# Supporting information

## Catalyst- and Additive-Free Three-Component Construction of Isoxazolidinyl Nucleosides and Azoles via 1,3-Dipolar Cycloaddition

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## 1. General Information

Unless otherwise noted, all reagents and solvents obtained from commercial sources were used without further purification. Some reagents such as pyrimidines, purines, imidazoles, and triazoles were purchased from Sigma-aldrich, Alfa Aesar, J&K, TCI, Acros, Fluka, Energy, and Aladdin. Deuterated solvents were purchased from Sigma-Aldrich. Column chromatography was performed on silica gel (200−300 mesh) using petroleum ether /ethyl acetate/dichloromethane. $^{1}$H NMR spectra were taken on a Bruker AVANCE III 600 MHz NMR spectrometer. The chemical shifts are reported in ppm downfield to the $CDCl_3$ resonance (δ = 7.27). Spectra are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration, and assignment. $^{13}C\{^{1}H\}$ NMR data were collected at 150 MHz with complete proton decoupling. The chemical shifts are reported in ppm downfield to the central $CDCl_3$ resonance (δ = 77.0). High-resolution mass spectra (HRMS) 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. Substrates such as diazo compounds **1**[1], nitrosoarenes **2**[2], N1-vinylpyrimidines **3**[3], purine nucleobase acrylates **5**[4] and imidazole- or triazole-substituted acrylates **7**[4a] were synthesized according to the corresponding literature procedures. Among these starting materials, *tert*-butyl 2,6-dioxo-5-phenyl-3-vinyl-3,6-dihydropyrimidine-1(2*H*)-carboxylate (**3g**) is a new compound. Other starting materials are all known compounds and the analytical data ($^{1}$HNMR) matches with the literatures. In most reactions, only one single isomer (*cis*- or *endo*-) product were obtained and the other isomer (*trans*- or *exo*-) product cannot be observed. The structures of stereochemistry for these products have been mentioned clearly throughout in the manuscript and Supporting Information. Notably, only several reactions provided two isomeric products, and the diastereomeric mixture and the structures of stereochemistry have also been mentioned clearly throughout in the manuscript and Supporting Information.

## 2. General procedures

### 2.1 General procedure for the synthesis of isoxazolidinyl nucleosides and oxazoles via catalyst-free one-pot three-component cycloadditions of diazo compounds, nitrosoarenes and vinyl pyrimidines, or vinyl purines, or vinyl imidazoles, or vinyl triazoles

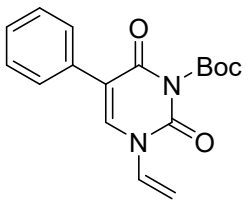
To a reaction system of nitrosoarene **2** (0.15 mmol, 1.5 equiv) and α-diazo compound **1** (0.15 mmol, 1.5 equiv) in DCE (1.2 mL) was added alkene **3**, **5** or **7** (0.1 mmol) under air atmosphere. Subsequently, the resulting mixture was stirred under 70 °C (oil bath) and monitored by TLC. Upon completion of the consumption of the olefin **3**, **5** or **7**, the reaction mixture was directly purified by silica gel column chromatography without any treatment to give the desired cycloaddition products **4**, **6** and **8**.

### 2.2 3 mmol-Scale preparation of 4a

To a round-bottom flask equipped with a magnetic stir bar were added nitrosobenzene **2a** (0.496 g, 4.5 mmol, 1.5 equiv), ethyl diazoacetate **1a** (0.521 g, 4.5 mmol, 1.5 equiv), Boc-protected N1-vinylthymine **3a** (0.757 g, 3 mmol) and DCE (25 mL) in turn. Subsequently, the reaction system was heated to 70 °C (oil bath) and stirred until Boc-protected N1-vinylthymine **3a** was completely consumed as determined by TLC. At last, the reaction mixture was concentrated in vacuum and then purified by silica gel column chromatography to give the desired product **4a** (1.068 g, 80% yield).

## 3. Characterization data of substrate 3g

***tert*-butyl 2,6-dioxo-5-phenyl-3-vinyl-3,6-dihydropyrimidine-1(2*H*)-carboxylate (3g)**

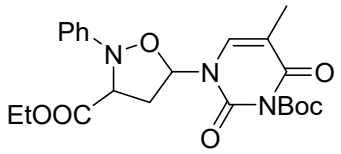



White solid, m.p. = 136−138 °C; **$^1$H NMR** (600 MHz, $CDCl_3$) $\delta$ 7.59 (s, 1H), 7.52 (d, $J$ = 6.0 Hz,

2H), 7.43−7.36 (m, 3H), 7.26−7.21 (m, 1H), 5.19 (dd, *J* = 18.0, 6.0 Hz, 1H), 5.03 (dd, *J* = 9.0, 6.0 Hz, 1H), 1.62 (s, 9H) ppm; $^{13}C$ {$^{1}H$} NMR ($CDCl_3$, 150 MHz) *δ* 159.7, 147.5, 147.2, 135.3, 131.5, 129.7, 128.7, 128.7, 128.5, 116.4, 102.3, 87.3, 27.5 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{19}N_2O_4^+$ , 315.1339; found, 315.1346.

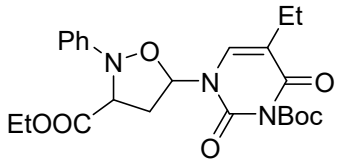
## 4. Characterization data of products 4

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4a)**



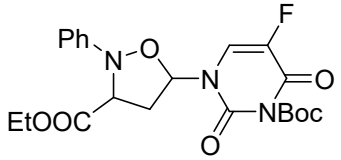

Yellow oil, Yield: 85% (37.8 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^{1}H$ NMR ($CDCl_3$, 400 MHz) *δ* 7.80 (s, 1H), 7.29−7.25 (m, 2H), 7.07−7.01 (m, 3H), 6.41 (dd, *J* = 7.8, 3.8 Hz, 1H), 4.25−4.18 (m, 3H), 3.06−2.97 (m, 1H), 2.70 (dt, *J* = 14.0, 4.4 Hz, 1H), 1.90 (s, 3H), 1.55 (s, 9H), 1.25 (t, *J* = 7.1 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) *δ* 170.3, 161.2, 148.8, 148.8, 147.8, 135.4, 129.2, 124.2, 115.9, 111.0, 86.8, 82.9, 67.0, 62.3, 38.7, 27.4, 14.0, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{28}N_3O_7^+$, 446.1922; found, 446.1938.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-ethyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4b)**




Yellow oil, Yield: 88% (40.4 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^{1}H$ NMR ($CDCl_3$, 400 MHz) *δ* 7.85 (s, 1H), 7.37−7.32 (m, 2H), 7.15−7.09 (m, 3H), 6.51 (dd, *J* = 7.8, 3.9 Hz, 1H), 4.32−4.26 (m, 3H), 3.12−3.03 (m, 1H), 2.77 (dt, *J* = 14.0, 4.4 Hz, 1H), 2.38 (q, *J* = 7.4 Hz, 2H), 1.62 (s, 9H), 1.32 (t, *J* = 7.1 Hz, 3H), 1.18 (t, *J* = 7.4 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) *δ* 170.3, 160.8, 148.8, 148.8, 147.9, 134.8, 129.2, 124.2, 116.8, 116.0, 86.8, 82.9, 67.1, 62.3, 38.4, 27.4, 20.3, 14.0, 12.5 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{30}N_3O_7^+$, 460.2078; found, 460.2080.

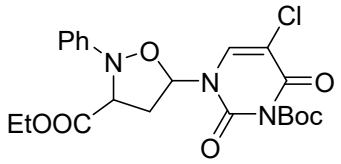
**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4c)**




Yellow oil, Yield: 77% (34.6 mg); $R_f$ = 0.35 (PE/EA = 3:1, v/v); $^{1}H$ NMR ($CDCl_3$, 400 MHz) *δ* 8.23 (d, *J* = 6.3 Hz, 1H), 7.38−7.33 (m, 2H), 7.16−7.11 (m, 3H), 6.45 (dd, *J* = 7.6, 2.0 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 4.21 (dd, *J* = 9.8, 5.0 Hz, 1H) 3.21−3.12 (m, 1H), 2.84−2.77 (m, 1H),

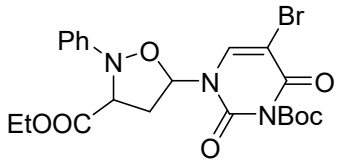
1.62 (s, 9H), 1.32 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ ($CDCl_3$, 100 MHz) $\delta$ 170.1, 154.6 (d, $J$ = 28.1 Hz), 148.3, 147.3, 146.4, 141.2, 138.8, 129.2, 124.7 (d, $J$ = 32.8 Hz), 116.4, 87.8, 83.4, 66.7, 62.5, 39.4, 27.4, 14.0 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{25}FN_3O_7^+$, 450.1671; found, 450.1678.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-chloro-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4d)**



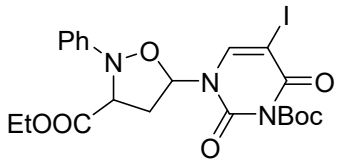

Yellow oil, Yield: 90% (41.9 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.31 (s, 1H), 7.39−7.34 (m, 2H), 7.17−7.12 (m, 3H), 6.44 (dd, $J$ = 7.5, 2.9 Hz, 1H), 4.27 (q, $J$ = 7.2 Hz, 2H), 4.22 (dd, $J$ = 9.8, 4.8 Hz, 1H), 3.22−3.13 (m, 1H), 2.87−2.81 (m, 1H), 1.62 (s, 9H), 1.32 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 170.0, 156.6, 148.4, 147.8, 146.6, 137.0, 129.2, 124.6, 116.4, 108.9, 87.7, 83.7, 66.7, 62.6, 39.7, 27.4, 14.0 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{25}ClN_3O_7^+$, 466.1376; found, 466.1373.

**Ethyl 5-(5-bromo-3-(*tert*-butoxycarbonyl)-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4e)**



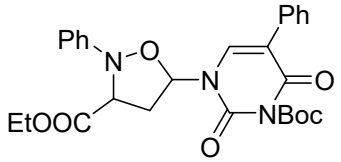

Yellow oil, Yield: 85% (43.4 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.40 (s, 1H), 7.39−7.34 (m, 2H), 7.17−7.12 (m, 3H), 6.43 (dd, $J$ = 7.5, 2.9 Hz, 1H), 4.27 (q, $J$ = 7.2 Hz, 2H), 4.22 (dd, $J$ = 9.8, 4.8 Hz, 1H), 3.22−3.13 (m, 1H), 2.88−2.81 (m, 1H), 1.62 (s, 9H), 1.32 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 170.0, 156.5, 148.4, 148.1, 146.7, 139.6, 129.2, 124.6, 116.4, 96.4, 87.7, 83.8, 66.8, 62.6, 39.7, 27.4, 14.1 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{25}BrN_3O_7^+$, 510.0870; found, 510.0861.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-iodo-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4f)**



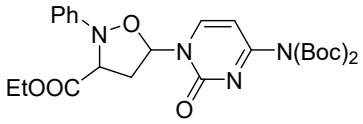

Yellow oil, Yield: 82% (45.7 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.47 (s, 1H), 7.39−7.34 (m, 2H), 7.17−7.12 (m, 3H), 6.42 (dd, $J$ = 7.5, 2.9 Hz, 1H), 4.28 (q, $J$ = 7.2 Hz, 2H), 4.23 (dd, $J$ = 9.8, 4.7 Hz, 1H), 3.20−3.11 (m, 1H), 2.87−2.81 (m, 1H), 1.61 (s, 9H), 1.33 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 170.0, 157.4, 148.5, 148.4, 146.7, 144.6, 129.2, 124.6, 116.4, 87.6, 83.7, 66.8, 62.6, 39.6, 27.3, 14.1 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{25}IN_3O_7^+$, 558.0732; found, 558.0729.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-2,4-dioxo-5-phenyl-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4g)**




Yellow oil, Yield: 88% (44.7 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.25 (s, 1H), 7.61−7.57 (m, 2H), 7.41−7.32 (m, 2H), 7.15−7.11 (m, 3H), 6.54 (dd, $J$ = 7.6, 3.3 Hz, 1H), 4.31−4.21 (m, 3H), 3.20−3.11 (m, 1H), 2.94−2.86 (m, 1H), 1.63 (s, 9H), 1.23 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 170.1, 159.7, 148.7, 148.4, 147.7, 137.0, 132.0, 129.2, 128.5, 128.2, 128.1, 124.4, 116.2, 115.2, 87.1, 83.4, 66.9, 62.4, 39.2, 27.4, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{30}N_3O_7^+$, 508.2078; found, 508.2078.

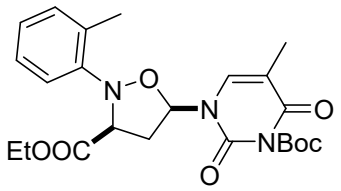
**Ethyl 5-(4-((*ditert*-butoxycarbonyl)amino)-2-oxopyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4h)**




Yellow oil, Yield: 72% (38.2 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.24 (d, $J$ = 7.6 Hz, 1H), 7.38−7.33 (m, 2H), 7.12 (t, $J$ = 8.5 Hz, 4H), 6.39 (dd, $J$ = 7.2, 2.3 Hz, 1H), 4.23−4.17 (m, 3H), 3.31−3.22 (m, 1H), 2.90−2.84 (m, 1H), 1.57 (s, 18H), 1.25 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 170.0, 162.6, 154.5, 149.5, 148.9, 144.0, 129.1, 124.2, 116.2, 95.9, 85.0, 84.9, 66.5, 62.2, 40.6, 27.7, 14.0 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{35}N_4O_8^+$, 531.2449; found, 531.2457.

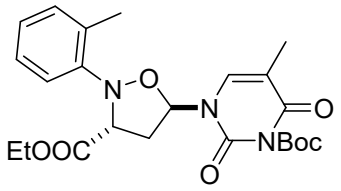
## dr (*cis*-4i/*trans*-4i) = 2:1

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(*o*-tolyl)isoxazolidine-3-carboxylate (*cis*-4i)**



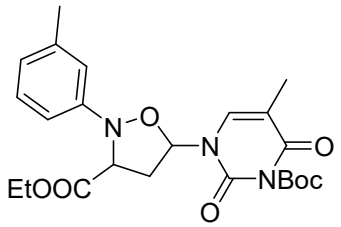

Yellow oil, Yield: 53% (24.5 mg); $R_f$ = 0.22 (PE/EA = 3:1, v/v); dr (*trans*/*cis*) = 2:1, $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.10 (d, $J$ = 1.2 Hz, 1H), 7.36 (d, $J$ = 7.8 Hz, 1H), 7.25−7.17 (m, 3H), 6.49 (dd, $J$ = 7.8, 3.6 Hz, 1H), 4.20 (dd, $J$ = 9.0, 6.6 Hz, 1H), 4.15 (q, $J$ = 7.2 Hz, 2H), 3.30−3.25 (m, 1H), 2.84−2.80 (m, 1H), 2.37 (s, 3H), 1.99 (s, 3H), 1.61 (s, 9H), 1.20 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 150 MHz) $\delta$ 169.3, 161.4, 149.0, 148.0, 145.1, 136.1, 134.4, 131.4, 127.8, 126.9, 120.5, 110.6, 86.9, 83.1, 66.6, 62.1, 40.7, 27.6, 18.3, 14.1, 12.8 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{30}N_3O_7^+$, 460.2078; found, 460.2075.

**Ethyl-5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(*o*-tolyl)isoxazolidine-3-carboxylate (*trans*-4i)**



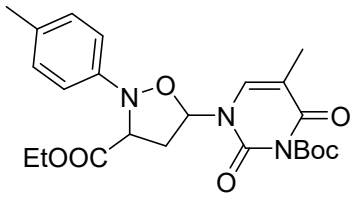
Yellow oil, Yield: 27% (12.3 mg); $R_f$ = 0.20 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 600 MHz) $\delta$ 7.48 (d, $J$ = 1.2 Hz, 1H), 7.39 (d, $J$ = 7.8 Hz, 1H), 7.19 (d, $J$ = 7.2 Hz, 2H), 7.13−7.10 (m, 1H), 6.47 (dd, $J$ = 7.8, 3.6 Hz, 1H), 4.51 (dd, $J$ = 7.8, 1.8 Hz, 1H), 3.85−3.76 (m, 2H), 3.39−3.35 (m, 1H), 2.76−2.71 (m, 1H), 2.31 (s, 3H), 1.90 (s, 3H), 1.61 (s, 9H), 0.84 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 150 MHz) $\delta$ 168.3, 148.8, 148.0, 143.8, 134.8, 130.7, 126.6, 126.1, 118.9, 110.6, 87.0, 83.2, 63.6, 61.2, 40.9, 29.8, 27.6, 18.4, 13.7, 12.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{30}N_3O_7^+$, 460.2078; found, 460.2075.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(*m*-tolyl)isoxazolidine-3-carboxylate (4j)**



Yellow oil, Yield: 86% (39.5 mg); $R_f$ = 0.20 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.80 (d, $J$ = 1.2 Hz, 1H), 7.15 (t, $J$ = 7.8 Hz, 1H), 6.87−6.83 (m, 3H), 6.40 (dd, $J$ = 7.8, 3.8 Hz, 1H), 4.25−4.16 (m, 3H), 3.06−2.98 (m, 1H), 2.74−2.67 (m, 1H), 2.28 (s, 3H), 1.90 (d, $J$ = 1.2 Hz, 3H), 1.54 (s, 9H), 1.25 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 170.4, 161.2, 148.8, 148.8, 147.8, 139.2, 135.5, 129.0, 125.1, 116.7, 113.0, 110.9, 86.8, 83.0, 66.9, 62.3, 38.9, 27.4, 21.6, 14.0, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{30}N_3O_7^+$, 460.2078; found, 460.2075.

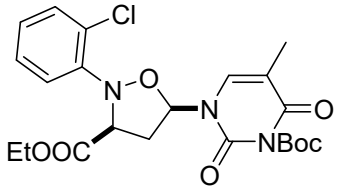
**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(*p*-tolyl)isoxazolidine-3-carboxylate (4k)**



Yellow oil, Yield: 88% (40.4 mg); $R_f$ = 0.20 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.81 (d, $J$ = 1.2 Hz, 1H), 7.06 (d, $J$ = 8.1 Hz, 2H), 6.96 (d, $J$ = 8.6 Hz, 2H), 6.37 (dd, $J$ = 7.8, 3.8 Hz, 1H), 4.17 (q, $J$ = 7.2 Hz, 2H), 4.12 (dd, $J$ = 9.5, 5.3 Hz, 1H), 3.08−2.99 (m, 1H), 2.73−2.66 (m, 1H), 2.25 (s, 3H), 1.90 (d, $J$ = 1.2 Hz, 3H), 1.54 (s, 9H), 1.23 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 170.2, 161.2, 148.8, 147.8, 146.2, 135.5, 134.3, 129.7, 116.6, 110.9, 86.8, 82.9, 67.2, 62.2, 39.1, 27.4, 14.0, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{30}N_3O_7^+$, 460.2078; found, 460.2075.

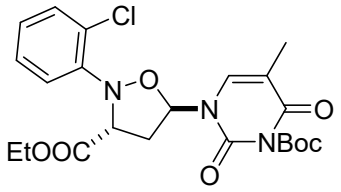
**dr (*cis*-4n/*trans*-4n) = 2:1**

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(2-chlorophenyl)isoxazolidine-3-carboxylate (*cis*-4n)**



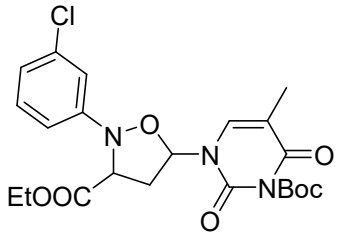

Yellow oil, Yield: 55% (26.3 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); dr (*trans*/*cis*) = 2:1, $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.06 (d, $J$ = 1.2 Hz, 1H), 7.46 (dd, $J$ = 8.4, 1.8 Hz, 1H), 7.38 (dd, $J$ = 7.8, 1.2 Hz, 1H), 7.32−7.29 (m, 1H), 7.20−7.17 (m, 1H), 6.55 (dd, $J$ = 7.8, 3.6 Hz, 1H), 4.37 (dd, $J$ = 9.0, 5.4 Hz, 1H), 4.16 (q, $J$ = 7.2 Hz, 2H), 3.21−3.16 (m, 1H), 2.85−2.81 (m, 1H), 1.98 (s, 3H), 1.61 (s, 9H), 1.18 (t, $J$ = 6.6 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 150 MHz) $\delta$ 169.0, 161.4, 149.0, 148.0, 144.3, 135.9, 130.7, 128.0, 127.9, 121.2, 110.8, 87.0, 86.9, 83.6, 66.5, 62.2, 39.7, 27.6, 14.0, 12.8 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{27}ClN_3O_7^+$, 480.1532; found, 480.1529.

**Ethyl(3*S*,5*S*)-5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(2-chlorophenyl)isoxazolidine-3-carboxylate (*trans*-4n)**




Yellow oil, Yield: 27% (13.1 mg); $R_f$ = 0.26 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 600 MHz) $\delta$ 7.55 (d, $J$ = 1.2 Hz, 1H), 7.44 (dd, $J$ = 7.8, 1.2 Hz, 1H), 7.38 (dd, $J$ = 8.4, 1.8 Hz, 1H), 7.27−7.24 (m, 1H), 7.14−7.11 (m, 1H), 6.59 (dd, $J$ = 7.8, 3.6 Hz, 1H), 5.03 (d, $J$ = 7.8 Hz, 1H), 3.86−3.80 (m, 2H), 3.38−3.34 (m, 1H), 2.76−2.72 (m, 1H), 1.92 (s, 3H), 1.61 (s, 9H), 0.85 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 150 MHz) $\delta$ 168.1, 161.4, 148.8, 148.0, 142.5, 134.9, 127.5, 124.8, 120.4, 111.2, 87.0, 82.3, 63.1, 61.3, 40.1, 27.6, 13.8, 12.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{27}ClN_3O_7^+$, 480.1532; found, 480.1529.

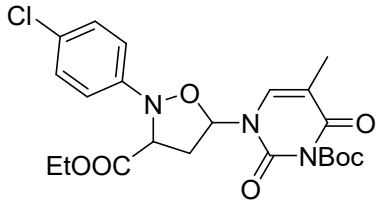
**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(3-chlorophenyl)isoxazolidine-3-carboxylate (4o)**




Yellow oil, Yield: 83% (39.8 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.72 (d, $J$ = 1.2 Hz, 1H), 7.19 (t, $J$ = 8.1 Hz, 1H), 7.05 (t, $J$ = 2.1 Hz, 1H), 7.01−6.98 (m, 1H), 6.93−6.90 (m, 1H), 6.40 (dd, $J$ = 7.7, 3.9 Hz, 1H), 4.26−4.16 (m, 3H), 3.07−2.98 (m, 1H), 2.72 (dt, $J$ = 14.0, 4.4 Hz, 1H), 1.92 (d, $J$ = 1.1 Hz, 3H), 1.54 (s, 9H), 1.26 (t, $J$ = 7.1 Hz, 3H) ppm;

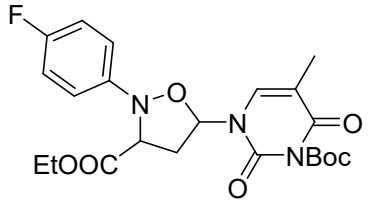
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 170.0, 161.1, 150.0, 148.8, 147.7, 135.2, 130.3, 124.0, 116.0, 113.8, 111.1, 86.9, 83.0, 66.7, 62.5, 38.5, 27.4, 14.0, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{27}ClN_3O_7^+$, 480.1532; found, 480.1535.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(4-chlorophenyl)isoxazolidine-3-carboxylate (4p)**



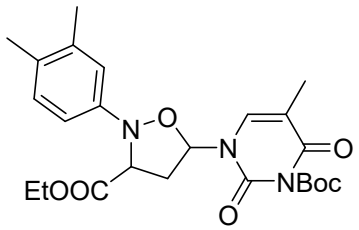

Yellow oil, Yield: 87% (41.7 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^{1}H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 7.75 (d, *J* = 1.2 Hz, 1H), 7.21 (d, *J* = 9.0 Hz, 1H), 6.98 (d, *J* = 9.0 Hz, 2H), 6.40 (dd, *J* = 7.8, 4.0 Hz, 1H), 4.19 (q, *J* = 7.1 Hz, 2H), 4.13 (dd, *J* = 9.6, 5.0Hz, 1H), 3.07−2.98 (m, 1H), 2.76−2.69 (m, 1H), 1.90 (d, *J* = 1.2 Hz, 3H), 1.54 (s, 9H), 1.24 (t, *J* = 7.1 Hz, 3H), ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 170.0, 161.1, 148.8, 147.7, 147.4, 135.2, 129.5, 129.2, 117.4, 111.1, 86.9, 82.9, 67.0, 62.5, 38.6, 27.4, 14.0, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{27}ClN_3O_7^+$, 480.1532; found, 480.1540.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(4-fluorophenyl)isoxazolidine-3-carboxylate (4q)**




Yellow oil, Yield: 72% (33.3 mg); $R_f$ = 0.20 (PE/EA = 3:1, v/v); $^{1}H$ NMR ($CDCl_3$, 600 MHz) $\delta$ 7.86 (d, *J* = 1.2 Hz, 1H), 7.14−7.12 (m, 2H), 7.05−7.02 (m, 2H), 6.48 (dd, *J* = 7.8, 3.6 Hz, 1H), 4.27 (q, *J* = 7.2 Hz, 2H), 4.16 (dd, *J* = 9.0, 5.4 Hz, 1H), 3.17−3.12 (m, 1H), 2.81−2.77 (m, 1H), 1.98 (s, 3H), 1.61 (s, 9H), 1.30 (t, *J* = 7.2 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 150 MHz) $\delta$ 170.0, 161.3, 160.9, 159.3, 149.0, 147.9, 144.8, 135.5, 118.9, 116.2, 116.0, 111.2, 87.1, 83.0, 67.7, 62.5, 39.5, 27.6, 14.2, 12.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{27}FN_3O_7^+$, 464.1828; found, 464.1825.

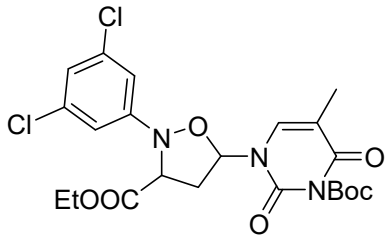
**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(3,4-dimethylphenyl)isoxazolidine-3-carboxylate (4r)**




Yellow oil, Yield: 72% (34.1 mg); $R_f$ = 0.20 (PE/EA = 3:1, v/v); $^{1}H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 7.82 (d, *J* = 1.1 Hz, 1H), 7.01 (d, *J* = 8.2 Hz, 1H), 6.86 (d, *J* = 2.1 Hz, 1H), 6.78 (dd, *J* = 8.1, 2.4

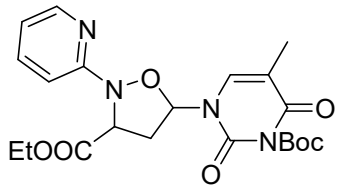
Hz, 1H), 6.38 (dd, *J* = 7.8, 3.7 Hz, 1H), 4.18 (q, *J* = 7.0 Hz, 2H), 4.12 (dd, *J* = 9.5, 5.3 Hz, 1H), 3.08−3.00 (m, 1H), 2.72−2.65 (m, 1H), 2.19 (s, 3H), 2.15 (s, 3H), 1.90 (d, *J* = 1.0 Hz, 3H), 1.54 (s, 9H), 1.24 (t, *J* = 7.2 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 170.3, 161.2, 148.8, 147.8, 146.5, 137.6, 135.6, 133.0, 130.2, 118.1, 113.9, 110.8, 86.8, 82.9, 67.1, 62.2, 39.3, 27.4, 20.1, 19.1, 14.0, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{32}N_3O_7^+$, 474.2235; found, 474.2205.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(3,5-dichlorophenyl)isoxazolidine-3-carboxylate (4s)**



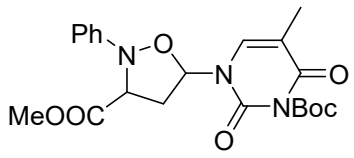

Yellow oil, Yield: 74% (38.0 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 7.66 (d, *J* = 1.2 Hz, 1H), 7.01 (t, *J* = 1.8 Hz, 1H), 6.92 (d, *J* = 1.7 Hz, 2H), 6.40 (dd, *J* = 7.7, 3.9 Hz, 1H), 4.29−4.20 (m, 2H), 4.16 (dd, *J* = 9.8, 4.6 Hz, 1H), 3.07−2.99 (m, 1H), 2.75 (dt, *J* = 14.1, 4.3 Hz, 1H), 1.90 (d, *J* = 1.1 Hz, 3H), 1.55 (s, 9H), 1.27 (t, *J* = 7.2 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 169.7, 161.0, 150.6, 148.7, 147.6, 135.7, 134.9, 123.7, 114.1, 111.3, 87.0, 83.0, 66.4, 62.7, 38.3, 27.4, 14.0, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{26}Cl_2N_3O_7^+$, 514.1142; found, 514.1137.

**Ethyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(pyridin-2-yl)isoxazolidine-3-carboxylate (4t)**



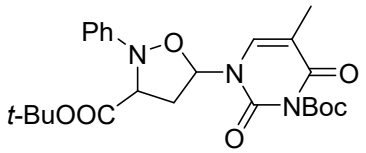

Yellow oil, Yield: 71% (31.7 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.21−8.19 (m, 1H), 7.78 (d, *J* = 1.2 Hz, 1H), 7.63−7.58 (m, 1H), 7.15 (d, *J* = 8.3 Hz, 1H), 6.94−6.90 (m, 1H), 6.34 (dd, *J* = 8.2, 4.5 Hz, 1H), 5.16 (dd, *J* = 9.7, 4.4 Hz, 1H), 4.24 (q, *J* = 7.2Hz, 2H), 2.93−2.84 (m, 1H), 2.62 (dt, *J* = 14.0, 4.4 Hz, 1H), 1.91 (d, *J* = 1.2 Hz, 3H), 1.55 (s, 9H), 1.28 (t, *J* = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 171.2, 161.0, 159.5, 148.9, 147.7, 147.4, 138.5, 135.3, 119.0, 111.6, 110.8, 86.9, 83.2, 62.2, 36.6, 27.4, 14.1, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{27}N_4O_7^+$, 447.1874; found, 447.1871.

**Methyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4u)**



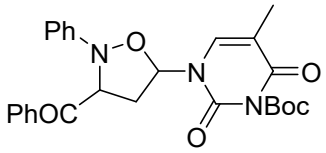
Yellow oil, Yield: 86% (37.1 mg); $R_f$ = 0.20 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.78 (d, $J$ = 1.2 Hz, 1H), 7.25 (dd, $J$ = 8.8, 7.2 Hz, 2H), 7.04 (d, $J$ = 7.8 Hz, 3H), 6.42 (dd, $J$ = 7.9, 4.1 Hz, 1H), 4.22 (dd, $J$ = 9.6, 4.9 Hz, 1H), 3.78 (s, 3H), 3.05−2.96 (m, 1H), 2.69 (dt, $J$ = 14.0, 4.6 Hz, 1H), 1.91 (d, $J$ = 1.0 Hz, 3H), 1.55 (s, 9H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 170.9, 161.1, 148.8, 148.7, 147.8, 135.3, 129.3, 124.3, 115.9, 111.1, 86.9, 82.9, 66.9, 53.2, 38.4, 27.4, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{26}N_3O_7^+$, 432.1765; found, 432.1752.

***tert*-Butyl 5-(3-(*tert*-butoxycarbonyl)-5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-phenylisoxazolidine-3-carboxylate (4v)**




Yellow oil, Yield: 80% (37.9 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.78 (d, $J$ = 1.2 Hz, 1H), 7.25 (dd, $J$ = 8.7, 7.4 Hz, 2H), 7.07−7.01 (m, 3H), 6.37 (dd, $J$ = 7.6, 3.6 Hz, 1H), 4.05 (dd, $J$ = 9.6, 5.0 Hz, 1H), 3.04−2.96 (m, 1H), 2.73−2.67 (m, 1H), 1.89 (d, $J$ = 1.2 Hz, 3H), 1.55 (s, 9H), 1.42 (s, 9H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.3, 161.2, 149.0, 148.8, 147.8, 135.6, 129.1, 124.0, 116.0, 110.8, 86.6, 83.2, 83.0, 67.7, 39.1, 27.8, 27.4, 12.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{32}N_3O_7^+$, 474.2235; found, 474.2232.

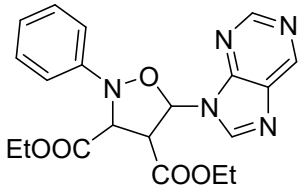
***tert*-Butyl 3-(3-benzoyl-2-phenylisoxazolidin-5-yl)-5-methyl-2,6-dioxo-3,6-dihydropyrimidine-1(2*H*)-carboxylate (4w)**




Yellow oil, Yield: 61% (29.1 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.96−7.93 (m, 2H), 7.86 (d, $J$ = 1.2 Hz, 1H), 7.57 (t, $J$ = 7.4 Hz, 1H), 7.44 (t, $J$ = 7.5 Hz, 2H), 7.25 (dd, $J$ = 8.7, 7.4 Hz, 2H), 7.09−7.02 (m, 3H), 6.42 (dd, $J$ = 8.2, 4.2 Hz, 1H), 5.13 (dd, $J$ = 9.3, 5.0 Hz, 1H), 3.08−2.99 (m, 1H), 2.77 (dt, $J$ = 13.9, 4.6 Hz, 1H), 1.94 (d, $J$ = 1.2 Hz, 3H), 1.55 (s, 9H), 1.53 (s, 9H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 195.4, 161.1, 149.0, 148.3, 147.8, 135.7, 135.0, 134.2, 129.4, 129.0, 128.8, 124.3, 116.1, 111.2, 86.8, 82.8, 68.4, 37.5, 27.4, 12.8 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{28}N_3O_6^+$, 478.1973; found, 478.1986.

## 5. Characterization data of products 6

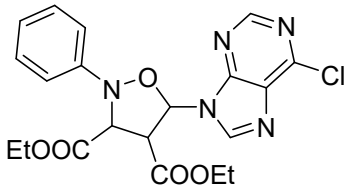
**Diethyl 2-phenyl-5-(9*H*-purin-9-yl)isoxazolidine-3,4-dicarboxylate (6a)**




Yellow oil, Yield: 83% (34.1 mg); $R_f$ = 0.20 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$

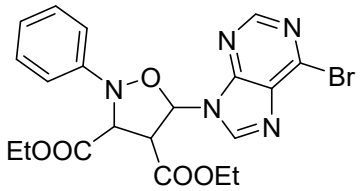
9.19 (s, 1H), 9.04 (s, 1H), 8.85 (s, 1H), 7.39−7.34 (m, 2H), 7.21 (d, *J* = 7.7 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.07 (d, *J* = 3.7 Hz, 1H), 4.75 (d, *J* = 5.1 Hz, 1H), 4.50 (dd, *J* = 5.0, 3.8 Hz, 1H), 4.29 (d, *J* = 7.1 Hz, 2H), 4.18 (d, *J* = 7.1 Hz, 2H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 169.0, 168.1, 153.0, 151.3, 148.9, 148.9, 147.6, 144.0, 133.9, 129.2, 125.1, 117.2, 82.8, 70.3, 62.8, 62.7, 57.9, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{22}N_5O_5^+$, 412.1615; found, 412.1628.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (6b)**



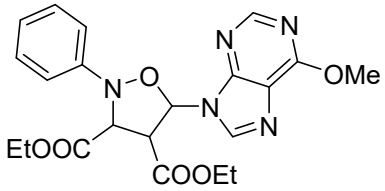

Yellow oil, Yield: 85% (37.9 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.90 (s, 1H), 8.81 (s, 1H), 7.35 (dd, *J* = 8.6 , 7.4 Hz, 2H), 7.24−7.20 (m, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.06 (d, *J* = 3.4 Hz, 1H), 4.71 (d, *J* = 5.2 Hz, 1H), 4.48 (dd, *J* = 5.1, 3.6 Hz, 1H), 4.30 (d, *J* = 7.1 Hz, 2H), 4.21 (d, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.23 (t, *J* = 7.2 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 168.8, 167.9, 152.4, 151.6, 151.3, 147.4, 144.1, 131.5, 129.2, 125.4, 117.5, 83.3, 70.3, 62.8, 62.8, 58.2, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{21}ClN_5O_5^+$, 446.1226; found, 446.1223.

**Diethyl 5-(6-bromo-9*H*-purin-9-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (6c)**




Yellow oil, Yield: 84% (41.2 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.90 (s, 1H), 8.75 (s, 1H), 7.34 (dd, *J* = 8.7, 7.4 Hz, 2H), 7.20 (dd, *J* = 8.6, 1.0 Hz, 2H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.04 (d, *J* = 3.4 Hz, 1H), 4.70 (d, *J* = 5.2 Hz, 1H), 4.47 (dd, *J* = 5.2, 3.4 Hz, 1H), 4.28 (d, *J* = 7.1 Hz, 2H), 4.20 (d, *J* = 7.1 Hz, 2H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.22 (t, *J* = 7.2 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 168.8, 167.9, 152.3, 150.4, 147.4, 143.9, 143.3, 134.1, 129.2, 125.4, 117.5, 83.3, 70.7, 62.8, 62.8, 58.2, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{21}BrN_5O_5^+$, 490.0721; found, 490.0720.

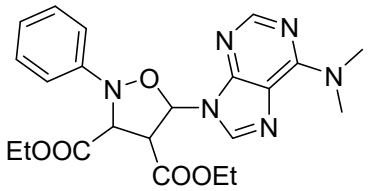
**Diethyl 5-(6-methoxy-9*H*-purin-9-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (6d)**




Yellow oil, Yield: 99% (43.7 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.62 (s, 1H), 8.59 (s, 1H), 7.38−7.33 (m, 2H), 7.20 (d, *J* = 7.8 Hz, 1H), 7.14 (t, *J* = 7.3 Hz, 1H), 6.99 (d, *J* = 3.9 Hz, 1H), 4.76 (d, *J* = 5.0 Hz, 1H), 4.54−4.50 (m, 1H), 4.29 (d, *J* = 7.1 Hz, 2H),

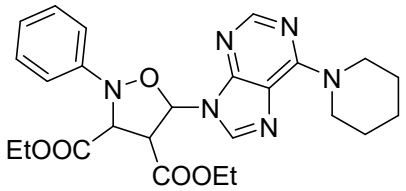
4.21 (s, 3H), 4.20−4.16 (m, 2H), 1.30 (t, $J$ = 7.2 Hz, 3H), 1.18 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 169.0, 168.2, 161.1, 152.5, 151.9, 147.9, 140.9, 129.2, 124.8, 121.3, 116.9, 83.2, 70.3, 62.7, 62.6, 57.8, 54.3, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{24}N_5O_6^+$, 442.1721; found, 442.1734.

**Diethyl 5-(6-(dimethylamino)-9*H*-purin-9-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (6e)**



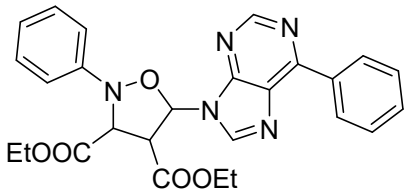

Yellow oil, Yield: 85% (38.6 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.40 (s, 1H), 8.37 (s, 1H), 7.32 (dd, $J$ = 8.5, 7.4 Hz, 2H), 7.19 (d, $J$ = 7.7 Hz, 2H), 7.11 (t, $J$ = 7.4 Hz, 1H), 6.93 (d, $J$ = 4.2 Hz, 1H), 4.77 (d, $J$ = 4.9 Hz, 1H), 4.48 (t, $J$ = 4.5 Hz, 1H), 4.29 (d, $J$ = 7.0 Hz, 2H), 4.14 (d, $J$ = 7.1 Hz, 2H), 3.54 (s, 6H), 1.30 (t, $J$ = 7.2 Hz, 3H), 1.16 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 169.2, 168.4, 154.9, 152.7, 150.6, 148.2, 136.7, 129.1, 124.5, 119.8, 116.7, 83.1, 70.4, 62.6, 62.5, 57.6, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{27}N_6O_5^+$, 455.2037; found, 455.2040.

**Diethyl 2-phenyl-5-(6-(piperidin-1-yl)-9*H*-purin-9-yl)isoxazolidine-3,4-dicarboxylate (6f)**




Yellow oil, Yield: 83% (41.0 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 8.41 (s, 1H), 8.35 (s, 1H), 7.32 (dd, $J$ = 8.6, 7.4 Hz, 2H), 7.22−7.18 (m, 2H), 7.11 (t, $J$ = 7.4 Hz, 1H), 6.93 (d, $J$ = 4.2 Hz, 1H), 4.77 (d, $J$ = 5.0 Hz, 1H), 4.48 (t, $J$ = 4.8 Hz, 1H), 4.35−4.28 (m, 3H), 4.26−4.25 (m, 3H), 4.14 (d, $J$ = 7.1 Hz, 2H), 1.75−1.69 (m, 6H), 1.30 (t, $J$ = 7.1 Hz, 3H), 1.16 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 169.2, 168.4, 153.8, 152.8, 150.9, 148.1, 136.5, 129.1, 124.5, 119.4, 116.7, 83.0, 70.4, 62.6, 62.5, 57.6, 26.5, 24.8, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{31}N_6O_5^+$, 495.2350; found, 495.2356.

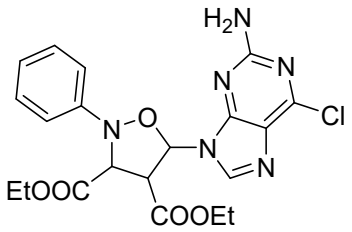
**Diethyl 2-phenyl-5-(6-phenyl-9*H*-purin-9-yl)isoxazolidine-3,4-dicarboxylate (6g)**




Yellow oil, Yield: 79% (38.5 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1H$ NMR ($CDCl_3$, 400 MHz) $\delta$ 9.06 (s, 1H), 8.86 (s, 1H), 8.82−8.79 (m, 2H), 7.60−7.53 (m, 3H), 7.34 (dd, $J$ = 8.5, 7.4 Hz, 2H), 7.22−7.18 (m, 2H), 7.15 (t, $J$ = 7.3 Hz, 1H), 7.10 (d, $J$ = 3.8 Hz, 1H), 4.77 (d, $J$ = 5.0 Hz, 1H), 4.54 (dd, $J$ = 5.0, 3.8 Hz, 1H), 4.29 (d, $J$ = 7.1 Hz, 2H), 4.18 (d, $J$ = 7.1 Hz, 2H), 1.29 (t, $J$ = 7.2 Hz, 3H), 1.20 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) $\delta$ 169.0, 168.2, 155.1,

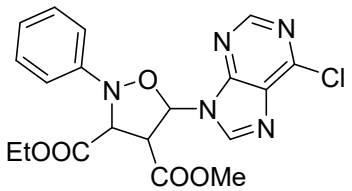
152.7, 147.8, 143.0, 135.4, 131.1, 130.8, 129.8, 129.2, 128.7, 125.0, 117.1, 83.1, 70.4, 62.7, 57.9, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{26}N_5O_5^+$, 488.1928; found, 488.1936.

**Diethyl 5-(2-amino-6-chloro-9*H*-purin-9-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (6h)**



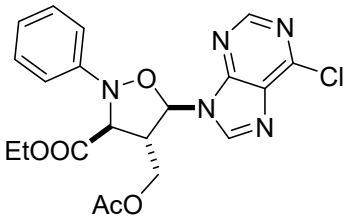

Yellow oil, Yield: 83% (38.3 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.47 (s, 1H), 7.32 (dd, $J$ = 8.6, 7.4 Hz, 2H), 7.18 (d, $J$ = 7.7 Hz, 2H), 7.14 (t, $J$ = 7.4 Hz, 1H), 6.78 (d, $J$ = 3.9 Hz, 1H), 5.33 (s, 2H), 4.69 (d, $J$ = 5.2 Hz, 1H), 4.43 (dd, $J$ = 5.1, 4.0 Hz, 1H), 4.29 (d, $J$ = 7.1 Hz, 2H), 4.17 (d, $J$ = 7.1 Hz, 2H), 1.30 (t, $J$ = 7.2 Hz, 3H), 1.20 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.9, 168.2, 159.3, 153.7, 151.5, 147.7, 140.8, 129.2, 125.0, 124.9, 117.1, 82.8, 70.3, 62.8, 62.6, 57.5, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{22}ClN_6O_5^+$, 461.1335; found, 461.1332.

**3-Ethyl 4-methyl 5-(6-chloro-9*H*-purin-9-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (6i)**




Yellow oil, Yield: 81% (35.0 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz), δ 8.88 (s, 1H), 8.80 (s, 1H), 7.34 (dd, $J$ = 8.6, 7.4 Hz, 2H), 7.23−7.19 (m, 2H), 7.19 (t, $J$ = 7.4 Hz, 1H), 7.03 (d, $J$ = 3.4 Hz, 1H), 5.33 (s, 2H), 4.69 (d, $J$ = 5.3 Hz, 1H), 4.52 (dd, $J$ = 5.3, 3.4 Hz, 1H), 4.28 (d, $J$ = 7.1 Hz, 2H), 3.79 (s, 3H), 1.28 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz), δ 168.7, 168.4, 152.3, 151.6, 151.3, 147.3, 144.0, 131.5, 129.2, 125.4, 117.6, 83.2, 70.1, 62.9, 58.0, 53.5, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{19}ClN_5O_5^+$, 432.1069; found, 432.1074.

**Ethyl 4-(acetoxymethyl)-5-(6-chloro-9*H*-purin-9-yl)-2-phenylisoxazolidine-3-carboxylate**

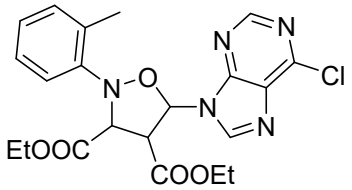



**(6k)**

Yellow oil, Yield: 52% (23.1 mg); $^1$H NMR ($CDCl_3$, 600 MHz) $\delta$ 8.93 (s, 1H), 8.76 (s, 1H), 7.36−7.34 (m, 2H), 7.17−7.13 (m, 3H), 6.59 (d, $J$ = 2.4 Hz, 1H), 4.45−4.43 (m, 1H), 4.39−4.36 (m, 1H), 4.32−4.27 (m, 2H), 4.03 (d, $J$ = 6.0 Hz, 1H), 3.75−3.71 (m, 1H), 1.99 (s, 3H), 1.28 (t, $J$ = 6.6 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 150 MHz) $\delta$ 170.6, 169.2, 152.3, 151.6, 151.3, 147.8, 144.3, 131.5, 129.3, 125.2, 117.4, 83.7, 69.9, 62.8, 62.6, 55.0, 29.8, 20.6, 14.1 ppm; HRMS (ESI)

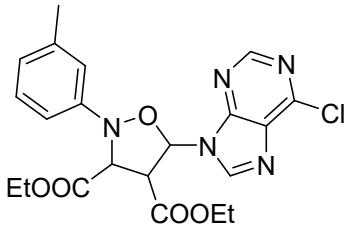
*m/z*: $[M + H]^+$ Calcd for $C_{20}H_{21}ClN_5O_5^+$, 446.1226; found, 446.1222.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(*o*-tolyl)isoxazolidine-3,4-dicarboxylate (6l)**



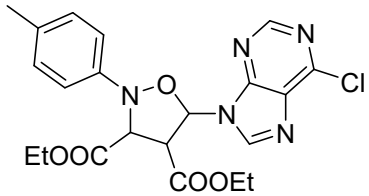

Yellow oil, Yield: 56% (25.7 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.80 (s, 1H), 8.42 (s, 1H), 7.32 (dd, $J$ = 7.8, 3.0 Hz, 1H), 7.17 (dd, $J$ = 7.2, 1.8 Hz, 1H), 7.13−7.12 (m, 2H), 7.10−7.07 (m, 1H), 5.01−4.99 (m, 1H), 4.97−4.95 (m, 1H), 4.26−4.18 (m, 2H), 3.92−3.83 (m, 2H), 2.35 (s, 3H), 1.23 (t, $J$ = 7.2 Hz, 3H), 0.89 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 150 MHz) $\delta$ 167.4, 166.7, 152.3, 151.8, 151.5, 144.4, 143.6, 132.1, 130.8, 129.6, 126.6, 126.3, 118.5, 83.4, 66.9, 62.3, 61.4, 56.2, 18.1, 14.0, 13.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{23}ClN_5O_5^+$, 460.1382; found, 460.1388.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(*m*-tolyl)isoxazolidine-3,4-dicarboxylate (6m)**




Yellow oil, Yield: 84% (38.6 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.90 (s, 1H), 8.80 (s, 1H), 7.24 (t, $J$ = 7.7 Hz, 1H), 7.04 (d, $J$ = 3.3 Hz, 1H), 7.03−6.97 (m, 3H), 4.67 (d, $J$ = 5.4 Hz, 1H), 4.45 (dd, $J$ = 5.4, 3.4 Hz, 1H), 4.35−4.28 (m, 2H), 4.21 (q, $J$ = 7.1 Hz, 2H), 2.35 (s, 3H), 1.30 (t, $J$ = 7.1 Hz, 3H), 1.23 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.9, 167.9, 152.3, 151.6, 151.2, 147.3, 144.1, 139.2, 131.4, 129.0, 126.2, 118.3, 114.6, 83.1, 70.2, 62.8, 62.7, 58.3, 21.5, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{23}ClN_5O_5^+$, 460.1382; found, 460.1379.

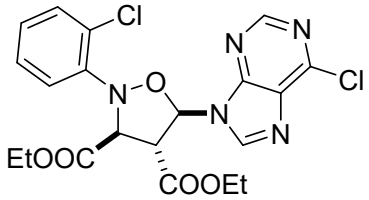
**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(*p*-tolyl)isoxazolidine-3,4-dicarboxylate (6n)**




Yellow oil, Yield: 88% (40.4 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.91 (s, 1H), 8.79 (s, 1H), 7.18−7.11 (m, 4H), 7.03 (d, $J$ = 3.2 Hz, 1H), 4.61 (d, $J$ = 5.7 Hz, 1H), 4.44 (dd, $J$ = 5.7, 3.3 Hz, 1H), 4.33−4.21 (m, 4H), 2.33 (s, 3H), 1.28 (t, $J$ = 7.2 Hz, 3H), 1.24 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.7, 168.0, 152.3, 151.6, 151.2, 144.7, 144.2, 135.7, 131.4, 129.7, 118.4, 83.1, 70.5, 62.7, 58.6, 20.8, 14.0, 14.0 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{23}ClN_5O_5^+$, 460.1382; found, 460.1390.

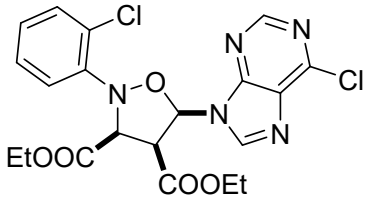
## dr (*endo*-6q/*exo*-6q) = 9:1

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(2-chlorophenyl)isoxazolidine-3,4-dicarboxylate (*endo*-6q)**



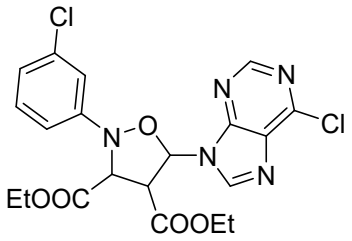

Yellow oil, Yield: 70% (33.7 mg), dr (*trans*/*cis*) = 9:1; $R_f$ = 0.31 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 600 MHz) $\delta$ 8.82 (s, 1H), 8.79 (s, 1H), 7.27 (t, $J$ = 7.8 Hz, 1H), 7.20 (t, $J$ = 1.8 Hz, 1H), 7.12−7.10 (m, 1H), 7.06−7.05 (m, 1H), 7.02 (d, $J$ = 3.6 Hz, 1H), 4.71 (d, $J$ = 4.8 Hz, 1H), 4.53−4.52 (m, 1H), 4.34−4.28 (m, 2H), 4.23 (q, $J$ = 7.2 Hz, 2H), 1.29 (t, $J$ = 7.2 Hz, 3H), 1.22 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 150 MHz) $\delta$ 168.6, 167.8, 152.4, 151.6, 151.4, 148.9, 143.9, 135.0, 131.6, 130.3, 125.1, 117.3, 115.1, 83.5, 70.0, 63.1, 63.0, 57.9, 14.0, 14.0 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{20}Cl_2N_5O_5^+$, 480.0836; found, 480.0830.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(2-chlorophenyl)isoxazolidine-3,4-dicarboxylate (*exo*-6q)**



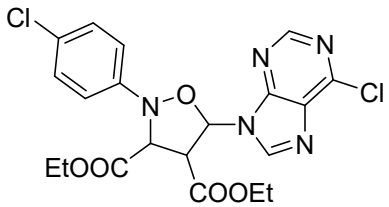

Yellow oil, Yield: 8% (3.7 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 600 MHz) $\delta$ 8.69 (s, 1H), 8.35 (s, 1H), 7.16 (t, $J$ = 8.4 Hz, 1H), 7.05 (d, $J$ = 5.4 Hz, 1H), 7.02−6.98 (m, 2H), 6.87 (d, $J$ = 10.2 Hz, 1H), 5.14−5.10 (m, 2H), 4.21 (q, $J$ = 7.2 Hz, 2H), 4.16−4.09 (m, 2H), 1.24 (t, $J$ = 7.2 Hz, 3H), 1.13 (t, $J$ = 7.2 Hz, 3H) ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{20}Cl_2N_5O_5^+$, 480.0836; found, 480.0830.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(3-chlorophenyl)isoxazolidine-3,4-dicarboxylate (6r)**



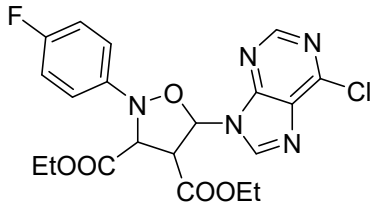

Yellow oil, Yield: 81% (38.8 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.74 (s, 1H), 8.73 (s, 1H), 7.20 (d, $J$ = 8.0 Hz, 1H), 7.14 (t, $J$ = 2.1 Hz, 1H), 7.08−7.04 (m, 1H), 7.01−6.98 (m, 1H), 6.94 (d, $J$ = 3.5 Hz, 1H), 4.63 (d, $J$ = 4.9 Hz, 1H), 4.43 (dd, $J$ = 4.8, 3.6 Hz, 1H), 4.22 (m, 2H), 4.14 (q, $J$ = 7.1 Hz, 2H), 1.23 (t, $J$ = 7.2 Hz, 3H), 1.16 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 167.5, 166.7, 151.4, 150.5, 150.3, 147.8, 142.8, 134.0, 130.5, 129.3, 124.0, 116.2, 114.0, 82.4, 68.9, 62.0, 61.9, 56.8, 12.9, 12.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{20}Cl_2N_5O_5^+$, 480.0836; found, 480.0833.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(4-chlorophenyl)isoxazolidine-3,4-dicarboxylate (6s)**



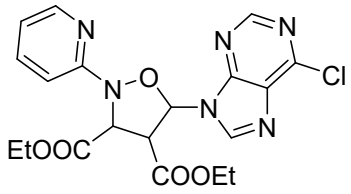

Yellow oil, Yield: 86% (41.2 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.84 (s, 1H), 8.80 (s, 1H), 7.32 (d, $J$ = 8.9 Hz, 1H), 7.14 (d, $J$ = 8.9 Hz, 2H), 7.01 (d, $J$ = 3.4 Hz, 1H), 4.65 (d, $J$ = 5.2 Hz, 1H), 4.49 (dd, $J$ = 5.2, 3.4 Hz, 1H), 4.28 (q, $J$ = 7.1 Hz, 2H), 4.22 (q, $J$ = 7.1 Hz, 2H), 1.30 (t, $J$ = 7.2 Hz, 3H), 1.24 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.5, 167.8, 152.4, 151.6, 151.3, 146.0, 143.9, 131.5, 130.7, 129.3, 118.9, 83.3, 70.2, 63.0, 62.9, 58.0, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{20}Cl_2N_5O_5^+$, 480.0836; found, 480.0833.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(4-fluorophenyl)isoxazolidine-3,4-dicarboxylate (6t)**



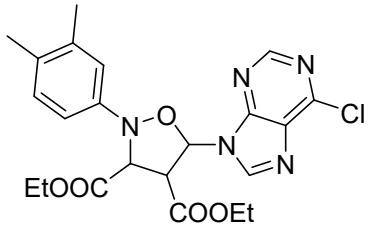

Yellow oil, Yield: 78% (36.1 mg); $^1$H NMR ($CDCl_3$, 600 MHz) $\delta$ 8.87 (s, 1H), 8.77 (s, 1H), 7.23−7.21 (m, 2H), 7.05−7.02 (m, 2H), 7.01 (d, $J$ = 3.0 Hz, 1H), 4.53 (d, $J$ = 6.0 Hz, 1H), 4.46−4.45 (m, 1H), 4.28−4.23 (m, 4H), 1.24 (td, $J$ = 7.2, 4.8 Hz, 6H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 150 MHz) $\delta$ 168.4, 168.0, 152.4, 151.7, 151.3, 144.1, 131.5, 120.9, 120.9, 116.1, 116.0, 83.1, 70.9, 62.9, 62.9, 58.6, 14.1, 14.0 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{20}ClFN_5O_5^+$, 464.1132; found, 464.1137.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(pyridin-2-yl)isoxazolidine-3,4-dicarboxylate (6u)**



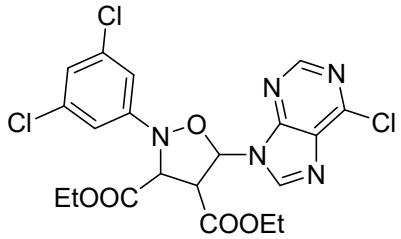

Yellow oil, Yield: 74% (33.0 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.84 (s, 1H), 8.80 (s, 1H), 8.27 (dq, $J$ = 4.9, 0.8 Hz, 1H), 7.73−7.68 (m, 1H), 7.22 (d, $J$ = 8.3 Hz, 1H), 7.02 (ddd, $J$ = 7.3, 4.9, 0.8 Hz, 1H), 6.99 (d, $J$ = 4.1 Hz, 1H), 5.64 (d, $J$ = 4.2 Hz, 1H), 4.49 (dd, $J$ = 5.2, 3.4 Hz, 1H), 4.44−4.37 (m, 2H), 4.24−4.14 (m, 2H), 1.37 (t, $J$ = 7.1 Hz, 3H), 1.22 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.8, 168.1, 159.1, 152.5, 151.7, 151.4, 147.5, 144.0, 138.6, 131.5, 119.5, 111.0, 84.1, 66.1, 62.7, 62.6, 56.2, 14.1, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{20}ClN_6O_5^+$, 447.1178; found, 447.1174.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(3,4-dimethylphenyl)isoxazolidine-3,4-dicarboxylate (6v)**



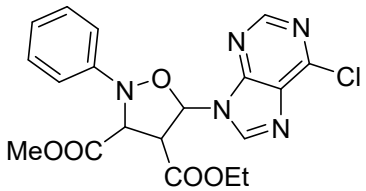

Yellow oil, Yield: 70% (33.1 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.93 (s, 1H), 8.79 (s, 1H), 7.09 (d, $J$ = 8.1 Hz, 1H), 7.02 (d, $J$ = 3.2 Hz, 1H), 7.01 (s, 1H), 6.95 (dd, $J$ = 8.1, 2.4 Hz, 1H), 4.58 (d, $J$ = 5.9 Hz, 1H), 4.42 (dd, $J$ = 5.9, 3.2 Hz, 1H), 4.33−4.27 (m, 2H), 4.23 (q, $J$ = 7.1 Hz, 2H), 2.25 (s, 3H), 2.23 (s, 3H), 1.31−1.23 (m, 6H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.7, 168.0, 152.3, 151.6, 151.2, 144.8, 144.2, 137.6, 134.5, 131.4, 130.1, 119.9, 115.8, 83.0, 70.3, 62.7, 62.7, 58.8, 14.0, 14.0 ppm; HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{22}H_{25}ClN_5O_5^+$, 474.1539; found, 474.1535.

**Diethyl 5-(6-chloro-9*H*-purin-9-yl)-2-(3,5-dichlorophenyl)isoxazolidine-3,4-dicarboxylate (6w)**



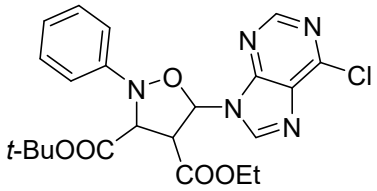

Yellow oil, Yield: 68% (34.9 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.81 (s, 1H), 8.75 (s, 1H), 7.13 (t, $J$ = 1.7 Hz, 1H), 7.07 (d, $J$ = 1.7 Hz, 2H), 6.98 (d, $J$ =3.5 Hz, 1H), 4.71 (d, $J$ = 4.6 Hz, 1H), 4.54 (dd, $J$ = 4.5, 3.8 Hz, 1H), 4.38−4.30 (m, 2H), 4.23 (q, $J$ = 7.1 Hz, 2H), 1.32 (t, $J$ = 7.1 Hz, 3H), 1.25 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.3, 167.5, 152.5, 151.5, 151.5, 149.6, 143.6, 135.7, 131.6, 124.6, 115.1, 83.6, 69.5, 63.2, 63.1, 57.5, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{20}H_{19}Cl_3N_5O_5^+$, 514.0446; found, 514.0443.

**4-Ethyl 3-methyl 5-(6-chloro-9*H*-purin-9-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (6x)**



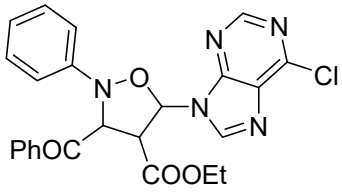

Yellow oil, Yield: 81% (35.0 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.86 (s, 1H), 8.80 (s, 1H), 7.39−7.34 (m, 2H), 7.19 (d, $J$ = 8.5 Hz, 2H), 7.15 (d, $J$ = 7.4 Hz, 1H), 7.04 (d, $J$ = 3.5 Hz, 1H), 4.78 (d, $J$ = 5.0 Hz, 1H), 4.49 (dd, $J$ = 5.0, 3.7 Hz, 1H), 4.19 (q, $J$ = 7.1 Hz, 2H), 3.87 (s, 3H), 1.21 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.4, 167.8, 152.4, 151.6, 151.3, 147.4, 144.0, 131.5, 129.3, 125.3, 117.2, 83.4, 70.1, 62.8, 58.0, 53.6, 13.9 ppm; HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{19}H_{19}ClN_5O_5^+$, 432.1069; found, 432.1065.

**3-(*tert*-Butyl) 4-ethyl 5-(6-chloro-9*H*-purin-9-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (6y)**




Yellow oil, Yield: 62% (29.3 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.92 (s, 1H), 8.80 (s, 1H), 7.34 (dd, $J$ = 8.6, 7.4 Hz, 2H), 7.23−7.20 (m, 2H), 7.17 (t, $J$ = 7.4 Hz, 1H), 7.04 (d, $J$ = 3.2 Hz, 1H), 4.51 (d, $J$ = 5.6 Hz, 1H), 4.41 (dd, $J$ = 5.6, 3.2 Hz, 1H), 4.21 (q, $J$ = 7.2 Hz, 2H), 1.47 (s, 9H), 1.24 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.1, 167.6, 152.3, 151.6, 151.2, 147.5, 144.2, 131.4, 129.1, 125.4, 117.9, 84.0, 83.0, 71.2, 62.7, 58.4, 27.8, 14.0 ppm; HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{22}H_{25}ClN_5O_5^+$, 474.1539; found, 474.1535.

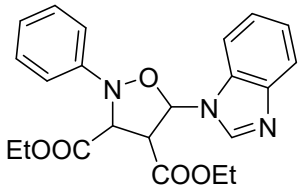
**Ethyl 3-benzoyl-5-(6-chloro-9*H*-purin-9-yl)-2-phenylisoxazolidine-4-carboxylate (6z)**




Yellow oil, Yield: 59% (28.2 mg); $R_f$ = 0.3 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 9.03 (s, 1H), 8.78 (s, 1H), 8.04 (d, $J$ = 7.4 Hz, 2H), 7.63 (t, $J$ = 7.4 Hz, 1H), 7.52−7.47 (m, 2H), 7.39−7.34 (m, 2H), 7.24 (d, $J$ = 7.9 Hz, 2H), 7.15 (d, $J$ = 7.3 Hz, 1H), 7.07 (d, $J$ = 4.2 Hz, 1H), 5.83 (d, $J$ = 4.1 Hz, 1H), 4.68 (t, $J$ = 4.1 Hz, 1H), 4.12 (q, $J$ = 7.1 Hz, 2H), 1.12 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 194.2, 168.6, 152.4, 151.2, 147.1, 144.4, 134.7, 134.4, 131.4, 129.5, 129.3, 128.9, 125.1, 116.7, 83.4, 71.2, 62.7, 56.4, 13.9 ppm; HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{24}H_{21}ClN_5O_4^+$, 478.1277; found, 478.1264.

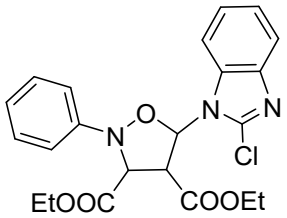
## 6. Characterization data of products 8

**Diethyl 5-(1*H*-benzo[*d*]imidazol-1-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (8a)**



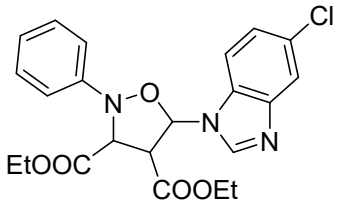

Yellow oil, Yield: 84% (34.4 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.38 (s, 1H), 7.86−7.83 (m, 1H), 7.71 (d, $J$ = 7.1 Hz, 1H), 7.40−7.32 (m, 4H), 7.20 (d, $J$ = 7.9 Hz, 1H), 7.13 (t, $J$ = 7.4 Hz, 1H), 6.63 (d, $J$ = 5.3 Hz, 1H), 4.84 (d, $J$ = 5.2 Hz, 1H), 4.47 (t, $J$ = 1.3 Hz, 1H), 4.31 (q, $J$ = 7.2 Hz, 2H), 4.13 (q, $J$ = 7.1 Hz, 2H), 1.31 (t, $J$ = 7.1 Hz, 3H), 1.18 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.0, 168.4, 148.3, 144.0, 141.6, 132.5, 129.3, 124.4, 123.7, 123.0, 120.7, 116.1, 110.5, 85.5, 70.4, 62.8, 62.6, 56.5, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{22}H_{24}N_3O_5^+$, 410.1710; found, 410.1716.

**Diethyl 5-(2-chloro-1*H*-benzo[*d*]imidazol-1-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (8b)**



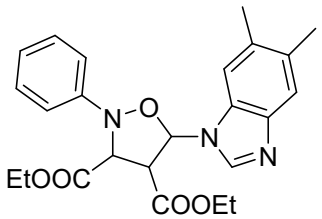

Yellow oil, Yield: 73% (32.3 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.10−8.07 (m, 1H), 7.75−7.72 (m, 1H), 7.41−7.33 (m, 4H), 7.22 (d, $J$ = 7.9 Hz, 2H), 7.13 (t, $J$ = 7.4 Hz, 1H), 6.64 (d, $J$ = 7.8 Hz, 1H), 4.88 (d, $J$ = 6.7 Hz, 1H), 4.75 (t, $J$ = 7.2 Hz, 1H), 4.37 (q, $J$ = 7.2 Hz, 2H), 4.19−4.09 (m, 2H), 1.31 (t, $J$ = 7.2 Hz, 3H), 1.17 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.2, 168.0, 148.9, 142.1, 140.1, 132.4, 129.5, 124.2, 124.1, 123.8, 119.8, 115.4, 112.5, 86.0, 70.6, 62.8, 62.6, 53.5, 14.1, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{23}ClN_3O_5^+$, 444.1321; found, 444.1312.

**Diethyl 5-(5-chloro-1*H*-benzo[*d*]imidazol-1-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (8c)**




Yellow oil, Yield: 83% (36.8 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.38 (s, 1H), 7.82 (d, $J$ = 1.8 Hz, 1H), 7.67 (d, $J$ = 8.6 Hz, 1H), 7.39−7.35 (m, 2H), 7.35−7.32 (m, 1H), 7.22−7.19 (m, 2H), 7.14 (t, $J$ = 7.4 Hz, 1H), 6.60 (d, $J$ = 5.1 Hz, 1H), 4.80 (d, $J$ = 5.4 Hz, 1H), 4.43 (t, $J$ = 4.1 Hz, 1H), 4.30 (q, $J$ = 7.1 Hz, 2H), 4.14 (q, $J$ = 7.1 Hz, 2H), 1.31 (t, $J$ = 7.1 Hz, 3H), 1.19 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.9, 168.3, 148.0, 144.8, 142.9, 131.1, 129.3, 128.7, 124.2, 120.4, 116.4, 111.5, 85.5, 70.3, 62.8, 62.7, 56.7, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{23}ClN_3O_5^+$, 444.1321; found, 444.1313.

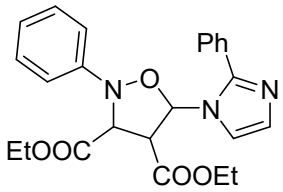
**Diethyl 5-(5,6-dimethyl-1*H*-benzo[*d*]imidazol-1-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (8d)**




Yellow oil, Yield: 73% (31.9 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.23 (s, 1H), 7.59 (s, 1H), 7.47 (s, 1H), 7.34 (dd, $J$ = 8.7, 7.4 Hz, 2H), 7.22−7.19 (m, 2H), 7.12 (t, $J$ = 7.4 Hz, 1H), 6.55 (d, $J$ = 5.5 Hz, 1H), 4.85 (d, $J$ = 5.3 Hz, 1H), 4.47 (t, $J$ = 5.4 Hz, 1H), 4.38−4.31 (m, 2H), 4.12 (q, $J$ = 7.2 Hz, 2H), 2.42 (s, 3H), 2.39 (s, 3H), 1.32 (t, $J$ = 7.2 Hz, 3H), 1.17 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.1, 168.6, 148.5, 142.6, 140.9, 132.9, 131.9, 131.0, 129.3, 124.2, 120.6, 115.9, 110.7, 85.6, 70.3, 62.7, 62.5, 56.2, 20.6, 20.2, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{28}N_3O_5^+$, 438.2023; found,

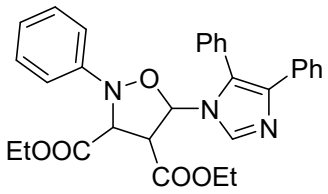
438.2026.

**Diethyl 2-phenyl-5-(2-phenyl-1*H*-imidazol-1-yl)isoxazolidine-3,4-dicarboxylate (8e)**



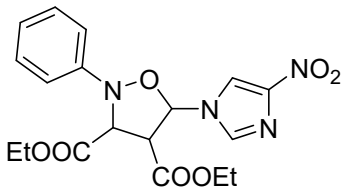

Yellow oil, Yield: 79% (34.4 mg); $R_f$ = 0.30 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.74 (d, $J$ = 1.5 Hz, 1H), 7.67−7.64 (m, 2H), 7.48−7.45 (m, 3H), 7.26 (dd, $J$ = 8.7, 7.4 Hz, 2H), 7.22 (d, $J$ = 1.1 Hz, 1H), 7.12−7.08 (m, 2H), 7.04 (d, $J$ = 7.4 Hz, 1H), 6.42 (d, $J$ = 5.1 Hz, 1H), 4.77 (d, $J$ = 4.8 Hz, 1H), 4.38−4.31 (m, 3H), 4.04−3.98 (m, 2H), 1.33 (t, $J$ = 7.2 Hz, 3H), 1.10 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.3, 168.5, 149.2, 148.0, 129.9, 129.4, 129.1, 128.6, 124.3, 118.1, 116.2, 85.6, 70.5, 62.7, 62.3, 57.2, 14.0, 13.7 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{26}N_3O_5^+$, 436.1867; found, 436.1868.

**Diethyl 5-(4,5-diphenyl-1*H*-imidazol-1-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (8f)**



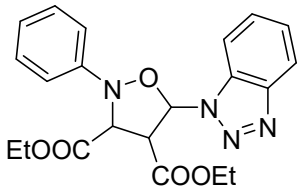

Yellow oil, Yield: 74% (37.9 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.28 (s, 1H), 7.45−7.41 (m, 3H), 7.41 (d, $J$ = 2.8 Hz, 2H), 7.38−7.34 (m, 2H), 7.16−7.11 (m, 4H), 7.10−7.06 (m, 1H), 6.95 (t, $J$ = 7.4 Hz, 1H), 6.88 (d, $J$ = 7.7 Hz, 2H), 5.96 (d, $J$ = 5.2 Hz, 1H), 4.65 (d, $J$ = 4.7 Hz, 1H), 4.35 (t, $J$ = 4.9 Hz, 1H), 4.30−4.23 (m, 2H), 3.92 (q, $J$ = 7.1 Hz, 2H), 1.31 (t, $J$ = 7.2 Hz, 3H), 0.97 (t, $J$ = 7.1 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.0, 168.4, 148.0, 138.2, 135.5, 134.0, 131.3, 129.7, 129.2, 129.0, 128.6, 128.1, 126.7, 126.6, 124.2, 116.1, 84.2, 70.8, 62.8, 62.3, 56.8, 14.1, 13.8 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{30}N_3O_5^+$, 512.2180; found, 512.2183.

**Diethyl 5-(4-nitro-1*H*-imidazol-1-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (8g)**



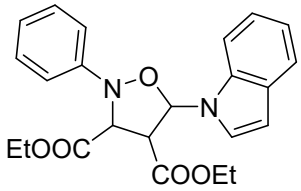

Yellow oil, Yield: 89% (36.0 mg); $R_f$ = 0.20 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.89 (d, $J$ = 1.6 Hz, 1H), 7.39−7.34 (m, 2H), 7.21−7.18 (m, 2H), 7.18−7.17 (m, 1H), 6.45 (d, $J$ = 3.6 Hz, 1H), 6.42 (d, $J$ = 5.1 Hz, 1H), 4.61 (d, $J$ = 5.6 Hz, 1H), 4.30 (q, $J$ = 7.1 Hz, 2H), 4.28−4.20 (m, 3H), 1.31 (t, $J$ = 7.2 Hz, 3H), 1.25 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.4, 167.7, 146.9, 135.4, 129.3, 125.7, 118.1, 117.7, 86.4, 70.2, 63.0, 59.1, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{18}H_{21}N_4O_7^+$, 405.1405; found, 405.1407.

**Diethyl 5-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (8h)**




Yellow oil, Yield: 98% (40.2 mg); $R_f$ = 0.25 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.09 (d, $J$ = 8.4 Hz, 1H), 8.05 (d, $J$ = 8.4 Hz, 1H), 7.60−7.55 (m, 1H), 7.32 (dd, $J$ = 8.7, 7.4 Hz, 2H), 7.23−7.19 (m, 2H), 7.12 (t, $J$ = 7.4 Hz, 1H), 7.08 (d, $J$ = 4.5 Hz, 1H), 7.03−6.97 (m, 3H), 5.14 (dd, $J$ = 5.6, 4.5 Hz, 1H), 4.85 (d, $J$ = 5.6 Hz, 1H), 4.39−4.30 (m, 2H), 4.16 (q, $J$ = 7.1 Hz, 2H), 1.32 (t, $J$ = 7.2 Hz, 3H), 1.19 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 168.6, 168.4, 148.3, 146.8, 132.0, 129.1, 128.3, 124.6, 124.6, 120.2, 116.7, 111.0, 87.6, 70.3, 62.6, 62.6, 55.8, 14.0, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{23}N_4O_5^+$, 411.1663; found, 411.1667.

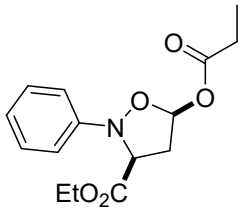
**Diethyl 5-(1*H*-indol-1-yl)-2-phenylisoxazolidine-3,4-dicarboxylate (8i)**




Yellow oil, Yield: 71% (29.0 mg); $R_f$ = 0.35 (PE/EA = 3:1, v/v); $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.63 (d, $J$ = 7.8 Hz, 1H), 7.58 (d, $J$ = 3.4 Hz, 1H), 7.54 (d, $J$ = 8.3 Hz, 1H), 7.33 (dd, $J$ = 8.6, 7.4 Hz, 2H), 7.29−7.26 (m, 1H), 7.21−7.17 (m, 3H), 7.08 (t, $J$ = 7.3 Hz, 1H), 6.67 (d, $J$ = 6.2 Hz, 1H), 6.64 (d, $J$ = 3.4 Hz, 1H), 4.93 (d, $J$ = 4.7 Hz, 1H), 4.41 (dd, $J$ = 6.2, 4.8 Hz, 1H), 4.45−4.32 (m, 2H), 4.13−4.04 (m, 2H), 1.35 (t, $J$ = 7.2 Hz, 3H), 1.10 (t, $J$ = 7.2 Hz, 3H) ppm; $^{13}$C{$^1$H} NMR ($CDCl_3$, 100 MHz) $\delta$ 169.7, 169.1, 149.2, 136.2, 129.3, 129.2, 125.0, 123.5, 122.4, 121.2, 120.7, 115.0, 109.6, 104.7, 86.4, 70.6, 62.6, 62.2, 55.8, 14.1, 13.9 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{25}N_2O_5^+$, 409.1758; found, 409.1762.

## 7. Characterization data of products 11

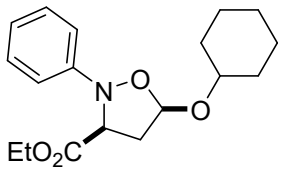
## Ethyl 2-phenyl-5-(propionyloxy)isoxazolidine-3-carboxylate (11a)




Yellow oil, 16.7 mg, 57% yield. Silica gel TLC $R_f$ = 0.20 (PE:EA = 15:1); **$^1$H NMR** (600 MHz, $CDCl_3$) $\delta$ 7.29 (t, $J$ = 8.4 Hz, 2H), 7.23 (d, $J$ = 8.4 Hz, 2H), 7.04 (t, $J$ = 7.2 Hz, 1H), 6.63 (d, $J$ = 5.4 Hz, 2H), 4.36−4.30 (m, 2H), 4.21 (dd, $J$ = 9.3, 3.0 Hz, 2H), 2.83−2.75 (m, 2H), 2.41−2.32 (m, 2H), 1.35 (t, $J$ = 7.2 Hz, 3H), 1.14 (t, $J$ = 7.2 Hz, 3H) ppm; **$^{13}$C{$^1$H} NMR** (150 MHz, $CDCl_3$) $\delta$

172.4, 169.2, 149.0, 127.8, 127.5, 122.4, 114.9, 112.9, 93.4, 65.6, 60.9, 37.4, 26.6, 13.1, 7.6 ppm; HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{20}NO_5^+$, 294.1336; found, 294.1341.

### Ethyl 5-(cyclohexyloxy)-2-phenylisoxazolidine-3-carboxylate (11b)




Yellow oil, 16.2 mg, 51% yield. Silica gel TLC $R_f$ = 0.20 (PE:EA = 10:1); **$^1$H NMR** (600 MHz, $CDCl_3$) $\delta$ 7.27−7.25 (m, 2H), 7.06 (d, $J$ = 7.8 Hz, 2H), 6.99 (t, $J$ = 7.2, 1H), 5.59 (dd, J = 5.4, 1.2), 4.36-4.30 (m, 1H), 4.29-4.24 (m, 1H), 4.20 (dd, J = 6, 2.4, 1H), 3.75-3.71(m, 1H), 2.68-2.65(m, 1H), 2.52-2.48(m, 1H), 1.92-1.91(m, 2H), 1.73-1.71(m, 2H), 1.53-1.51 (m, 1H), 1.43-1.37 (m, 1H), 1.33 (t, J = 14.4, 3H), 1.30-1.26(m, 3H), 1.23-1.91(m, 1H); **$^{13}$C{$^1$H} NMR** (150 MHz, $CDCl_3$) $\delta$ 170.9, 151.1, 128.7, 122.5, 115.5, 98.8, 67.3, 61.6, 61.6, 38.4, 33.3, 31.4, 25.7, 24.0, 23.9, 14.27 ppm; HRMS (ESI) m/z: [M + H]+ Calcd for $C_{18}H_{26}NO_4^+$, 320.1856; found, 320.1851.

## 8. References

(1) (a) Shi, T.; Teng, S.; Wei, Y.; Guo, X.; Hu, W. Synthesis of Spiro[2,3-dihydrofuran-3,3'-oxindole] Derivatives via a Multi-component Cascade Reaction of α-Diazo Esters, Water, Isatins and Malononitrile/Ethyl Cyanoacetate. *Green Chem.* **2019**, *21*, 4936. (b) Gallo, R. D. C.; Burtoloso, A. C. B. Silica-supported $HClO_4$ Promotes Catalytic Solvent- and Metal-Free O-H Insertion Reactions with Diazo Compounds. *Green Chem.* **2018**, *20*, 4547.

(2) Synthesis of nitrosoarenes, See: (a) Priewisch, B.; Rück-Braun, K. Efficient Preparation of Nitrosoarenes for the Synthesis of Azobenzenes. *J. Org. Chem.* **2005**, *70*, 2350. (b) Hu, W.; Yu, J.-T.; Liu, S.; Jiang, Y.; Cheng, J. Copper-mediated Annulation of 2-(1-Arylvinyl) Anilines and Aryl Nitrosos towards 2,3-Diaryl-2*H*-indazoles. *Org. Chem. Front.* **2017**, *4*, 22. (c) Wang, Q.; Li, X. Synthesis of 1*H*-Indazoles from Imidates and Nitrosobenzenes via Synergistic Rhodium/Copper Catalysis. *Org. Lett.* **2016**, *18*, 2102.

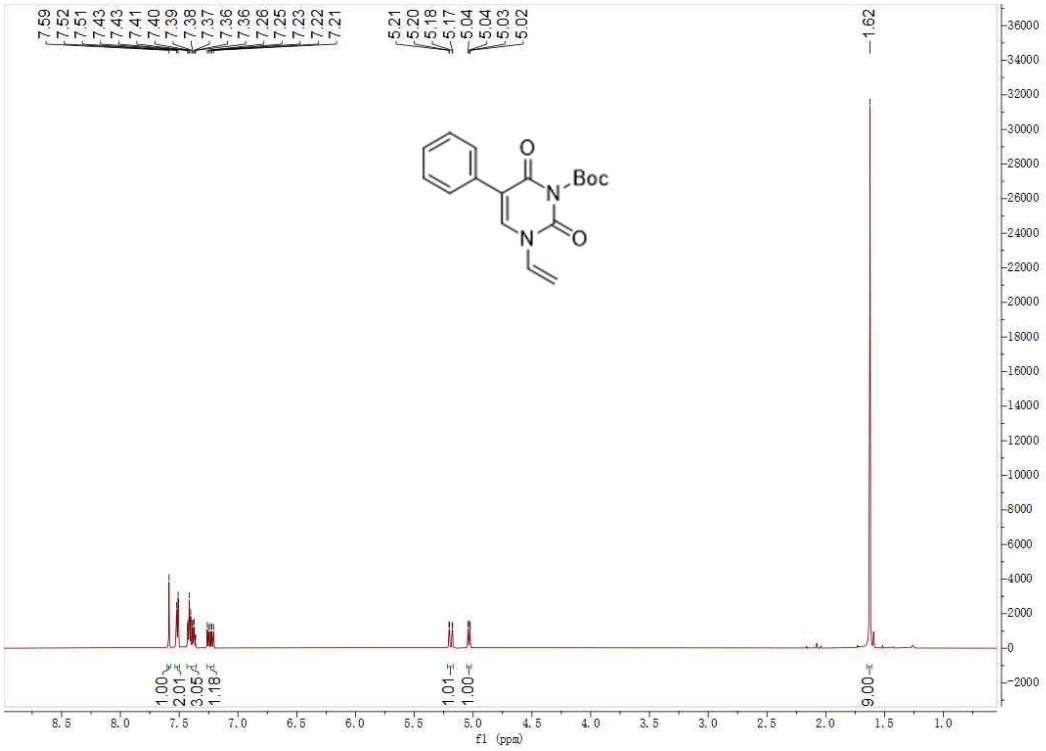
(3) (a) Buslov, I.; Hu, X. Transition-Metal-Free Intermolecular α-C-H Amination of Ethers at Room Temperature. *Adv. Synth. Catal.* **2014**, *356*, 3325. (b) Xie, M.-S.; Zhou, P.; Niu, H.-Y.; Qu, G.-R.; Guo, H.-M. Enantioselective Intermolecular Cyclopropanations for the Synthesis of Chiral Pyrimidine Carbocyclic Nucleosides. *Org. Lett.* **2016**, *18*, 4344.

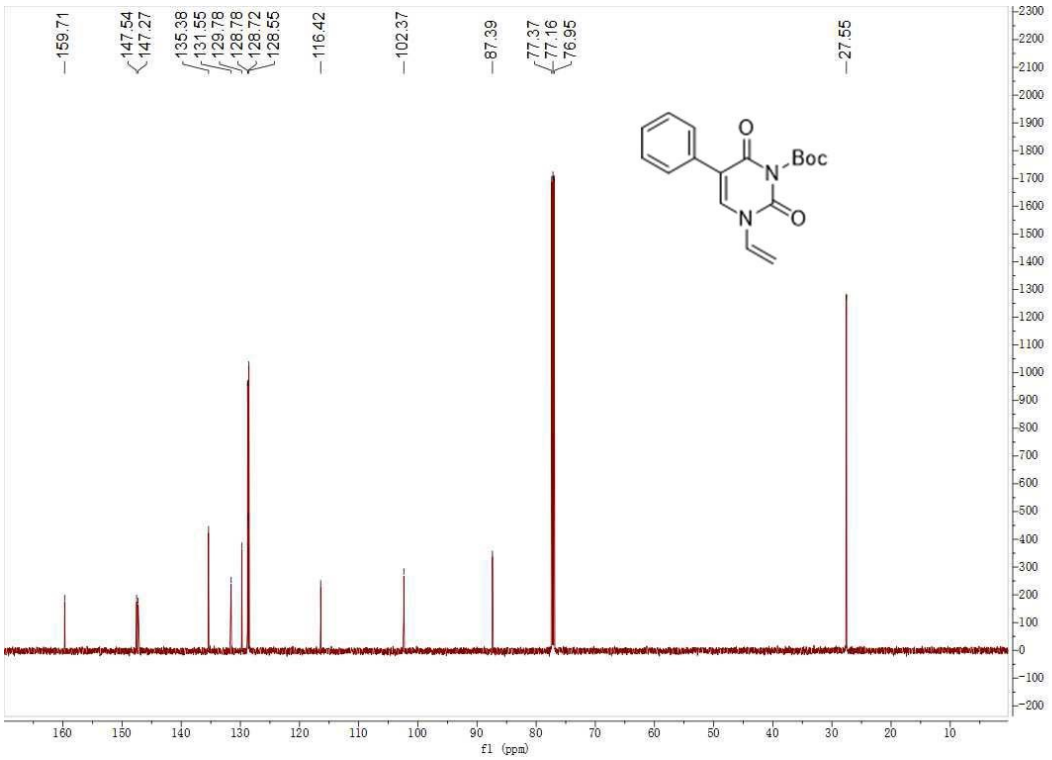
(4) (a) Yang, Q.-L.; Xie, M.-S.; Xia, C.; Sun, H.-L.; Zhang, D.-J.; Huang, K.-X.; Guo, Z.; Qu, G.-R.; Guo, H.-M. A Rapid and Divergent access to Chiral Azacyclic Nucleoside Analogues via Highly Enantioselective 1,3-Dipolar Cycloaddition of *β*-Nucleobase Substituted Acrylates. *Chem. Commun.* **2014**, *50*, 14809. (b) Gao, Y.-W.; Niu, H.-Y.; Zhang, Q.-Y.; Xie, M.-S.; Qu, G.-R.; Guo, H.-M. Regio- and Enantioselective [3+2] Cycloaddition of

α-Purine Substituted Acrylates with Allenes: An Approach to Chiral Carbocyclic Nucleosides. *Adv. Synth. Catal.* **2018**, *360*, 2813. (c) Huang, K.-X.; Xie, M.-S.; Zhao, G.-F.; Qu, G.-R.; Guo, H.-M. Synthesis of Chiral Cyclopropyl Carbocyclic Purine Nucleosides via Asymmetric Intramolecular Cyclopropanations Catalyzed by a Chiral Ruthenium(II) Complex. *Adv. Synth. Catal.* **2016**, *358*, 3627. (d) Wei, T.; Xie, M.-S.; Qu, G.-R.; Niu, H.-Y.; Guo, H.-M. A New Strategy To Construct Acyclic Nucleosides via Ag(I)-Catalyzed Addition of Pronucleophiles to 9-Allenyl-9*H*-Purines. *Org. Lett.* **2014**, *16*, 900.

## 9. $^{1}$H-NMR and $^{13}$C-NMR spectra of substrate 3g

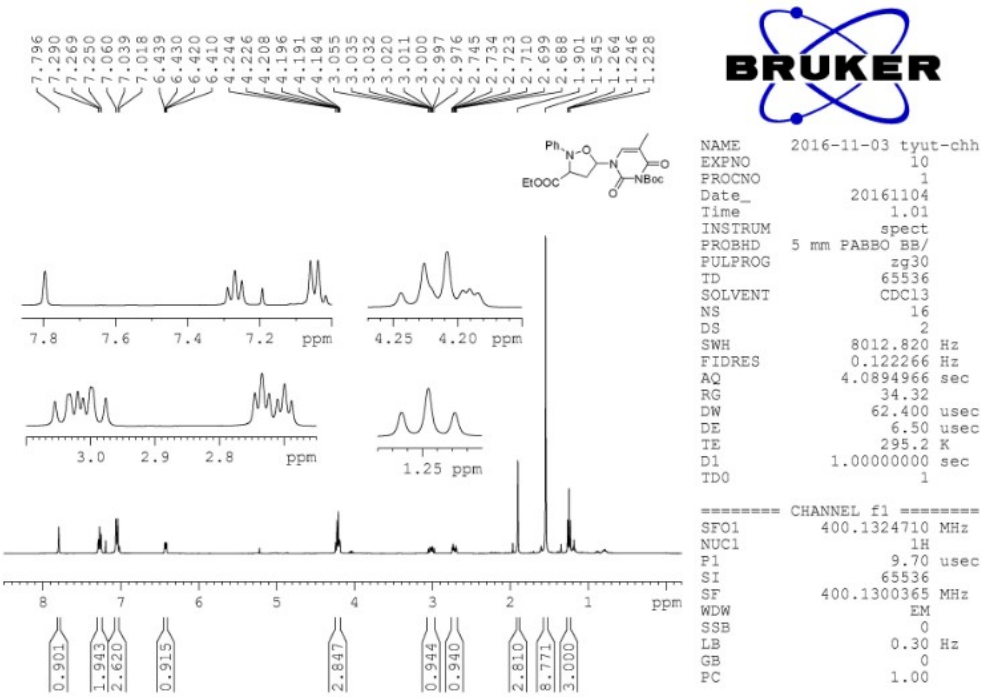
**3g**

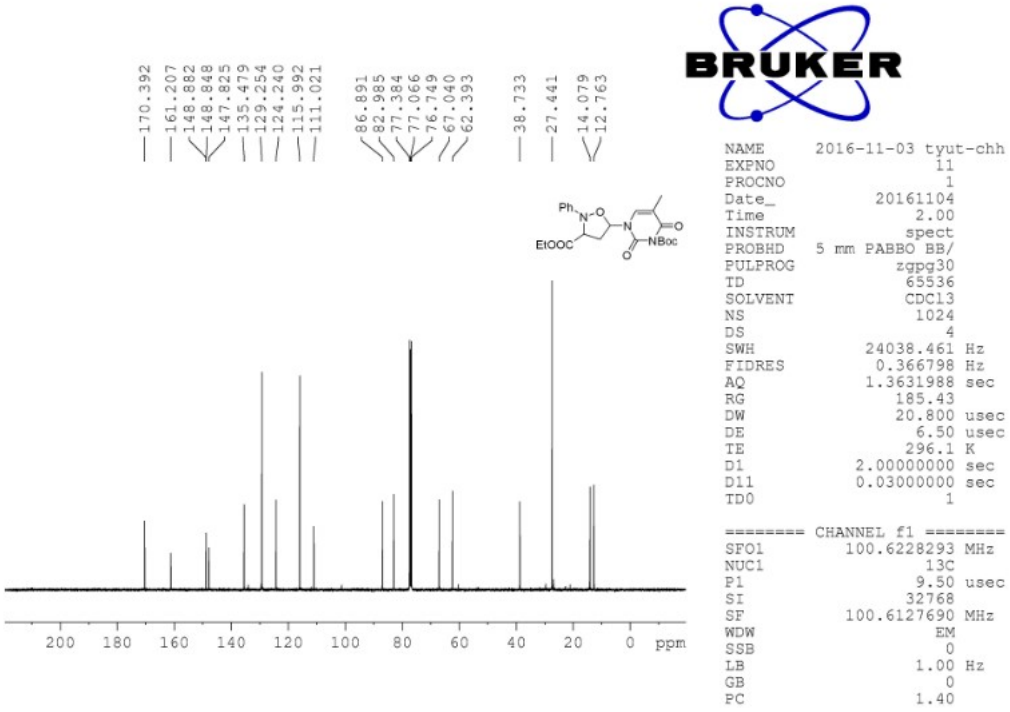





## 10. $^{1}$H- and $^{13}$C-NMR spectra of products 4

### 4a

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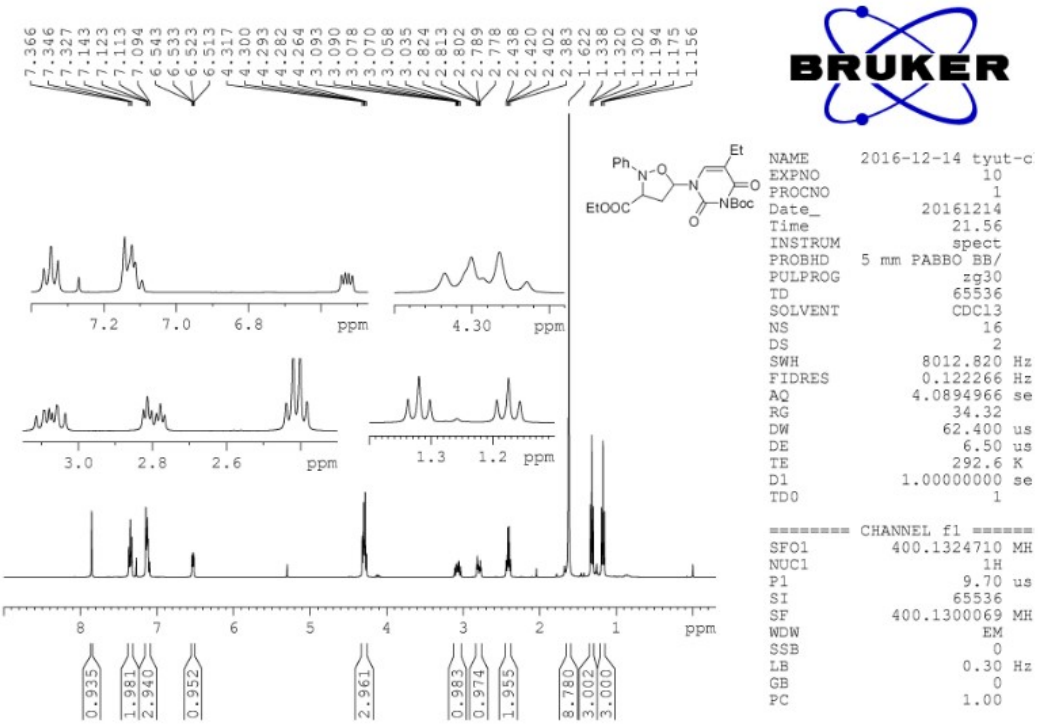
**4b**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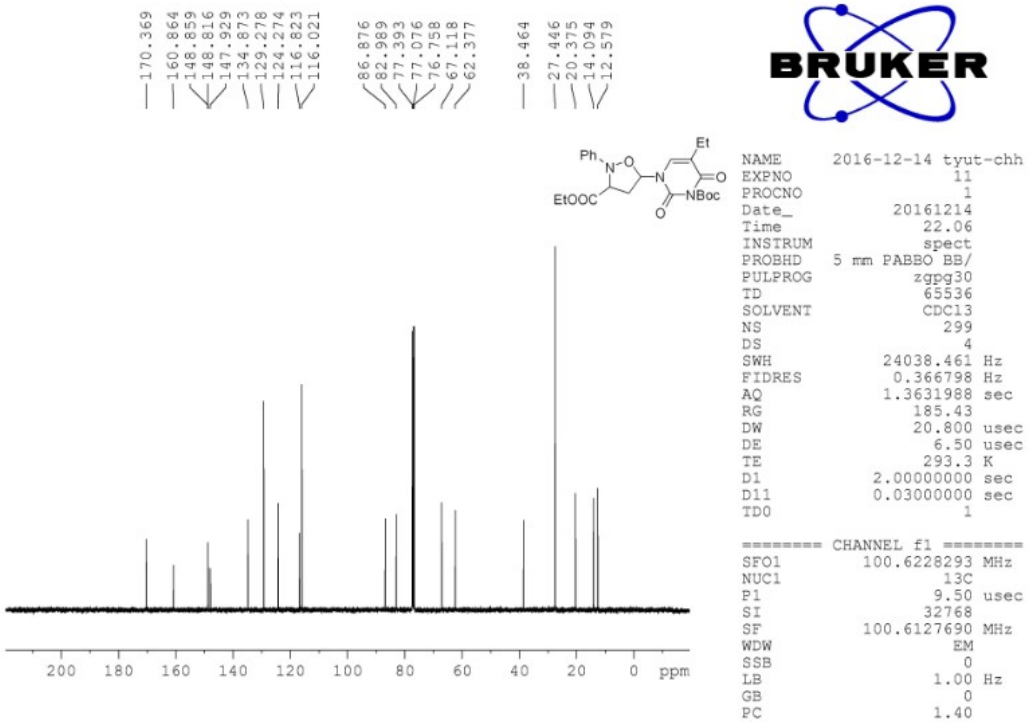
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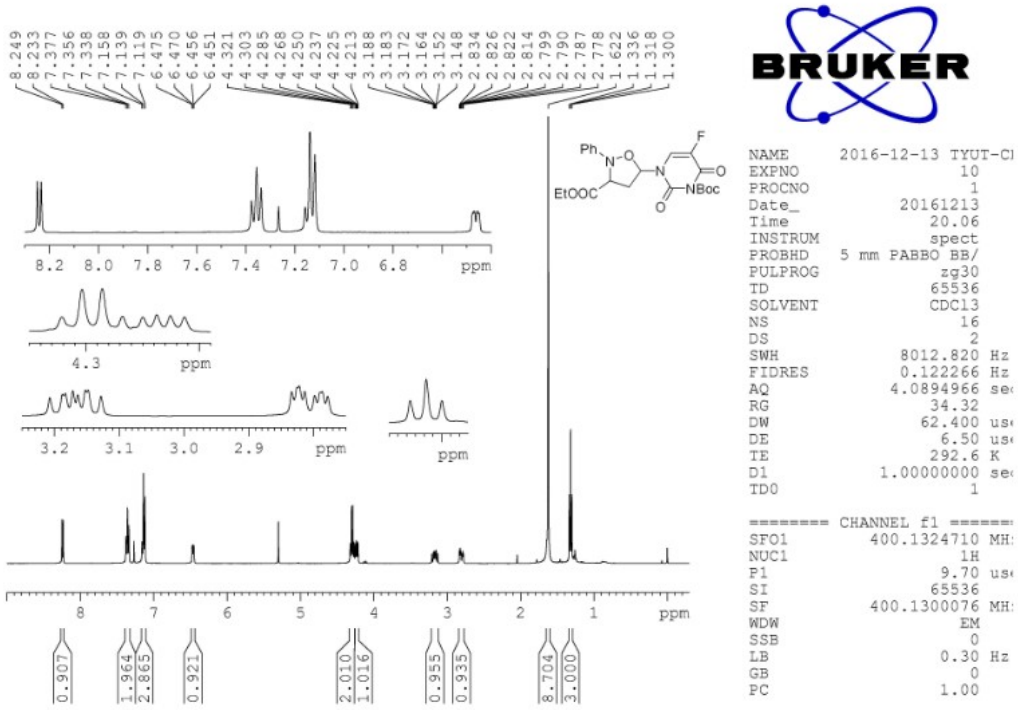
**4c**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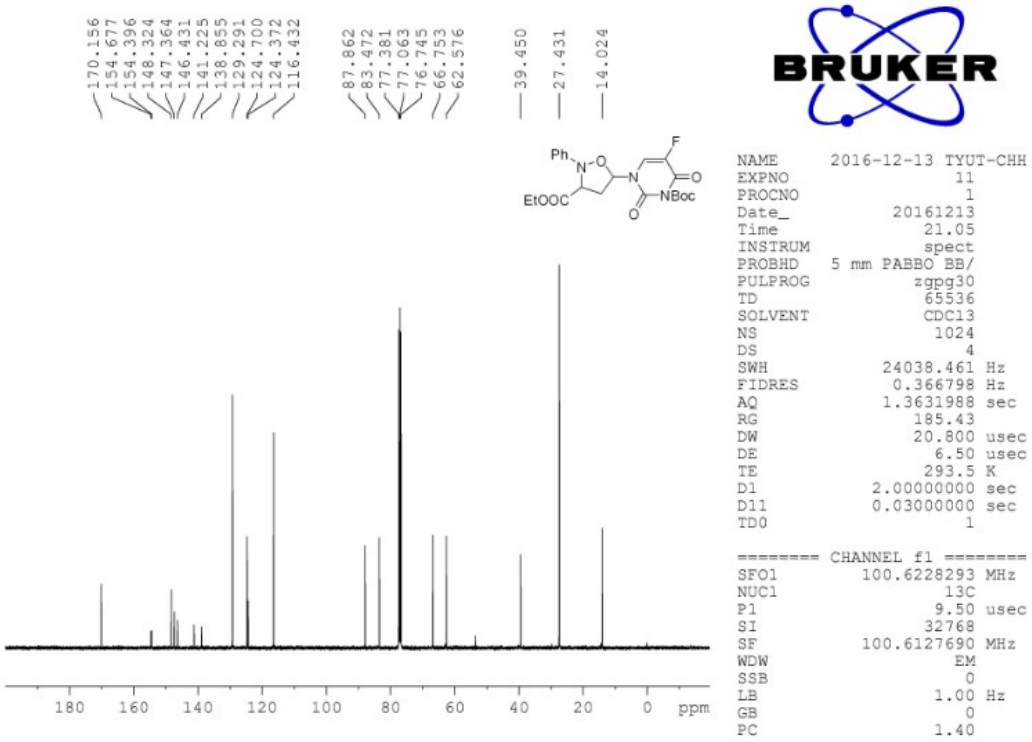
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FIDRES 0.366798 Hz
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RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 293.5 K
D1 2.00000000 sec
D11 0.03000000 sec
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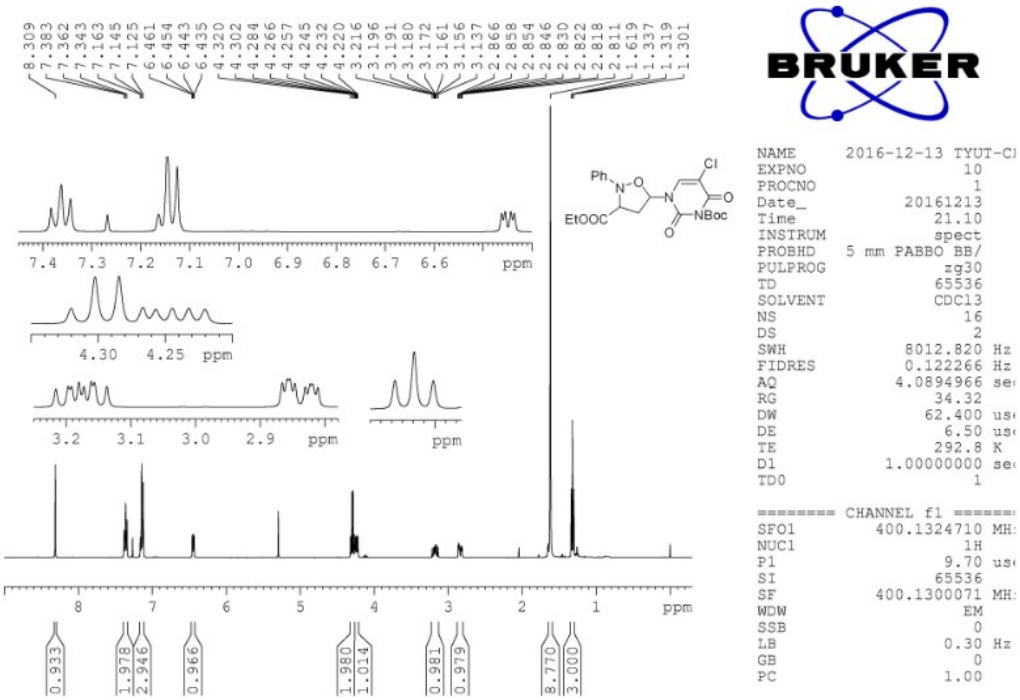
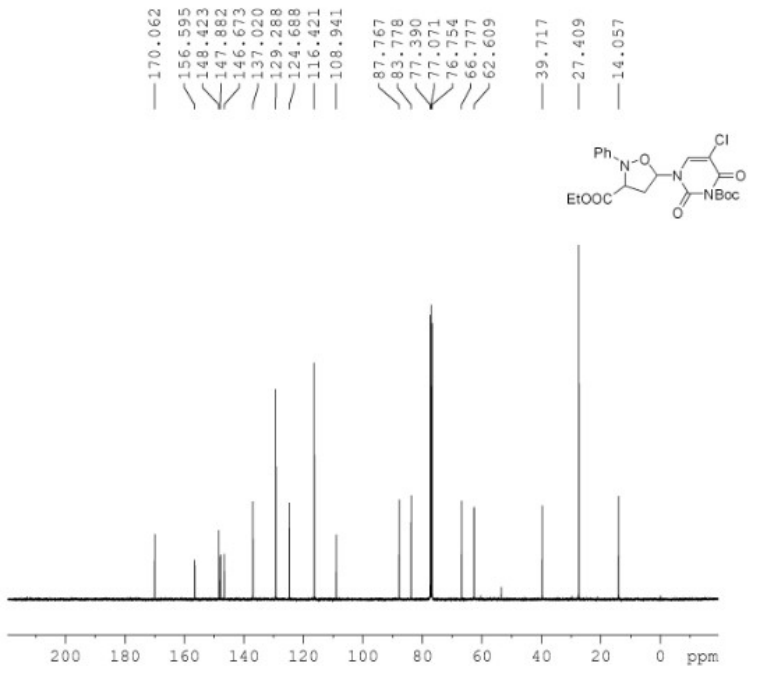
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

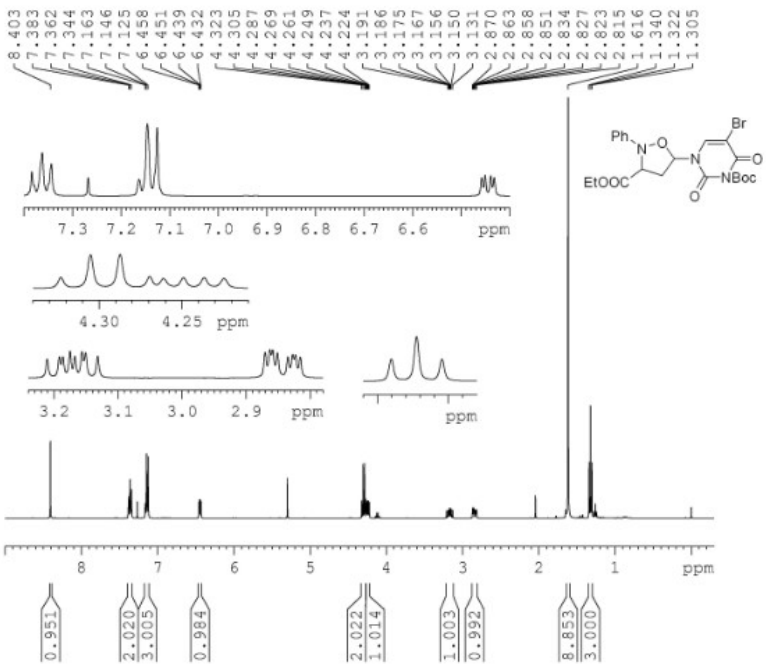
**4d**


8.309
7.383
7.362
7.343
7.163
7.145
7.125
6.461
6.454
6.443
6.435
4.320
4.302
4.284
4.266
4.257
4.245
4.232
4.220
3.216
3.196
3.191
3.180
3.172
3.161
3.156
3.137
2.866
2.858
2.854
2.846
2.830
2.822
2.818
2.811
1.619
1.337
1.319
1.301
Ph
EtOOC
Cl
NBoc
7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 ppm
4.30 4.25 ppm
3.2 3.1 3.0 2.9 ppm
ppm
8 7 6 5 4 3 2 1 ppm
0.933
1.978
2.946
0.966
1.980
1.014
0.981
0.979
8.770
3.000
BRUKER
NAME 2016-12-13 TYUT-CI
EXPNO 10
PROCNO 1
Date_ 20161213
Time 21.10
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 se
RG 34.32
DW 62.400 us
DE 6.50 us
TE 292.8 K
D1 1.00000000 se
TD0 1
======== CHANNEL f1 ======
SFO1 400.1324710 MH
NUC1 1H
P1 9.70 us
SI 65536
SF 400.1300071 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

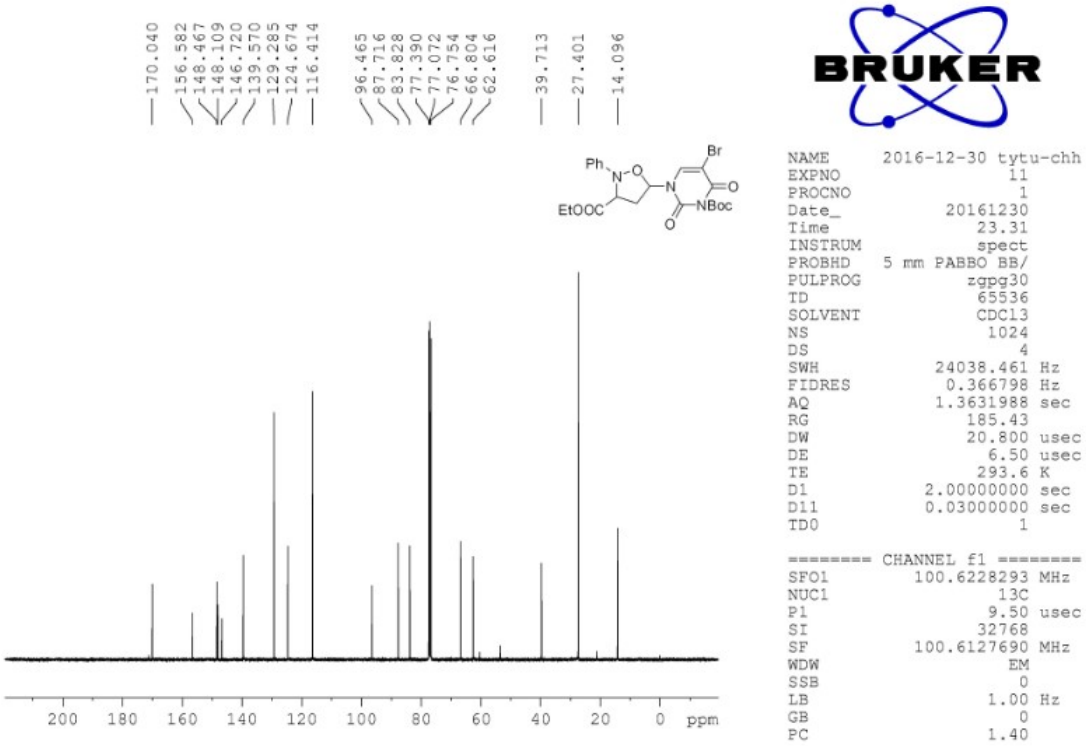



```
NAME          2016-12-13 TYUT-CHH
EXPNO                     11
PROCNO                     1
Date_                 20161213
Time                     22.09
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  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                       293.5 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
```

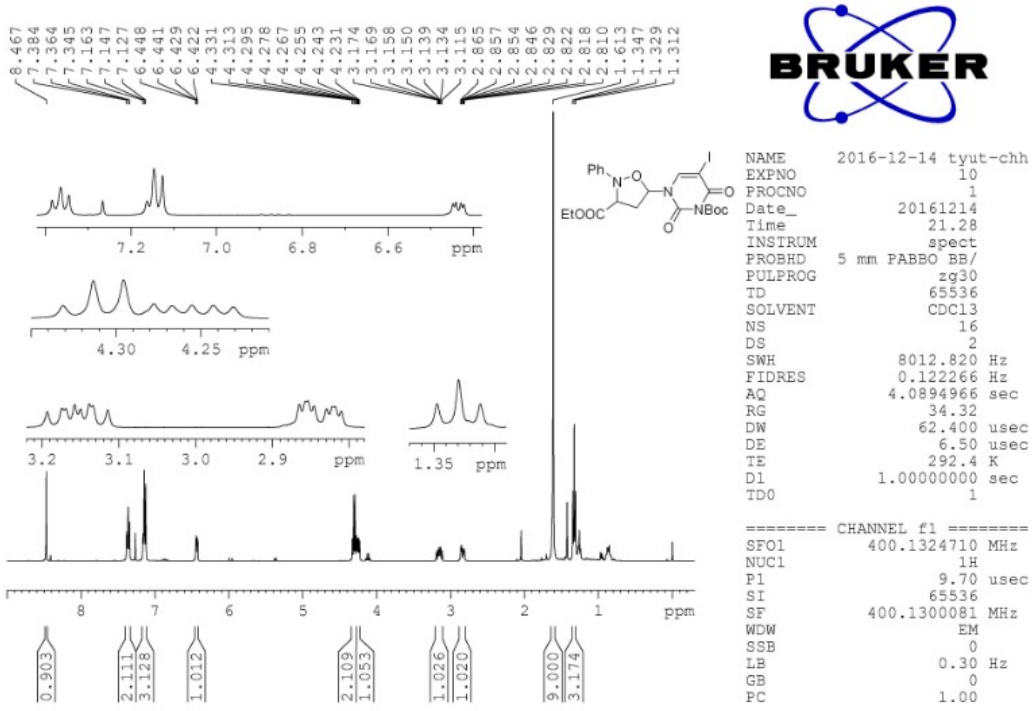
**4e**

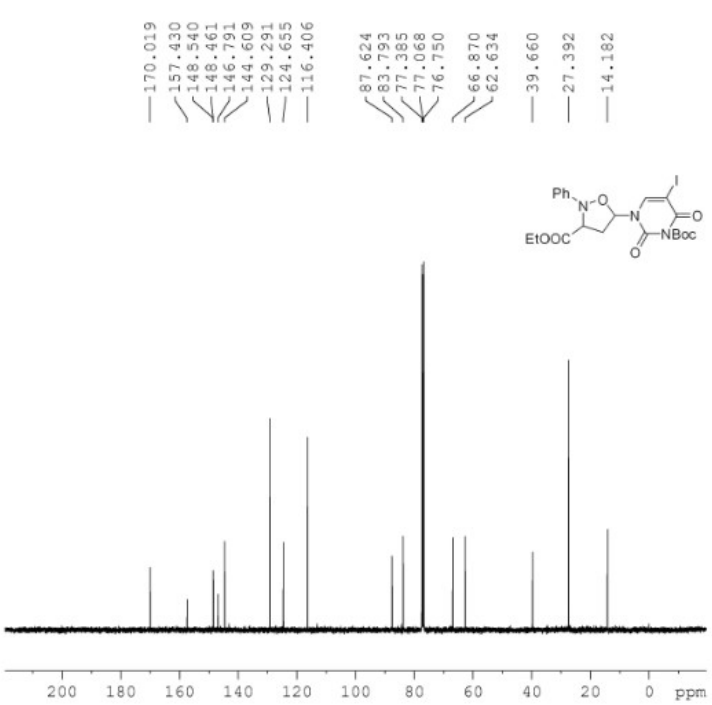



```
NAME          2016-12-30 tytu-chh
EXPNO                     10
PROCNO                     1
Date_                 20161230
Time                     22.32
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  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                       292.7 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                        9.70 usec
SI                       65536
SF                  400.1300069 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```


170.040
156.582
148.467
148.109
146.720
139.570
129.285
124.674
116.414
96.465
87.716
83.828
77.390
77.072
76.754
66.804
62.616
39.713
27.401
14.096
Br
Ph
N
O
N
O
NBoc
O
EtOOC
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
NAME 2016-12-30 tytu-chh
EXPNO 11
PROCNO 1
Date_ 20161230
Time 23.31
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 293.6 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

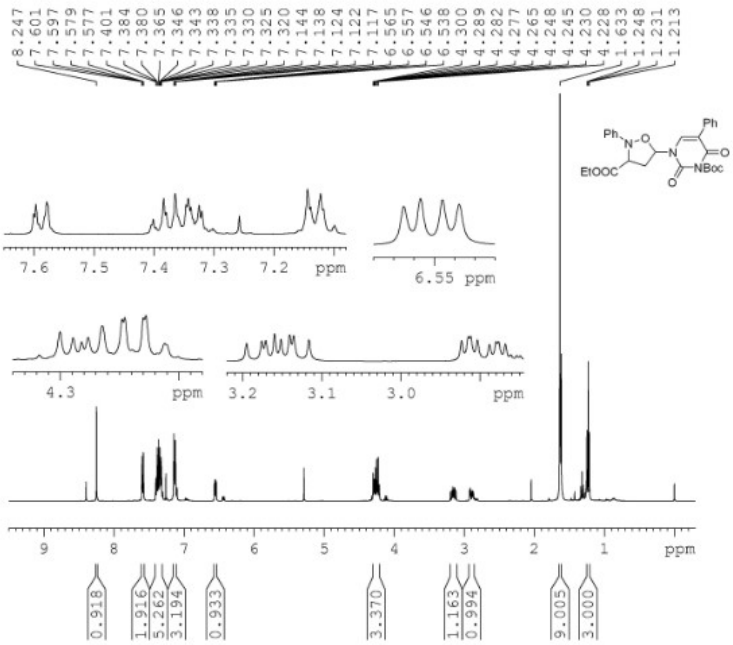
**4f**


8.467
7.384
7.364
7.345
7.163
7.147
7.127
6.448
6.441
6.429
6.422
4.331
4.313
4.295
4.278
4.267
4.255
4.243
4.231
3.174
3.169
3.158
3.150
3.139
3.134
3.115
2.865
2.857
2.854
2.846
2.829
2.822
2.818
2.810
1.613
1.347
1.329
1.312
Ph
N
O
N
O
NBoc
O
EtOOC
I
7.2 7.0 6.8 6.6 ppm
4.30 4.25 ppm
3.2 3.1 3.0 2.9 ppm
1.35 ppm
8 7 6 5 4 3 2 1 ppm
0.903
2.111
3.128
1.012
2.109
1.053
1.026
1.020
9.000
3.174
BRUKER
NAME 2016-12-14 tyut-chh
EXPNO 10
PROCNO 1
Date_ 20161214
Time 21.28
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 292.4 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

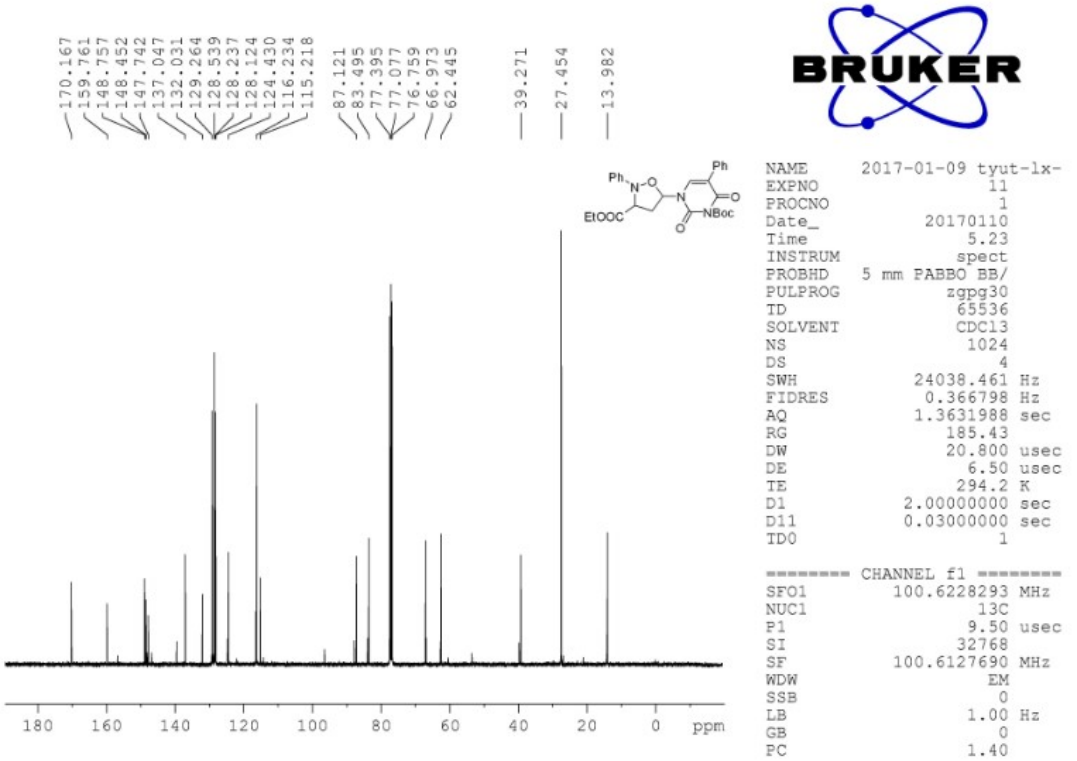



```
NAME          2016-12-14 tyut-chh
EXPNO                 11
PROCNO                 1
Date_           20161214
Time              21.30
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  399
DS                    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                292.8 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
```

**4g**

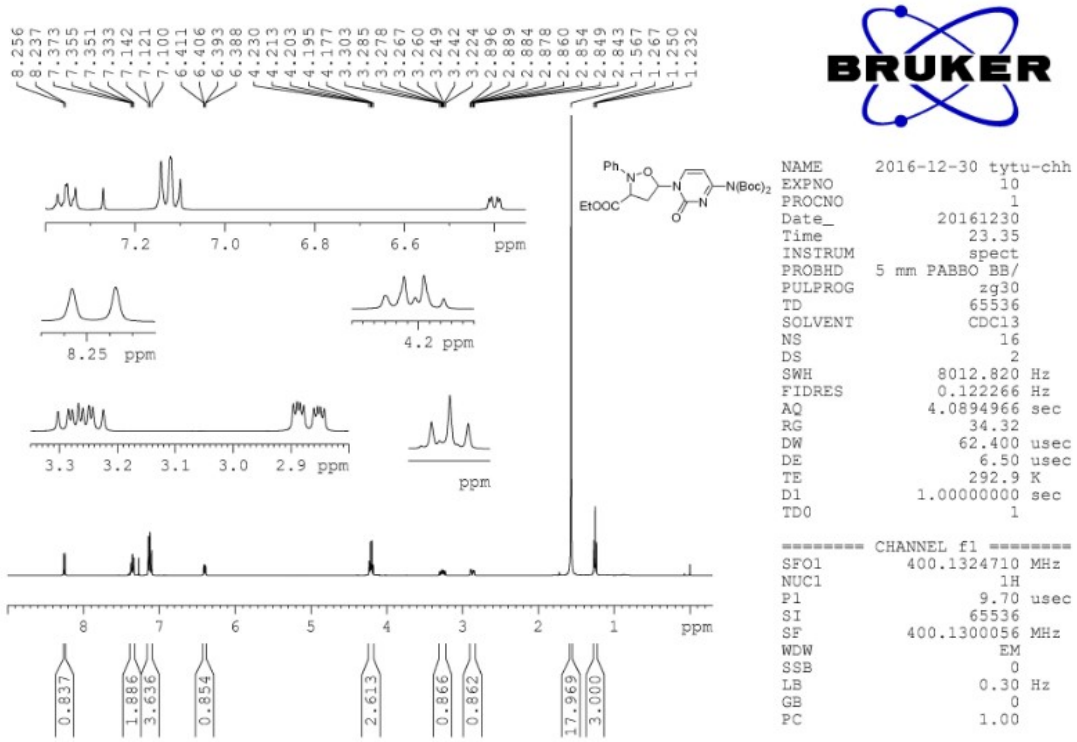



```
NAME          2017-01-09 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20170110
Time                4.24
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    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                293.6 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                 9.70 usec
SI                65536
SF           400.1300104 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

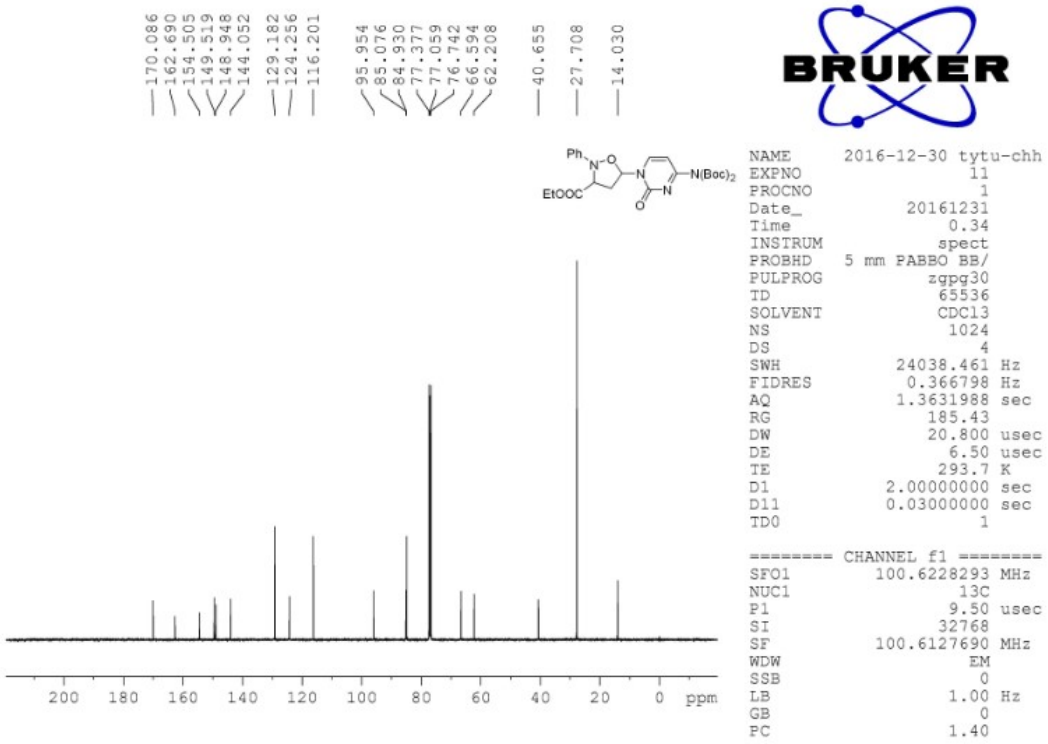



| | |
|---|---|
| NAME | 2017-01-09 tyut-lx- |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20170110 |
| Time | 5.23 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 1024 |
| DS | 4 |
| SWH | 24038.461 Hz |
| FIDRES | 0.366798 Hz |
| AQ | 1.3631988 sec |
| RG | 185.43 |
| DW | 20.800 usec |
| DE | 6.50 usec |
| TE | 294.2 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 |

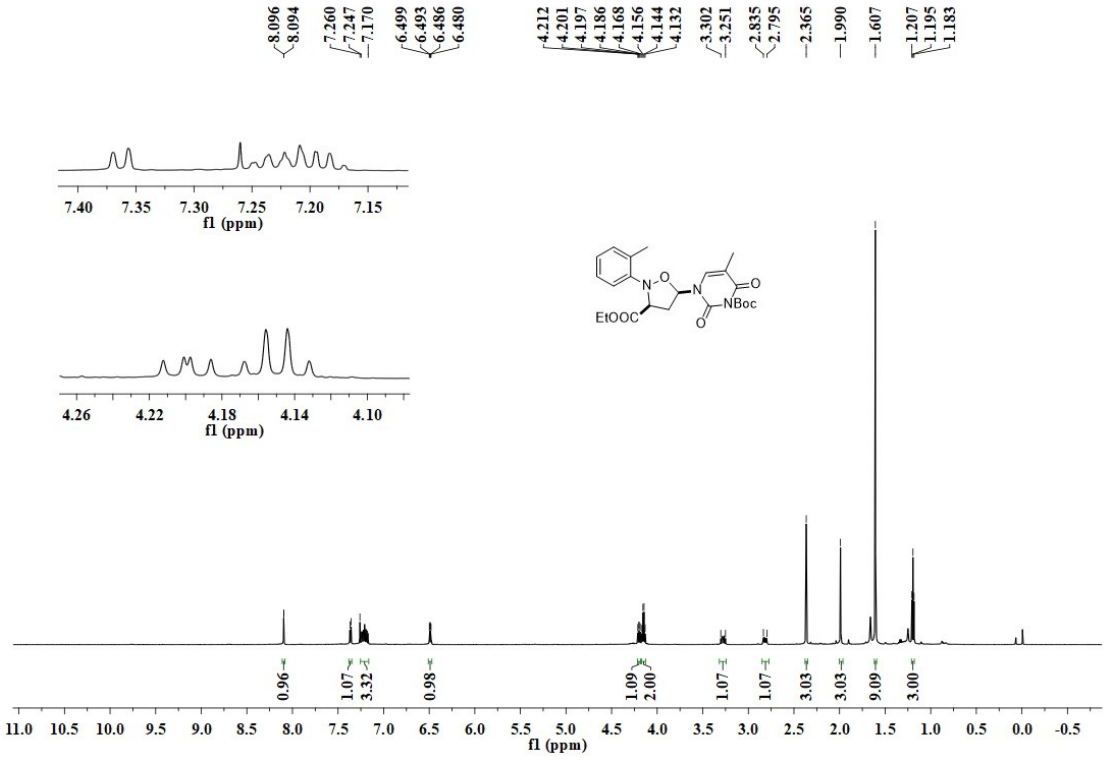
**4h**

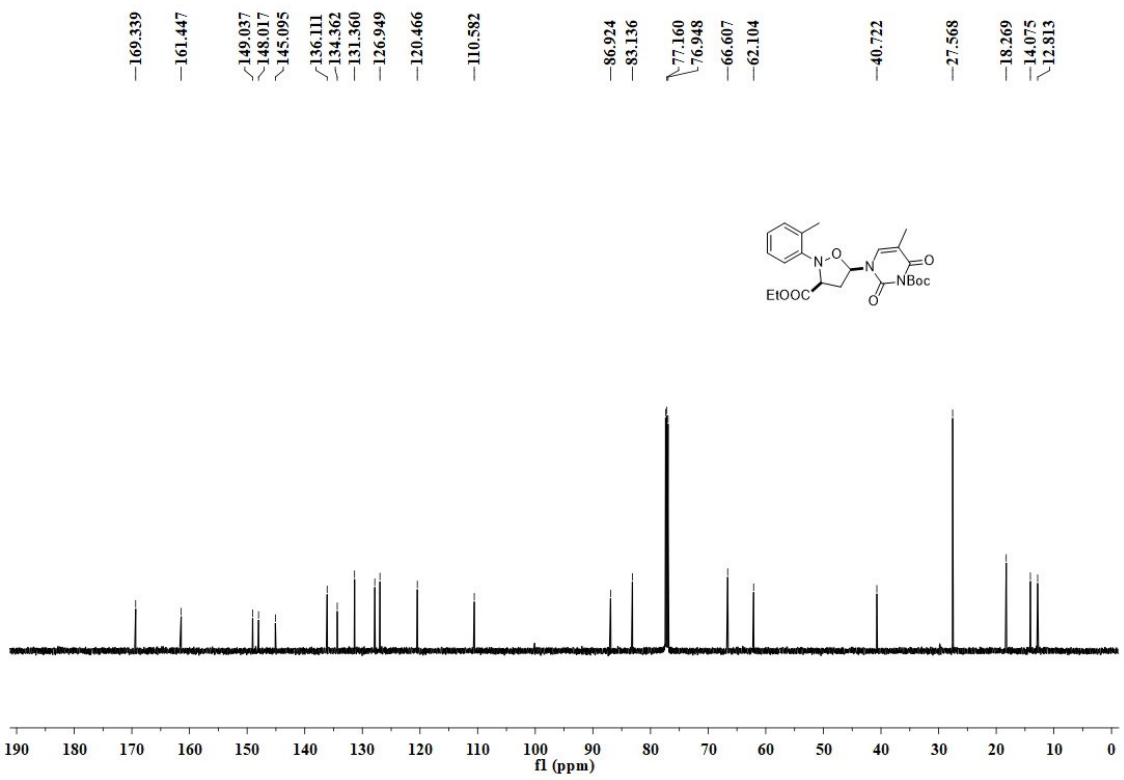



| | |
|---|---|
| NAME | 2016-12-30 tytu-chh |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20161230 |
| Time | 23.35 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 8012.820 Hz |
| FIDRES | 0.122266 Hz |
| AQ | 4.0894966 sec |
| RG | 34.32 |
| DW | 62.400 usec |
| DE | 6.50 usec |
| TE | 292.9 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300056 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

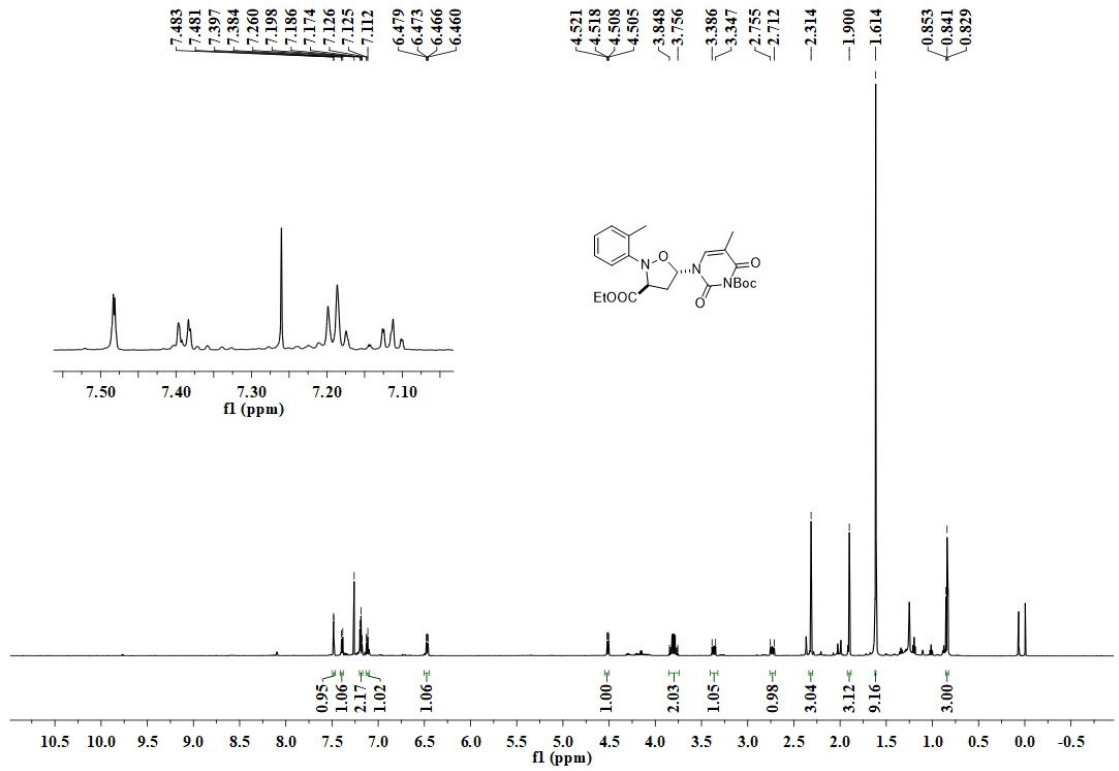

170.086
162.690
154.505
149.519
148.948
144.052
129.182
124.256
116.201
95.954
85.076
84.930
77.377
77.059
76.742
66.594
62.208
40.655
27.708
14.030
Ph
N(Boc)2
EtOOC
200 180 160 140 120 100 80 60 40 20 0 ppm
NAME 2016-12-30 tytu-chh
EXPNO 11
PROCNO 1
Date_ 20161231
Time 0.34
INSTRUM spect
PROBHD 5 mm 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 293.7 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

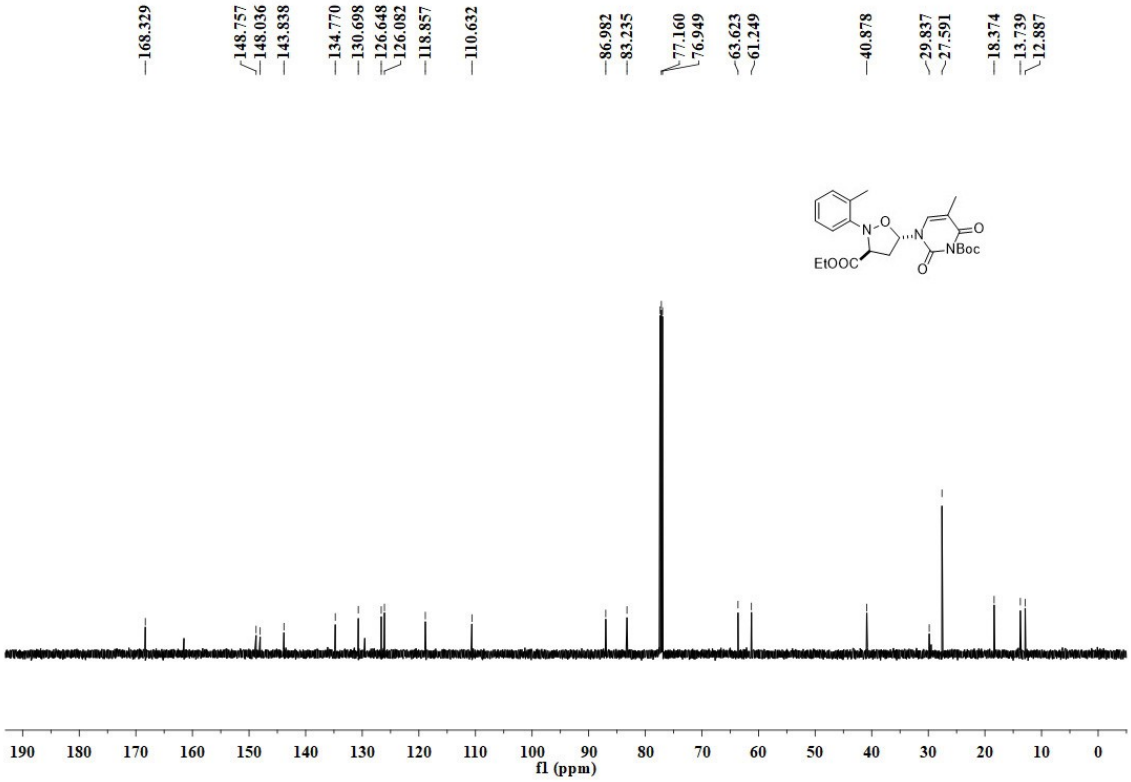
*cis*-**4i**


8.096
8.094
7.260
7.247
7.170
6.499
6.493
6.486
6.480
4.212
4.201
4.197
4.186
4.168
4.156
4.144
4.132
3.302
3.251
2.835
2.795
2.365
1.990
1.607
1.207
1.195
1.183
7.40 7.35 7.30 7.25 7.20 7.15
f1 (ppm)
4.26 4.22 4.18 4.14 4.10
f1 (ppm)
EtOOC
NBoc
0.96
1.07
3.32
0.98
1.09
2.00
1.07
1.07
3.03
3.03
9.09
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

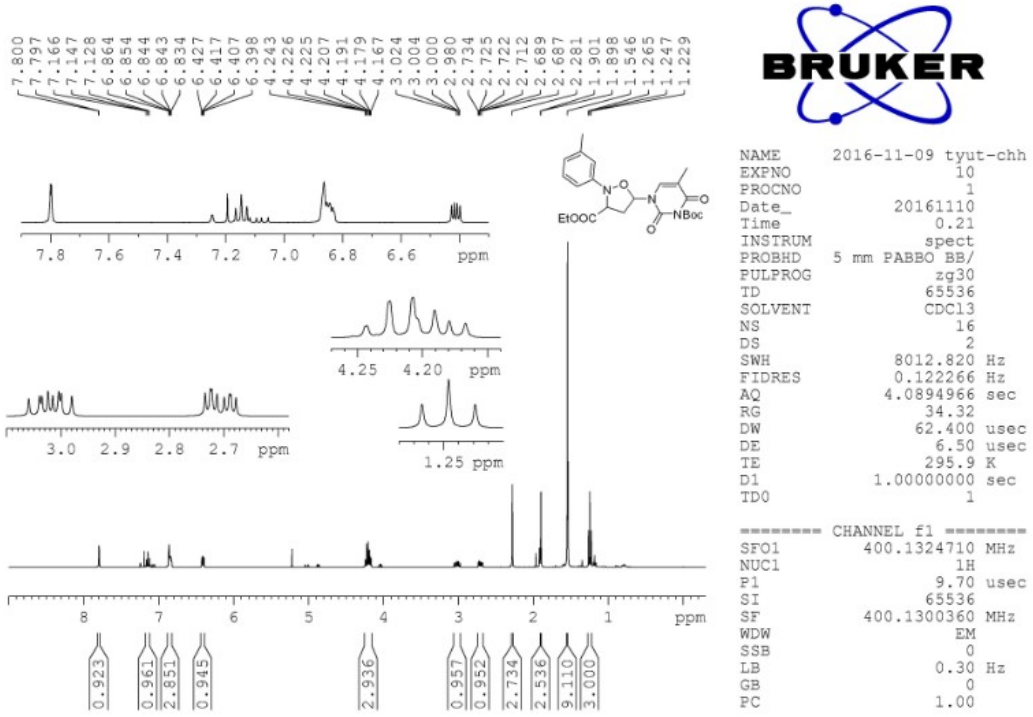

169.339
161.447
149.037
148.017
145.095
136.111
134.362
131.360
126.949
120.466
110.582
86.924
83.136
77.160
76.948
66.607
62.104
40.722
27.568
18.269
14.075
12.813
EtOOC
NBoc
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

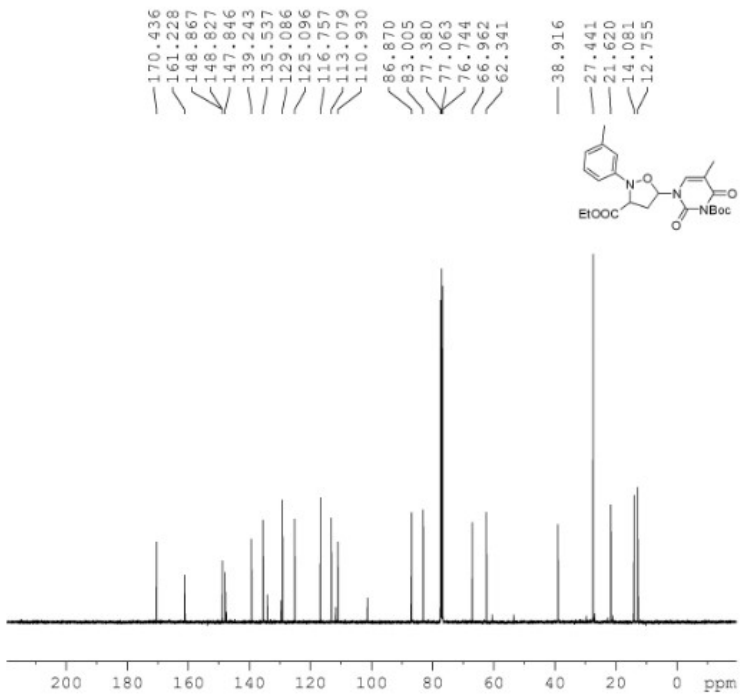
*trans*-**4i**


7.483
7.481
7.397
7.384
7.260
7.198
7.186
7.174
7.126
7.125
7.112
6.479
6.473
6.466
6.460
4.521
4.518
4.508
4.505
3.848
3.756
3.386
3.347
2.755
2.712
2.314
1.900
1.614
0.853
0.841
0.829
EtOOC
NBoc
7.50 7.40 7.30 7.20 7.10
f1 (ppm)
0.95 1.06 2.17 1.02 1.06 1.00 2.03 1.05 0.98 3.04 3.12 9.16 3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


168.329
148.757
148.036
143.838
134.770
130.698
126.648
126.082
118.857
110.632
86.982
83.235
77.160
76.949
63.623
61.249
40.878
29.837
27.591
18.374
13.739
12.887
EtOOC
NBoc
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

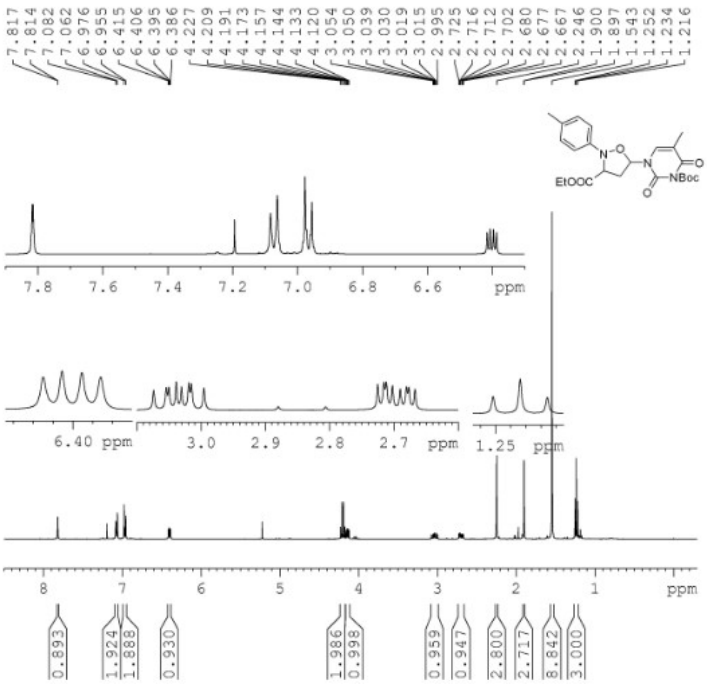
**4j**


7.800 7.797 7.166 7.147 7.128 6.864 6.854 6.844 6.843 6.834 6.427 6.417 6.407 6.398 4.243 4.226 4.225 4.207 4.191 4.179 4.167 3.024 3.004 3.000 2.980 2.734 2.725 2.722 2.712 2.689 2.687 2.281 1.901 1.898 1.546 1.265 1.247 1.229
EtOOC
NBoc
7.8 7.6 7.4 7.2 7.0 6.8 6.6 ppm
4.25 4.20 ppm
3.0 2.9 2.8 2.7 ppm
1.25 ppm
8 7 6 5 4 3 2 1 ppm
0.923 0.961 2.851 0.945 2.936 0.957 0.952 2.734 2.536 9.110 3.000
BRUKER
NAME 2016-11-09 tyut-chh
EXPNO 10
PROCNO 1
Date_ 20161110
Time 0.21
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 295.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.70 usec
SI 65536
SF 400.1300360 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

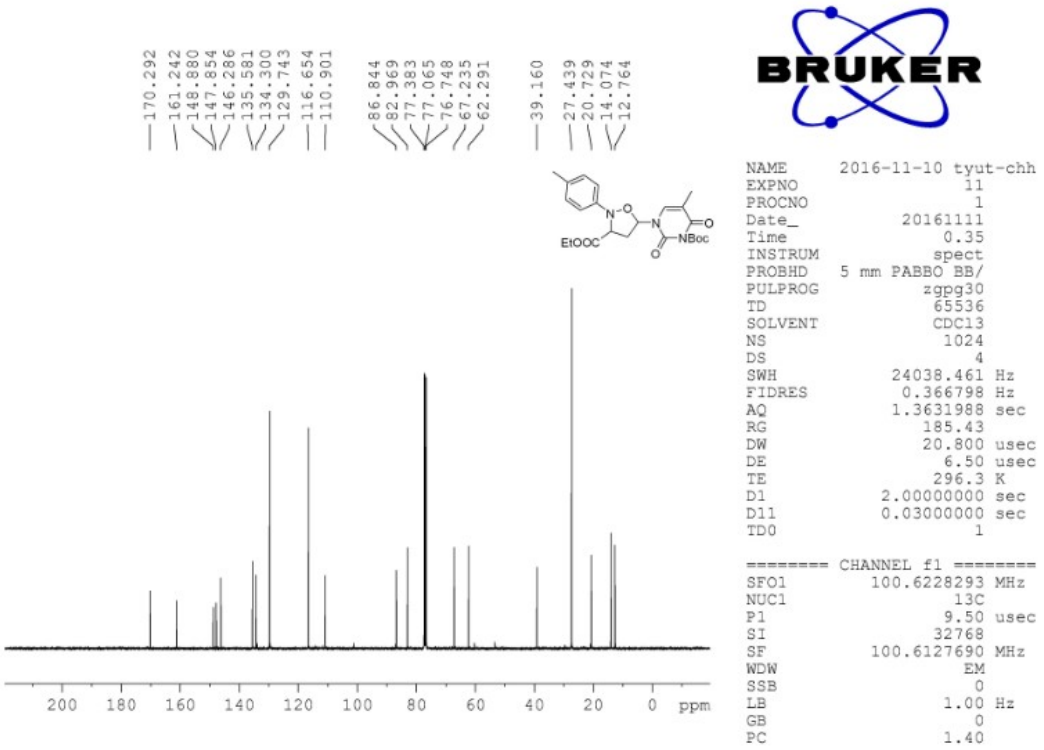



```
NAME          2016-11-09 tyut-chh
EXPNO                 11
PROCNO                 1
Date_           20161110
Time               1.20
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    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                296.5 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
```

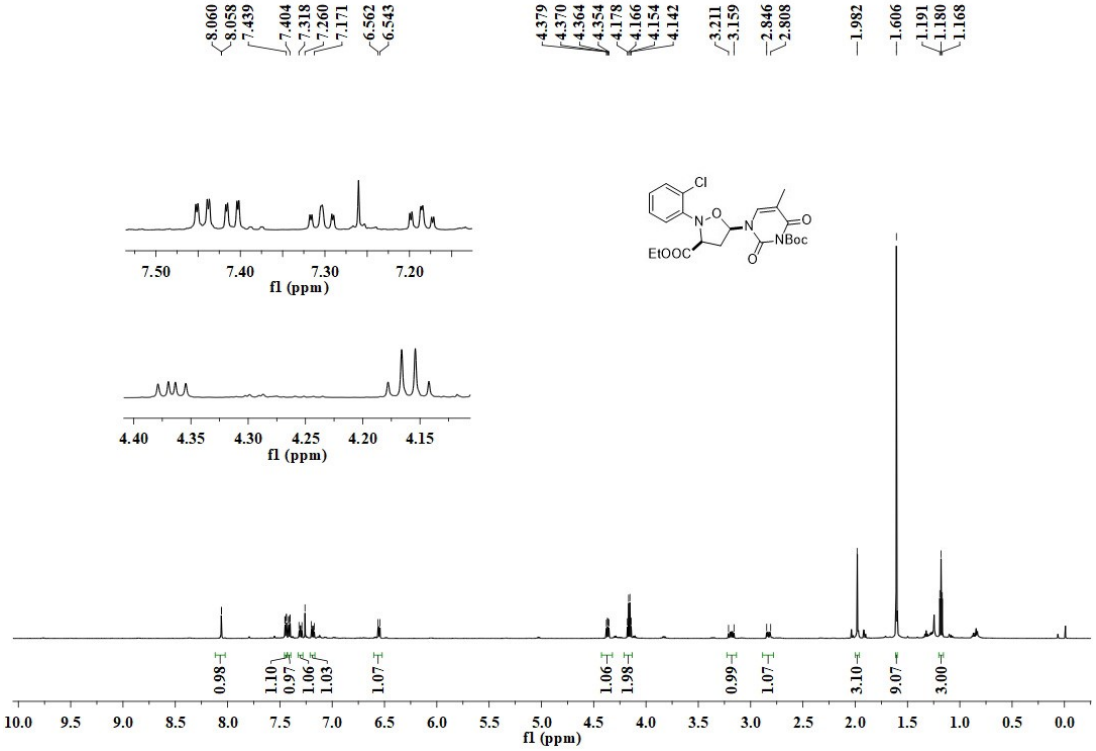
**4k**

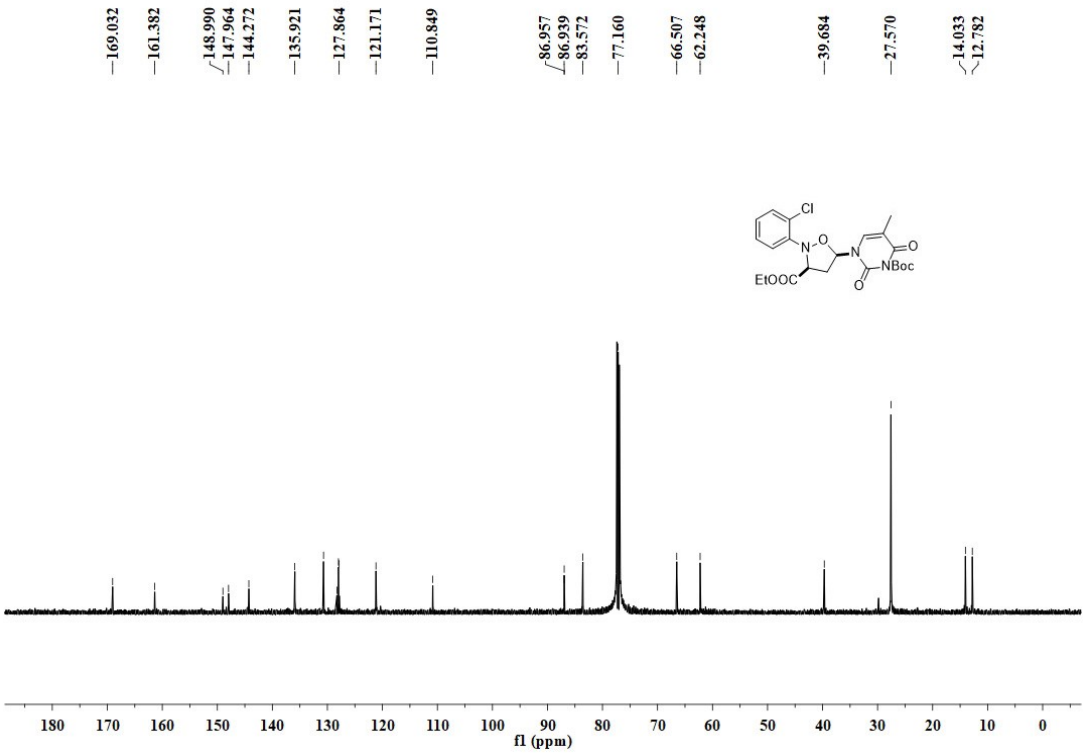



```
NAME          2016-11-10 tyut-chh
EXPNO                 10
PROCNO                 1
Date_           20161110
Time              23.37
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    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                295.6 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                 9.70 usec
SI                65536
SF           400.1300363 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

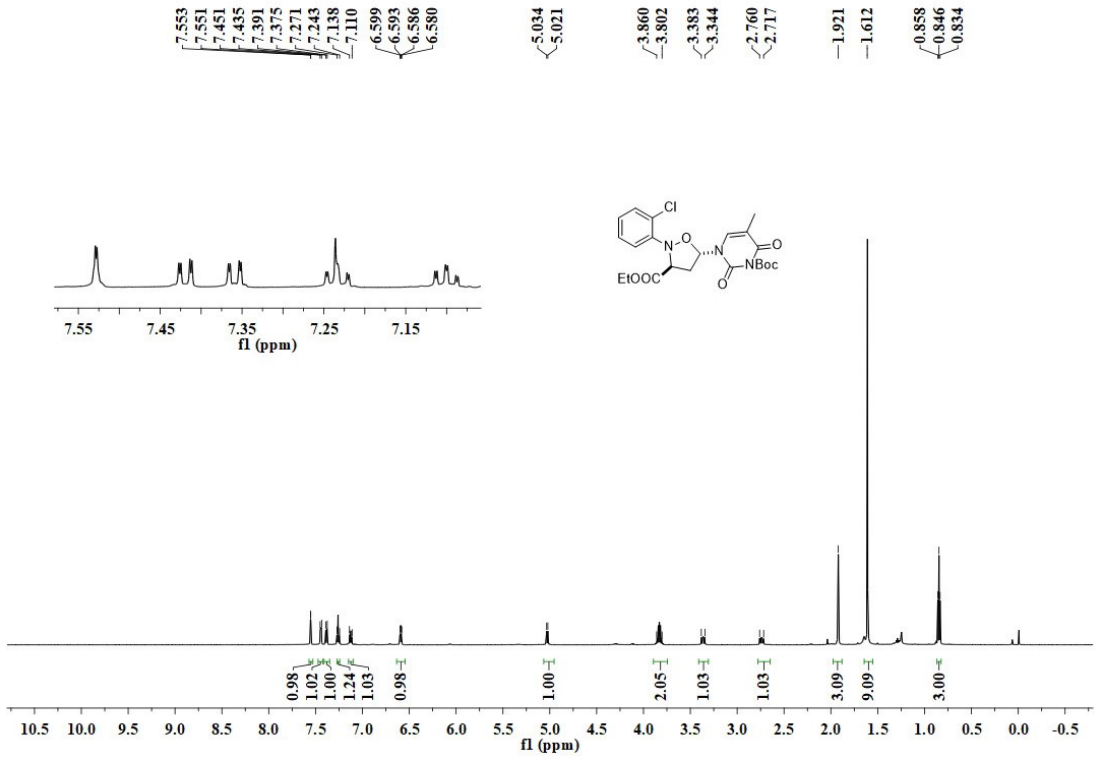

170.292
161.242
148.880
147.854
146.286
135.581
134.300
129.743
116.654
110.901
86.844
82.969
77.383
77.065
76.748
67.235
62.291
39.160
27.439
20.729
14.074
12.764
EtOOC
NBoc
200 180 160 140 120 100 80 60 40 20 0 ppm
NAME 2016-11-10 tyut-chh
EXPNO 11
PROCNO 1
Date_ 20161111
Time 0.35
INSTRUM spect
PROBHD 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 296.3 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

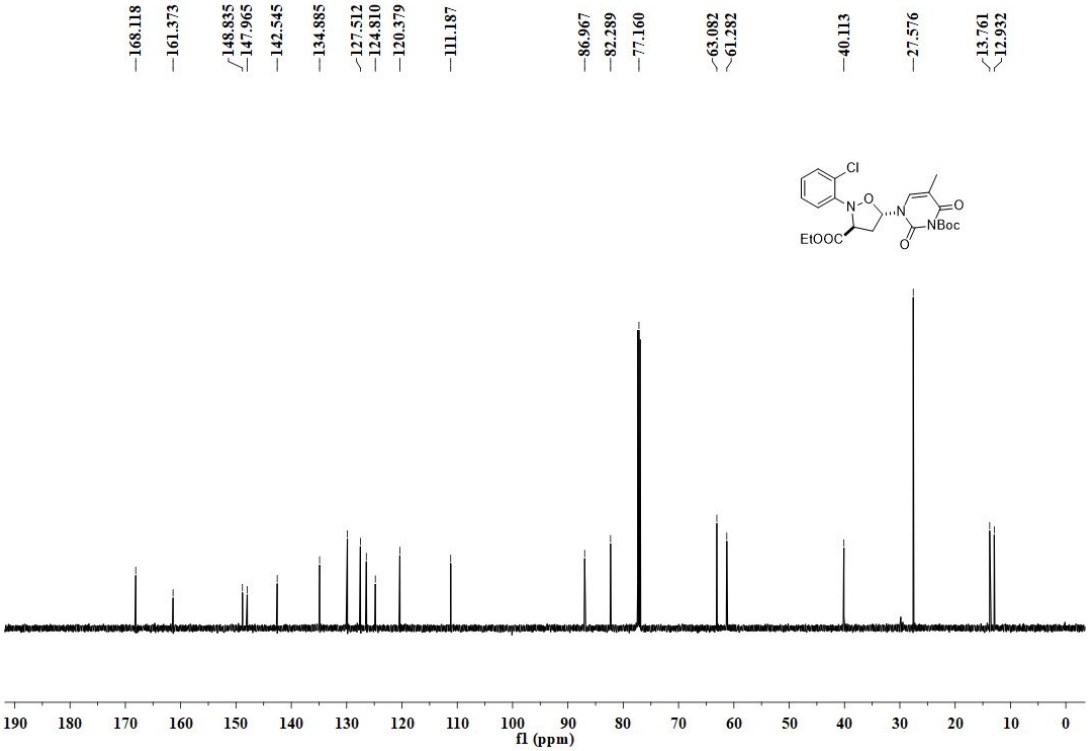
*cis*-**4n**


8.060
8.058
7.439
7.404
7.318
7.260
7.171
6.562
6.543
4.379
4.370
4.364
4.354
4.178
4.166
4.154
4.142
3.211
3.159
2.846
2.808
1.982
1.606
1.191
1.180
1.168
Cl
EtOOC
NBoc
7.50 7.40 7.30 7.20
f1 (ppm)
4.40 4.35 4.30 4.25 4.20 4.15
f1 (ppm)
0.98
1.10
0.97
1.06
1.03
1.07
1.06
1.98
0.99
1.07
3.10
9.07
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

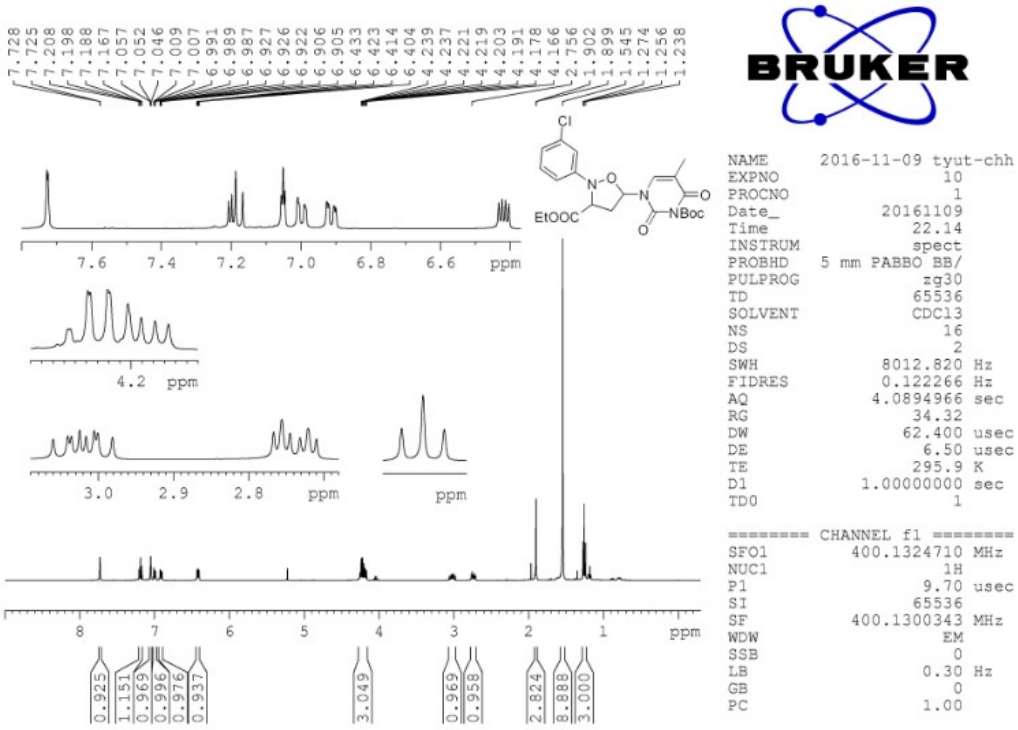

169.032
161.382
148.990
147.964
144.272
135.921
127.864
121.171
110.849
86.957
86.939
83.572
77.160
66.507
62.248
39.684
27.570
14.033
12.782
Cl
N
O
N
O
NBoc
O
EtOOC
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

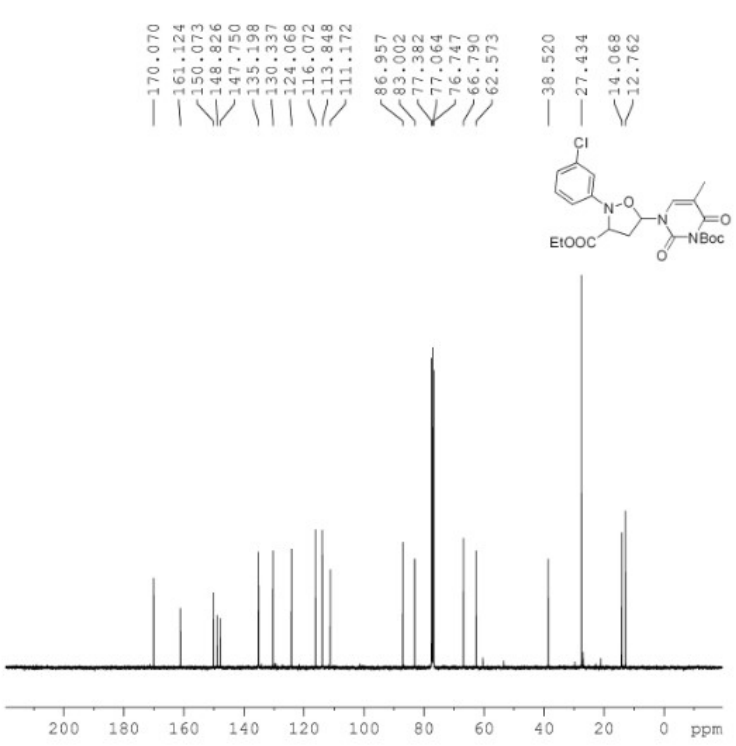
*trans*-**4n**


7.553
7.551
7.451
7.435
7.391
7.375
7.271
7.243
7.138
7.110
6.599
6.593
6.586
6.580
5.034
5.021
3.860
3.802
3.383
3.344
2.760
2.717
1.921
1.612
0.858
0.846
0.834
Cl
N
O
N
O
NBoc
O
EtOOC
7.55 7.45 7.35 7.25 7.15
f1 (ppm)
0.98
1.02
1.00
1.24
1.03
0.98
1.00
2.05
1.03
1.03
3.09
9.09
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


168.118
161.373
148.835
147.965
142.545
134.885
127.512
124.810
120.379
111.187
86.967
82.289
77.160
63.082
61.282
40.113
27.576
13.761
12.932
Cl
EtOOC
NBoc
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

**4o**

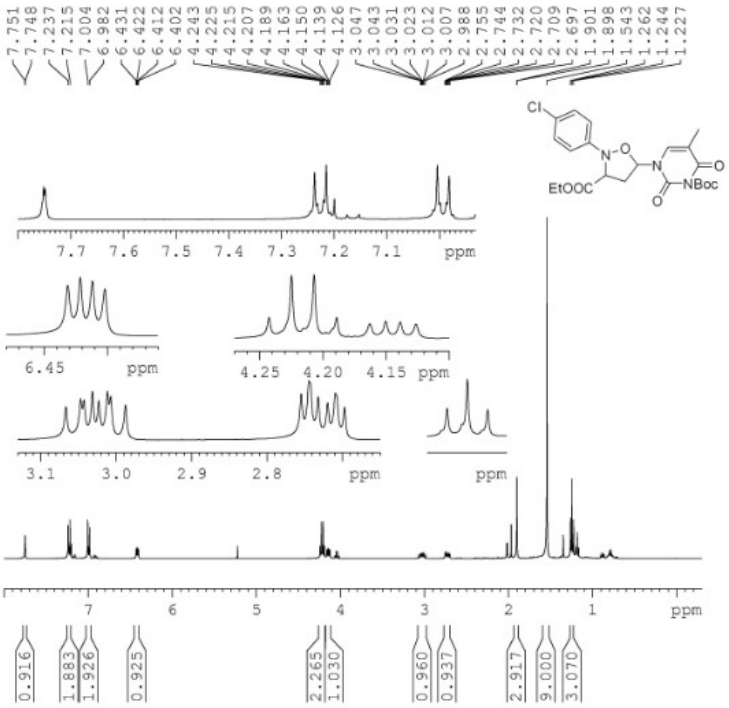

7.728 7.725 7.208 7.198 7.188 7.167 7.057 7.052 7.046 7.009 7.007 6.991 6.989 6.987 6.927 6.926 6.922 6.906 6.905 6.433 6.423 6.414 6.404 6.239 4.237 4.221 4.219 4.203 4.191 4.178 4.166 2.756 1.902 1.899 1.545 1.274 1.256 1.238
Cl
EtOOC
NBoc
7.6 7.4 7.2 7.0 6.8 6.6 ppm
4.2 ppm
3.0 2.9 2.8 ppm
ppm
8 7 6 5 4 3 2 1 ppm
0.925 1.151 0.969 0.996 0.976 0.937 3.049 0.969 0.958 2.824 8.888 3.000
BRUKER
NAME 2016-11-09 tyut-chh
EXPNO 10
PROCNO 1
Date_ 20161109
Time 22.14
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 295.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.70 usec
SI 65536
SF 400.1300343 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




BRUKER

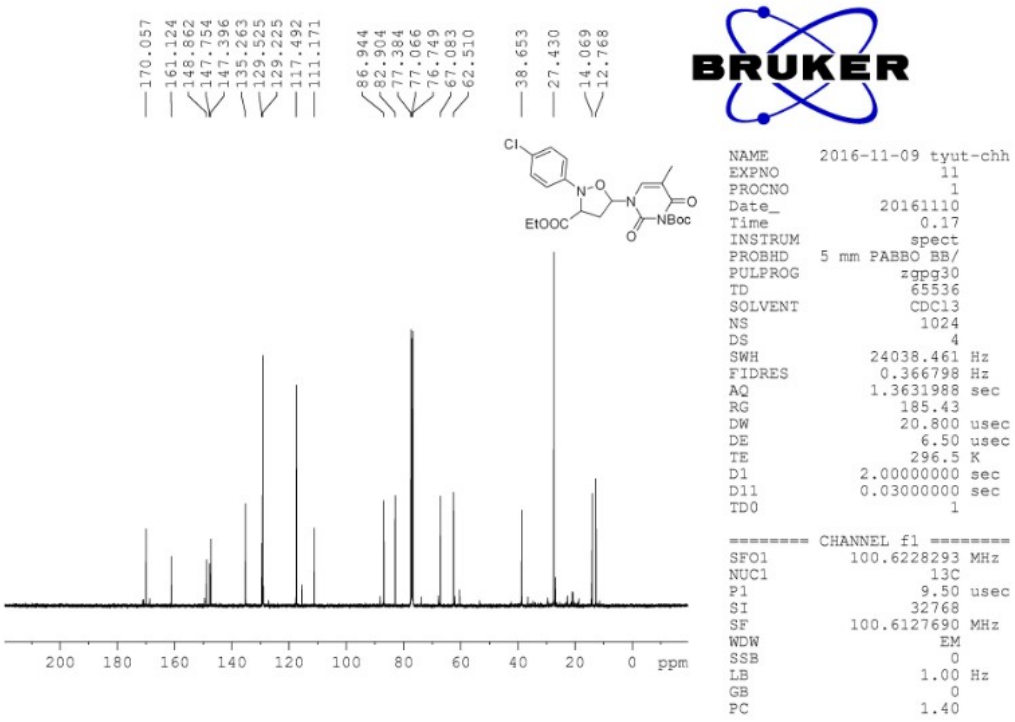
| | |
|---|---|
| NAME | 2016-11-09 tyut-chh |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20161109 |
| Time | 23.13 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 1024 |
| DS | 4 |
| SWH | 24038.461 Hz |
| FIDRES | 0.366798 Hz |
| AQ | 1.3631988 sec |
| RG | 185.43 |
| DW | 20.800 usec |
| DE | 6.50 usec |
| TE | 296.6 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 |

**4p**

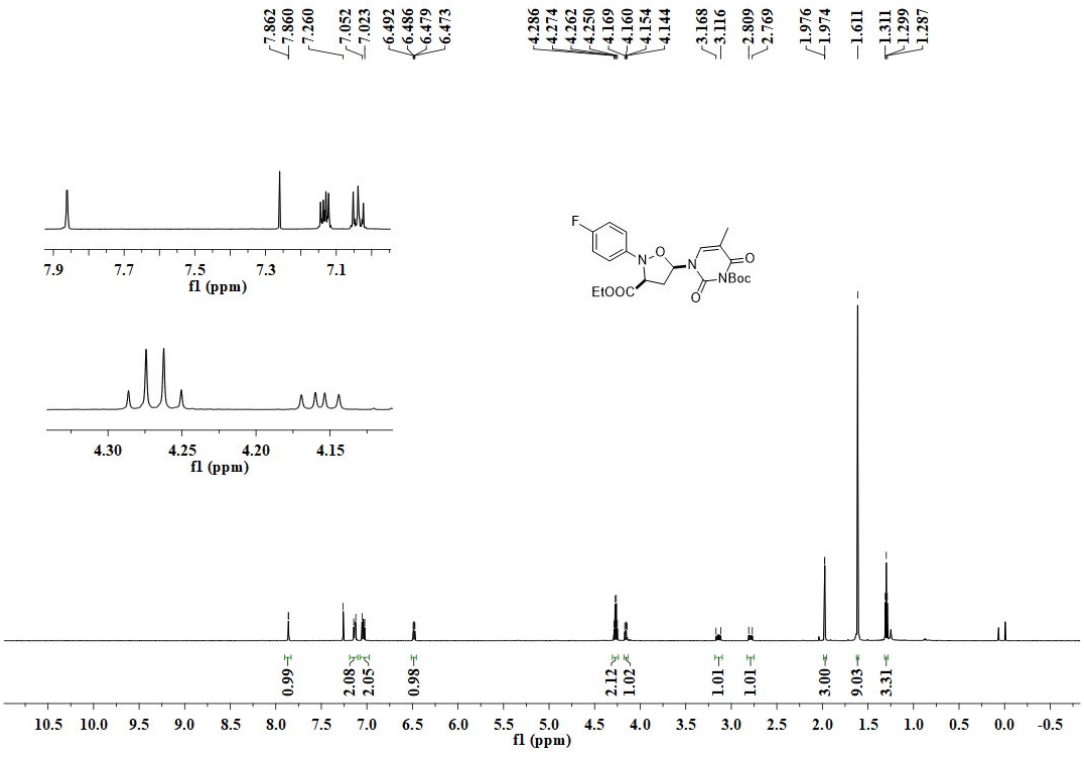


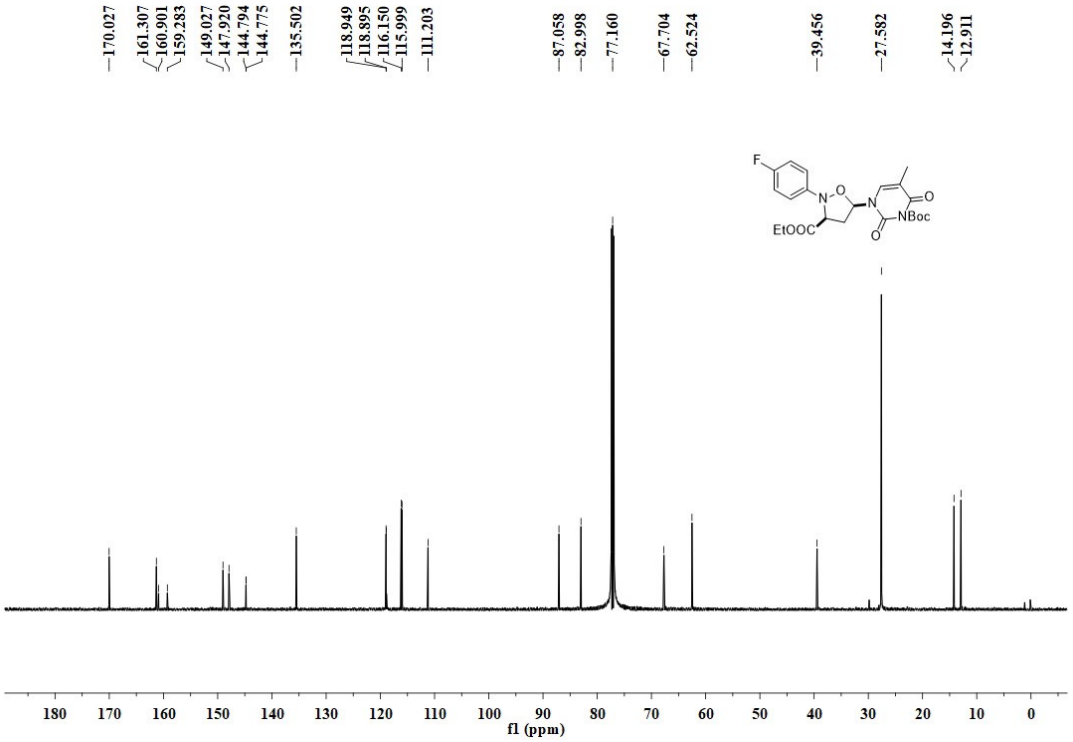

BRUKER

| | |
|---|---|
| NAME | 2016-11-09 tyut-chh |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20161109 |
| Time | 23.18 |
| 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 | 295.9 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== | CHANNEL f1 ======== |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300338 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

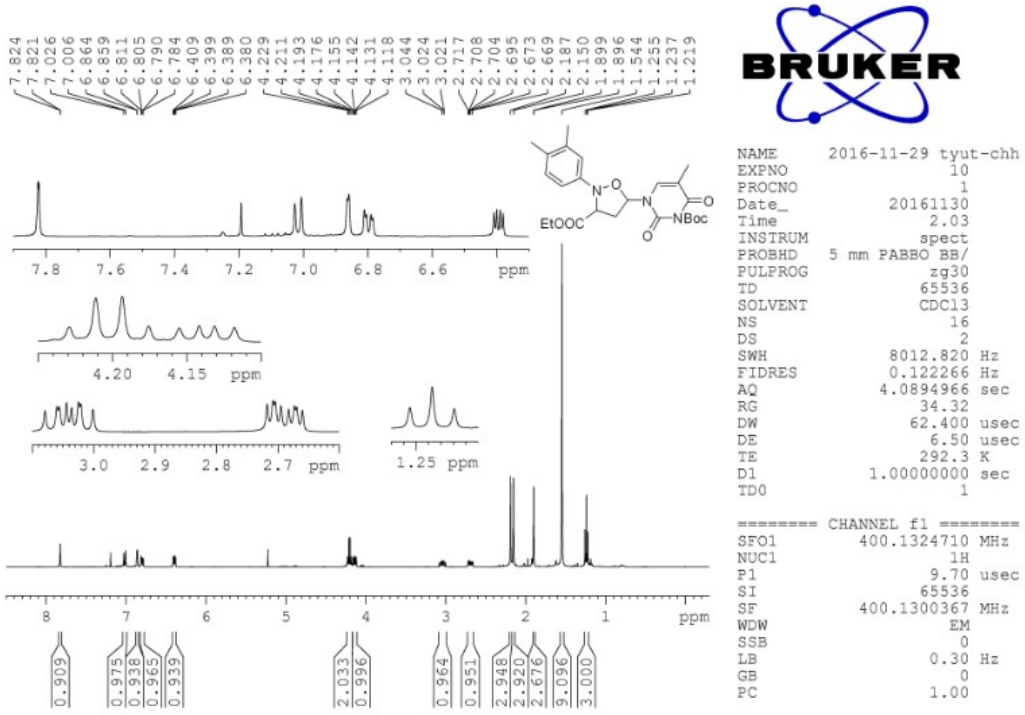

170.057
161.124
148.862
147.754
147.396
135.263
129.525
129.225
117.492
111.171
86.944
82.904
77.384
77.066
76.749
67.083
62.510
38.653
27.430
14.069
12.768
BRUKER
Cl
EtOOC
NBoc
NAME 2016-11-09 tyut-chh
EXPNO 11
PROCNO 1
Date_ 20161110
Time 0.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
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 296.5 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
200 180 160 140 120 100 80 60 40 20 0 ppm

**4q**


7.862
7.860
7.260
7.052
7.023
6.492
6.486
6.479
6.473
4.286
4.274
4.262
4.250
4.169
4.160
4.154
4.144
3.168
3.116
2.809
2.769
1.976
1.974
1.611
1.311
1.299
1.287
F
EtOOC
NBoc
7.9 7.7 7.5 7.3 7.1
f1 (ppm)
4.30 4.25 4.20 4.15
f1 (ppm)
0.99
2.08
2.05
0.98
2.12
1.02
1.01
1.01
3.00
9.03
3.31
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

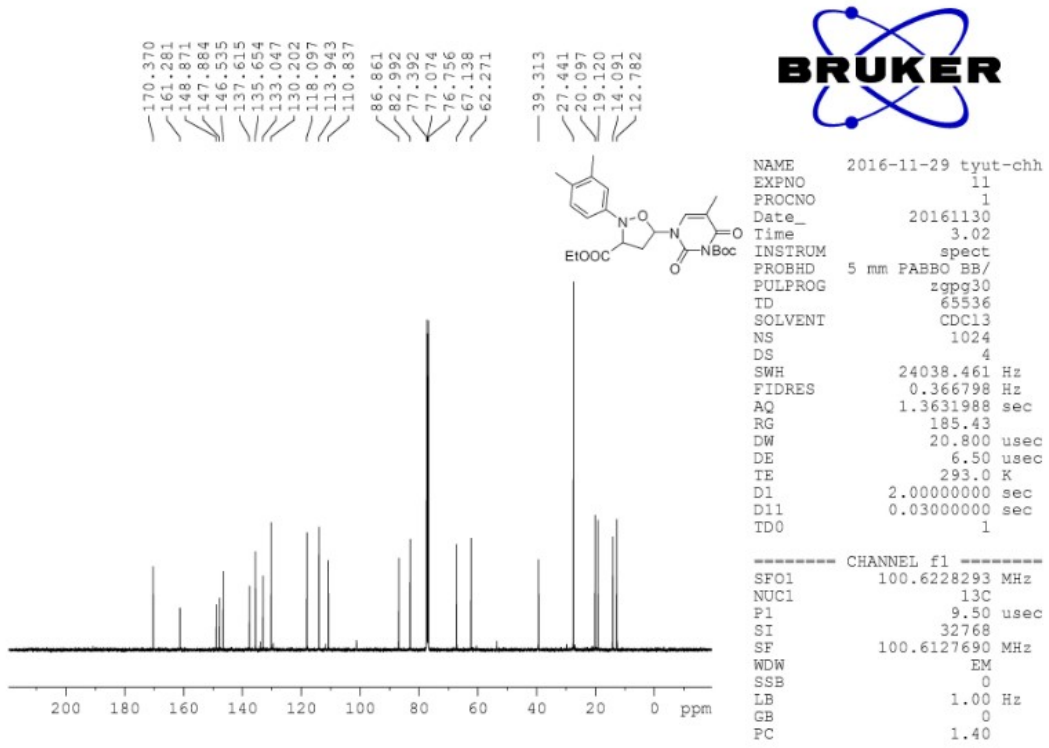



**4r**

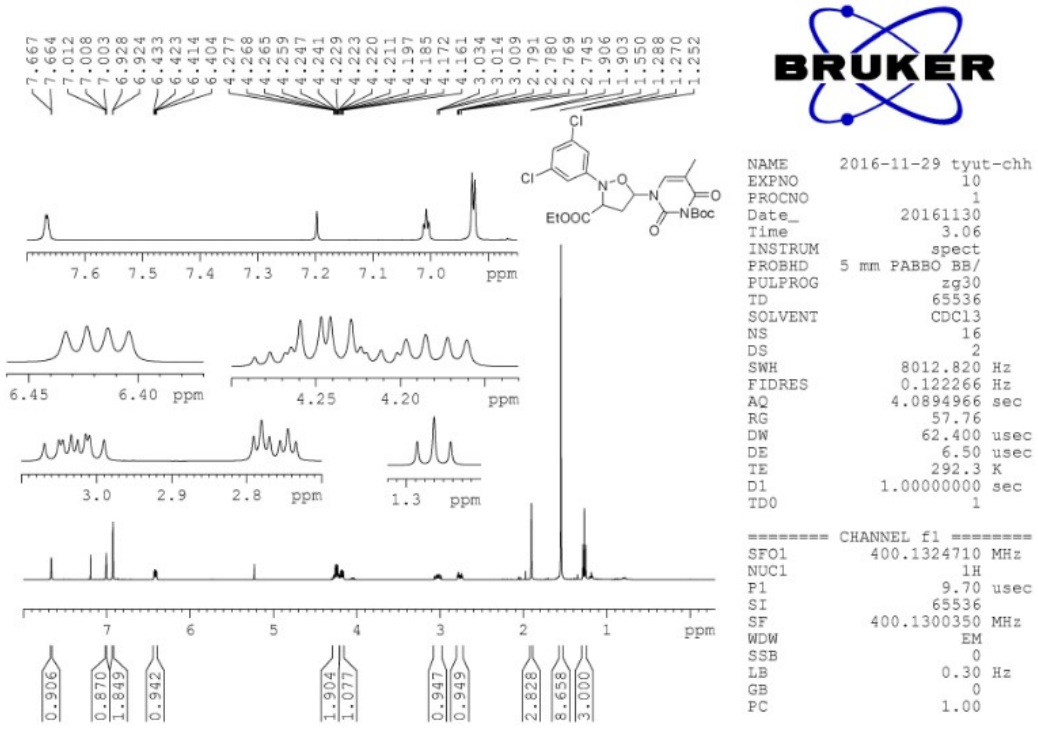


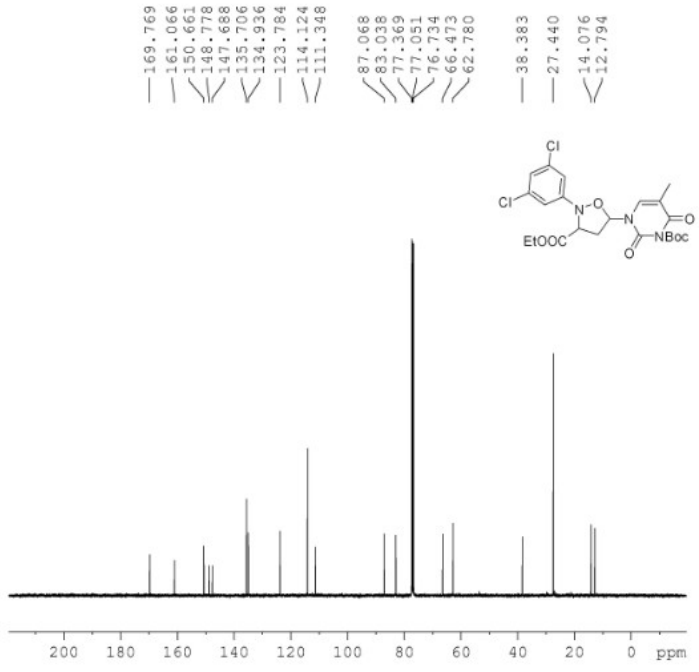

BRUKER

| | |
|---|---|
| NAME | 2016-11-29 tyut-chh |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20161130 |
| Time | 2.03 |
| 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 | 292.3 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300367 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |


170.370
161.281
148.871
147.884
146.535
137.615
135.654
133.047
130.202
118.097
113.943
110.837
86.861
82.992
77.392
77.074
76.756
67.138
62.271
39.313
27.441
20.097
19.120
14.091
12.782
EtOOC
NBoc
200 180 160 140 120 100 80 60 40 20 0 ppm
NAME 2016-11-29 tyut-chh
EXPNO 11
PROCNO 1
Date_ 20161130
Time 3.02
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 293.0 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

**4s**

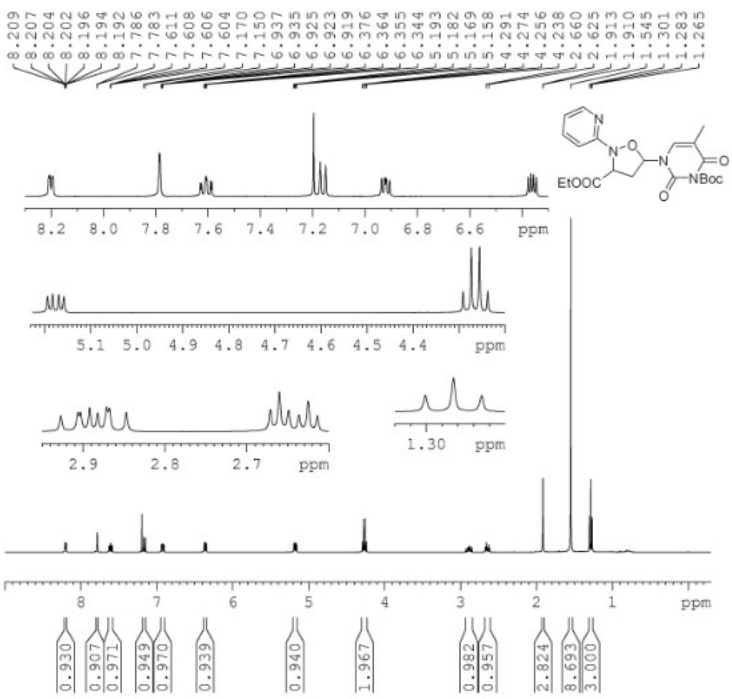

7.667
7.664
7.012
7.008
7.003
6.928
6.924
6.433
6.423
6.414
6.404
4.277
4.268
4.265
4.259
4.247
4.241
4.229
4.223
4.220
4.211
4.197
4.185
4.172
4.161
3.034
3.014
3.009
2.791
2.780
2.769
2.745
1.906
1.903
1.550
1.288
1.270
1.252
Cl
Cl
EtOOC
NBoc
7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
6.45 6.40 ppm
4.25 4.20 ppm
3.0 2.9 2.8 ppm
1.3 ppm
7 6 5 4 3 2 1 ppm
0.906
0.870
1.849
0.942
1.904
1.077
0.947
0.949
2.828
8.658
3.000
NAME 2016-11-29 tyut-chh
EXPNO 10
PROCNO 1
Date_ 20161130
Time 3.06
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 57.76
DW 62.400 usec
DE 6.50 usec
TE 292.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.70 usec
SI 65536
SF 400.1300350 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




BRUKER

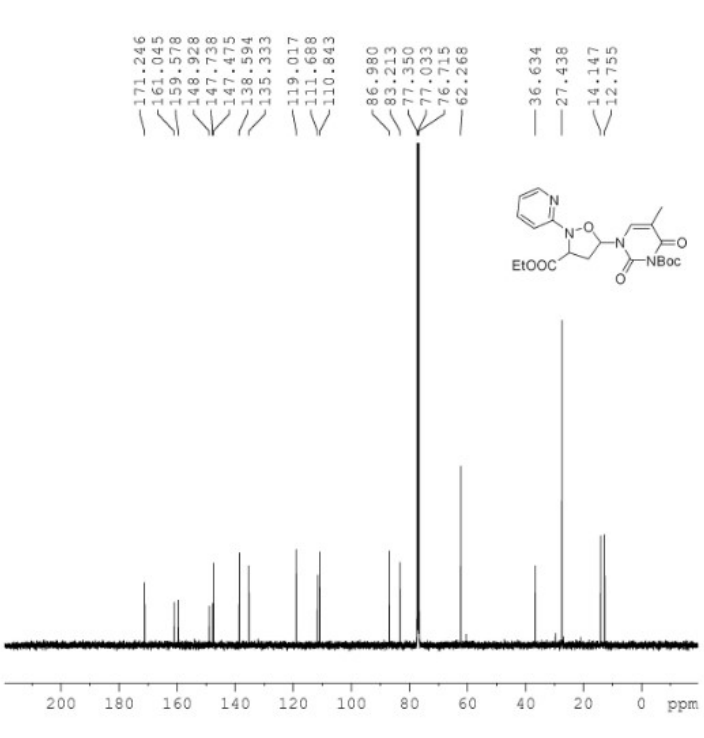
```
NAME          2016-11-29 tyut-chh
EXPNO                 11
PROCNO                 1
Date_           20161130
Time                4.05
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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              293.0 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
```

**4t**



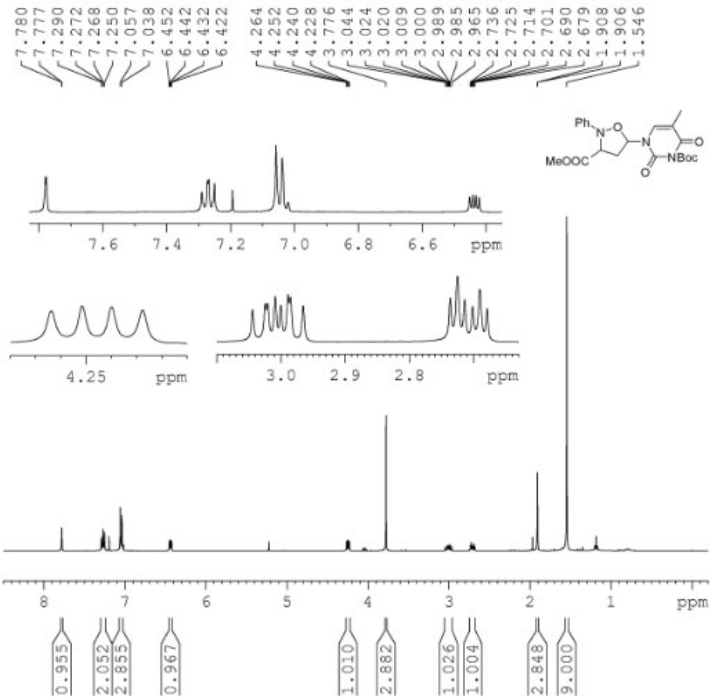

BRUKER

```
NAME          2016-11-10 tyut-chh
EXPNO                 10
PROCNO                 1
Date_           20161111
Time                0.40
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                 67.58
DW              62.400 usec
DE               6.50 usec
TE              295.6 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1               1H
P1                9.70 usec
SI                65536
SF            400.1300354 MHz
WDW                EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

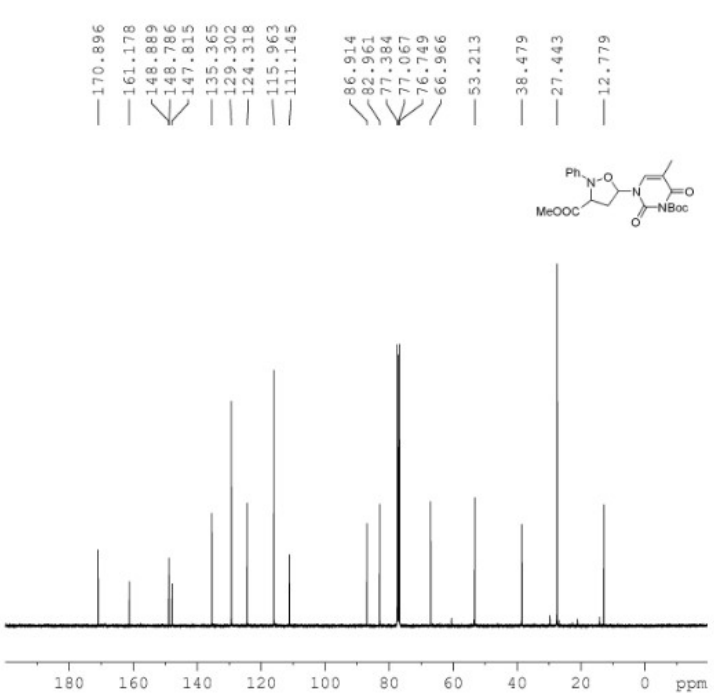



```
NAME          2016-11-10 tyut-chh
EXPNO                 11
PROCNO                 1
Date_           20161111
Time                1.39
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDC13
NS                 1024
DS                    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                296.2 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
```

**4u**

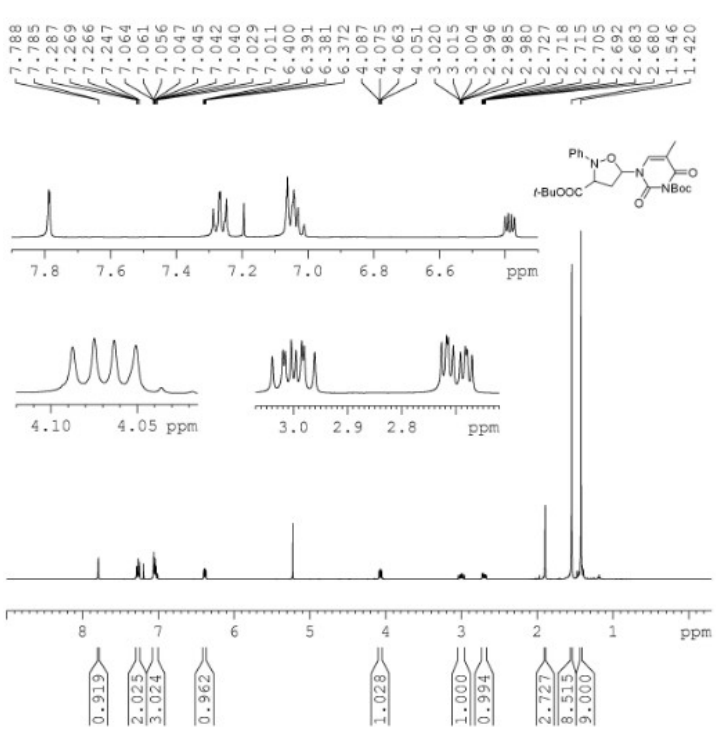



```
NAME          2016-11-08 tyut-chh
EXPNO                 10
PROCNO                 1
Date_           20161109
Time               10.26
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDC13
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894966 sec
RG                34.32
DW                62.400 usec
DE                 6.50 usec
TE                295.4 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1               1H
P1                9.70 usec
SI               65536
SF          400.1300361 MHz
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```

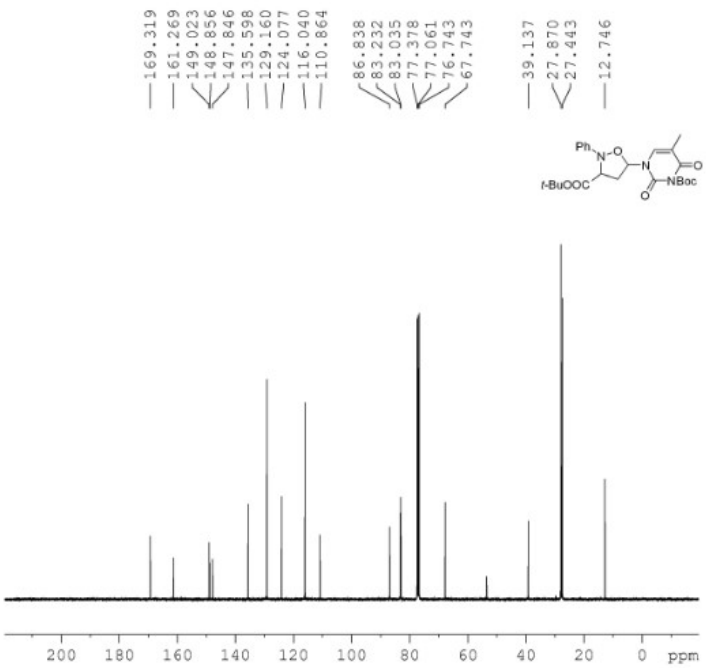



```
NAME          2016-11-08 tyut-chh
EXPNO                 11
PROCNO                 1
Date_           20161109
Time               11.25
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    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              296.3 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
```

**4v**

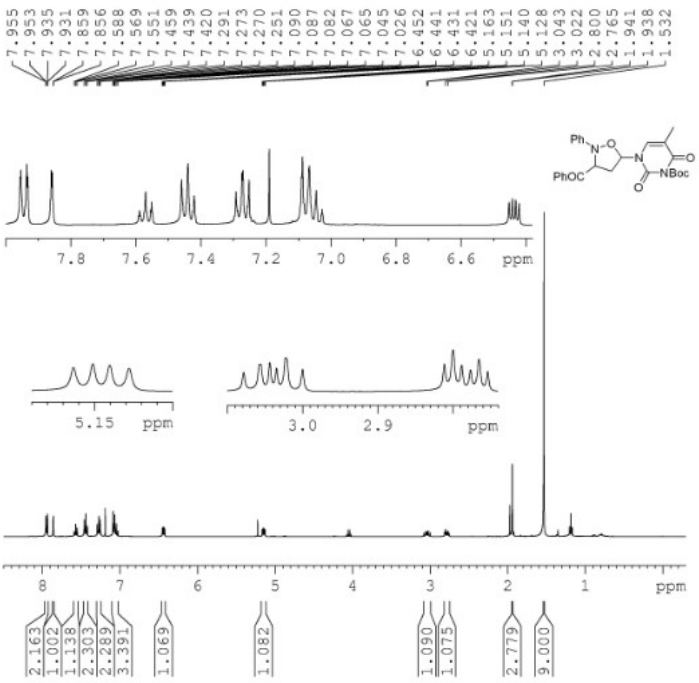



```
NAME          2016-11-08 tyut-chh
EXPNO                 10
PROCNO                 1
Date_           20161109
Time               11.29
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    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              295.6 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1               1H
P1                9.70 usec
SI               65536
SF          400.1300361 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

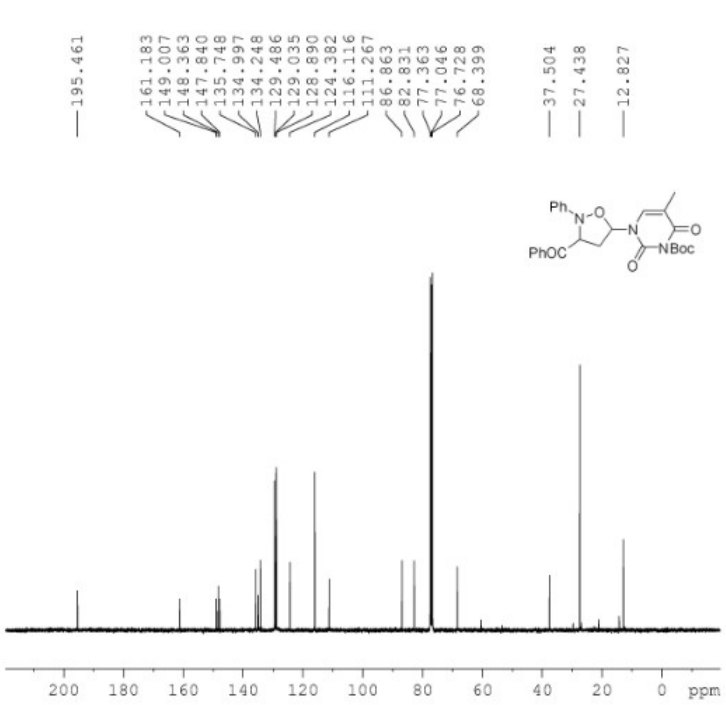



```
NAME          2016-11-08 tyut-chh
EXPNO                   11
PROCNO                   1
Date_               20161109
Time                   12.28
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     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                    296.3 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
```

**4w**



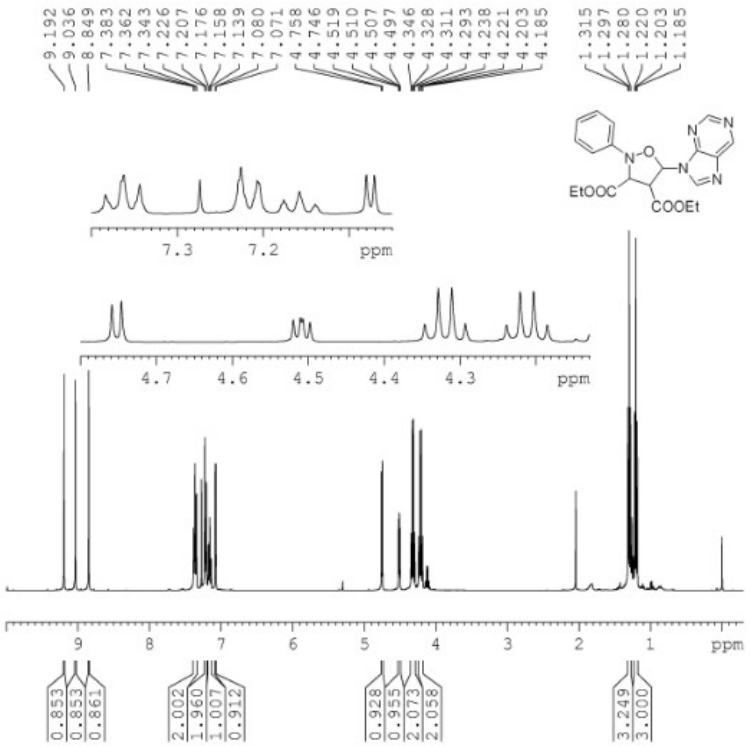

```
NAME          2016-11-08 tyut-chh
EXPNO                   10
PROCNO                   1
Date_               20161109
Time                   12.32
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       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                    295.7 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                    1H
P1                     9.70 usec
SI                    65536
SF               400.1300381 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



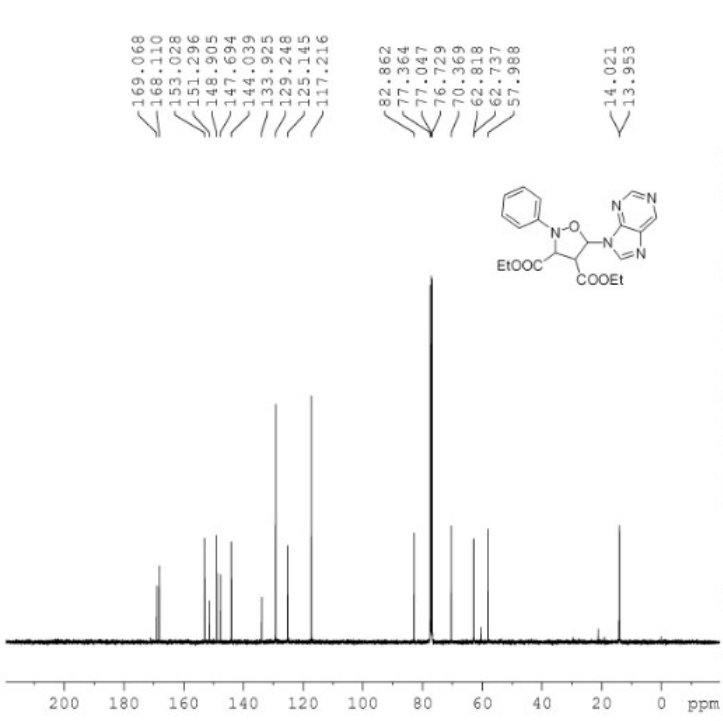

```
NAME          2016-11-08 tyut-chh
EXPNO                 11
PROCNO                 1
Date_           20161109
Time              13.31
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    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               296.4 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
```

## 11. $^{1}$H- and $^{13}$C-NMR spectra of products 6

### 6a

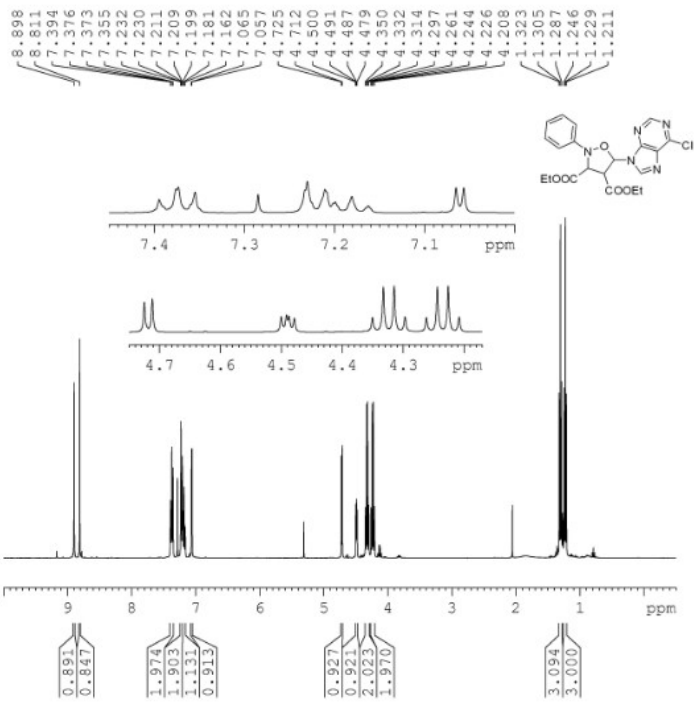



```
NAME          2017-03-17 tyut-lix
EXPNO                 10
PROCNO                 1
Date_           20170318
Time              18.25
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894966 sec
RG                57.76
DW               62.400 usec
DE                6.50 usec
TE               295.5 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1               1H
P1                9.70 usec
SI               65536
SF           400.1300046 MHz
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```

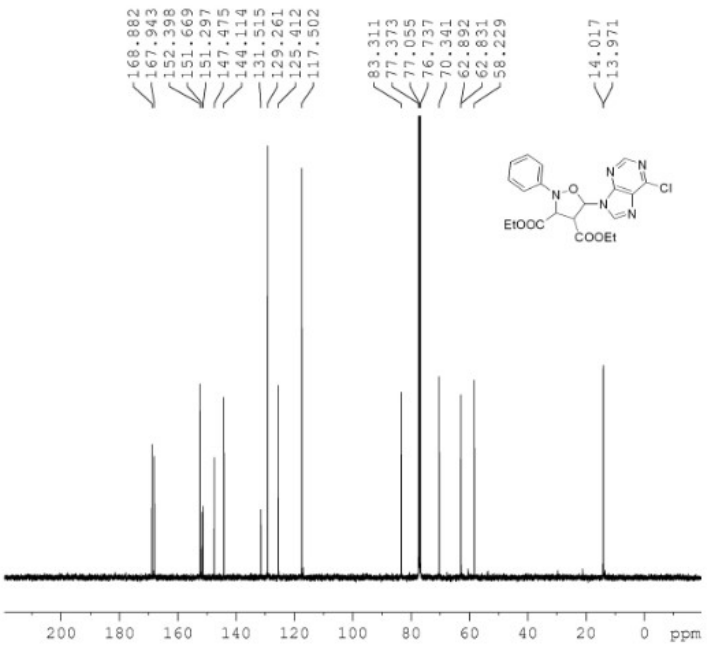



```
NAME        2017-03-17 tyut-lix
EXPNO                   11
PROCNO                   1
Date_             20170319
Time                  3.31
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
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                   296.3 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
```

**6b**

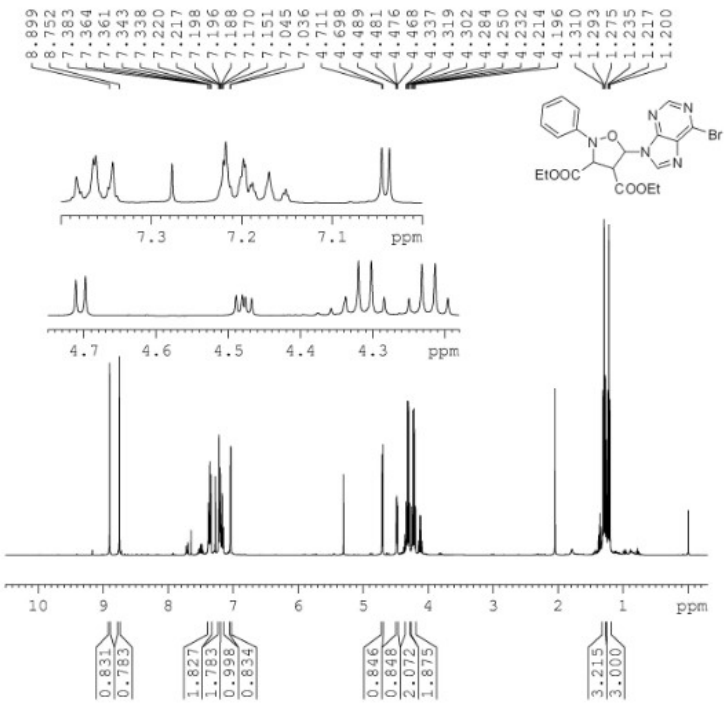



```
NAME        2016-09-22 tyuy-chh
EXPNO                   10
PROCNO                   1
Date_             20160922
Time                 18.45
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                   57.76
DW                   62.400 usec
DE                    6.50 usec
TE                   295.4 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
```

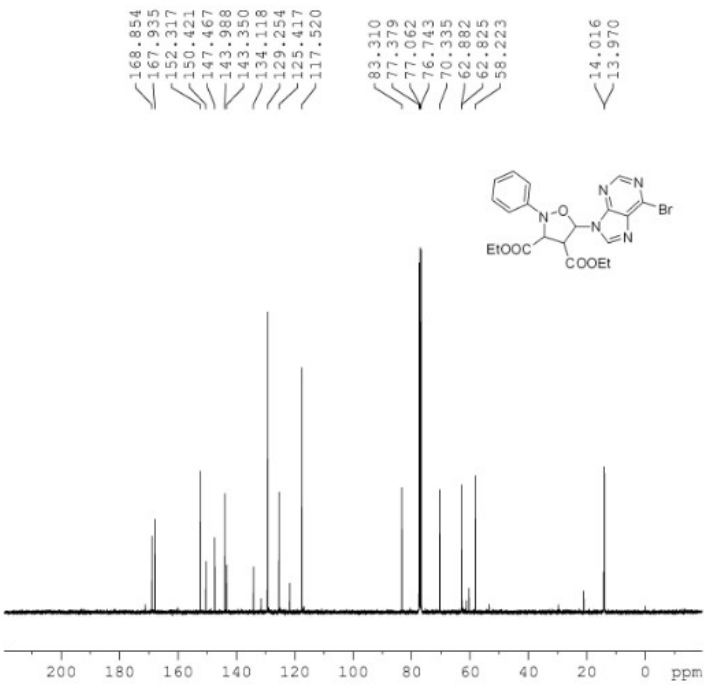



```
NAME          2016-09-22 tyuy-chh
EXPNO                 11
PROCNO                 1
Date_           20160922
Time                19.44
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      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                 296.2 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
```

**6c**

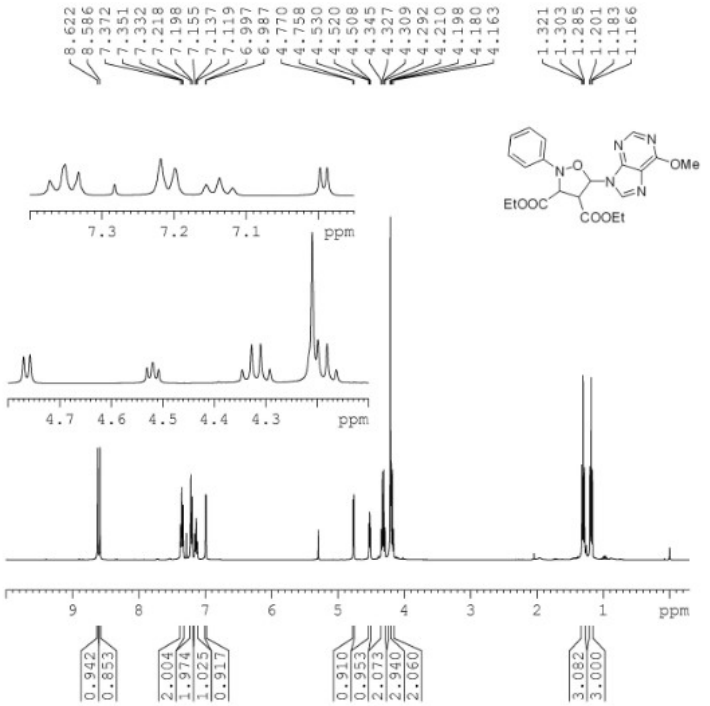



```
NAME          2017-03-16 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20170317
Time                1.46
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      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                 295.4 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.70 usec
SI                 65536
SF            400.1300031 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

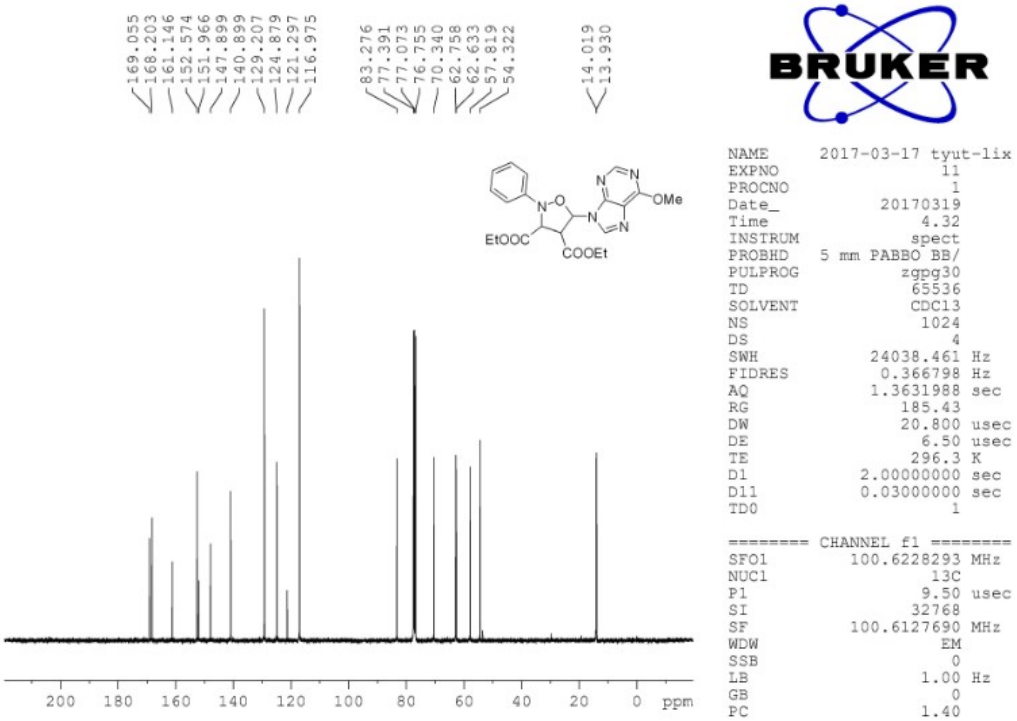



```
NAME          2017-03-16 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20170317
Time                2.45
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    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              296.4 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
```

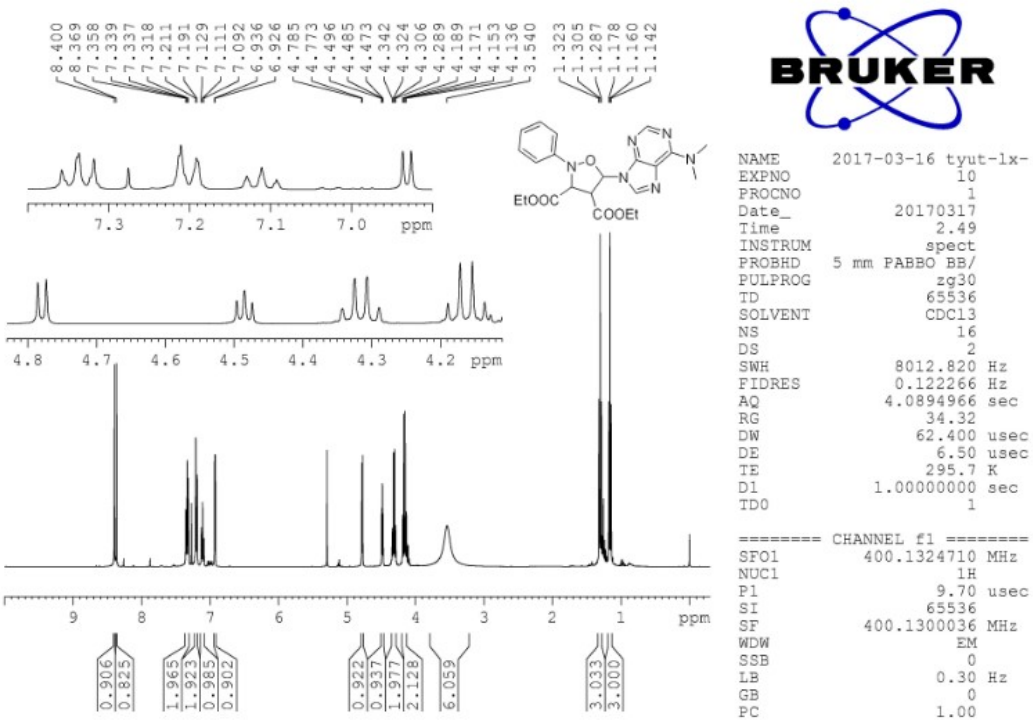
**6d**

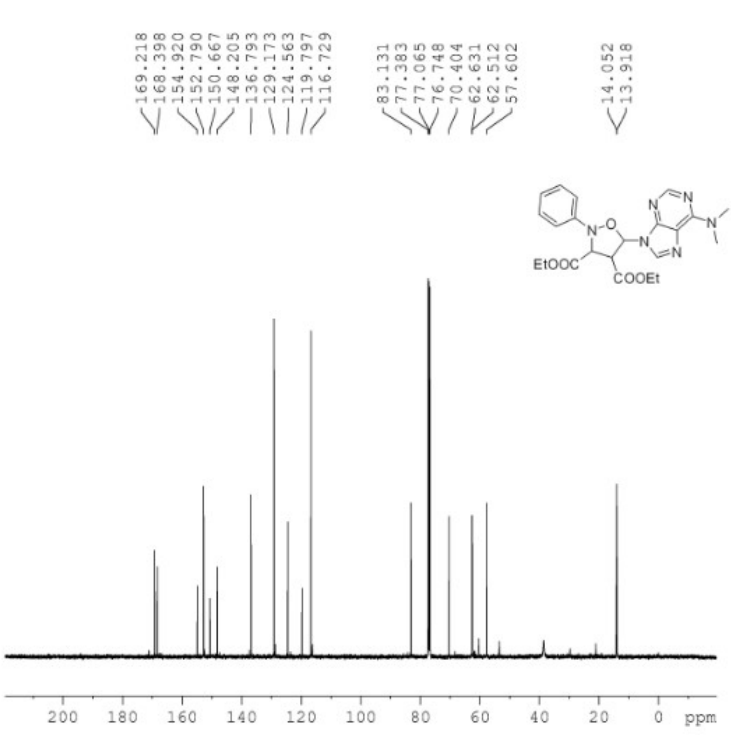



```
NAME          2017-03-17 tyut-lix
EXPNO                 10
PROCNO                 1
Date_           20170318
Time               18.29
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    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              295.5 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1               1H
P1                9.70 usec
SI               65536
SF          400.1300010 MHz
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```


169.055
168.203
161.146
152.574
151.966
147.899
140.899
129.207
124.879
121.297
116.975
83.276
77.391
77.073
76.755
70.340
62.758
62.633
57.819
54.322
14.019
13.930
OMe
EtOOC
COOEt
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
NAME 2017-03-17 tyut-lix
EXPNO 11
PROCNO 1
Date_ 20170319
Time 4.32
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 296.3 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

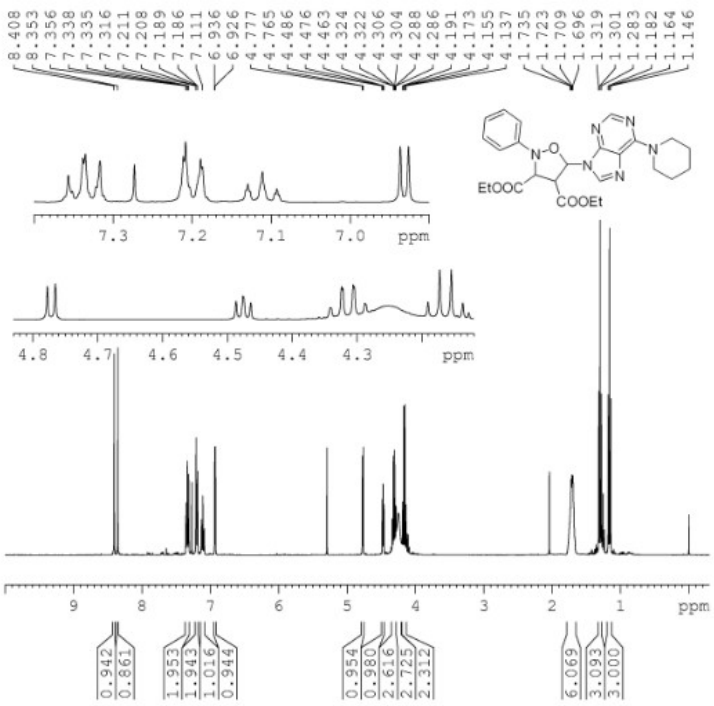
**6e**


8.400
8.369
7.358
7.339
7.337
7.318
7.211
7.191
7.129
7.111
7.092
6.936
6.926
4.785
4.773
4.496
4.485
4.473
4.342
4.324
4.306
4.289
4.189
4.171
4.153
4.136
3.540
1.323
1.305
1.287
1.178
1.160
1.142
EtOOC
COOEt
7.3 7.2 7.1 7.0 ppm
4.8 4.7 4.6 4.5 4.4 4.3 4.2 ppm
9 8 7 6 5 4 3 2 1 ppm
0.906
0.825
1.965
1.923
0.985
0.902
0.922
0.937
1.977
2.128
6.059
3.033
3.000
BRUKER
NAME 2017-03-16 tyut-lx-
EXPNO 10
PROCNO 1
Date_ 20170317
Time 2.49
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 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.70 usec
SI 65536
SF 400.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

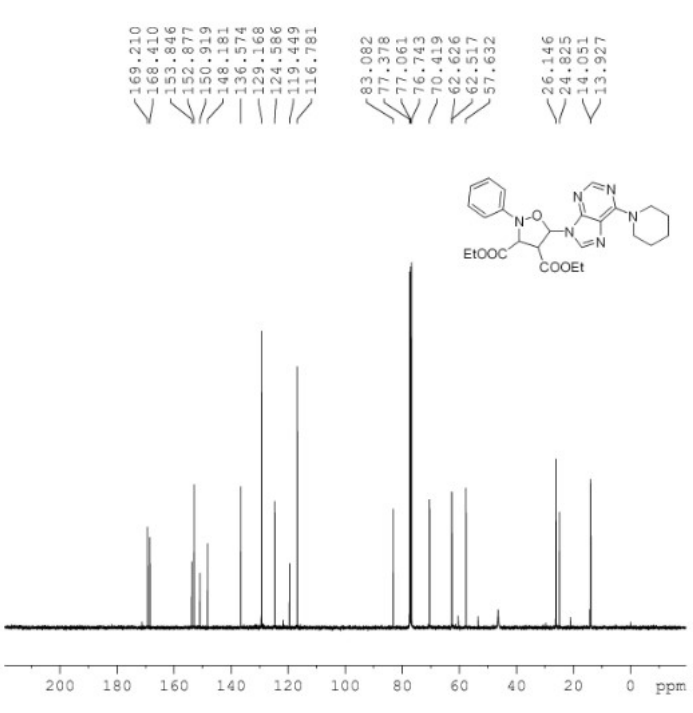



```
NAME          2017-03-16 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20170317
Time                3.48
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                296.4 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
```

**6f**

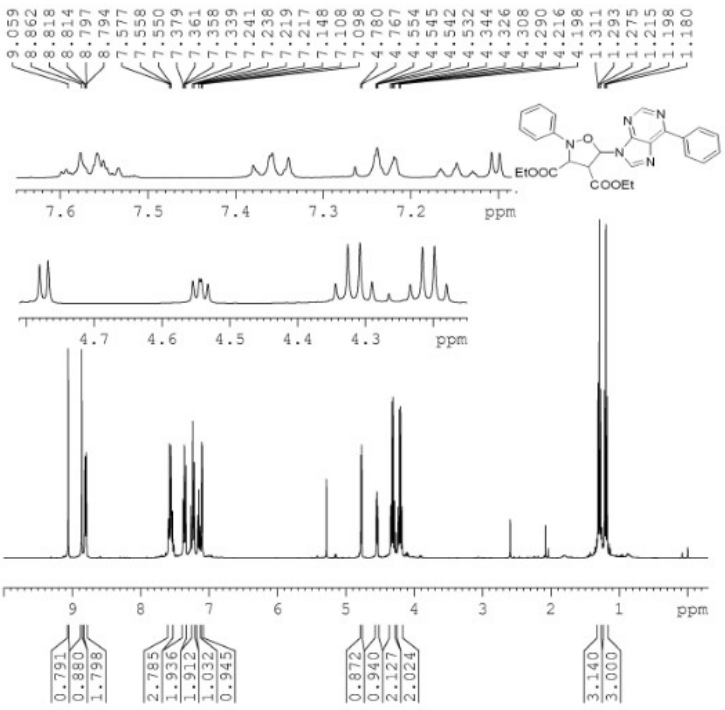



```
NAME          2017-03-16 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20170317
Time                3.52
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     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                295.7 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                   1H
P1                  9.70 usec
SI                 65536
SF            400.1300047 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

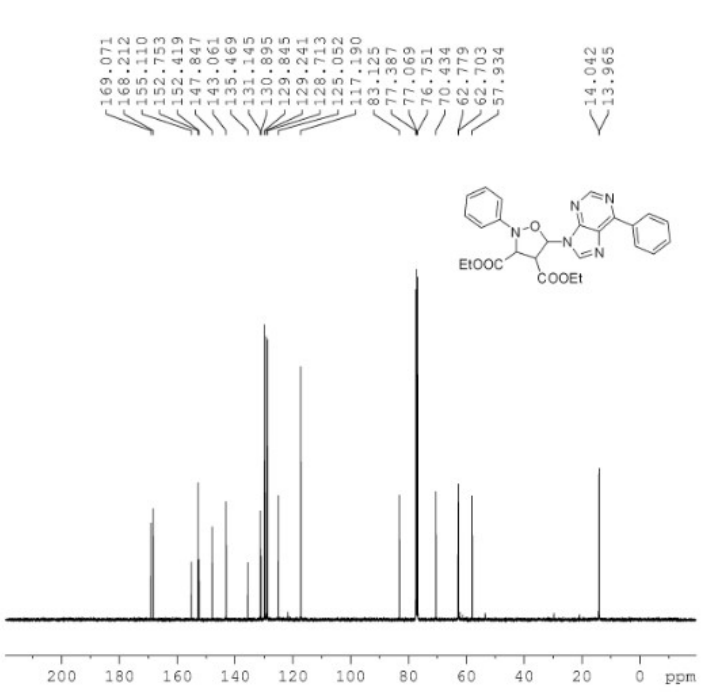



```
NAME          2017-03-16 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20170317
Time                4.51
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                296.3 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
```

**6g**

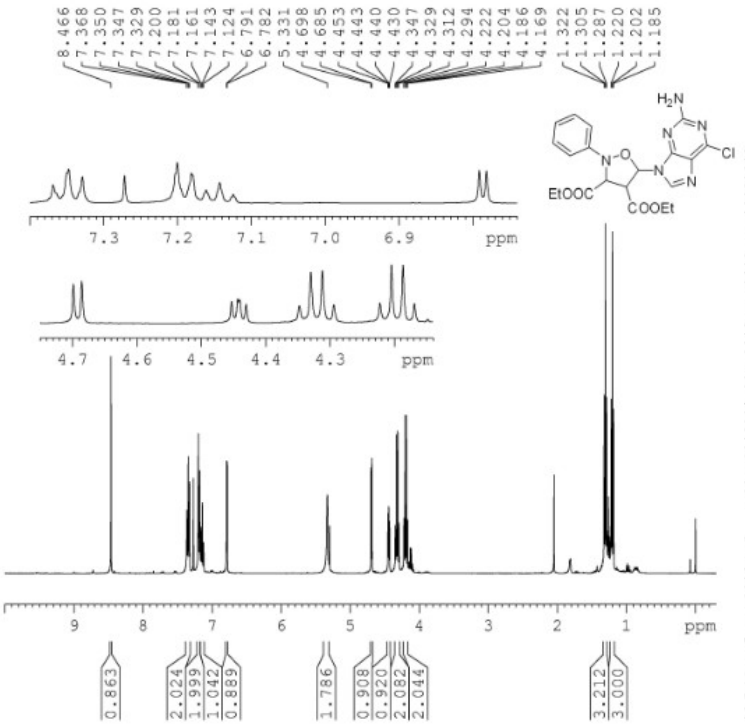



```
NAME          2017-04-28 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20170428
Time               21.11
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     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                297.6 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.70 usec
SI                 65536
SF           400.1300086 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

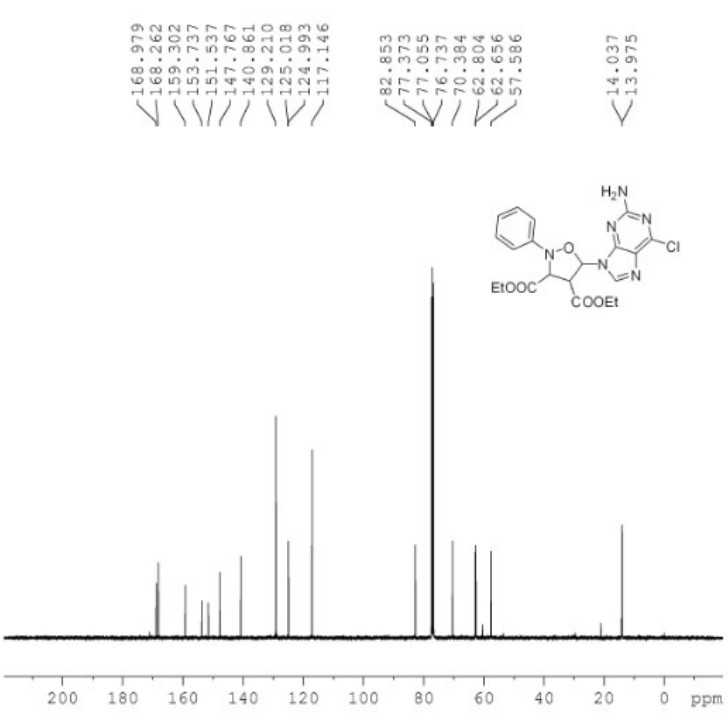



```
NAME        2017-05-02 tyut-lx-
EXPNO                   10
PROCNO                   1
Date_             20170502
Time                 21.51
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     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                   298.0 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
```

**6h**

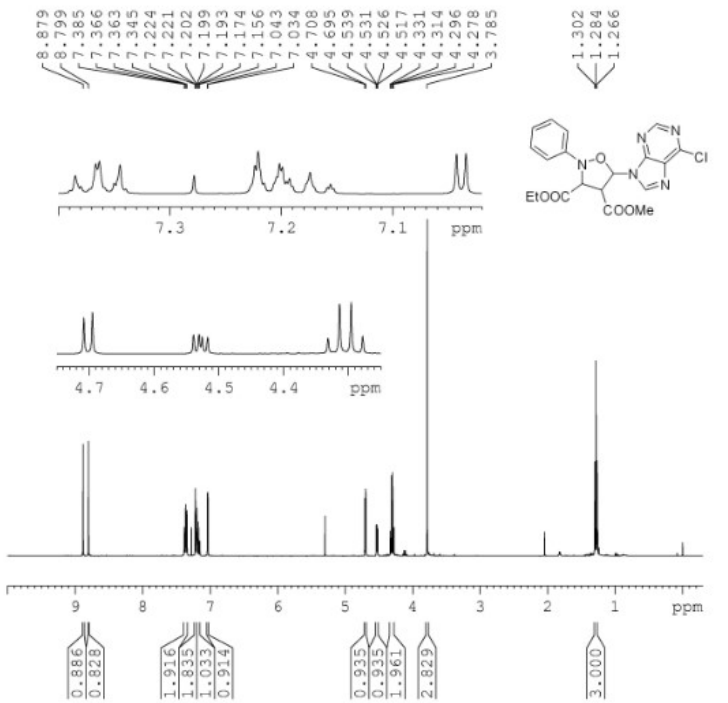



```
NAME        2017-03-17 tyut-lix
EXPNO                   10
PROCNO                   1
Date_             20170318
Time                 18.33
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                   57.76
DW                   62.400 usec
DE                    6.50 usec
TE                   295.5 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                     1H
P1                    9.70 usec
SI                   65536
SF              400.1300053 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

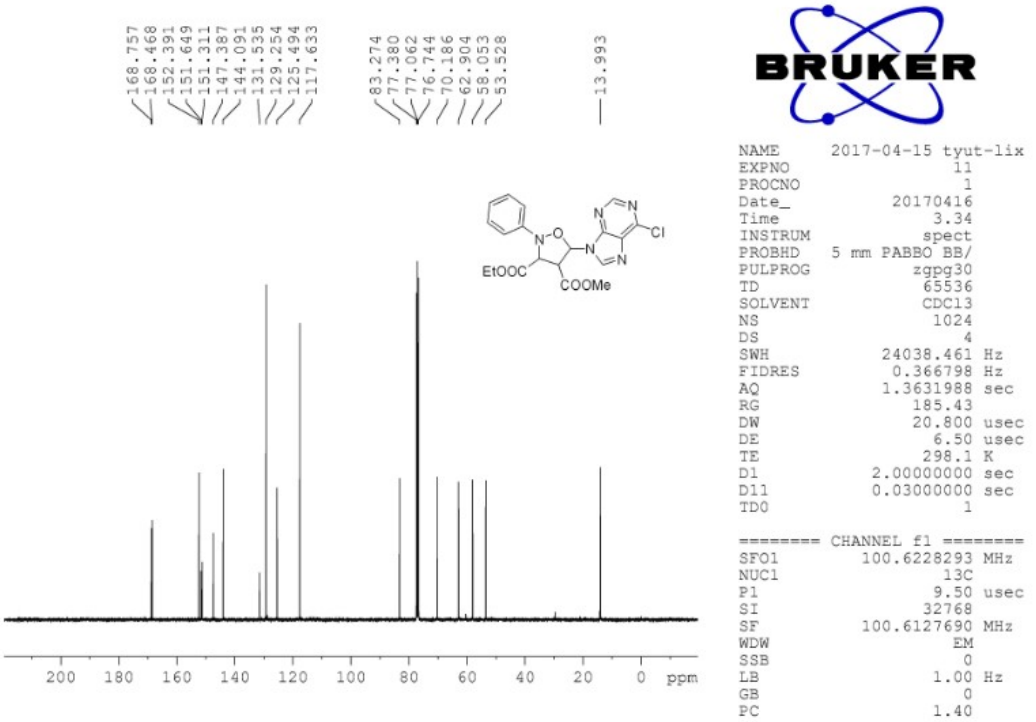



```
NAME          2017-03-17 tyut-lix
EXPNO                 11
PROCNO                 1
Date_           20170319
Time                5.33
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    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                296.3 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
```

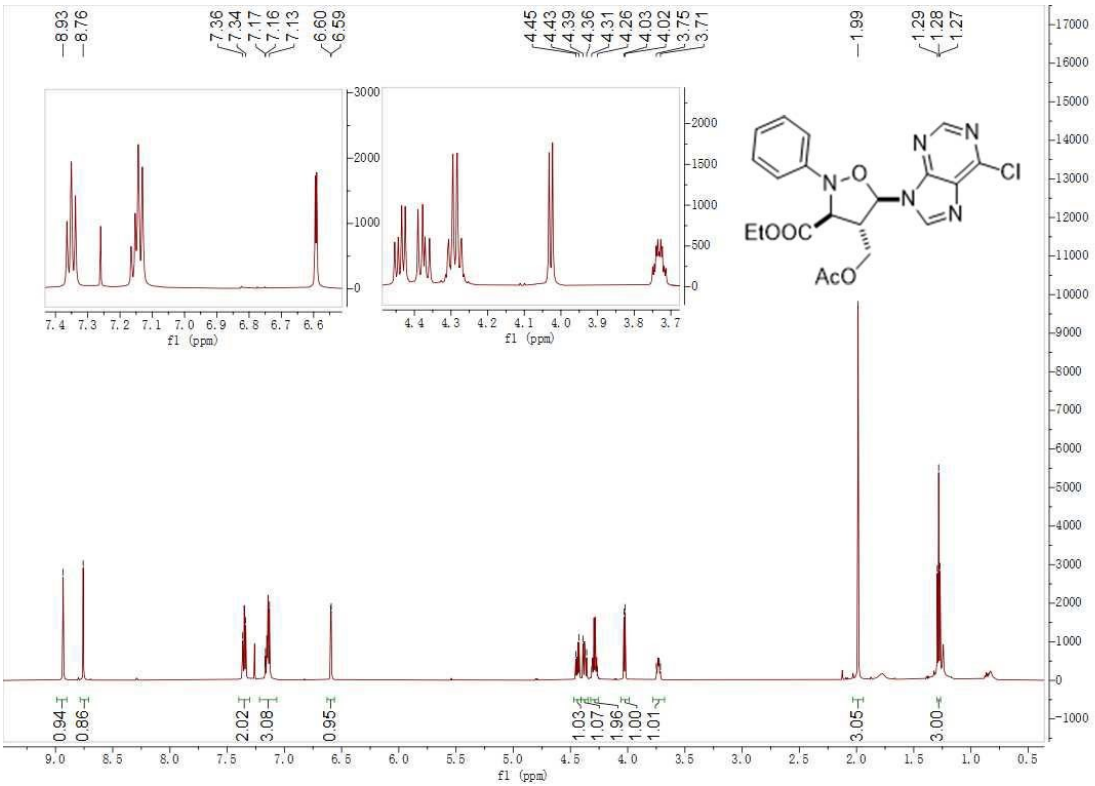
**6i**

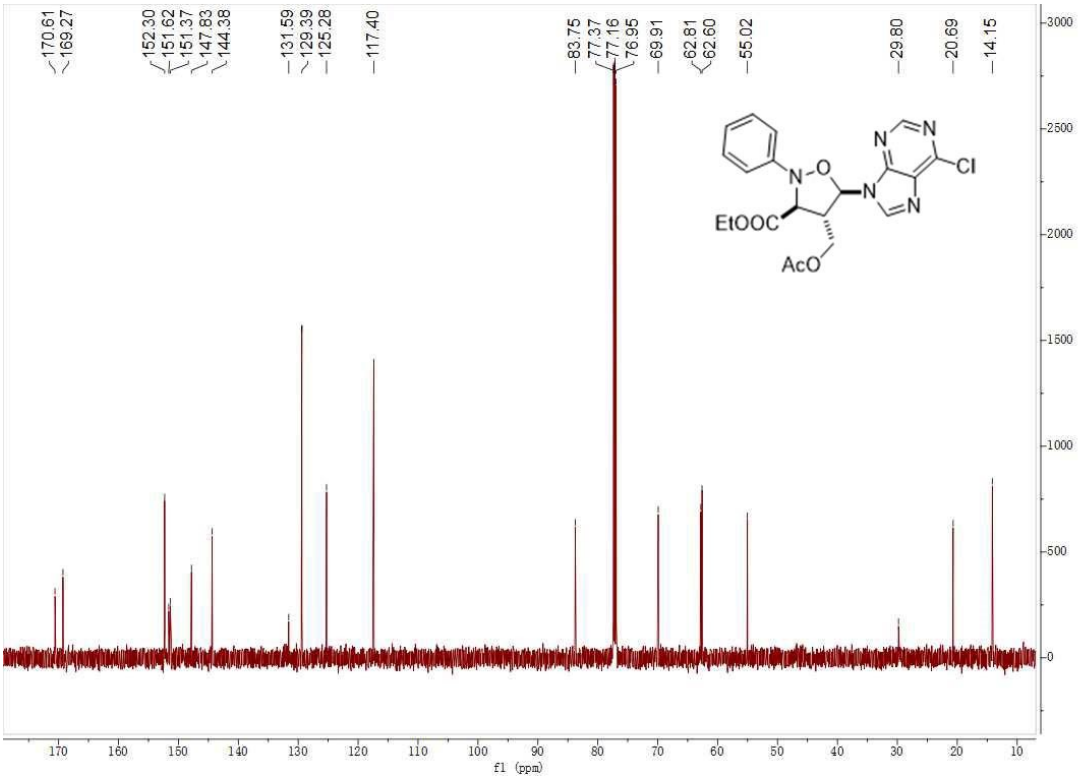



```
NAME          2017-04-15 tyut-lix
EXPNO                 10
PROCNO                 1
Date_           20170416
Time                2.35
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    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                297.4 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                   1H
P1                  9.70 usec
SI                 65536
SF           400.1300024 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

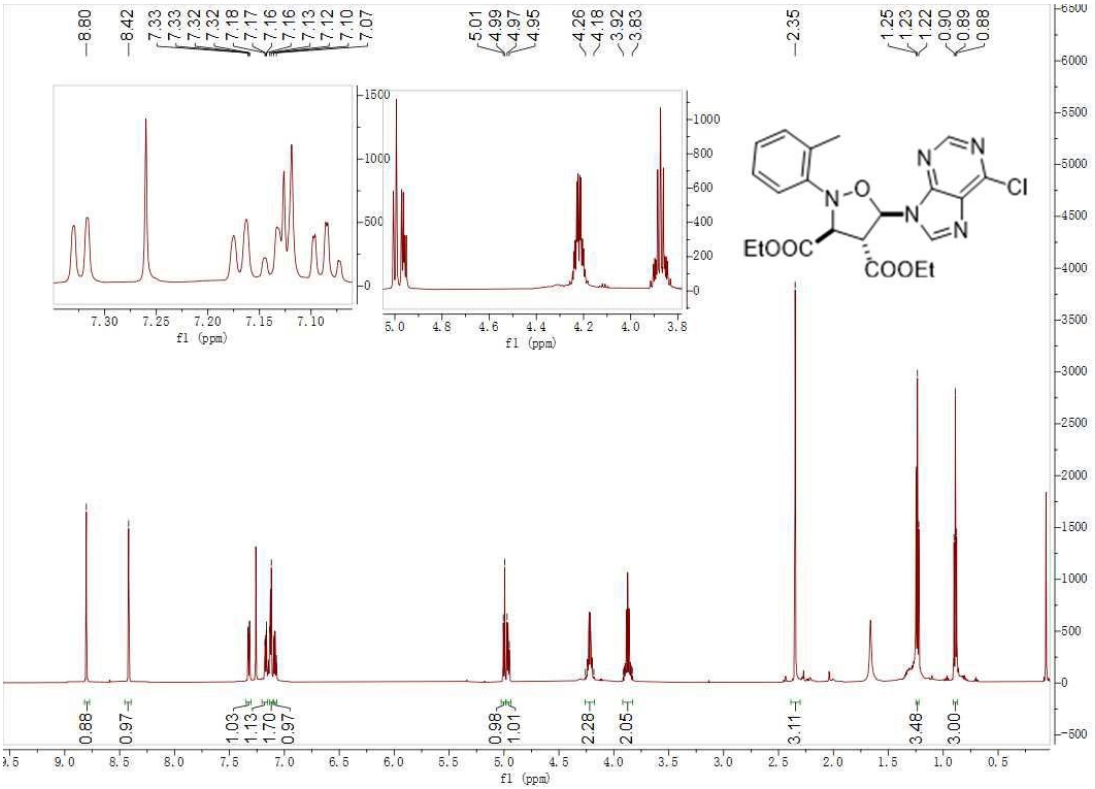

168.757
168.468
152.391
151.649
151.311
147.387
144.091
131.535
129.254
125.494
117.633
83.274
77.380
77.062
76.744
70.186
62.904
58.053
53.528
13.993
BRUKER
NAME 2017-04-15 tyut-lix
EXPNO 11
PROCNO 1
Date_ 20170416
Time 3.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 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 298.1 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
EtOOC
COOMe
Cl
200 180 160 140 120 100 80 60 40 20 0 ppm

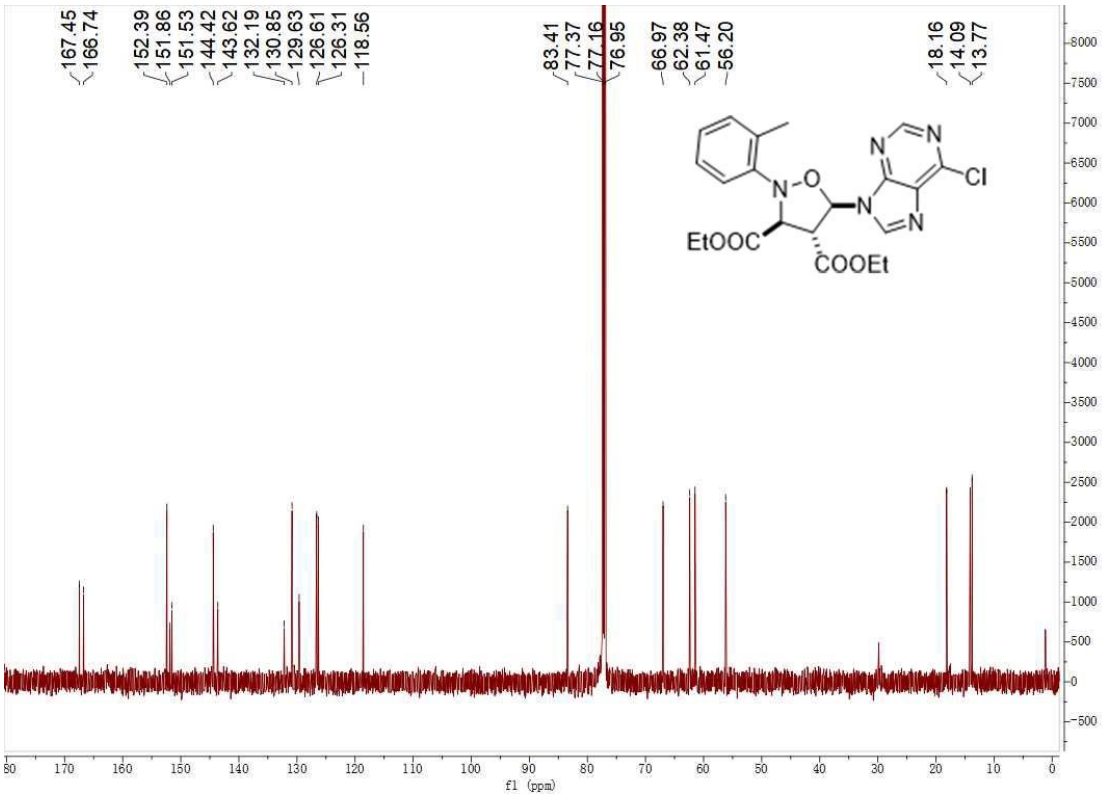
**6k**


8.93
8.76
7.36
7.34
7.17
7.16
7.13
6.60
6.59
4.45
4.43
4.39
4.36
4.31
4.26
4.03
4.02
3.75
3.71
1.99
1.29
1.28
1.27
EtOOC
AcO
Cl
f1 (ppm)
0.94
0.86
2.02
3.08
0.95
1.03
1.07
1.96
1.00
1.01
3.05
3.00

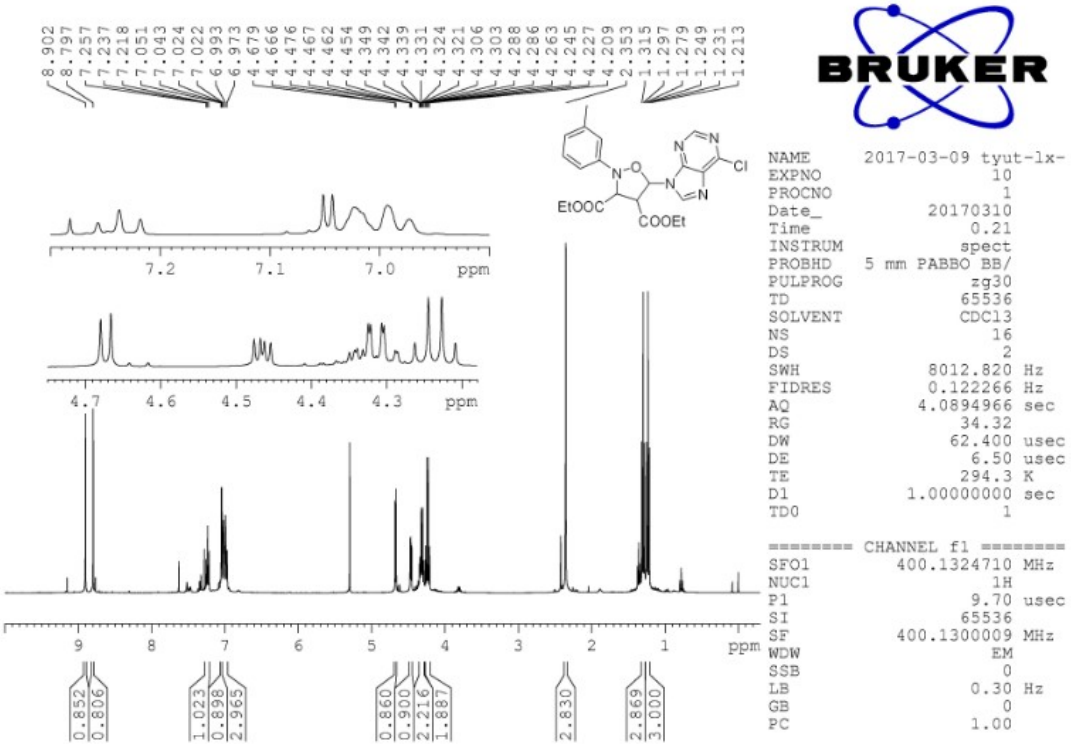

170.61
169.27
152.30
151.62
151.37
147.83
144.38
131.59
129.39
125.28
117.40
83.75
77.37
77.16
76.95
69.91
62.81
62.60
55.02
29.80
20.69
14.15
EtOOC
AcO
Cl
f1 (ppm)

**6l**


8.80
8.42
7.33
7.33
7.32
7.32
7.18
7.17
7.16
7.16
7.13
7.12
7.10
7.07
5.01
4.99
4.97
4.95
4.26
4.18
3.92
3.83
2.35
1.25
1.23
1.22
0.90
0.89
0.88
EtOOC
COOEt
Cl
0.88
0.97
1.03
1.13
1.70
0.97
0.98
1.01
2.28
2.05
3.11
3.48
3.00
f1 (ppm)

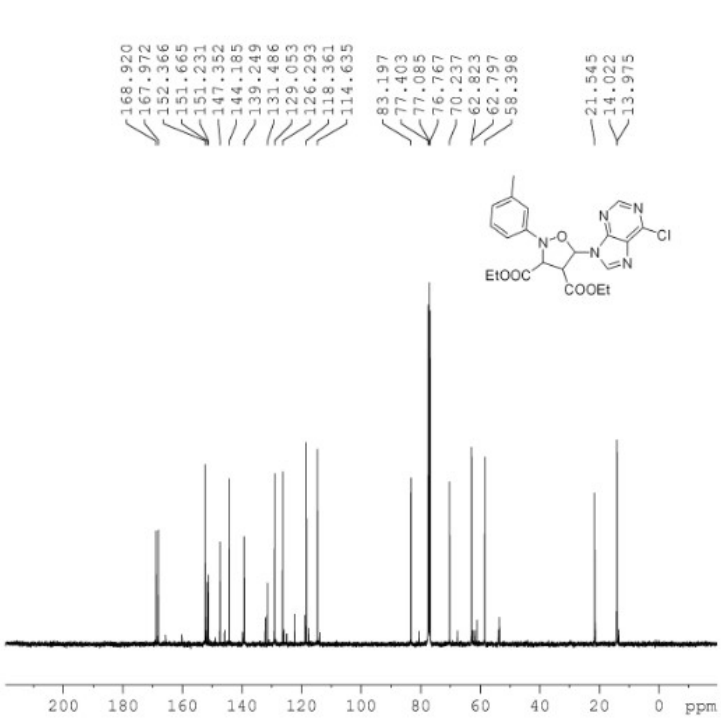



**6m**



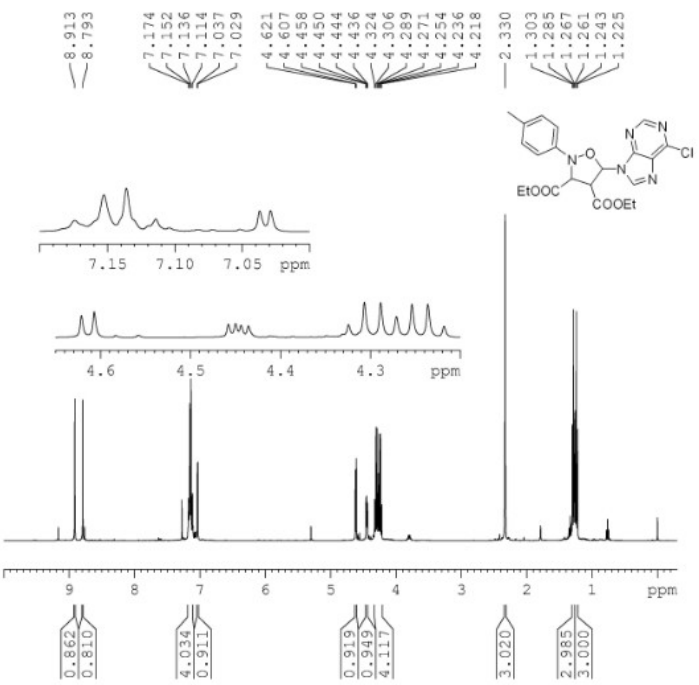

BRUKER

| | |
|---|---|
| NAME | 2017-03-09 tyut-lx- |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20170310 |
| Time | 0.21 |
| 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 | 294.3 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300009 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

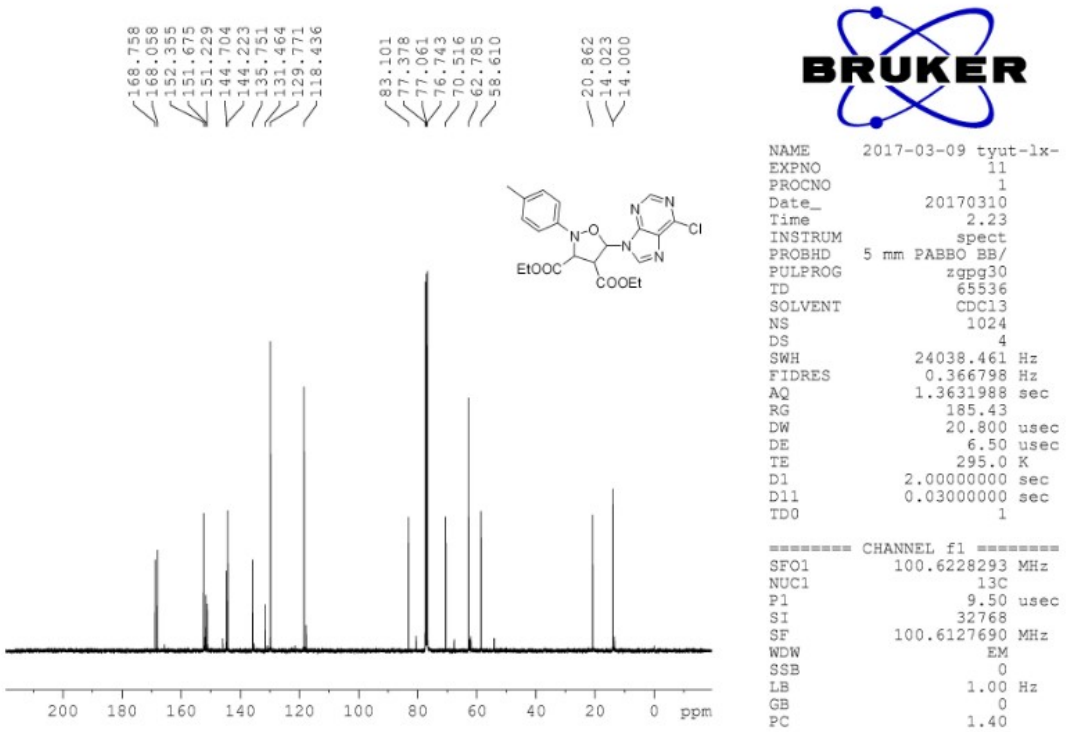



```
NAME          2017-03-09 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20170310
Time                1.20
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                295.0 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
```

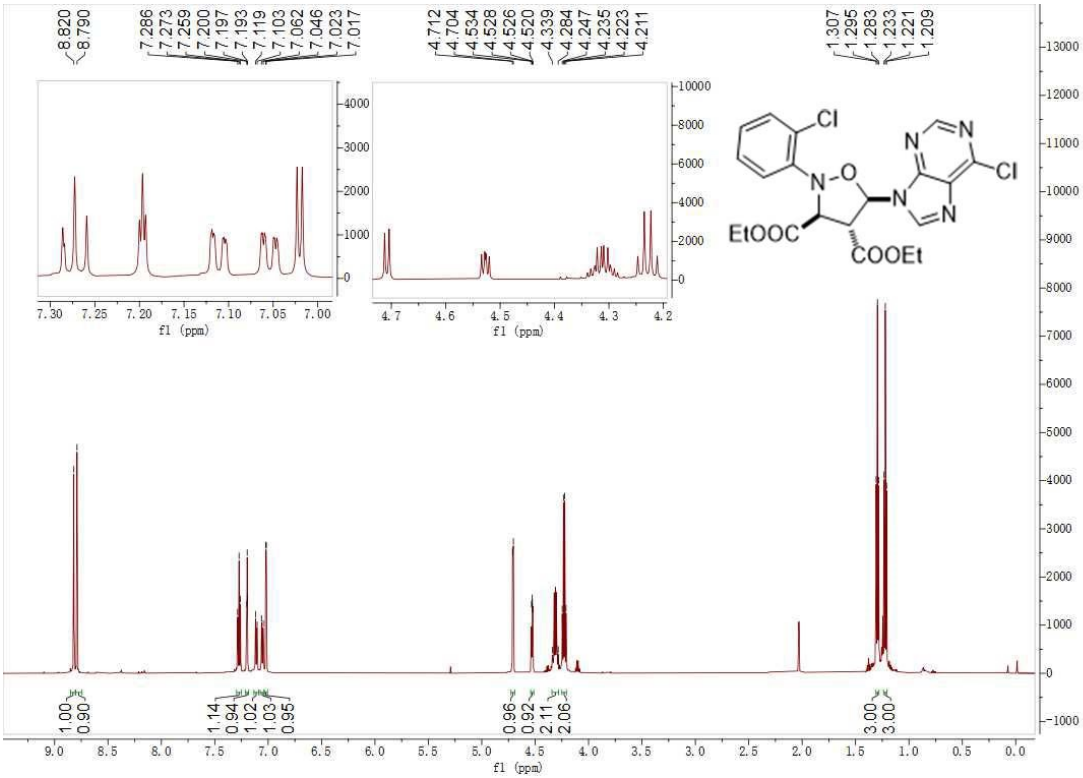
**6n**

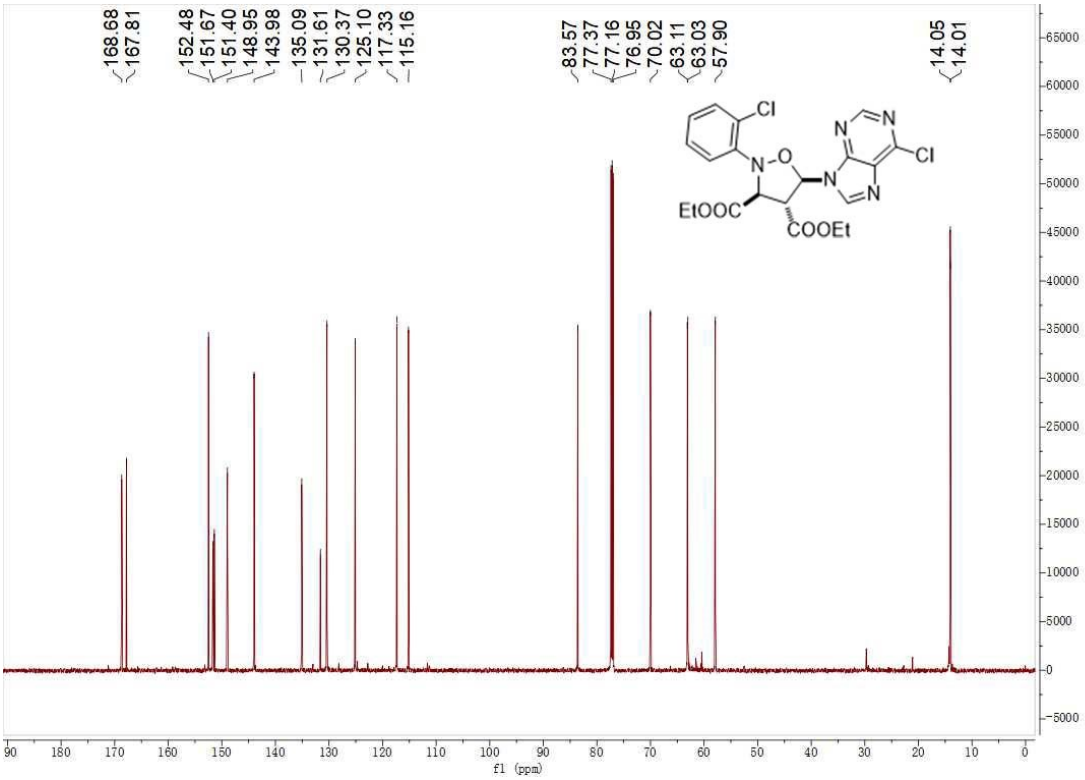



```
NAME          2017-03-09 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20170310
Time                1.24
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                   16
DS                     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                294.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1               1H
P1                 9.70 usec
SI                65536
SF            400.1300040 MHz
WDW                EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

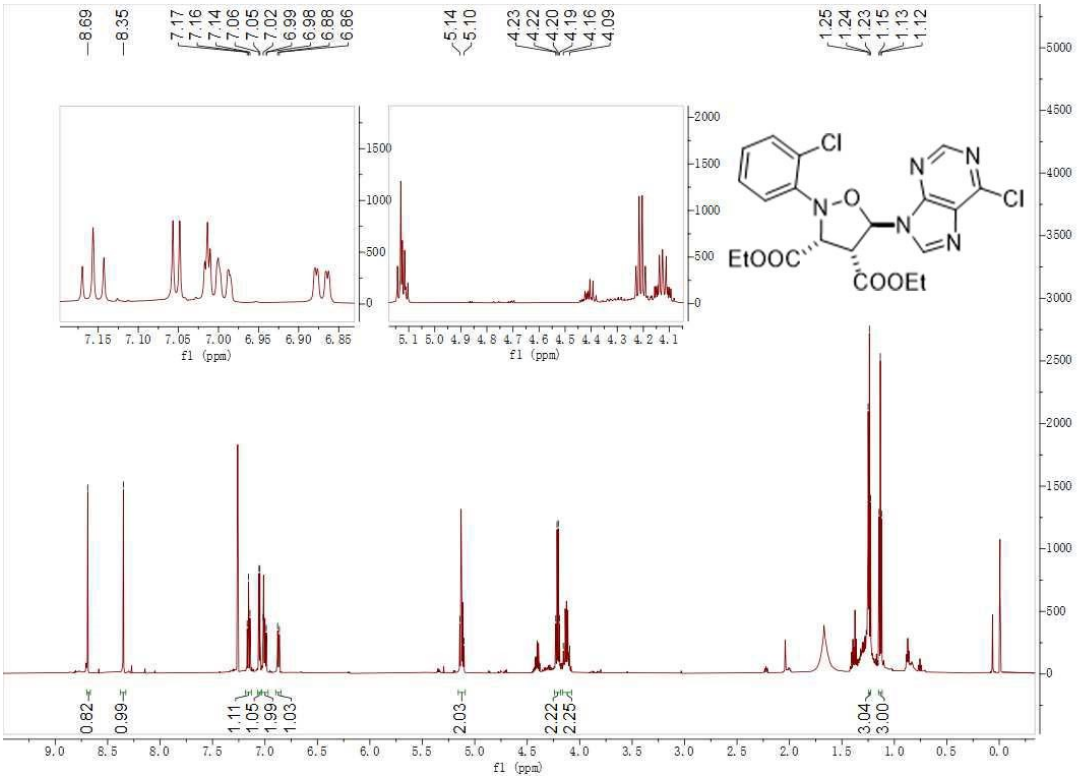

168.758
168.058
152.355
151.675
151.229
144.704
144.223
135.751
131.464
129.771
118.436
83.101
77.378
77.061
76.743
70.516
62.785
58.610
20.862
14.023
14.000
EtOOC
COOEt
Cl
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
NAME 2017-03-09 tyut-lx-
EXPNO 11
PROCNO 1
Date_ 20170310
Time 2.23
INSTRUM spect
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 295.0 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

*endo*-**6q**

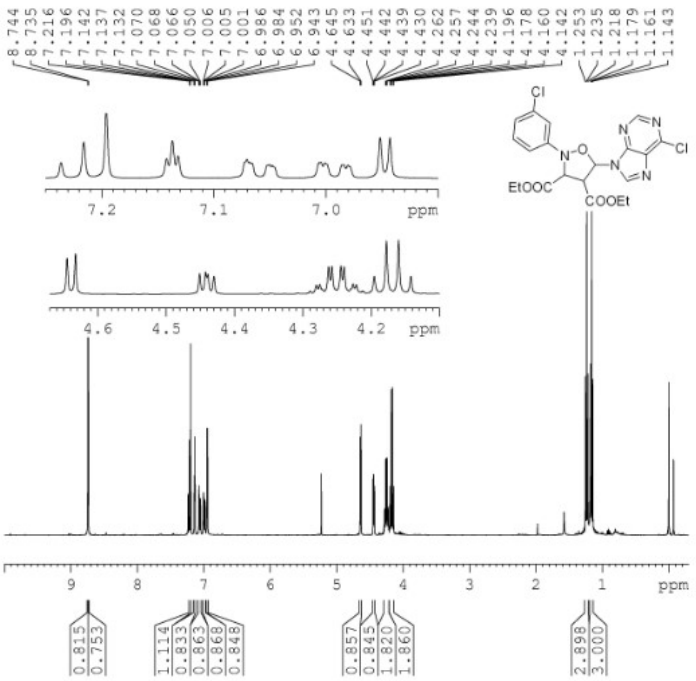

8.820
8.790
7.286
7.273
7.259
7.200
7.197
7.193
7.119
7.103
7.062
7.046
7.023
7.017
4.712
4.704
4.534
4.528
4.526
4.520
4.339
4.284
4.247
4.235
4.223
4.211
1.307
1.295
1.283
1.233
1.221
1.209
Cl
EtOOC
COOEt
f1 (ppm)
1.00
0.90
1.14
0.94
1.02
1.03
0.95
0.96
0.92
2.11
2.06
3.00
3.00


168.68
167.81
152.48
151.67
151.40
148.95
143.98
135.09
131.61
130.37
125.10
117.33
115.16
83.57
77.37
77.16
76.95
70.02
63.11
63.03
57.90
14.05
14.01
Cl
N
N
Cl
N-O
N
N
EtOOC
COOEt
f1 (ppm)

*exo*-**6q**

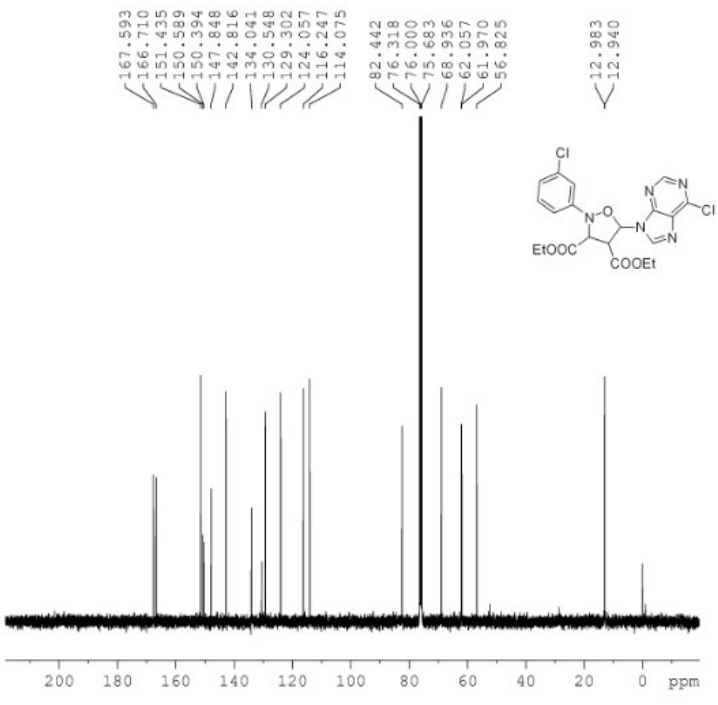

8.69
8.35
7.17
7.16
7.14
7.06
7.05
7.02
6.99
6.98
6.88
6.86
5.14
5.10
4.23
4.22
4.20
4.19
4.16
4.09
1.25
1.24
1.23
1.15
1.13
1.12
Cl
N
N
Cl
N-O
N
N
EtOOC
COOEt
0.82
0.99
1.11
1.05
1.99
1.03
2.03
2.22
2.25
3.04
3.00
f1 (ppm)

**6r**





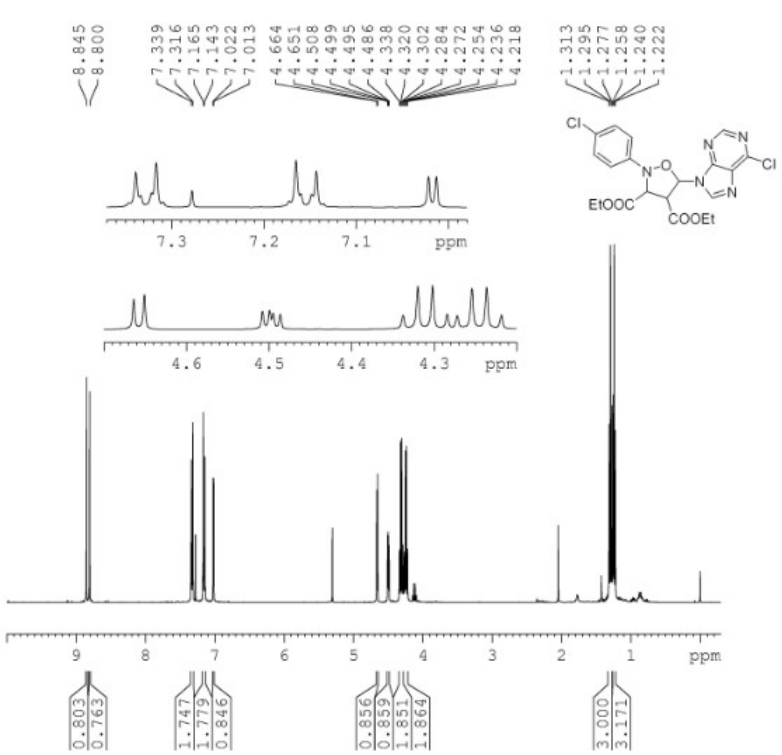
| | |
|---|---|
| NAME | 2017-03-10 tyut-chh |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20170311 |
| Time | 0.22 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 8012.820 Hz |
| FIDRES | 0.122266 Hz |
| AQ | 4.0894966 sec |
| RG | 74.25 |
| DW | 62.400 usec |
| DE | 6.50 usec |
| TE | 294.7 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300353 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |



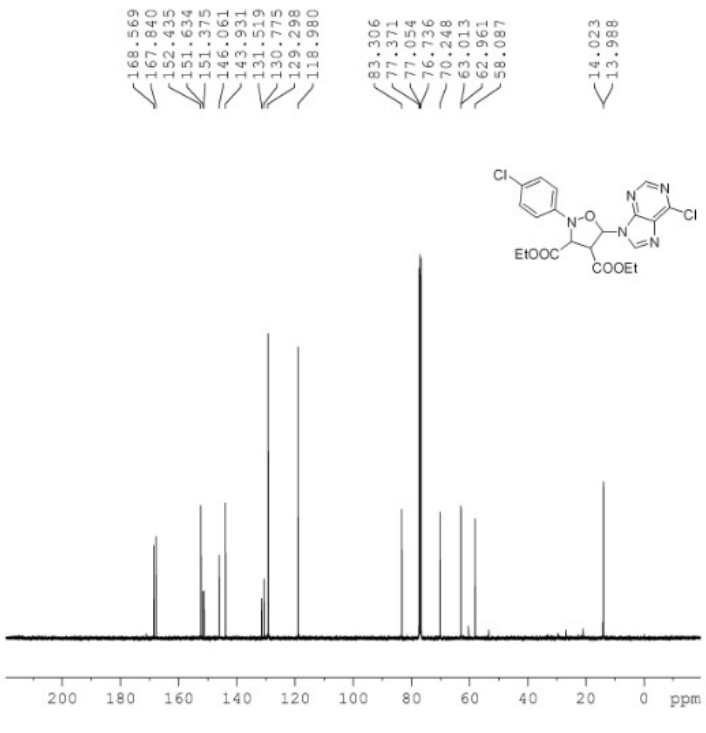


| | |
|---|---|
| NAME | 2017-03-10 tyut-chh |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20170311 |
| Time | 1.21 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 1024 |
| DS | 4 |
| SWH | 24038.461 Hz |
| FIDRES | 0.366798 Hz |
| AQ | 1.3631988 sec |
| RG | 185.43 |
| DW | 20.800 usec |
| DE | 6.50 usec |
| TE | 295.3 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 | 100.6128730 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |

**6s**

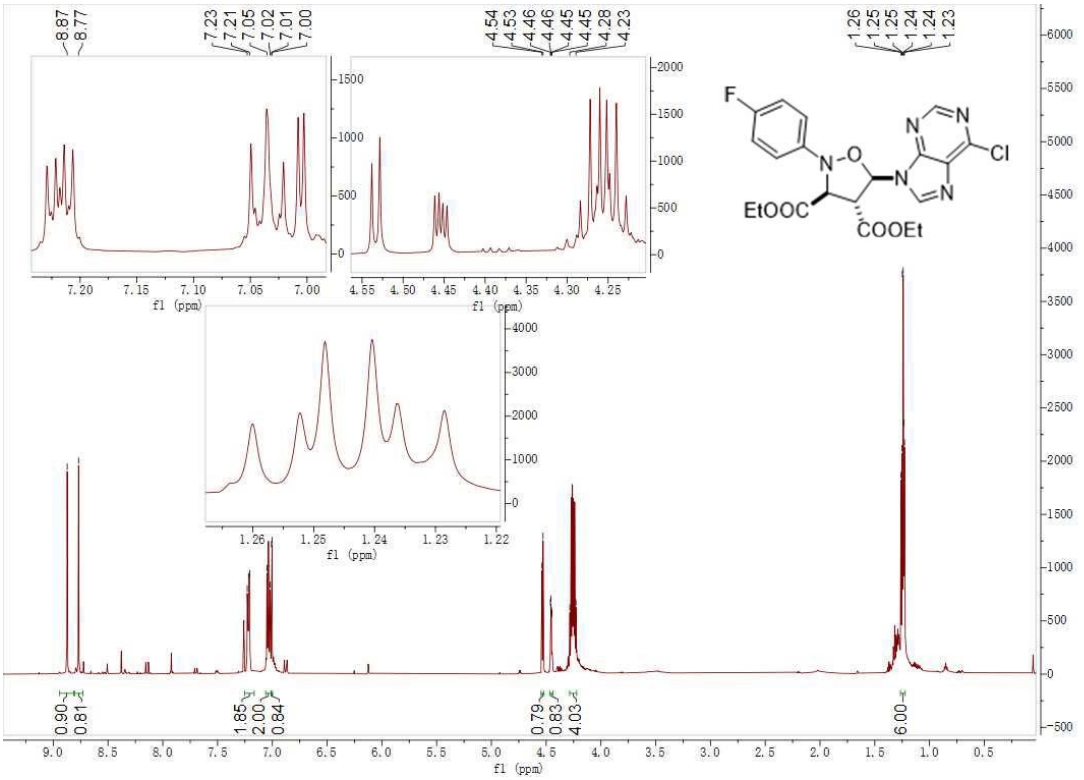


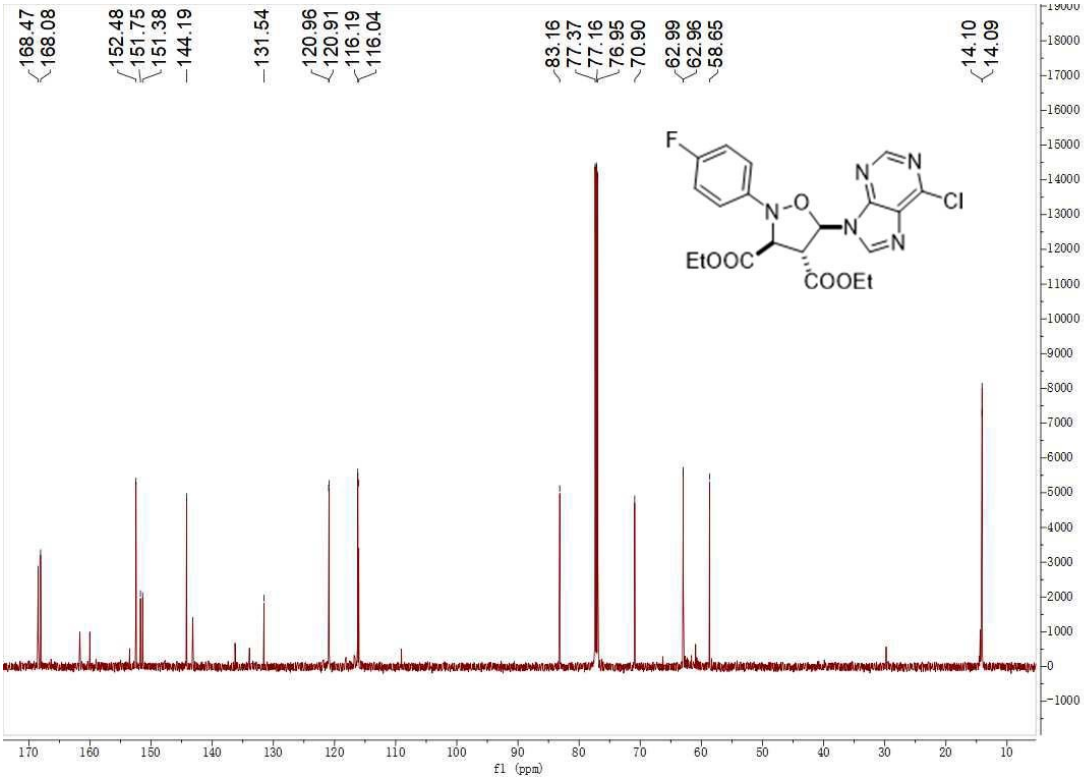

```
NAME          2017-03-10 tyut-chh
EXPNO                   10
PROCNO                   1
Date_             20170311
Time                  1.25
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   54.19
DW                 62.400 usec
DE                  6.50 usec
TE                 294.6 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                   9.70 usec
SI                   65536
SF            400.1300024 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



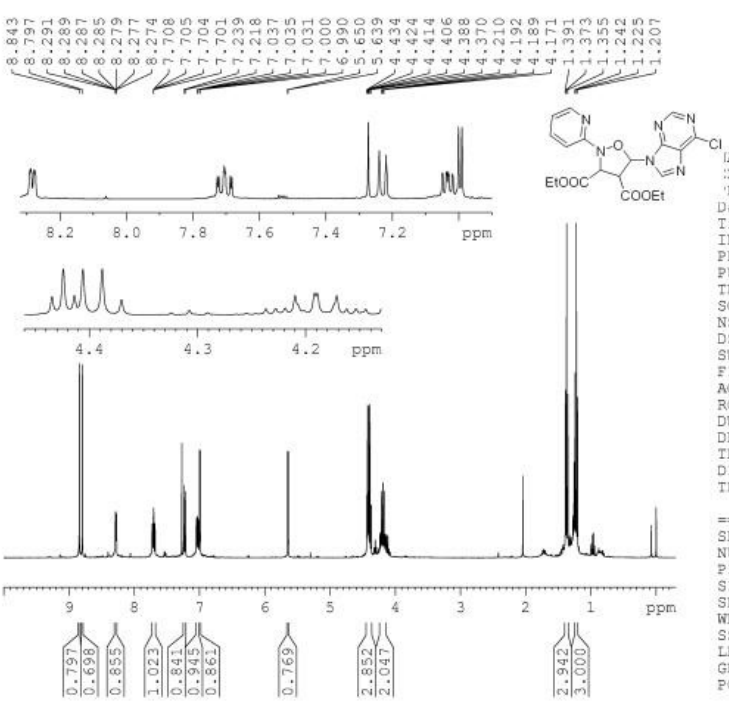

```
NAME          2017-03-10 tyut-chh
EXPNO                   11
PROCNO                   1
Date_             20170311
Time                  2.24
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    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                 295.2 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
```

**6t**


8.87
8.77
7.23
7.21
7.05
7.02
7.01
7.00
4.54
4.53
4.46
4.46
4.45
4.45
4.28
4.23
1.26
1.25
1.25
1.24
1.24
1.23
F
N
N
Cl
N
O
N
N
EtOOC
COOEt
f1 (ppm)
0.90
0.81
1.85
2.00
0.84
0.79
0.83
4.03
6.00

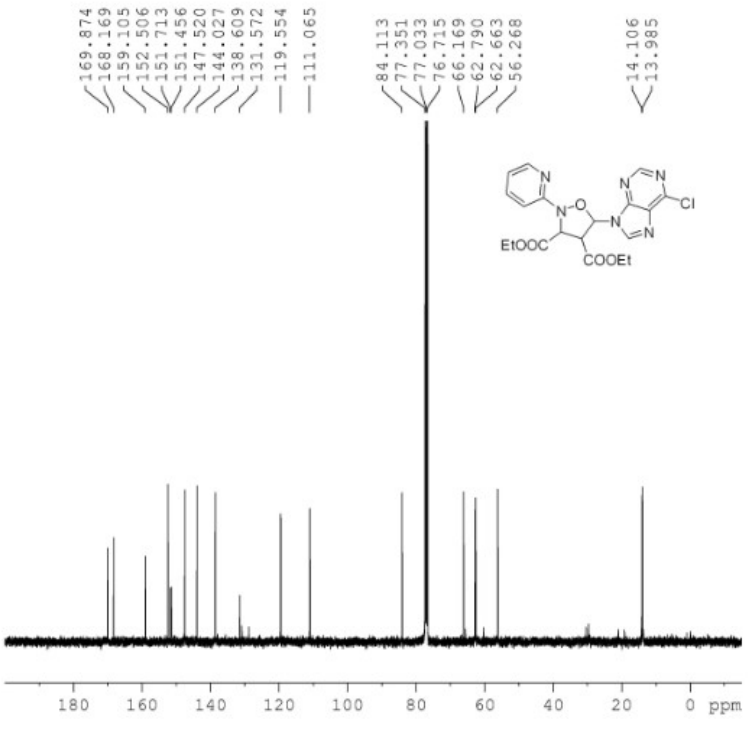

168.47
168.08
152.48
151.75
151.38
144.19
131.54
120.96
120.91
116.19
116.04
83.16
77.37
77.16
76.95
70.90
62.99
62.96
58.65
14.10
14.09
F
N
N
Cl
N
O
N
N
EtOOC
COOEt
f1 (ppm)

**6u**




BRUKER

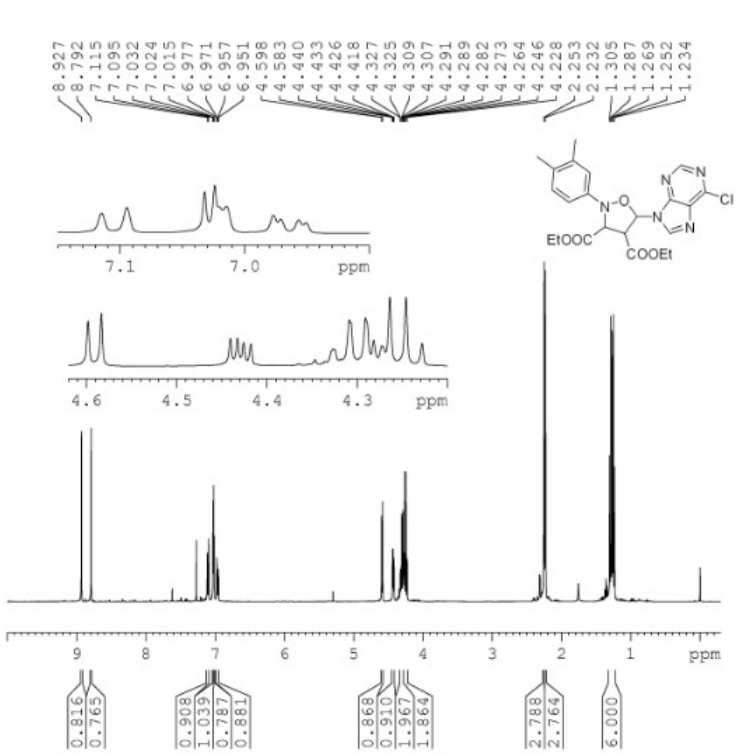
| | |
|---|---|
| NAME | 2014-04-06 tyut-lix |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20170407 |
| Time | 1.15 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 8012.820 Hz |
| FIDRES | 0.122266 Hz |
| AQ | 4.0894966 sec |
| RG | 67.58 |
| DW | 62.400 usec |
| DE | 6.50 usec |
| TE | 298.3 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300050 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |



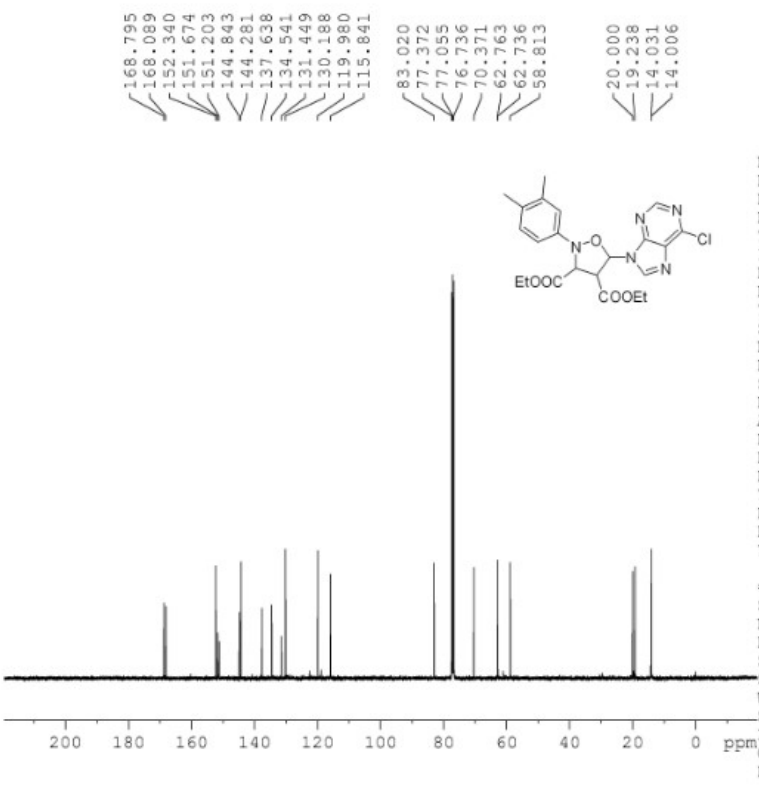

BRUKER

| | |
|---|---|
| NAME | 2014-04-06 tyut-lix |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20170407 |
| Time | 2.14 |
| 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 | 298.9 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 |

**6v**

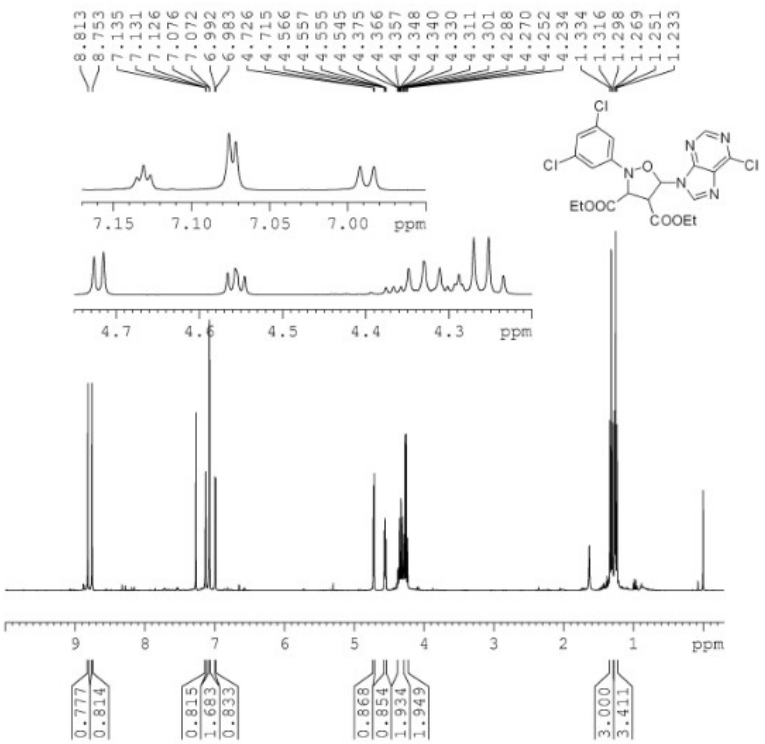



```
NAME          2017-03-11 tyut-lix
EXPNO                 10
PROCNO                 1
Date_           20170311
Time               18.54
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     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                294.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.70 usec
SI                 65536
SF           400.1300046 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



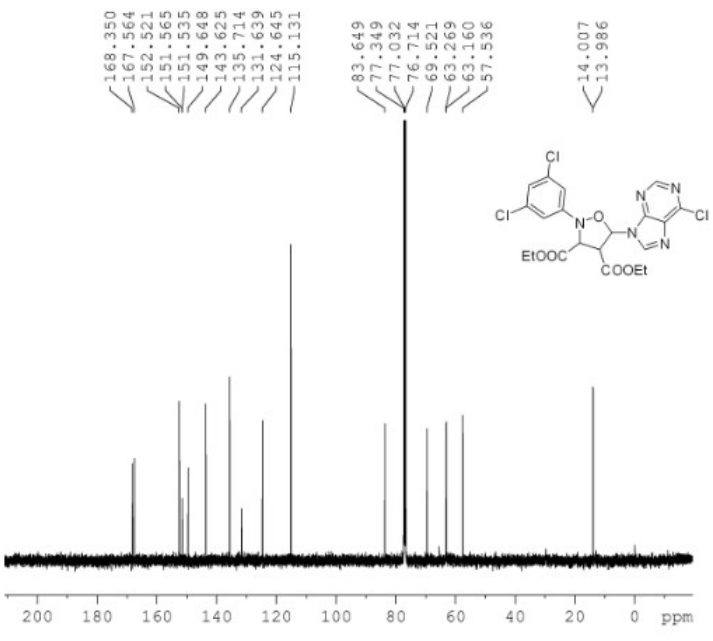

```
NAME          2017-03-11 tyut-lix
EXPNO                 11
PROCNO                 1
Date_           20170311
Time               19.53
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                295.2 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
```

**6w**





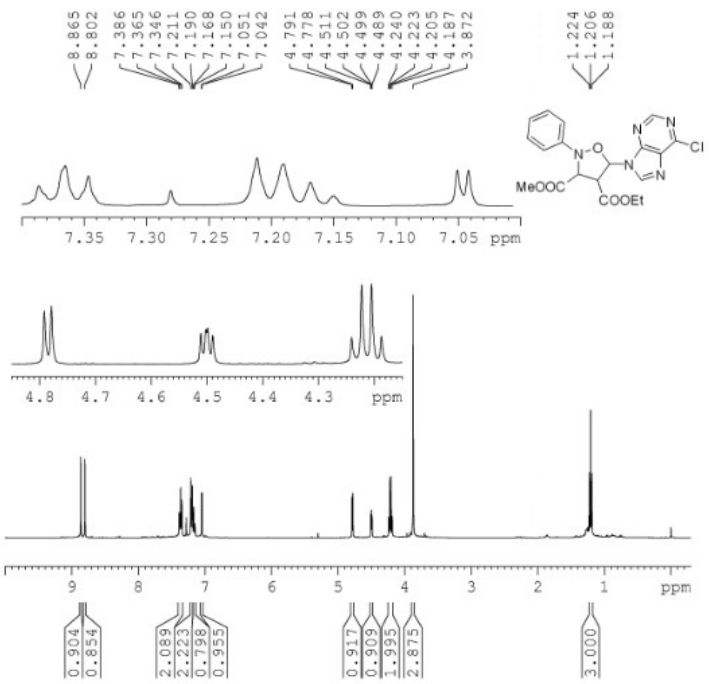
```
NAME          2017-03-11 tyut-lix
EXPNO                 10
PROCNO                 1
Date_           20170311
Time               19.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894966 sec
RG                 87.46
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           400.1300066 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



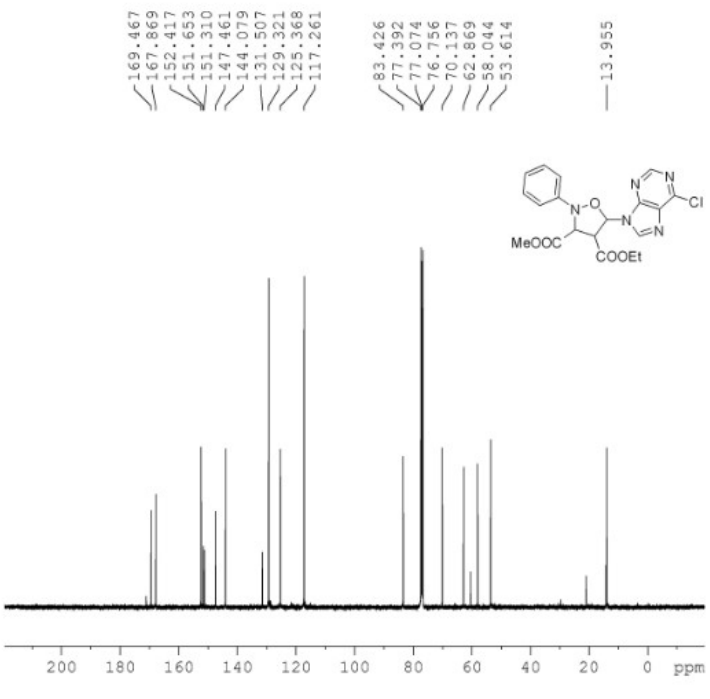


```
NAME          2017-03-11 tyut-lix
EXPNO                 11
PROCNO                 1
Date_           20170311
Time               20.56
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                295.2 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
```

**6x**

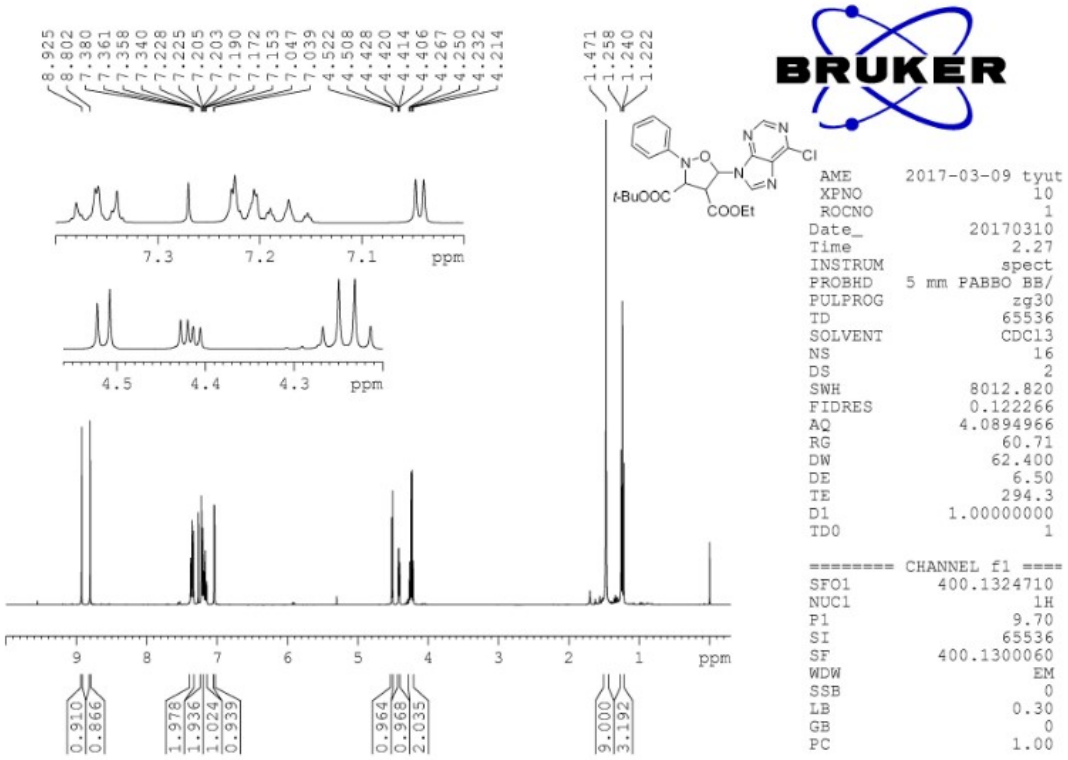


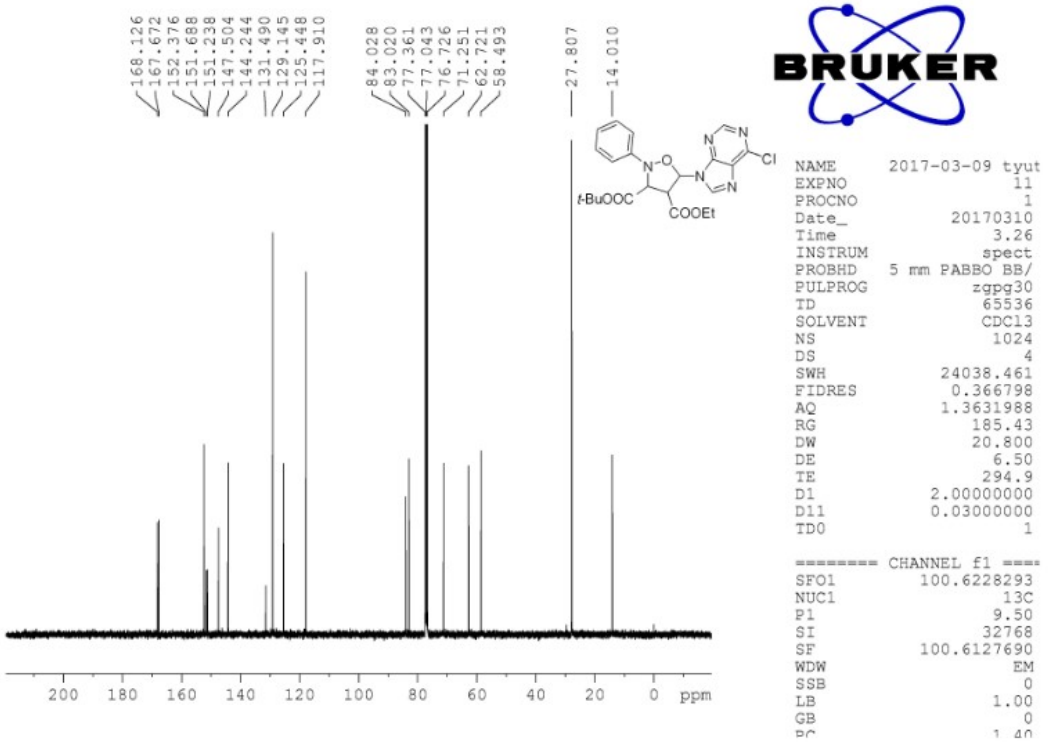

```
NAME          2017-03-08 tyut-chh
EXPNO                 10
PROCNO                 1
Date_           20170309
Time                9.00
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     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                293.5 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.70 usec
SI                 65536
SF            400.1300014 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



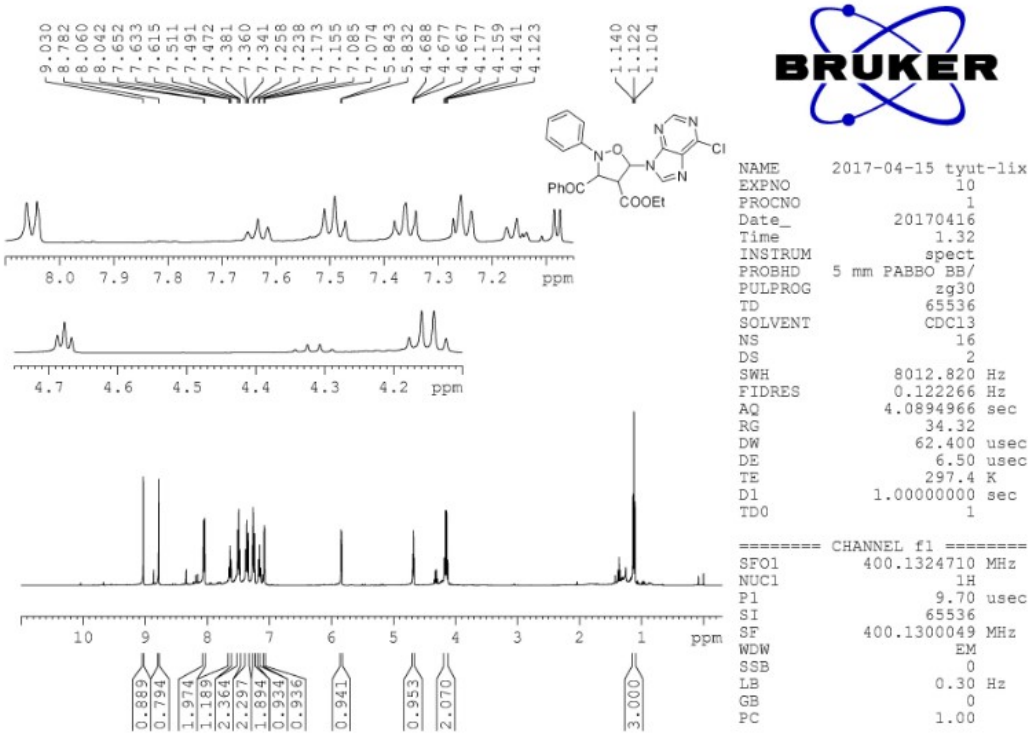

```
NAME          2017-03-08 tyut-chh
EXPNO                 11
PROCNO                 1
Date_           20170309
Time                9.59
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                294.4 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
```

**6y**


8.925
8.802
7.380
7.361
7.358
7.340
7.228
7.225
7.205
7.203
7.190
7.172
7.153
7.047
7.039
4.522
4.508
4.428
4.420
4.414
4.406
4.267
4.250
4.232
4.214
1.471
1.258
1.240
1.222
t-BuOOC
COOEt
Cl
7.3
7.2
7.1
ppm
4.5
4.4
4.3
ppm
9
8
7
6
5
4
3
2
1
ppm
0.910
0.866
1.978
1.936
1.024
0.939
0.964
0.968
2.035
9.000
3.192
BRUKER
AME 2017-03-09 tyut
XPNO 10
ROCNO 1
Date_ 20170310
Time 2.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820
FIDRES 0.122266
AQ 4.0894966
RG 60.71
DW 62.400
DE 6.50
TE 294.3
D1 1.00000000
TD0 1
======== CHANNEL f1 ====
SFO1 400.1324710
NUC1 1H
P1 9.70
SI 65536
SF 400.1300060
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

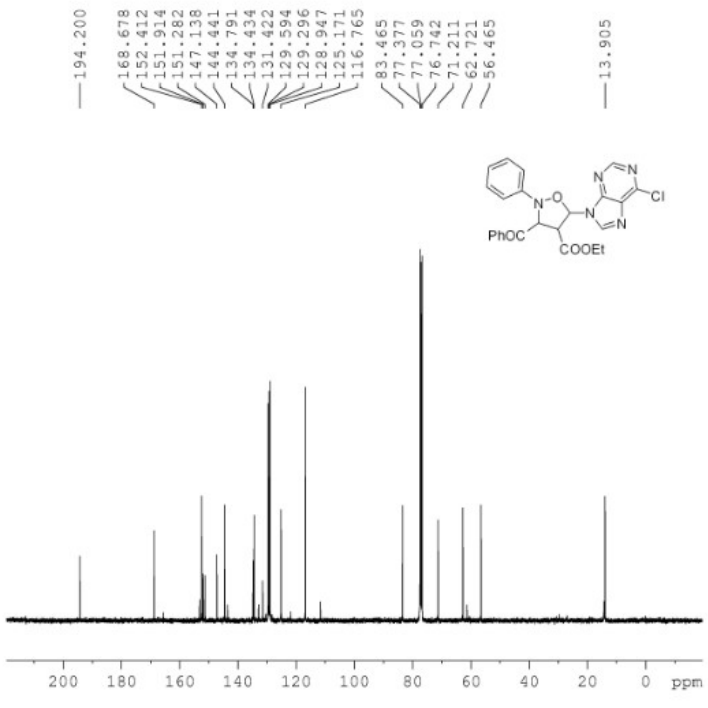

168.126
167.672
152.376
151.688
151.238
147.504
144.244
131.490
129.145
125.448
117.910
84.028
83.020
77.361
77.043
76.726
71.251
62.721
58.493
27.807
14.010
t-BuOOC
COOEt
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
NAME 2017-03-09 tyut
EXPNO 11
PROCNO 1
Date_ 20170310
Time 3.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461
FIDRES 0.366798
AQ 1.3631988
RG 185.43
DW 20.800
DE 6.50
TE 294.9
D1 2.00000000
D11 0.03000000
TD0 1
======== CHANNEL f1 ====
SFO1 100.6228293
NUC1 13C
P1 9.50
SI 32768
SF 100.6127690
WDW EM
SSB 0
LB 1.00
GB 0

**6z**




BRUKER

```
NAME          2017-04-15 tyut-lix
EXPNO                 10
PROCNO                 1
Date_           20170416
Time                1.32
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                297.4 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.70 usec
SI                 65536
SF            400.1300049 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

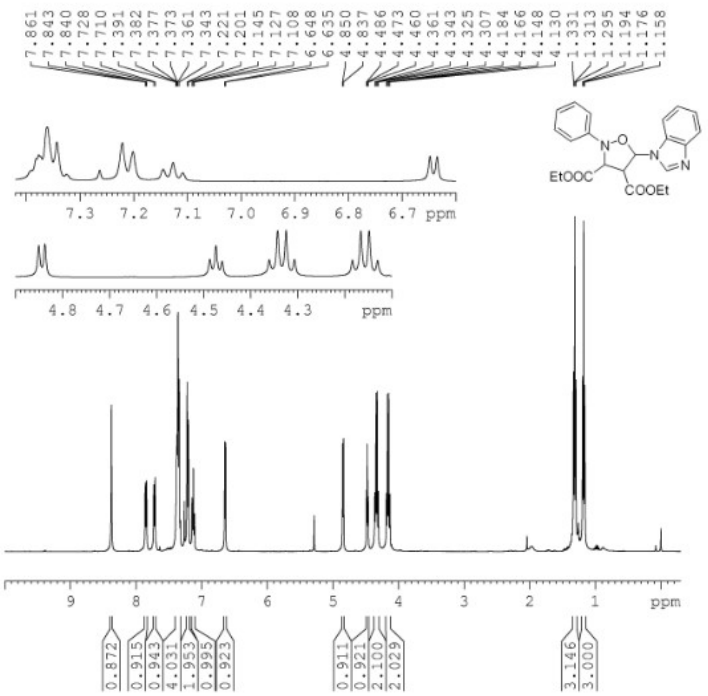



BRUKER

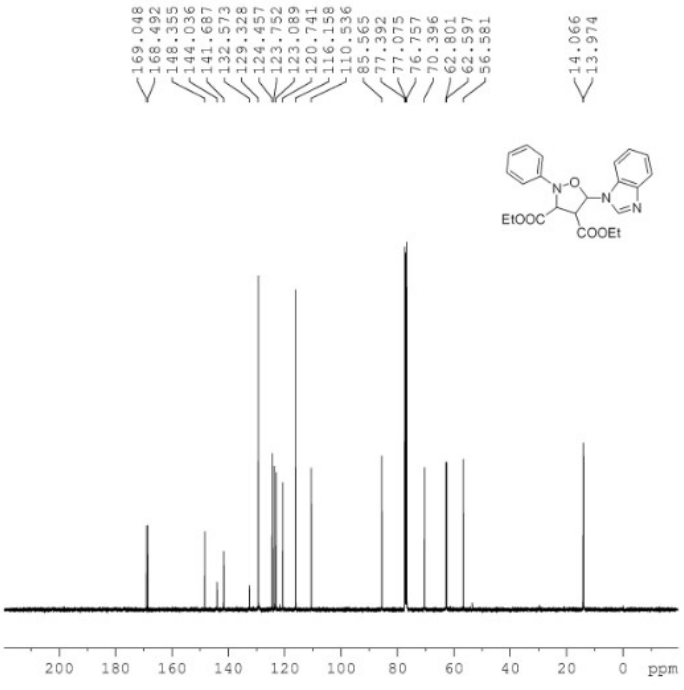
```
NAME          2017-04-15 tyut-lix
EXPNO                 11
PROCNO                 1
Date_           20170416
Time                2.30
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                298.1 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
```

## 12. $^{1}$H-NMR and $^{13}$C-NMR spectra of products 8

### 8a

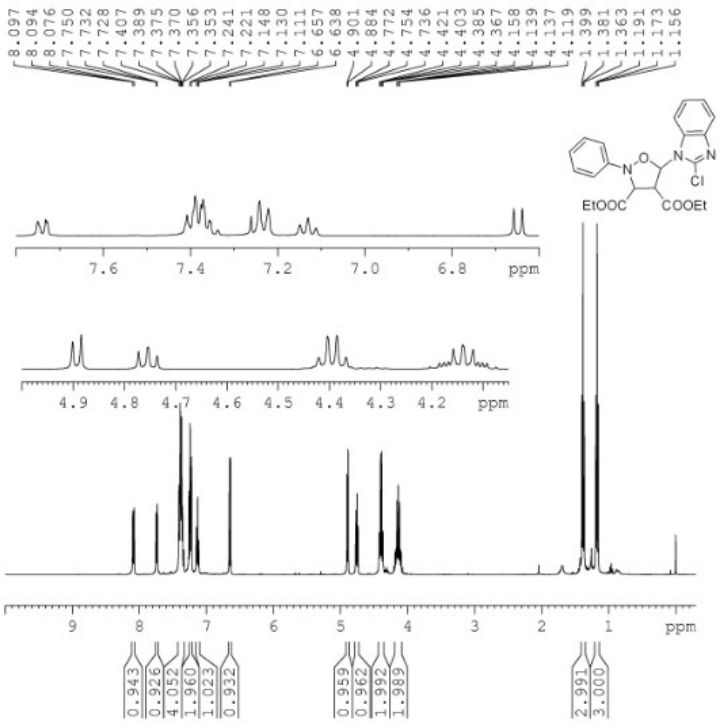



```
NAME          2017-03-11 tyut-lix
EXPNO                 10
PROCNO                 1
Date_           20170311
Time               21.00
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     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            400.1300082 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

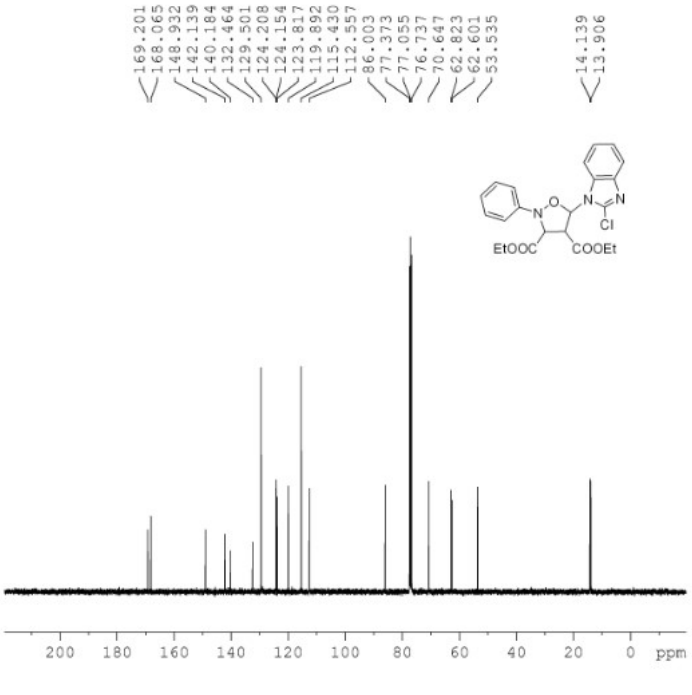



```
NAME          2017-03-11 tyut-lix
EXPNO                 11
PROCNO                 1
Date_           20170311
Time               21.59
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                295.3 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
```

**8b**

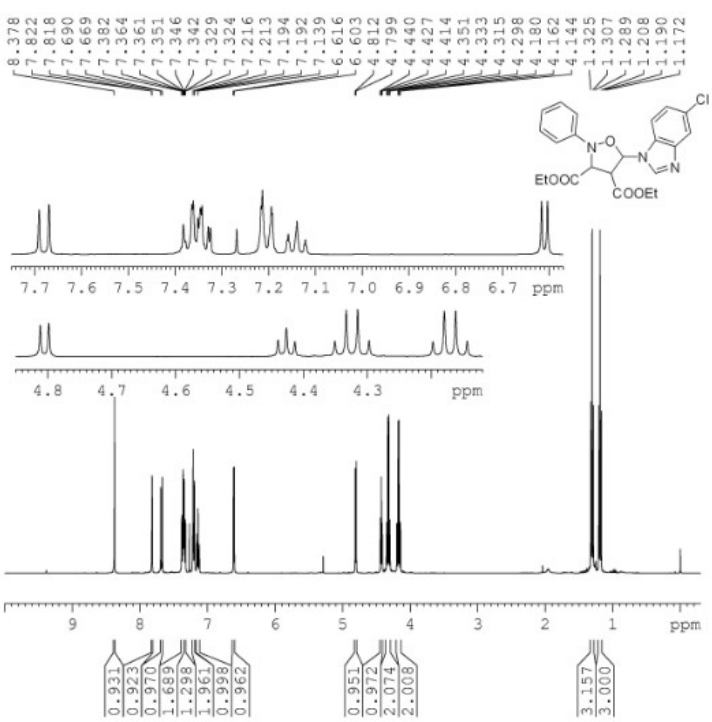



```
NAME        2017-03-24 tyut-lix
EXPNO                   10
PROCNO                   1
Date_             20170324
Time                 21.55
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       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                   295.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                    1H
P1                    9.70 usec
SI                   65536
SF             400.1300093 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



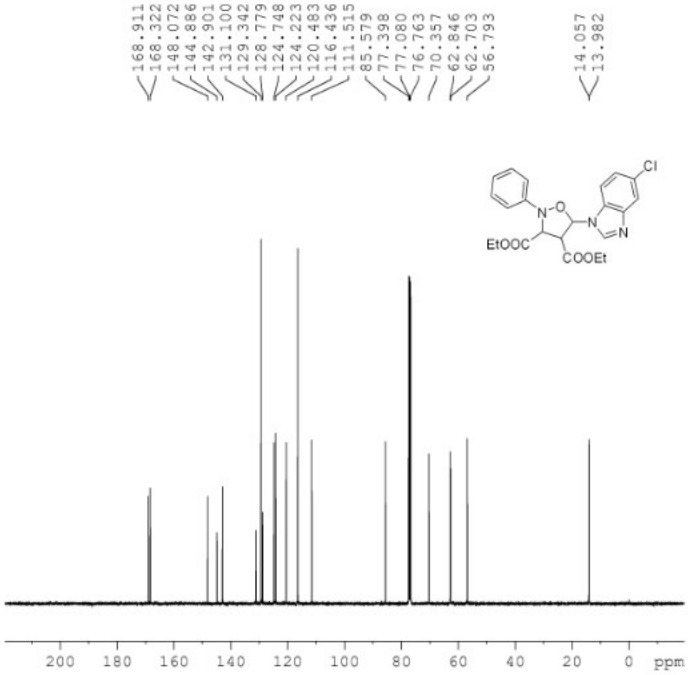

```
NAME        2017-03-24 tyut-lix
EXPNO                   11
PROCNO                   1
Date_             20170324
Time                 22.12
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      399
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                   295.9 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
```

**8c**





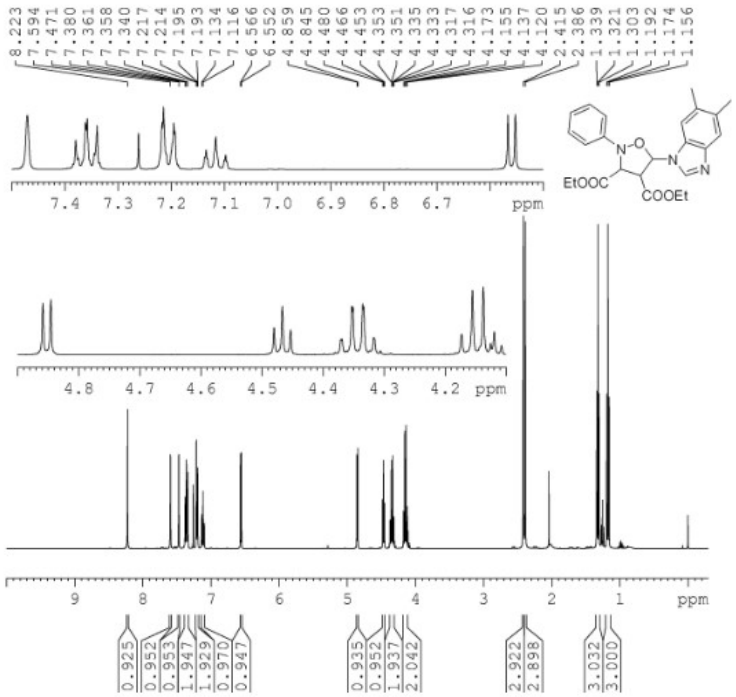
| | |
|---|---|
| NAME | 2017-03-24 tyut-lix |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20170324 |
| Time | 22.22 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 8012.820 Hz |
| FIDRES | 0.122266 Hz |
| AQ | 4.0894966 sec |
| RG | 34.32 |
| DW | 62.400 usec |
| DE | 6.50 usec |
| TE | 295.3 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300063 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |





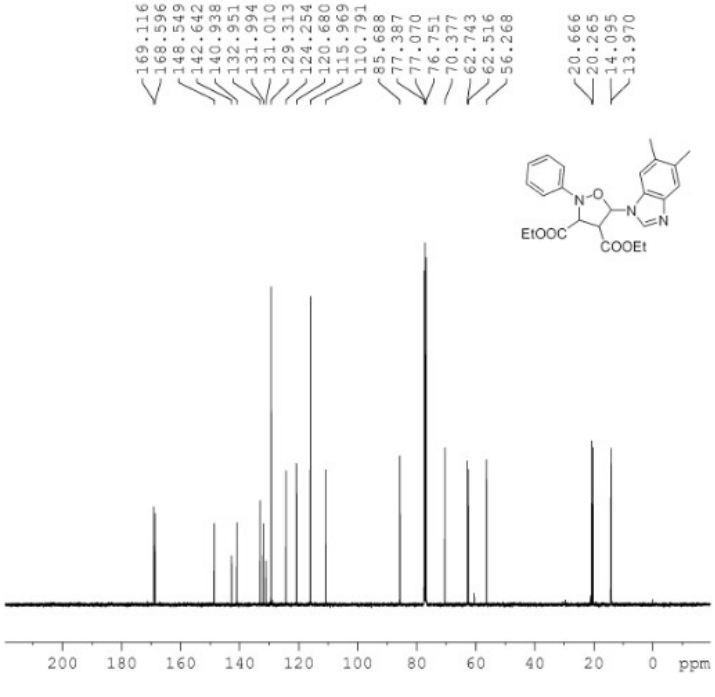
| | |
|---|---|
| NAME | 2017-03-24 tyut-lix |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20170324 |
| Time | 23.21 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 1024 |
| DS | 4 |
| SWH | 24038.461 Hz |
| FIDRES | 0.366798 Hz |
| AQ | 1.3631988 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 ======== | |
| 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 |

**8d**




BRUKER

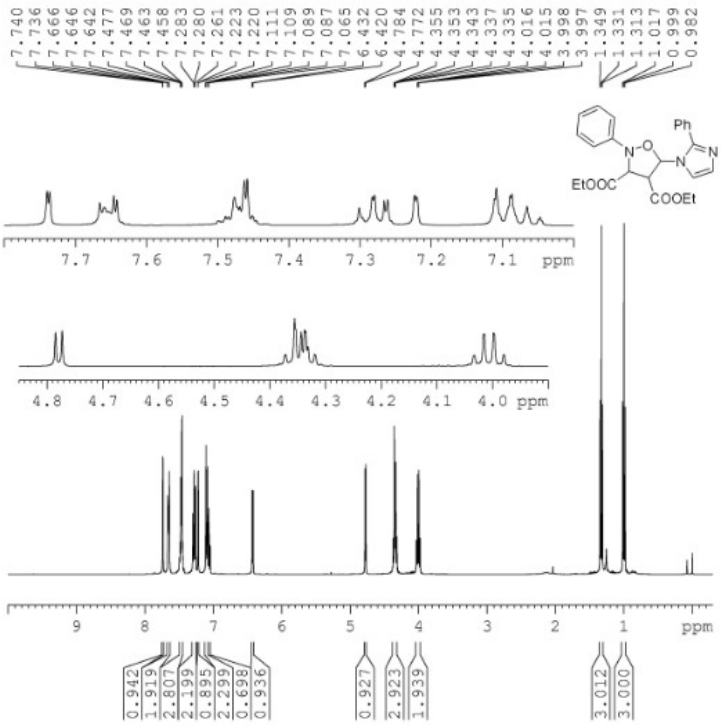
| | |
|---|---|
| NAME | 2017-03-23 tyut-lix |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20170323 |
| Time | 23.01 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 8012.820 Hz |
| FIDRES | 0.122266 Hz |
| AQ | 4.0894966 sec |
| RG | 34.32 |
| DW | 62.400 usec |
| DE | 6.50 usec |
| TE | 295.5 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300092 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |



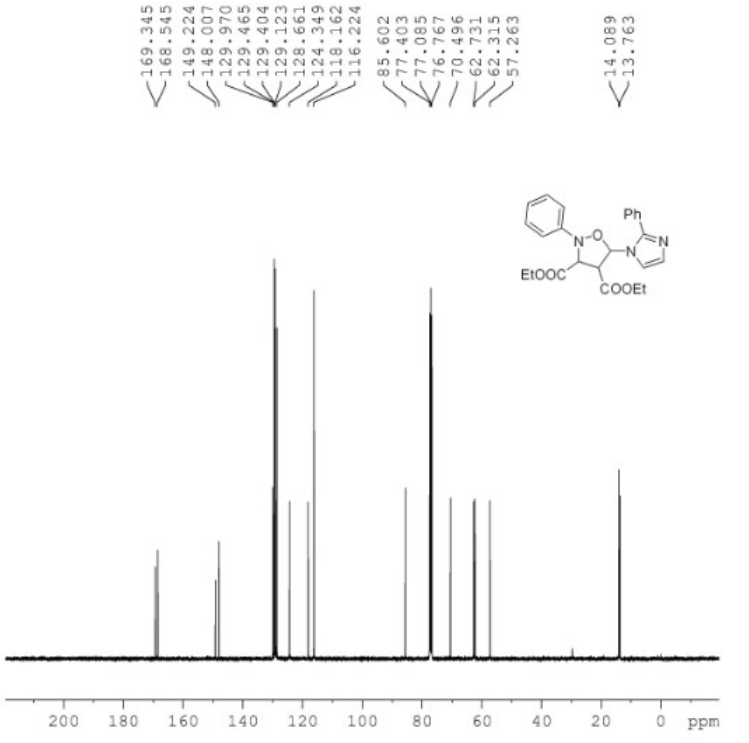

BRUKER

| | |
|---|---|
| NAME | 2017-03-23 tyut-lix |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20170324 |
| Time | 0.00 |
| 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 | 296.5 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 |

**8e**

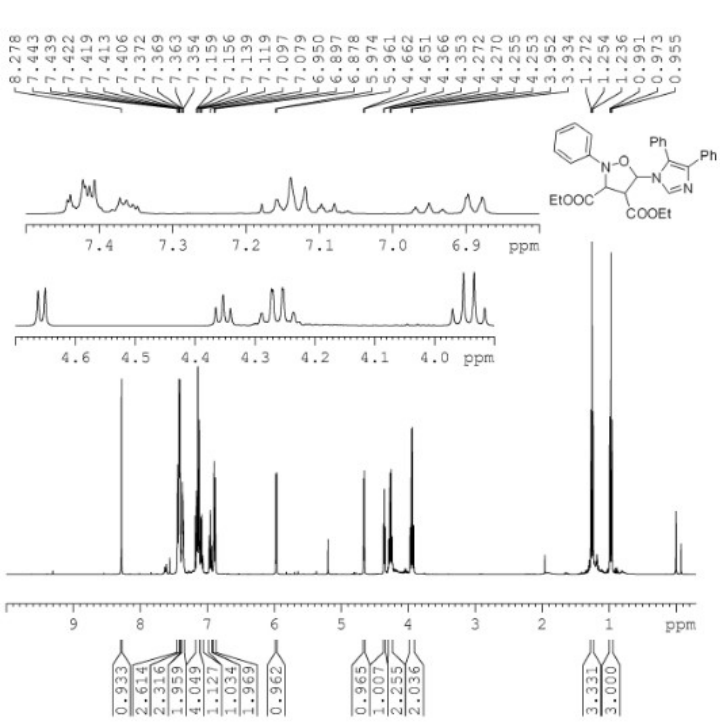



```
NAME        2017-03-24 tyut-lix
EXPNO                   10
PROCNO                   1
Date_             20170324
Time                 23.25
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      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                  295.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                   1H
P1                   9.70 usec
SI                  65536
SF             400.1300072 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



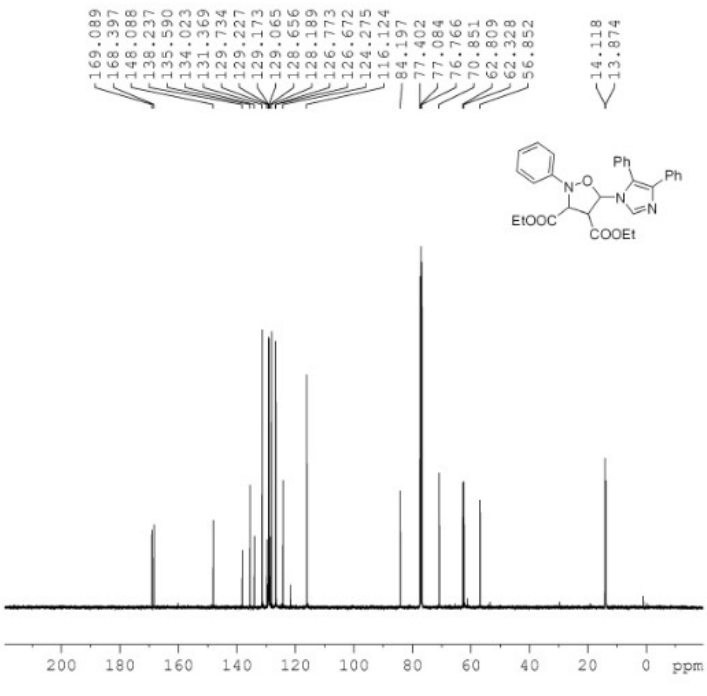

```
NAME        2017-03-24 tyut-lix
EXPNO                   11
PROCNO                   1
Date_             20170325
Time                 0.24
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
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                  295.7 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
```

**8f**





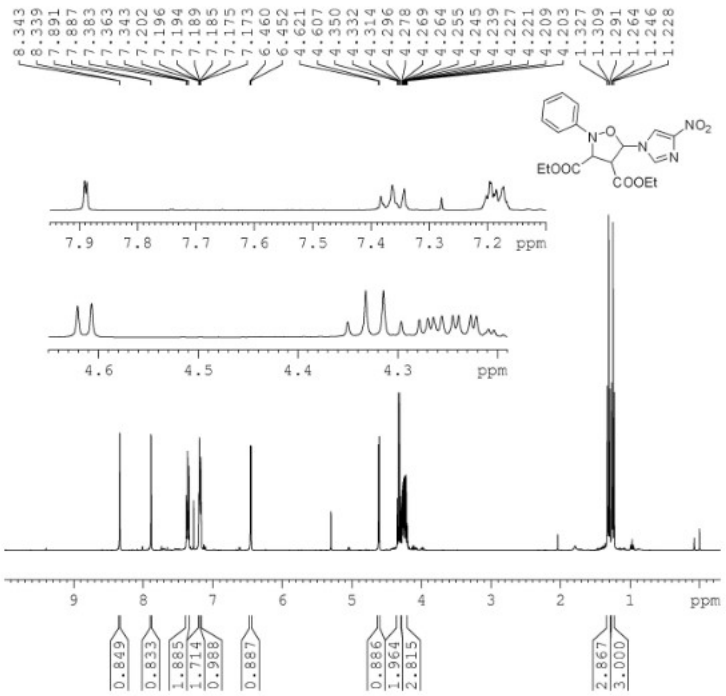
| | |
|---|---|
| NAME | 2017-03-27 tyut-lix |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20170327 |
| Time | 23.01 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 8012.820 Hz |
| FIDRES | 0.122266 Hz |
| AQ | 4.0894966 sec |
| RG | 34.32 |
| DW | 62.400 usec |
| DE | 6.50 usec |
| TE | 297.3 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |
| ======== | CHANNEL f1 ======== |
| SFO1 | 400.1324710 MHz |
| NUC1 | 1H |
| P1 | 9.70 usec |
| SI | 65536 |
| SF | 400.1300422 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |



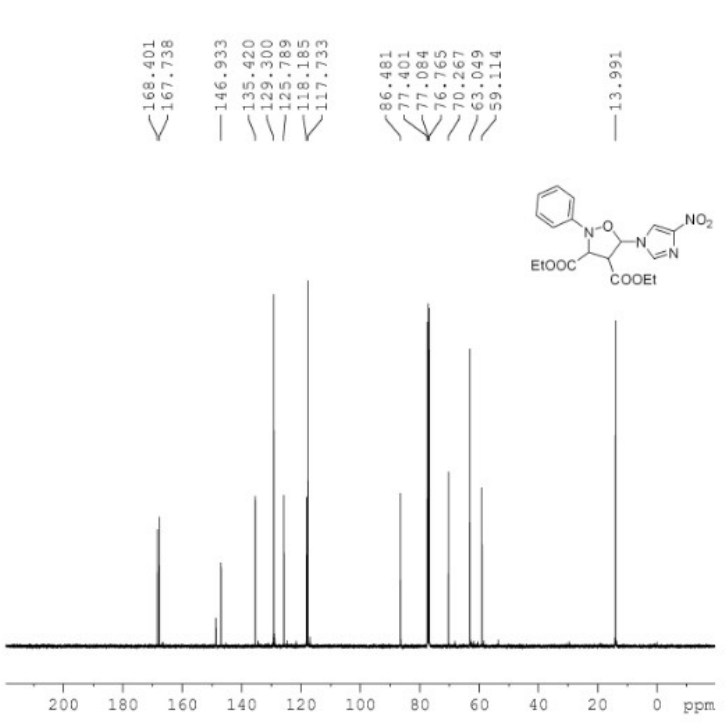


| | |
|---|---|
| NAME | 2017-03-27 tyut-lix |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20170328 |
| Time | 0.00 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB/ |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 1024 |
| DS | 4 |
| SWH | 24038.461 Hz |
| FIDRES | 0.366798 Hz |
| AQ | 1.3631988 sec |
| RG | 185.43 |
| DW | 20.800 usec |
| DE | 6.50 usec |
| TE | 295.7 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 |

**8g**

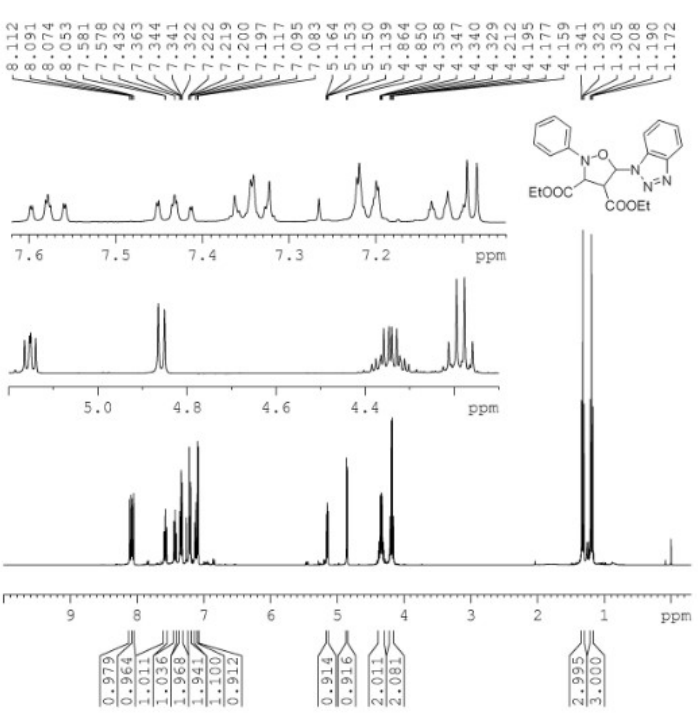



```
NAME          2017-03-27 tyut-lix
EXPNO                 10
PROCNO                 1
Date_           20170328
Time                5.19
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     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                294.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 9.70 usec
SI                 65536
SF            400.1300020 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

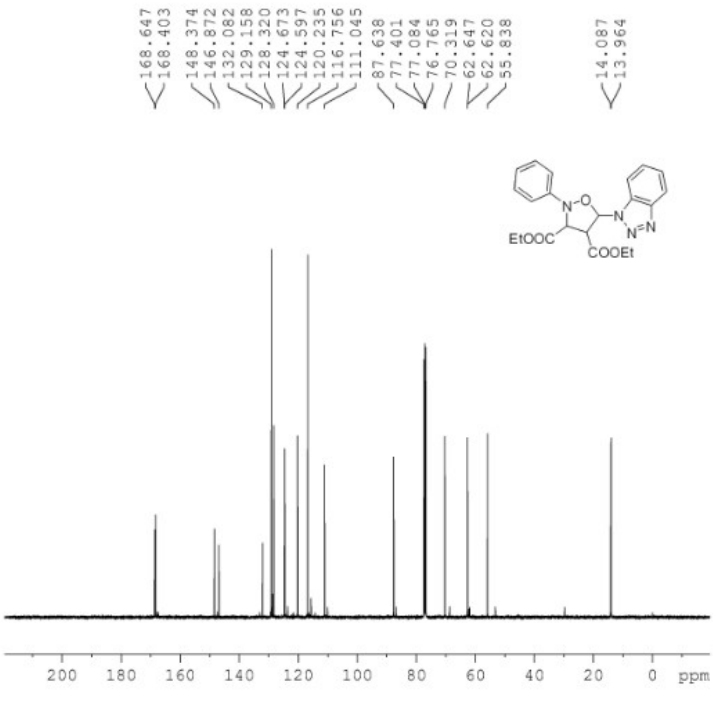



```
NAME          2017-03-27 tyut-lix
EXPNO                 11
PROCNO                 1
Date_           20170328
Time                6.18
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                294.7 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
```

**8h**

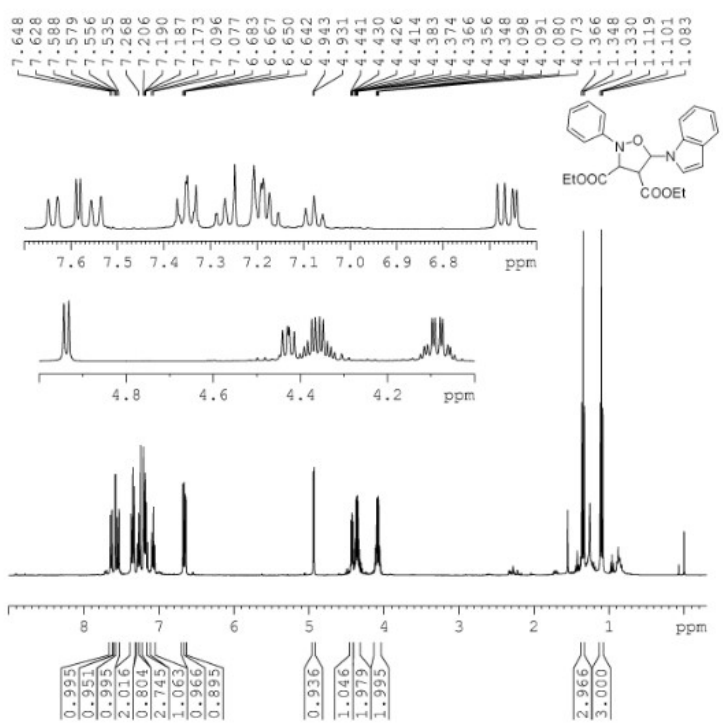



```
NAME          2017-03-23 tyut-lix
EXPNO                   10
PROCNO                   1
Date_             20170324
Time                  0.04
INSTRUM              spect
PROBHD     5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
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 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                   9.70 usec
SI                  65536
SF              400.1300076 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



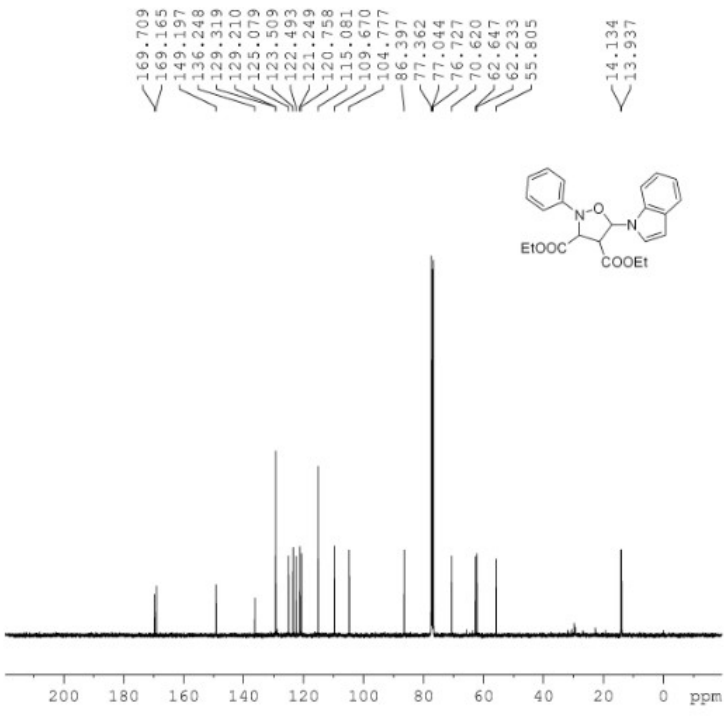

```
NAME          2017-03-23 tyut-lix
EXPNO                   11
PROCNO                   1
Date_             20170324
Time                  1.03
INSTRUM              spect
PROBHD     5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
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                  296.5 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
```

**8i**





```
NAME        2017-04-19 tyut-lx-
EXPNO                   10
PROCNO                   1
Date_             20170419
Time                  21.16
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                   297.4 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                    9.70 usec
SI                   65536
SF            400.1300150 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

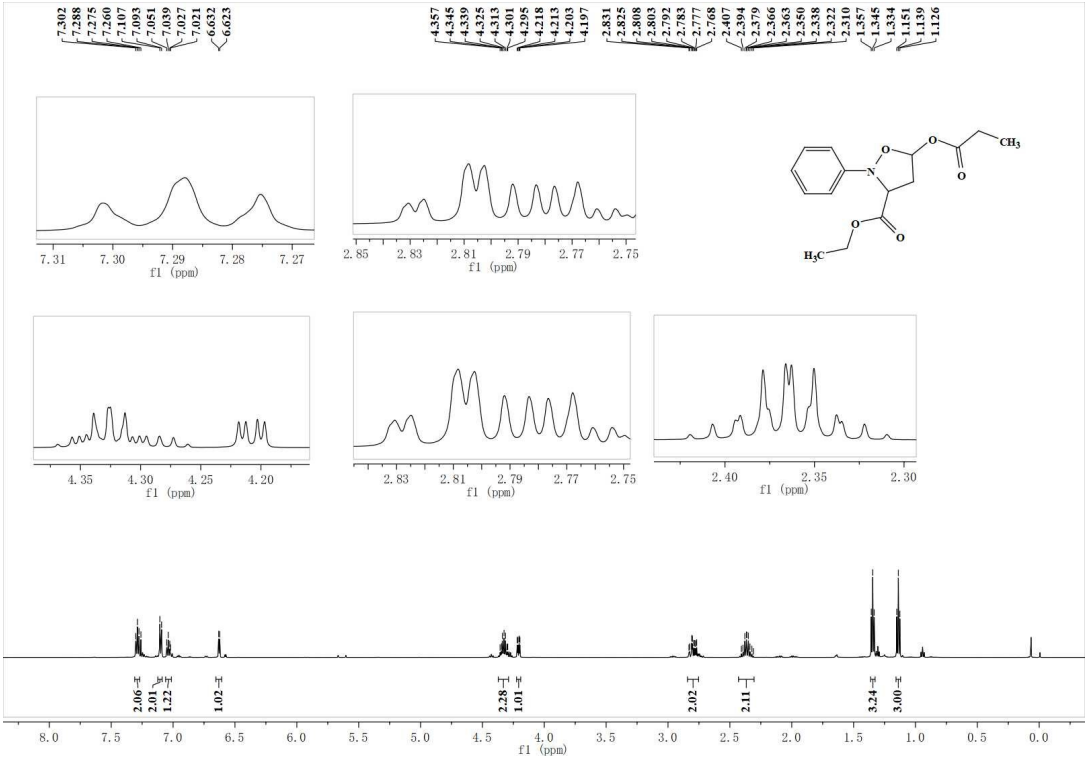


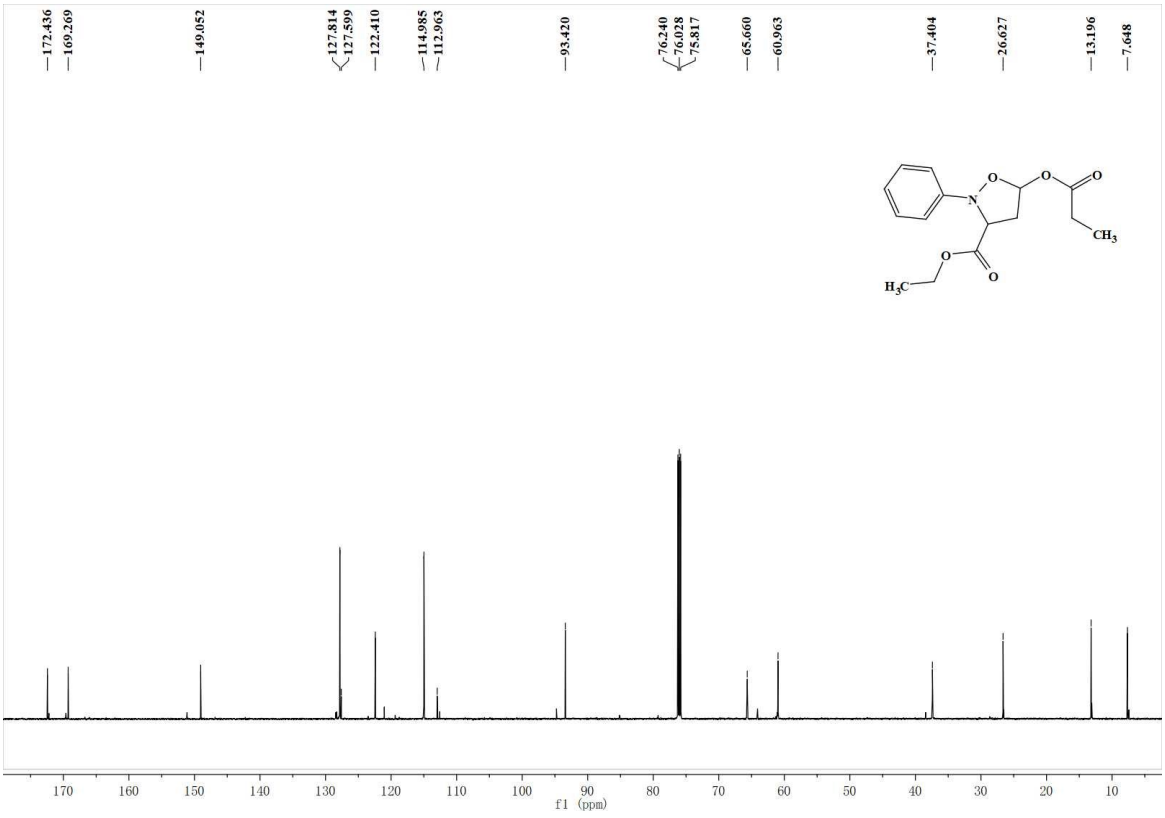


```
NAME        2017-04-19 tyut-lx-
EXPNO                   10
PROCNO                   1
Date_             20170420
Time                  11.12
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     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                   297.7 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
```

## 13. $^{1}$H-NMR and $^{13}$C-NMR spectra of products 11

### 11a



# 11b