

Nanocomposite CuCO₃-CuO as a novel and environmentally friendly catalyst for triazole synthesis.

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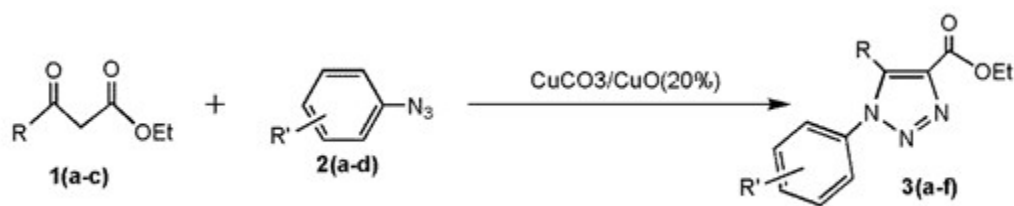
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Supporting Information



Tables 1S

Entry	Condition	Yields (%)
1	DMF, rt	no products
2	DMF, 60°C	no products
3	DMF, 80°C	no products
4	DMF, 100°C	no products
5	DMF /H ₂ O, rt	no products
6	Et ₂ O, rt	no products
7	THF, rt	no products
8	EtOH, rt	no products

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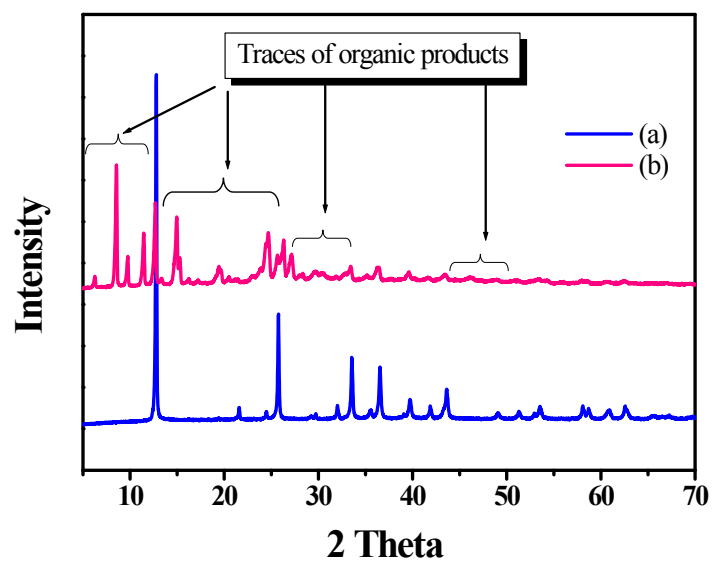


Fig.S1: XRD patterns of MB1 catalyst; (a) MB1 before reaction, (b) MB1 after reaction.

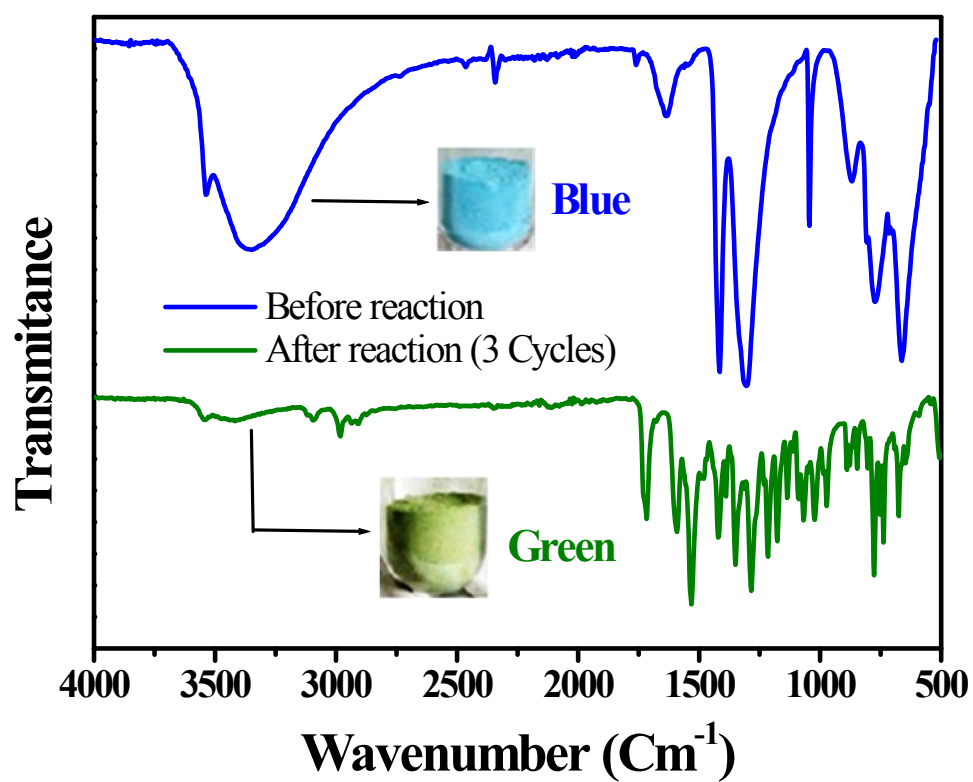


Fig.S2: FT-IR spectra of MB1 catalyst.

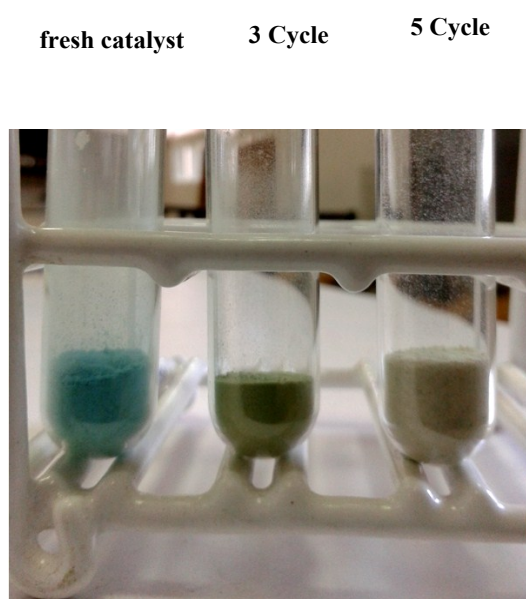
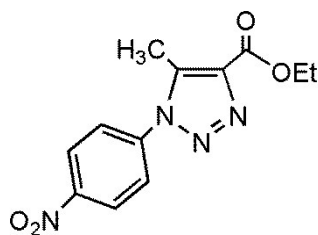


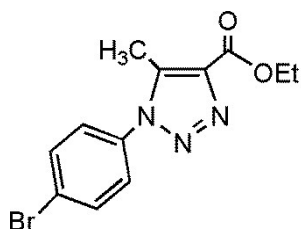
Fig.S3: color change of catalyst during five reuse

1. Analytical Data



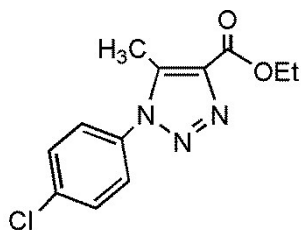
Ethyl 5-methyl-1-(4-nitrophenyl)-1H-1,2,3-triazole-4-carboxylate(3a).

Yield: 90% (procedure 1), 96% (procedure 2). Yellow powder, mp 176-180°C. IR (KBr): 1118, 1530, 1718, 2919. ¹H NMR (400 MHz, CDCl₃): 1.47 (t, 3H, J = 7.1 Hz), 2.70 (s, 3H), 4.49 (q, 2H, J = 7.1 Hz), 7.75 (d, 2H, J = 8.9 Hz), 8.48 (d, 2H, J = 8.9 Hz). ¹³C NMR (75 MHz, CDCl₃): 10.20 (CH₃), 14.33 (CH₃), 61.33 (CH₂), 125.18 (2 CH), 125.85 (2 CH), 137.46 (C), 138.86 (C), 140.11 (C), 148.22 (C), 161.34 (C O).



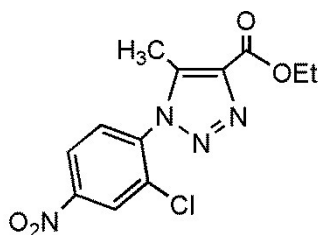
Ethyl 5-methyl-1-(4-bromophenyl)-1H-1,2,3-triazole-4-carboxylate(3b).

Yield: 64% (procedure 1), 40% (procedure 2). White powder, mp 170-175°C. IR (KBr): 833, 1100, 1494, 1710, 3010. ¹H NMR (300 MHz, CDCl₃): 1.43 (t, 3H, J = 7.1 Hz), 2.60 (s, 3H), 4.46 (q, 2H, J = 7.1 Hz), 7.35 (d, 2H, J = 8.7 Hz), 7.72 (d, 2H, J = 8.7 Hz). ¹³C NMR (75 MHz, CDCl₃): 9.95 (CH₃), 14.33 (CH₃), 61.14 (CH₂), 124.27 (2 CH), 126.76 (2 CH), 132.90 (C), 134.36 (C), 136.89 (C), 138.74 (C), 161.56 (C O).



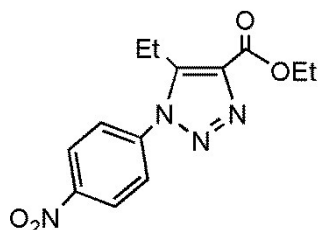
Ethyl 5-methyl-1-(4-chlorophenyl)-1H-1,2,3-triazole-4-carboxylate(3c).

Yield: 61% (procedure 1), 60% (procedure 2). White powder, mp 163-168 °C. IR (KBr): 837, 1101, 1561, 1713, 2916. ¹H NMR (300 MHz, CDCl₃): 1.45 (t, 3H, J = 7.1 Hz), 2.60 (s, 3H), 4.47 (q, 2H, J = 7.1 Hz), 7.42 (d, 2H, J = 8.9 Hz), 7.57 (d, 2H, J = 8.9 Hz). ¹³C NMR (75 MHz, CDCl₃): 9.96 (CH₃), 14.32 (CH₃), 61.16 (CH₂), 126.52 (2 CH), 129.90 (2 CH), 133.77 (C), 136.27 (C), 136.77 (C), 138.75 (C), 161.59 (C O).



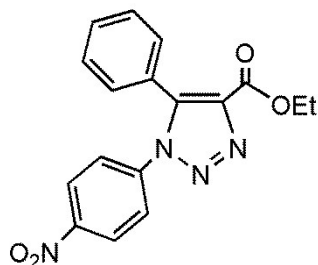
Ethyl 5-methyl-1-(2-chloro,4-nitrophenyl)-1H-1,2,3-triazole-4-carboxylate(3d).

Yield: 90% (procedure 1), 90% (procedure 2). Beige powder, mp 125-128 °C. IR (KBr): 744, 1206, 1526, 1732, 3050. ¹H NMR (300 MHz, CDCl₃): 1.48 (t, 3H, J = 7.1 Hz), 2.52 (s, 3H), 4.50 (q, 2H, J = 7.1 Hz), 7.70 (d, 1H, J = 7.5 Hz), 8.38 (d, 1H, J = 7.5 Hz), 8.5 (s, 1H). ¹³C NMR (75 MHz, CDCl₃): 09.46 (CH₃), 14.25 (CH₃), 61.39 (CH₂), 123.13 (CH), 125.93 (CH), 130.34 (CH), 133.34 (C), 136.73 (C), 138.13 (C), 140.57 (C), 149.31 (C), 161.26 (C=O).



Ethyl 5-ethyl-1-(4-nitrophenyl)-1H-1,2,3-triazole-4-carboxylate(3e).

Yield: 80% (procedure 1), 79% (procedure 2). Brown powder, mp 120-125 °C. IR (KBr): 1106, 1525, 1714, 2988. ¹H NMR (300 MHz, CDCl₃): 1.24 (t, 3H, J = 7.5 Hz), 1.47 (t, 3H, J = 7.1 Hz), 3.08 (q, 2H, J = 7.5 Hz), 4.50 (q, 2H, J = 7.1 Hz), 7.73 (d, 2H, J = 9.1 Hz), 8.49 (d, 2H, J = 9.1 Hz). ¹³C NMR (75 MHz, CDCl₃): 13.32 (CH₃), 14.30 (CH₃), 17.05 (CH₂), 61.35 (CH₂), 125.20 (2 CH), 126.28 (2 CH), 136.76 (C), 140.34 (C), 144.47 (C), 148.38 (C), 161.08 (C=O).

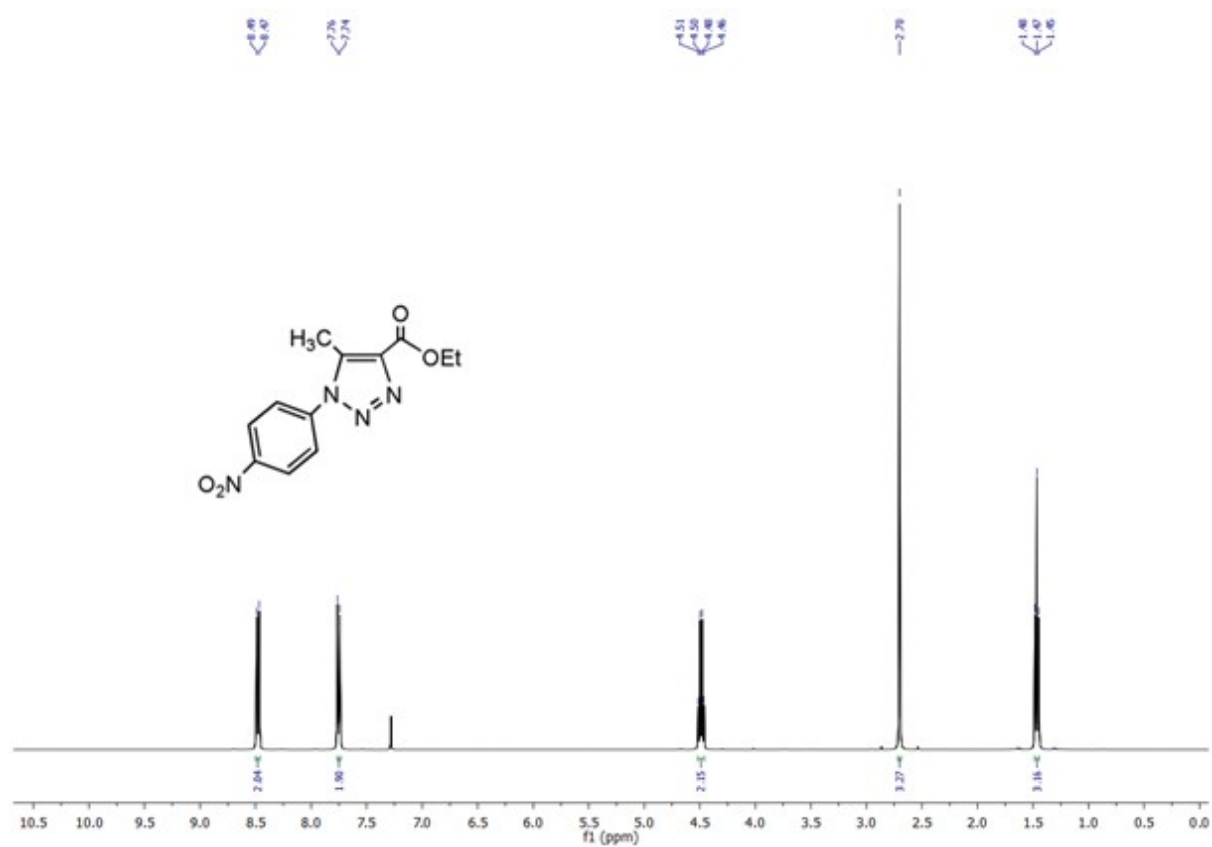


Ethyl 5-phenyl-1-(4-nitrophenyl)-1H-1,2,3-triazole-4-carboxylate(3f).

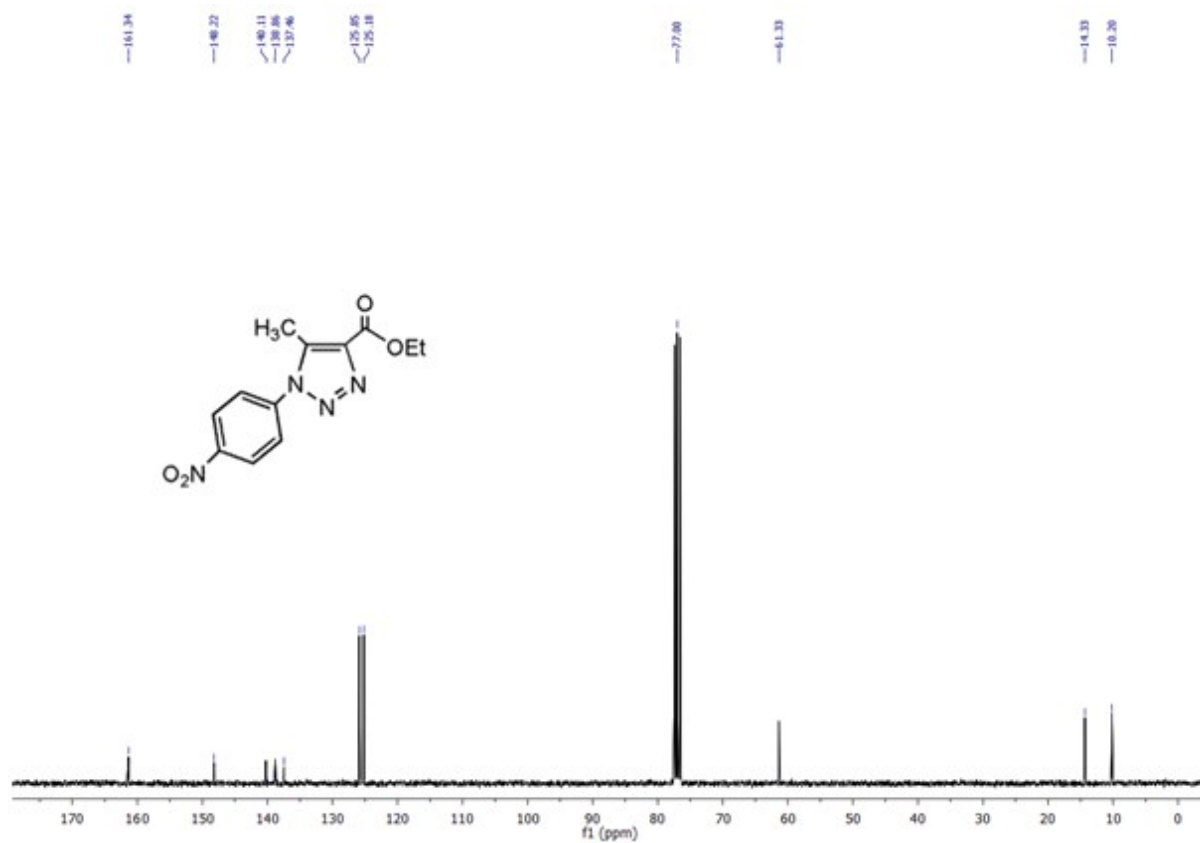
Yield: 89% (procedure 1), 93% (procedure 2). Orange powder, mp 162-167 °C. IR (KBr): 1107, 1521, 1711, 2900. ¹H NMR (300 MHz, CDCl₃): 1.32 (t, 3H, J = 7.1 Hz), 4.36 (q, 2H, J = 7.1 Hz), 7.30-7.48 (m, 5H), 7.50 (d, 2H, J = 8.9 Hz), 8.26 (d, 2H, J = 8.9 Hz). ¹³C NMR (75 MHz, CDCl₃): 14.02 (CH₃), 61.39 (CH₂), 124.73 (2 CH), 125.01 (2 CH), 125.48 (CH), 128.76 (2 CH), 130.04 (2 CH), 130.50 (C), 137.49 (C), 140.41 (C), 140.89 (C), 147.59 (C), 160.43 (C=O).

2. ¹H and ¹³C NMR spectra of products 3(a-f)

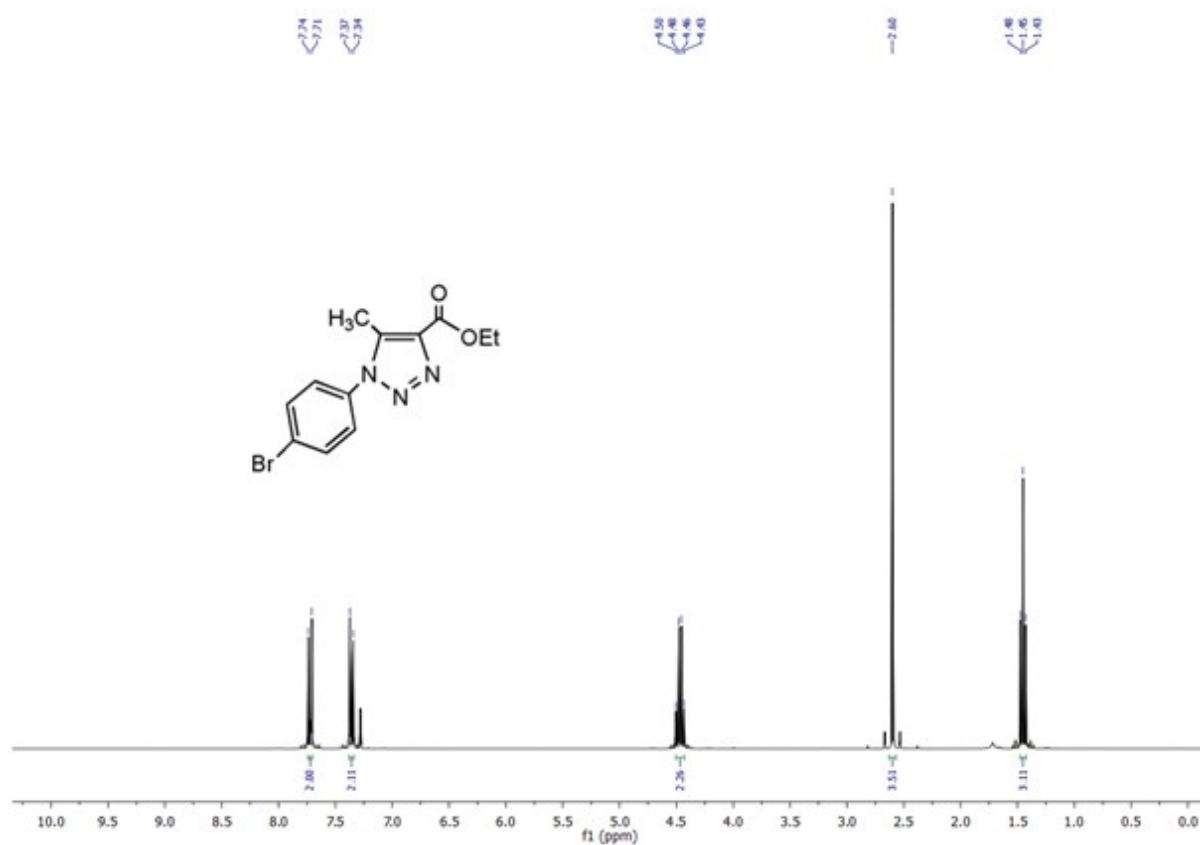
^1H NMR Spectra of **3a** (400 MHz, CDCl_3)



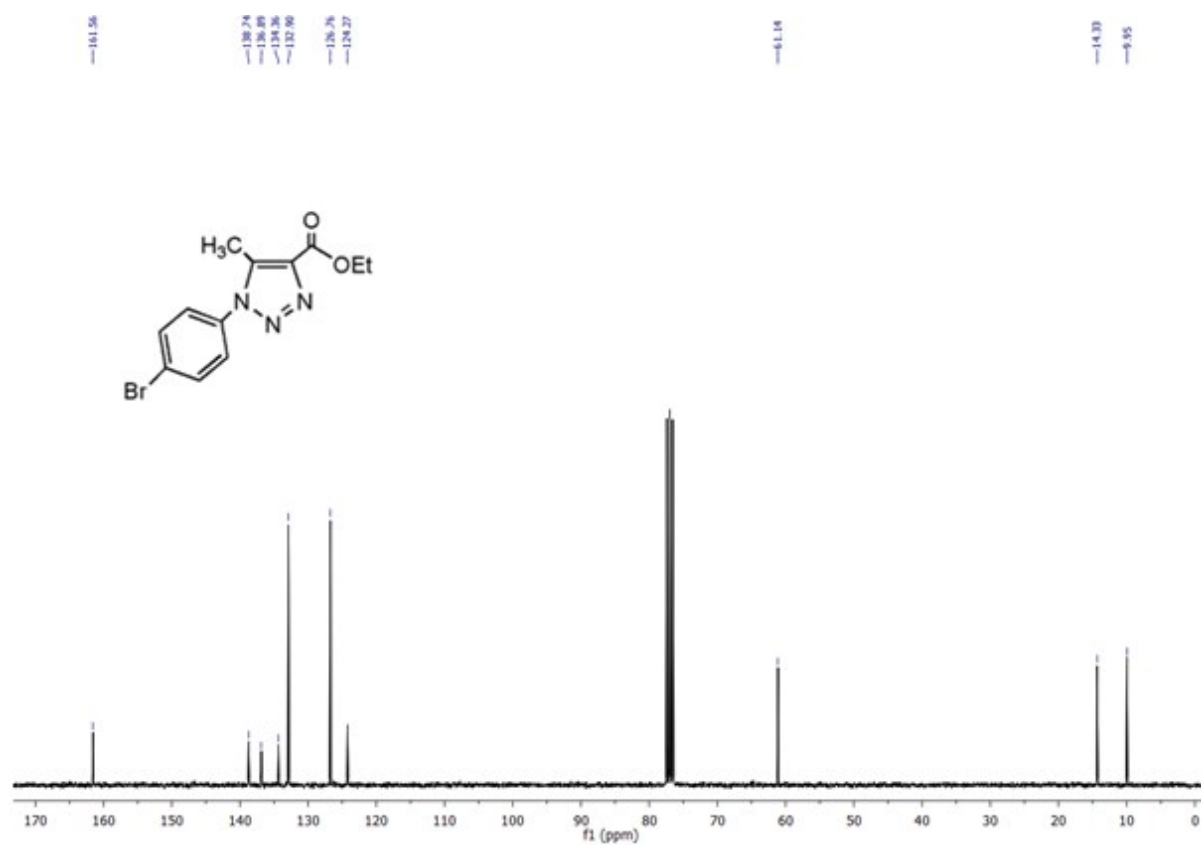
^{13}C NMR Spectra of **3a** (75 MHz, CDCl_3)



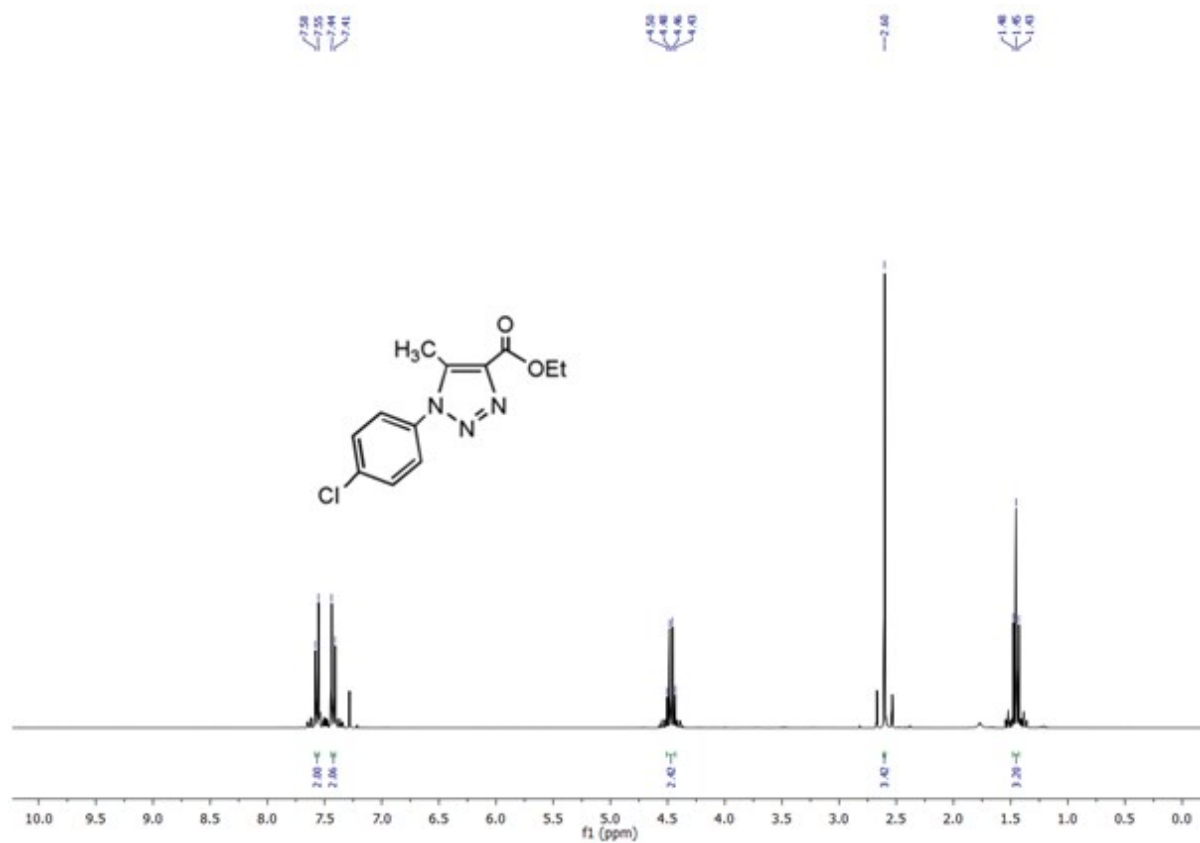
¹H NMR Spectra of **3b** (300 MHz, CDCl₃)



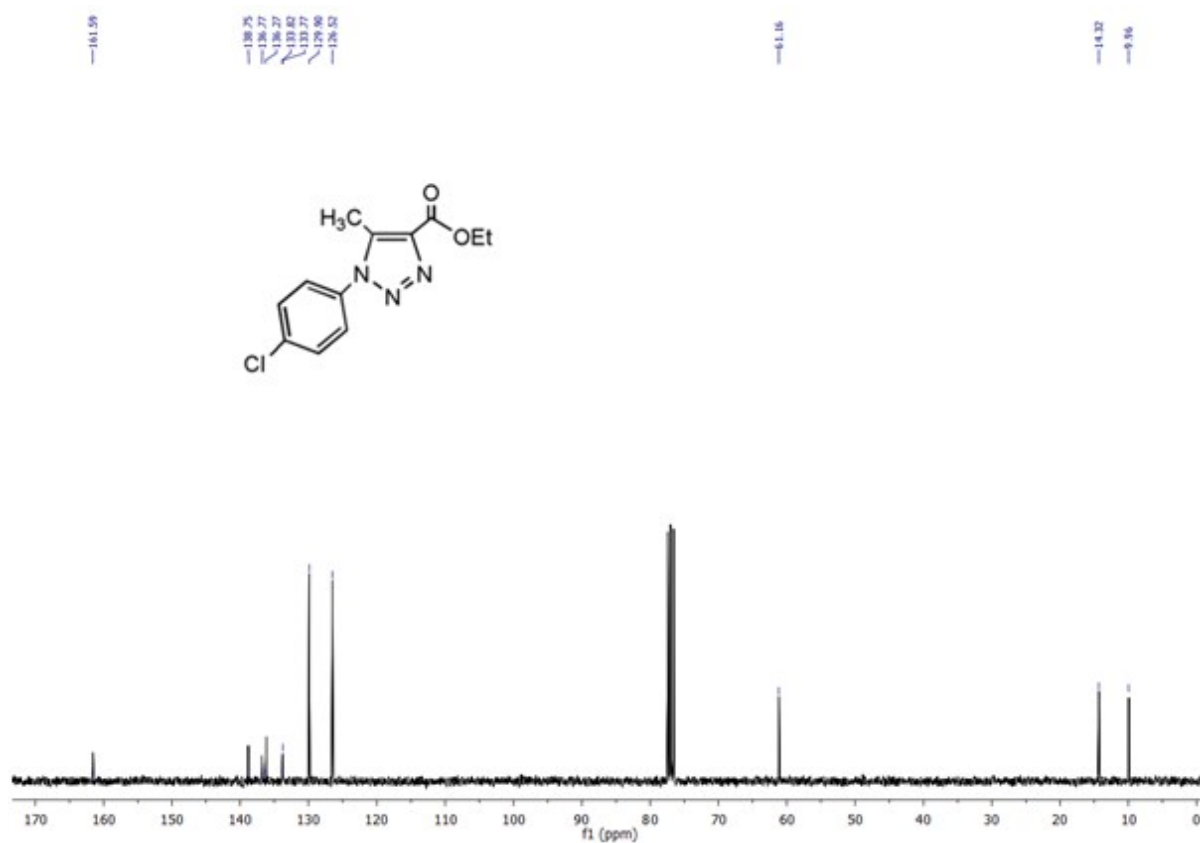
^{13}C NMR Spectra of **3b** (75 MHz, CDCl_3)



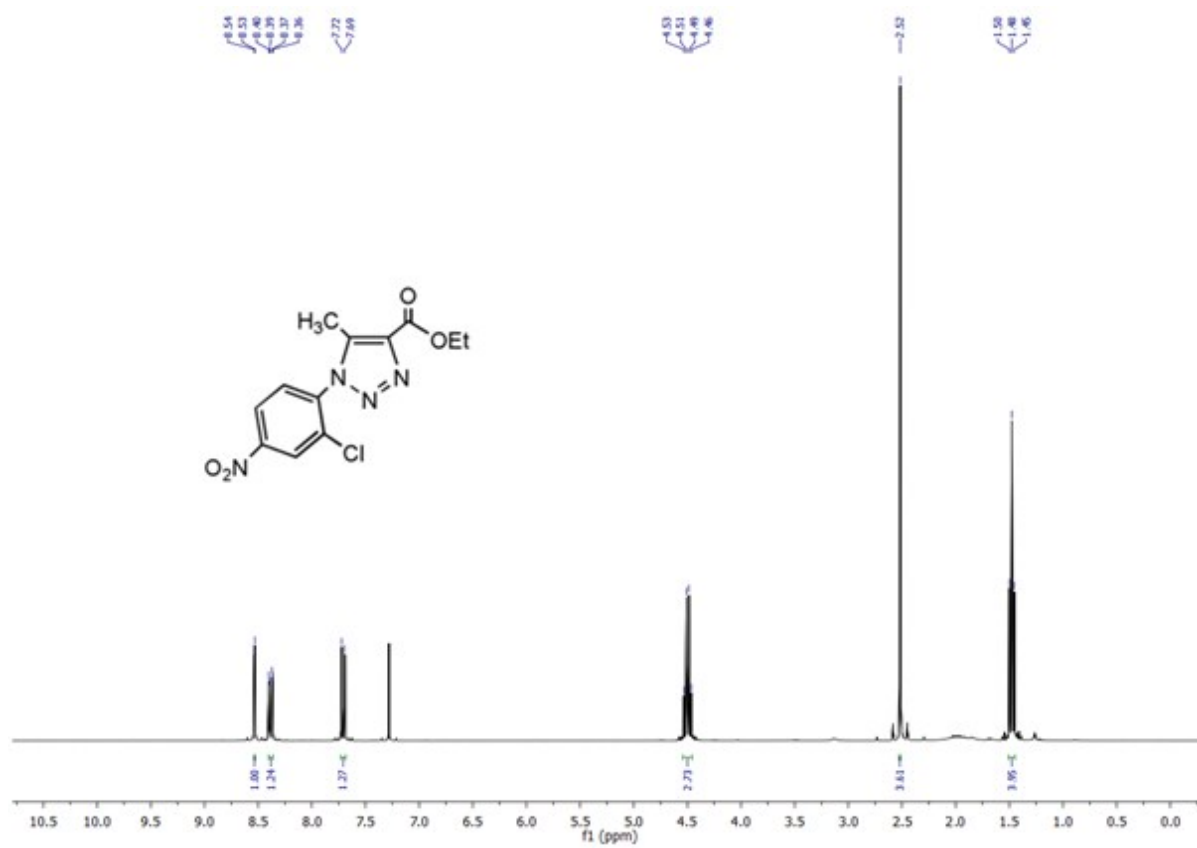
^1H NMR Spectra of **3c** (300 MHz, CDCl_3)



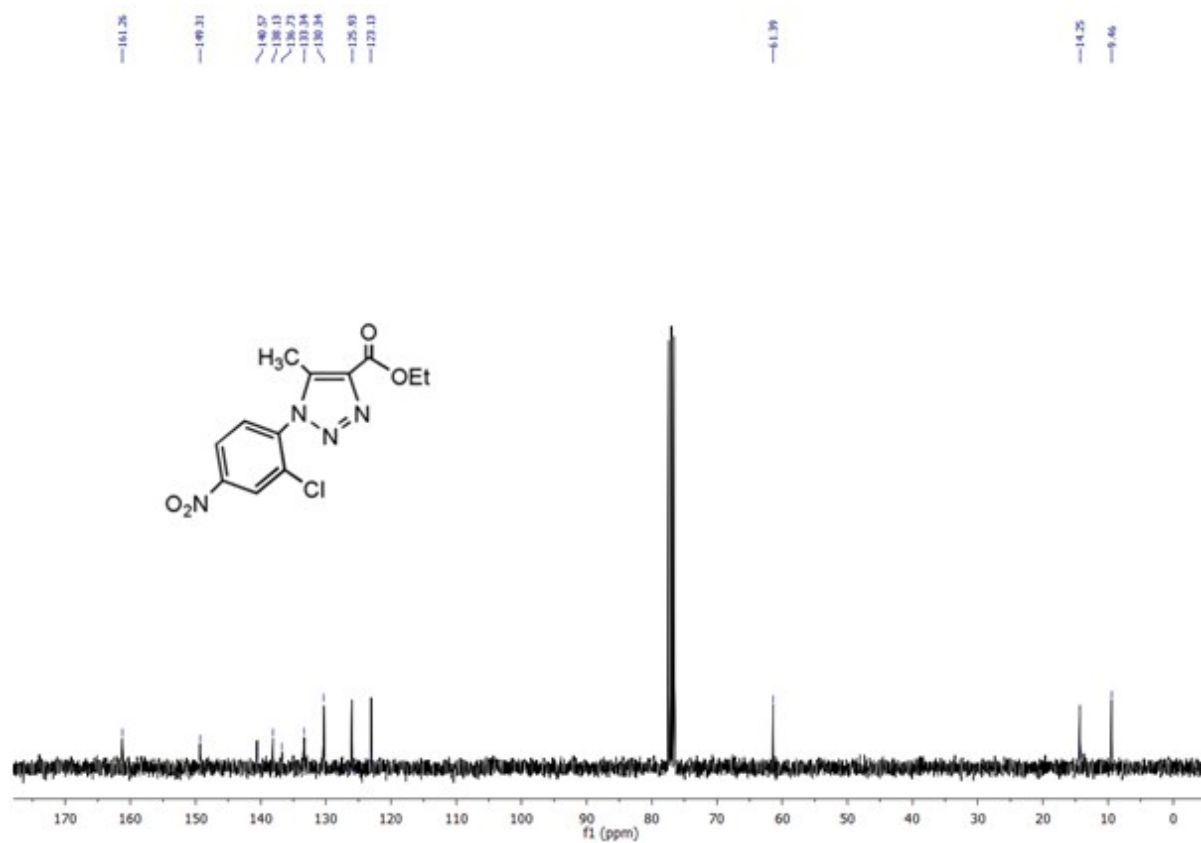
¹³C NMR Spectra of **3c** (75 MHz, CDCl₃)



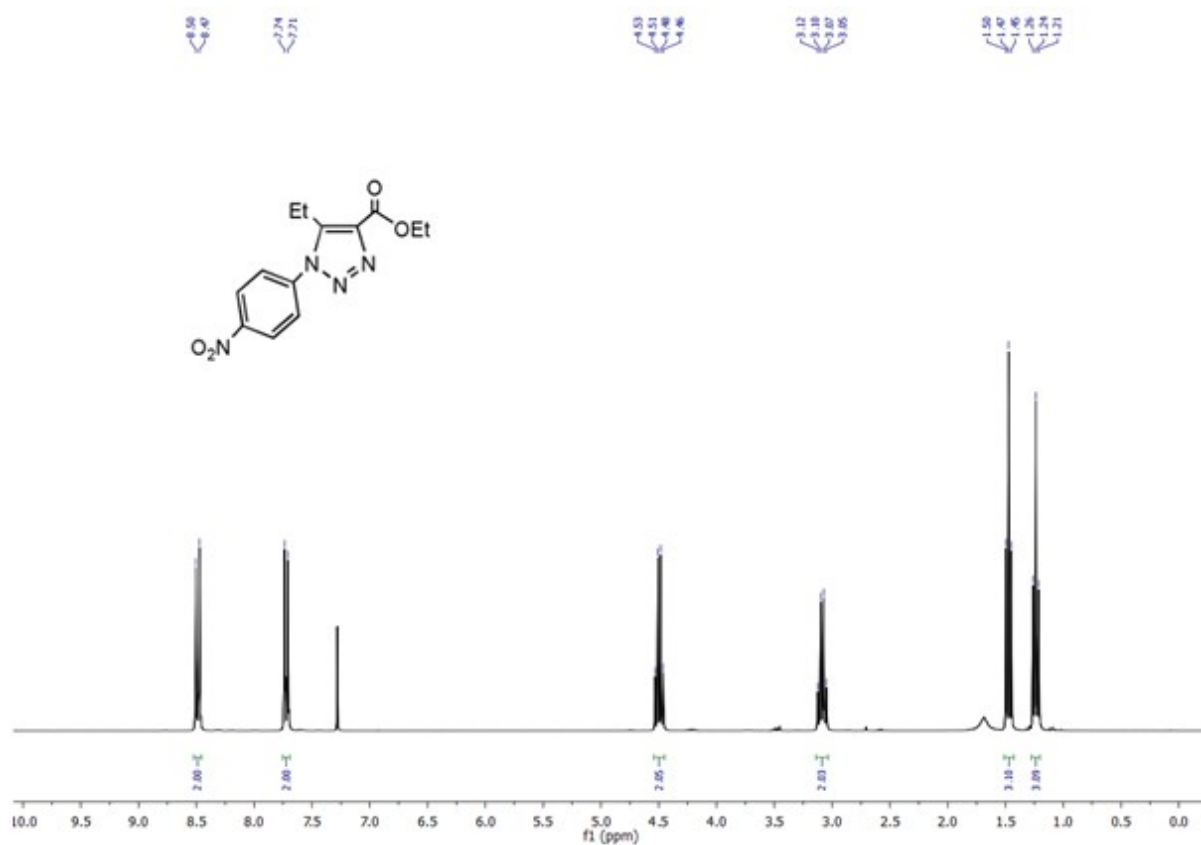
^1H NMR Spectra of **3d** (300 MHz, CDCl_3)



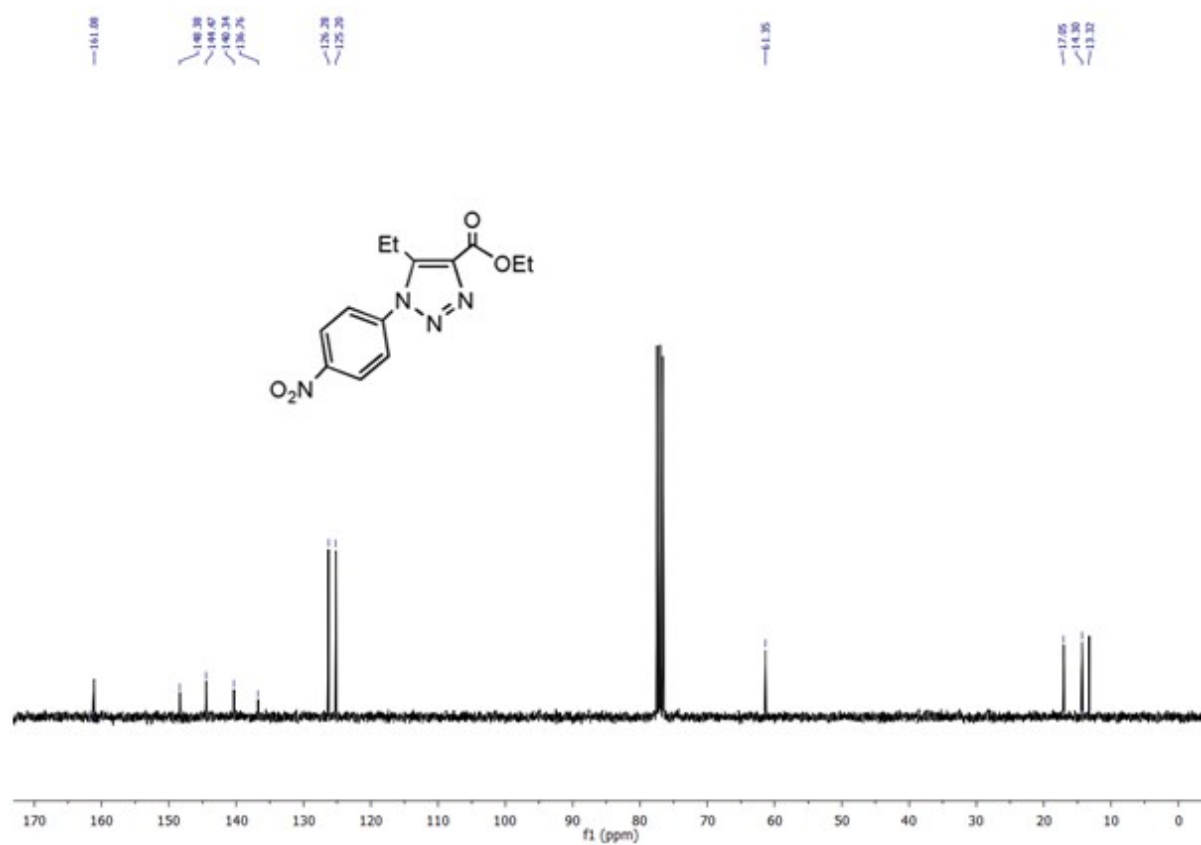
^{13}C NMR Spectra of **3d** (75 MHz, CDCl_3)



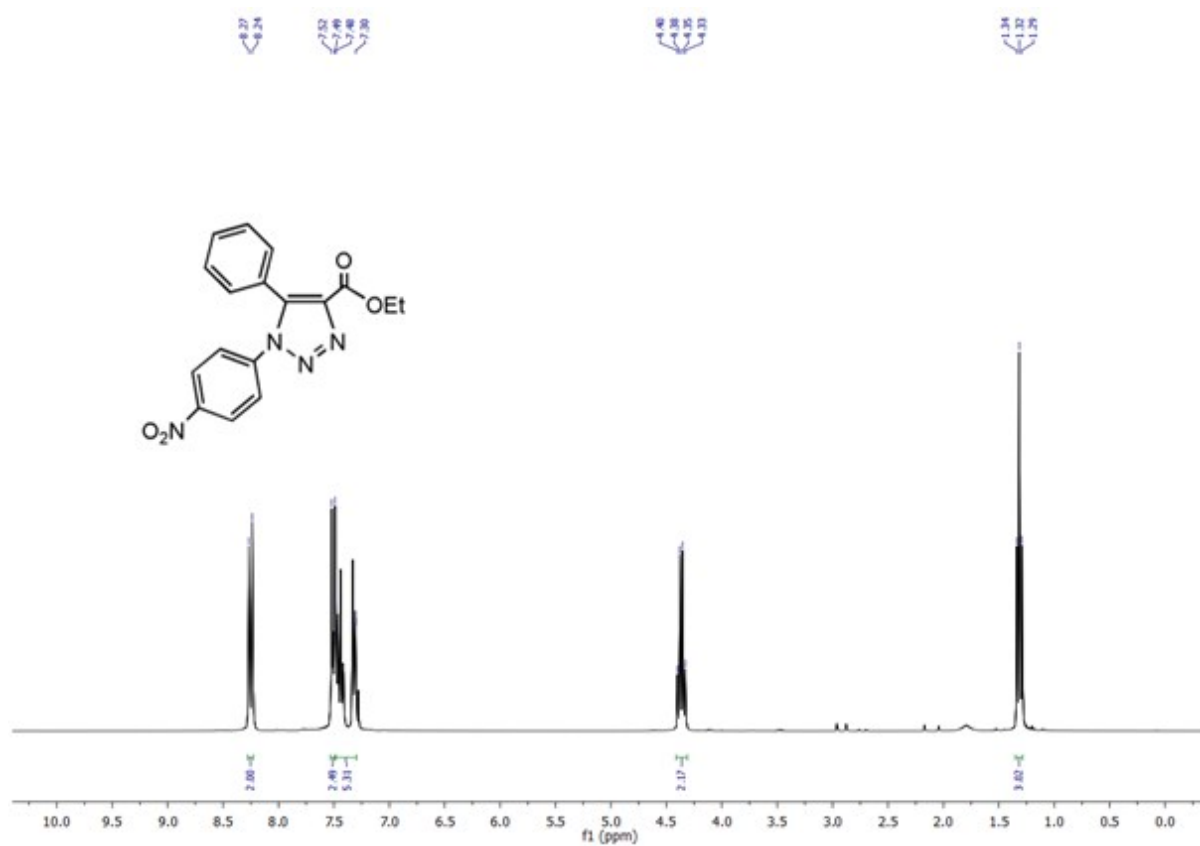
¹H NMR Spectra of **3e** (300 MHz, CDCl₃)



^{13}C NMR Spectra of **3e** (75 MHz, CDCl_3)



^1H NMR Spectra of **3f** (300 MHz, CDCl_3)



¹³C NMR Spectra of **3f** (75 MHz, CDCl₃)

