Supporting Information

Catalytic Intermolecular Cross-Couplings of Azides and LUMO Activated Unsaturated Acyl Azoliums

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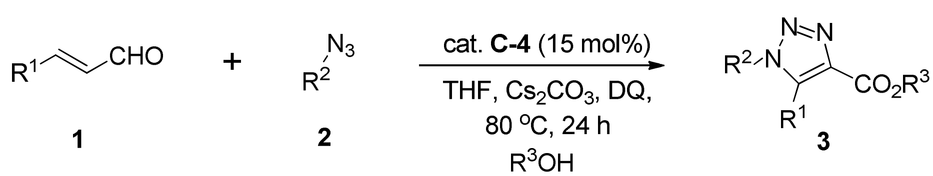
A: General Information and Starting Materials.

General Information. Proton nuclear magnetic resonance (^{1}H NMR) spectra and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker ACF300 spectrometer (400 MHz and 100 MHz). Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26, $(CD_3)_2CO$: δ 2.05, DMSO-d_6: δ 2.50). Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.16, $(CD_3)_2CO$: δ 29.87, DMSO-d_6: δ 39.52). Data are represented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz). All high resolution mass spectra were obtained on a Finnigan/MAT 95XL-T mass spectrometer. For thin layer chromatography (TLC), Merck pre-coated TLC plates (Merck 60 F254) were used, and compounds were visualized with a UV light at 254 nm. Flash chromatography separations were performed on Merck 60 (0.040-0.063 mm) mesh silica gel.

Starting Materials. All solvents and inorganic reagents were from commercial sources and used without purification unless otherwise noted. The azides were prepared following literature reported procedures.[1] α,β-Unsaturated aldehyde **1a**, **1b**, **1c**, **1d**, **1f**, **1g**, **1h**, **1k**, **1l** were purchased from commercial resources, **1e**, **1i** and **1j** were prepared following the literature procedures.[2]

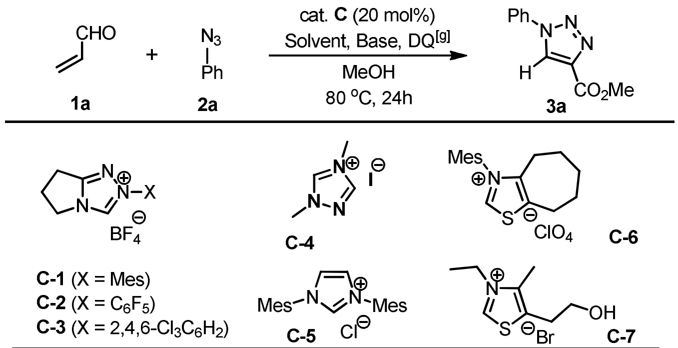
B: General Procedure for NHC-Catalyzed [3+2] Cycloaddition Reaction



To a solution of THF (0.3 mL) in a sealed tube (25.0 mL) was added α,β-unsaturated aldehyde **1** (0.20 mmol), azides **2** (0.10 mmol), catalyst **C-4** (0.015 mmol), Cs_2CO_3 (0.02 mmol), alcohol (0.50 mmol) and oxidant DQ (0.10 mmol). The reaction tube was placed in an oil bath and stirred at 80 °C for 24h. After the completion of the reaction, reaction mixture was dried under vacuum and residue was purified by silica gel chromatography to yield the desired product **3**.

C Comprehensive Optimization

Table S1. Optimization of the reaction conditions.[a]



entry	cat.	solvent	base	yield (%)[b]
1	**C-1**	$CHCl_3$	K_2CO_3	13
2	**C-2**	$CHCl_3$	K_2CO_3	22
3	**C-3**	$CHCl_3$	K_2CO_3	25
4	**C-4**	$CHCl_3$	K_2CO_3	47
5	**C-5**	$CHCl_3$	K_2CO_3	17
6	**C-6**	$CHCl_3$	K_2CO_3	34
7	**C-7**	$CHCl_3$	K_2CO_3	29
8	**C-4**	DMSO	K_2CO_3	19
9	**C-4**	Toluene	K_2CO_3	52
10	**C-4**	THF	K_2CO_3	73
11	**C-4**	1,4-Dioxane	K_2CO_3	21
12	**C-4**	DCE	K_2CO_3	48
13	**C-4**	MeOH	K_2CO_3	<5
14	**C-4**	THF	KO^tBu	58
15	**C-4**	THF	NaOAc	37
16	**C-4**	THF	Na_2CO_3	42
17	**C-4**	THF	Cs_2CO_3	94
18[c]	**C-4**	**THF**	**Cs_2CO_3**	**91**
19[h]	--[h]	THF	Cs_2CO_3	0
20[d]	**C-4**	THF	Cs_2CO_3	82
21[c,e]	**C-4**	THF	Cs_2CO_3	79
22[c,f]	**C-4**	THF	Cs_2CO_3	81

Further Investigation on Oxidant

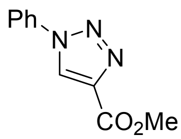
Oxidant	Solvent	Sealed Tube	Result
DQ (1.0 eq.)	THF (Degassing)	Filled with O_2	**3a**: 12 h, 94%
no DQ	THF (Degassing)	Filled with O_2	**3a**: 24 h, <5%
DQ (1.0 eq.)	THF (Degassing)	Glovebox	**3a**: 24 h, <5%
DQ (2.0 eq.)	THF (Degassing)	Glovebox	**3a**: 24 h, <5%

Conditions: cat. **C-4** (15 mmol%), THF, 80 °C, Cs_2CO_3, oxidant

[a] Reaction conditions: A mixture of **1a** (0.20 mmol), **2a** (0.10 mmol), MeOH (0.5 mmol), cat. (20 mol%), DQ as oxidant (0.10 mmol), base (20 mol%) and **3a** (0.5 mmol) in the solvent (0.3 mL, without degasing) was stirred at 80 °C for 24h in a sealed tube (25 mL). [b] Isolated yield. [c] cat. **C-4** (15 mol%) was used. [d] cat. **C-4** (10 mol%) was used. [e] **1a** (0.1 mmol) was used. [f] MeOH (0.3 mmol) was used. [g] DQ = 3,3',5,5'-Tetra-*tert*-butyldiphenoquinone; If other oxidants (e.g. PCC, DDQ) used, none of **3a** was detected by either GC or TLC. [h] None of **3a** was observed without catalyst.

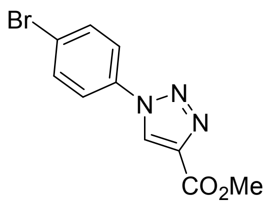
D: Characterization Data.

Methyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3a)



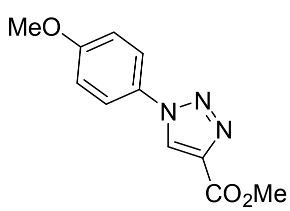
Yellow solid, 91% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.54 (s, 1H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.60-7.56 (m, 2H), 7.53-7.50 (m, 1H), 4.02 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.0, 140.6, 136.3, 129.9, 129.5, 125.6, 120.8, 52.3. HRMS (EI): exact mass calculated for M ($C_{10}H_9N_3O_2$) requires m/z 203.0695, found m/z 203.0692.

Methyl 1-(4-bromophenyl)-1H-1,2,3-triazole-4-carboxylate (3b)



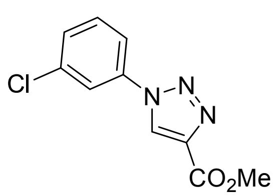
Yellow solid, 92% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.54 (s, 1H), 7.72-7.67 (m, 4H), 4.01 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 160.8, 140.8, 135.3, 133.1, 125.4, 123.4, 122.2, 52.4. HRMS (EI): exact mass calculated for M ($C_{10}H_8N_3O_2Br$) requires m/z 280.9800, found m/z 280.9805.

Methyl 1-(4-methoxyphenyl)-1H-1,2,3-triazole-4-carboxylate (3c)



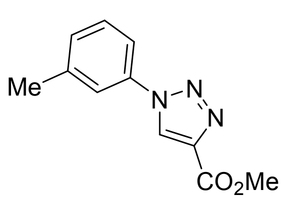
Yellow solid, 94% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.45 (s, 1H), 7.67 (d, *J* = 9.0 Hz, 2H), 7.06 (d, *J* = 9.0 Hz, 2H), 4.01 (s, 3H), 3.90 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.1, 160.4, 140.3, 129.7, 125.6, 122.4, 114.9, 55.7, 52.3. HRMS (EI): exact mass calculated for M ($C_{11}H_{11}N_3O_3$) requires m/z 233.0800, found m/z 233.0796.

Methyl 1-(3-chlorophenyl)-1H-1,2,3-triazole-4-carboxylate (3d)



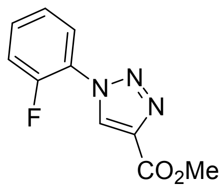
Yellow solid, 91% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.55 (s, 1H), 7.86-7.85 (m, 1H), 7.70-7.68 (m, 1H), 7.55-7.50 (m, 2H), 4.03 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 160.8, 140.7, 137.1, 135.8, 131.0, 129.6, 125.5, 121.1, 118.7, 52.4. HRMS (EI): exact mass calculated for M ($C_{10}H_8N_3O_2Cl$) requires m/z 237.0305, found m/z 237.0303.

Methyl 1-m-tolyl-1H-1,2,3-triazole-4-carboxylate (3e)



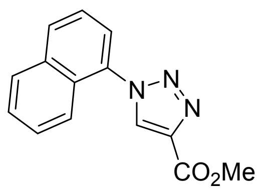
Yellow oil, 85% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.52 (s, 1H), 7.62 (s, 1H), 7.56-7.54 (m, 1H), 7.47-7.43 (m, 1H), 7.33-7.31 (m, 1H), 4.02 (s, 3H), 2.48 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.0, 140.4, 140.3, 136.3, 130.3, 129.7, 125.5, 121.5, 117.8, 52.3, 21.4. HRMS (EI): exact mass calculated for M ($C_{11}H_{11}N_3O_2$) requires m/z 217.0851, found m/z 217.0849.

Methyl 1-(2-fluorophenyl)-1H-1,2,3-triazole-4-carboxylate (3f)



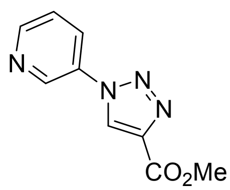
Yellow solid, 84% yield. [1]H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.64 (s, 1H), 8.04-8.00 (m, 1H), 7.52-7.49 (m, 1H), 7.39-7.35 (m, 2H), 4.02 (s, 3H). [13]C NMR ($CDCl_3$, 100 MHz): δ (ppm) 160.9, 153.3 (d, J = 1000.0 Hz), 140.4, 131.0 (d, J = 32.0 Hz), 128.6 (d, J = 34.0 Hz), 125.4 (d, J = 16.0 Hz), 124.9, 117.2 (d, J = 80.0 Hz), 52.3. HRMS (EI): exact mass calculated for M ($C_{10}H_8N_3O_2F$) requires m/z 221.0601, found m/z 221.0609.

Methyl 1-(naphthalen-1-yl)-1H-1,2,3-triazole-4-carboxylate (3g)



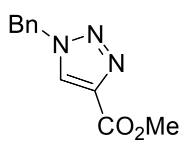
Yellow solid, 83% yield. [1]H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.49 (s, 1H), 8.10-8.08 (m, 1H), 8.02-8.00 (m, 1H), 7.65-7.61 (m, 3H), 7.60-7.58 (m, 2H), 4.06 (s, 3H). [13]C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.8, 140.7, 134.8, 133.5, 131.7, 130.7, 129.1, 129.0, 128.9, 128.8, 125.6, 124.4, 122.5, 53.0. HRMS (EI): exact mass calculated for M ($C_{14}H_{11}N_3O_2$) requires m/z 253.0851, found m/z 253.0846.

Methyl 1-(pyridin-3-yl)-1H-1,2,3-triazole-4-carboxylate (3h)



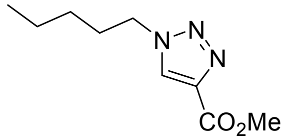
Yellow solid, 85% yield. [1]H NMR ($CDCl_3$, 400 MHz): δ (ppm) 9.07-9.06 (m, 1H), 8.79-8.78 (m, 1H), 8.61 (s, 1H), 8.21-8.19 (m, 1H), 7.58-7.56 (m, 1H), 4.03 (s, 3H). [13]C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.3, 151.4, 142.4, 141.7, 133.7, 129.2, 126.2, 125.0, 53.2. HRMS (EI): exact mass calculated for M ($C_9H_8N_4O_2$) requires m/z 204.0647, found m/z 204.0650.

Methyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate (3i)



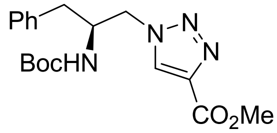
Yellow oil, 83% yield. [1]H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.01 (s, 1H), 7.40-7.38 (m, 3H), 7.30-7.28 (m, 2H), 5.58 (s, 2H), 3.91 (s, 3H). [13]C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.1, 140.3, 133.7, 129.3, 129.1, 128.3, 127.4, 54.5, 52.2. HRMS (EI): exact mass calculated for M ($C_{11}H_{11}N_3O_2$) requires m/z 217.0851, found m/z 217.0846.

Methyl 1-pentyl-1H-1,2,3-triazole-4-carboxylate (3j)



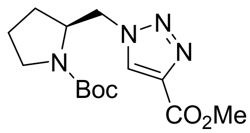
Yellow solid, 93% yield. [1]H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.09 (s, 1H), 4.42 (t, J = 8.0 Hz, 2H), 3.96 (s, 3H), 1.98-1.91 (m, 2H), 1.38-1.29 (m, 4H), 0.91 (t, J = 8.0 Hz, 3H). [13]C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.2, 139.9, 127.2, 52.1, 50.7, 29.8, 28.4, 22.0, 13.8. HRMS (EI): exact mass calculated for M ($C_9H_{15}N_3O_2$) requires m/z 197.1164, found m/z 197.1160.

(*S*)-Methyl 1-(2-(tert-butoxycarbonyl)-3-phenylpropyl)-1H-1,2,3-triazole-4-carboxylate (3k)



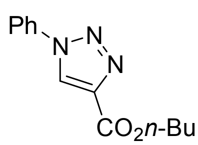
Yellow solid, 74% yield. ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.09 (s, 1H), 7.37-7.34 (m, 2H), 7.30-7.27 (m, 1H), 7.24-7.22 (m, 2H), 4.69-4.55 (m, 3H), 4.25-4.20 (m, 1H), 3.97 (s, 3H), 2.91-2.80 (m, 2H), 1.40 (s, 9H). ^{13}C NMR ($(CD_3)_2CO$), 100 MHz): δ (ppm) 160.9, 154.8, 139.1, 137.9, 129.2, 129.0, 128.3, 126.4, 78.2, 53.1, 52.3, 50.9, 37.8, 27.5. HRMS (EI): exact mass calculated for M ($C_{18}H_{24}N_4O_4$) requires m/z 360.1798, found m/z 360.1793.

(*S*)-Methyl 1-((1-(tert-butoxycarbonyl)pyrrolidin-2-yl)methyl)-1H-1,2,3-triazole-4-carboxylate (3l)



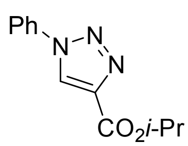
Yellow solid, 78% yield. ^1H NMR ((DMSO-d_6, 400 MHz, 80°C): δ (ppm) 8.57 (s, 1H), 4.53-4.51 (m, 2H), 4.19-4.17 (m, 1H), 3.85 (s, 3H), 3.34-3.27 (m, 1H), 3.18-3.09 (m, 1H), 1.97-1.88 (m, 1H), 1.75-1.72 (m, 2H), 1.63-1.56 (m, 1H), 1.37 (s, 9H). ^{13}C NMR ((DMSO-d_6, 100 MHz, 80°C): δ (ppm) 161.2, 154.1, 139.0, 129.9, 79.3, 56.9, 52.5, 51.9, 46.6, 28.5, 22.9. HRMS (EI): exact mass calculated for M ($C_{14}H_{22}N_4O_4$) requires m/z 310.1641, found m/z 310.1635.

Butyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3m)



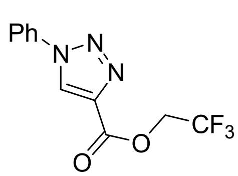
Yellow solid, 87% yield. ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.52 (s, 1H), 7.79-7.77 (m, 2H), 7.60-7.56 (m, 2H), 7.53-7.51 (m, 1H), 4.43 (t, *J* = 7.0 Hz, 2H), 1.85-1.78 (m, 2H), 1.53-1.47 (m, 2H), 1.00 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 160.7, 140.8, 136.4, 129.9, 129.5, 125.4, 120.8, 65.3, 30.7, 19.1, 13.7. HRMS (EI): exact mass calculated for M ($C_{13}H_{15}N_3O_2$) requires m/z 245.1164, found m/z 245.1160.

Isopropyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3n)



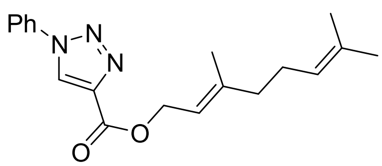
Yellow solid, 78% yield. ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.51 (s, 1H), 7.79-7.77 (m, 2H), 7.60-7.56 (m, 2H), 7.53-7.51 (m, 1H), 5.37 (septets, *J* = 7.0 Hz, 1H), 1.43 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 160.2, 141.2, 136.4, 129.9, 129.5, 125.4, 120.8, 69.2, 21.9. HRMS (EI): exact mass calculated for M ($C_{12}H_{13}N_3O_2$) requires m/z 231.1008, found m/z 231.1003.

2,2,2-Trifluoroethyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3o)



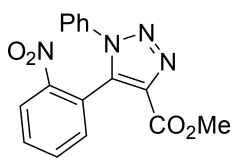
Yellow oil, 85% yield. ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.59 (s, 1H), 7.81-7.79 (m, 2H), 7.63-7.55 (m, 3H), 4.82 (q, *J* = 8.0 Hz, 2H). ^{13}C NMR ($(CD_3)_2CO$), 100 MHz): δ (ppm) 158.7, 138.6, 136.6, 129.9, 129.4, 127.4, 122.2, 120.8, 60.3 (q, J = 145.0 Hz). HRMS (EI): exact mass calculated for M ($C_{11}H_8F_3N_3O_2$) requires m/z 271.0569, found m/z 271.0573.

(*E*)-3,7-Dimethylocta-2,6-dienyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3p)



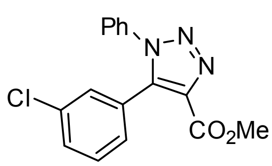
Yellow solid, 63% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.52 (s, 1H), 7.79-7.77 (m, 2H), 7.60-7.56 (m, 2H), 7.54-7.50 (m, 1H), 5.56-5.51 (m, 1H), 5.13-5.10 (m, 1H), 4.95 (d, J = 8.0 Hz, 2H), 2.17-2.08 (m, 4H), 1.80 (s, 3H), 1.70 (s, 3H), 1.63 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 160.6, 143.1, 140.9, 136.4, 131.9, 129.9, 129.5, 125.5, 123.7, 120.8, 117.9, 62.3, 39.6, 26.3, 25.6, 17.7, 16.6. HRMS (EI): exact mass calculated for M ($C_{19}H_{23}N_3O_2$) requires m/z 325.1790, found m/z 325.1795.

Methyl 5-(2-nitrophenyl)-1-phenyl-1H-1,2,3-triazole-4-carboxylate (3q)



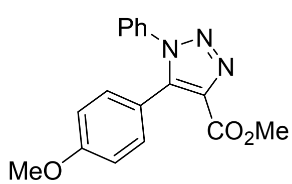
Yellow solid, 84% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.24-8.22 (m, 1H), 7.69-7.65 (m, 2H), 7.45-7.37 (m, 5H), 7.26-7.24 (m, 1H), 3.87 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.1, 148.6, 138.0, 136.5, 135.3, 133.4, 132.3, 131.3, 130.0, 129.5, 125.1, 124.9, 122.2, 52.3. HRMS (EI): exact mass calculated for M ($C_{16}H_{12}N_4O_4$) requires m/z 324.0859, found m/z 324.0863.

Methyl 1-(3-chlorophenyl)-5-phenyl-1H-1,2,3-triazole-4-carboxylate (3r)



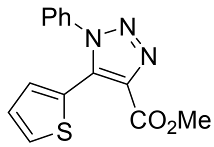
Yellow solid, 86% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.49-7.41 (m, 5H), 7.33-7.29 (m, 3H), 7.12-7.10 (m, 1H), 7.12-7.10 (m, 1H), 3.93 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.2, 141.0, 136.8, 136.7, 135.2, 130.3, 130.2, 130.1, 129.8, 128.6, 125.4, 125.2, 123.2, 52.2. HRMS (EI): exact mass calculated for M ($C_{16}H_{12}N_3ClO_2$) requires m/z 313.0618, found m/z 313.0611.

Methyl 5-(4-methoxyphenyl)-1-phenyl-1H-1,2,3-triazole-4-carboxylate (3s)



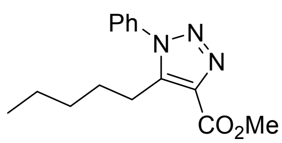
Yellow solid, 89% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.44-7.40 (m, 3H), 7.32-7.29 (m, 2H), 7.24 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 8.0 Hz, 2H), 3.95 (s, 3H), 3.84 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.6, 160.8, 140.9, 136.3, 135.9, 131.7, 129.5, 129.3, 125.3, 117.2, 113.9, 55.3, 52.1. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O_3$) requires m/z 309.1113, found m/z 309.1112.

Methyl 1-phenyl-5-(thiophen-2-yl)-1H-1,2,3-triazole-4-carboxylate (3t)



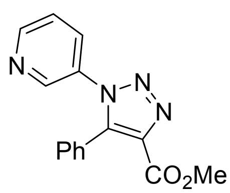
Yellow solid, 85% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.52-7.47 (m, 4H), 7.39-7.37 (m, 2H), 7.33-7.32 (m, 1H), 7.09-7.07 (m, 1H), 3.99 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.3, 136.6, 135.8, 135.3, 132.2, 130.1, 129.9, 129.5, 127.2, 125.9, 124.5, 52.3. HRMS (EI): exact mass calculated for M ($C_{14}H_{11}N_3O_2S$) requires m/z 285.0572, found m/z 285.0572.

Methyl 5-pentyl-1-phenyl-1H-1,2,3-triazole-4-carboxylate (3u)



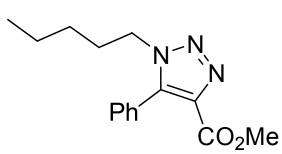
Yellow solid, 83% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.63-7.59 (m, 3H), 7.45-7.43 (m, 2H), 4.01 (s, 3H), 2.98 (t, J = 8.0 Hz, 2H), 1.54-1.47 (m, 2H), 1.27-1.22 (m, 4H), 0.82 (t, J = 8.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 162.0, 143.7, 136.0, 135.6, 130.3, 129.7, 125.8, 52.0, 31.3, 28.2, 23.2, 21.9, 13.7. HRMS (EI): exact mass calculated for M ($C_{15}H_{19}N_3O_2$) requires m/z 273.1477, found m/z 273.1481.

Methyl 5-phenyl-1-(pyridin-3-yl)-1H-1,2,3-triazole-4-carboxylate (3v)



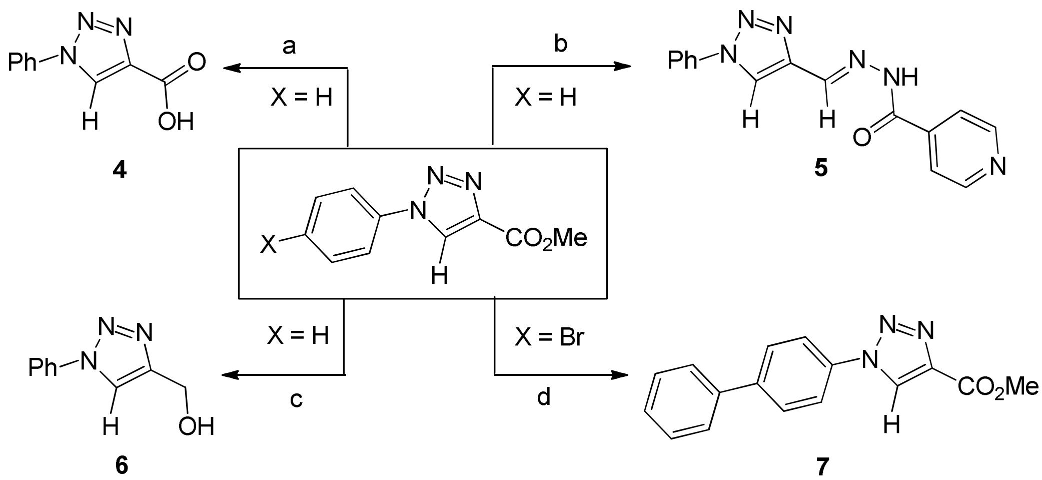
Yellow solid, 82% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.68-8.67 (m, 1H), 7.57-7.56 (m, 1H), 7.70-7.67 (m, 1H), 7.49-7.37 (m, 4H), 7.33-7.30 (m, 2H), 3.93 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.1, 150.5, 145.8, 141.3, 137.0, 132.6, 132.4, 130.5, 130.2, 128.8, 124.9, 123.8, 52.3. HRMS (EI): exact mass calculated for M ($C_{15}H_{12}N_4O_2$) requires m/z 280.0960, found m/z 280.0958.

Methyl 1-pentyl-5-phenyl-1H-1,2,3-triazole-4-carboxylate (3w)



Yellow solid, 86% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.56-7.53 (m, 3H), 7.40-7.37 (m, 2H), 4.24 (t, J = 8.0 Hz, 2H), 3.87 (s, 3H), 1.82-1.78 (m, 2H), 1.25-1.19 (m, 4H), 0.84 (t, J = 8.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.6, 141.3, 136.6, 130.2, 129.7, 128.9, 126.2, 52.1, 48.6, 29.8, 28.5, 22.0, 13.9. HRMS (EI): exact mass calculated for M ($C_{15}H_{19}N_3O_2$) requires m/z 273.1477, found m/z 273.1472.

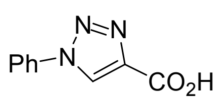
E: Synthetic Transformations.



a) Synthesis of 1-phenyl-1H-1,2,3-triazole-4-carboxylic acid

To a solution of **3a** (0.10 mmol) in THF (1.5 mL) and H_2O (0.3 mL) was added LiOH (0.20 mmol). The resulting mixture was stirred at room temperature for overnight. H_2O (2.0 mL) was then added to quench the reaction. After aqueous solution was extracted with Et_2O (3*5 mL), the aqueous layer was then acidified with 1N HCl until the pH=1. Then the solution was extracted with ethyl acetate for three times (3*10 mL), the combined organic layers was dried with anhydrous Na_2SO_4, filtered and concentrated in vacuum to yield the desired product **4** in 92% yield.

1-phenyl-1H-1,2,3-triazole-4-carboxylic acid (4)

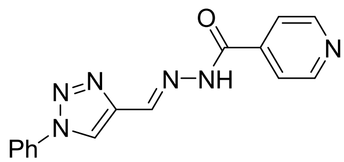


Yellow solid, 92% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 10.15 (br, 1H), 8.64 (s, 1H), 7.81-7.79 (m, 2H), 7.61-7.58 (m, 2H), 7.55-7.52 (m, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ (ppm) 162.0, 141.1, 136.6, 130.3, 129.6, 127.5, 120.9. HRMS (EI): exact mass calculated for M^+ ($C_9H_8N_3O_2$) requires m/z 190.0617, found m/z 190.0620.

b) Synthesis of (E)-N'-((1-phenyl-1H-1,2,3-triazol-4-yl)methylene) isonicotinohydrazide

To a solution of **3a** (0.10 mmol) in anhydrous THF was added DIBAL-H (0.2 mmol, 1.0 M in cyclohexane) in one portion. The reaction mixture was stirred at room temperature for 12h. Then the reaction was quenched by water (3.0 mL) and the aqueous phase was extracted with CH_2Cl_2 (3*5.0 mL). The organic phase was dried with anhydrous Na_2SO_4 and reduced in vacuum to yield the alcohol intermediate. To a solution of the alcohol intermediate in CH_2Cl_2 (3.0 mL) was added PCC (1.5 eq.) in one portion. The reaction mixture was stirred at room temperature for 2h. Then the reaction solution was reduced in vacuum to yield a residue, which was purified by silica gel to yield the desired product. To a solution of this desired product (0.10 mmol) in ethanol (1.0 mL) was added the solution of Isoniazid (0.10 mmol) in H_2O (1.0 mL). After stirring for 3h at room temperature, the resulting mixture was concentrated under reduced pressure to give a residue, which was purified by washing with cold ethanol and ethyl ether to yield the desired product **5** in 82% yield (3 steps).

(E)-N'-((1-phenyl-1H-1,2,3-triazol-4-yl)methylene)isonicotinohydrazide (5)

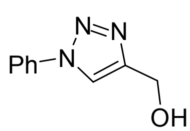


White solid, 82% yield. ^{1}H NMR (DMSO-d_6, 400 MHz): δ (ppm) 12.17 (s, 1H), 9.35 (s, 1H), 8.82 (d, J = 5.0 Hz, 2H), 8.66 (s, 1H), 8.04-8.02 (m, 2H), 7.85 (d, J = 5.0 Hz, 2H), 7.65-7.62 (m, 2H), 7.55-7.52 (m, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ (ppm) 162.1, 150.8, 144.4, 141.4, 140.8, 136.8, 130.4, 129.5, 122.0, 121.3, 120.8. HRMS (EI): exact mass calculated for M^- ($C_{15}H_{11}N_6O$) requires m/z 291.0994, found m/z 291.0996.

c) Synthesis of (1-phenyl-1H-1,2,3-triazol-4-yl)methanol

To a solution of **4a** (0.1 mmol) in anhydrous THF (2.0 mL) was added $LiAlH_4$ (0.15 mmol) at -20 ^{o}C. The resulting solution was stirred at -20 ^{o}C for 30 min, sat. NH_4Cl (2.0 mL) was added to quench the reaction. The aqueous solution was extracted with Et_2O (3*5 mL), the combined organic layers was dried with anhydrous Na_2SO_4, filtered and concentrated to yield the crude product, which was purified by column chromatography to afford **6** in 95% yield.

(1-phenyl-1H-1,2,3-triazol-4-yl)methanol (6)

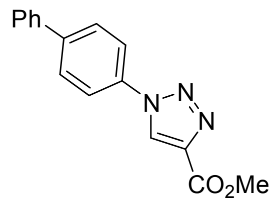


Yellow solid, 95% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.02 (s, 1H), 7.74-7.72 (m, 2H), 7.56-7.52 (m, 2H), 7.48-7.44 (m, 1H), 4.92 (d, J = 6.0 Hz, 2H), 3.06 (t, J = 6.0 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 148.4, 137.0, 129.8, 128.8, 120.6, 120.0, 56.5. HRMS (EI): exact mass calculated for M^+ ($C_9H_{10}N_3O$) requires m/z 176.0824, found m/z 176.0828.

d) Synthesis of methyl (4'- phenyl -1-phenyl-1H-1,2,3-triazole)-4-carboxylate

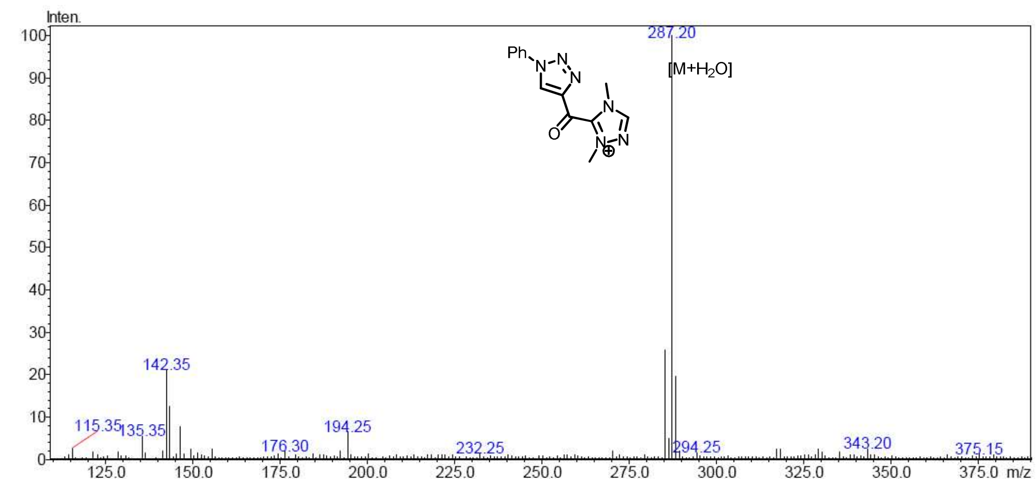
Under Ar atmosphere, to a solution of **4c** (0.10 mmol) and $Pd(PPh_3)_4$ (0.01 mmol) in dry toluene (5 mL) was added K_2CO_3 (0.30 mmol) and $PhB(OH)_2$ (0.30 mmol). The vigorously stirred mixture was heated to 90 ^{o}C for 2 h. After cooling, the mixture was filtered through a pad of celite, the filter cake was washed with ethyl acetate. The organic solvent was removed and the residue was purified by column chromatography to afford **7** in 88% yield.

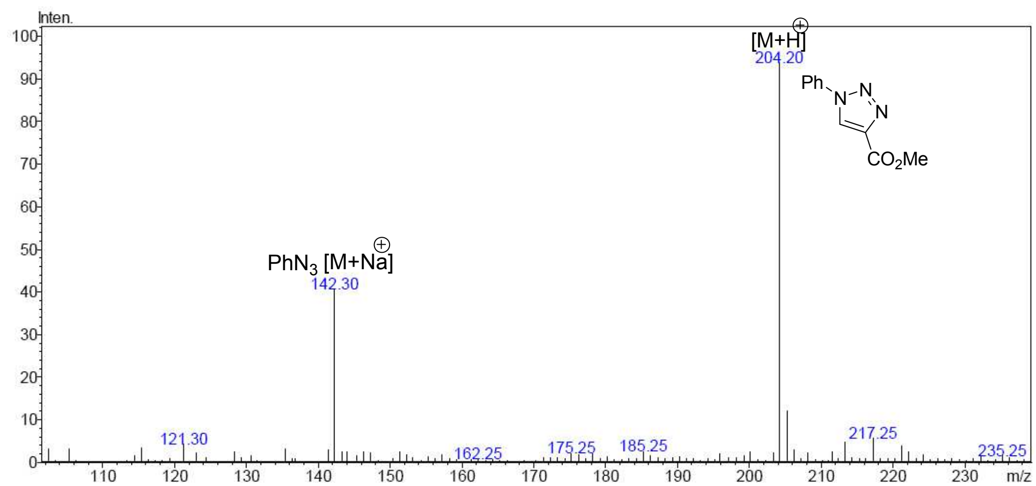
Methyl (4'- phenyl -1-phenyl-1H-1,2,3-triazole)-4-carboxylate (7)



Yellow solid, 88% yield. [1]H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.58 (s, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.66-7.64 (m, 2H), 7.53-7.49 (m, 2H), 7.45-7.42 (m, 1H), 4.03 (s, 3H). [13]C NMR ($CDCl_3$, 100 MHz): δ (ppm) 161.0, 142.6, 140.6, 139.3, 135.4, 129.0, 128.5, 128.2, 127.1, 125.4, 121.1, 52.4. HRMS (EI): exact mass calculated for M ($C_{16}H_{13}N_3O_2$) requires m/z 279.1008, found m/z 279.1012.

F: ESI-MS Studies.



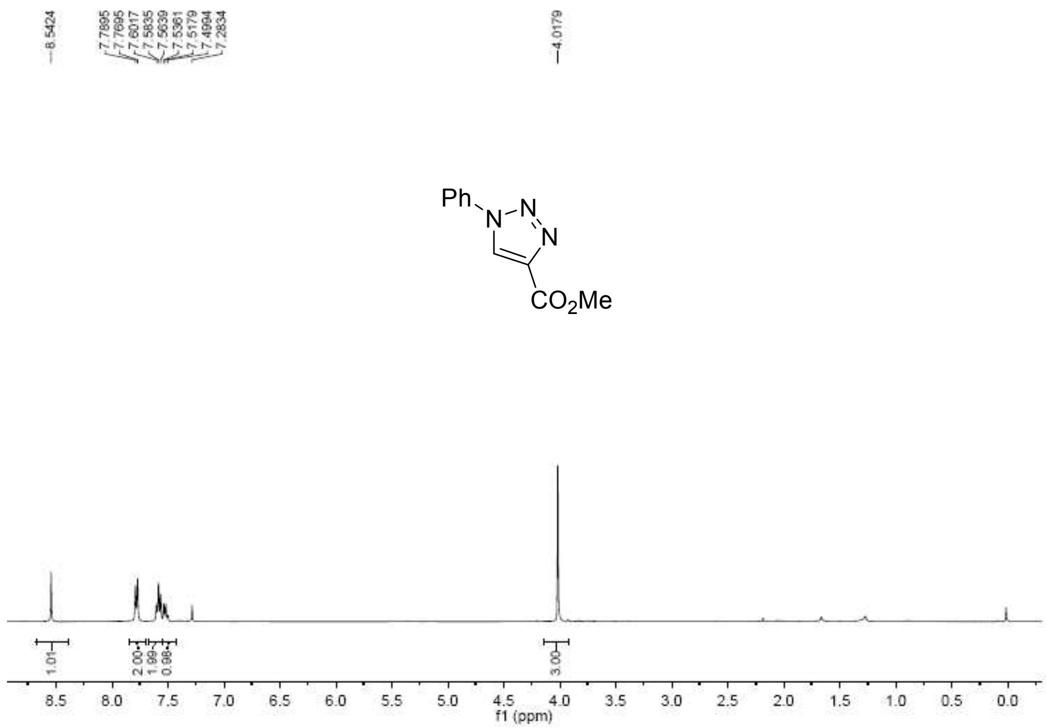


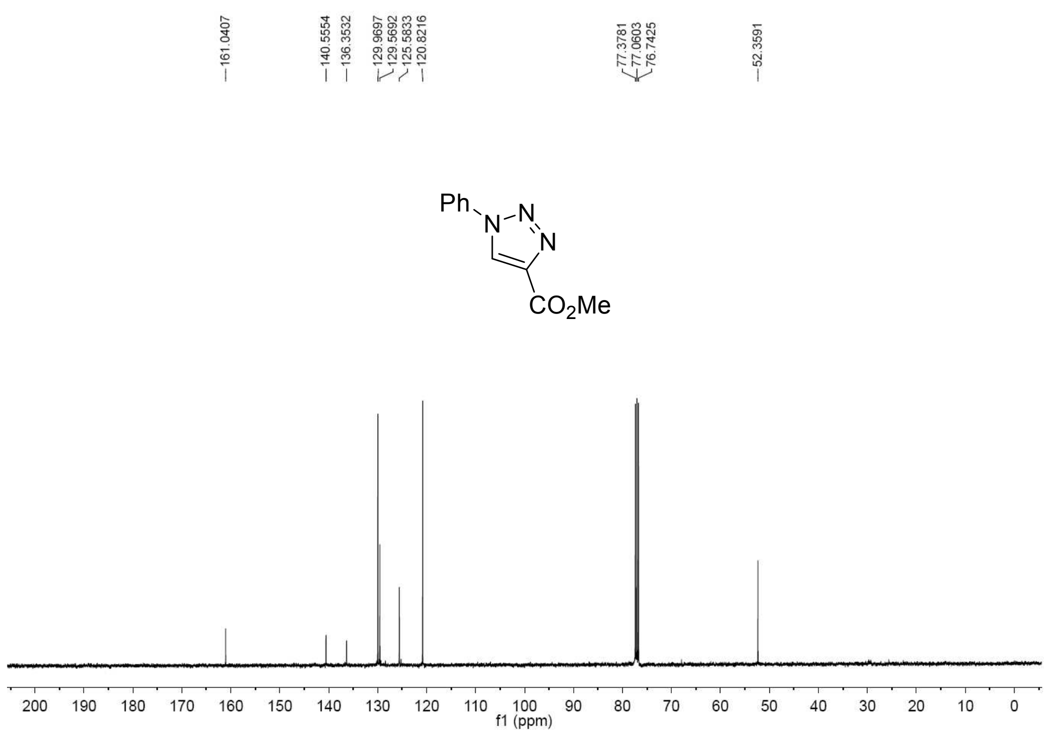
Reaction conditions: A mixture of **1a** (0.20 mmol), azide **2a** (0.10 mmol), NHC **C-4** (0.10 mmol), DQ (0.10 mmol), Cs_2CO_3 (0.15 mmol) and MeOH (0.50 mmol) in THF (0.3 mL) in a sealed tube (25 mL) was stirred at 80 ^oC for 4h.

Figure S1. ESI(+)-MS spectra for the reaction of 1a, 2a, and MeOH catalyzed by C-4 in a sealed tube for 4 hours. Other unidentified ions are likely to correspond to either impurities (favorably ionized under positive-ion ESI) or side-reaction products.

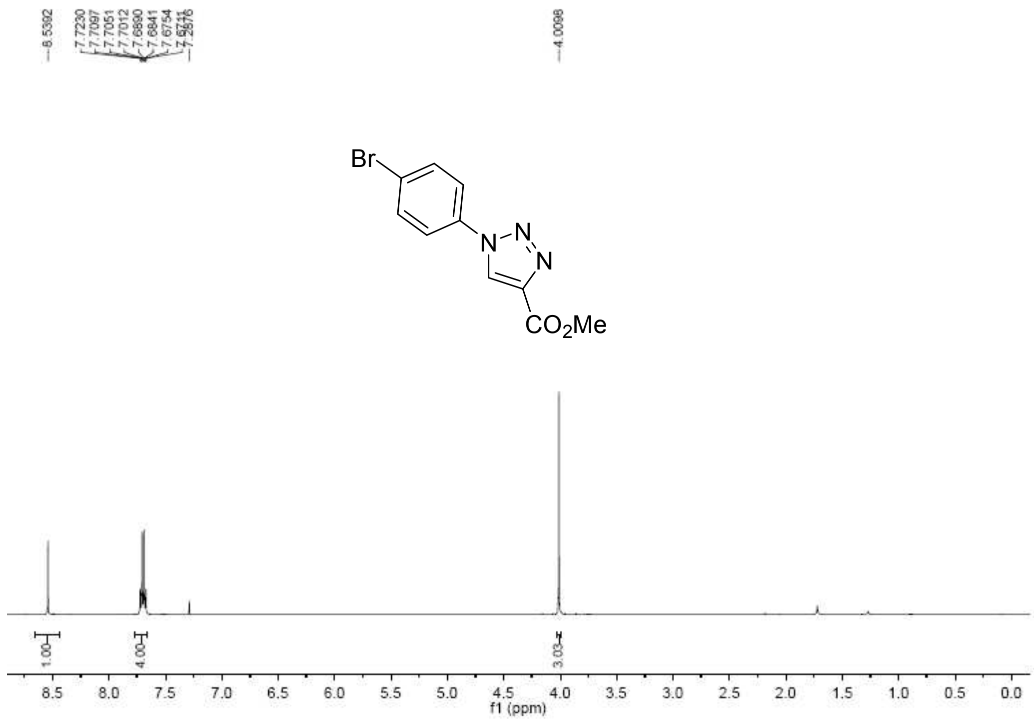
G: NMR Spectra.

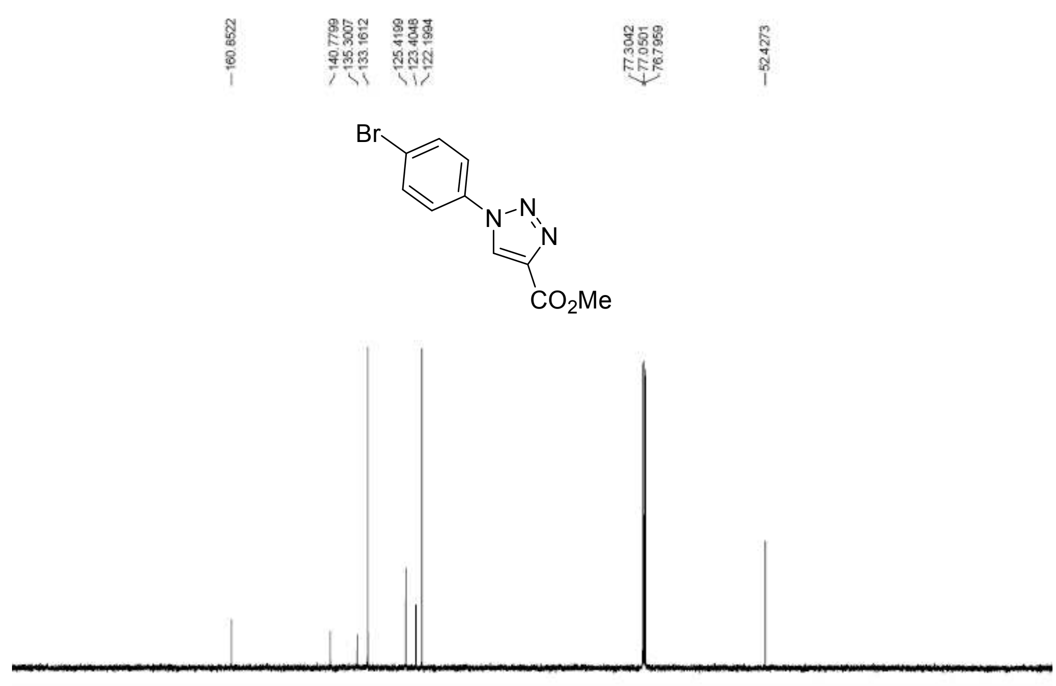
Methyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3a)



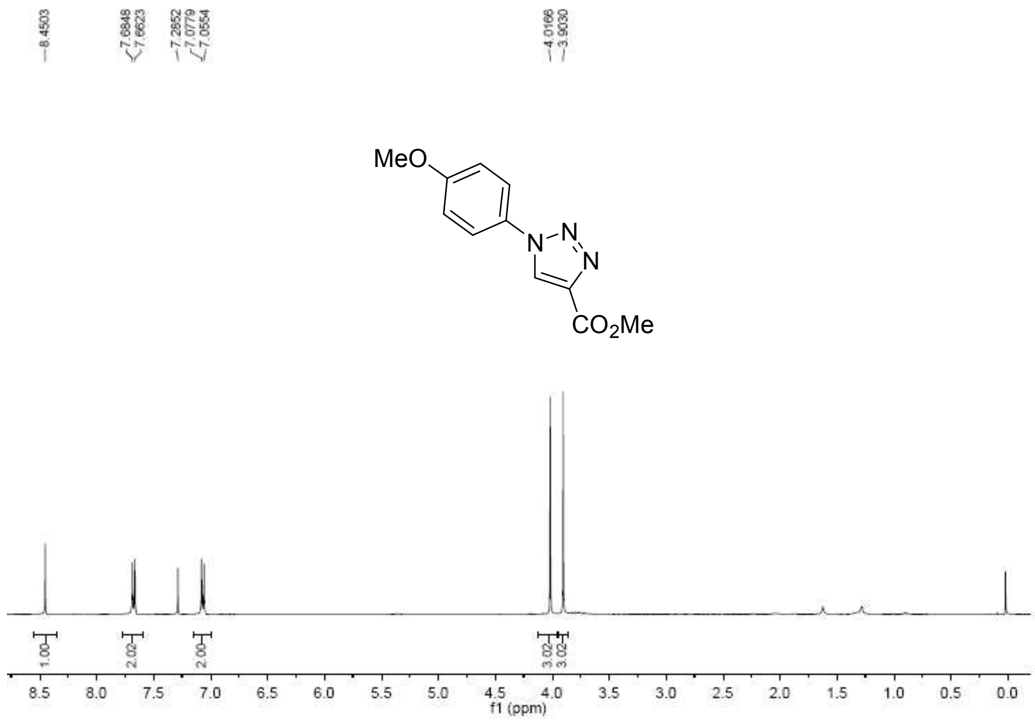


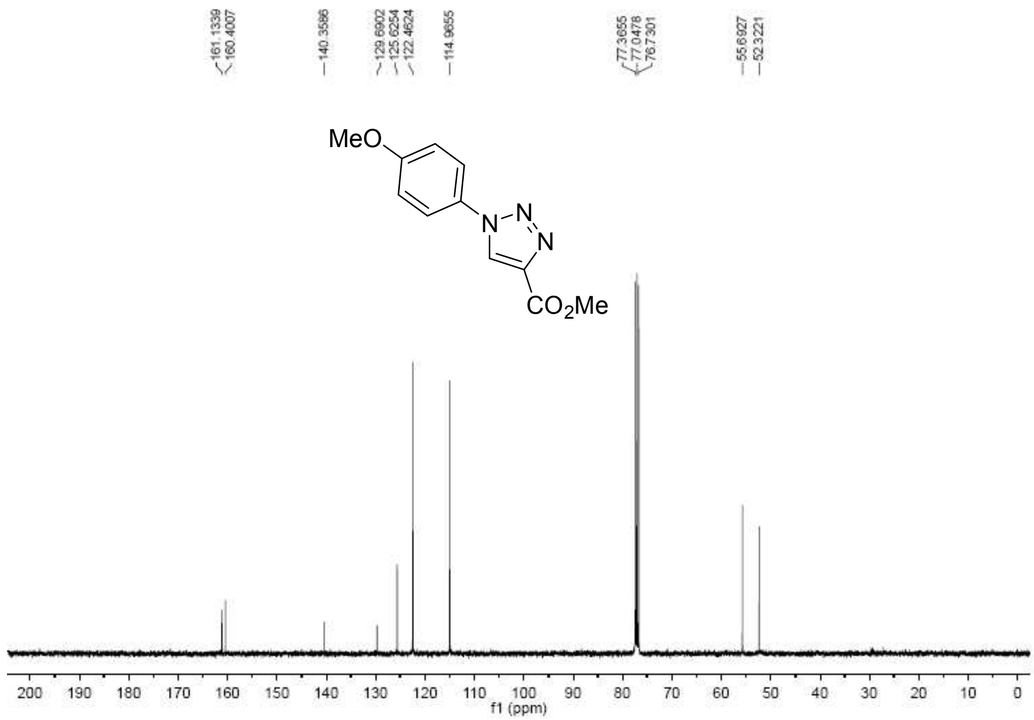
Methyl 1-(4-bromophenyl)-1H-1,2,3-triazole-4-carboxylate (3b)



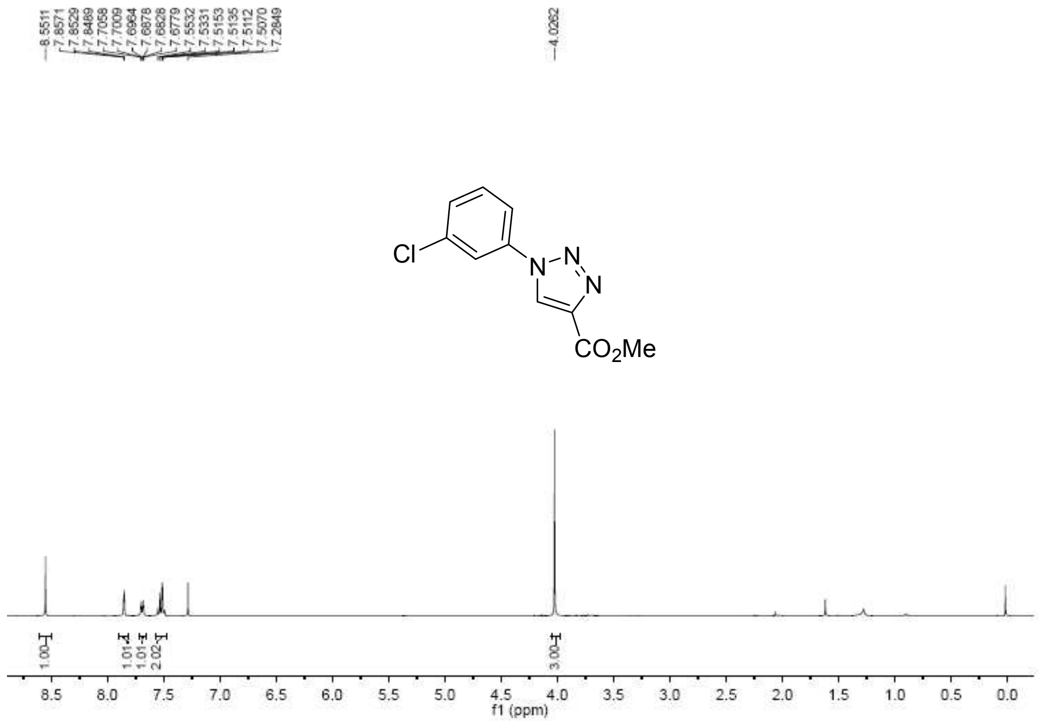


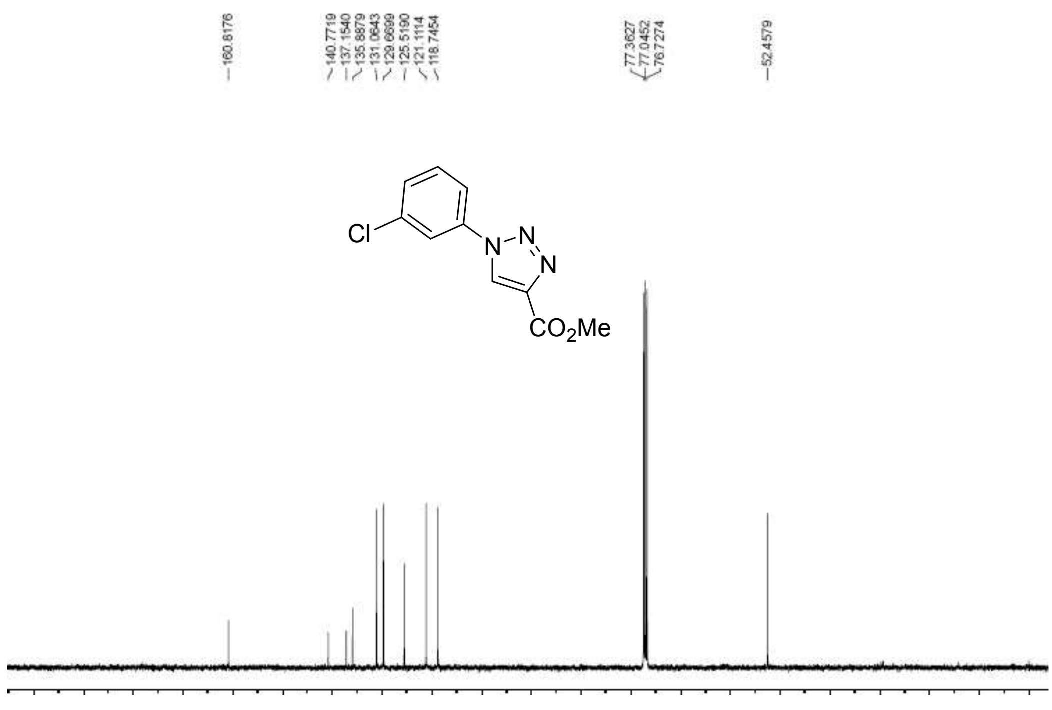
Methyl 1-(4-methoxyphenyl)-1H-1,2,3-triazole-4-carboxylate (3c)



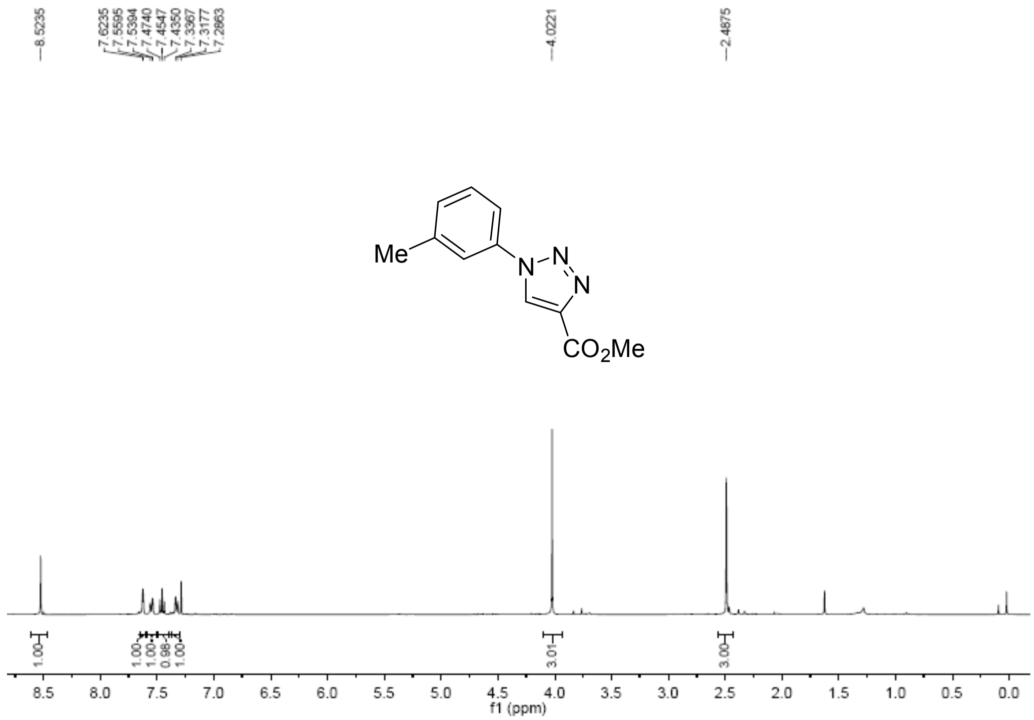


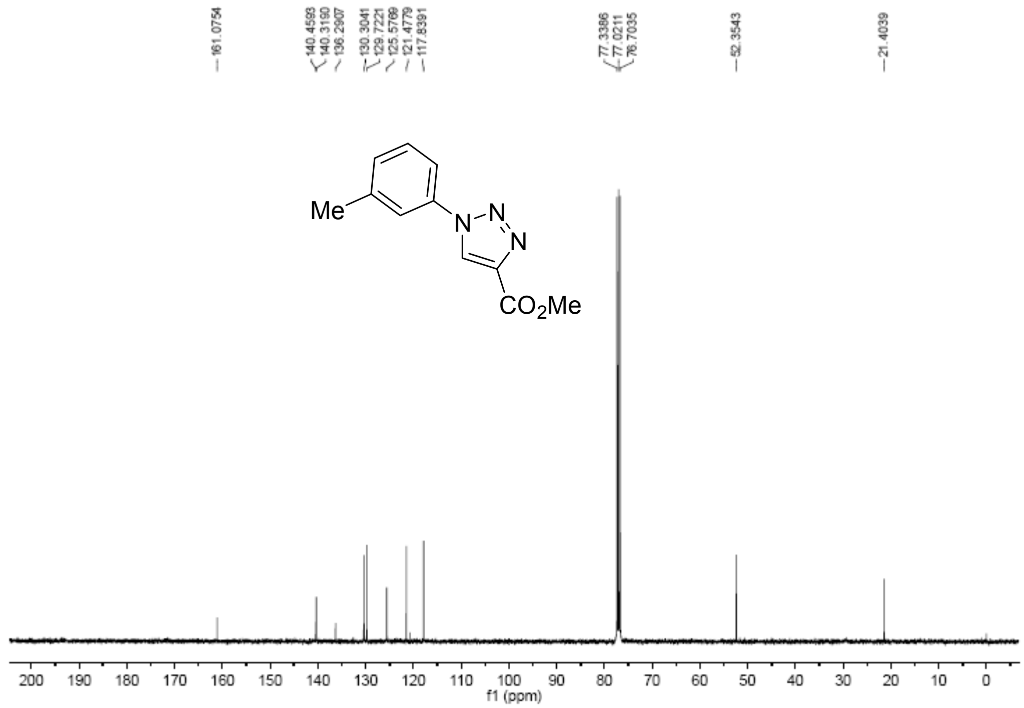
Methyl 1-(3-chlorophenyl)-1H-1,2,3-triazole-4-carboxylate (3d)



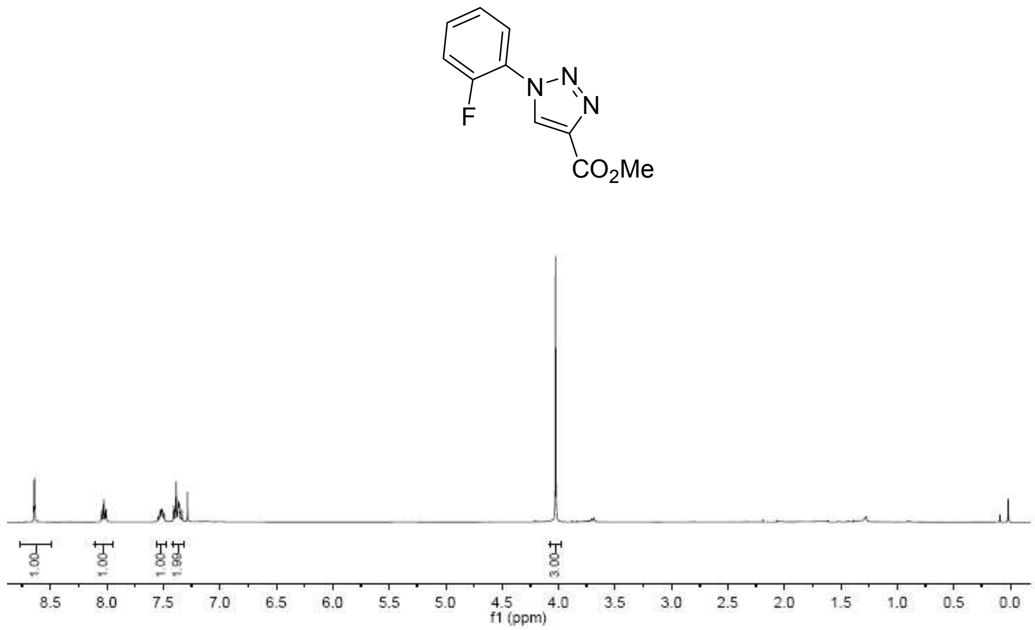


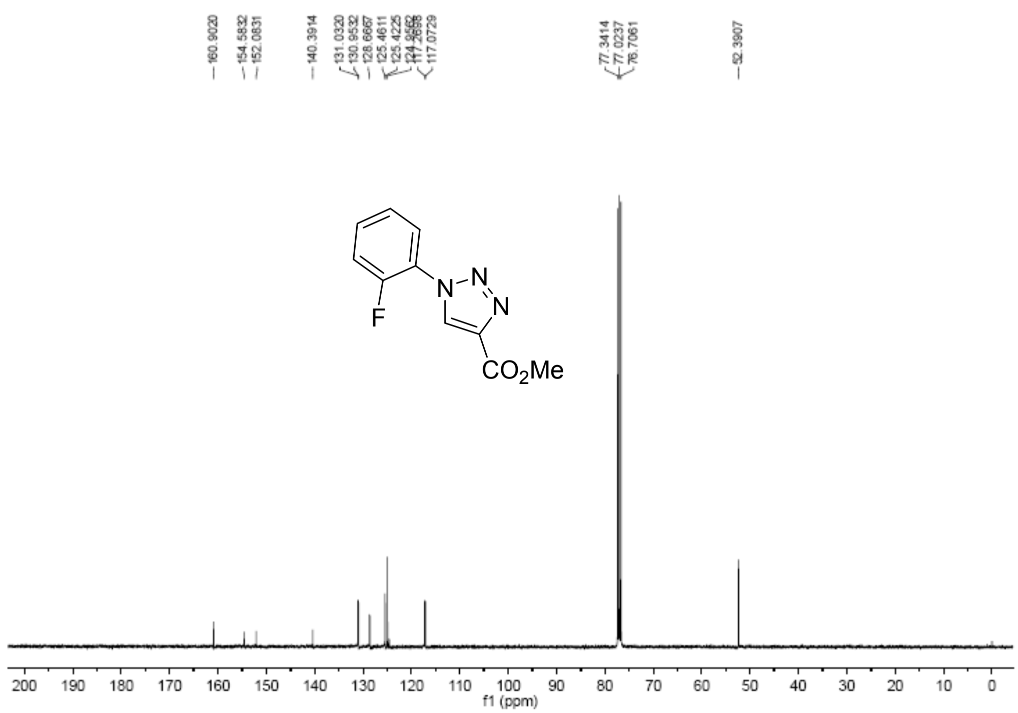
Methyl 1-m-tolyl-1H-1,2,3-triazole-4-carboxylate (3e)



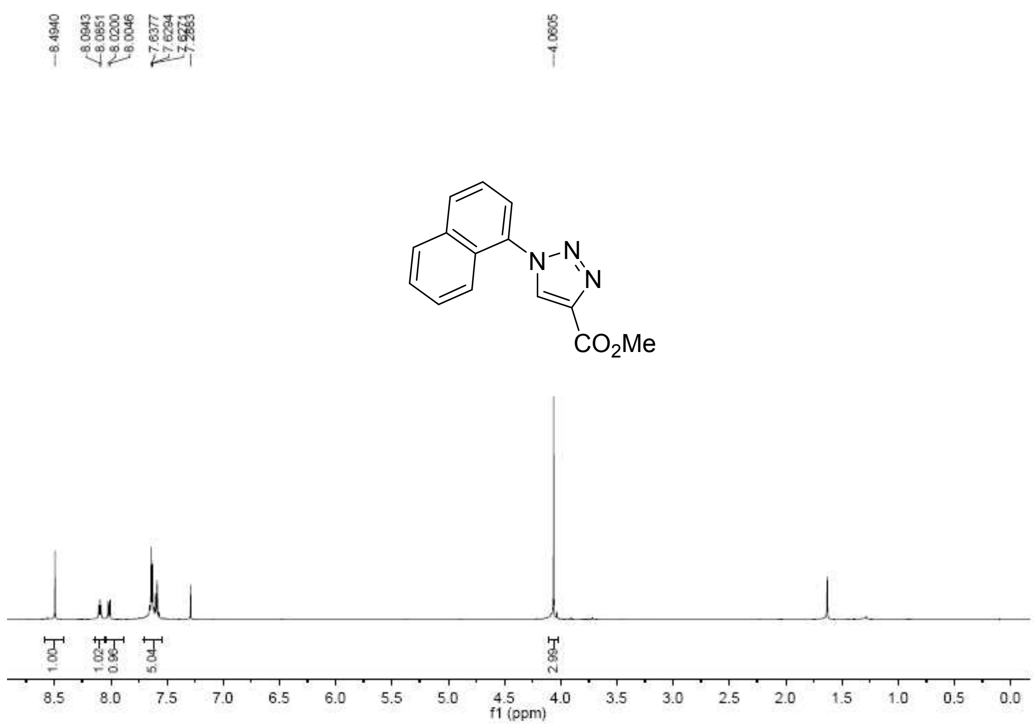


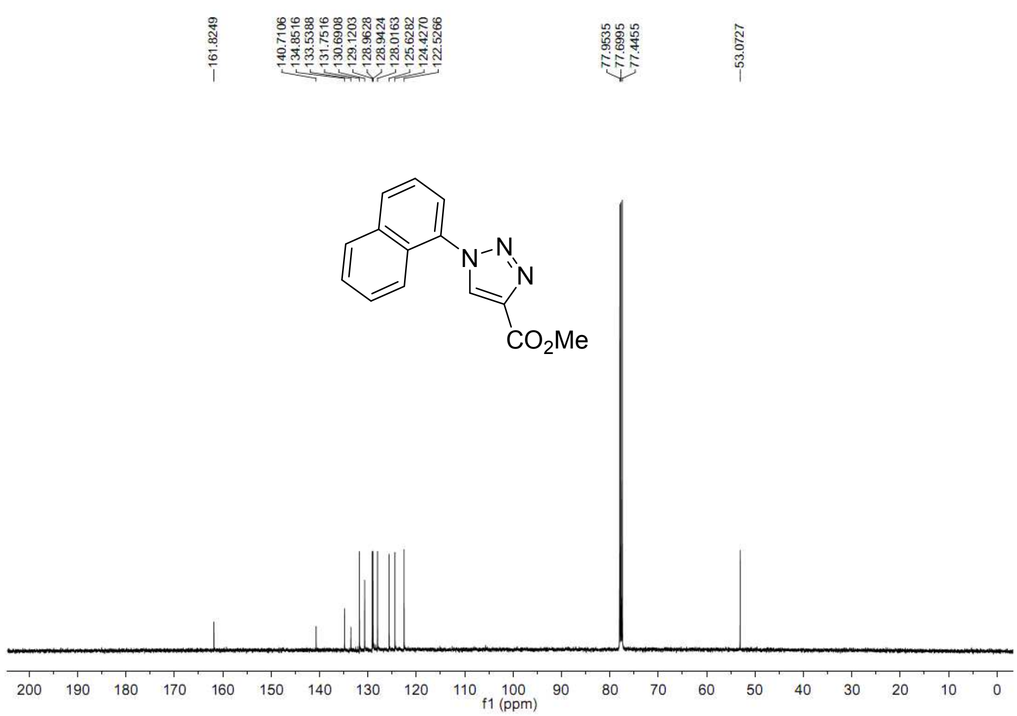
Methyl 1-(2-fluorophenyl)-1H-1,2,3-triazole-4-carboxylate (3f)



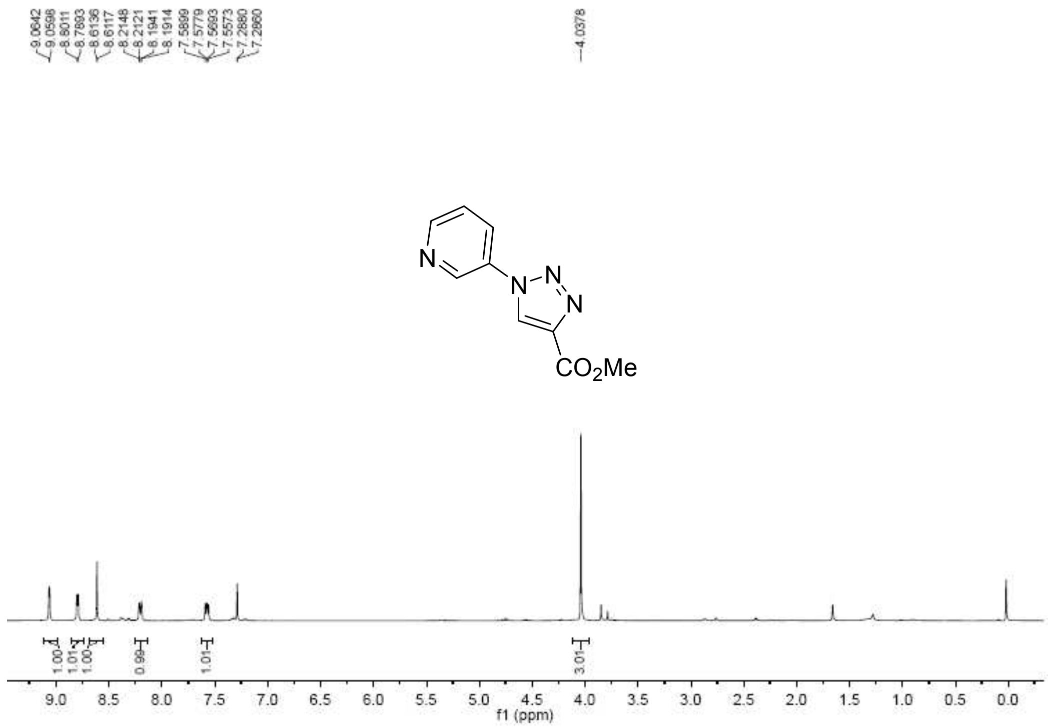


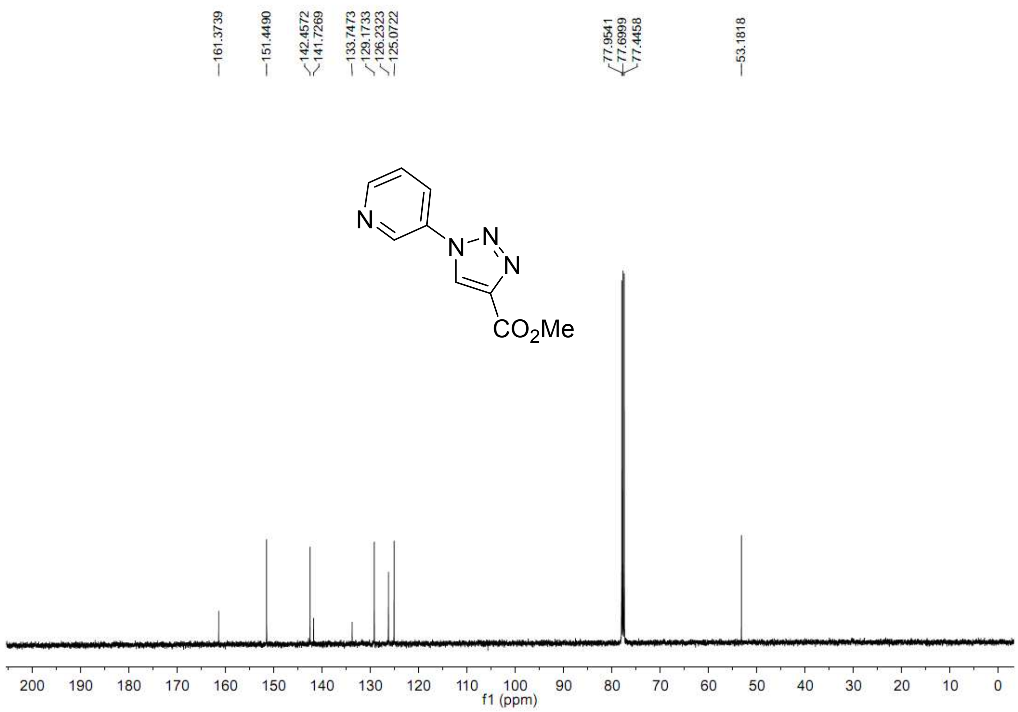
Methyl 1-(naphthalen-1-yl)-1H-1,2,3-triazole-4-carboxylate (3g)



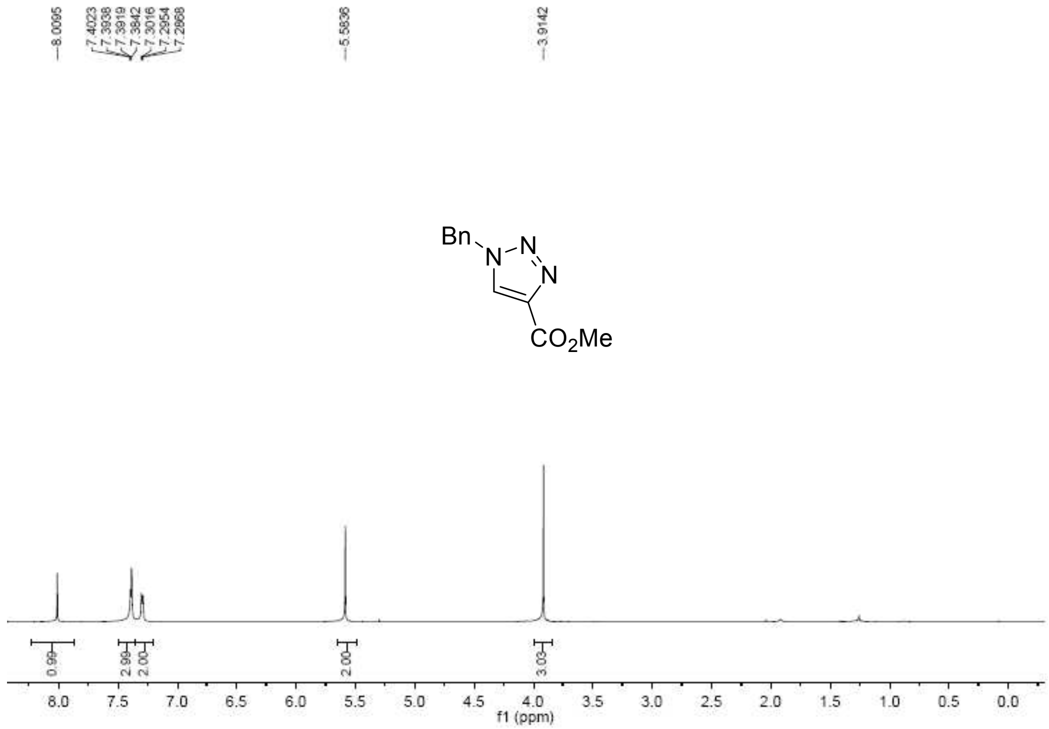


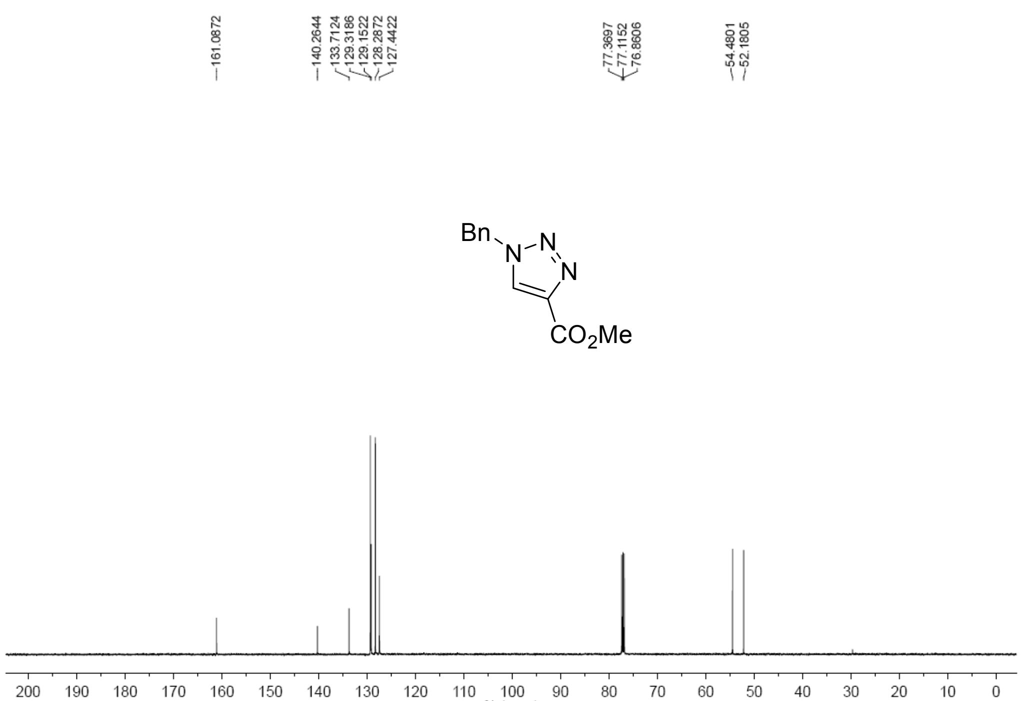
Methyl 1-(pyridin-3-yl)-1H-1,2,3-triazole-4-carboxylate (3h)



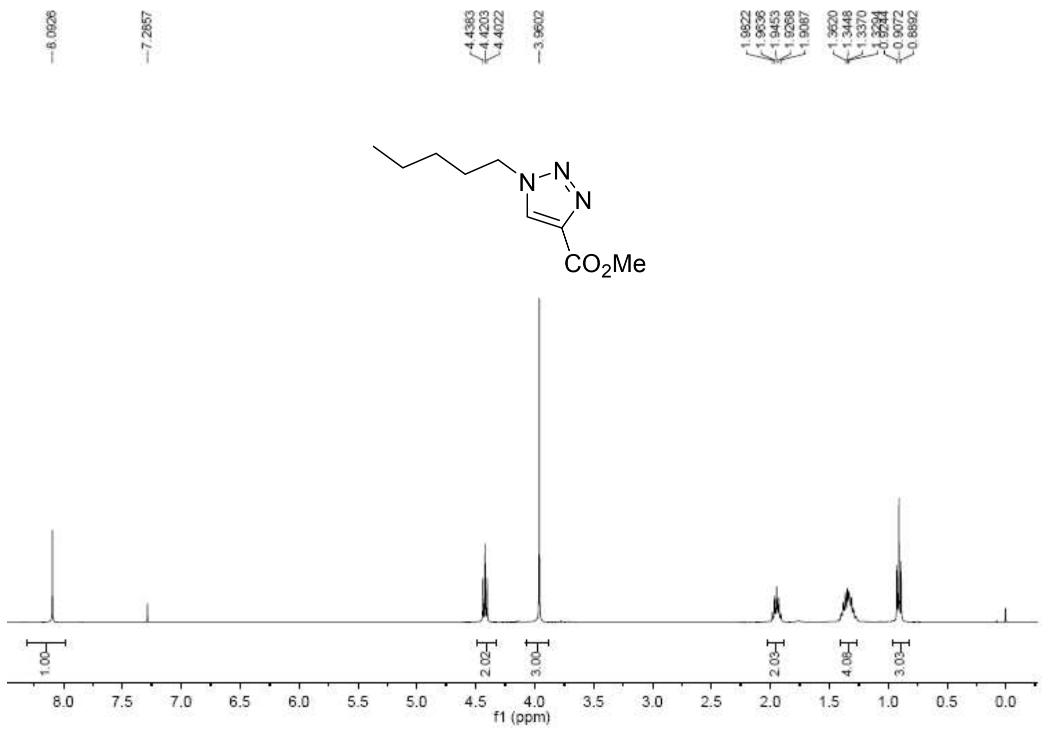


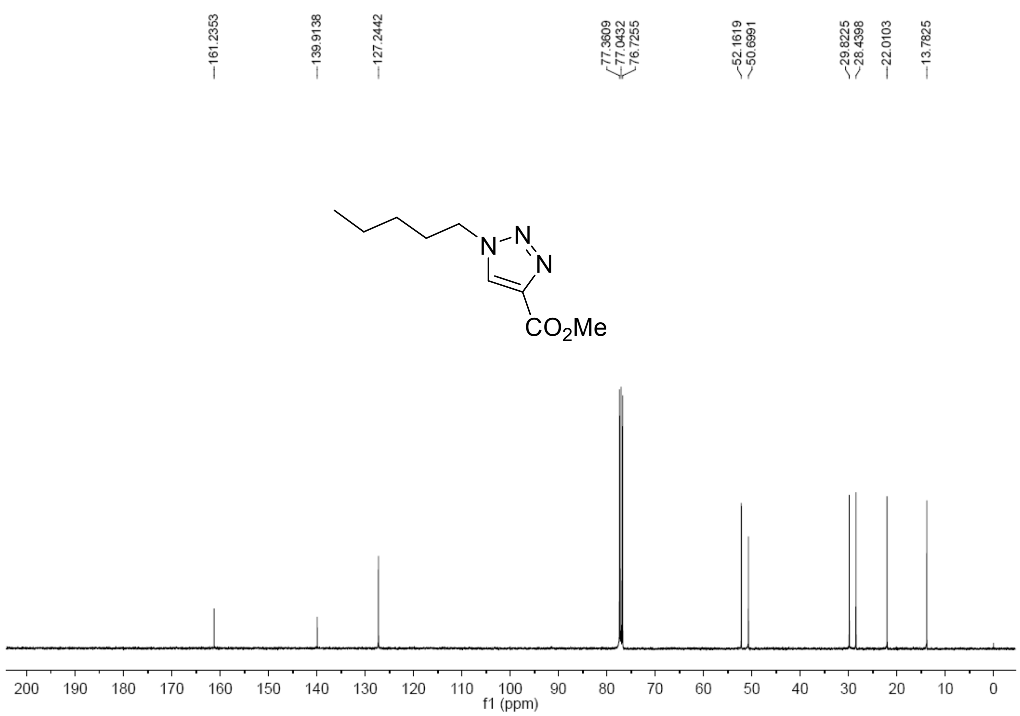
Methyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate (3i)



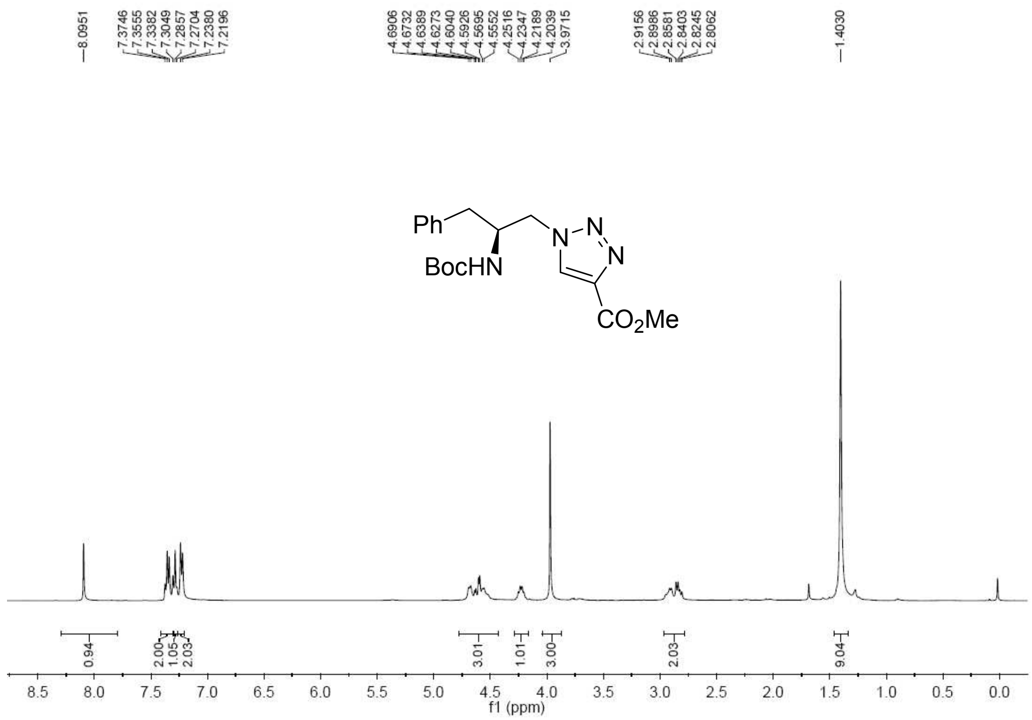


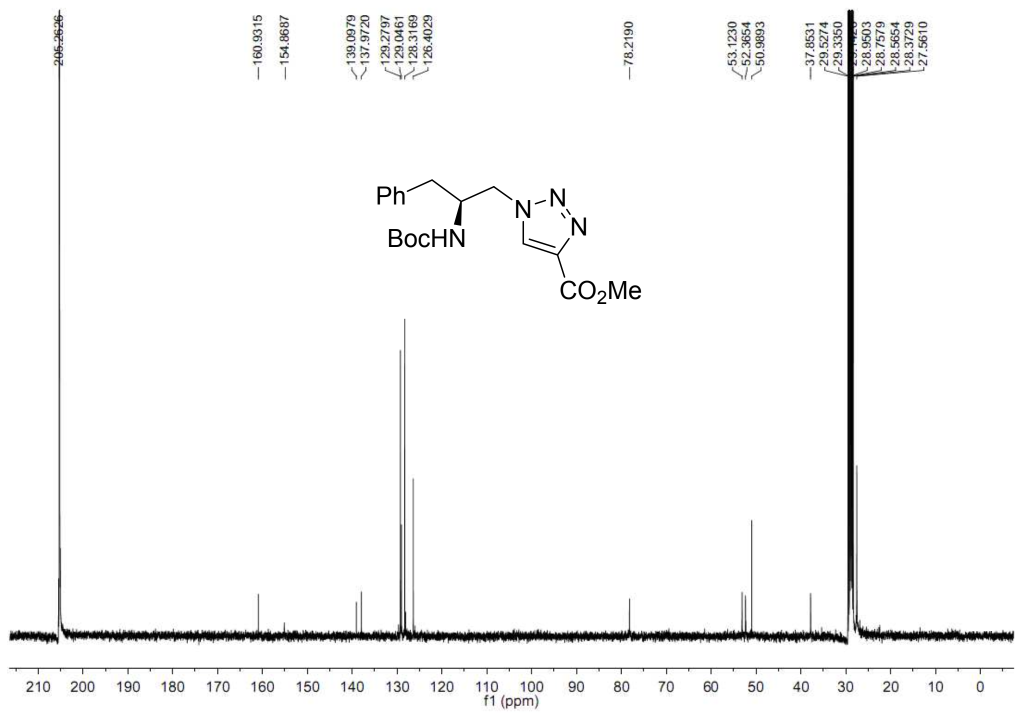
Methyl 1-pentyl-1H-1,2,3-triazole-4-carboxylate (3j)



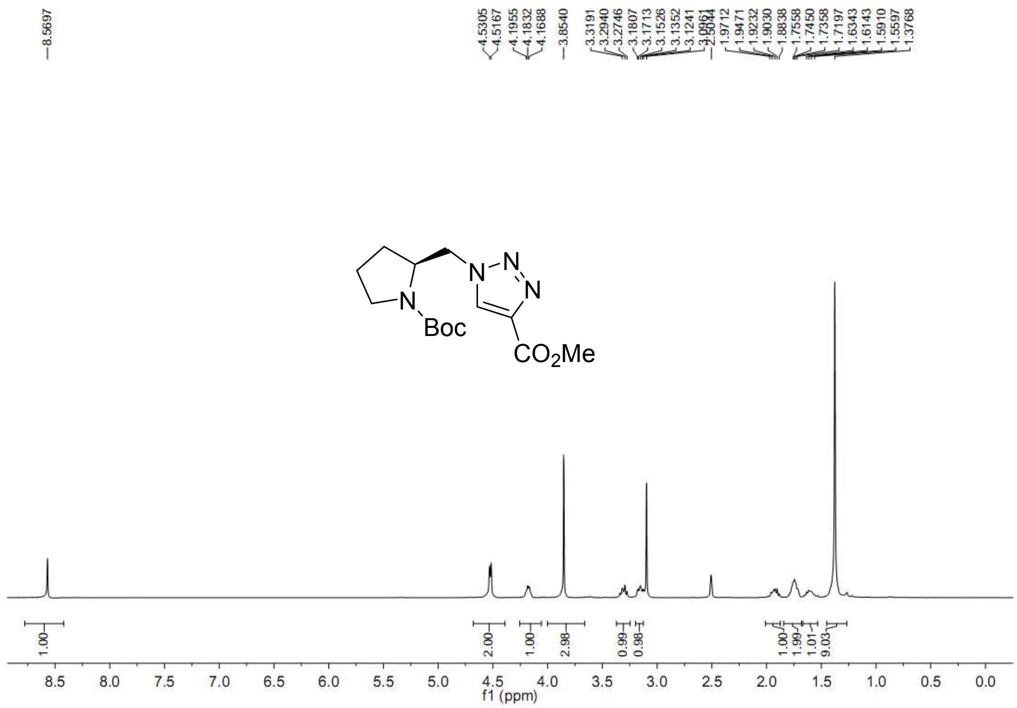


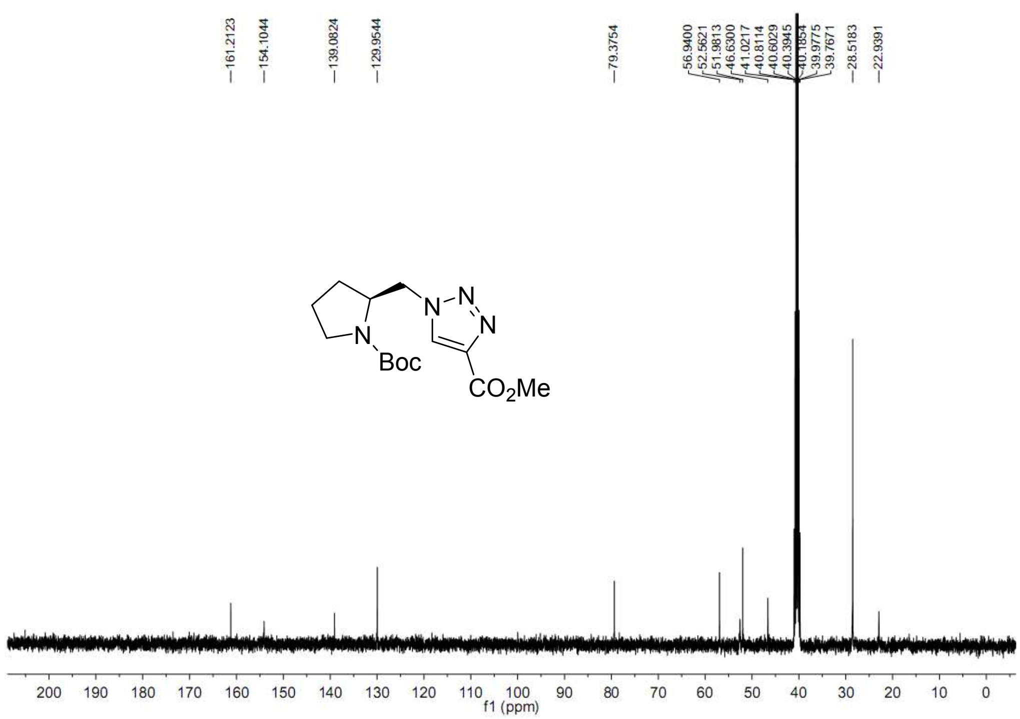
(*S*)-methyl 1-(2-(tert-butoxycarbonyl)-3-phenylpropyl)-1H-1,2,3-triazole-4-carboxylate (3k)



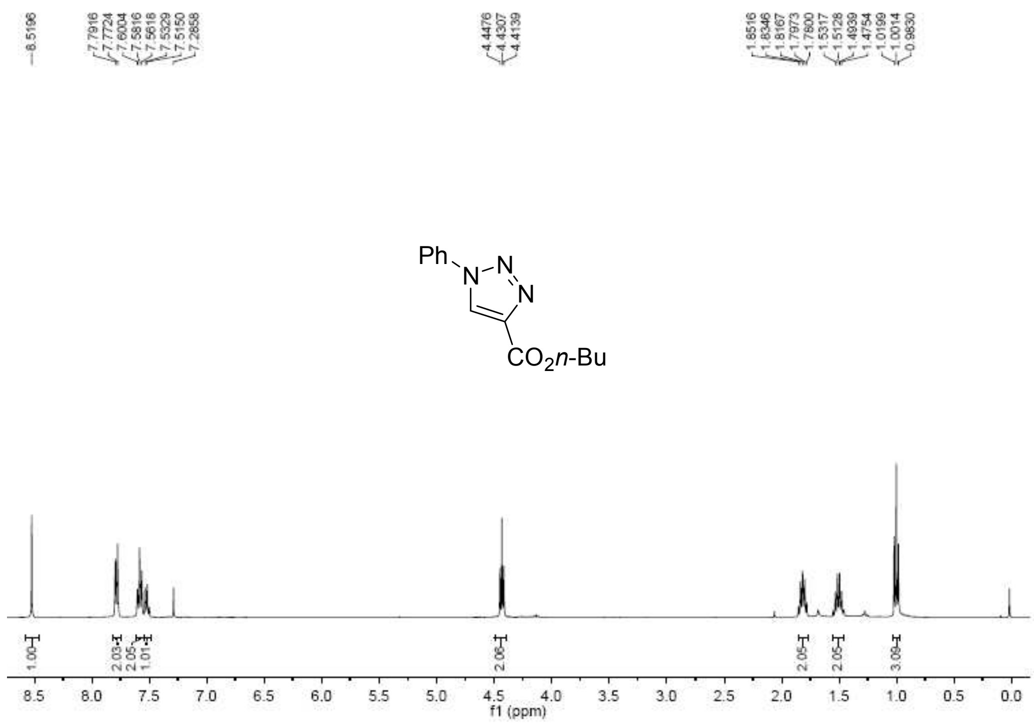


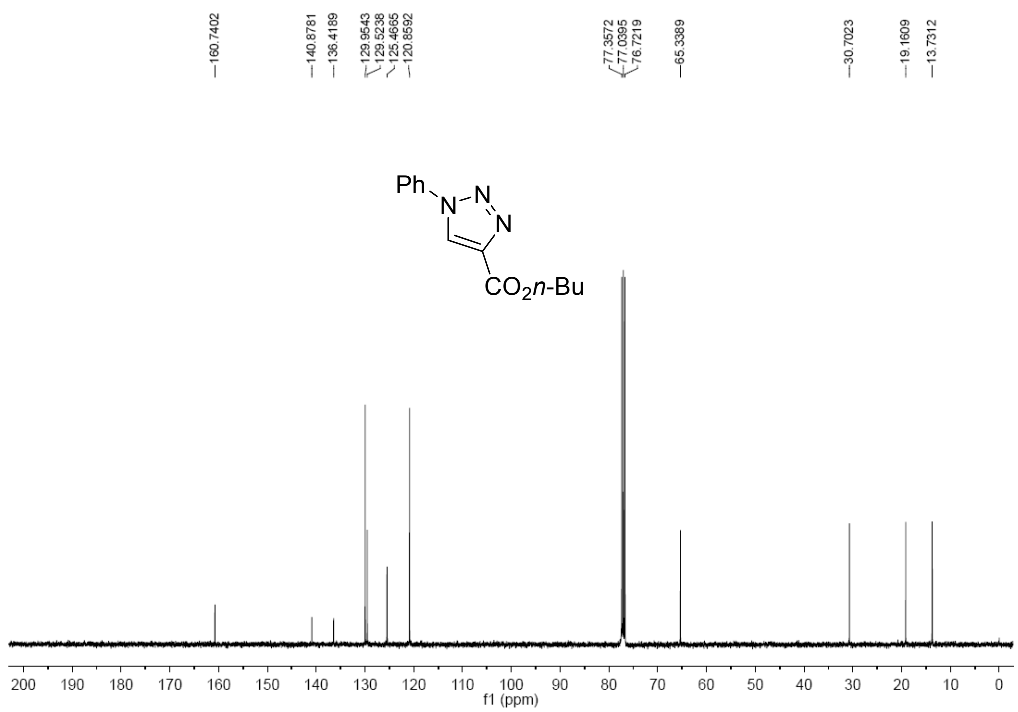
(*S*)-Methyl 1-((1-(tert-butoxycarbonyl)pyrrolidin-2-yl)methyl)-1H-1,2,3-triazole-4-carboxylate (3l)



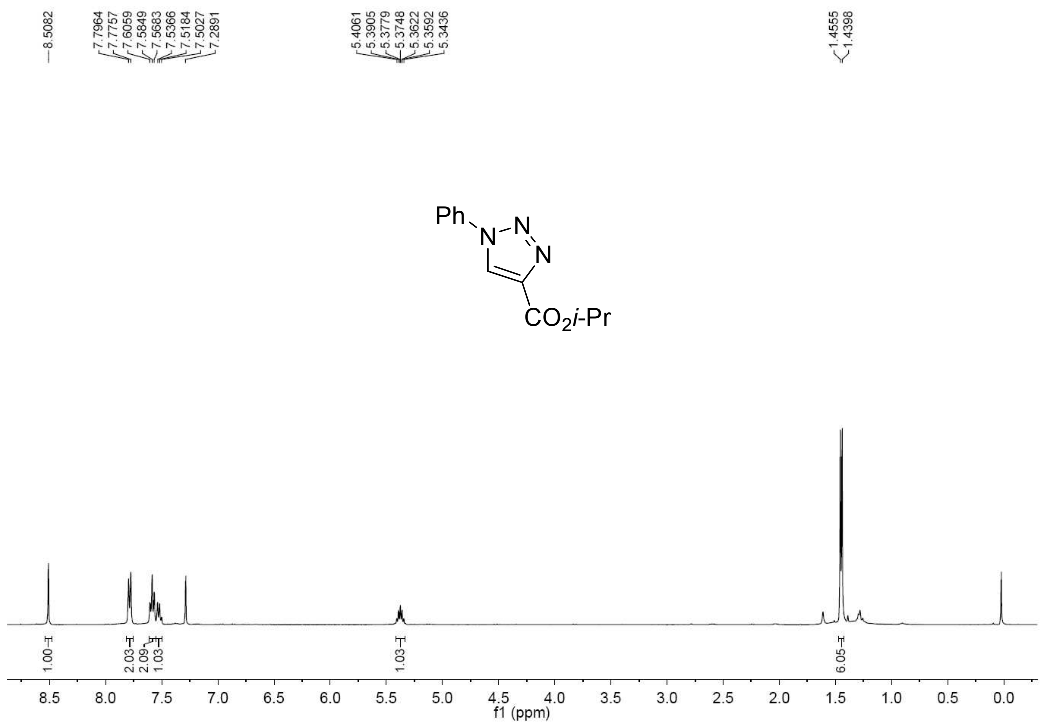


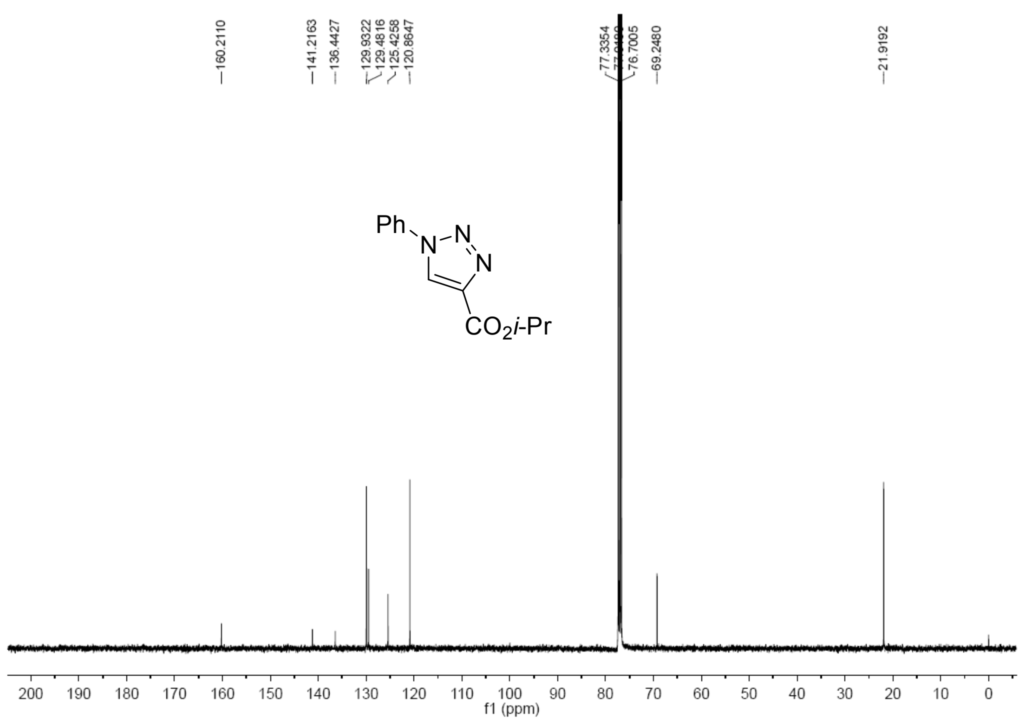
Butyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3m)



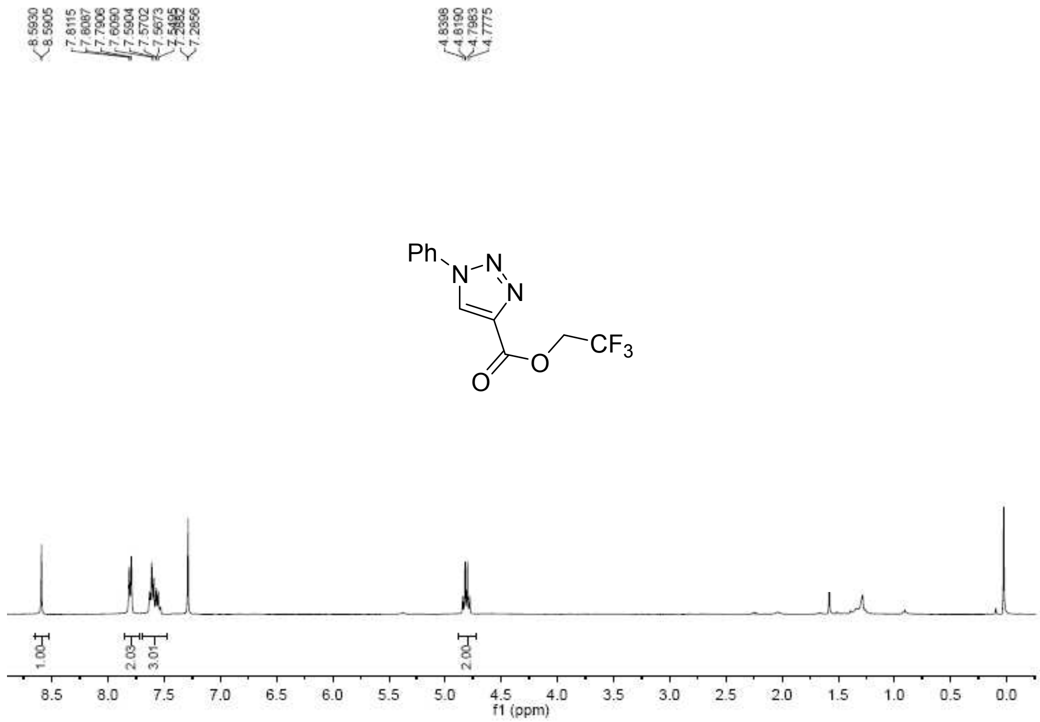


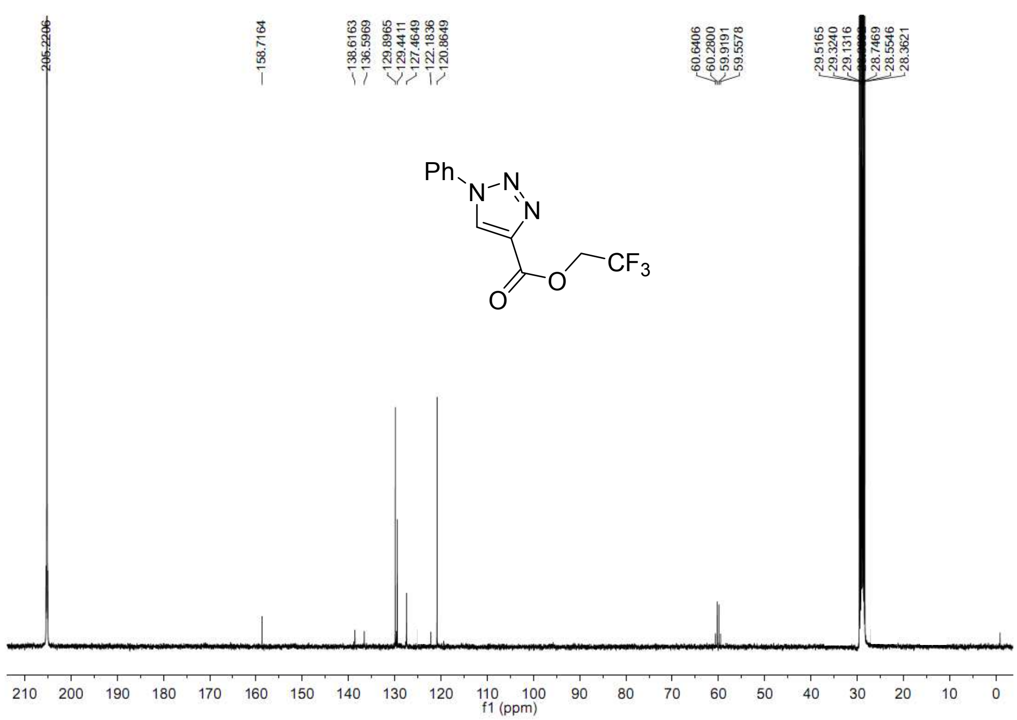
Isopropyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3n)



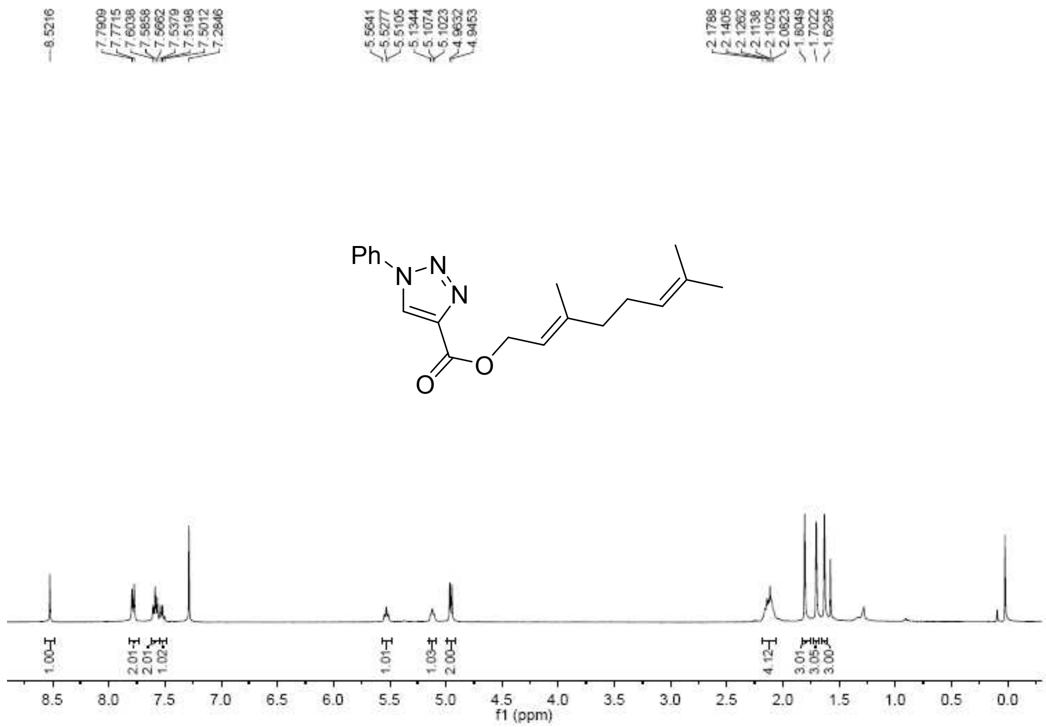


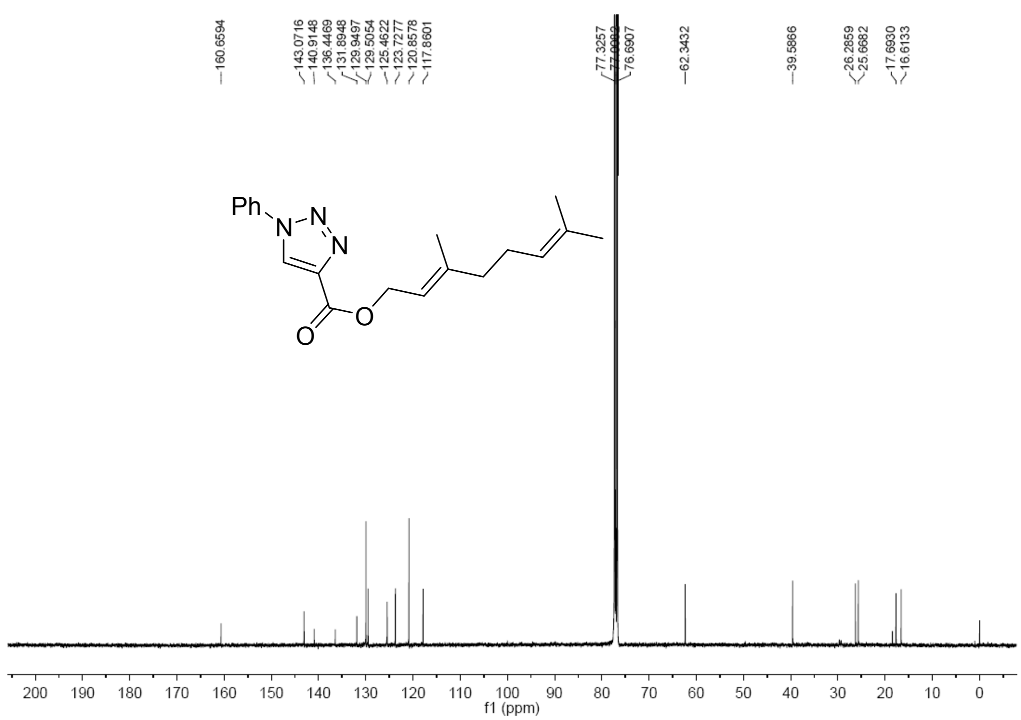
2,2,2-Trifluoroethyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3o)



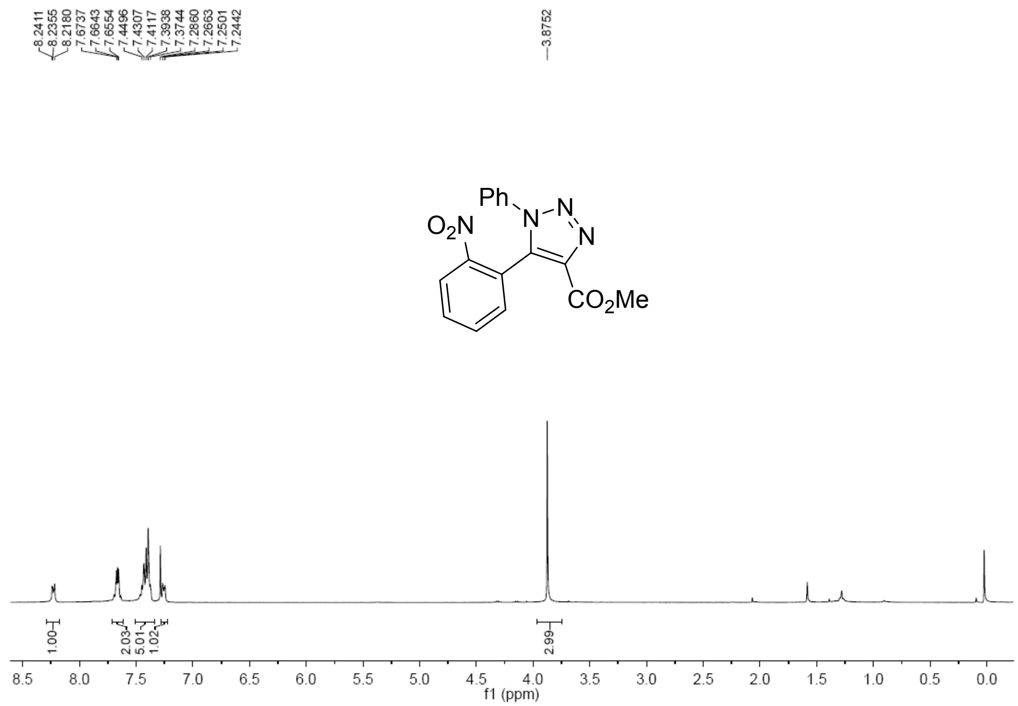


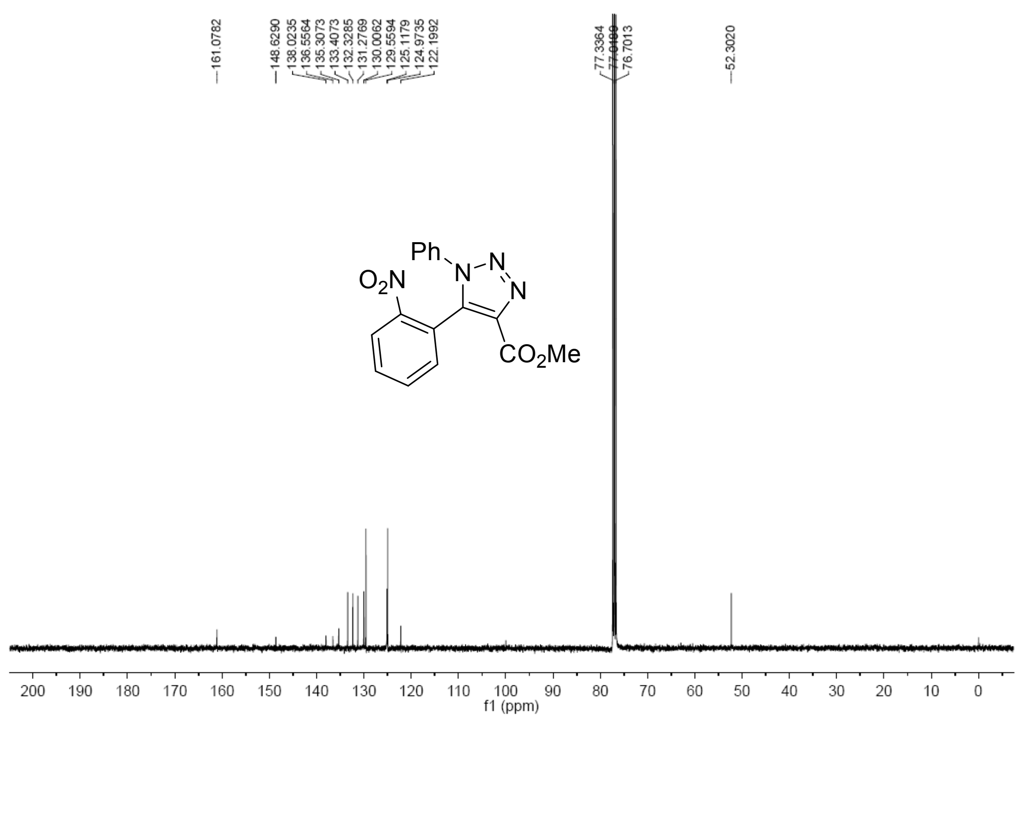
(*E*)-3,7-dimethylocta-2,6-dienyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (3p)



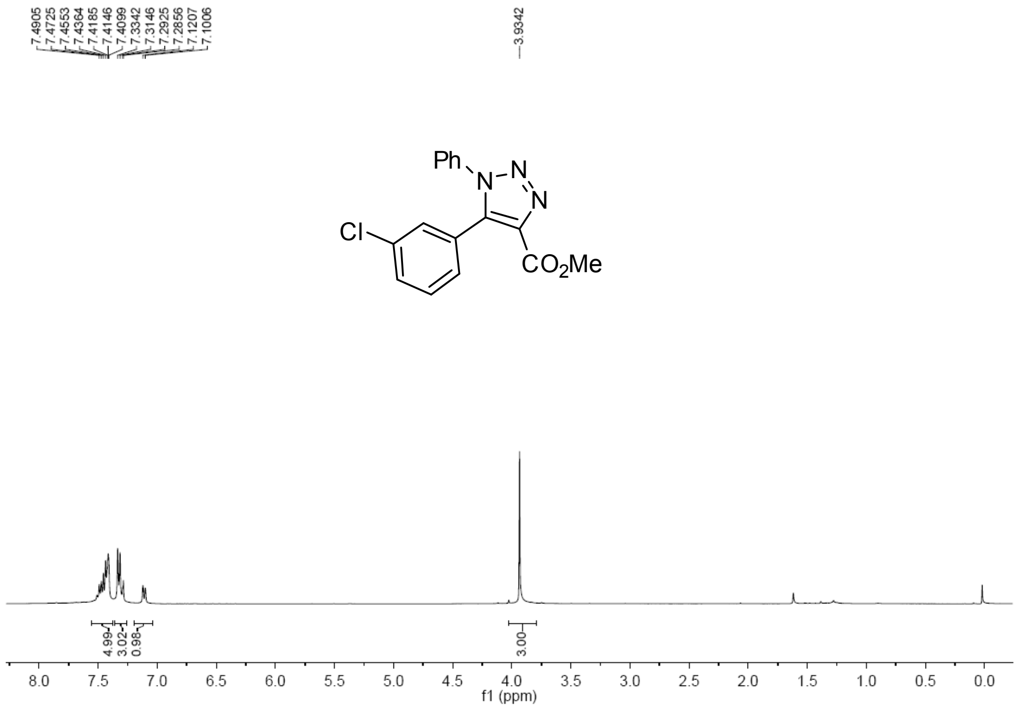


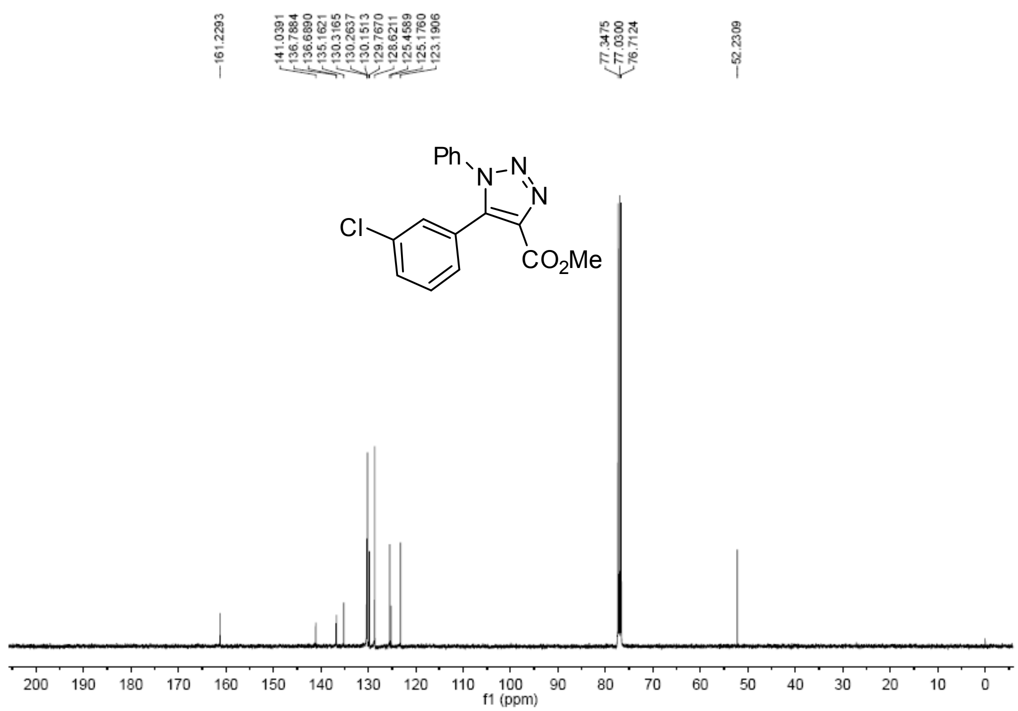
Methyl 5-(2-nitrophenyl)-1-phenyl-1H-1,2,3-triazole-4-carboxylate (3q)



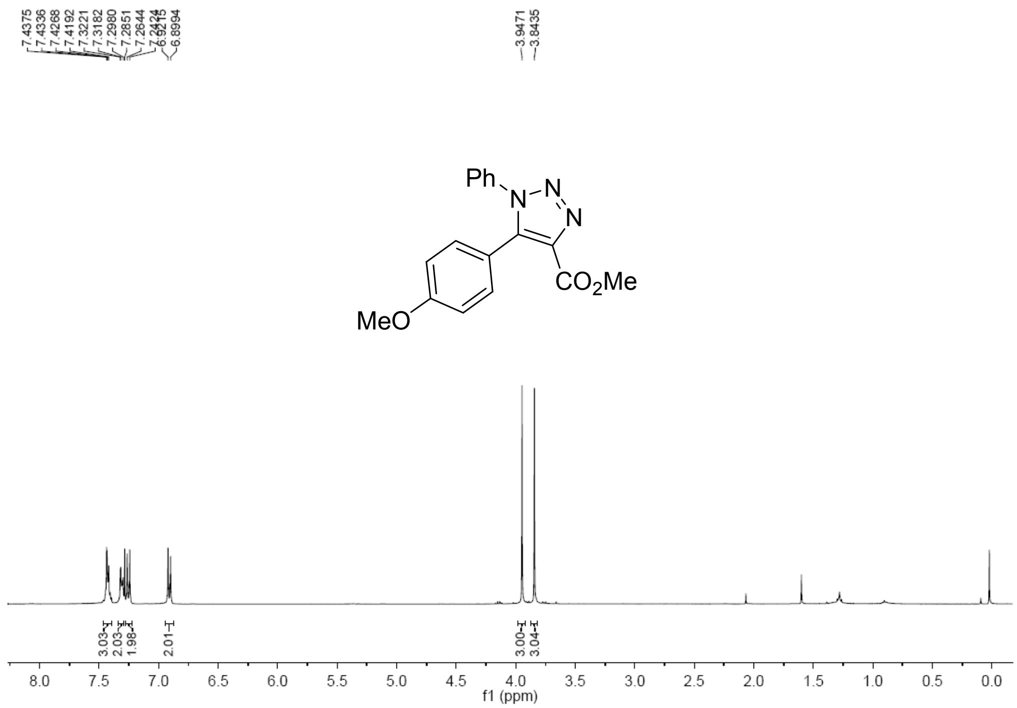


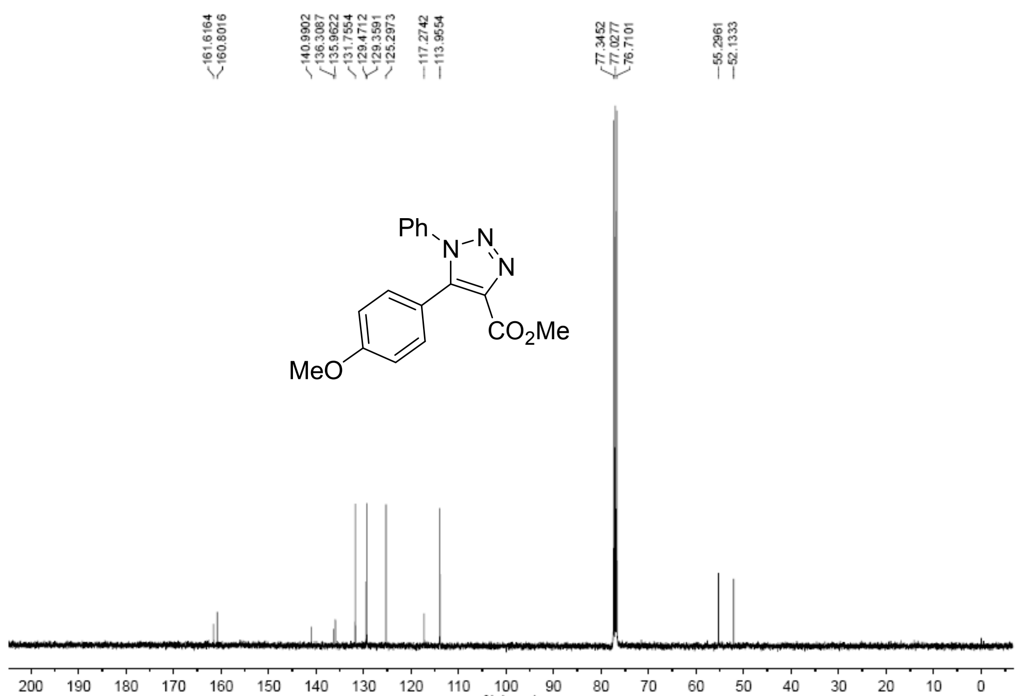
Methyl 1-(3-chlorophenyl)-5-phenyl-1H-1,2,3-triazole-4-carboxylate (3r)



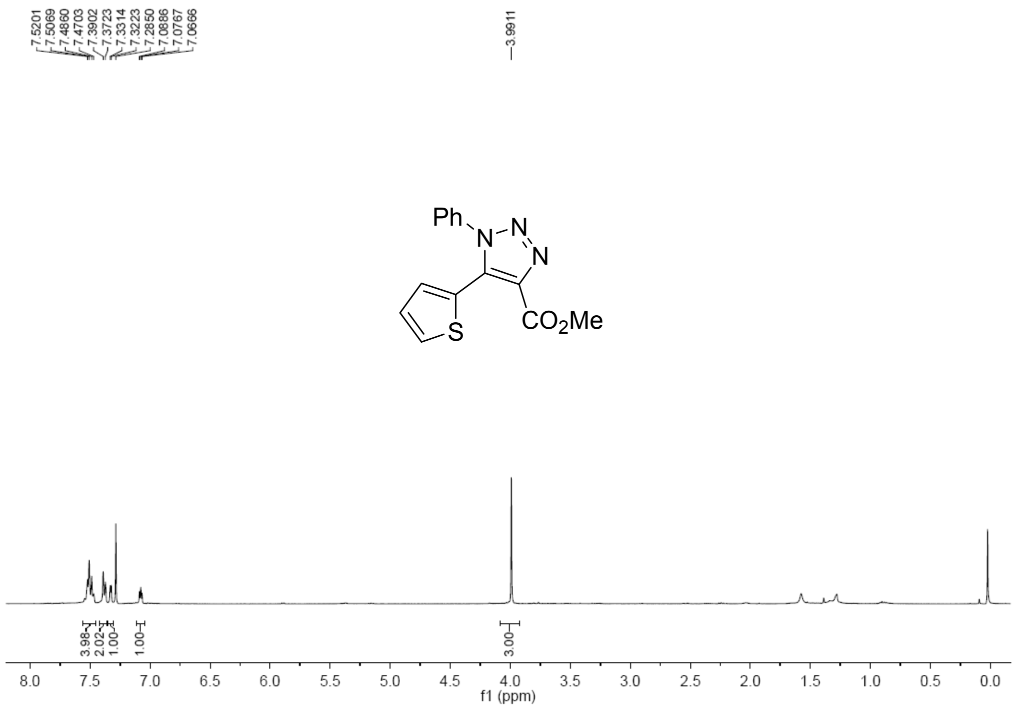


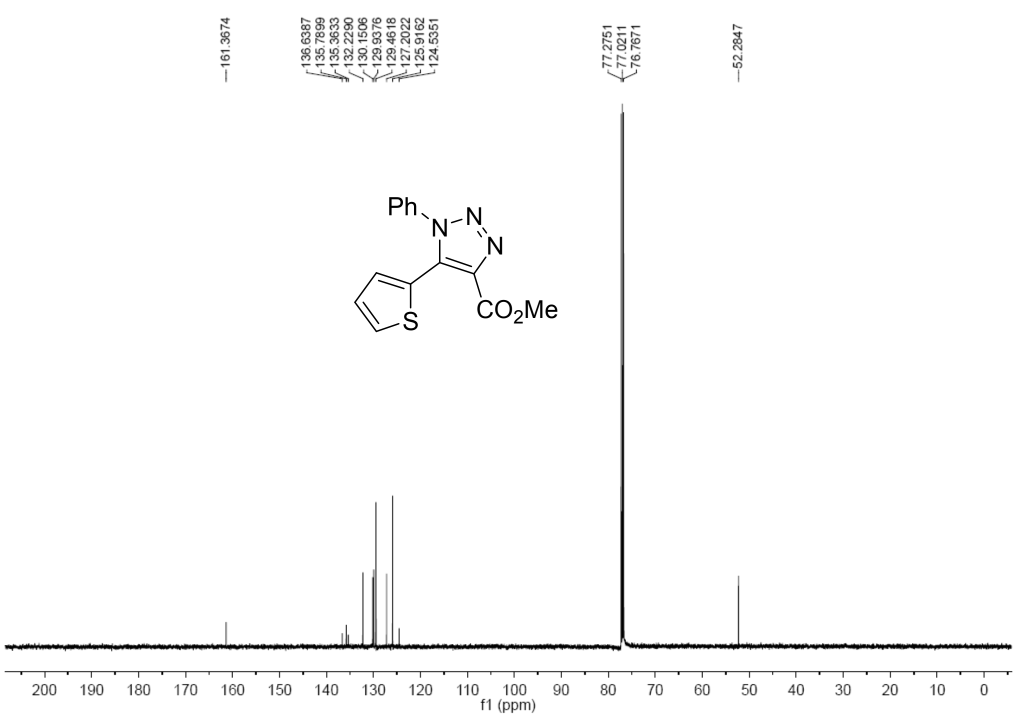
Methyl 5-(4-methoxyphenyl)-1-phenyl-1H-1,2,3-triazole-4-carboxylate (3s)



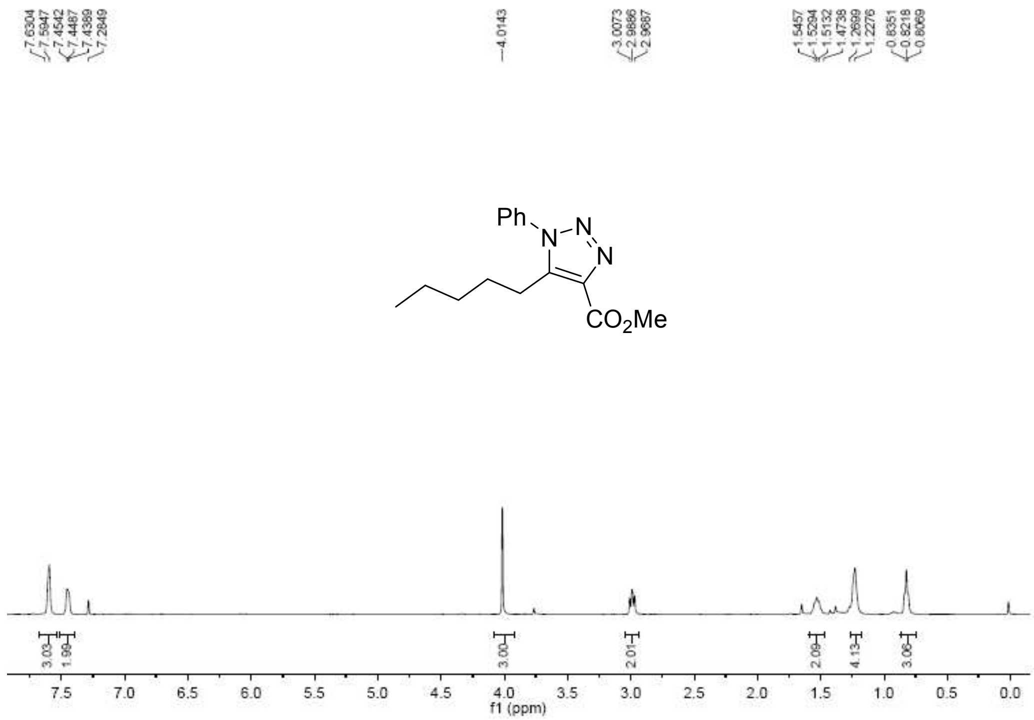


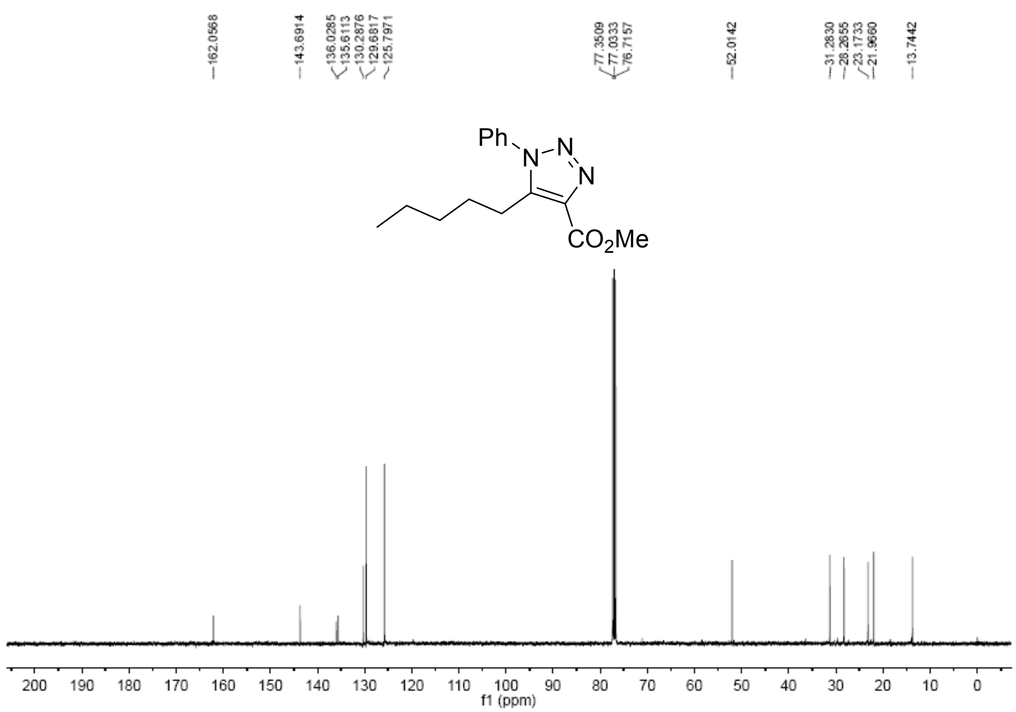
Methyl 1-phenyl-5-(thiophen-2-yl)-1H-1,2,3-triazole-4-carboxylate (3t)



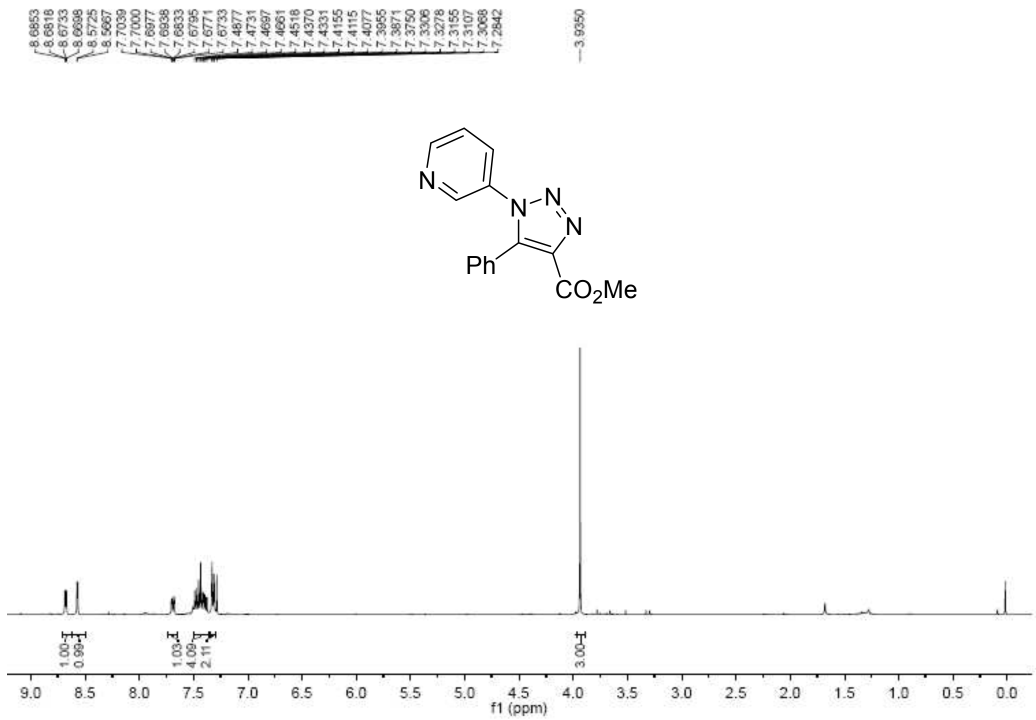


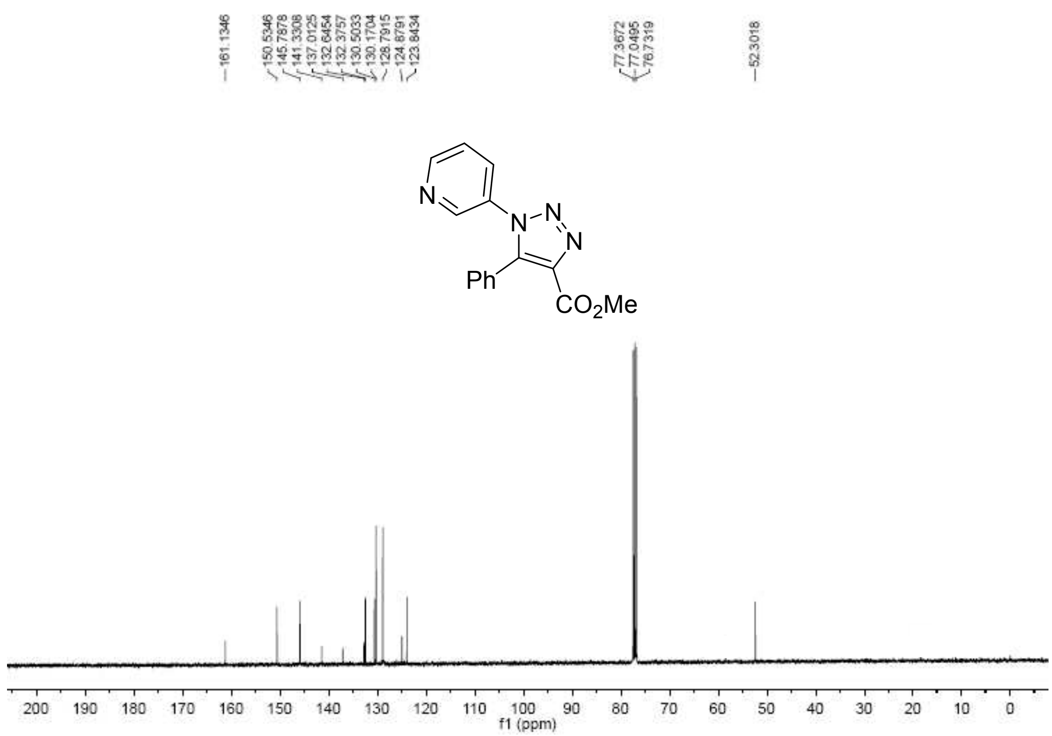
Methyl 5-pentyl-1-phenyl-1H-1,2,3-triazole-4-carboxylate (3u)



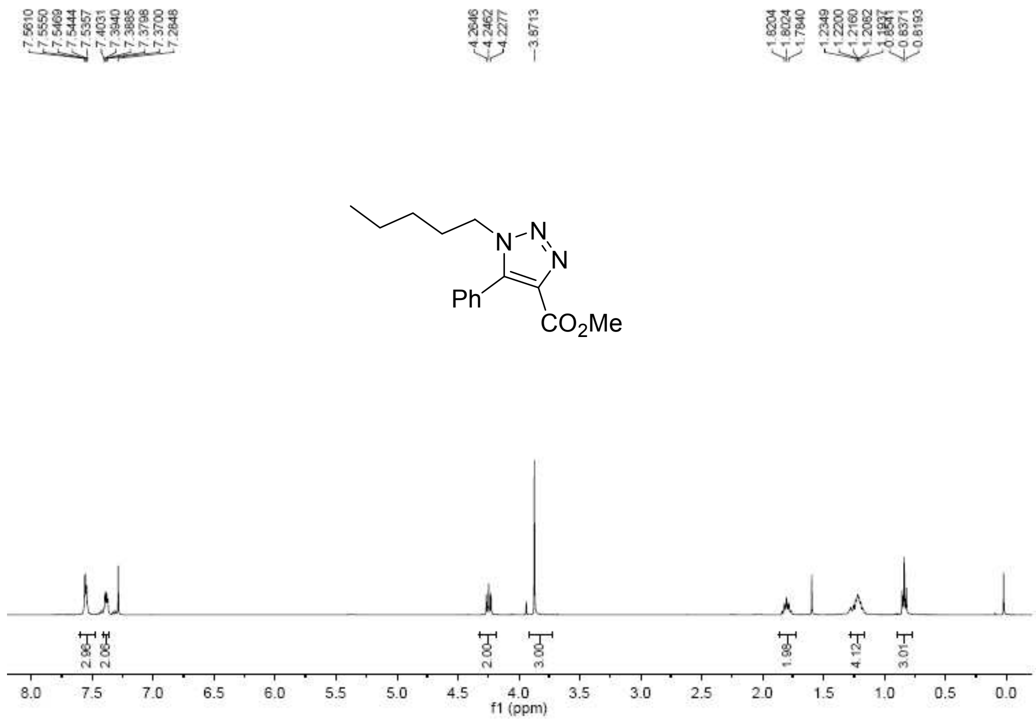


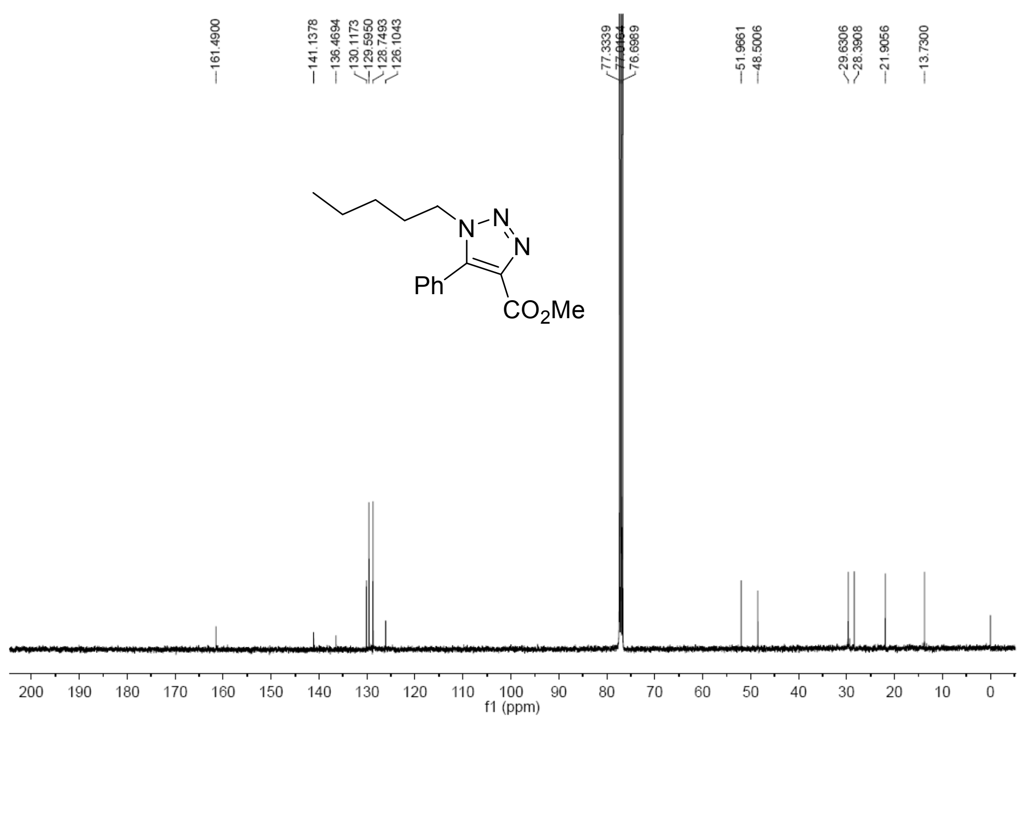
Methyl 5-phenyl-1-(pyridin-3-yl)-1H-1,2,3-triazole-4-carboxylate (3v)



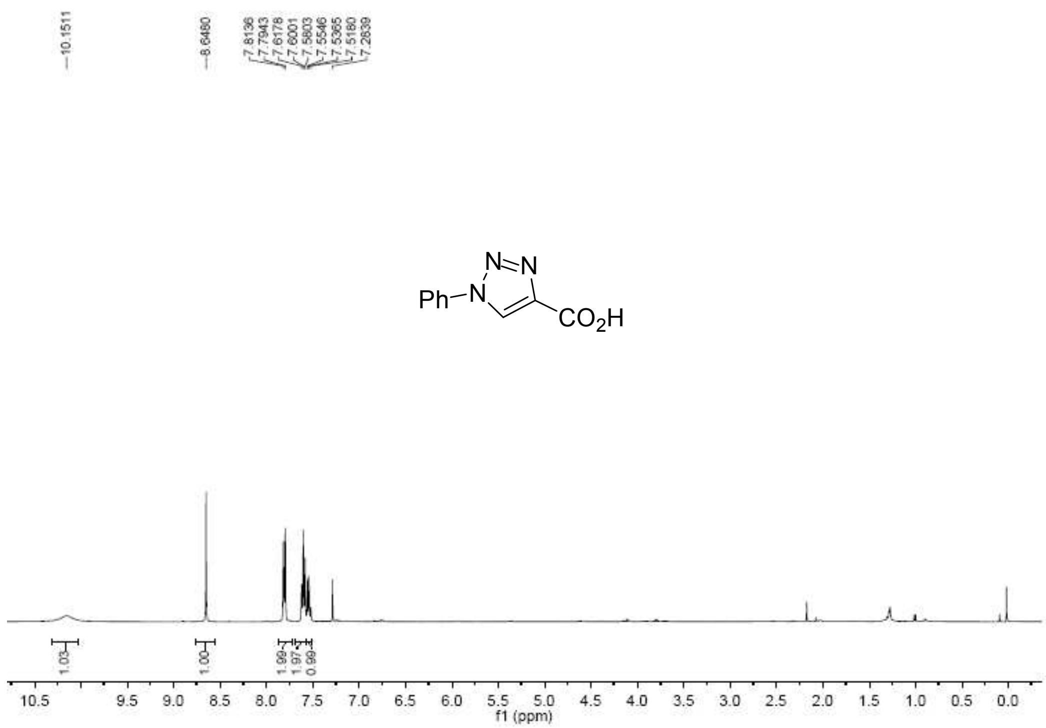


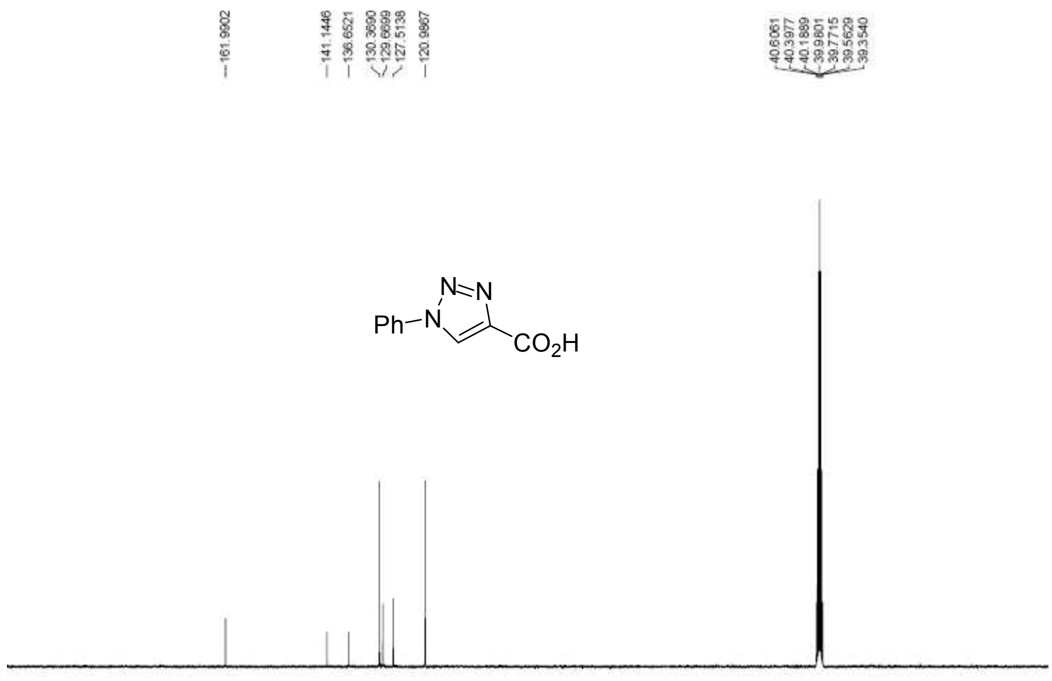
Methyl 1-pentyl-5-phenyl-1H-1,2,3-triazole-4-carboxylate (3w)



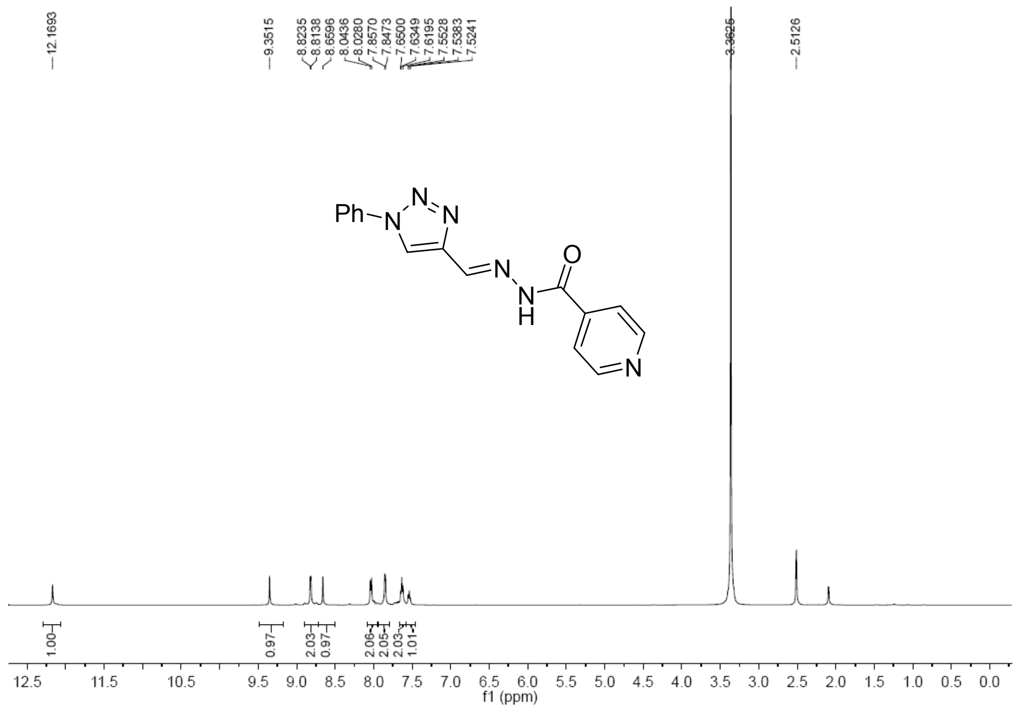


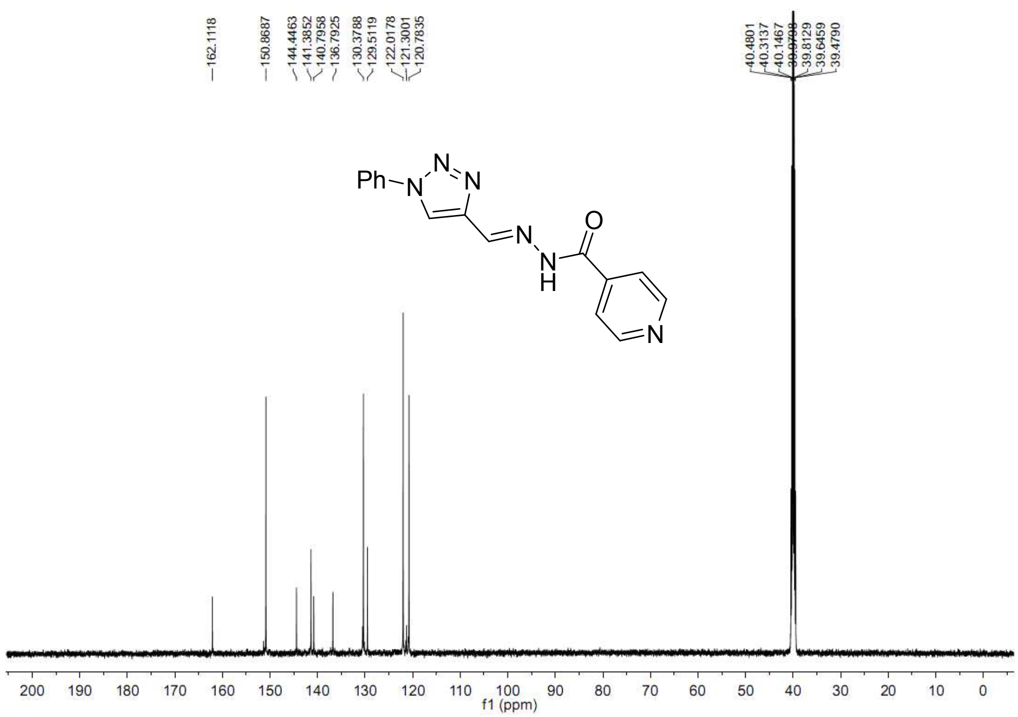
1-phenyl-1H-1,2,3-triazole-4-carboxylic acid (4)



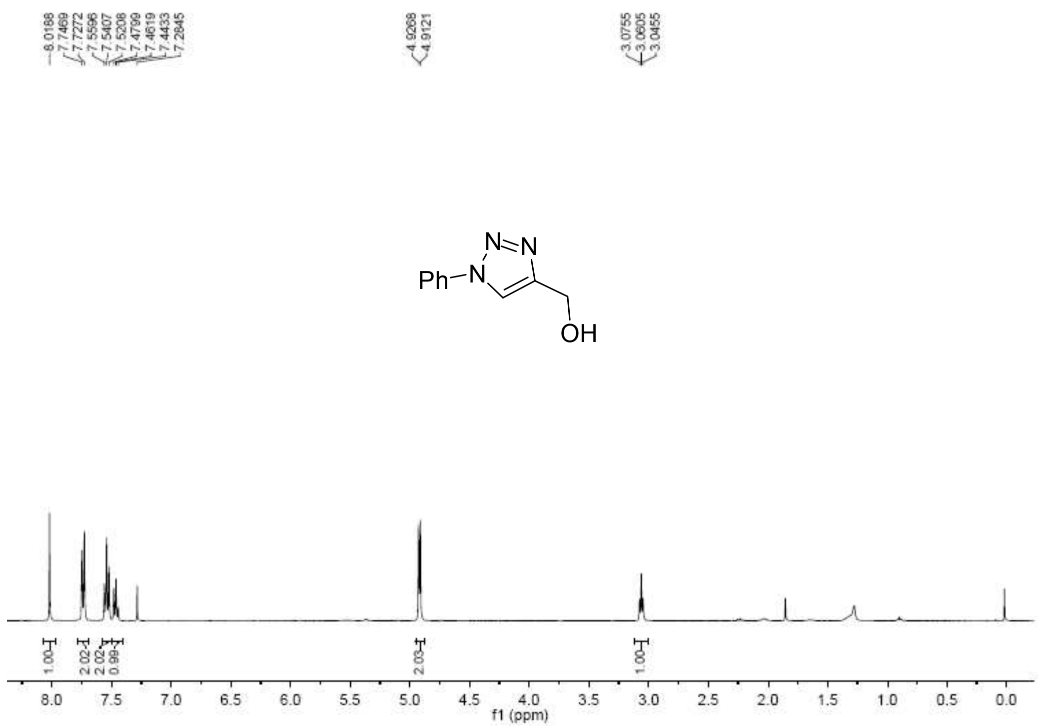


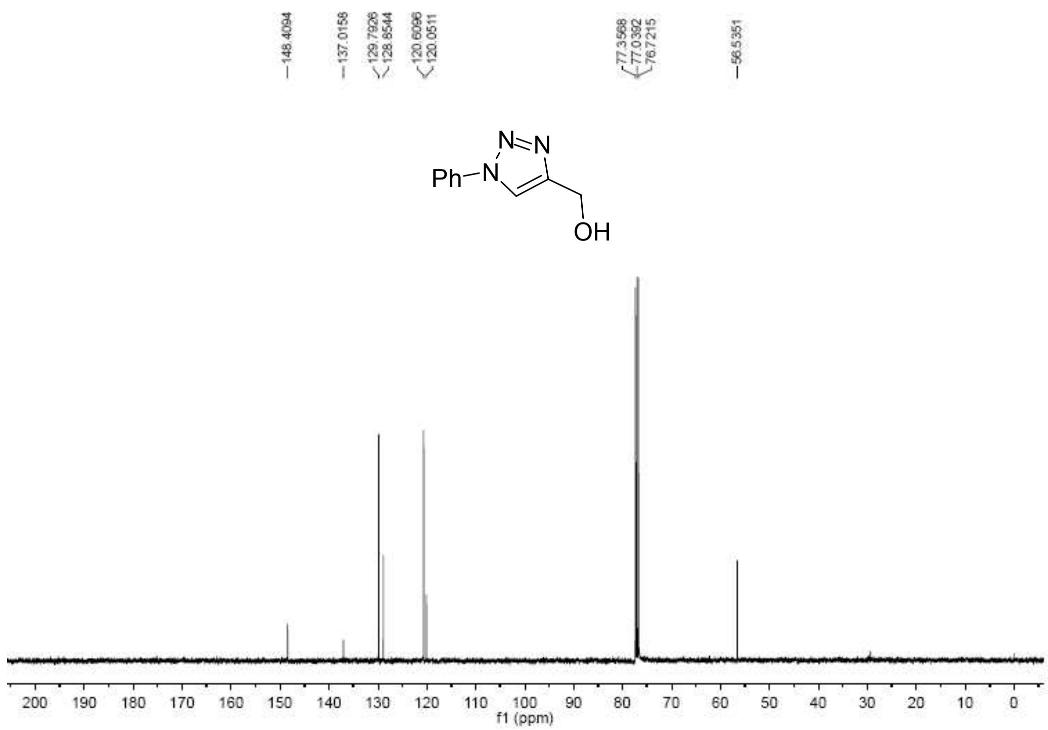
(*E*)-N'-((1-phenyl-1H-1,2,3-triazol-4-yl)methylene)isonicotinohydrazide (5)



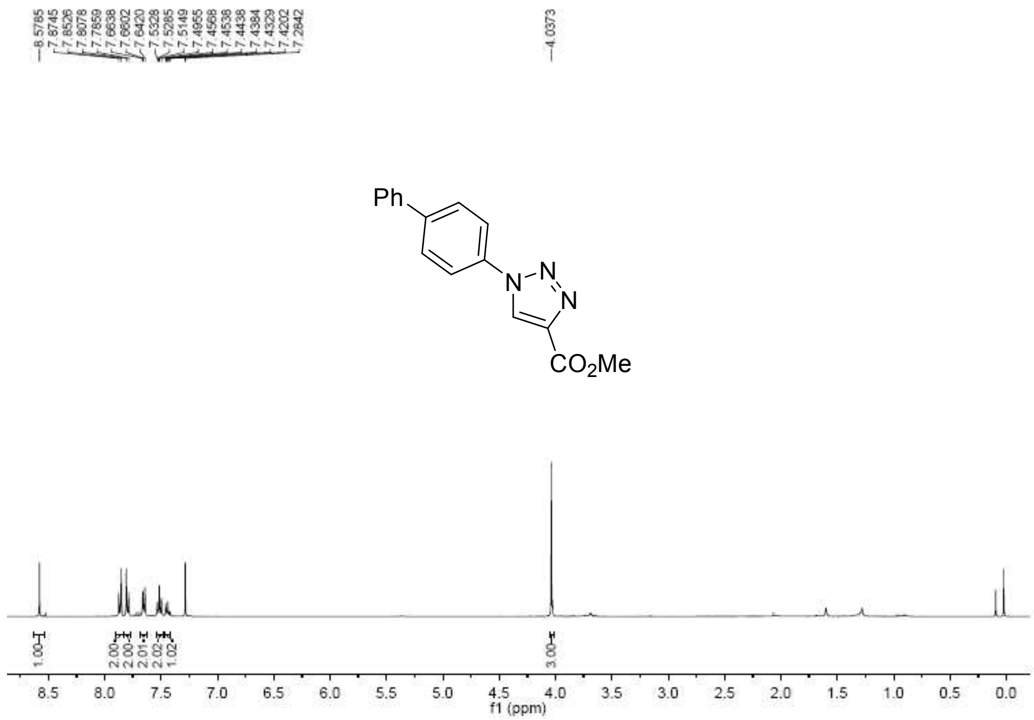


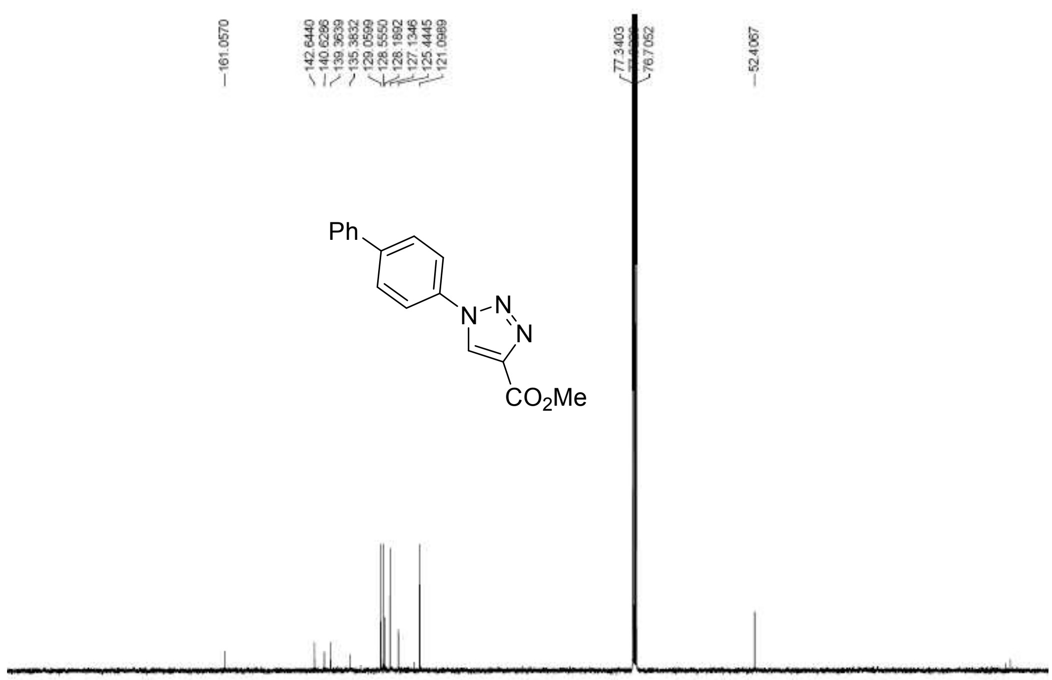
(1-phenyl-1H-1,2,3-triazol-4-yl)methanol (6)





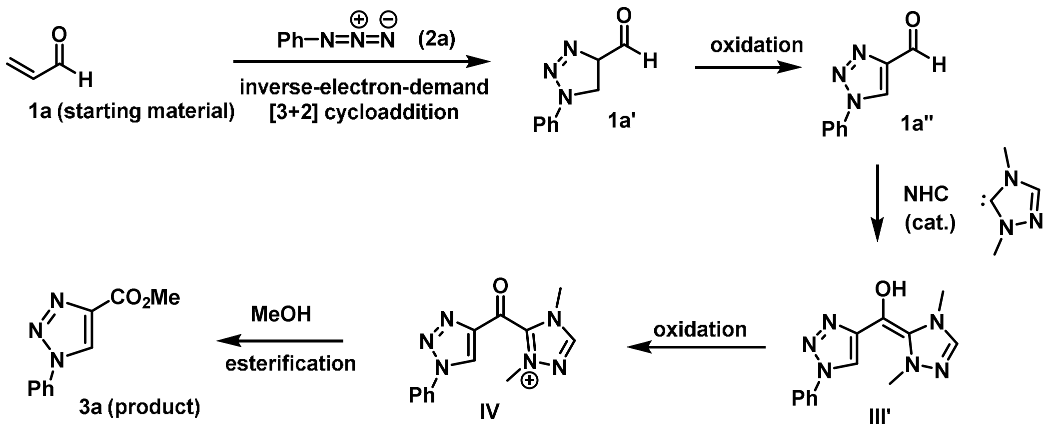
Methyl (4'- phenyl -1-phenyl-1H-1,2,3-triazole)-4-carboxylate (7)

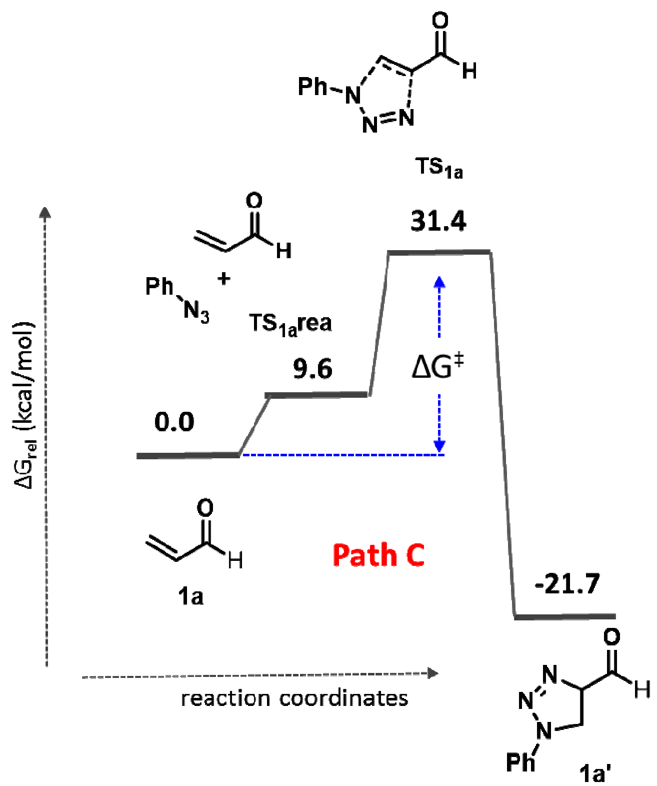




H: Additional pathways of the reaction mechanism

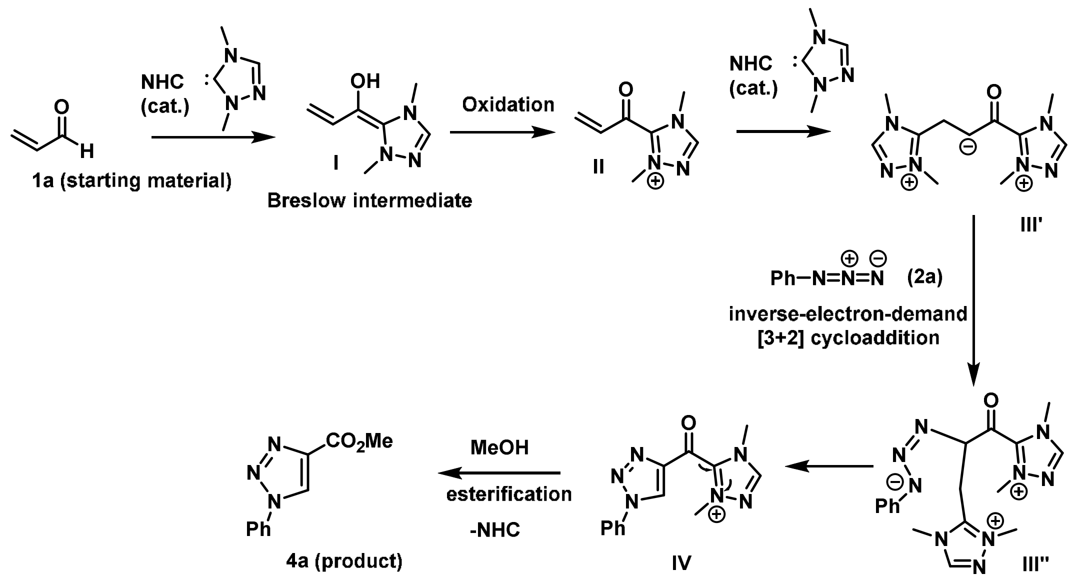
Path C: 1,3-dipolar cycloaddition without the assistance from NHC

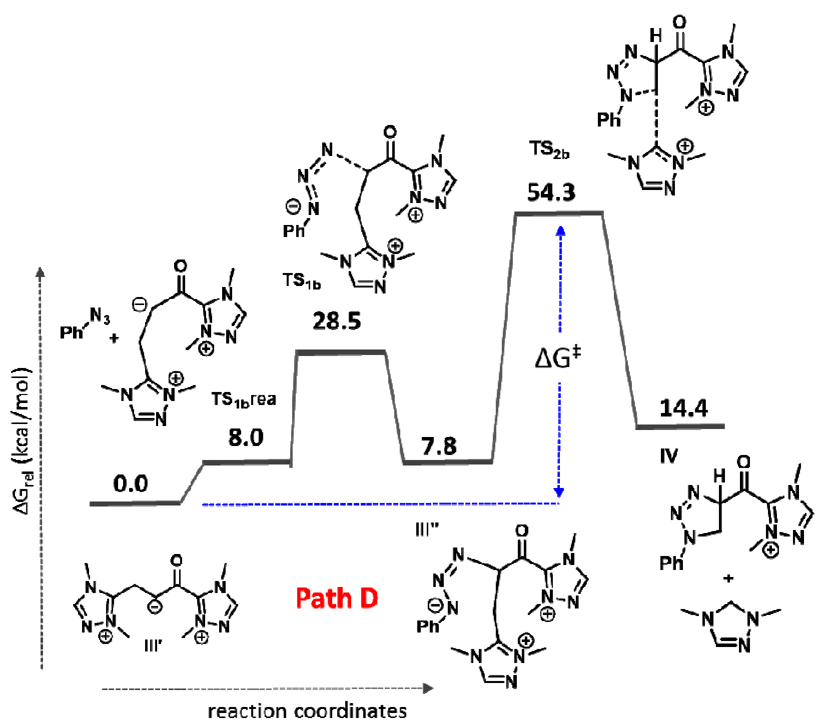




Activation energy barrier of 1,3 dipolar cycoladdition via path C.

Path D:





Activation energy barrier of 1,3 dipolar cycloaddition via path D

I: Computational Details

All the calculations were carried out by using Gaussian 09 suite of computational programs.[2] Geometry optimization of all the key stationary points were performed in the gas phase using Pople's 6-31+G** basis set at the M06-2X level of theory.[3-5] The stationary points were characterized by frequency calculations. The transition states were verified by single imaginary frequency pertaining to the desired reaction coordinate and by intrinsic reaction coordinate (IRC) calculations.[6-8] All calculations were performed at the standard temperature (298.15 K) and pressure (1 atm). Solvent effects were incorporated using the solvation model based on density (SMD).[9] Since the reaction was performed in tetrahydrofuran, a continuum solvent dielectric of ε= 7.426 was employed in our calculations. Energies were further refined by doing a single point calculation using 6-311+G** basis set. The energetics of the reaction mechanisms are discussed on the basis of SMD-M06-2X/6-311+G**//M06-2X/6-31+G** level relative Gibbs free energy (ΔG_{rel}) values. Activation free energy, $\Delta G^{\ddagger}$ is the difference in Gibbs free energy between a transition state and the corresponding lower energy reactants.

J: Optimized Cartesian Coordinates

Optimized Cartesian coordinates (Å) along with number of imaginary frequencies (N_{Img}) and energy parameters (a.u).

II

At no.	X	Y	Z
7	2.484705000	-0.139897000	-0.131979000
6	2.135507000	1.112315000	-0.019467000
7	0.778221000	1.239985000	0.065097000
6	0.281127000	-0.012028000	0.003675000
7	1.328480000	-0.824145000	-0.109446000
6	1.358172000	-2.293008000	-0.185667000
1	1.229640000	-2.703128000	0.815467000
1	0.550889000	-2.635784000	-0.830159000
1	2.330795000	-2.553614000	-0.597217000
6	0.052771000	2.507466000	0.242780000
1	-0.277979000	2.885606000	-0.725073000
1	-0.797547000	2.347737000	0.904516000
1	0.737367000	3.219336000	0.701978000
1	2.821362000	1.946893000	0.010896000
6	-1.151025000	-0.497541000	0.109807000
6	-2.224554000	0.347902000	-0.440317000
8	-1.303216000	-1.581138000	0.627101000
6	-3.500495000	0.036928000	-0.184548000
1	-4.316126000	0.623754000	-0.593029000
1	-3.744717000	-0.817532000	0.440796000
1	-1.956803000	1.192042000	-1.068263000

$N_{Img} = 0$
E_{ele} (M06-2X/6-311++G**) = -511.97324
E_{ele} (M06-2X /6-31+G**) = -511.76658
$G_{corr} = 0.13703$

TS_1rea

At no.	X	Y	Z
7	-4.218392000	0.931597000	0.388647000
6	-4.370932000	-0.350510000	0.566002000
7	-3.275879000	-1.041939000	0.130379000
6	-2.413743000	-0.117691000	-0.340770000
7	-3.006919000	1.060075000	-0.181778000
6	-2.521678000	2.407260000	-0.502950000
1	-2.529598000	2.987681000	0.418689000
1	-1.518697000	2.330327000	-0.911233000
1	-3.202107000	2.837643000	-1.237311000
6	-3.133954000	-2.505411000	0.134860000
1	-2.569010000	-2.817121000	-0.742475000
1	-2.631348000	-2.827848000	1.047342000
1	-4.132988000	-2.937291000	0.089759000
1	-5.247631000	-0.818140000	0.990833000
6	-1.055094000	-0.344739000	-0.977411000
6	-0.192358000	-1.381721000	-0.386050000
8	-0.761444000	0.363908000	-1.914317000
6	0.956692000	-1.706733000	-0.992137000
7	1.734444000	0.151298000	1.811988000
1	1.232776000	-1.243025000	-1.935537000
7	-0.256460000	1.337842000	1.389941000
7	0.727428000	0.793985000	1.549708000
6	2.794400000	0.177389000	0.852435000
6	2.729012000	0.903628000	-0.338954000
6	3.913457000	-0.594238000	1.162443000
6	3.801966000	0.848807000	-1.226101000
6	4.975293000	-0.643017000	0.264581000
6	4.923443000	0.074849000	-0.930804000
1	1.857053000	1.508752000	-0.577334000
1	3.937880000	-1.138898000	2.100382000
1	3.759957000	1.418188000	-2.148948000
1	5.849496000	-1.239150000	0.504270000
1	5.756433000	0.038362000	-1.624348000
1	1.641179000	-2.428708000	-0.558910000
1	-0.480436000	-1.819293000	0.566304000

$N_{Img} = 0$
E_{ele} (M06-2X/6-311++G**) = -907.76513

E_{ele} (M06-2X /6-31+G**) = -907.47074
G_{corr} = 0.22937

TS_1

At no.	X	Y	Z
7	-4.479743000	1.213469000	0.189355000
6	-4.790899000	-0.003004000	-0.157718000
7	-3.671192000	-0.746181000	-0.411937000
6	-2.619335000	0.071964000	-0.204891000
7	-3.132869000	1.244857000	0.151057000
6	-2.426045000	2.491139000	0.466731000
1	-3.137203000	3.117440000	1.001037000
1	-1.560834000	2.259401000	1.084952000
1	-2.098438000	2.960053000	-0.460078000
6	-3.657894000	-2.142838000	-0.861668000
1	-3.552331000	-2.809393000	-0.004900000
1	-4.601601000	-2.339646000	-1.368990000
1	-2.830181000	-2.285701000	-1.554748000
1	-5.797517000	-0.385231000	-0.244502000
6	-1.140442000	-0.178049000	-0.400499000
6	-0.620277000	-1.431136000	-0.023187000
8	-0.494281000	0.784172000	-0.842858000
6	0.768980000	-1.665737000	-0.319261000
7	1.769154000	-0.859740000	0.739780000
1	1.105427000	-1.191336000	-1.243475000
7	0.090057000	-0.012591000	2.094844000
7	1.086827000	-0.222998000	1.599879000
6	2.991012000	-0.256633000	0.240121000
6	2.910605000	0.916787000	-0.506367000
6	4.190427000	-0.919000000	0.469242000
6	4.089419000	1.454735000	-1.015904000
6	5.359879000	-0.370763000	-0.054044000
6	5.307785000	0.812591000	-0.789347000
1	1.940921000	1.373769000	-0.690923000
1	4.203330000	-1.834537000	1.051443000
1	4.055952000	2.370344000	-1.596414000
1	6.309695000	-0.865886000	0.116060000
1	6.222054000	1.235253000	-1.192583000
1	1.108286000	-2.694226000	-0.219777000
1	-1.228233000	-2.181711000	0.465680000

N_{Img} = 1
E_{ele} (M06-2X/6-311++G**) = -907.75039
E_{ele} (M06-2X /6-31+G**) = -907.45235
G_{corr} = 0.23079

III

At no.	X	Y	Z
7	-4.101175000	-1.709246000	0.261141000
6	-4.780622000	-0.631365000	-0.011625000
7	-3.963276000	0.461955000	-0.066352000
6	-2.718757000	0.010003000	0.171429000
7	-2.822232000	-1.296520000	0.373455000
6	-1.790115000	-2.282999000	0.718320000
1	-1.426367000	-2.746063000	-0.197860000
1	-0.972928000	-1.777549000	1.229468000
1	-2.265624000	-3.008959000	1.375445000
6	-4.360904000	1.858210000	-0.296692000
1	-4.119703000	2.451959000	0.584690000
1	-3.844641000	2.245319000	-1.175962000
1	-5.434854000	1.873314000	-0.474614000
1	-5.848589000	-0.593959000	-0.170908000
6	-1.516685000	0.945127000	0.282053000
6	-0.466810000	0.858052000	-0.807127000
8	-1.521476000	1.733611000	1.189388000
6	0.904979000	1.400745000	-0.403546000
7	1.666408000	0.148699000	-0.430695000
1	0.905159000	1.847631000	0.595285000
7	-0.250347000	-0.577749000	-1.119800000
7	0.943139000	-0.870718000	-0.859565000
6	3.046632000	0.020570000	-0.142230000
6	3.690435000	-1.211265000	-0.294201000
6	3.749600000	1.143661000	0.294651000
6	5.045334000	-1.304318000	-0.000536000
6	5.108779000	1.029876000	0.582964000
6	5.761352000	-0.189754000	0.438620000
1	3.136998000	-2.075659000	-0.640607000
1	3.256235000	2.102573000	0.413171000
1	5.545718000	-2.259543000	-0.120372000
1	5.653388000	1.905293000	0.920689000
1	6.818885000	-0.273605000	0.663194000
1	1.312141000	2.115470000	-1.123497000
1	-0.890932000	1.350690000	-1.693013000

N_{Img} = 0

E_{ele} (M06-2X/6-311++G**) = -907.81895

E_{ele} (M06-2X /6-31+G**) = -907.50371

G_{corr} = 0.23494

VI

At no.	X	Y	Z
7	-3.136464000	0.620091000	-0.433510000
6	-2.273864000	1.592750000	-0.439853000
7	-1.067066000	1.203677000	0.066572000
6	-1.178301000	-0.106431000	0.386135000
7	-2.441784000	-0.427797000	0.089541000
6	-3.078682000	-1.729101000	0.229376000
1	-3.992856000	-1.697171000	-0.360315000
1	-2.411305000	-2.500009000	-0.158213000
1	-3.316541000	-1.929130000	1.275448000
6	0.179690000	1.962318000	0.040263000
1	0.774879000	1.718527000	0.919500000
1	0.750397000	1.663339000	-0.843130000
1	-0.068831000	3.023378000	0.020917000
1	-2.475151000	2.591475000	-0.797217000
6	-0.076964000	-1.022992000	0.799176000
1	0.492377000	-0.556071000	1.608688000
1	-0.525449000	-1.942761000	1.200582000
6	0.785671000	-1.200871000	-0.410141000
1	0.431097000	-1.808346000	-1.232826000
6	2.084730000	-0.685758000	-0.497043000
8	2.465208000	0.040668000	0.654319000
8	2.894521000	-0.780115000	-1.421951000
6	3.810072000	0.485206000	0.642070000
1	3.995912000	1.166284000	-0.194210000
1	3.968317000	0.999812000	1.592475000
1	4.502407000	-0.356275000	0.551248000

N_{Img} = 0
E_{ele} (M06-2X/6-311++G**) = -627.27083
E_{ele} (M06-2X /6-31+G**) = -627.06931
G_{corr} = 0.17520

TS_2rea

At no.	X	Y	Z
7	-4.091739000	-0.535796000	0.503466000
6	-3.323962000	-1.477245000	0.971316000
7	-2.128501000	-1.522241000	0.315013000
6	-2.146271000	-0.526329000	-0.589966000
7	-3.343842000	0.042181000	-0.467999000
6	-3.828679000	1.196883000	-1.206727000
1	-4.665399000	1.608416000	-0.645423000
1	-3.004948000	1.913484000	-1.272475000
1	-4.157847000	0.894606000	-2.203187000
6	-0.947949000	-2.302675000	0.680842000

1	-0.176301000	-1.591614000	0.993430000
1	-1.224448000	-2.962964000	1.503010000
1	-0.611940000	-2.895854000	-0.170254000
1	-3.586417000	-2.141093000	1.780501000
6	-1.033220000	-0.088319000	-1.485231000
1	-0.280512000	-0.892783000	-1.466765000
1	-1.426272000	-0.045351000	-2.508501000
6	-0.522806000	1.260837000	-1.058804000
1	-0.375535000	2.047595000	-1.785188000
6	-0.273655000	1.444671000	0.294518000
8	0.193064000	2.699510000	0.631977000
8	-0.437877000	0.586720000	1.198955000
6	0.472912000	2.883350000	2.009247000
1	1.226607000	2.168826000	2.352997000
1	0.850480000	3.903279000	2.101723000
1	-0.429838000	2.761031000	2.615758000
7	2.658579000	2.659611000	-1.373632000
7	2.675145000	1.865532000	-0.575277000
7	2.734312000	1.084199000	0.384376000
6	2.561424000	-0.285543000	0.084844000
6	2.646139000	-1.162966000	1.170991000
6	2.344376000	-0.786237000	-1.202835000
6	2.537846000	-2.533372000	0.964636000
6	2.230615000	-2.162018000	-1.395638000
6	2.332741000	-3.043142000	-0.319578000
1	2.795567000	-0.746900000	2.161661000
1	2.252661000	-0.104239000	-2.043955000
1	2.616276000	-3.208256000	1.811889000
1	2.072189000	-2.545532000	-2.399697000
1	2.259443000	-4.114257000	-0.480283000

N_{Img} = 0

E_{ele} (M06-2X/6-311++G**) = -1023.06506

E_{ele} (M06-2X /6-31+G**) = -1022.78724

G_{corr} = 0.27031

TS$_2$

At no.	X	Y	Z
7	-3.884410000	-2.014364000	0.289049000
6	-2.791704000	-2.501476000	0.803174000
7	-1.679872000	-1.950162000	0.236368000
6	-2.113352000	-1.043830000	-0.656546000
7	-3.441239000	-1.110714000	-0.618129000
6	-4.371257000	-0.290638000	-1.378971000
1	-5.350919000	-0.412884000	-0.921709000

1	-4.042611000	0.749361000	-1.317539000
1	-4.399086000	-0.619842000	-2.419682000
6	-0.299994000	-2.078445000	0.707175000
1	-0.043039000	-1.148224000	1.220565000
1	-0.253583000	-2.940631000	1.372533000
1	0.368717000	-2.224871000	-0.141527000
1	-2.756293000	-3.247911000	1.581853000
6	-1.294504000	-0.106334000	-1.476911000
1	-0.271856000	-0.500754000	-1.494252000
1	-1.670404000	-0.146192000	-2.505454000
6	-1.368540000	1.316797000	-0.958086000
1	-1.768204000	2.074550000	-1.618349000
6	-1.520004000	1.516619000	0.440403000
8	-1.735068000	2.821134000	0.772844000
8	-1.462464000	0.644616000	1.322436000
6	-1.785928000	3.091365000	2.166566000
1	-0.847025000	2.809727000	2.650758000
1	-1.948499000	4.165678000	2.253402000
1	-2.602928000	2.542668000	2.643077000
7	0.628256000	2.049706000	-1.398201000
7	1.446558000	1.346734000	-0.963726000
7	1.664569000	0.296563000	-0.255436000
6	3.029585000	-0.024133000	-0.124169000
6	3.338363000	-1.080000000	0.745328000
6	4.077812000	0.616681000	-0.803367000
6	4.655170000	-1.486489000	0.929564000
6	5.392791000	0.205560000	-0.609330000
6	5.694897000	-0.847909000	0.253262000
1	2.529333000	-1.562453000	1.286368000
1	3.854586000	1.436545000	-1.479236000
1	4.871350000	-2.303652000	1.611760000
1	6.190941000	0.715442000	-1.141318000
1	6.722734000	-1.163506000	0.398487000

N_{Img} = 1
E_{ele} (M06-2X/6-311++G**) = -1023.04554
E_{ele} (M06-2X /6-31+G**) = -1022.76343
G_{corr} = 0.34483

VII

At no.	X	Y	Z
7	-4.758726000	-1.064851000	0.116295000
6	-4.695761000	-0.132060000	1.022026000
7	-3.400211000	0.219564000	1.288010000
6	-2.623911000	-0.552378000	0.502387000

7	-3.464351000	-1.309276000	-0.200448000
6	-3.109236000	-2.285393000	-1.230370000
1	-3.168593000	-3.290753000	-0.810318000
1	-3.825177000	-2.177432000	-2.043892000
1	-2.096425000	-2.073358000	-1.588348000
6	-2.919578000	1.241949000	2.223706000
1	-3.757619000	1.894952000	2.464902000
1	-2.551330000	0.761192000	3.131506000
1	-2.120478000	1.809405000	1.739645000
1	-5.549010000	0.320426000	1.504290000
6	-1.159473000	-0.508980000	0.349847000
1	-0.704727000	0.028615000	1.181099000
1	-0.756738000	-1.525147000	0.344379000
6	-0.791898000	0.166184000	-1.017891000
1	-1.709798000	0.356305000	-1.593556000
6	-0.211885000	1.544873000	-0.713687000
8	0.495009000	2.031377000	-1.724150000
8	-0.485028000	2.188326000	0.287239000
6	1.164801000	3.265248000	-1.465502000
1	1.876195000	3.127556000	-0.647100000
1	1.687734000	3.513369000	-2.387105000
1	0.447248000	4.045270000	-1.201351000
7	0.008051000	-0.721754000	-1.852345000
7	1.194505000	-0.924821000	-1.386920000
7	1.501669000	-0.306676000	-0.288803000
6	2.811187000	-0.527922000	0.157523000
6	3.204191000	0.182028000	1.303928000
6	3.740260000	-1.398527000	-0.442047000
6	4.479363000	0.030036000	1.839243000
6	5.012771000	-1.543086000	0.100860000
6	5.396208000	-0.835515000	1.242598000
1	2.483466000	0.859669000	1.755254000
1	3.447073000	-1.947770000	-1.329287000
1	4.759605000	0.592719000	2.725715000
1	5.718028000	-2.220098000	-0.374376000
1	6.391898000	-0.956582000	1.657569000

N_{Img} = 0
E_{ele} (M06-2X/6-311++G**) = -1023.10309
E_{ele} (M06-2X /6-31+G**) = -1022.79873
G_{corr} = 0.27561

1a

At no. X Y Z

6	-1.756690000	0.144651000	0.000101000
1	-1.834202000	1.230037000	0.000042000
1	-2.684924000	-0.416595000	0.000347000
6	-0.564022000	-0.454537000	-0.000107000
1	-0.446537000	-1.534740000	-0.000055000
6	0.675776000	0.350845000	-0.000433000
8	1.788899000	-0.121863000	0.000222000
1	0.524091000	1.450448000	0.000521000

N_{Img} = 0
E_{ele} (M06-2X/6-311++G**) = -191.89192
E_{ele} (M06-2X /6-31+G**) = -191.83317
G_{corr} = 0.03571

TS$_{1a}$rea

At no.	X	Y	Z
6	-3.008031000	1.025825000	0.029164000
6	-2.785574000	0.188940000	-1.178175000
8	-2.133590000	1.660903000	0.580117000
6	-1.604583000	0.185691000	-1.802637000
7	0.091471000	-1.712619000	0.069498000
1	-0.791204000	0.809546000	-1.437454000
7	-1.824724000	-1.467052000	1.425913000
7	-0.885071000	-1.529756000	0.802506000
6	1.105603000	-0.713358000	0.097822000
6	0.963602000	0.514403000	0.749992000
6	2.276259000	-1.016739000	-0.599666000
6	2.011656000	1.430799000	0.705876000
6	3.313327000	-0.091029000	-0.635380000
6	3.187720000	1.135046000	0.018569000
1	0.036738000	0.770257000	1.256973000
1	2.356377000	-1.977051000	-1.098341000
1	1.897492000	2.387017000	1.206553000
1	4.223804000	-0.329951000	-1.175790000
1	3.997977000	1.855932000	-0.012166000
1	-1.422014000	-0.426086000	-2.679902000
1	-3.621060000	-0.413655000	-1.524900000
1	-4.040990000	1.045286000	0.425295000

N_{Img} = 0
E_{ele} (M06-2X/6-311++G**) = -587.67698
E_{ele} (M06-2X /6-31+G**) = -587.52690
G_{corr} = 0.12630

TS$_{1a}$

At no.	X	Y	Z

6	-2.916936000	1.026899000	-0.388573000
6	-2.701707000	-0.392042000	-0.690516000
8	-2.026118000	1.859831000	-0.395830000
6	-1.499643000	-0.774470000	-1.274332000
7	-0.282200000	-1.157254000	0.246782000
1	-0.855271000	0.012092000	-1.661012000
7	-2.128411000	-0.662582000	1.503763000
7	-1.028843000	-0.880919000	1.240000000
6	0.985750000	-0.495036000	0.179953000
6	1.118456000	0.853472000	0.517363000
6	2.060018000	-1.218427000	-0.331342000
6	2.358695000	1.467014000	0.371965000
6	3.293576000	-0.589444000	-0.486851000
6	3.445697000	0.748785000	-0.128649000
1	0.250185000	1.413425000	0.856009000
1	1.918794000	-2.262892000	-0.590138000
1	2.471932000	2.513656000	0.635186000
1	4.136793000	-1.147795000	-0.880650000
1	4.408905000	1.234777000	-0.246141000
1	-1.412486000	-1.748895000	-1.741935000
1	-3.548418000	-1.068029000	-0.636895000
1	-3.948741000	1.319789000	-0.115705000

N_{Img} = 1
E_{ele} (M06-2X/6-311++G**) = -587.64612
E_{ele} (M06-2X /6-31+G**) = -587.49690
G_{corr} = 0.13025

1a'

At no.	X	Y	Z
6	-3.516975000	-0.273568000	-0.447217000
6	-2.521784000	0.144488000	0.628405000
8	-3.465452000	-1.328934000	-1.025311000
6	-1.253867000	-0.704740000	0.672222000
7	-0.289434000	0.281238000	0.191317000
1	-1.322231000	-1.563271000	-0.003020000
7	-2.059986000	1.522849000	0.301997000
7	-0.838345000	1.503261000	0.061246000
6	1.090259000	0.086849000	0.055292000
6	1.930446000	1.144868000	-0.319094000
6	1.628689000	-1.181665000	0.294448000
6	3.294941000	0.919998000	-0.445842000
6	3.000829000	-1.386499000	0.161469000
6	3.842354000	-0.342057000	-0.207177000

1	1.506526000	2.124455000	-0.502995000
1	0.985581000	-2.008089000	0.577219000
1	3.938403000	1.744896000	-0.735573000
1	3.407673000	-2.375559000	0.347597000
1	4.909527000	-0.506524000	-0.310066000
1	-0.990735000	-1.043126000	1.680054000
1	-3.064712000	0.187512000	1.579444000
1	-4.301397000	0.473697000	-0.667127000

N_{Img} = 0
E_{ele} (M06-2X/6-311++G**) = -587.73546
E_{ele} (M06-2X /6-31+G**) = -587.56791
G_{corr} = 0.13494

III'

At no.	X	Y	Z
7	3.850501000	-1.274555000	0.389363000
6	4.193974000	-0.030353000	0.233889000
7	3.110187000	0.749506000	-0.067825000
6	2.037071000	-0.073751000	-0.090516000
7	2.515953000	-1.286754000	0.177128000
6	1.787911000	-2.550511000	0.299399000
1	1.725287000	-2.815029000	1.355680000
1	0.805393000	-2.409393000	-0.145878000
1	2.355901000	-3.307282000	-0.239986000
6	3.157723000	2.181815000	-0.369531000
1	2.400142000	2.407671000	-1.118581000
1	2.971968000	2.763552000	0.534272000
1	4.149263000	2.410783000	-0.759103000
1	5.201440000	0.350203000	0.316681000
6	0.602610000	0.246786000	-0.427465000
6	0.086348000	1.419351000	0.058140000
8	-0.006767000	-0.620798000	-1.125216000
6	-1.339831000	1.742143000	-0.319009000
1	-1.433477000	1.958301000	-1.390417000
1	-1.697782000	2.625065000	0.220021000
1	0.645544000	2.106523000	0.679396000
7	-3.445819000	-0.889644000	1.136550000
6	-3.612033000	-1.096751000	-0.137899000
7	-2.911599000	-0.192232000	-0.885204000
6	-2.264679000	0.604598000	-0.017333000
7	-2.607411000	0.170628000	1.192292000
6	-2.203852000	0.725190000	2.478991000
1	-2.351798000	-0.054246000	3.223863000

1	-1.151196000	1.004952000	2.421416000
1	-2.821372000	1.592047000	2.721318000
6	-2.763183000	-0.189926000	-2.341758000
1	-1.710301000	-0.373681000	-2.565780000
1	-3.387967000	-0.988020000	-2.740578000
1	-3.100584000	0.765173000	-2.745362000
1	-4.221347000	-1.880424000	-0.562806000

N_{Img} = 0
E_{ele} (M06-2X/6-311++G**) = -832.853132
E_{ele} (M06-2X /6-31+G**) = -832.5672578
G_{corr} = 0.248224

TS$_{1b}$rea

At no.	X	Y	Z
7	2.215325000	1.705448000	1.807289000
6	1.660141000	2.776653000	1.321550000
7	0.489233000	2.481372000	0.680757000
6	0.323521000	1.142055000	0.777070000
7	1.378089000	0.701737000	1.464852000
6	1.693504000	-0.662044000	1.904996000
1	1.245340000	-0.824930000	2.885394000
1	1.274531000	-1.365012000	1.191570000
1	2.780253000	-0.729900000	1.947605000
6	-0.381661000	3.459161000	0.031877000
1	-0.156834000	3.502648000	-1.035175000
1	-1.418254000	3.163151000	0.189265000
1	-0.197988000	4.429781000	0.491941000
1	2.058686000	3.776502000	1.410396000
6	-0.786982000	0.253672000	0.282540000
6	-1.423539000	0.585747000	-0.889648000
8	-1.003212000	-0.773884000	0.989391000
6	-2.373747000	-0.455977000	-1.429799000
1	-1.861331000	-1.416597000	-1.568601000
1	-2.780036000	-0.154701000	-2.400933000
1	-1.142919000	1.426018000	-1.510756000
7	-4.895954000	-1.620896000	0.981814000
6	-5.330266000	-0.431709000	0.683809000
7	-4.513373000	0.174081000	-0.230293000
6	-3.519185000	-0.697464000	-0.499981000
7	-3.775979000	-1.771240000	0.237538000
6	-2.981500000	-2.994198000	0.347635000
1	-3.000816000	-3.529034000	-0.602926000
1	-1.967839000	-2.704870000	0.629631000

1	-3.453115000	-3.594984000	1.122224000
6	-4.680174000	1.493393000	-0.832386000
1	-5.471524000	2.016782000	-0.297555000
1	-3.740683000	2.040525000	-0.742430000
1	-4.956327000	1.391144000	-1.883382000
1	-6.218420000	0.025157000	1.094346000
7	1.524765000	1.842360000	-2.185669000
7	1.765302000	0.751788000	-1.998181000
7	1.922107000	-0.456283000	-1.835356000
6	3.065426000	-0.849372000	-1.076870000
6	3.212127000	-2.220585000	-0.862670000
6	3.980990000	0.058611000	-0.540461000
6	4.272577000	-2.681481000	-0.090611000
6	5.039640000	-0.416513000	0.231362000
6	5.186794000	-1.782817000	0.463718000
1	2.490744000	-2.902734000	-1.300416000
1	3.876047000	1.126173000	-0.717320000
1	4.388764000	-3.747340000	0.076536000
1	5.750650000	0.288276000	0.649902000
1	6.014166000	-2.146357000	1.063499000

$N_{Img} = 0$
E_{ele} (M06-2X/6-311++G**) = -1228.646392
E_{ele} (M06-2X /6-31+G**) = -1228.269547
$G_{corr} = 0.344412$

TS_{1b}

At no.	X	Y	Z
7	-3.566698000	3.541791000	-0.665886000
6	-2.432346000	3.609209000	-1.300644000
7	-1.671527000	2.498946000	-1.079405000
6	-2.391271000	1.699546000	-0.256723000
7	-3.530977000	2.357545000	-0.025170000
6	-4.683071000	1.993113000	0.814165000
1	-5.137559000	1.082360000	0.430598000
1	-4.347162000	1.825433000	1.835338000
1	-5.364334000	2.838637000	0.750180000
6	-0.341177000	2.292224000	-1.661155000
1	0.404369000	2.182926000	-0.874196000
1	-0.351486000	1.409997000	-2.301803000
1	-0.112295000	3.170366000	-2.263441000
1	-2.120300000	4.434056000	-1.924120000
6	-2.074760000	0.361696000	0.366707000
6	-0.748724000	-0.121595000	0.290177000
8	-2.995030000	-0.140951000	1.030630000

6	-0.455618000	-1.402822000	1.044140000
1	-1.089798000	-1.449444000	1.932545000
1	0.589197000	-1.406824000	1.372689000
1	-0.128950000	0.079304000	-0.577653000
7	-1.591976000	-4.416232000	-0.728083000
6	-0.411321000	-4.220352000	-1.238578000
7	0.189673000	-3.121814000	-0.688315000
6	-0.677260000	-2.622232000	0.215609000
7	-1.743561000	-3.415979000	0.171204000
6	-2.959967000	-3.354202000	0.984589000
1	-2.851850000	-4.026143000	1.837329000
1	-3.117437000	-2.322714000	1.300913000
1	-3.782571000	-3.686272000	0.353512000
6	1.539067000	-2.618441000	-0.976926000
1	1.592968000	-1.556009000	-0.724440000
1	2.270103000	-3.173112000	-0.385941000
1	1.736850000	-2.758605000	-2.039484000
1	0.044067000	-4.836305000	-2.000263000
7	0.187458000	1.167417000	1.467007000
7	1.335129000	1.116987000	1.144517000
7	1.979068000	0.535973000	0.203227000
6	3.385367000	0.713206000	0.226926000
6	4.076543000	0.305795000	-0.918717000
6	4.097937000	1.225798000	1.317515000
6	5.463610000	0.410788000	-0.976597000
6	5.483548000	1.331731000	1.248152000
6	6.174314000	0.924188000	0.106511000
1	3.513503000	-0.073444000	-1.768007000
1	3.564795000	1.536155000	2.210774000
1	5.989313000	0.097943000	-1.873361000
1	6.028716000	1.732663000	2.097024000
1	7.254765000	1.008306000	0.062186000

N_{Img} = 1

E_{ele} (M06-2X/6-311++G**) = -1228.614405

E_{ele} (M06-2X /6-31+G**) = -1228.233353

G_{corr} = 0.345155

III"

At no.	X	Y	Z
7	-3.549948000	3.586291000	-0.536605000
6	-2.333998000	3.828566000	-0.943865000
7	-1.520798000	2.752026000	-0.763199000
6	-2.290699000	1.789564000	-0.210711000

7	-3.512475000	2.319966000	-0.092425000
6	-4.745596000	1.737180000	0.453435000
1	-5.108219000	0.958753000	-0.215613000
1	-4.542904000	1.315676000	1.436433000
1	-5.452908000	2.560823000	0.519779000
6	-0.080313000	2.779187000	-1.069710000
1	0.463622000	3.090454000	-0.178109000
1	0.270618000	1.792672000	-1.367173000
1	0.055303000	3.480770000	-1.892455000
1	-1.999178000	4.763626000	-1.368875000
6	-1.996033000	0.354340000	0.178551000
6	-0.568177000	-0.023499000	0.386065000
8	-2.952618000	-0.372566000	0.349405000
6	-0.414900000	-1.398524000	1.080583000
1	-1.064942000	-1.428531000	1.957426000
1	0.624013000	-1.444063000	1.423703000
1	-0.076832000	-0.065872000	-0.606933000
7	-1.621680000	-4.403985000	-0.644270000
6	-0.511819000	-4.151924000	-1.275726000
7	0.102293000	-3.038094000	-0.773984000
6	-0.681535000	-2.583869000	0.224400000
7	-1.713900000	-3.423474000	0.282601000
6	-2.821628000	-3.435281000	1.239092000
1	-2.461504000	-3.788681000	2.206645000
1	-3.236838000	-2.432260000	1.314774000
1	-3.561330000	-4.128211000	0.843644000
6	1.411553000	-2.507236000	-1.182588000
1	2.191968000	-3.198881000	-0.861179000
1	1.422892000	-2.407122000	-2.268372000
1	1.568260000	-1.529072000	-0.714472000
1	-0.115772000	-4.739054000	-2.091487000
7	-0.001341000	1.030439000	1.218663000
7	1.292341000	1.150884000	1.104989000
7	1.901332000	0.406516000	0.256796000
6	3.305968000	0.592396000	0.229631000
6	3.974858000	0.205158000	-0.937339000
6	4.046584000	1.090949000	1.310233000
6	5.359563000	0.321734000	-1.032129000
6	5.429087000	1.206108000	1.207185000
6	6.093647000	0.823020000	0.040758000
1	3.393654000	-0.163159000	-1.779906000
1	3.528376000	1.379437000	2.218072000
1	5.864594000	0.026678000	-1.946861000
1	5.995369000	1.592284000	2.049353000

1	7.172572000	0.913068000	-0.028777000

N_{Img} = 0

E_{ele} (M06-2X/6-311++G**) = -1228.650228

E_{ele} (M06-2X /6-31+G**) = -1228.253295

G_{corr} = 0.347958

TS_{2b}

At no.	X	Y	Z
7	3.722447000	-2.475779000	-0.493205000
6	3.211044000	-3.278963000	0.398974000
7	1.871817000	-3.060879000	0.552054000
6	1.560109000	-2.068125000	-0.296782000
7	2.682230000	-1.736248000	-0.921254000
6	2.876596000	-0.689356000	-1.930440000
1	2.403153000	-0.997440000	-2.862404000
1	2.440647000	0.239205000	-1.557519000
1	3.951850000	-0.583399000	-2.056395000
6	0.971921000	-3.757277000	1.480877000
1	0.710957000	-3.072086000	2.288419000
1	0.081324000	-4.079497000	0.939710000
1	1.497156000	-4.634370000	1.856414000
1	3.763470000	-4.026664000	0.948764000
6	0.209846000	-1.437702000	-0.605429000
6	-0.601449000	-0.884449000	0.569656000
8	-0.130047000	-1.404326000	-1.761750000
6	-1.016779000	0.516092000	0.148458000
1	-0.990179000	0.821937000	-0.887874000
1	-1.299655000	1.249259000	0.895293000
1	-1.429881000	-1.561938000	0.792248000
7	-5.193116000	-0.035347000	-0.917239000
6	-5.275484000	0.204001000	0.356680000
7	-4.026822000	0.325531000	0.910369000
6	-3.098710000	0.159187000	-0.069271000
7	-3.851255000	-0.058794000	-1.151196000
6	-3.388744000	-0.298782000	-2.511385000
1	-3.625402000	0.565119000	-3.134179000
1	-2.313492000	-0.472394000	-2.481585000
1	-3.897265000	-1.180212000	-2.902275000
6	-3.732347000	0.623054000	2.309330000
1	-3.563889000	1.693482000	2.443371000
1	-4.576946000	0.310991000	2.923729000
1	-2.845002000	0.068335000	2.617042000
1	-6.199112000	0.288991000	0.910767000
7	0.274081000	-0.791924000	1.746125000

7	1.056321000	0.201866000	1.589383000
7	0.840645000	0.845728000	0.461897000
6	1.466670000	2.102161000	0.294662000
6	1.344317000	2.708229000	-0.961259000
6	2.173012000	2.751369000	1.315473000
6	1.920766000	3.953983000	-1.197403000
6	2.754342000	3.990060000	1.063224000
6	2.631138000	4.598324000	-0.186901000
1	0.798189000	2.197891000	-1.751587000
1	2.260989000	2.282531000	2.288796000
1	1.815775000	4.417881000	-2.172948000
1	3.302681000	4.489617000	1.855627000
1	3.083088000	5.567442000	-0.368753000

N_{Img} = 1

E_{ele} (M06-2X/6-311++G**) = -1228.571134

E_{ele} (M06-2X /6-31+G**) = -1228.185615

G_{corr} = 0.342953

IV

At no.	X	Y	Z
7	-2.864895000	2.874718000	0.997494000
6	-2.805569000	2.896196000	-0.306066000
7	-1.943020000	1.956610000	-0.782829000
6	-1.451382000	1.318430000	0.297313000
7	-2.017806000	1.892751000	1.359079000
6	-1.845460000	1.594650000	2.787529000
1	-2.260907000	0.610821000	3.002541000
1	-0.785905000	1.605428000	3.037190000
1	-2.381949000	2.377525000	3.318673000
6	-1.726131000	1.658588000	-2.202607000
1	-0.689561000	1.876937000	-2.458697000
1	-1.974007000	0.606017000	-2.363221000
1	-2.400530000	2.295011000	-2.774660000
1	-3.365405000	3.569655000	-0.938726000
6	-0.438800000	0.203806000	0.412929000
6	0.501048000	-0.017966000	-0.760552000
8	-0.329138000	-0.343383000	1.482860000
6	1.710081000	-0.881456000	-0.405717000
1	1.617003000	-1.344156000	0.580905000
1	1.926368000	-1.645851000	-1.158647000
1	-0.072820000	-0.384806000	-1.615735000
7	-3.528066000	-3.232705000	0.254419000
6	-4.502354000	-2.386111000	0.121564000
7	-4.035835000	-1.185999000	-0.350413000

6	-2.682504000	-1.257454000	-0.536186000
7	-2.438082000	-2.521488000	-0.153285000
6	-1.140257000	-3.174086000	-0.093412000
1	-0.498559000	-2.740741000	-0.860782000
1	-0.694623000	-3.038242000	0.895032000
1	-1.281742000	-4.235796000	-0.291702000
6	-4.847107000	-0.003449000	-0.593854000
1	-5.898208000	-0.289882000	-0.643379000
1	-4.716790000	0.724589000	0.211743000
1	-4.560009000	0.440639000	-1.548819000
1	-5.538901000	-2.598144000	0.340449000
7	1.070665000	1.330231000	-1.066365000
7	2.301266000	1.319051000	-0.819904000
7	2.753354000	0.147034000	-0.409354000
6	4.123788000	-0.070197000	-0.138365000
6	4.540859000	-1.344744000	0.247886000
6	5.043981000	0.976264000	-0.257050000
6	5.889733000	-1.570980000	0.517805000
6	6.383930000	0.730414000	0.015836000
6	6.815129000	-0.539134000	0.403937000
1	3.830794000	-2.159316000	0.343026000
1	4.708929000	1.960631000	-0.560437000
1	6.210790000	-2.562753000	0.818263000
1	7.098717000	1.541277000	-0.078088000
1	7.863457000	-0.719823000	0.614346000

N_{Img} = 0

E_{ele} (M06-2X/6-311++G**) = -1228.637985

E_{ele} (M06-2X /6-31+G**) = -1228.252564

G_{corr} = 0.346332

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