Supporting Information

1,2,3-Triazoles from Carbonyl Azides and Alkynes: Filling the Gap

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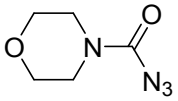
General Methods. All manipulations were carried out under a nitrogen atmosphere using standard Schlenk techniques. Reagents were purchased from commercial suppliers and used without further purification. Solvents were dried and degassed before use. The complex [Tpa*Cu]PF_6[1] was prepared according to the literature procedures. ^{1}H and ^{13}C{^{1}H} NMR spectra were recorded on a Varian Mercury 400 MHz spectrometer. ^{1}H chemical shifts were measured relative to partially deuterated solvents peaks but are reported relatively to tetramethylsilane. IR data were collected in a Varian Scmitar 1000 Fourier transform IR spectrophotometer. Elemental Analyses were performed at the Unidad de Analisis Elemental of the Universidad de Huelva. High-resolution mass spectra were performed at the CITIUS (Universidad de Sevilla). ESI mass spectrum was performed at the Instituto de Invstigaciones Químicas (Sevilla).

General procedure for the synthesis of N-carbamoyl azides. A 250-mL round-bottomed flask equipped with magnetic stirring bar was charged with NaN_3 (0.29 mol) and H_2O (50 mL) and stirred until the sodium azide was dissolved. The mixture was cooled in an ice bath and a solution of carbonyl chloride (0.57 mol) in THF (20 mL) was added over 15 min. The resulting mixture was stirred at the same temperature for a further 1 h. Then, it was extracted with diethyl ether (2 x 100 mL) and the organic phases were collected and washed with H_2O (50 mL), saturated aq Na_2CO_3 (50 mL) and brine (50 mL). After drying over $MgSO_4$ the solvent was rotary evaporated and the products were purified by column chromatography on silica gel using hexane/EtOAc (30:1) as eluent to afford the desired products.

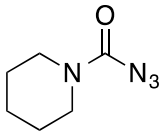
Characterization of N-carbamoyl azides



N-morpholinocarbamoyl azide

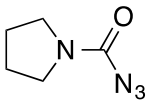
Following the general procedure, the azide was isolated as a colorless oil (31.7 g, 70%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.56 (d, J = 3.6 Hz, 2H), 3.51 (d, J = 3.6 Hz, 2H), 3.43 (br s, 2H), 3.32 (br s, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 155.4, 66.2, 45.5, 43.8. HRMS calcd for $C_5H_8N_4O_2$: 156.0647; found: 156.0646 $[M]^+$.

[1] K. Fujisawa; S. Chiba, Y. Miyashita, K. Okamoto, *Eur. J. Inorg. Chem*. **2009**, 3921.



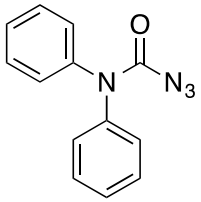
N-Piperidinocarbamoyl azide

Following the general procedure, the azide was isolated as a colorless oil (37.1 g, 83%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.40 (m, 2H), 3.29 (m, 2H), 1.48 (m, 6H). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 155.1, 46.4, 44.7, 25.8, 25.3, 24.1. FABMS: *m/z* = 177.2 ($[M+Na]^+$).



N-Pyrrolidinocarbamoyl azide

Following the general procedure, the azide was isolated as a colorless oil (25.7 g, 63%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.40 (t, *J* = 8.0 Hz, 2H), 3.29 (t, *J* = 8.0 Hz, 2H), 1.74 (m, 4H). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 154.4, 46.6, 46.3, 25.4, 24.6. HRMS calcd for $C_5H_9N_4O$: 141.0776; found: 141.0778 $[M+H]^+$.



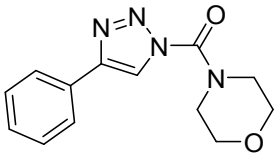
N,N-Diphenylcarbamoyl azide

Following the general procedure, the azide was isolated as a white solid (59.4 g, 86 %) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.27 (m, 10H). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 156.2, 149.1, 142.2, 141.6, 129.4, 129.2, 128.6, 127.3, 125.9. This azide has a fluxional behavior at room temperature since, the broad resonances that appeared at ca. 142.2 and at 128.6-125.9 in the $^{13}C\{^{1}H\}$ NMR spectrum at room temperature sharpen when the spectrum was recorded at 50 ºC in $CDCl_3$. HRMS calcd for $C_{13}H_{10}N_4O$: 238.0855; found: 238.0850 $[M]^+$.

General catalytic procedure for the [3+2] cycloaddition of N-carbamoyl azides and 1-alkynes catalyzed by [Tpa*Cu]PF$_6$. The catalyst (0.028 mg, 0.05 mmol,) and the N-carbamoyl azide (1 mmol) were dissolved in dichloroethane (1 mL) under a nitrogen atmosphere. The alkyne (1.2

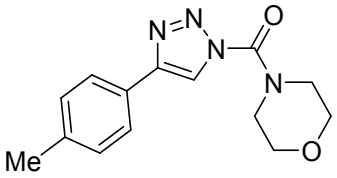
mmol) was added and the reaction mixture was stirred at 40 ºC for 24 h. Volatiles were removed under vacuum and the residue was dissolved in $CDCl_3$. An exactly weighted amount of trimethylvinylsilane was added as internal standard and the mass balance was then determined by ^1H NMR. The sample was recovered and the reaction crude was then purified by flash chromatography on silica gel using diethyl ether/petroleum ether (1:3) as eluent to afford the desired products.

Characterization data for compounds shown in Scheme 2 and 3:



1-(N-Morpholinocarbamoyl)-4-phenyl-1H-1,2,3-triazol (Scheme 2, 1)

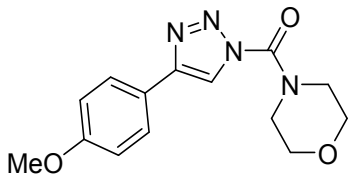
Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and phenylacetylene (132 μL) the title compound **1** was isolated as a yellow pale solid (0.180 g, 70%) after chromatographic purification. ^1H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.86 (dd, *J* = 7.0, 1.4 Hz, 2H), 7.48–7.40 (m, 2H), 7.40–7.32 (m, 1H), 4.04 (br s, 2H), 3.82 (br s, 6H). IR (nujol), ν(CO) (cm^{-1}): 1685. 9. Spectroscopic data for **1** were consistent with those previously reported for this compound.[2]



1-(N-Morpholinocarbamoyl)-4-(4-methylphenyl)-1H-1,2,3-triazol (Scheme 2, 2)

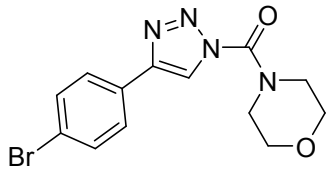
Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and 1-ethynyl-4-methylbenzene (152 μL) the title compound **2** was isolated as a yellow pale solid (0.207 g, 76%) after chromatographic purification. ^1H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 4.04 (br s, 2H), 3.82 (br s, 6H), 2.37 (s, 3H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 148.1, 146.9, 138.8, 129.6, 126.5, 125.8, 120.3, 66.6, 48.5, 45.8, 21.3. IR (nujol), ν(CO) (cm^{-1}): 1709.6. Anal.Calcd. for $C_{14}H_{16}N_4O_2$: C, 61.75; H, 5.92; N, 20.58. Found: C, 61.96; H, 6.11; N, 20.01.

[2] L. E. Kiss, D. A. Learmonth, C. P. D. C. P. Rosa, R. Gusmao de Noronha, P. N. L. Palma, P. M. V. A. Soares da Silva, A. Beliaev, PCT Int. Appl.(2010), WO 2010074588 A2 20100701



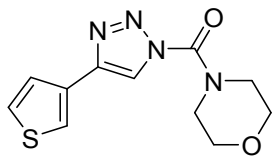
1-(N-Morpholinocarbamoyl)-4-(4-methoxyphenyl)-1H-1,2,3-triazol (**Scheme 2, 3)**

Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and 1-ethynyl-4-methoxybenzene (156 μL) the title compound **3** was isolated as a yellow pale solid (0.208 g, 72%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.78 (d, *J* = 8.3 Hz, 2H), 6.96 (d, *J* = 8.3 Hz, 2H), 4.04 (br s, 2H), 3.83 (br s, 9H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.0, 148.1, 146.7, 127.2, 121.9, 119.9, 114.4, 66.6, 48.5, 45.8. IR (nujol), ν(CO) (cm^{-1}): 1709.9. Anal. Calcd. for $C_{14}H_{16}N_4O_3$: C, 58.33; H, 5.56; N, 19.44. Found: C, 58.94; H, 5.74; N, 18.64.



1-(N-Morpholinocarbamoyl)-4-(4-bromophenyl)-1H-1,2,3-triazol (**Scheme 2, 4)**

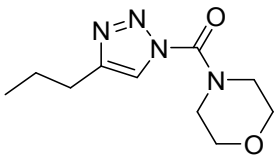
Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and 1-ethynyl-4-bromobenzene (217 mg) the title compound **4** was isolated as a yellow pale solid (0.219 g, 65%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 8.2 Hz, 2H), 4.07 (br s, 2H), 3.84 (br s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 147.9, 145.8, 132.2, 128.3, 127.4, 122.8, 121.1, 66.6, 48.5, 45.8. IR (nujol), ν(CO) (cm^{-1}): 1717.6. Anal. Calcd. for $C_{13}H_{13}BrN_4O_2$: C, 46.31; H, 3.89; N, 16.62. Found: C, 46.13; H, 3.50; N, 16.28.



1-(N-Morpholinocarbamoyl)-4-(thien-3-yl)-1H-1,2,3-triazol (**Scheme 2, 5)**

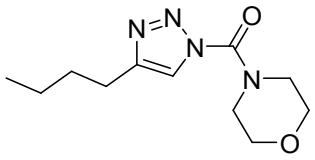
Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and 3-ethynyl-thiophene (118 μL) the title compound **5** was isolated as a yellow pale solid (0.185 g, 70%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 7.77–7.72 (m, 1H), 7.45 (d, *J*= 5.0 Hz, 1H), 7.40 (dd, *J*= 5.0, 3.0 Hz, 1H), 4.03 (br s, 2H), 3.82 (br s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 148.0, 143.1, 130.5, 126.8, 125.7, 122.1, 120.6, 120.5, 66.6, 48.5, 45.8. IR (nujol),

ν(CO) (cm^{-1}): 1701.2. Anal. Calcd. for $C_{11}H_{12}N_4O_2S$: C, 49.99; H, 4.58; N, 21.20. Found: C, 50.37; H, 4.56; N, 20.76.



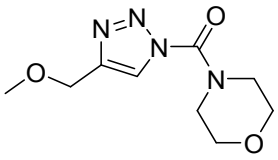
1-(N-Morpholinocarbamoyl)-4-*n*-propyl-1H-1,2,3-triazol (Scheme 2, 6)

Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and 1-pentyne (118 μL) the title compound **6** was isolated as a yellow pale oil (0.184 g, 82%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 3.91 (br s, 2H), 3.72 (br s, 6H), 2.63 (t, *J* = 7.5 Hz, 2H), 1.68–1.58 (m, 2H), 0.89 (t, *J* = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 148.1, 147.3, 122.1, 66.5, 48.3, 45.6, 27.2, 22.2, 13.6. IR (nujol), ν(CO) (cm^{-1}): 1709.9. Anal. Calcd. for $C_{10}H_{16}N_4O_2$: C, 53.56; H, 7.19; N, 24.98. Found: C, 53.84; H, 7.39; N, 24.71.



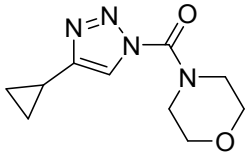
1-(N-Morpholinocarbamoyl)-4-*n*-butyl-1H-1,2,3-triazol (Scheme 2, 7)

Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and 1-hexyne (138 μL) the title compound **7** was isolated as a yellow pale oil (0.184 g, 77%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 3.98 (br s, 2H), 3.78 (br s, 6H), 2.72 (t, *J* = 7.7 Hz, 2H), 1.70 – 1.60 (m, 2H), 1.42 – 1.31 (m, 2H), 0.91 (td, *J* = 7.3, 1.4 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 148.3, 147.6, 122.0, 66.6, 48.3, 45.5, 31.1, 24.9, 22.2, 13.7. IR (nujol), ν(CO) (cm^{-1}): 1702.5. Anal. Calcd. for $C_{11}H_{18}N_4O_2$: C, 55.45; H, 7.61; N, 23.51. Found: C, 55.18; H, 7.79; N, 23.57.



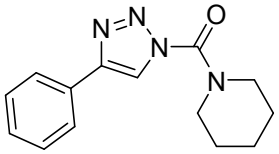
1-(N-Morpholinocarbamoyl)-4-(methoxymethyl)-1H-1,2,3-triazol (Scheme 2, 8)

Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and methylpropargyl ether (101 μL) the title compound **8** was isolated as a yellow pale oil (0.195 g, 86%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 4.48 (s, 2H), 3.84 (br s, 2H), 3.68 (br s, 6H), 3.30 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 147.9, 144.2, 124.0, 123.9, 66.3, 65.2, 58.3, 48.2, 45.6. IR (nujol), ν(CO) (cm^{-1}): 1716.5. Anal. Calcd. for $C_9H_{14}N_4O_3$: C, 47.78; H, 6.24; N, 24.77. Found: C, 47.72; H, 6.37; N, 24.85.



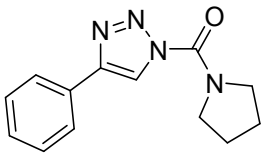
1-(N-Morpholinocarbamoyl)-4-cyclopropyl-1H-1,2,3-triazol (Scheme 2, 9)

Following the general procedure from N-morpholinocarbamoyl azide (0.156 g) and cyclopropylacetylene (102μL) the title compound **9** was isolated as a yellow pale oil (0.187 g, 84%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (s, 1H), 3.86 (br s, 2H), 3.68 (br s, 6H), 1.93–1.81 (m, 1H), 0.93-0.84 (m, 2H), 0.80-0.73 (m, 2H) . ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 149.2, 148.0, 120.9, 120.9, 66.4, 48.2, 45.4, 39.6, 7.7, 6.3. IR (nujol), ν(CO) (cm^{-1}): 1703.9. Anal. Calcd. for $C_{10}H_{14}N_4O_2$·C, 54.05; H, 6.31; N, 25.23. Found: C, 54.42; H, 6.43; N, 23.86.



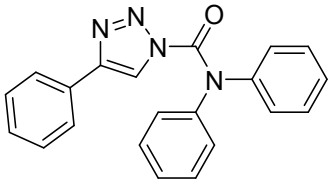
1-(N-Piperidinocarbamoyl)-4-phenyl-1H-1,2,3-triazol (Scheme 3, 10)

Following the general procedure from N-piperidinocarbamoyl azide (0.154 g) and phenylacetylene (132 μL) the title compound **10** was isolated as a yellow pale oil (0.128 g, 50%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.83 (d, J = 7.7 Hz, 2H), 7.39 (t, J = 7.7 Hz, 2H), 7.30 (t, J = 7.7 Hz, 1H), 3.75-3.69 (m, 4H), 1.67 (s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ 148.1, 146.7, 129.6, 128.9, 128.6, 125.8, 120.8, 49.1, 46.8, 26.2, 25.5, 24.1. IR (nujol), ν(CO) (cm^{-1}): 1685.1. Anal. Calcd. for $C_{14}H_{16}N_4O$: C, 65.63; H, 6.25; N, 21.88. Found: C, 65.54; H, 6.65; N, 19.81.



1-(N-Pyrrolidinocarbamoyl)-4-phenyl-1H-1,2,3-triazol (Scheme 3, 11)

Following the general procedure from N-pyrrolidinocarbamoyl azide (0.140 g) and phenylacetylene (132 μL) the title compound **11** was isolated as a yellow pale oil (0.073g, 30%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 7.88 (d, *J*= 7.6 Hz, 2H), 7.45 (d, *J*= 7.3 Hz, 2H), 7.37 (t, *J*= 7.4 Hz, 1H), 4.07 (t, *J*= 6.4 Hz, 2H), 3.75 (t, *J*= 6.5 Hz, 2H), 2.01 (dt, *J*= 13.2, 6.6 Hz, 4H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 147.1, 146.4, 129.6, 128.9, 128.6, 125.9, 120.2, 50.3, 49.0, 29.7, 26.5, 23.9. IR (nujol), ν(CO) (cm^{-1}): 1686.06. Anal. Calcd. for $C_{13}H_{14}N_4O$: C, 64.46; H, 5.79; N, 23.14. Found: C, 63.22; H, 5.60; N, 22.61.



N,N,4-Triphenyl-1H-1,2,3-triazole-1-carboxamide (Scheme 3, 12)

Following the general procedure from N-diphenylcarbamoyl azide (0.238 g) and phenylacetylene (110 μL) the title compound **12** was isolated as a yellow pale solid (0.187g, 55%) after chromatographic purification. ^{1}H NMR (400 MHz, $CDCl_3$). δ 8.37 (s, 1H), 7.84 (d, *J*= 6.7 Hz, 2H), 7.44–7.37 (m, 7H), 7.32-7.28 (m, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ 148.8, 146.6, 142.4, 129.6, 129.3, 128.9, 128.7, 127.5, 126.6, 125.9, 120.0. IR (nujol), ν(CO) (cm^{-1}): 1724.3.

Selected X-ray crystal data for compounds 1, 4, 5 and 8

1-(N-Morpholinocarbamoyl)-4-phenyl-1H-1,2,3-triazol (Scheme 2, 1)

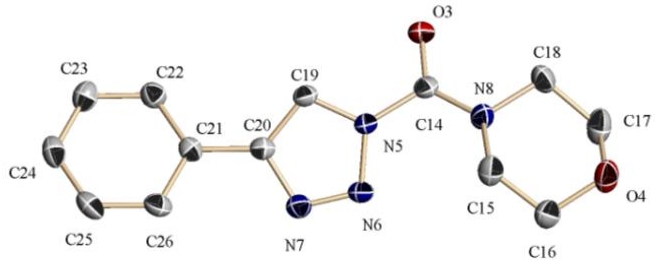


Table S1. Crystal data and structure refinement for 1.

Empirical formula	$C_{13}H_{14}N_4O_2$	
Formula weight	258.28	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1	
Unit cell dimensions	a = 8.1976(5) Å	α= 90°.
	b = 12.7958(7) Å	β= 104.2270(10)°.
	c = 11.9888(6) Å	γ = 90°.
Volume	1218.99(12) $Å^3$	
Z	4	
Density (calculated)	1.407 Mg/m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	544	
Crystal size	0.50 x 0.40 x 0.35 mm^3	
Theta range for data collection	3.02 to 25.25°.	
Index ranges	-9<=h<=9, -14<=k<=15, -11<=l<=14	
Reflections collected	11401	
Independent reflections	2164 [R(int) = 0.0246]	
Completeness to theta = 25.25°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9662 and 0.9542	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	2164 / 1 / 344
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0295, wR2 = 0.0727
R indices (all data)	R1 = 0.0332, wR2 = 0.0744
Largest diff. peak and hole	0.131 and -0.270 e.Å^{-3}

Table S2. Bond lengths [Å] and angles [°] for 1.

O(1)-C(1)	1.215(3)	C(11)-C(12)	1.381(4)
O(2)-C(4)	1.416(3)	C(11)-H(11)	0.9500
O(2)-C(3)	1.422(3)	C(12)-C(13)	1.384(4)
N(1)-C(6)	1.357(3)	C(12)-H(12)	0.9500
N(1)-N(2)	1.370(3)	C(13)-H(13)	0.9500
N(1)-C(1)	1.442(3)	O(3)-C(14)	1.216(3)
N(2)-N(3)	1.298(3)	O(4)-C(16)	1.419(3)
N(3)-C(7)	1.372(3)	O(4)-C(17)	1.420(3)
N(4)-C(1)	1.334(3)	N(5)-C(19)	1.352(3)
N(4)-C(5)	1.468(3)	N(5)-N(6)	1.370(3)
N(4)-C(2)	1.469(3)	N(5)-C(14)	1.441(3)
C(2)-C(3)	1.515(3)	N(6)-N(7)	1.296(3)
C(2)-H(2A)	0.9900	N(7)-C(20)	1.373(3)
C(2)-H(2B)	0.9900	N(8)-C(14)	1.338(3)
C(3)-H(3A)	0.9900	N(8)-C(18)	1.467(3)
C(3)-H(3B)	0.9900	N(8)-C(15)	1.475(3)
C(4)-C(5)	1.507(4)	C(15)-C(16)	1.503(4)
C(4)-H(4A)	0.9900	C(15)-H(15A)	0.9900
C(4)-H(4B)	0.9900	C(15)-H(15B)	0.9900
C(5)-H(5A)	0.9900	C(16)-H(16A)	0.9900
C(5)-H(5B)	0.9900	C(16)-H(16B)	0.9900
C(6)-C(7)	1.361(3)	C(17)-C(18)	1.504(4)
C(6)-H(6)	0.9500	C(17)-H(17A)	0.9900
C(7)-C(8)	1.474(3)	C(17)-H(17B)	0.9900
C(8)-C(13)	1.391(3)	C(18)-H(18A)	0.9900
C(8)-C(9)	1.397(3)	C(18)-H(18B)	0.9900
C(9)-C(10)	1.386(4)	C(19)-C(20)	1.366(3)
C(9)-H(9)	0.9500	C(19)-H(19)	0.9500
C(10)-C(11)	1.385(4)	C(20)-C(21)	1.467(3)
C(10)-H(10)	0.9500	C(21)-C(22)	1.387(3)

C(21)-C(26)	1.401(4)	C(5)-C(4)-H(4B)	109.5
C(22)-C(23)	1.385(4)	H(4A)-C(4)-H(4B)	108.1
C(22)-H(22)	0.9500	N(4)-C(5)-C(4)	109.6(2)
C(23)-C(24)	1.384(4)	N(4)-C(5)-H(5A)	109.7
C(23)-H(23)	0.9500	C(4)-C(5)-H(5A)	109.7
C(24)-C(25)	1.375(4)	N(4)-C(5)-H(5B)	109.7
C(24)-H(24)	0.9500	C(4)-C(5)-H(5B)	109.7
C(25)-C(26)	1.382(4)	H(5A)-C(5)-H(5B)	108.2
C(25)-H(25)	0.9500	N(1)-C(6)-C(7)	105.16(19)
C(26)-H(26)	0.9500	N(1)-C(6)-H(6)	127.4
C(4)-O(2)-C(3)	109.95(19)	C(7)-C(6)-H(6)	127.4
C(6)-N(1)-N(2)	109.92(19)	C(6)-C(7)-N(3)	108.3(2)
C(6)-N(1)-C(1)	124.42(19)	C(6)-C(7)-C(8)	130.1(2)
N(2)-N(1)-C(1)	125.01(18)	N(3)-C(7)-C(8)	121.6(2)
N(3)-N(2)-N(1)	107.16(18)	C(13)-C(8)-C(9)	119.0(2)
N(2)-N(3)-C(7)	109.45(18)	C(13)-C(8)-C(7)	120.9(2)
C(1)-N(4)-C(5)	117.6(2)	C(9)-C(8)-C(7)	120.1(2)
C(1)-N(4)-C(2)	130.1(2)	C(10)-C(9)-C(8)	120.2(2)
C(5)-N(4)-C(2)	112.3(2)	C(10)-C(9)-H(9)	119.9
O(1)-C(1)-N(4)	125.2(2)	C(8)-C(9)-H(9)	119.9
O(1)-C(1)-N(1)	116.4(2)	C(11)-C(10)-C(9)	120.4(2)
N(4)-C(1)-N(1)	118.3(2)	C(11)-C(10)-H(10)	119.8
N(4)-C(2)-C(3)	109.9(2)	C(9)-C(10)-H(10)	119.8
N(4)-C(2)-H(2A)	109.7	C(12)-C(11)-C(10)	119.5(2)
C(3)-C(2)-H(2A)	109.7	C(12)-C(11)-H(11)	120.2
N(4)-C(2)-H(2B)	109.7	C(10)-C(11)-H(11)	120.2
C(3)-C(2)-H(2B)	109.7	C(11)-C(12)-C(13)	120.6(2)
H(2A)-C(2)-H(2B)	108.2	C(11)-C(12)-H(12)	119.7
O(2)-C(3)-C(2)	112.6(2)	C(13)-C(12)-H(12)	119.7
O(2)-C(3)-H(3A)	109.1	C(12)-C(13)-C(8)	120.3(2)
C(2)-C(3)-H(3A)	109.1	C(12)-C(13)-H(13)	119.8
O(2)-C(3)-H(3B)	109.1	C(8)-C(13)-H(13)	119.8
C(2)-C(3)-H(3B)	109.1	C(16)-O(4)-C(17)	109.69(19)
H(3A)-C(3)-H(3B)	107.8	C(19)-N(5)-N(6)	110.33(19)
O(2)-C(4)-C(5)	110.8(2)	C(19)-N(5)-C(14)	124.74(19)
O(2)-C(4)-H(4A)	109.5	N(6)-N(5)-C(14)	124.46(18)
C(5)-C(4)-H(4A)	109.5	N(7)-N(6)-N(5)	106.85(18)
O(2)-C(4)-H(4B)	109.5	N(6)-N(7)-C(20)	109.73(18)

C(14)-N(8)-C(18)	116.6(2)	C(26)-C(21)-C(20)	120.2(2)
C(14)-N(8)-C(15)	127.9(2)	C(23)-C(22)-C(21)	120.6(2)
C(18)-N(8)-C(15)	112.5(2)	C(23)-C(22)-H(22)	119.7
O(3)-C(14)-N(8)	125.9(2)	C(21)-C(22)-H(22)	119.7
O(3)-C(14)-N(5)	116.8(2)	C(24)-C(23)-C(22)	120.1(3)
N(8)-C(14)-N(5)	117.3(2)	C(24)-C(23)-H(23)	120.0
N(8)-C(15)-C(16)	109.2(2)	C(22)-C(23)-H(23)	120.0
N(8)-C(15)-H(15A)	109.8	C(25)-C(24)-C(23)	119.8(2)
C(16)-C(15)-H(15A)	109.8	C(25)-C(24)-H(24)	120.1
N(8)-C(15)-H(15B)	109.8	C(23)-C(24)-H(24)	120.1
C(16)-C(15)-H(15B)	109.8	C(24)-C(25)-C(26)	120.6(2)
H(15A)-C(15)-H(15B)	108.3	C(24)-C(25)-H(25)	119.7
O(4)-C(16)-C(15)	111.0(2)	C(26)-C(25)-H(25)	119.7
O(4)-C(16)-H(16A)	109.4	C(25)-C(26)-C(21)	120.1(3)
C(15)-C(16)-H(16A)	109.4	C(25)-C(26)-H(26)	119.9
O(4)-C(16)-H(16B)	109.4	C(21)-C(26)-H(26)	119.9
C(15)-C(16)-H(16B)	109.4		
H(16A)-C(16)-H(16B)	108.0		
O(4)-C(17)-C(18)	112.8(2)		
O(4)-C(17)-H(17A)	109.0		
C(18)-C(17)-H(17A)	109.0		
O(4)-C(17)-H(17B)	109.0		
C(18)-C(17)-H(17B)	109.0		
H(17A)-C(17)-H(17B)	107.8		
N(8)-C(18)-C(17)	110.2(2)		
N(8)-C(18)-H(18A)	109.6		
C(17)-C(18)-H(18A)	109.6		
N(8)-C(18)-H(18B)	109.6		
C(17)-C(18)-H(18B)	109.6		
H(18A)-C(18)-H(18B)	108.1		
N(5)-C(19)-C(20)	105.0(2)		
N(5)-C(19)-H(19)	127.5		
C(20)-C(19)-H(19)	127.5		
C(19)-C(20)-N(7)	108.0(2)		
C(19)-C(20)-C(21)	130.2(2)		
N(7)-C(20)-C(21)	121.8(2)		
C(22)-C(21)-C(26)	118.8(2)		
C(22)-C(21)-C(20)	121.0(2)		

1-(N-Morpholinocarbamoyl)-4-(4-bromophenyl)-1H-1,2,3-triazol (Scheme 2, 4)

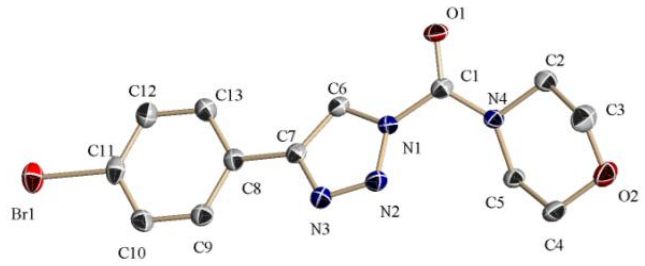


Table S3. Crystal data and structure refinement for 4.

Empirical formula	$C_{13}H_{13}BrN_4O_2$	
Formula weight	337.18	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 28.3878(14) Å	α= 90°.
	b = 5.0616(3) Å	β= 95.781(3)°.
	c = 18.7871(12) Å	γ = 90°.
Volume	2685.7(3) $Å^3$	
Z	8	
Density (calculated)	1.668 Mg/m^3	
Absorption coefficient	3.068 mm^{-1}	
F(000)	1360	
Crystal size	0.50 x 0.15 x 0.10 mm^3	
Theta range for data collection	2.49 to 25.25°.	
Index ranges	-34<=h<=34, -5<=k<=6, -10<=l<=22	
Reflections collected	12029	
Independent reflections	2248 [R(int) = 0.0418]	
Completeness to theta = 25.25°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7359 and 0.5807	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2248 / 0 / 181	
Goodness-of-fit on F^2	1.007	
Final R indices [I>2sigma(I)]	R1 = 0.0351, wR2 = 0.0905	
R indices (all data)	R1 = 0.0420, wR2 = 0.0939	

Largest diff. peak and hole	0.871 and -0.622 e.Å^{-3}

Table S4. Bond lengths [Å] and angles [°] for 4.

Br(1)-C(11)	1.902(3)	C(12)-H(12)	0.9500
O(1)-C(1)	1.213(3)	C(13)-H(13)	0.9500
O(2)-C(4)	1.421(4)	C(4)-O(2)-C(3)	110.3(2)
O(2)-C(3)	1.423(4)	C(6)-N(1)-N(2)	110.4(2)
N(1)-C(6)	1.349(3)	C(6)-N(1)-C(1)	125.2(2)
N(1)-N(2)	1.368(3)	N(2)-N(1)-C(1)	124.0(2)
N(1)-C(1)	1.433(4)	N(3)-N(2)-N(1)	106.8(2)
N(2)-N(3)	1.297(4)	N(2)-N(3)-C(7)	109.7(2)
N(3)-C(7)	1.374(4)	C(1)-N(4)-C(2)	116.4(2)
N(4)-C(1)	1.346(3)	C(1)-N(4)-C(5)	124.7(2)
N(4)-C(2)	1.462(4)	C(2)-N(4)-C(5)	112.7(2)
N(4)-C(5)	1.471(3)	O(1)-C(1)-N(4)	125.6(3)
C(2)-C(3)	1.512(4)	O(1)-C(1)-N(1)	117.6(2)
C(2)-H(2A)	0.9900	N(4)-C(1)-N(1)	116.7(2)
C(2)-H(2B)	0.9900	N(4)-C(2)-C(3)	108.5(2)
C(3)-H(3A)	0.9900	N(4)-C(2)-H(2A)	110.0
C(3)-H(3B)	0.9900	C(3)-C(2)-H(2A)	110.0
C(4)-C(5)	1.508(4)	N(4)-C(2)-H(2B)	110.0
C(4)-H(4A)	0.9900	C(3)-C(2)-H(2B)	110.0
C(4)-H(4B)	0.9900	H(2A)-C(2)-H(2B)	108.4
C(5)-H(5A)	0.9900	O(2)-C(3)-C(2)	111.2(3)
C(5)-H(5B)	0.9900	O(2)-C(3)-H(3A)	109.4
C(6)-C(7)	1.365(4)	C(2)-C(3)-H(3A)	109.4
C(6)-H(6)	0.9500	O(2)-C(3)-H(3B)	109.4
C(7)-C(8)	1.473(4)	C(2)-C(3)-H(3B)	109.4
C(8)-C(9)	1.384(4)	H(3A)-C(3)-H(3B)	108.0
C(8)-C(13)	1.392(4)	O(2)-C(4)-C(5)	111.3(2)
C(9)-C(10)	1.384(4)	O(2)-C(4)-H(4A)	109.4
C(9)-H(9)	0.9500	C(5)-C(4)-H(4A)	109.4
C(10)-C(11)	1.381(4)	O(2)-C(4)-H(4B)	109.4
C(10)-H(10)	0.9500	C(5)-C(4)-H(4B)	109.4
C(11)-C(12)	1.377(4)	H(4A)-C(4)-H(4B)	108.0
C(12)-C(13)	1.376(4)	N(4)-C(5)-C(4)	109.4(2)

N(4)-C(5)-H(5A)	109.8
C(4)-C(5)-H(5A)	109.8
N(4)-C(5)-H(5B)	109.8
C(4)-C(5)-H(5B)	109.8
H(5A)-C(5)-H(5B)	108.2
N(1)-C(6)-C(7)	105.2(2)
N(1)-C(6)-H(6)	127.4
C(7)-C(6)-H(6)	127.4
C(6)-C(7)-N(3)	107.9(2)
C(6)-C(7)-C(8)	130.3(2)
N(3)-C(7)-C(8)	121.8(2)
C(9)-C(8)-C(13)	119.0(3)
C(9)-C(8)-C(7)	120.6(2)
C(13)-C(8)-C(7)	120.4(3)
C(10)-C(9)-C(8)	120.9(3)
C(10)-C(9)-H(9)	119.5
C(8)-C(9)-H(9)	119.5
C(11)-C(10)-C(9)	118.9(3)
C(11)-C(10)-H(10)	120.6
C(9)-C(10)-H(10)	120.6
C(12)-C(11)-C(10)	121.2(3)
C(12)-C(11)-Br(1)	120.1(2)
C(10)-C(11)-Br(1)	118.6(2)
C(13)-C(12)-C(11)	119.4(3)
C(13)-C(12)-H(12)	120.3
C(11)-C(12)-H(12)	120.3
C(12)-C(13)-C(8)	120.6(3)
C(12)-C(13)-H(13)	119.7
C(8)-C(13)-H(13)	119.7

1-(N-Morpholinocarbamoyl)-4-(thien-3-yl)-1H-1,2,3-triazol (Scheme 2, 5)

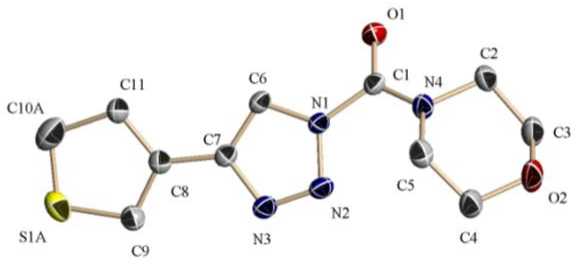


Table S5. Crystal data and structure refinement for 5.

Empirical formula	$C_{11}H_{12}N_4O_2S$	
Formula weight	264.31	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P $2_1/n$	
Unit cell dimensions	a = 5.2958(3) Å	α= 90°.
	b = 11.8997(6) Å	β= 93.808(2)°.
	c = 18.8466(10) Å	γ = 90°.
Volume	1185.06(11) $Å^3$	
Z	4	
Density (calculated)	1.481 Mg/m^3	
Absorption coefficient	0.273 mm^{-1}	
F(000)	552	
Crystal size	0.50 x 0.45 x 0.40 mm^3	
Theta range for data collection	2.76 to 25.25°.	
Index ranges	-5<=h<=6, -14<=k<=14, -22<=l<=19	
Reflections collected	19721	
Independent reflections	2145 [R(int) = 0.0210]	
Completeness to theta = 25.25°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8966 and 0.8715	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2145 / 37 / 163	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0434, wR2 = 0.1159	
R indices (all data)	R1 = 0.0469, wR2 = 0.1202	

Largest diff. peak and hole 0.444 and -0.620 e.Å^{-3}

Table S6. Bond lengths [Å] and angles [°] for 5.

O(1)-C(1)	1.216(2)	C(6)-N(1)-C(1)	124.85(14)
O(2)-C(3)	1.425(2)	N(2)-N(1)-C(1)	123.05(13)
O(2)-C(4)	1.428(2)	N(3)-N(2)-N(1)	106.83(13)
N(1)-C(6)	1.356(2)	N(2)-N(3)-C(7)	109.29(14)
N(1)-N(2)	1.3679(19)	C(1)-N(4)-C(5)	128.22(14)
N(1)-C(1)	1.437(2)	C(1)-N(4)-C(2)	118.57(14)
N(2)-N(3)	1.302(2)	C(5)-N(4)-C(2)	112.95(14)
N(3)-C(7)	1.375(2)	O(1)-C(1)-N(4)	125.67(16)
N(4)-C(1)	1.337(2)	O(1)-C(1)-N(1)	117.81(15)
N(4)-C(5)	1.466(2)	N(4)-C(1)-N(1)	116.49(14)
N(4)-C(2)	1.470(2)	N(4)-C(2)-C(3)	107.74(15)
C(2)-C(3)	1.511(3)	N(4)-C(2)-H(2A)	110.2
C(2)-H(2A)	0.9900	C(3)-C(2)-H(2A)	110.2
C(2)-H(2B)	0.9900	N(4)-C(2)-H(2B)	110.2
C(3)-H(3A)	0.9900	C(3)-C(2)-H(2B)	110.2
C(3)-H(3B)	0.9900	H(2A)-C(2)-H(2B)	108.5
C(4)-C(5)	1.510(3)	O(2)-C(3)-C(2)	111.86(16)
C(4)-H(4A)	0.9900	O(2)-C(3)-H(3A)	109.2
C(4)-H(4B)	0.9900	C(2)-C(3)-H(3A)	109.2
C(5)-H(5A)	0.9900	O(2)-C(3)-H(3B)	109.2
C(5)-H(5B)	0.9900	C(2)-C(3)-H(3B)	109.2
C(6)-C(7)	1.359(2)	H(3A)-C(3)-H(3B)	107.9
C(6)-H(6)	0.9500	O(2)-C(4)-C(5)	111.09(16)
C(7)-C(8)	1.464(2)	O(2)-C(4)-H(4A)	109.4
C(8)-C(9)	1.381(2)	C(5)-C(4)-H(4A)	109.4
C(8)-C(11)	1.400(2)	O(2)-C(4)-H(4B)	109.4
C(9)-S(1A)	1.6819(19)	C(5)-C(4)-H(4B)	109.4
C(9)-H(9)	0.9500	H(4A)-C(4)-H(4B)	108.0
S(1A)-C(10A)	1.5537(14)	N(4)-C(5)-C(4)	109.16(15)
C(10A)-C(11)	1.617(2)	N(4)-C(5)-H(5A)	109.8
C(10A)-H(10A)	0.9500	C(4)-C(5)-H(5A)	109.8
C(11)-H(11)	0.9500	N(4)-C(5)-H(5B)	109.8
C(3)-O(2)-C(4)	110.47(14)	C(4)-C(5)-H(5B)	109.8
C(6)-N(1)-N(2)	110.46(14)	H(5A)-C(5)-H(5B)	108.3

N(1)-C(6)-C(7)	104.90(14)
N(1)-C(6)-H(6)	127.5
C(7)-C(6)-H(6)	127.5
C(6)-C(7)-N(3)	108.50(15)
C(6)-C(7)-C(8)	129.40(15)
N(3)-C(7)-C(8)	122.03(15)
C(9)-C(8)-C(11)	112.24(16)
C(9)-C(8)-C(7)	124.41(16)
C(11)-C(8)-C(7)	123.27(15)
C(8)-C(9)-S(1A)	111.06(14)
C(8)-C(9)-H(9)	124.5
S(1A)-C(9)-H(9)	124.5
C(10A)-S(1A)-C(9)	100.67(8)
S(1A)-C(10A)-C(11)	105.85(9)
S(1A)-C(10A)-H(10A)	127.1
C(11)-C(10A)-H(10A)	127.1
C(8)-C(11)-C(10A)	110.17(14)
C(8)-C(11)-H(11)	124.9
C(10A)-C(11)-H(11)	124.9

1-(N-Morpholinocarbamoyl)-4-(methoxymethyl)-1H-1,2,3-triazol (Scheme 2, 8)

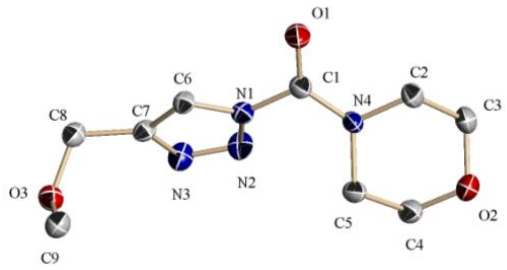


Table S7. Crystal data and structure refinement for 8.

Empirical formula	$C_9H_{14}N_4O_3$	
Formula weight	226.24	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P n	
Unit cell dimensions	a = 4.7202(3) Å	α= 90°.
	b = 13.9971(8) Å	β= 92.621(2)°.
	c = 8.1756(6) Å	γ = 90°.
Volume	539.59(6) $Å^3$	
Z	2	
Density (calculated)	1.392 Mg/m^3	
Absorption coefficient	0.107 mm^{-1}	
F(000)	240	
Crystal size	0.50 x 0.45 x 0.40 mm^3	
Theta range for data collection	2.89 to 25.24°.	
Index ranges	-4<=h<=5, -16<=k<=10, -9<=l<=9	
Reflections collected	5133	
Independent reflections	965 [R(int) = 0.0178]	
Completeness to theta = 25.24°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9584 and 0.9485	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	965 / 2 / 147	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0257, wR2 = 0.0708	

R indices (all data)	R1 = 0.0269, wR2 = 0.0717
Largest diff. peak and hole	0.130 and -0.153 e.Å^{-3}

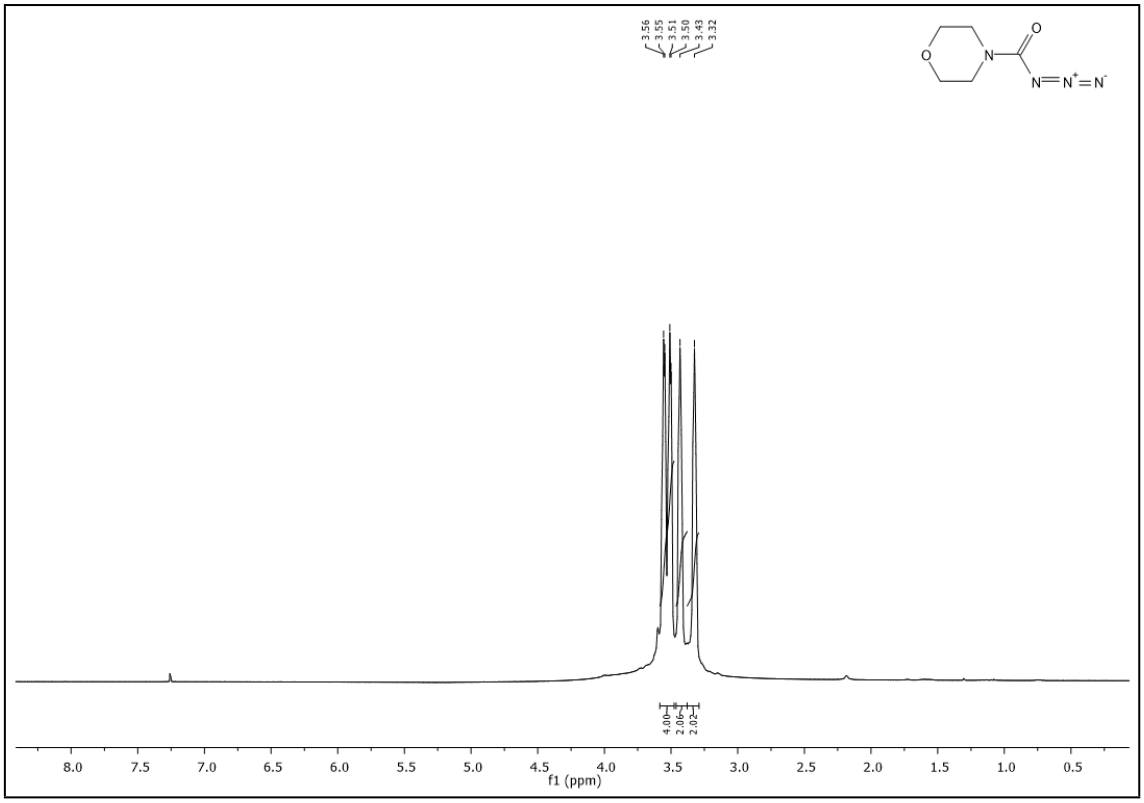
Table S8. Bond lengths [Å] and angles [°] for 8.

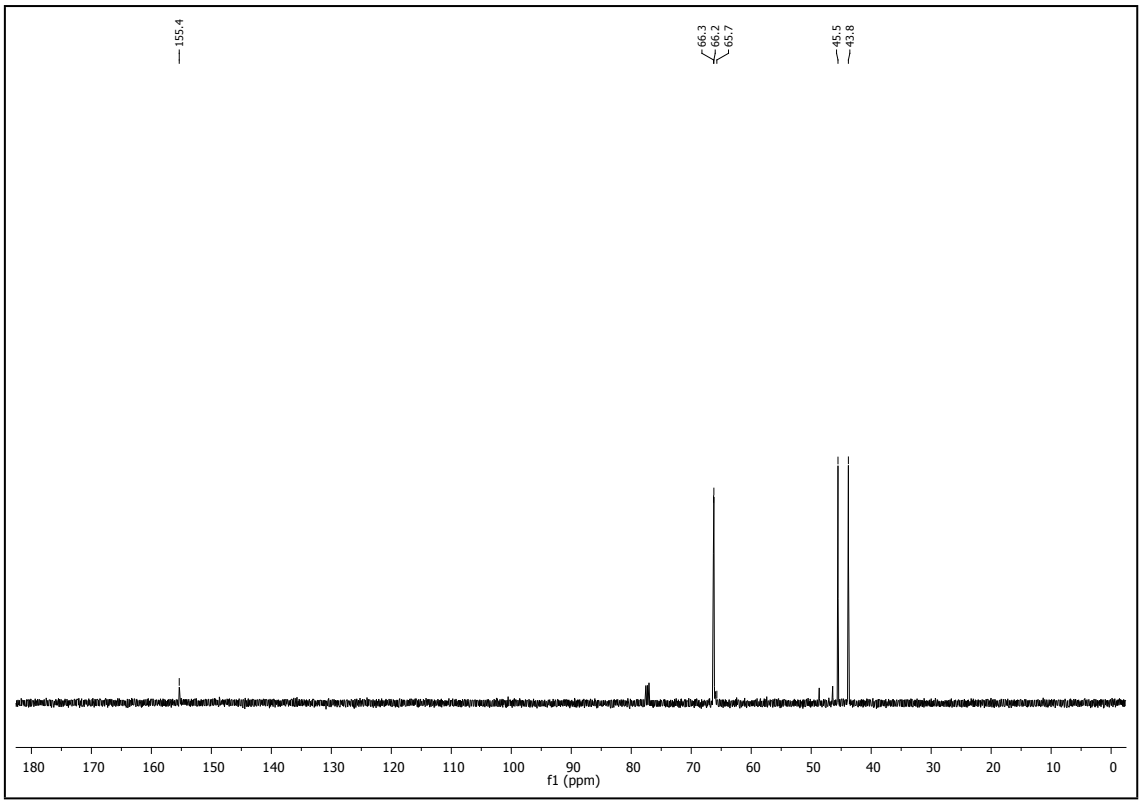
O(1)-C(1)	1.206(3)	C(4)-O(2)-C(3)	109.65(15)
O(2)-C(4)	1.421(2)	C(9)-O(3)-C(8)	112.16(16)
O(2)-C(3)	1.427(3)	C(6)-N(1)-N(2)	110.53(14)
O(3)-C(9)	1.418(3)	C(6)-N(1)-C(1)	125.74(16)
O(3)-C(8)	1.425(2)	N(2)-N(1)-C(1)	123.34(14)
N(1)-C(6)	1.348(2)	N(3)-N(2)-N(1)	106.67(14)
N(1)-N(2)	1.361(2)	N(2)-N(3)-C(7)	109.35(15)
N(1)-C(1)	1.452(2)	C(1)-N(4)-C(2)	116.51(16)
N(2)-N(3)	1.306(2)	C(1)-N(4)-C(5)	125.53(16)
N(3)-C(7)	1.368(3)	C(2)-N(4)-C(5)	112.57(15)
N(4)-C(1)	1.347(3)	O(1)-C(1)-N(4)	126.9(2)
N(4)-C(2)	1.468(2)	O(1)-C(1)-N(1)	117.73(18)
N(4)-C(5)	1.473(3)	N(4)-C(1)-N(1)	115.34(17)
C(2)-C(3)	1.511(3)	N(4)-C(2)-C(3)	108.93(16)
C(2)-H(2A)	0.9900	N(4)-C(2)-H(2A)	109.9
C(2)-H(2B)	0.9900	C(3)-C(2)-H(2A)	109.9
C(3)-H(3A)	0.9900	N(4)-C(2)-H(2B)	109.9
C(3)-H(3B)	0.9900	C(3)-C(2)-H(2B)	109.9
C(4)-C(5)	1.507(3)	H(2A)-C(2)-H(2B)	108.3
C(4)-H(4A)	0.9900	O(2)-C(3)-C(2)	111.91(17)
C(4)-H(4B)	0.9900	O(2)-C(3)-H(3A)	109.2
C(5)-H(5A)	0.9900	C(2)-C(3)-H(3A)	109.2
C(5)-H(5B)	0.9900	O(2)-C(3)-H(3B)	109.2
C(6)-C(7)	1.358(3)	C(2)-C(3)-H(3B)	109.2
C(6)-H(6)	0.9500	H(3A)-C(3)-H(3B)	107.9
C(7)-C(8)	1.498(3)	O(2)-C(4)-C(5)	111.12(17)
C(8)-H(8A)	0.9900	O(2)-C(4)-H(4A)	109.4
C(8)-H(8B)	0.9900	C(5)-C(4)-H(4A)	109.4
C(9)-H(9A)	0.9800	O(2)-C(4)-H(4B)	109.4
C(9)-H(9B)	0.9800	C(5)-C(4)-H(4B)	109.4
C(9)-H(9C)	0.9800	H(4A)-C(4)-H(4B)	108.0
		N(4)-C(5)-C(4)	109.37(15)

N(4)-C(5)-H(5A)	109.8
C(4)-C(5)-H(5A)	109.8
N(4)-C(5)-H(5B)	109.8
C(4)-C(5)-H(5B)	109.8
H(5A)-C(5)-H(5B)	108.2
N(1)-C(6)-C(7)	105.21(17)
N(1)-C(6)-H(6)	127.4
C(7)-C(6)-H(6)	127.4
C(6)-C(7)-N(3)	108.22(17)
C(6)-C(7)-C(8)	130.46(18)
N(3)-C(7)-C(8)	121.31(17)
O(3)-C(8)-C(7)	113.19(15)
O(3)-C(8)-H(8A)	108.9
C(7)-C(8)-H(8A)	108.9
O(3)-C(8)-H(8B)	108.9
C(7)-C(8)-H(8B)	108.9
H(8A)-C(8)-H(8B)	107.8
O(3)-C(9)-H(9A)	109.5
O(3)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
O(3)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5

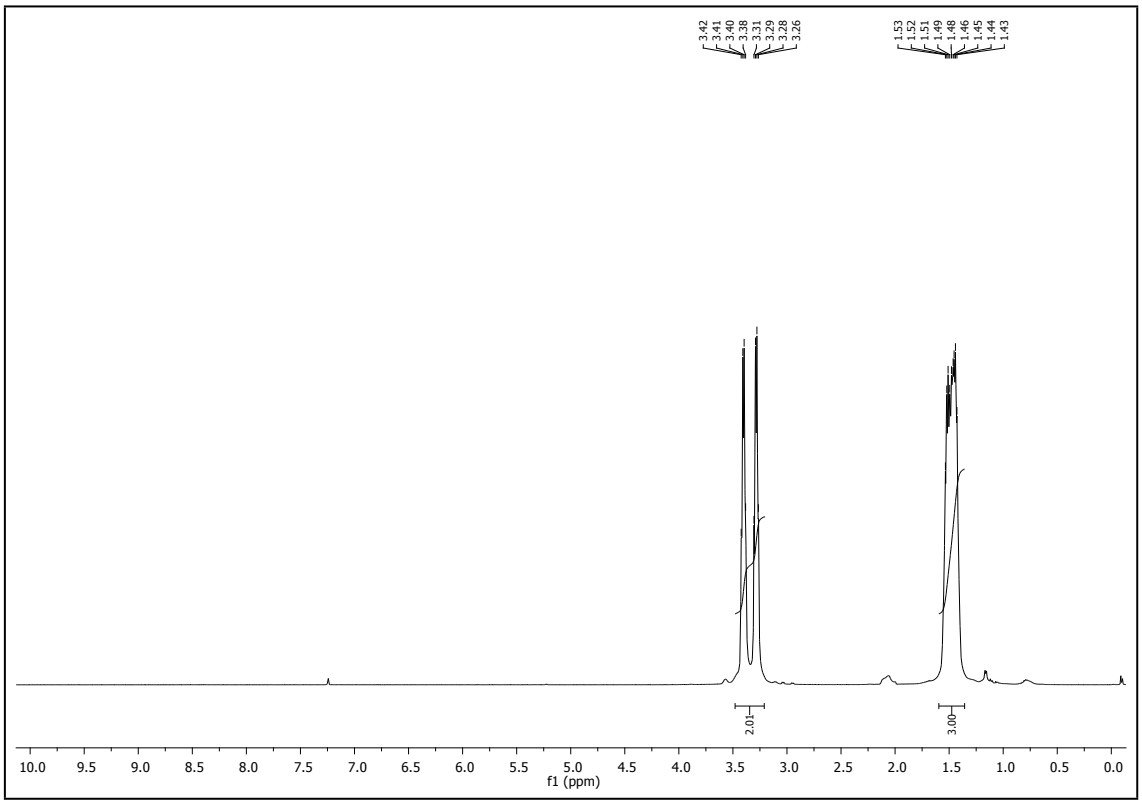
NMR spectra of compounds.

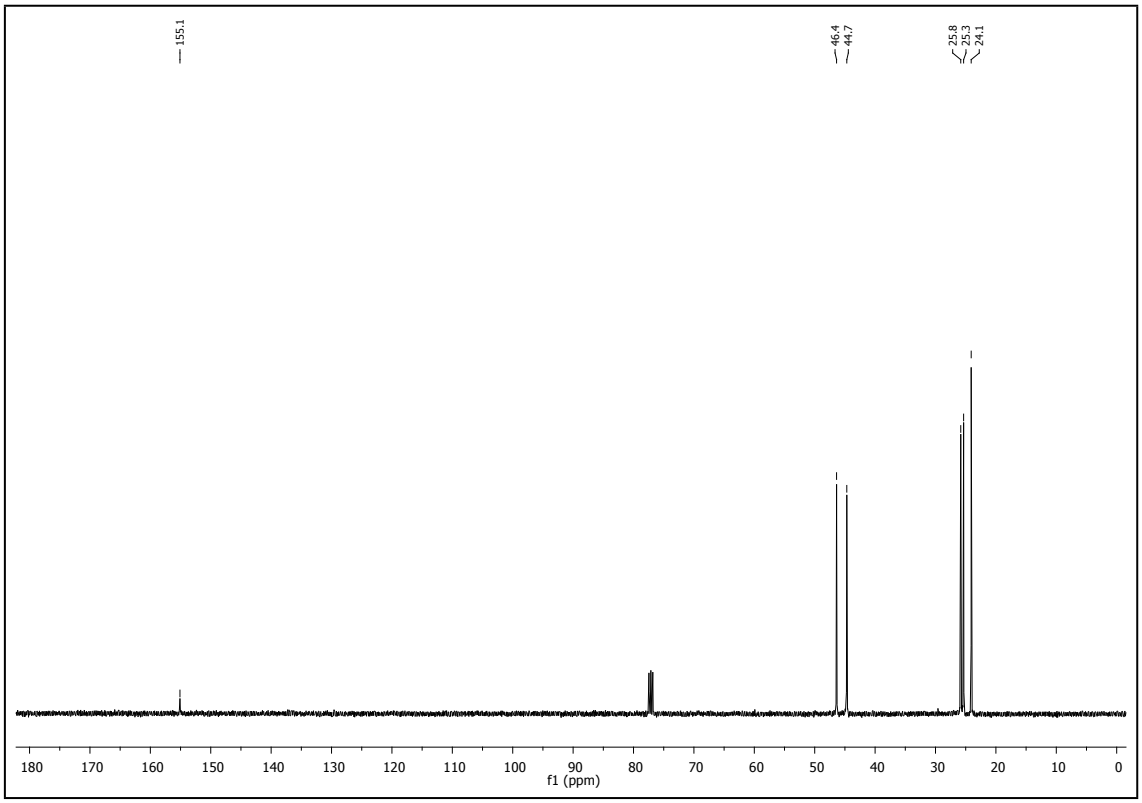
N-Morpholino-carbamoyl azide



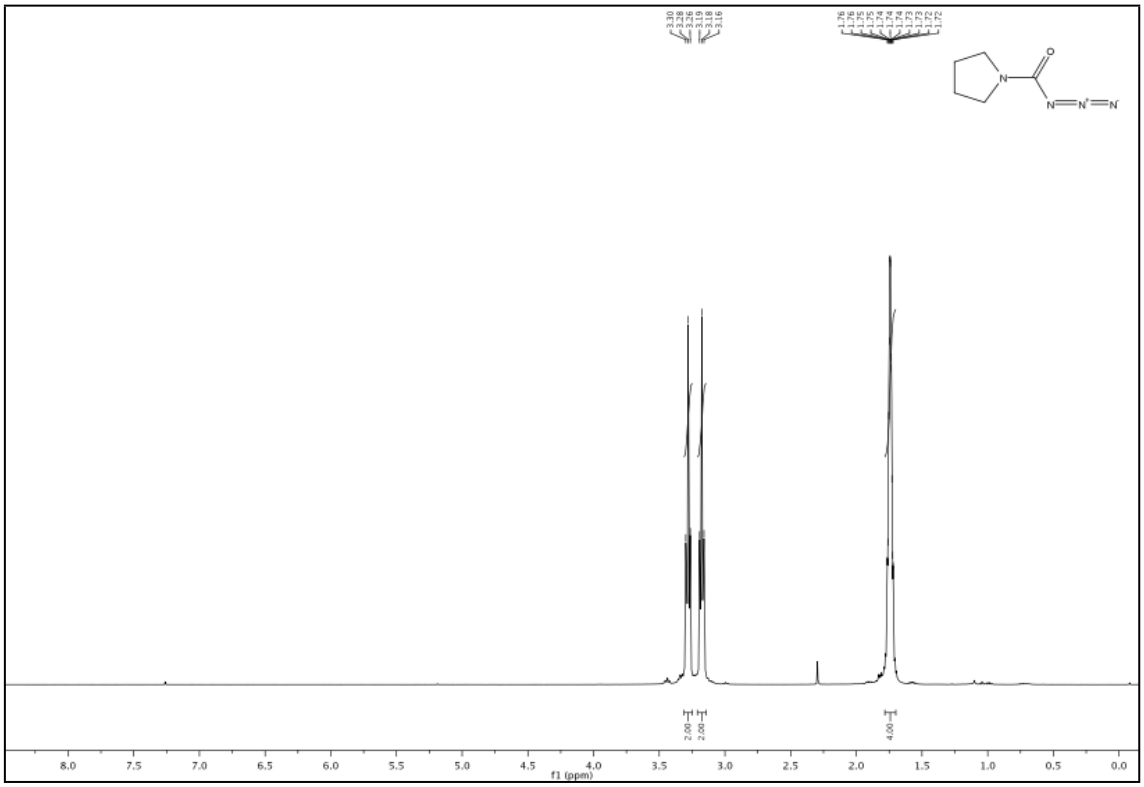


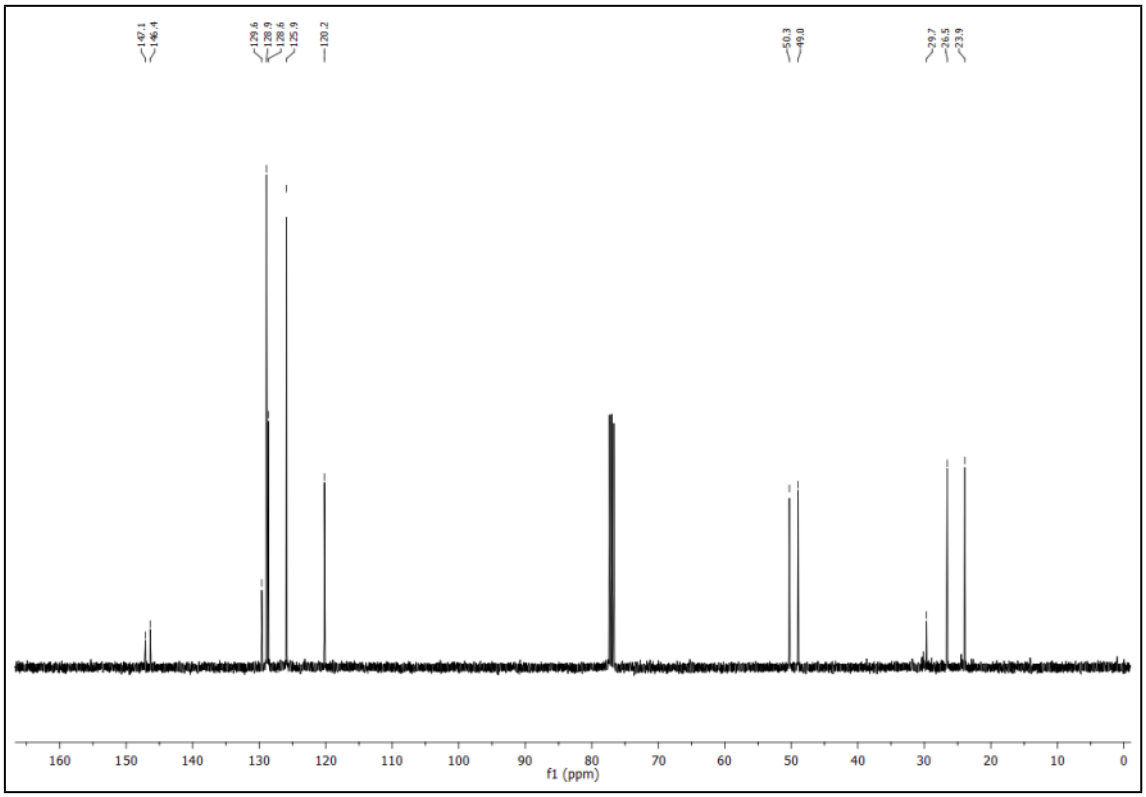
N-Piperidino-carbamoyl azide



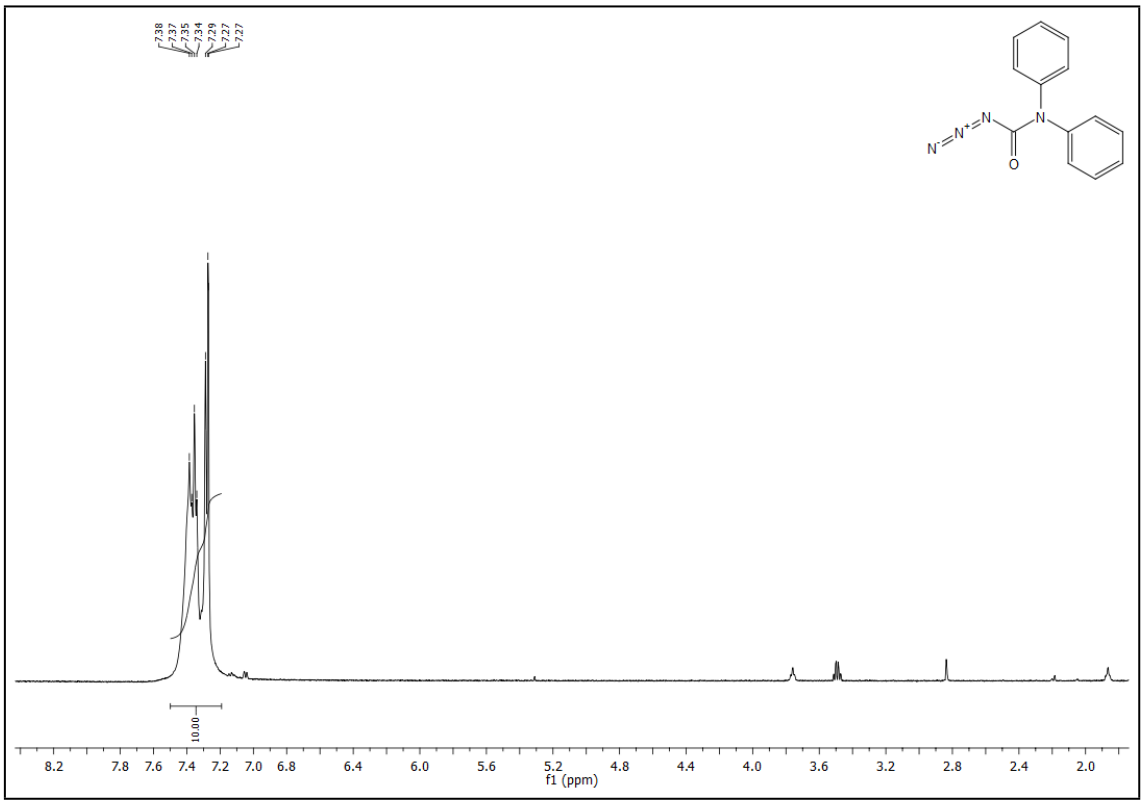


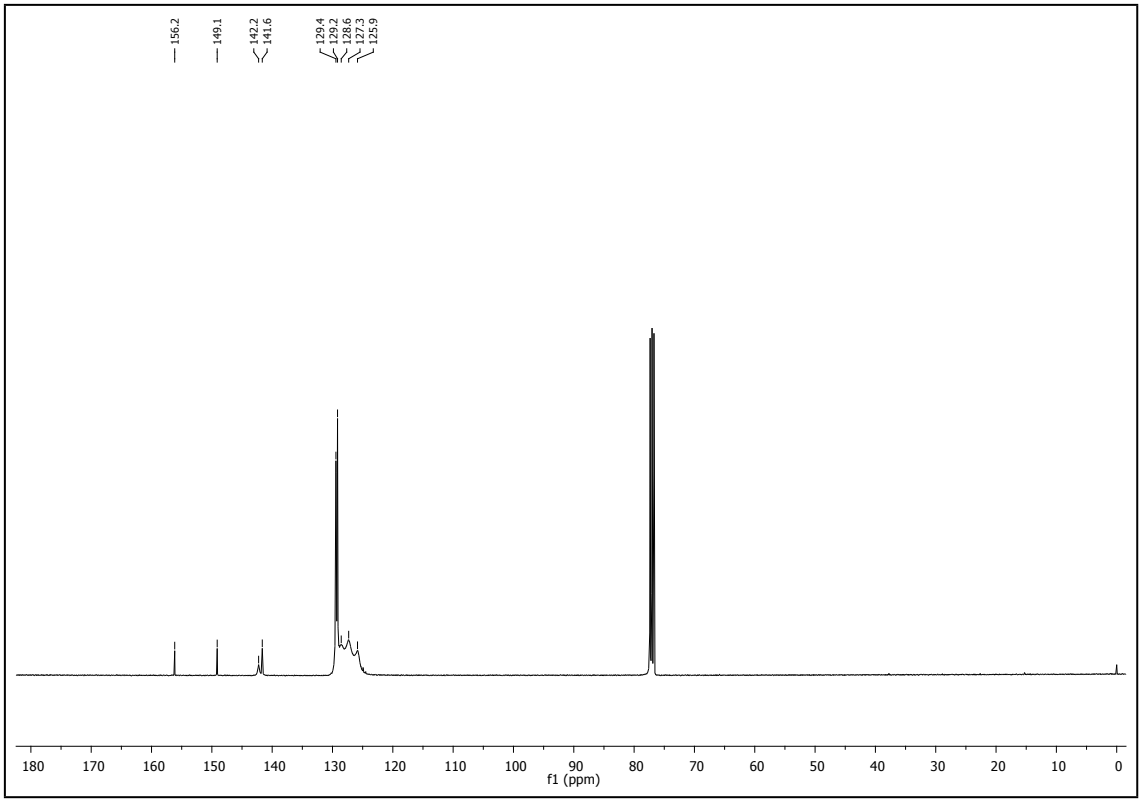
N-Pyrrolidinocarbamoyl azide



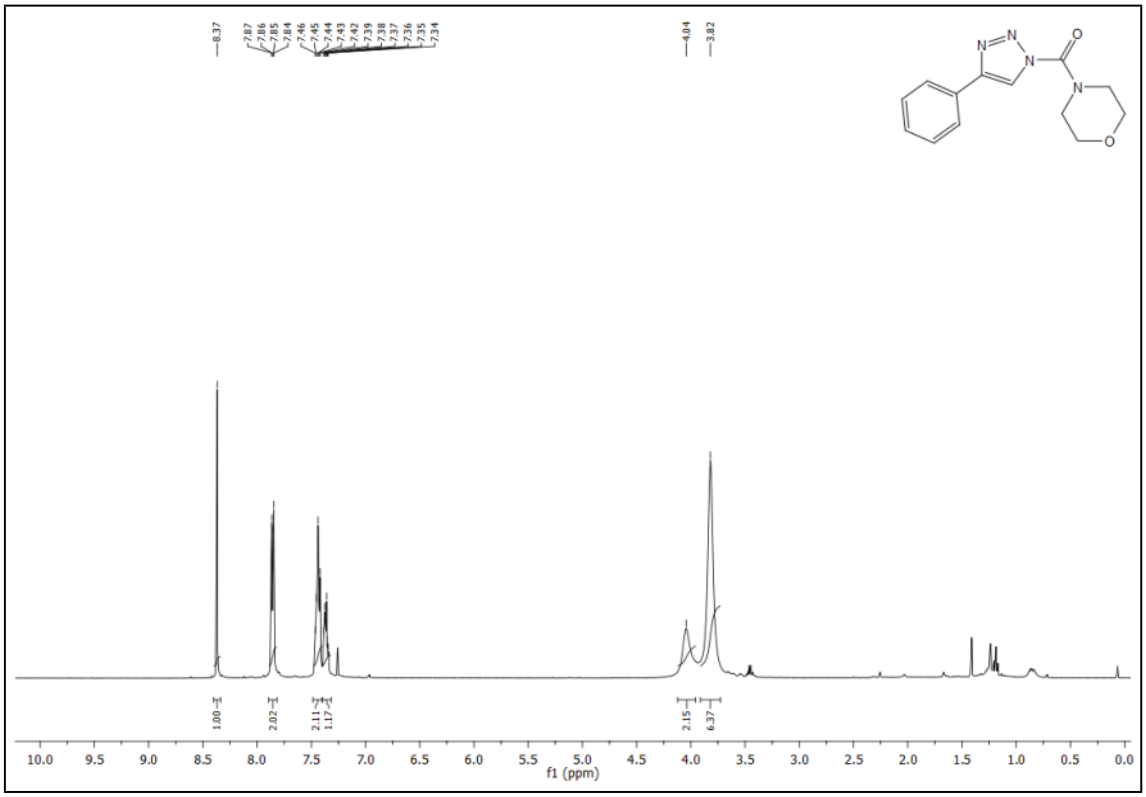


N,N-Diphenylcarbamoyl azide

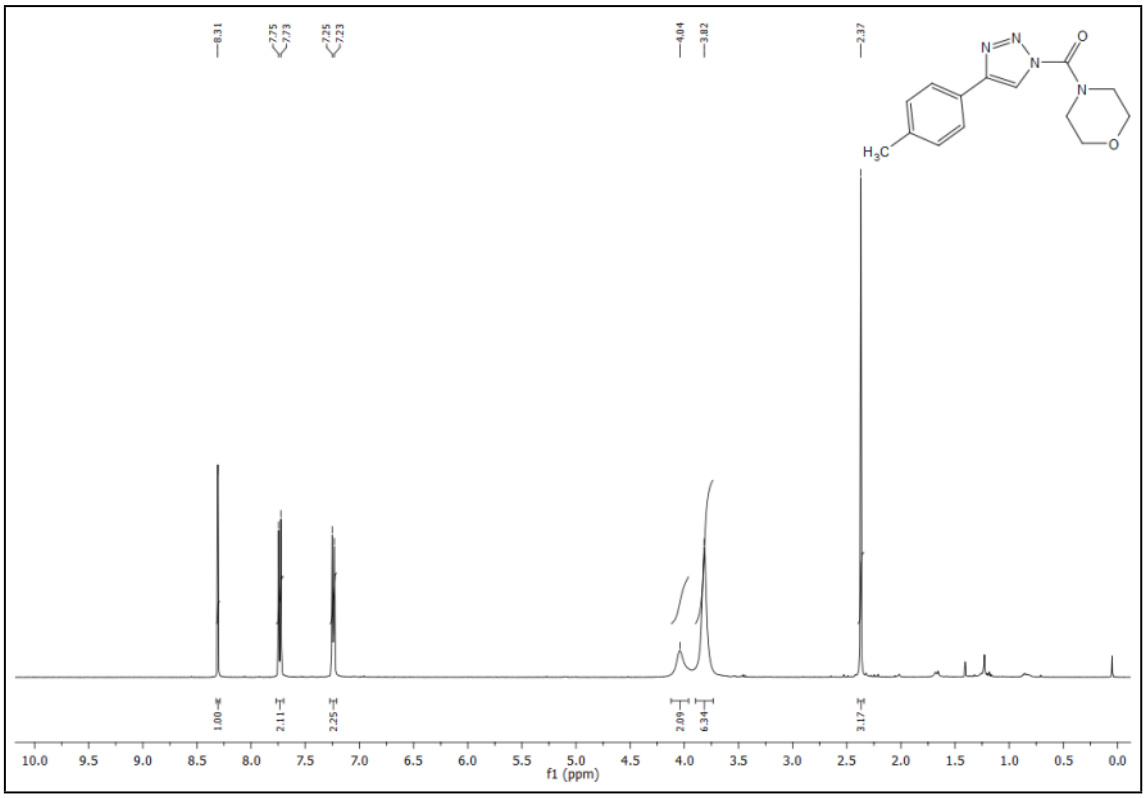


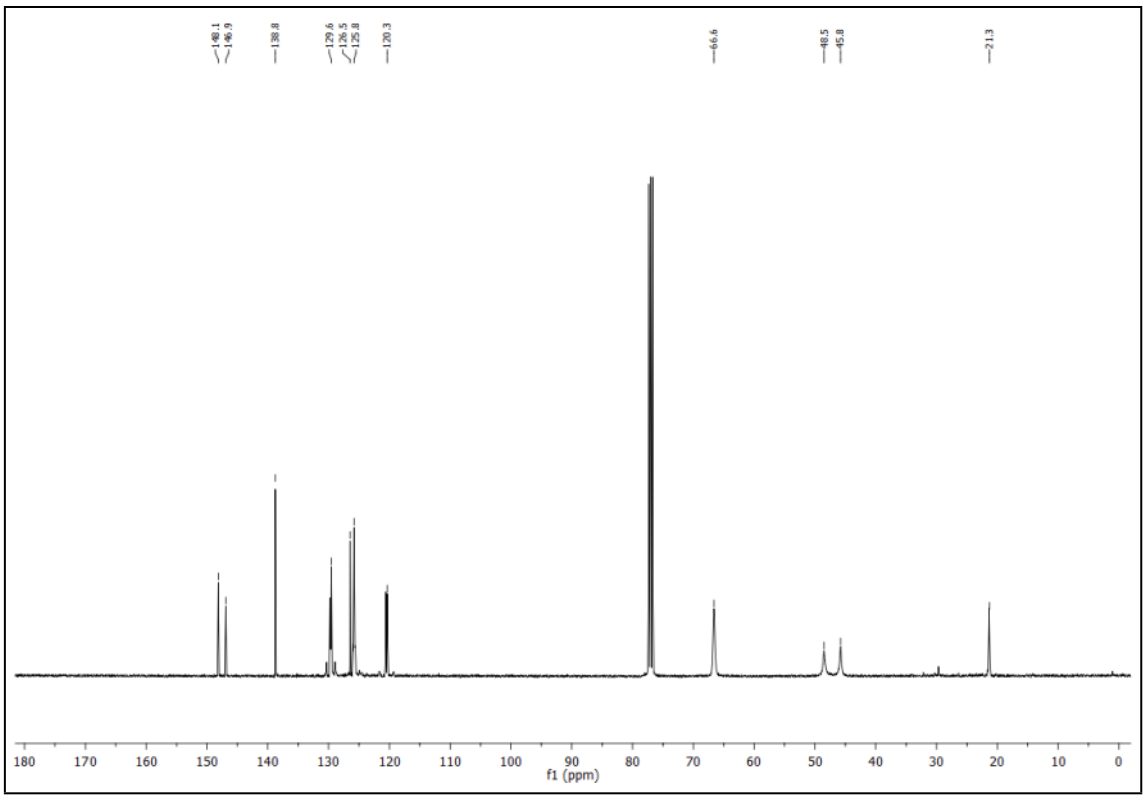


1-(N-Morpholinocarbamoyl)-4-phenyl-1H-1,2,3-triazol (Scheme 2, 1)

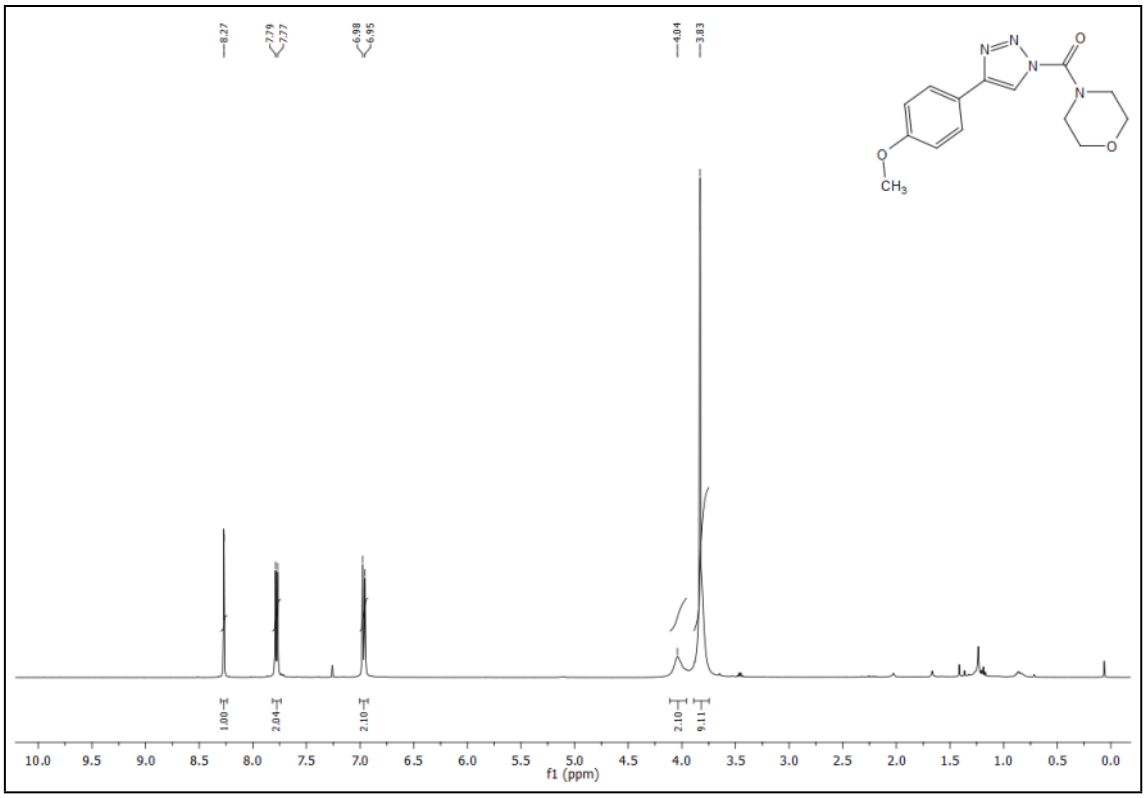


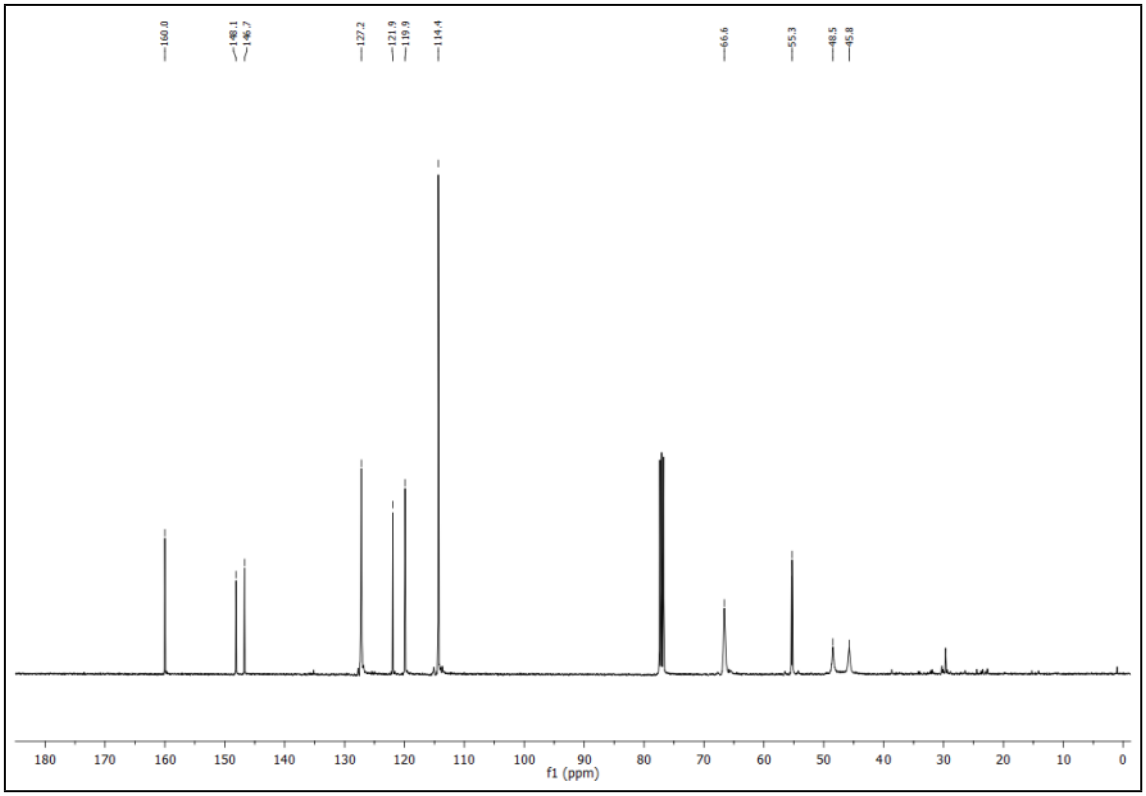
1-(N-Morpholinocarbamoyl)-4-(4-methylphenyl)-1H-1,2,3-triazol (Scheme 2, 2)



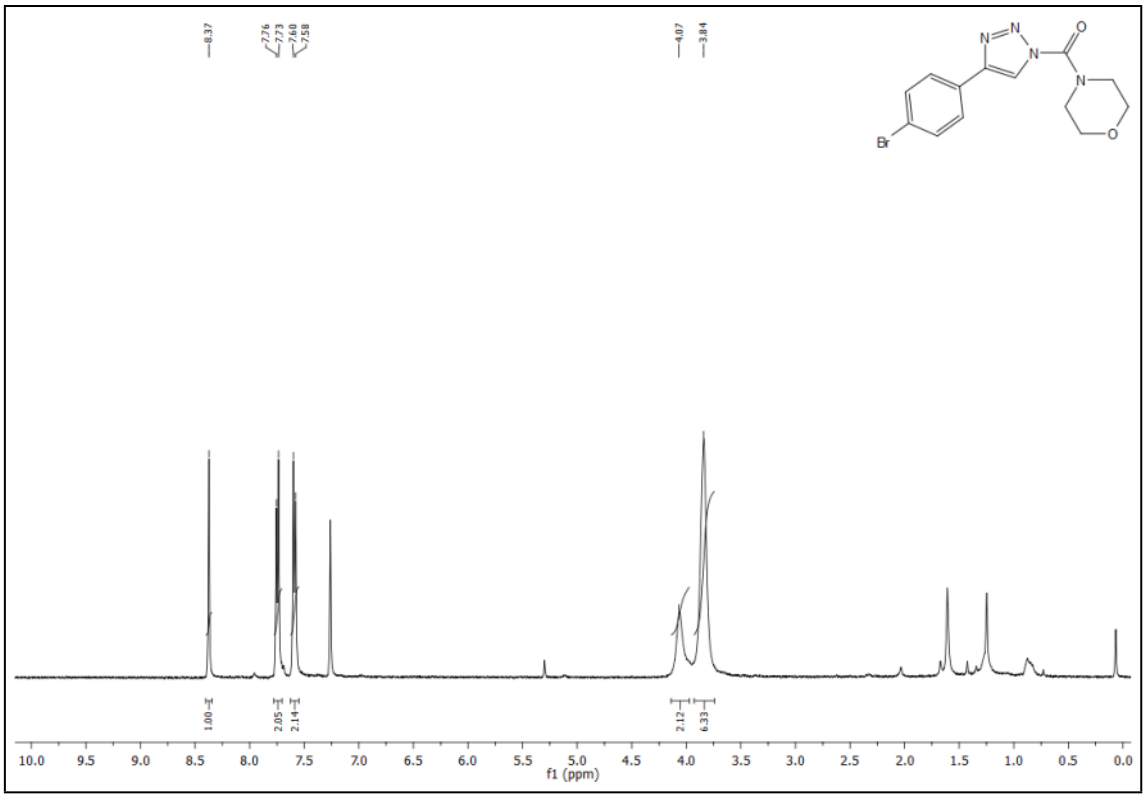


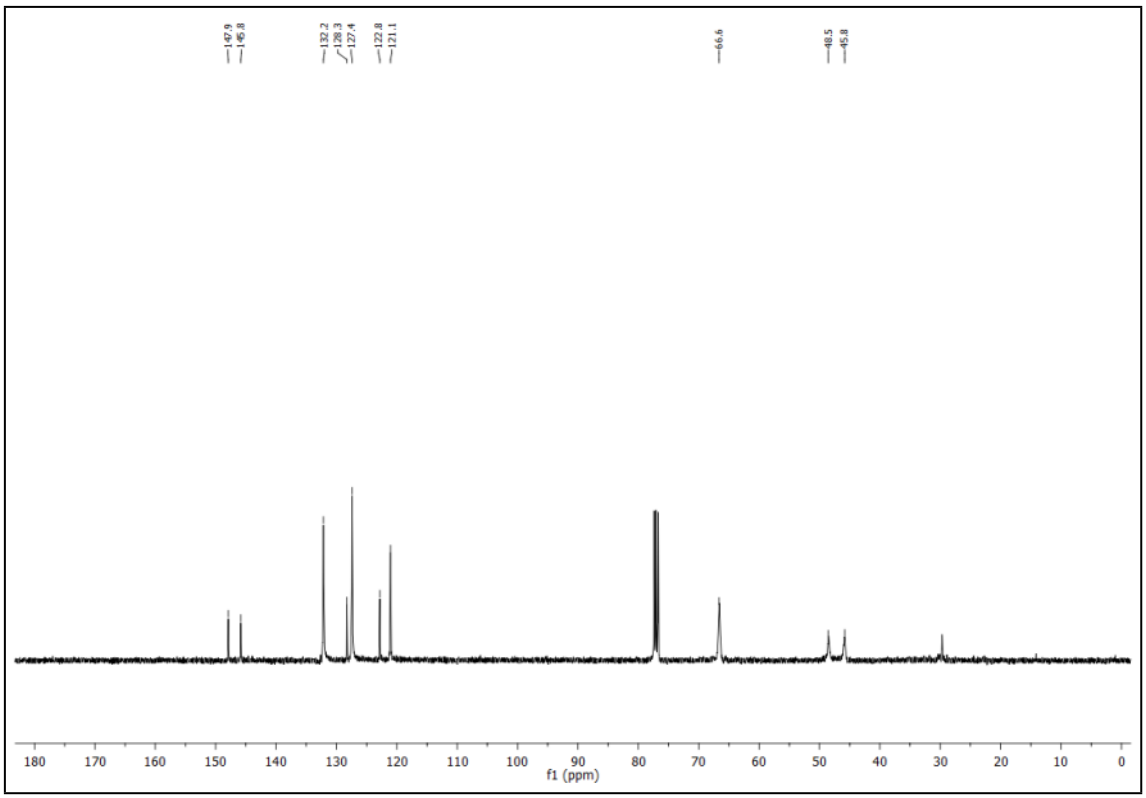
1-(N-Morpholinocarbamoyl)-4-(4-methoxyphenyl)-1H-1,2,3-triazol (Scheme 2, 3)



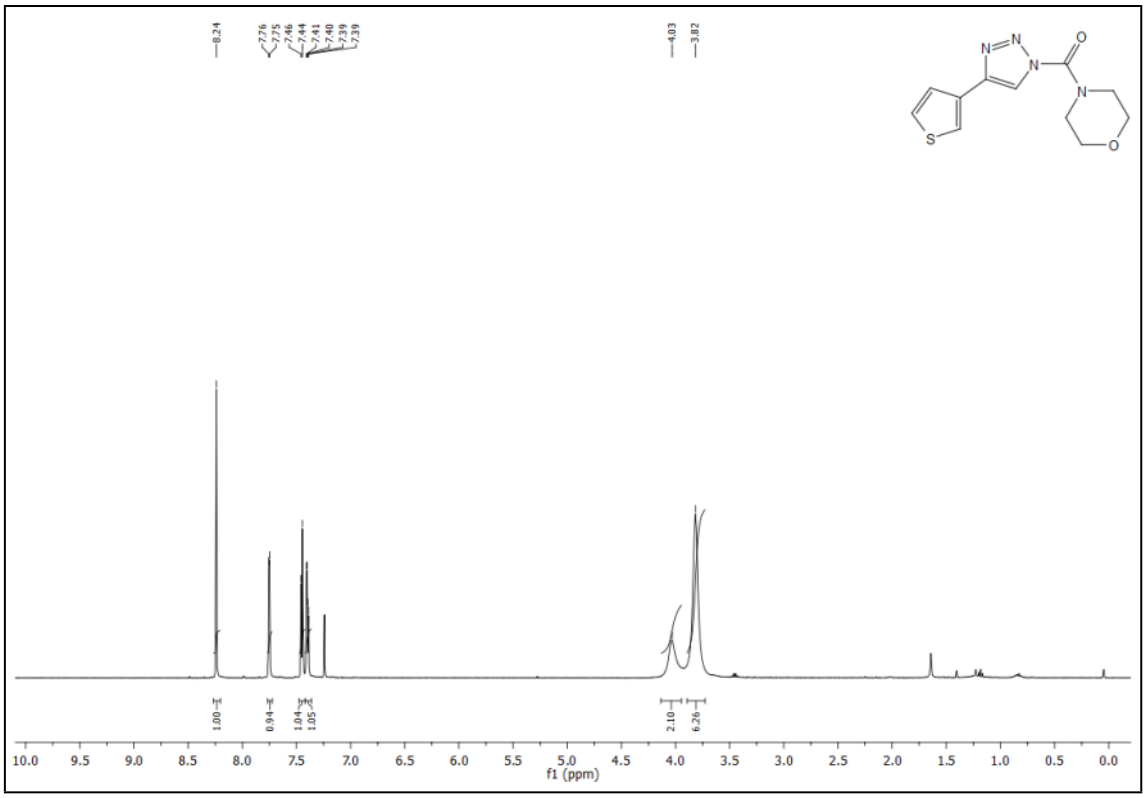


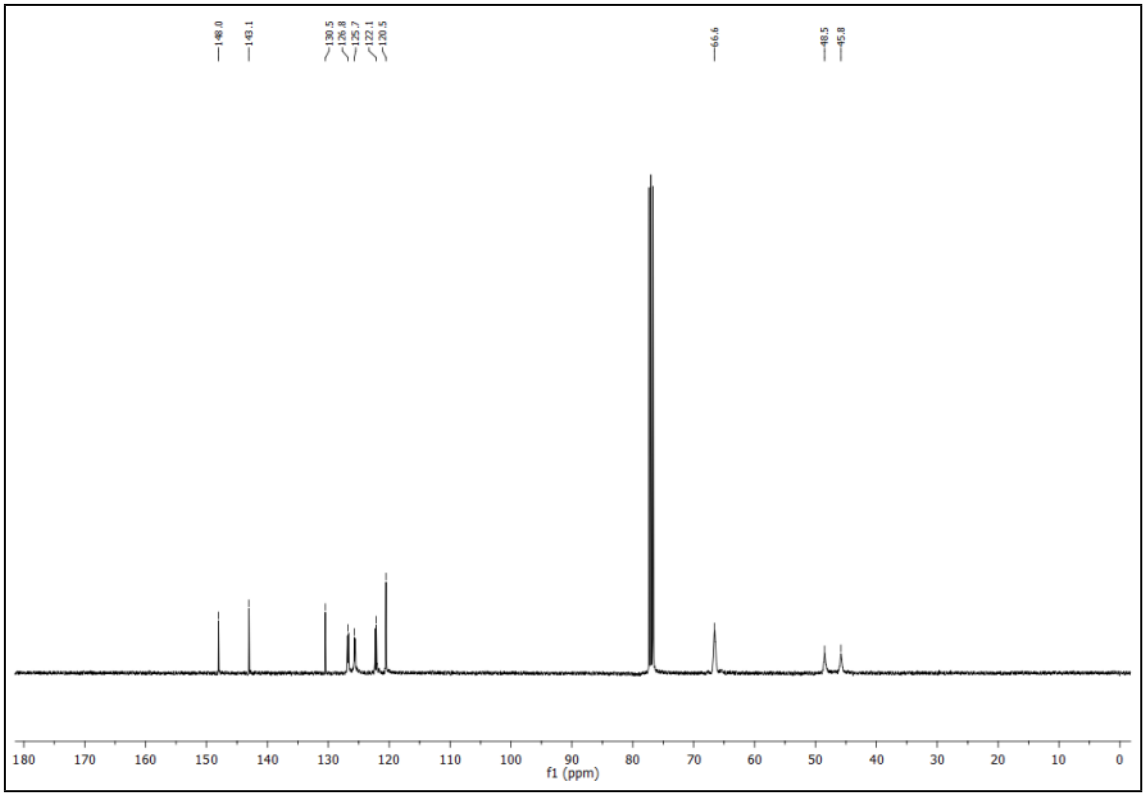
1-(N-Morpholinocarbamoyl)-4-(4-bromophenyl)-1H-1,2,3-triazol (Scheme 2, 4)



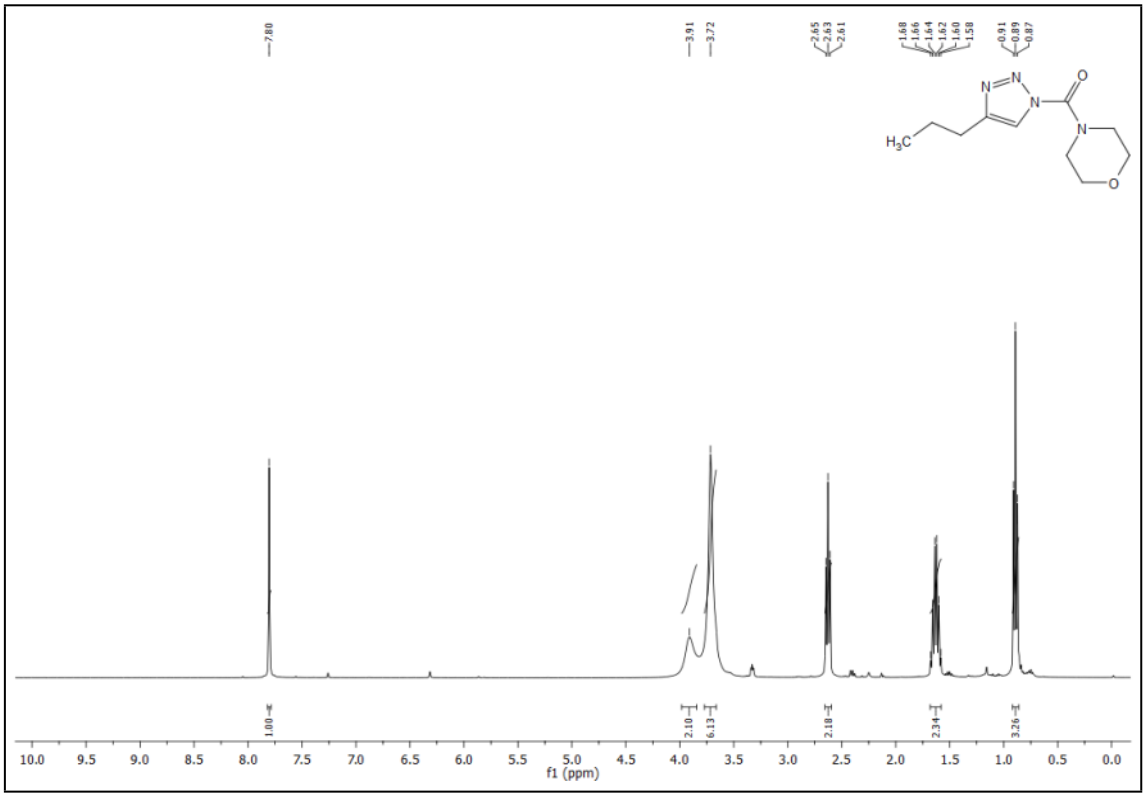


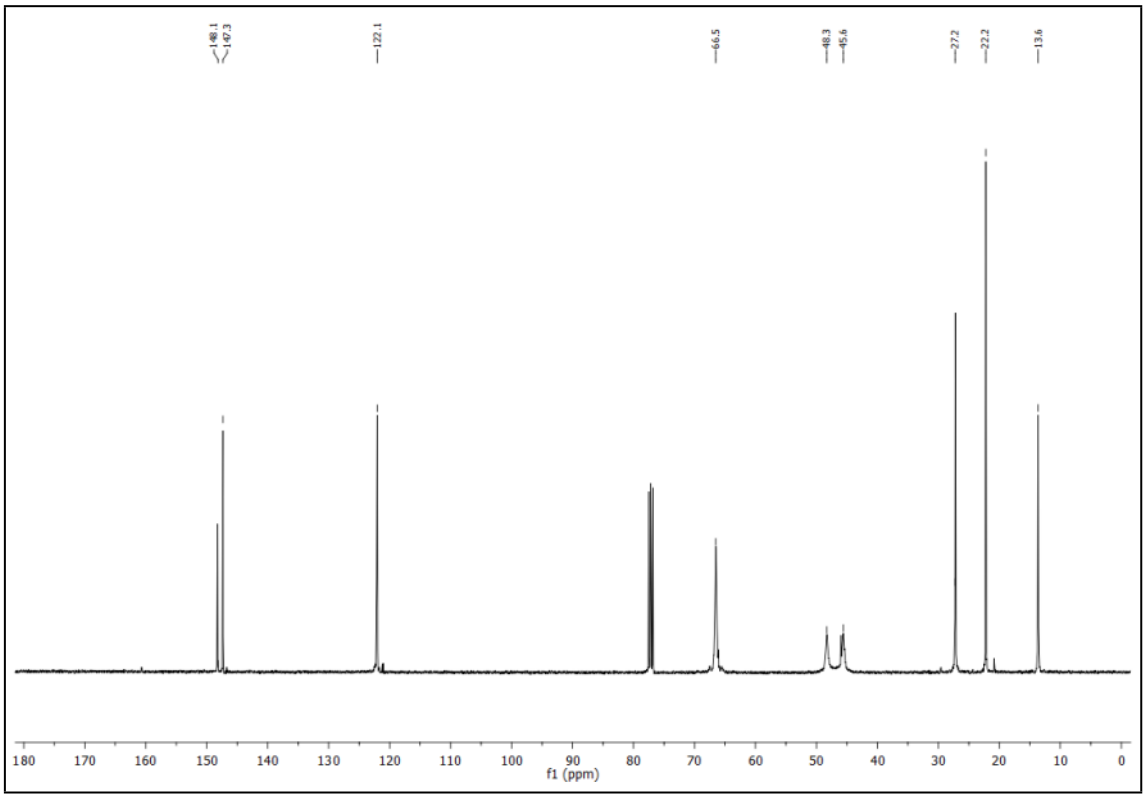
1-(N-Morpholinocarbamoyl)-4-(thien-3-yl)-1H-1,2,3-triazol (Scheme 2, 5)


8.24
7.76
7.75
7.46
7.44
7.41
7.40
7.39
7.39
4.03
3.82
N
N
N
O
N
O
S
1.00
0.94
1.04
1.05
2.10
6.26
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)

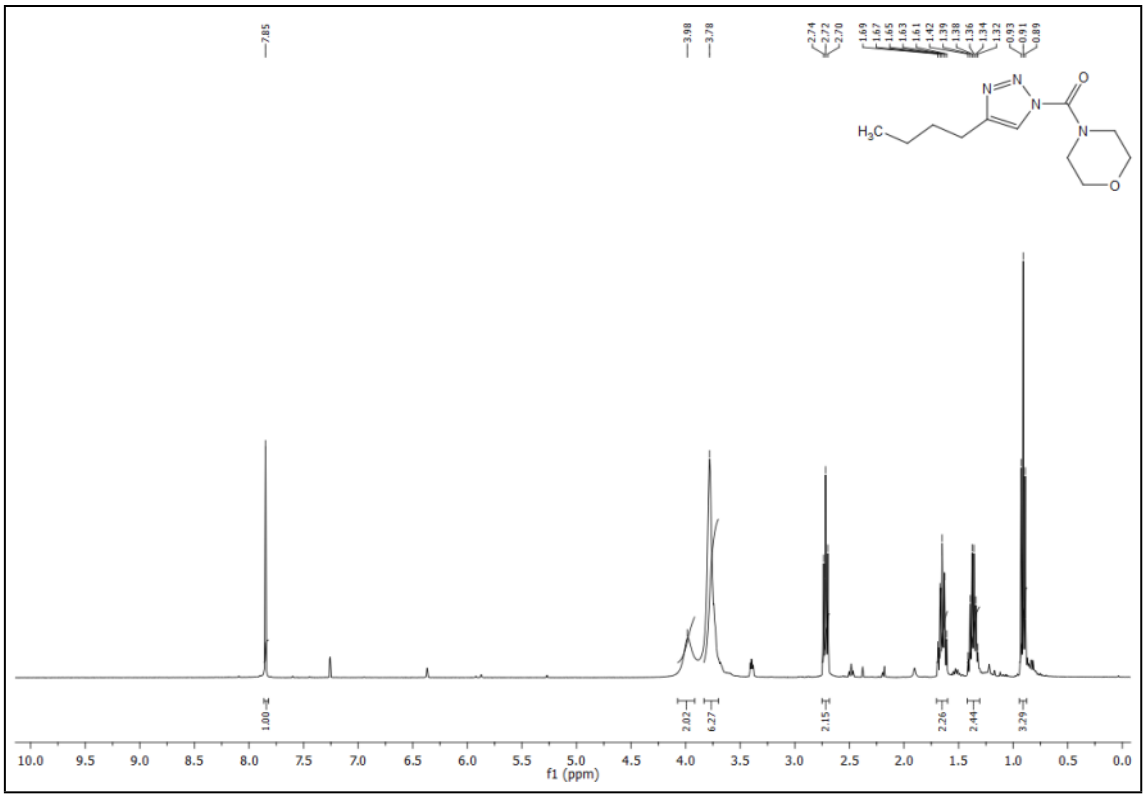

148.0
143.1
130.5
126.8
125.7
122.1
120.5
66.6
48.5
45.8
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

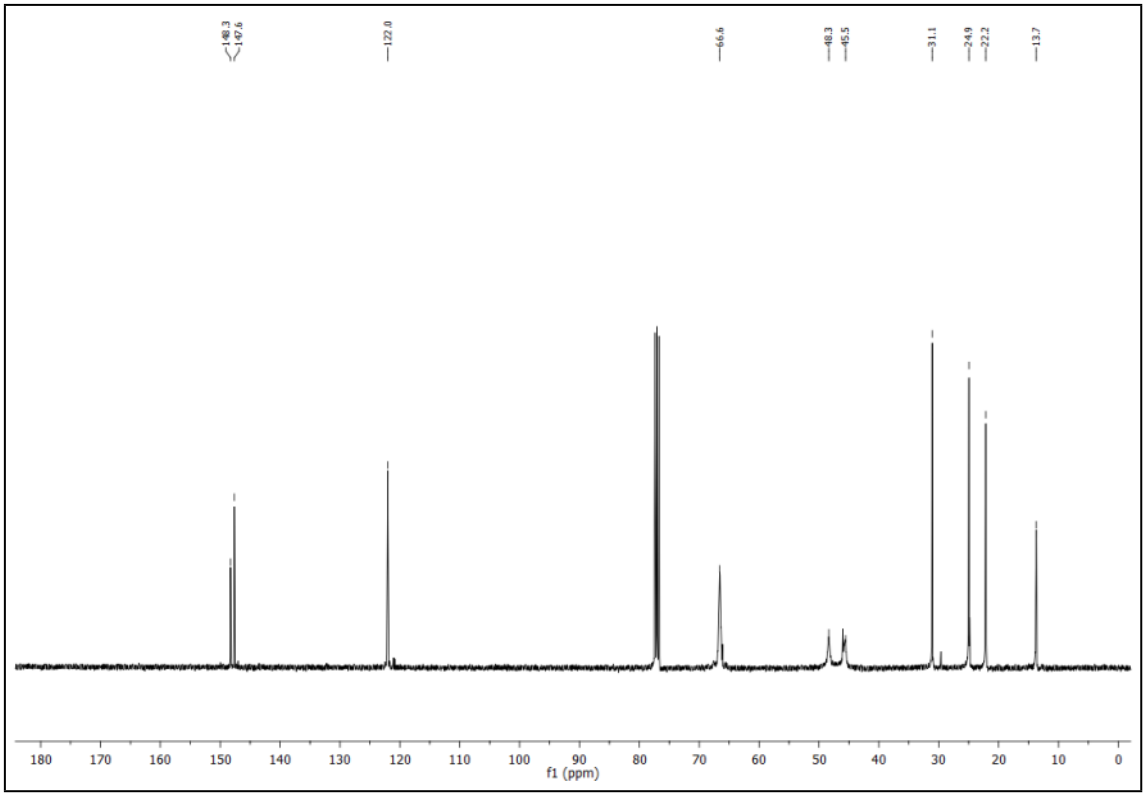
1-(N-Morpholinocarbamoyl)-4-*n*-propyl-1H-1,2,3-triazol (Scheme 2, 6)



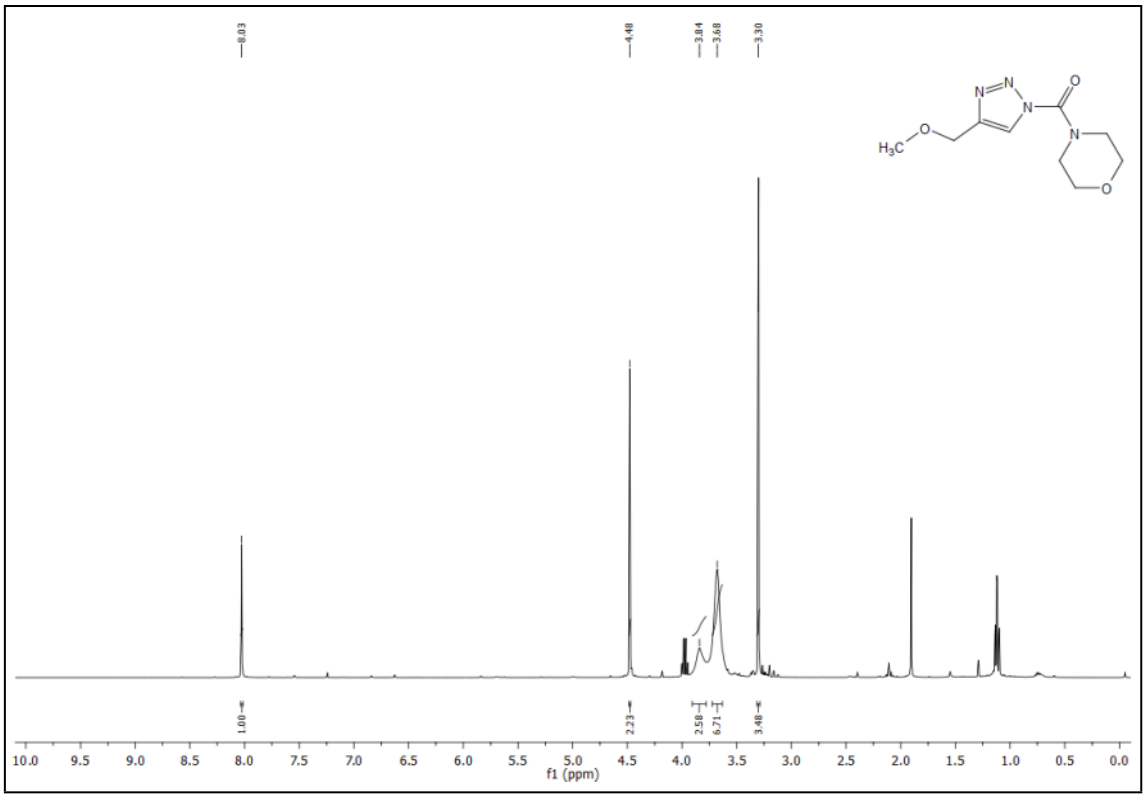


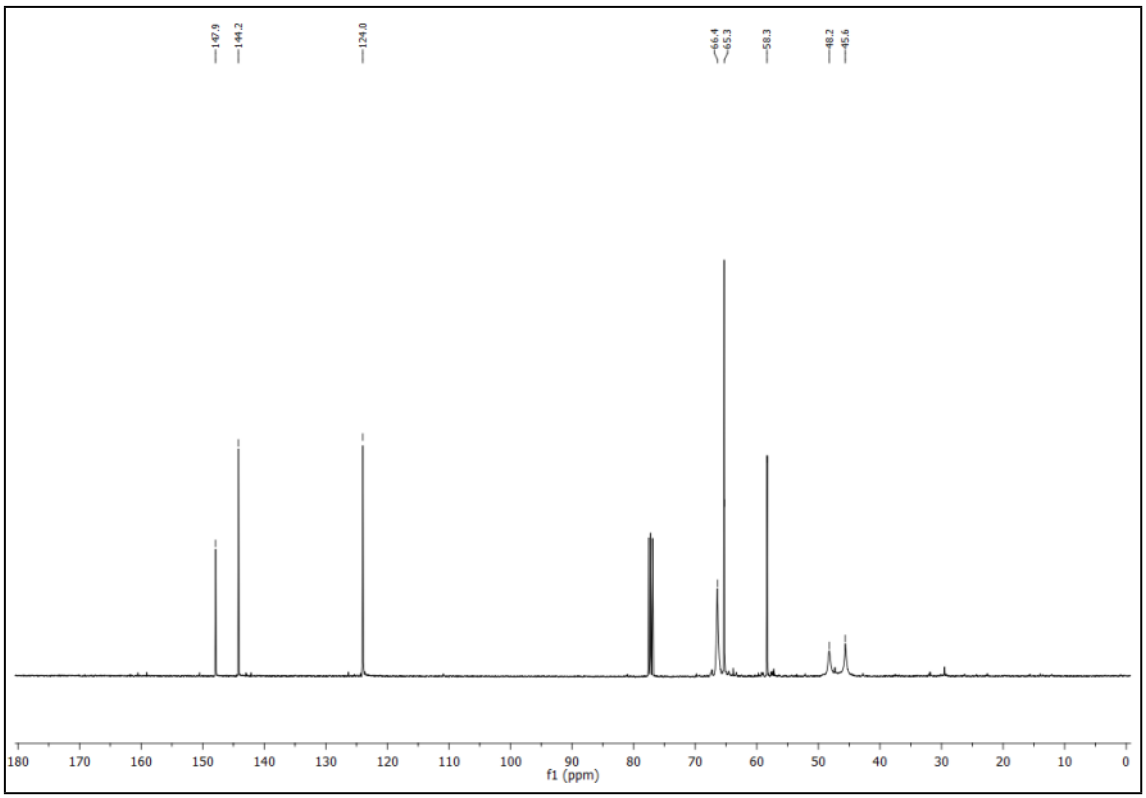
1-(N-Morpholinocarbamoyl)-4-*n*-butyl-1H-1,2,3-triazol (Scheme 2, 7)



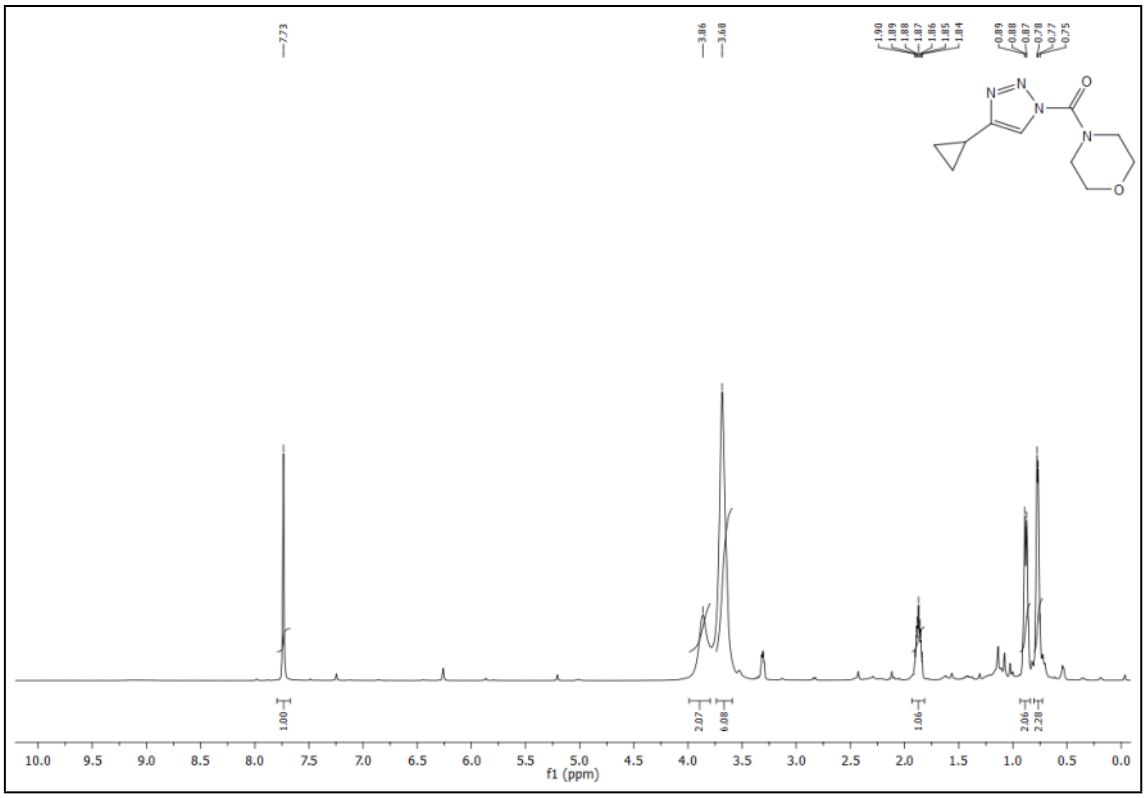


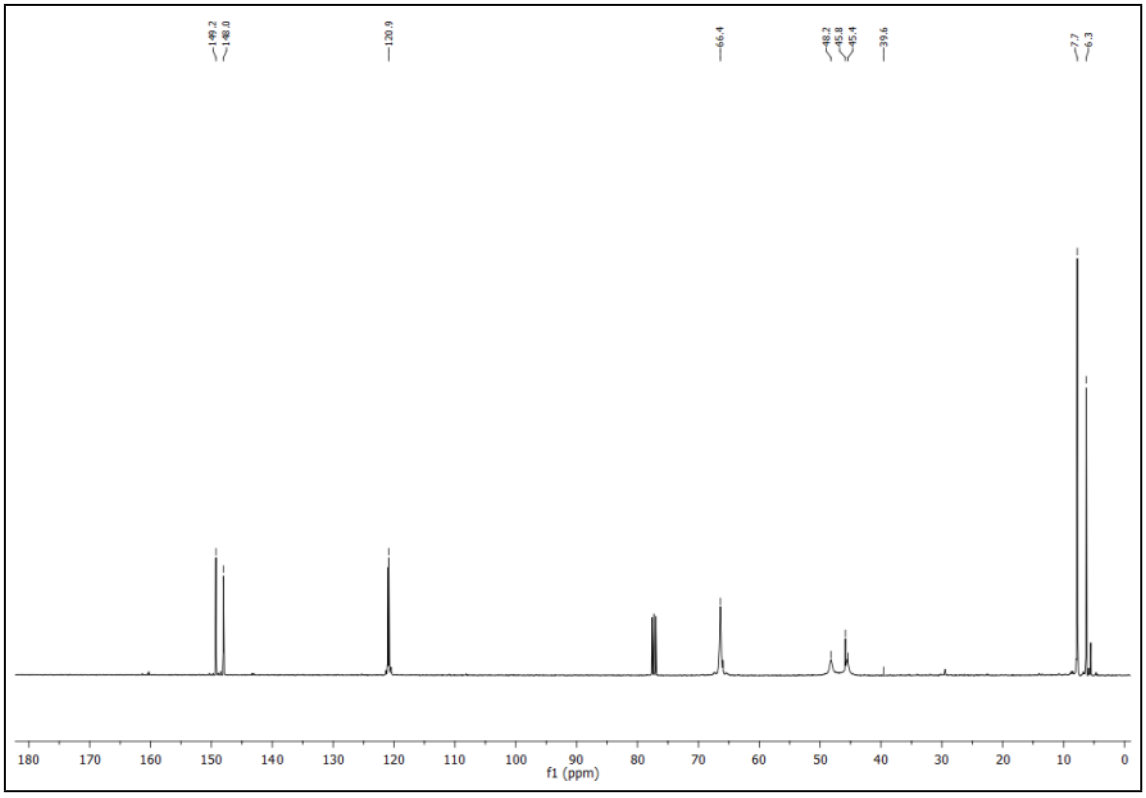
1-(N-Morpholinocarbamoyl)-4-(methoxymethyl)-1H-1,2,3-triazol (Scheme 2, 8)



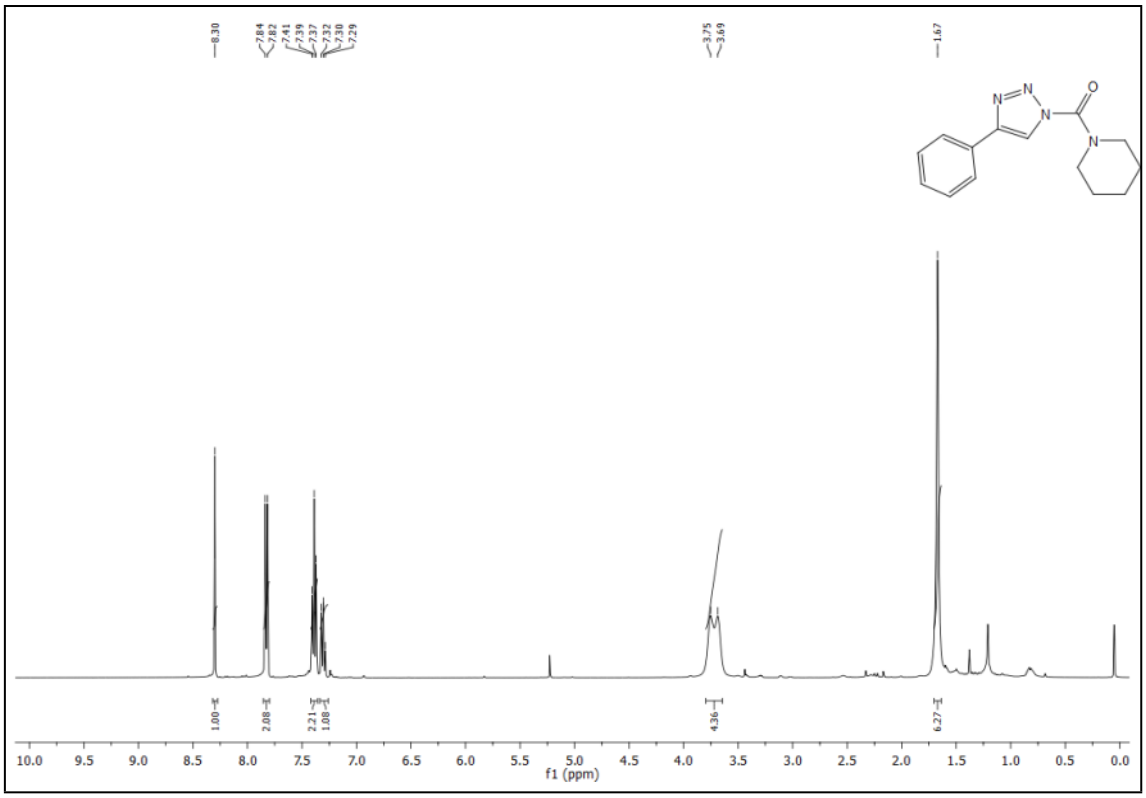


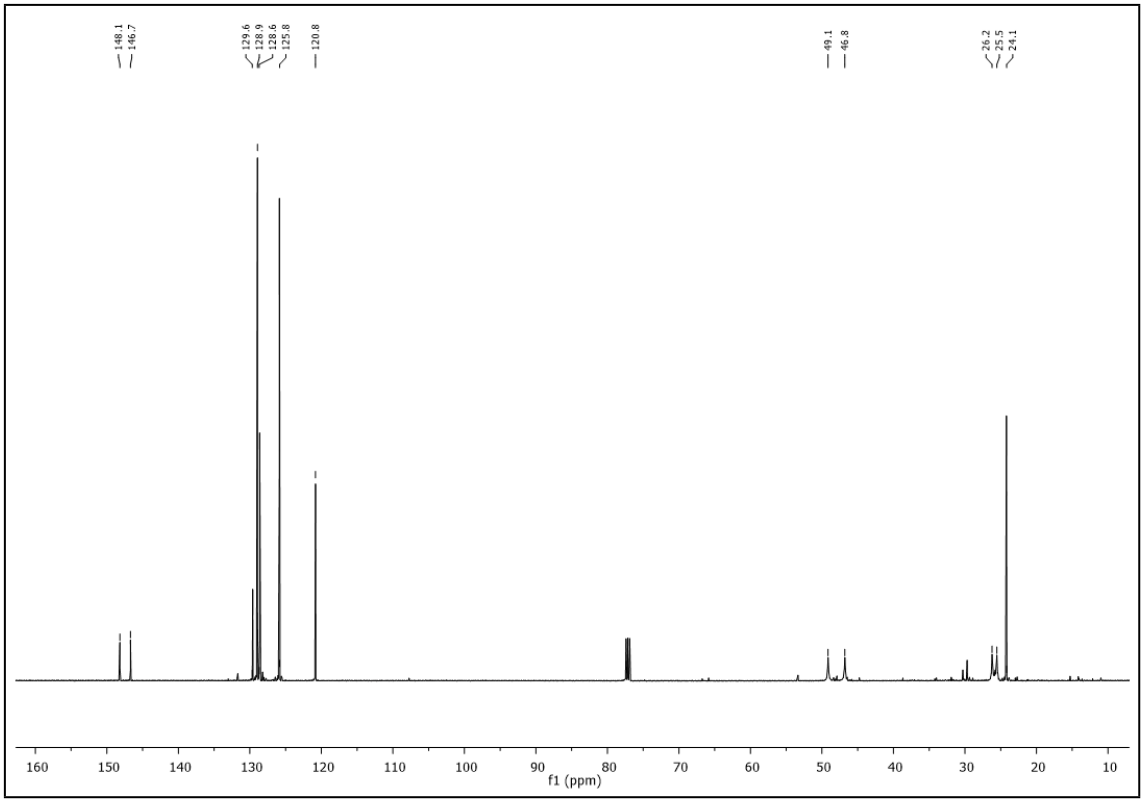
1-(N-Morpholinocarbamoyl)-4-cyclopropyl-1H-1,2,3-triazol (Scheme 2, 9)



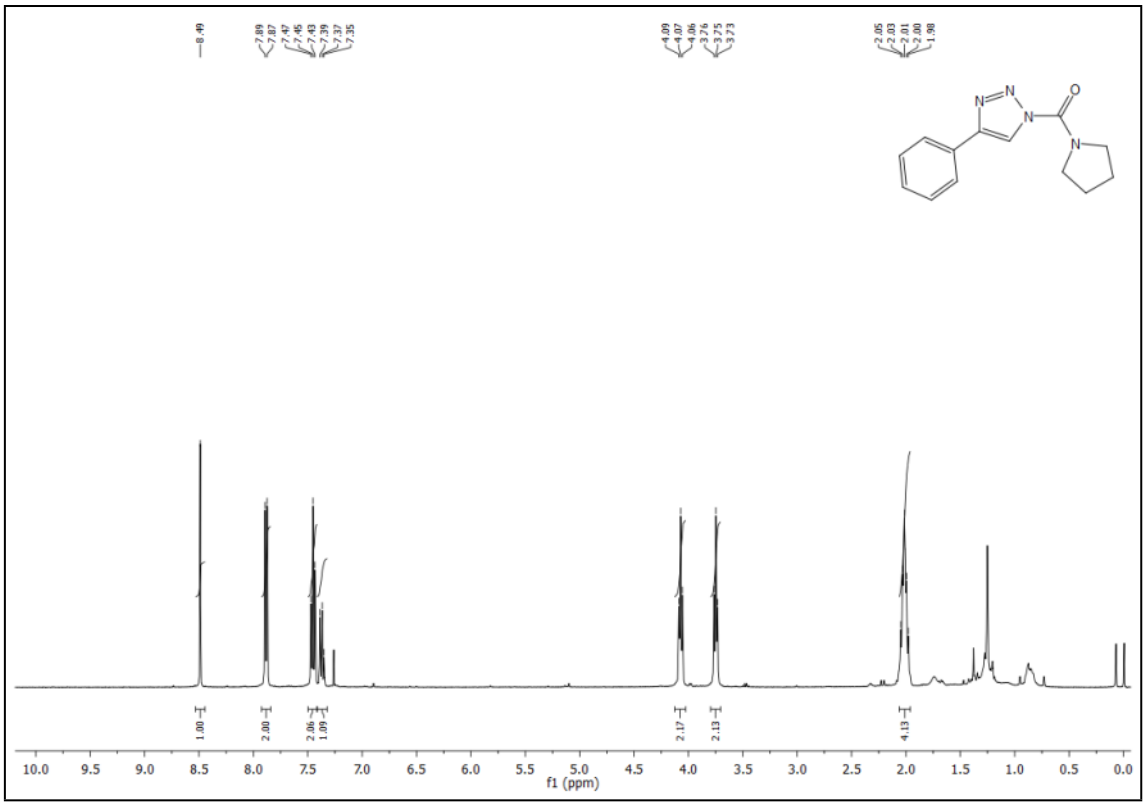


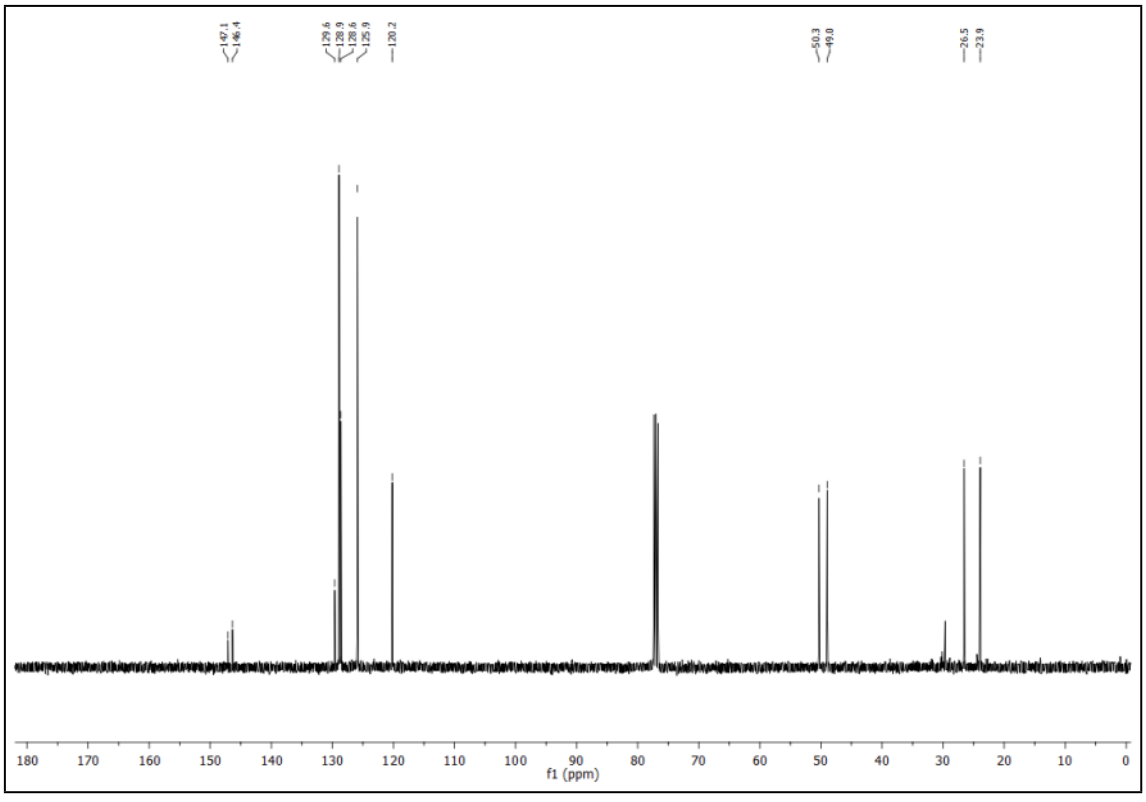
1-(N-Piperidinocarbamoyl)-4-phenyl-1H-1,2,3-triazol (Scheme 2, 10)



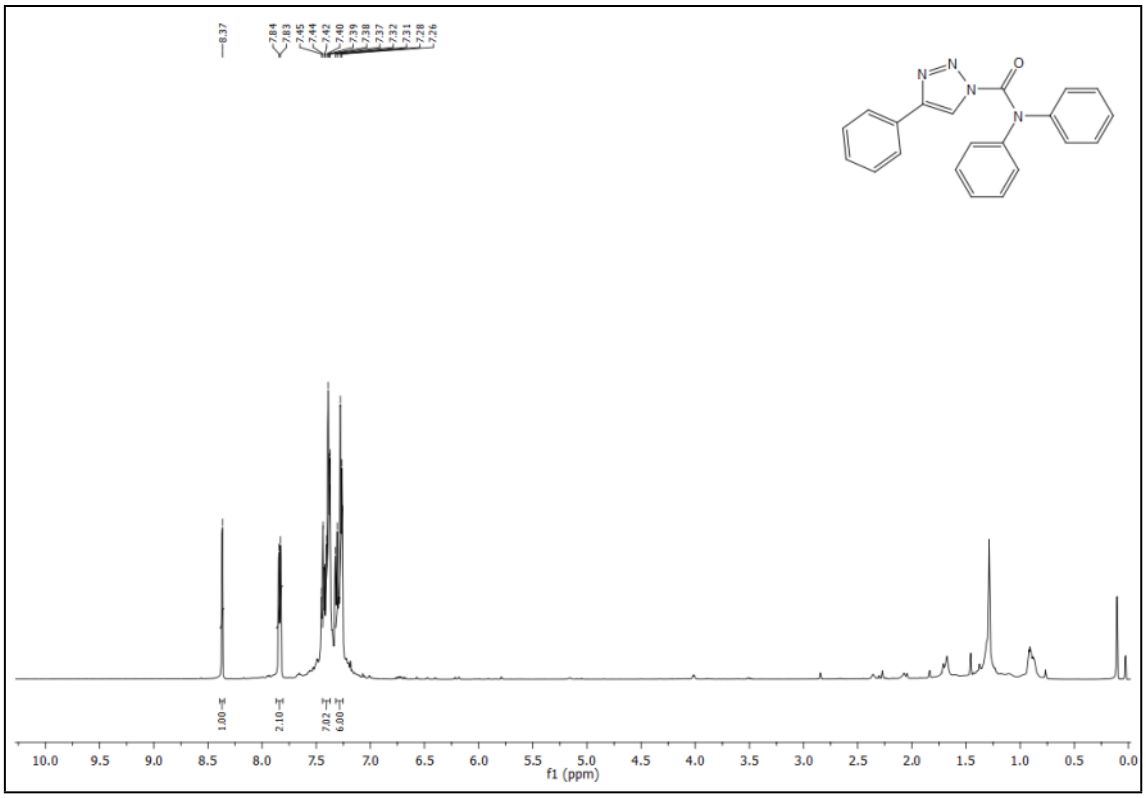


1-(N-Pyrrolidinocarbamoyl)-4-phenyl-1H-1,2,3-triazol (Scheme 3, 11)





N,N,4-Triphenyl-1H-1,2,3-triazole-1-carboxamide (Scheme 2, 12)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7.83
7.45
7.44
7.42
7.40
7.39
7.38
7.37
7.32
7.31
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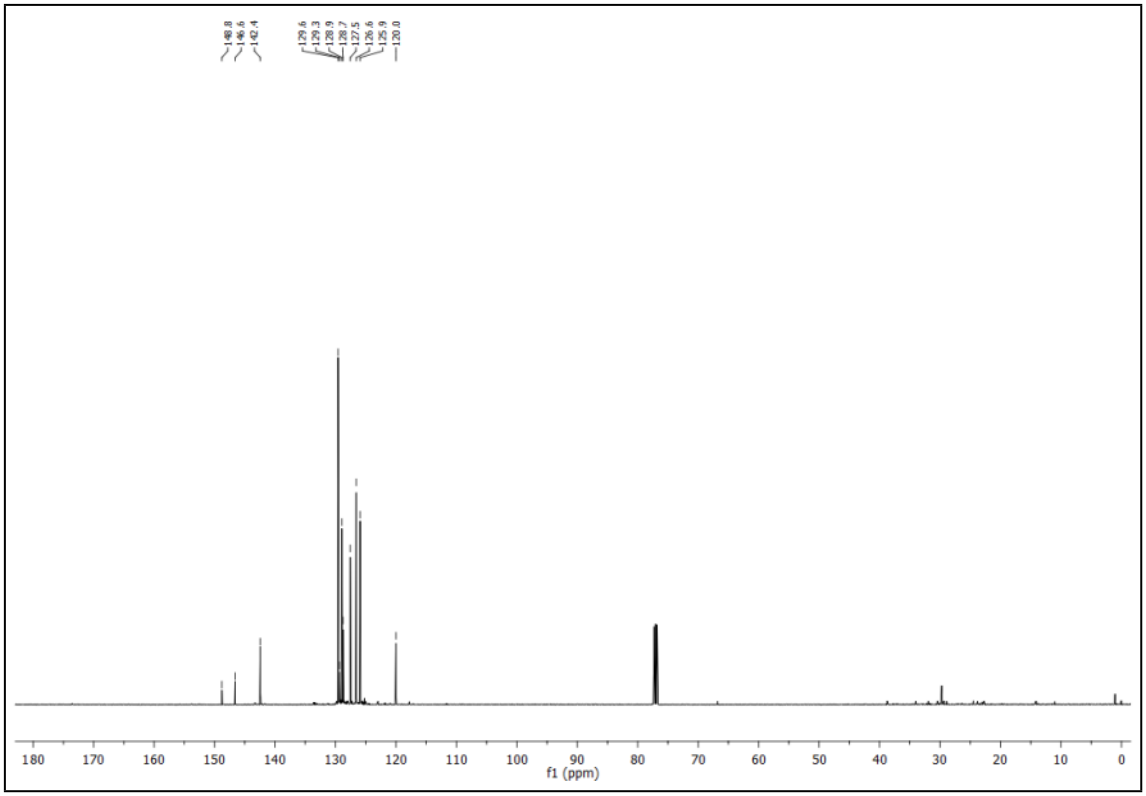
7.26
N
N
N
O
N
1.00
2.10
7.02
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


148.8
146.6
142.4
129.6
129.3
128.9
128.7
127.5
126.6
125.9
120.0
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)