrometry Sample Analysis Report

#### Analysis Info

Analysis Name FTMS-22050052\_Pos\_20220511\_000013.d  
Sample 0509-12  
Comment

Acquisition Date 5/11/2022 3:10:27 PM  
Instrument Bruker Solarix XR FTMS  
Operator Peking University



Bruker Compass DataAnalysis 5.0

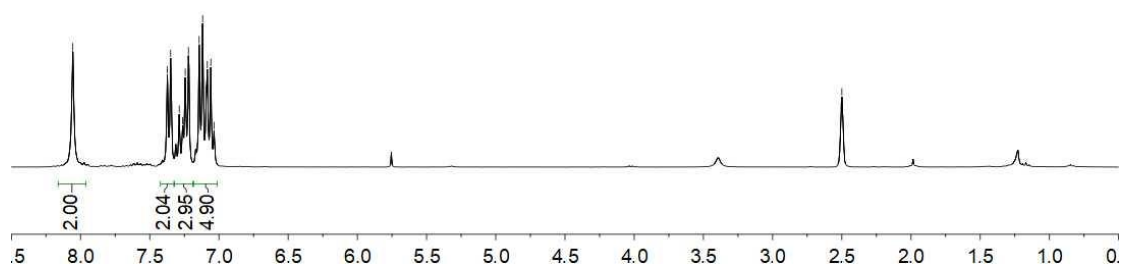
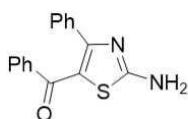
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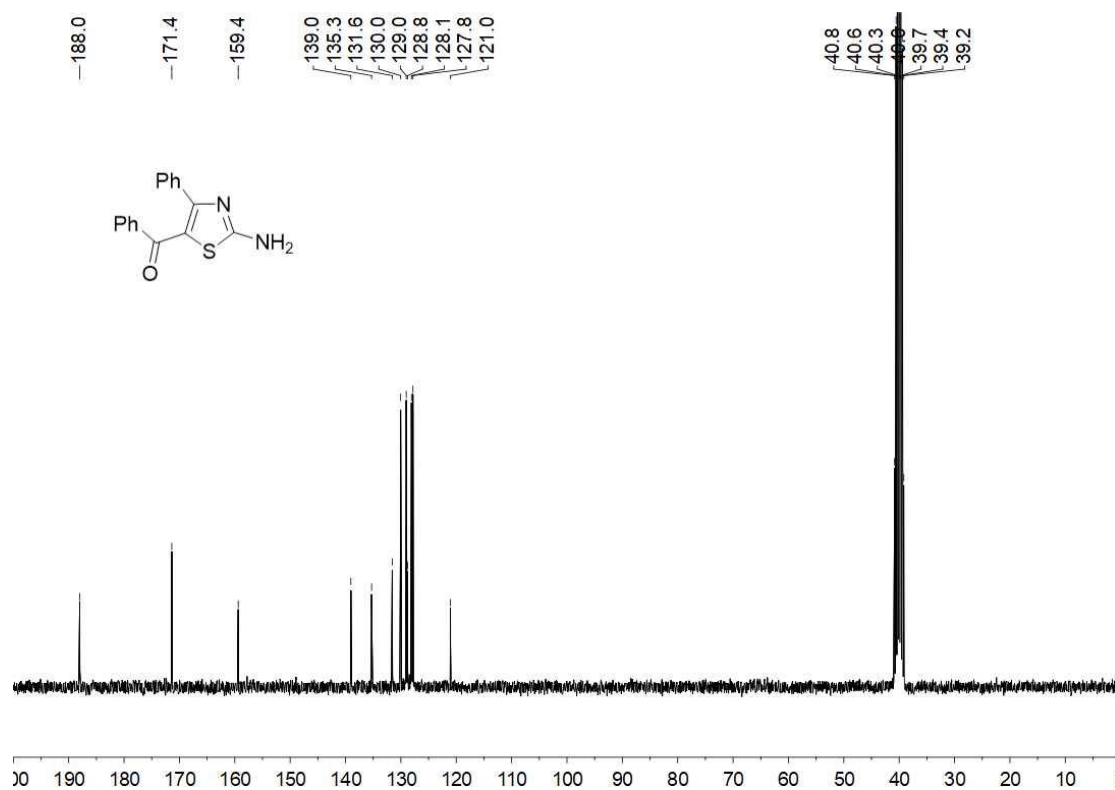
## <sup>1</sup>H NMR of (2-amino-4-phenylthiazol-5-yl) (phenyl)methanone (3z)

8.06  
7.37  
7.35  
7.29  
7.26  
7.24  
7.22  
7.22  
7.14  
7.12  
7.09  
7.08  
7.06  
7.04

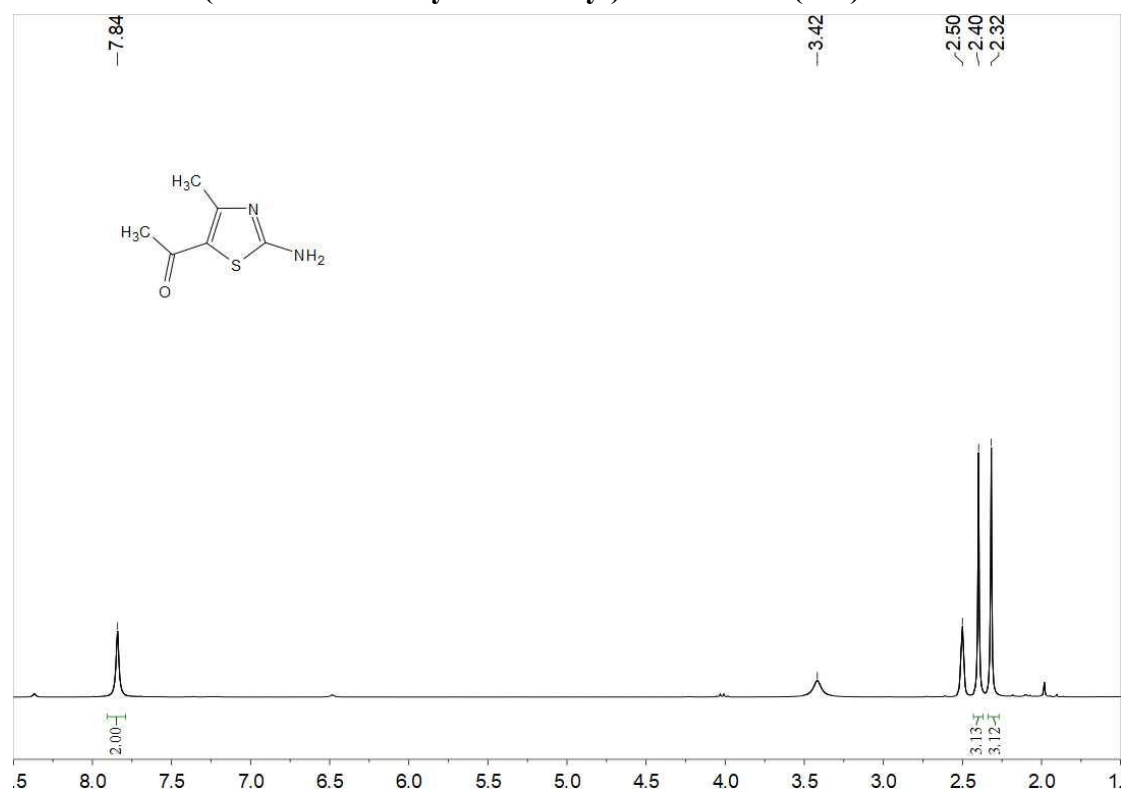
2.51  
2.50  
2.49



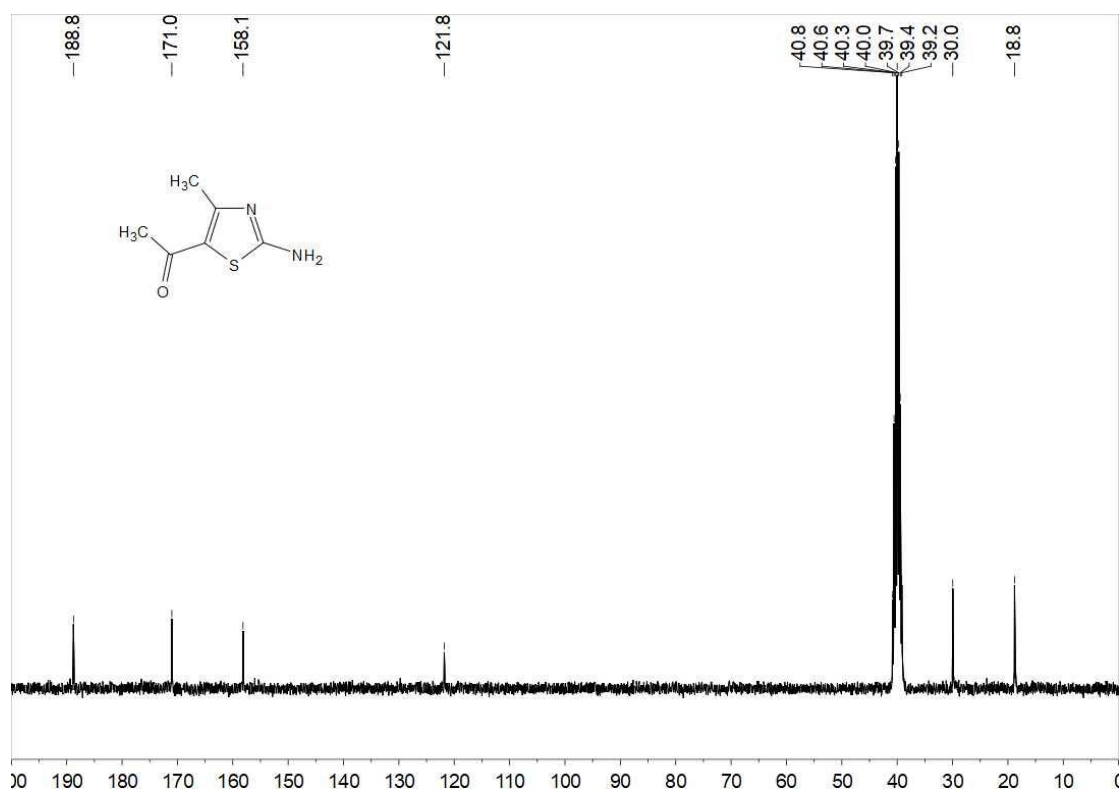
**$^{13}\text{C}$  NMR of (2-amino-4-phenylthiazol-5-yl) (phenyl)methanone (3z)**



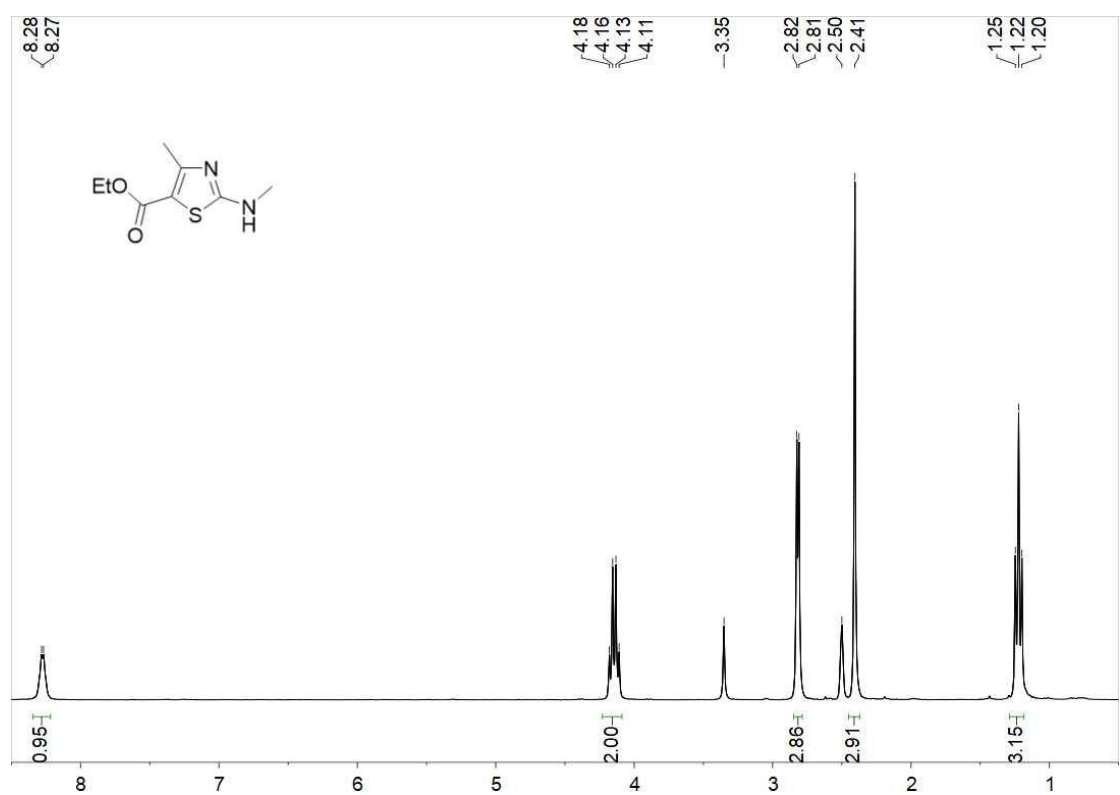
**$^1\text{H}$  NMR of 1-(2-amino-4-methylthiazol-5-yl)ethan-1-one (3aa)**



**<sup>13</sup>C NMR of 1-(2-amino-4-methylthiazol-5-yl)ethan-1-one (3aa)**

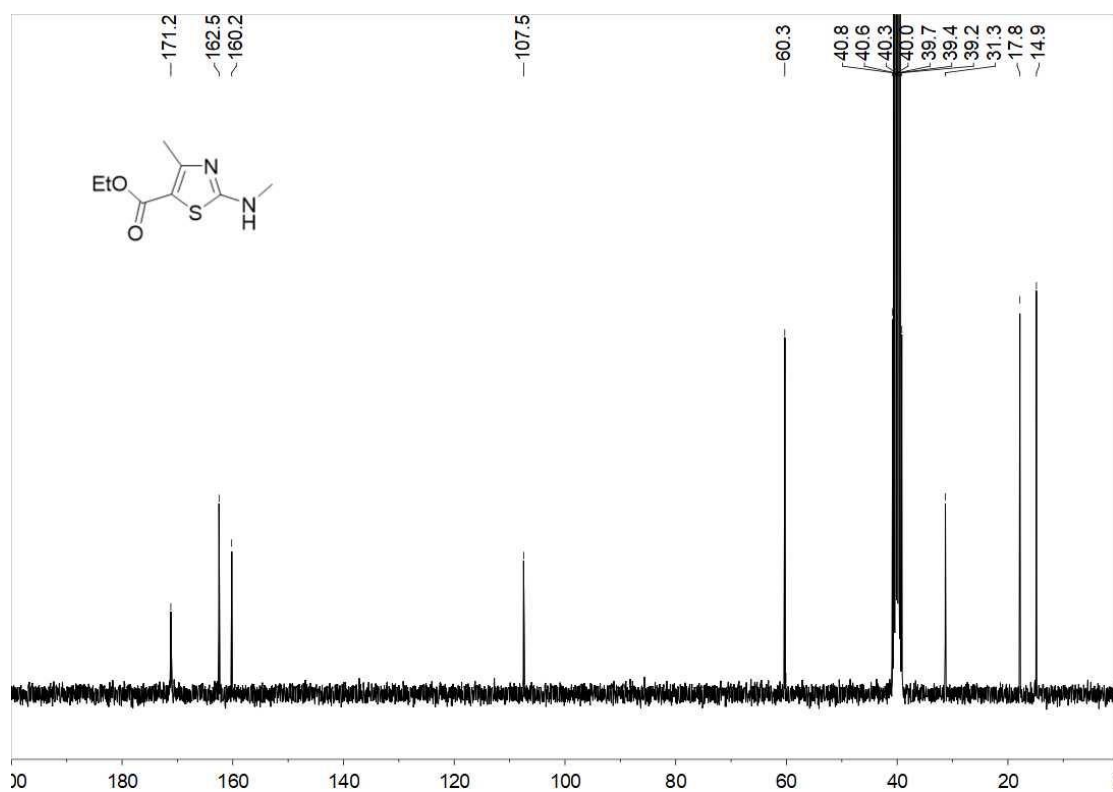


**<sup>1</sup>H NMR of ethyl 4-methyl-2-(methylamino) thiazole-5-carboxylate (3bb)**

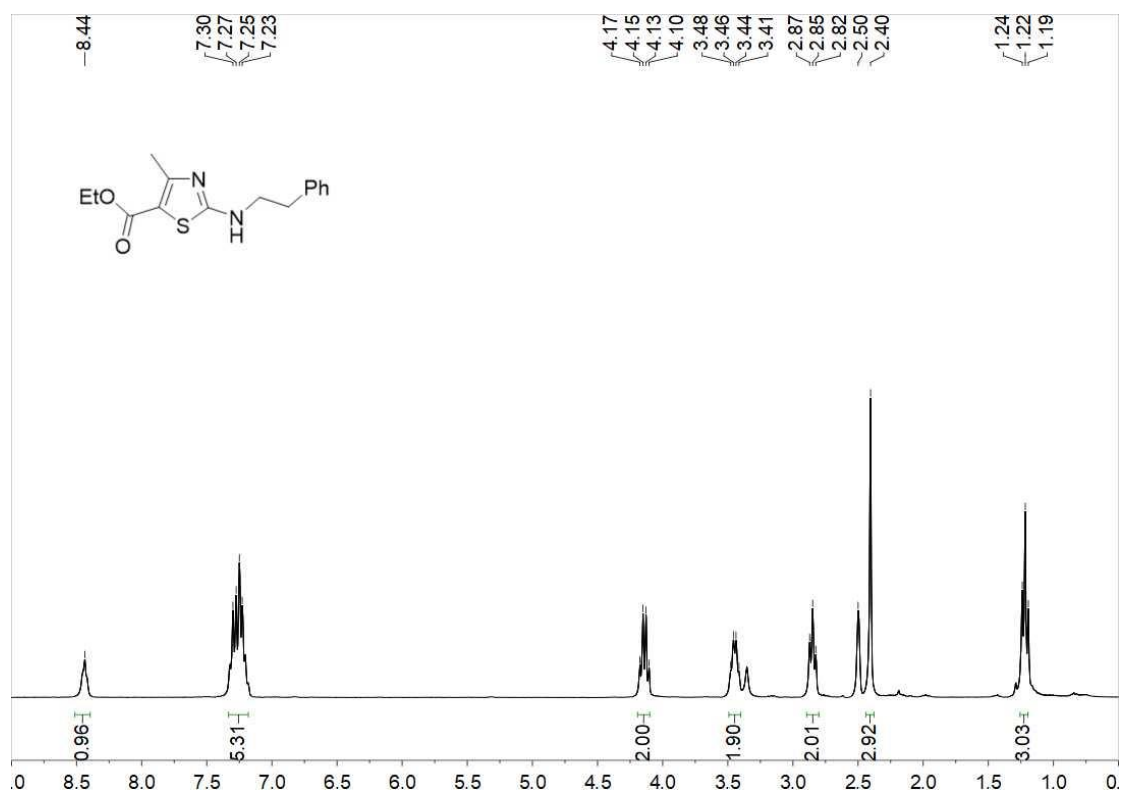




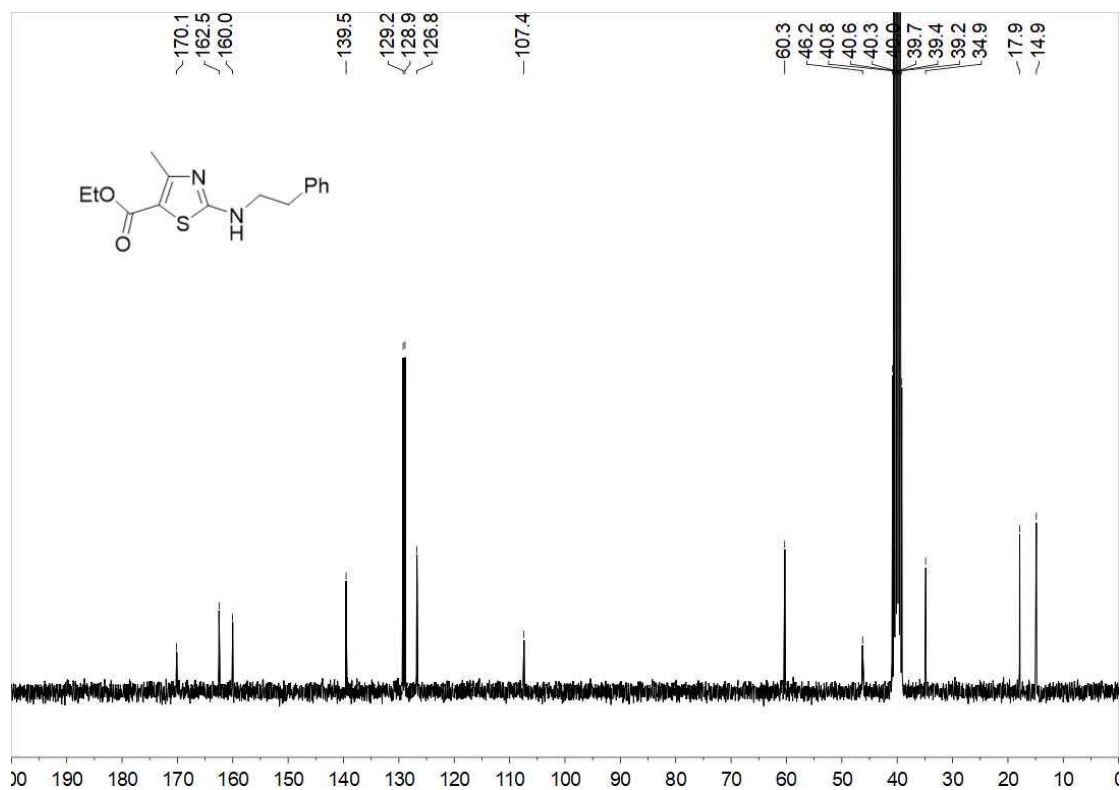
**$^{13}\text{C}$  NMR of ethyl 4-methyl-2-(methylamino) thiazole-5-carboxylate (3bb)**



**$^1\text{H}$  NMR of ethyl 4-methyl-2-(phenethylamino) thiazole-5-carboxylate (3cc)**



### <sup>13</sup>C NMR of ethyl 4-methyl-2-(phenethylamino) thiazole-5-carboxylate (3cc)



### HRMS of ethyl 4-methyl-2-(phenethylamino) thiazole-5-carboxylate (3cc)

#### Peking University Mass Spectrometry Sample Analysis Report

##### Analysis Info

Analysis Name FTMS-22050052\_Pos\_20220511\_000011.d  
 Sample 0509-11  
 Comment

Acquisition Date 5/11/2022 3:07:49 PM  
 Instrument Bruker Solarix XR FTMS  
 Operator Peking University

