Supporting Information

Endogenous water-triggered and ultrasound accelerated synthesis of 1,5-disubstituted tetrazoles *via* solvent and catalyst-free Ugi-azide reaction

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General information

All reactions were carried out in 10 ml stoppered glass tube. Reactions were monitored by silica gel TLC plates, using mixture of hexane and ethyl acetate as eluents. Flash column chromatography was performed using silica gel (230–400 mesh) and mixtures in different proportions of hexanes with ethyl acetate as mobile phase. Melting points were determined on a Fisher-Johns apparatus and were uncorrected. All solvents were distilled prior use. Aldehydes and amines were purchased from Sigma Aldrich.

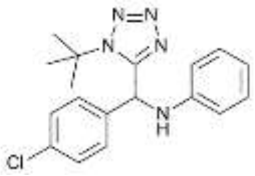
^{1}H NMR spectra were recorded on Bruker Advance III spectrometer (500 MHz) at 295 K in $CDCl_3$; chemical shifts (δ in ppm) and coupling constants (J in Hz) are reported in standard fashion with reference to either internal standard tetramethylsilane (TMS) (δ_H = 0 ppm) or $CHCl_3$ (δ_H = 7.25 ppm). ^{13}C NMR spectra were recorded on Bruker Advance III spectrometer (126 MHz) at room temperature in $CDCl_3$; chemical shifts (δ in ppm) are reported relative to $CHCl_3$ (δ_C = 77.00 ppm). In ^{1}H NMR, the following abbreviations were used throughout: s = singlet, d = doublet, m = multiplet and bs = broad singlet. The assignment of signals were confirmed by ^{1}H and ^{13}C spectral data. IR spectra were recorded by ATR method using neat compounds. The wavelengths are reported in reciprocal centimeters (ν_{max} /cm^{-1}). HRMS spectra were acquired via electrospray ionization ESI (+) and recorded via the TOF method on Bruker mass spectrometer. Ultrasound irradiated reactions were performed in 10 ml stoppered glass tube placed into a water bath of a Branson 1510 sonicator cleaner working at 42 kHz ± 6% frequencies. GC-MS experiment was carried out on Scion GC-MS 456 TQ.

General procedure for the synthesis of 1,5-disubstituted tetrazole (4)

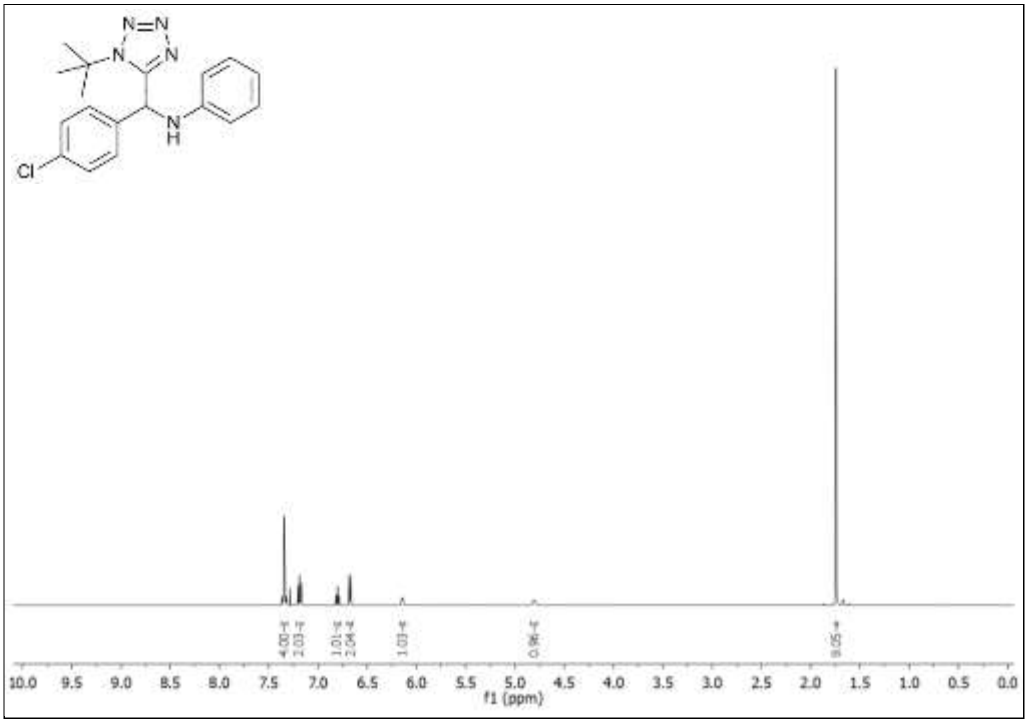
A dry 10 ml tube was charged with aldehyde (1 mmol), amine (1 mmol), an isocyanide (1 mmol) and $TMSN_3$ (1 mmol). The reaction was then sonicated in an ultrasonic cleaner water bath at room temperature for 30 mins. The resulting crude products were purified by column chromatography using Hexane - AcOEt (7/3 V/V) as eluent.

Spectral data

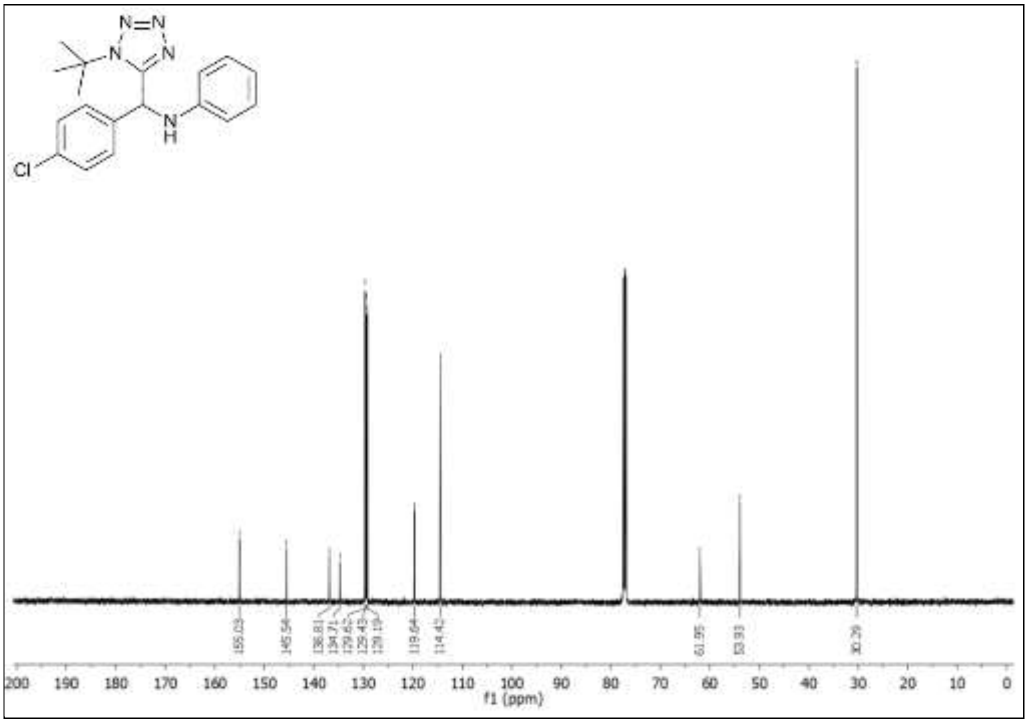
N-((1-(tert-butyl)-1H-tetrazol-5-yl)(4-chlorophenyl)methyl)aniline (4a)



Based on *GP*, 100 mg 4-Chlorobenzaldehyde (0.71 mmol), 0.065 cm^3 aniline (0.71 mmol), 0.080 cm^3 ter. Butyl isocyanide (0.71 mmol), and 0.093 cm^3 TMS-azide (0.71 mmol) were reacted together to afford 237 mg (97%) as a white solid. Melting range 144-145°C, $R_f = 0.45$ (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 – 7.29 (m, 4H), 7.18 – 7.13 (m, 2H), 6.79 – 6.75 (m, 1H), 6.65 (d, *J* = 7.6 Hz, 2H), 6.11 (d, *J* = 6.2 Hz, 1H), 4.78 (d, *J* = 5.6 Hz, 1H), 1.71 (s, 9H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.03, 145.54, 136.81, 134.71, 129.62, 129.43, 129.19, 119.64, 114.42, 61.95, 53.93, 30.29; **FT-IR** (ATR) ν_{max}/cm^{-1} 3330.5, 3052.5, 2940.9, 1603.6, 1284.1; **HRMS** (ESI+): *m/z* calcd. for $C_{18}H_{20}ClN_5^+$ 342.1480, found 342.1474.

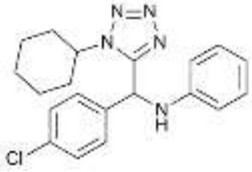


^{1}H NMR spectra of the compound **4a**

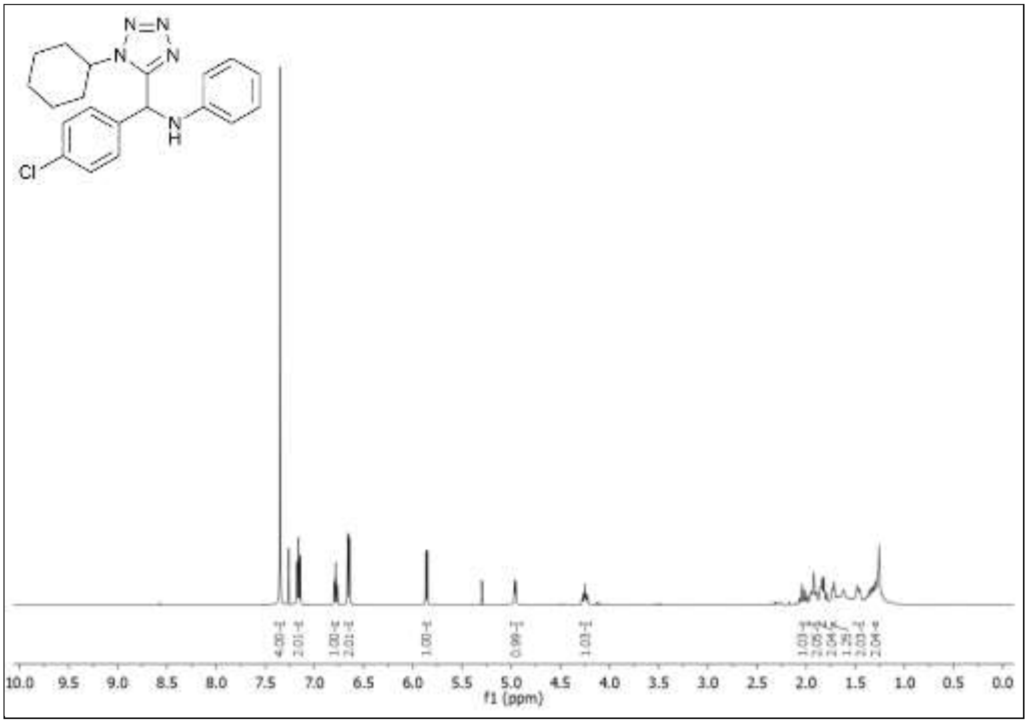


^{13}C NMR spectra of the compound **4a**

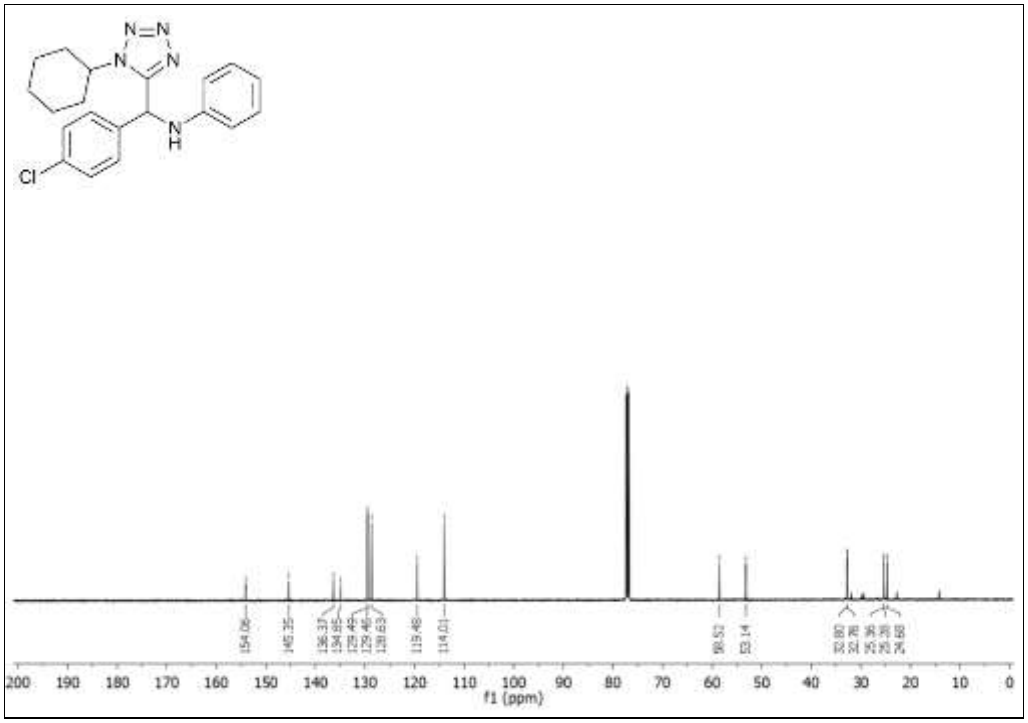
N-((4-chlorophenyl)(1-cyclohexyl-1H-tetrazol-5-yl)methyl)aniline (4b)



Based on *GP*, 100 mg 4-Chlorobenzaldehyde (0.71 mmol), 0.065 cm^3 aniline (0.71 mmol), 0.088 cm^3 cyclohexyl isocyanide (0.71 mmol), and 0.093 cm^3 TMS-azide (0.71 mmol) were reacted together to afford 212 mg (81%) as a brown white solid. Melting range 127-129^{o}C, R$_f$ = 0.45 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.35 (s, 4H), 7.19 – 7.13 (m, 2H), 6.80 - 6.76 (m, 1H), 6.65 (d, *J* = 7.7 Hz, 2H), 5.86 (d, *J* = 6.6 Hz, 1H), 4.96 (d, *J* = 6.6 Hz, 1H), 4.25 (m, 1H), 2.06 – 1.99 (m, 1H), 1.96 – 1.89 (m, 2H), 1.87 – 1.80 (m, 2H), 1.75 – 1.70 (m, 1H), 1.51 – 1.42 (m, 2H), 1.33 – 1.28 (m, 2H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 154.06, 145.35, 136.37, 134.85, 129.49, 129.46, 128.63, 119.48, 114.01, 58.52, 53.14, 32.80, 32.78, 25.36, 25.28, 24.68; **FT-IR** (ATR) ν_{max}/cm^{-1} 3369.8, 3054.2, 2932.6, 1601.9, 1093.4; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{22}ClN_5^+$ 368.1636, found 368.1622.

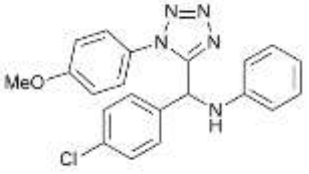


^{1}H NMR spectra of the compound **4b**

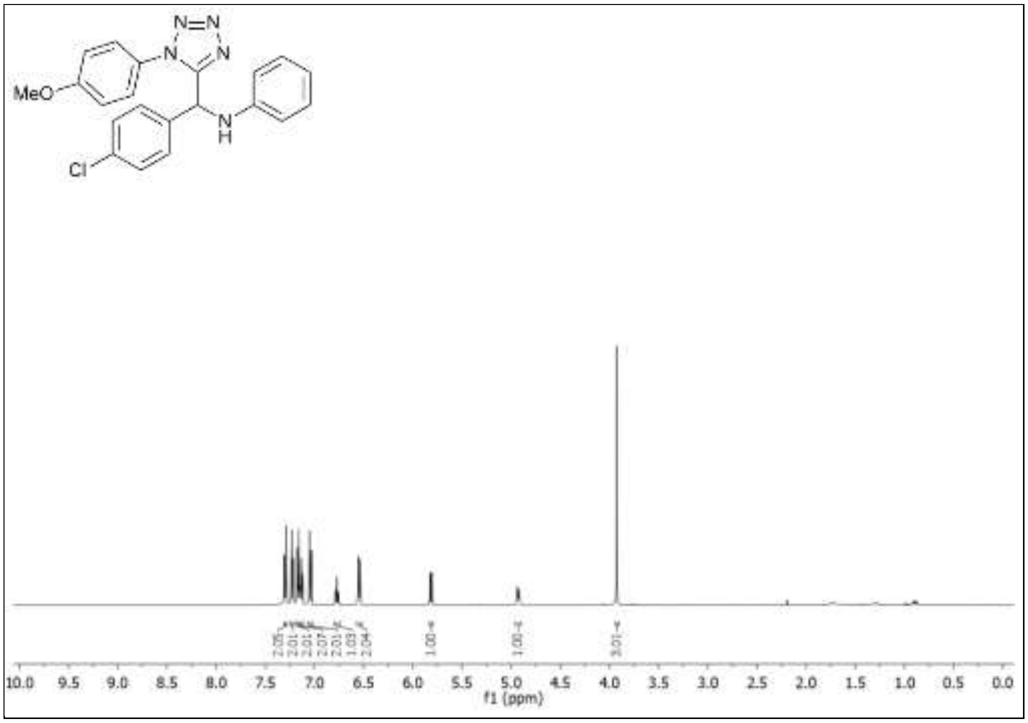


^{13}C NMR spectra of the compound **4b**

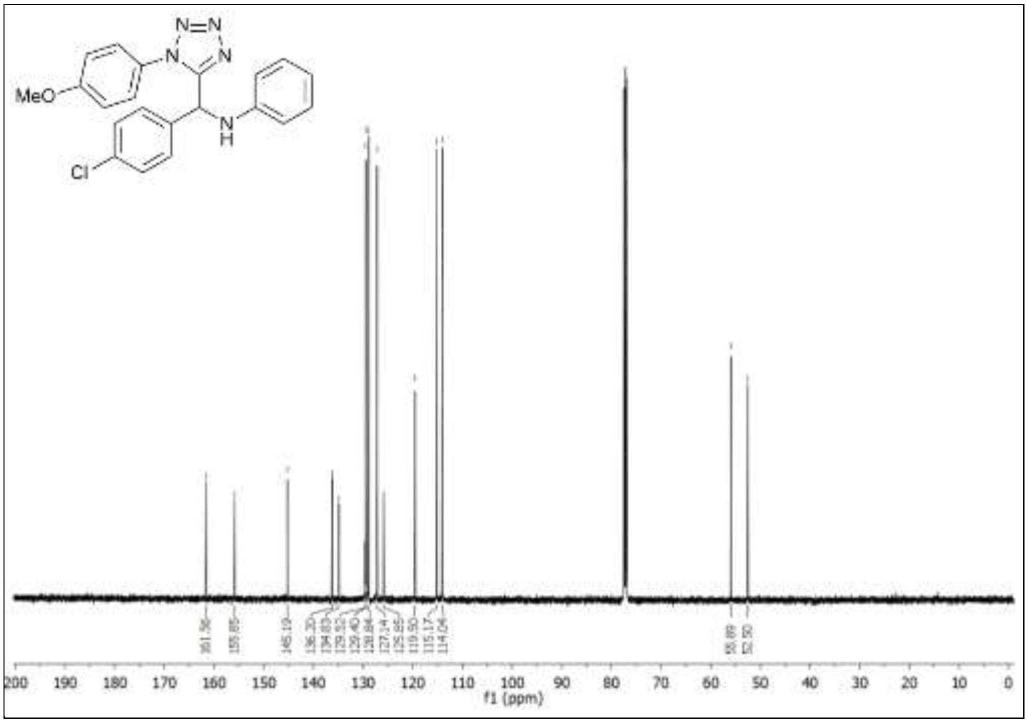
N-((4-chlorophenyl)(1-(4-methoxyphenyl)-1H-tetrazol-5-yl)methyl)aniline (4c)



Based on *GP*, 100 mg 4-Chlorobenzaldehyde (0.71 mmol), 0.065 cm^3 aniline (0.71 mmol), 94 mg. 4-methoxyphenyl isocyanide (0.71 mmol), and 0.093 cm^3 TMS-azide (0.71 mmol) were reacted together to afford 241 mg (86%) as a light yellow solid. Melting range 153-155°C, R_f = 0.51 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 2H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.18 – 7.15 (m, 2H), 7.15 – 7.11 (m, 2H), 7.06 – 7.02 (m, 2H), 6.77 (t, *J* = 7.3 Hz, 1H), 6.54 (d, *J* = 7.9 Hz, 2H), 5.81 (d, *J* = 8.2 Hz, 1H), 4.93 (d, *J* = 8.2 Hz, 1H), 3.92 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.56, 155.85, 145.19, 136.20, 134.83, 129.52, 129.40, 128.84, 127.14, 125.85, 119.50, 115.17, 114.04, 55.89, 52.50; **FT-IR** (ATR) ν_{max}/cm^{-1} 3306.1, 3026.4, 2966.1, 1600.0, 1259.2; **HRMS** (ESI+): *m/z* calcd. for $C_{21}H_{18}ClN_5O^+$ 392.1272, found 392.1263.

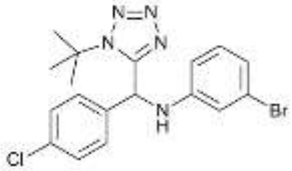


^{1}H NMR spectra of the compound **4c**

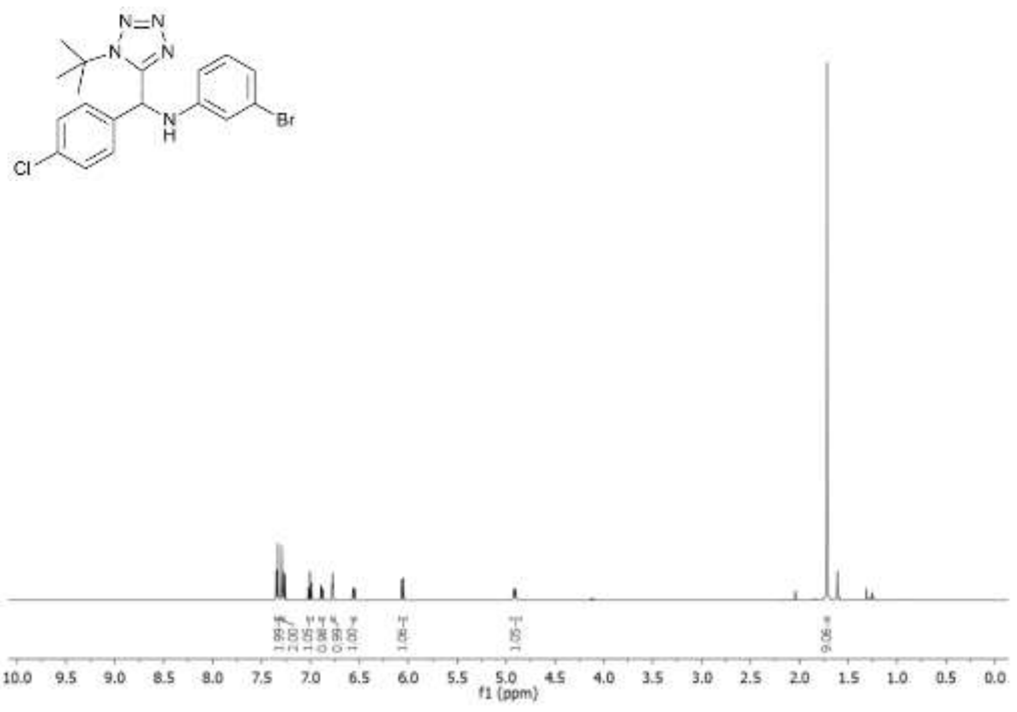


^{13}C NMR spectra of the compound **4c**

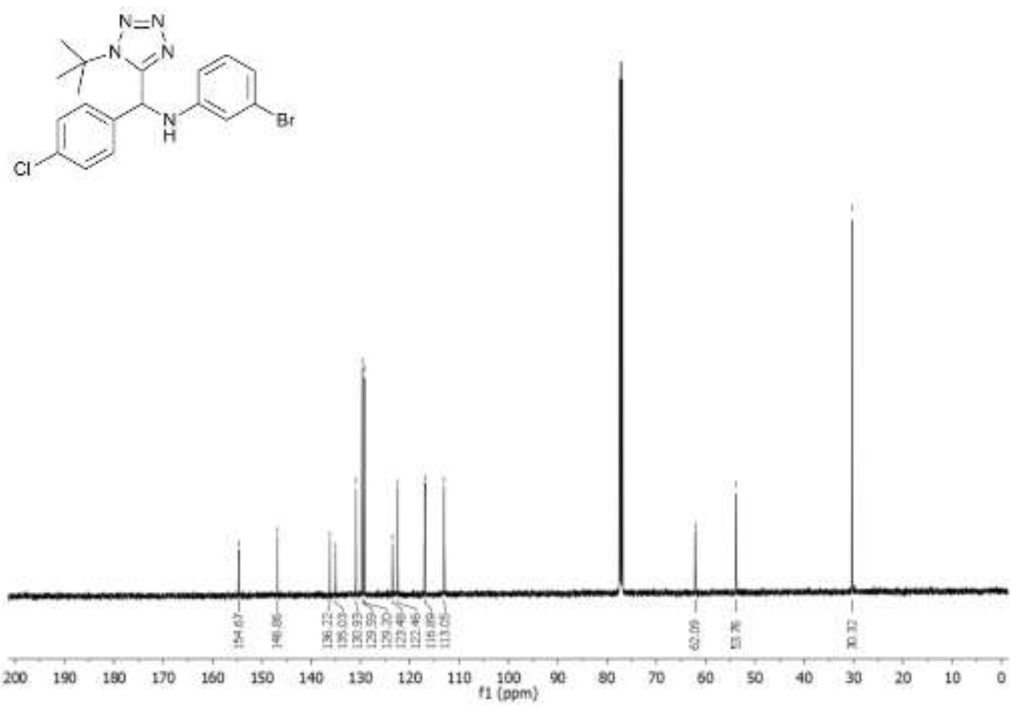
3-bromo-N-((1-(tert-butyl)-1H-tetrazol-5-yl)(4-chlorophenyl)methyl)aniline (4d)



Based on *GP*, 100 mg 4-Chlorobenzaldehyde (0.71 mmol), 0.076 cm^3 3-bromoaniline (0.71 mmol), 0.080 cm^3 ter. butyl isocyanide (0.71 mmol), and 0.093 cm^3 TMS-azide (0.71 mmol) were reacted together to afford 223 mg (74%) as a white solid. Melting range 165-168°C, R_f = 0.45 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.35 – 7.32 (m, 2H), 7.30 – 7.27 (m, 2H), 7.02 – 6.98 (m, 1H), 6.88 (d, *J* = 7.9 Hz, 1H), 6.78 – 6.77 (m, 1H), 6.55 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.06 (d, *J* = 9.2 Hz, 1H), 4.91 (d, *J* = 9.2 Hz, 1H), 1.72 (s, 9H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.67, 146.86, 136.22, 135.03, 130.93, 129.59, 129.20, 123.48, 122.46, 116.89, 113.05, 62.09, 53.76, 30.32; **FT-IR** (ATR) ν_{max}/cm^{-1} 3296.7, 2979.9, 2921.6, 1595.4, 1089.3; **HRMS** (ESI+): *m/z* calcd. for $C_{18}H_{19}BrClN_5^+$ 420.0585, found 420.0573.

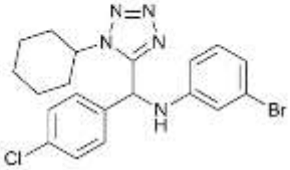


^{1}H NMR spectra of the compound **4d**

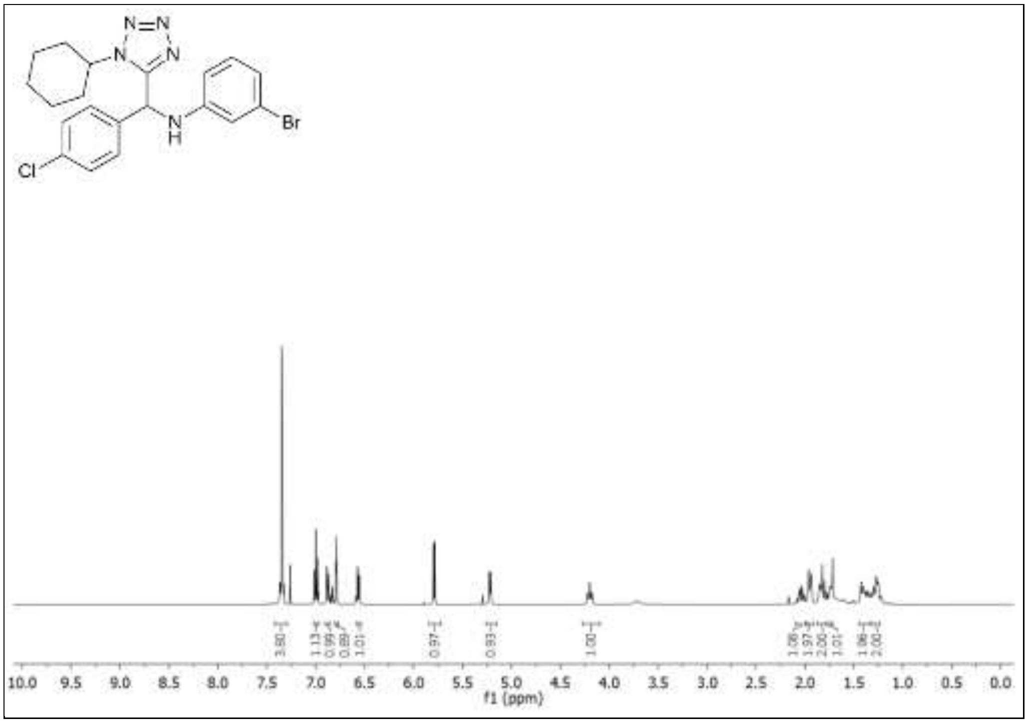


^{13}C NMR spectra of the compound **4d**

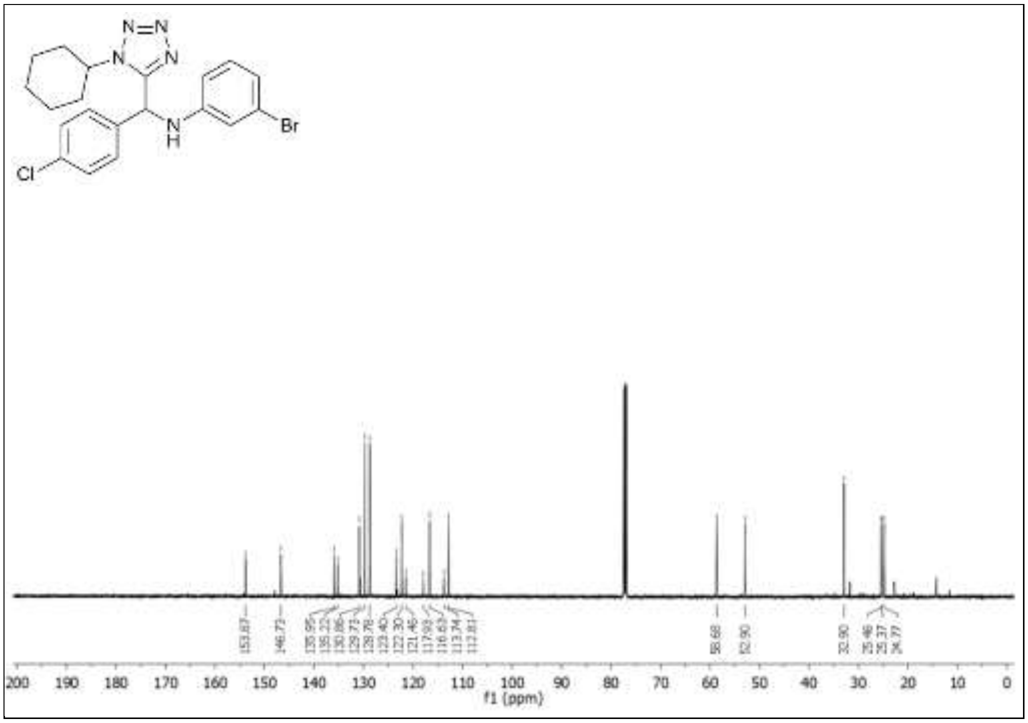
3-bromo-N-((4-chlorophenyl)(1-cyclohexyl-1H-tetrazol-5-yl)methyl)aniline (4e)



Based on *GP*, 100 mg 4-Chlorobenzaldehyde (0.71 mmol), 0.076 cm^3 3-bromoaniline (0.71 mmol), 0.088 cm^3 cyclohexyl isocyanide (0.71 mmol), and 0.093 cm^3 TMS-azide (0.71 mmol) were reacted together to afford 200 mg (83%) as a light yellow oil. R$_f$ = 0.46 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.38 – 7.31 (m, 4H), 7.10 - 6.97 (m, 1H), 6.90 – 6.86 (m, 1H), 6.79 (t, *J* = 2.0 Hz, 1H), 6.56 (dd, *J* = 8.3, 2.0 Hz, 1H), 5.79 (d, *J* = 6.8 Hz, 1H), 5.22 (d, *J* = 6.8 Hz, 1H), 4.23 – 4.16 (m, 1H), 2.09 – 1.99 (m, 1H), 1.95 (d, *J* = 11.6 Hz, 2H), 1.87 – 1.78 (m, 2H), 1.76 – 1.72 (m, 1H), 1.43 - 1.34 (m, 2H), 1.31 – 1.23 (m, 2H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 153.87, 146.73, 135.95, 135.22, 130.86, 129.73, 128.78, 123.40, 122.30, 121.46, 117.93, 116.63, 113.74, 112.81, 58.68, 52.90, 32.90, 25.46, 25.37, 24.77; **FT-IR** (ATR) ν_{max}/cm^{-1} 3323.2, 3065.6, 2931.0, 1594.1, 1479.3; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{21}BrClN_5^+$ 446.0741, found 446.0731.

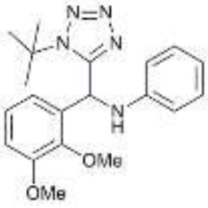


^{1}H NMR spectra of the compound **4e**

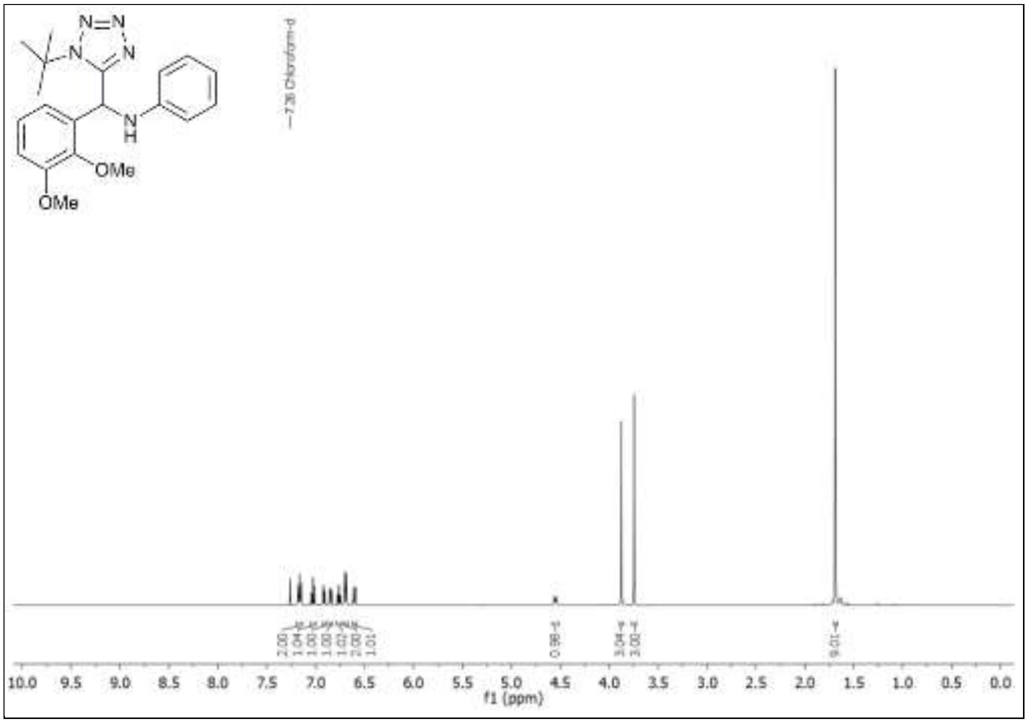


^{13}C NMR spectra of the compound **4e**

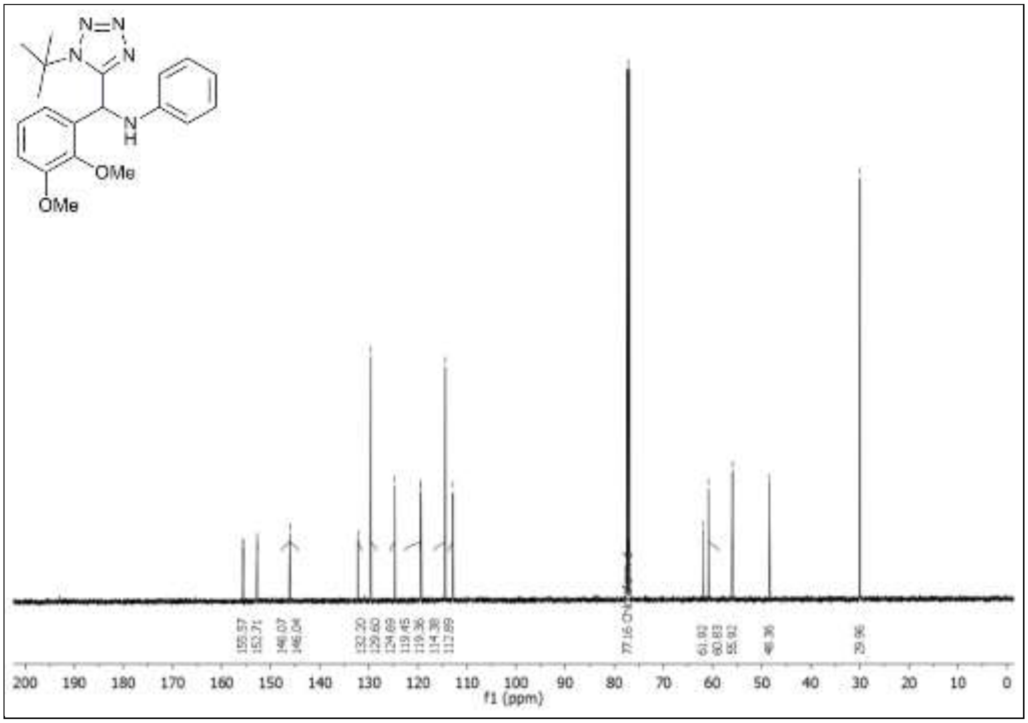
N-((1-(tert-butyl)-1H-tetrazol-5-yl)(2,3-dimethoxyphenyl)methyl)aniline (4f)



Based on *GP*, 100 mg 2,3-dimethoxybenzaldehyde (0.60 mmol), 0.060 cm^3 aniline (0.60 mmol), 0.068 cm^3 ter. Butyl isocyanide (0.60 mmol), and 0.079 cm^3 TMS-azide (0.60 mmol) were reacted together to afford 200 mg (90%) as a light yellow solid. Melting range 149-150°C, R$_f$ = 0.50 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.19 – 7.14 (m, 2H), 7.03 (t, *J* = 8.0 Hz, 1H), 6.91 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.84 (dd, *J* = 7.8, 1.0 Hz, 1H), 6.78 – 6.73 (m, 1H), 6.69 (d, *J* = 7.7 Hz, 2H), 6.60 (d, *J* = 10.2 Hz, 1H), 4.55 (d, *J* = 10.1 Hz, 1H), 3.87 (s, 3H), 3.74 (s, 3H), 1.69 (s, 9H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 155.57, 152.71, 146.07, 146.04, 132.20, 129.60, 124.69, 119.45, 119.36, 114.38, 112.89, 61.92, 60.83, 55.92, 48.36, 29.96; **FT-IR** (ATR) ν_{max}/cm^{-1} 3402.6, 3005.6, 2942.4, 1601.3, 1269.0; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{25}N_5O_2^+$ 368.2081, found 368.2072.

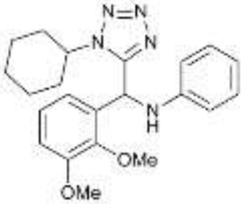


^{1}H NMR spectra of the compound **4f**

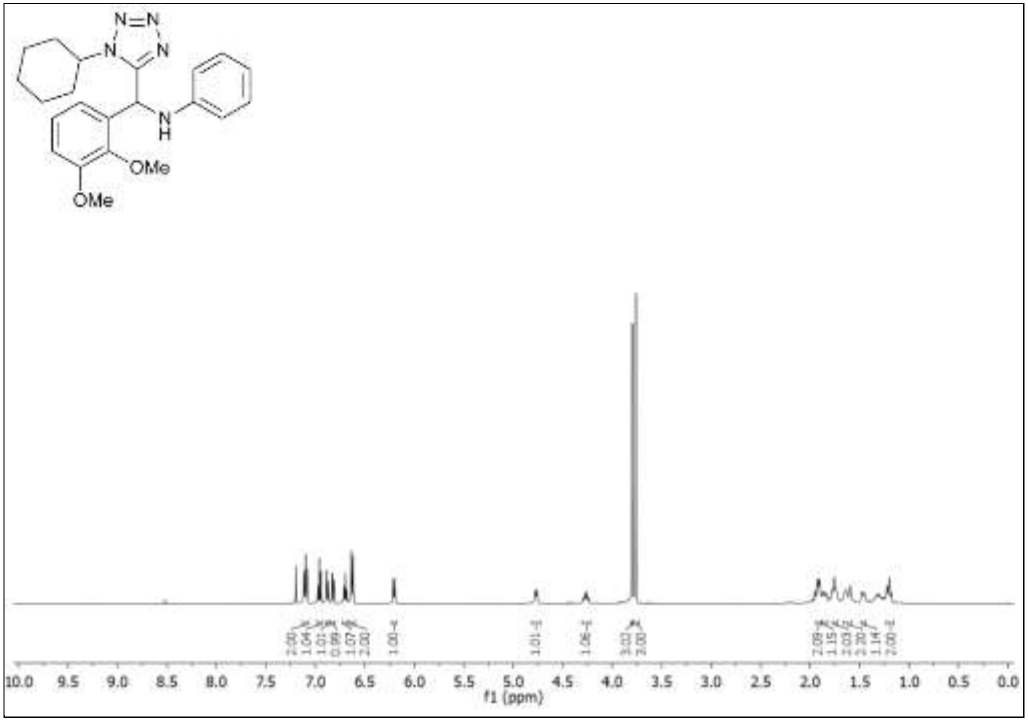


^{13}C NMR spectra of the compound **4f**

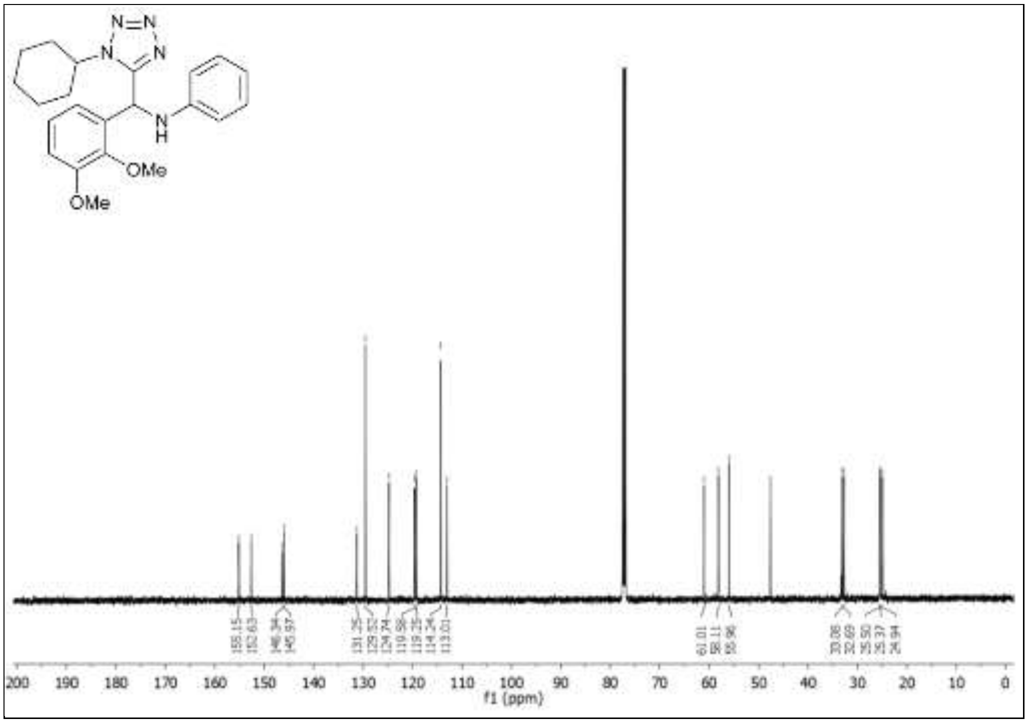
N-((1-cyclohexyl-1H-tetrazol-5-yl)(2,3-dimethoxyphenyl)methyl)aniline (4g)



Based on *GP*, 100 mg 2,3-dimethoxybenzaldehyde (0.60 mmol), 0.060 cm^3 aniline (0.60 mmol), 0.074 cm^3 cyclohexyl isocyanide (0.60 mmol), and 0.079 cm^3 TMS-azide (0.60 mmol) were reacted together to afford 220 mg (93%) as a cream white solid. Melting range 111-113°C, R_f = 0.52 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.18 – 7.13 (m, 2H), 7.04 – 7.00 (m, 1H), 6.94 (dd, *J* = 7.9, 1.4 Hz, 1H), 6.88 (dd, *J* = 8.1, 1.4 Hz, 1H), 6.78 – 6.74 (m, 1H), 6.69 (d, *J* = 7.7 Hz, 2H), 6.27 (d, *J* = 8.4 Hz, 1H), 4.83 (d, *J* = 8.4 Hz, 1H), 4.36 – 4.29 (m, 1H), 3.86 (s, 3H), 3.82 (s, 3H), 2.0 - 1.95 (m, 2H), 1.94-1.89 (m, 1H), 1.84 – 1.78 (m, 2H), 1.73 – 1.64 (m, 2H), 1.55-1.50 (m, 1H), 1.29 – 1.22 (m, 2H). **^{13}C NMR** (126 MHz, CDCl$_3$) δ 155.15, 152.63, 146.34, 145.97, 131.25, 129.52, 124.74, 119.58, 119.25, 114.24, 113.01, 61.01, 58.11, 55.96, 47.59, 33.08, 32.69, 25.50, 25.37, 24.94; **FT-IR** (ATR) ν_{max}/cm^{-1} 3353.1, 3020.3, 2935.8, 1601.2, 1280.5; **HRMS** (ESI+): *m/z* calcd. for $C_{22}H_{27}N_5O_2^+$ 394.2237, found 394.2227.

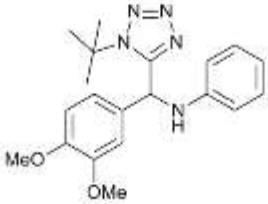


^{1}H NMR spectra of the compound **4g**

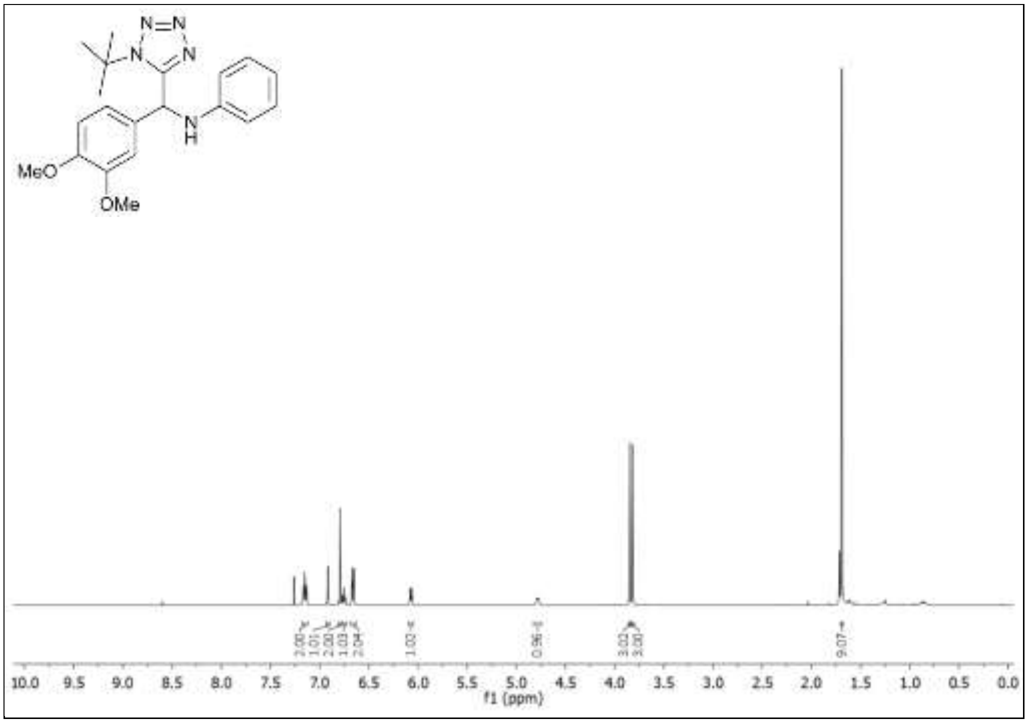


^{13}C NMR spectra of the compound **4g**

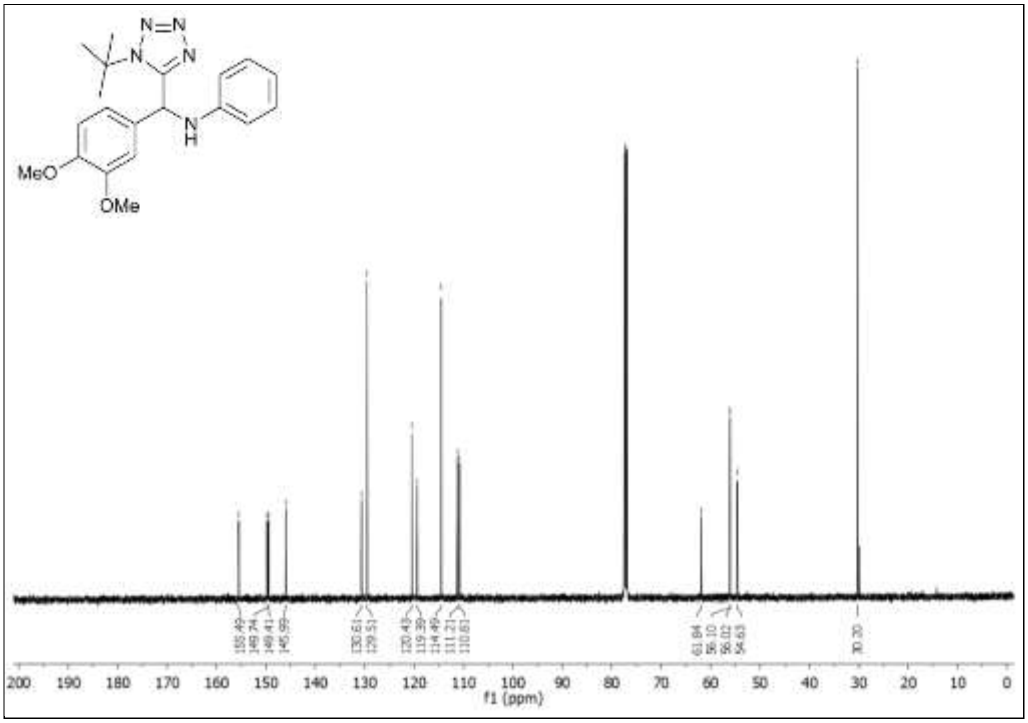
N-((1-(tert-butyl)-1H-tetrazol-5-yl)(3,4-dimethoxyphenyl)methyl)aniline (4h)



Based on *GP*, 100 mg 3,4-dimethoxybenzaldehyde (0.60 mmol), 0.060 cm^3 aniline (0.60 mmol), 0.068 cm^3 ter. Butyl isocyanide (0.60 mmol), and 0.079 cm^3 TMS-azide (0.60 mmol) were reacted together to afford 193 mg (87%) as a light yellow solid. Melting range113-115°C, R_f = 0.47 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.15 (dd, *J* = 11.3, 4.6 Hz, 2H), 6.92 (s, 1H), 6.79 (s, 2H), 6.78 – 6.73 (m, 1H), 6.68 – 6.63 (m, 2H), 6.07 (d, *J* = 8.9 Hz, 1H), 4.78 (d, *J* = 8.7 Hz, 1H), 3.85 (s, 3H), 3.82 (s, 3H), 1.69 (s, 9H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 155.49, 149.74, 149.41, 145.99, 130.61, 129.51, 120.43, 119.39, 114.49, 111.21, 110.81, 61.84, 56.10, 56.02, 54.63, 30.20; **FT-IR** (ATR) v_{max}/cm^{-1} 3387.4, 3001.4, 2955.4, 1603.4, 1253.3; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{25}N_5O_2^+$ 368.2081, found 368.2075.

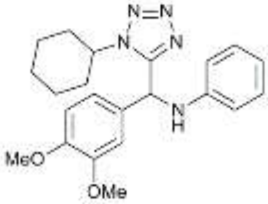


^{1}H NMR spectra of the compound **4h**

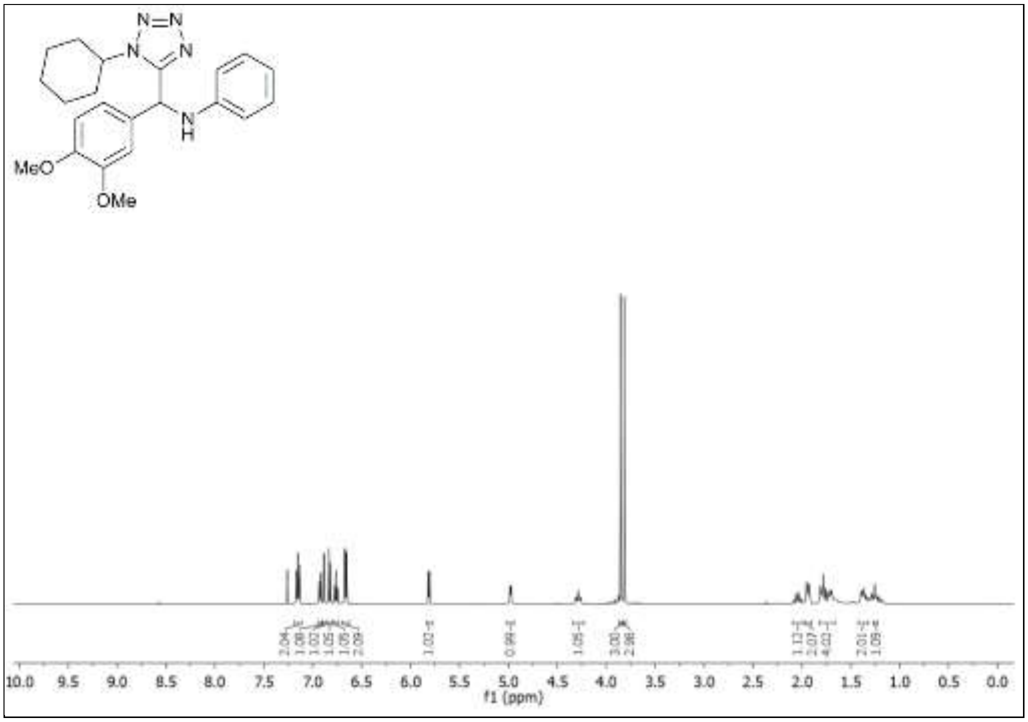


^{13}C NMR spectra of the compound **4h**

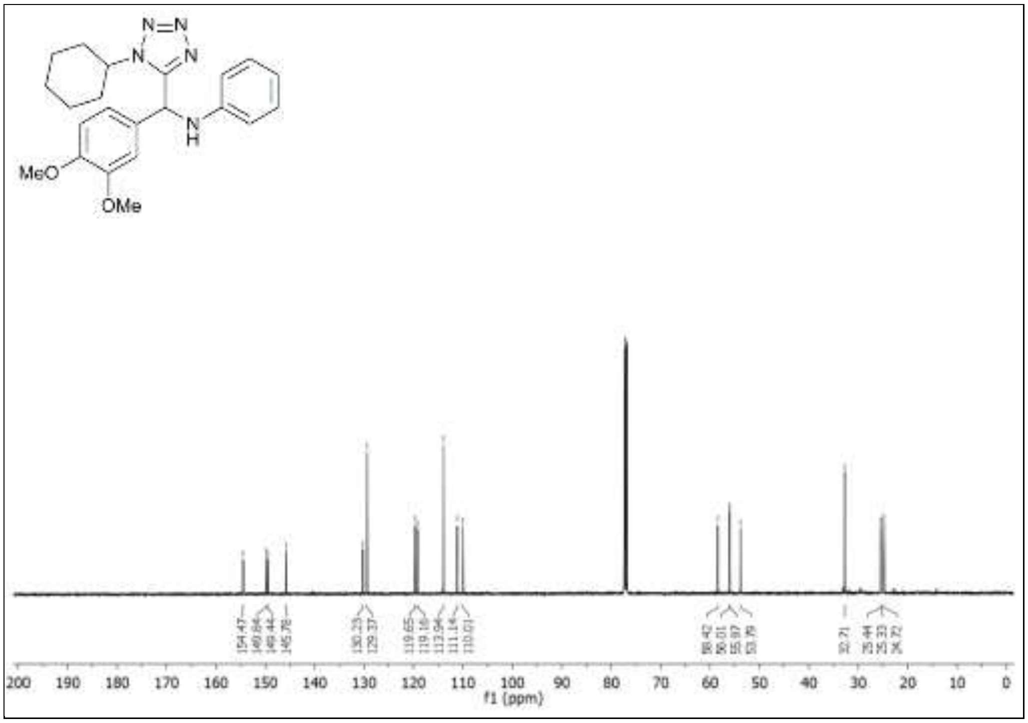
N-((1-cyclohexyl-1H-tetrazol-5-yl)(3,4-dimethoxyphenyl)methyl)aniline (4i)



Based on *GP*, 100 mg 3,4-dimethoxybenzaldehyde (0.60 mmol), 0.060 cm^3 aniline (0.60 mmol), 0.074 cm^3 cyclohexyl isocyanide (0.60 mmol), and 0.079 cm^3 TMS-azide (0.60 mmol) were reacted together to afford 200 mg (84%) as a light yellow solid. Melting range 135-138°C, R_f = 0.51 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.18 – 7.12 (m, 2H), 6.93 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.88 (d, *J* = 2.1 Hz, 1H), 6.82 (d, *J* = 10 Hz, 1H), 6.76 (t, *J* = 7.4 Hz, 1H), 6.66 (dd, *J* = 8.5, 0.9 Hz, 2H), 5.81 (d, *J* = 6.1 Hz, 1H), 4.98 (d, *J* = 6.0 Hz, 1H), 4.29 (m, 1H), 3.85 (s, 3H), 3.81 (s, 3H), 2.08 – 2.0 (m, 1H), 1.94 (d, *J* = 11.7 Hz, 2H), 1.82 – 1.71 (m, 3H), 1.42 – 1.34 (m, 2H), 1.28 – 1.22 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.47, 149.84, 149.44, 145.78, 130.23, 129.37, 119.65, 119.16, 113.94, 111.14, 110.01, 58.42, 56.01, 55.97, 53.79, 32.71, 25.44, 25.33, 24.72; **FT-IR** (ATR) v_{max}/cm^{-1} 3379.5, 3004.2, 2929.9, 1605.1, 1239.1; **HRMS** (ESI+): *m/z* calcd. for $C_{22}H_{27}N_5O_2^+$ 394.2237, found 394.2229.

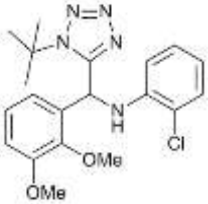


^{1}H NMR spectra of the compound **4i**

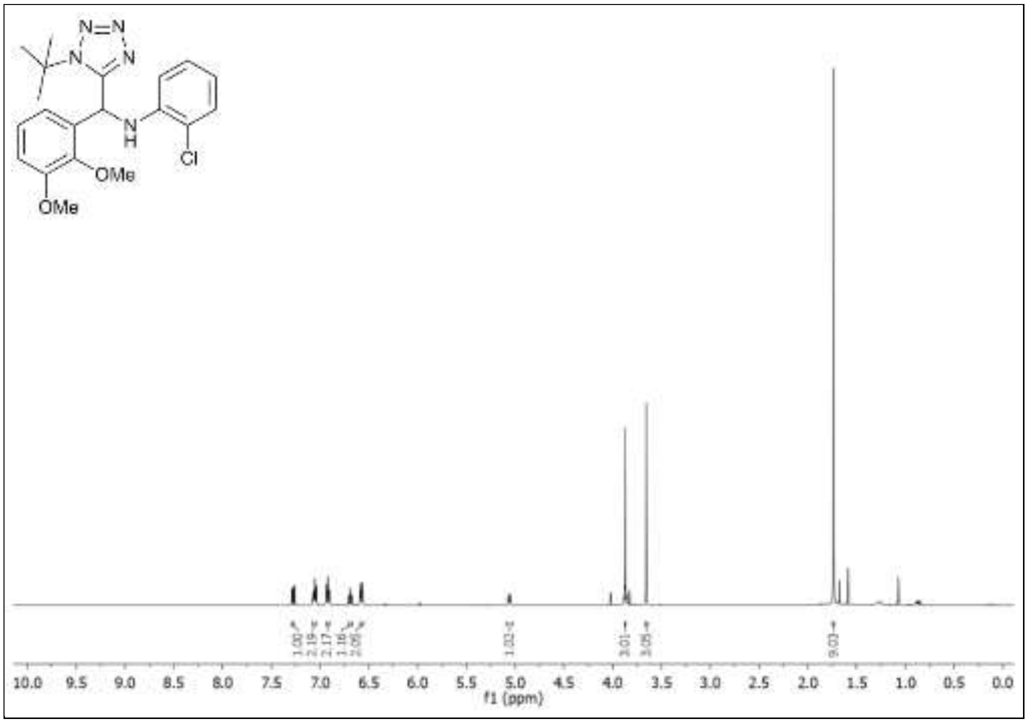


^{13}C NMR spectra of the compound **4i**

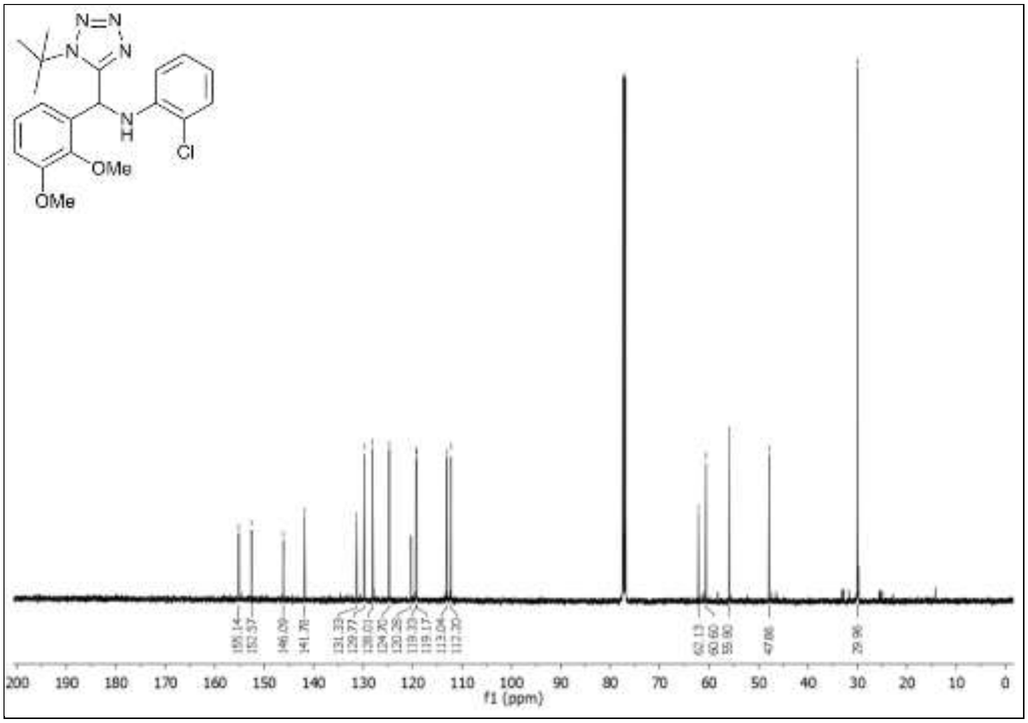
N-((1-(tert-butyl)-1H-tetrazol-5-yl)(2,3-dimethoxyphenyl)methyl)-2-chloroaniline (4j)



Based on *GP*, 100 mg 2,3-dimethoxybenzaldehyde (0.60 mmol), 0.056 cm^3 2-chloroaniline (0.60 mmol), 0.068 cm^3 ter. butyl isocyanide (0.60 mmol), and 0.079 cm^3 TMS-azide (0.60 mmol) were reacted together to afford 163 mg (67%) as a white solid. Melting range 131-133°C, R_f = 0.49 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.28 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.08 – 7.03 (m, 2H), 6.94 – 6.90 (m, 2H), 6.69 (td, *J* = 7.7, 1.3 Hz, 1H), 6.58 (dd, *J* = 5.3, 4.1 Hz, 2H), 5.06 (d, *J* = 9.4 Hz, 1H), 3.87 (s, 3H), 3.66 (s, 3H), 1.74 (s, 9H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 155.14, 152.57, 146.09, 141.78, 131.33, 129.77, 128.01, 124.70, 120.28, 119.33, 119.17, 113.04, 112.20, 62.13, 60.60, 55.90, 47.86, 29.96; **FT-IR** (ATR) ν_{max}/cm^{-1} 3407.1, 2937.9, 2834.7, 1595.9, 1275.5; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{24}ClN_5O_2^+$ 402.1691, found 402.1686.

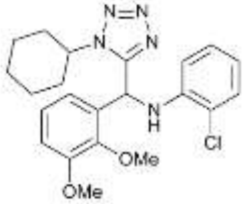


^{1}H NMR spectra of the compound **4j**

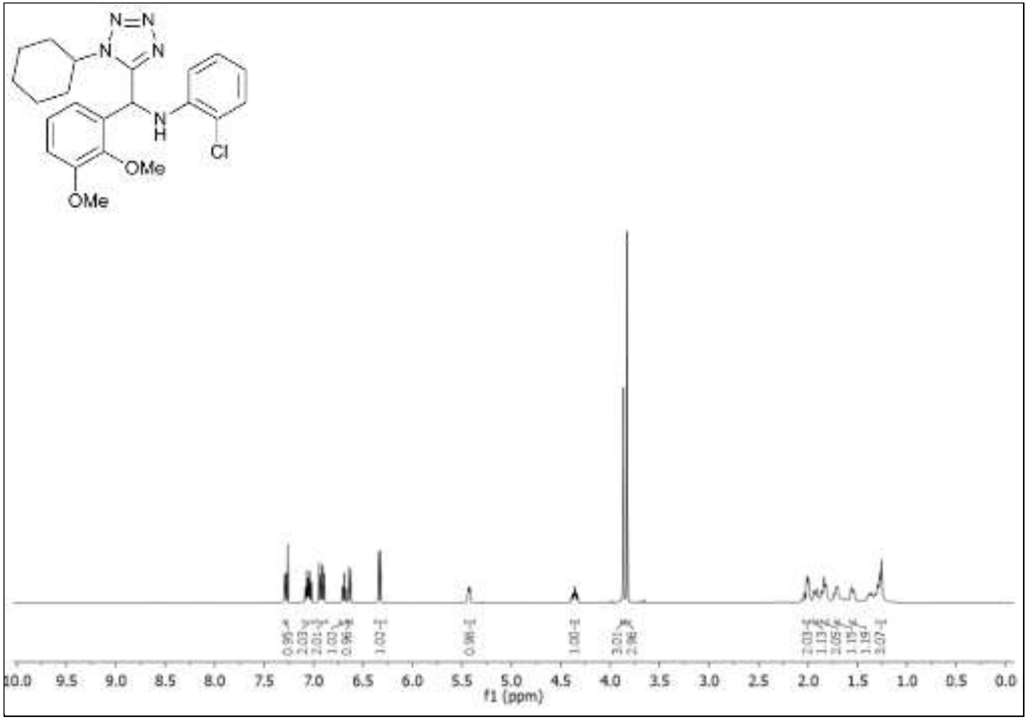


^{13}C NMR spectra of the compound **4j**

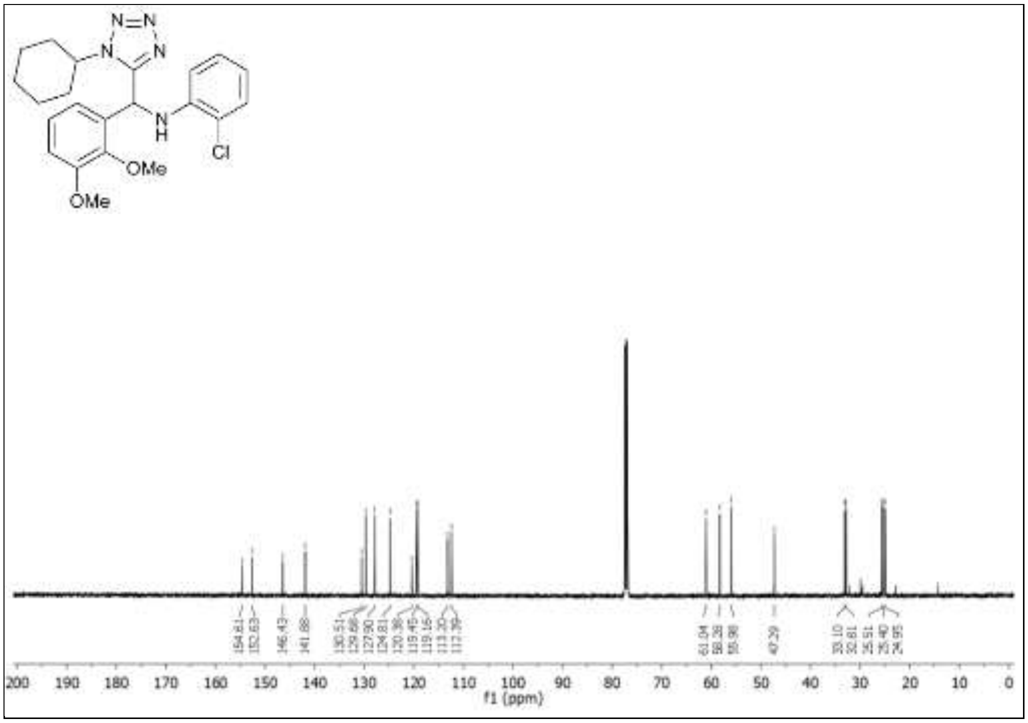
2-chloro-N-((1-cyclohexyl-1H-tetrazol-5-yl)(2,3-dimethoxyphenyl)methyl)aniline (4k)



Based on *GP*, 100 mg 2,3-dimethoxybenzaldehyde (0.60 mmol), 0.056 cm^3 2-chloroaniline (0.60 mmol), 0.074 cm^3 cyclohexyl isocyanide (0.60 mmol), and 0.079 cm^3 TMS-azide (0.60 mmol) were reacted together to afford 203 mg (79%) as a creamy white solid. Melting range 115-117°C, R_f = 0.50 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.9 Hz, 1H), 7.10 – 7.01 (m, 2H), 6.92 (dd, *J* = 17.1, 7.6 Hz, 2H), 6.69 (dd, *J* = 11.1, 4.2 Hz, 1H), 6.63 (d, *J* = 8.1 Hz, 1H), 6.33 (d, *J* = 8.0 Hz, 1H), 5.43 (d, *J* = 7.7 Hz, 1H), 4.39 – 4.32 (m, 1H), 3.86 (s, 3H), 3.83 (s, 3H), 2.05 – 1.97 (m, 2H), 1.92 (d, *J* = 12.6 Hz, 1H), 1.86 – 1.80 (m, 2H), 1.71 (bs, 1H), 1.55 (d, *J* = 11.2 Hz, 1H), 1.30 – 1.21 (m, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.61, 152.63, 146.43, 141.88, 130.51, 129.68, 127.90, 124.81, 120.38, 119.45, 119.16, 113.20, 112.39, 61.04, 58.28, 55.98, 47.29, 33.10, 32.81, 25.51, 25.40, 24.95; **FT-IR** (ATR) ν_{max}/cm^{-1} 3414.4, 3015.7, 2935.8, 1590.1, 1267.7; **HRMS** (ESI+): *m/z* calcd. for $C_{22}H_{26}ClN_5O_2^+$ 428.1847, found 428.1835.

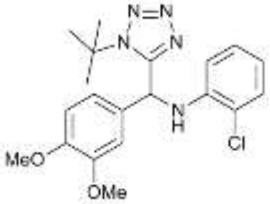


^{1}H NMR spectra of the compound **4k**

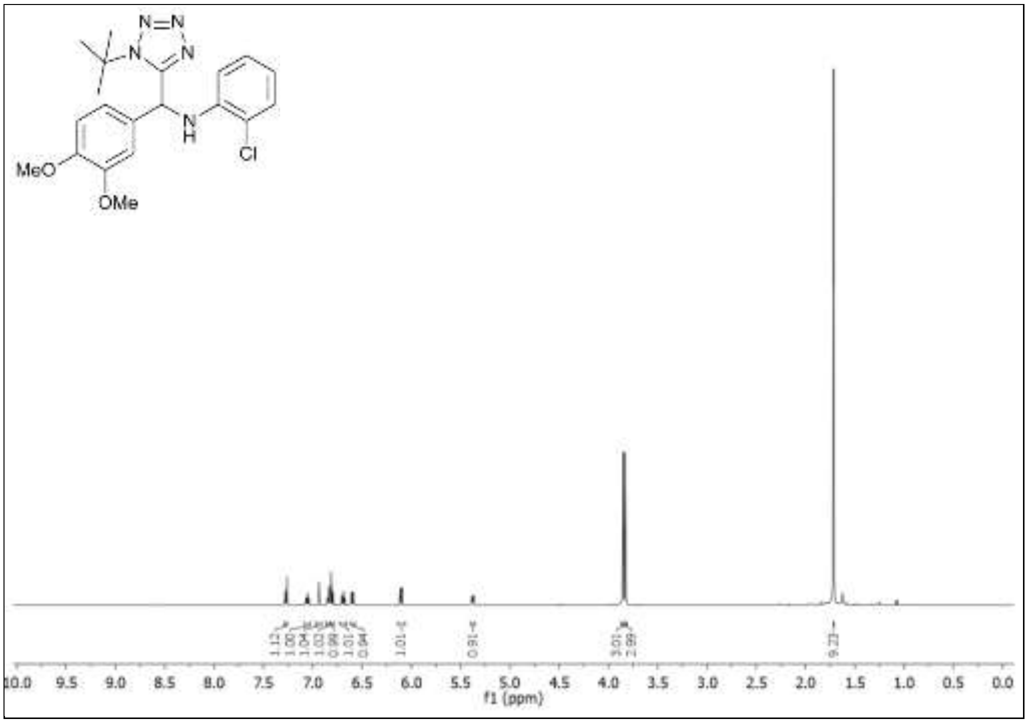


^{13}C NMR spectra of the compound **4k**

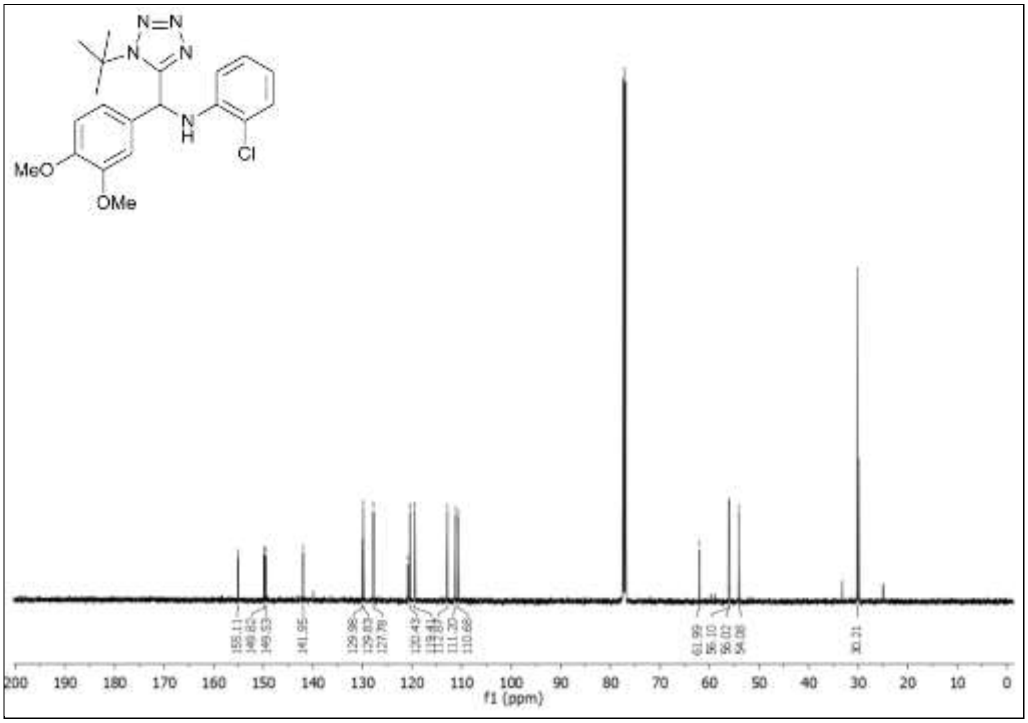
N-((1-(tert-butyl)-1H-tetrazol-5-yl)(3,4-dimethoxyphenyl)methyl)-2-chloroaniline (4l)



Based on *GP*, 100 mg 3,4-dimethoxybenzaldehyde (0.60 mmol), 0.076 cm^3 2-chloroaniline (0.60 mmol), 0.068 cm^3 ter. butyl isocyanide (0.60 mmol), and 0.079 cm^3 TMS-azide (0.60 mmol) were reacted together to afford 137 mg (57%) as a white semisolid, R_f = 0.57 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.27 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.07 – 7.03 (m, 1H), 6.94 (d, *J* = 2.0 Hz, 1H), 6.84 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.80 (d, *J* = 8.3 Hz, 1H), 6.71 – 6.67 (m, 1H), 6.60 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.10 (d, *J* = 8.6 Hz, 1H), 5.38 (d, *J* = 8.7 Hz, 1H), 3.85 (s, 3H), 3.83 (s, 3H), 1.72 (s, 9H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 155.11, 149.82, 149.53, 141.95, 129.98, 129.83, 127.78, 120.84, 120.43, 119.41, 112.87, 111.20, 110.68, 61.99, 56.10, 56.02, 54.08, 30.21; **FT-IR** (ATR) ν_{max}/cm^{-1} 3385.3, 3002.4, 2960.7, 1593.8, 1262.3; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{24}ClN_5O_2^+$ 402.1691, found 402.1683.

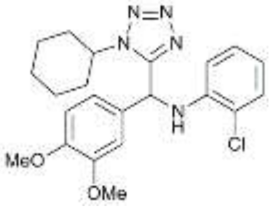


^{1}H NMR spectra of the compound **4l**

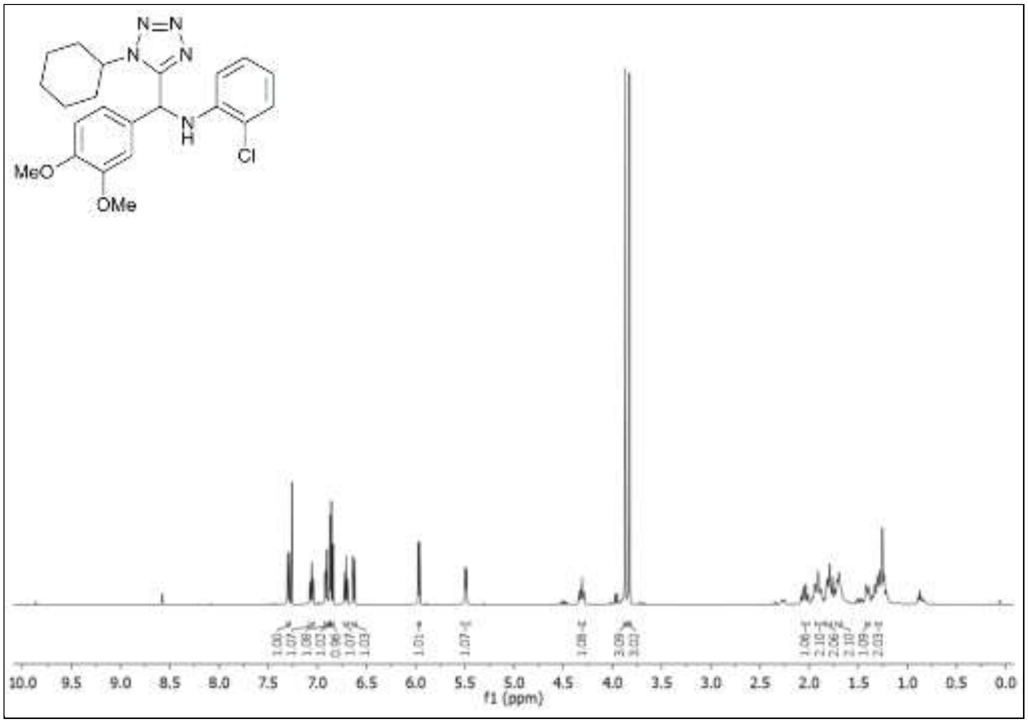


^{13}C NMR spectra of the compound **4l**

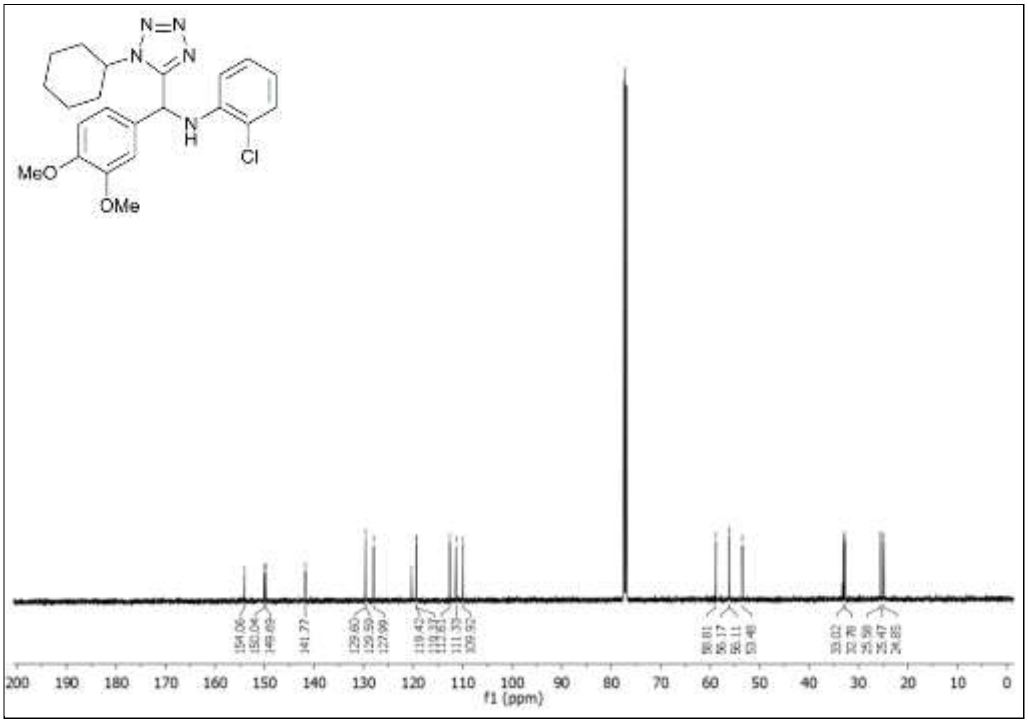
2-chloro-N-((1-cyclohexyl-1H-tetrazol-5-yl)(3,4-dimethoxyphenyl)methyl)aniline (4m)



Based on *GP*, 100 mg 3,4-dimethoxybenzaldehyde (0.60 mmol), 0.076 cm^3 2-chloroaniline (0.60 mmol), 0.074 cm^3 cyclohexyl isocyanide (0.60 mmol), and 0.079 cm^3 TMS-azide (0.60 mmol) were reacted together to afford 162 mg (63%) as a white solid. Melting range 146-148°C, R_f = 0.55 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.08 – 7.03 (m, 1H), 6.91 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.87 (d, *J* = 2.1 Hz, 1H), 6.84 (d, *J* = 8 Hz,1H), 6.73 – 6.68 (m, 1H), 6.63 (dd, *J* = 8.2, 1.1 Hz, 1H), 5.97 (d, *J* = 5.8 Hz, 1H), 5.49 (d, *J* = 5.7 Hz, 1H), 4.34 – 4.27 (m, 1H), 3.87 (s, 3H), 3.83 (s, 3H), 2.09 – 2.00 (m, 1H), 1.95 – 1.86 (m, 2H), 1.83 – 1.77 (m, 2H), 1.72 – 1.66 (m, 2H), 1.44 – 1.38 (m, 1H), 1.34 – 1.25 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.06, 150.04, 149.69, 141.77, 129.60, 129.59, 127.99, 120.37, 119.42, 119.37, 112.61, 111.33, 109.92, 58.81, 56.17, 56.11, 53.48, 33.02, 32.78, 25.58, 25.47, 24.85, **FT-IR** (ATR) ν_{max}/cm^{-1} 3394.6, 3027.2, 2939.0, 1594.3, 1255.6; **HRMS** (ESI+): *m/z* calcd. for $C_{22}H_{26}ClN_5O_2^+$ 428.1847, found 428.1832.

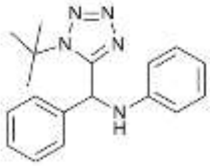


^{1}H NMR spectra of the compound **4m**

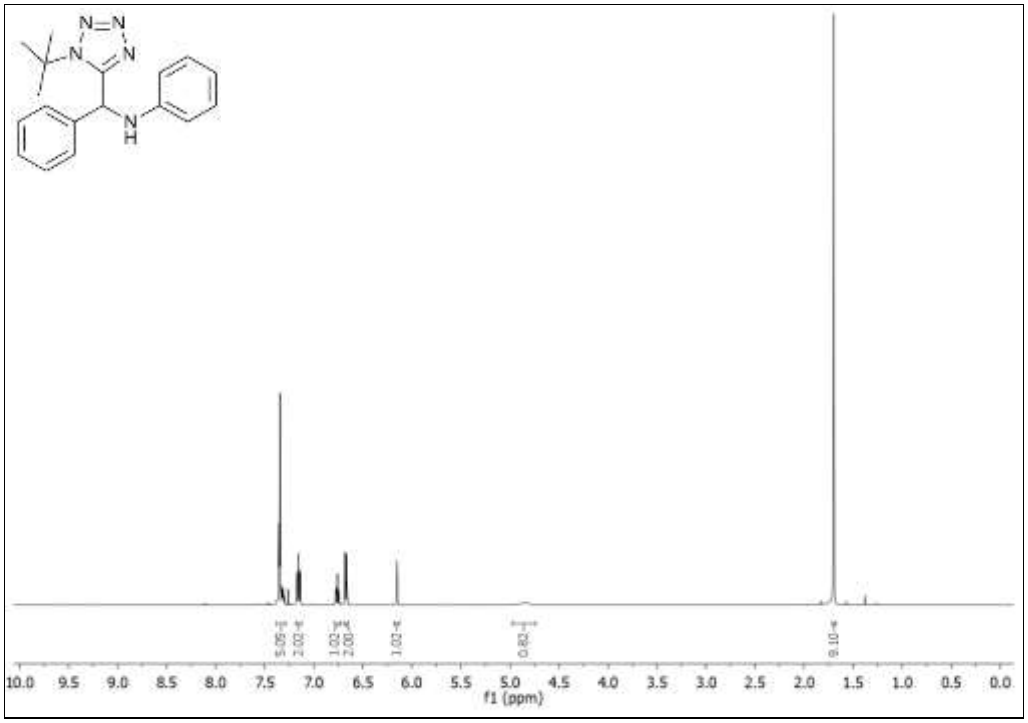


^{13}C NMR spectra of the compound **4m**

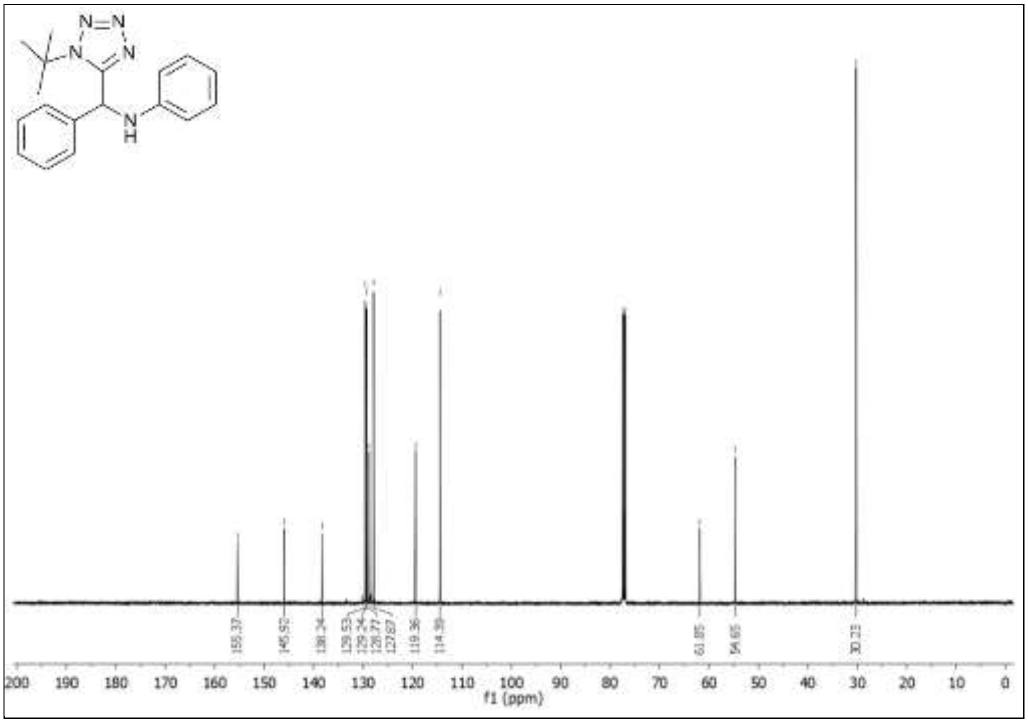
N-((1-(tert-butyl)-1H-tetrazol-5-yl)(phenyl)methyl)aniline (4n)



Based on *GP*, 0.096 cm^3 benzaldehyde (0.94 mmol), 0.090 cm^3 aniline (0.94 mmol), 0.106 cm^3 ter. Butyl isocyanide (0.94 mmol), and 0.123 cm^3 TMS-azide (0.94 mmol) were reacted together to afford 229 mg (79%) as a light yellow solid. Melting range 127-128^{o}C, R_f = 0.40 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.38 – 7.29 (m, 5H), 7.16 (dd, *J* = 8.4, 7.5 Hz, 2H), 6.76 (t, *J* = 7.4 Hz, 1H), 6.67 (d, *J* = 7.7 Hz, 2H), 4.85 (bs, 1H), 1.70 (s, 9H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 155.37, 145.92, 138.24, 129.53, 129.24, 128.77, 127.87, 119.36, 114.39, 61.85, 54.65, 30.23; **FT-IR** (ATR) ν_{max}/cm^{-1} 3320.0, 3004.7, 2988.7, 1598.6, 1320.3; **HRMS** (ESI+): *m/z* calcd. for $C_{18}H_{21}N_5^+$ 308.1869, found 308.1864.

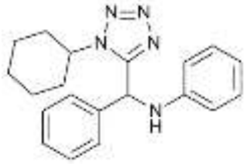


^{1}H NMR spectra of the compound **4n**

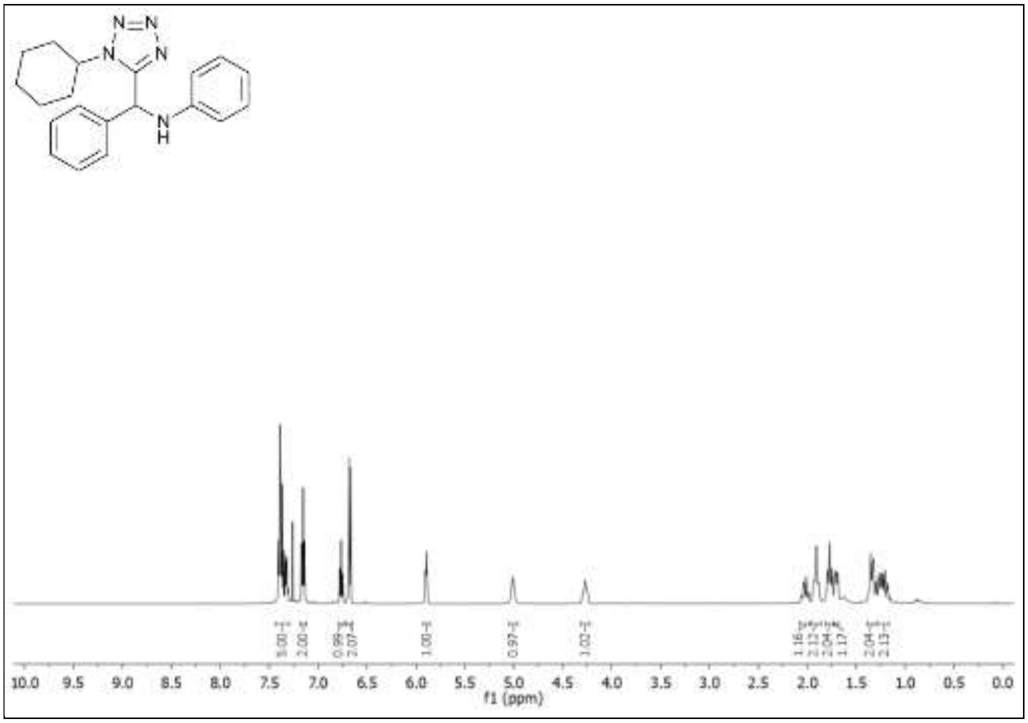


^{13}C NMR spectra of the compound **4n**

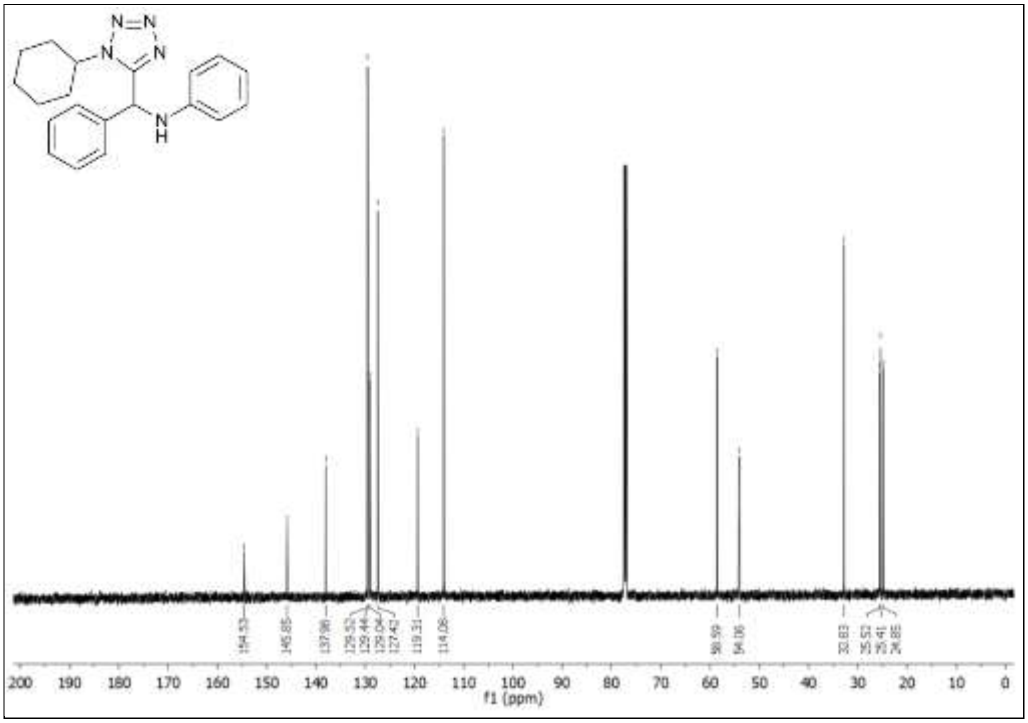
N-((1-cyclohexyl-1H-tetrazol-5-yl)(phenyl)methyl)aniline (4o)



Based on *GP*, 0.096 cm^3 benzaldehyde (0.94 mmol), 0.090 cm^3 aniline (0.94 mmol), 0.117 cm^3 cyclohexyl isocyanide (0.94 mmol), and 0.123 cm^3 TMS-azide (0.94 mmol) were reacted together to afford 217 mg (70%) as a white solid. Melting range 112-124°C, R$_f$ = 0.45 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.42 – 7.30 (m, 5H), 7.15 (t, *J* = 7.7 Hz, 2H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.67 (d, *J* = 7.7 Hz, 2H), 5.90 (d, *J* = 5.4 Hz, 1H), 5.01 (bs, 1H), 4.31 – 4.23 (m, 1H), 2.08 – 1.97 (m, 1H), 1.95 – 1.86 (m, 2H), 1.77 (t, *J* = 11.0 Hz, 2H), 1.72 – 1.68 (m, 1H), 1.39 – 1.30 (m, 2H), 1.28 – 1.16 (m, 2H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 154.53, 145.85, 137.98, 129.52, 129.44, 129.04, 127.42, 119.31, 114.08, 58.59, 54.06, 32.83, 25.52, 25.41, 24.85; **FT-IR** (ATR) ν_{max}/cm^{-1} 3406.9, 3026.5, 2941.4, 1602.0, 1262.8; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{23}N_5^+$ 334.2026, found 334.2021.

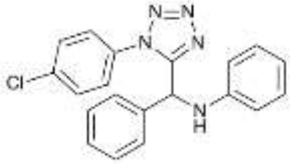


^{1}H NMR spectra of the compound **4o**

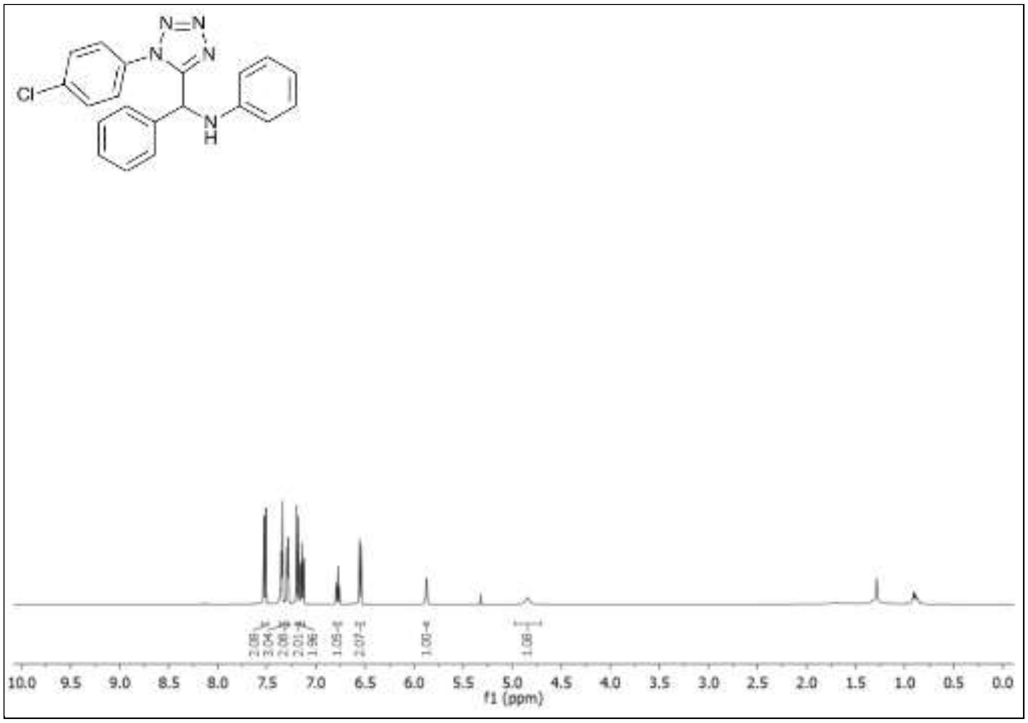


^{13}C NMR spectra of the compound **4o**

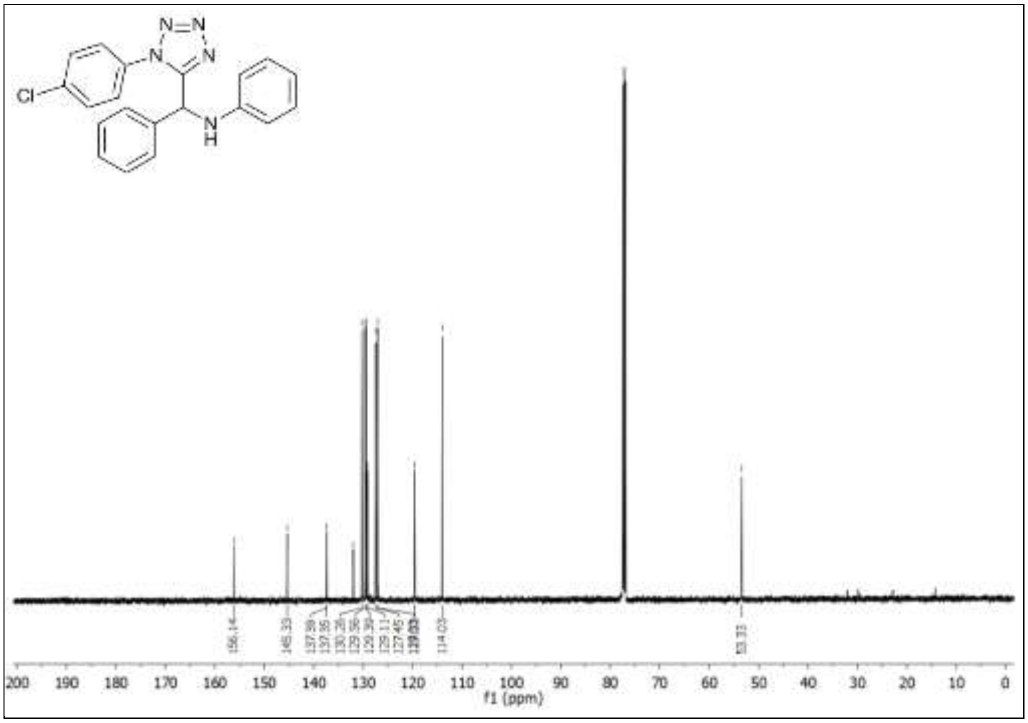
N-((1-(4-chlorophenyl)-1H-tetrazol-5-yl)(phenyl)methyl)aniline (4p)



Based on *GP*, 0.096 cm^3 benzaldehyde (0.94 mmol), 0.090 cm^3 aniline (0.94 mmol), 130 mg 4-chlorophenyl isocyanide (0.94 mmol), and 0.123 cm^3 TMS-azide (0.94 mmol) were reacted together to afford 285 mg (83%) as an orange solid. Melting range 140-143^{o}C, R_f = 0.41 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.54 – 7.50 (m, 2H), 7.37 – 7.33 (m, 3H), 7.30 - 7.27 (m, 2H), 7.21 – 7.17 (m, 2H), 7.16 – 7.11 (m, 2H), 6.78 (t, *J* = 7.4 Hz, 1H), 6.55 (d, *J* = 7.7 Hz, 2H), 5.87 (s, 1H), 4.84 (bs, 1H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 156.14, 145.33, 137.39, 137.35, 132.00, 130.26, 129.56, 129.39, 129.11, 127.45, 127.03, 119.53, 114.03, 53.33; **FT-IR** (ATR) ν_{max}/cm^{-1} 3414.5, 3052.6, 2921.5, 1601.1, 1484.5; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{16}ClN_5^+$ 362.1167, found 362.1155.

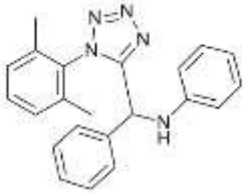


^{1}H NMR spectra of the compound **4p**

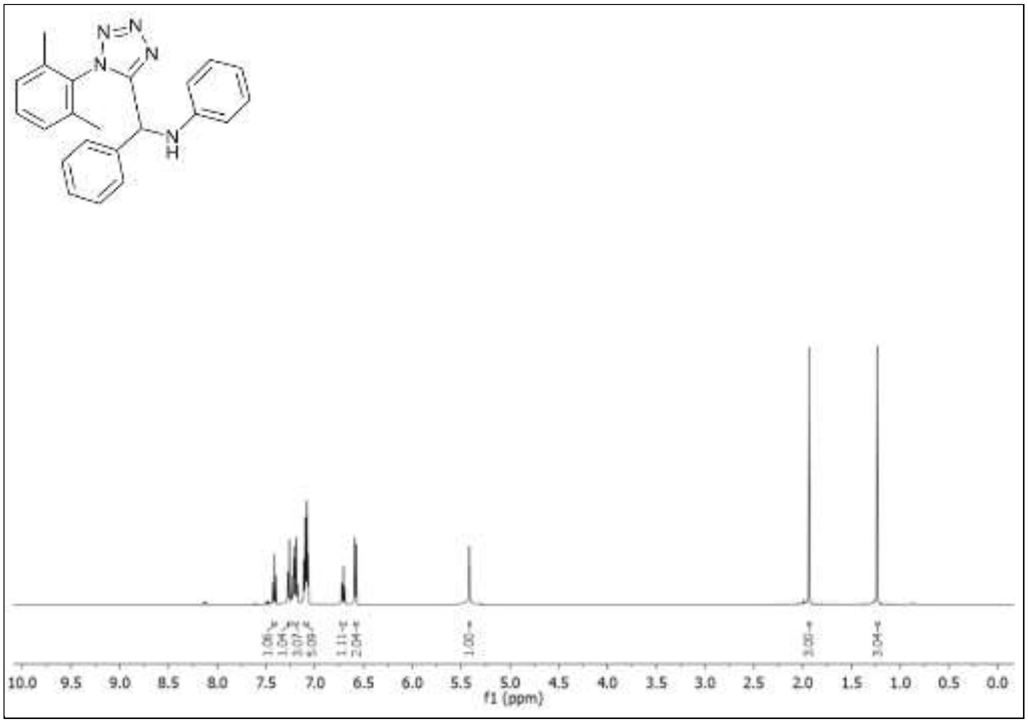


^{13}C NMR spectra of the compound **4p**

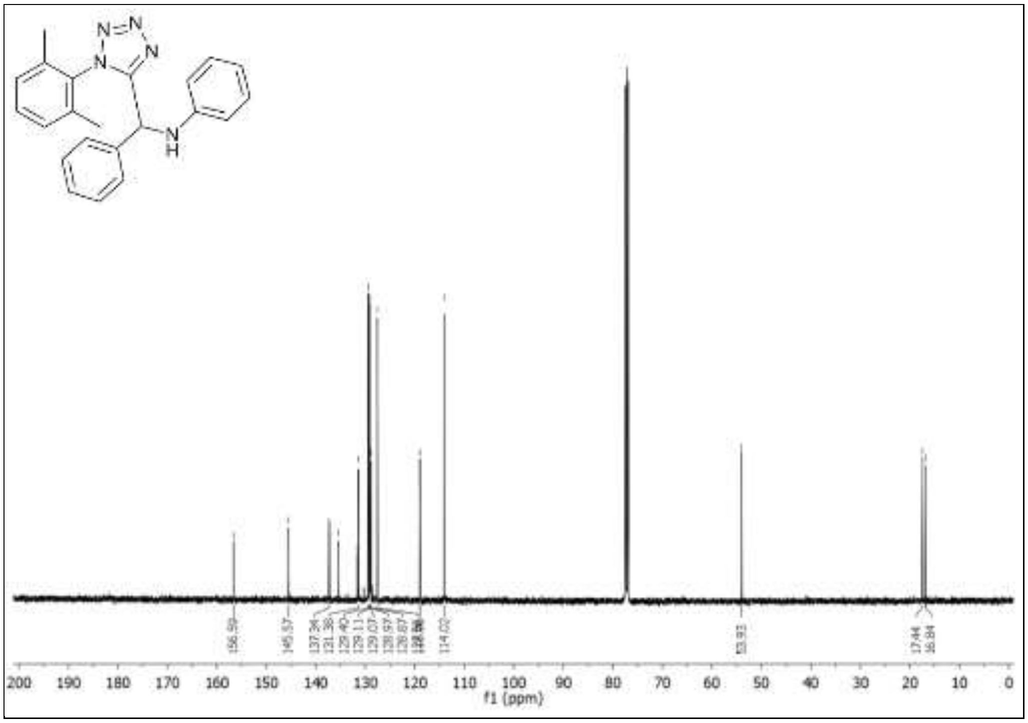
N-((1-(2,6-dimethylphenyl)-1H-tetrazol-5-yl)(phenyl)methyl)aniline (4q)



Based on *GP*, 0.096 cm^3 benzaldehyde (0.94 mmol), 0.090 cm^3 aniline (0.94 mmol), 125 mg 2,6-dimethylphenyl isocyanide (0.94 mmol), and 0.123 cm^3 TMS-azide (0.94 mmol) were reacted together to afford 310 mg (95%) as a white solid. Melting range 135-136°C, R_f = 0.46 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 7.41 (dd, *J* = 9.6, 5.7 Hz, 1H), 7.27 (s, 1H), 7.23 – 7.17 (m, 3H), 7.12 – 7.06 (m, 5H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.58 (d, *J* = 7.7 Hz, 2H), 5.42 (s, 1H), 1.93 (s, 3H), 1.23 (s, 3H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 156.59, 145.57, 137.34, 137.23, 135.43, 131.55, 131.38, 129.40, 129.11, 129.07, 128.97, 128.87, 127.56, 118.96, 114.02, 53.93, 17.44, 16.84; **FT-IR** (ATR) ν_{max}/cm^{-1} 3363.9, 3062.1, 2923.4, 1601.1, 1240; **HRMS** (ESI+): *m/z* calcd. for $C_{22}H_{21}N_5^+$ 356.1869, found 356.1860.

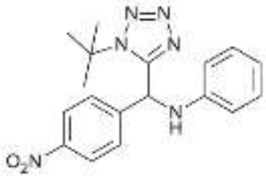


^{1}H NMR spectra of the compound **4q**

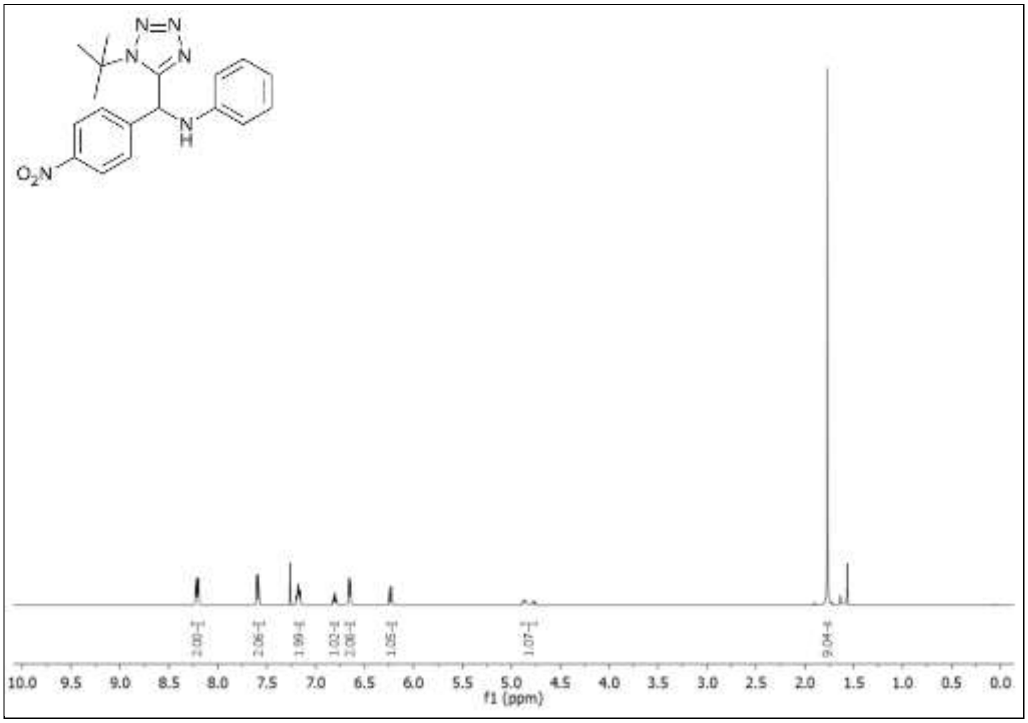


^{13}C NMR spectra of the compound **4q**

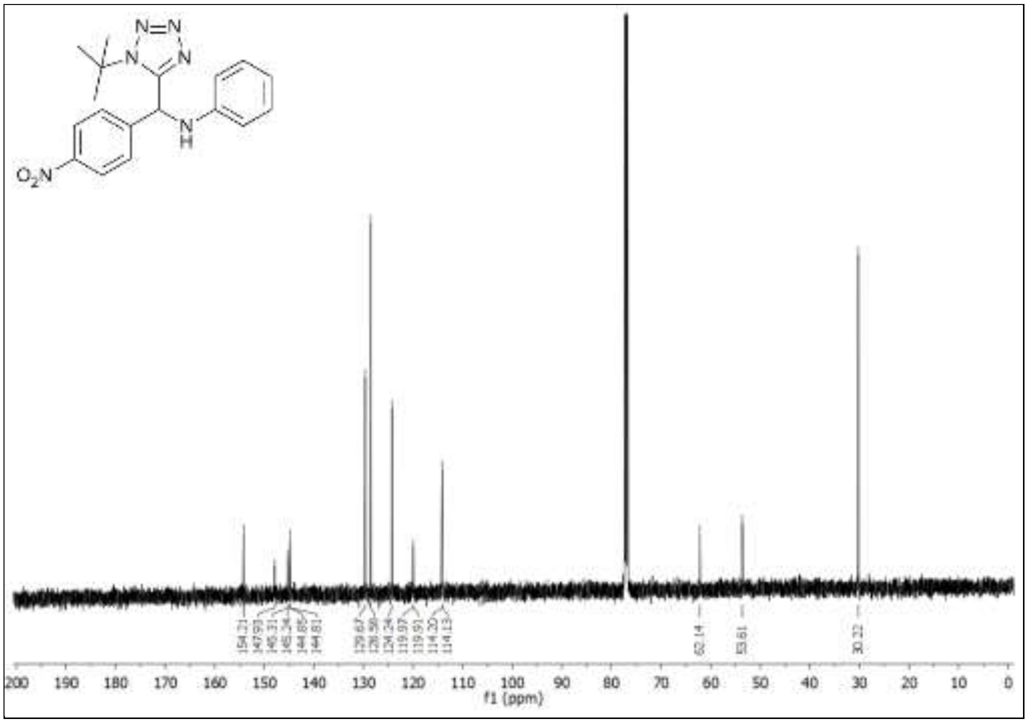
N-((1-(tert-butyl)-1H-tetrazol-5-yl)(4-nitrophenyl)methyl)aniline (4r)



Based on *GP*, 100 mg 4-nitrobenzaldehyde (0.66 mmol), 0.061 cm^3 aniline (0.66 mmol), 0.075 cm^3 ter. Butyl isocyanide (0.66 mmol), and 0.086 cm^3 TMS-azide (0.66 mmol) were reacted together to afford 221 mg (94%) as a reddish solid. Melting range 136-138°C, R_f = 0.45 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.23 -8.19 (m, 2H), 7.59 (d, *J* = 6.8 Hz, 2H), 7.21 – 7.13 (m, 2H), 6.84 – 6.77 (m, 1H), 6.65 (d, *J* = 6.6 Hz, 2H), 6.24 (d, *J* = 9.2 Hz, 1H), 4.82 (dd, *J* = 52.8, 9.3 Hz, 1H), 1.77 (s, 9H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.21, 147.93, 145.31, 145.24, 144.85, 144.81, 129.67, 128.58, 124.24, 119.97, 119.91, 114.20, 114.13, 62.14, 53.61, 30.22; **FT-IR** (ATR) ν_{max}/cm^{-1} 3328.9, 3051.4, 2990.4, 1598.3, 1524.9, 1348.7; **HRMS** (ESI+): *m/z* calcd. for $C_{18}H_{20}N_6O_2^+$ 353.1720, found 353.1711.

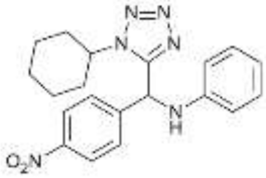


^{1}H NMR spectra of the compound **4r**

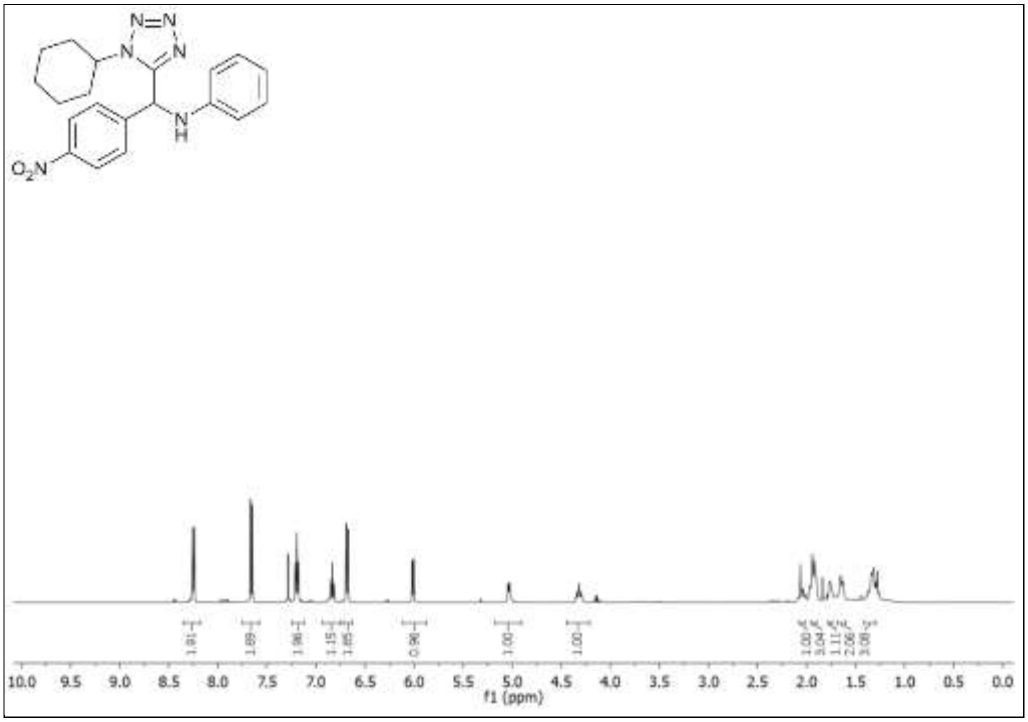


^{13}C NMR spectra of the compound **4r**

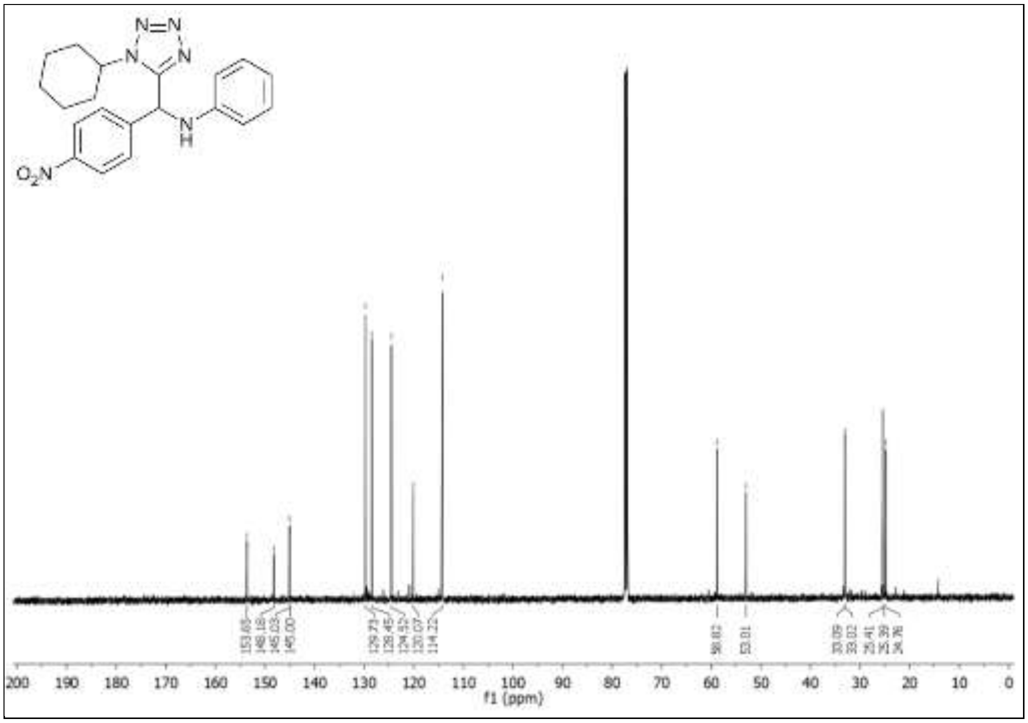
N-((1-cyclohexyl-1H-tetrazol-5-yl)(4-nitrophenyl)methyl)aniline (4s)



Based on *GP*, 100 mg 4-nitrobenzaldehyde (0.66 mmol), 0.061 cm^3 aniline (0.66 mmol), 0.082 cm^3 cyclohexyl isocyanide (0.66 mmol), and 0.086 cm^3 TMS-azide (0.66 mmol) were reacted together to afford 217 mg (86%) as a yellow semisolid. R_f = 0.48 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.7 Hz, 2H), 7.67 – 7.64 (m, 2H), 7.20 (t, *J* = 7.9 Hz, 2H), 6.83 (t, *J* = 7.4 Hz, 1H), 6.68 (d, *J* = 7.8 Hz, 2H), 6.01 (d, *J* = 7.2 Hz, 1H), 5.03 (d, *J* = 7.0 Hz, 1H), 4.3 – 4.28 (m, 1H), 2.08 – 2.01 (m, 1H), 1.95 – 1.89 (m, 3H), 1.77 (bs, 1H), 1.64 (d, *J* = 12.3 Hz, 1H), 1.42 – 1.29 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.65, 148.18, 145.03, 145.00, 129.73, 128.45, 124.52, 120.07, 114.22, 58.82, 53.01, 33.09, 33.02, 25.41, 25.39, 24.76; **FT-IR** (ATR) ν_{max}/cm^{-1} 3411.8, 3059.2, 2934.8, 1599.5, 1519.6, 1345.0; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{22}N_6O_2^+$ 379.1877, found 379.1866.

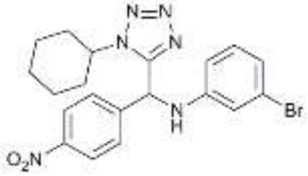


^{1}H NMR spectra of the compound **4s**

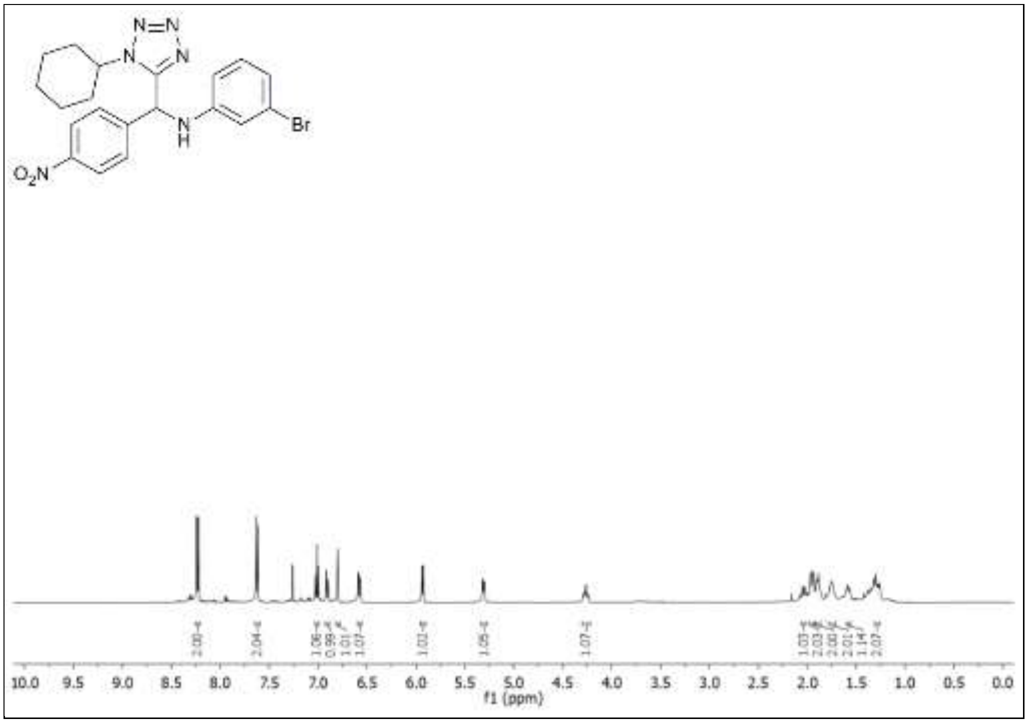


^{13}C NMR spectra of the compound **4s**

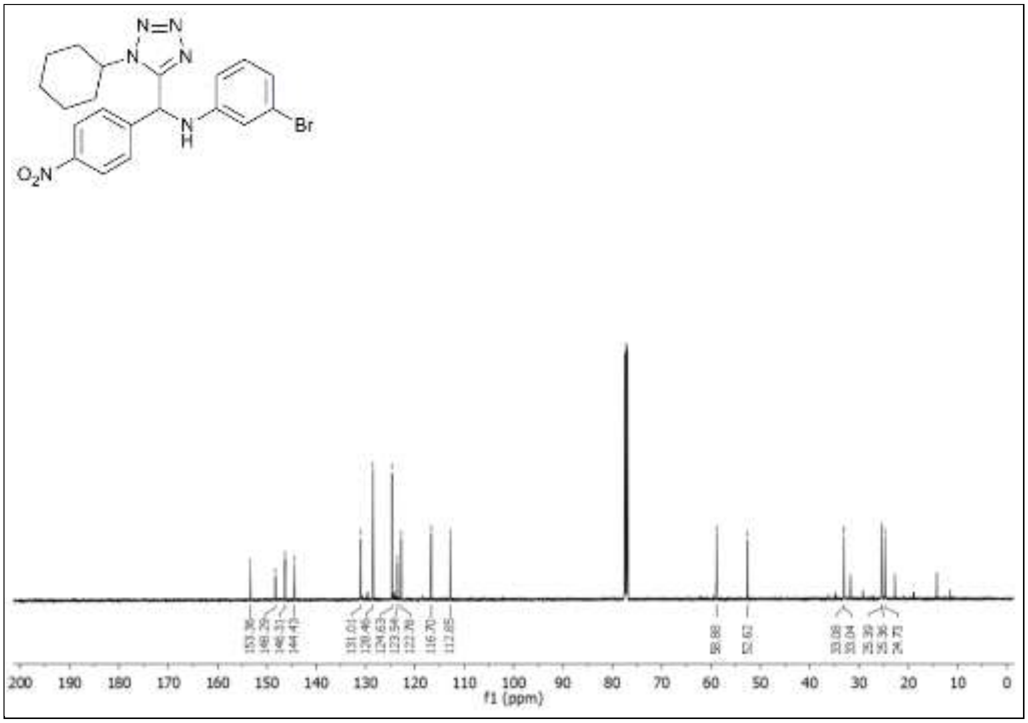
3-bromo-N-((1-cyclohexyl-1H-tetrazol-5-yl)(4-nitrophenyl)methyl)aniline (4t)



Based on *GP*, 100 mg 4-nitrobenzaldehyde (0.66 mmol), 0.070 cm^3 3-bromoaniline (0.71 mmol), 0.082 cm^3 cyclohexyl isocyanide (0.71 mmol), and 0.086 cm^3 TMS-azide (0.71 mmol) were reacted together to afford 181 mg (55%) as a reddish solid. Melting range 103-106°C, $R_f = 0.45$ (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 8.25 – 8.21 (m, 2H), 7.65 – 7.60 (m, 2H), 7.01 (t, *J* = 8.0 Hz, 1H), 6.92 – 6.89 (m, 1H), 6.80 (t, *J* = 2.0 Hz, 1H), 6.58 (dd, *J* = 8.0, 2.0 Hz, 1H), 5.93 (d, *J* = 7.2 Hz, 1H), 5.31 (d, *J* = 7.2, 1H), 4.30 - 4.23 (m, 1H), 2.06 - 2.01 (m, 1H), 1.95 (d, *J* = 11.6 Hz, 2H), 1.91 – 1.86 (m, 2H), 1.79 – 1.70 (m, 2H), 1.58 (d, *J* = 11.1 Hz, 1H), 1.33 – 1.25 (m, 2H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 153.36, 148.29, 146.31, 144.43, 131.01, 128.46, 124.63, 123.54, 122.78, 116.70, 112.85, 58.88, 52.62, 33.08, 33.04, 25.39, 25.36, 24.73; **FT-IR** (ATR) ν_{max}/cm^{-1} 3305.1, 3079.8, 2935.3, 2857.8, 1593.3, 1345.0; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{21}BrN_6O_2^+$ 457.0982, found 457.0965.

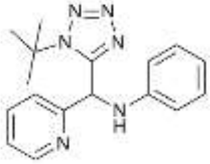


^{1}H NMR spectra of the compound **4t**

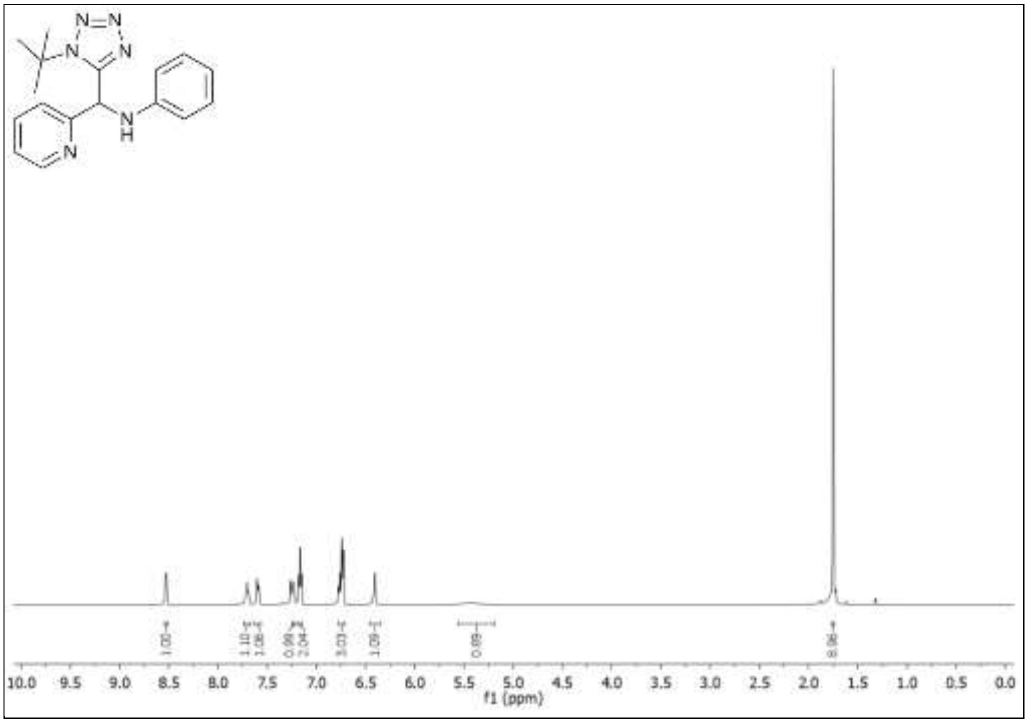


^{13}C NMR spectra of the compound **4t**

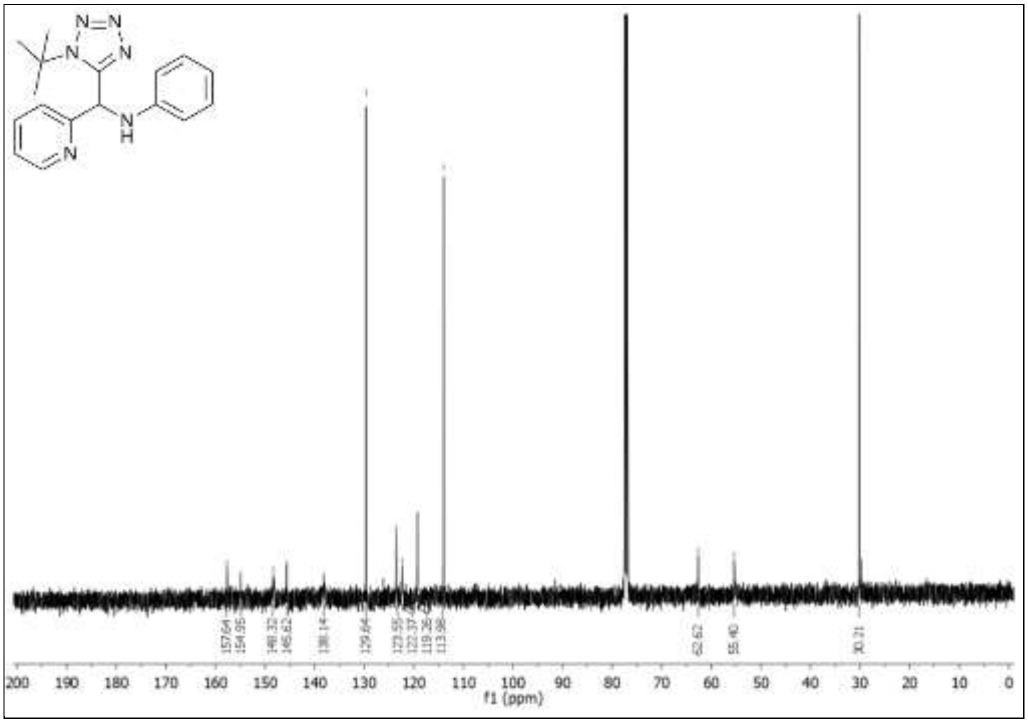
N-((1-(tert-butyl)-1H-tetrazol-5-yl)(pyridin-2-yl)methyl)aniline (4u)



Based on *GP*, 100 mg 2-pyridinecarboxaldehyde (0.93 mmol), 0.085 cm^3 aniline (0.93 mmol), 0.105 cm^3 ter. butyl isocyanide (0.85 mmol), and 0.122 cm^3 TMS-azide (0.93 mmol) were reacted together to afford 266 mg (92%) as a white solid. melting range 147-149°C, R$_f$ = 0.47 (Hexane-AcOEt = 7/3 V/V), **^{1}H NMR** (500 MHz, CDCl$_3$) δ 8.53 (s, 1H), 7.70 (d, *J* = 7.3 Hz, 1H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.24 (s, 1H), 7.19 – 7.14 (m, 2H), 6.77 – 6.71 (m, 3H), 6.41 (s, 1H), 5.43 (s, 1H), 1.75 (s,9H); **^{13}C NMR** (126 MHz, CDCl$_3$) δ 157.64, 154.95, 148.32, 145.62, 138.14, 129.64, 123.55, 122.37, 119.26, 113.98, 62.62, 55.40, 30.21; **FT-IR** (ATR) ν_{max}/cm^{-1} 3273.6, 3054.6, 2958.2, 1604.4, 1254.1; **HRMS** (ESI+): *m/z* calcd. for $C_{17}H_{20}N_6^+$ 309.1822, found 309.1810.

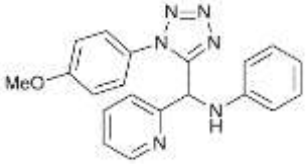


^{1}H NMR spectra of the compound **4u**

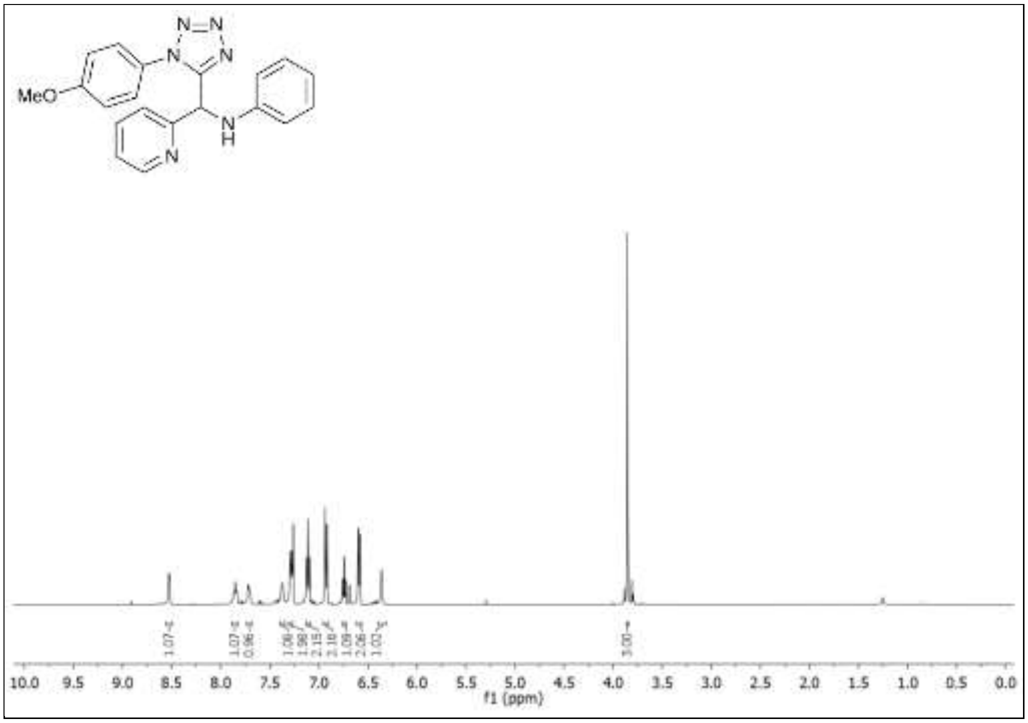


^{13}C NMR spectra of the compound **4u**

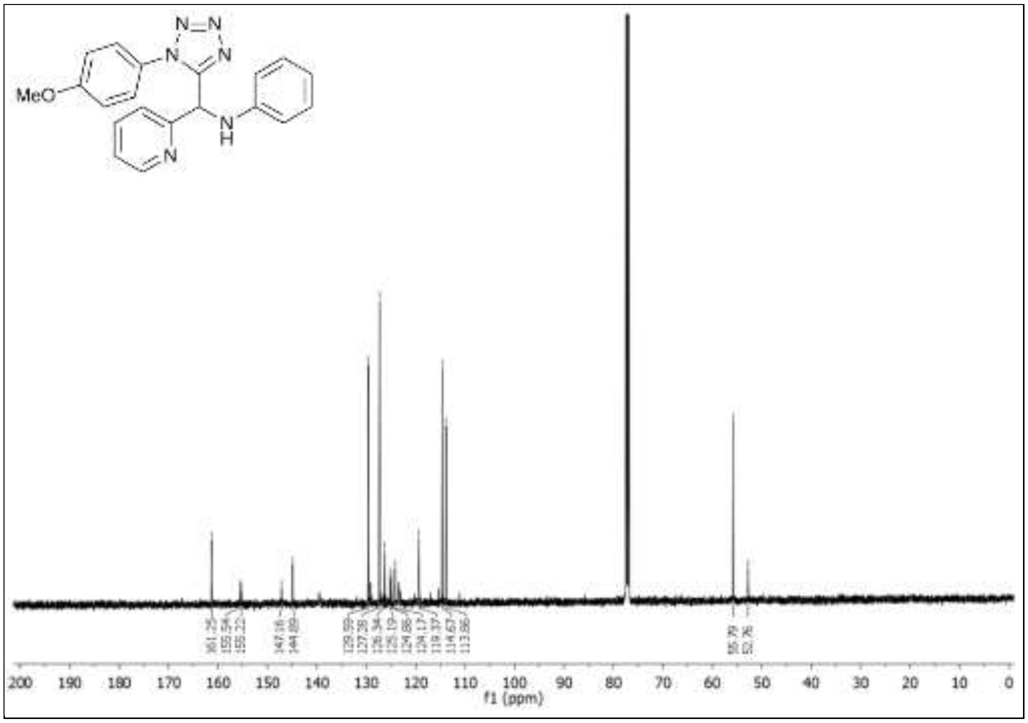
N-((1-(4-methoxyphenyl)-1H-tetrazol-5-yl)(pyridin-2-yl)methyl)aniline (4v)



Based on *GP*, 100 mg 2-pyridinecarboxaldehyde (0.93 mmol), 0.085 cm^3 aniline (0.93 mmol), 124 mg 4-methoxyphenyl isocyanide (0.85 mmol), and 0.122 cm^3 TMS-azide (0.93 mmol) were reacted together to afford 288 mg (86%) as a light yellow solid. Melting range 182-183°C, $R_f = 0.50$ (Hexane-AcOEt = 7/3 V/V); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.52 (d, *J* = 4.5 Hz, 1H), 7.89 – 7.82 (m, 1H), 7.70 (d, *J* = 7.0 Hz, 1H), 7.38 (d, *J* = 4.9 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.13 – 7.09 (m, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 6.76 – 6.72 (m, 1H), 6.59 (d, *J* = 8.0 Hz, 2H), 6.36 (s, 1H), 3.85 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.25, 155.54, 155.22, 147.16, 144.89, 129.59, 127.28, 126.34, 125.19, 124.86, 124.17, 119.37, 114.67, 113.86, 55.79, 52.76; **FT-IR** (ATR) ν_{max}/cm^{-1} 3273.6, 3054.6, 2968.4, 1604.4, 1254.1; **HRMS** (ESI+): *m/z* calcd. for $C_{20}H_{18}N_6O^+$ 359.1614, found 359.1606.

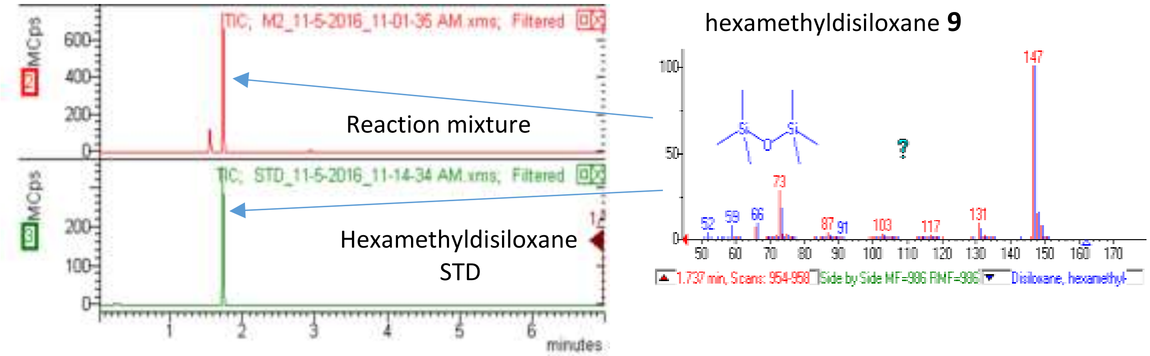


^{1}H NMR spectra of the compound **4v**



^{13}C NMR spectra of the compound **4v**

GC-MS experiment


hexamethyldisiloxane **9**

Reaction mixture

Hexamethyldisiloxane
STD

Column SGE 5-MS 30m x 0.25mm x 0.25µm
Horno 60-260°C, 30°C/min, TIC 60-400 m/z, injector 250°C, flow of He 1ml/min
Sample 1-5µl vapours, temperature 23°C, split 1:25

X-ray data of the compound 4q

Table 1 Crystal data and structure refinement for **4q**.

Identification code	**4q**
Empirical formula	$C_{22}H_{21}N_5$
Formula weight	355.44
Temperature/K	293
Crystal system	Triclinic
Space group	P-1
a/Å	9.2637(4)
b/Å	10.3529(4)
c/Å	10.4849(5)
α/°	86.787(4)
β/°	75.671(4)
γ/°	82.064(4)
Volume/Å^3	964.70(8)
Z	2
ρ_{calc}g/cm^3	1.224
μ/mm^{-1}	0.075
F(000)	376.0
Crystal size/mm^3	0.54 × 0.223 × 0.207
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.778 to 59.126
Index ranges	$12 \le h \le 7$, $13 \le k \le 13$, $14 \le l \le 11$
Reflections collected	8194
Independent reflections	4432 [R_{int} = 0.0191, R_{sigma} = 0.0282]
Data/restraints/parameters	4432/0/251
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0533, wR_2 = 0.1293
Final R indexes [all data]	R_1 = 0.0699, wR_2 = 0.1424
Largest diff. peak/hole / e Å^{-3}	0.15/0.17

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **4q**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*Y*	*Z*	U(eq)
N(0AA)	-104.7(15)	8110.9(13)	4050.9(15)	61.5(4)
N(1)	1790.2(14)	6757.9(12)	3093.2(13)	50.3(3)
N(2)	647.3(16)	6636.5(14)	2528.5(15)	63.0(4)
N(3)	-478.0(17)	7448.9(15)	3110.0(17)	68.8(4)
N(4)	1369.3(17)	8845.9(13)	5970.3(13)	62.0(4)
C(0AA)	1302.9(17)	7670.1(14)	4023.9(15)	48.0(4)
C(3)	3426.9(17)	8922.0(15)	4016.6(14)	48.8(4)
C(5)	633.8(17)	8285.2(16)	7143.1(15)	50.6(4)
C(6)	3258.4(17)	6035.7(15)	2625.3(16)	52.4(4)
C(8)	2257.4(17)	8112.5(15)	4849.1(14)	50.5(4)
C(10)	4939.8(18)	8467.9(18)	3766.9(17)	61.5(4)
C(11)	21(2)	9086.3(18)	8214.8(16)	65.3(5)
C(12)	2980(2)	10128.8(16)	3500.2(16)	55.7(4)
C(13)	4038(2)	10861.6(18)	2749.2(18)	66.7(5)
C(15)	471(2)	6965.9(17)	7304.8(17)	63.7(5)
C(16)	3647.8(19)	4892.8(16)	3299.0(18)	59.8(4)
C(17)	4205(2)	6526.6(19)	1504.4(17)	66.7(5)
C(18)	5088(2)	4252(2)	2839(2)	79.9(6)
C(19)	-813(2)	7262(2)	9570.7(19)	79.4(6)
C(20)	5993(2)	9204(2)	3015(2)	73.4(5)
C(21)	-246(2)	6467(2)	8518.8(19)	73.3(5)
C(22)	5545(2)	10400(2)	2511(2)	73.5(5)
C(23)	2569(2)	4355.3(19)	4455(2)	81.4(6)
C(24)	-697(2)	8577(2)	9407.6(18)	80.9(6)
C(25)	5621(2)	5824(3)	1087(2)	88.5(7)
C(26)	6062(2)	4721(3)	1751(3)	93.6(8)
C(27)	3718(3)	7740(2)	782(2)	92.7(7)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for **4q**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(0AA)	56.1(8)	55.6(8)	69.0(9)	-3.2(7)	-12.6(7)	1.8(6)
N(1)	51.1(7)	46.4(7)	52.2(7)	-4.3(6)	-12.9(6)	-0.4(5)
N(2)	62.4(9)	57.4(8)	73.3(10)	-4.3(7)	-25.9(7)	-3.7(7)
N(3)	59.3(9)	62.8(9)	86.5(11)	-3.1(8)	-25.3(8)	-0.4(7)
N(4)	82.6(10)	49.1(7)	44.8(7)	-3.7(6)	1.5(7)	-5.2(7)

C(0AA)	51.0(8)	40.4(7)	46.9(8)	1.8(6)	-5.0(6)	-0.8(6)
C(3)	50.4(8)	56.1(9)	38.7(7)	-3.2(7)	-10.5(6)	-2.9(7)
C(5)	50.0(8)	57.3(9)	43.8(8)	0.8(7)	-10.1(6)	-7.5(7)
C(6)	52.0(9)	52.6(9)	51.2(8)	-13.4(7)	-9.9(7)	-1.9(7)
C(8)	56.3(9)	48.2(8)	43.0(8)	-2.1(6)	-8.0(7)	0.5(7)
C(10)	54.5(10)	70.3(11)	57.5(10)	4.2(8)	-16.8(8)	3.1(8)
C(11)	83.1(12)	66.5(11)	46.9(9)	-8.2(8)	-8.8(8)	-21.6(9)
C(12)	51.4(9)	57.7(10)	54.1(9)	0.4(8)	-8.7(7)	-1.8(7)
C(13)	73.7(12)	59.2(10)	64.8(11)	6.8(9)	-13.7(9)	-9.3(9)
C(15)	72.5(11)	58.7(10)	54.7(10)	-4.7(8)	-6.4(8)	-6.3(8)
C(16)	59.9(10)	53.6(9)	65.7(10)	-11.6(8)	-18.9(8)	3.6(7)
C(17)	71.8(12)	72.5(12)	52.8(10)	-15.3(9)	-3.1(8)	-14.9(9)
C(18)	68.8(12)	76.4(13)	94.9(15)	-23.2(11)	-30.1(12)	16.2(10)
C(19)	92.6(15)	97.7(15)	49.7(10)	5.4(10)	-5.7(9)	-42.6(12)
C(20)	46.1(9)	96.0(15)	73.9(12)	2.6(11)	-10.1(8)	-5.2(9)
C(21)	85.4(13)	67.1(11)	66.2(11)	7.3(9)	-10.3(10)	-24(1)
C(22)	62.3(11)	84.2(13)	71.6(12)	8.2(10)	-7.6(9)	-21.5(10)
C(23)	91.7(15)	58.3(11)	84.7(14)	10.2(10)	-13.2(11)	2.7(10)
C(24)	99.2(15)	93.9(15)	47.5(10)	-14.6(10)	0.2(10)	-33.6(12)
C(25)	67.3(13)	119.4(19)	71.5(13)	-32.0(13)	9.4(10)	-22.8(13)
C(26)	53.8(11)	118(2)	105.4(18)	-46.3(16)	-15.2(12)	12.2(12)
C(27)	131(2)	86.6(15)	52.4(11)	3.4(10)	-0.9(12)	-26.7(14)

Table 4 Bond Lengths for **4q**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N(0AA)	N(3)	1.368(2)	C(6)	C(17)	1.398(2)
N(0AA)	C(0AA)	1.3146(19)	C(10)	C(20)	1.383(3)
N(1)	N(2)	1.3575(18)	C(11)	C(24)	1.377(2)
N(1)	C(0AA)	1.3474(19)	C(12)	C(13)	1.383(2)
N(1)	C(6)	1.4421(19)	C(13)	C(22)	1.377(3)
N(2)	N(3)	1.2909(19)	C(15)	C(21)	1.390(2)
N(4)	C(5)	1.388(2)	C(16)	C(18)	1.387(2)
N(4)	C(8)	1.4437(19)	C(16)	C(23)	1.502(3)
C(0AA)	C(8)	1.508(2)	C(17)	C(25)	1.389(3)
C(3)	C(8)	1.529(2)	C(17)	C(27)	1.504(3)
C(3)	C(10)	1.380(2)	C(18)	C(26)	1.379(3)
C(3)	C(12)	1.385(2)	C(19)	C(21)	1.366(3)
C(5)	C(11)	1.390(2)	C(19)	C(24)	1.378(3)
C(5)	C(15)	1.391(2)	C(20)	C(22)	1.370(3)
C(6)	C(16)	1.394(2)	C(25)	C(26)	1.371(3)

Table 5 Bond Angles for **4q**

Atom	Atom	Atom	Angle/˚
C(0AA)	N(0AA)	N(3)	106.18(13)
N(2)	N(1)	C(6)	121.14(13)
C(0AA)	N(1)	N(2)	108.37(12)
C(0AA)	N(1)	C(6)	130.37(13)
N(3)	N(2)	N(1)	106.34(14)
N(2)	N(3)	N(0AA)	110.77(14)
C(5)	N(4)	C(8)	124.15(13)
N(0AA)	C(0AA)	N(1)	108.33(14)
N(0AA)	C(0AA)	C(8)	127.11(14)
N(1)	C(0AA)	C(8)	124.53(13)
C(10)	C(3)	C(8)	120.86(14)
C(10)	C(3)	C(12)	118.87(15)
C(12)	C(3)	C(8)	120.26(14)
N(4)	C(5)	C(11)	118.23(15)
N(4)	C(5)	C(15)	123.65(15)
C(11)	C(5)	C(15)	118.11(15)
C(16)	C(6)	N(1)	118.72(14)
C(16)	C(6)	C(17)	123.90(15)
C(17)	C(6)	N(1)	117.37(15)
N(4)	C(8)	C(0AA)	112.29(13)
N(4)	C(8)	C(3)	109.90(13)
C(0AA)	C(8)	C(3)	110.74(12)
C(3)	C(10)	C(20)	120.65(16)
C(24)	C(11)	C(5)	120.64(17)
C(13)	C(12)	C(3)	120.25(16)
C(22)	C(13)	C(12)	120.31(17)
C(21)	C(15)	C(5)	120.46(17)
C(6)	C(16)	C(23)	122.37(15)
C(18)	C(16)	C(6)	116.75(18)
C(18)	C(16)	C(23)	120.87(17)
C(6)	C(17)	C(27)	122.08(17)
C(25)	C(17)	C(6)	116.20(19)
C(25)	C(17)	C(27)	121.71(19)
C(26)	C(18)	C(16)	120.9(2)
C(21)	C(19)	C(24)	119.17(17)
C(22)	C(20)	C(10)	120.23(17)
C(19)	C(21)	C(15)	120.69(18)
C(20)	C(22)	C(13)	119.68(17)
C(11)	C(24)	C(19)	120.87(18)
C(26)	C(25)	C(17)	121.5(2)
C(25)	C(26)	C(18)	120.61(19)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4q.**

Atom	*x*	*y*	*z*	U(eq)
H(4)	1291	9683	5908	74
H(8)	2794	7334	5179	61
H(10)	5254	7659	4107	74
H(11)	97	9975	8125	78
H(12)	1940(20)	10445(16)	3661(17)	64(5)
H(13)	3730	11670	2403	80
H(15)	845	6414	6595	76
H(18)	5400	3495	3271	96
H(19)	-1271	6921	10387	95
H(20)	7010	8887	2851	88
H(21)	-340	5582	8616	88
H(22)	6255	10897	2011	88
H(23A)	2764	4609	5257	122
H(23B)	2696	3421	4420	122
H(23C)	1558	4692	4427	122
H(24)	-1109	9128	10113	97
H(25)	6285	6109	340	106
H(26)	7027	4284	1465	112
H(27A)	2839	7623	494	139
H(27B)	4512	7904	32	139
H(27C)	3492	8467	1359	139

ORTEP diagram of the compound 4q