

# Supporting Information

## Access to highly functionalized imidazolones bearing $\alpha$ - amino acid esters via KOH-promoted annulation of amidines, nitrosoarenes and malonic esters

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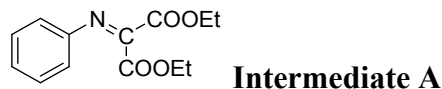
## 1. General

<sup>1</sup>H NMR spectra were taken on a Bruker AVANCE III 600 MHz NMR spectrometer. The chemical shifts are reported in ppm downfield to the CDCl<sub>3</sub> resonance ( $\delta = 7.27$ ). Spectra are reported as follows: chemical shift ( $\delta$  ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration, and assignment. <sup>13</sup>C NMR data were collected at 100 MHz with complete proton decoupling. The chemical shifts are reported in ppm downfield to the central CDCl<sub>3</sub> resonance ( $\delta = 77.0$ ). High-resolution mass spectra were performed on a micrOTOF-Q II instrument with an ESI source. Melting points were measured with a RD-II melting point apparatus and are uncorrected. Unless otherwise noted, all reagents and solvents obtained from commercial sources were used without further purification. Deuterated solvents were purchased from Sigma–Aldrich. The purity of the KOH is 95%. Column chromatography was performed on silica gel (200–300 mesh). All yields were referred to isolated yields (average of two runs) of compounds.

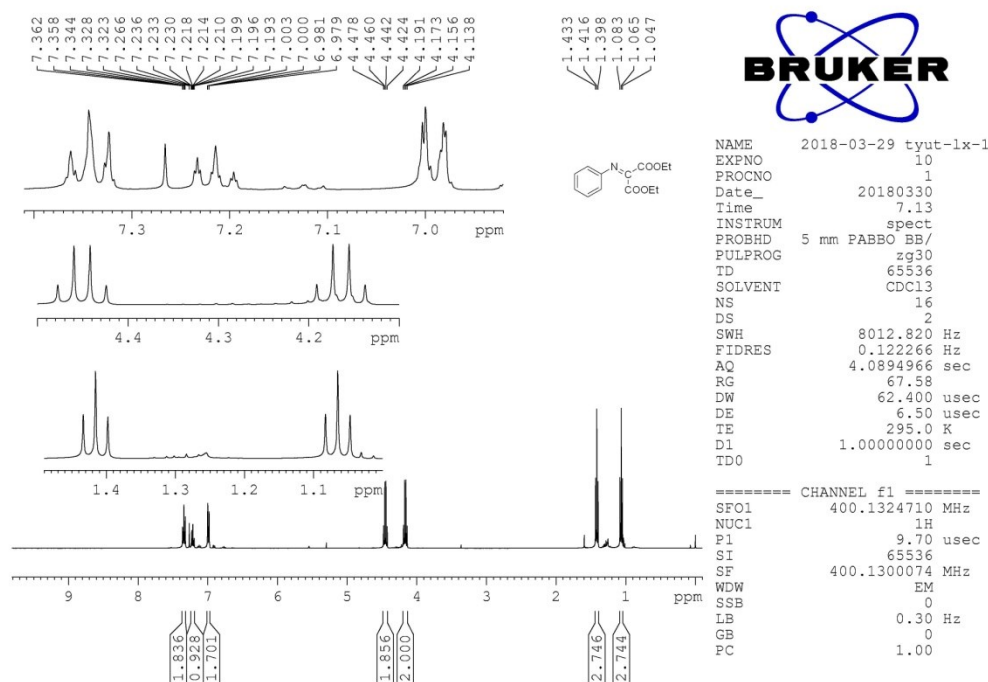
## 2. General procedure for KOH-mediated three-component annulation of amidines, nitrosoarenes, and malonic acid diesters

To a reaction system of amidine **1** (0.2 mmol), nitrosoarene **2** (0.26 mmol, 1.3 equiv) and KOH (0.1 mmol, 0.5 equiv) in CHCl<sub>3</sub> (1.2 mL) was added malonic acid diester **3** (0.34 mmol, 1.7 equiv) under air atmosphere. Subsequently, the resulting mixture was stirred under 60 °C (oil bath) and monitored by TLC. Upon completion of the consumption of the amidine **1**, the reaction mixture was purified by silica gel column chromatography to give the cycloaddition product **4**.

### 3. Characterization data and <sup>1</sup>H-NMR spectra of intermediate A

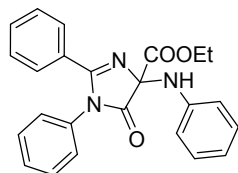


Yellow oil;  $R_f = 0.3$  (PE:EA = 20:1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.37–7.32 (m, 2H), 7.24–7.19 (m, 1H), 7.01–6.97 (m, 2H), 4.44 (q,  $J = 7.2$  Hz, 2H), 4.15 (q,  $J = 7.2$  Hz, 2H), 1.41 (t,  $J = 6.8$  Hz, 3H), 1.07 (t,  $J = 7.2$  Hz, 3H); HRMS (ESI)  $m/z$  [M + H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>16</sub>NO<sub>4</sub> 250.1074; found 250.1078.



### 4. Characterization data of products

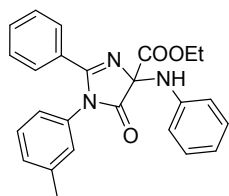
#### Ethyl 5-oxo-1,2-diphenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4aaa)



Yellow solid (75.0 mg, 94% yield); mp 156–158 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz,

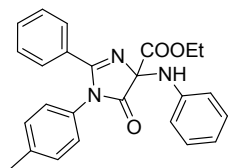
CDCl<sub>3</sub>)  $\delta$  7.44–7.41 (m, 3H), 7.40–7.35 (m, 3H), 7.30–7.25 (m, 2H), 7.19–7.13 (m, 2H), 7.10–7.07 (m, 2H), 6.83 (t,  $J = 7.2$  Hz, 1H), 6.78 (m, 2H), 5.54 (s, 1H), 4.37–4.25 (m, 2H), 1.28 (t,  $J = 7.2$  Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  177.2 (O–C=O), 165.6 (N–C=O), 165.2 (C=N), 143.5, 134.0, 131.8, 129.6, 129.3, 128.8, 128.5, 128.4, 126.9, 120.4, 116.3, 84.2 (C), 63.6 (CH<sub>2</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI)  $m/z$  [M + H]<sup>+</sup> Calcd for C<sub>24</sub>H<sub>22</sub>N<sub>3</sub>O<sub>3</sub> 400.1656; found 400.1645.

**Ethyl 5-oxo-2-phenyl-4-(phenylamino)-1-(*m*-tolyl)-4,5-dihydro-1H-imidazole-4-carboxylate (4baa)**



Yellow solid (79.3 mg, 96% yield); mp 132–134 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.38–7.33 (m, 3H), 7.24–7.17 (m, 3H), 7.09 (t,  $J = 8.0$  Hz, 3H), 6.87 (s, 1H), 6.76 (t,  $J = 7.6$  Hz, 2H), 6.68 (d,  $J = 7.6$  Hz, 2H), 5.44 (s, 1H), 4.31–4.19 (m, 2H), 2.26 (s, 3H), 1.22 (t,  $J = 7.2$  Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  177.3 (O–C=O), 165.6 (N–C=O), 165.2 (C=N), 143.5, 139.8, 134.0, 131.7, 129.7, 129.3, 129.2, 128.9, 128.5, 128.4, 127.4, 124.0, 120.4, 116.3, 84.1 (C), 63.6 (CH<sub>2</sub>), 21.3 (CH<sub>3</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI)  $m/z$  [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1818.

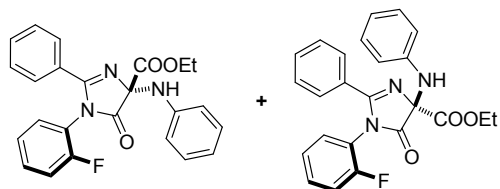
**Ethyl 5-oxo-2-phenyl-4-(phenylamino)-1-(*p*-tolyl)-4,5-dihydro-1H-imidazole-4-carboxylate (4caa)**



Yellow solid (80.2 mg, 97% yield); mp 145–147 °C; Column chromatography on

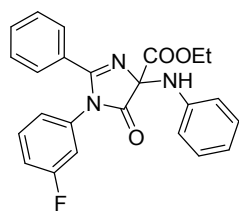
silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.46–7.40 (m, 3H), 7.29 (t,  $J = 7.6$  Hz, 2H), 7.21 (m, 4H), 6.97 (d,  $J = 8.4$  Hz, 2H), 6.83 (t,  $J = 7.2$  Hz, 1H), 6.75 (d,  $J = 7.6$  Hz, 2H), 5.52 (s, 1H), 4.38–4.25 (m, 2H), 2.36 (s, 3H), 1.29 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.4 (O–C=O), 165.6 (N–C=O), 165.3 (C=N), 143.5, 138.9, 131.7, 131.4, 130.2, 129.2, 128.9, 128.5, 128.4, 126.7, 120.4, 116.3, 84.1 (C), 63.5 ( $\text{CH}_2$ ), 21.2 ( $\text{CH}_3$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{25}\text{H}_{24}\text{N}_3\text{O}_3$  414.1812; found 414.1816.

**Ethyl 1-(2-fluorophenyl)-5-oxo-2-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4daa+4d'aa)**



Yellow solid (62.6 mg, 75% yield); mp 149–151 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.50–7.45 (m, 6H), 7.45–7.40 (m, 2H), 7.37–7.29 (m, 6H), 7.27–7.13 (m, 8H), 6.90–6.84 (m, 2H), 6.83–6.77 (m, 4H), 5.63 (s, 1H), 5.60 (s, 1H), 4.45–4.29 (m, 4H), 1.38–1.28 (m, 6H) ppm;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -119.60, -119.70 ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{21}\text{FN}_3\text{O}_3$  418.1561; found 418.1576.

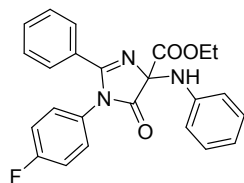
**Ethyl 1-(3-fluorophenyl)-5-oxo-2-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4eaa)**



Yellow solid (64.2 mg, 77% yield); mp 118–120 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,

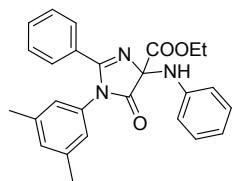
CDCl<sub>3</sub>)  $\delta$  7.52–7.44 (m, 3H), 7.42–7.33 (m, 3H), 7.23–7.18 (m, 2H), 7.15–7.09 (m, 1H), 6.90–6.85 (m, 3H), 6.78 (d,  $J$  = 7.6 Hz, 2H), 5.54 (s, 1H), 4.42–4.30 (m, 2H), 1.32 (t,  $J$  = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  176.8 (O–C=O), 165.3 (N–C=O), 164.6 (C=N), 162.7, (d,  $J$  = 247.8 Hz), 143.3, 135.3 (d,  $J$  = 9.8 Hz), 132.0, 130.7 (d,  $J$  = 9.0 Hz), 129.3, 128.7 (d,  $J$  = 12.9 Hz), 128.1, 122.6, 120.7, 116.4, 115.9 (d,  $J$  = 20.8 Hz), 114.4 (d,  $J$  = 23.5 Hz), 84.3 (C), 63.7 (CH<sub>2</sub>), 14.0 (CH<sub>3</sub>) ppm; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -110.03 ppm; HRMS (ESI)  $m/z$  [M + H]<sup>+</sup> Calcd for C<sub>24</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>3</sub> 418.1561; found 418.1568.

**Ethyl 1-(4-fluorophenyl)-5-oxo-2-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4faa)**



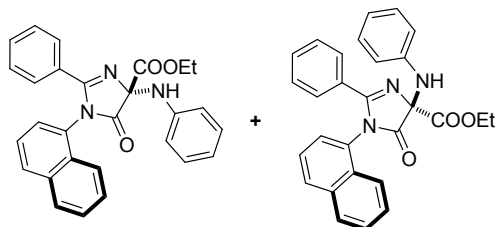
Yellow solid (72.6 mg, 87% yield); mp 136–138 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.51–7.43 (m, 3H), 7.35 (t,  $J$  = 7.2 Hz, 2H), 7.20 (t,  $J$  = 7.2 Hz, 2H), 7.15–7.06 (m, 4H), 6.88 (t,  $J$  = 7.6 Hz, 1H), 6.79 (d,  $J$  = 8.4 Hz, 2H), 5.53 (s, 1H), 4.43–4.49 (m, 2H), 1.32 (t,  $J$  = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  177.2 (O–C=O), 165.4 (N–C=O), 164.8 (C=N), 162.3 (d,  $J$  = 248.1 Hz), 143.4, 131.9, 130.0 (d,  $J$  = 3.2 Hz), 129.2, 128.8, 128.7 (d,  $J$  = 8.8 Hz), 128.5, 128.2, 120.6, 116.7 (d,  $J$  = 22.9 Hz), 116.5, 84.2 (C), 63.6 (CH<sub>2</sub>), 14.0 (CH<sub>3</sub>) ppm; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -111.19 ppm; HRMS (ESI)  $m/z$  [M + H]<sup>+</sup> Calcd for C<sub>24</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>3</sub> 418.1561; found 418.1568.

**Ethyl 1-(3,5-dimethylphenyl)-5-oxo-2-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4gaa)**



Yellow solid (73.5 mg, 86% yield); mp 150–152 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.53–7.43 (m, 3H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.24–7.17 (m, 2H), 7.03 (s, 1H), 6.87 (t, *J* = 7.2 Hz, 1H), 6.80 (d, *J* = 7.6 Hz, 2H), 6.72 (s, 2H), 5.54 (s, 1H), 4.42–4.29 (m, 2H), 2.31 (s, 6H), 1.33 (t, *J* = 6.8 Hz, 3H) ppm; <sup>13</sup>C {<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 177.4 (O–C=O), 165.7 (N–C=O), 165.2 (C=N), 143.5, 139.4, 133.9, 131.7, 130.7, 129.2, 128.9, 128.5, 128.4, 124.6, 120.4, 116.3, 84.1 (C), 63.5 (CH<sub>2</sub>), 21.2 (CH<sub>3</sub> X 2), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) *m/z* [M + H]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>26</sub>N<sub>3</sub>O<sub>3</sub> 428.1969; found 428.1967.

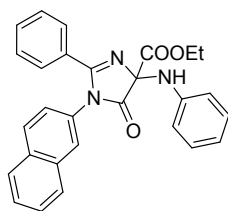
**Ethyl 1-(naphthalen-1-yl)-5-oxo-2-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4haa+4h'aa)**



Yellow solid (62.9 mg, 70% yield); mp 152–154 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.06–8.00 (m, 1H), 7.92–7.83 (m, 3H), 7.56–7.51 (m, 2H), 7.48–7.44 (m, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.39–7.34 (m, 2H), 7.33–7.25 (m, 4H), 7.25–7.19 (m, 3H), 7.14–7.08 (m, 4H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.98 (t, *J* = 7.2 Hz, 1H), 6.90–6.83 (m, 3H), 5.61 (s, 1H), 5.47 (s, 1H), 4.53–4.44 (m, 1H), 4.42–4.32 (m, 2H), 1.42 (t, *J* = 7.2 Hz, 3H), 1.32 (t, *J* = 7.2 Hz, 1H) ppm; HRMS (ESI) *m/z* [M + H]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 450.1812; found 450.1815.

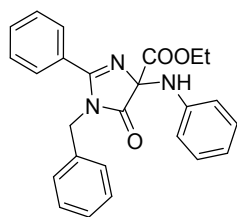
**Ethyl 1-(naphthalen-2-yl)-5-oxo-2-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-**

**carboxylate (4iaa)**



Yellow solid (67.4 mg, 75% yield); mp 135–137 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90–7.83 (m, 3H), 7.70 (d,  $J = 1.6$  Hz, 1H), 7.59–7.54 (m, 2H), 7.53–7.50 (m, 2H), 7.44 (t,  $J = 7.2$  Hz, 1H), 7.29 (t,  $J = 8.4$  Hz, 2H), 7.24–7.21 (m, 2H), 7.09 (dd,  $J = 8.8, 2.0$  Hz, 1H), 6.90 (t,  $J = 7.2$  Hz, 1H), 6.85 (d,  $J = 7.6$  Hz, 2H), 5.58 (s, 1H), 4.45–4.33 (m, 2H), 1.36 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.4 (O–C=O), 165.6 (N–C=O), 165.1 (C=N), 143.5, 133.3, 132.8, 131.8, 131.4, 129.6, 129.3, 128.9, 128.5, 128.4, 128.2, 127.9, 127.2, 127.1, 125.8, 124.2, 120.5, 116.4, 84.3 (C), 63.7 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{28}\text{H}_{24}\text{N}_3\text{O}_3$  450.1812; found 450.1815.

**Ethyl 1-benzyl-5-oxo-2-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4kaa)**

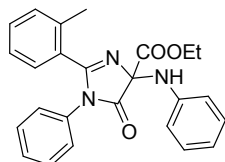


Yellow solid (75.2 mg, 91% yield); mp 119–121 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59–7.54 (m, 1H), 7.50–7.42 (m, 4H), 7.33–7.28 (m, 3H), 7.14–7.06 (m, 4H), 6.84 (t,  $J = 8.0$  Hz, 1H), 6.64 (d,  $J = 7.6$  Hz, 2H), 5.52 (s, 1H), 4.92 (d,  $J = 15.6$  Hz, 1H), 4.82 (d,  $J = 15.6$  Hz, 1H), 4.39–4.26 (m, 2H), 1.30 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  178.6 (O–C=O), 167.2 (N–C=O), 165.6 (C=N), 143.4, 135.6, 131.7, 129.2, 129.0, 128.9, 128.8, 128.1, 128.0, 127.3, 120.2, 116.2,



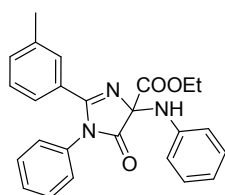
83.8 (C), 63.5 (CH<sub>2</sub>), 45.7 (CH<sub>2</sub>), 13.9 (CH<sub>3</sub>) ppm; HRMS (ESI) m/z [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1810.

**Ethyl 5-oxo-1-phenyl-4-(phenylamino)-2-(o-tolyl)-4,5-dihydro-1H-imidazole-4-carboxylate (4laa)**



Yellow solid (74.4 mg, 90% yield); mp 141–143 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.32–7.25 (m, 4H), 7.23–7.15 (m, 3H), 7.11 (d, *J* = 8.4 Hz, 2H), 7.02–6.98 (m, 2H), 6.88 (t, *J* = 7.6 Hz, 1H), 6.81 (d, *J* = 7.6 Hz, 2H), 5.50 (s, 1H), 4.42–4.30 (m, 2H), 2.18 (s, 3H), 1.34 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 176.6 (O–C=O), 166.4 (N–C=O), 165.5 (C=N), 143.4, 136.8, 133.3, 130.8, 130.7, 129.2, 129.1, 128.9, 128.8, 128.3, 126.0, 125.8, 120.8, 116.9, 84.5 (C), 63.6 (CH<sub>2</sub>), 19.5 (CH<sub>3</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) m/z [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1818.

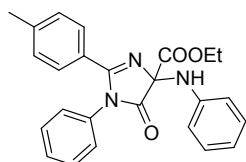
**Ethyl 5-oxo-1-phenyl-4-(phenylamino)-2-(m-tolyl)-4,5-dihydro-1H-imidazole-4-carboxylate (4maa)**



Yellow solid (76.0 mg, 92% yield); mp 154–156 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.35–7.27 (m, 4H), 7.17 (d, *J* = 9.2 Hz, 1H), 7.13–7.06 (m, 3H), 7.04–6.98 (m, 3H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.68 (d, *J* = 7.6 Hz, 2H), 5.47 (s, 1H), 4.31–4.19 (m, 2H), 2.19 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 177.2 (O–C=O), 165.6 (N–C=O), 165.3 (C=N), 143.5, 138.5, 134.1, 132.6, 129.5,

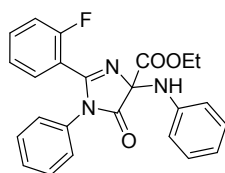
129.4, 129.2, 128.7, 128.3, 128.1, 126.9, 125.9, 120.3, 116.2, 84.1 (C), 63.6 (CH<sub>2</sub>), 21.3 (CH<sub>3</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) m/z [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1818.

**Ethyl 5-oxo-1-phenyl-4-(p-tolyl)-2-(p-tolyl)-4,5-dihydro-1H-imidazole-4-carboxylate (4naa)**



Yellow solid (77.7 mg, 94% yield); mp 163–165 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.44–7.36 (m, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.19–7.14 (m, 2H), 7.09 (d, *J* = 7.6 Hz, 4H), 6.83 (t, *J* = 7.2 Hz, 1H), 6.75 (d, *J* = 7.6 Hz, 2H), 5.54 (s, 1H), 4.38–4.26 (m, 2H), 2.33 (s, 3H), 1.29 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 177.3 (O–C=O), 165.7 (N–C=O), 165.0 (C=N), 143.5, 142.4, 134.2, 129.5, 129.2, 129.5, 129.1, 128.8, 128.7, 127.0, 125.5, 120.4, 116.3, 84.1 (C), 63.5 (CH<sub>2</sub>), 21.5 (CH<sub>3</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) m/z [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1814.

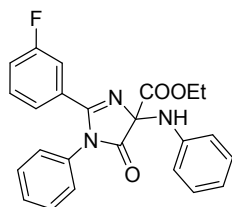
**Ethyl 2-(2-fluorophenyl)-5-oxo-1-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4oaa)**



Yellow solid (58.4 mg, 70% yield); mp 145–147 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.57–7.52 (m, 1H), 7.49–7.42 (m, 1H), 7.39–7.33 (m, 3H), 7.26–7.20 (m, 3H), 7.12–7.07 (m, 2H), 6.95 (t, *J* = 8.8 Hz, 1H), 6.89 (t, *J* = 7.2 Hz, 1H), 6.80 (d, *J* = 7.6 Hz, 2H), 5.59 (s, 1H), 4.44–4.32 (m, 2H), 1.36 (t, *J* = 6.8 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H}

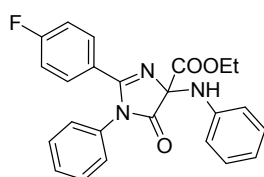
NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  176.3 (O=C=O), 165.1 (N=C=O), 163.2 (C=N), 159.5 (d,  $J = 251.4$  Hz), 143.3, 133.5 (d,  $J = 8.2$  Hz), 133.2 (d,  $J = 1.4$  Hz), 130.4 (d,  $J = 2.4$  Hz), 129.2 (d,  $J = 9.2$  Hz), 128.6, 126.1, 124.7 (d,  $J = 3.6$  Hz), 120.5, 117.8 (d,  $J = 14.6$  Hz), 116.2, 116.1, 116.0, 84.3 (C), 63.7 (CH<sub>2</sub>), 13.9 (CH<sub>3</sub>) ppm; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -110.34 ppm; HRMS (ESI)  $m/z$  [M + H]<sup>+</sup> Calcd for C<sub>24</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>3</sub> 418.1561; found 418.1564.

**Ethyl 2-(3-fluorophenyl)-5-oxo-1-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4paa)**



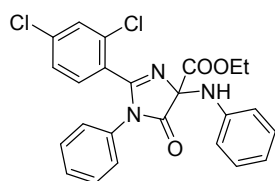
Yellow solid (60.9 mg, 73% yield); mp 137–139 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.48–7.40 (m, 3H), 7.32–7.27 (m, 1H), 7.23–7.18 (m, 4H), 7.17–7.10 (m, 3H), 6.88 (t,  $J = 7.6$  Hz, 1H), 6.78 (d,  $J = 7.6$  Hz, 2H), 5.54 (s, 1H), 4.44–4.32 (m, 2H), 1.36 (t,  $J = 6.8$  Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  177.0 (O=C=O), 165.3 (N=C=O), 164.0 (C=N), 162.3 (d,  $J = 246.5$  Hz), 143.3, 133.7, 130.4 (d,  $J = 8.0$  Hz), 130.2 (d,  $J = 8.0$  Hz), 129.7, 129.3, 129.1, 126.8, 124.6 (d,  $J = 3.2$  Hz), 120.6, 118.9 (d,  $J = 21.0$  Hz), 116.4, 116.0 (d,  $J = 23.8$  Hz), 115.9, 84.2 (C), 63.7 (CH<sub>2</sub>), 14.0 (CH<sub>3</sub>) ppm; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -111.18 ppm; HRMS (ESI)  $m/z$  [M + H]<sup>+</sup> Calcd for C<sub>24</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>3</sub> 418.1561; found 418.1572.

**Ethyl 2-(4-fluorophenyl)-5-oxo-1-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4qaa)**



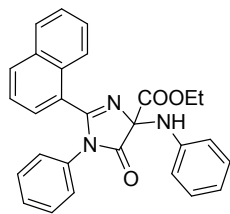
Yellow solid (70.1 mg, 84% yield); mp 170–171 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.49–7.40 (m, 5H), 7.23–7.17 (m, 2H), 7.13–7.09 (m, 2H), 7.01 (t,  $J = 8.8$  Hz, 2H), 6.87 (t,  $J = 7.6$  Hz, 1H), 6.78 (d,  $J = 7.6$  Hz, 2H), 5.53 (s, 1H), 4.42–4.29 (m, 2H), 1.32 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.1 (O–C=O), 165.5 (N–C=O), 164.7 (d,  $J = 252.4$  Hz), 164.1 (C=N), 143.4, 133.9, 131.2 (d,  $J = 8.9$  Hz), 129.5 (d,  $J = 45.6$  Hz), 129.0, 127.0, 124.6 (d,  $J = 3.2$  Hz), 120.5, 116.3, 115.8 (d,  $J = 21.9$  Hz), 84.2 (C), 63.6 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm;  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -106.48 ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{21}\text{FN}_3\text{O}_3$  418.1561; found 418.1568.

**Ethyl 2-(2,4-dichlorophenyl)-5-oxo-1-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4raa)**



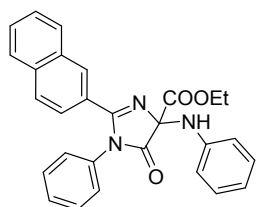
Yellow oil (66.3 mg, 71% yield); Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.35–7.28 (m, 6H), 7.23–7.18 (m, 2H), 7.06–7.02 (m, 2H), 6.88 (t,  $J = 7.2$  Hz, 1H), 6.80 (d,  $J = 8.0$  Hz, 2H), 5.54 (s, 1H), 4.43–4.30 (m, 2H), 1.34 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.0 (O–C=O), 165.0 (N–C=O), 163.9 (C=N), 143.1, 137.8, 133.6, 132.8, 131.5, 130.0, 129.3, 129.2, 128.7, 127.6, 126.2, 120.8, 116.6, 84.5 (C), 63.8 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{20}\text{Cl}_2\text{N}_3\text{O}_3$  468.0876; found 468.0888.

**Ethyl 2-(naphthalen-1-yl)-5-oxo-1-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4saa)**



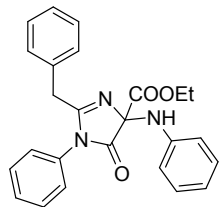
Yellow oil (78.2 mg, 87% yield); Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 (d,  $J = 8.0$  Hz, 1H), 7.88 (m, 1H), 7.79 (d,  $J = 8.0$  Hz, 1H), 7.48–7.38 (m, 2H), 7.35–7.30 (m, 2H), 7.25 (t,  $J = 8.0$  Hz, 2H), 7.20–7.14 (m, 3H), 7.00–6.94 (m, 2H), 6.91 (t,  $J = 6.4$  Hz, 3H), 5.56 (s, 1H), 4.48–4.35 (m, 2H), 1.40 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.8 (O–C=O), 165.5 (N–C=O), 165.4 (C=N), 143.5, 133.4, 133.3, 131.4, 130.7, 129.3, 129.2, 128.5, 128.4, 127.7, 127.4, 126.6, 126.3, 126.1, 124.8, 124.5, 121.1, 117.3, 84.9 (C), 63.8 ( $\text{CH}_2$ ), 14.1 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{28}\text{H}_{24}\text{N}_3\text{O}_3$  450.1812; found 450.1820.

**Ethyl 2-(naphthalen-2-yl)-5-oxo-1-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4taa)**



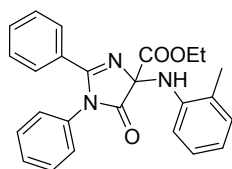
Yellow solid (79.1 mg, 88% yield); mp 138–140 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 (s, 1H), 7.79 (d,  $J = 8.0$  Hz, 1H), 7.74 (t,  $J = 8.8$  Hz, 2H), 7.56–7.38 (m, 1H), 7.50–7.44 (m, 2H), 7.41–7.37 (m, 3H), 7.21–7.17 (m, 2H), 7.16–7.13 (m, 2H), 6.86–6.78 (m, 3H), 5.58 (s, 1H), 4.41–4.28 (m, 2H), 1.33 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.2 (O–C=O), 165.6 (N–C=O), 165.1 (C=N), 143.5, 134.6, 134.2, 132.3, 130.1, 129.6, 129.3, 128.9, 128.8, 128.2, 128.1, 127.8, 127.0, 126.9, 125.7, 124.7, 120.4, 116.3, 84.2 (C), 63.7 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{28}\text{H}_{24}\text{N}_3\text{O}_3$  450.1812; found 450.1814.

**Ethyl 2-benzyl-5-oxo-1-phenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4uaa)**



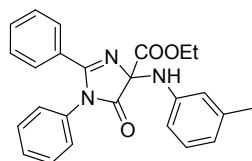
Yellow solid (62.0 mg, 75% yield); mp 101–103 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.42–7.33 (m, 3H), 7.22–7.10 (m, 5H), 6.92–6.88 (m, 2H), 6.85 (d, *J* = 8.4 Hz, 3H), 6.68 (dd, *J* = 8.4, 0.8 Hz, 2H), 5.45 (s, 1H), 4.37–4.25 (m, 2H), 3.84–3.75 (m, 2H), 1.27 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 176.9 (O–C=O), 166.5 (N–C=O), 165.6 (C=N), 143.3, 132.8, 132.7, 129.6, 129.2, 129.0, 128.5, 127.7, 127.4, 120.5, 116.5, 84.0 (C), 63.6 (CH<sub>2</sub>), 36.4 (CH<sub>2</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) *m/z* [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1820.

**Ethyl 5-oxo-1,2-diphenyl-4-(*o*-tolylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4aba)**



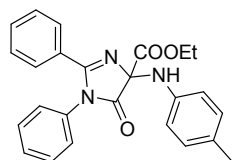
Yellow solid (68.6 mg, 83% yield); mp 109–111 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.45–7.40 (m, 4H), 7.39–7.36 (m, 2H), 7.31–7.26 (m, 2H), 7.13–7.08 (m, 3H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.75 (t, *J* = 7.2 Hz, 1H), 6.53 (d, *J* = 8.0 Hz, 1H), 5.57 (s, 1H), 4.39–4.27 (m, 2H), 2.36 (s, 3H), 1.30 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 177.3 (O–C=O), 165.8 (N–C=O), 165.1 (C=N), 141.8, 134.1, 131.8, 130.7, 129.6, 128.8, 128.7, 128.5, 128.4, 126.9, 126.8, 125.0, 120.0, 113.2, 84.1 (C), 63.7 (CH<sub>2</sub>), 17.7 (CH<sub>3</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) *m/z* [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1820.

**Ethyl 5-oxo-1,2-diphenyl-4-(*m*-tolylamino)-4,5-dihydro-1*H*-imidazole-4-carboxylate (4aca)**



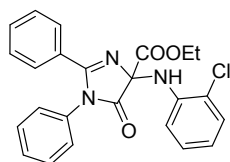
Yellow solid (71.9 mg, 87% yield); mp 109–111 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.45–7.39 (m, 4H), 7.39–7.35 (m, 2H), 7.32–7.26 (m, 2H), 7.11–7.06 (m, 2H), 7.04 (d, *J* = 8.8 Hz, 1H), 6.67 (d, *J* = 7.6 Hz, 1H), 6.56 (d, *J* = 7.2 Hz, 2H), 5.50 (s, 1H), 4.39–4.26 (m, 2H), 2.23 (s, 3H), 1.29 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 177.3 (O–C=O), 165.6 (N–C=O), 165.1 (C=N), 143.4, 138.9, 134.1, 131.7, 129.6, 129.1, 128.8, 128.7, 128.5, 128.4, 126.9, 121.3, 116.9, 113.3, 84.2 (C), 63.6 (CH<sub>2</sub>), 21.6 (CH<sub>3</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) *m/z* [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1818.

**Ethyl 5-oxo-1,2-diphenyl-4-(*p*-tolylamino)-4,5-dihydro-1*H*-imidazole-4-carboxylate (4ada)**



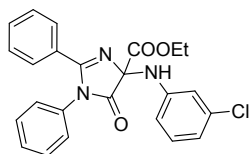
Yellow solid (73.5 mg, 89% yield); mp 141–143 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.45–7.33 (m, 6H), 7.31–7.24 (m, 2H), 7.07 (m, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.70 (d, *J* = 8.4 Hz, 2H), 5.38 (s, 1H), 4.38–4.26 (m, 2H), 2.22 (s, 3H), 1.29 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 177.3 (O–C=O), 165.7 (N–C=O), 165.0 (C=N), 140.9, 134.1, 131.7, 130.0, 129.7, 129.5, 128.8, 128.7, 128.5, 128.4, 126.9, 117.0, 84.6 (C), 63.5 (CH<sub>2</sub>), 20.6 (CH<sub>3</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) *m/z* [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub> 414.1812; found 414.1814.

**Ethyl 4-((2-chlorophenyl)amino)-5-oxo-1,2-diphenyl-4,5-dihydro-1*H*-imidazole-4-carboxylate (4aea)**



Yellow oil (72.8 mg, 84% yield); Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47–7.42 (m, 3H), 7.42–7.36 (m, 3H), 7.32–7.26 (m, 3H), 7.13 (dd,  $J = 6.4, 1.6$  Hz, 2H), 7.08–7.02 (m, 1H), 6.75–6.69 (m, 1H), 6.63 (dd,  $J = 8.0, 1.2$  Hz, 1H), 6.36 (s, 1H), 4.36–4.27 (m, 2H), 1.27 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.8 (O–C=O), 165.5 (N–C=O), 165.2 (C=N), 140.1, 134.0, 132.0, 129.7, 129.6, 129.0, 128.9, 128.5, 128.2, 127.6, 126.8, 121.4, 120.1, 113.6, 83.6 (C), 63.8 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{21}\text{ClN}_3\text{O}_3$  434.1266; found 434.1274.

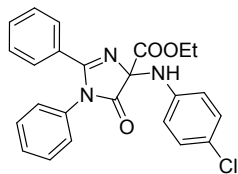
**Ethyl 4-((3-chlorophenyl)amino)-5-oxo-1,2-diphenyl-4,5-dihydro-1H-imidazole-4-carboxylate (4afa)**



Yellow solid (74.5 mg, 86% yield); mp 137–140 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47–7.41 (m, 4H), 7.41–7.38 (m, 2H), 7.31 (t,  $J = 7.6$  Hz, 2H), 7.14 (dd,  $J = 8.0, 1.6$  Hz, 2H), 7.08 (t,  $J = 8.0$  Hz, 1H), 6.78 (dd,  $J = 8.0, 0.8$  Hz, 1H), 6.68–6.63 (m, 2H), 5.68 (s, 1H), 4.40–4.27 (m, 2H), 1.30 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.9 (O–C=O), 165.6 (N–C=O), 165.2 (C=N), 144.8, 134.9, 133.9, 131.9, 130.3, 129.7, 129.0, 128.8, 128.5, 128.3, 127.0, 120.0, 115.0, 114.2, 83.7 (C), 63.8 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{21}\text{ClN}_3\text{O}_3$  434.1266; found 434.1268.

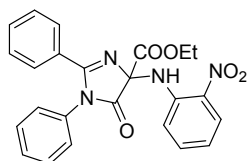
**Ethyl 4-((4-chlorophenyl)amino)-5-oxo-1,2-diphenyl-4,5-dihydro-1H-imidazole-4-carboxylate (4aga)**





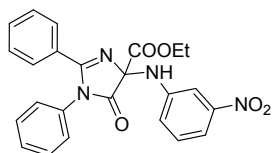
Yellow solid (80.6 mg, 93% yield); mp 122–124 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47–7.40 (m, 4H), 7.40 (s, 2H), 7.30 (t,  $J = 7.2$  Hz, 2H), 7.13 (d,  $J = 8.8$  Hz, 2H), 7.08 (dd,  $J = 8.0, 2.0$  Hz, 2H), 6.71 (d,  $J = 8.8$  Hz, 2H), 5.54 (s, 1H), 4.38–4.26 (m, 2H), 1.30 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.9 (O–C=O), 165.4 (N–C=O), 165.3 (C=N), 142.3, 134.0, 131.9, 129.6, 129.2, 128.9, 128.8, 128.5, 128.2, 126.8, 125.2, 117.4, 84.1 (C), 63.7 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{21}\text{ClN}_3\text{O}_3$  434.1266; found 434.1279.

**Ethyl 4-((2-nitrophenyl)amino)-5-oxo-1,2-diphenyl-4,5-dihydro-1H-imidazole-4-carboxylate (4aha)**



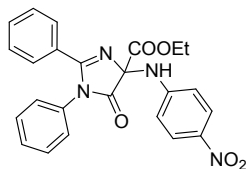
Yellow solid (65.7 mg, 74% yield); mp 129–134 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.53 (s, 1H), 8.22 (dd,  $J = 8.8, 1.6$  Hz, 1H), 7.49 (d,  $J = 8.0$  Hz, 3H), 7.47–7.39 (m, 4H), 7.33 (t,  $J = 7.6$  Hz, 2H), 7.17 (dd,  $J = 8.4, 2.0$  Hz, 2H), 6.84–6.77 (m, 2H), 4.42–4.30 (m, 2H), 1.31 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.1 (O–C=O), 166.0 (N–C=O), 164.5 (C=N), 141.6, 135.8, 134.4, 133.8, 132.2, 129.7, 129.1, 128.9, 128.6, 128.0, 127.1, 126.8, 118.1, 115.5, 83.2 (C), 64.1 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{21}\text{N}_4\text{O}_5$  445.1506; found 445.1512.

**Ethyl 4-((3-nitrophenyl)amino)-5-oxo-1,2-diphenyl-4,5-dihydro-1H-imidazole-4-carboxylate (4aia)**



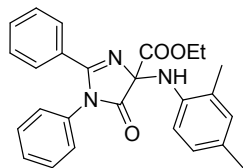
Yellow solid (79.9 mg, 90% yield); mp 119–121 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.65 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.51–7.45 (m, 3H), 7.45–7.40 (m, 3H), 7.38 (d, *J* = 2.4 Hz, 1H), 7.35–7.30 (m, 3H), 7.26–7.22 (m, 2H), 7.11 (dd, *J* = 7.6, 2.0 Hz, 1H), 6.06 (s, 1H), 4.44–4.32 (m, 2H), 1.34 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 176.5 (O–C=O), 166.5 (N–C=O), 164.9 (C=N), 149.1, 144.4, 133.7, 132.0, 130.0, 129.7, 129.1, 128.8, 128.6, 128.1, 127.1, 122.3, 114.4, 107.1, 83.2 (C), 64.1 (CH<sub>2</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) *m/z* [M + H]<sup>+</sup> Calcd for C<sub>24</sub>H<sub>21</sub>N<sub>4</sub>O<sub>5</sub> 445.1506; found 445.1510.

**Ethyl 4-((4-nitrophenyl)amino)-5-oxo-1,2-diphenyl-4,5-dihydro-1H-imidazole-4-carboxylate (4aja)**



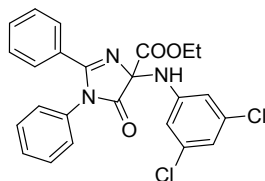
Yellow solid (80.8 mg, 91% yield); mp 198–200 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.09 (d, *J* = 9.2 Hz, 2H), 7.52–7.43 (m, 6H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.15 (dd, *J* = 8.0, 2.0 Hz, 2H), 6.70 (d, *J* = 9.2 Hz, 2H), 6.25 (s, 1H), 4.42–4.30 (m, 2H), 1.31 (t, *J* = 7.2 Hz, 3H) ppm; <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 176.0 (O–C=O), 166.2 (N–C=O), 164.8 (C=N), 149.4, 140.1, 133.7, 132.3, 129.8, 129.2, 128.8, 128.7, 127.9, 126.7, 126.0, 113.7, 83.9 (C), 64.2 (CH<sub>2</sub>), 14.0 (CH<sub>3</sub>) ppm; HRMS (ESI) *m/z* [M + H]<sup>+</sup> Calcd for C<sub>24</sub>H<sub>21</sub>N<sub>4</sub>O<sub>5</sub> 445.1506; found 445.1516.

**Ethyl 4-((2,4-dimethylphenyl)amino)-5-oxo-1,2-diphenyl-4,5-dihydro-1H-imidazole-4-carboxylate (4aka)**



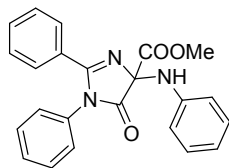
Yellow oil (58.1 mg, 68% yield); Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45–7.35 (m, 6H), 7.29 (t,  $J = 7.2$  Hz, 2H), 7.09 (dd,  $J = 8.0, 2.0$  Hz, 2H), 6.92 (s, 1H), 6.81 (d,  $J = 8.0$  Hz, 1H), 6.49 (d,  $J = 8.0$  Hz, 1H), 5.42 (s, 1H), 4.39–4.27 (m, 2H), 2.33 (s, 3H), 2.20 (s, 3H), 1.30 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.4 (O–C=O), 165.9 (N–C=O), 164.9 (C=N), 139.3, 134.1, 131.7, 131.5, 129.5, 129.4, 128.8, 128.7, 128.6, 128.4, 127.1, 126.9, 125.6, 114.0, 84.5 (C), 63.5 ( $\text{CH}_2$ ), 20.5 ( $\text{CH}_3$ ), 17.7 ( $\text{CH}_3$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{26}\text{H}_{26}\text{N}_3\text{O}_3$  428.1969; found 428.1973.

**Ethyl 4-((3,5-dichlorophenyl)amino)-5-oxo-1,2-diphenyl-4,5-dihydro-1H-imidazole-4-carboxylate (4a)**



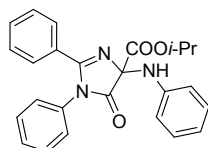
Yellow solid (59.8 mg, 64% yield); mp 60–62 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.48–7.45 (m, 2H), 7.44 (s, 1H), 7.43 (s, 1H), 7.42–7.39 (m, 2H), 7.32 (t,  $J = 7.6$  Hz, 2H), 7.15 (dd,  $J = 8.8, 2.0$  Hz, 2H), 6.78 (t,  $J = 1.6$  Hz, 1H), 6.59 (d,  $J = 2.0$  Hz, 2H), 5.82 (s, 1H), 4.40–4.27 (m, 2H), 1.30 (t,  $J = 7.2$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.6 (O–C=O), 166.0 (N–C=O), 165.0 (C=N), 145.5, 135.5, 133.7, 132.0, 129.7, 129.1, 128.8, 128.6, 128.2, 127.0, 119.6, 113.5, 83.3 (C), 64.0 ( $\text{CH}_2$ ), 14.0 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{20}\text{Cl}_2\text{N}_3\text{O}_3$  468.0876; found 468.0879.

**Methyl 5-oxo-1,2-diphenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4a)**



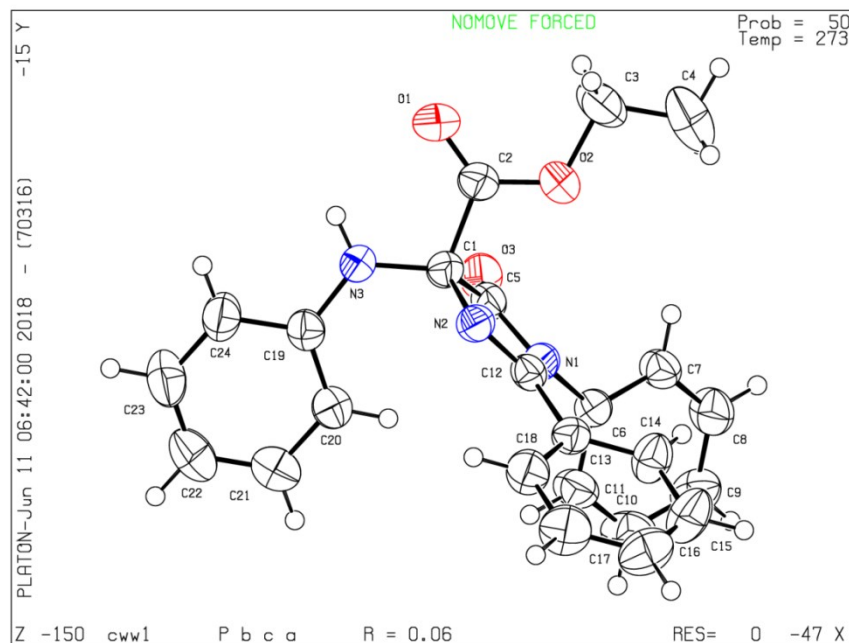
Yellow solid (73.2 mg, 95% yield); mp 145–147 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.46–7.41 (m, 3H), 7.41–7.37 (m, 3H), 7.31–7.27 (m, 2H), 7.20–7.15 (m, 2H), 7.10–7.06 (m, 2H), 6.85 (t,  $J = 7.2$  Hz, 1H), 6.78 (dd,  $J = 8.8, 1.2$  Hz, 2H), 5.49 (s, 1H), 3.87 (s, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.1 (O–C=O), 166.3 (N–C=O), 165.2 (C=N), 143.3, 133.9, 131.8, 129.5, 129.2, 128.9, 128.8, 128.4, 128.3, 126.9, 120.7, 116.7, 84.1 (C), 54.3 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_3$  386.1499; found 386.1499.

**Isopropyl 5-oxo-1,2-diphenyl-4-(phenylamino)-4,5-dihydro-1H-imidazole-4-carboxylate (4aac)**



Yellow solid (72.7 mg, 88% yield); mp 145–147 °C; Column chromatography on silicagel (Eluent: V/V, petroleum ether/ethyl acetate, 8/1);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45–7.36 (m, 6H), 7.31–7.25 (m, 2H), 7.18–7.14 (dd,  $J = 7.6, 0.8$  Hz, 2H), 7.10–7.07 (dd,  $J = 6.4, 2.0$  Hz, 2H), 6.84 (t,  $J = 7.6$  Hz, 1H), 6.75 (d,  $J = 7.6$  Hz, 2H), 5.54 (s, 1H), 5.15–5.11 (m, 1H), 1.30 (d,  $J = 6.4$  Hz, 3H), 1.27 (d,  $J = 6.0$  Hz, 3H) ppm;  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.1 (O–C=O), 164.9 (N–C=O), 164.8 (C=N), 143.5, 134.1, 131.7, 129.5, 129.2, 128.7, 128.4, 126.8, 120.2, 115.9, 84.2 (C), 71.8 ( $\text{CH}_2$ ), 21.6 ( $\text{CH}_3$ ), 21.5 ( $\text{CH}_3$ ) ppm; HRMS (ESI)  $m/z$   $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{25}\text{H}_{24}\text{N}_3\text{O}_3$  414.1812; found 414.1814.

## 5. Crystal structure of compound 4aaa (CCDC 2092223)



### Crystal data

Chemical formula	<u>C<sub>24</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub></u>
<i>M</i> <sub>r</sub>	<u>399.44</u>
Crystal system, space group	<u>Orthorhombic, <i>Pbca</i></u>
Temperature (K)	<u>273</u>
<i>a</i> , <i>b</i> , <i>c</i> (Å)	<u>12.1633 (9), 16.9191 (14), 20.7850 (16)</u>
<i>V</i> (Å <sup>3</sup> )	<u>4277.4 (6)</u>
<i>Z</i>	<u>8</u>
Radiation type	<u>Mo <i>K</i>α</u>
μ (mm <sup>-1</sup> )	<u>0.08</u>
Crystal size (mm)	<u>0.35 × 0.27 × 0.21</u>

### Data collection

Diffractometer	<u>CCD area detector</u>
Absorption correction	<u>Multi-scan</u> <u>SADABS-2016/2 (Bruker,2016/2) was used for</u> <u>absorption correction. wR2(int) was 0.1052 before</u>

	<u>and 0.0562 after correction. The Ratio of minimum to maximum transmission is 0.9453. The <math>\lambda/2</math> correction factor is Not present.</u>
$T_{\min}, T_{\max}$	<u>0.705, 0.746</u>
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	<u>73985, 5330, 3383</u>
$R_{\text{int}}$	<u>0.054</u>
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	<u>0.055, 0.148, 1.05</u>
No. of reflections	<u>5330</u>
No. of parameters	<u>272</u>
H-atom treatment	<u>H-atom parameters constrained</u>
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	<u>0.29, -0.32</u>

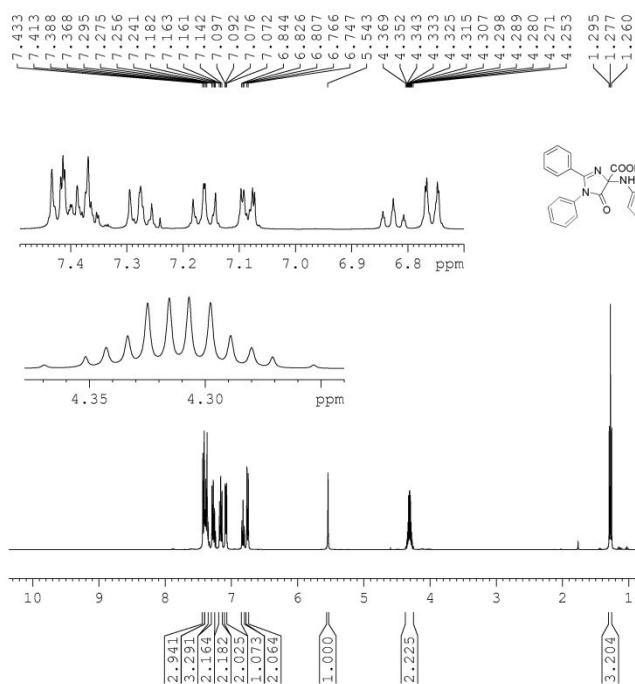
Computer programs: SAINT v8.37A (Bruker, 2015), ShelXT (Sheldrick, 2015), ShelXL (Sheldrick, 2015), Olex2 (Dolomanov *et al.*, 2009).

## 6. References

Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. J. *Appl. Cryst.* **2009**, *42*, 339–341.

Sheldrick, G. M. *Acta Cryst.* 2015, **C71**, 3–8.

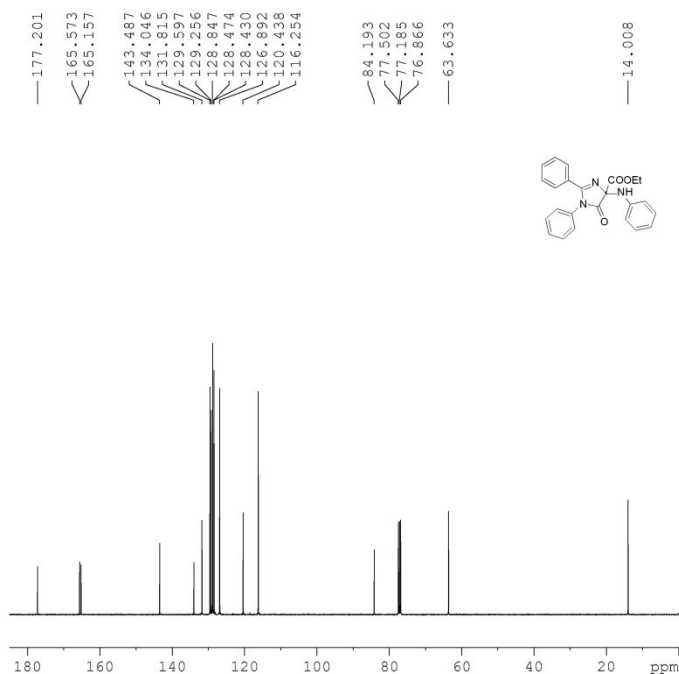
## 7. <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of products 4aaa



```

NAME      2018-11-23 tyut-lx-0
EXPNO    10
PROCNO   1
Date_    20181123
Time     18.33
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       19.58
DW       62.400 usec
DE       6.50 usec
TE       293.6 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI      65536
SF      400.1300176 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

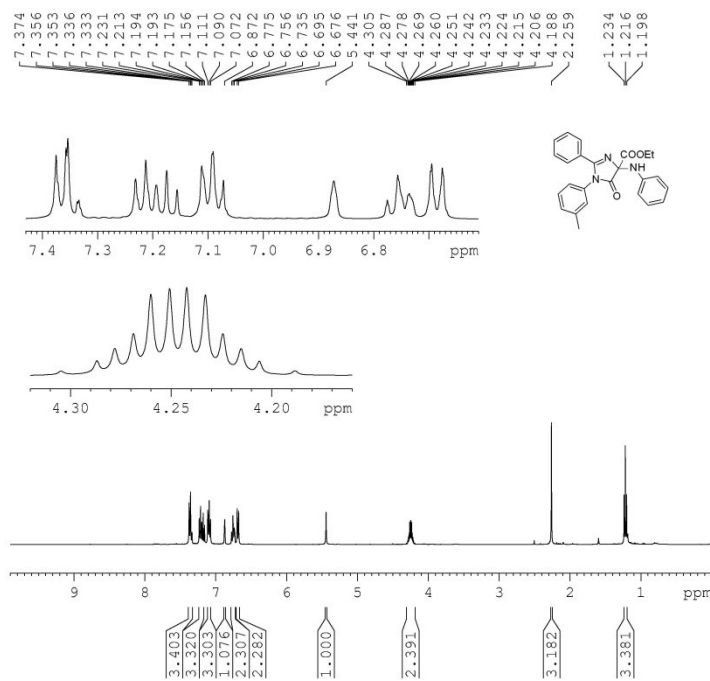


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NAME      2018-11-24 tyut-lx-6c
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PROCNO   1
Date_    20181125
Time     4.21
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631988 sec
RG       185.43
DW       20.800 usec
DE       6.50 usec
TE       294.1 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    100.6228293 MHz
NUC1    13C
P1       9.50 usec
SI      32768
SF      100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

# 4baa

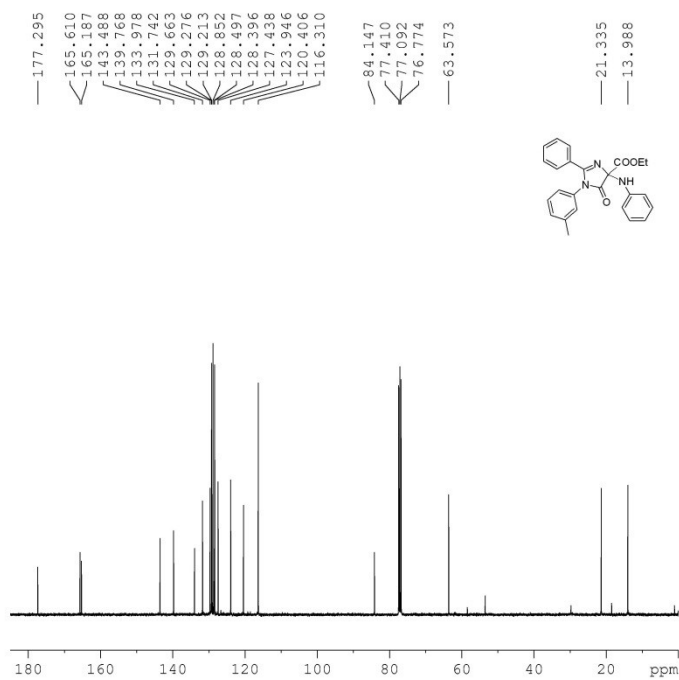


```

NAME      2018-11-14 tyut-lx-
EXPNO     10
PROCNO    1
Date_     20181114
Time      17.37
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        34.32
DW        62.400 usec
DE        6.50 usec
TE        296.0 K
D1        1.00000000 sec
TD0       1
    
```

```

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1      1H
P1       9.70 usec
SI       65536
SF       400.1300445 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



```

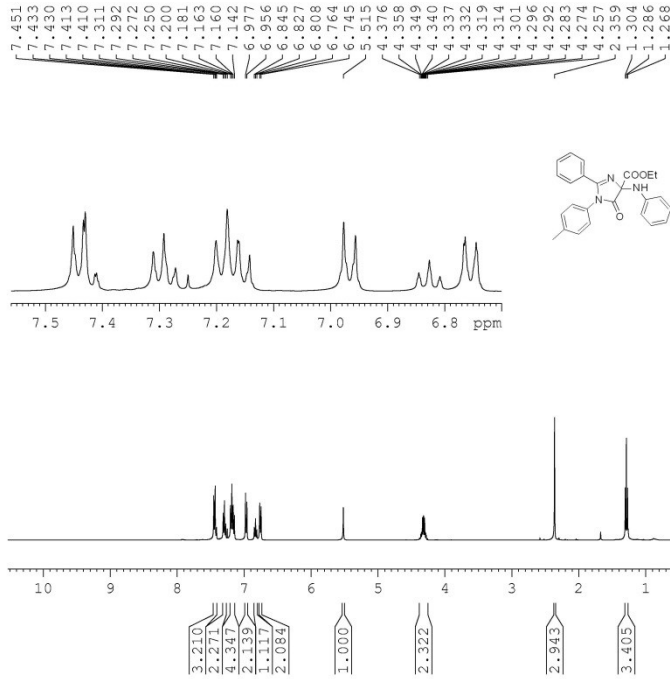
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EXPNO     10
PROCNO    1
Date_     20181116
Time      10.46
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   CDC13
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        296.8 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
    
```

```

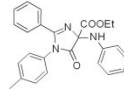
===== CHANNEL f1 =====
SFO1     100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```



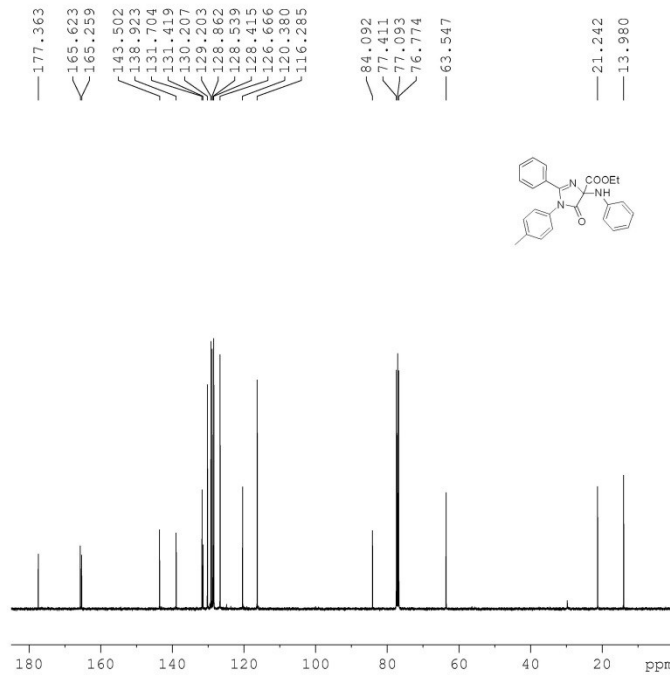
4caa



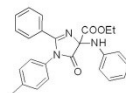
NAME 2018-11-14 tyut-lx-(  
EXPNO 10  
PROCNO 1  
Date\_ 20181114  
Time 17.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 34.32  
DW 62.400 usec  
DE 6.50 usec  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
SF01 400.1324710 MHz  
NUC1 1H  
P1 9.70 usec  
SI 65536  
SF 400.1300140 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

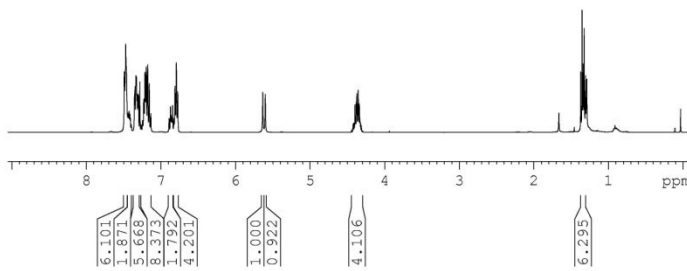
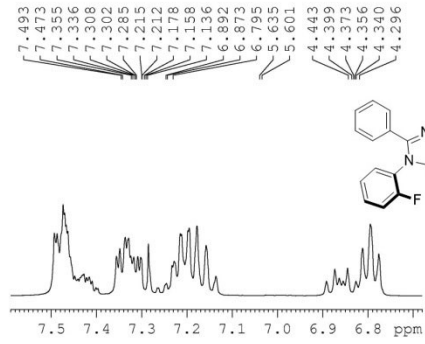


NAME 2018-11-14 tyut-lx-06C  
EXPNO 10  
PROCNO 1  
Date\_ 20181116  
Time 11.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 185.43  
DW 20.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1



===== CHANNEL f1 =====  
SF01 100.6228293 MHz  
NUC1 13C  
P1 9.50 usec  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

4daa

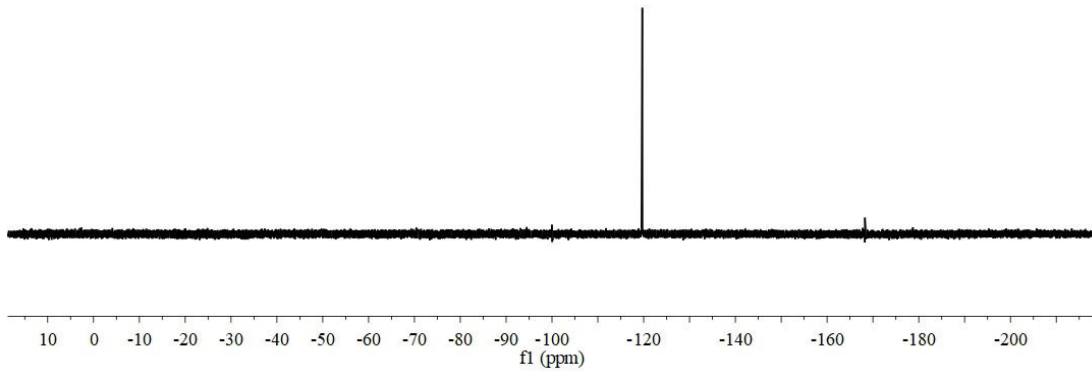
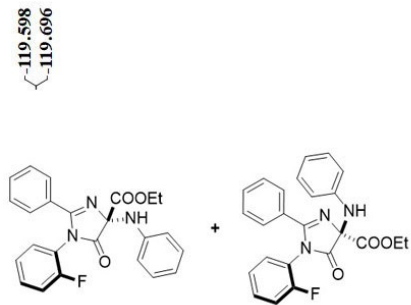
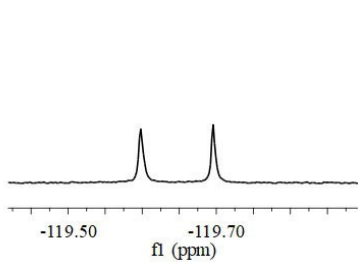


```

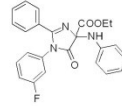
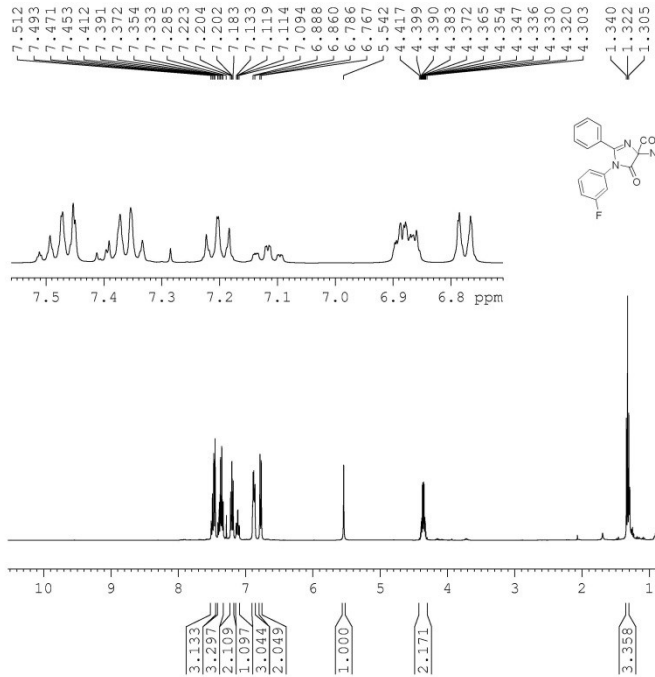
NAME      2018-11-15 tyut-lx-1
EXPNO    10
PROCNO   1
Date_    20181116
Time     2.12
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       34.32
DW       62.400 usec
DE       6.50 usec
TE       296.6 K
D1       1.00000000 sec
TD0      1
    
```

```

===== CHANNEL f1 =====
SF01    400.1324710 MHz
NUC1     1H
P1      9.70 usec
SI      65536
SF      400.1300000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
    
```

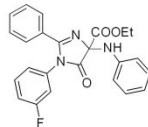
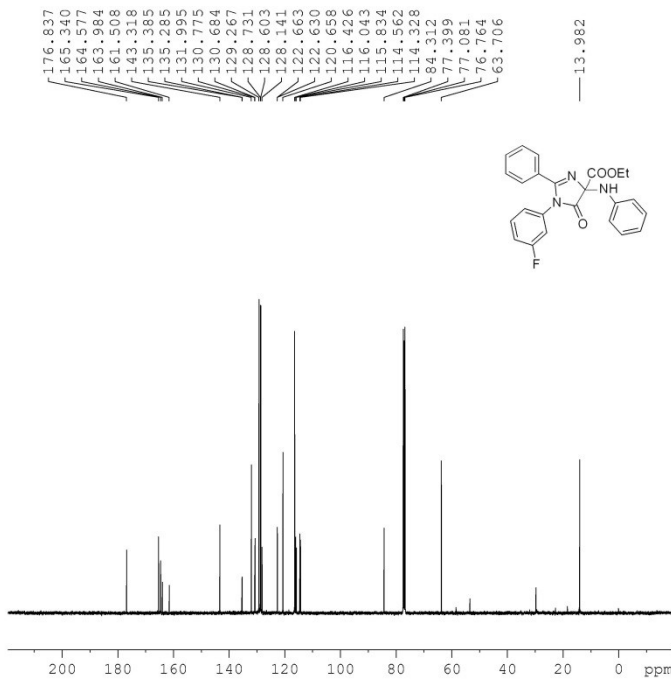


4eaa



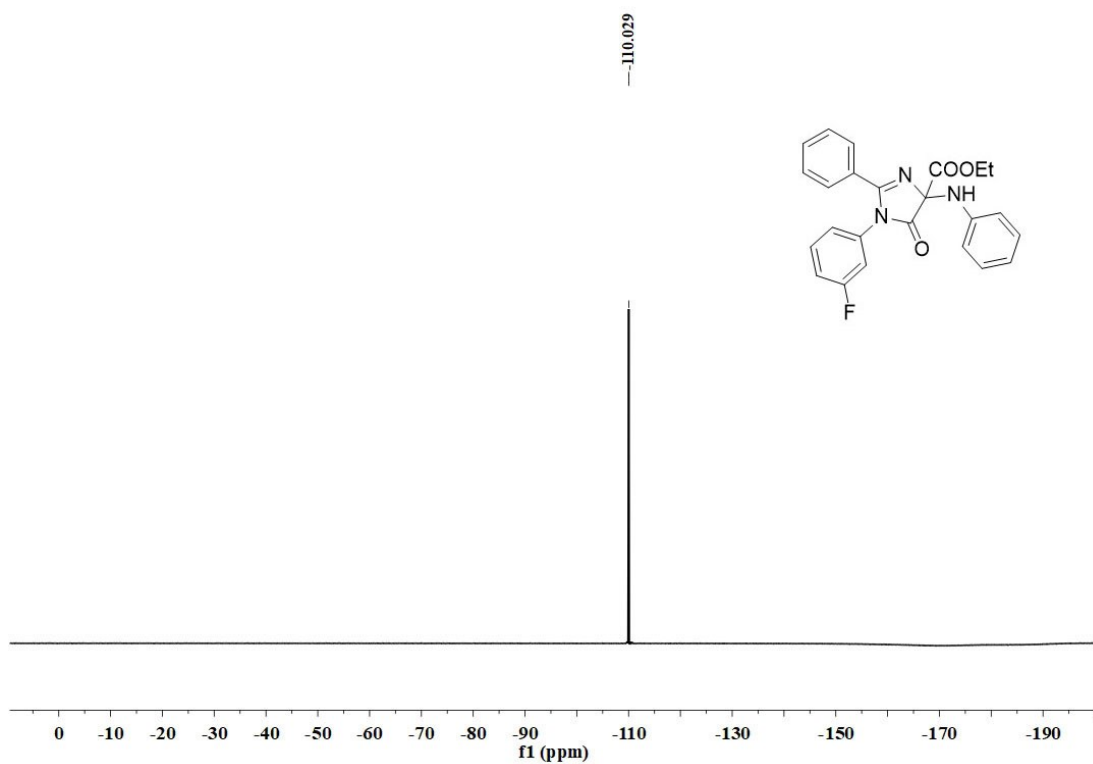
NAME 2018-11-15 tyut-lx  
EXPNO 10  
PROCNO 1  
Date\_ 20181116  
Time 2.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 34.32  
DW 62.400 usec  
DE 6.50 usec  
TE 296.6 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.1324710 MHz  
NUC1 1H  
P1 9.70 usec  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

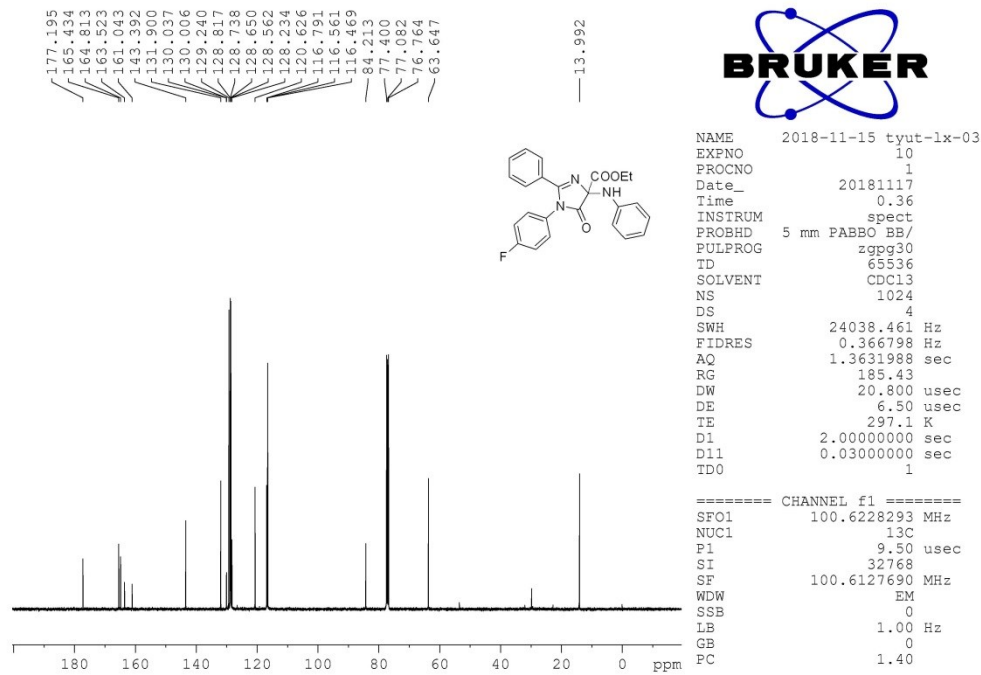
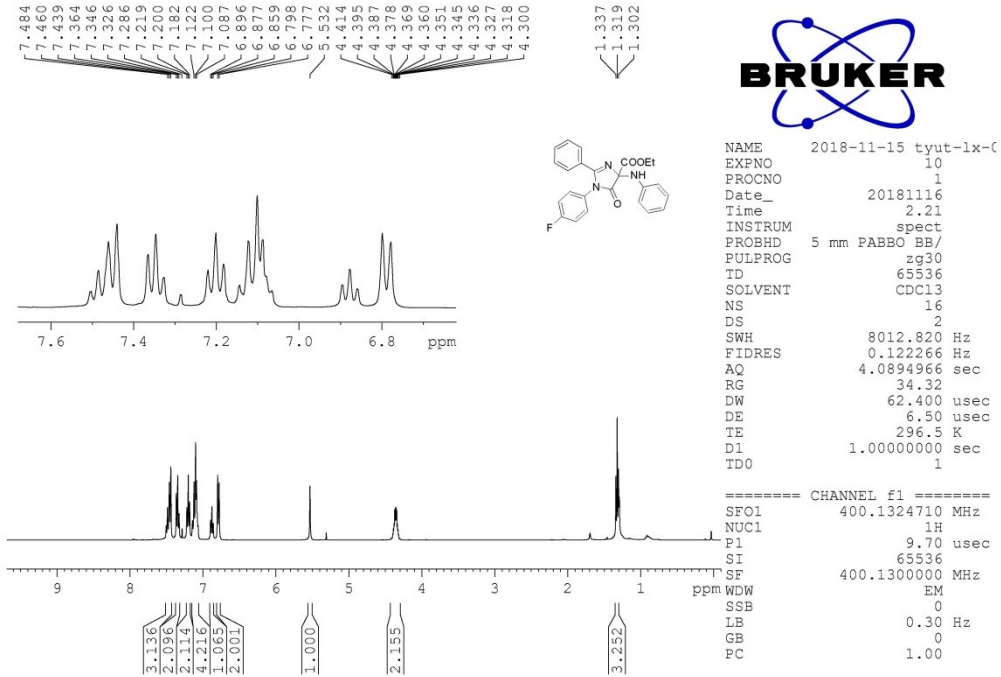


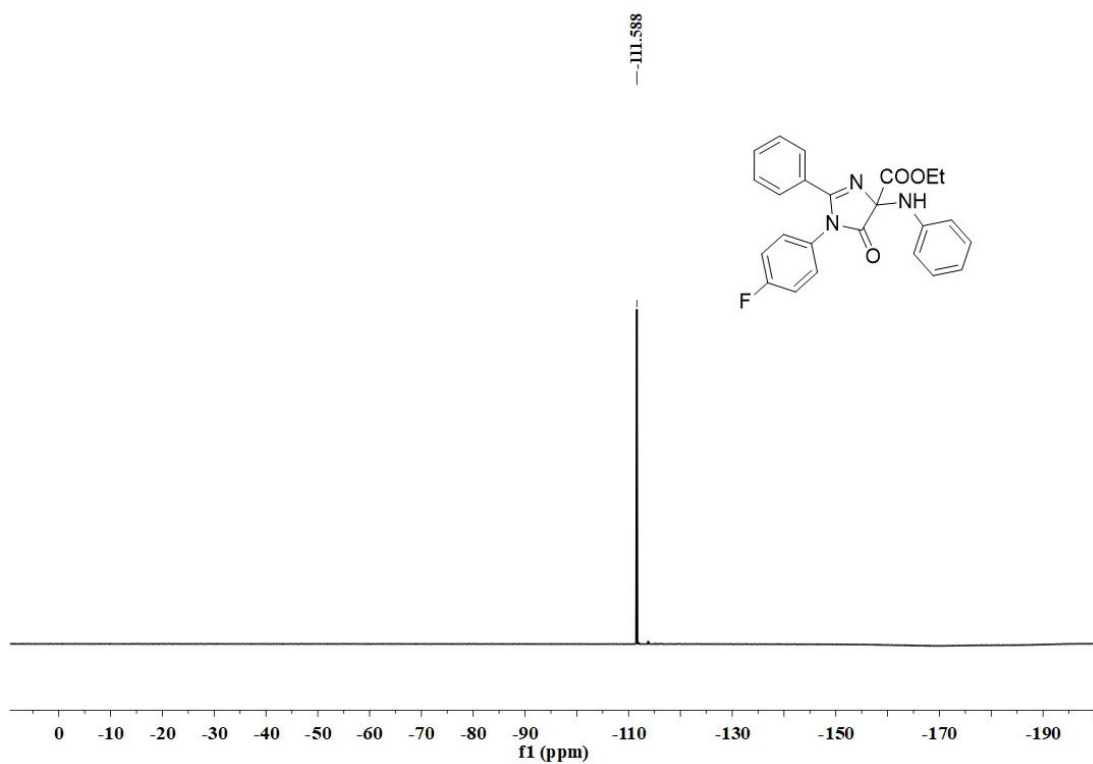
NAME 2018-11-15 tyut-lx-02  
EXPNO 10  
PROCNO 1  
Date\_ 20181116  
Time 23.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 185.43  
DW 20.800 usec  
DE 6.50 usec  
TE 297.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6228293 MHz  
NUC1 13C  
P1 9.50 usec  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

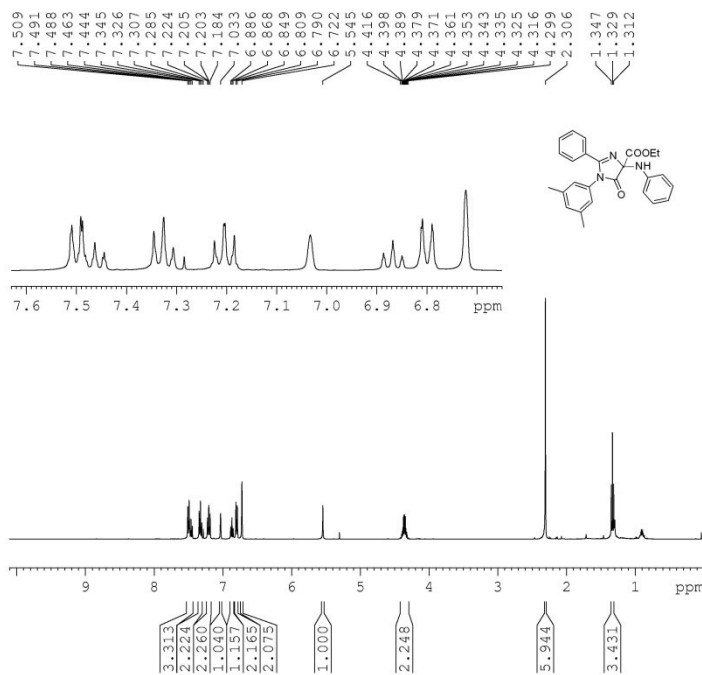


4faa



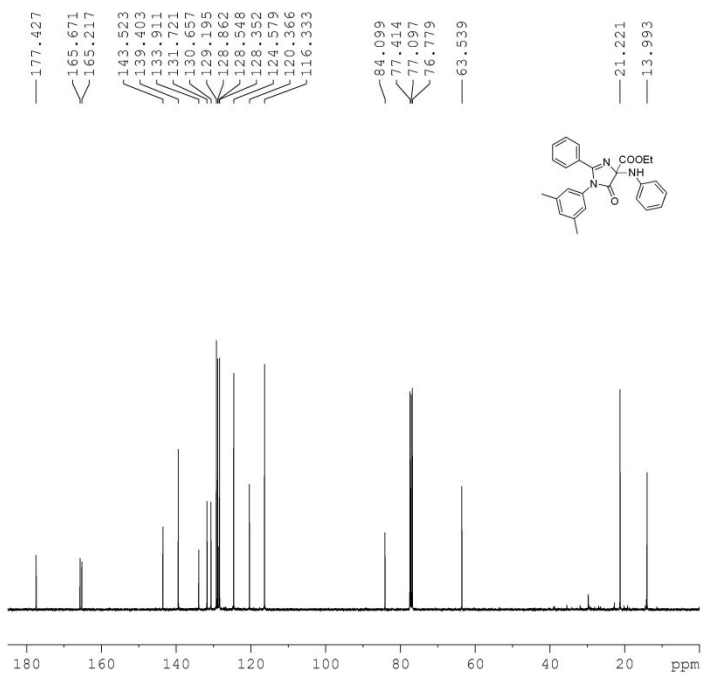


# 4gaa



NAME 2018-11-16 tyut-lx  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20181117  
 Time 6.11  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 34.32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.8 K  
 D1 1.00000000 sec  
 TD0 1

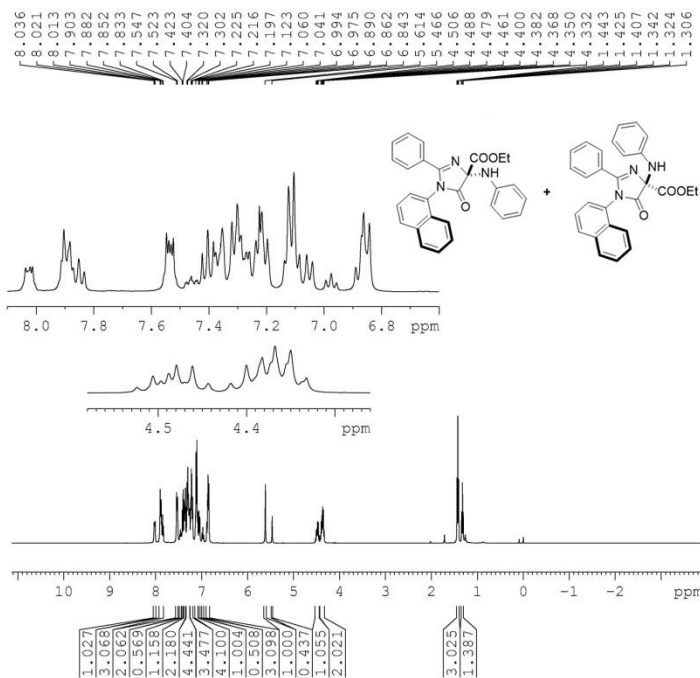
===== CHANNEL f1 =====  
 SF01 400.1324710 MHz  
 NUC1 1H  
 P1 9.70 usec  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME 2018-11-17 tyut-lx-7  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20181117  
 Time 22.24  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 185.43  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 100.6228293 MHz  
 NUC1 13C  
 P1 9.50 usec  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

# 4haa

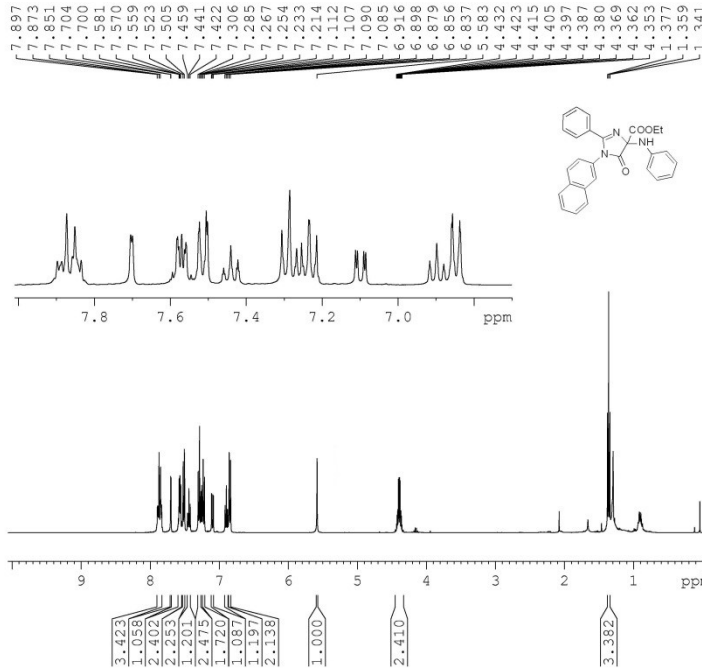


```

NAME      2018-11-23 tyut-1x-0
EXPNO    10
PROCNO   1
Date_    20181123
Time     18.44
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       19.58
DW       62.400 usec
DE       6.50 usec
TE       293.7 K
D1       1.00000000 sec
TD0      1
===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300239 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

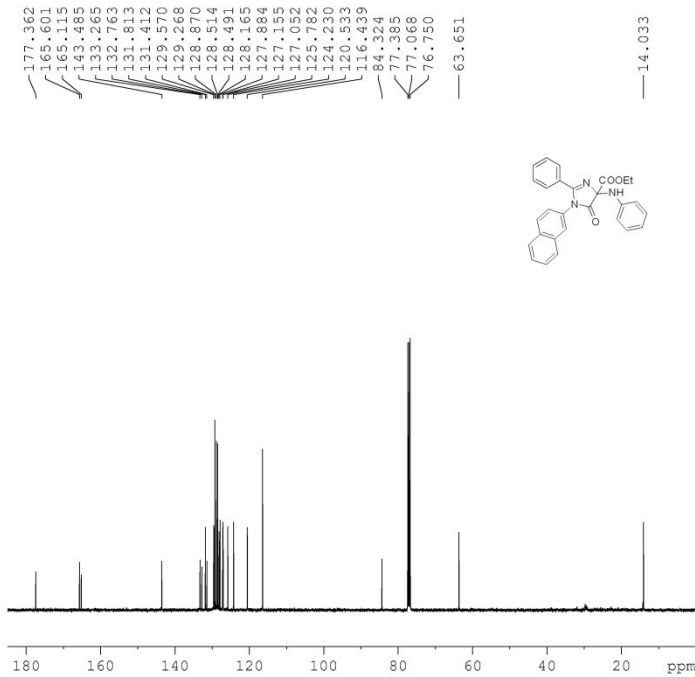


4iaa



NAME 2018-11-16 tyut-lx  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20181117  
 Time 6.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 34.32  
 DW 62.400 use  
 DE 6.50 use  
 TE 295.8 K  
 D1 1.00000000 sec  
 TD0 1

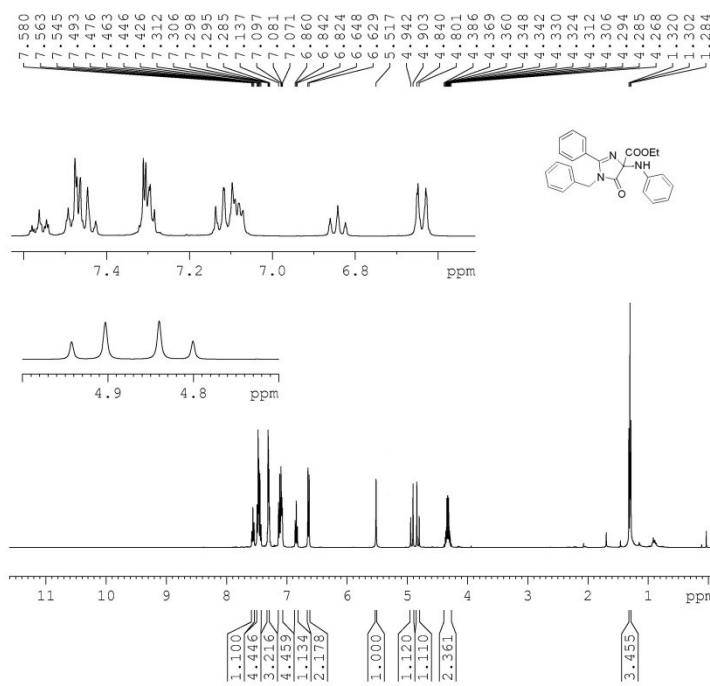
===== CHANNEL f1 =====  
 SF01 400.1324710 MHz  
 NUC1 1H  
 P1 9.70 use  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



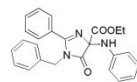
NAME 2018-11-17 tyut-lx-9  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20181117  
 Time 23.25  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 185.43  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 100.6228293 MHz  
 NUC1 13C  
 P1 9.50 usec  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

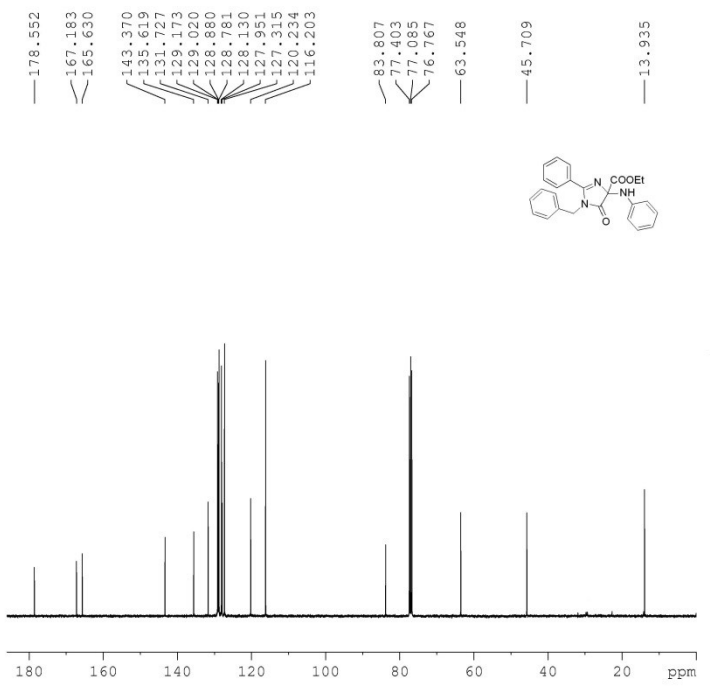
4kaa



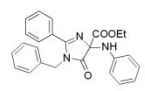
NAME 2018-11-16 tyut-lx-  
EXPNO 10  
PROCNO 1  
Date\_ 20181117  
Time 6.03  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 34.32  
DW 62.400 usec  
DE 6.50 usec  
TE 295.8 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
SFO1 400.1324710 MHz  
NUC1 1H  
P1 9.70 usec  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

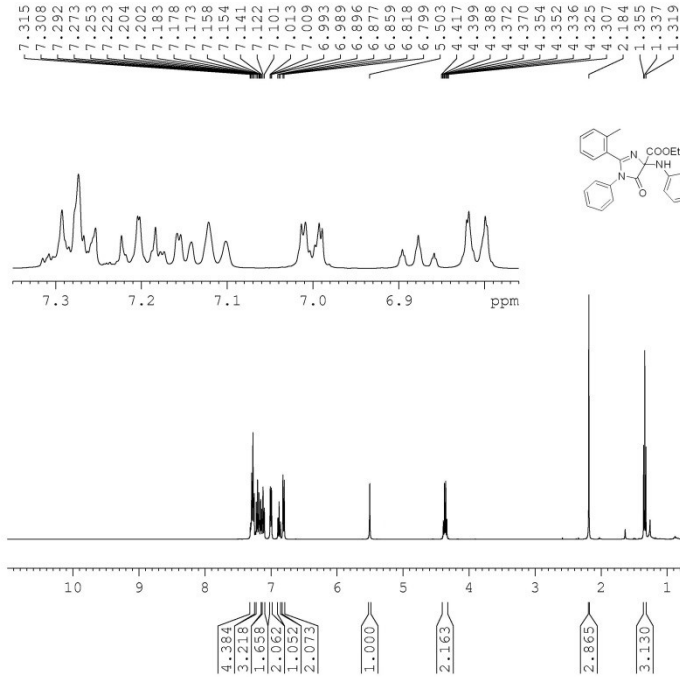


NAME 2018-11-17 tyut-lx-5c  
EXPNO 10  
PROCNO 1  
Date\_ 20181117  
Time 21.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 185.43  
DW 20.800 usec  
DE 6.50 usec  
TE 296.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1



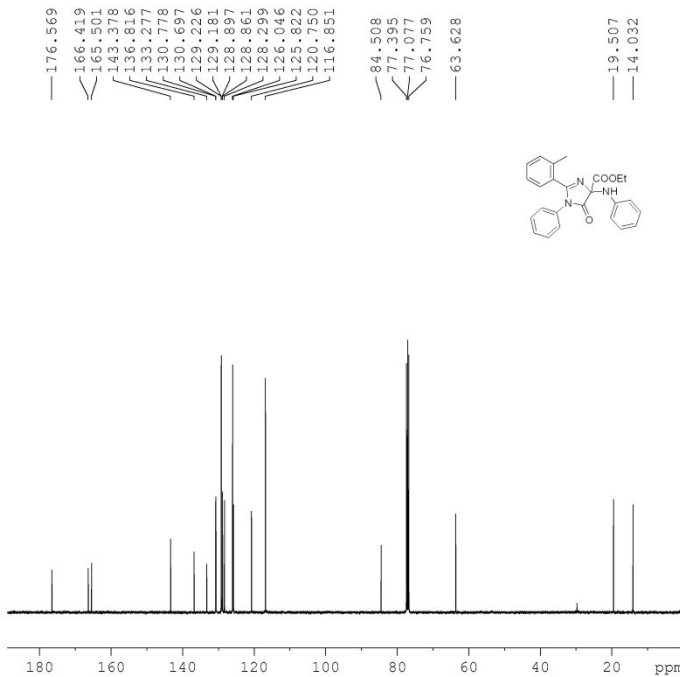
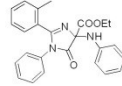
===== CHANNEL f1 =====  
SFO1 100.6228293 MHz  
NUC1 13C  
P1 9.50 usec  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

4laa



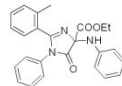
NAME 2018-11-14 tyut-lx  
EXPNO 10  
PROCNO 1  
Date\_ 20181114  
Time 17.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 34.32  
DW 62.400 use  
DE 6.50 use  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 400.1324710 MHz  
NUC1 1H  
P1 9.70 use  
SI 65536  
SF 400.1300128 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

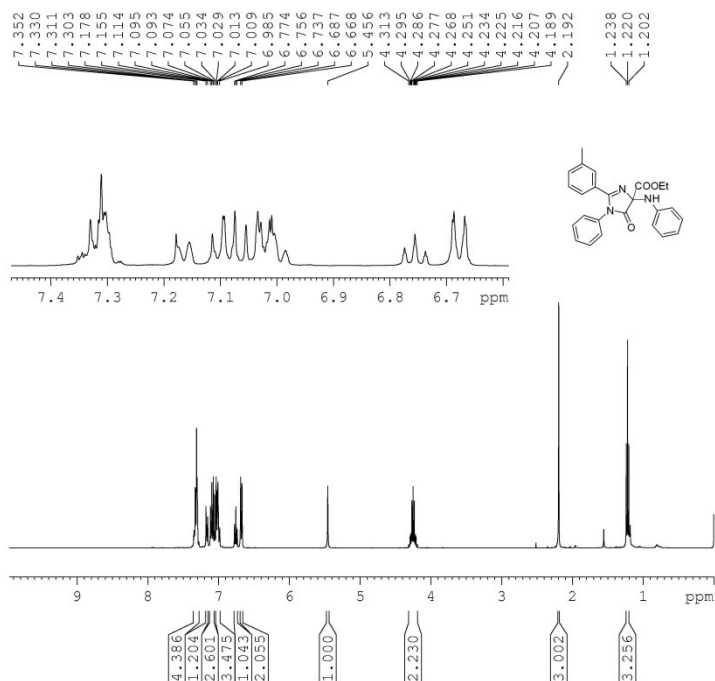


NAME 2018-11-14 tyut-lx-07  
EXPNO 10  
PROCNO 1  
Date\_ 20181116  
Time 12.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 185.43  
DW 20.800 usec  
DE 6.50 usec  
TE 297.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 100.6228293 MHz  
NUC1 13C  
P1 9.50 usec  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

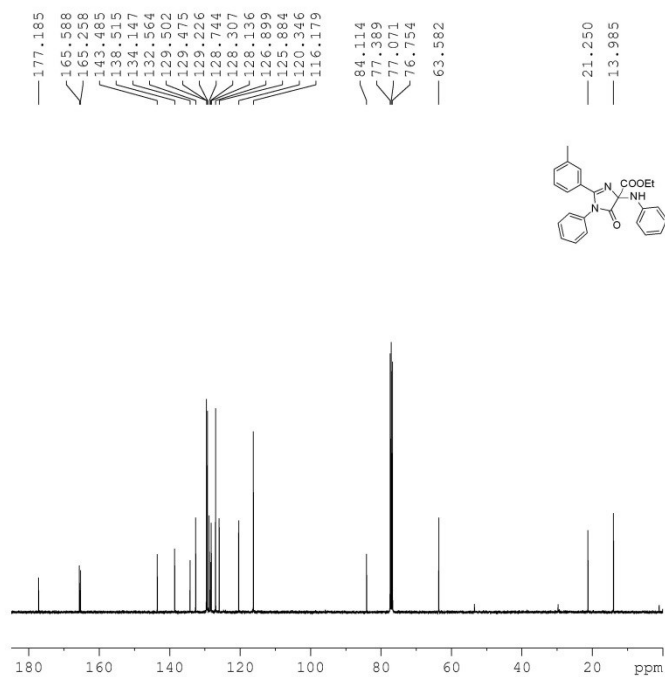


# 4maa



NAME 2018-11-14 tyut-lx-  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20181114  
 Time 17.49  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 34.32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 1.00000000 sec  
 TD0 1

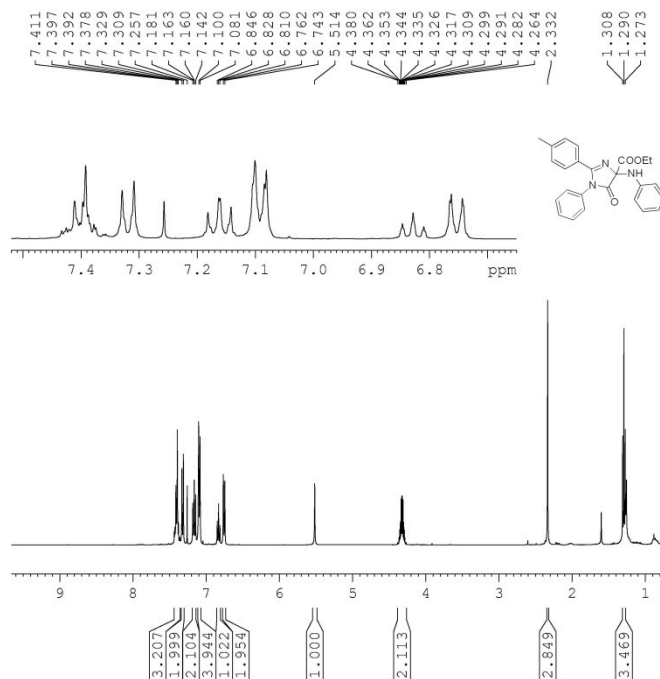
===== CHANNEL f1 =====  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 9.70 usec  
 SI 65536  
 SF 400.1300426 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME 2018-11-14 tyut-lx-080  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20181116  
 Time 13.49  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 185.43  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 9.50 usec  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

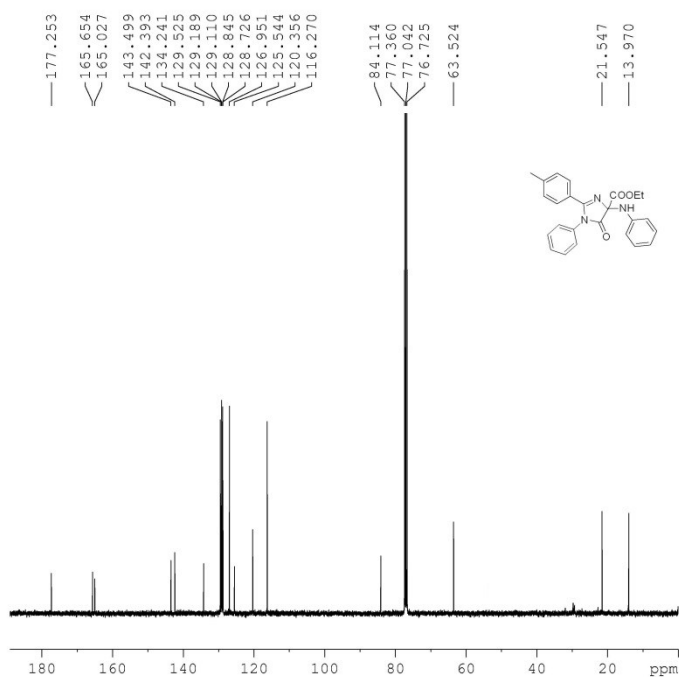
# 4naa



```

NAME      2018-11-14 tyut-lx-
EXPNO     10
PROCNO    1
Date_     20181114
Time      17.53
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        67.58
DW        62.400 usec
DE        6.50 usec
TE        296.1 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300111 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

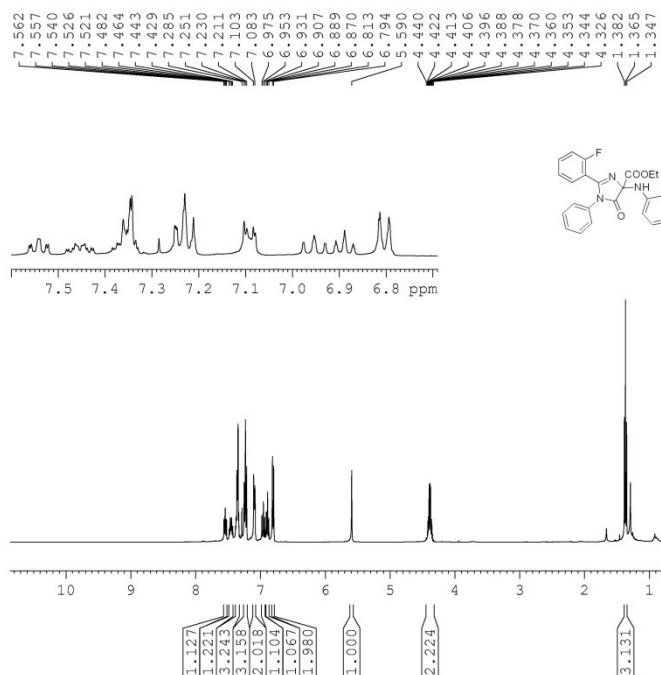


```

NAME      2018-11-14 tyut-lx-09C
EXPNO     10
PROCNO    1
Date_     20181116
Time      14.51
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   CDC13
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        297.2 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

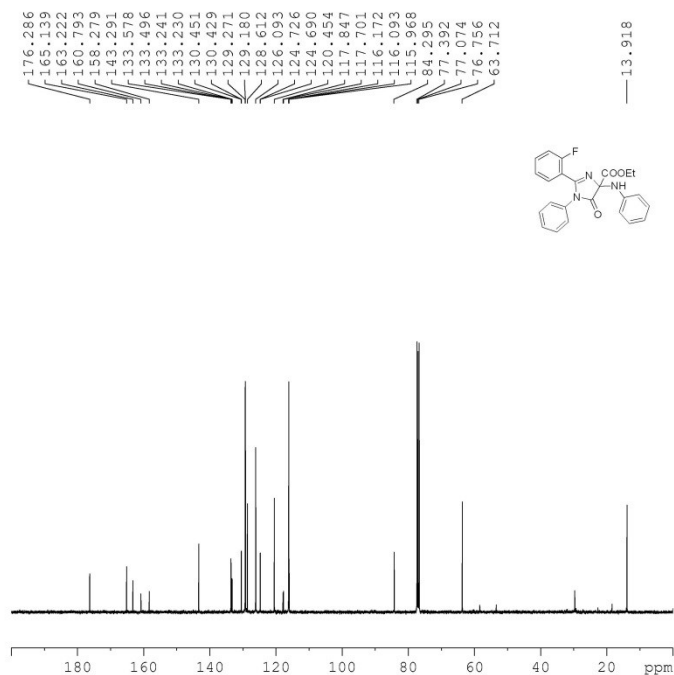
40aa



```

NAME      2018-11-15 tyut-lx-(
EXPNO     10
PROCNO    1
Date_     20181116
Time      2.25
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        34.32
DW        62.400 usec
DE        6.50 usec
TE        296.5 K
D1        1.00000000 sec
TD0       1

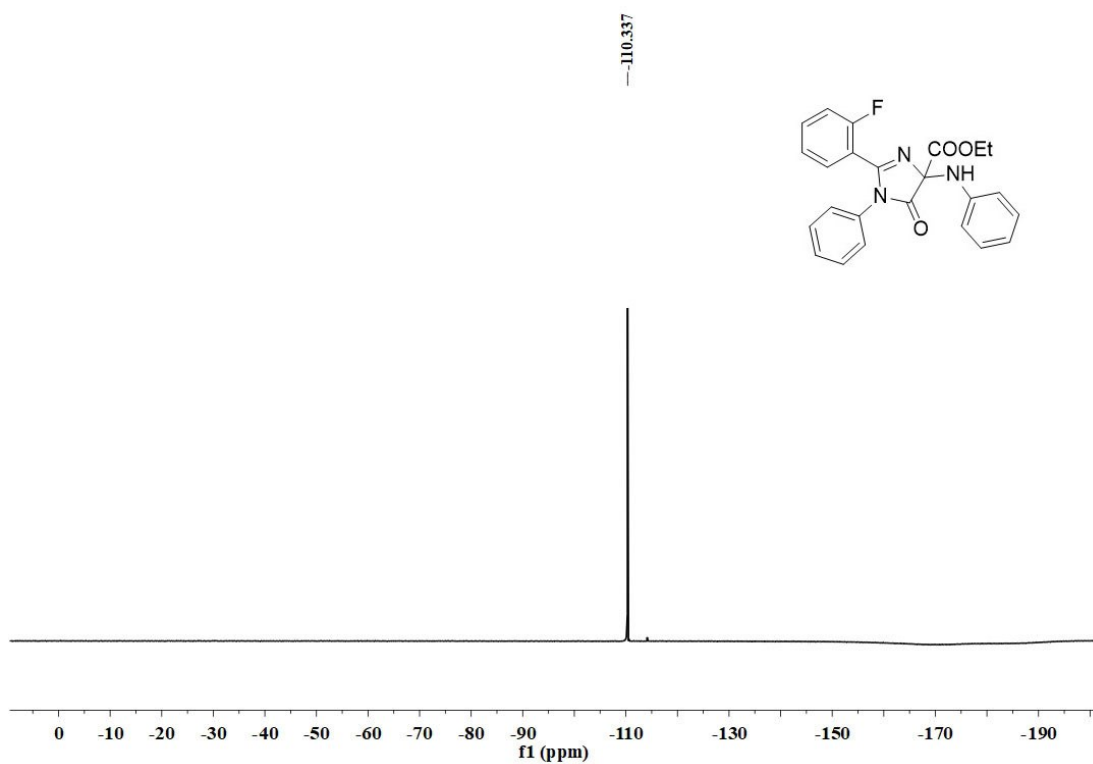
===== CHANNEL f1 =====
SF01     400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



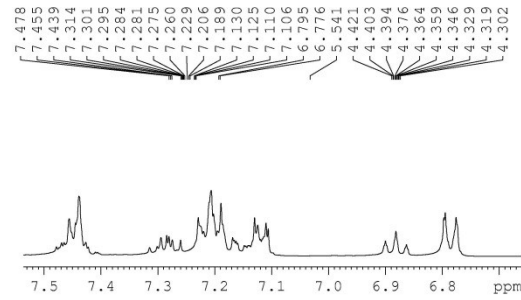
```

NAME      2018-11-15 tyut-lx-04c
EXPNO     10
PROCNO    1
Date_     20181117
Time      1.37
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        297.0 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

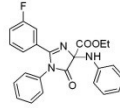
===== CHANNEL f1 =====
SF01     100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```



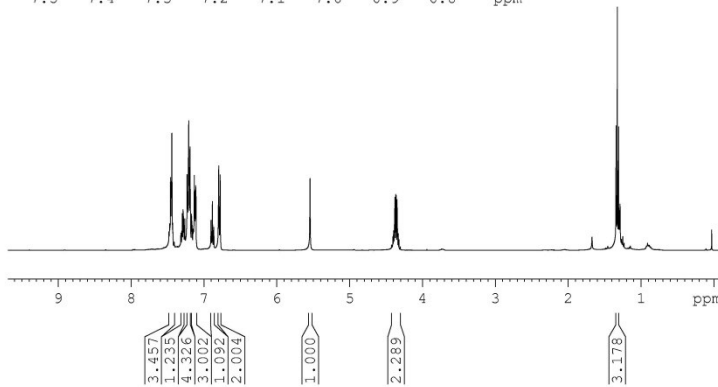
4paa



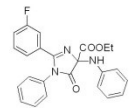
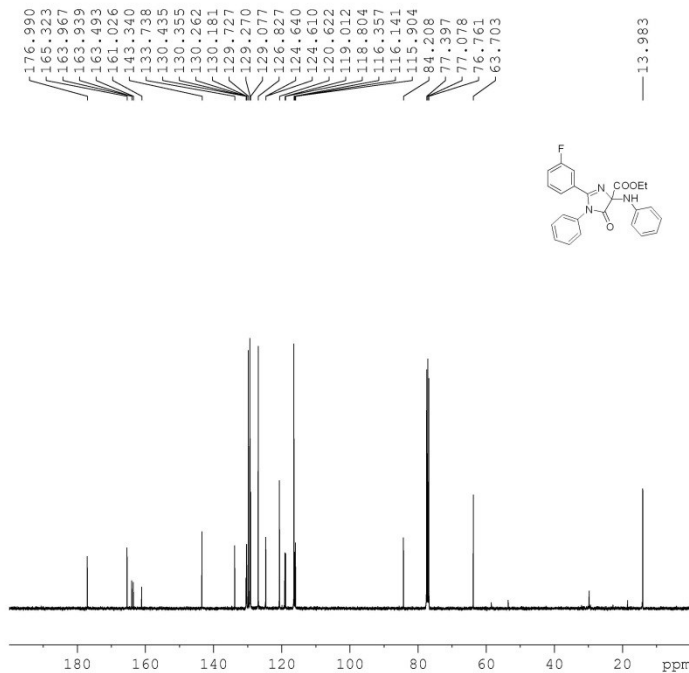
7.478  
7.455  
7.439  
7.414  
7.301  
7.295  
7.284  
7.281  
7.275  
7.260  
7.229  
7.206  
7.189  
7.130  
7.125  
7.110  
7.106  
6.795  
6.776  
6.541  
6.261  
4.503  
4.394  
4.376  
4.364  
4.359  
4.346  
4.329  
4.319  
4.302



NAME 2018-11-15 tyut-lx-  
EXPNO 10  
PROCNO 1  
Date\_ 20181116  
Time 2.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 34.32  
DW 62.400 usec  
DE 6.50 usec  
TE 296.5 K  
D1 1.00000000 sec  
TD0 1



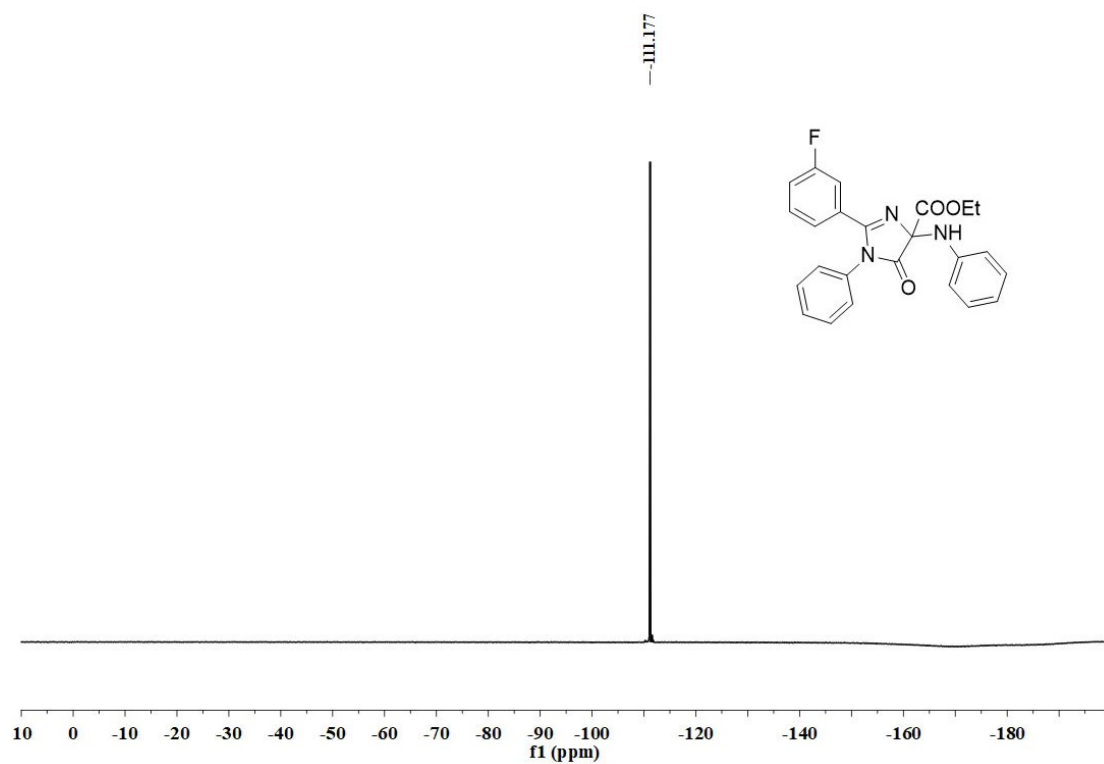
==== CHANNEL f1 =====  
SF01 400.1324710 MHz  
NUC1 1H  
P1 9.70 usec  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



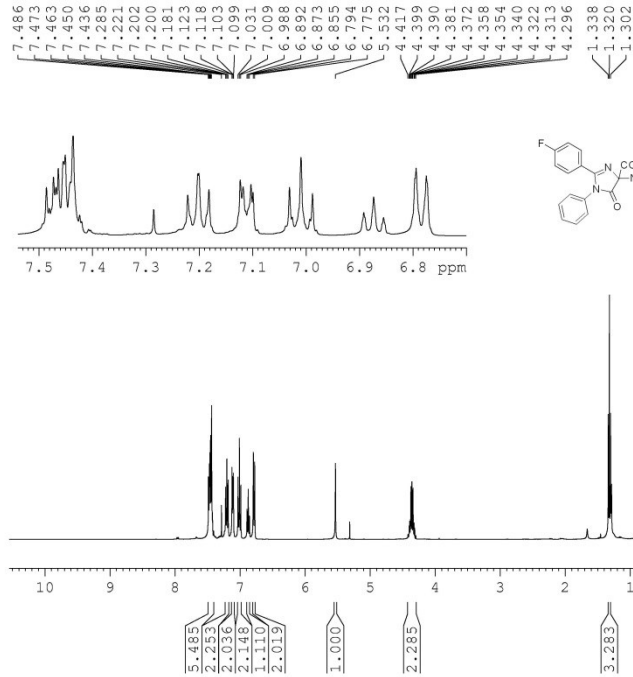
NAME 2018-11-15 tyut-lx-05  
EXPNO 10  
PROCNO 1  
Date\_ 20181117  
Time 2.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 185.43  
DW 20.800 usec  
DE 6.50 usec  
TE 297.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SF01 100.6228293 MHz  
NUC1 13C  
P1 9.50 usec  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





# 4qaa

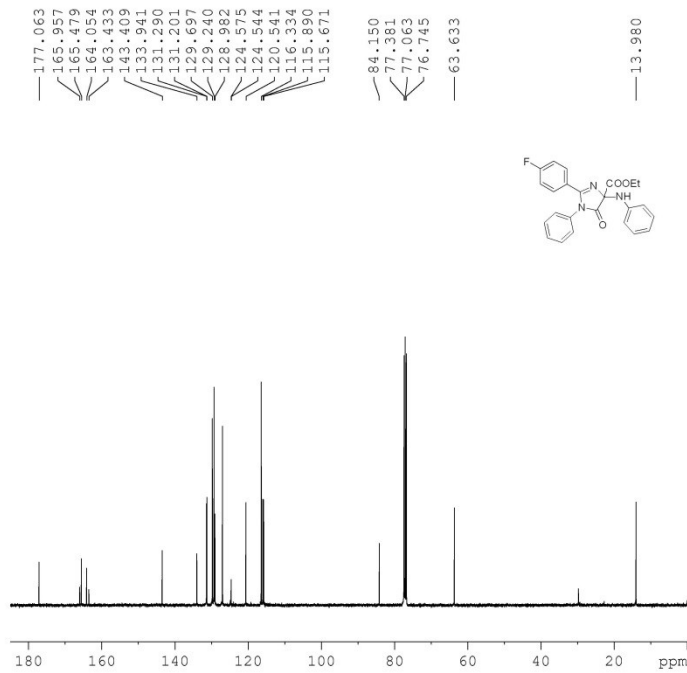


```

NAME      2018-11-15 tyut-lx-
EXPNO     10
PROCNO    1
Date_     20181116
Time      2.33
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        34.32
DW        62.400 usec
DE        6.50 usec
TE        296.5 K
D1        1.00000000 sec
TD0       1
    
```

```

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

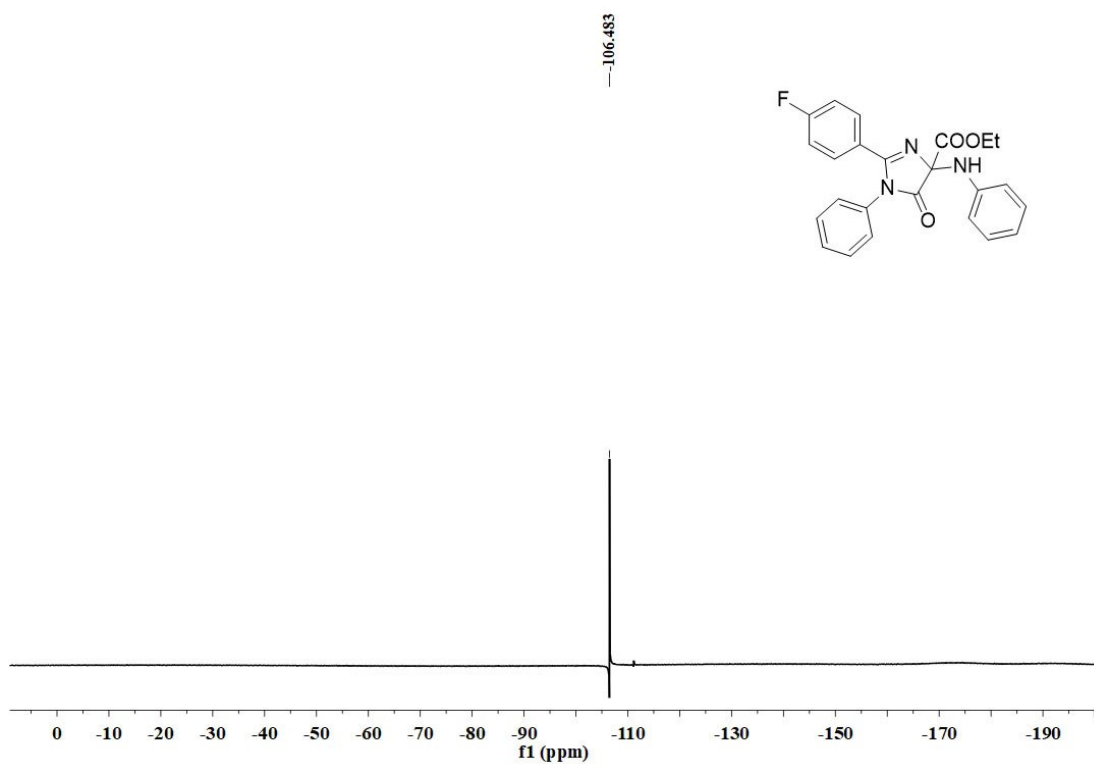


```

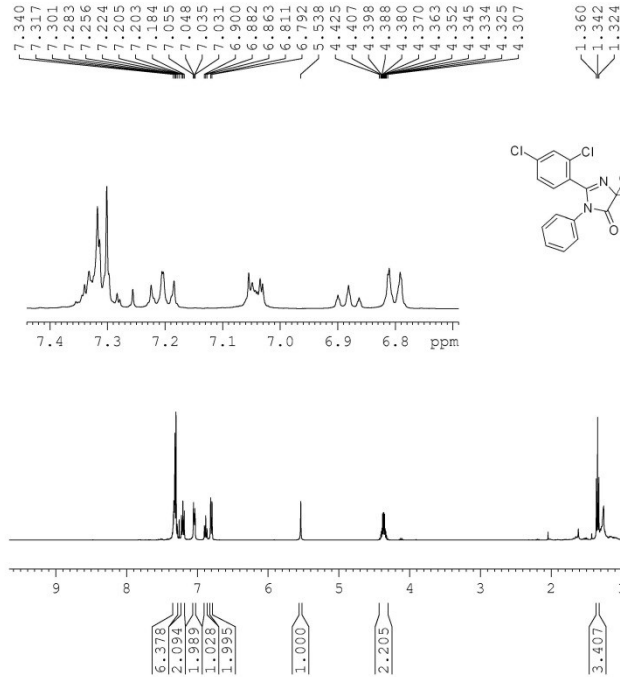
NAME      2018-11-15 tyut-lx-06
EXPNO     10
PROCNO    1
Date_     20181117
Time      3.40
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        296.9 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
    
```

```

===== CHANNEL f1 =====
SFO1     100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```



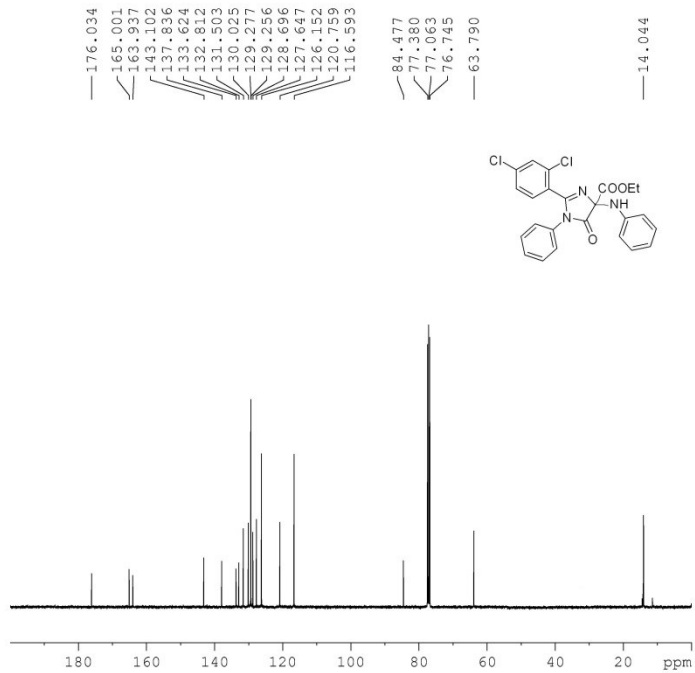
4raa



```

NAME      2018-11-19 tyut-lx-3
EXPNO     10
PROCNO    1
Date_     20181119
Time      20.10
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        34.32
DW        62.400 usec
DE        6.50 usec
TE        294.8 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
SF01     400.1324710 MHz
NUC1      1H
P1        9.70 usec
SI        65536
SF        400.1300115 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

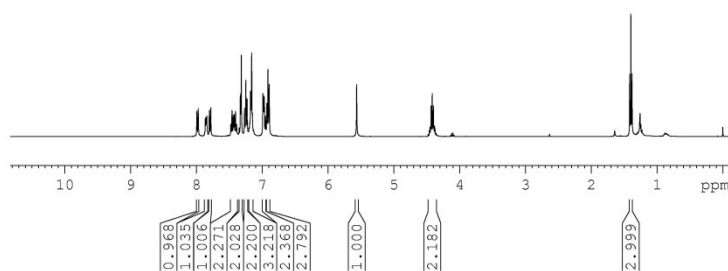
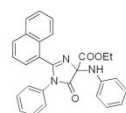
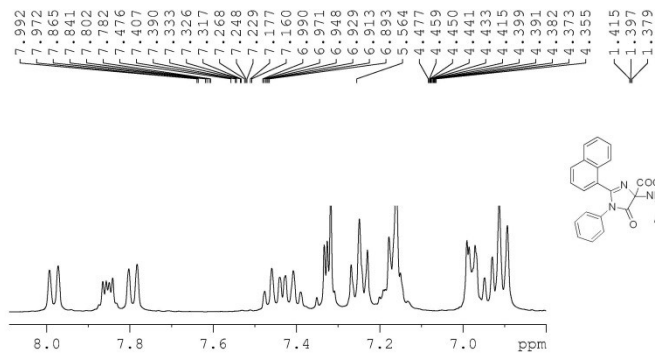


```

NAME      2018-11-19 tyut-lx-3
EXPNO     10
PROCNO    1
Date_     20181121
Time      4.18
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   CDC13
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        295.8 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SF01     100.6228293 MHz
NUC1      13C
P1        9.50 usec
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
    
```

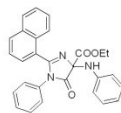
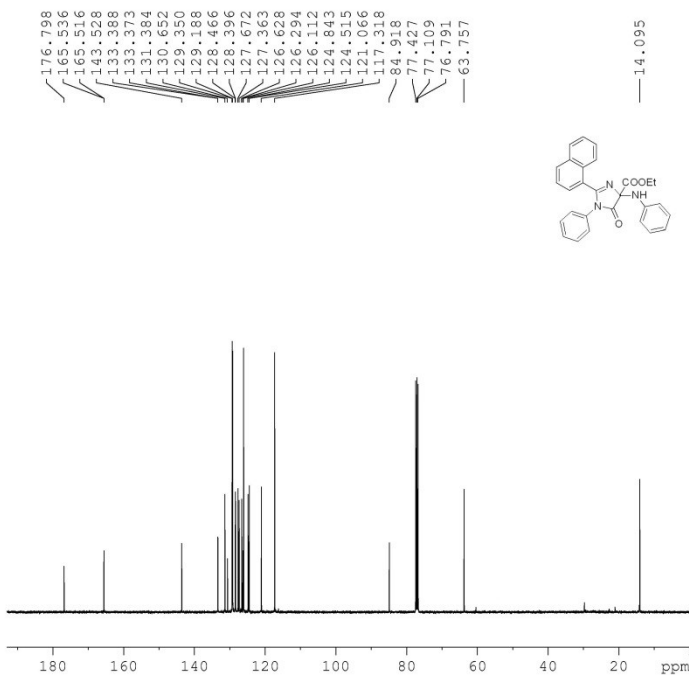
4saa



```

NAME      2018-11-19 tyut-lx
EXPNO    10
PROCNO    1
Date_     20181119
Time      20.02
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         34.32
DW         62.400 use
DE         6.50 use
TE         294.8 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      400.1324710 MHz
NUC1       1H
P1         9.70 use
SI         65536
SF         400.1300172 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

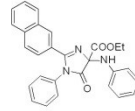
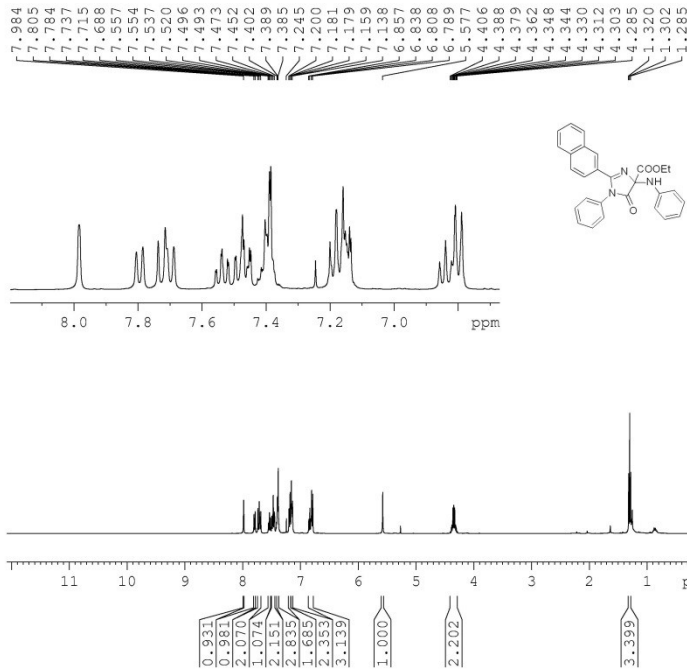


```

NAME      2018-11-19 tyut-lx-
EXPNO    10
PROCNO    1
Date_     20181121
Time      2.16
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         1024
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         185.43
DW         20.800 usec
DE         6.50 usec
TE         295.8 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      100.6228293 MHz
NUC1      13C
P1         9.50 usec
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

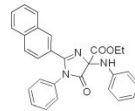
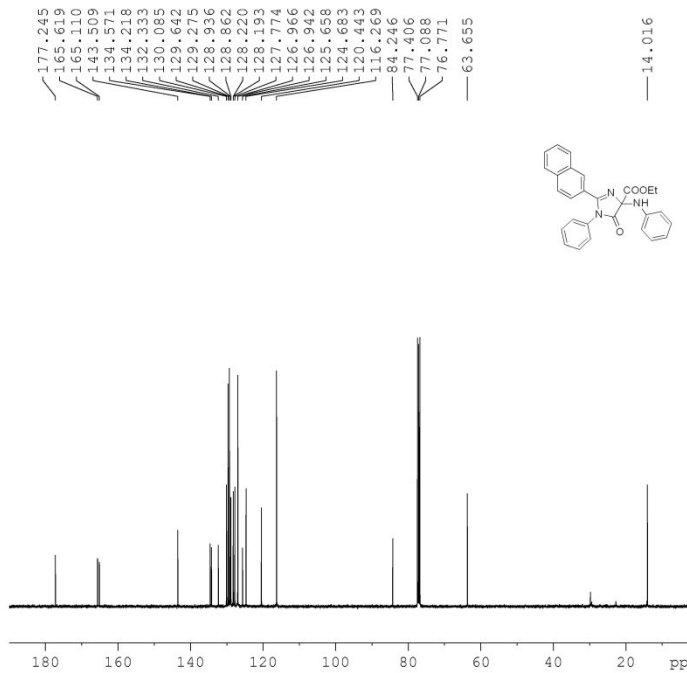
4taa



```

NAME      2018-11-19 tyut-lx-
EXPNO     10
PROCNO    1
Date_     20181119
Time      20.06
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG         34.32
DW        62.400 usec
DE         6.50 usec
TE        294.8 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1      1H
P1        9.70 usec
SI        65536
SF        400.1300159 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

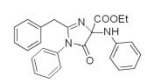
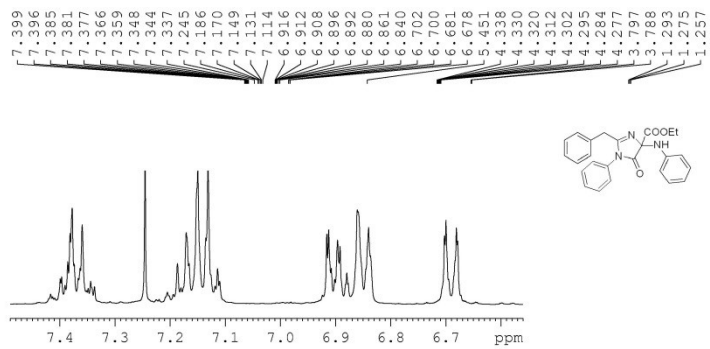


```

NAME      2018-11-19 tyut-lx-
EXPNO     10
PROCNO    1
Date_     20181121
Time      3.17
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG         185.43
DW        20.800 usec
DE         6.50 usec
TE        295.8 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     100.6228293 MHz
NUC1     13C
P1        9.50 usec
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```

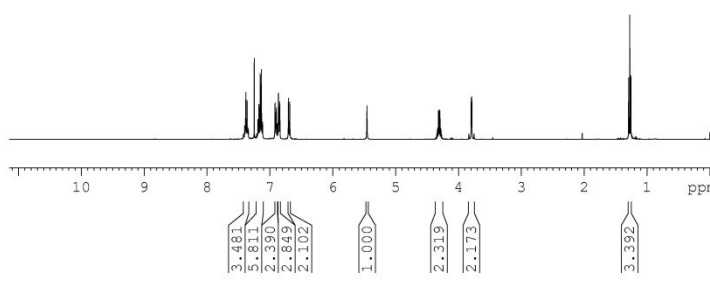
# 4uaa



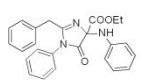
```

NAME      2018-11-23 tyut-lx-(
EXPNO     1
PROCNO    1
Date_     20181123
Time      18.40
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        34.32
DW        62.400 usec
DE        6.50 usec
TE        293.7 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1      400.1324710 MHz
NUC1      1H
P1        9.70 usec
SI        65536
SF        400.1300159 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```



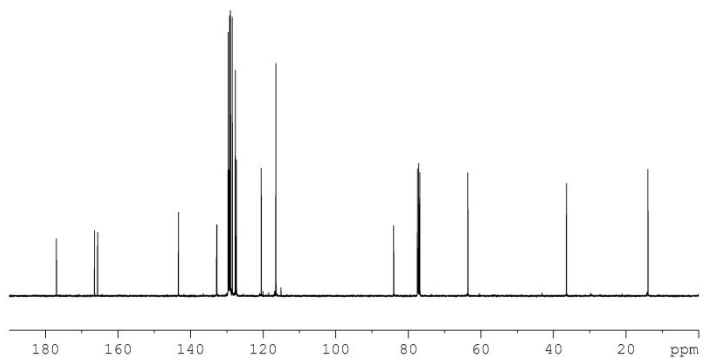
176.888  
 166.457  
 165.624  
 143.341  
 132.820  
 132.735  
 129.627  
 129.459  
 129.239  
 129.006  
 128.503  
 127.575  
 127.266  
 120.505  
 116.477  
 84.028  
 77.455  
 77.137  
 76.819  
 63.560  
 36.414  
 13.937



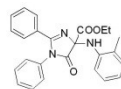
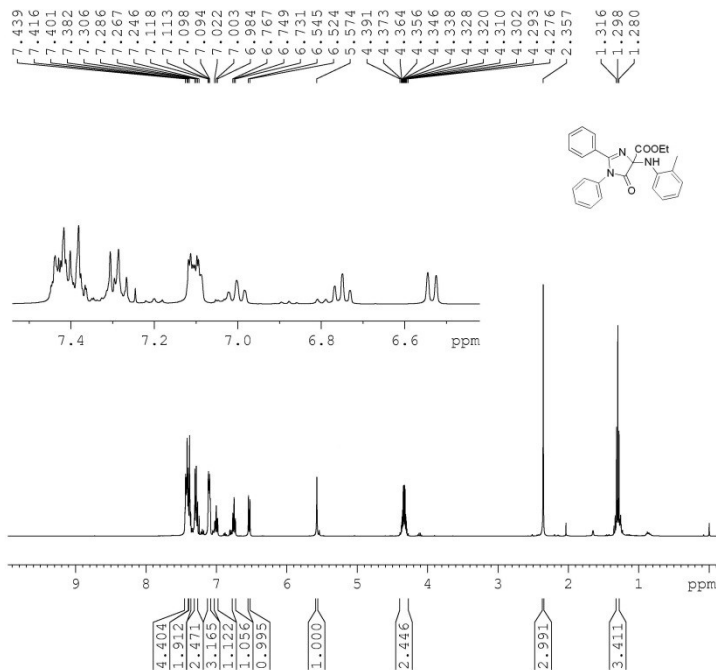
```

NAME      2018-11-24 tyut-lx-
EXPNO     1
PROCNO    1
Date_     20181125
Time      5.26
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        294.1 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1      100.6228293 MHz
NUC1      13C
P1        9.50 usec
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```



# 4aba

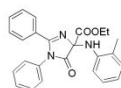
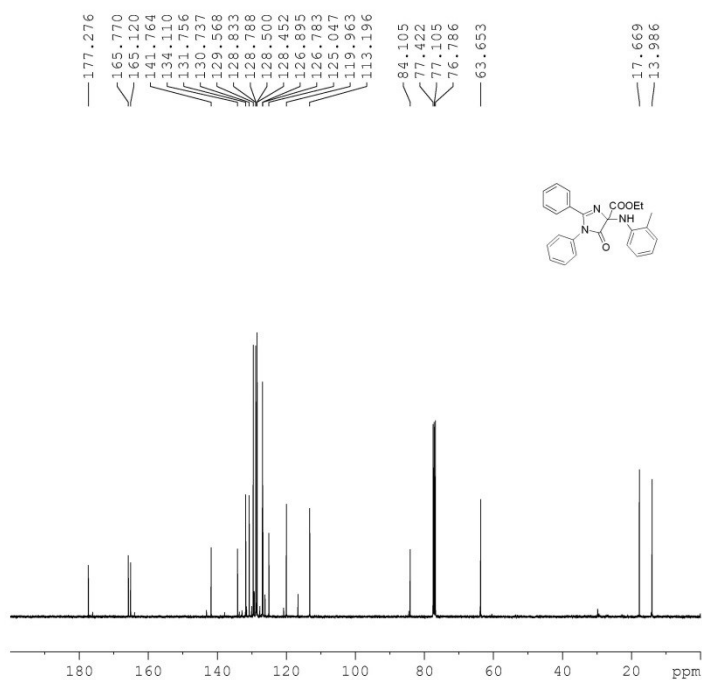


```

NAME      2018-11-19 tyut-lx-!
EXPNO    10
PROCNO   1
Date_    20181119
Time     20.18
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       34.32
DW       62.400 usec
DE       6.50 usec
TE       294.8 K
D1       1.00000000 sec
TD0      1
    
```

```

===== CHANNEL f1 =====
SF01    400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300155 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



```

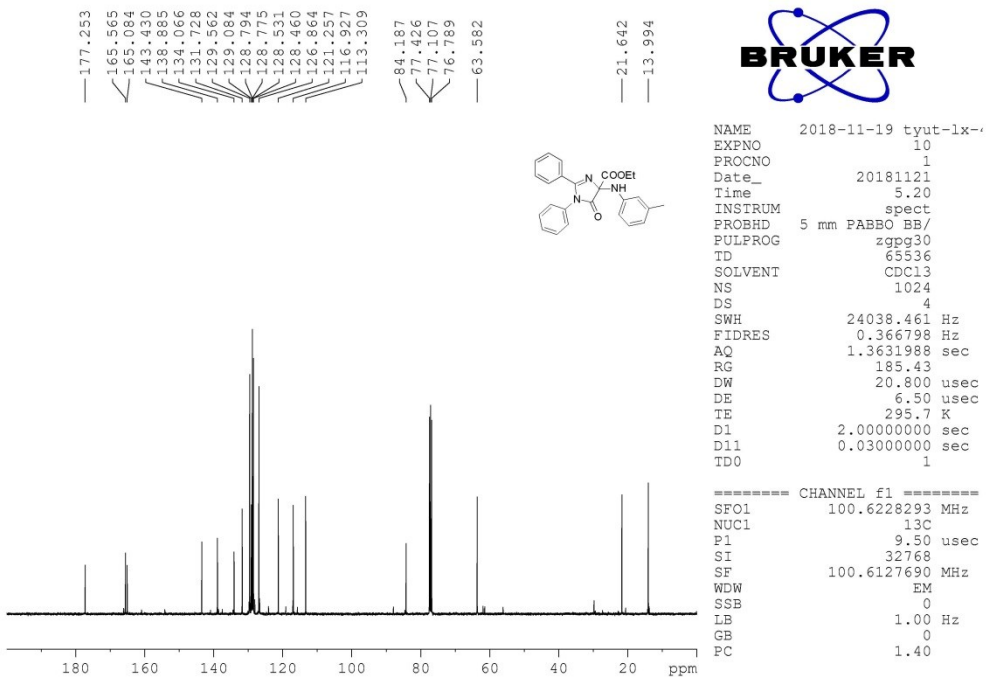
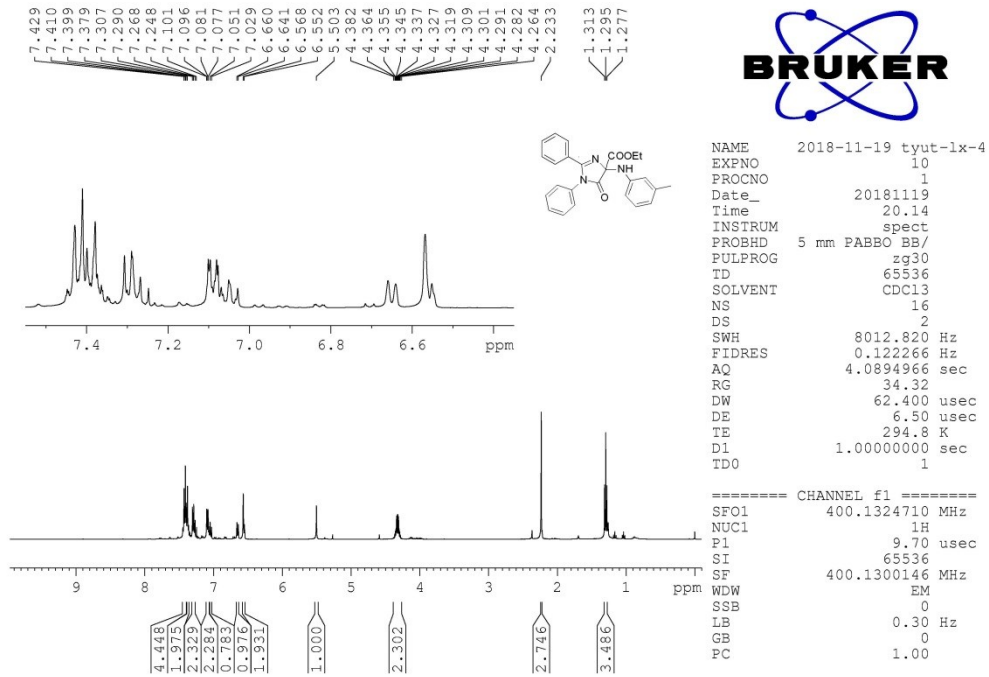
NAME      2018-11-19 tyut-lx-
EXPNO    10
PROCNO   1
Date_    20181121
Time     6.21
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631988 sec
RG       185.43
DW       20.800 usec
DE       6.50 usec
TE       295.7 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
    
```

```

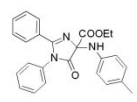
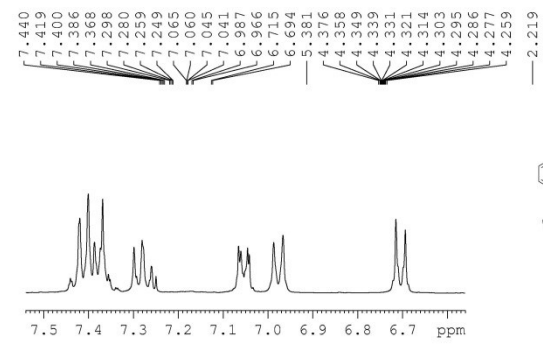
===== CHANNEL f1 =====
SF01    100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```



4aca

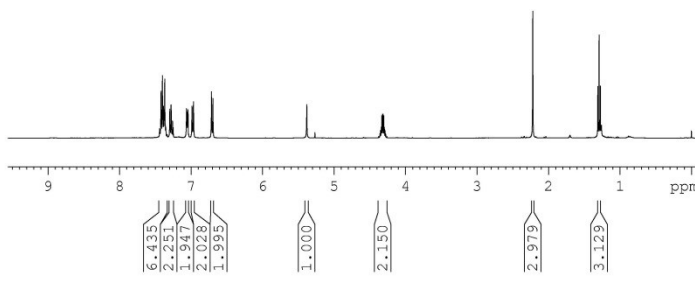


4ada



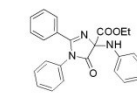
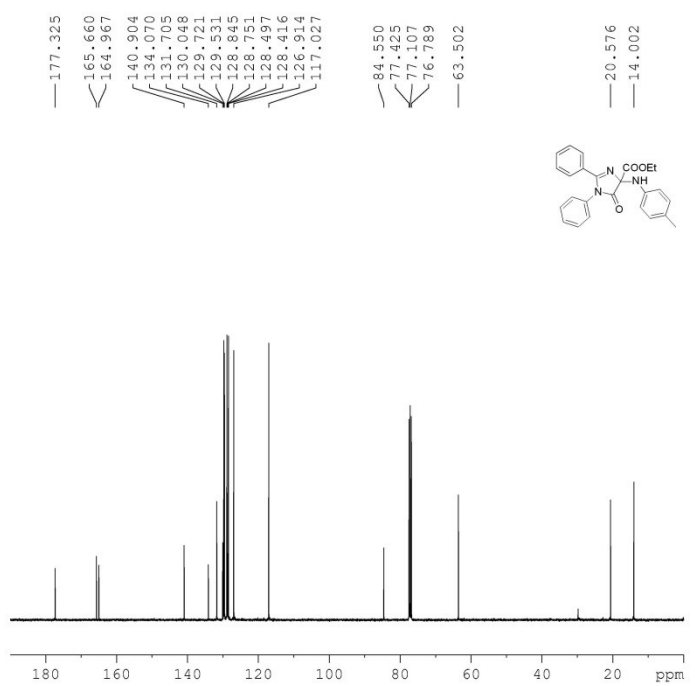
```

NAME      2018-11-19 tyut-1x-6
EXPNO    10
PROCNO   1
Date_    20181119
Time     20.22
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       34.32
DW       62.400 usec
DE       6.50 usec
TE       294.8 K
D1       1.00000000 sec
TD0      1
    
```



```

===== CHANNEL f1 =====
SFO1    400.1324710 MHz
NUC1    1H
P1      9.70 usec
SI      65536
SF      400.1300142 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
    
```



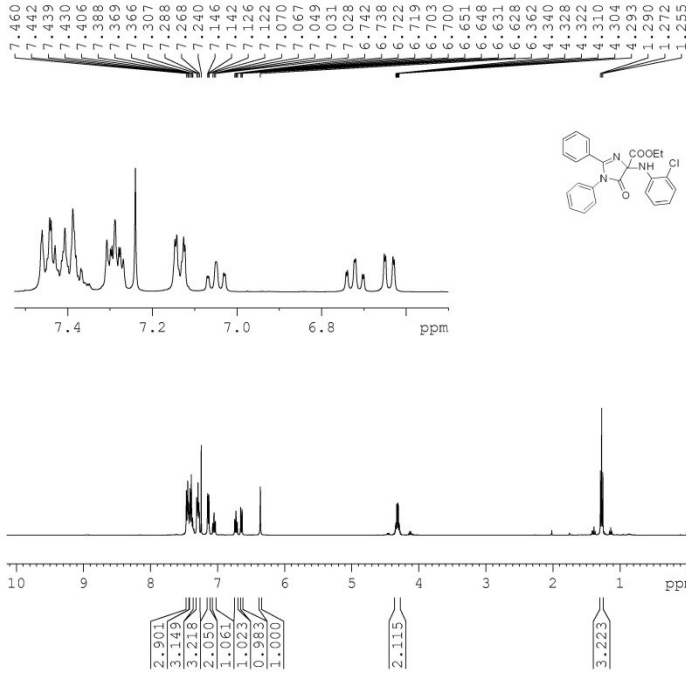
```

NAME      2018-11-19 tyut-1x-6
EXPNO    10
PROCNO   1
Date_    20181121
Time     7.22
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631988 sec
RG       185.43
DW       20.800 usec
DE       6.50 usec
TE       295.6 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
    
```

```

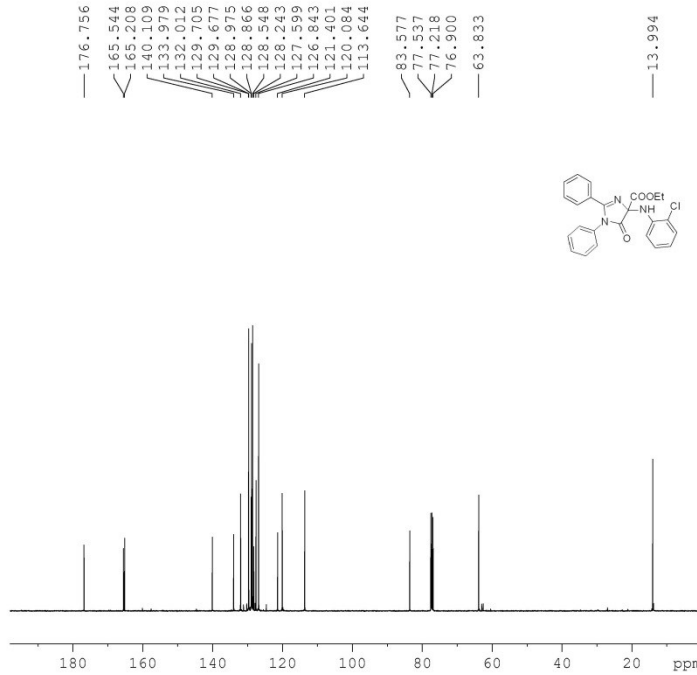
===== CHANNEL f1 =====
SFO1    100.6228293 MHz
NUC1    13C
P1      9.50 usec
SI      32768
SF      100.6127690 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
    
```

4aea



NAME 2018-12-06 tyut-lx-  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20181206  
 Time 22.42  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 14.45  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.2 K  
 D1 1.00000000 sec  
 TD0 1

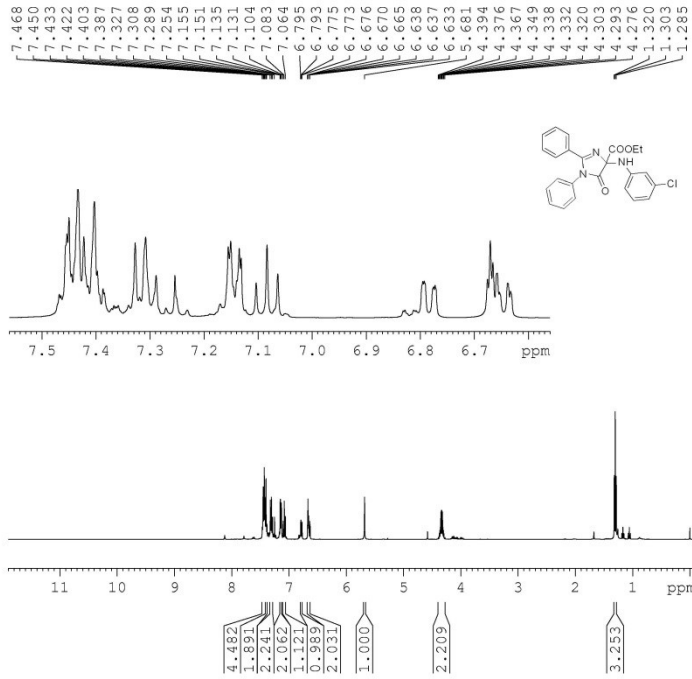
===== CHANNEL f1 =====  
 SF01 400.1324710 MHz  
 NUC1 1H  
 P1 9.70 usec  
 SI 65536  
 SF 400.1300175 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME 2018-12-07 tyut-lx-1  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20181207  
 Time 17.23  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 185.43  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

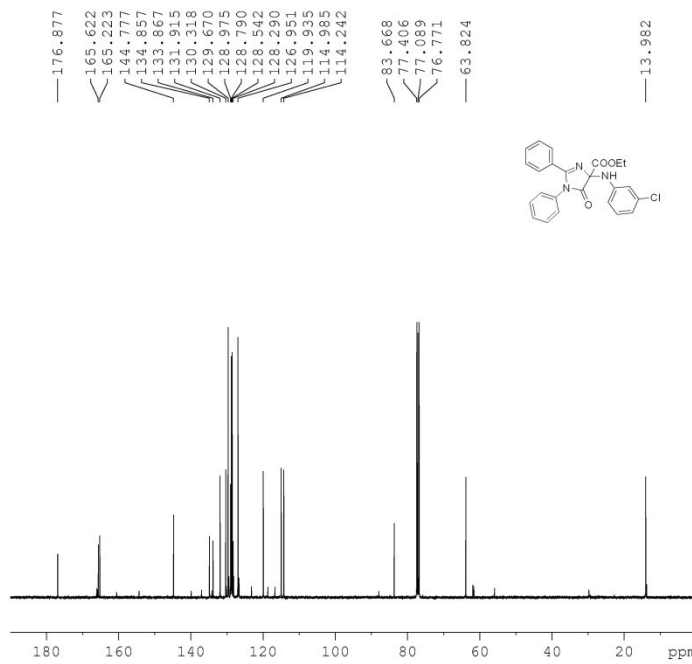
===== CHANNEL f1 =====  
 SF01 100.6228293 MHz  
 NUC1 13C  
 P1 9.50 usec  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4afa



NAME 2018-11-19 tyut-lx-  
EXPNO 10  
PROCNO 1  
Date\_ 20181119  
Time 20.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 34.32  
DW 62.400 usec  
DE 6.50 usec  
TE 294.8 K  
D1 1.00000000 sec  
TD0 1

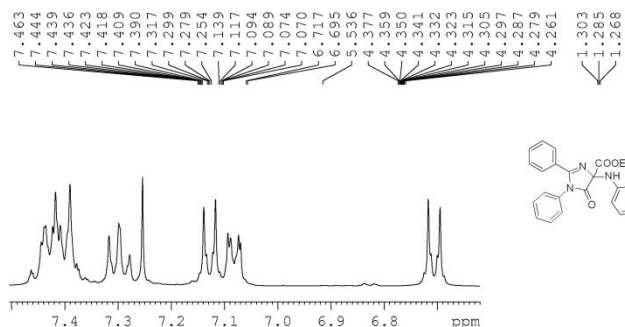
===== CHANNEL f1 =====  
SF01 400.1324710 MHz  
NUC1 1H  
P1 9.70 usec  
SI 65536  
SF 400.1300123 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



NAME 2018-11-19 tyut-lx-1  
EXPNO 10  
PROCNO 1  
Date\_ 20181121  
Time 9.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 185.43  
DW 20.800 usec  
DE 6.50 usec  
TE 295.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

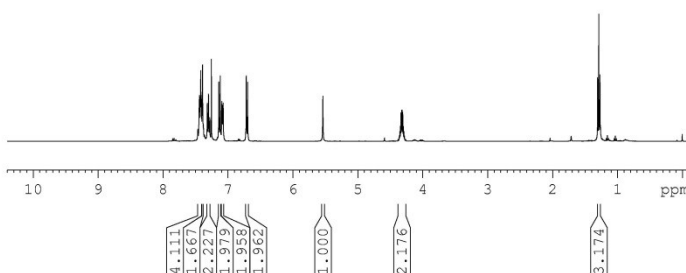
===== CHANNEL f1 =====  
SF01 100.6228293 MHz  
NUC1 13C  
P1 9.50 usec  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# 4aga



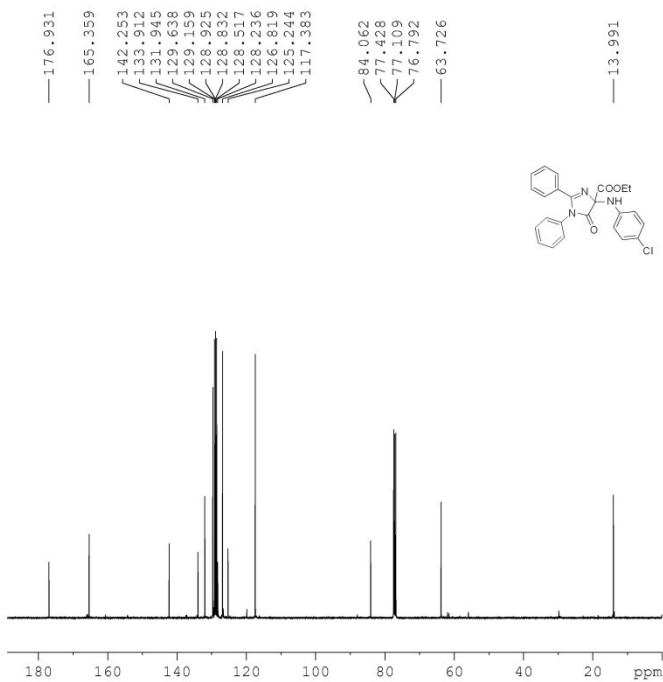
```

NAME      2018-11-20 tyut-lx-01
EXPNO     10
PROCNO    1
Date_     20181120
Time      20.47
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        34.32
DW        62.400 usec
DE        6.50 usec
TE        294.7 K
D1        1.00000000 sec
TD0       1
  
```



```

===== CHANNEL f1 =====
SF01     400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300125 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



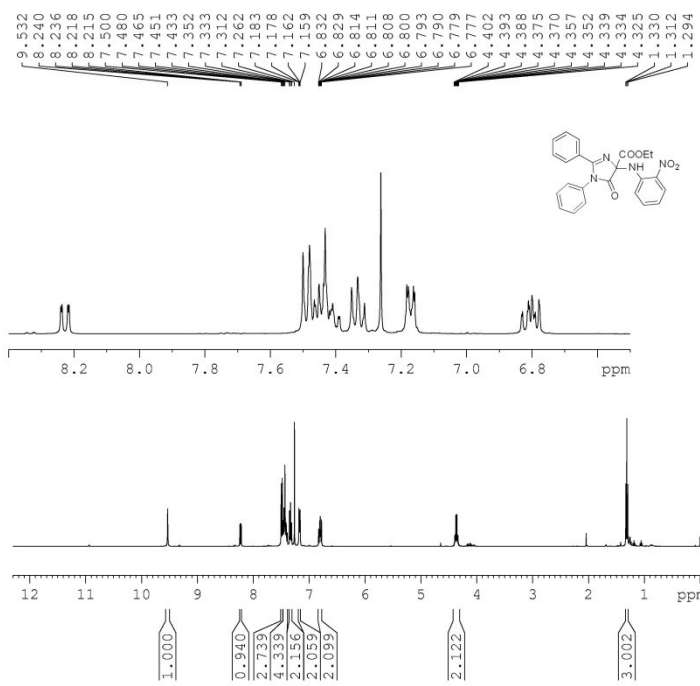
```

NAME      2018-11-20 tyut-lx-1C
EXPNO     10
PROCNO    1
Date_     20181121
Time      15.38
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        295.5 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
SF01     100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

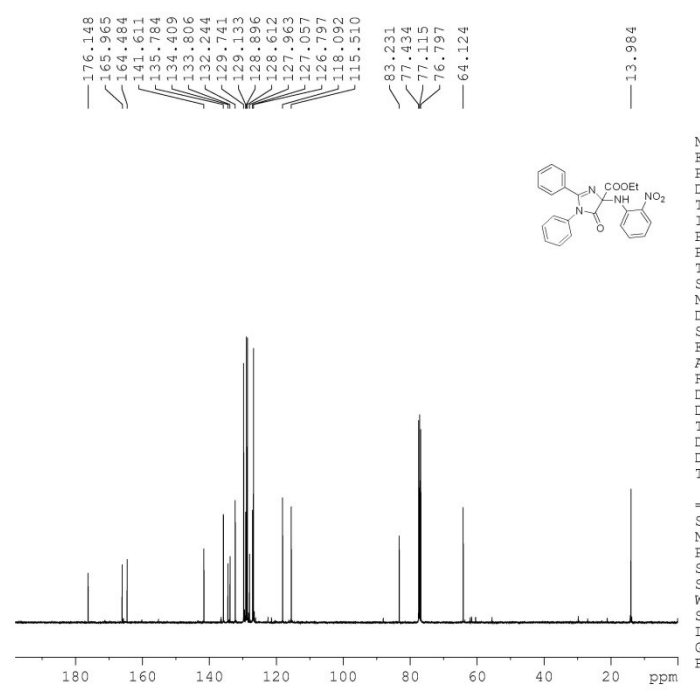
### 4aha



```

NAME      2018-12-06 tyut-lx-3
EXPNO    10
PROCNO   1
Date_    20181206
Time     22.50
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ        4.0894966 sec
RG        34.32
DW        62.400 usec
DE        6.50 usec
TE        293.3 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300088 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

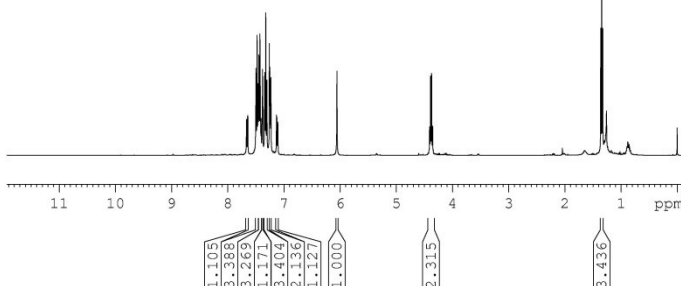
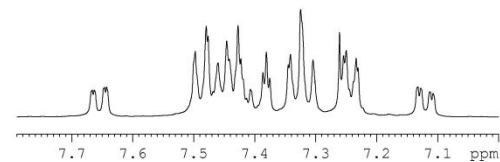
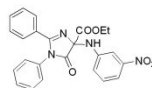
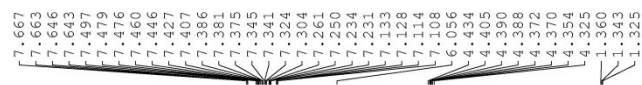


```

NAME      2018-12-07 tyut-lx-3C
EXPNO    10
PROCNO   1
Date_    20181207
Time     18.24
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        294.9 K
D1        2.00000000 sec
D11      0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

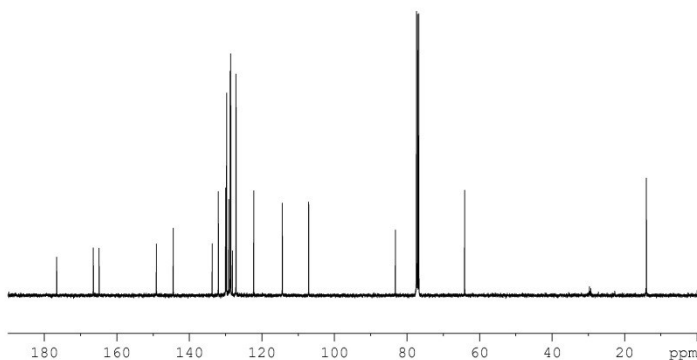
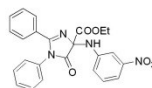
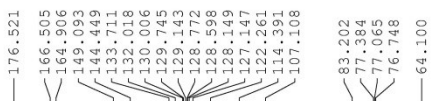
4aia



```

NAME      2018-11-19 tyut-lx-7
EXPNO    10
PROCNO   1
Date_    20181119
Time     20.26
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD        65536
SOLVENT  CDC13
NS        16
DS        2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ        4.0894966 sec
RG        54.19
DW        62.400 usec
DE        6.50 usec
TE        294.8 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300094 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

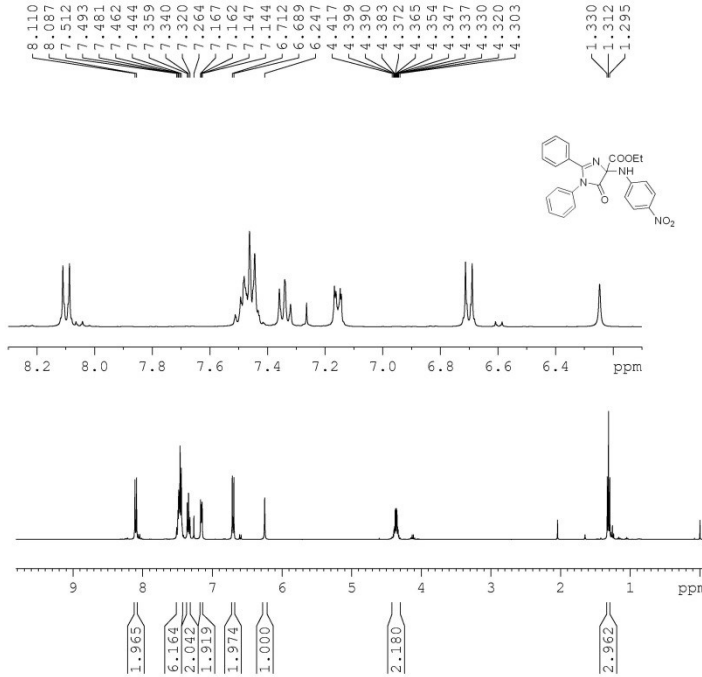


```

NAME      2018-11-19 tyut-lx-7
EXPNO    10
PROCNO   1
Date_    20181121
Time     8.23
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDC13
NS        1024
DS        4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ        1.3631988 sec
RG        185.43
DW        20.800 usec
DE        6.50 usec
TE        295.6 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

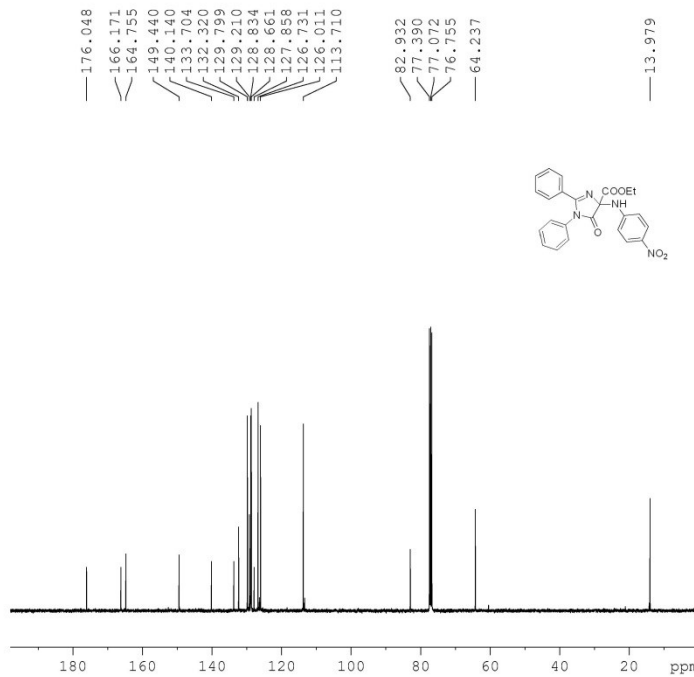
4aja



```

NAME      2018-12-06 tyut-lx-4
EXPNO    10
PROCNO   1
Date_    20181206
Time     22.54
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       54.19
DW       62.400 usec
DE       6.50 usec
TE       293.3 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI       65536
SF       400.1300081 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



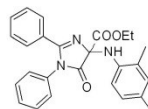
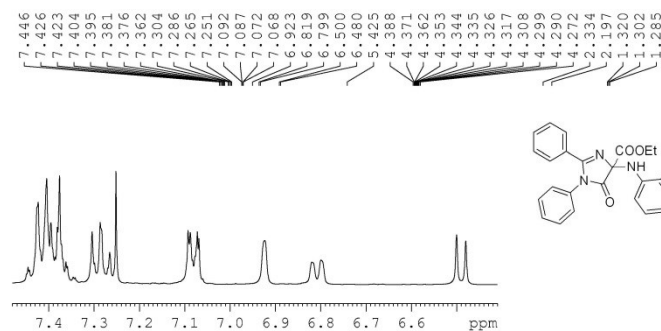
```

NAME      2018-12-07 tyut-lx-4
EXPNO    10
PROCNO   1
Date_    20181207
Time     21.23
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631988 sec
RG       185.43
DW       20.800 usec
DE       6.50 usec
TE       294.8 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     100.6228293 MHz
NUC1     13C
P1       9.50 usec
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

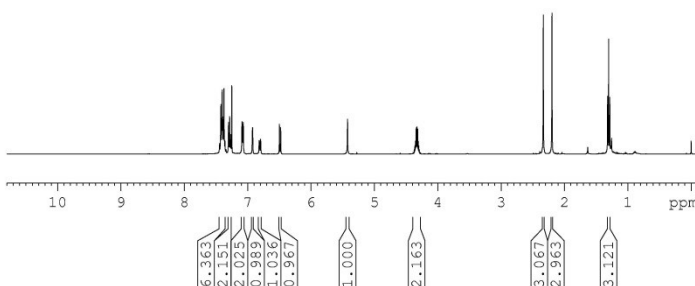


# 4aka



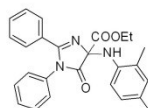
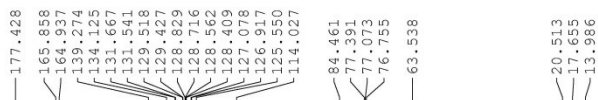
```

NAME      2018-11-20 tyut-lx-02
EXPNO    10
PROCNO    1
Date_    20181120
Time     21.14
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       34.32
DW       62.400 usec
DE       6.50 usec
TE       294.5 K
D1       1.00000000 sec
TD0      1
    
```



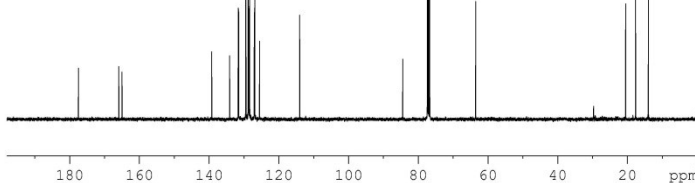
```

===== CHANNEL f1 =====
SFO1    400.1324710 MHz
NUC1     1H
P1       9.70 usec
SI      65536
SF      400.1300136 MHz
WDW      EM
SSB      0
LB      0.30 Hz
GB      0
PC      1.00
    
```



```

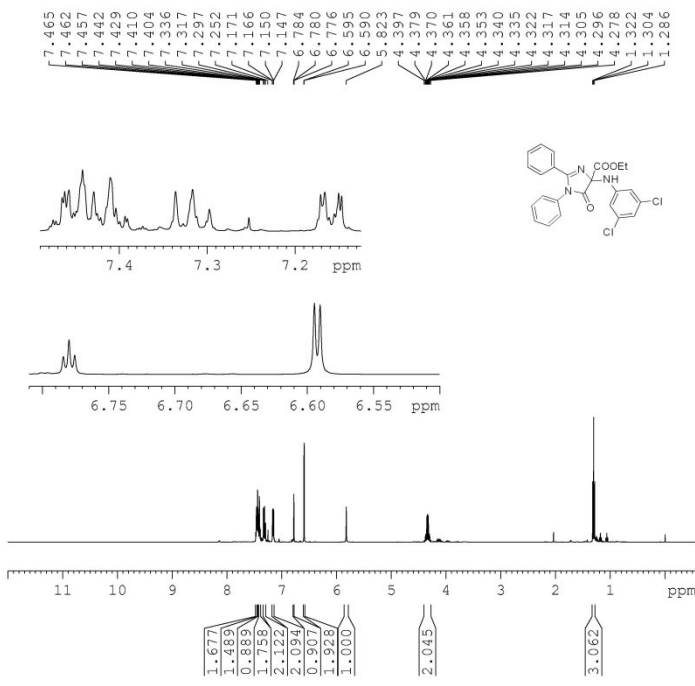
NAME      2018-11-20 tyut-lx-2
EXPNO    10
PROCNO    1
Date_    20181121
Time     16.39
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631988 sec
RG       185.43
DW       20.800 usec
DE       6.50 usec
TE       295.5 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
    
```



```

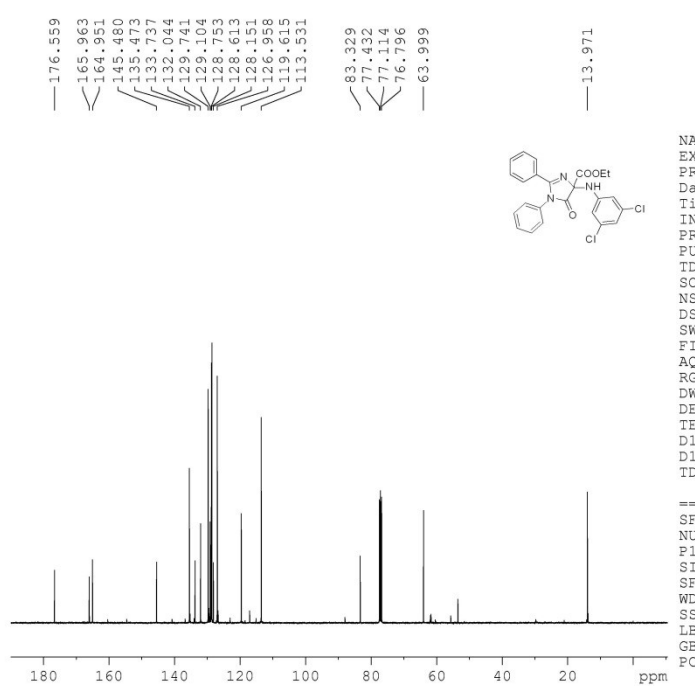
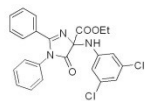
===== CHANNEL f1 =====
SFO1    100.6228293 MHz
NUC1    13C
P1       9.50 usec
SI      32768
SF      100.6127690 MHz
WDW      EM
SSB      0
LB      1.00 Hz
GB      0
PC      1.40
    
```

4ala



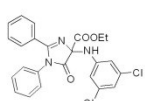
NAME 2019-03-16 tyut-lx-0  
EXPNO 10  
PROCNO 1  
Date\_ 20190316  
Time 19.17  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 34.32  
DW 62.400 usec  
DE 6.50 usec  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 400.1324710 MHz  
NUC1 1H  
P1 9.59 usec  
SI 65536  
SF 400.1300129 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

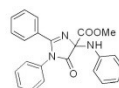
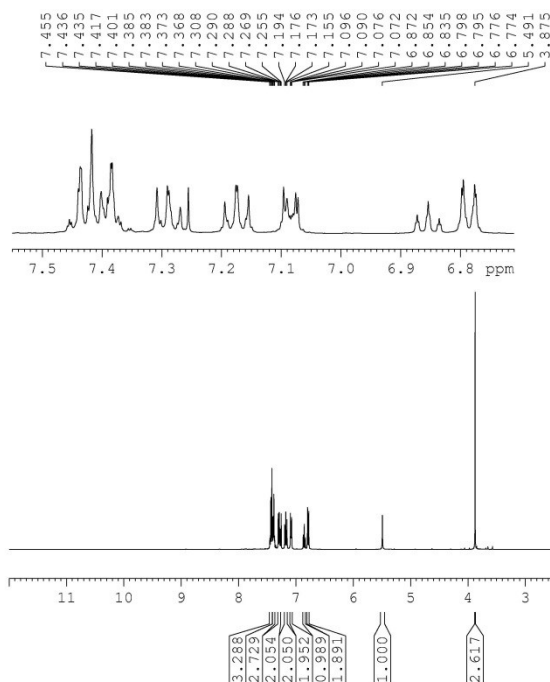


NAME 2019-03-18 tyut-lx-C-03  
EXPNO 10  
PROCNO 1  
Date\_ 20190318  
Time 19.00  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 185.43  
DW 20.800 usec  
DE 6.50 usec  
TE 297.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 100.6228293 MHz  
NUC1 13C  
P1 10.27 usec  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



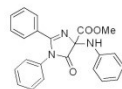
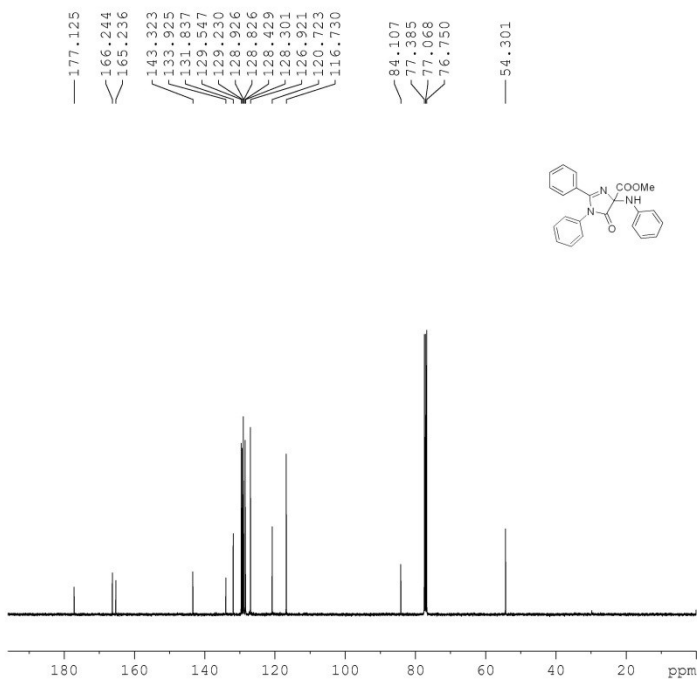
4aab



```

NAME      2018-11-23 tyut-lx-1
EXPNO     10
PROCNO    1
Date_     20181123
Time      18.48
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         57.76
DW         62.400 usec
DE         6.50 usec
TE         293.7 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
SF01      400.1324710 MHz
NUC1       1H
P1         9.70 usec
SI         65536
SF         400.1300118 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

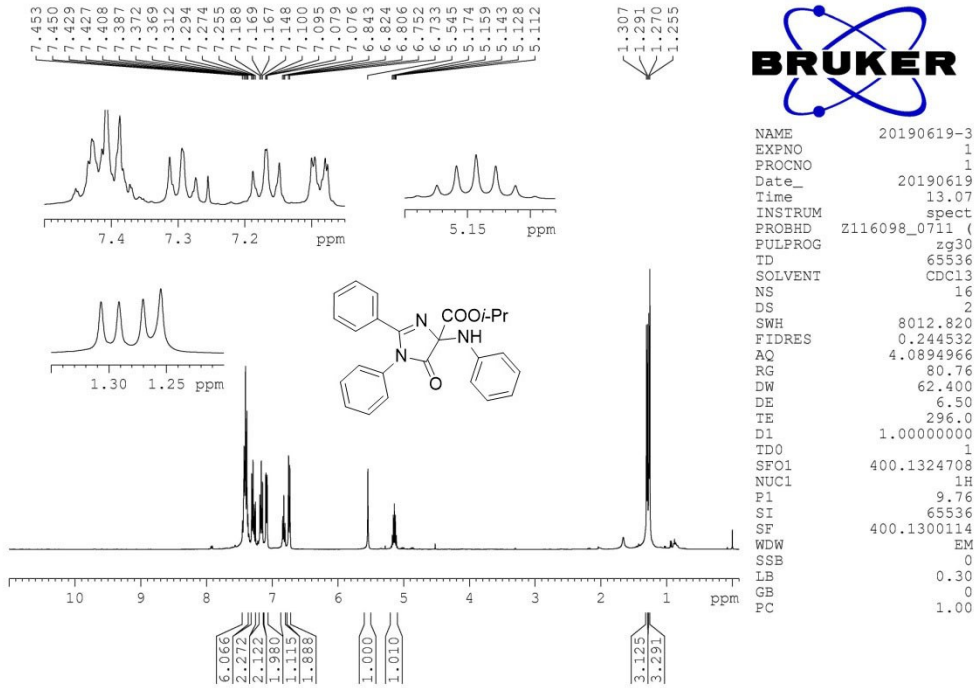


```

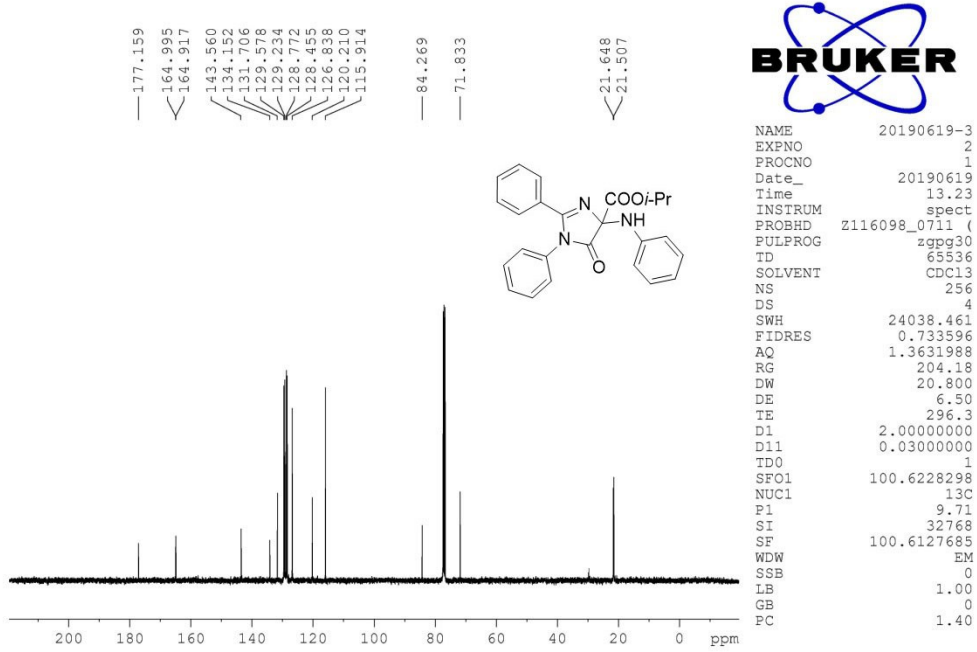
NAME      2018-11-24 tyut-lx-1
EXPNO     10
PROCNO    1
Date_     20181125
Time      6.31
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         185.43
DW         20.800 usec
DE         6.50 usec
TE         294.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SF01      100.6228293 MHz
NUC1       13C
P1         9.50 usec
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

4aac



NAME 20190619-3  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20190619  
 Time\_ 13.07  
 INSTRUM spect  
 PROBHD Z116098\_0711 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820  
 FIDRES 0.244532  
 AQ 4.0894966  
 RG 80.76  
 DW 62.400  
 DE 6.50  
 TE 296.0  
 D1 1.00000000  
 TD0 1  
 SFO1 400.1324708  
 NUC1 1H  
 P1 9.76  
 SI 65536  
 SF 400.1300114  
 WDW EM  
 SSB 0  
 LB 0.30  
 GB 0  
 PC 1.00



NAME 20190619-3  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20190619  
 Time\_ 13.23  
 INSTRUM spect  
 PROBHD Z116098\_0711 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 4  
 SWH 24038.461  
 FIDRES 0.733596  
 AQ 1.3631988  
 RG 204.18  
 DW 20.800  
 DE 6.50  
 TE 296.3  
 D1 2.00000000  
 D11 0.03000000  
 TD0 1  
 SFO1 100.6228298  
 NUC1 13C  
 P1 9.71  
 SI 32768  
 SF 100.6127685  
 WDW EM  
 SSB 0  
 LB 1.00  
 GB 0  
 PC 1.40