Supporting Information

Understanding the Regioselectivity of 5-Substituted 1*H*-Tetrazoles Alkylation

Guillaume Reynard, Julien Moisan-Labelle, Étienne Parent and Hélène Lebel*.

Department of Chemistry and Center in Green Chemistry and Catalysis (CGCC), Université de Montréal, P.O. Box 6128, Station Downtown, Montréal, QC H3C 3J7, Canada

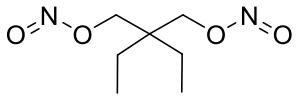
Table of Contents

General Information

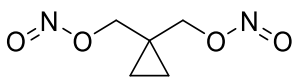
Analytical thin-layer chromatography was performed using 0.25 mm silica gel 60-F plates. Visualization of the developed chromatogram was performed by UV absorbance, cerium ammonium molybdate, or aqueous potassium permanganate. Flash chromatography was performed using silica gel (230−400 mesh) with the indicated solvent system. Infrared spectra are reported in reciprocal centimeters (cm^{-1}). Only the most important and relevant frequencies are reported. Chemical shifts for ^1H NMR spectra were recorded in parts per million with the solvent resonance as the reference $CDCl_3$ (δ = 7.26 ppm) unless otherwise indicated. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qn = quintuplet, sx=sextet, sept = septet, m = multiplet and br = broad), coupling constant in Hz and integration. Chemical shifts for 13C(1H) NMR spectra are recorded in parts per million using the central peak of $CDCl_3$ (δ = 77.16 ppm) as the reference unless otherwise indicated. All 13C(1H) NMR spectra were obtained with complete proton decoupling. All NMR yields were determined using quantitative 1H NMR spectra using tetrachloroethane as an internal standard with a 10-sec relaxation time. High resolution mass spectra analysis was performed by the Centre régional de spectroscopie de masse de l'Université de Montréal.

Dinitrite Reagents Synthesis

1,3-Propanedinitrite and 1,3-(2,2-Dimethyl)propanedinitrite were synthesized according to previously reported methods.[1,2] *DSC-TGA spectra of dinitrite reagents in a sealed stainless-steel crucible revealed an important, strong exothermic event from ~120 to 175 °C, with an important loss of mass and a significant modification of temperature setpoint, consistent with a decomposition. Heating dinitrite reagents concentrated or neat is thus not recommended, as autocatalytic decomposition may occur and overpressure might develop, due to the formation of gases. Distillation should also be avoided.*



2,2-Diethylpropane-1,3-diyl dinitrite. In a 100 mL round bottom flask with magnetic stirring bar, sodium nitrite (4.43 g, 64.3 mmol, 2.40 equiv) was dissolved in H_2O (15 mL) under ambient atmosphere. 2,2-diethyl-1,3-propanediol (3.54 g, 26.8 mmol, 1.00 equiv) was added and the solution was cooled to 0 °C. A solution of H_2SO_4 (4.89 mL, 64.3 mmol, 2.40 equiv) diluted in H_2O (15 mL) was added dropwise with an addition funnel over a period of 30 min. The reaction was stirred 60 min at 0 °C after the end of addition. The reaction was transferred in a separatory funnel and brine (15 mL) was added. The two layers were separated, and the organic layer was washed with brine, then dried over Na_2SO_4. The title compound was isolated as a yellow liquid (4.94 g, 26.0 mmol, 97% yield). 2,2-diethylpropane-1,3-diyl dinitrite was stored on Na_2SO_4 at rt during few months without significant decomposition. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 4.56 (s, 4H), 1.38 (q, *J* = 5.2 Hz, 4H), 0.87 (t, *J* = 7.5 Hz, 6H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 69.5, 40.7, 23.1, 7.0.

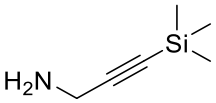


Cyclopropane-1,1-diylbis(methylene) dinitrite. In a 100 mL round bottom flask with magnetic stirring bar, sodium nitrite (4.49 g, 67.9 mmol, 2.40 equiv) was dissolved in H_2O (15 mL) under ambient atmosphere. Cyclopropane-1,1-diyldimethanol (2.89 g, 28.3 mmol, 1.00 equiv) was added and the solution was cooled to 0 °C. A solution of H_2SO_4 (5.17 mL, 67.9 mmol, 2.40 equiv) diluted in H_2O (15 mL) was added dropwise with an addition funnel over a period of 30 min. The reaction was stirred 60 min at 0 °C after the end of addition. The reaction was transferred in a separatory funnel and brine (15 mL)

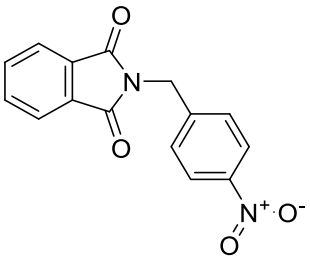
[1] G. Reynard, E.-M. Joseph-Valcin and H. Lebel, *Chem. Commun.*, 2020, **56**, 10938-10941.
[2] C. Audubert and H. Lebel, *Org. Lett.*, 2017, **19**, 4407-4410.

was added. The two layers were separated, and the organic layer was washed with brine, then dried over Na_2SO_4. The title compound was isolated as a bright orange liquid (4.40 g, 27.5 mmol, 97% yield). Cyclopropane-1,1-diylbis(methylene) dinitrite was stored on Na_2SO_4 in the fridge during few weeks without significant decomposition. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 4.66 (s, 4H), 0.73 (s, 4H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 71.9, 20.9, 9.8.

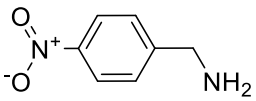
Starting Material Synthesis



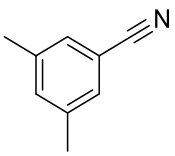
3-(Trimethylsilyl)prop-2-yn-1-amine. 3-(trimethylsilyl)prop-2-yn-1-amine was prepared from propargylamine, lithium bis(trimethylsilyl)amide, and chlorotrimethylsilane according to the literature procedure affording the hydrochloride salt.[3] It was then dissolved in sat. $NaHCO_3$, extracted three times with $CHCl_3$. The combined organic layers were dried over Na_2SO_4, and concentrated under vacuum at room temperature. Distillation afforded the free base as a clear oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.43 (s, 2H), 1.31 (br.s., 2H), 0.16 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 107.5, 86.7, 32.5, 0.1.



2-(4-Nitrobenzyl)isoindoline-1,3-dione. 2-(4-nitrobenzyl)isoindoline-1,3-dione was prepared from 4-nitrobenzyl bromide according to literature procedure.[4] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.8 Hz, 2H), 7.87 (dd, *J* = 5.5 Hz, 3.0 Hz, 2H), 7.75 (dd, *J* = 5.5 Hz, 3.1 Hz, 2H), 7.58 (d, *J* = 8.8 Hz, 2H), 4.93 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 167.9, 147.7, 143.4, 134.5, 132.0, 129.5, 124.1, 123.8, 41.0.



4-Nitrobenzylamine. 4-nitrobenzylamine was prepared from 2-(4-nitrobenzyl)isoindoline-1,3-dione according to literature procedure.[5] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.6 Hz, 2H), 7.50 (d, *J* = 8.7 Hz, 2H), 4.00 (s, 2H), 1.50 (br.s., 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.7, 147.0, 127.8, 123.9, 45.9.



3,5-Dimethylbenzonitrile. 3,5-dimethylbenzonitrile was prepared from 1-bromo-3,5-dimethylbenzene according to literature procedure.[6] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.26 (s, 2H), 7.21 (s, 1H), 2.35 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 139.1, 134.7, 129.8, 119.3, 21.1.

---

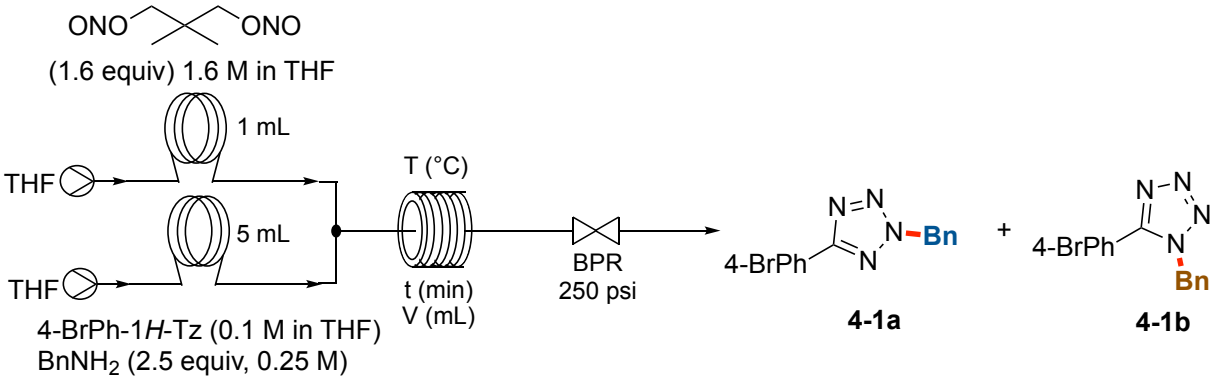
[3] J. Derosa, A. L. Cantu, M. N. Boulous, M. L. O'Duill, J. L. Turnbull, Z. Liu, D. M. De La Torre, K. M. Engle, *J. Am. Chem. Soc.,* 2017, **139**, 5183-5193.

[4] Y. Katsura, T. Tomishi, Y. Inoue, K. Sakane, Y. Matsumoto, C. Morinaga, H. Ishikawa, H. Takasugi, *J. Med. Chem.,* 2000, **43**, 3315-3321.

[5] P. Liu, Y. Du, L. Song, J. Shen, Q. Li, *Bioorg. Med. Chem.,* 2015, **23**, 7079-7088.

[6] J. Zanon, A. Klapars, S. L. Buchwald, *J. Am. Chem. Soc.,* 2003, **125**, 2890-2891.

Procedure for the Optimization of the Continuous Flow Alkylation of 1*H*-Tz



A 5 mL sample loop A was charged with a 0.1 M solution of the tetrazole (0.50 mmol, 1.00 equiv) in THF and a 0.25 M solution of the amine (1.25 mmol, 2.50 equiv). A 1 mL sample loop B was charged with a 1.6 M solution of the 1,3-(2,2-dimethyl)-propanedinitrite (0.800 mmol, 1.6 equiv). The solutions were prepared in a 10 mL gauge flask. The 2 loops were injected in the system with the calculated flowrate in a reactor at the desired temperature with a back-pressure regulator at 250 psi. When more than one 10 mL reactor was used, the reactors were connected head-to-head. After the desired residence time, the product was collected in an opened flask (25 mL collection volume).

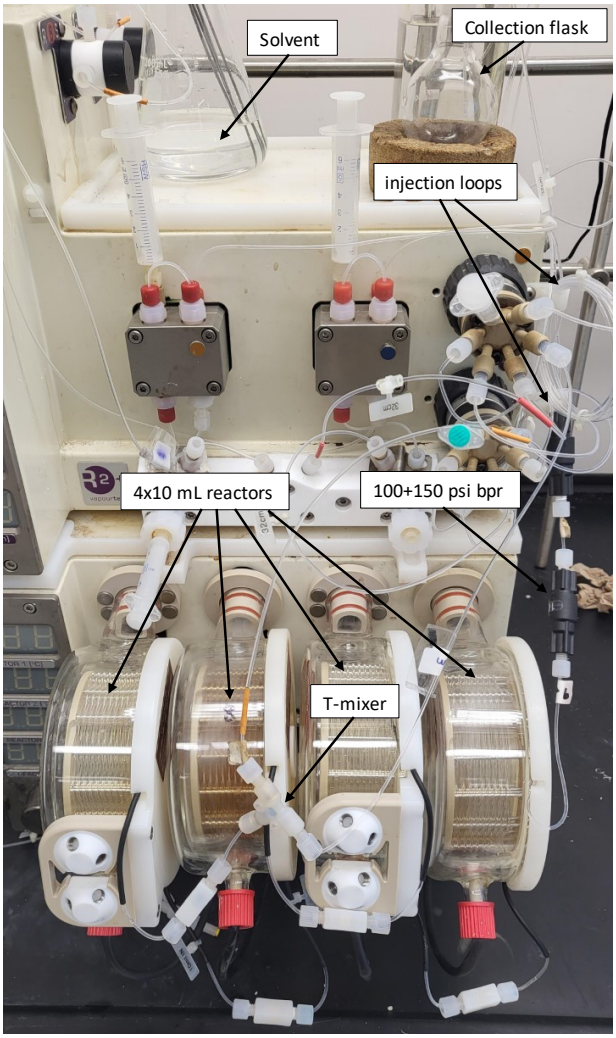


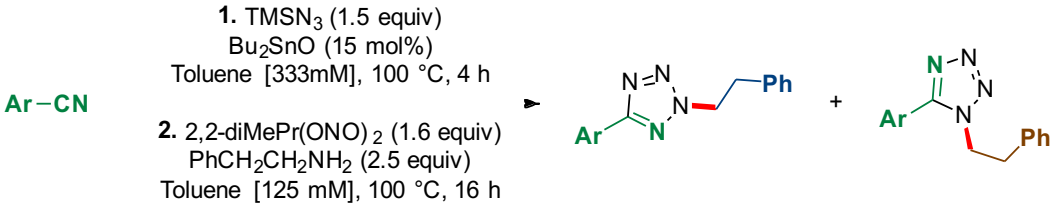
Figure S1. Continuous Flow Reactor Set-up

Table S1. Optimization of the Continuous Flow Alkylation of 1*H*-Tz via Amine Diazotization

Entry	T (°C)	t (min)	V (mL)	1a yield	1a : 1b ratio
1	70	30	40	41%	76 : 24
2	100	30	40	40%	74 : 26
3	100	15	40	43%	77 : 23
4	100	15	20	45%	78 : 22
5	120	30	40	52%	79 : 21
6	120	15	20	49%	79 : 21
7	120	5	20	47%	78 : 22
8	120	60	20	45%	80 : 20
9	140	15	20	57%	78 : 22
10	140	5	10	42%	78 : 22
11	160	15	20	46%	78 : 22
12	160	5	20	46%	79 : 21

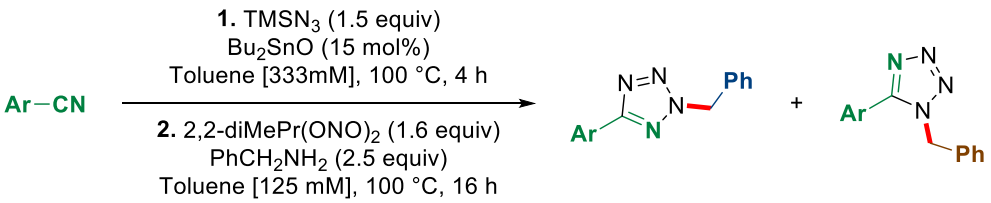
Notes: Reactions were performed on a 1 mmol scale. PFA tubings were used for temperature up to 120 °C. For temperature of 140 °C and above, stainless still reactors were used. Both reactors were tested at 120 °C without a significant modification of the yield. Yields were calculated by NMR using 1,1,2,2-tetrachloroethane as the internal standard.

Table S2. Alkylation of Various Tetrazoles with Phenethylamine



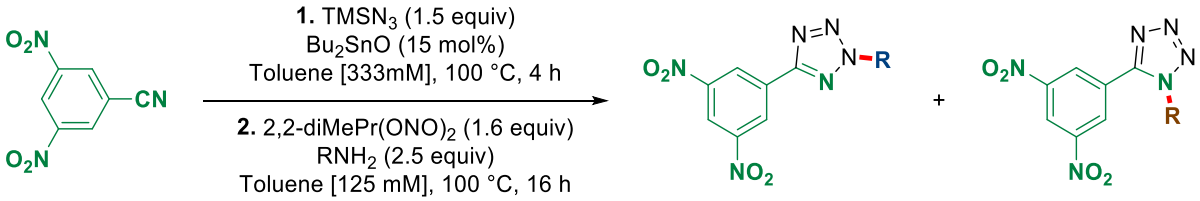
Entry	Ar	Yield (2,5-Tz)	Yield (1,5-Tz)	Ratio	substrate
1	3,5-diMePh	59%	22%	73 : 27	**35**
2	Ph	70%	17%	80 : 20	**36**
3	3-BrPh	77%	18%	81 : 19	**37**
4	3-NO_2Ph	73%	12%	86 : 14	**38**
5	4-NO_2Ph	80%	8%	91 : 9	**39**
6	3,5-diNO_2Ph	87%	Not isolated	93 : 7	**40**

Table S3. Alkylation of Various Tetrazoles with Benzylamine



Entry	Ar	Yield (2,5-Tz)	Yield (1,5-Tz)	Ratio	substrate
1	3,5-diMePh	55%	24%	70 : 30	**41**
2	Ph	59%	24%	71 : 29	**6**
3	3-BrPh	65%	26%	71 : 29	**42**
4	3-NO_2Ph	66%	24%	73 : 27	**43**
5	4-NO_2Ph	67%	18%	79 : 31	**44**
6	3,5-diNO_2Ph	70%	22%	76 : 24	**45**

Table S4. Alkylation of 5-(3,4-dinitrophenyl)-1H-tetrazole with Various Amines



Entry	R	Yield (2,5-Tz)	Yield (1,5-Tz)	Ratio	Substrate
1	(S)-1-phenylethyl	50%	19%	72 : 28	**46**
2	4-OMePhCH$_2$	64%	24%	73 : 27	**47**
4	4-NO$_2$PhCH$_2$	69%	14%	83 : 17	**48**
6	Me	86%	6%	94 : 6	**49**

General procedures

General procedure A for the alkylation of 5-monosubstituted tetrazoles

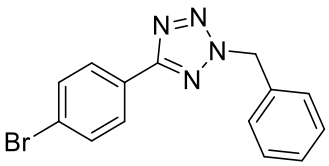
In a round bottom flask with a magnetic stirring bar, the 5-monosubstituted tetrazole (0.500 mmol, 1.00 equiv) was suspended in EtOAc (4 mL). The resulting suspension was stirred at room temperature. 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) was added, followed by the amine (1.25 mmol, 2.50 equiv.). The flask was placed in an oil bath, and the mixture was heated to reflux for 16 hours. The solvent was removed under reduced pressure, and the crude mixture was purified by flash chromatography.

General procedure B for the sequential one-pot cycloaddition-diazotisation reaction

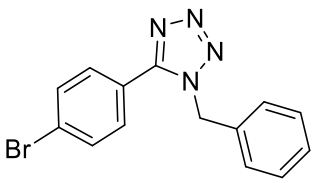
In a round bottom flask with a magnetic stirring bar, the nitrile (0.500 mmol, 1.00 equiv) was diluted in toluene (1.5 mL). The resulting mixture was stirred at room temperature. Dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv) was added, followed by azidotrimethylsilane (0.099 mL, 0.750 mmol, 1.50 equiv). The flask was placed in an oil bath, and the mixture was heated to reflux for 4 h (procedure **B1**) or 16 hours (procedure **B2**). The mixture was cooled to room temperature, and toluene (2.5 mL) was added. 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) was added, followed by the amine (1.25 mmol, 2.50 equiv.). The flask was placed in an oil bath, and the mixture was heated to reflux for 16 hours. The mixture was stirred at room temperature. The solvent was removed under reduced pressure, and the crude mixture was purified by flash chromatography.

Characterization data

The synthesis of 2,5-Tz **1a**, **2**, **3a**, **4**, **6a**, **8a**, **9a**, **10a**, **11**, **13a**, **15**, **16**, **18a**, **19a**, **20a**, **23**, **24**, **31**, **32a**, **33a**, **37a**, **39a** and **49a** has been previously described.[7]



1a



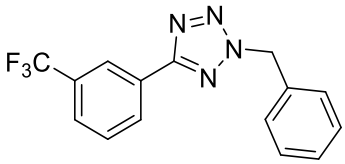
1b

2-Benzyl-5-(4-bromophenyl)-2H-tetrazole (1a) and 1-benzyl-5-(4-bromophenyl)-1H-tetrazole (1b). The title compounds were prepared according to the general procedure **A** using 5-(4-bromophenyl)-1H-tetrazole (113 mg, 0.500 mmol, 1.00 equiv), benzylamine (0.137 ml, 1.25 mmol, 2.50 equiv) and 1,3-

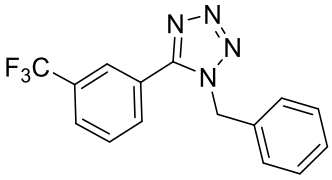
[7] G. Reynard and H. Lebel, *J. Org. Chem.*, 2021, **86**, 12452-12459.

(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 10%, then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **1a** (112 mg, 0.36 mmol, 71% yield) was isolated as a white solid as previously reported.[7] $\mathbf{R_f}$ 0.53 (20% EtOAc/hexanes); **mp** 103-107 °C (litt. 105-107 °C);[8] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01 (dt, *J* = 8.7 Hz, 2.1 Hz, 2H), 7.60 (dt, *J* = 8.7 Hz, 2.0 Hz, 2H), 7.45-7.34 (m, 5H), 5.80 (s, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 164.8, 133.3, 132.2, 129.2, 128.6, 128.5, 126.5, 124.8, 57.1. Tetrazole **1b** (36.8 mg, 0.12 mmol, 23% yield) was isolated as a white solid. Spectral data matched those reported in the literature.[8] $\mathbf{R_f}$ 0.28 (20% EtOAc/hexanes); **mp** 92-94 °C; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 87.64 (d, *J* = 9 Hz, 2H), 7.45 (d, *J* = 9 Hz, 2H), 7.37-7.34 (m, 3H), 7.17-7.12 (m, 2H), 5.61 (s, 2H); **^{13}C** NMR (75 MHz, $CDCl_3$) δ154.0, 133.8, 132.7, 130.4, 129.4, 129.1, 127.2, 126.3, 122.8, 51.6.

The title compounds were also prepared according to the general procedure **B1** using 4-bromobenzonitrile (91.0 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step) leading to tetrazole **1a** (102 mg, 0.324 mmol, 65% yield) as a white solid and tetrazole **1b** (37.8 mg, 0.120 mmol, 24% yield) as a white solid.



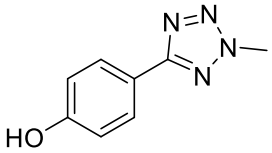
3a



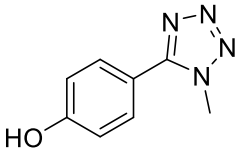
3b

2-Benzyl-5-(3-(trifluoromethyl)phenyl)-2H-tetrazole (3a) and 1-benzyl-5-(3-(trifluoromethyl)phenyl)-1H-tetrazole (3b). The title compounds were prepared according to the general procedure **A** using 5-(3-(trifluoromethyl)phenyl)-1H-tetrazole (107 mg, 0.500 mmol, 1.00 equiv), benzylamine (0.137 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **3a** (85.1 mg, 0.36 mmol, 72% yield) was isolated as a white solid as previously reported.[7] $\mathbf{R_f}$ 0.54 (20% EtOAc/hexanes); **mp** 69-74 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 8.33 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.46-7.33 (m, 5H), 5.82 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 133.2, 131.5 (q, *J* = 32.8 Hz), 130.1 (d, *J* = 0.8 Hz), 129.6, 129.2, 128.6, 128.4, 128.0, 127.0 (q, *J* = 3.7 Hz), 123.9 (q, *J* = 3.9 Hz), 123.9 (d, *J* = 272.4 Hz), 57.1; **^{19}F NMR** (375 MH, $CDCl_3$) δ 62.82 (s).

Tetrazole **3b** (42.6 mg, 0.14 mmol, 28% yield) was isolated as a pale-yellow oil. $\mathbf{R_f}$ 0.24 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84-7.77 (m, 3H), 7.64 (t, *J* = 8.1 Hz, 1H), 7.40-7.32 (m, 3H), 7.19-7.13 (m, 2H), 5.64 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.6, 133.6, 132.3, 131.9 (d, *J* = 33.2 Hz), 131.4, 130.0, 129.2, 128.1 (q, *J* = 3.6 Hz), 127.3, 126.0 (q, *J* = 3.6 Hz), 124.8, 123.7 (d, *J* = 272.7 Hz), 51.9; **^{19}F NMR** (375 MH, $CDCl_3$) δ 62.93 (s); **FTIR** (cm^{-1}) (neat) 3200-2800, 1498, 1332, 1125, 747, 725, 697; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{12}F_3N_4Na$ 305.1009, found 305.1008.



5a



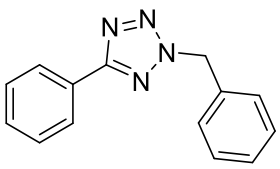
5b

4-(2-Methyl-2H-tetrazol-5-yl)phenol (5a) and 4-(1-methyl-1H-tetrazol-5-yl)phenol (5b). The title compounds were prepared according to the general procedure **A** using 4-(1H-tetrazol-5-yl)phenol (81.1

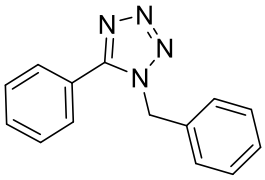
[8] Y.-J. Ding, Y. Li, S.-Y. Dai, Q. Lan, X.-S. Wang, *Org. Biomol. Chem.,* 2015, **13**, 3198-3201.

mg, 0.500 mmol, 1.00 equiv), methylamine (0.625 ml, 1.25 mmol, 2.50 equiv, 2 M in THF) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 30% then 300 mL 50% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **5a** (38.7 mg, 0.22 mmol, 44% yield) was isolated as a white solid. Spectral data matched those reported in the literature.[9] **R_f** 0.53 (50% EtOAc/hexanes); **mp** 197-202 °C (litt. 210-212 °C);[9] **^{1}H NMR** (400 MHz, acetone-d6) δ 8.85-8.81 (br. s., 1H), 7.96 (dt, J = 8.8 Hz, 2.4 Hz, 2H), 6.99 (dt, J = 8.8 Hz, 2.3 Hz, 2H), 4.39 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.2, 160.6, 129.4, 120.5, 117.1, 40.1.

Tetrazole **5b** (10.6 mg, 0.06 mmol, 12% yield) was isolated as a pale-yellow sticky oil. Spectral data matched those reported in the literature.[10] **R_f** 0.48 (50% EtOAc/hexanes); **^{1}H NMR** (400 MHz, dmso-d6) δ 10.18 (br. s., 1H), 7.70 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.7 Hz, 2H), 4.13 (s, 3H); **^{13}C NMR** (100 MHz, dmso-d6) δ 159.9, 153.9, 130.3, 115.9, 114.3, 35.0.



6a



6b

2-Benzyl-5-phenyl-2H-tetrazole (6a) and 1-benzyl-5-phenyl-1H-tetrazole (6b). The title compounds were prepared according to the general procedure **A** using 5-phenyl-1H-tetrazole (73.1 mg, 0.500 mmol, 1.00 equiv), benzylamine (0.137 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **6a** (85.1 mg, 0.36 mmol, 72% yield) was isolated as a white solid as previously reported.[7] **R_f** 0.57 (20% EtOAc/hexanes); **mp** 88-90 °C (litt. 90-92 °C);[12] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.19-8.11 (m, 2H), 7.51-7.44 (m, 3H), 7.44-7.32 (m, 5H), 5.80 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ165.5, 133.5, 130.4, 129.1, 129.0, 128.9, 128.5, 127.5, 127.0, 56.9.

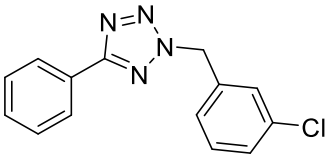
Tetrazole **6b** (30.7 mg, 0.13 mmol, 26% yield) was isolated as a pale-yellow oil. Spectral data matched those reported in the literature.[11] **R_f** 0.23 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61-7.53 (m, 3H), 7.52-7.46 (m, 2H), 7.38-7.31 (m, 3H), 7.18-7.11 (m, 2H), 5.61 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.8, 134.0, 131.5, 129.31, 129.29, 129.0, 128.9, 127.3, 123.9, 51.5.

The title compounds were also prepared according to the general procedure **B1** using benzonitrile (0.516 mL, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step) leading to tetrazole **6a** (70.0 mg, 0.296 mmol, 59% yield) as a white solid and tetrazole **6b** (28.0 mg, 0.12 mmol, 24% yield) as a clear oil.

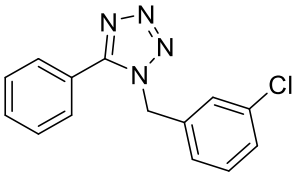
[9] S. Graßmann, B. Sadek, X. Ligneau, S. Elz, C. R. Ganellin, J.-M. Arrang, J.-C. Schwartz, H. Stark, W. Schunack, *Eur. J. Pharm. Sci.* **2002**, *15*, 367-378.

[10] A. Xie, Q. Zhang, Y. Liu, L. Feng, X. Hu, W. Dong, *J. Heterocycl. Chem.* **2015**, *52*, 1483-1487.

[11] K. Livingstone, S. Bertrand, C. Jamieson, *J. Org. Chem.* **2020**, *85*, 7413-7423.



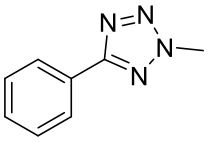
7a



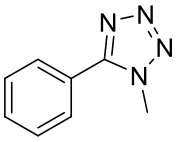
7b

2-(3-Chlorobenzyl)-5-phenyl-2H-tetrazole (7a) and 1-(3-chlorobenzyl)-5-phenyl-1H-tetrazole (7b). The title compounds were prepared according to the general procedure **A** using 5-phenyl-1H-tetrazole (73.1 mg, 0.500 mmol, 1.00 equiv), 3-chlorobenzylamine (0.153 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **7a** (82.6 mg, 0.31 mmol, 61% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.48 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.18-8.11 (m, 2H), 7.52-7.45 (m, 3H), 7.41 (s, 1H), 7.36-7.27 (m, 3H), 5.77 (s, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 165.7, 135.2, 135.0, 130.5, 130.4, 129.3, 129.0, 128.6, 127.3, 127.0, 126.6, 56.4; **FTIR** (cm^{-1}) (neat) 3200-2800, 1600, 1472, 1404, 1079, 775, 734, 695; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{14}H_{12}ClN_4$ 271.0745, found 271.0740.

Tetrazole **7b** (23.0 mg, 0.085 mmol, 17% yield) was isolated as a pale-yellow oil. $\mathbf{R_f}$ 0.18 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61-7.49 (m, 5H), 7.35-7.25 (m, 2H), 7.15 (s, 1H), 7.02 (d, *J* = 7.1 Hz, 1H), 5.58 (s, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 154.9, 135.8, 135.3, 131.7, 130.6, 129.4, 129.2, 128.9, 127.5, 125.4, 123.6, 50.8; **FTIR** (cm^{-1}) (neat) 3200-2800, 1600, 1448, 759, 731, 691; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{14}H_{11}N_4Na$ 293.0564, found 293.0561.



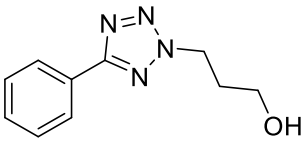
8a



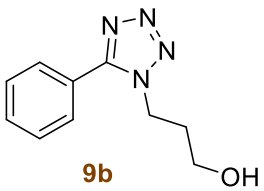
8b

2-Methyl-5-phenyl-2H-tetrazole (8a) and 1-methyl-5-phenyl-1H-tetrazole (8b). The title compounds were prepared according to the general procedure **A** using 5-phenyl-1H-tetrazole (73.1 mg, 0.500 mmol, 1.00 equiv), methylamine (0.625 ml, 1.25 mmol, 2M solution in THF, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (3.35 mL). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 30% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **8a** (57.6 mg, 0.36 mmol, 72% yield) was isolated as a white solid as previously reported.[7] $\mathbf{R_f}$ 0.53 (25% EtOAc/hexanes); **mp** 49-52 °C (litt: 50-52 °C);[14] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.16-8.10 (m, 2H), 7.51-7.44 (m, 3H), 4.39 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 165.39, 130.4, 129.0, 127.5, 126.9, 39.6.

Tetrazole **8b** (17.0 mg, 0.11 mmol, 21% yield) was isolated as a white solid. Spectral data matched those reported in the literature.[12] $\mathbf{R_f}$ 0.51 (50% EtOAc/hexanes); **mp** 101-105 °C (litt. 100-101 °C);[12] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76-7.69 (m, 2H), 7.61-7.53 (m, 3H), 4.17 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.6, 131.4, 129.4, 128.8, 123.9, 35.1.



9a



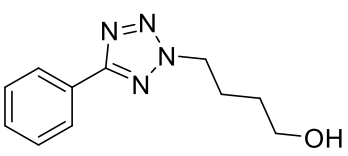
9b

3-(5-Phenyl-2H-tetrazol-2-yl)propan-1-ol (9a) and 3-(5-phenyl-1H-tetrazol-1-yl)propan-1-ol (9b). The title compounds were prepared according to the general procedure **A** using 5-phenyl-1H-tetrazole (73.1 mg, 0.500 mmol, 1.00 equiv), 3-aminopropan-1-ol (0.099 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-

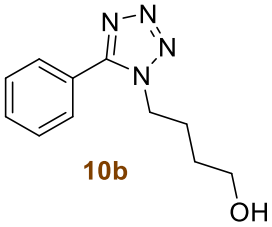
[12] K. Ishihara, T. Shioiri, M. Matsugi, *Org. Lett.* **2020**, *22*, 6244-6247.

dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 50% then 300 mL 75% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **9a** (74.5 mg, 0.37 mmol, 73% yield) was isolated as a clear oil as previously reported.[7] **R_f** 0.56 (75% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10-8.05 (m, 2H), 7.46-7.39 (m, 3H), 4.78 (t, *J* = 6.9 Hz, 2H), 3.70 (t, *J* = 5.9 HZ, 2H), 3.31-3.25 (br.s., 1H), 2.25 (qn, *J* = 6.4 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 165.0, 130.4, 128.9, 127.2, 126.7, 58.7, 50.1, 31.9; **FTIR** (cm^{-1}) (neat) 3600-3200, 3200-2800, 1611, 1530, 1450, 1044; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{10}H_{13}N_4O$ 205.1084, found 205.1082.

Tetrazole **9b** (24.5 mg, 0.12 mmol, 24% yield) was isolated as a clear oil. **R_f** 0.25 (75% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75-7.71 (m, 2H), 7.62-7.55 (m, 3H), 4.60 (t, *J* = 6.9 Hz, 2H), 3.71 (q, *J* = 5.3 Hz, 2H), 2.21 (qn, *J* = 6.3 Hz, 2H), 1.61 (br. t, *J* = 4.7 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.7, 131.4, 129.5, 128.9, 124.1, 58.9, 45.0, 32.1; **FTIR** (cm^{-1}) (neat) 3600-3200, 3200-2800, 1609, 1536, 1470, 1060, 779, 736, 697; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for Calcd for $C_{10}H_{13}N_4O$ 205.1084, found 205.1081.



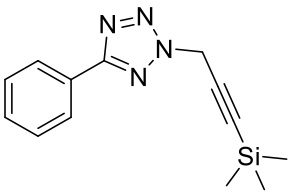
10a



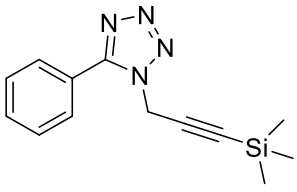
10b

4-(5-Phenyl-2H-tetrazol-2-yl)butan-1-ol (10a) and 4-(5-phenyl-1H-tetrazol-1-yl)butan-1-ol (10b). The title compounds were prepared according to the general procedure **A** using 5-phenyl-1H-tetrazole (73.1 mg, 0.500 mmol, 1.00 equiv), 4-amino-1-butanol (0.115 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in $CHCl_3$ (4 mL). The crude mixture was purified by flash chromatography (300 mL 50% then 300 mL 80% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **10a** (78.6 mg, 0.36 mmol, 72% yield) was isolated as a clear oil as previously reported.[7] **R_f** 0.46 (80% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15-8.11 (m, 2H), 7.51-7.43 (m, 3H), 4.70 (t, *J* = 7.0 Hz, 2H), 3.71 (t, *J* = 6.2 Hz, 2H), 2.17 (quint., *J* = 7.3 Hz, 2H), 1.84-1.76 (br.s., 1H), 1.68-1.60 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 165.2, 130.4, 129.0, 127.5, 126.9, 61.9, 53.1, 29.4, 26.1; **FTIR** (cm^{-1}) (neat) 3600-3200, 3100-2800, 1469, 1536, 1609, 1062, 697, 736; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{11}H_{15}N_4O$ 219.1240, found 219.1238.

Tetrazole **10b** (16.4 mg, 0.075 mmol, 15% yield) was isolated as a pale-yellow oil; **R_f** 0.28 (80% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69-7.66 (m, 2H), 7.62-7.54 (m, 3H), 4.48 (t, *J* = 7.3 Hz, 2H), 3.66 (t, *J* = 5.8 Hz, 2H), 2.06 (quint., 7.5 Hz, 2H), 1.62-1.55 (m, 2H), 1.45-1.39 (br.s., 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.5, 131.4, 129.5, 128.9, 124.2, 61.9, 48.0, 29.3, 26.6; **FTIR** (cm^{-1}) (neat) 3600-3200, 3100-2800, 1449, 1539, 1611, 1046, 692, 731; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{11}H_{15}N_4O$ 219.1240, found 219.1237.



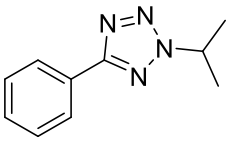
12a



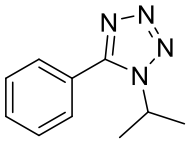
12b

5-Phenyl-2-(3-(trimethylsilyl)prop-2-yn-1-yl)-2H-tetrazole (12a) and 5-phenyl-1-(3-(trimethylsilyl)-prop-2-yn-1-yl)-1H-tetrazole (12b). The title compounds were prepared according to the general procedure **A** using 5-phenyl-1H-tetrazole (73.1 mg, 0.500 mmol, 1.00 equiv), 3-(trimethylsilyl)prop-2-yn-1-amine (159 mg, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 5% then 300 mL 20% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **12a** (43.6 mg,

0.17 mmol, 34% yield) was isolated as a pale-yellow oil. R_f 0.64 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.19-8.15 (m, 2H), 7.52-7.46 (m, 3H), 5.44 (s, 2H), 0.19 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 165. 6, 130.6, 129.0, 127.3, 127.1, 94.9, 93.4, 43.7, -0.3; **FTIR** (cm^{-1}) (neat) 3100-2800, 2190, 1530, 1450, 1250, 732, 693; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{17}N_4Si$ 257.1217, found 257.1216.
Tetrazole **12b** (17.9 mg, 0.070 mmol, 14% yield) was isolated as a pale-yellow oil. R_f 0.29 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90-7.86 (m, 2H), 7.62-7.55 (m, 3H), 5.22 (s, 2H), 0.14 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.4, 131.6, 129.4, 129.0, 123.6, 95.9, 93.9, 39.1, -0.4; **FTIR** (cm^{-1}) (neat) 3100-2800, 2190, 1610, 1537, 1462, 1250, 731, 695; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{17}N_4Si$ 257.1217, found 257.1220.

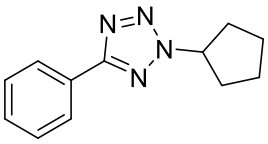


13a

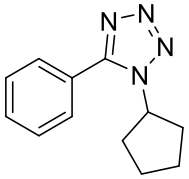


13b

2-Isopropyl-5-phenyl-2H-tetrazole (13a) and 1-isopropyl-5-phenyl-1H-tetrazole (13b). The title compounds were prepared according to the general procedure **A** using 5-phenyl-1H-tetrazole (73.1 mg, 0.500 mmol, 1.00 equiv), isopropylamine (0.107 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **13a** (64.0 mg, 0.34 mmol, 68% yield) was isolated as a pale-yellow oil as previously reported.[7] R_f 0.39 (10% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.18-8.12 (m, 2H), 7.52-7.41 (m, 3H), 5.11 (hept, *J* = 6.7 Hz, 1H), 1.70 (d, *J* = 6.7 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.9, 130.2, 128.9, 127.8, 126.9, 56.7, 22.3.
Tetrazole **13b** (25.4 mg, 0.14 mmol, 27% yield) was isolated as a pale-yellow oil. Spectral data matched those reported in the literature.[13] R_f 0.32 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64-7.53 (m, 5H), 4.77 (hept, *J* =6.7 Hz, 1H), 2.50 (d, *J* = 6.7 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.7, 131.3, 129.4, 129.0, 124.5, 51.3, 23.1.



14a

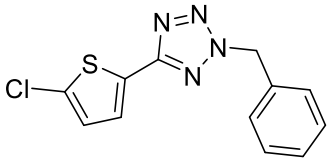


14b

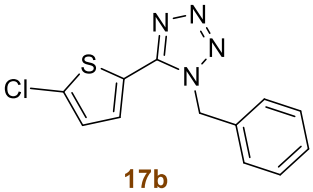
2-Cyclopentyl-5-phenyl-2H-tetrazole (14a) and 1-cyclopentyl-5-phenyl-1H-tetrazole (14b). The title compounds were prepared according to the general procedure **A** using 5-phenyl-1H-tetrazole (73.1 mg, 0.500 mmol, 1.00 equiv), cyclopentylamine (0.123 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **14a** (47.7 mg, 0.22 mmol, 45% yield) was isolated as a pale-yellow oil. R_f 0.68 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 7.9 Hz, 1.8 Hz, 2H), 7.51-7.43 (m, 3H), 5.26 (quint, *J* = 6.6 Hz, 1H), 2.28 (q, *J* = 6.5 Hz, 4H), 2.05-1.93 (m, 2H), 1.84-1.72 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.9, 130.2, 127.8, 126.9, 65.1, 33.1, 24.5; **FTIR** (cm^{-1}) (neat) 3200-2800, 1528, 1465, 1449, 733, 694; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{15}N_4$ 215.1291, found 215.1296.
Tetrazole **14b** (11.5 mg, 0.054 mmol, 11% yield) was isolated as a light-brown sticky oil. R_f 0.33 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.66-7.61 (m, 2H), 7.59-7.52 (m, 3H), 4.86 (quint, *J* = 6.9 Hz, 1H), 2.19 (q, *J* = 6.5 Hz, 4H), 2.12-2.01 (m, 2H), 1.79-1.69 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.2,

[13] A. O. Koren, P. N. Gaponik, V. A. Ostrovskii, *Int. J. Chem. Kinet.* **1993**, *25*, 1043-1051.

131.2, 129.3, 129.1, 124.6, 59.6, 34.0, 24.8; **FTIR** (cm^{-1}) (neat) 3200-2800, 1533, 1467, 1454, 737, 697; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{15}N_4$ 215.1291, found 215.1291.



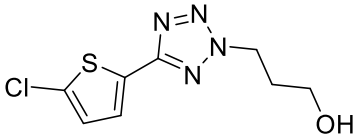
17a



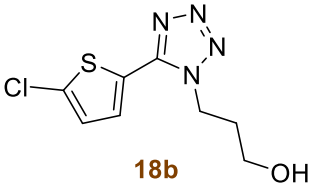
17b

2-Benzyl-5-(5-chlorothiophen-2-yl)-2H-tetrazole (17a) and 1-benzyl-5-(5-chlorothiophen-2-yl)-1H-tetrazole (17b). The title compounds were prepared according to the general procedure **A** using 5-(5-chlorothiophen-2-yl)-1H-tetrazole (93.3 mg, 0.500 mmol, 1.00 equiv), benzylamine (0.147 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole 1**7a** (92.6 mg, 0.34 mmol, 67% yield) was isolated as a white solid. $\mathbf{R_f}$ 0.35 (10% EtOAc/hexanes); **mp** 71-76 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 3.9 Hz, 1H), 7.42-7.35 (m, 5H), 6.94 (d, *J*) 3.9 Hz, 1H), 5.76 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.8, 133.1, 133.0, 129.21, 129.20, 128.6, 127.7, 127.3, 127.2, 57.0; **FTIR** (cm^{-1}) (neat) 3200-2800, 1571, 1488, 1457, 1068, 749, 719, 695; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{10}N_4S$ 277.0309, found 277.0308.

Tetrazole 1**7b** (44.2 mg, 0.16 mmol, 32% yield) was isolated as a sticky pale-yellow oil. $\mathbf{R_f}$ 0.42 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42-7.34 (m, 3H), 7.20 (d, *J* = 3.9 Hz, 1H), 7.18-7.13 (m, 2H), 6.96 (d, *J* = 4.0 Hz, 1H), 5.73 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.1, 136.1, 133.4, 129.7, 129.5, 129.1, 127.6, 126.9, 122.7, 51.6; **FTIR** (cm^{-1}) (neat) 3200-2800, 1607, 1492, 1449, 1073, 725, 692; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{12}H_9N_4S$ 299.0129, found 299.0126.



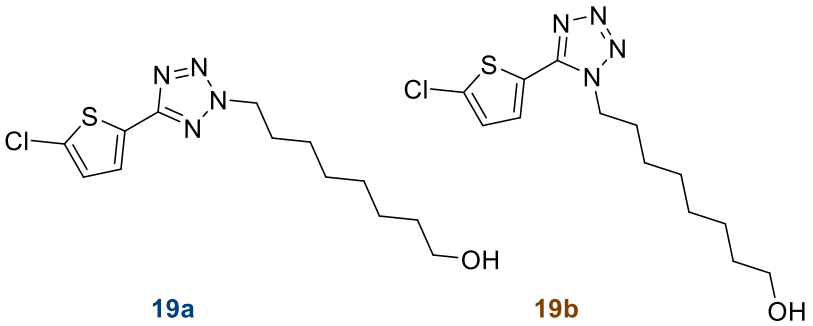
18a



18b

3-(5-(5-Chlorothiophen-2-yl)-2H-tetrazol-2-yl)propan-1-ol (18a) and 3-(5-(5-chlorothiophen-2-yl)-1H-tetrazol-1-yl)propan-1-ol (18b). The title compound was prepared according to the general procedure **A** using 5-(5-chloro-2-thienyl)-1H-tetrazole (93.3 mg, 0.500 mmol, 1.00 equiv), 3-amino-1-propanol (0.101 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 50% then 300 mL 75% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **18a** (93.0 mg, 0.38 mmol, 76% yield) was isolated as a pale-yellow oil as previously reported.[7] $\mathbf{R_f}$ 0.52 (75% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 3.9 Hz, 1H), 6.90 (d, *J* = 3.9 Hz, 1H), 4.75 (t, *J* = 6.9 Hz, 2H), 3.69 (t, *J* = 5.7 Hz, 2H), 3.02 (br.s., 1H), 2.23 (qn, *J* = 6.4 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.2, 132.9, 127.4, 127.2, 127.1, 58.6, 50.2, 31.8.; **FTIR** (cm^{-1}) (neat) 3600-3200, 3200-2800, 1575, 1485, 1415, 1058, 1032, 1007; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_8H_{10}ClN_4OS$ 245.0258, found 245.0262.

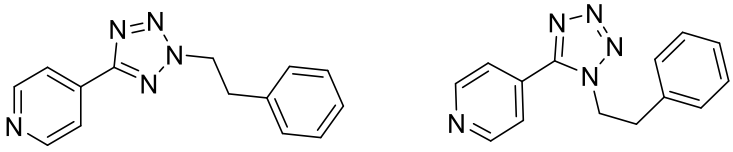
Tetrazole **18b** (26.9 mg, 0.11 mmol, 22% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.21 (75% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 4.0 Hz, 1H), 7.04 (d, *J* = 4.0 Hz, 1H), 4.67 (t, *J* = 7.1 Hz, 2H), 5.30 (q, *J* = 5.3 Hz, 2H), 2.28-2.19 (m, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.8, 135.9, 129.5, 127.7, 122.9, 58.6, 45.4, 31.8; **FTIR** (cm^{-1}) (neat) 3600-3200, 3200-2800, 1576, 1490, 1403, 1053, 1041, 1001; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_8H_{10}ClN_4OS$ 245.0258, found 245.0257.



19a 19b

8-(5-(5-Chlorothiophen-2-yl)-2H-tetrazol-2-yl)octan-1-ol (19a) and 8-(5-(5-chlorothiophen-2-yl)-1H-tetrazol-1-yl)octan-1-ol (19b). The title compound was prepared according to the general procedure **A** using 5-(5-chloro-2-thienyl)-1H-tetrazole (93.3 mg, 0.500 mmol, 1.00 equiv), 8-amino-1-octanol (0.210 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 40% then 300 mL 50% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **19a** (120.0 mg, 0.38 mmol, 76% yield) was isolated as a pale-yellow oil as previously reported.[7] $\mathbf{R_f}$ 0.48 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 3.9 Hz, 1H), 6.90 (d, *J* = 3.9 Hz, 1H), 4.54 (t, *J* = 7.2 Hz, 2H), 3.55 (t, *J* = 6.7 Hz, 2H), 2.38 (br.s., 1H), 1.96 (qn, *J* = 6.9 Hz, 2H), 1.53-1.44 (m, 2H), 1.34-1.21 (m, 8H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.1, 132.6, 127.6, 127.1, 126.9, 62.6, 53.3, 32.6, 29.2, 29.1, 28.8, 26.2, 25.6; **FTIR** (cm^{-1}) (neat) 3600-3200, 3200-2800, 1576, 1486, 1034, 1007; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{20}ClN_4OS$ 315.1041, found 315.1046.

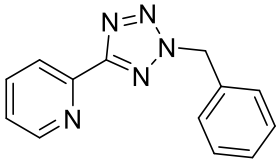
Tetrazole **19b** (28.6 mg, 0.91 mmol, 18% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.27 (50% EtOAc/hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 4.0 Hz, 1H), 7.06 (d, *J* = 4.0 Hz, 1H), 4.48 (t, *J* = 7.4 Hz, 2H), 3.62 (t, *J* = 6.6 Hz, 2H), 1.95 (qn, *J* = 7.4 Hz, 2H), 1.54 (qn, *J* = 6.8 Hz, 2H), 1.46 (br.s., 1H), 1.40-1.27 (m, 8H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 148.6, 135.7, 129.3, 127.6, 123.0, 63.0, 48.5, 32.7, 29.5, 29.2, 29.0, 26.4, 25.7; **FTIR** (cm^{-1}) (neat) 3600-3200, 3200-2800, 1577, 1491, 1056, 1017, 805; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{20}ClN_4OS$ 315.1041, found 315.1043.



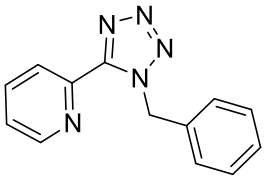
20a 20b

4-(2-Phenethyl-2H-tetrazol-5-yl)pyridine (20a) and 4-(1-phenethyl-1H-tetrazol-5-yl)pyridine (20b). The title compounds were prepared according to the general procedure **A** using 5-(4-pyridyl)-1H-tetrazole (73.6 mg, 0.500 mmol, 1.00 equiv), phenethylamine (0.157 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 50% then 300 mL 80% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **20a** (106 mg, 0.42 mmol, 84% yield) was isolated as an off-white solid as previously reported.[7] $\mathbf{R_f}$ 0.38 (50% EtOAc/hexanes); **mp** 60-69 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 5.6 Hz, 2H), 7.99 (d, *J* = 5.6 Hz, 2H), 7.33-7.21 (m, 3H), 7.18 (d, *J* = 7.2 Hz, 2H), 4.90 (t, *J* = 7.6 Hz, 2H), 3.37 (t, *J* = 7.6 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.1, 150.7, 136.2, 134.8, 129.0, 128.7, 127.3, 120.8, 54.5, 35.7; **FTIR** (cm^{-1}) (neat) 3200-2800, 1611, 1497, 1457, 753, 716, 699; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{14}H_{14}N_5$ 252.1244, found 252.1237.

Tetrazole **20b** (19.0 mg, 0.08 mmol, 15% yield) was isolated as a pale-yellow oil. $\mathbf{R_f}$ 0.21 (75% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.6 Hz, 2H), 7.24-7.15 (m, 3H), 7.08 (d, *J* = 5.6 Hz, 2H), 6.86 (d, *J* = 6.7 Hz, 2H), 4.65 (t, *J* = 6.7 Hz, 2H), 3.26 (t, *J* = 6.7 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.0, 150.7, 135.9, 131.8, 129.2, 128.8, 127.7, 122.7, 49.7, 36.4; **FTIR** (cm^{-1}) (neat) 3200-2800, 1683, 1609, 1496, 1454, 751, 701; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{14}H_{14}N_5$ 252.1244, found 252.1243.



21a



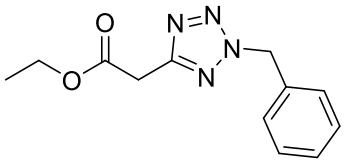
21b

2-(2-Benzyl-2H-tetrazol-5-yl)pyridine (21a) and 2-(1-benzyl-1H-tetrazol-5-yl)pyridine (21b). The title compounds were prepared according to the general procedure **A** using 2-(1H-tetrazol-5-yl)pyridine (73.6 mg, 0.500 mmol, 1.00 equiv), benzylamine (0.137 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 30% then 300 mL 50% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **21a** (51.0 mg, 0.22 mmol, 41% yield) was isolated as a yellow solid. $\mathbf{R_f}$ 0.27 (50% EtOAc/hexanes); **mp** 70-76 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.76-8.72 (m, 1H), 8.20 (d, J=8 Hz, 1H), 7.80 (td, J=8 Hz, 2Hz, 1H), 7.45-739 (m, 2H), 7.37-7.29 (m, 4H), 5.83 (s, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 165.1, 150.3, 146.8, 137.1, 133.1, 129.1, 128.6, 124.9, 122.5, 57.1; **FTIR** (cm^{-1}) (neat) 3200-2800, 1593, 1497, 1456, 1043, 729, 711, 693; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{12}N_5$ 238.1087, found 238.1080.

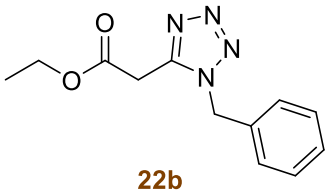
Tetrazole **21b** (66.0 mg, 0.28 mmol, 52% yield) was isolated as a bright yellow oil. Spectral data matched those reported in the literature.[14] $\mathbf{R_f}$ 0.48 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.76-8.73 (m, 1H), 8.34 (dt, J= 8Hz, 1 Hz, 1H), 7.88 (td, J=8Hz, 2Hz), 7.46-7.42 (m, 1H), 7.37-7.33 (m, 2H), 7.31-7.25 (m, 3H), 6.25 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.7, 149.4, 144.9, 137.6, 134.9, 128.8, 128.5, 128.4, 125.6, 124.7, 52.7.

The title compounds were also obtained doing the reaction in toluene (4 mL); leading to the tetrazole **21a** (70.0 mg, 0.30 mmol, 59% yield) as an off-white solid, and tetrazole **21b** (38.0 mg, 0.16 mmol, 32% yield) as a pale-yellow oil.

The title compounds were also prepared according to the general procedure **B1** using 2-pyridine-carbonitrile (60.1 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step) leading to tetrazole **21a** (67.1 mg, 0.28 mmol, 49% yield) as an off-white solid and tetrazole **21b** (35.6 mg, 0.15 mmol, 26% yield) as a bright yellow oil.



22a



22b

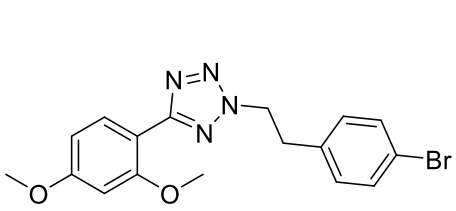
Ethyl 2-(2-benzyl-2H-tetrazol-5-yl)acetate (22a) and Ethyl 2-(1-benzyl-1H-tetrazol-5-yl)acetate (22b). The title compounds were prepared according to the general procedure **A** using ethyl 1H-tetrazole-5-acetate (78.1 mg, 0.500 mmol, 1.00 equiv), benzylamine (0.147 ml, 1.25 mmol, 2.50 equiv) and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in EtOAc (4 mL). The crude mixture was purified by flash chromatography (300 mL 20% then 300 mL 40% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **22a** (76.0 mg, 0.31 mmol, 62% yield) was isolated as a clear oil. Spectral data matched those reported in the literature.[15] $\mathbf{R_f}$ 0.47 (40% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38-7.33 (m, 5H), 5.75 (s, 2H), 4.19 (q, J = 7.1 Hz, 2H), 3.95 (s, 2H), 1.24 (t, J = 7.1 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 168.4, 160.2, 133.3, 129.2, 129.1, 128.5, 61.7, 56.9, 32.0, 14.2.

Tetrazole **22b** (31.0 mg, 0.13 mmol, 25% yield) was isolated as a pale-yellow oil. Spectral data matched those reported in the literature.[15] $\mathbf{R_f}$ 0.25 (40% EtOAc/hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39-7.35

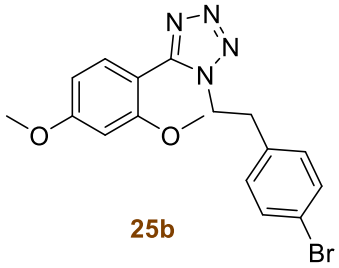
[14] C. Behloul, M. Benlahrech, F. Foubelo, C. Nájera, M. Yus, *Synthesis* **2018**, *50*, 3430-3435.

[15] H. Kanno, H. Yamaguchi, Y. Ichikawa, S. Isoda, *Chem. Pharm. Bull.* **1991**, *39*, 1099-1105.

(m, 3H), 7.21-7.18 (m, 2H), 5.61 (s, 2H), 4.13 (q, J=7 Hz, 2H), 3.81 (s, 2H), 1.22 (t, J=7 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 166.6, 149.2, 132.8, 129.4, 129.3, 127.9, 62.4, 51.7, 30.1, 14.1.



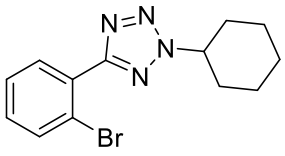
25a



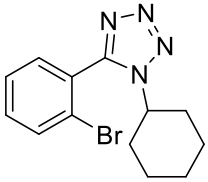
25b

2-(4-Bromophenethyl)-5-(2,4-dimethoxyphenyl)-2H-tetrazole (25a) and 1-(4-bromophenethyl)-5-(2,4-dimethoxyphenyl)-1H-tetrazole (25b). The title compounds were prepared according to the general procedure **B2** using 3,5-dimethoxybenzonitrile (81.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), 4-bromophenethylamine (250 mg, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 25% then 300 mL 50% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **25a** (101 mg, 0.26 mmol, 52% yield) was isolated as a sticky light-brown oil. **R_f** 0.20 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.4 Hz, 1H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.04 (d, *J* = 8.3 Hz, 2H), 6.62-6.56 (m, 2H), 4.84 (t, *J* = 7.5 Hz, 2H), 3.90 (s, 3H), 3.85 (s, 3H), 3.31 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.3, 162.2, 158.8, 135.7, 131.9, 131.7, 130.5, 121.1, 109.4, 105.1, 99.2, 56.1, 55.5, 53.8, 35.2; **FTIR** (cm^{-1}) (neat) 3200-2800, 1613, 1536, 1453, 1262, 1209, 1162, 766, 686; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{17}H_{17}BrN_4O_2Na$ 411.0427, found 411.0422.

Tetrazole **25b** (35.0 mg, 0.090 mmol, 18% yield) was isolated as a pale-yellow oil. **R_f** 0.28 (50% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.3 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 1H), 6.76 (d, *J* = 8.3 Hz, 2H), 6.54 (dd, *J* = 8.4 Hz, 2.2 Hz, 1H), 6.51 (d, *J* = 2.1 Hz, 1H), 4.44 (t, *J* = 7.1 Hz, 2H), 3.87 (s, 3H), 3.77 (s, 3H), 3.10 (t, *J* = 7.1 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.6, 157.9, 153.0, 135.8, 132.8, 131.9, 130.4, 121.2, 105.4, 99.0, 55.9, 55.8, 49.0, 35.4; **FTIR** (cm^{-1}) (neat) 3200-2800, 1615, 1548, 1437, 1290, 1210, 1162, 771; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{17}H_{17}BrN_4O_2Na$ 411.0427, found 411.0414.



26a

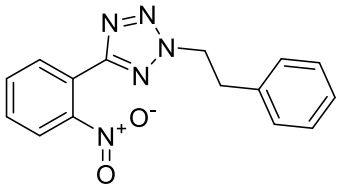


26b

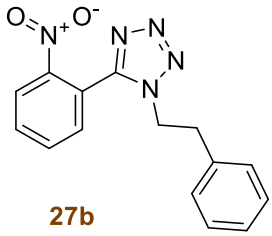
5-(2-Bromophenyl)-2-cyclohexyl-2H-tetrazole (26a) and 5-(2-bromophenyl)-1-cyclohexyl-1H-tetrazole (26b). The title compounds were prepared according to the general procedure **B2** using 2-bromobenzonitrile (91.0 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), cyclohexylamine (124 mg, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **26a** (49.2 mg, 0.16 mmol, 32% yield) was isolated as a pale-yellow oil. **R_f** 0.59 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 7.7 Hz, 1.6 Hz, 1H), 7.73 (dd, *J* = 8.0 Hz, 0.8 Hz, 1H), 7.42 (td, *J* = 7.6 Hz, 1.0 Hz, 1H), 7.32 (td, *J* = 7.7 Hz, 1.6 Hz, 1H), 4.79 (tt, *J* = 11.2 Hz, 3.9 Hz, 1H), 2.36-2.27 (m, 2H), 2.06 (td, *J* = 12.1 Hz, 3.4 Hz, 2H), 2.01-1.92 (m, 2H), 1.81-1.73 (m, 1H), 1.51 (qt, *J* = 12.7 Hz, 3.4 Hz, 2H), 1.36 (tt, *J* = 12.2 Hz, 3.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.7, 134.2, 131.8,

131.2, 129.1, 127.5, 122.3, 63.5, 32.6, 25.1, 24.9; **FTIR** (cm^{-1}) (neat) 3200-2800, 1600, 1519, 1452, 823, 746; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{16}BrN_4$ 307.0553, found 307.0548.

Tetrazole **26b** (20.0 mg, 0.065 mmol, 13% yield) was isolated as a light-brown oil. R_f 0.23 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78-7.73 (m, 1H), 7.53-7.44 (m, 2H), 7.39-7.35 (m, 1H), 4.00 (quint, *J* = 7.8 Hz, 1H), 2.08-1.97 (m, 4H), 1.94-1.83 (m, 2H), 1.74-1.56 (m, 2H), 1.36-1.20 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.0, 133.6, 132.7, 132.0, 128.0, 126.8, 123.6, 58.7, 32.9, 25.3, 24.9; **FTIR** (cm^{-1}) (neat) 3200-2800, 1451, 1532, 1600, 1401, 767, 707; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{16}BrN_4$ 307.0553, found 307.0548.



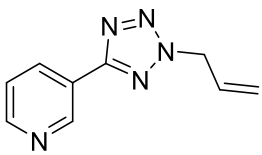
27a



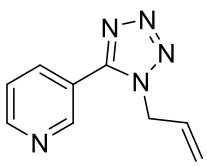
27b

2-Phenethyl-5-(2-nitrophenyl)-2H-tetrazole (27a) and 1-phenethyl-5-(2-nitrophenyl)-1H-tetrazole (27b). The title compounds were prepared according to the general procedure **B2** using 2-nitrobenzonitrile (74.1 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), phenethylamine (0.157 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 20% then 300 mL 35% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **27a** (100 mg, 0.34 mmol, 68% yield) was isolated as a clear oil. R_f 0.57 (35% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 7.7 Hz, 1.4 Hz, 1H), 7.87 (dd, *J* = 8.0 Hz, 1.2 Hz, 1H), 7.69 (td, *J* = 7.6 Hz, 1.3 Hz, 1H), 7.62 (td, *J* = 7.8 Hz, 1.4 Hz, 1H), 7.33-7.28 (m, 2H), 7.24 (tt, *J* = 7.3 Hz, 2.6 Hz, 1H), 7.18-7.14 (m, 2H), 4.88 (t, *J* = 7.5 Hz, 2H), 3.35 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.4, 149.1, 136.3, 132.4, 131.2, 131.1, 128.9, 128.7, 127.3, 124.2, 121.6, 54.6, 35.7; **FTIR** (cm^{-1}) (neat) 3200-2800, 1529, 1454, 1355, 738, 699; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}N_5O_2$ 296.1142, found 296.1144.

Tetrazole **27b** (29.5 mg, 0.10 mmol, 20% yield) was isolated as a clear oil. R_f 0.27 (35% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.25 (dd, *J* = 8.3 Hz, 1.0 Hz, 1H), 7.74-7.69 (m, 1H), 7.56 (td, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.27-7.22 (m, 1H), 7.21-7.16(m, 2H), 6.88-6.85 (m, 2H), 6.52 (dd, *J* = 7.6 Hz, 1.3 Hz, 1H), 4.34 (t, *J* = 6.8 Hz, 2H), 3.24 (t, *J* = 6.78 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.5, 147.6, 136.5, 134.0, 132.8, 132.3, 129.1, 128.9, 127.4, 125.3, 119.8, 49.4, 35.8; **FTIR** (cm^{-1}) (neat) 3200-2800, 1529, 1455, 1346, 745, 700; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}N_5O_2$ 296.1142, found 296.1150.



28a

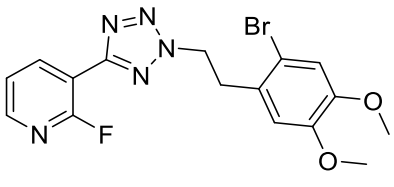


28b

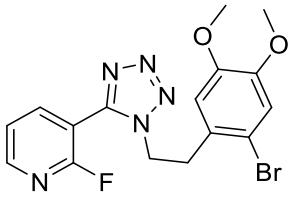
3-(2-Allyl-2H-tetrazol-5-yl)pyridine (28a) and 3-(1-allyl-1H-tetrazol-5-yl)pyridine (28b). The title compounds were prepared according to the general procedure **B1** using 3-pyridinecarbonitrile (52.1 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), allylamine (71.4 mg, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 50% then 300 mL 100% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **28a** (38.0 mg, 0.20 mmol, 41% yield) was isolated as a pale-yellow oil. R_f 0.39 (50% EtOAc/hexanes); **^{1}H NMR** (400 MHz,

$CDCl_3$) δ 9.37 (d, *J* = 1.4 Hz, 1H), 8.70 (dd, *J* = 4.8 Hz, 1.6 Hz, 1H), 8.41 (dt, *J* = 7.9 Hz, 1.9 Hz, 1H), 7.42 (ddd, *J* = 7.9 Hz, 4.9 Hz, 0.7 Hz, 1H), 6.13 (m, 1H), 5.45 (s, 1H), 5.41 (dd, *J* = 5.5 Hz, 0.5 Hz, 1H), 5.28 (dd, *J* = 6.3 Hz, 1.3 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.1, 151.4, 148.3, 134.2, 129.7, 123.8, 123.7, 121.4, 55.7; **FTIR** (cm^{-1}) (neat) 3200-2800, 1689, 1647, 1603, 1519, 1432, 791, 707; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_9H_{10}N_5$ 188.0930, found 188.0923.

Tetrazole **28b** (11.0 mg, 0.059 mmol, 12% yield) was isolated as a yellow oil; **R_f** 0.30 (100% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.96 (d, *J* = 1.8 Hz, 1H), 8.83 (dd, *J* = 4.8 Hz, 1.4 Hz, 1H), 8.10 (dt, *J* = 8.0 Hz, 1.9 Hz, 1H), 7.52 (dd, *J* = 7.9 Hz, 4.9 Hz, 1H), 6.12-6.00 (m, 1H), 5.41 (d, *J* = 10.4 Hz, 1H), 5.17-5.07 (m, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.5, 152.3, 149.1, 136.5, 130.4, 124.1, 120.6, 120.3, 50.4; **FTIR** (cm^{-1}) (neat) 3200-2800, 1688, 1647, 1602, 1529, 1446, 816, 708; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_9H_{10}N_5$ 188.0930, found 188.0922.



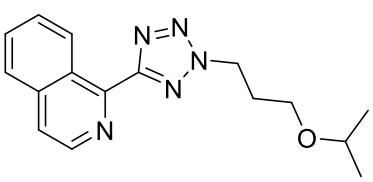
29a



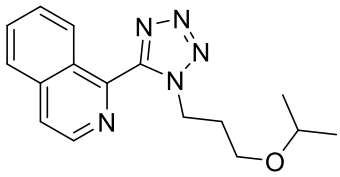
29b

3-(2-(2-Bromo-4,5-dimethoxyphenethyl)-2H-tetrazol-5-yl)-2-fluoropyridine (29a) and (3-(1-(2-bromo-4,5-dimethoxyphenethyl)-1H-tetrazol-5-yl)-2-fluoropyridine (29b). The title compounds were prepared according to the general procedure **B1** using 3-cyano-2-fluoropyridine (61.0 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), 2-bromo-4,5-dimethoxyphenethylamine (325 mg, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 30% then 300 mL 50% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **29a** (148 mg, 0.36 mmol, 60% yield) was isolated as an off-white solid. **R_f** 0.60 (50% EtOAc/hexanes); **mp** 130-134 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.56 (ddd, *J* = 2.0 Hz, 7.6 Hz, 9.3 Hz, 1H), 8.34 (qd, *J* = 1.0 Hz, 4.8 Hz, 1H), 7.36 (ddd, *J* = 1.7 Hz, 4.9 Hz, 6.2 Hz, 1H), 7.01 (s, 1H), 6.56 (s, 1H), 4.95 (t, *J* = 7.3 Hz, 2H), 3.84 (s, 3H), 3.72 (s, 3H), 3.45 (t, *J* = 7.2 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.2 (d, *J* = 246.0 Hz), 160.0 (d, *J* = 9.3 Hz), 149.4 (d, *J* = 14.7 Hz), 148.8 (d, *J* = 48.1 Hz), 140.5 (d, *J*) 2.9 Hz), 127.5, 121.9 (d, *J* = 4.6 Hz), 115.8, 114.3, 113.4, 111.2, 111.0, 56.3, 56.1, 53.0, 35.8; **^{19}F NMR** (375 MHz, $CDCl_3$) δ -64.88 (d, *J* = 9.1 Hz); **FTIR** (cm^{-1}) (neat) 3200-2800, 1604, 1508, 1446, 1259, 1214, 1101, 730, 700; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{16}H_{15}BrN_5O_2Na$ 430.0285, found 430.0284.

Tetrazole **29b** (69.3 mg, 0.17 mmol, 28% yield) was isolated as a red-brownish sticky oil; **R_f** 0.29 (50% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 4.8 Hz, 1H), 7.54 (ddd, *J* = 9.2 Hz, 7.6 Hz, 1.9 Hz, 1H), 7.22 (ddd, *J* = 7.1 Hz, 5.0 Hz, 2.0 Hz, 1H), 6.68 (s, 1H), 6.10 (s, 1H), 4.74 (t, *J* = 6.5 Hz, 2H), 3.79 (s, 3H), 3.67 (s, 3H), 3.19 (t, *J* = 6.5 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.1 (d, *J* = 240.1 Hz), 150.8 (d, *J* = 15.1 Hz), 150.1 (d, *J* = 5.4 Hz), 148.9 (d, *J* = 33.3 Hz), 142.5 (d, *J* = 2.8 Hz), 127.0, 121.7 (d, *J* = 4.5 Hz), 115.6, 114.1, 113.0, 107.7, 107.4, 56.3, 56.2, 47.9 (d, *J* = 6.1 Hz), 36.5; **^{19}F NMR** (375 MHz, $CDCl_3$) δ -65.44 (d, *J* = 9.0 Hz); **FTIR** (cm^{-1}) (neat) 3200-2800, 1603, 1509, 1457, 1259, 1222, 1099, 732; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{16}BrN_5O_2$ 408.0466, found 408.0468.



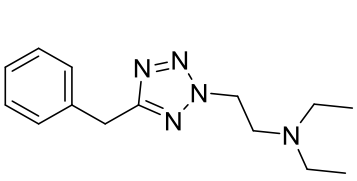
30a



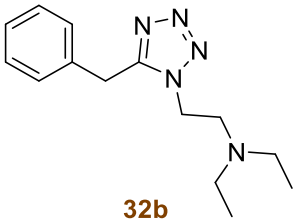
30b

1-(2-(3-Isopropoxypropyl)-2H-tetrazol-5-yl)isoquinoline (30a) and 1-(1-(3-isopropoxypropyl)-1H-tetrazol-5-yl)isoquinoline (30b) . The title compounds were prepared according to the general procedure **B1** using 1-isoquinolinecarbonitrile (77.1 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), 3-isopropoxypropylamine (146 mg, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 25% then 300 mL 40% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **30a** (46.1 mg, 0.16 mmol, 31% yield) was isolated as a pale-yellow oil. $\mathbf{R_f}$ 0.28 (50% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.17 (d, *J* = 8.4 Hz, 1H), 8.74 (d, *J* = 5.6 Hz, 1H), 7.91 (d, *J* = 7.9 Hz, 1H), 7.81-768 (m, 3H), 4.92 (t, *J* = 6.9 Hz, 2H), 3.57 (hept, *J* = 6.1 Hz, 1H), 3.51 (t, *J* = 5.8 Hz, 2H), 2.40 (quint, *J* = 6.4 Hz, 2H), 1.15 (d, *J* = 6.1 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.1, 146.6, 142.6, 137.1, 130.6, 128.6, 127.3, 127.2, 127.0, 122.7, 72.0, 64.2, 51.1, 30.1, 22.2; **FTIR** (cm^{-1}) (neat) 3200-2800, 1622, 1497, 1446, 1126, 1087, 799, 709; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{19}N_5O$ 320.1482, found 320.1483.

Tetrazole **30b** (78.8 mg, 0.27 mmol, 53% yield) was isolated as a pale-yellow oil; $\mathbf{R_f}$ 0.28 (50% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 8.5, 1H), 8.68 (d, *J* = 5.6 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.84 (d, *J* = 5.6 Hz, 1H), 7.79 (td, *J* = 7.5 Hz, 0.8 Hz, 1H), 7.75-7.69 (m, 1H), 4.91 (t, *J* = 6.9 Hz, 2H), 3.40-3.32 (m, 3H), 2.17 (quint, *J* = 6.4 Hz, 2H), 0.97 (d, *J* = 6.1 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.0, 144.7, 141.9, 137.0, 131.2, 129.1, 127.8, 127.2, 127.1, 123.3, 71.7, 64.3, 46.8, 30.5, 22.0; **FTIR** (cm^{-1}) (neat) 3200-2800, 1718, 1622, 1493, 1452, 1128, 1085, 801, 686; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{19}N_5O$ 320.1482, found 320.1476.



32a

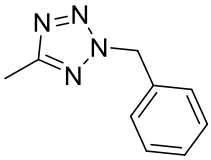


32b

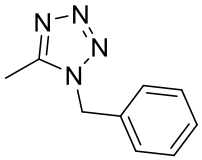
2-(5-Benzyl-2H-tetrazol-2-yl)-N,N-diethylethan-1-amine (32a) 2-(5-benzyl-1H-tetrazol-1-yl)-N,N-diethylethan-1-amine (32b). The title compounds were prepared according to the general procedure **B2** using benzyl cyanide (58.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), 2-diethylaminoethylamine (145 mg, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 75% then 300 mL 100% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **32a** (83.0 mg, 0.32 mmol, 64% yield) was isolated as a clear oil as previously reported.[7] $\mathbf{R_f}$ 0.37 (75% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32-7.25 (m, 4H), 7.24-7.18 (m, 1H), 4.59 (t, *J* = 6.9 Hz, 2H), 4.23 (s, 2H), 3.01 (t, *J* = 6.7 Hz, 2H), 2.52 (q, *J* = 7.1 Hz, 4H), 0.95 (t, *J* = 7.1 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.4, 136.9, 128.8, 128.7, 126.9, 51.8, 51.5, 47.4, 31.9, 12.1; **FTIR** (cm^{-1}) (neat) 3200-2800, 1604, 1495, 1454, 1137, 1073, 1028, 735, 697; **HRMS** (ESI-TOF) m/z:) $[M+H]^+$ Calcd for $C_{14}H_{26}N_5$ 260.1870, found 260.1857.

Tetrazole **32b** (25.9 mg, 0.10 mmol, 20% yield) was isolated as a clear oil; $\mathbf{R_f}$ 0.20 (100% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34-7.25 (m, 3H), 7.17 (d, *J* = 7.1 Hz, 2H), 4.36 (s, 2H), 4.13 (t, *J* = 6.3 Hz, 2H), 2.72 (t, *J* = 6.3 Hz, 2H), 2.43 (q, *J* = 7.1 Hz, 4H), 0.87 (t, *J* = 7.2 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.3, 134.4, 129.2, 128.5, 127.7, 52.7, 47.6, 46.6, 29.6, 11.9; **FTIR** (cm^{-1}) (neat) 3200-2800, 1604, 196,

1456, 1105, 1073, 1031, 732, 697; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{14}H_{26}N_5$ 260.1870, found 260.1866.



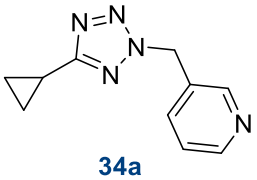
33a



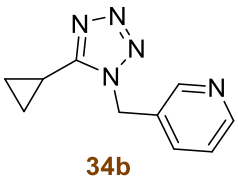
33b

2-Benzyl-5-methyl-2H-tetrazole (33a) and 1-benzyl-5-methyl-1H-tetrazole (33b). The title compounds were prepared according to the general procedure **B2** using acetonitrile (0.261 ml, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 ml, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 25% then 300 mL 60% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **33a** (47.0 mg, 0.27 mmol, 54% yield) was isolated as a clear oil as previously reported.[7] $\mathbf{R_f}$ 0.39 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 (s, 5H), 5.69 (s, 2H), 2.51 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.4, 133.5, 129.1, 129.0, 128.5, 56.6, 11.0; **FTIR** (cm^{-1}) (neat) 3200-2800, 1606, 1498, 1456, 802, 733; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_9H_{10}N_4Na$ 197.0798, found 197.0793.

Tetrazole **33b** (13.9 mg, 0.080 mmol, 16% yield) was isolated as a pale-yellow oil. Spectral data matched those reported in the literature.[12] $\mathbf{R_f}$ 0.50 (75% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39-7.34 (m, 3H), 7.22-7.17 (m, 2H), 5.50 (s, 2H), 2.44 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.8, 133.2, 129.4, 129.1, 127.6, 51.0, 9.1.



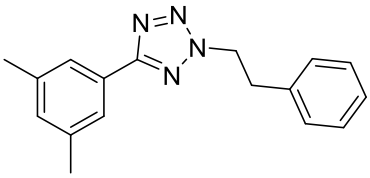
34a



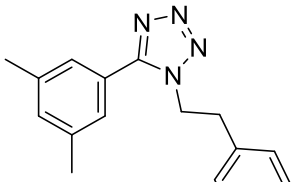
34b

4-((5-Cyclopropyl-2H-tetrazol-2-yl)methyl)pyridine (34a) and 4-((5-cyclopropyl-1H-tetrazol-1-yl)methyl)pyridine (34b). The title compounds were prepared according to the general procedure **B2** using cyclopropanecarbonitrile (33.5 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), 3-picolylamine (135 mg, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL EtOAc then 300 mL 5% MeOH/EtOAc) to separate the two tetrazole isomers. Tetrazole **34a** (50.3 mg, 0.25 mmol, 50% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.35 (100% EtOAc); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 5.9 Hz, 2H), 7.18 (d, *J* = 5.6 Hz, 2H), 5.69 (s, 2H), 2.22-2.14 (m, 1H), 1.12-1.05 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 150.6, 142.2, 122.6, 55.1, 8.6, 6.7; **FTIR** (cm^{-1}) (neat) 3200-2800, 1603, 1516, 1417, 771, 688; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{10}H_{12}N_5$ 202.1087, found 202.1088.

Tetrazole **34b** (26.2 mg, 0.13 mmol, 26% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.14 (100% EtOAc); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 5.9 Hz, 2H), 7.08 (d, *J* = 5.6 Hz, 2H), 5.60 (s, 2H), 1.75-1.66 (m, 1H), 1.24-1.18 (m, 2H), 1.17-1.10 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.5, 150.9, 142.5, 121.8, 49.3, 9.2, 4.1; **FTIR** (cm^{-1}) (neat) 3200-2800, 1603, 1542, 1416, 769, 722; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{10}H_{12}N_5$ 202.1087, found 202.1087.



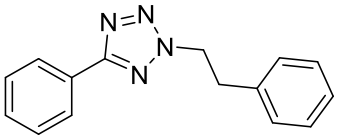
35a



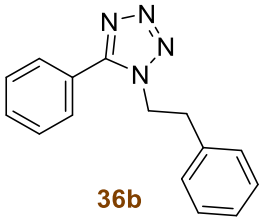
35b

2-Phenethyl-5-(3,5-dimehtylphenyl)-2H-tetrazole (35a) and 1-phenethyl-5-(3,5-dimehtylphenyl)-1H-tetrazole (35b). The title compounds were prepared according to the general procedure **B2** using 3,5-dimehtylbenzonitrile (65.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), phenethylamine (0.157 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **35a** (82.1 mg, 0.29 mmol, 59% yield) was isolated as a white solid. $\mathbf{R_f}$ 0.63 (25% EtOAc/hexanes); **mp** 95-98 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (s, 2H), 7.33-7.29 (m, 2H), 7.28-7.23 (m, 1H), 7.22-7.18 (m, 2H), 7.13-7.10 (m, 1H), 4.87 (t, *J* = 7.7 Hz, 2H), 3.38 (t, *J* = 7.7 Hz, 2H), 2.40 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) 165.5, 138.7, 136.6, 132.1, 129.0, 128.8, 127.3, 127.28, 124.7, 54.3, 35.9, 21.4.; **FTIR** (cm^{-1}) (neat) 3200-2800, 1607, 1498, 1362, 1031, 855, 736, 691; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{17}H_{19}N_4$ 279.1604, found 279.1608.

Tetrazole **35b** (30.6 mg, 0.11 mmol, 22% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.25 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25-7.21 (m, 3H), 7.12 (s, 2H), 6.97-6.92 (m, 2H), 6.80 (s, 2H), 4.57 (t, *J* = 7.0 Hz, 2H), 3.26 (t, *J* = 7.0 Hz, 2H), 2.31 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 155.2, 138.9, 136.5, 129.0, 128.9, 127.3, 126.5, 123.6, 49.2, 36.2, 21.3; **FTIR** (cm^{-1}) (neat) 3200-2800, 1605, 1455, 1397, 858, 752, 699; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{19}N_4$ 279.1604, found 279.1609.



36a

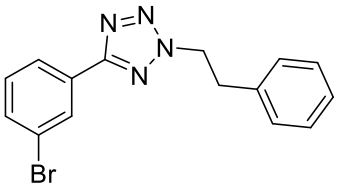


36b

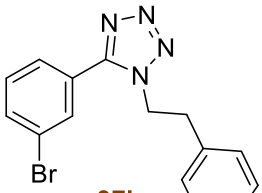
2-Phenethyl-5-phenyl-2H-tetrazole (36a) and 1-phenethyl-5-phenyl-1H-tetrazole (36b). The title compounds were prepared according to the general procedure **B2** using benzonitrile (0.47 mL, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), phenethylamine (0.157 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **36a** (87.6 mg, 0.35 mmol, 70% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.63 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.24-8.14 (m, 2H), 7.57-7.48 (m, 3H), 7.38-7.21 (m, 5H), 4.91 (t, *J* = 7.7 Hz, 2H), 3.42 (t, *J* = 7.7 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) 165.2, 136.6, 130.4, 129.0, 128.9, 127.5, 127.3, 126.9, 54.3, 35.8; **FTIR** (cm^{-1}) (neat) 3200-2800, 1997, 1450, 732, 694; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{15}N_4$ 251.1291, found 251.1294.

Tetrazole **36b** (21.3 mg, 0.085 mmol, 17% yield) was isolated as a clear oil. Spectral data matched those reported in the literature.[16] $\mathbf{R_f}$ 0.25 (25% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.50 (tt, *J* = 7.5 Hz, 1.3 Hz, 1H), 7.45-7.41 (m, 2H), 7.28-7.24 (m, 2H), 7.21-7.17 (m, 3H), 6.95-6.90 (m, 2H), 4.60 (t, *J* = 7.1 Hz, 2H), 3.23 (t, *J* = 7.1 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.8, 136.2, 131.1, 129.1, 128.9, 128.73, 128.70, 127.4, 123.8, 49.2, 36.1.

[16] A. L. Chandgude, A. Dömling, *Eur. J. Org. Chem.* **2016**, 2383-2387.



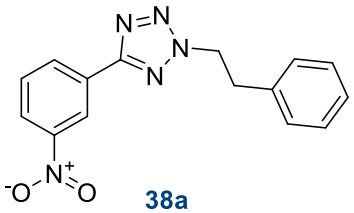
37a



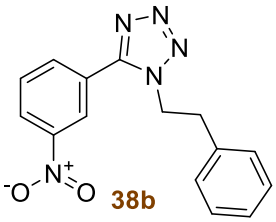
37b

2-Phenethyl-5-(3-bromophenyl)-2H-tetrazole (37a) and 1-phenethyl-5-(3-bromophenyl)-1H-tetrazole (37b). The title compounds were prepared according to the general procedure **B2** using 3-bromobenzonitrile (91.0 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), phenethylamine (0.157 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **37a** (127 mg, 0.39 mmol, 77% yield) was isolated as a white solid as previously reported.[7] **R_f** 0.64 (25% EtOAc/hexanes); **mp** 82-86 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.08 (d, *J* = 7.7 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.40-7.25 (m, 4H), 7.20 (d, *J* = 7.3 Hz, 2H), 4.88 (t, *J* = 7.7 Hz, 2H), 3.38 (t, *J* = 7.6 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) 163.9, 136.4, 133.4, 130.6, 129.9, 129.5, 129.0, 128.8, 127.4, 125.5, 123.1, 54.5, 35.8; **FTIR** (cm^{-1}) (neat) 3200-2800, 1604, 1517, 1439, 749, 681, 652; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}BrN_4$ 329.0396, found 329.0397.

Tetrazole **37b** (29.6 mg, 0.090 mmol, 18% yield) was isolated as a clear oil. **R_f** 0.26 (25% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65-7.61 (m, 1H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.27-7.19 (m, 4H), 7.17-7.14 (m, 1H), 6.90-6.87 (m, 2H), 4.60 (t, *J* = 6.8 Hz, 2H), 3.25 (t, *J* = 6.8 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.9, 136.1, 134.2, 131.8, 130.6, 129.2, 128.8, 127.6, 127.3, 125.8, 123.2, 49.5, 36.3; **FTIR** (cm^{-1}) (neat) 3200-2800, 1603, 1496, 1455, 740, 700, 669; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}BrN_4$ 329.0396, found 329.0404.



38a

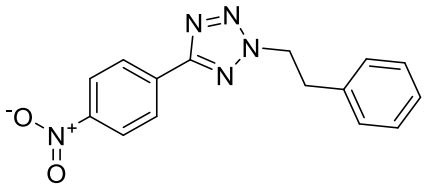


38b

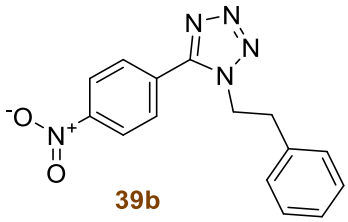
2-Phenethyl-5-(3-nitrophenyl)-2H-tetrazole (38a) and 1-phenethyl-5-(3-nitrophenyl)-1H-tetrazole (38b). The title compounds were prepared according to the general procedure **B2** using 3-nitrobenzonitrile (74.1 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), phenethylamine (0.157 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **38a** (108 mg, 0.37 mmol, 73% yield) was isolated as a white solid. **R_f** 0.54 (25% EtOAc/hexanes); **mp** 79-83 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.99 (t, *J* = 1.8 Hz, 1H), 8.48 (dt, *J* = 7.8 Hz, 1.2 Hz, 1H), 8.32 (ddd, *J* = 8.1 Hz, 2.1 Hz, 1.0 Hz, 1H), 7.69 (t, *J* = 8.0 Hz, 1H), 7.35-7.29 (m, 2H), 7.28-7.23 (m, 1H), 7.23-7.18 (m, 2H), 4.92 (t, *J* = 7.6 Hz, 2H), 3.40 (t, *J* = 7.6 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) 163.4, 148.8, 136.3, 132.6, 130.2, 129.3,129.0, 128.8, 127.5, 125.0, 122.0, 54.6, 35.8; **FTIR** (cm^{-1}) (neat) 3200-2800, 1541, 1512, 1344, 748, 723; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_5O_2$ 296.1142, found 296.1146.

Tetrazole **38b** (17.7 mg, 0.057 mmol, 12% yield) was isolated as a yellow sticky oil. **R_f** 0.15 (25% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.34 (ddd, *J* = 8.3 Hz, 2.2 Hz, 1.1 Hz, 1H), 8.02 (t, *J* = 1.9 Hz, 1H), 7.61 (t, *J* = 8.0 Hz, 1H), 7.53 (ddd, *J* = 7.7 Hz, 1.6 Hz, 1.1 Hz, 1H), 7.19-7.13 (m, 3H), 6.87-6.82 (m, 2H), 4.67 (t, *J* = 6.6 Hz, 2H), 3.27 (t, *J* = 6.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.2, 148.4, 135.8, 134.7, 130.4, 129.2, 128.8, 127.7, 125.7, 125.6, 123.7, 49.8, 36.4; **FTIR** (cm^{-1}) (neat) 3200-2800, 1717,

1641, 1515, 1496, 1364, 698; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_5O_2$ 296.1142, found 296.1143.



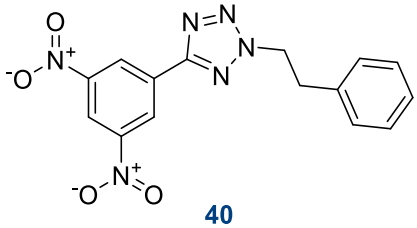
39a



39b

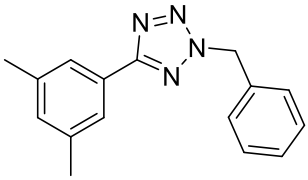
2-Phenethyl-5-(4-nitrophenyl)-2H-tetrazole (39a) and 1-phenethyl-5-(4-nitrophenyl)-1H-tetrazole (39b). The title compounds were prepared according to the general procedure **B2** using 4-nitrobenzonitrile (74.1 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), phenethylamine (0.157 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **39a** (118 mg, 0.40 mmol, 80% yield) was isolated as a white crystalline solid as previously reported.[7] $\mathbf{R}_f$ 0.55 (25% EtOAc/hexanes); **mp** 143-146 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.37-8.30 (m, 4H), 7.34-7.29 (m, 2H), 7.26 (tt, *J* = 7.3 Hz, 1.3 Hz, 1H), 7.22-7.18 (m, 2H), 4.92 (t, *J* = 7.7 Hz, 2H), 3.40 (t, *J* = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) 163.3, 149.0, 136.2, 133.4, 129.0, 128.7, 127.7, 127.4, 124.3, 54.6, 35.8; **FTIR** (cm^{-1}) (neat) 3200−2800, 1604, 1515, 1454, 1334, 1046; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_5O_2$ 296.1142, found 296.1152.

Tetrazole **39b** (11.7 mg, 0.40 mmol, 8% yield) was isolated as a white crystalline solid. $\mathbf{R}_f$ 0.21 (25% EtOAc/hexanes); **mp** 124-127 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.24 (dt, *J* = 8.9 Hz, 2.2 Hz, 2H), 7.30 (dt, *J* = 8.9 Hz, 2.2 Hz, 2H), 7.24-7.17 (m, 3H), 6.87-6.83 (m, 2H), 4.63 (t, *J* = 6.6 Hz, 2H), 3.28 (t, *J* = 6.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.5, 149.3, 136.0, 130.1, 130.0, 129.2, 128.8, 127.8, 124.2, 49.8, 36.4; **FTIR** (cm^{-1}) (neat) 3200−2800, 1611, 1523, 1452, 1340, 1105, 853, 689; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}N_5O_2$ 296.1142, found 296.1143.

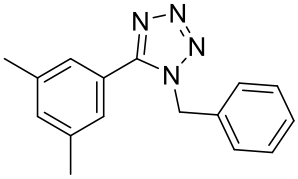


40

2-Phenethyl-5-(3,5-dinitrophenyl)-2H-tetrazole (40). The title compound was prepared according to the general procedure **B2** using 3,5-dinitrobenzonitrile (96.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), phenethylamine (0.157 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **40** (148 mg, 0.43 mmol, 87% yield) was isolated as an orange crystalline solid. $\mathbf{R}_f$ 0.50 (25% EtOAc/hexanes); **mp** 120-124 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (d, *J* = 2.0 Hz, 2H), 9.13 (t, *J* = 2.0 Hz, 1H), 7.35-7.25 (m, 3H), 7.23-7.18 (m, 2H), 4.97 (t, *J* = 7.6 Hz, 2H), 3.43 (t, *J* = 7.6 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) 161.7, 149.2, 136.0, 131.2, 129.1, 128.7, 127.6, 126.8, 119.9, 54.9, 35.8; **FTIR** (cm^{-1}) (neat) 3200-2800, 1598, 1543, 1519, 1496, 1455, 1383, 1342, 730, 704, 654; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}N_6O_4$ 341.0993 found 341.1000.

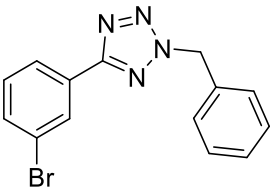


41a

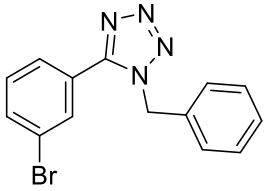


41b

2-Benzyl-5-(3,5-dimethylphenyl)-2H-tetrazole (41a) and 1-benzyl-5-(3,5-dimethyl phenyl)-1H-tetrazole (41b). The title compounds were prepared according to the general procedure **B2** using 3,5-dimethylbenzonitrile (65.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **41a** (72.7 mg, 0.28 mmol, 55% yield) was isolated as a white solid. $\mathbf{R_f}$ 0.71 (25% EtOAc/hexanes); **mp** 52-57 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79-7.76 (m, 2H), 7.43-7.35 (m, 5H), 7.10-7.08 (m, 1H), 5.80 (s, 2H), 2.38 (d, *J* = 0.5 Hz, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) 165.8, 138.6, 133.5, 132.1, 129.1, 129.0, 128.4, 127.2, 124.7, 56.8, 21.3; **FTIR** (cm^{-1}) (neat) 3200-2800, 1609, 1522, 1501, 1460, 1108, 872, 731, 698; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{17}N_4$ 265.1448 found 265.1451.
Tetrazole **41b** (31.7 mg, 0.12 mmol, 24% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.47 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37-7.32 (m, 3H), 7.21-7.14 (m, 5H), 5.59 (s, 2H), 2.33 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.1, 139.1, 134.3, 133.0, 129.2, 128.9, 127.5, 126.7, 123.6, 51.5, 21.3; **FTIR** (cm^{-1}) (neat) 3200-2800, 1606, 1524, 1498, 1456, 1111, 858, 725, 696; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{17}N_4$ 265.1448 found 265.1450.

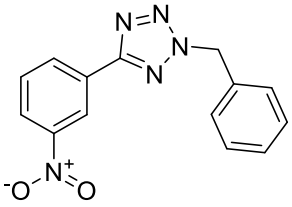


42a

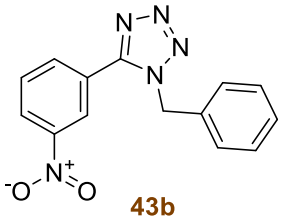


42b

2-Benzyl-5-(3-bromophenyl)-2H-tetrazole (42a) and 1-benzyl-5-(3-bromophenyl)-1H-tetrazole (42b). The title compounds were prepared according to the general procedure **B2** using 3-bromobenzonitrile (91.0 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 10% then 300 mL 25% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **42a** (102.5 mg, 0.33 mmol, 65% yield) was isolated as a white solid. Spectral data matched those reported in the literature.[9] $\mathbf{R_f}$ 0.60 (25% EtOAc/hexanes); **mp** 94-96 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.30 (t, *J* = 1.7 Hz, 1H), 8.09-8.05 (m, 1H), 7.58 (dq, *J* = 8.0 Hz, 1.0 Hz, 1H), 7.44-7.31 (m, 6H), 5.80 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) 164.3, 133.4, 133.3, 130.5, 129.9, 129.4, 129.19, 129.18, 128.5, 125.5, 123.0, 57.1.
Tetrazole **42b** (42.3 mg, 0.13 mmol, 26% yield) was isolated as a clear oil. $\mathbf{R_f}$ 0.31 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.72 (t, *J* = 1.7 Hz, 1H), 7.71-7.66 (m, 1H), 7.51 (dt, *J* = 7.8 Hz, 1.2 Hz, 1H), 7.40-7.34 (m, 4H), 7.20-7.14 (m, 2H), 5.62 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.5, 134.5, 133.7, 132.0, 130.8, 129.4, 129.1, 127.5, 127.4, 125.8, 123.3, 51.7; **FTIR** (cm^{-1}) (neat) 3200-2800, 1558, 1526, 1453, 1344, 722, 700, 658; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for C14H12BrN4 315.0245, found 315.0247.



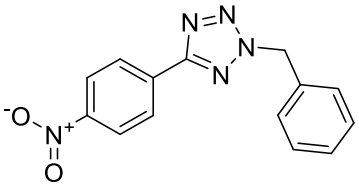
43a



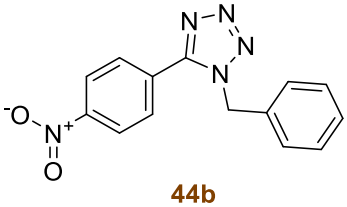
43b

2-Benzyl-5-(3-nitrophenyl)-2H-tetrazole (43a) and 1-benzyl-5-(3-nitrophenyl)-1H-tetrazole (43b). The title compounds were prepared according to the general procedure **B2** using 3-nitrobenzonitrile (74.1 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 20% then 300 mL 40% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **43a** (92.8 mg, 0.33 mmol, 66% yield) was isolated as a white crystalline solid. Spectral data matched those reported in the literature.[17] **R_f** 0.53 (25% EtOAc/hexanes); **mp** 98-100 °C (litt. 82-84 °C);[21] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.97 (t, *J* = 1.8 Hz, 1H), 8.47 (ddd, *J* = 7.8 Hz, 1.5 Hz, 1.1 Hz, 1H), 8.30 (ddd, *J* = 8.2 Hz, 2.3 Hz, 1.0 Hz, 1H), 7.66 (td, *J* = 8.0 Hz, 0.3 Hz, 1H), 7.46-7.43 (m, 2H), 7.42-7.35 (m, 3H), 5.83 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) 163.7, 148.7, 133.0, 132.6, 130.1, 129.3, 129.2, 128.6, 124.9, 122.0, 57.2.

Tetrazole **43b** (33.8 mg, 0.12 mmol, 24% yield) was isolated as a white solid. **R_f** 0.17 (25% EtOAc/hexanes); **mp** 115-119 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.43 (t, *J* = 1.8 Hz, 1H), 8.40 (ddd, *J* = 8.3 Hz, 2.2 Hz, 1.0 Hz, 1H), 8.01 (ddd, *J* = 7.8 Hz, 1.6 Hz, 1.1 Hz, 1H), 7.72 (t, *J* = 7.9 Hz, 1H), 7.41-7.35 (m, 3H), 7.22-7.18 (m, 2H), 5.70 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.8, 148.5, 134.9, 133.2, 130.7, 129.6, 129.3, 127.3, 126.1, 125.6, 123.8, 52.1; **FTIR** (cm^{-1}) (neat) 3200-2800, 1520, 1456, 1349, 719, 672; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{14}H_{12}N_5O_2$ 282.0986 found 282.0985.



44a

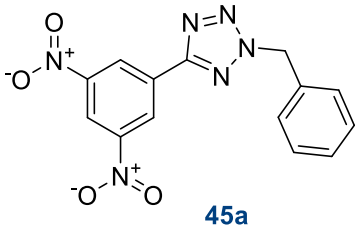


44b

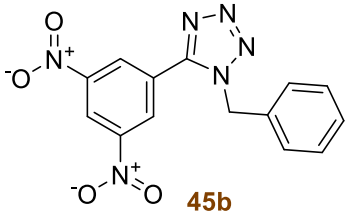
2-Benzyl-5-(4-nitrophenyl)-2H-tetrazole (44a) and 1-benzyl-5-(4-nitrophenyl)-1H-tetrazole (44b). The title compounds were prepared according to the general procedure **B2** using 4-nitrobenzonitrile (74.1 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 20% then 300 mL 35% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **44a** (94.2 mg, 0.34 mmol, 67% yield) was isolated as a white crystalline solid. Spectral data matched those reported in the literature.[8] **R_f** 0.59 (25% EtOAc/hexanes); **mp** 138-143 °C (litt. 140-141 °C); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.31 (s, 4H), 7.46-7.37 (m, 5H), 5.84 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) 163.7, 149.0, 133.3, 133.0, 129.3, 129.2, 128.6, 127.8, 124.3, 57.3.

Tetrazole **44b** (25.3 mg, 0.90 mmol, 18% yield) was isolated as a white crystalline solid. Spectral data matched those reported in the literature.[18] **R_f** 0.29 (35% EtOAc/hexanes); **mp** 124-127 °C (litt. 131-133 °C);[22] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.35 (dt, *J* = 8.9 Hz, 2.2 Hz, 2H), 7.79 (dt, *J* = 8.9 Hz, 2.2 Hz, 2H), 7.40-7.35 (m, 3H), 7.16-7.11 (m, 2H), 5.68 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.1, 149.6, 133.4, 130.2, 130.0, 129.6, 129.3, 127.1, 124.4, 52.0.

[17] L. Wang, K. Zhu, Q. Chen, M. He, *J. Org. Chem.* **2014**, *79*, 11780-11786.
[18] A. R. Katritzky, C. Cai, N. K. Meher, *Synthesis* **2007**, 1204-1208.

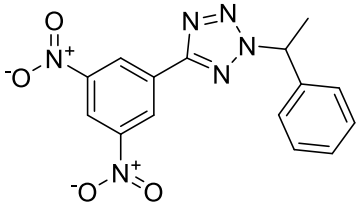


45a

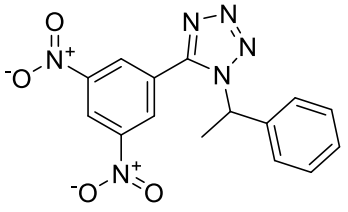


45b

2-Benzyl-5-(3,5-dinitrophenyl)-2H-tetrazole (45a) and 1-benzyl-5-(3,5-dinitrophenyl)-1H-tetrazole (45b). The title compounds were prepared according to the general procedure **B2** using 3,5-dinitrobenzonitrile (96.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), benzylamine (0.137 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 20% then 300 mL 40% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **45a** (114 mg, 0.35 mmol, 70% yield) was isolated as a white solid. Spectral data matched those reported in the literature.[19] **R_f** 0.35 (25% EtOAc/hexanes); **mp** 107-111 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.29 (d, *J* = 2.0 Hz, 2H), 9.10 (t, *J* = 1.9 Hz, 1H), 7.49-7.38 (m, 5H), 5.87 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ162.1, 149.2, 132.6, 131.2, 129.5, 129.4, 128.8, 126.8, 119.9, 57.6.
Tetrazole **45b** (36.2 mg, 0.11 mmol, 22% yield) was isolated as a clear oil. Spectral data matched those reported in the literature.[19] **R_f** 0.17 (25% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.16 (t, *J* = 1.9 Hz, 1H), 8.83 (d, *J* = 1.9 Hz, 2H), 7.45-7.38 (m, 3H), 7.27-7.21 (m, 2H), 5.80 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.1, 149.0, 132.5, 129.9, 129.8, 128.8, 127.5, 127.3, 121.0, 52.7.



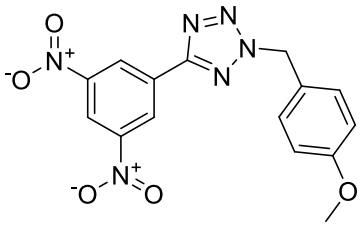
46a



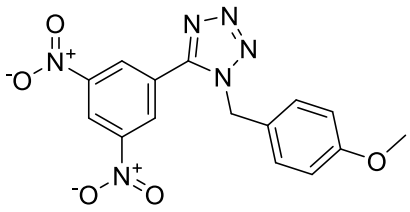
46b

5-(3,5-Dinitrophenyl)-2-(1-phenylethyl)-2H-tetrazole (46a) and 5-(3,5-dinitrophenyl)-1-(1-phenylethyl)-1H-tetrazole (46b). The title compounds were prepared according to the general procedure **B2** using 3,5-dinitrobenzonitrile (96.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), (R)-(+)-phenylethylamine (0.159 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 20% then 300 mL 30% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **46a** (85.1 mg, 0.25 mmol, 50% yield) was isolated as a clear sticky oil. **R_f** 0.57 (25% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.31 (d, *J* = 2.1 Hz, 2H), 9.11 (t, *J* = 2.1 Hz, 1H), 6.19 (q, *J* = 7.1 Hz, 1H), 2.16 (d, *J* = 7.1 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) 161.7, 149.2, 138.2, 131.4, 129.3, 126.9, 126.8, 119.9, 64.6, 21.1; **FTIR** (cm^{-1}) (neat) 3200-2800, 1556, 1519, 1345, 1077, 760, 725, 698; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{15}H_{12}N_6O_4Na$ 363.0812, found 363.0809.
Tetrazole **46b** (32.3 mg, 0.085 mmol, 19% yield) was isolated as a white solid. **R_f** 0.37 (25% EtOAc/hexanes); **mp** 163-165 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.16 (t, *J* = 2.1 Hz, 1H), 8.71 (d, *J* = 2.1 Hz, 2H), 7.43 (tt, *J* = 7.2 Hz, 1.6 Hz, 2H), 7.38 (tt, *J* = 7.3 Hz, 1.4 Hz, 1H), 7.27-7.26 (m, 1H), 7.25-7.24 (m, 1H), 5.72 (q, *J* = 6.9 Hz, 1H), 2.13 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.0, 148.9, 138.9, 130.0, 129.6, 129.2, 128.0, 126.1, 120.9, 60.6, 23.4; **FTIR** (cm^{-1}) (neat) 3200-2800, 1594, 1557, 1525, 1346, 1081, 756, 725, 702; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{15}H_{12}N_6O_4Na$ 363.0812, found 363.0812

[19] J. Němeček, P. Sychra, M. Macháček, M. Benková, G. Karabanovich, K. Konečná, V. Kavková, J. Stolaříková, A. Hrabálek, K. Vávrová, O. Soukup, J. Roh, V. Klimešová, *Eur. J. Med. Chem.* **2017**, *130*, 419-432.



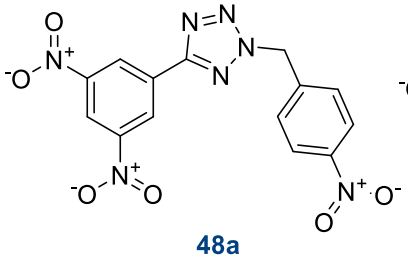
47a



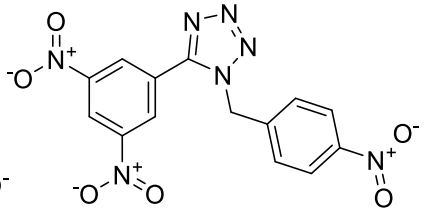
47b

5-(3,5-Dinitrophenyl)-2-(4-methoxybenzyl)-2H-tetrazole (47a) and 5-(3,5-dinitrophenyl)-1-(4-methoxybenzyl)-1H-tetrazole (47b). The title compounds were prepared according to the general procedure **B2** using 3,5-dinitrobenzonitrile (96.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), 4-methoxybenzylamine (0.163 mL, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 20% then 300 mL 30% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **47a** (114 mg, 0.32 mmol, 64% yield) was isolated as a yellow sticky oil. $\mathbf{R_f}$ 0.41 (25% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.27 (d, *J* = 2.1 Hz, 2H), 9.09 (t, *J* = 2.1 Hz, 1H), 7.42 (dt, *J* = 8.8 Hz, 2.5 Hz, 2H), 6.92 (dt, *J* = 8.8 Hz, 2.5 Hz, 2H), 5.80 (s, 2H), 3.80 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) 162.0, 160.5, 149.1, 131.2, 130.4, 126.7, 124.7, 119.8, 114.6, 57.2, 55.5; **FTIR** (cm^{-1}) (neat) 3200-2800, 1556, 1516, 1345, 1251, 1179, 782, 726; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{15}H_{12}N_6O_5Na$ 379.0761, found 379.0764.

Tetrazole **47b** (42.8 mg, 0.12 mmol, 24% yield) was isolated as a white solid; $\mathbf{R_f}$ 0.25 (25% EtOAc/hexanes); **mp**.160-164 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.17 (t, *J* = 1.8 Hz, 1H), 8.84 (d, *J* = 7.8 Hz, 2H), 7.18 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.6 Hz, 2H), 5.73 (s, 2H), 3.80 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.6, 151.0, 149.0, 129.0, 128.9, 127.6, 124.3, 121.0, 115.2, 55.6, 52.4; **FTIR** (cm^{-1}) (neat) 3200-2800, 1541, 1508, 1341, 1232, 1174, 779, 724; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{15}H_{12}N_6O_5Na$ 379.0761, found 379.0754.



48a

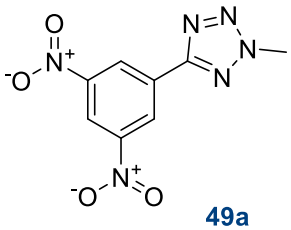


48b

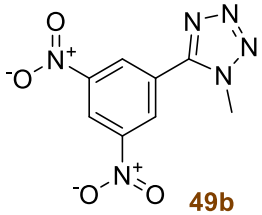
5-(3,5-Dinitrophenyl)-2-(4-nitrobenzyl)-2H-tetrazole (48a) and 5-(3,5-dinitrophenyl)-1-(4-nitrobenzyl)-1H-tetrazole (48b). The title compounds were prepared according to the general procedure **B2** using 3,5-dinitrobenzonitrile (96.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), 4-nitrobenzylamine (190 mg, 1.25 mmol, 2.50 equiv), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 30% then 300 mL 50% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **48a** (128 mg, 0.34 mmol, 69% yield) was isolated as a white solid. $\mathbf{R_f}$ 0.16 (25% EtOAc/hexanes); **mp** 165-168 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.29 (d, *J* = 2.1 Hz, 2H), 9.13 (t, *J* = 2.1 Hz, 1H), 8.29 (dt, *J* = 8.8 Hz, 2.2 Hz, 2H), 7.64 (dt, *J* = 8.8 Hz, 2.2 Hz, 2H), 6.00 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) 162.5, 149.2, 148.7, 139.1, 130.8, 129.7, 126.8, 124.6, 120.2, 59.5; **FTIR** (cm^{-1}) (neat) 3200-2800, 1533, 1518, 1341, 919, 789, 722; **HRMS** (ESI-TOF) m/z: $[M-H]^-$ calcd for $C_{14}H_8N_7O_6$ 370.0542, found 370.0539.

Tetrazole **48b** (26.0 mg, 0.070 mmol, 14% yield) was isolated as a white solid; $\mathbf{R_f}$ 0.12 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, dmso-d_6) δ 9.01 (t, *J* = 2.1 Hz, 1H), 8.92 (d, *J* = 2.1 Hz, 2H), 8.20 (d,

J = 8.2 Hz, 2H), 7.53 (d, *J* = 8.8 Hz, 2H), 5.97 (s, 2H); **^{13}C NMR** (125 MHz, dmso-d_6) δ 152.0, 148.4, 147.4, 141.3, 129.9, 129.5, 126.4, 123.9, 120.9, 50.4. *Due to the instability of tetrazole **48b**, melting point, infrared spectra, and HRMS could not be carried out.*



49a

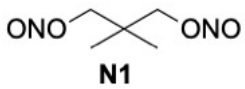


49b

2-Methyl-5-(3,5-dinitrophenyl)-2H-tetrazole (49a) and 1-meythl-5-(3,5-dinitrophenyl)-1H-tetrazole (49b). The title compounds were prepared according to the general procedure **B2** using 3,5-dinitrobenzonitrile (96.6 mg, 0.500 mmol, 1.00 equiv), dibutyltin oxide (18.7 mg, 0.075 mmol, 0.150 equiv), azidotrimethylsilane (0.986 mL, 0.750 mmol, 1.50 equiv), methylamine (0.625 mL, 1.25 mmol, 2.50 equiv, 2 M in THF), and 1,3-(2,2-dimethyl)propanedinitrite (0.093 mL, 0.800 mmol, 1.60 equiv) in toluene (4 mL, 1.5 mL for the first step + 2.5 mL for the second step). The crude mixture was purified by flash chromatography (300 mL 20% then 300 mL 50% EtOAc/hexanes) to separate the two tetrazole isomers. Tetrazole **49a** (108 mg, 0.43 mmol, 86% yield) was isolated as a white flaky as previously reported.[7] **R_f** 0.69 (50% EtOAc/hexanes); **mp** 141-142 °C (litt. 144-145 °C);[19] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.28 (d, *J* = 2.1 Hz, 2H), 9.10 (t, *J* = 2.1 Hz, 1H), 4.50 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) 161.9, 149.2, 131.1, 126.7, 119.9, 40.1.

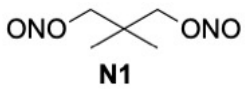
Tetrazole **49b** (7.51 mg, 0.027 mmol, 6% yield) was isolated as an off-white solid. **R_f** 0.44 (50% EtOAc/hexanes); **mp** 193-197 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.27 (t, *J* = 2.0 Hz, 1H), 9.02 (d, *J* = 2.0 Hz, 2H), 4.36 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$ + CD_3OD) δ 151.2, 149.2, 128.6, 127.5, 121.1, 35.7; **FTIR** (cm^{-1}) (neat) 3200-2800, 1595, 1530, 1347, 730; **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_8H_7N_6O_4$ 251.0523, found 251.0515.

1,3-(2,2-Dimethyl)Propanedinitrite - 1H - CDCl3 - 500 MHz



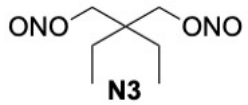
N1

1,3-(2,2-Dimethyl)propanedinitrite - 13C - CDCl3 - 125 MHz

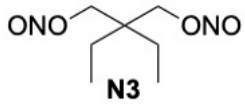


N1

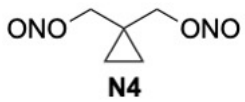
2,2-diethylpropane-1,3-diyl dinitrite - 1H - CDCl3 - 300 MHz



2,2-diethylpropane-1,3-diyl dinitrite - 13C - CDCl3 - 125 MHz

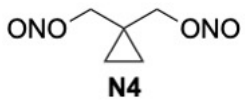


cyclopropane-1,1-diylbis(methylene) dinitrite - 1H - CDCl3 - 300 MHz



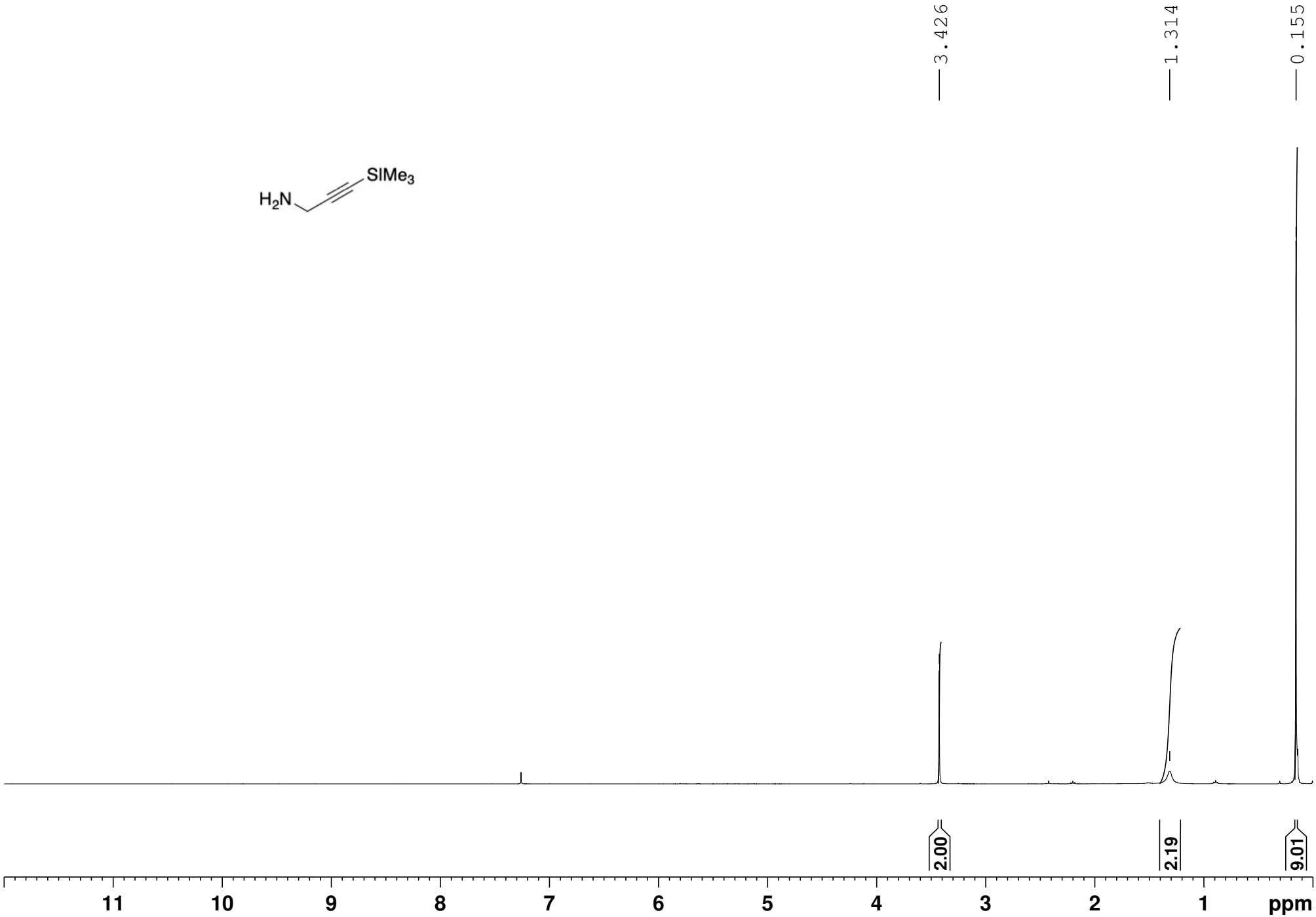
N4

cyclopropane-1,1-diylbis(methylene) dinitrite - 13C - CDCl3 - 75 MHz

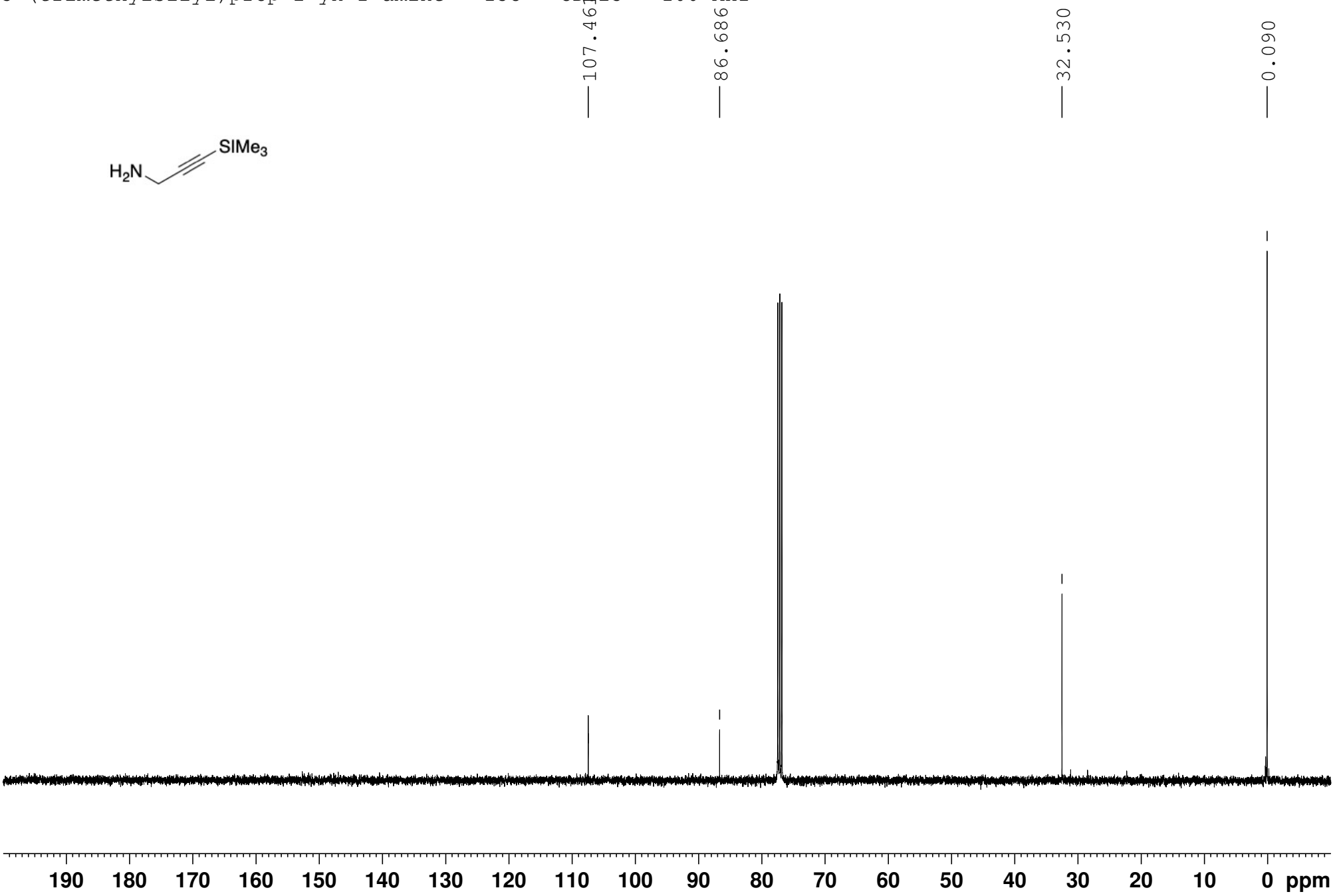


N4

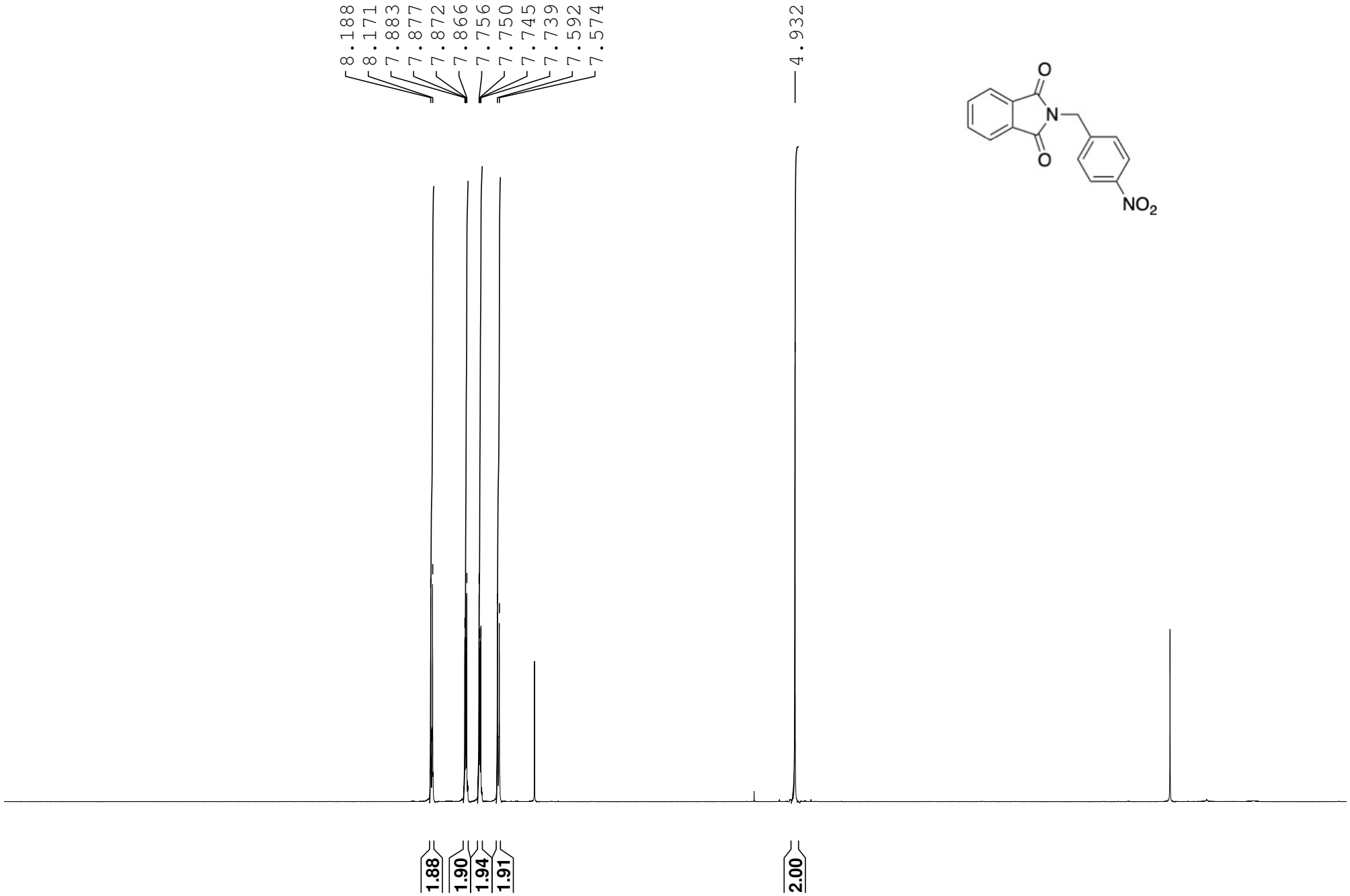
3-(trimethylsilyl)prop-2-yn-1-amine - 1H - CDCl3 - 400 MHz



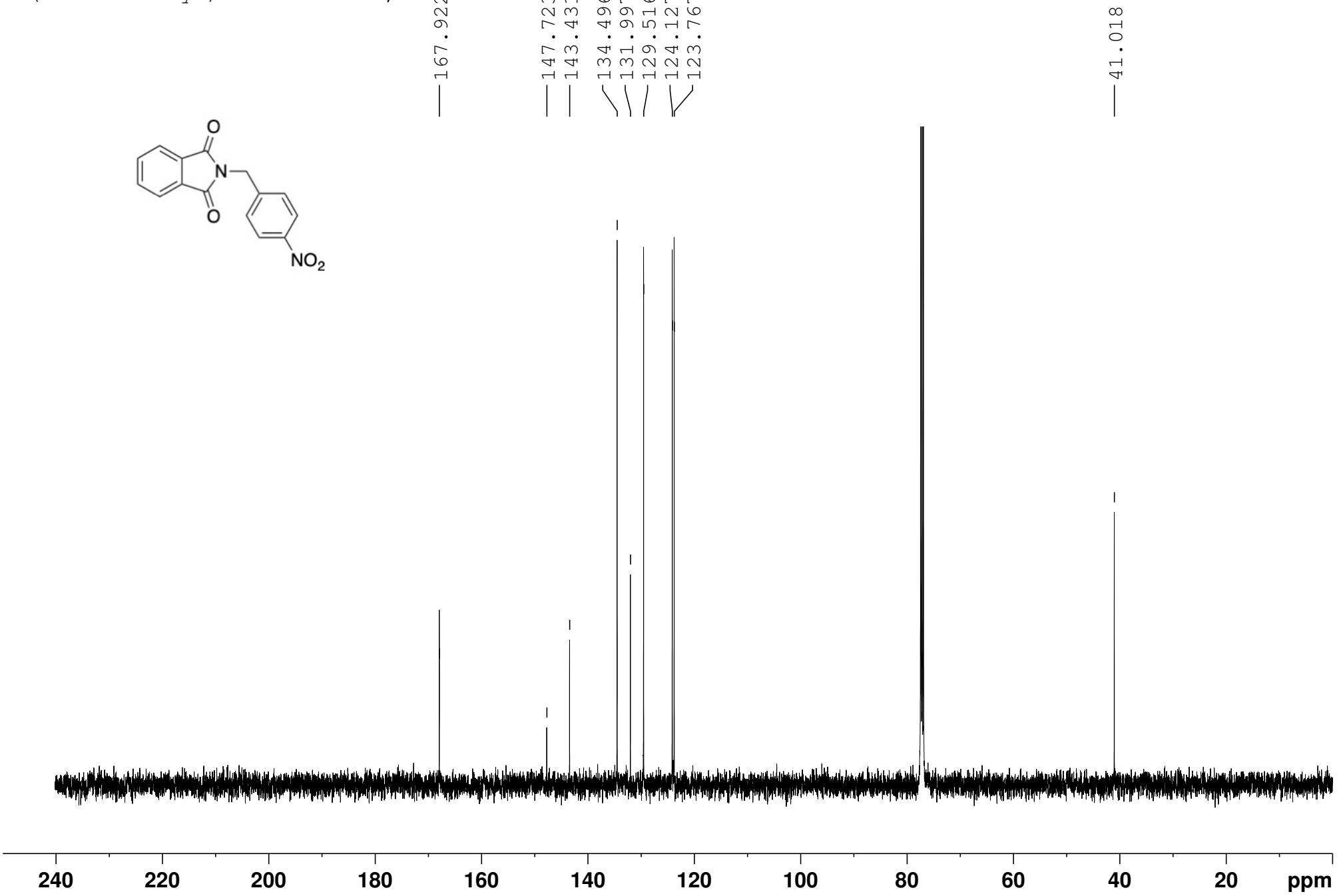
3-(trimethylsilyl)prop-2-yn-1-amine - 13C - CDCl3 - 100 MHz



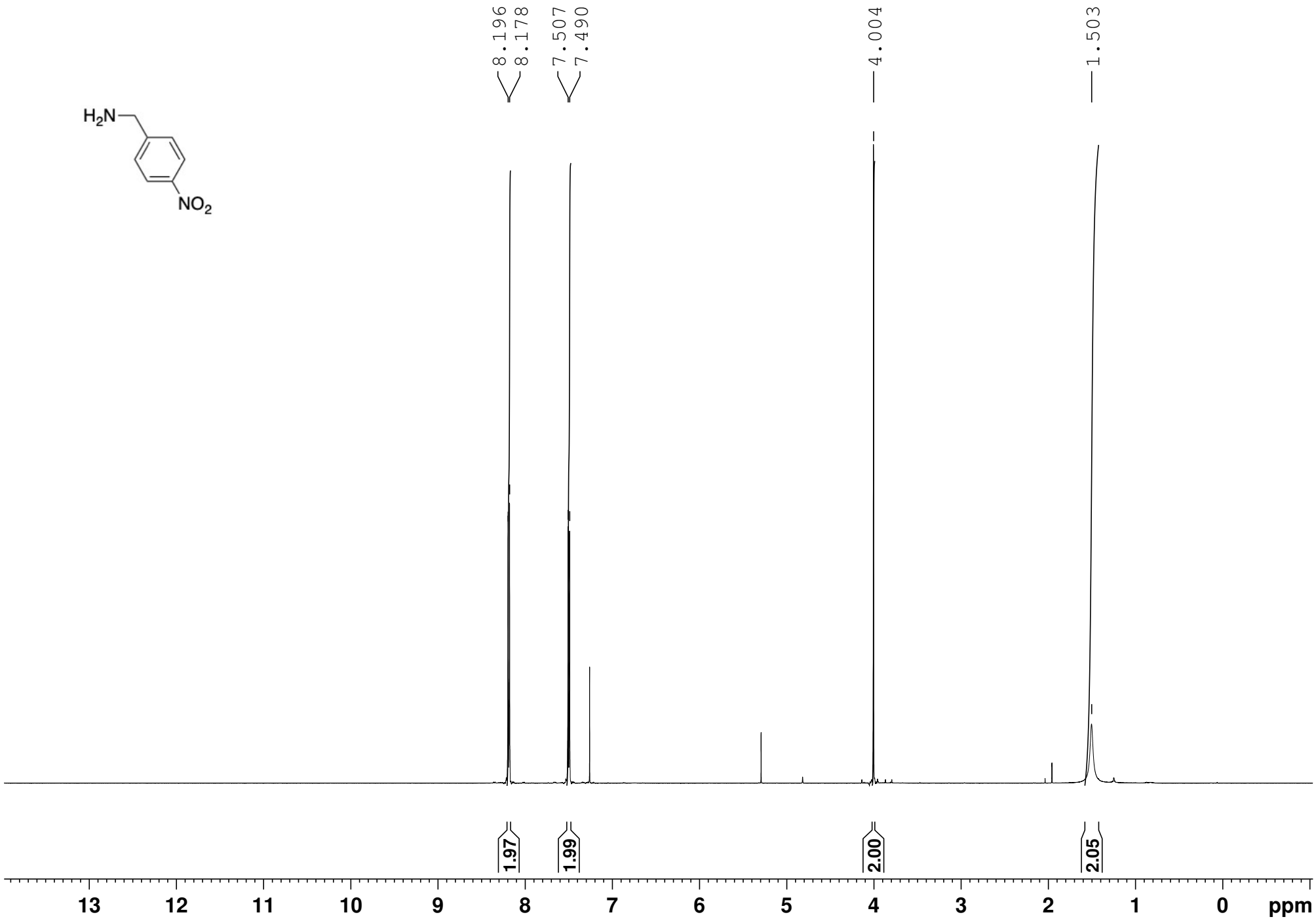
2-(4-nitrobenzyl)isoindoline-1,3-dione - 1H - CDCl3 - 500 MHz



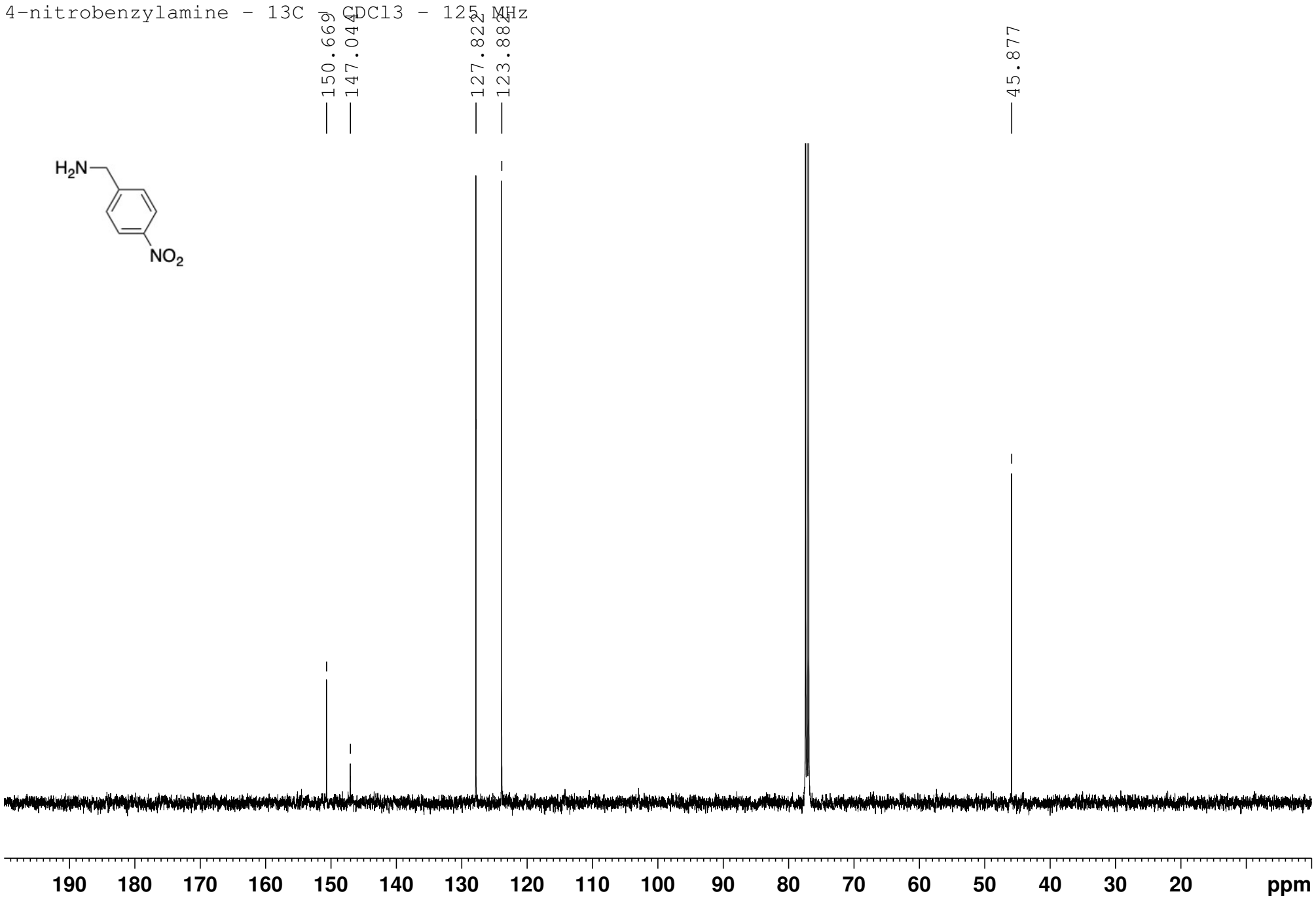
2-(4-nitrobenzyl)isoindoline-1,3-dione - 13C - CDCl3 - 125 MHz



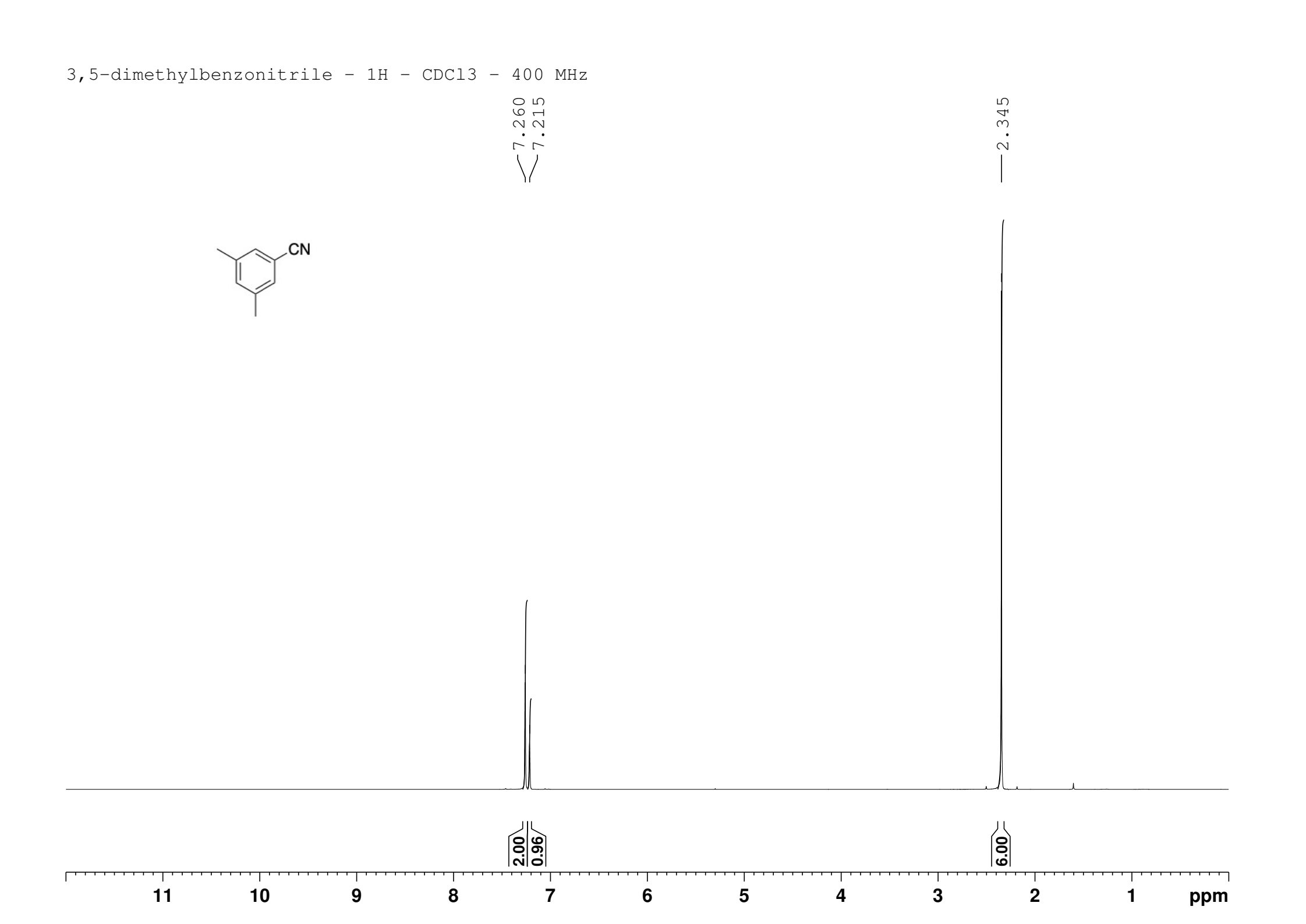
4-nitrobenzylamine - 1H - CDCl3 - 500 MHz



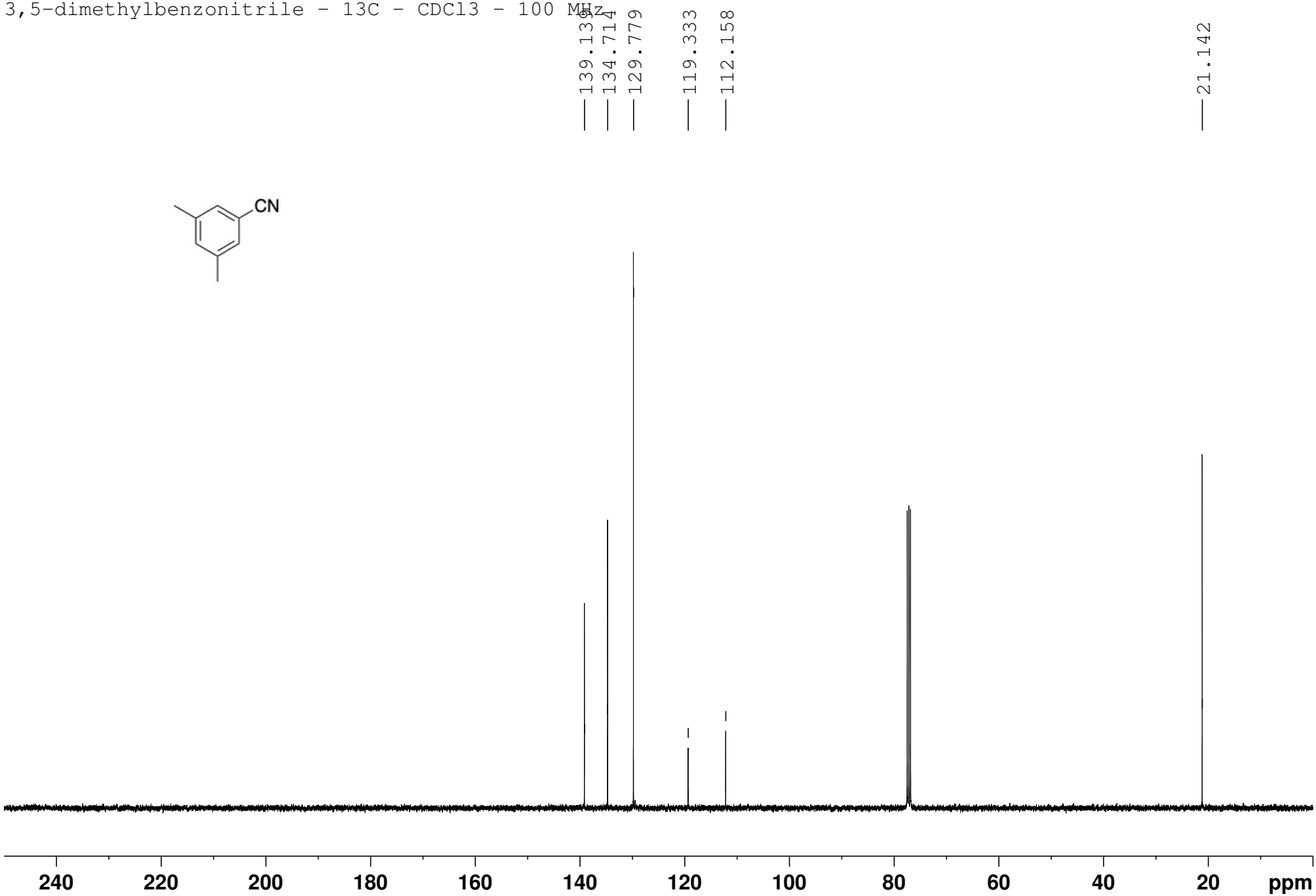
4-nitrobenzylamine - 13C - CDCl3 - 125 MHz



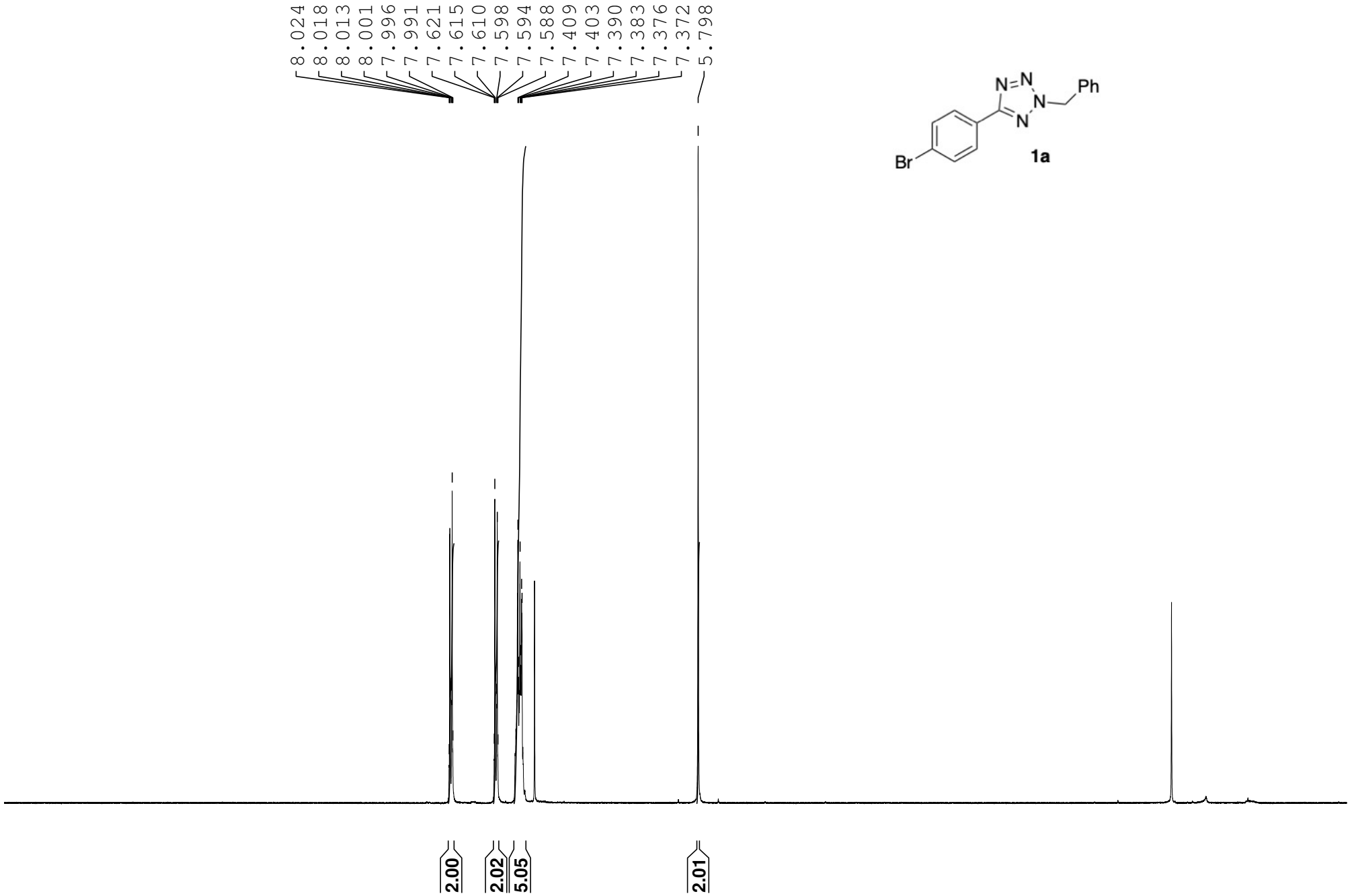
3,5-dimethylbenzonitrile - 1H - CDCl3 - 400 MHz



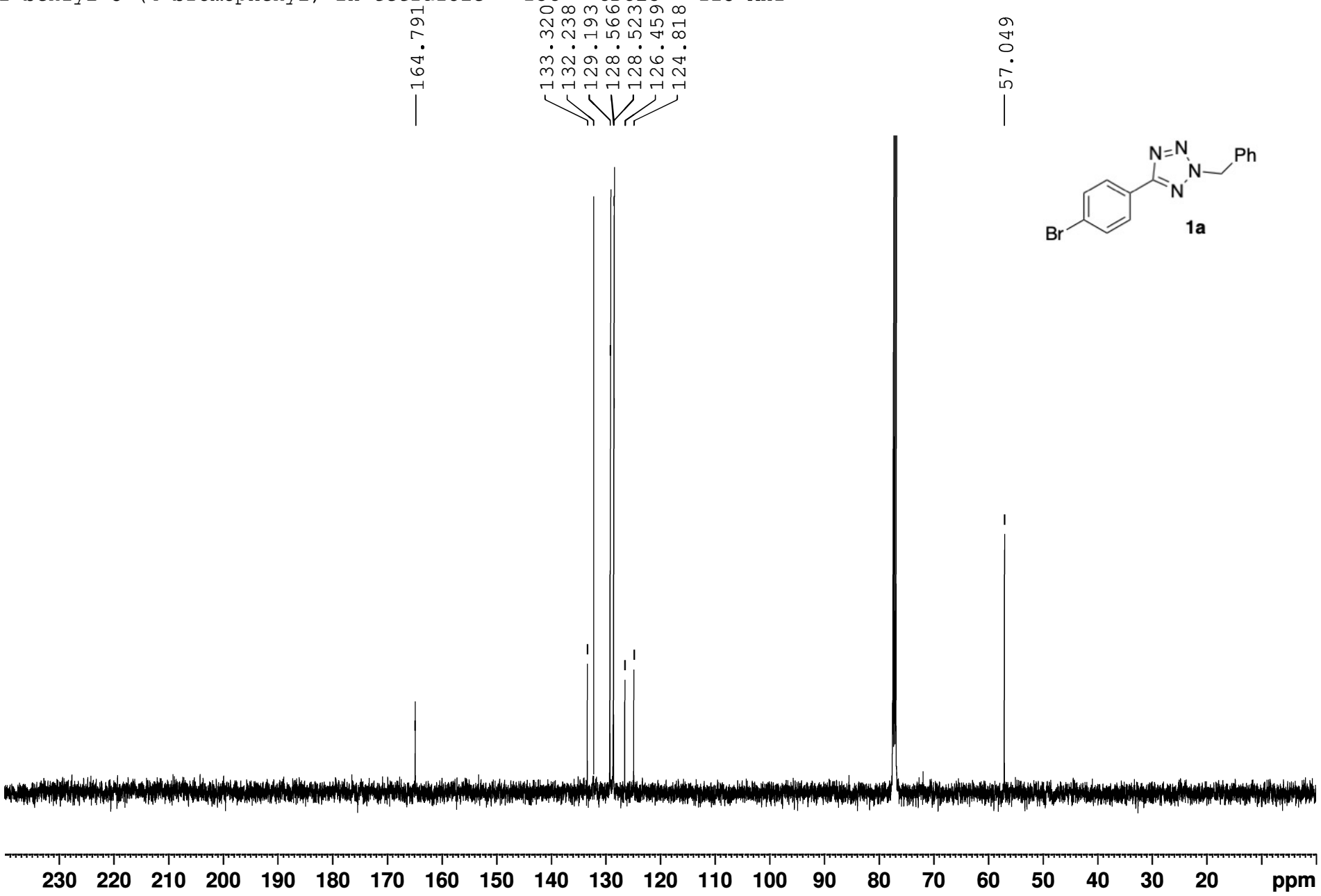
3,5-dimethylbenzonitrile - 13C - CDCl3 - 100 MHz



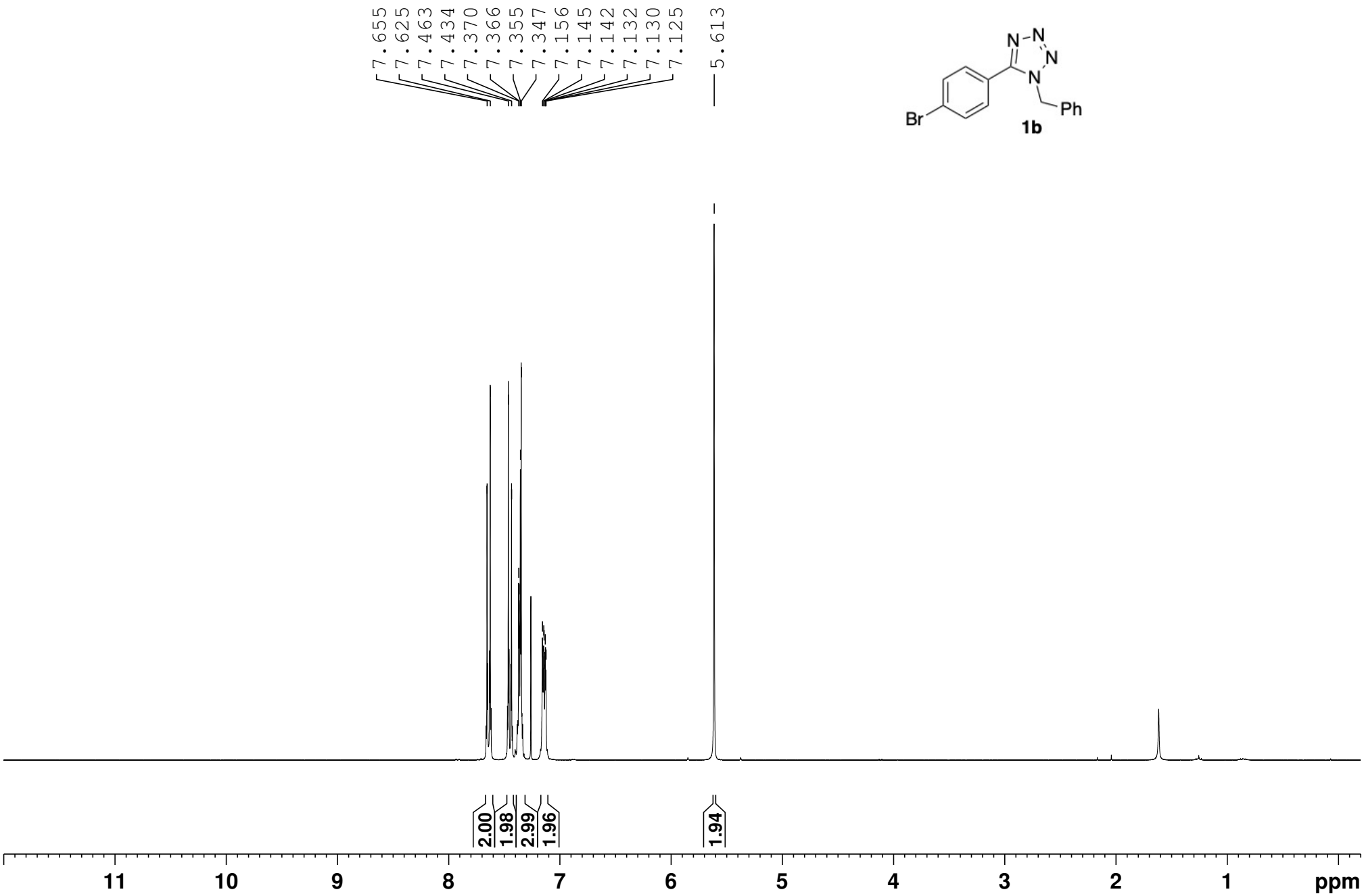
2-benzyl-5-(4-bromophenyl)-2H-tetrazole - 1H - CDCl3 - 400 MHz



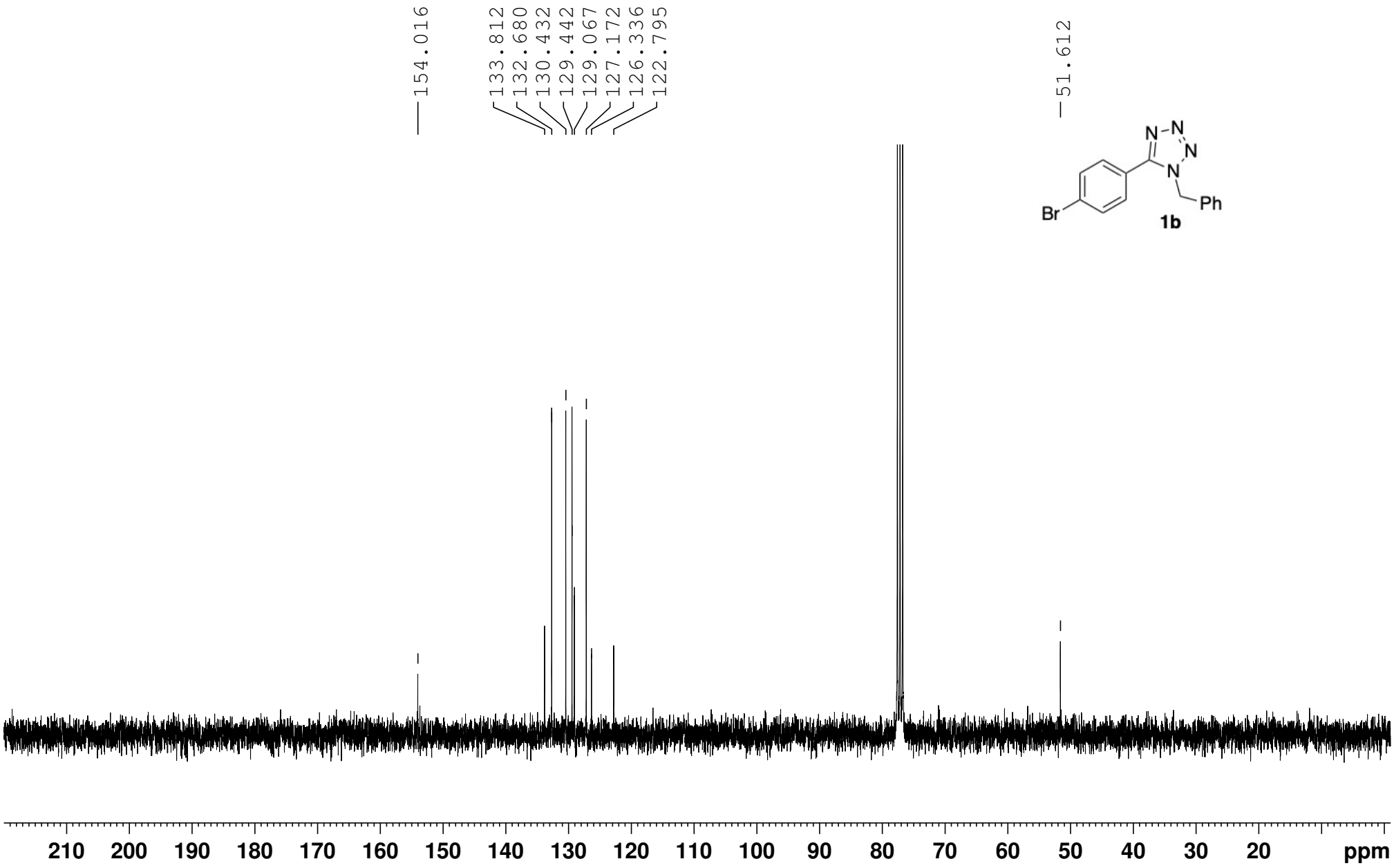
2-benzyl-5-(4-bromophenyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz



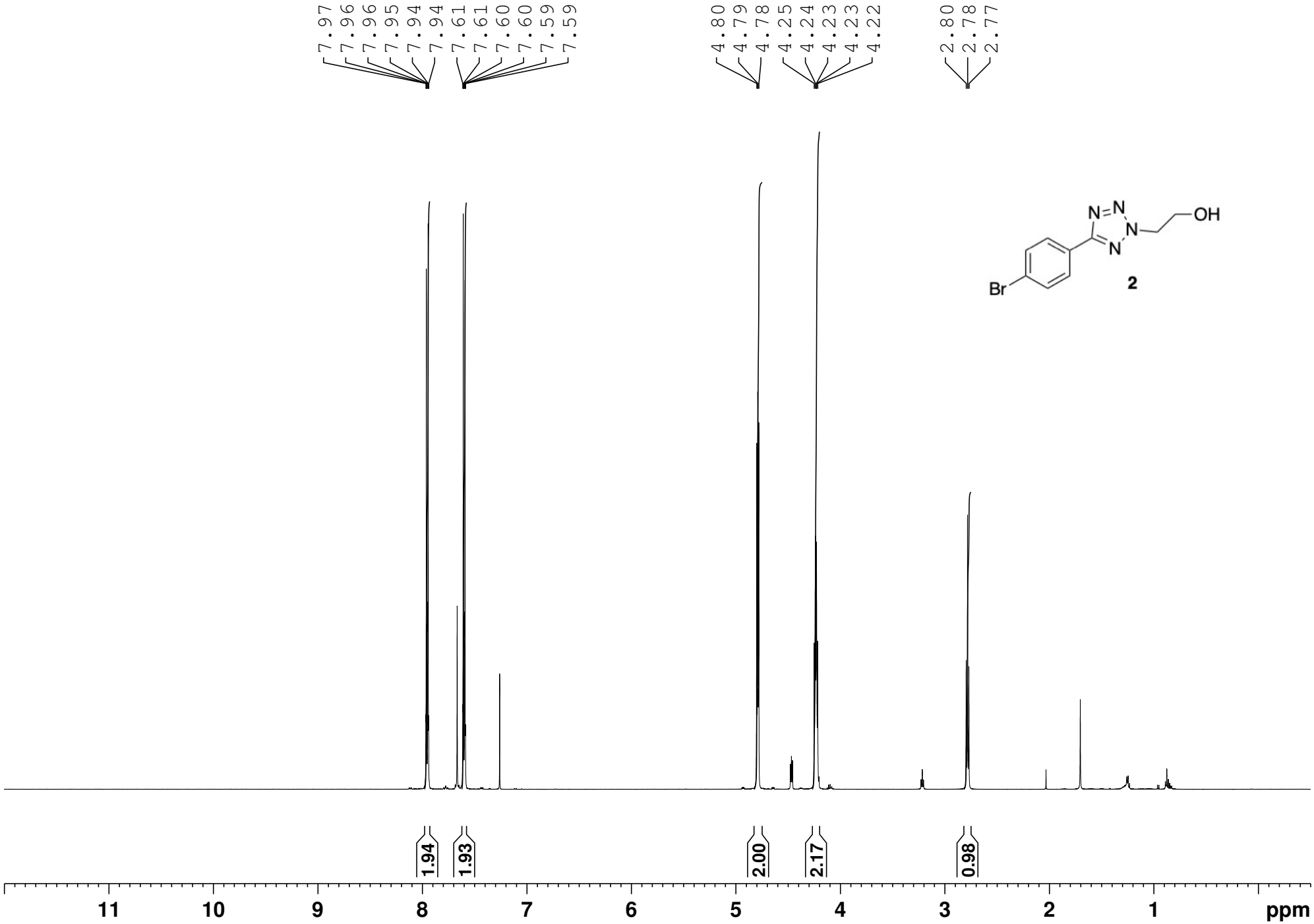
1-benzyl-5-(4-bromophenyl)-1H-tetrazole- 1H - CDCl3 - 300 MHz



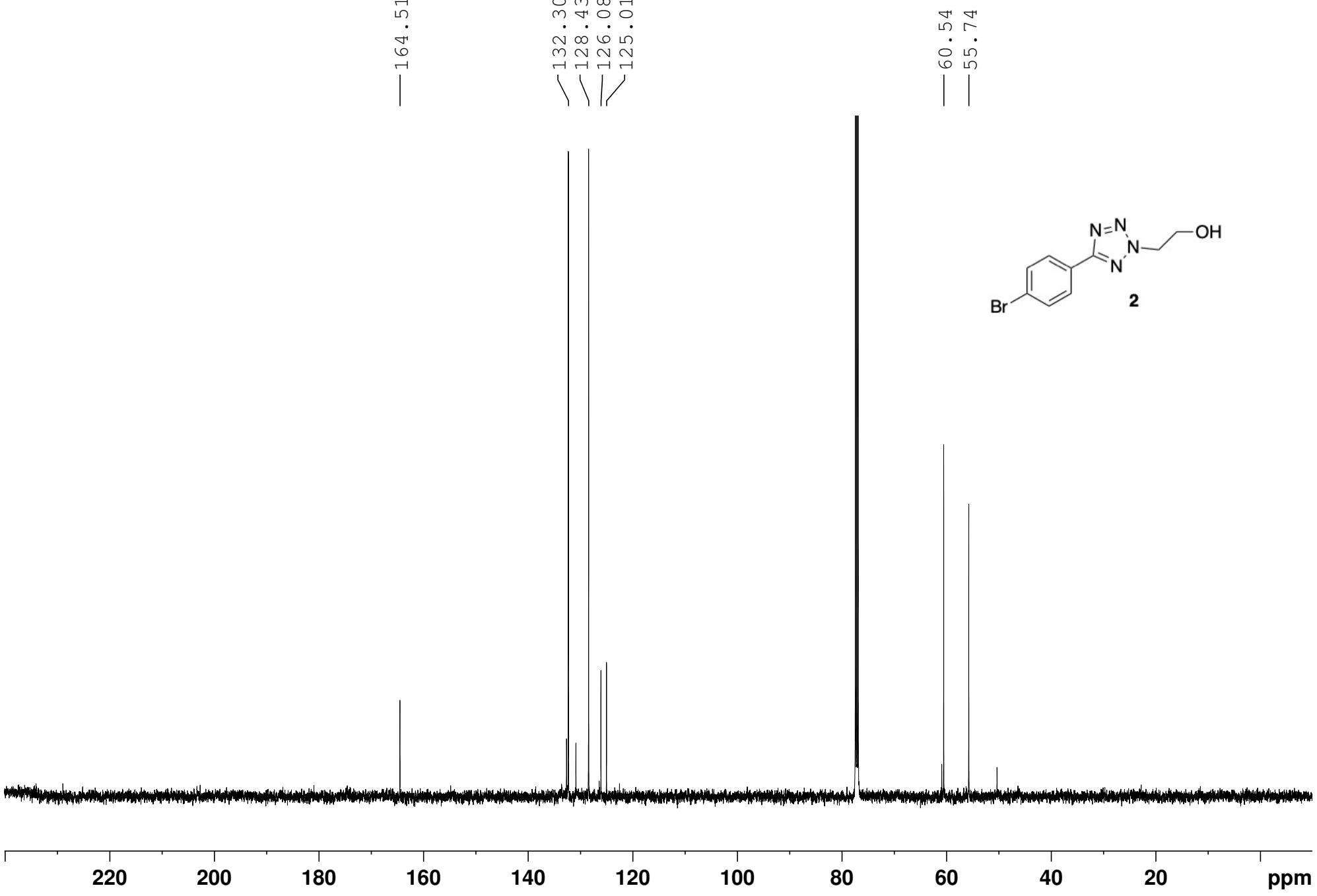
1-benzyl-5-(4-bromophenyl)-1H-tetrazole - 13C - CDCl3 - 75 MHz



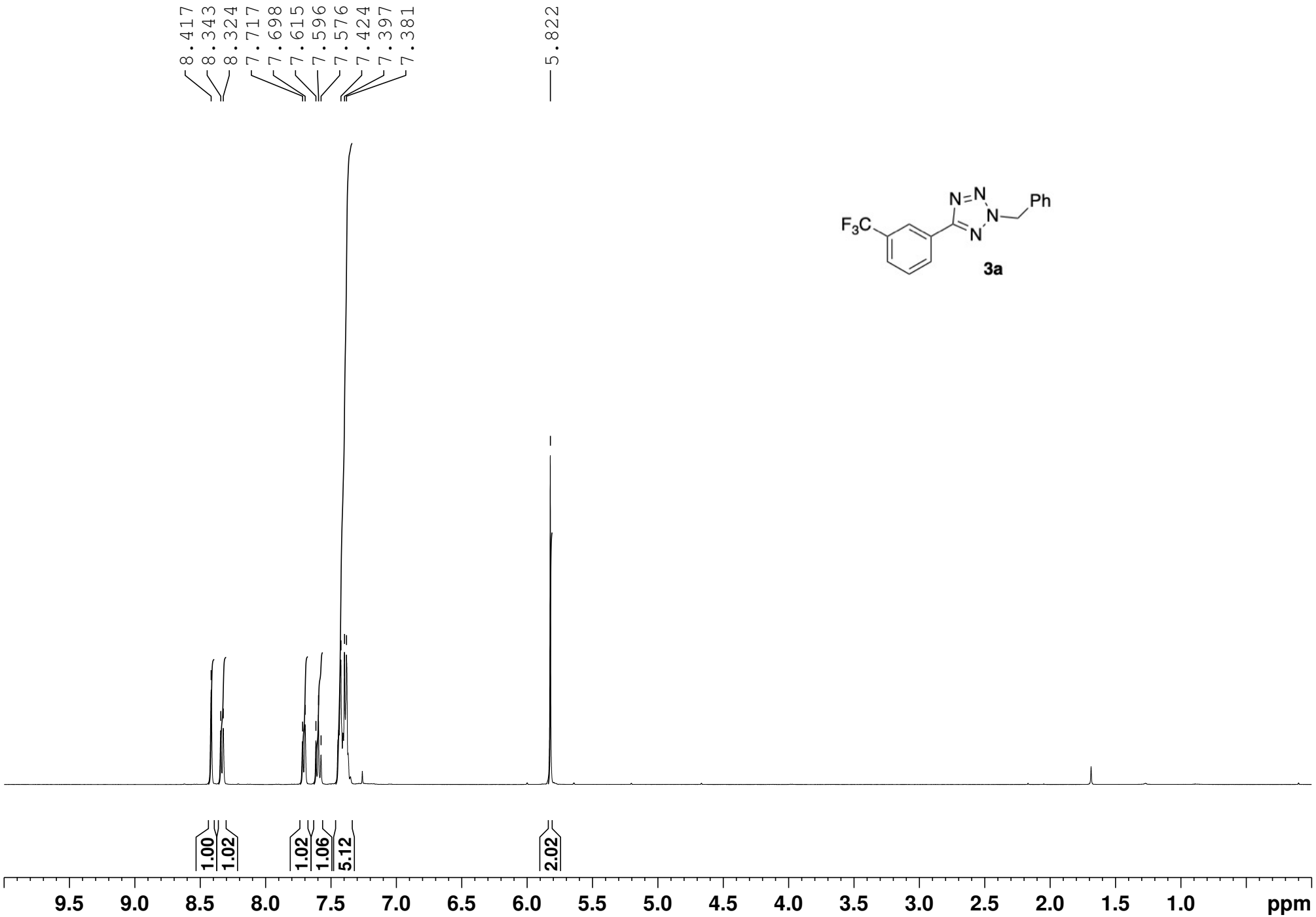
2-(5-(4-bromophenyl)-2H-tetrazol-2-yl)ethan-1-ol - 1H - CDCl3 - 500 MHz



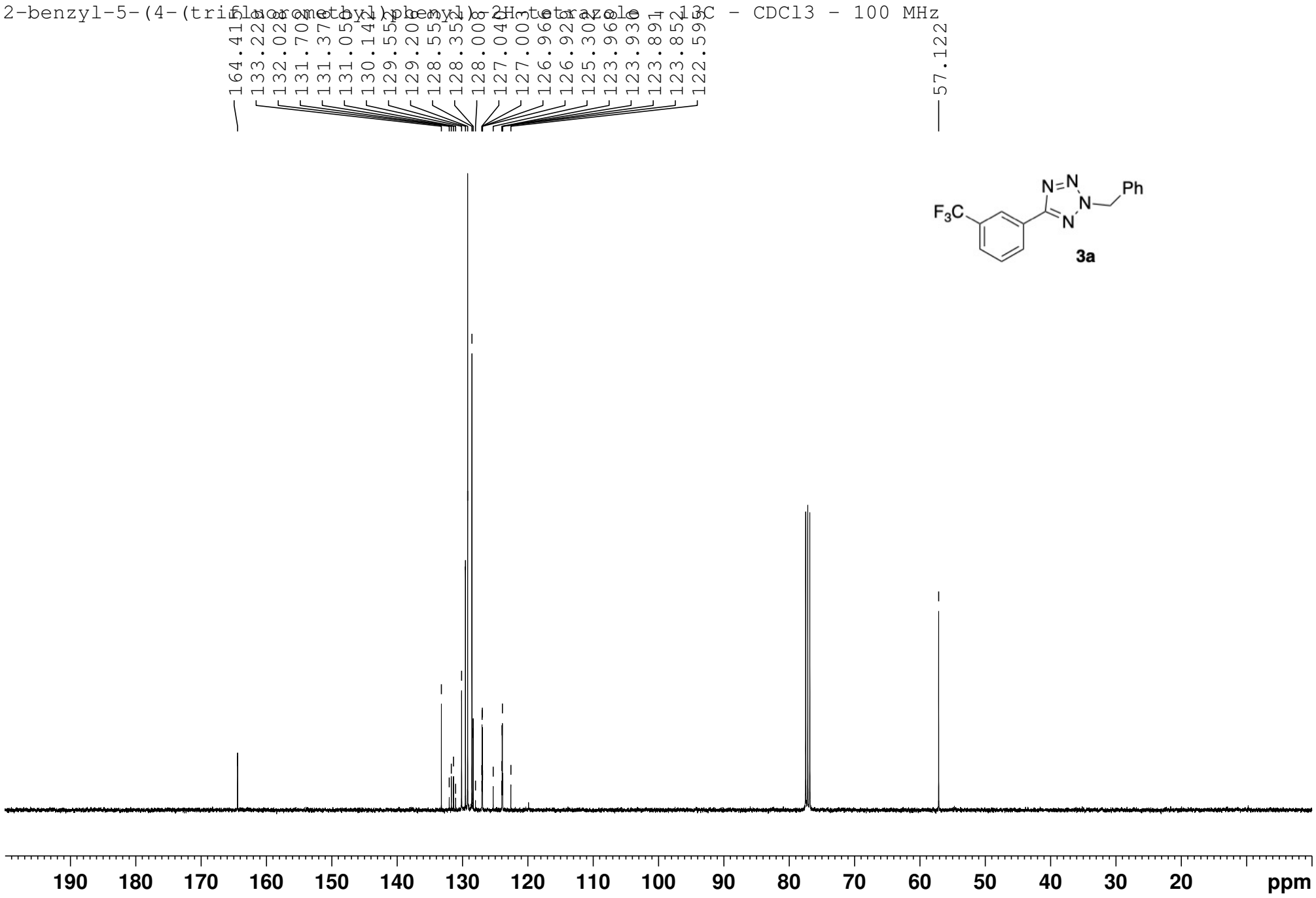
2-(5-(4-bromophenyl)-2H-tetrazol-2-yl)ethan-1-ol - 13C - CDCl3 - 125 MHz



2-benzyl-5-(3-(trifluoromethyl)phenyl)-2H-tetrazole - 1H - CDCl3 - 400 MHz

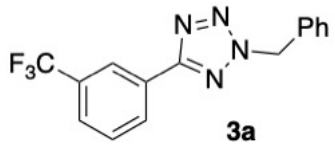


2-benzyl-5-(4-(trifluoromethyl)phenyl)-2H-tetrazole - 13C - CDCl3 - 100 MHz

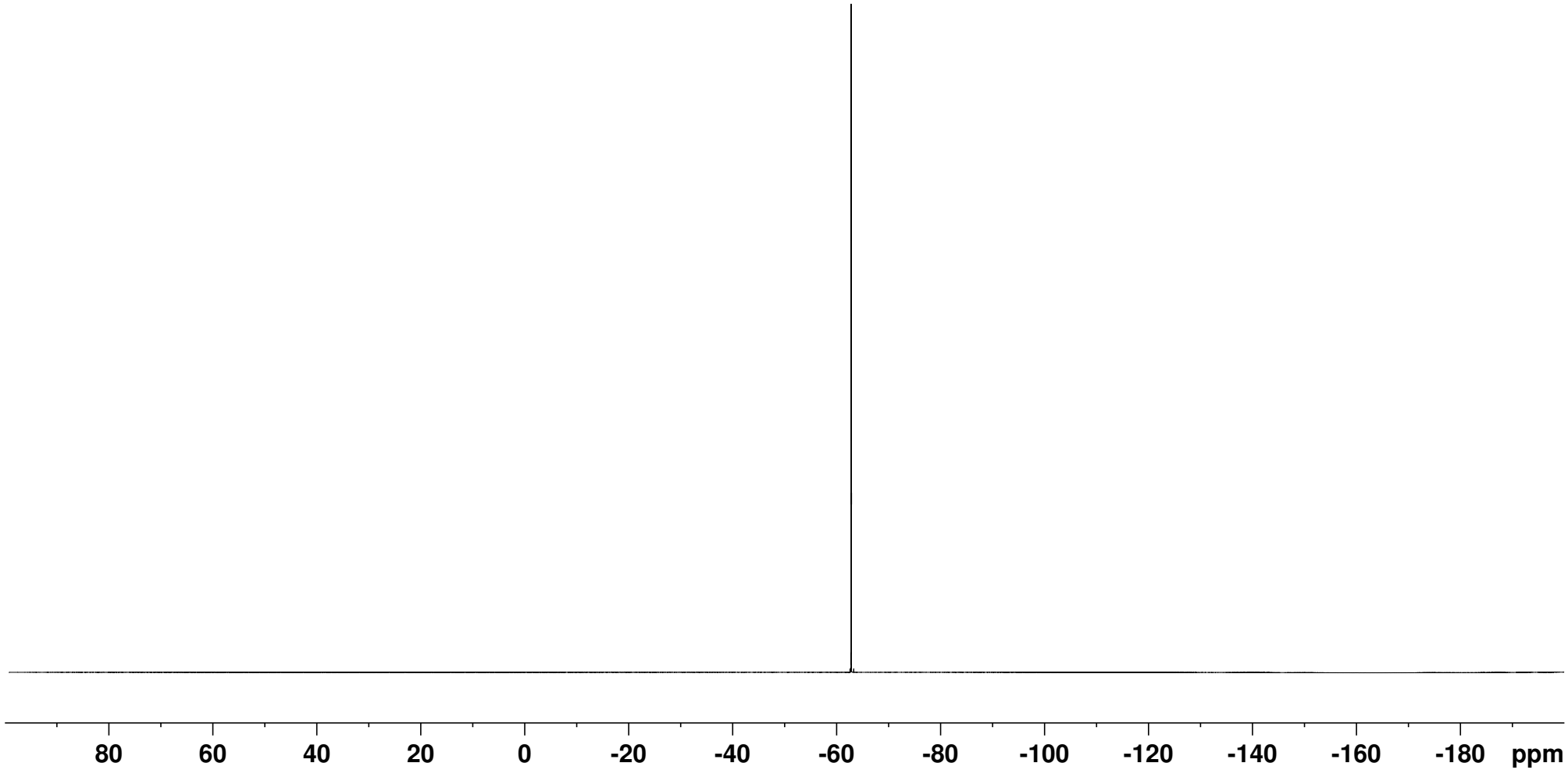


2-benzyl-5-(4-(trifluoromethyl)phenyl)-2H-tetrazole - ^{19}F - CDCl3 - 375 MHz

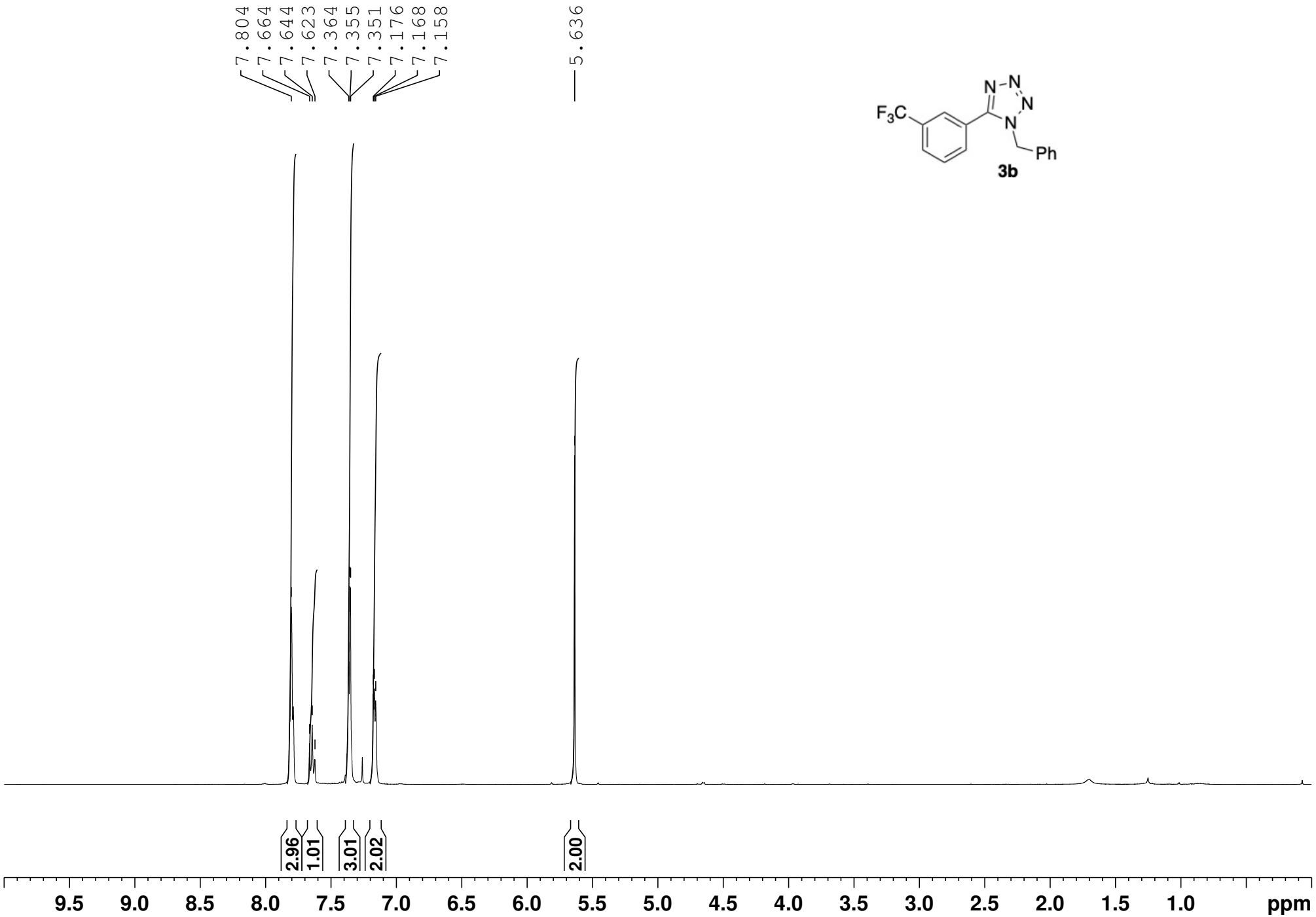
-62.827



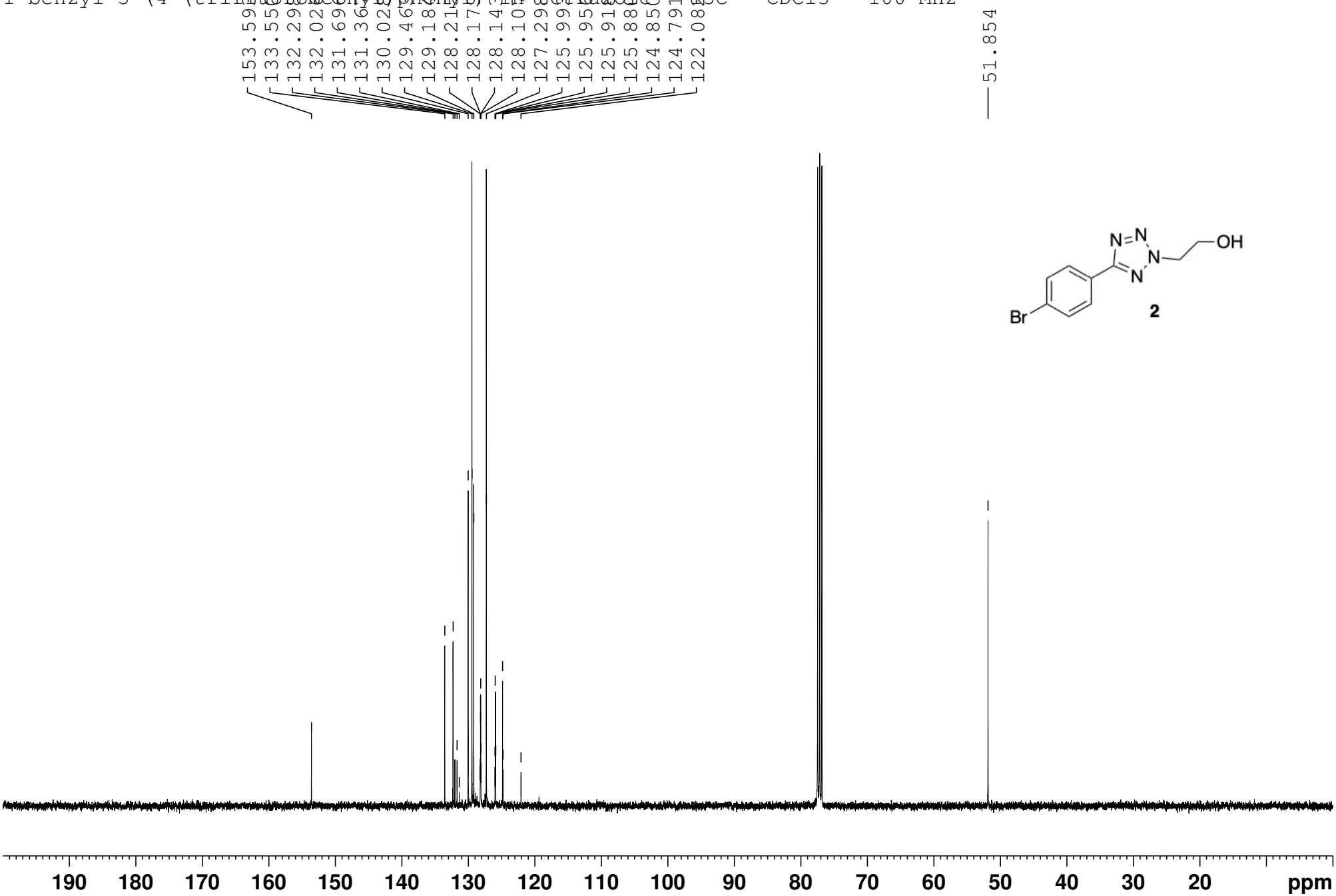
3a



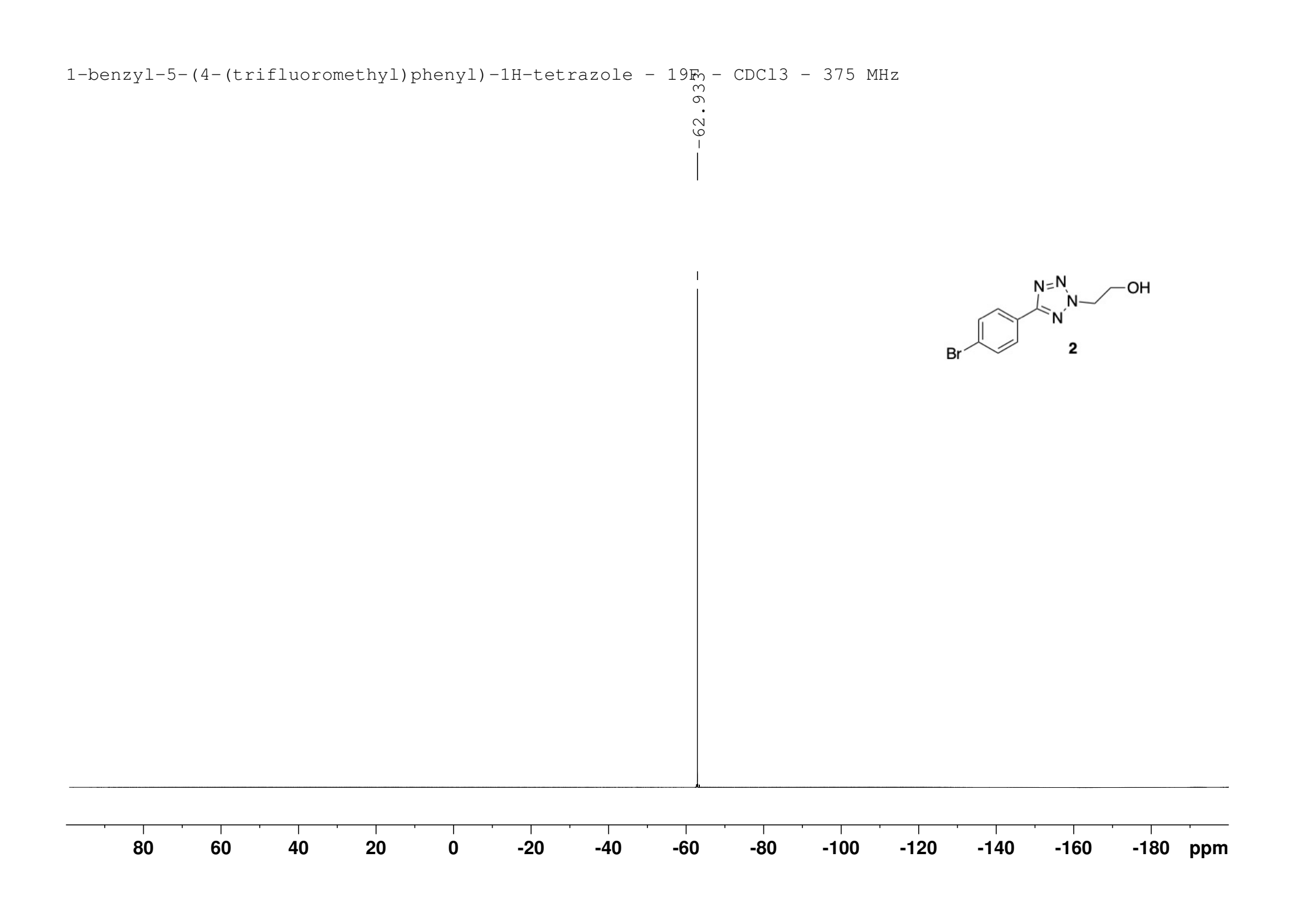
1-benzyl-5-(4-(trifluoromethyl)phenyl)-1H-tetrazole - 1H - CDCl3 - 400 MHz



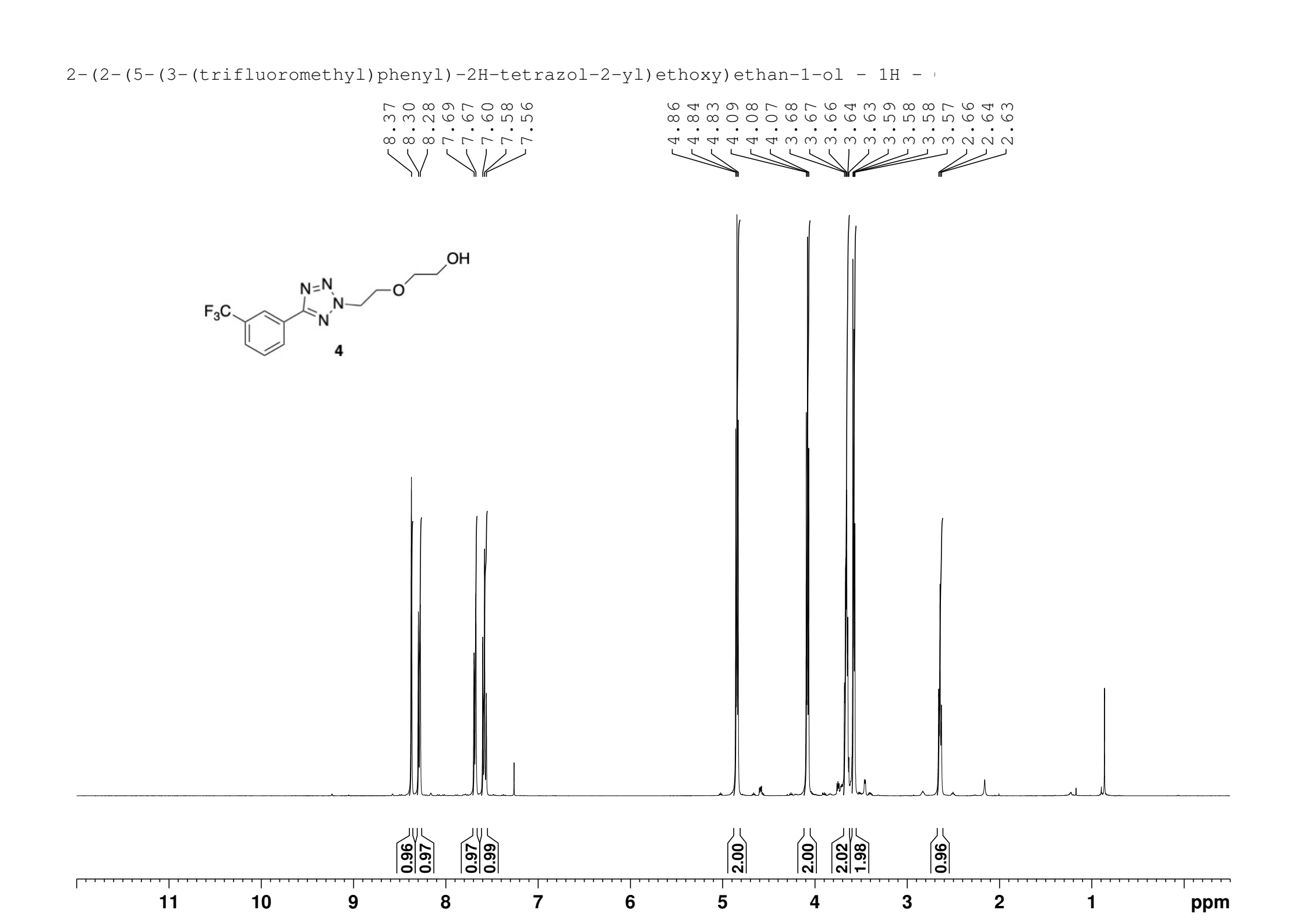
1-benzyl-5-(4-(trifluoromethyl)phenyl)-1H-tetrazole - 13C - CDCl3 - 100 MHz



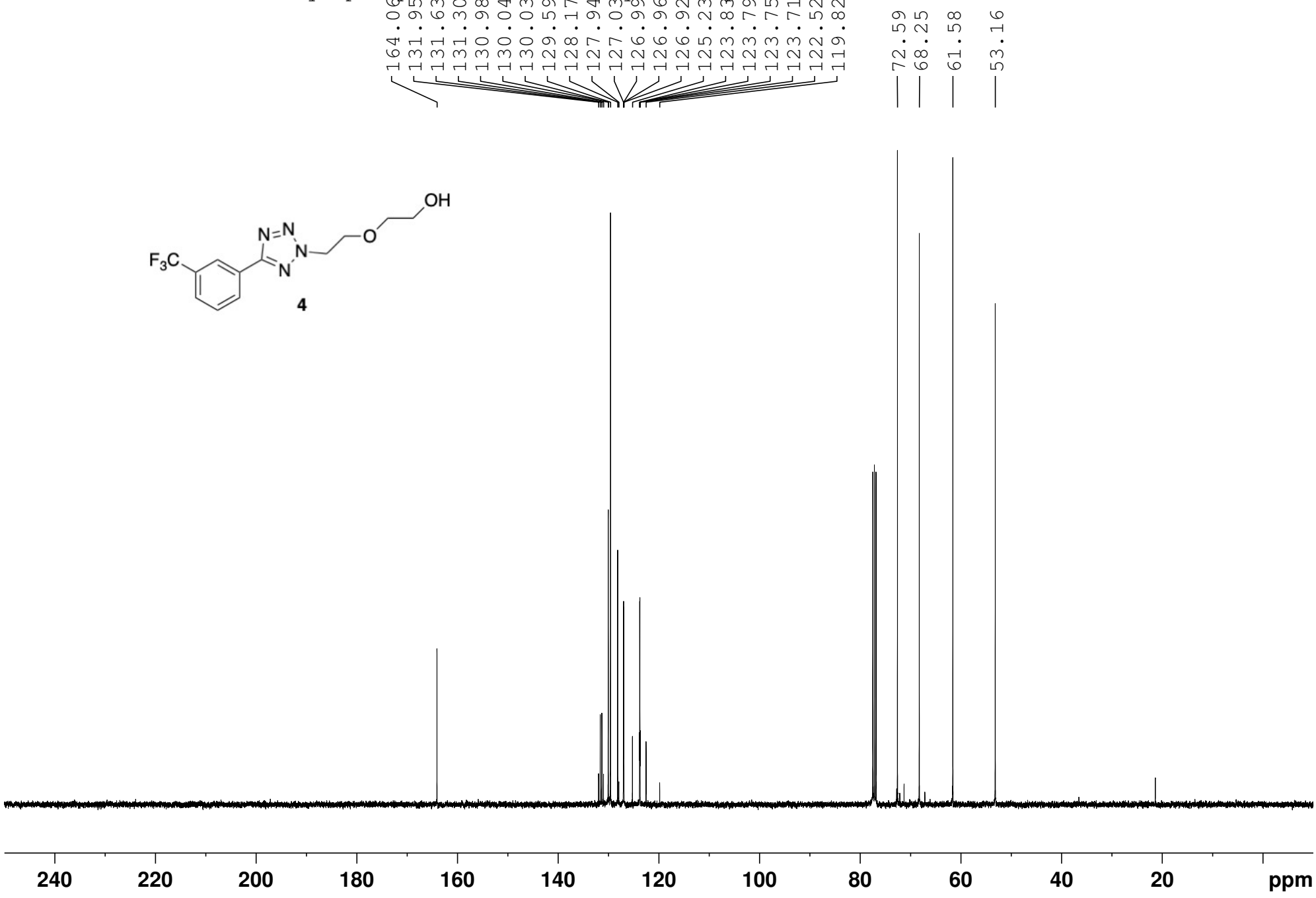
1-benzyl-5-(4-(trifluoromethyl)phenyl)-1H-tetrazole - 19F - CDCl3 - 375 MHz



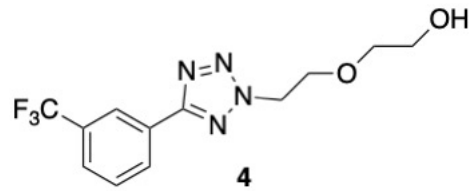
2-(2-(5-(3-(trifluoromethyl)phenyl)-2H-tetrazol-2-yl)ethoxy)ethan-1-ol - 1H -



2-(2-(5-(3-(trifluoromethyl)phenyl)-2H-tetrazol-2-yl)ethoxy)ethan-1-ol - 13C -

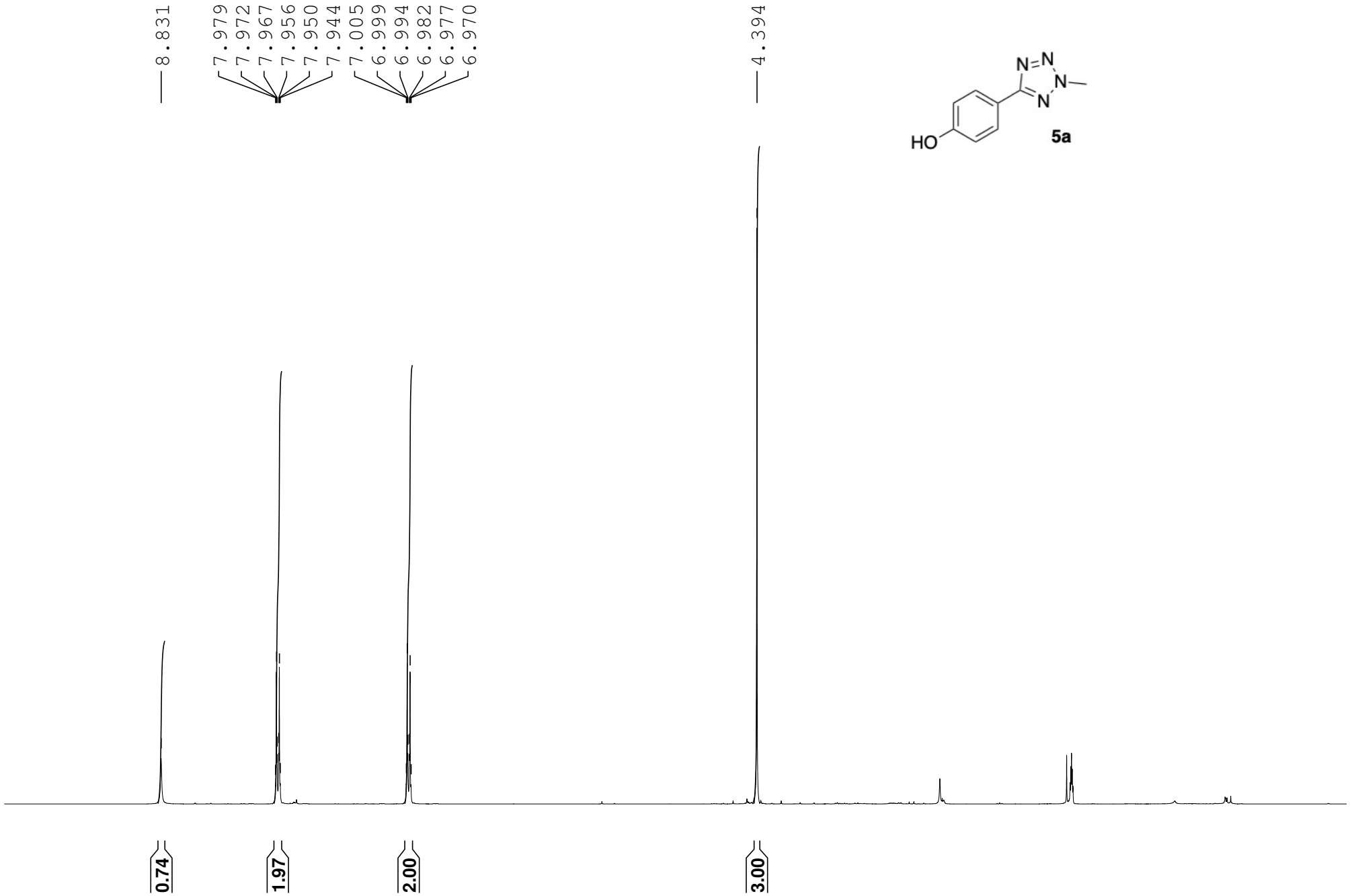


2-(2-(5-(3-(trifluoromethyl)phenyl)-2H-tetrazol-2-yl)ethoxy)ethan-1-ol - 19F - CDCl3 - 375 MHz



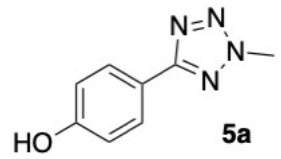
4

4-(2-methyl-2H-tetrazol-5-yl)phenol - 1H - acetone-d6 - 400 MHz



4-(2-methyl-2H-tetrazol-5-yl)phenol - 13C , acetone-d6, 100 MHz

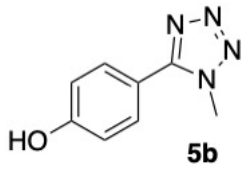
166.189
160.591
129.386
120.512
117.060
40.110



5a

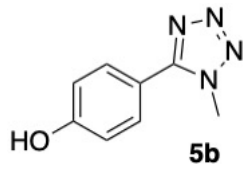
250 200 150 100 50 0 ppm

4-(1-methyl-1H-tetrazol-5-yl)phenol - 1H - dmso-d6 - 400 MHz



5b

4-(1-methyl-1H-tetrazol-5-yl)phenol - 13C - dmso-d6 - 100 MHz

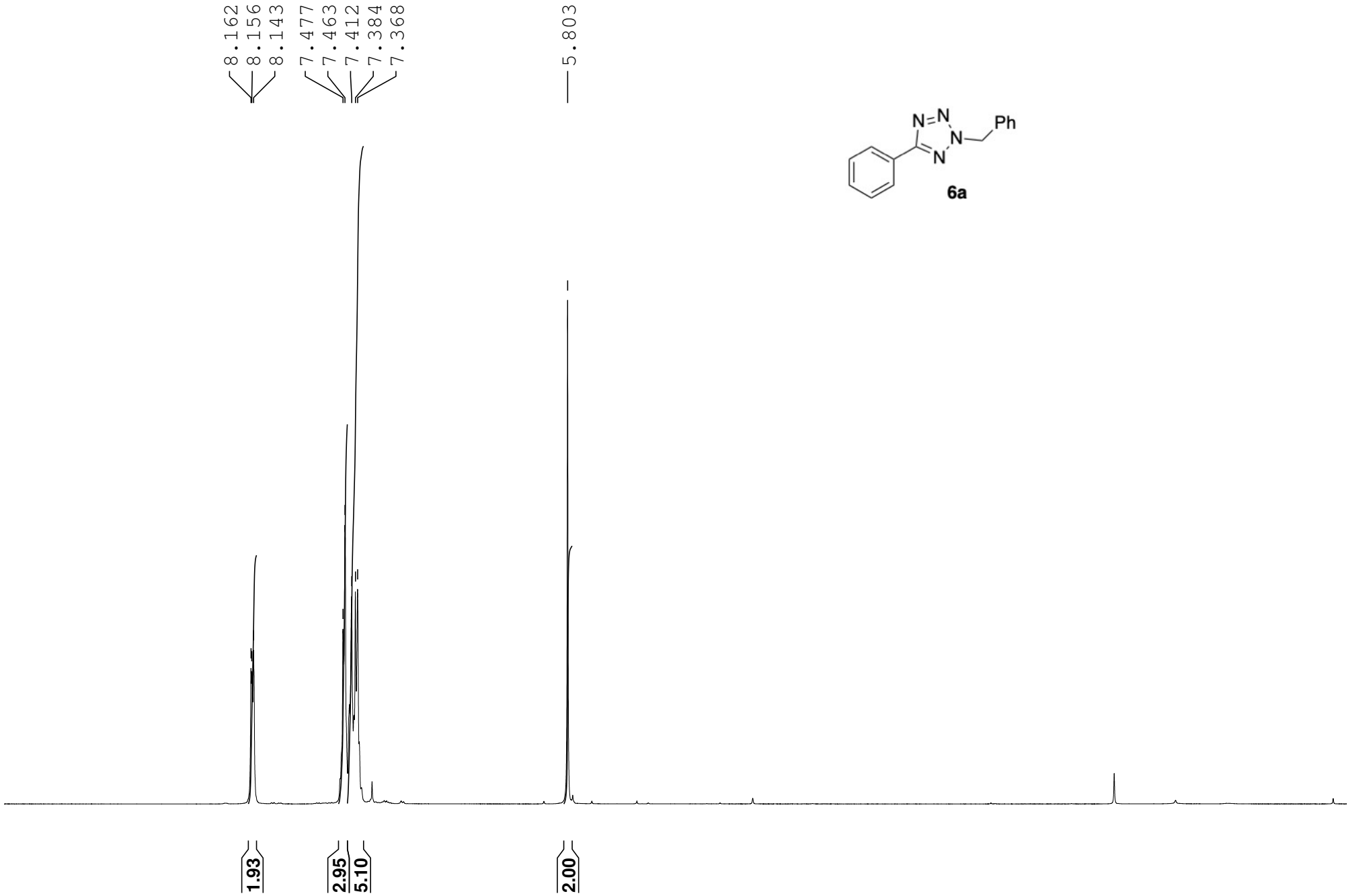


5b

159.921
153.944
130.341
115.911
114.034
35.007

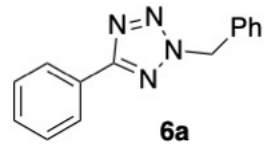
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

2-benzyl-5-phenyl-2H-tetrazole - 1H - CDCl3 - 400 MHz



2-benzyl-5-phenyl-2H-tetrazole - 13C - CDCl3 - 100 MHz

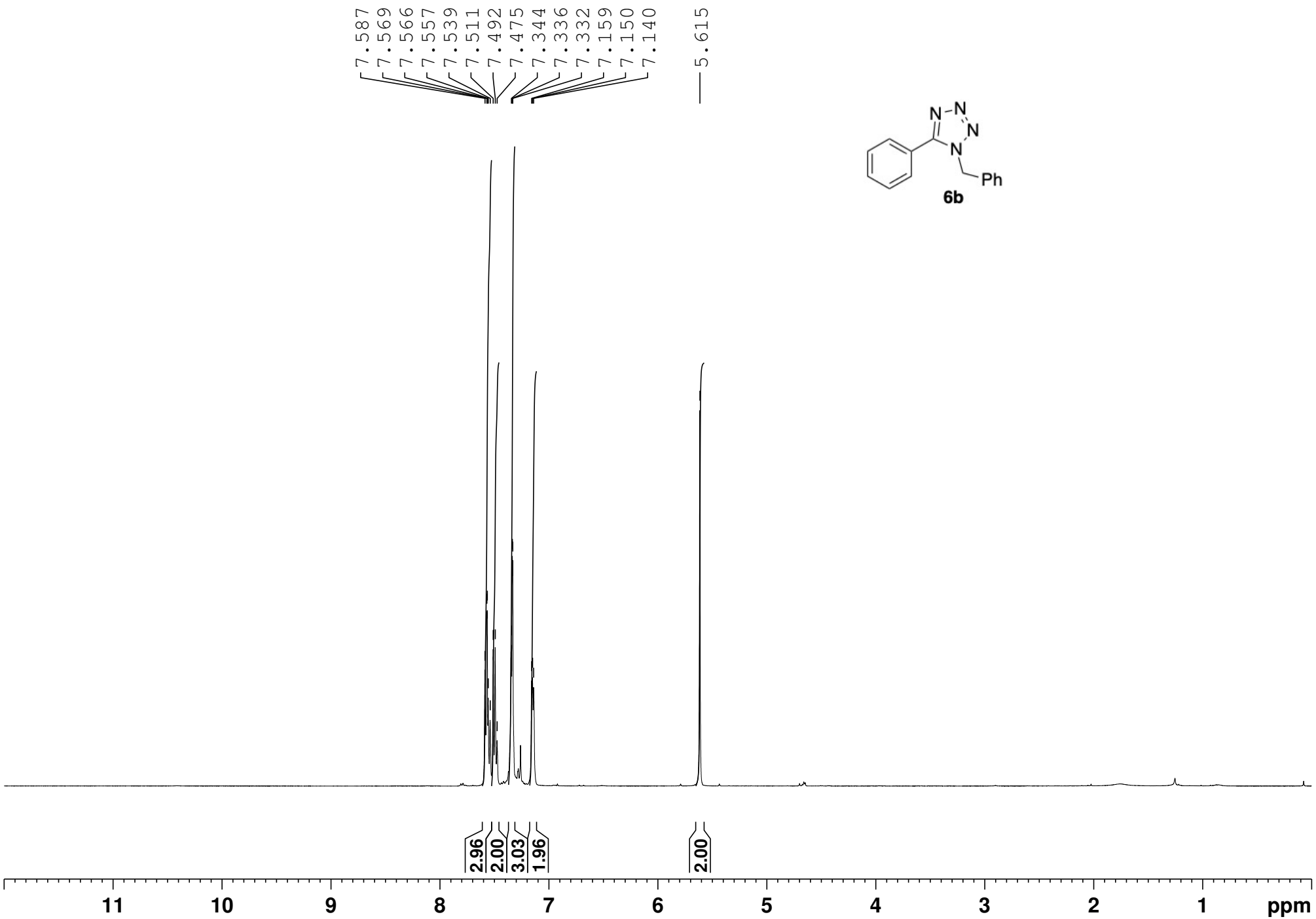
165.541
133.468
130.409
129.107
129.034
128.945
128.467
127.458
126.968
56.891

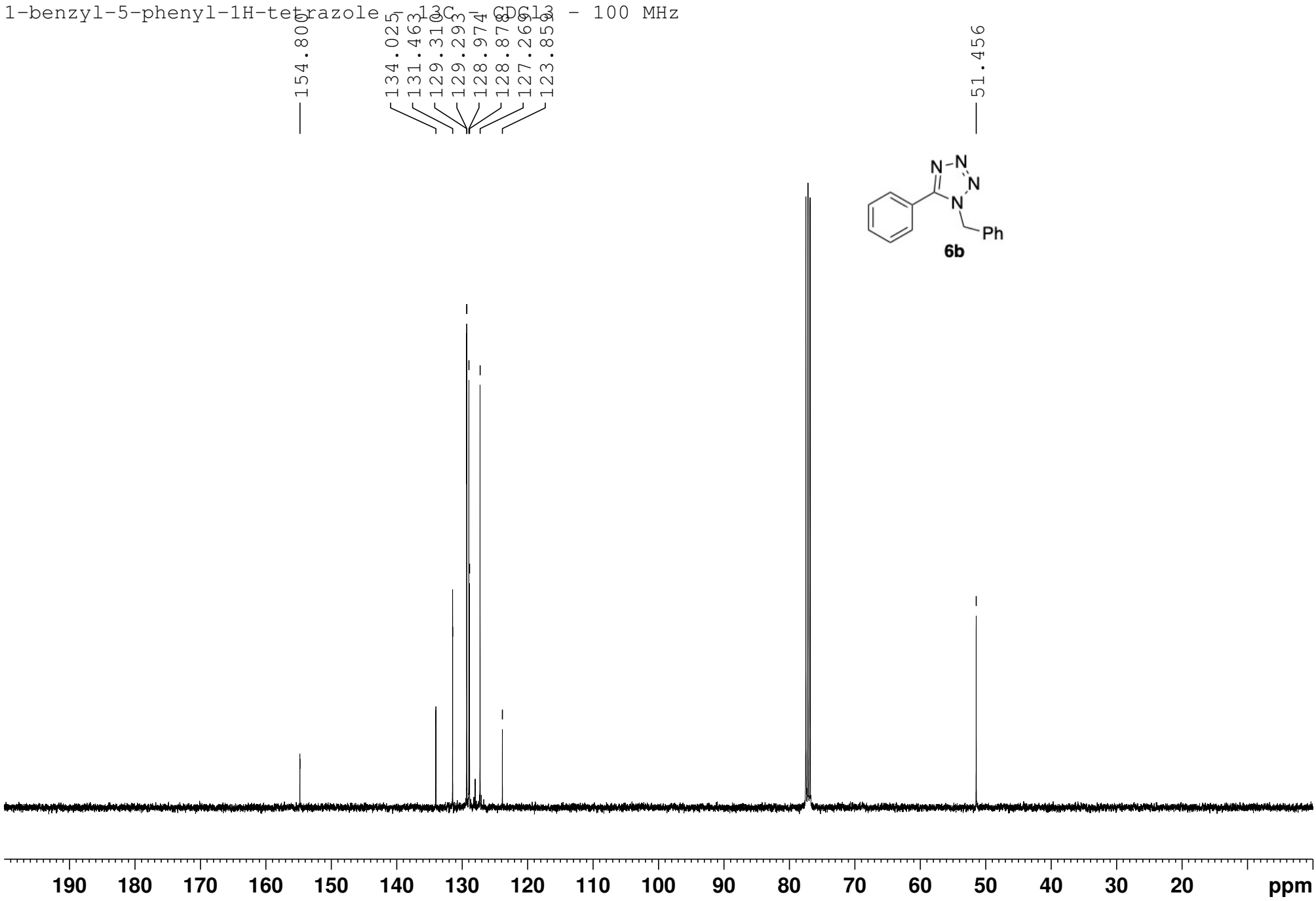


6a

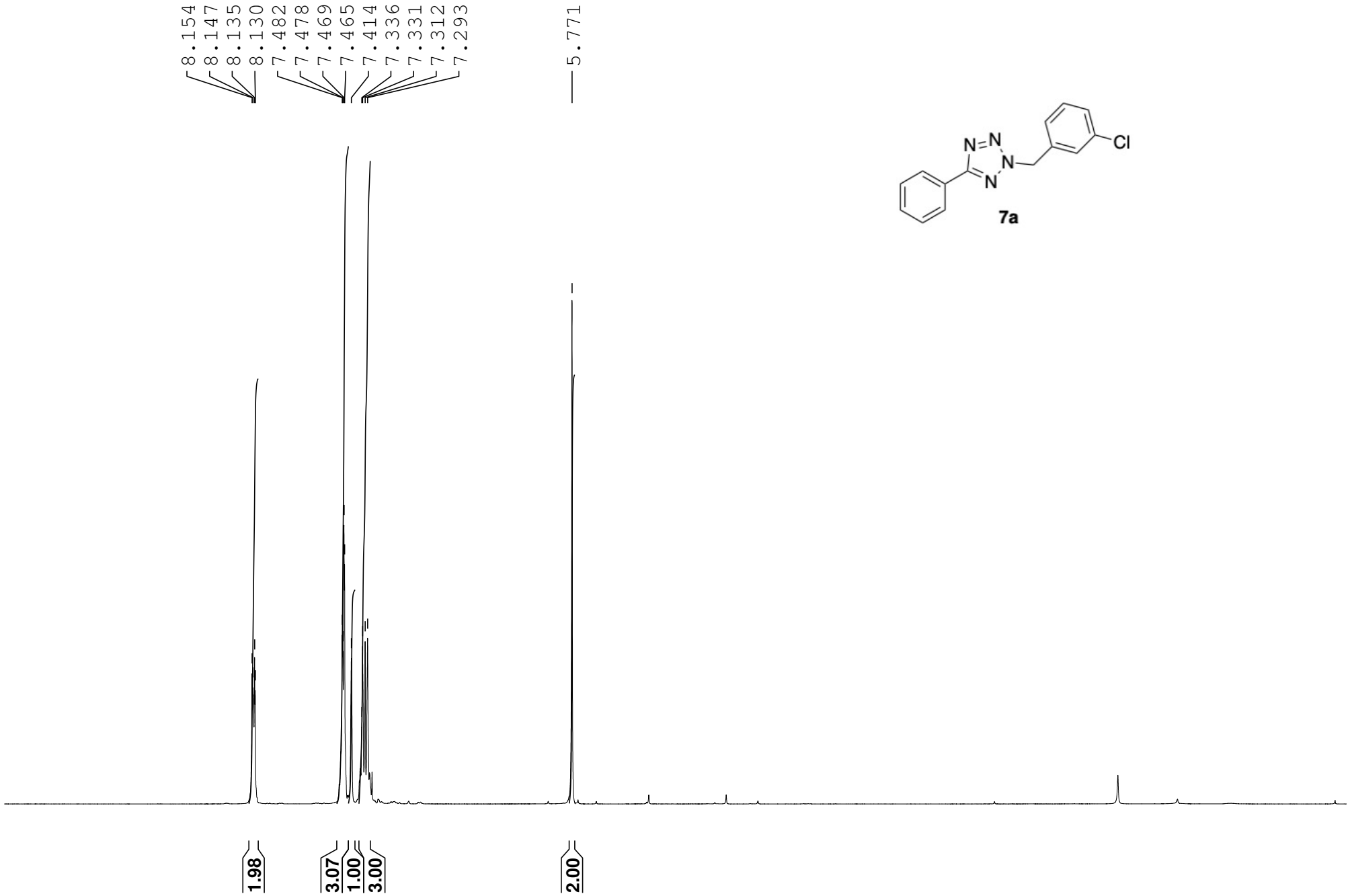
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

1-benzyl-5-phenyl-1H-tetrazole - 1H - CDCl3 - 400 MHz

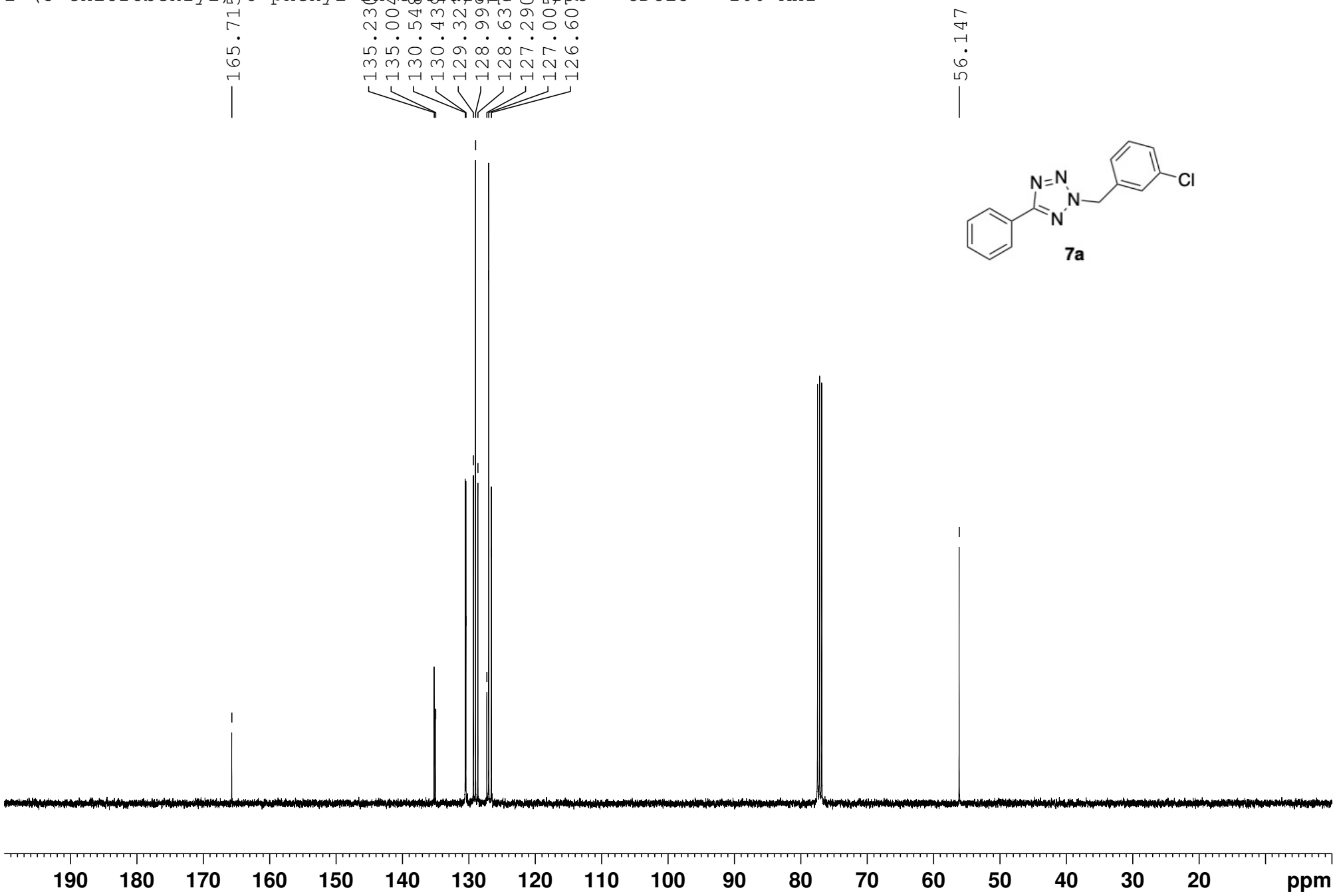



1-benzyl-5-phenyl-1H-tetrazole - 13C - CDCl3 - 100 MHz
154.800
134.025
131.463
129.310
129.293
128.974
128.878
127.269
123.853
51.456
N
N
N
N
Ph
6b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

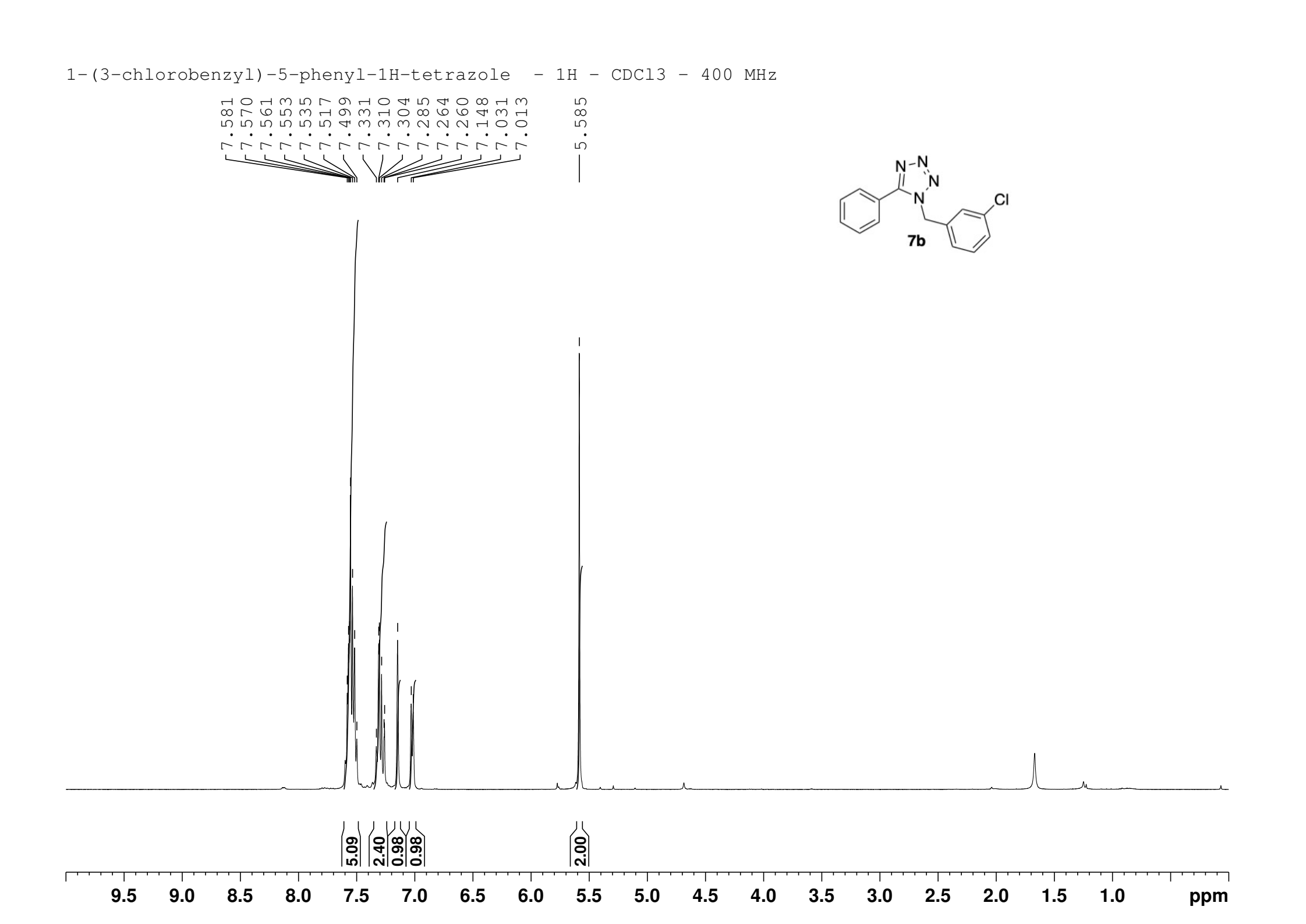
2-(3-chlorobenzyl)-5-phenyl-2H-tetrazole - 1H - CDCl3 - 400 MHz



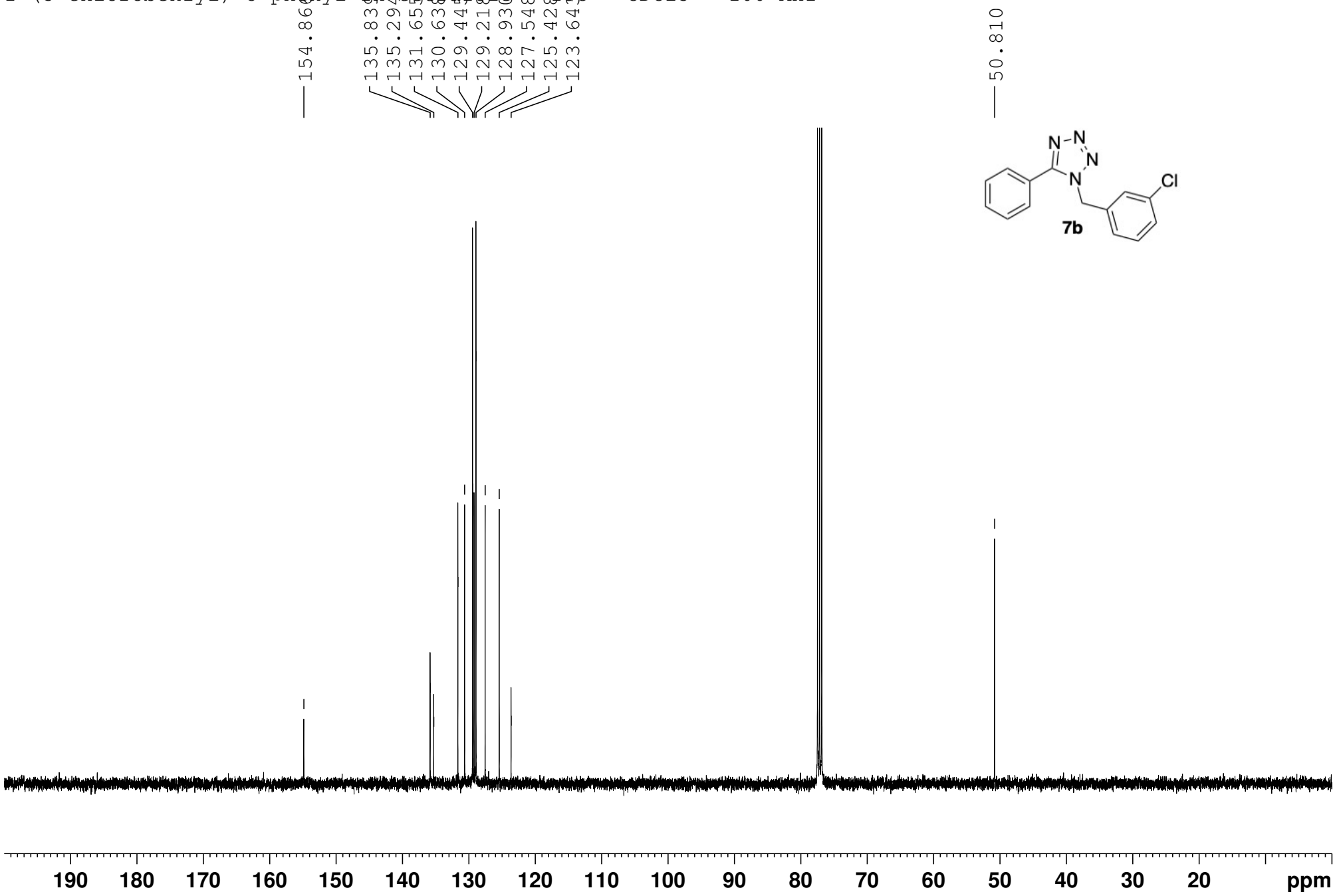
2-(3-chlorobenzyl)-5-phenyl-2H-tetrazole - 13C - CDCl3 - 100 MHz



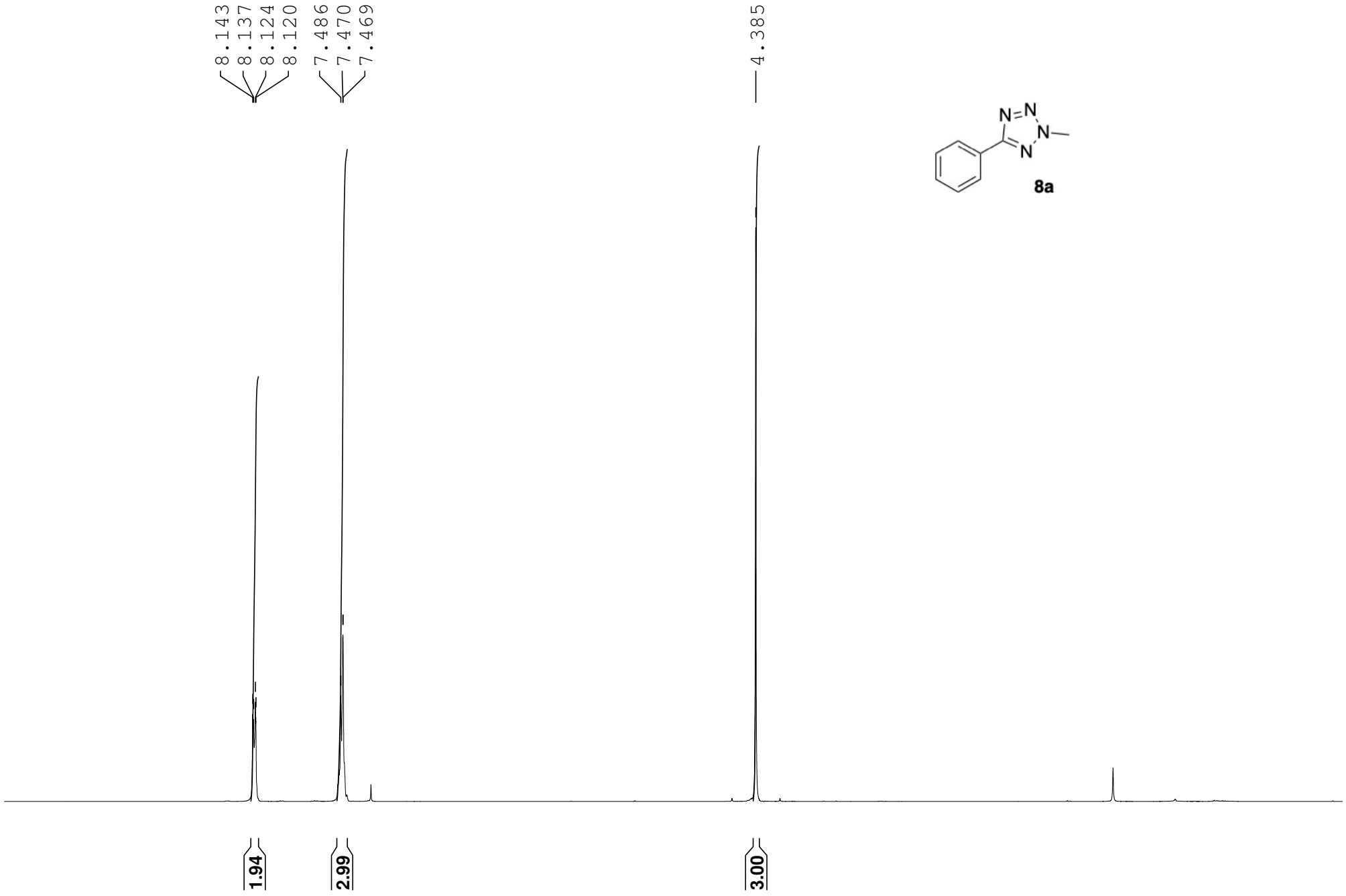
1-(3-chlorobenzyl)-5-phenyl-1H-tetrazole - 1H - CDCl3 - 400 MHz



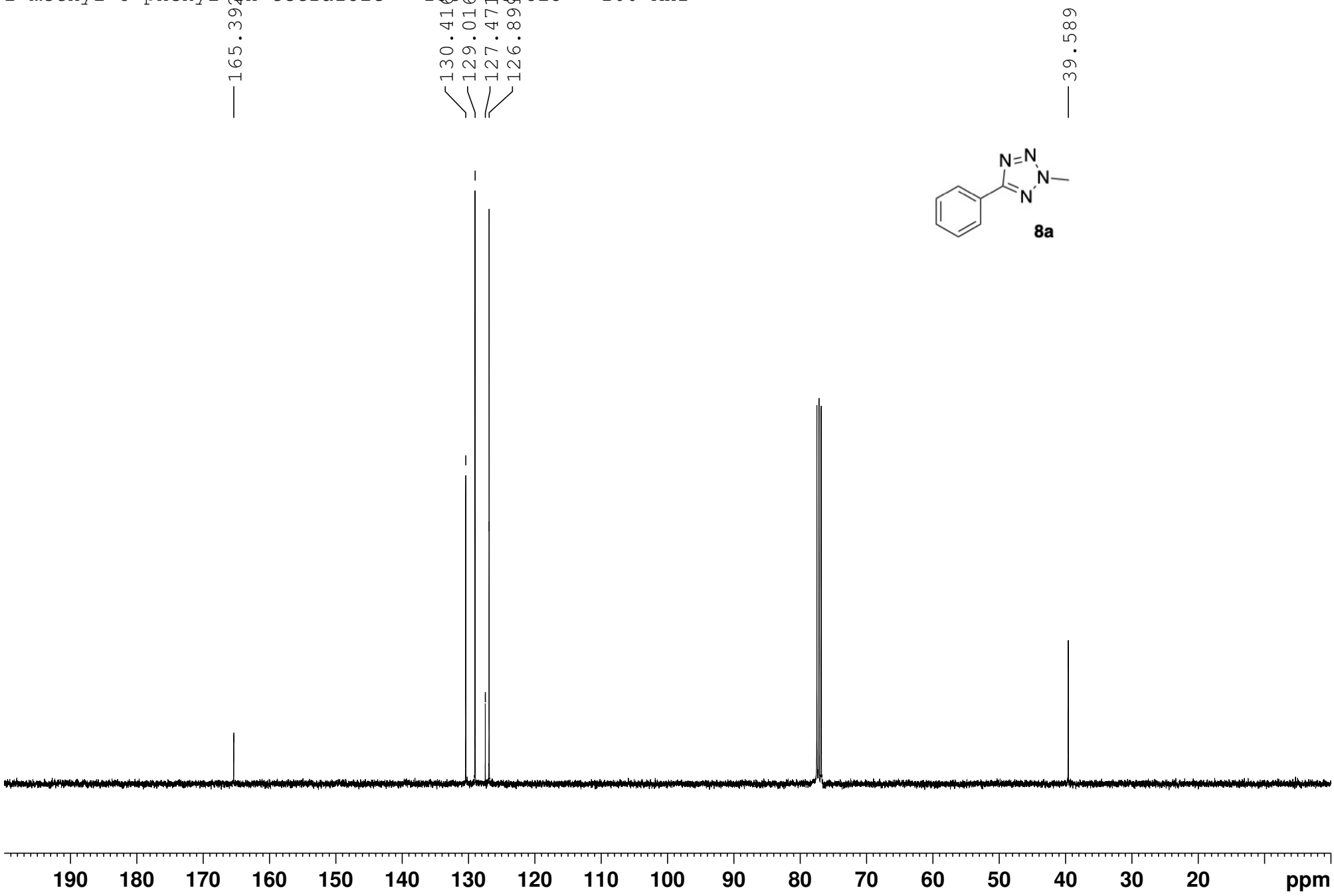
1-(3-chlorobenzyl)-5-phenyl-1H-tetrazole - 13C - CDCl3 - 100 MHz



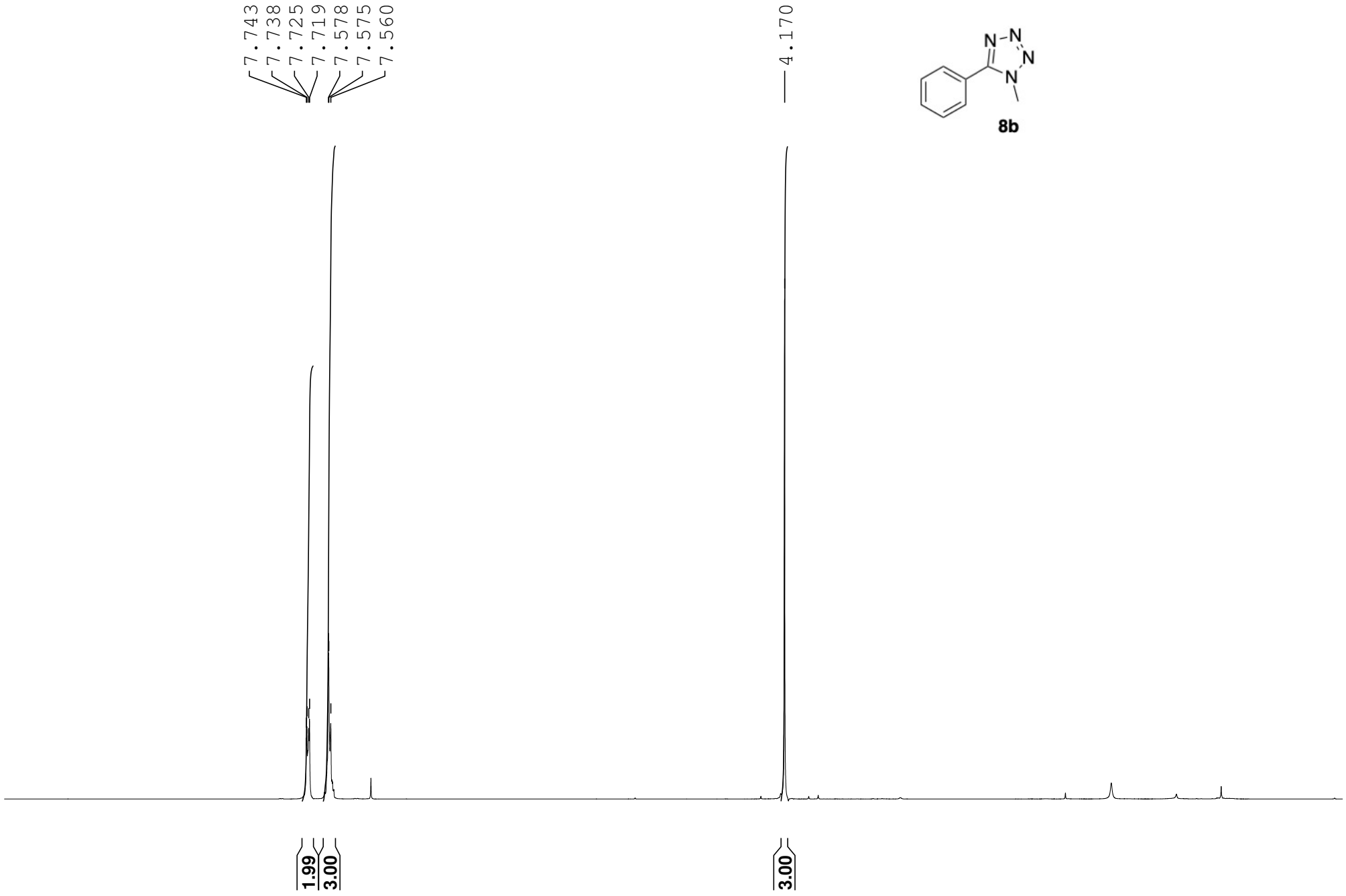
2-methyl-5-phenyl-2H-tetrazole - 1H - CDCl3 - 400MHz



2-methyl-5-phenyl-2H-tetrazole - 13C - CDCl3 - 100 MHz

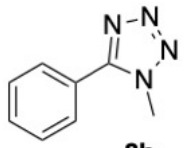


1-methyl-5-phenyl-1H-tetrazole - 1H - CDCl3 - 400 MHz



1-methyl-5-phenyl-1H-tetrazole - 13C - CDCl3 - 100 MHz

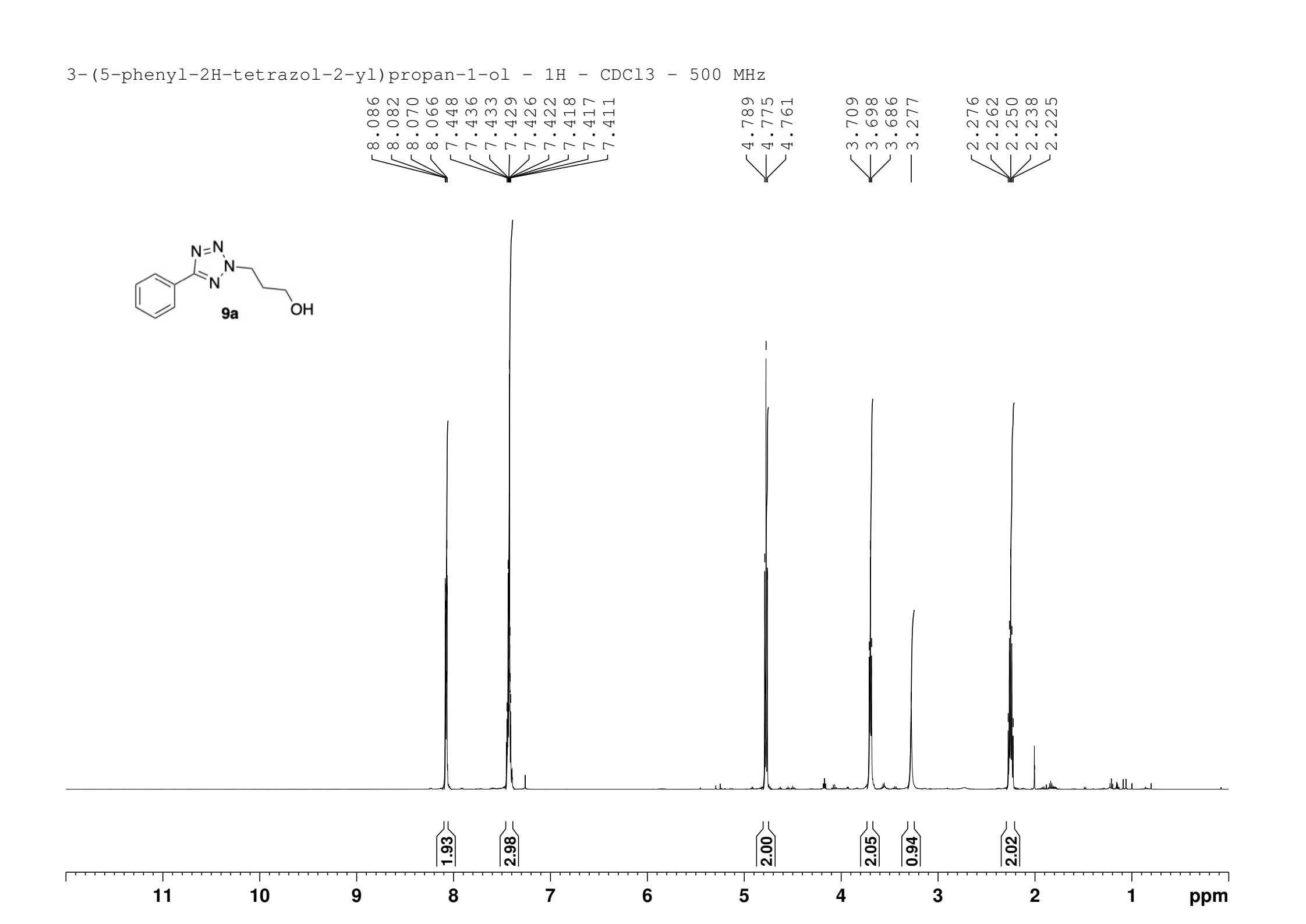
154.591
131.447
129.402
128.760
123.854
35.149



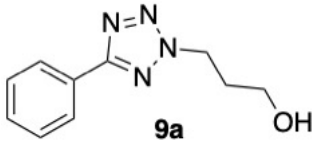
8b

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

3-(5-phenyl-2H-tetrazol-2-yl)propan-1-ol - 1H - CDCl3 - 500 MHz

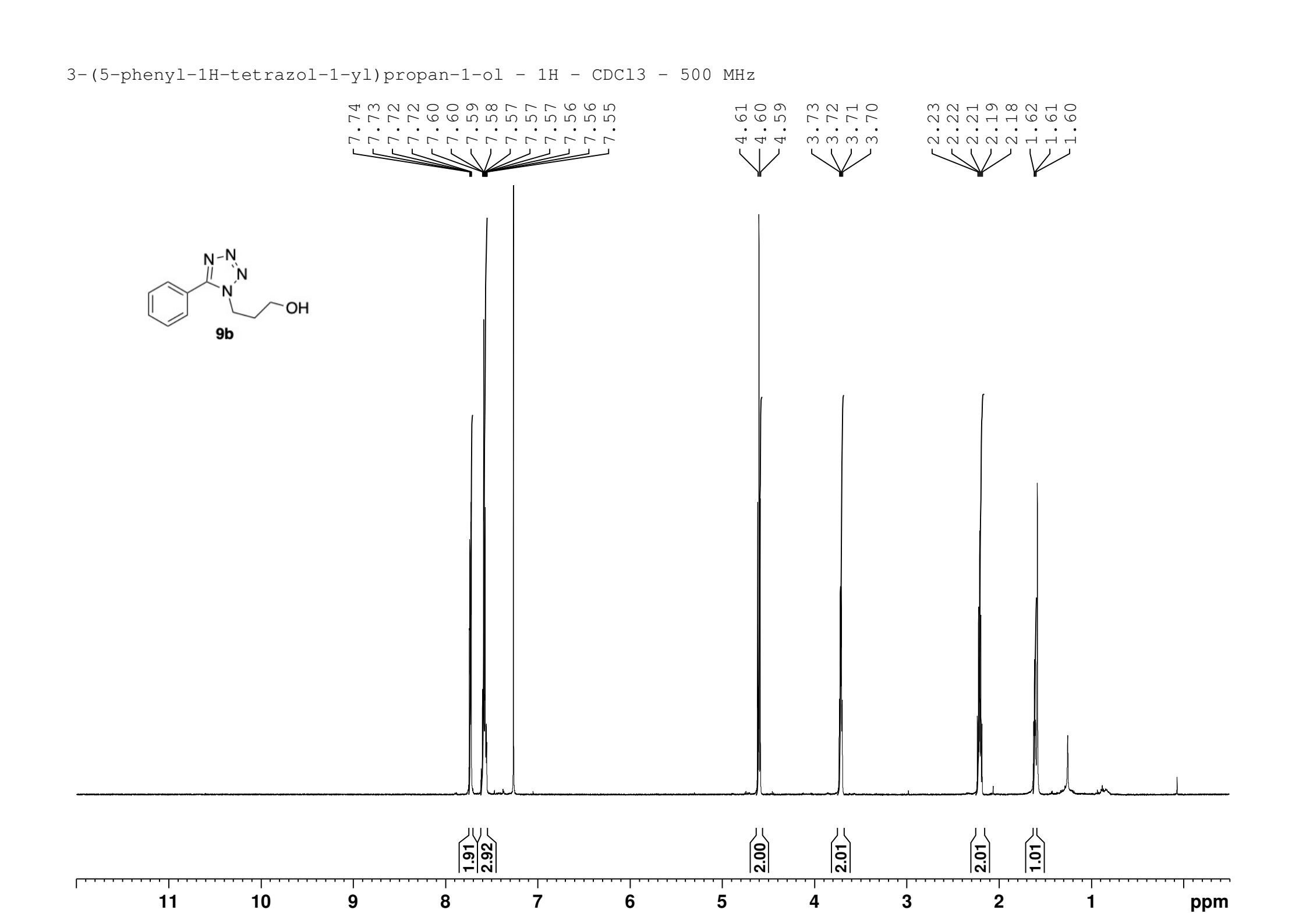


3-(5-phenyl-2H-tetrazol-2-yl)propan-1-ol - 13C - CDCl3 - 125 MHz

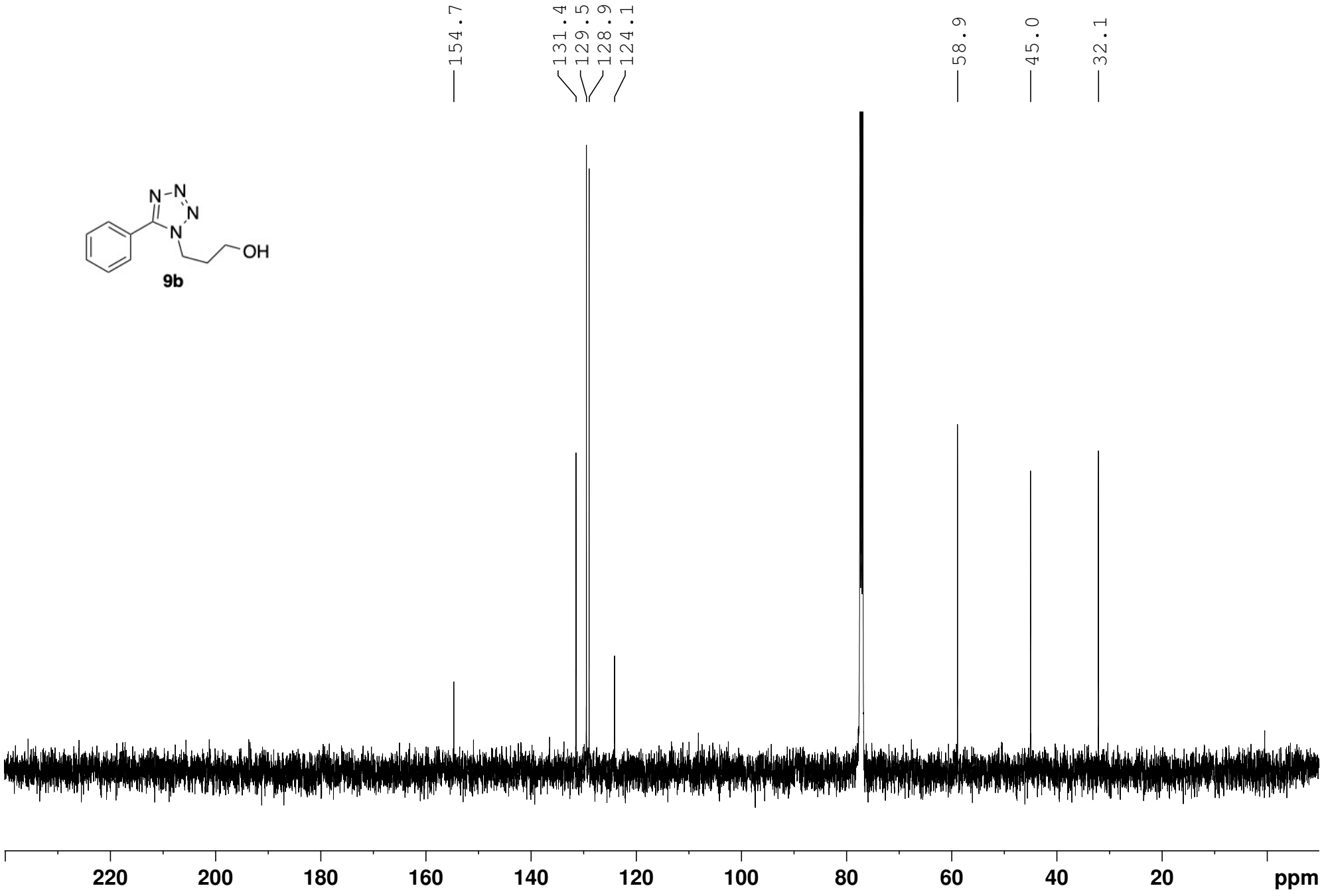


9a

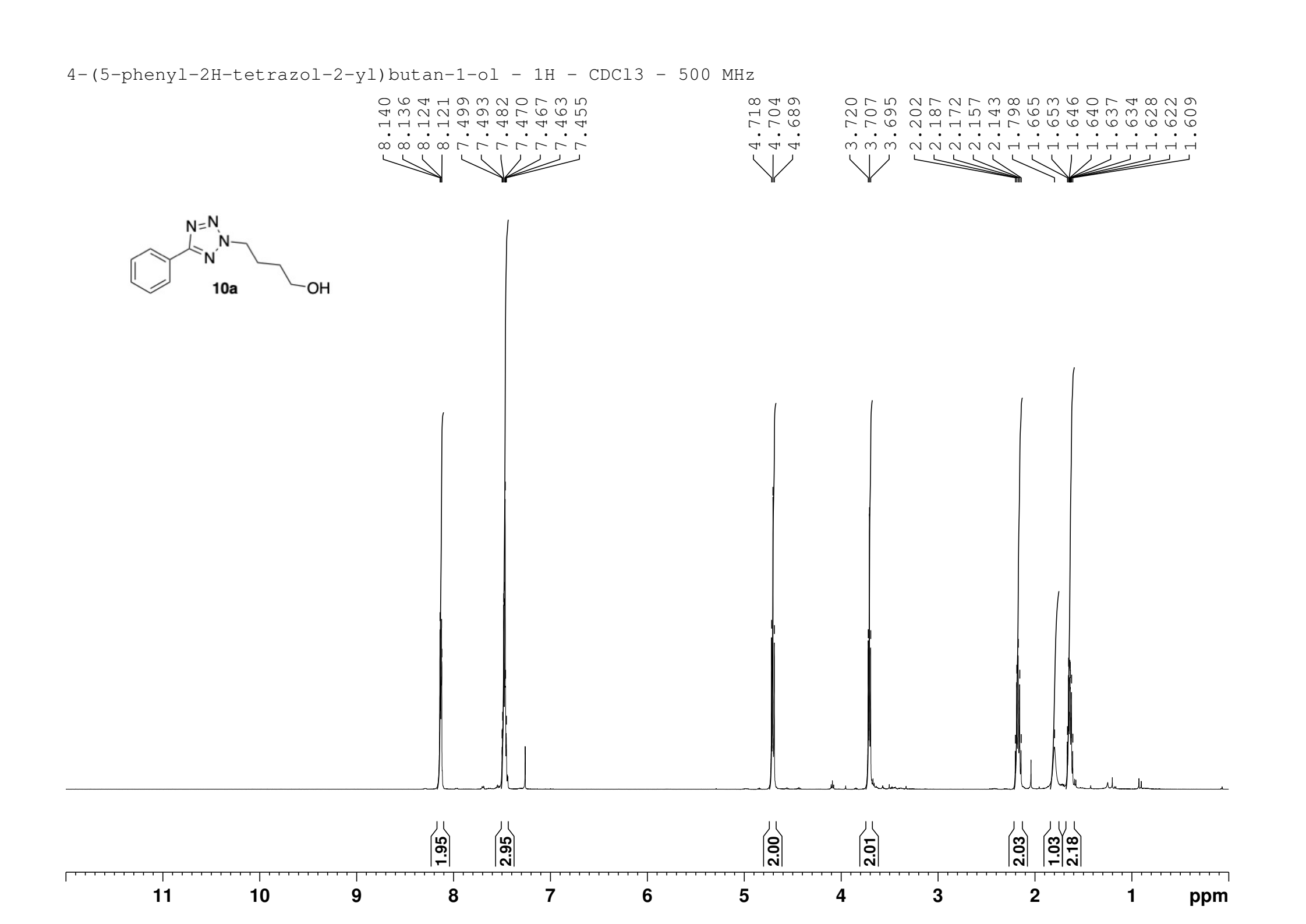
3-(5-phenyl-1H-tetrazol-1-yl)propan-1-ol - 1H - CDCl3 - 500 MHz



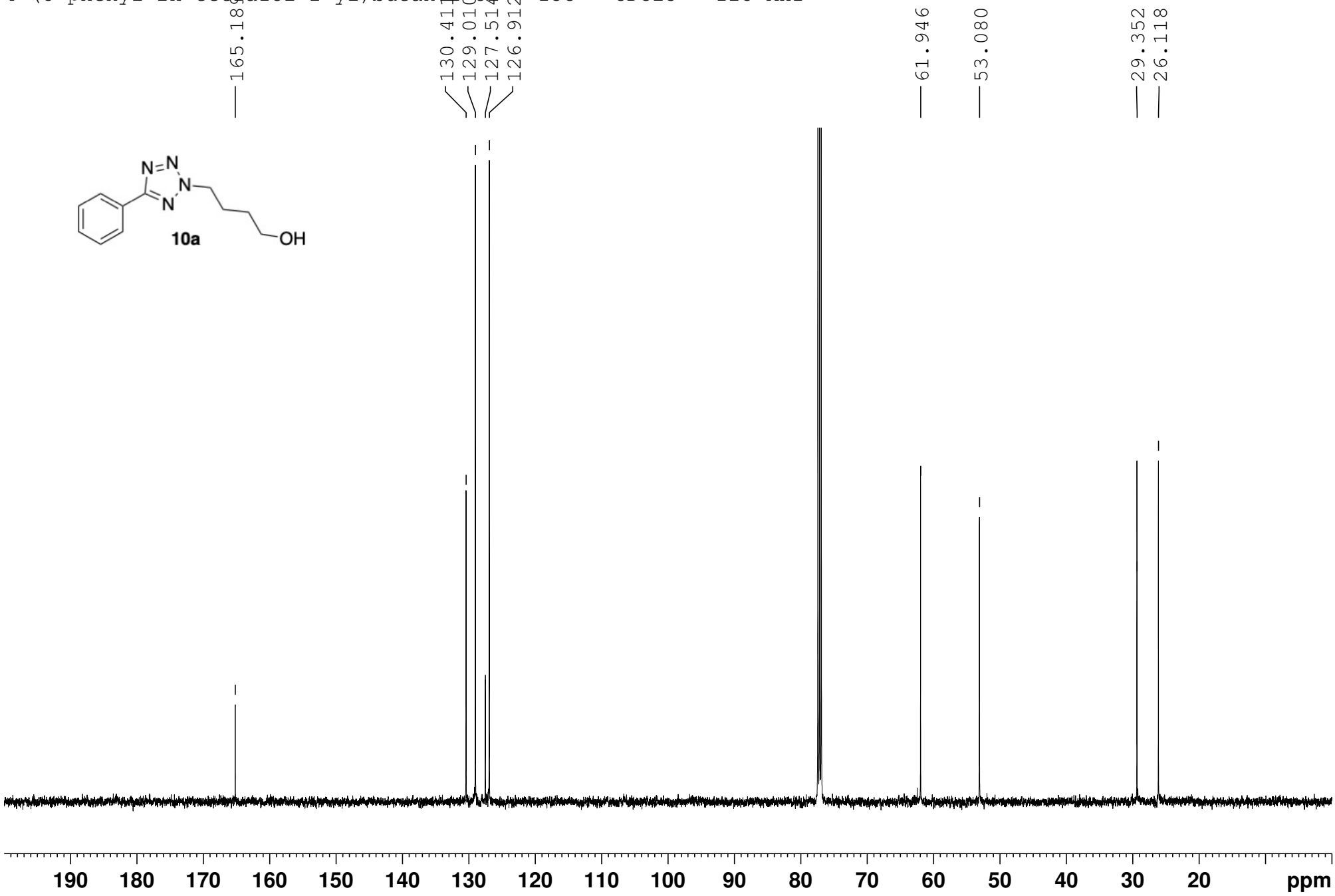
3-(5-phenyl-1H-tetrazol-1-yl)propan-1-ol - 13C - CDCl3 - 125 MHz



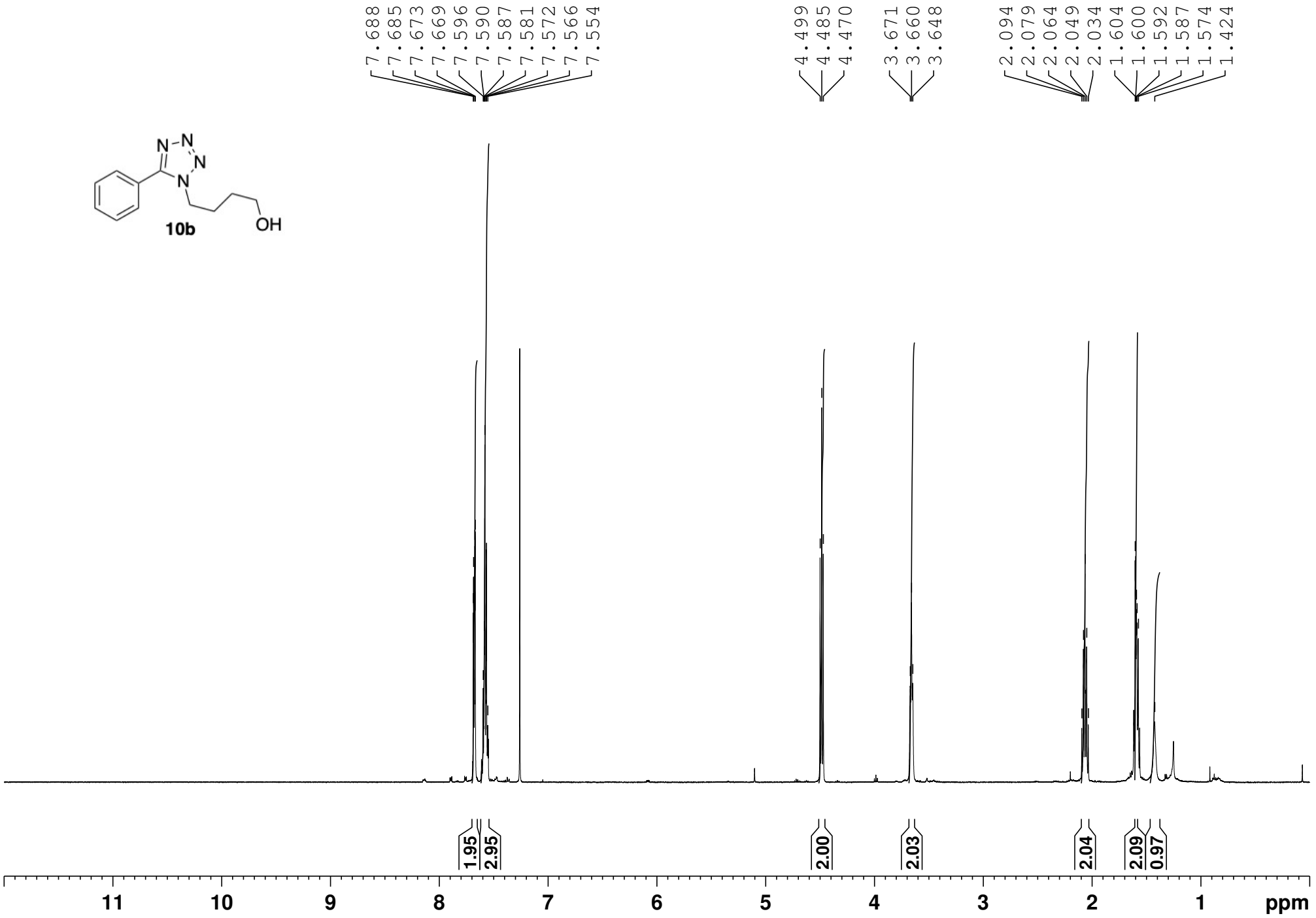
4-(5-phenyl-2H-tetrazol-2-yl)butan-1-ol - 1H - CDCl3 - 500 MHz



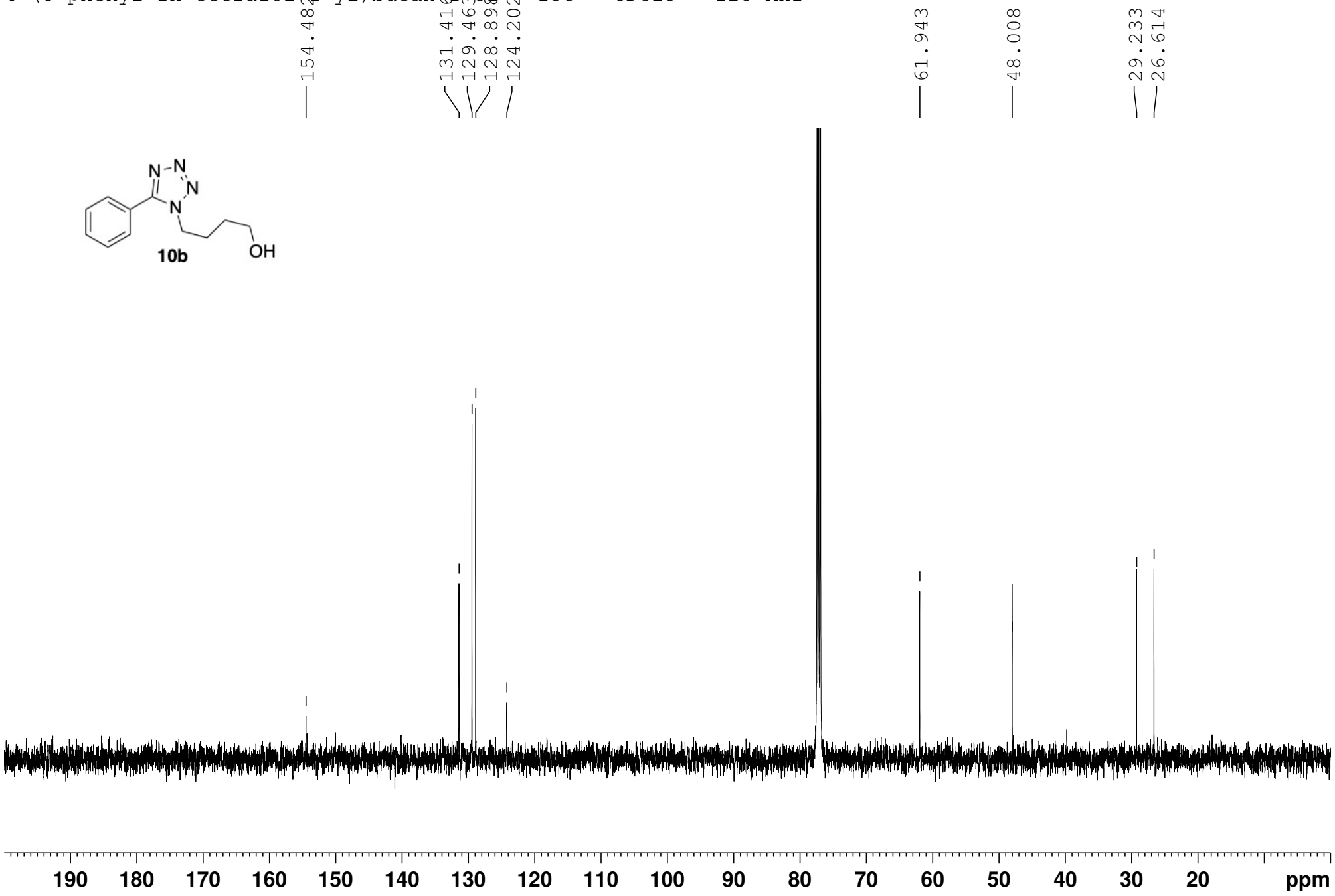
4-(5-phenyl-2H-tetrazol-2-yl)butan-1-ol 13C - CDCl3 - 125 MHz



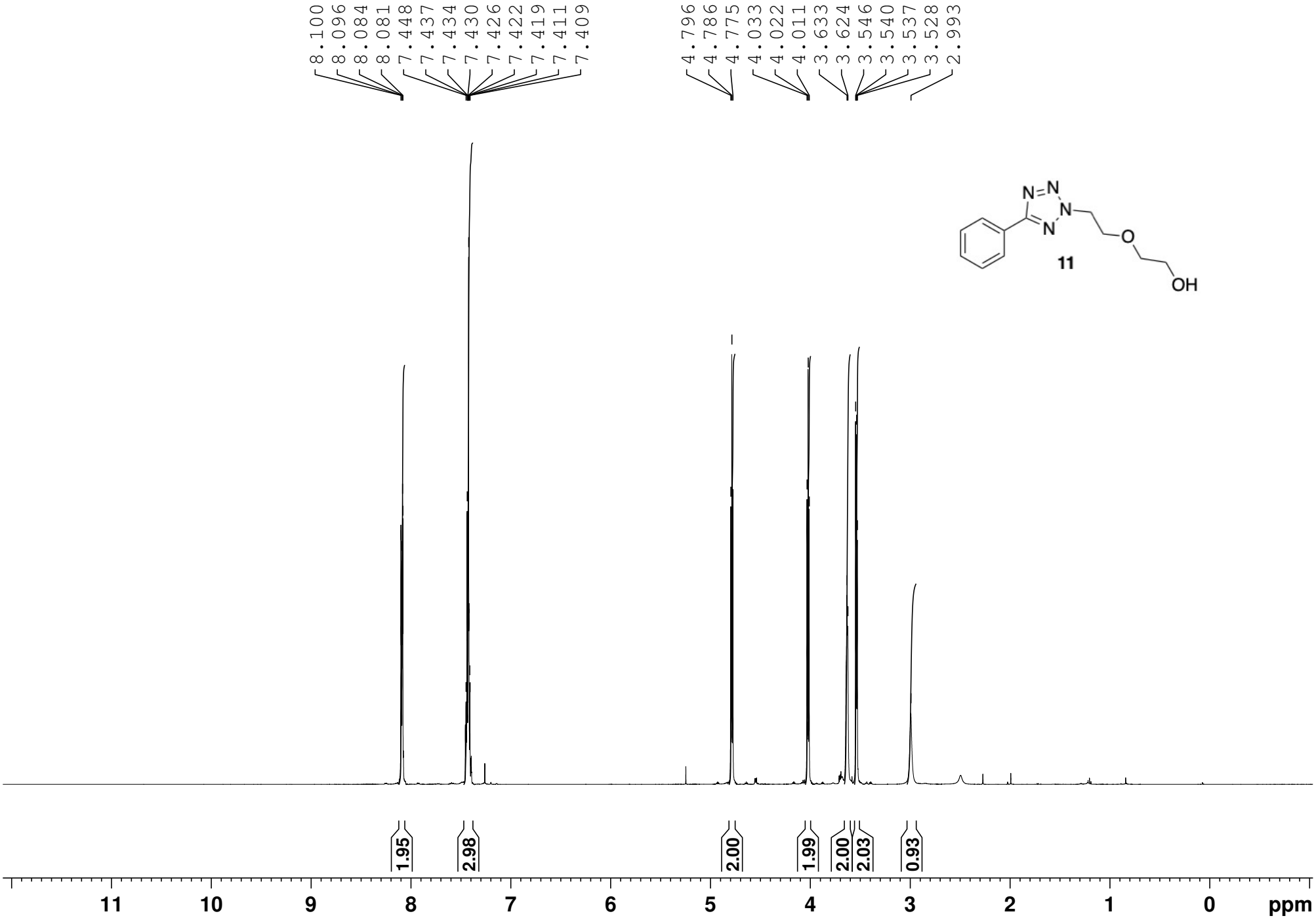
4-(5-phenyl-1H-tetrazol-1-yl)butan-1-ol - 1H - CDCl3 - 500 MHz



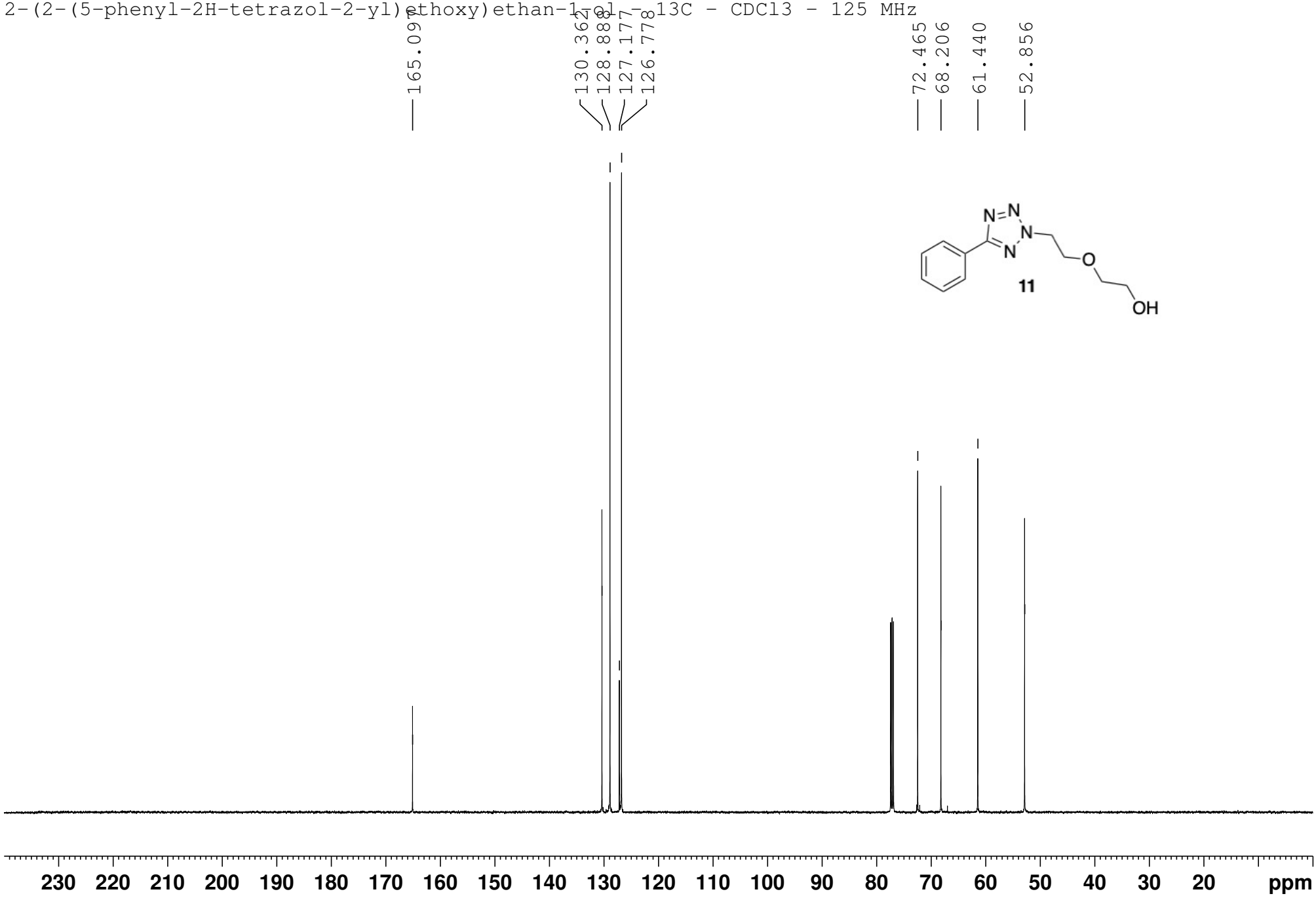
4-(5-phenyl-1H-tetrazol-1-yl)butan-1-ol - 13C - CDCl3 - 125 MHz



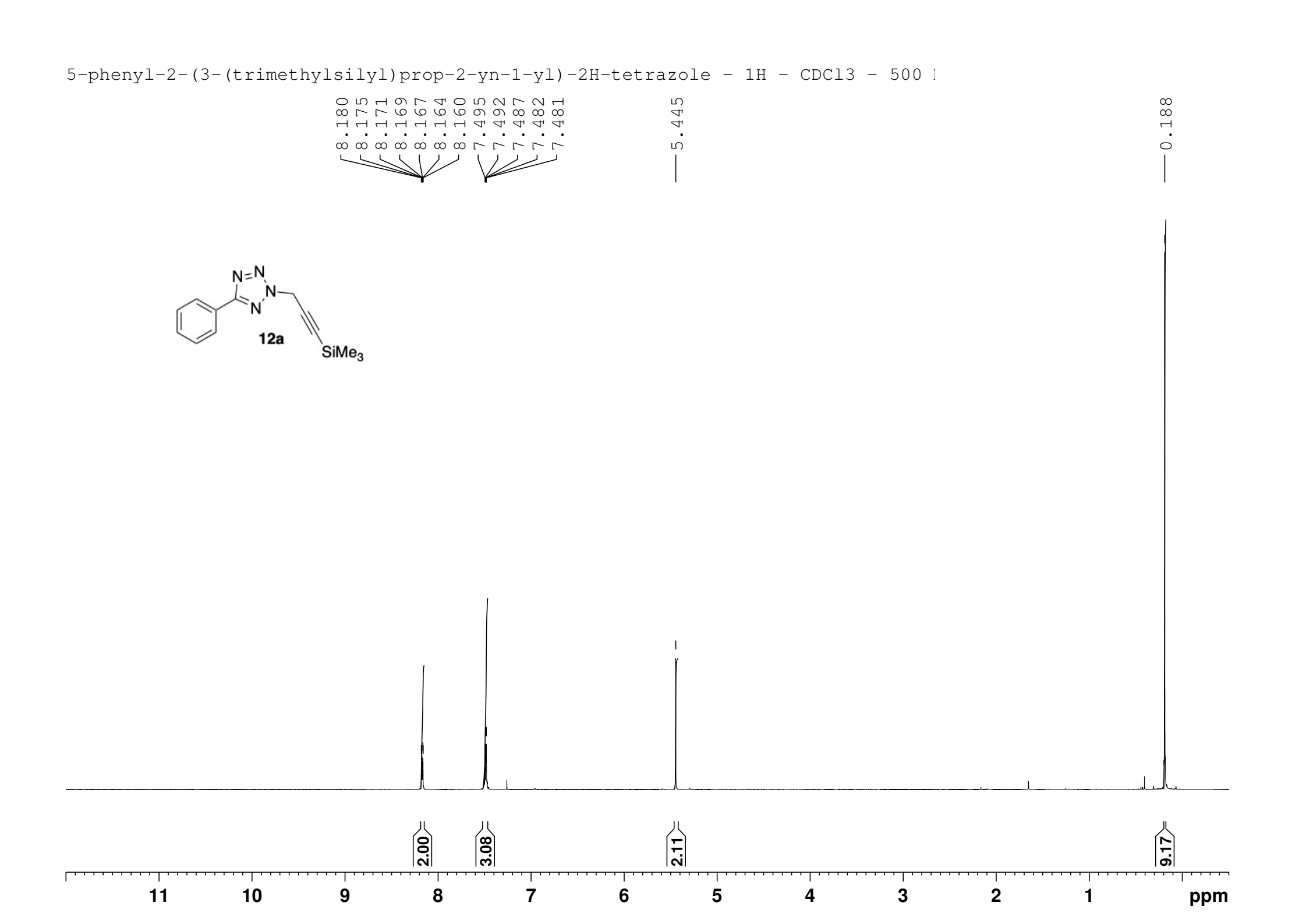
2-(2-(5-phenyl-2H-tetrazol-2-yl)ethoxy)ethan-1-ol - 1H - CDCl3 - 500 MHz



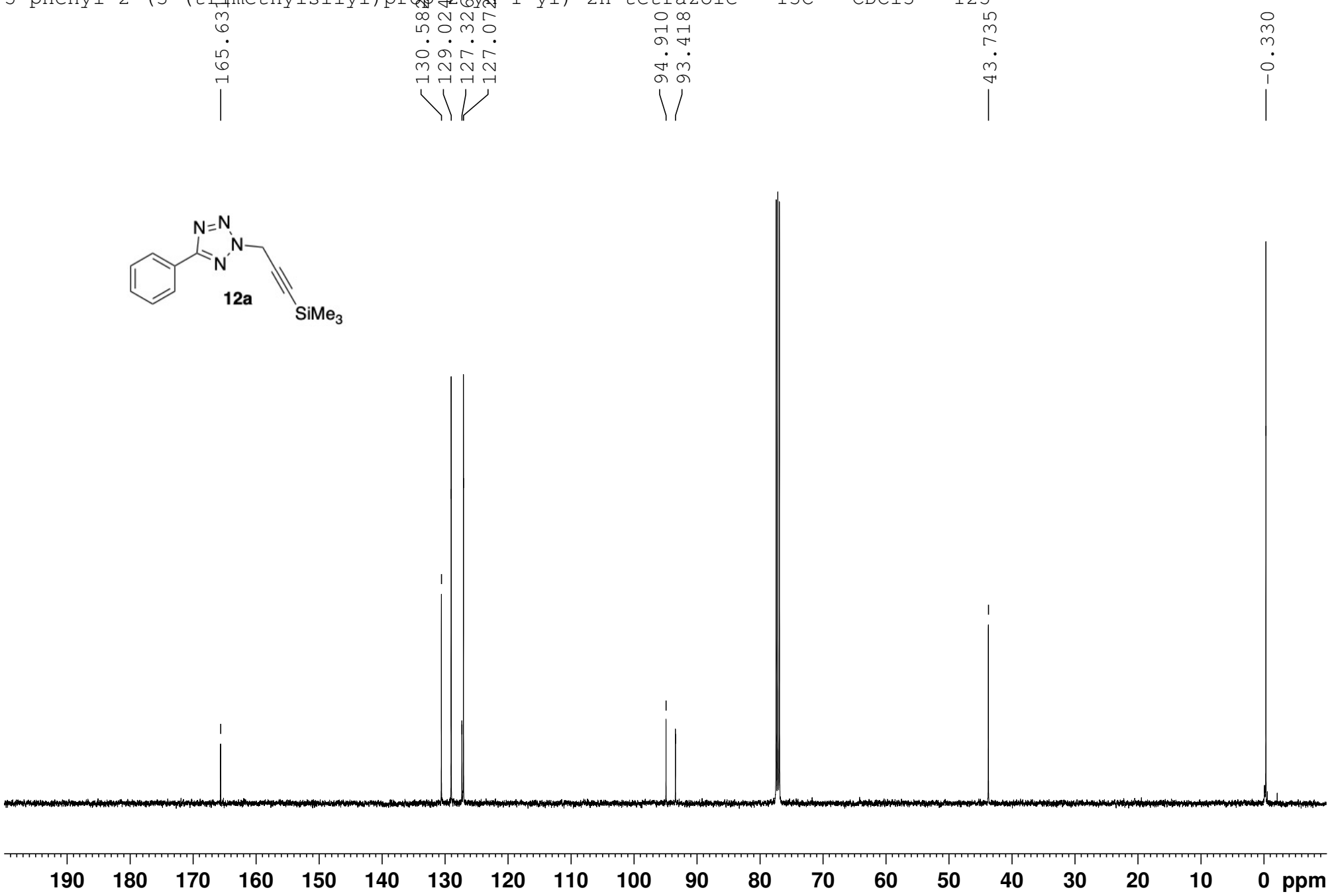
2-(2-(5-phenyl-2H-tetrazol-2-yl)ethoxy)ethan-1-ol - 13C - CDCl3 - 125 MHz



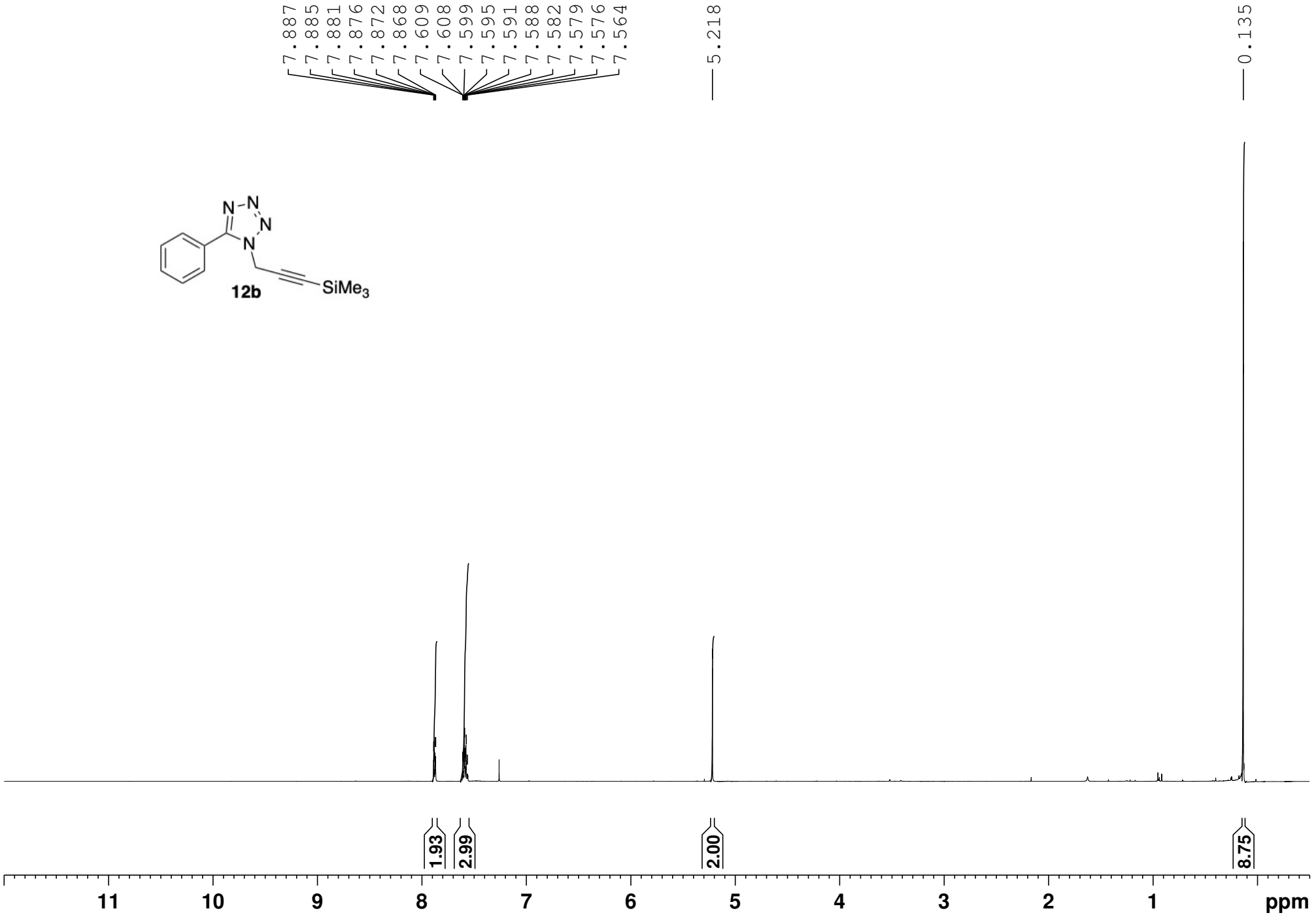
5-phenyl-2-(3-(trimethylsilyl)prop-2-yn-1-yl)-2H-tetrazole - 1H - CDCl3 - 500 I



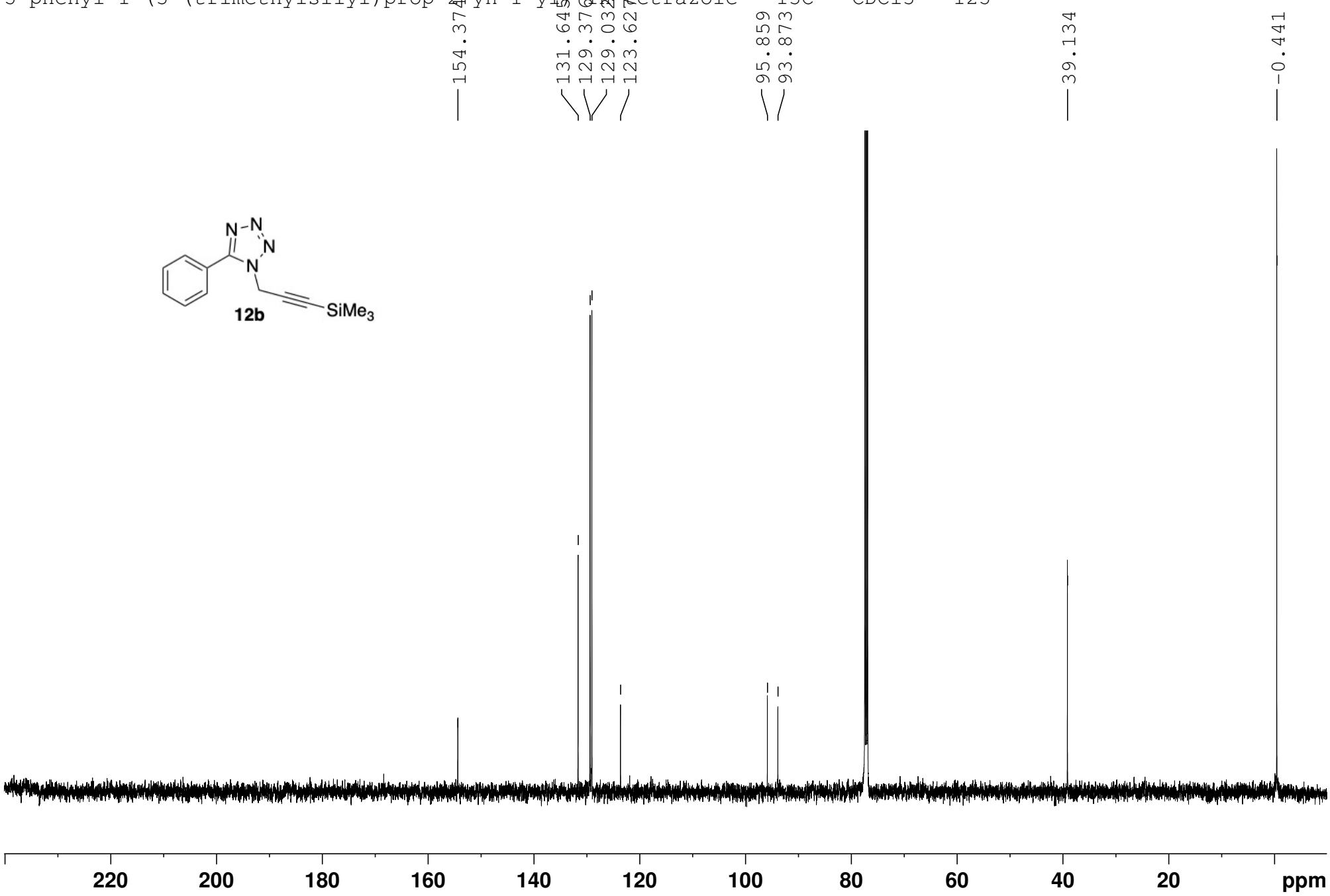
5-phenyl-2-(3-(trimethylsilyl)prop-2-yn-1-yl)-2H-tetrazole - 13C - CDCl3 - 125



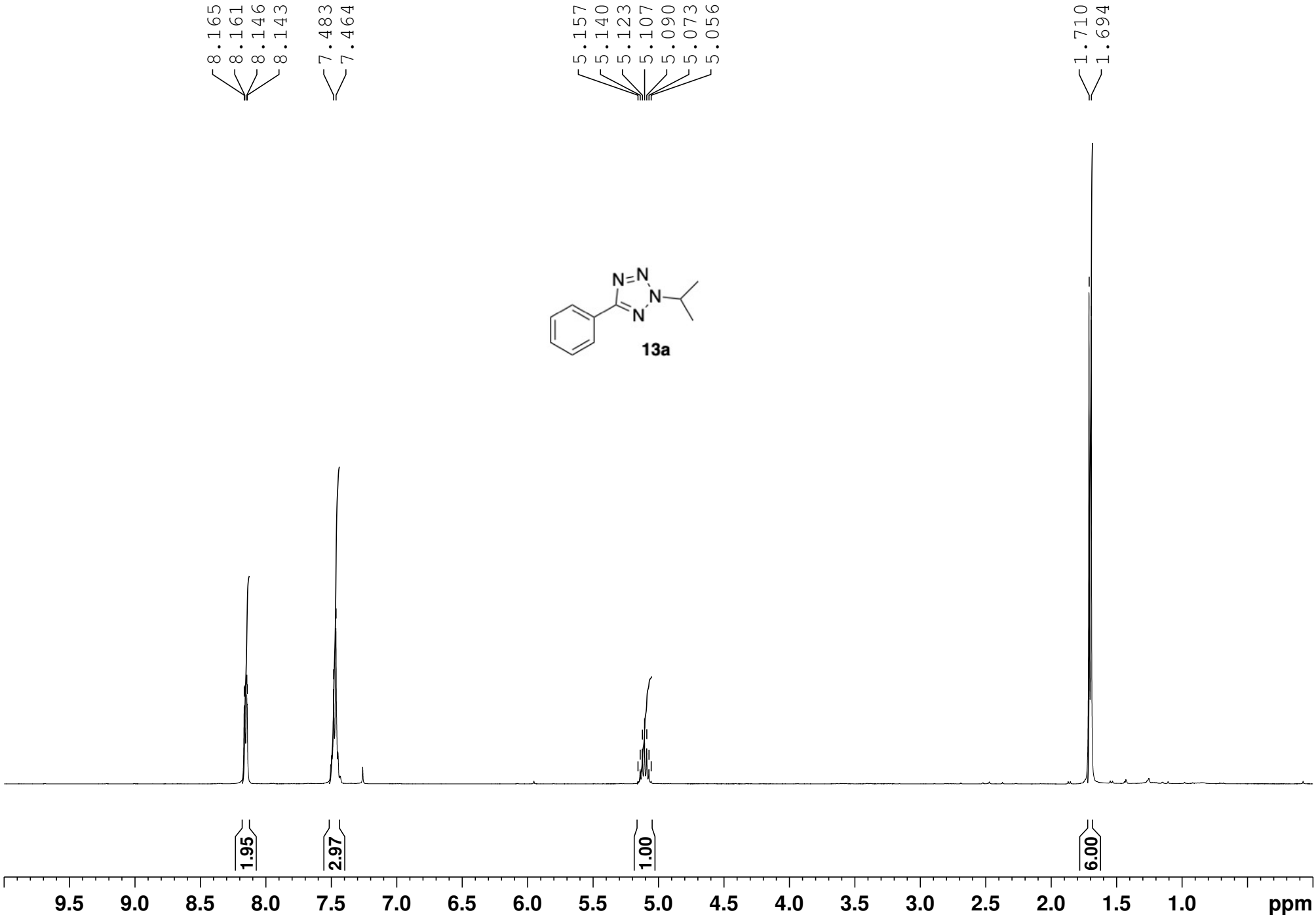
5-phenyl-1-(3-(trimethylsilyl)prop-2-yn-1-yl)-1H-tetrazole - 1H - CDCl3 - 500 I

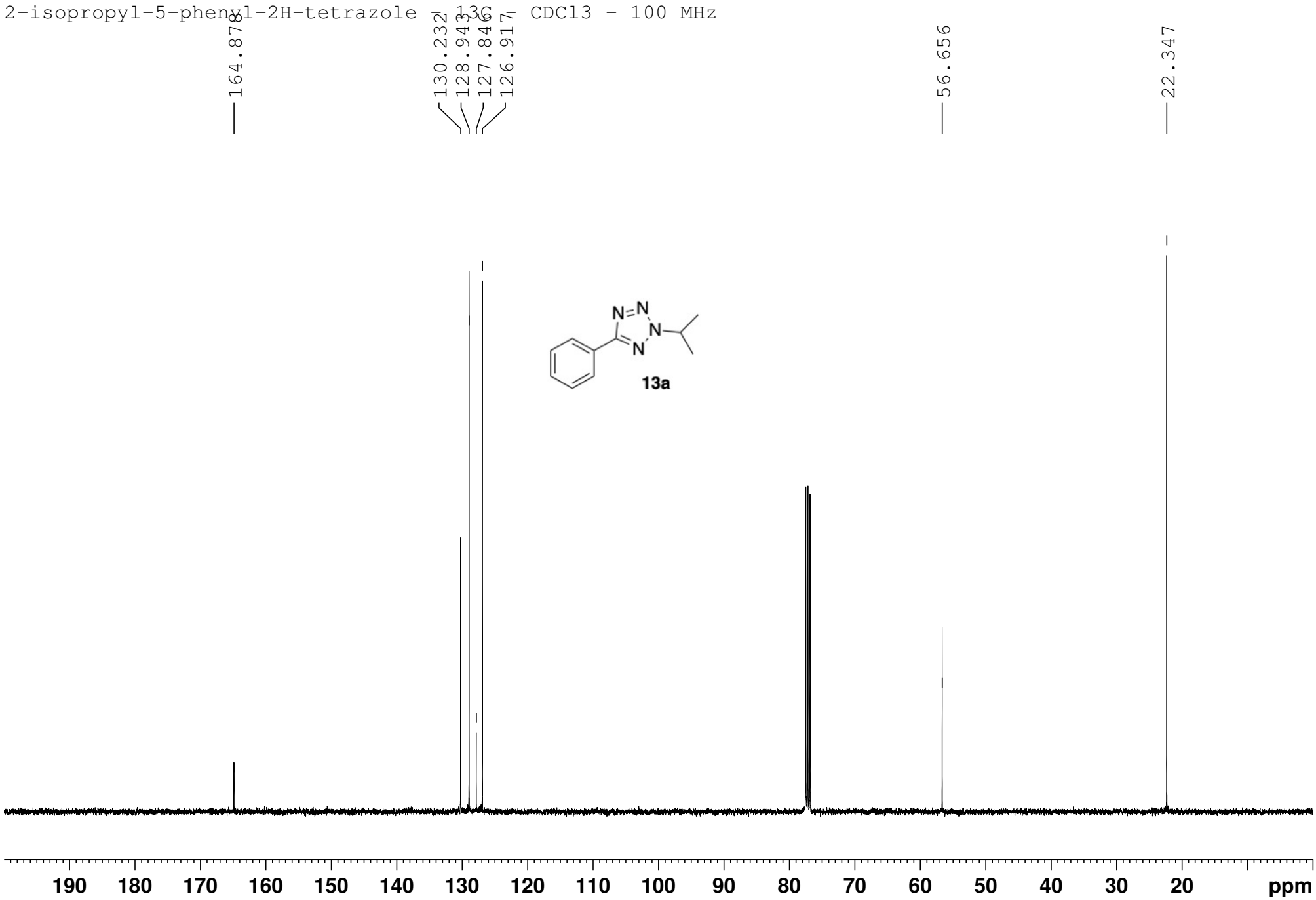


5-phenyl-1-(3-(trimethylsilyl)prop-2-yn-1-yl)-1H-tetrazole - 13C - CDCl3 - 125

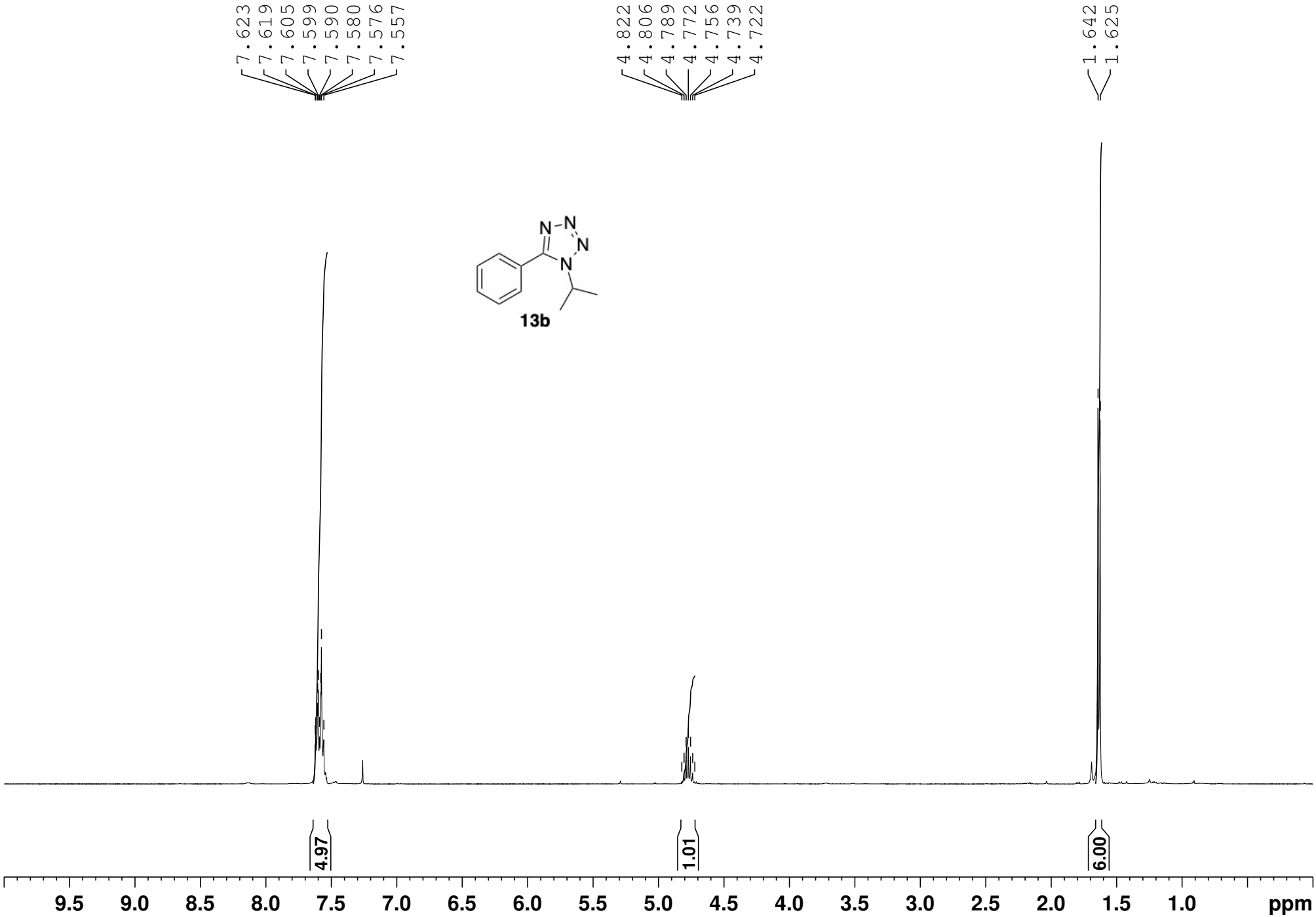


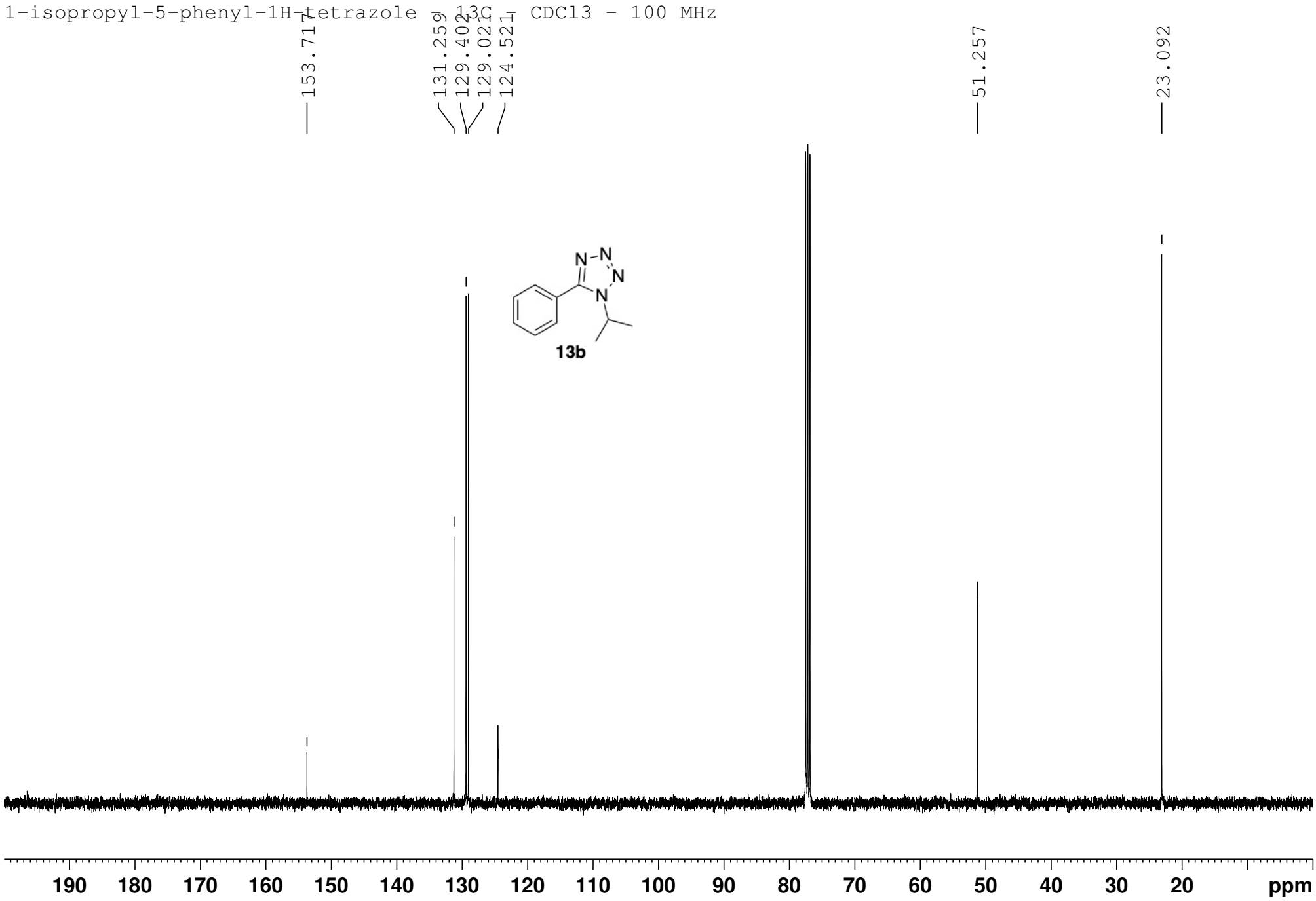
2-isopropyl-5-phenyl-2H-tetrazole - 1H - CDCl3 - 400 MHz



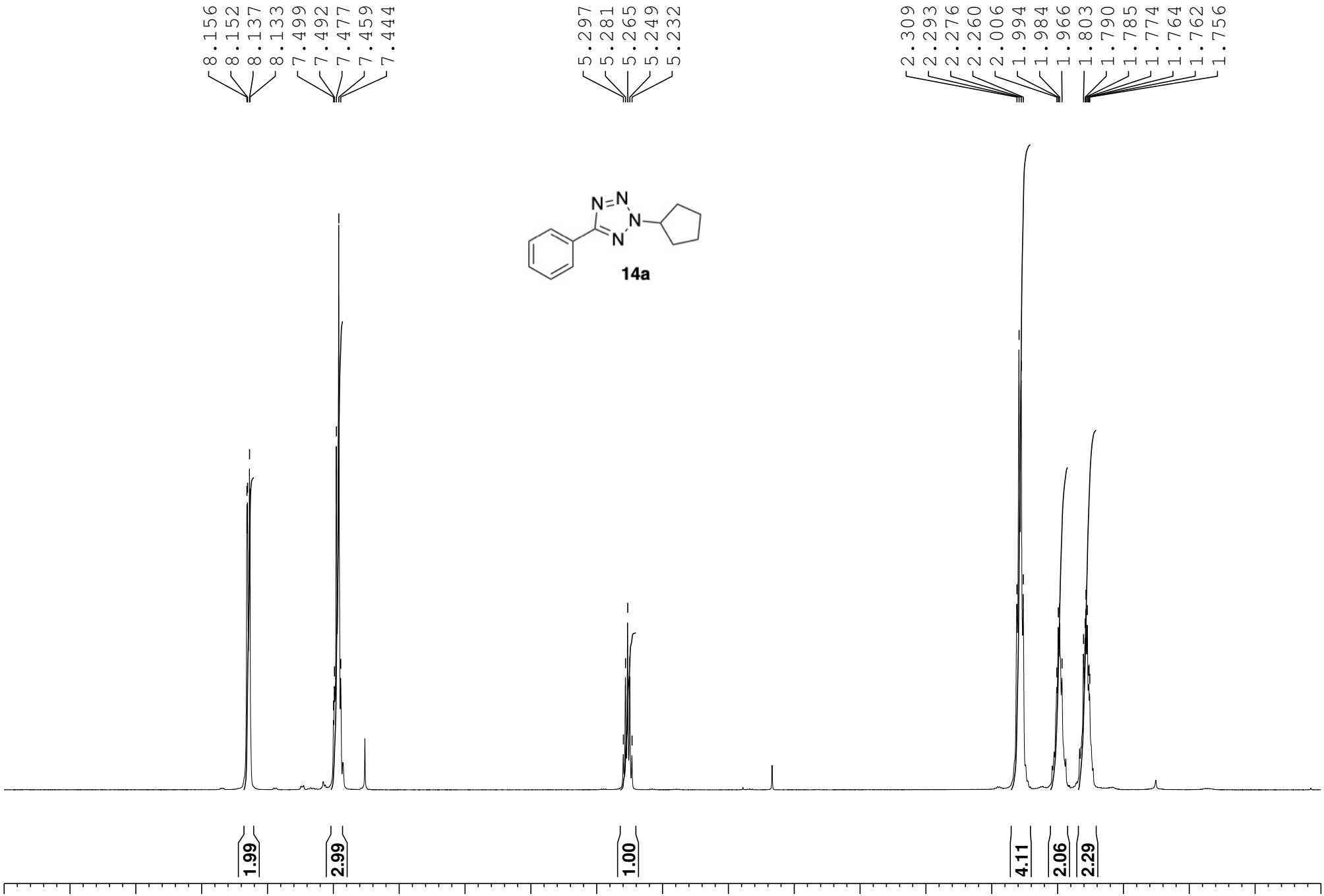

2-isopropyl-5-phenyl-2H-tetrazole - 13C - CDCl3 - 100 MHz
164.878
130.232
128.943
127.846
126.917
56.656
22.347
13a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

1-isopropyl-5-phenyl-1H-tetrazole - 1H - CDCl3 - 400 MHz

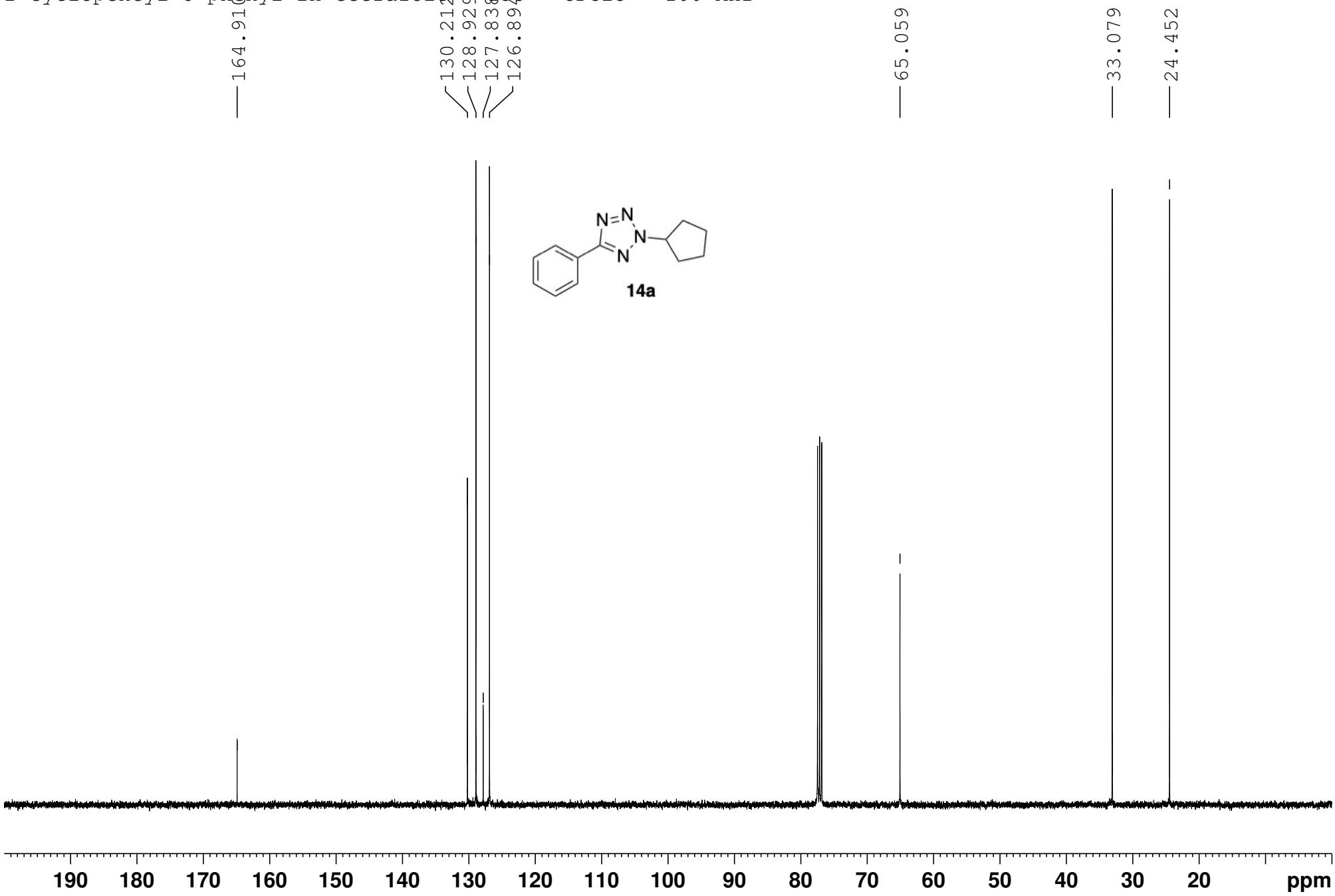



1-isopropyl-5-phenyl-1H-tetrazole - 13C - CDCl3 - 100 MHz
153.717
131.259
129.402
129.021
124.521
51.257
23.092
13b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

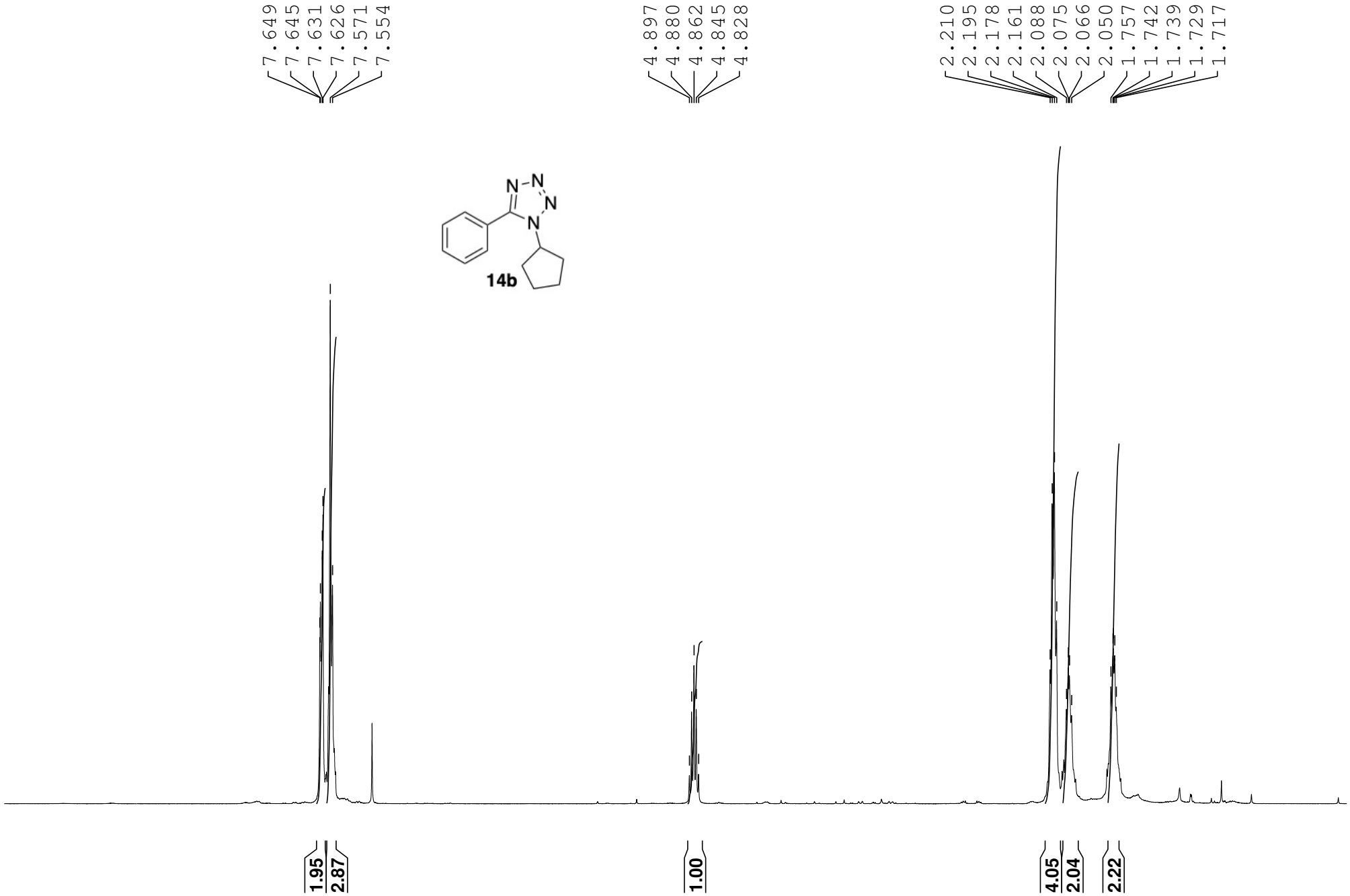
2-cyclopentyl-5-phenyl-2H-tetrazole - 1H - CDCl3 - 400 MHz



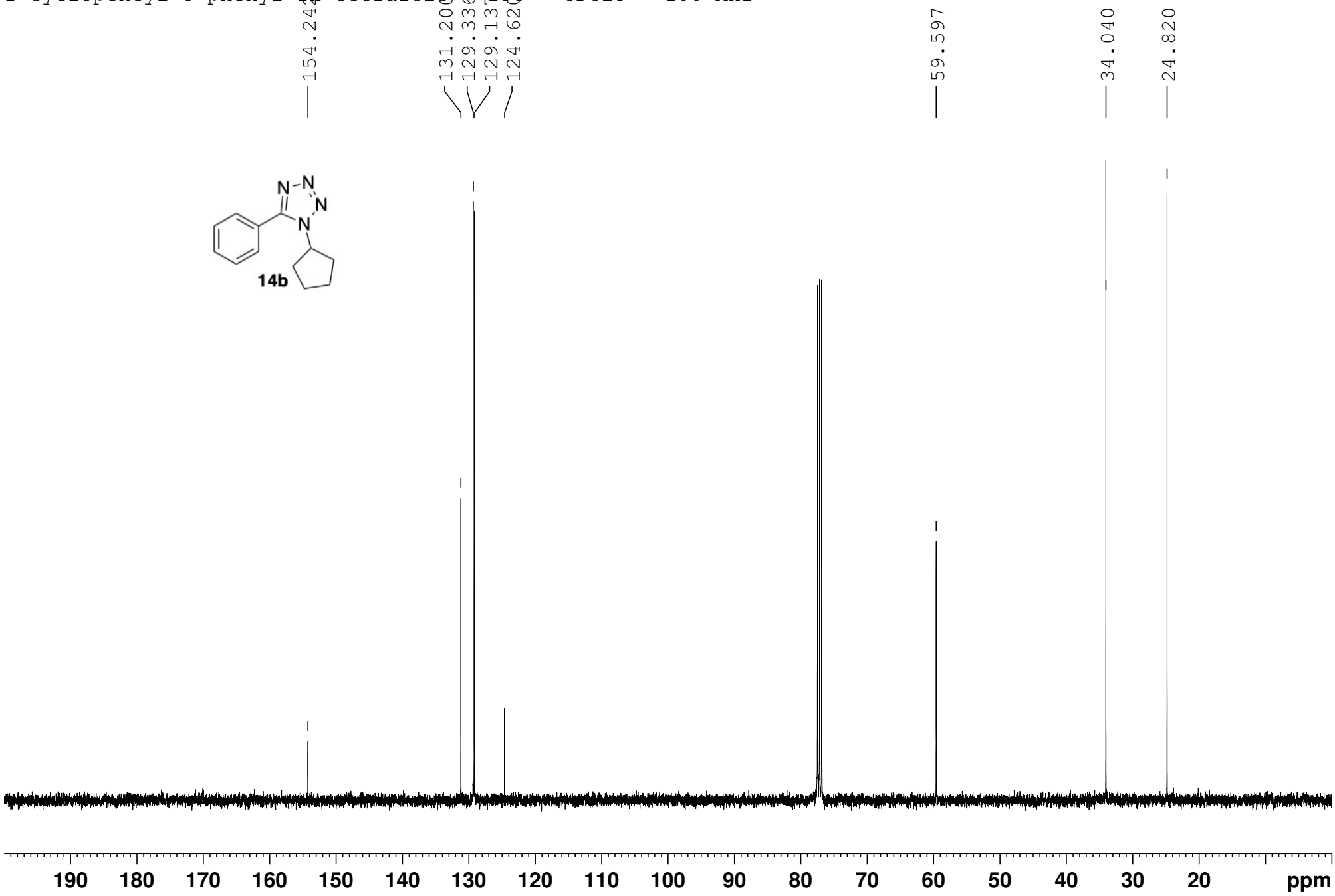
2-cyclopentyl-5-phenyl-2H-tetrazole, 13C - CDCl3 - 100 MHz



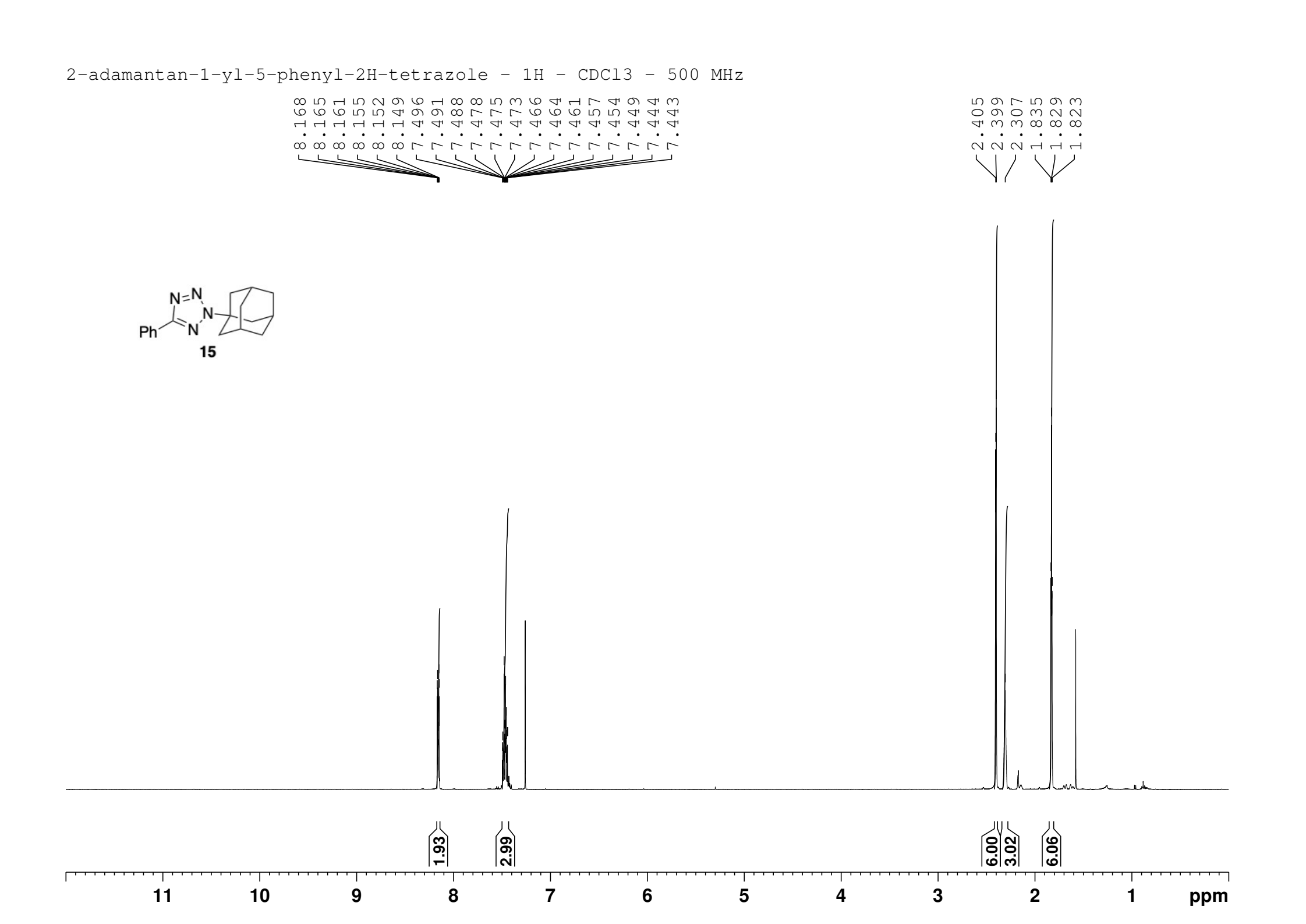
1-cyclopentyl-5-phenyl-1H-tetrazole - 1H - CDCl3 - 400 MHz

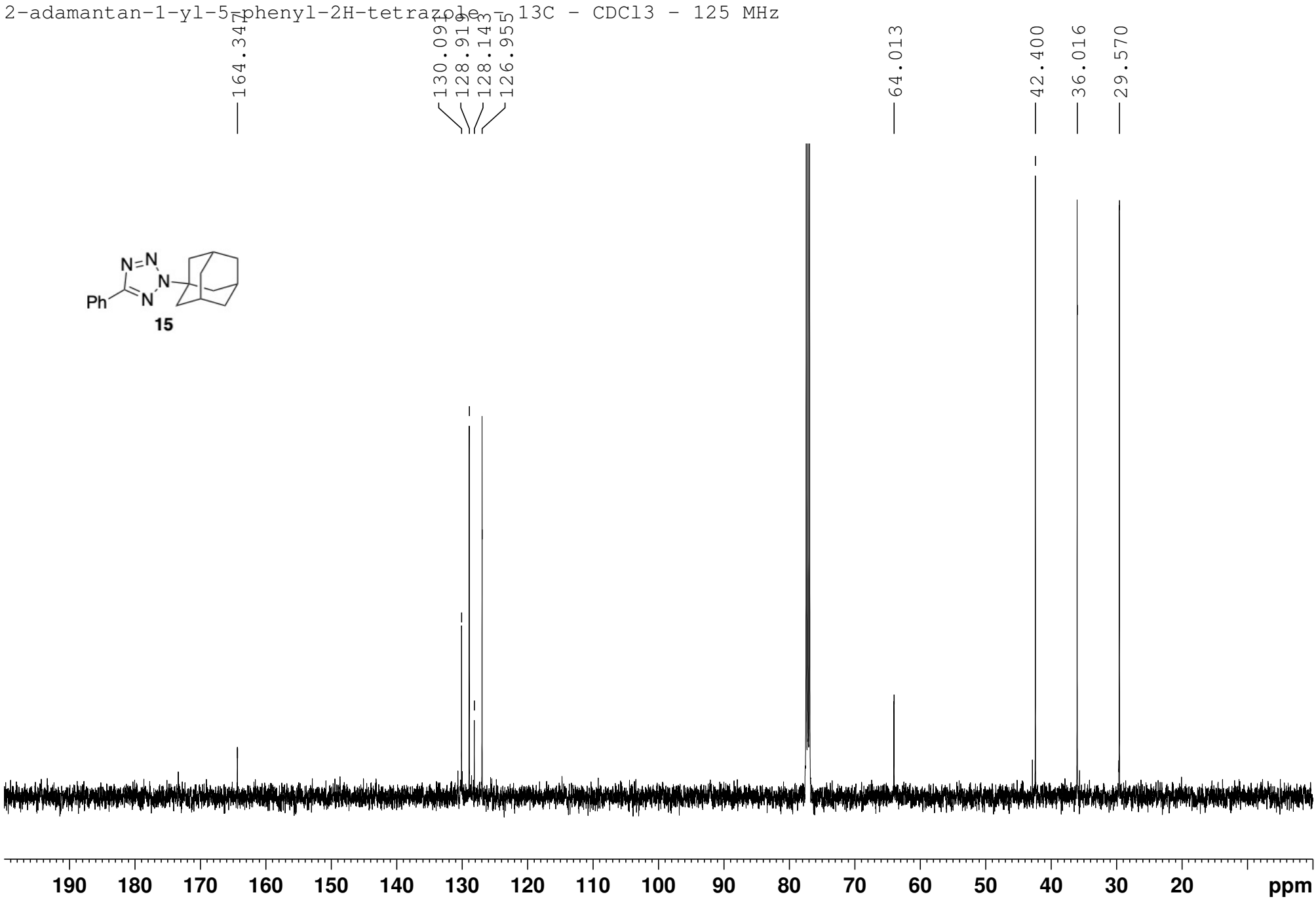


1-cyclopentyl-5-phenyl-1H-tetrazole, 13C - CDCl3 - 100 MHz



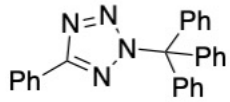
2-adamantan-1-yl-5-phenyl-2H-tetrazole - 1H - CDCl3 - 500 MHz




2-adamantan-1-yl-5-phenyl-2H-tetrazole - 13C - CDCl3 - 125 MHz
164.347
130.091
128.919
128.143
126.955
64.013
42.400
36.016
29.570
Ph
15
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

5-phenyl-2-triphenylmethyl-2H-tetrazole - 1H - CDCl3 - 400 MHz

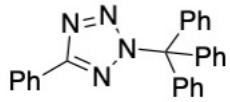
8.181
8.173
8.171
8.162
8.157
7.474
7.470
7.461
7.457
7.383
7.370
7.351
7.342
7.337
7.329
7.207
7.203
7.188
7.183



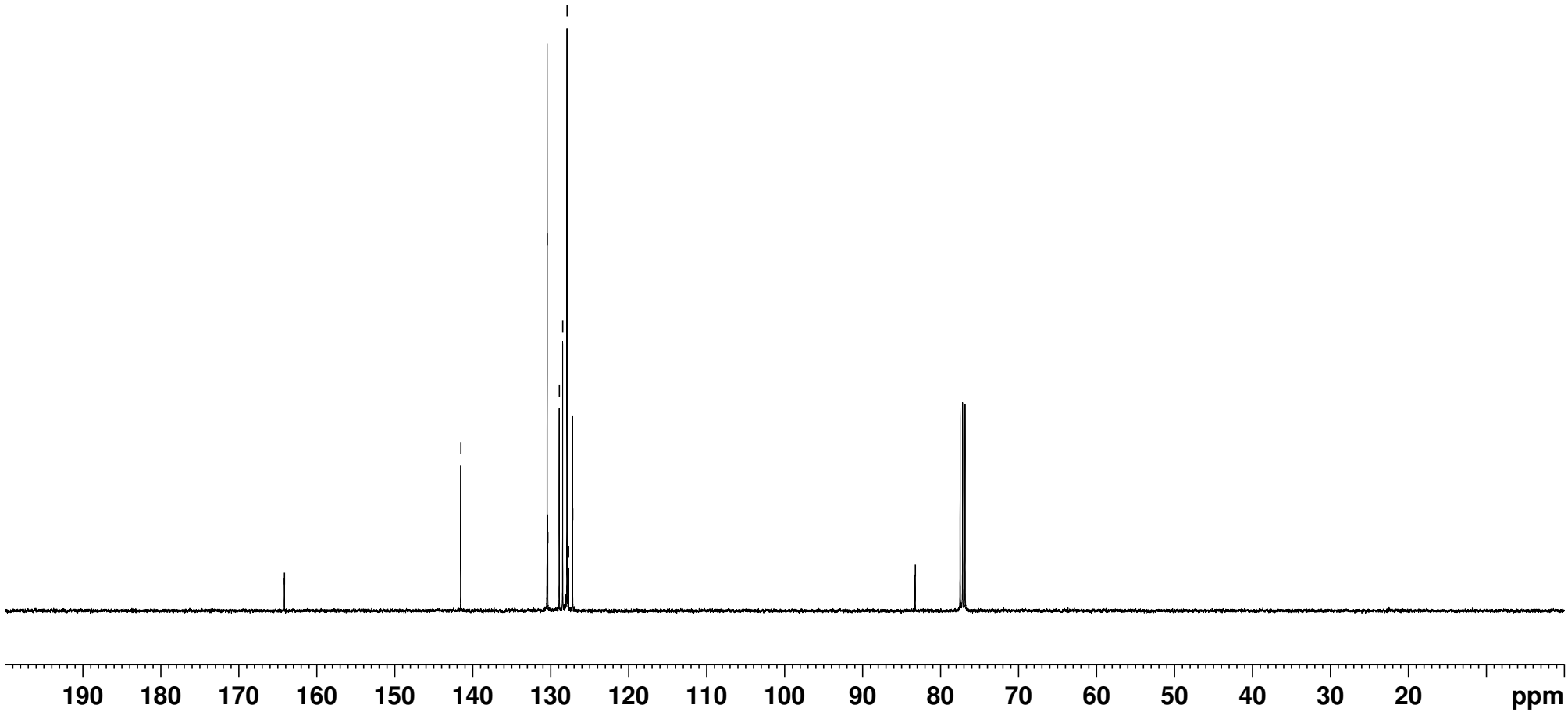
16

5-phenyl-2-triphenylmethyl-2H-tetrazole - 13C - CDCl3 - 100 MHz

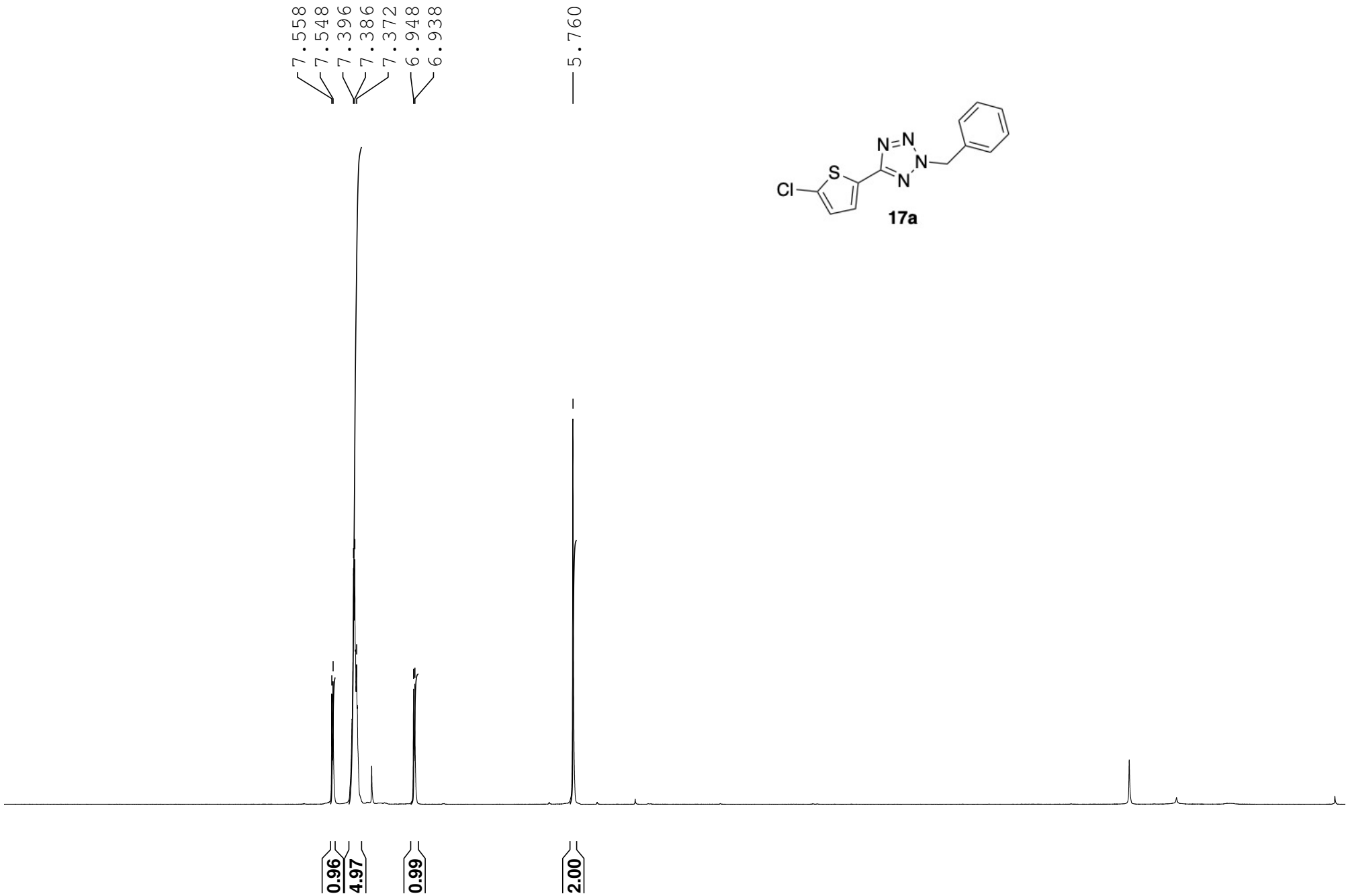
164.157
141.527
130.446
130.376
128.899
128.457
127.907
127.704
127.181
83.247



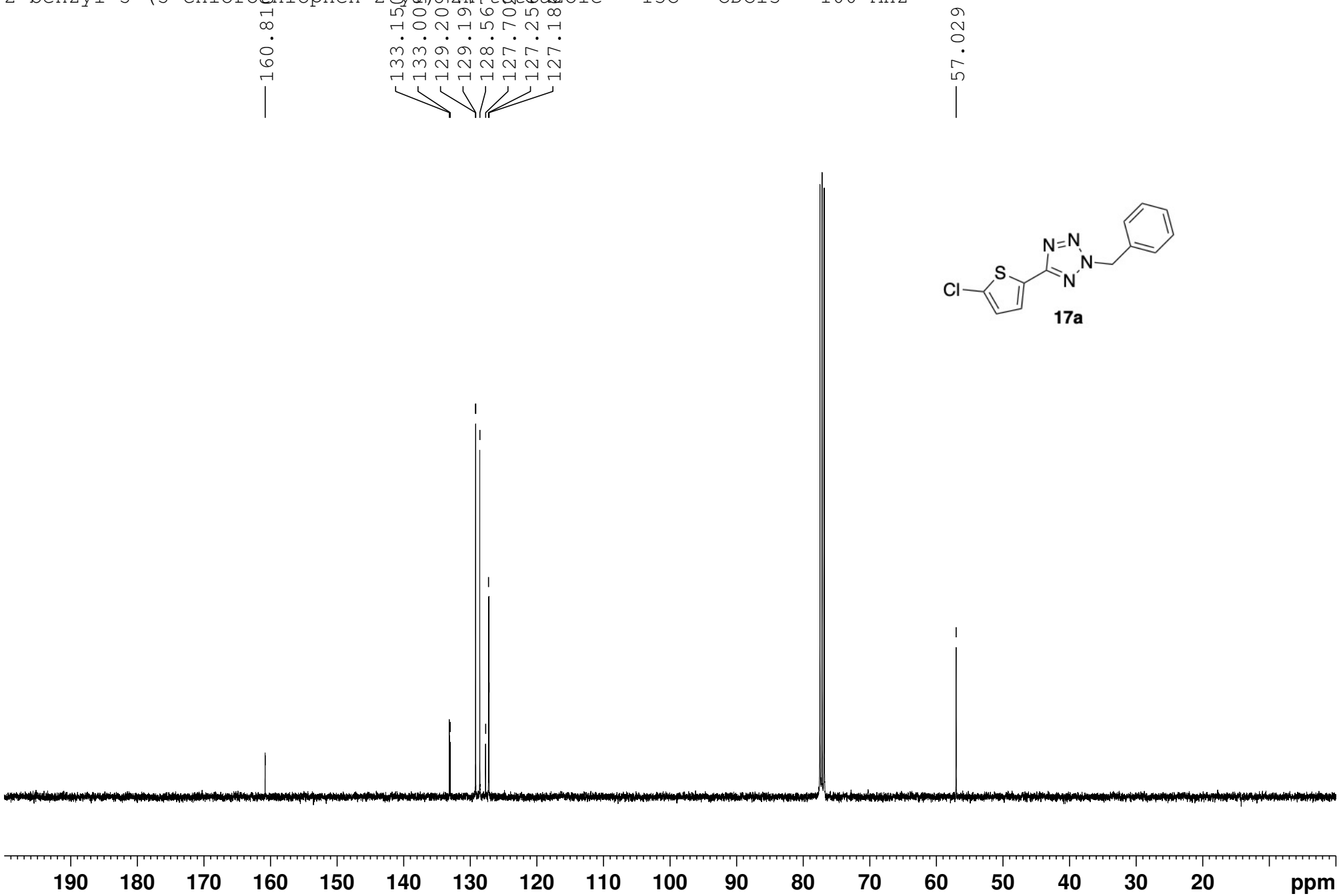
16



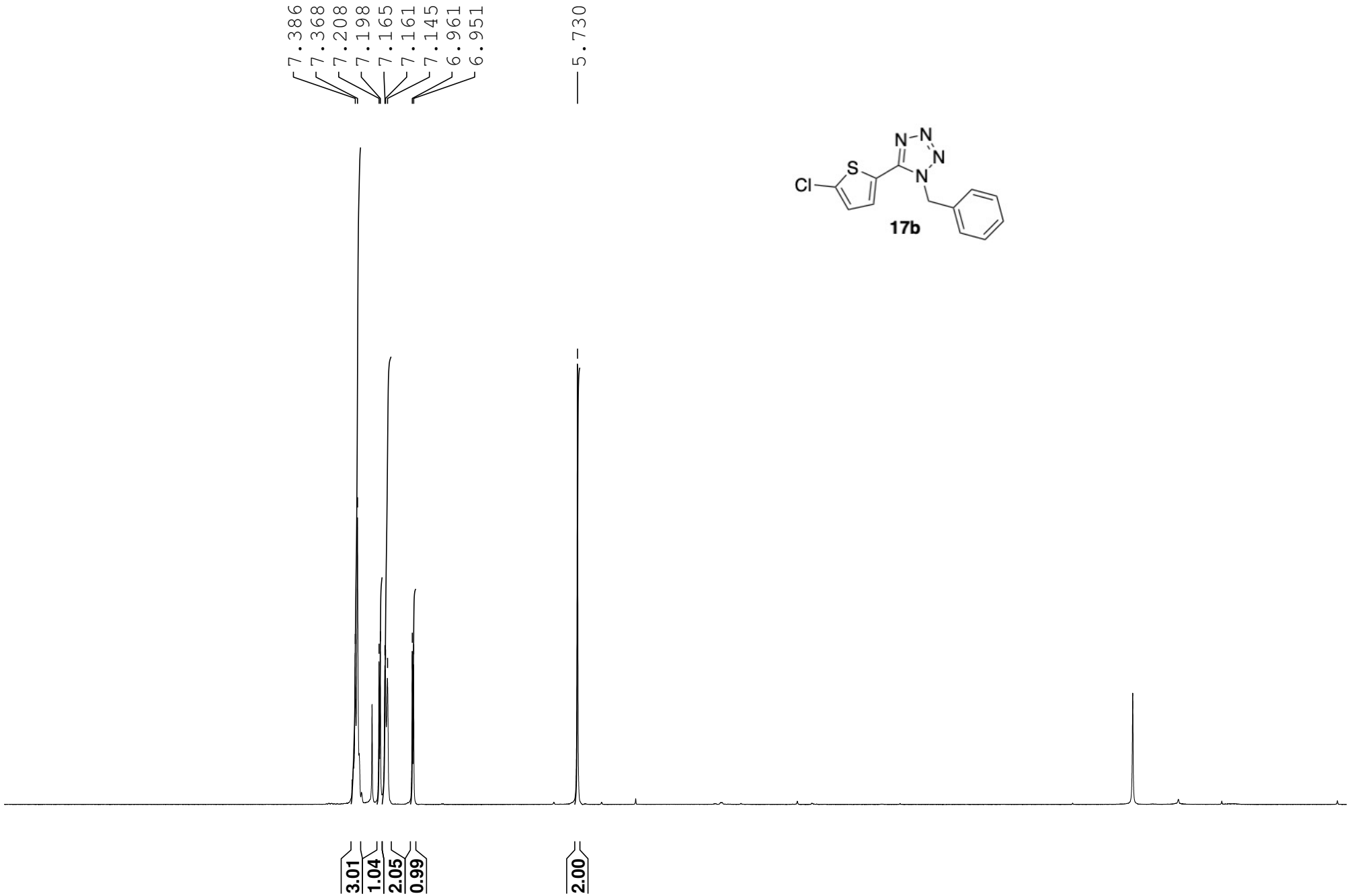
2-benzyl-5-(5-chlorothiophen-2-yl)-2H-tetrazole - 1H - CDCl3 - 400 MHz



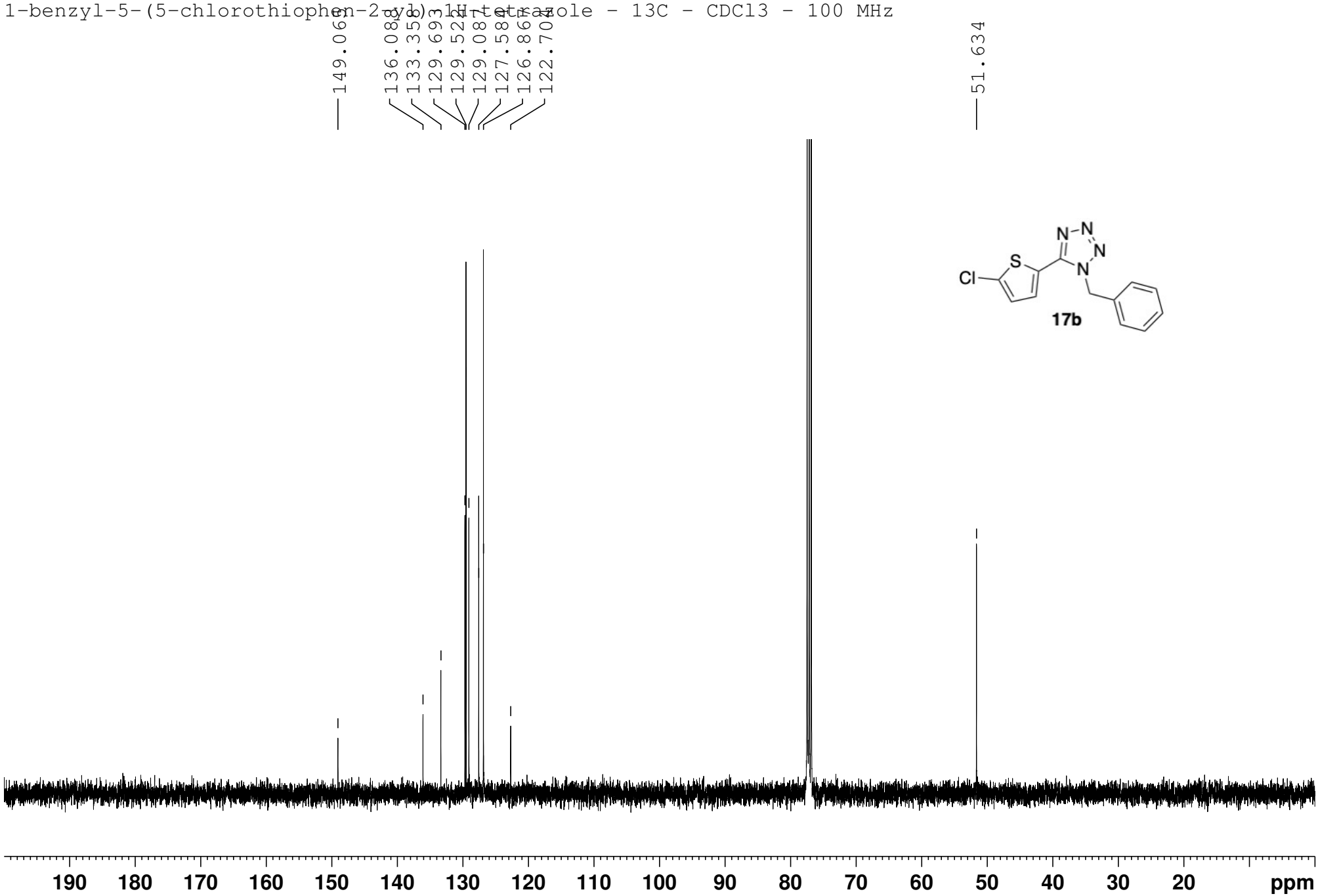
2-benzyl-5-(5-chlorothiophen-2-yl)-2H-tetrazole - 13C - CDCl3 - 100 MHz



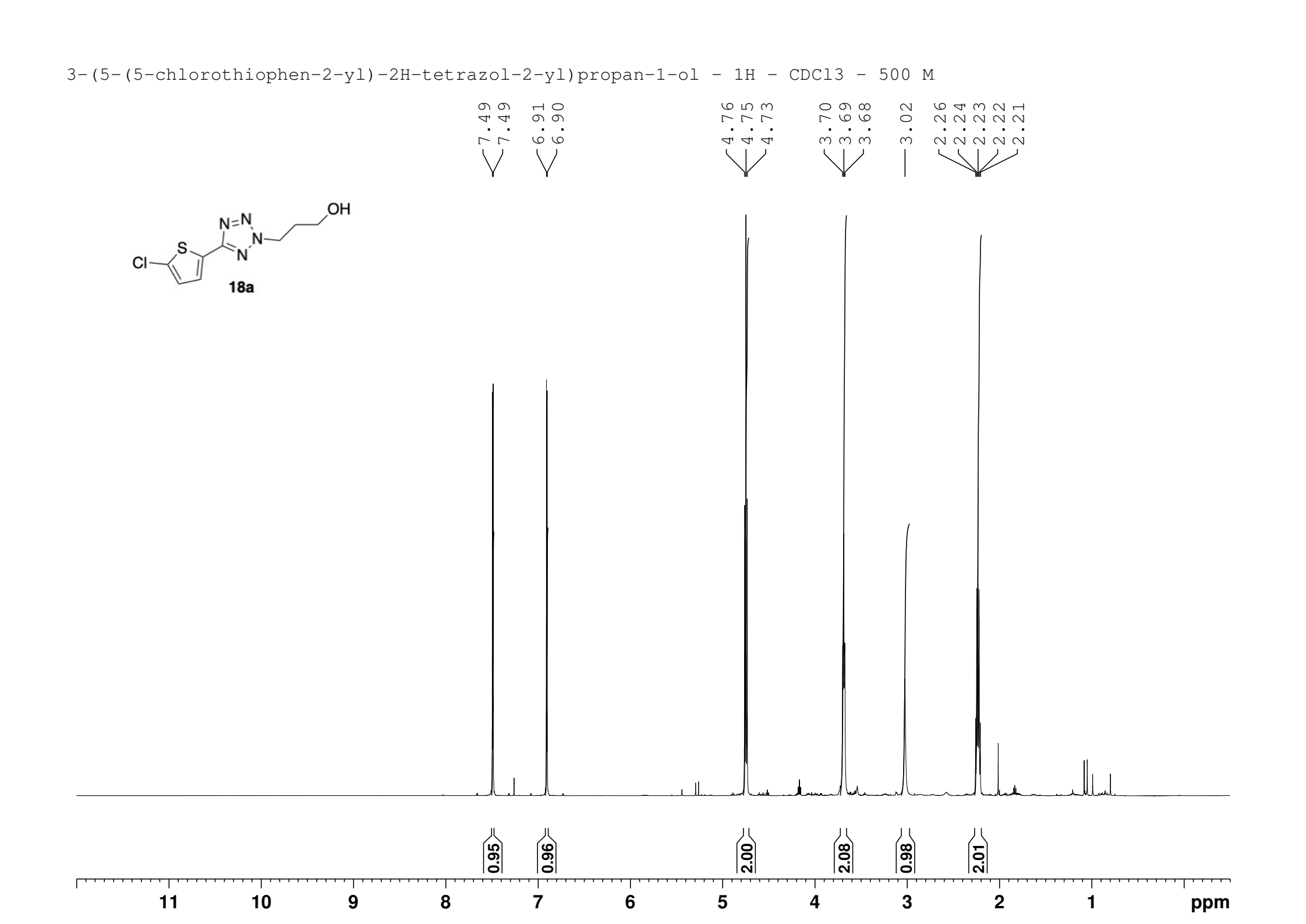
1-benzyl-5-(5-chlorothiophen-2-yl)-1H-tetrazole - 1H - CDCl3 - 400 MHz



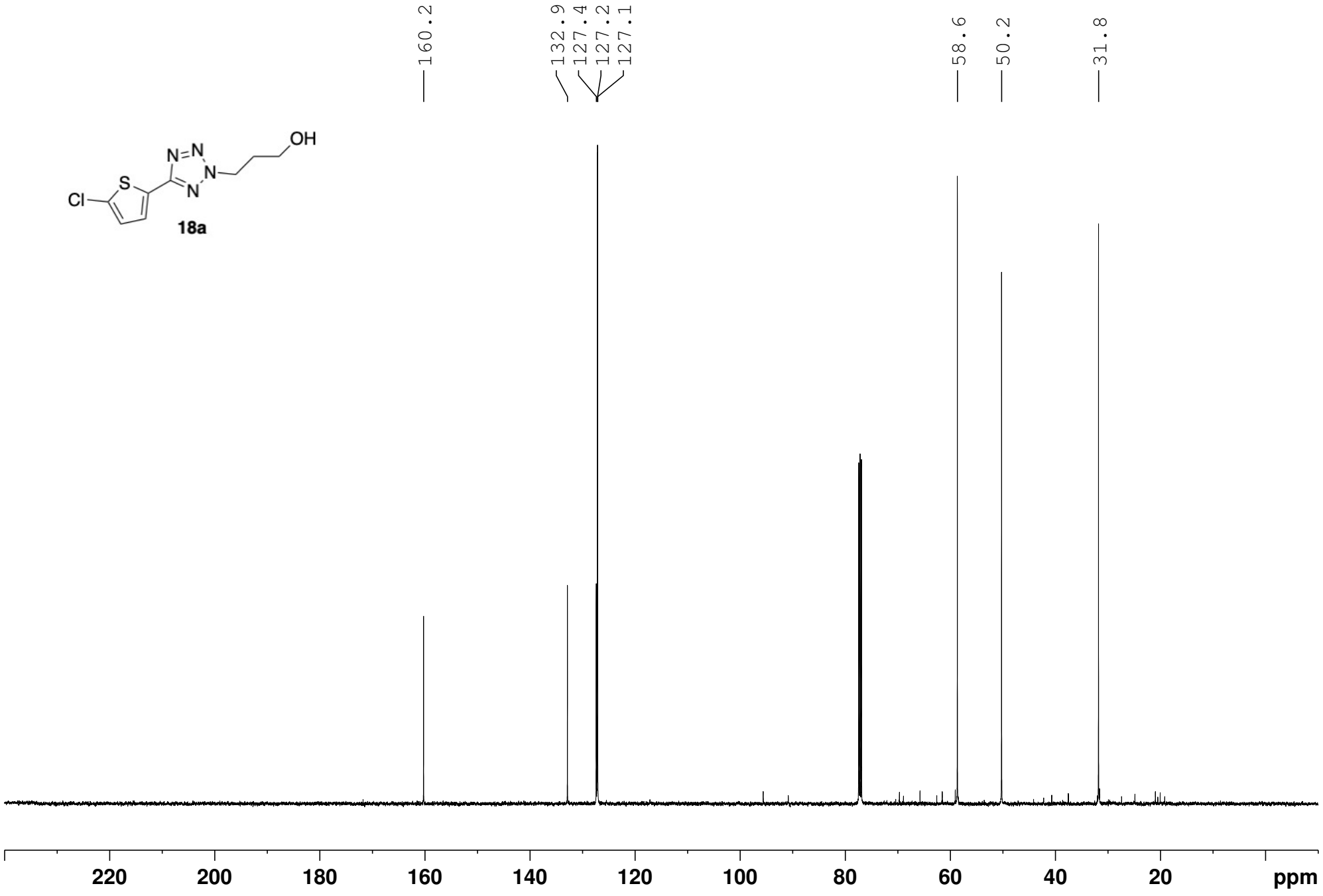
1-benzyl-5-(5-chlorothiophen-2-yl)-1H-tetrazole - 13C - CDCl3 - 100 MHz



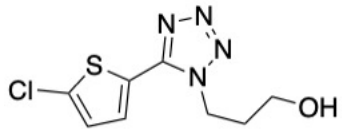
3-(5-(5-chlorothiophen-2-yl)-2H-tetrazol-2-yl)propan-1-ol - 1H - CDCl3 - 500 M



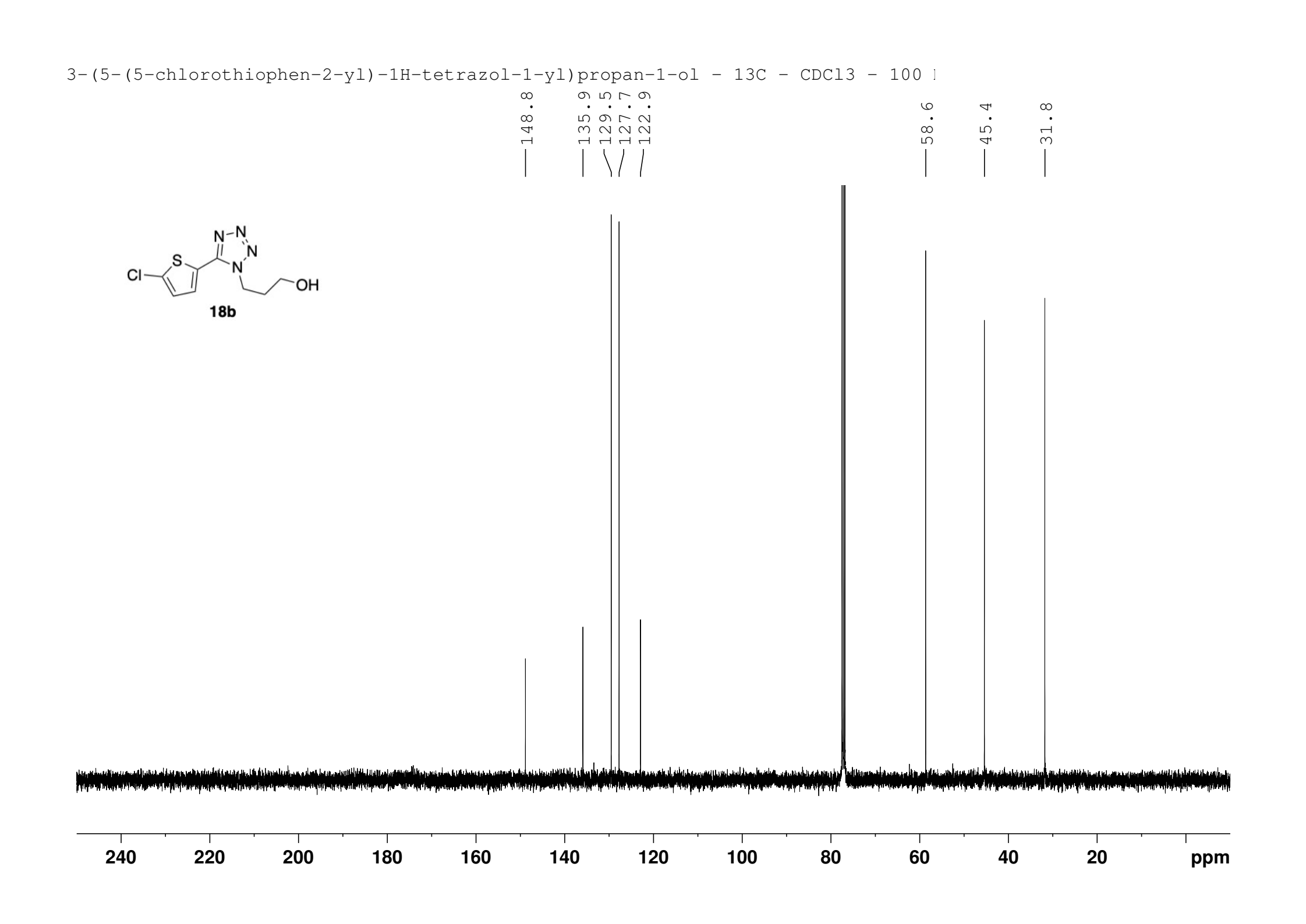
3-(5-(5-chlorothiophen-2-yl)-2H-tetrazol-2-yl)propan-1-ol - 13C - CDCl3 - 125 I



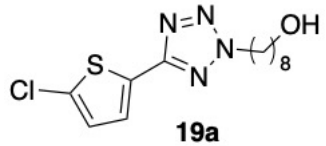
3-(5-(5-chlorothiophen-2-yl)-1H-tetrazol-1-yl)propan-1-ol - 1H - CDCl3 - 400 M



18b

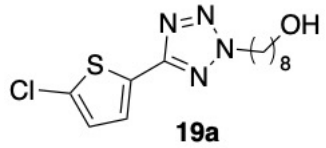

3-(5-(5-chlorothiophen-2-yl)-1H-tetrazol-1-yl)propan-1-ol - 13C - CDCl3 - 100
148.8
135.9
129.5
127.7
122.9
58.6
45.4
31.8
Cl
S
N
N
N
N
OH
18b
240
220
200
180
160
140
120
100
80
60
40
20
ppm

8-(5-(5-chlorothiophen-2-yl)-2H-tetrazol-2-yl)octan-1-ol - 1H - CDCl3 - 500 MH



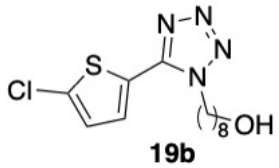
19a

8-(5-(5-chlorothiophen-2-yl)-2H-tetrazol-2-yl)octan-1-ol - 13C - CDCl3 - 125 M



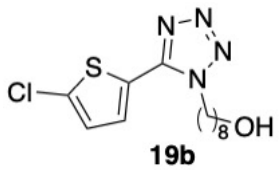
19a

8-(5-(5-chlorothiophen-2-yl)-1H-tetrazol-1-yl)octan-1-ol - 1H - CDCl3 - 500 MH



19b

8-(5-(5-chlorothiophen-2-yl)-1H-tetrazol-1-yl)octan-1-ol - 13C - CDCl3 - 125 M

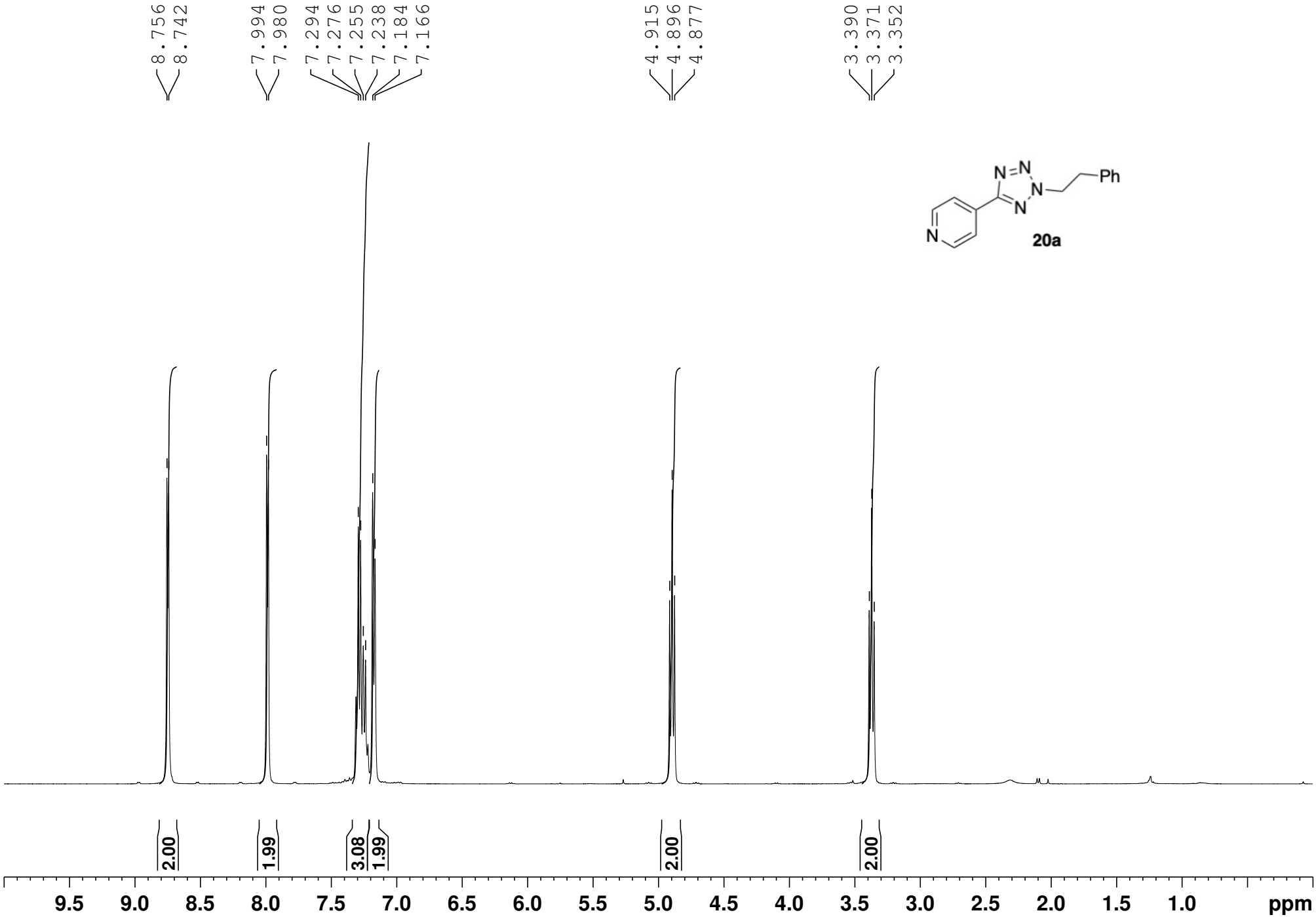


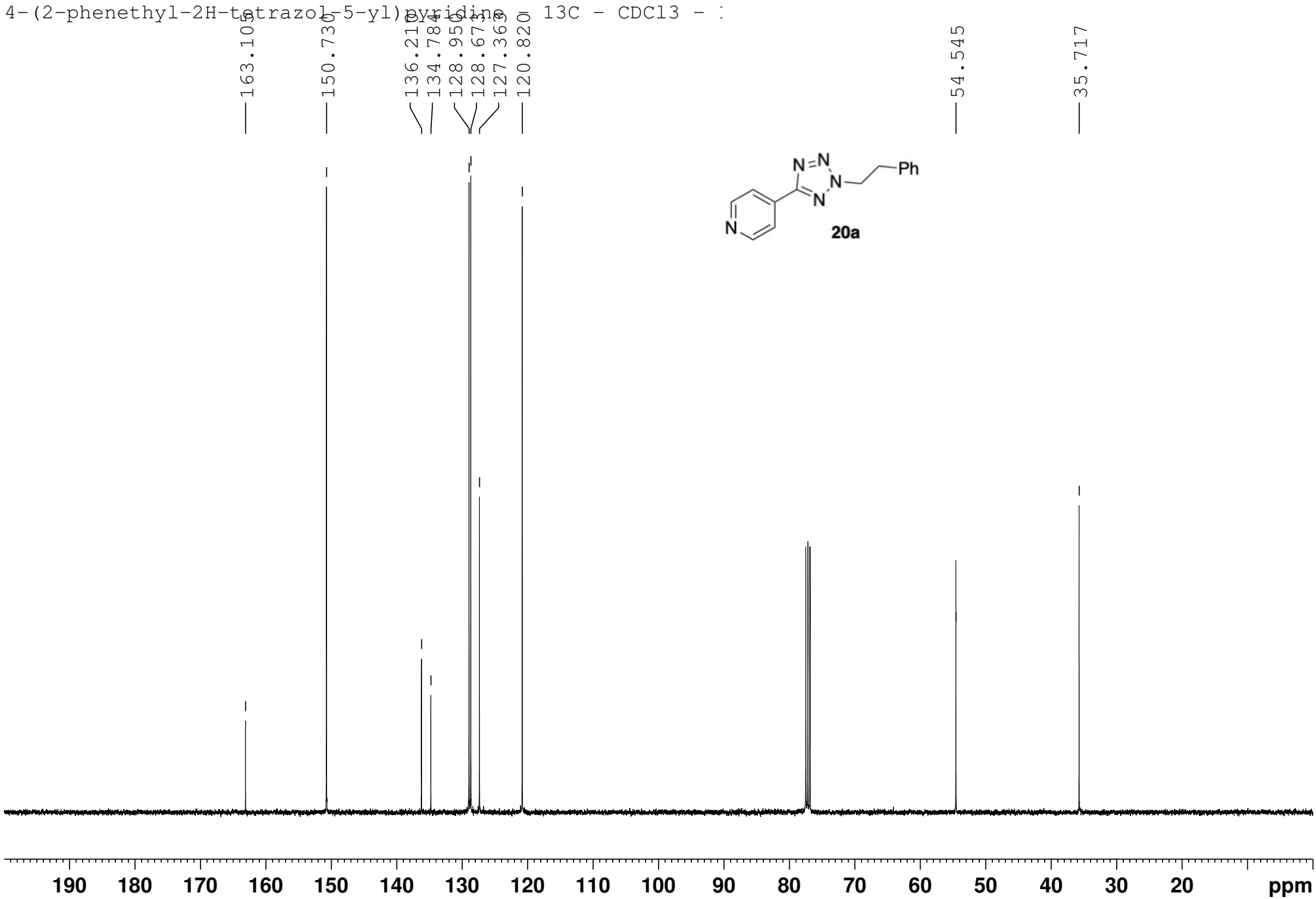
19b

148.6
135.7
129.3
127.6
123.0
63.0
48.5
32.7
29.5
29.2
29.0
26.4
25.7

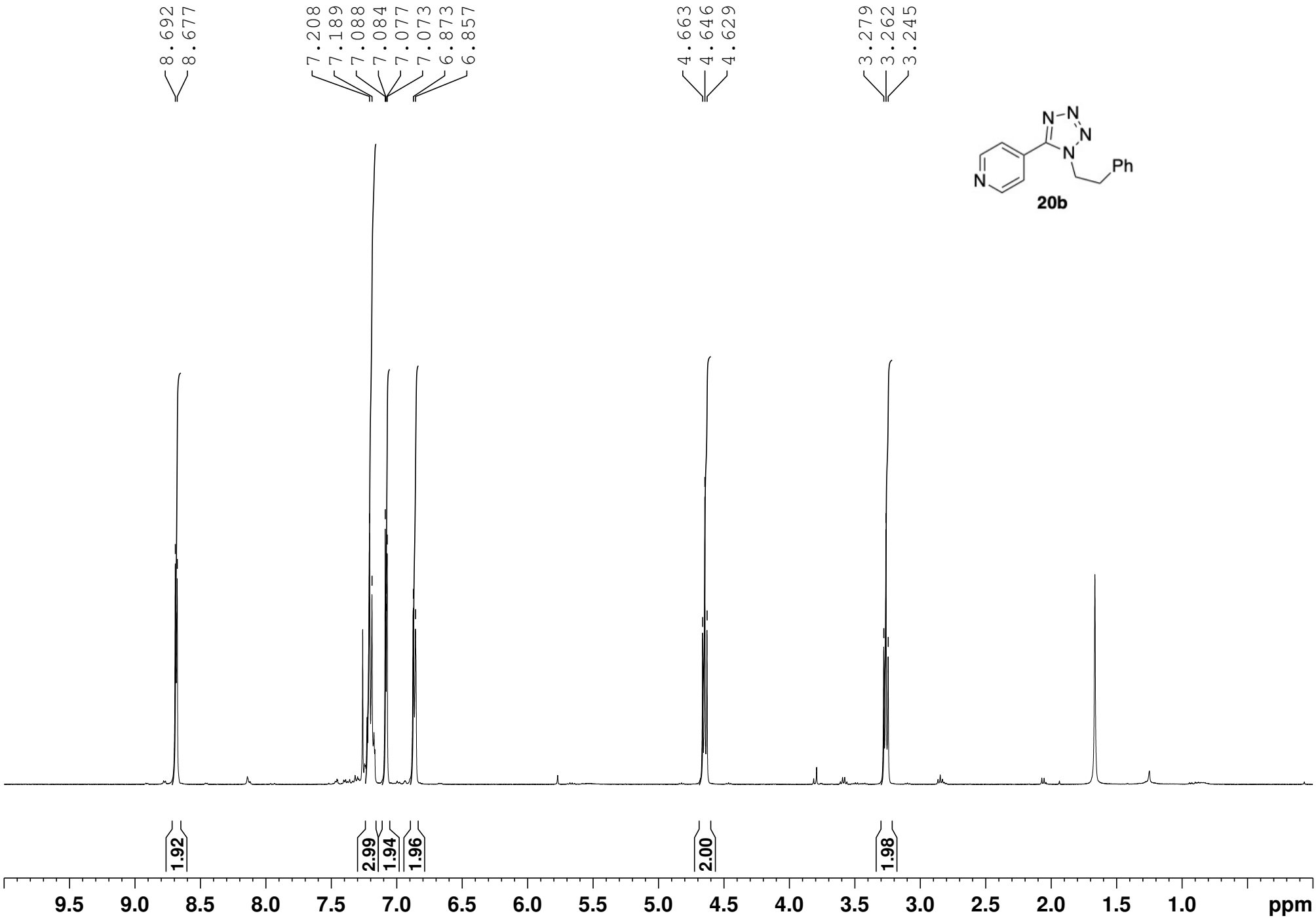
220 200 180 160 140 120 100 80 60 40 20 ppm

4-(2-phenethyl-2H-tetrazol-5-yl)pyridine - 1H - CDCl3 - 400 MHz



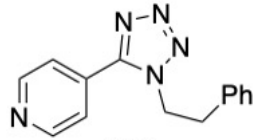

4-(2-phenethyl-2H-tetrazol-5-yl)pyridine - 13C - CDCl3 - 1
163.105
150.730
136.214
134.784
128.956
128.678
127.363
120.820
54.545
35.717
Ph
N
20a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

4-(1-phenethyl-1H-tetrazol-5-yl)pyridine - 1H - CDCl3 - 400 MHz



4-(1-phenethyl-1H-tetrazol-5-yl)pyridine 13C - CDCl3 - 100 MHz

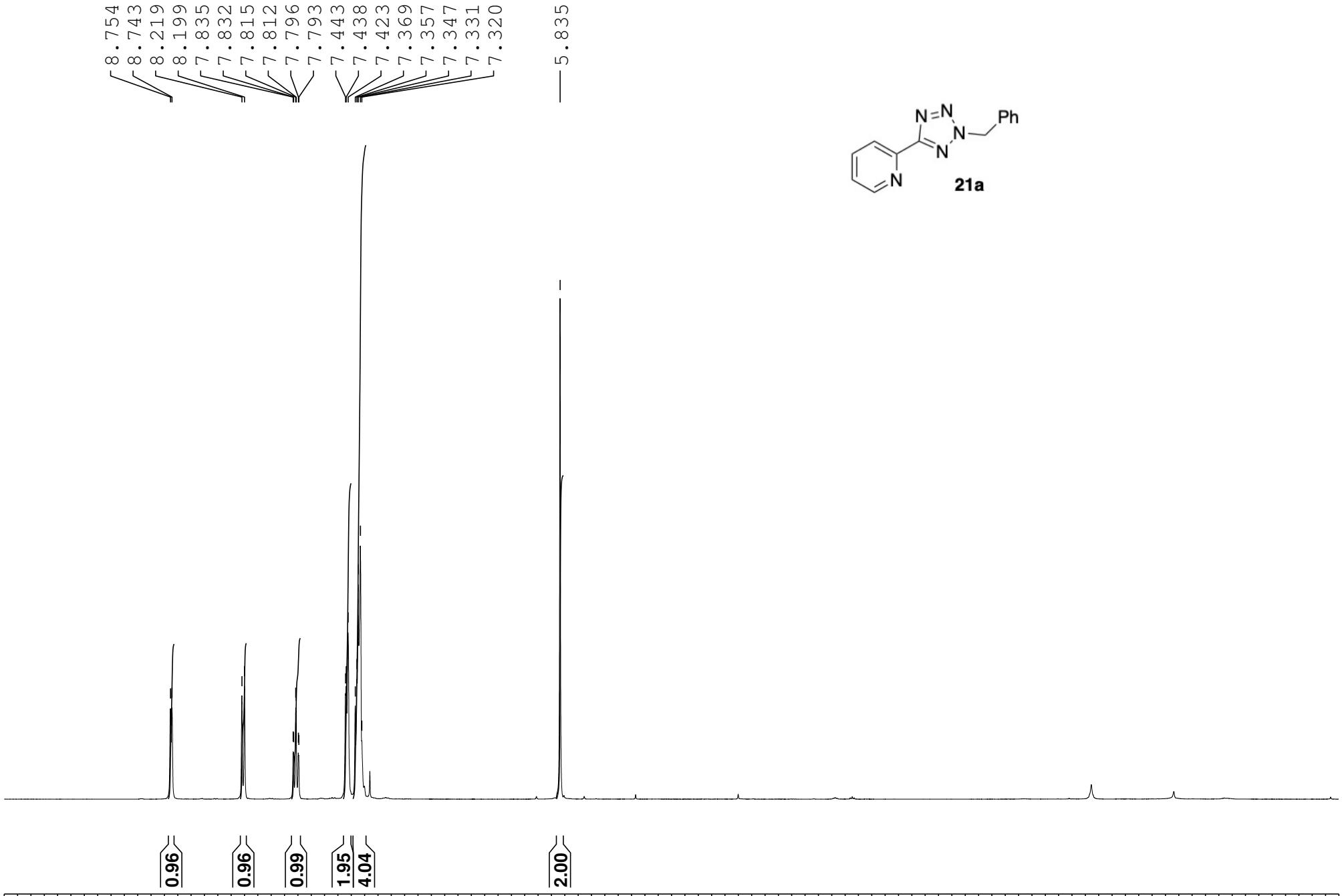
153.033
150.673
135.897
131.843
129.197
128.799
127.745
122.730
49.743
36.354



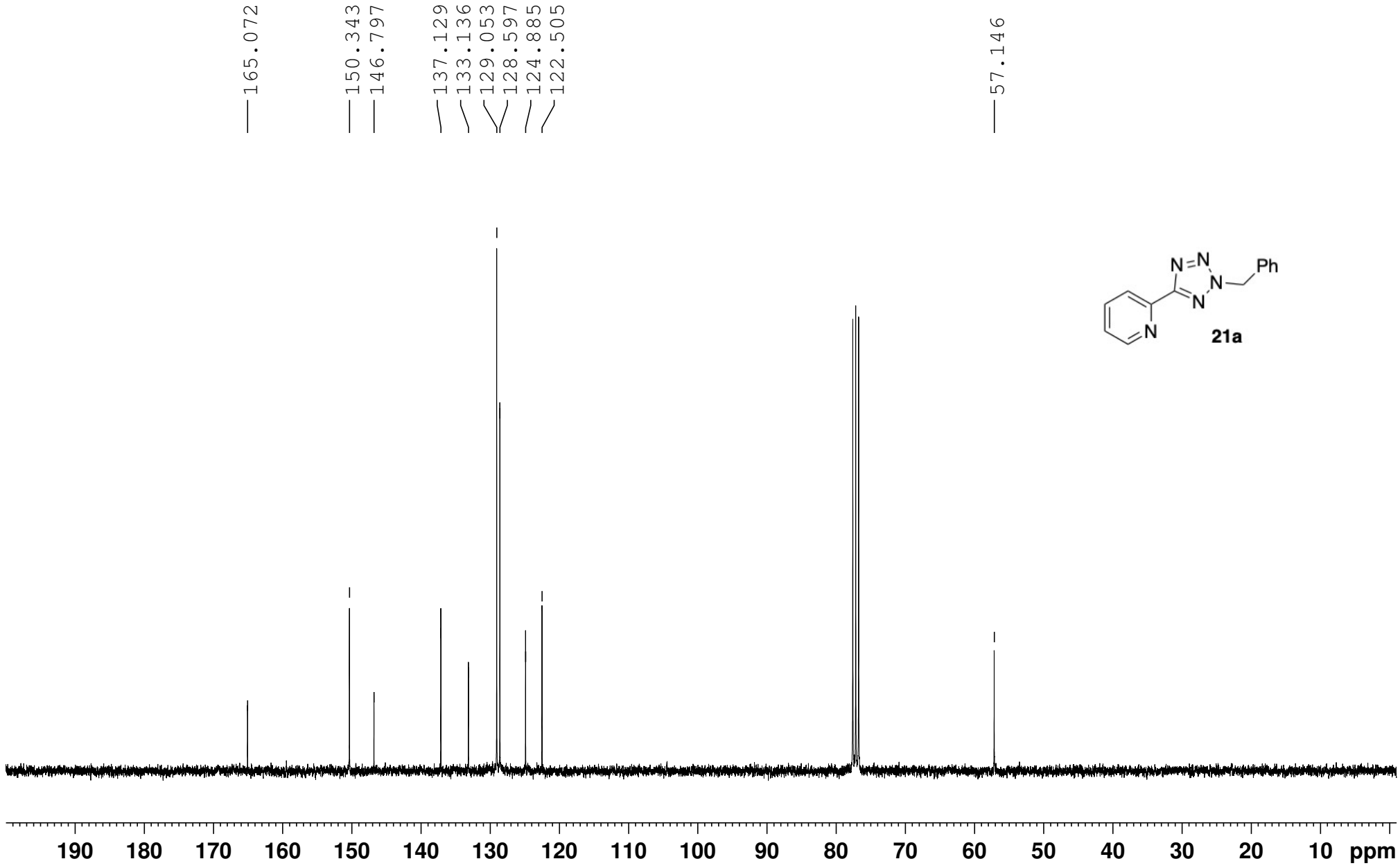
20b

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

2-(2-benzyl-2H-tetrazol-5-yl)pyridine - 1H - CDCl3 - 400 MHz

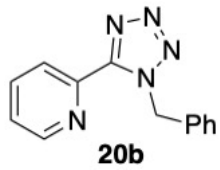


2-(2-benzyl-2H-tetrazol-5-yl)pyridine - 13C - CDCl3 - 75 MHz

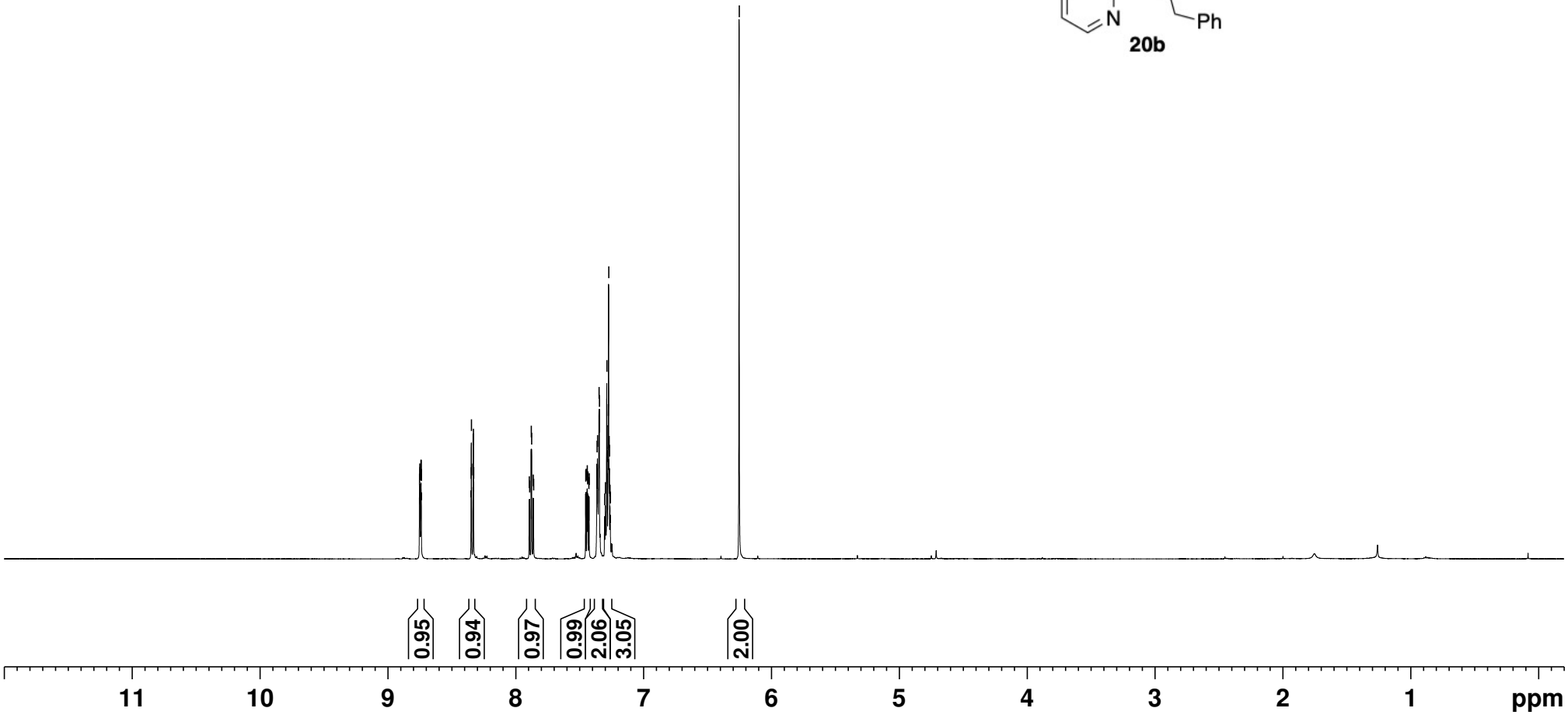


2-(1-benzyl-1H-tetrazol-5-yl)pyridine - 1H - CDCl3 - 500 MHz

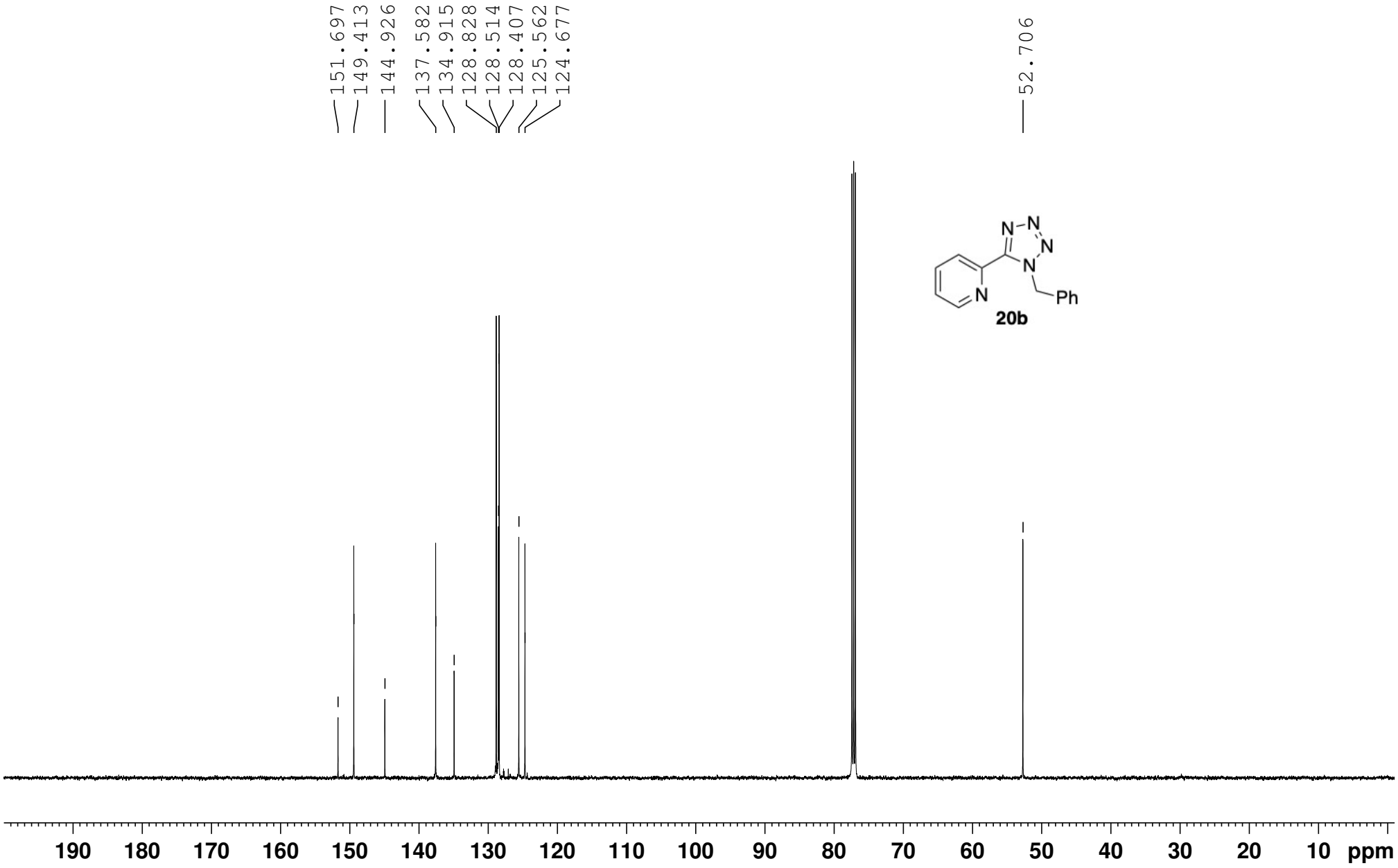
8.751
8.750
8.748
8.743
8.741
8.740
8.738
8.349
8.347
8.345
8.333
8.331
8.329
7.895
7.891
7.879
7.876
7.864
7.860
7.453
7.451
7.443
7.441
7.438
7.435
7.428
7.426
7.365
7.360
7.349
7.345
7.305
7.299
7.287
7.284
7.277
7.273
7.270
7.267
7.263
7.260
6.252



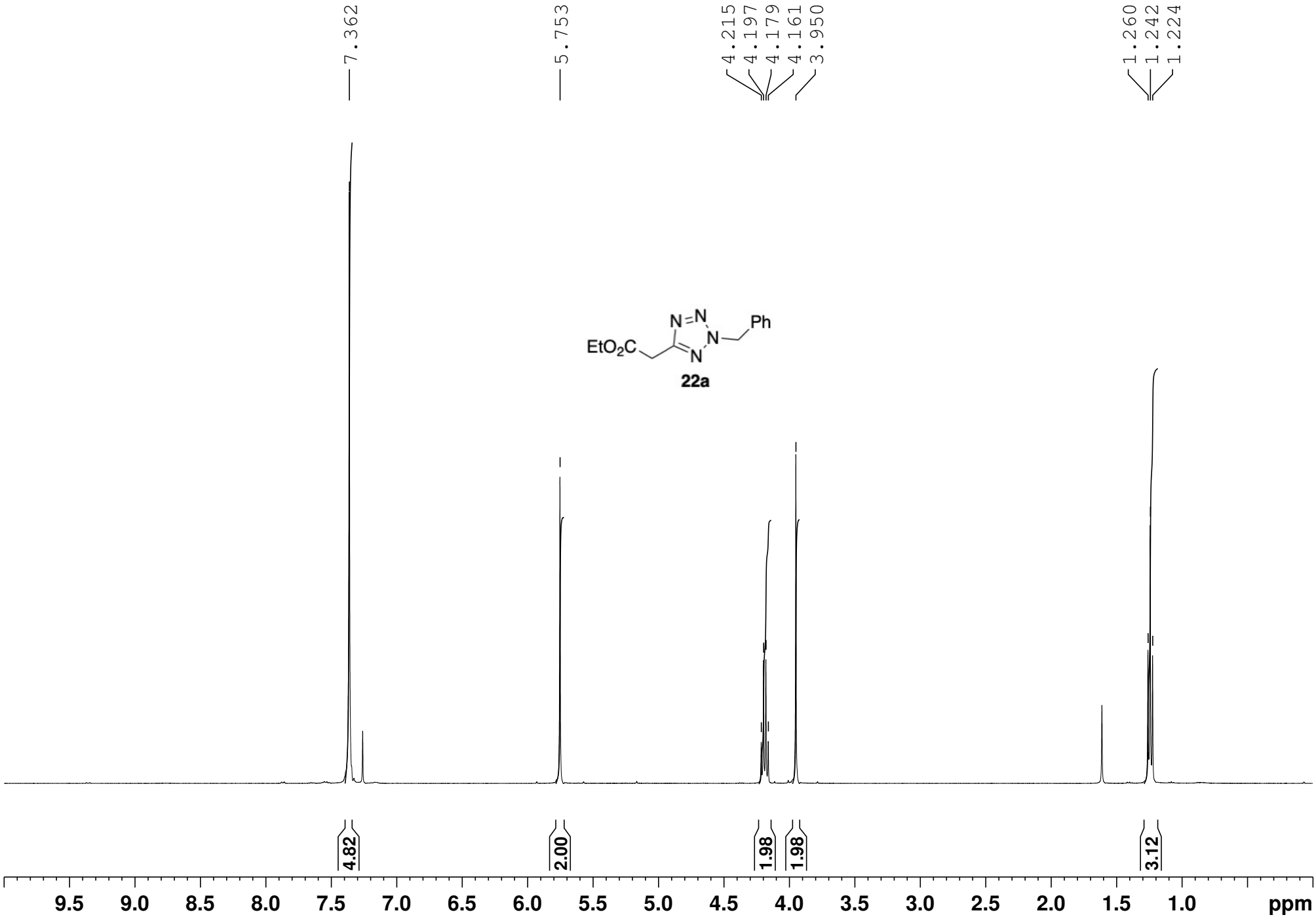
20b



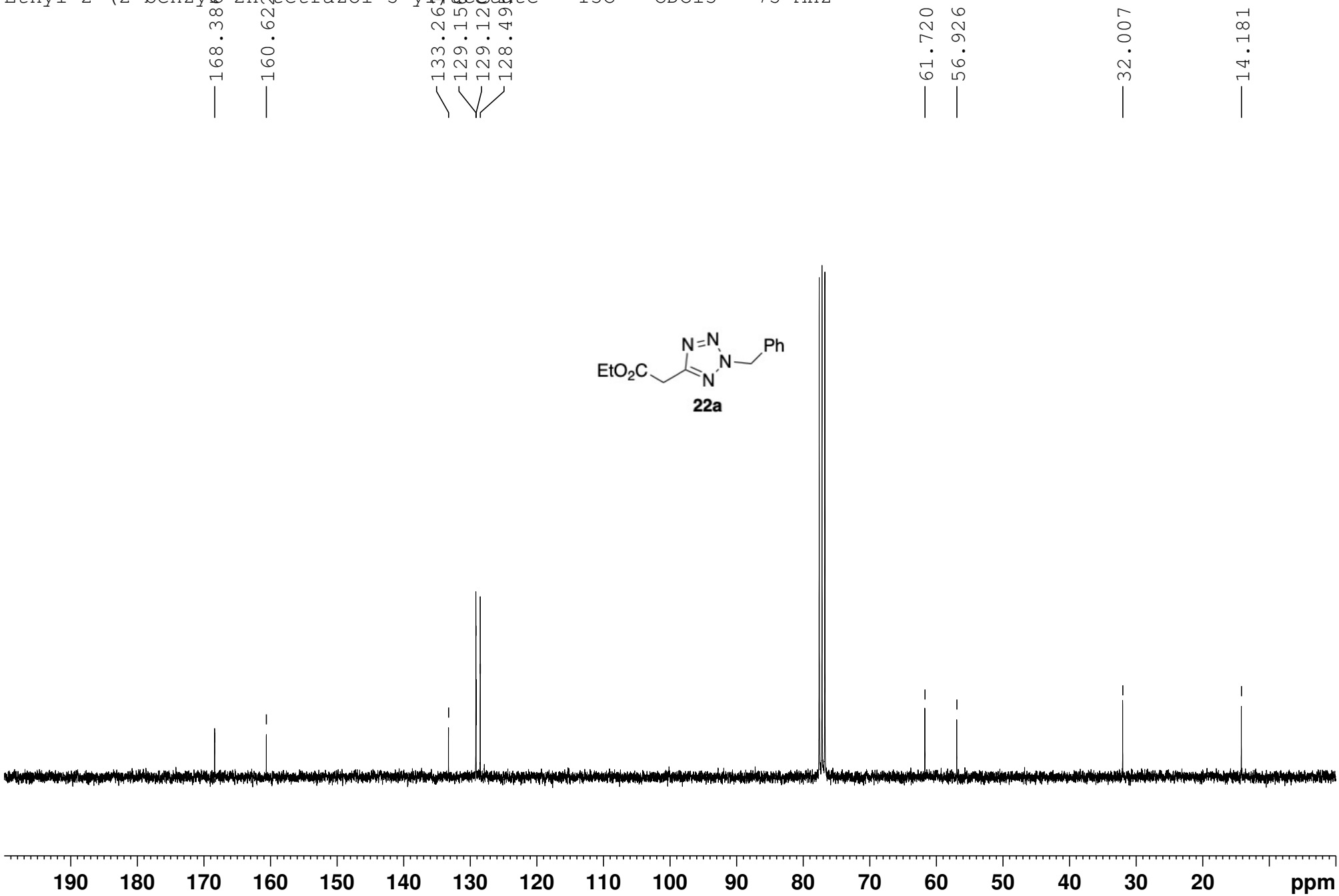
2-(1-benzyl-1H-tetrazol-5-yl)pyridine - 13C - CDCl3 - 125 MHz



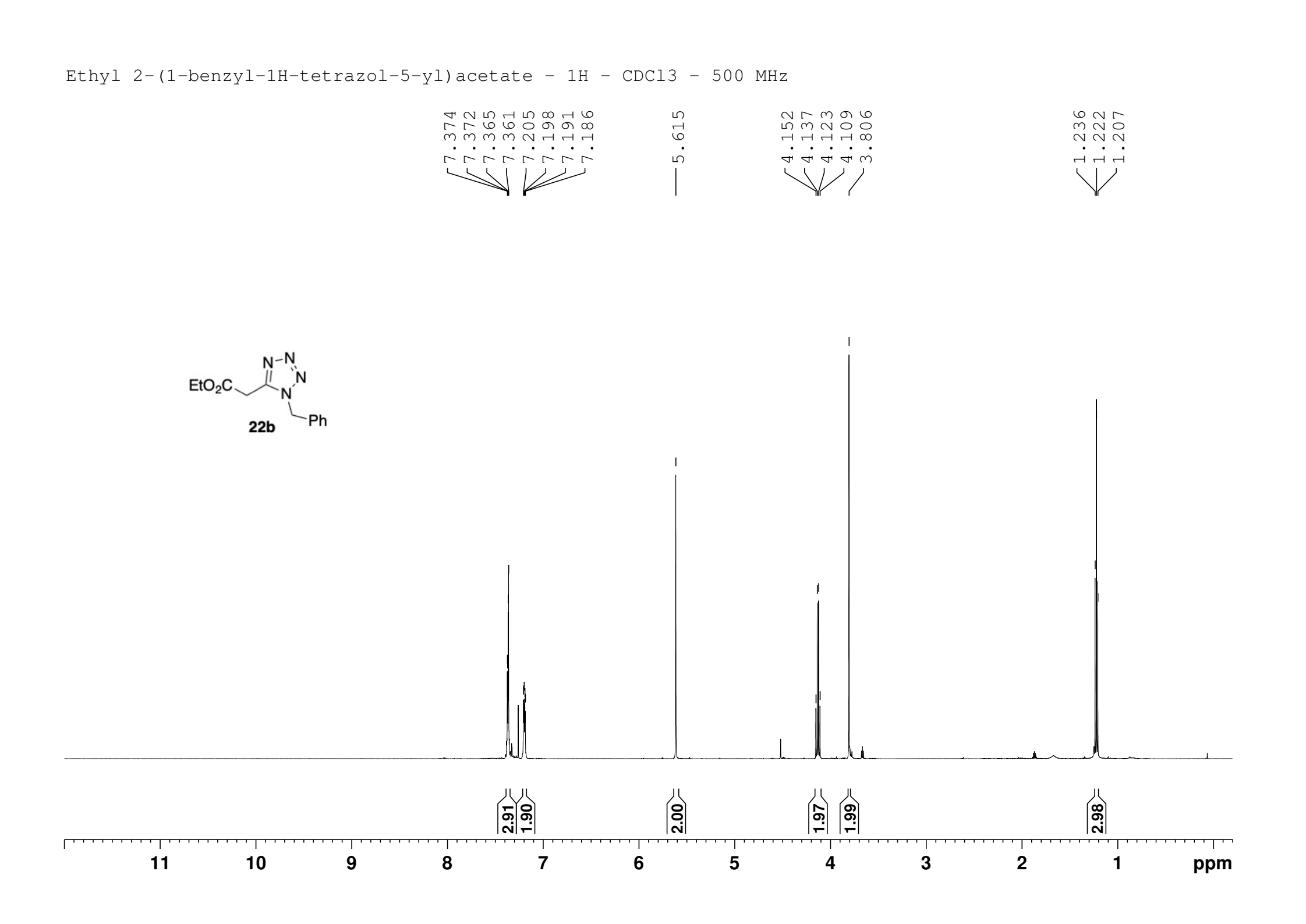
Ethyl 2-(2-benzyl-2H-tetrazol-5-yl)acetate - 1H - CDCl3 - 400 MHz



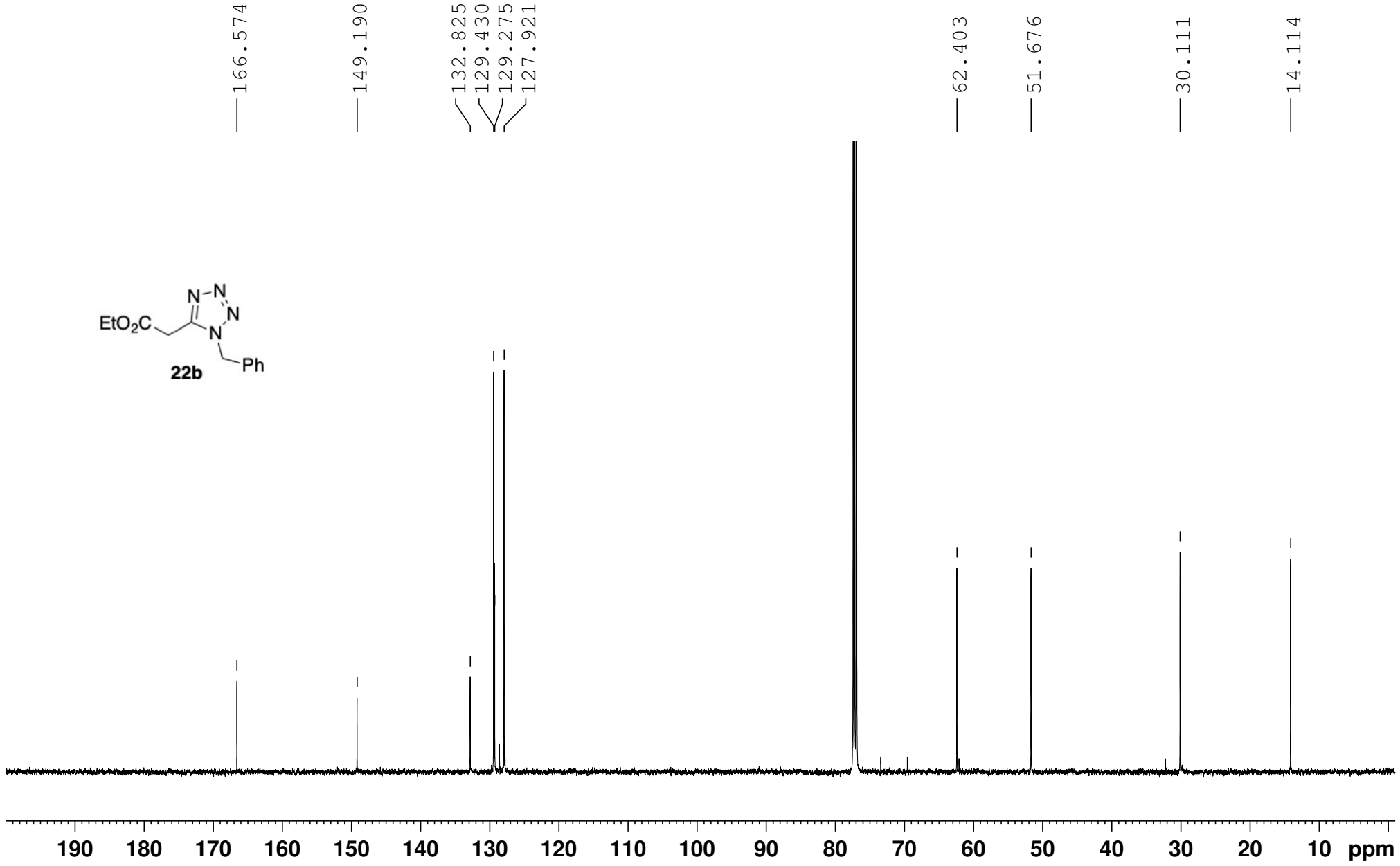
Ethyl 2-(2-benzyl-2H-tetrazol-5-yl)acetate - 13C - CDCl3 - 75 MHz



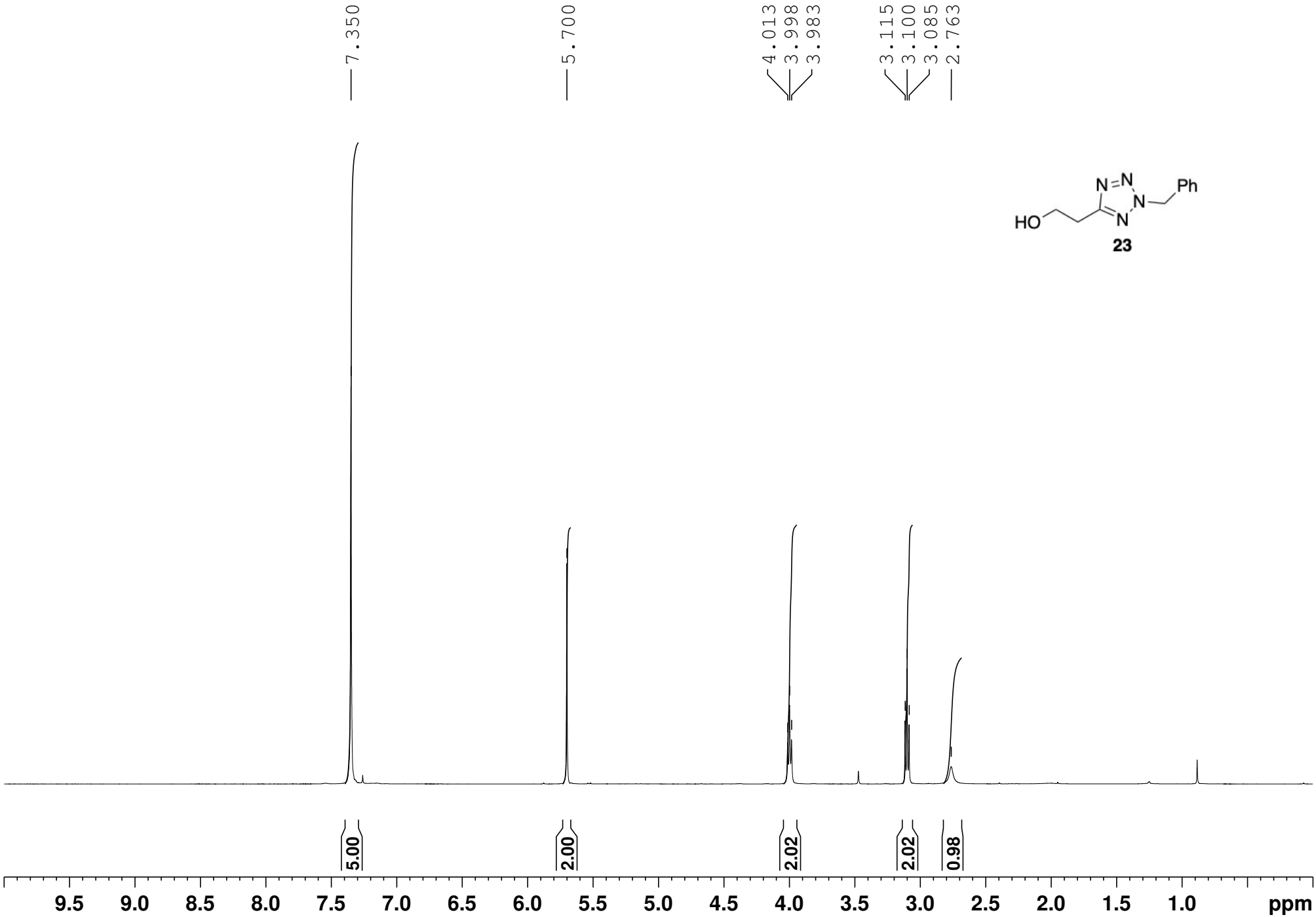
Ethyl 2-(1-benzyl-1H-tetrazol-5-yl)acetate - 1H - CDCl3 - 500 MHz



Ethyl 2-(1-benzyl-1H-tetrazol-5-yl)acetate - 13C - CDCl3 - 125 MHz

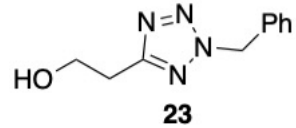


2-(2-benzyl-2H-tetrazol-5-yl)ethan-1-ol - 1H - CDCl3 - 400 MHz



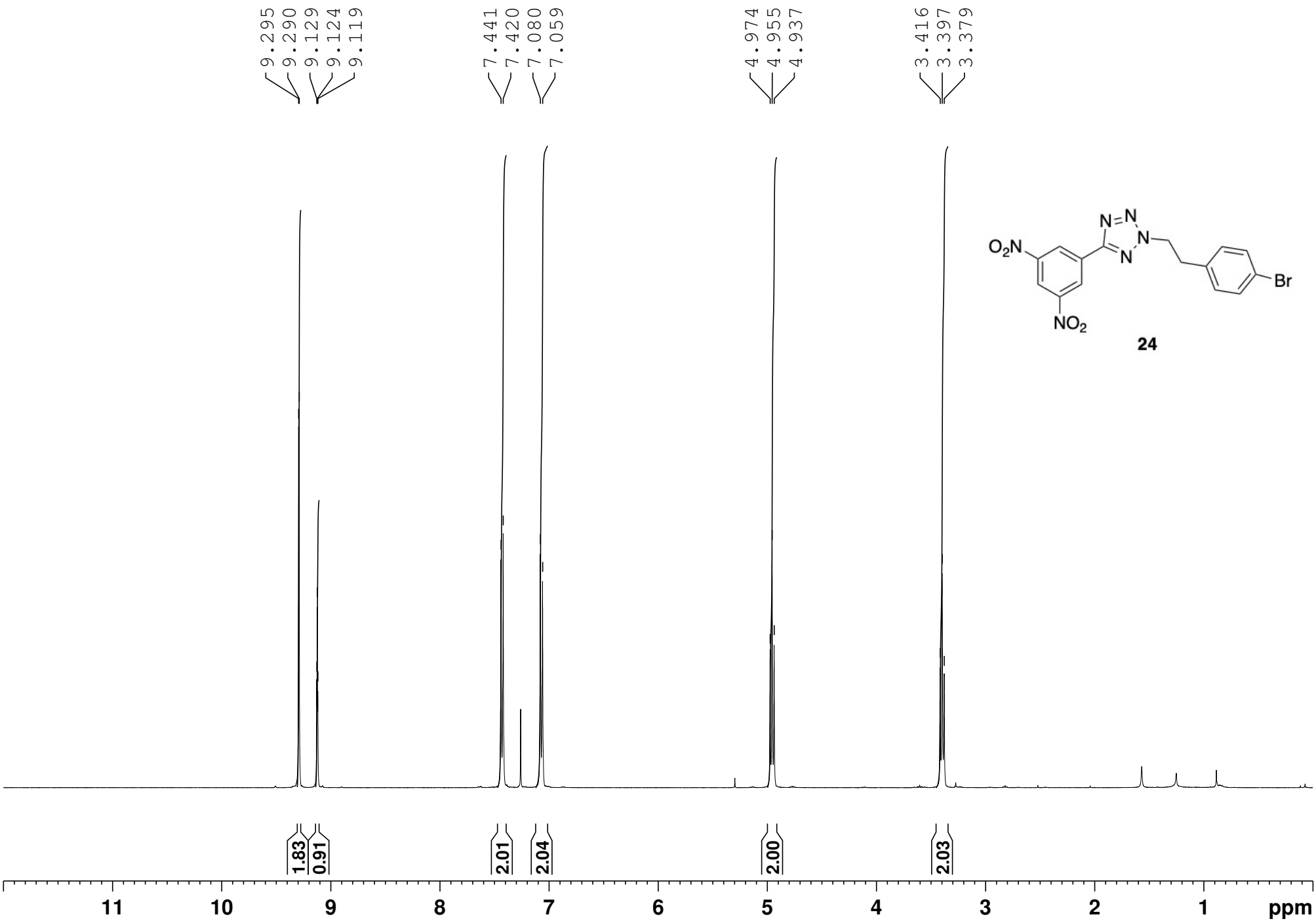
2-(2-benzyl-2H-tetrazol-5-yl)ethan-1-ol - 13C - CDCl3 - 100 MHz

165.038
133.241
129.108
129.076
128.505
60.260
56.772
28.887



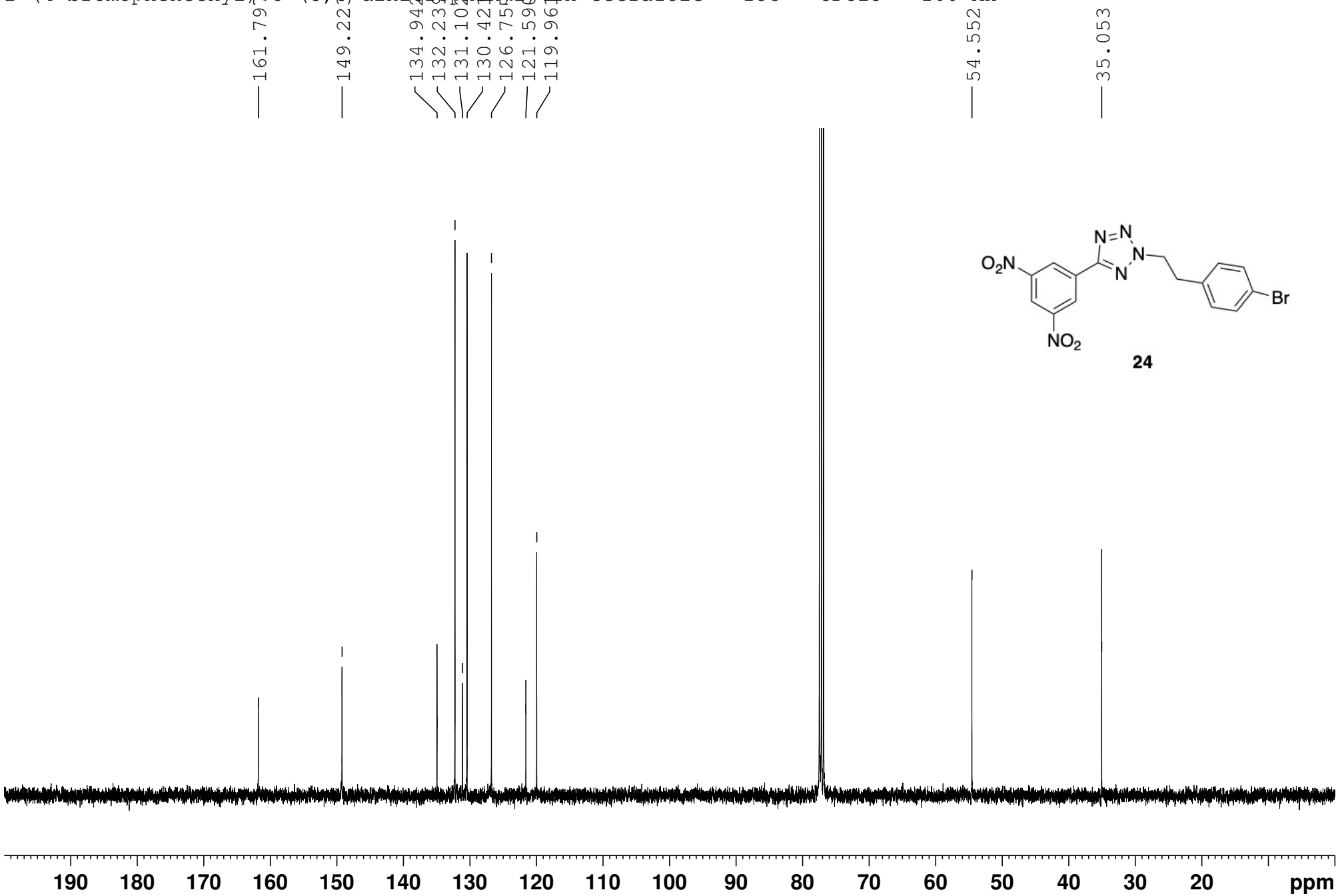
23

2-(4-bromophenethyl)-5-(3,5-dinitrophenyl)-2H-tetrazole - 1H - CDCl3 - 400 MHz

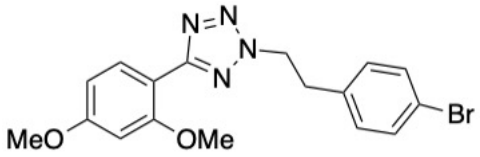


24

2-(4-bromophenethyl)-5-(3,5-dinitrophenyl)-2H-tetrazole - 13C - CDCl3 - 100 MH



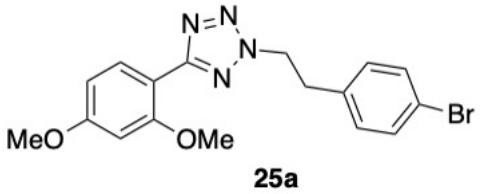
2-(4-bromophenethyl)-5-(2,4-dimethoxyphenyl)-2H-tetrazole - 1H - CDCl3 - 400 M



25a

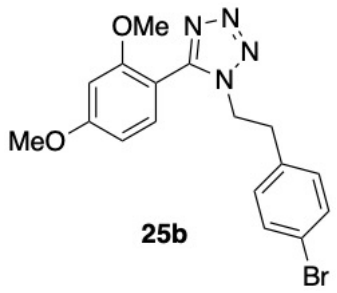
2-(4-bromophenethyl)-5-(2,4-dimethoxyphenyl)-2H-tetrazole - 13C - CDCl3 - 100

163.278
162.624
158.770
135.664
131.943
131.680
130.514
121.118
109.428
105.140
99.221
56.093
55.549
53.752
35.187



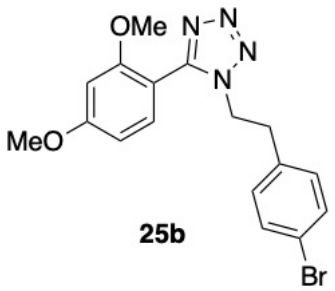
25a

1-(4-bromophenethyl)-5-(2,4-dimethoxyphenyl)-1H-tetrazole - 1H - CDCl3 - 400 M



25b

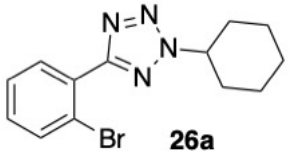
1-(4-bromophenethyl)-5-(2,4-dimethoxyphenyl)-1H-tetrazole - 13C - CDCl3 - 100



25b

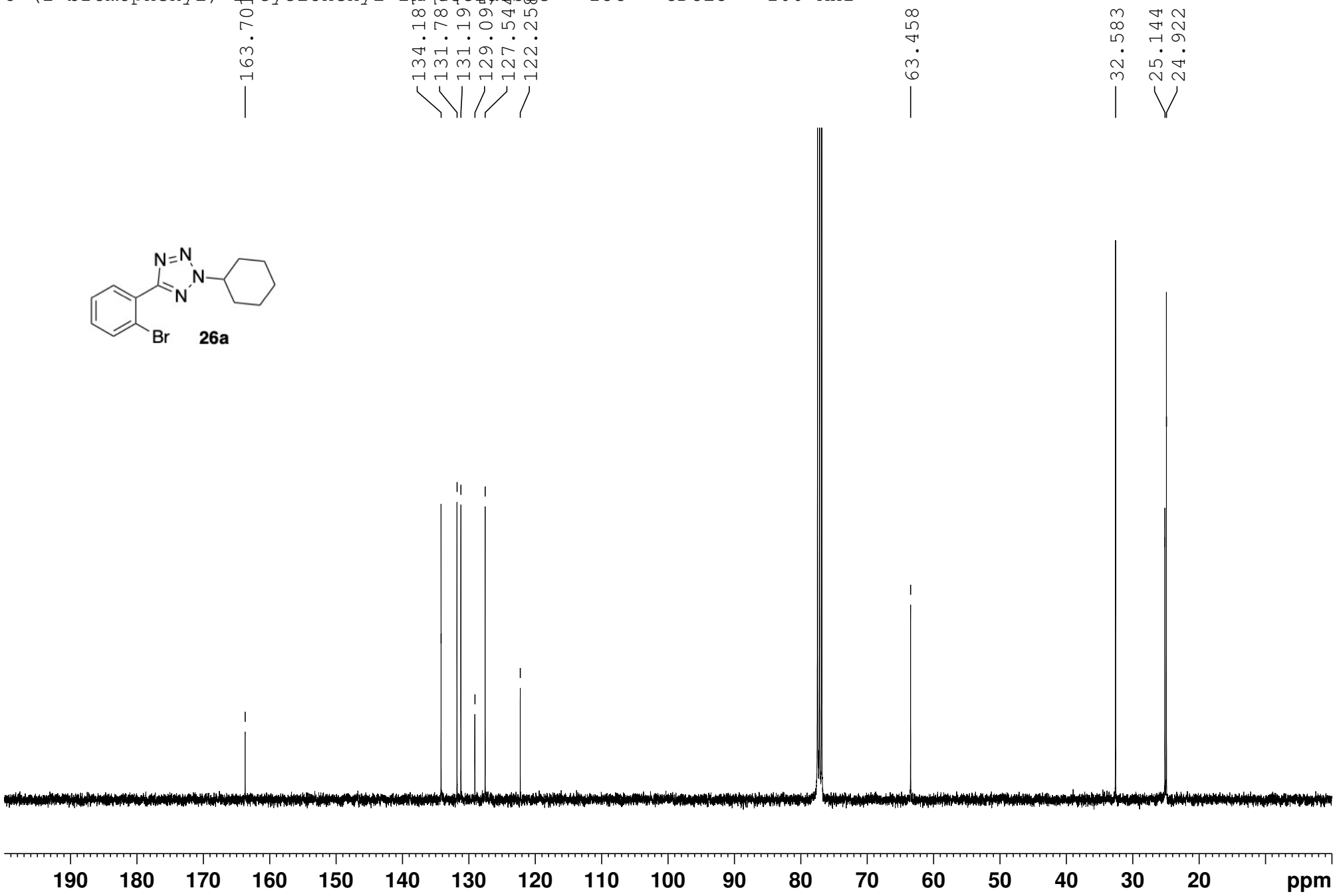
5-(2-bromophenyl)-2-cyclohexyl-2H-tetrazole - 1H - CDCl3 - 400 MHz

7.867
7.863
7.847
7.843
7.741
7.739
7.721
7.719
7.444
7.442
7.425
7.423
7.406
7.404
7.337
7.333
7.317
7.314
7.298
7.294
4.821
4.802
4.792
4.783
4.764
2.333
2.325
2.301
2.294
2.097
2.088
2.067
2.058
2.037
2.028
1.998
1.993
1.982
1.973
1.957
1.948
1.941
1.787
1.778
1.764
1.755
1.746
1.552
1.529
1.521
1.513
1.497
1.489
1.481
1.457
1.411
1.388
1.380
1.349

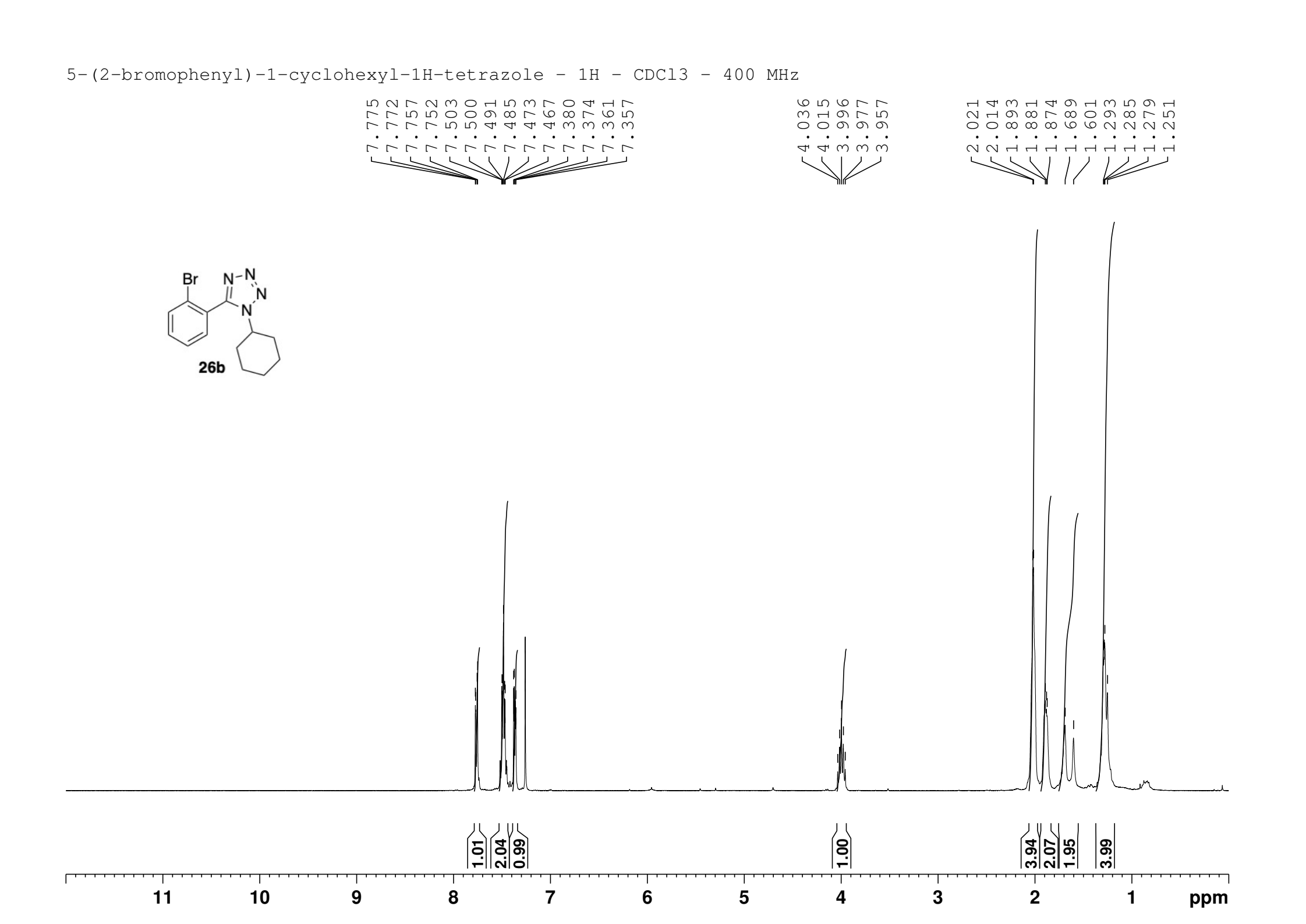


26a

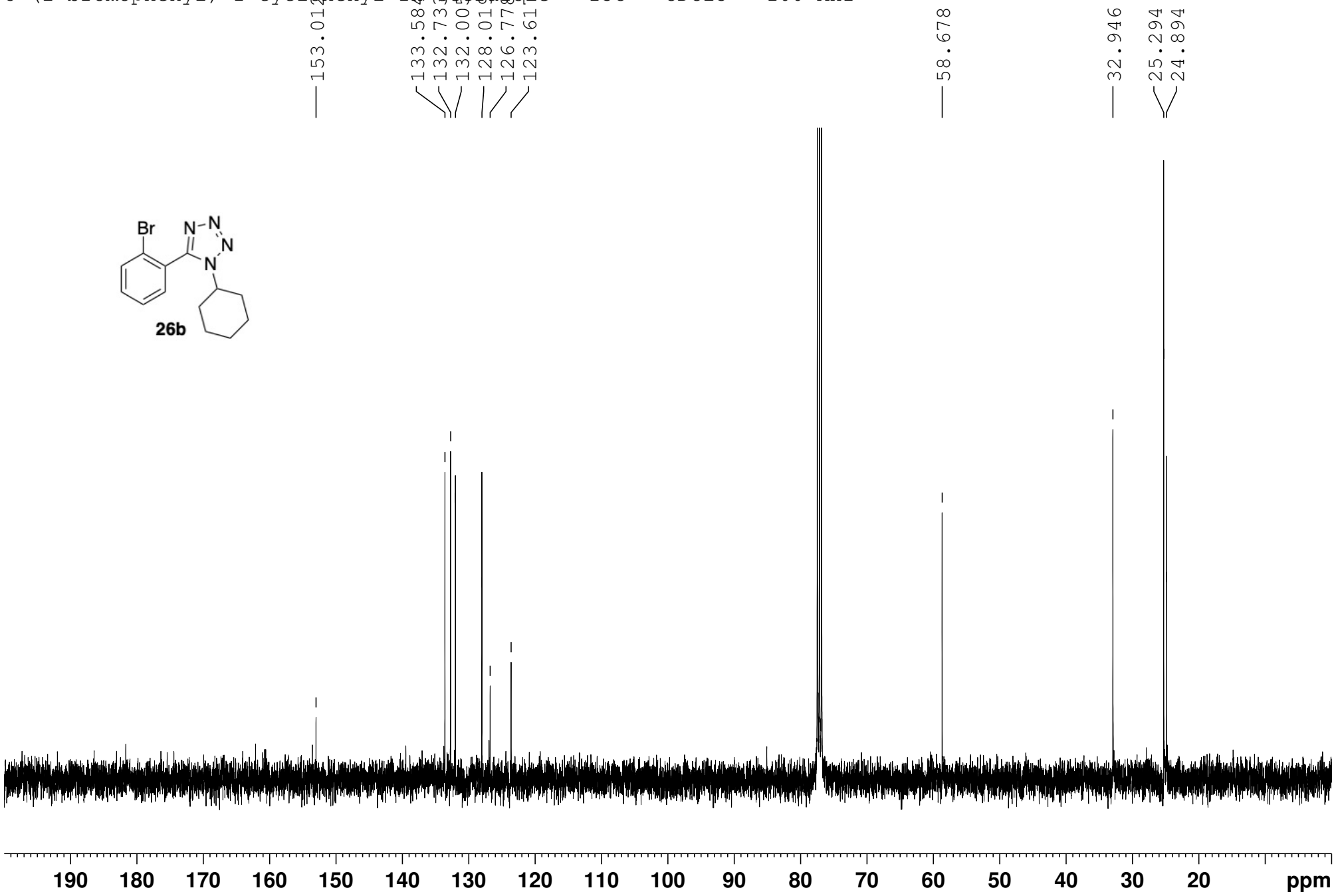
5-(2-bromophenyl)-2-cyclohexyl-2H-tetrazole - 13C - CDCl3 - 100 MHz



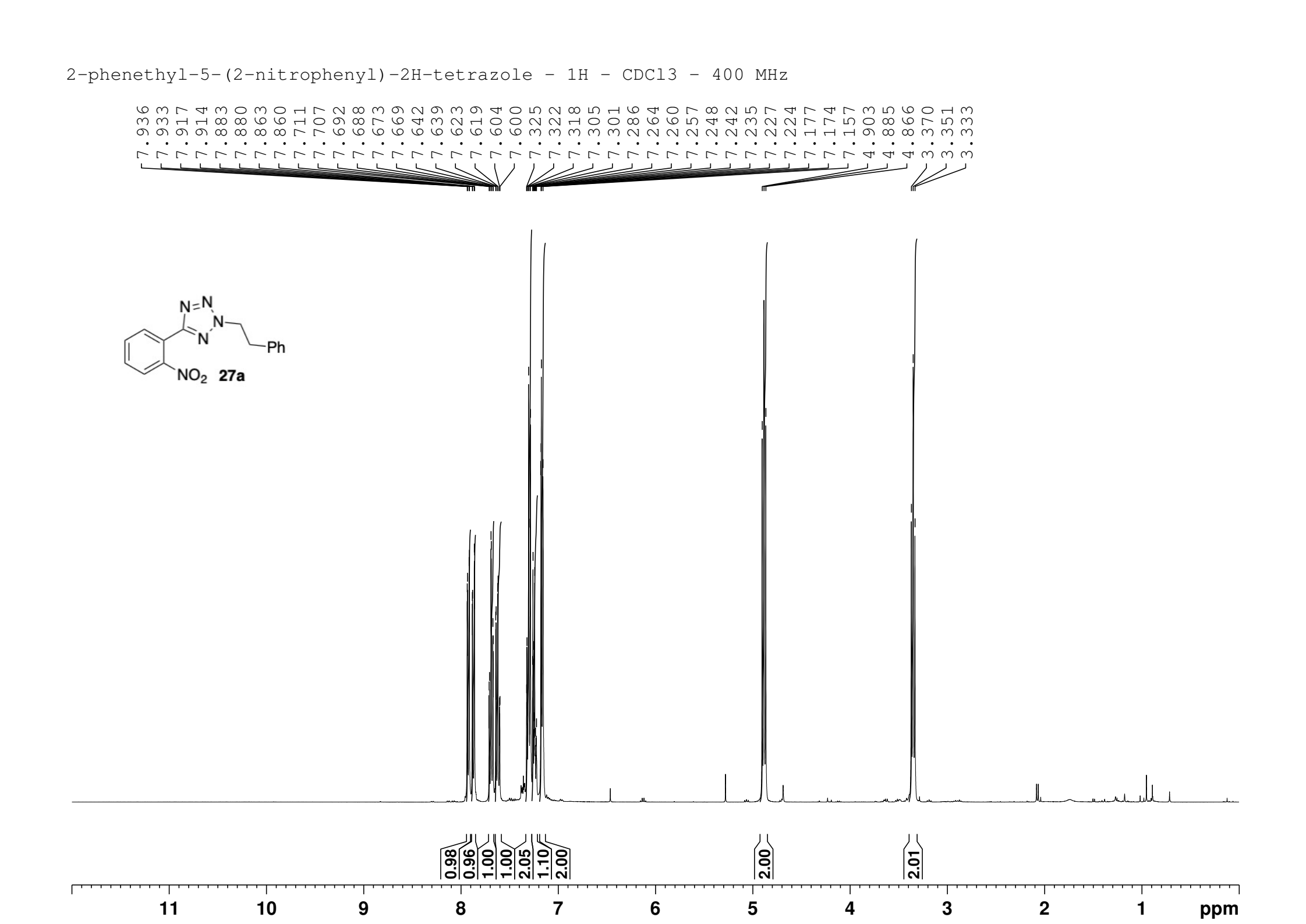
5-(2-bromophenyl)-1-cyclohexyl-1H-tetrazole - 1H - CDCl3 - 400 MHz



5-(2-bromophenyl)-1-cyclohexyl-1H-tetrazole - 13C - CDCl3 - 100 MHz

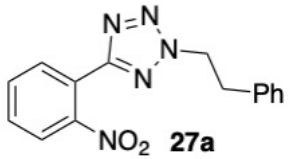


2-phenethyl-5-(2-nitrophenyl)-2H-tetrazole - 1H - CDCl3 - 400 MHz



2-phenethyl-5-(2-nitrophenyl)-2H-tetrazole - 13C - CDCl3 - 100 MHz

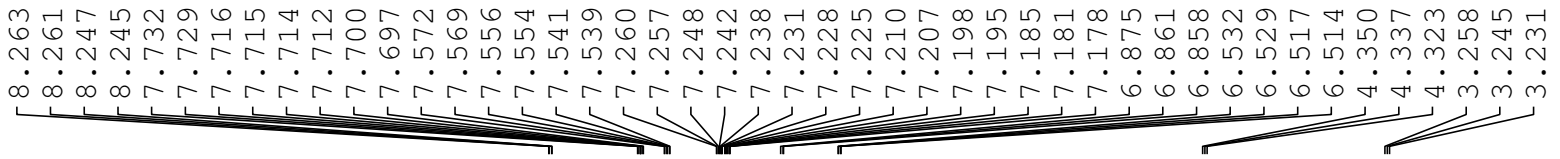
161.405
149.071
136.288
132.444
131.191
131.064
128.908
128.722
127.278
124.227
121.575
54.574
35.703

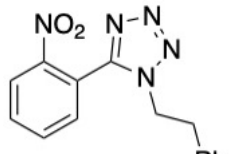


27a

240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

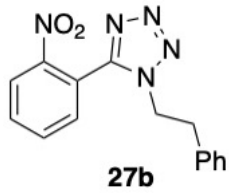
1-phenethyl-5-(2-nitrophenyl)-1H-tetrazole - 1H - CDCl3 - 500 MHz





27b

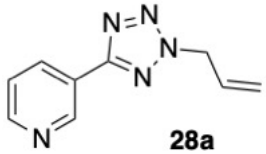
1-phenethyl-5-(2-nitrophenyl)-1H-tetrazole - 13C - CDCl3 - 125 MHz



27b

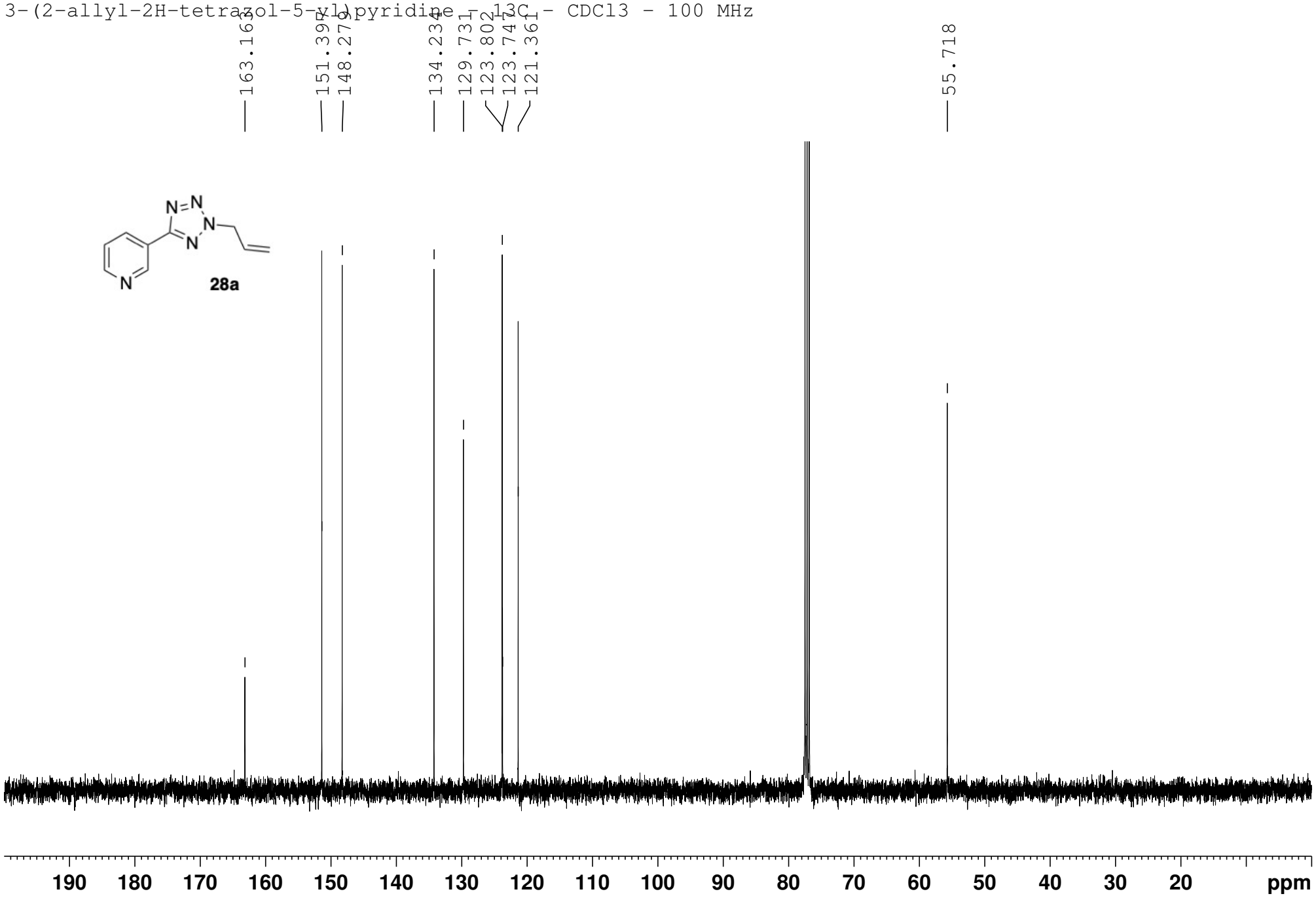
3-(2-allyl-2H-tetrazol-5-yl)pyridine - 1H - CDCl3 - 400 MHz

9.370
9.367
8.712
8.708
8.700
8.696
8.429
8.424
8.420
8.409
8.405
8.400
7.438
7.436
7.425
7.424
7.418
7.416
7.406
7.404
6.180
6.164
6.155
6.148
6.139
6.121
6.112
6.105
6.096
6.080
5.448
5.421
5.420
5.407
5.405
5.293
5.290
5.286
5.277
5.274
5.271

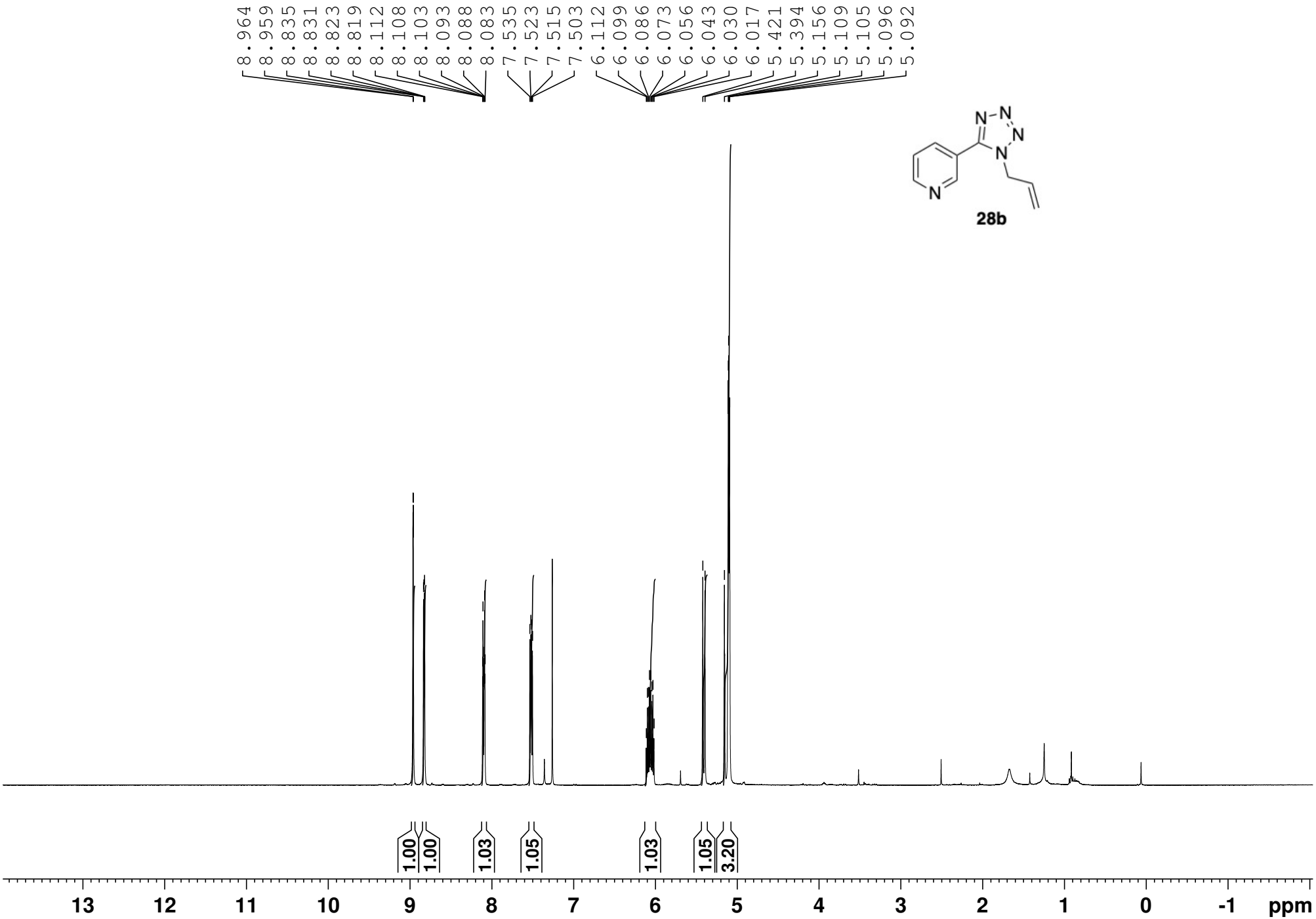


28a

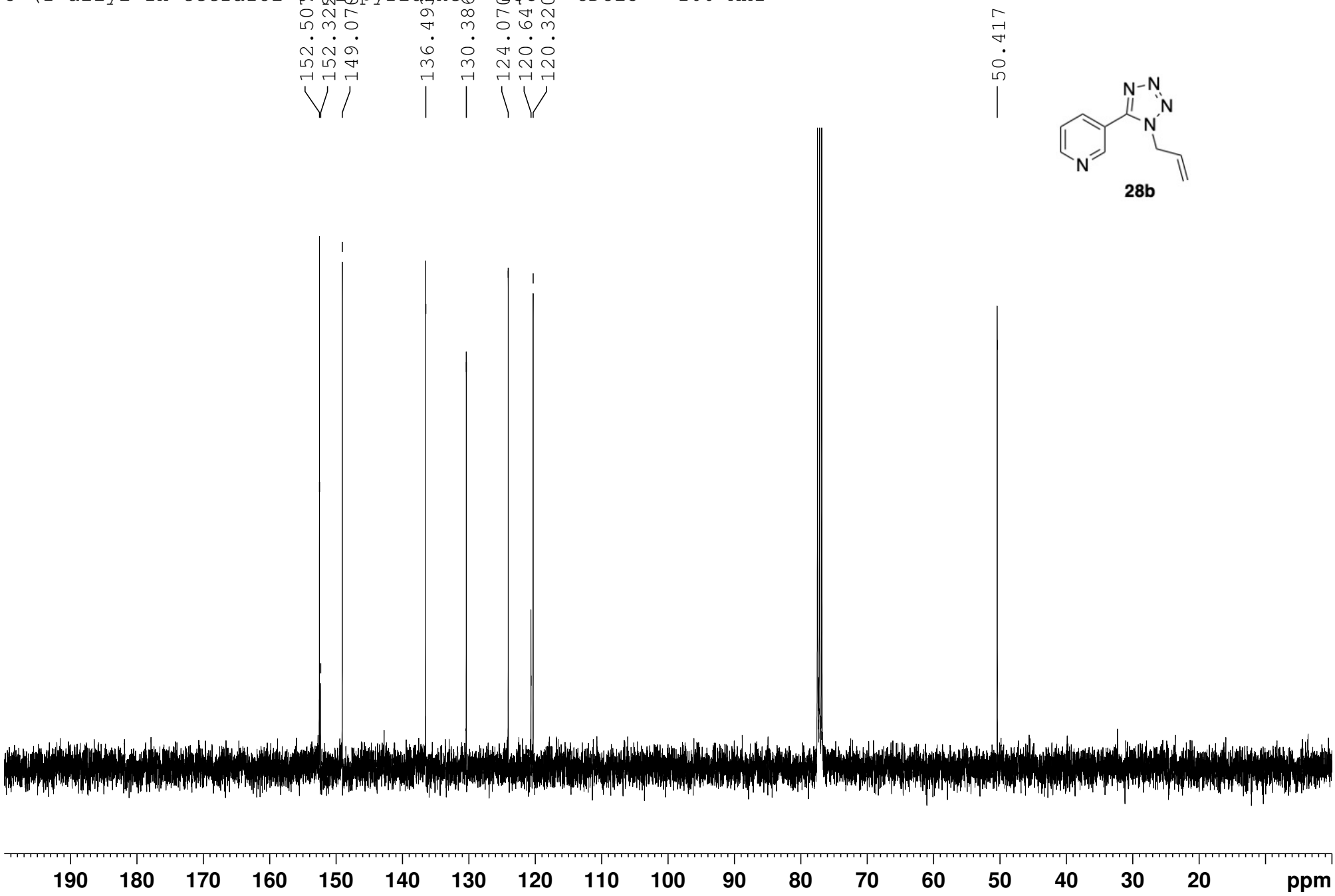
3-(2-allyl-2H-tetrazol-5-yl)pyridine - 13C - CDCl3 - 100 MHz



3-(1-allyl-1H-tetrazol-5-yl)pyridine - 1H - CDCl3 - 400 MHz

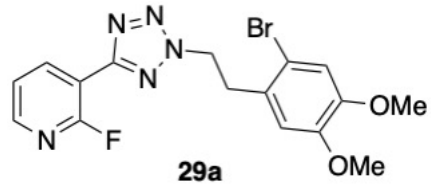


3-(1-allyl-1H-tetrazol-5-yl)pyridine - 13C - CDCl3 - 100 MHz



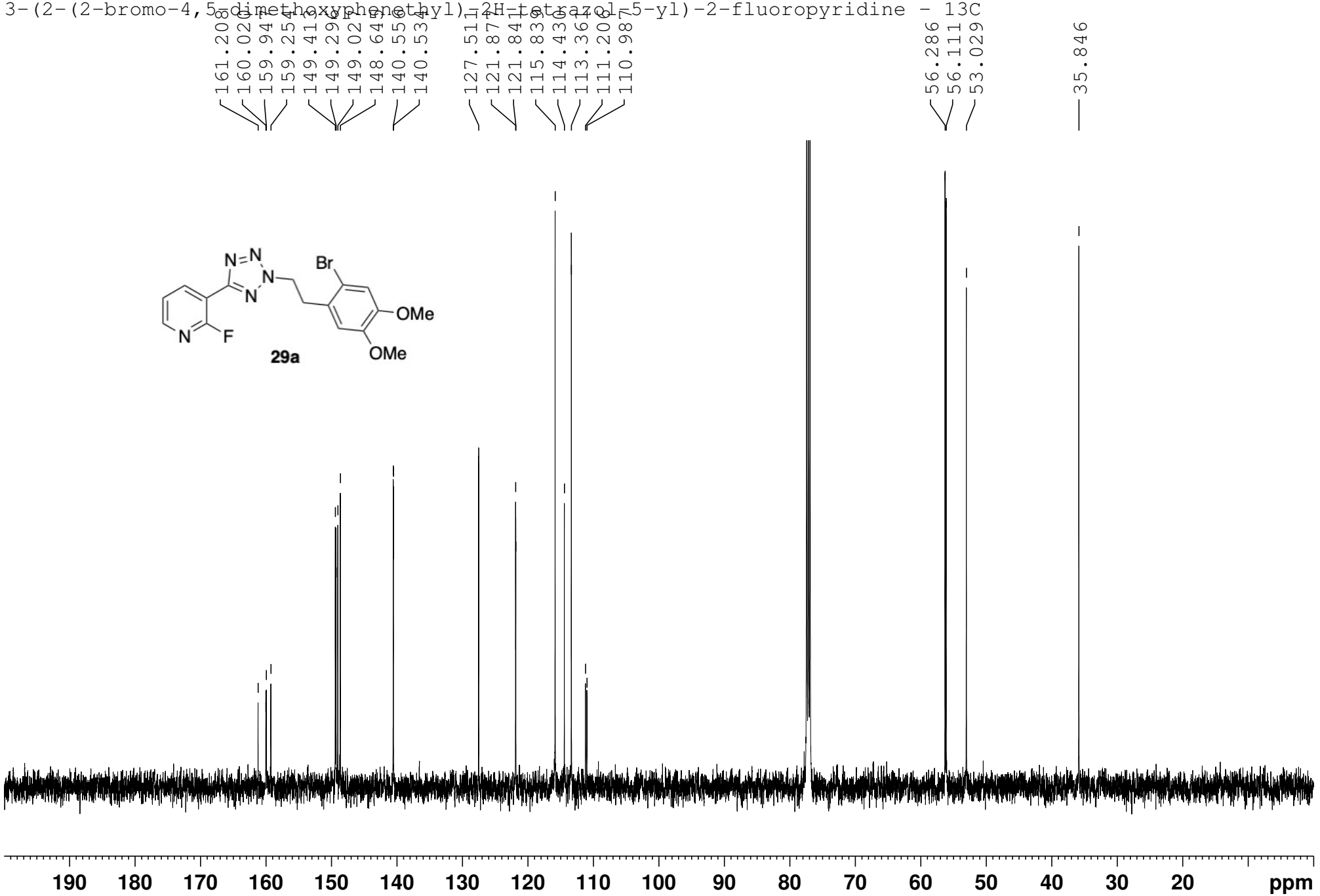
3-(2-(2-bromo-4,5-dimethoxyphenethyl)-2H-tetrazol-5-yl)-2-fluoropyridine - 1H

8.578
8.574
8.563
8.559
8.556
8.545
8.541
8.352
8.350
8.348
8.346
8.342
8.340
8.339
8.337
7.373
7.370
7.363
7.360
7.358
7.354
7.348
7.345
7.013
6.564
4.965
4.951
4.936
3.840
3.723
3.461
3.447
3.432

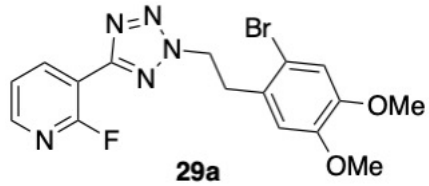


29a

3-(2-(2-bromo-4,5-dimethoxyphenethyl)-2H-tetrazol-5-yl)-2-fluoropyridine - 13C

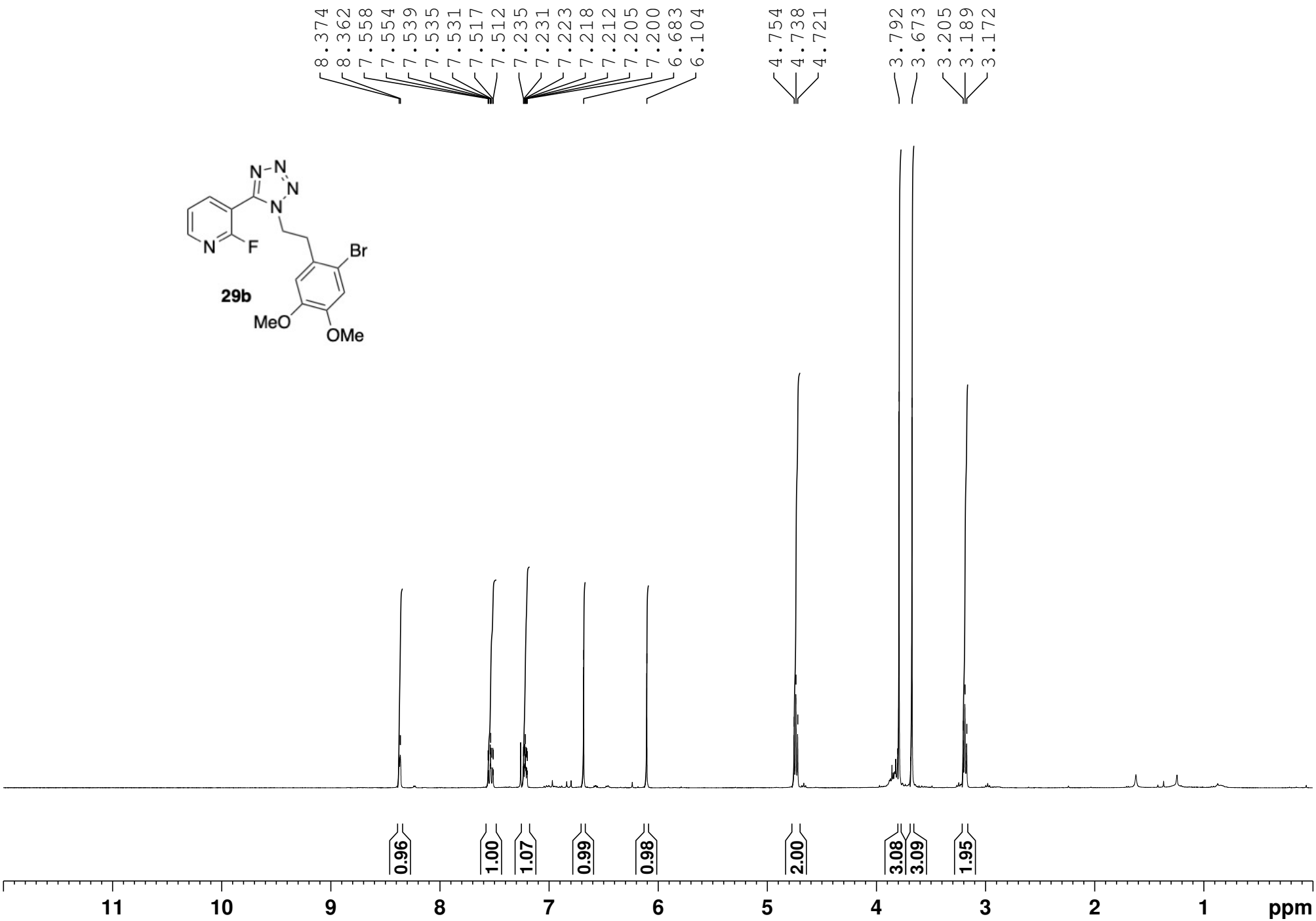


3-(2-(2-bromo-4,5-dimethoxyphenethyl)-2H-tetrazol-5-yl)-2-fluoropyridine - 19F

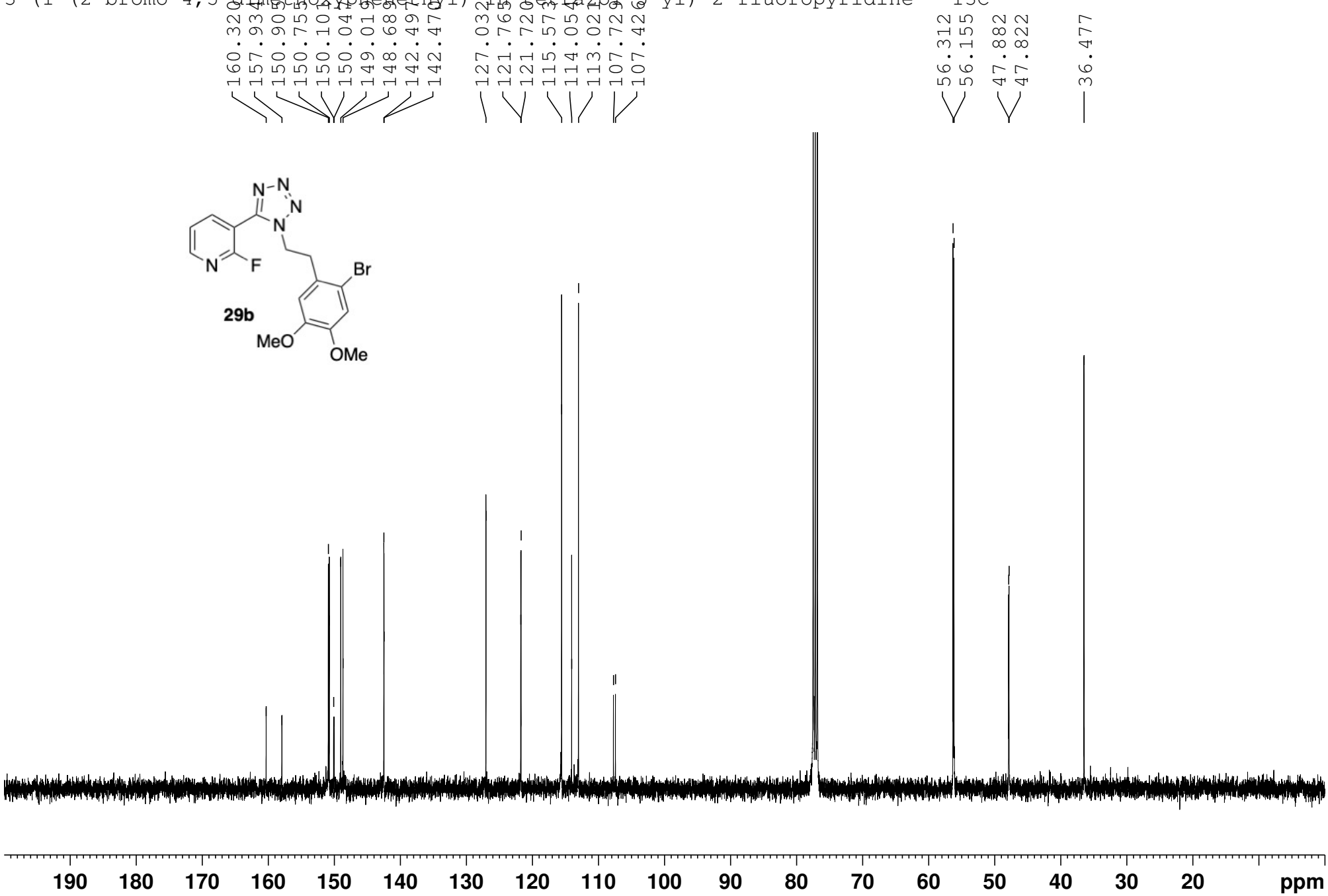


29a

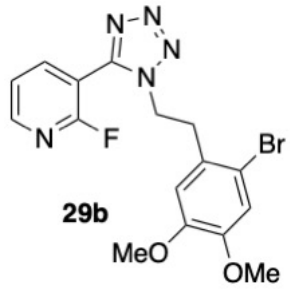
3-(1-(2-bromo-4,5-dimethoxyphenethyl)-1H-tetrazol-5-yl)-2-fluoropyridine - 1H



3-(1-(2-bromo-4,5-dimethoxyphenethyl)-1H-tetrazol-5-yl)-2-fluoropyridine - 13C



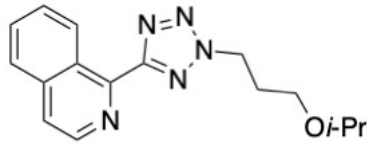
3-(1-(2-bromo-4,5-dimethoxyphenethyl)-1H-tetrazol-5-yl)-2-fluoropyridine - 19F



29b

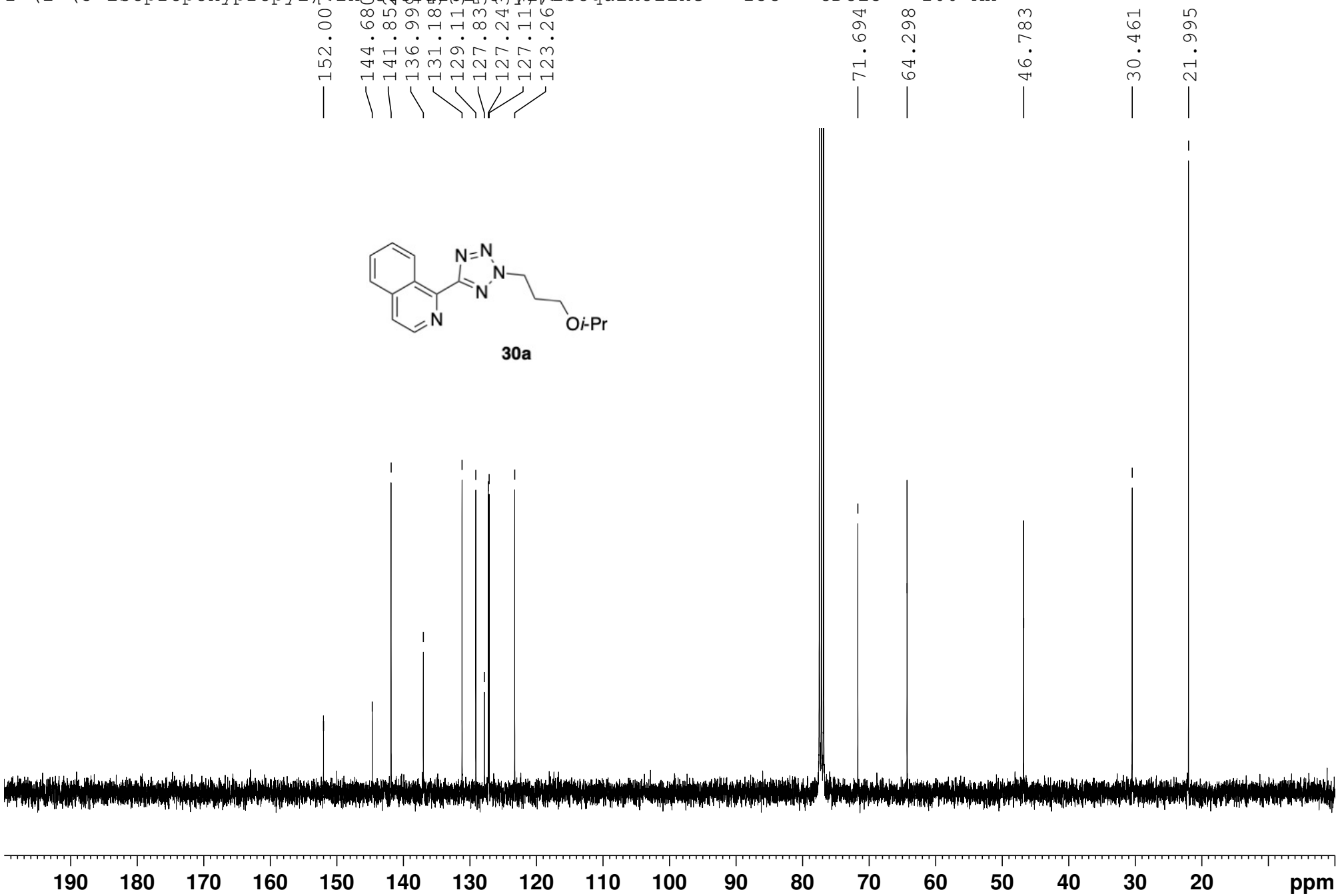
1-(2-(3-isopropoxypropyl)-2H-tetrazol-5-yl)isoquinoline - 1H - CDCl3 - 400 MHz

8.858
8.837
8.682
8.668
7.947
7.926
7.846
7.832
7.811
7.809
7.794
7.791
7.773
7.771
7.738
7.736
7.717
7.700
7.697
4.925
4.908
4.891
3.396
3.389
3.381
3.375
3.366
3.360
3.351
3.335
2.203
2.187
2.171
2.155
2.139
0.974
0.959



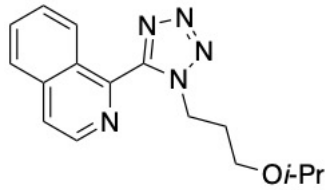
30a

1-(2-(3-isopropoxypropyl)-2H-tetrazol-5-yl)isoquinoline - 13C - CDCl3 - 100 MH



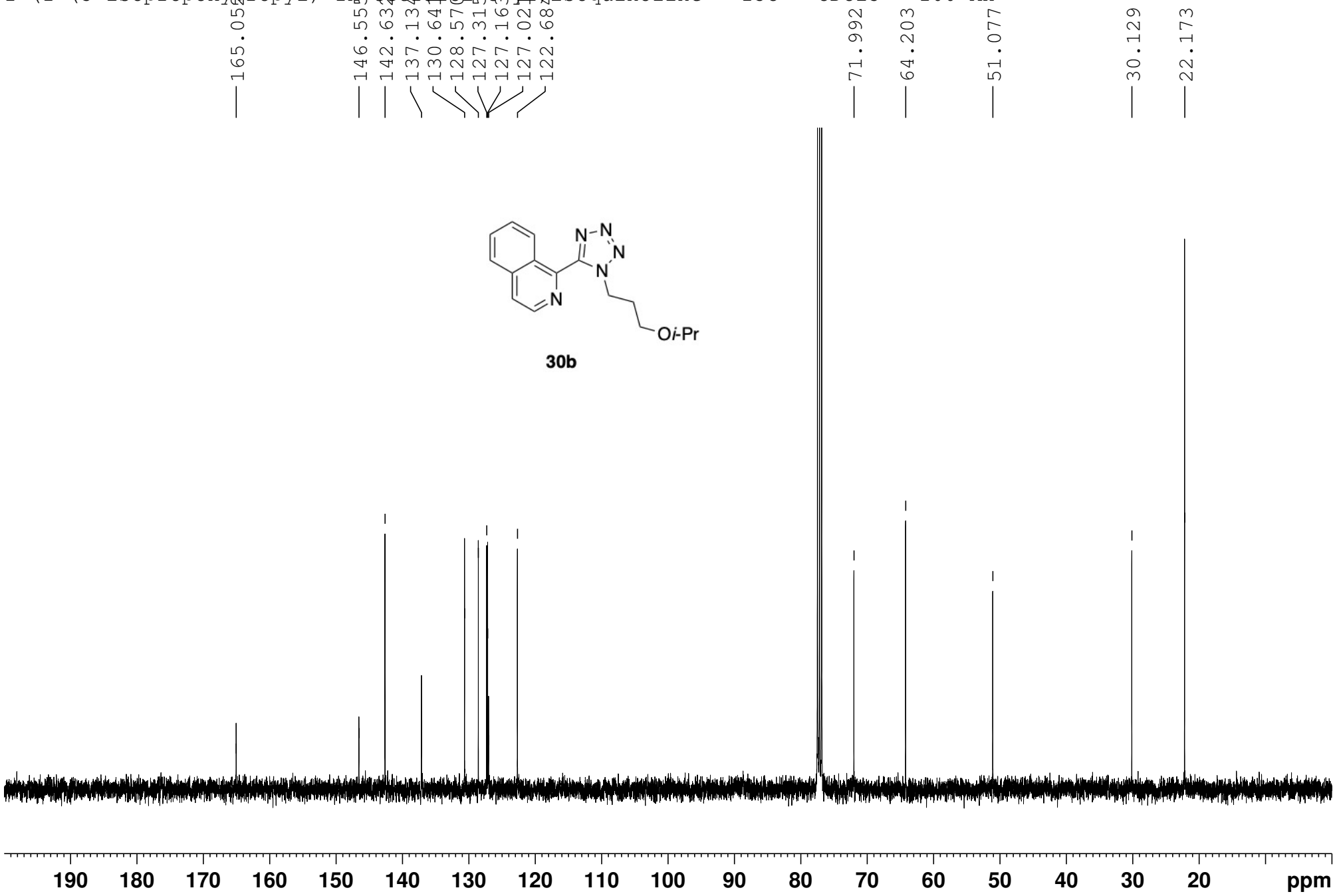
1-(1-(3-isopropoxypropyl)-1H-tetrazol-5-yl)isoquinoline - 1H - CDCl3 - 400 MHz

9.176
9.155
8.742
8.728
7.925
7.905
7.797
7.783
7.777
7.774
7.757
7.740
7.737
7.729
7.725
7.708
7.705
7.690
7.687
4.936
4.918
4.901
3.612
3.597
3.582
3.567
3.552
3.536
3.524
3.510
3.495
2.422
2.405
2.390
2.375
2.358
1.160
1.145

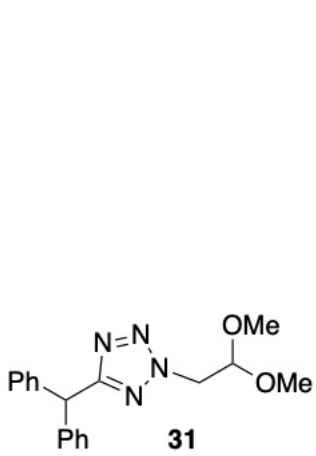


30b

1-(1-(3-isopropoxypropyl)-1H-tetrazol-5-yl)isoquinoline - 13C - CDCl3 - 100 MH

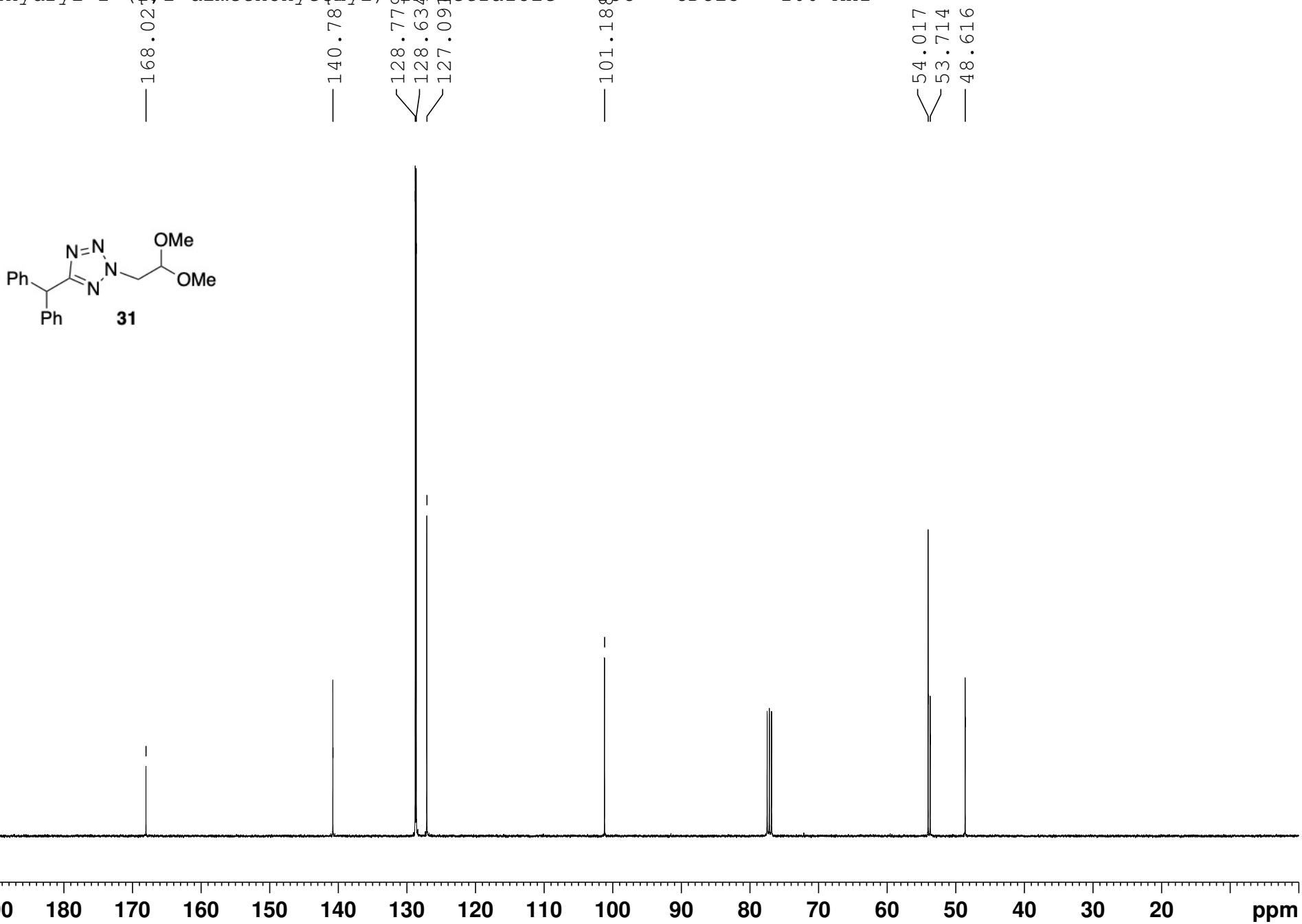


5-benzhydryl-2-(2,2-dimethoxyethyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz

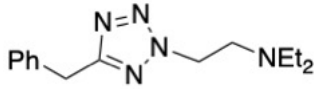


31

5-benzhydryl-2-(2,2-dimethoxyethyl)-2H-tetrazole - 13C - CDCl3 - 100 MHz

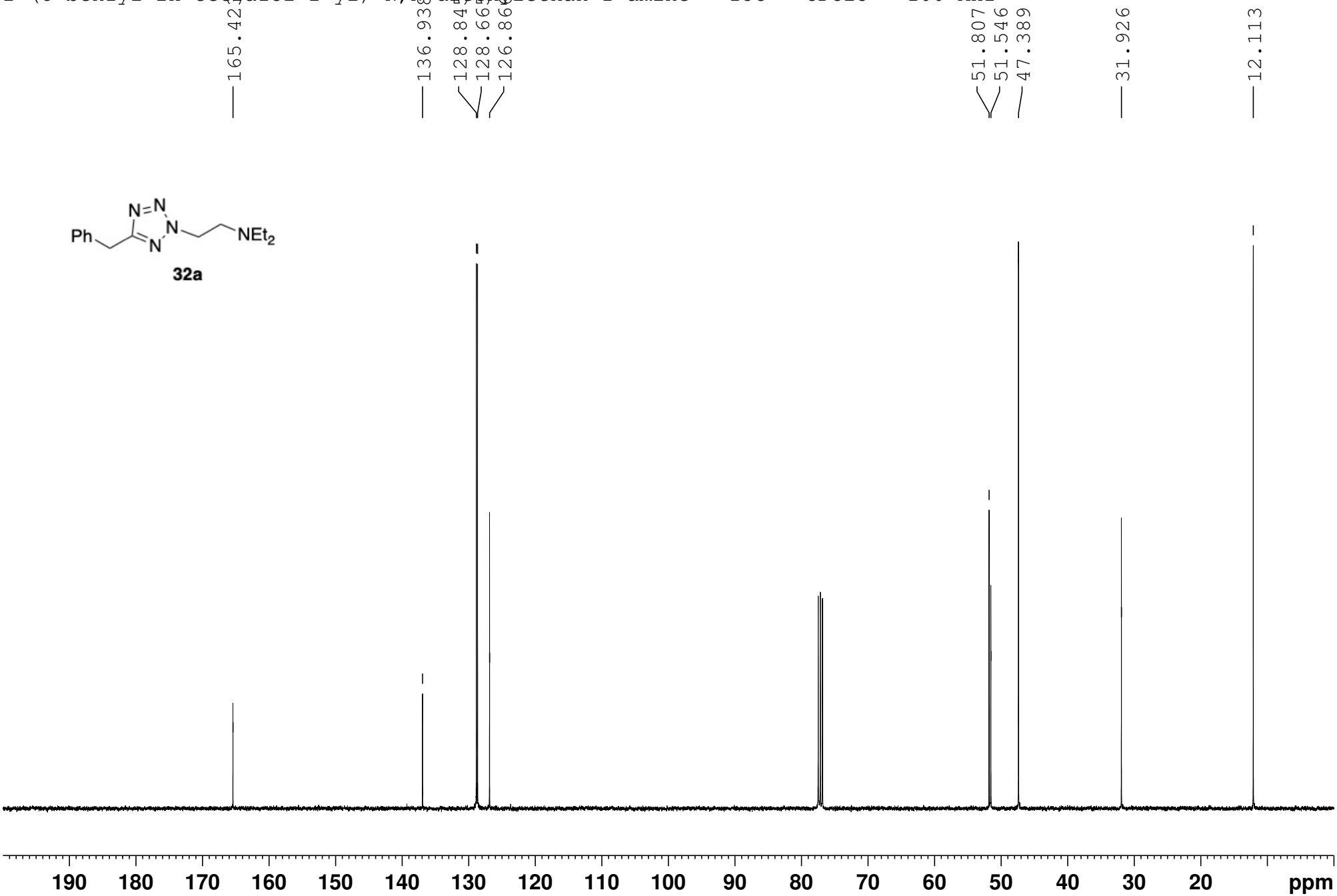


2-(5-benzyl-2H-tetrazol-2-yl)-N,N-diethylethan-1-amine - 1H - CDCl3 - 400 MHz

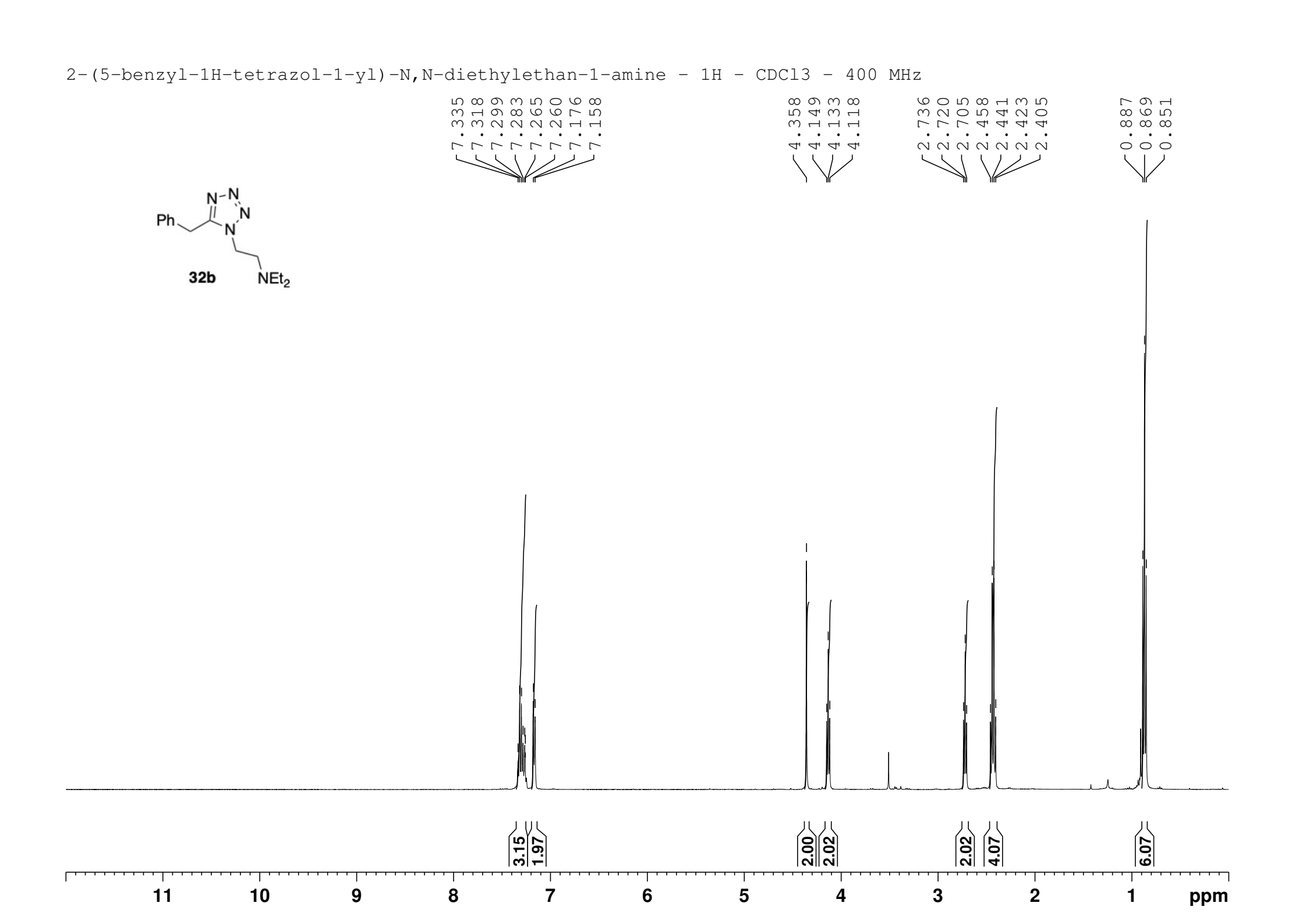


32a

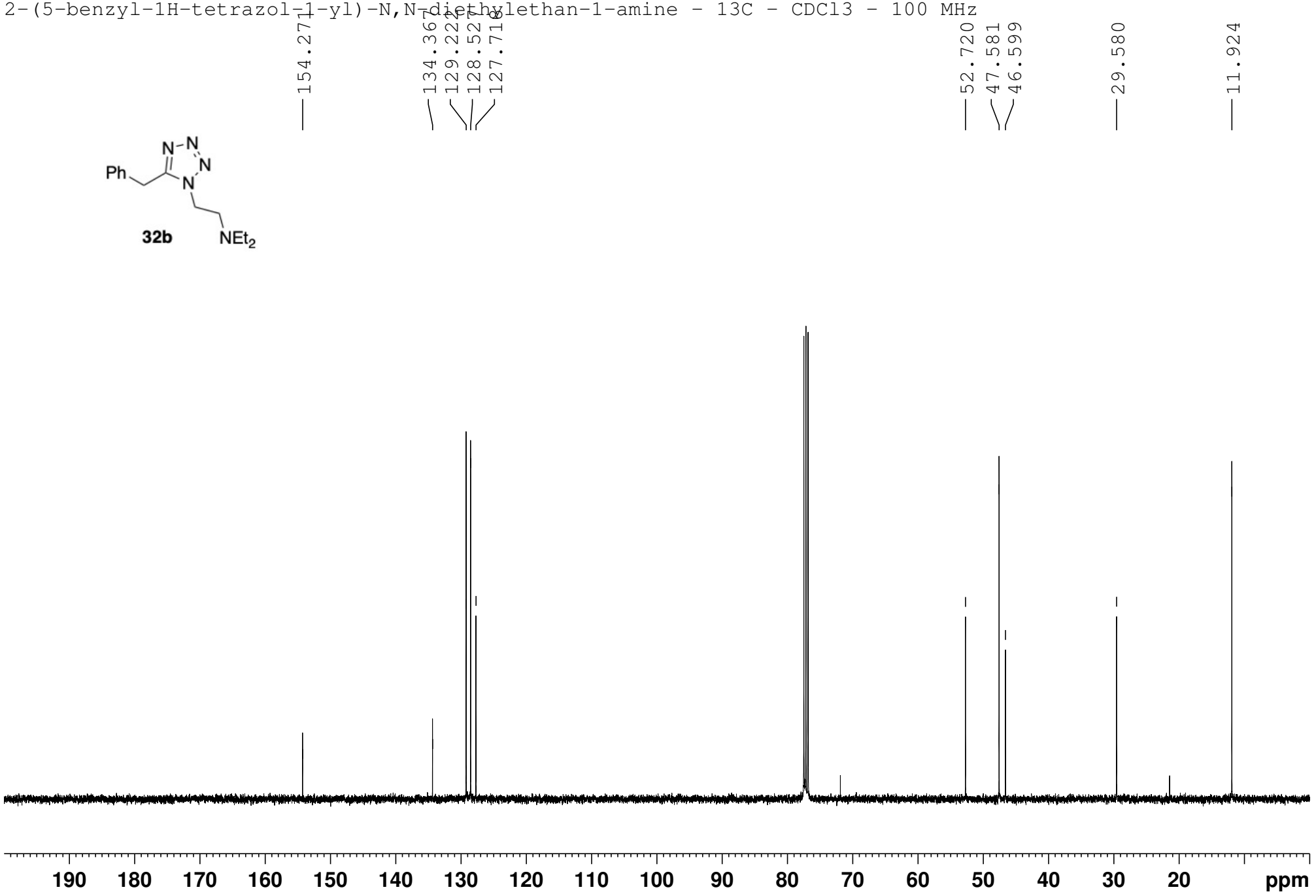
2-(5-benzyl-2H-tetrazol-2-yl)-N,N-diethylethan-1-amine - 13C - CDCl3 - 100 MHz



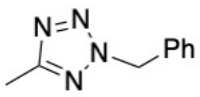
2-(5-benzyl-1H-tetrazol-1-yl)-N,N-diethylethan-1-amine - 1H - CDCl3 - 400 MHz



2-(5-benzyl-1H-tetrazol-1-yl)-N,N-diethylethan-1-amine - 13C - CDCl3 - 100 MHz

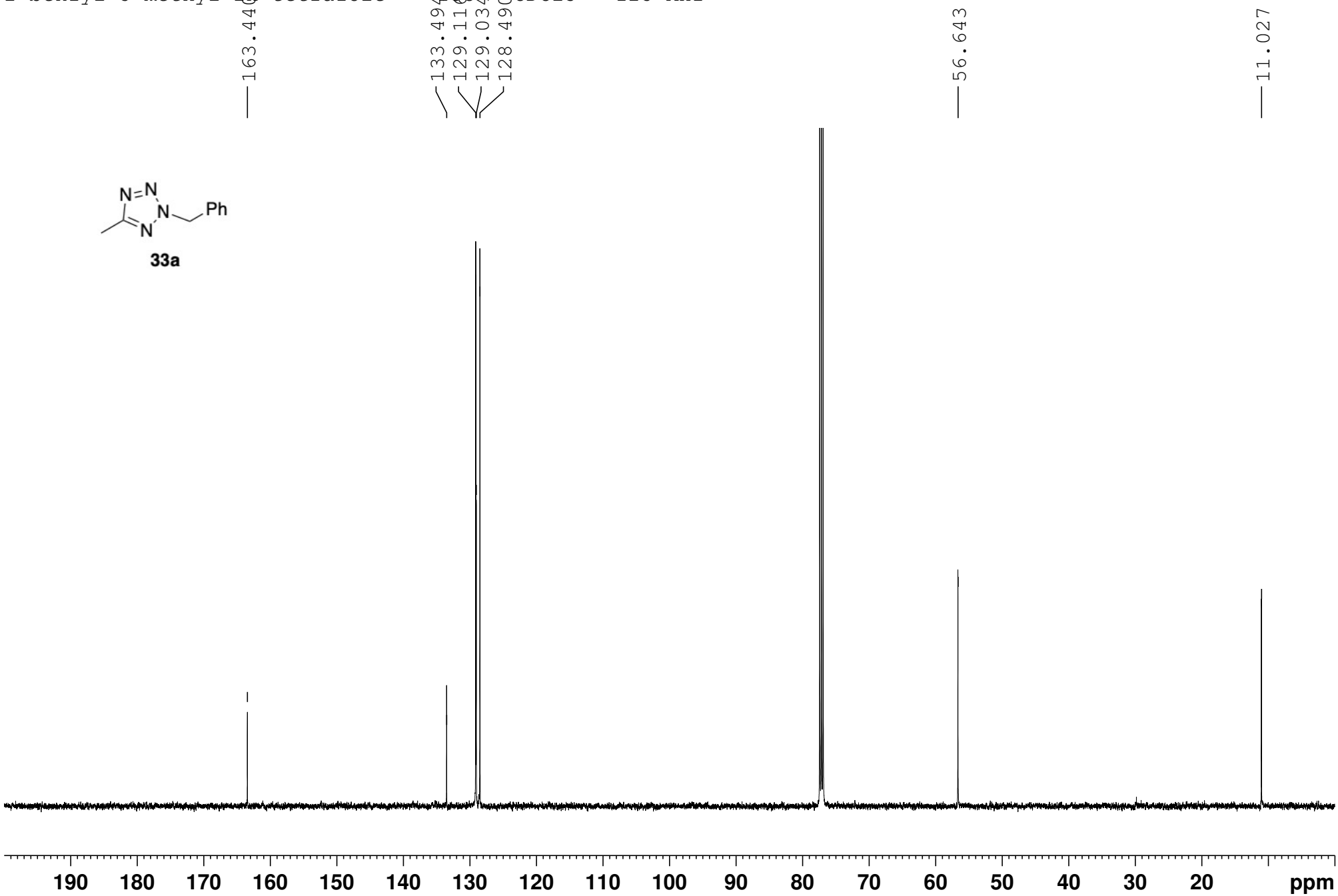


2-benzyl-5-methyl-2H-tetrazole - 1H - CDCl3 - 500 MHz

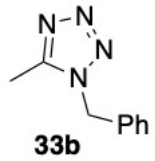


33a

2-benzyl-5-methyl-2H-tetrazole - 13C - CDCl3 - 125 MHz

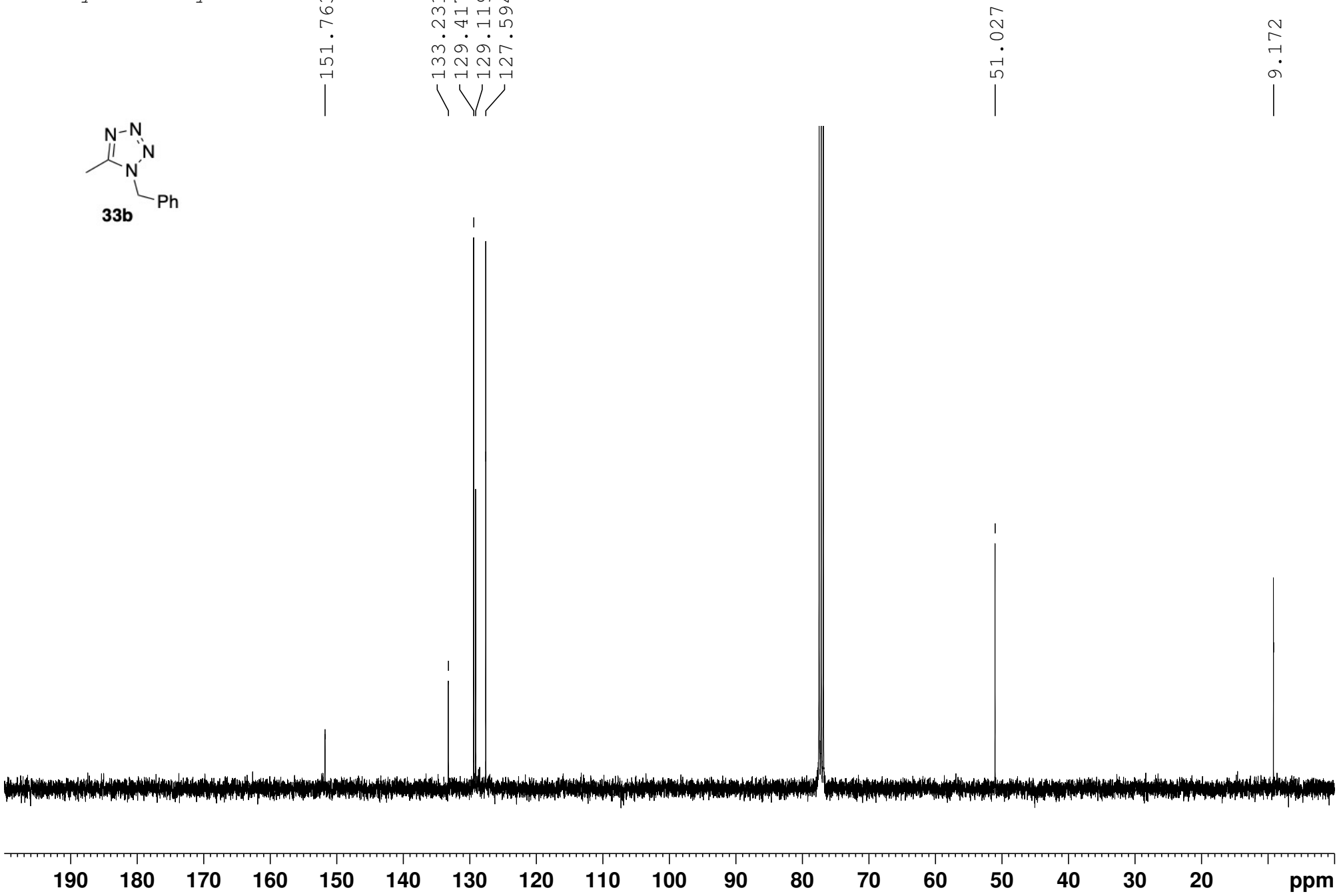


1-benzyl-5-methyl-1H-tetrazole - 1H - CDCl3 - 500 MHz

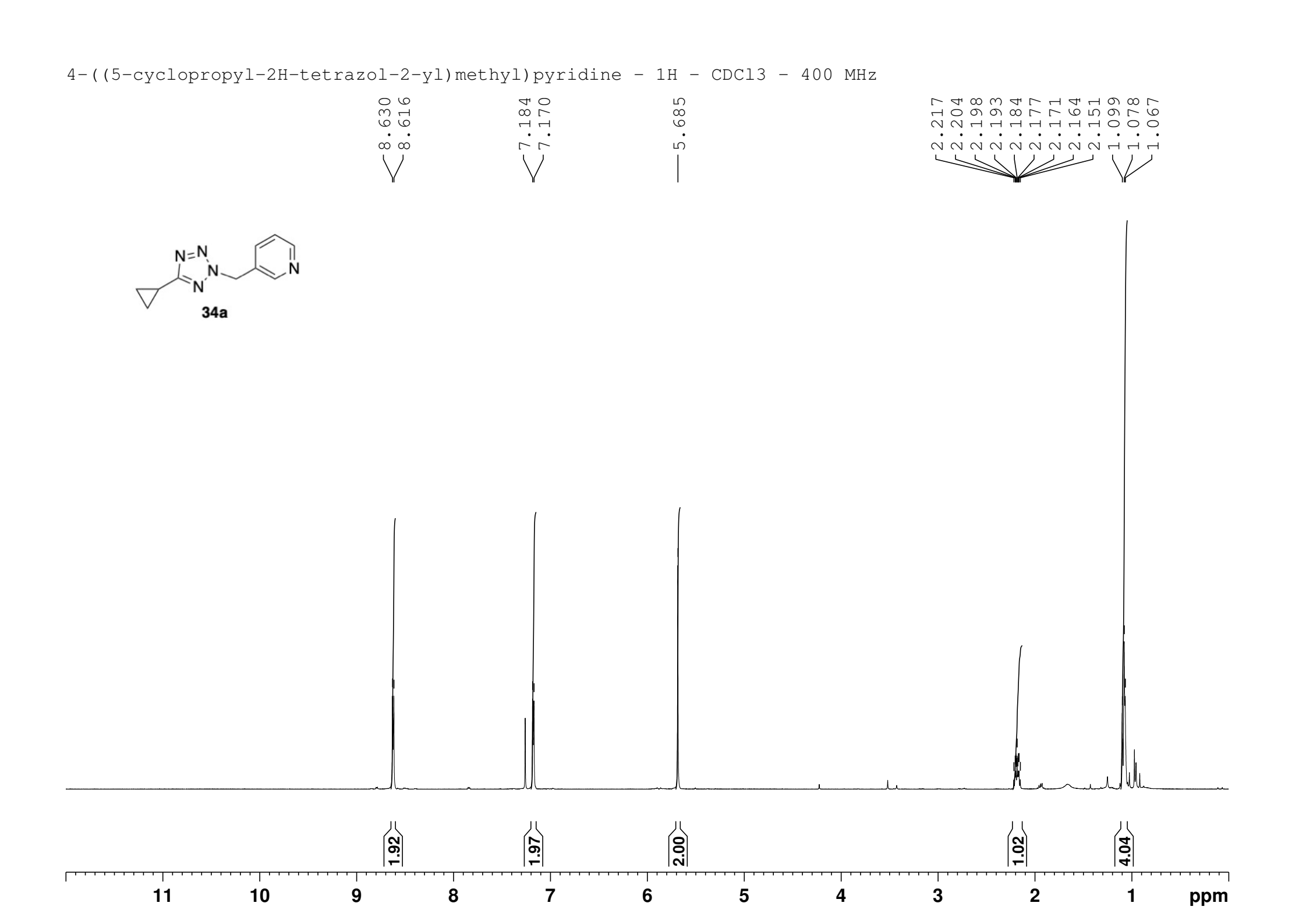


33b

1-benzyl-5-methyl-1H-tetrazole - 13C - CDCl3 - 100 MHz

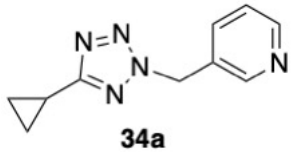


4-((5-cyclopropyl-2H-tetrazol-2-yl)methyl)pyridine - 1H - CDCl3 - 400 MHz

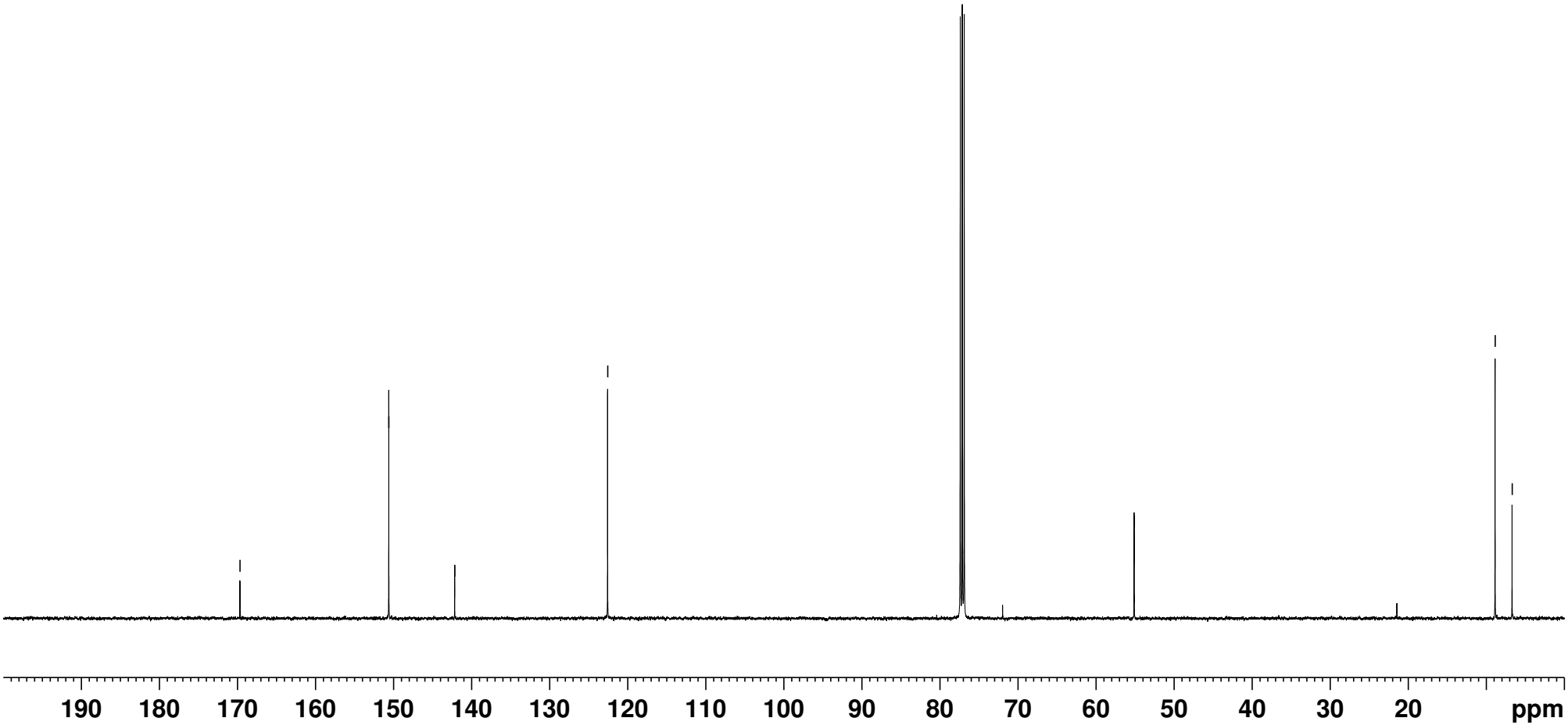


4-((5-cyclopropyl-2H-tetrazol-2-yl)methyl)pyridine - 13C - CDCl3 - 125 MHz

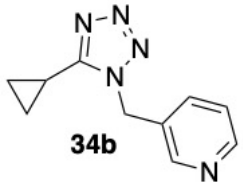
169.67
150.60
142.16
122.57
55.105
8.858
6.682



34a



4-((5-cyclopropyl-1H-tetrazol-1-yl)methyl)pyridine - 1H - CDCl3 - 400 MHz



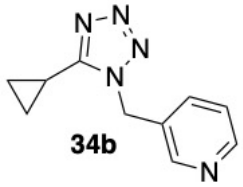
8.644
8.629
7.086
7.072
5.603
1.737
1.725
1.716
1.705
1.692
1.684
1.672
1.214
1.208
1.198
1.187
1.158
1.149
1.144
1.138
1.129
1.123

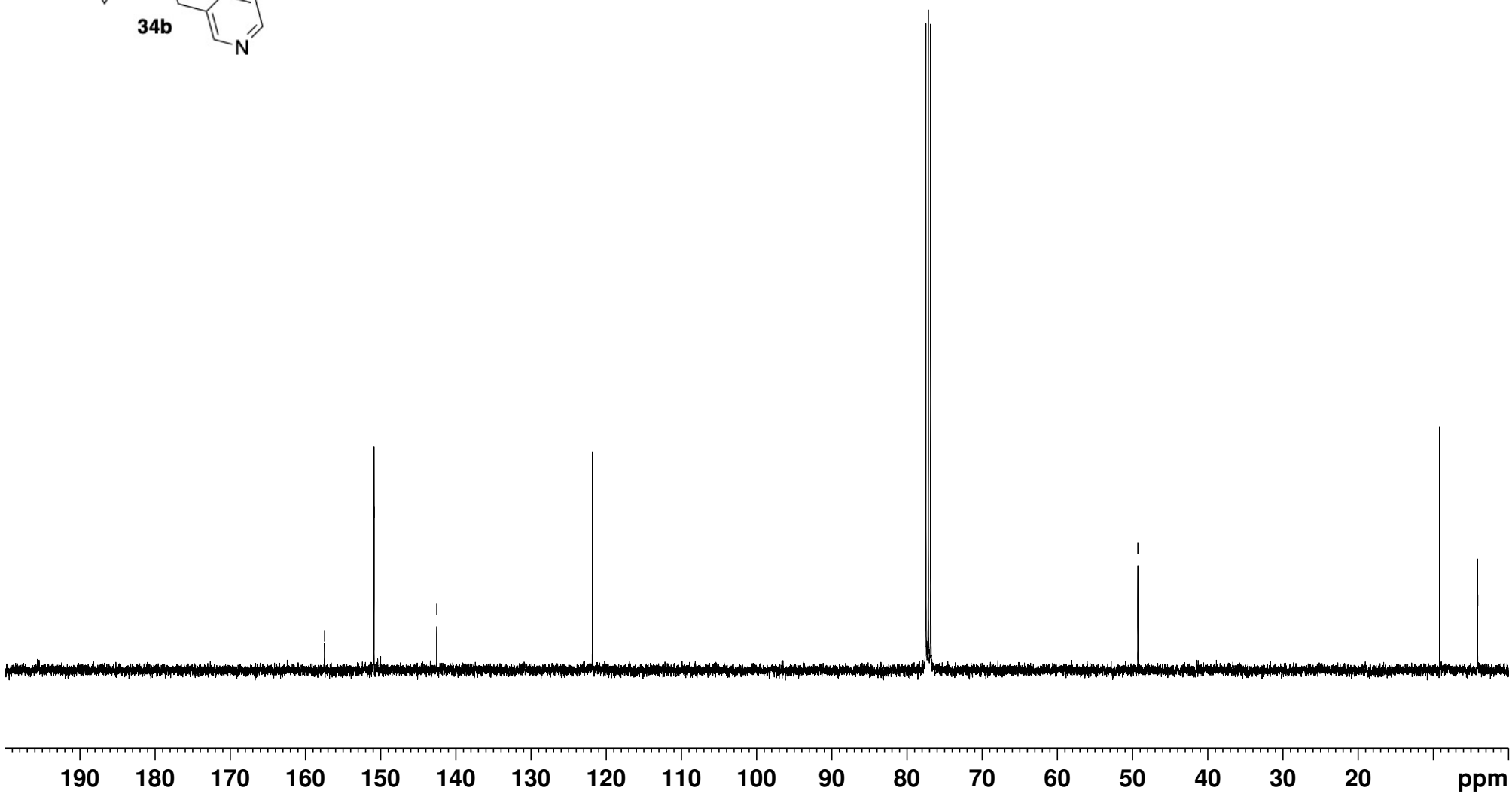
2.02
1.96
2.00
1.42
1.97
2.18

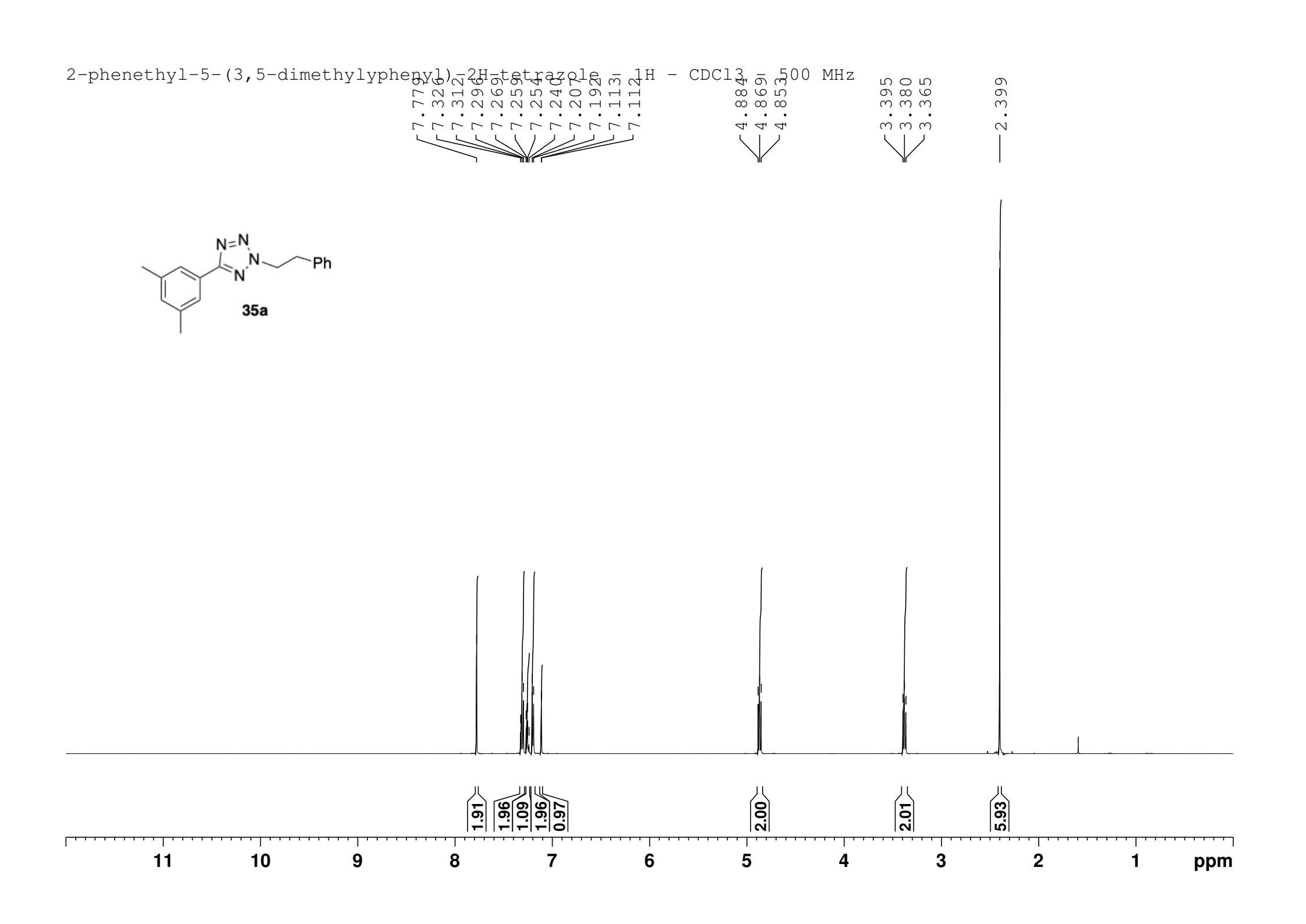
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm

4-((5-cyclopropyl-1H-tetrazol-1-yl)methyl)pyridine - 13C - CDCl3 - 100 MHz

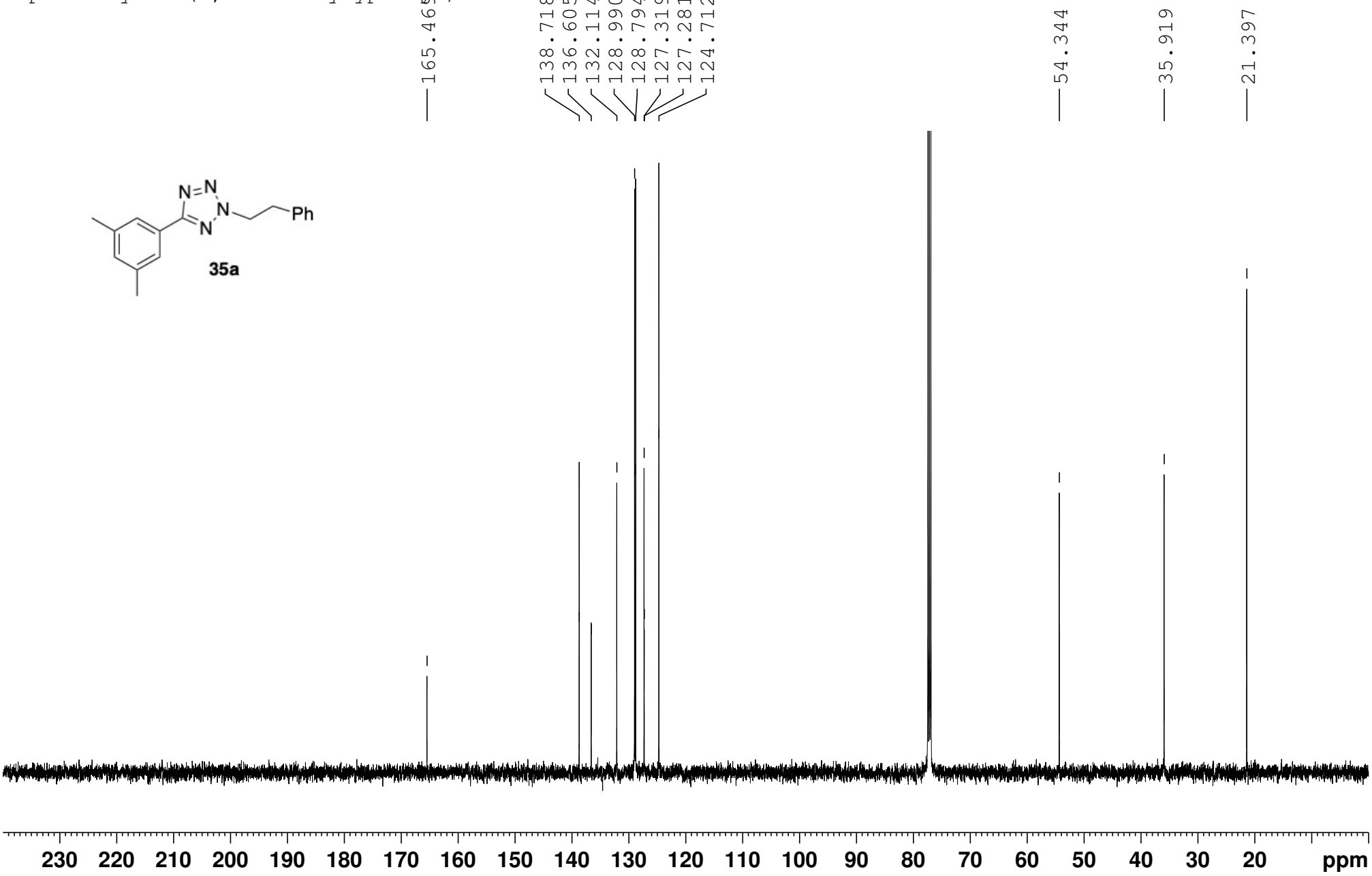
157.458
150.870
142.520
121.831
49.289
9.169
4.107

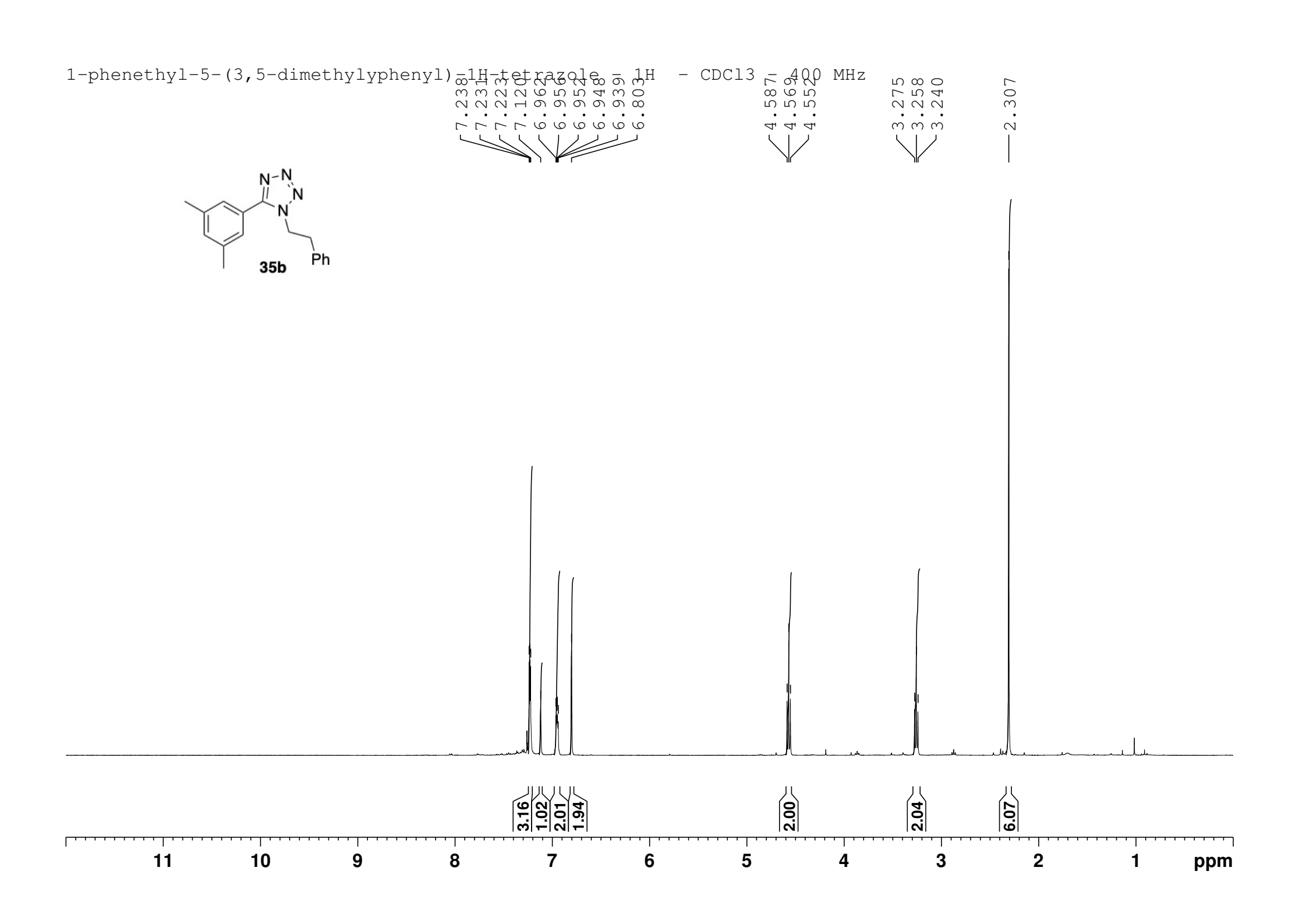




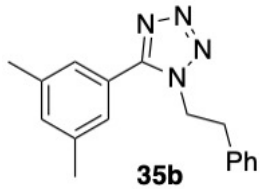

2-phenethyl-5-(3,5-dimethylyphenyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz
7.776
7.326
7.312
7.296
7.269
7.259
7.254
7.240
7.207
7.192
7.113
7.112
4.884
4.869
4.853
3.395
3.380
3.365
2.399
N=N
N
N
Ph
35a
1.91
1.96
1.09
1.96
0.97
2.00
2.01
5.93
11
10
9
8
7
6
5
4
3
2
1
ppm

2-phenethyl-5-(3,5-dimethylyphenyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz



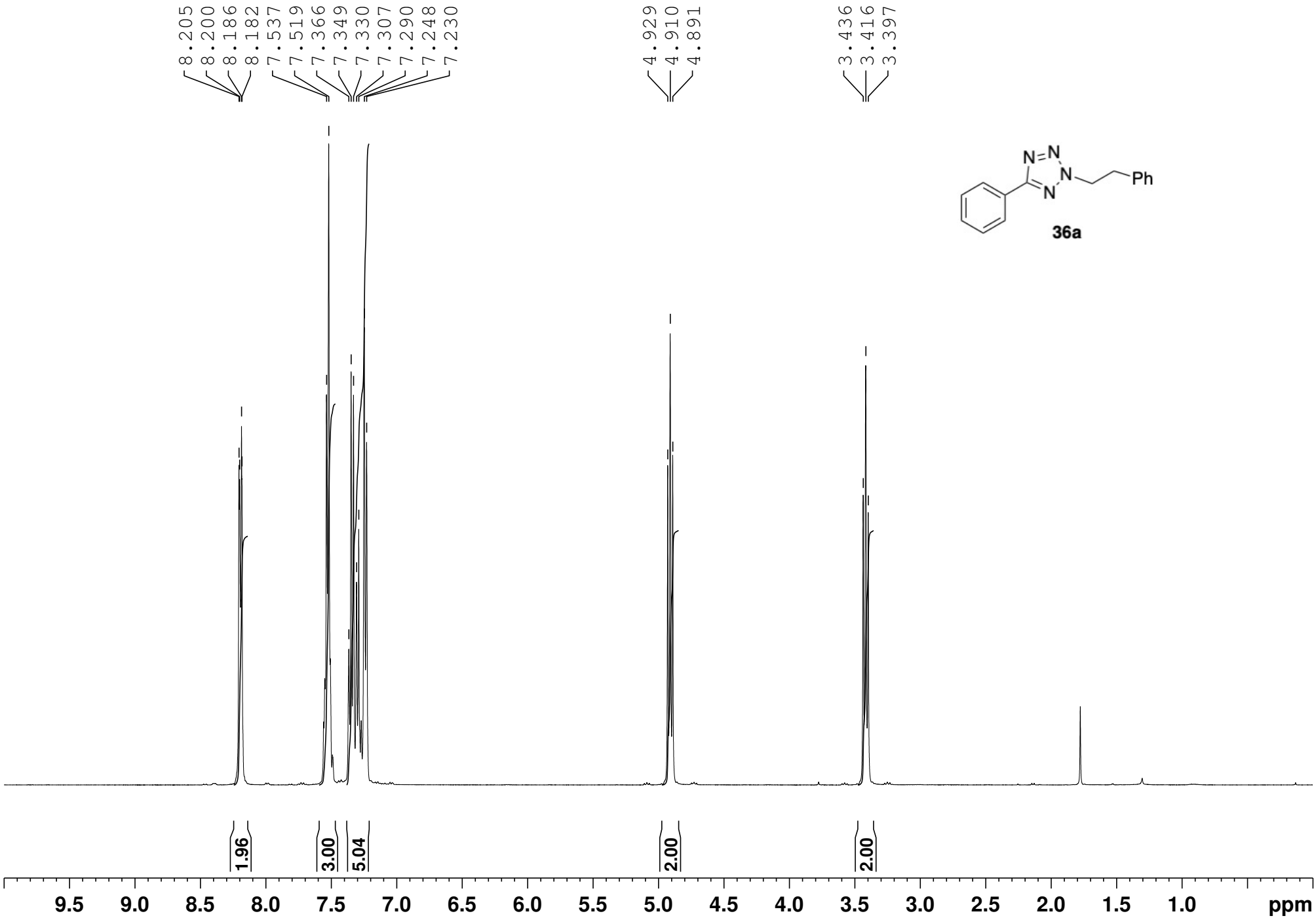

1-phenethyl-5-(3,5-dimethylyphenyl)-1H-tetrazole 1H - CDCl3 400 MHz
7.238
7.231
7.223
7.120
6.962
6.956
6.954
6.948
6.939
6.803
4.587
4.569
4.552
3.275
3.258
3.240
2.307
35b
Ph
3.16
1.02
2.01
1.94
2.00
2.04
6.07
11
10
9
8
7
6
5
4
3
2
1
ppm

1-phenethyl-5-(3,5-dimethylyphenyl)-1H-tetrazole - 13C - CDCl3 - 100 MHz

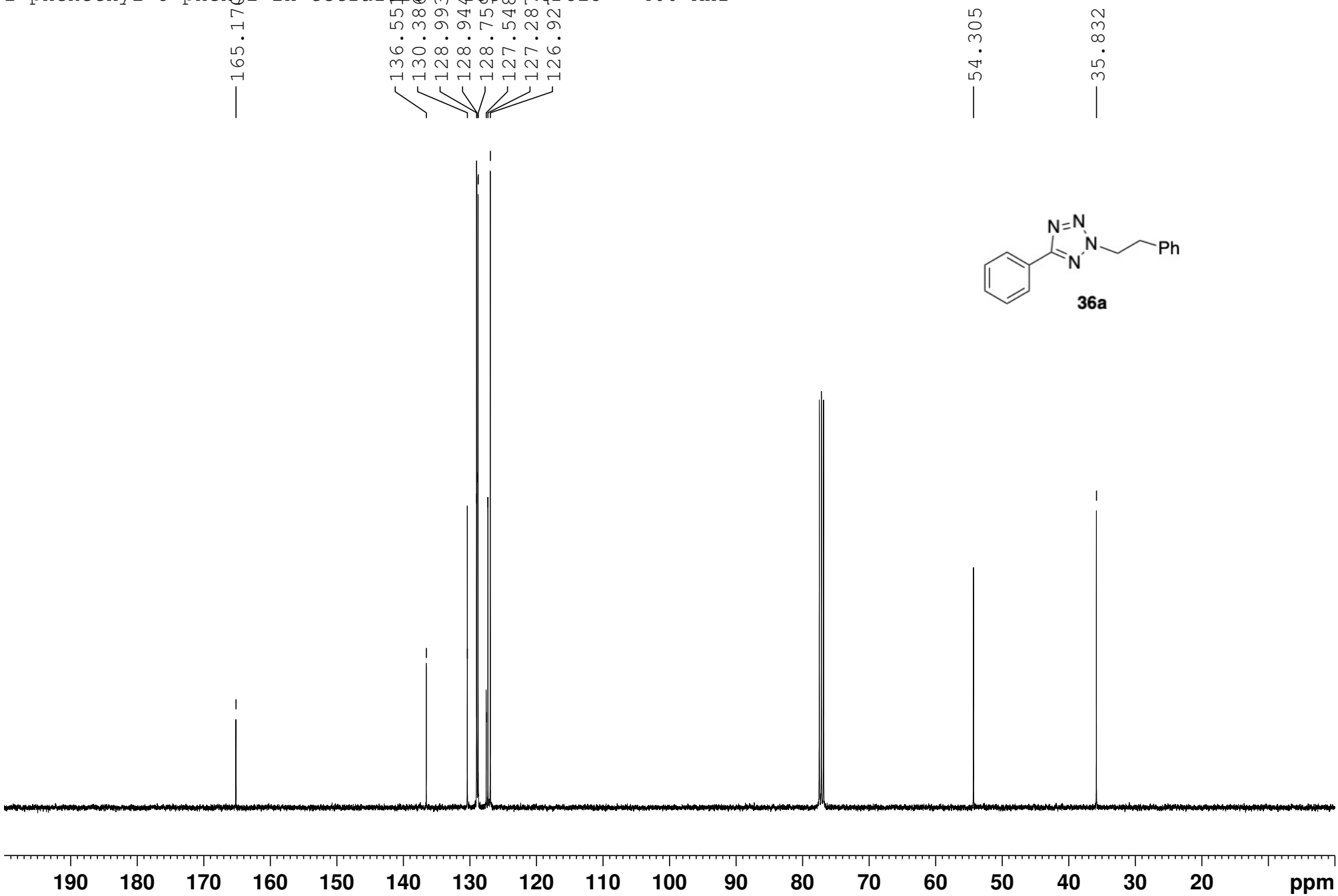


35b

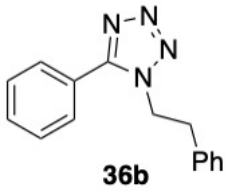
2-phenethyl-5-phenyl-2H-tetrazole - 1H - CDCl3 - 400 MHz



2-phenethyl-5-phenyl-2H-tetrazole - 13C - CDCl3 - 400 MHz

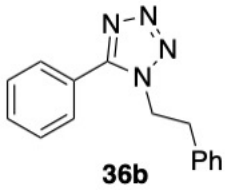


1-phenethyl-5-phenyl-1H-tetrazole - 1H - CDCl3 - 500 MHz



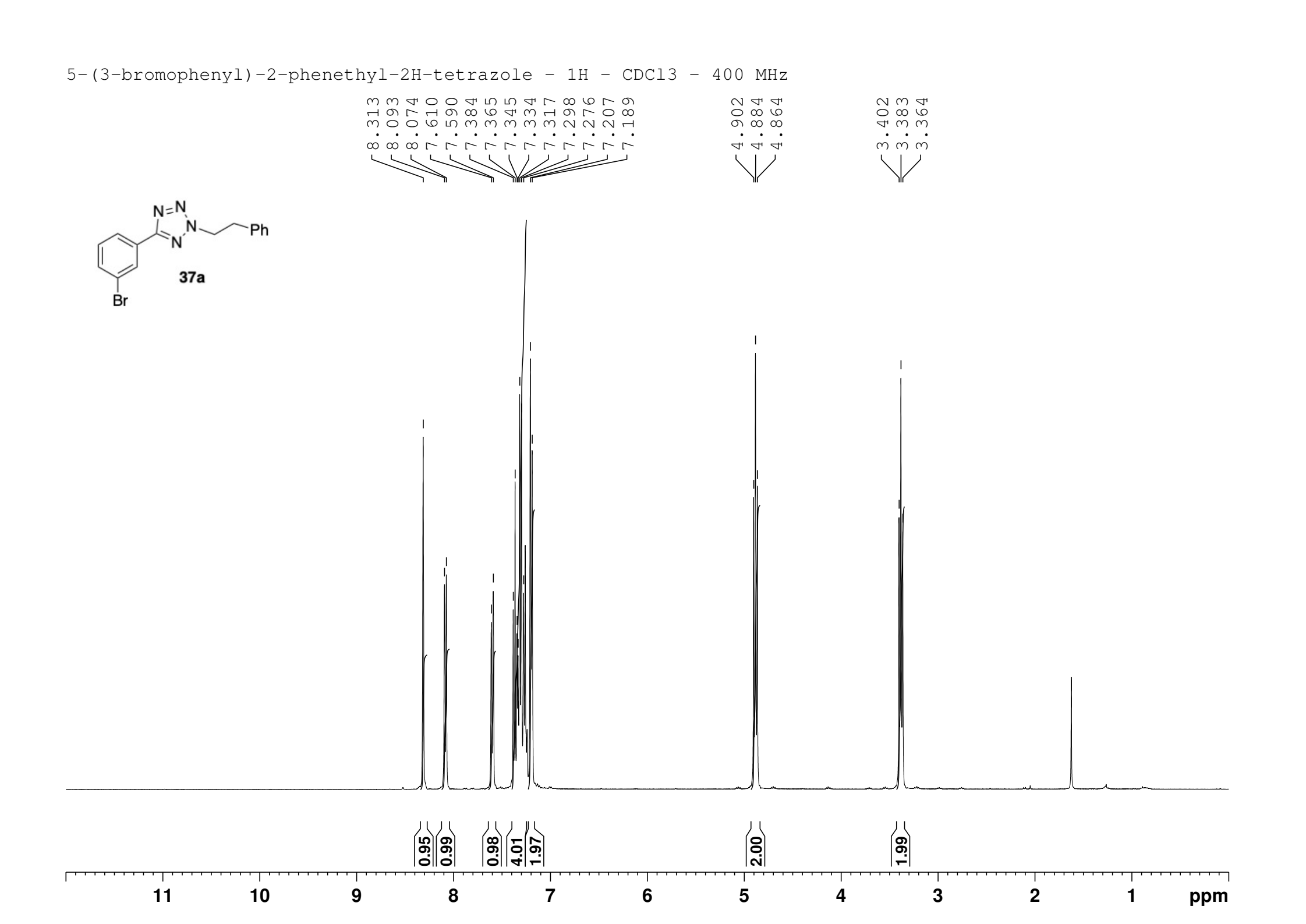
36b

1-phenethyl-5-phenyl-1H-tetrazole - 13C - CDCl3 - 125 MHz

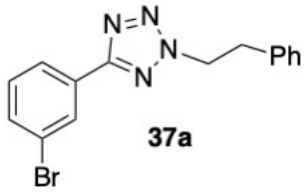


36b

5-(3-bromophenyl)-2-phenethyl-2H-tetrazole - 1H - CDCl3 - 400 MHz



5-(3-bromophenyl)-2-phenethyl-2H-tetrazole_-_13C_CDCl3_-_100 MHz

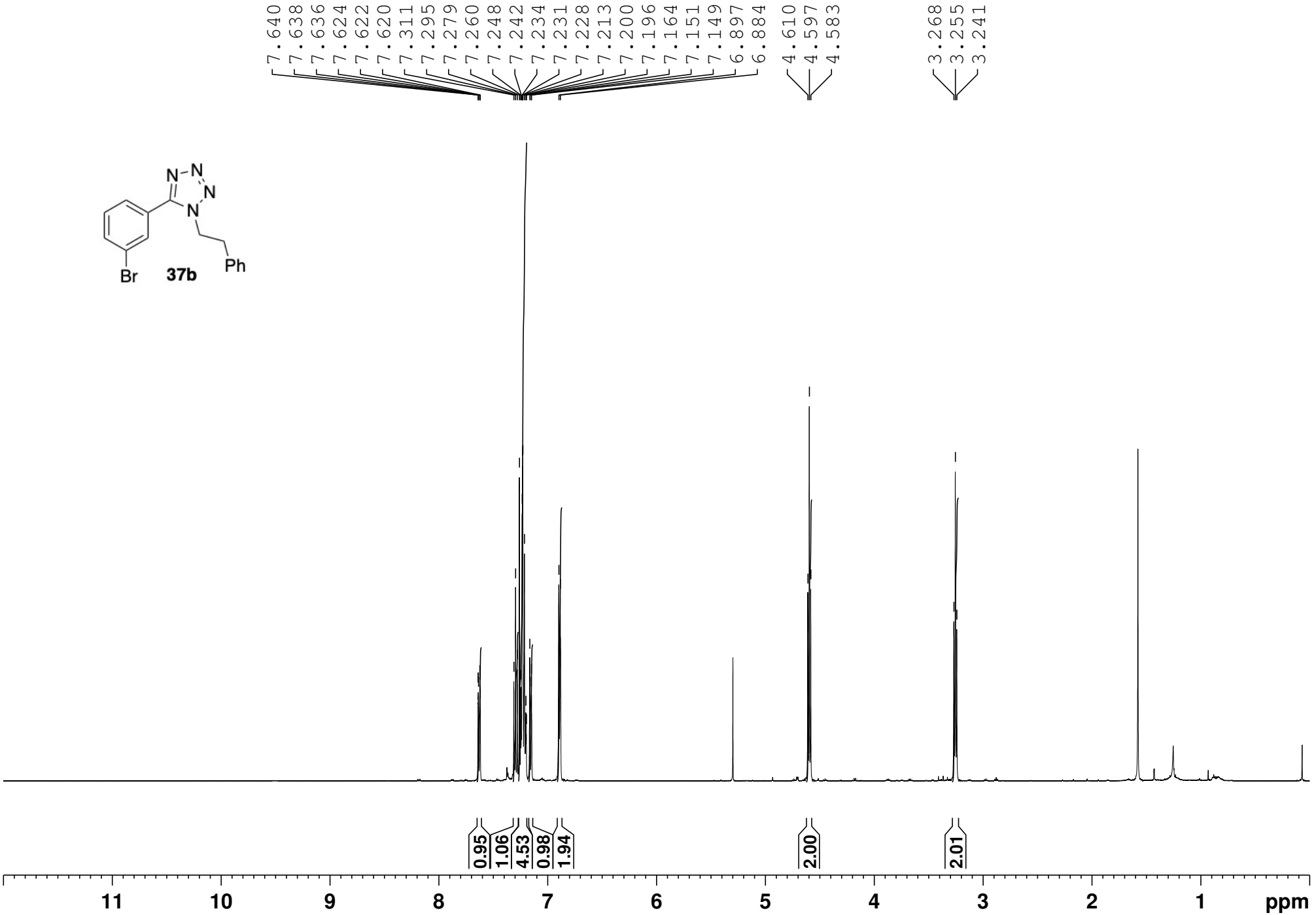


37a

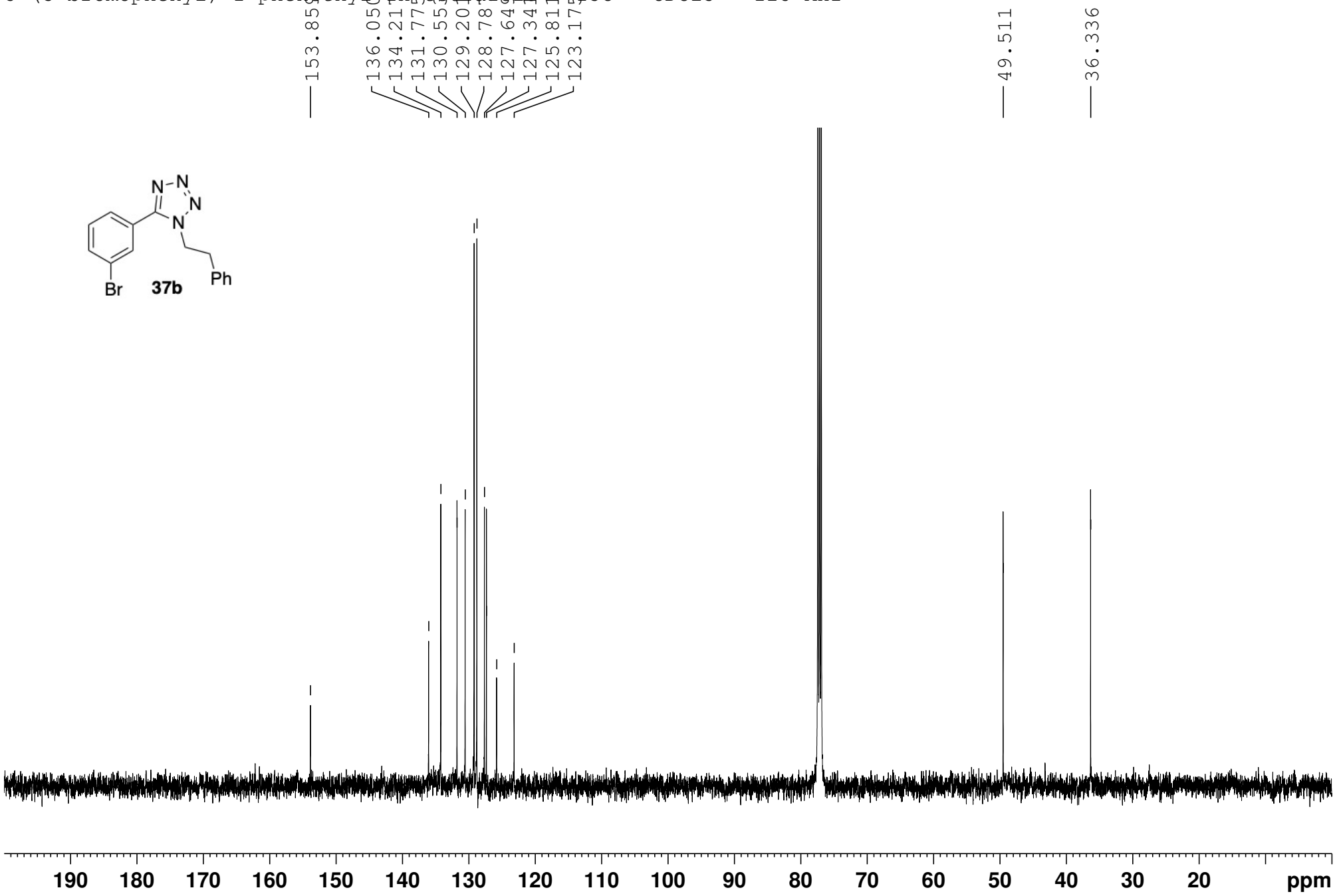
163.947
136.431
133.369
130.590
129.928
129.500
129.004
128.757
127.377
125.477
123.099
54.459
35.828

240 220 200 180 160 140 120 100 80 60 40 20 ppm

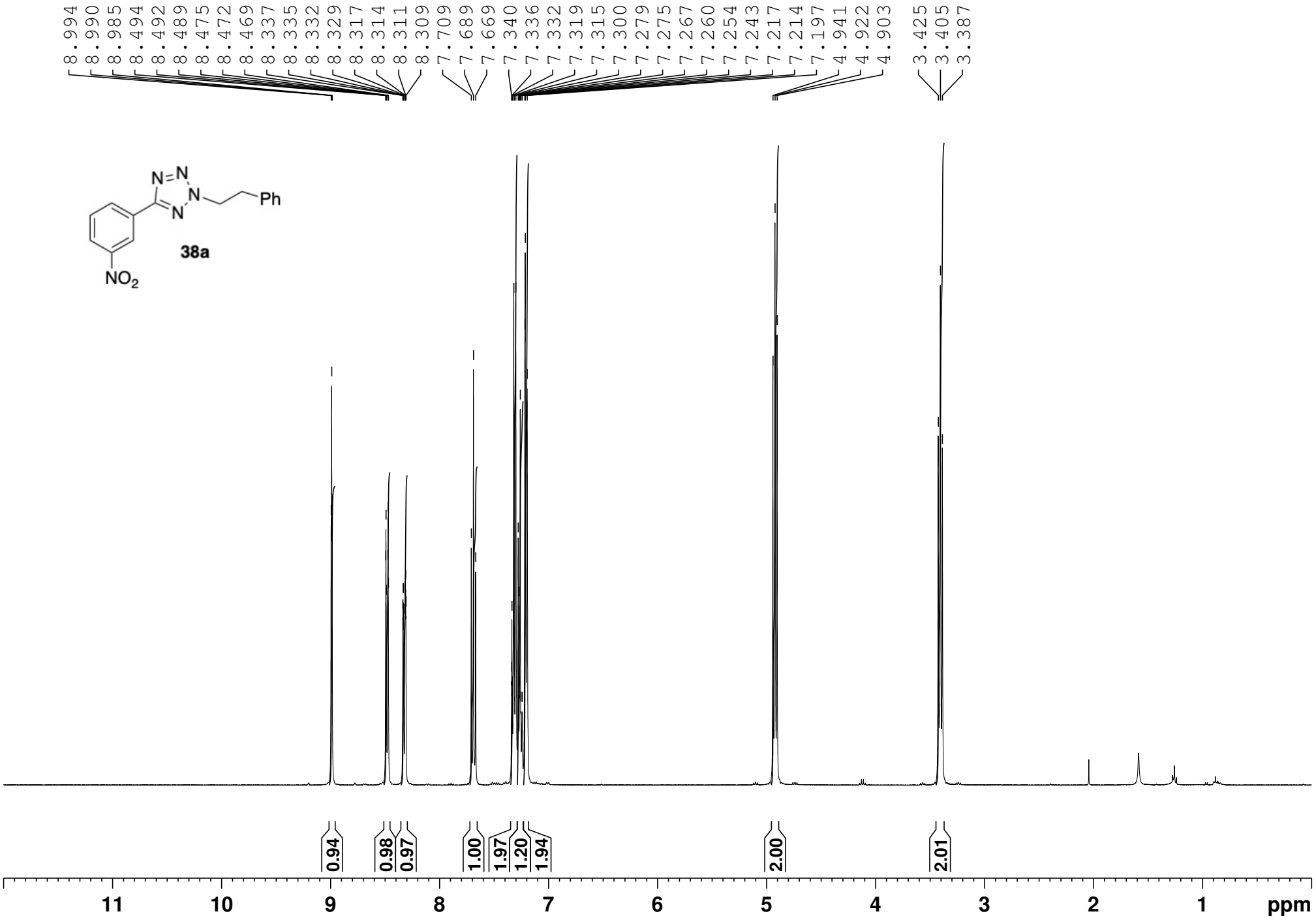
5-(3-bromophenyl)-1-phenethyl-1H-tetrazole - 1H - CDCl3 - 500 MHz



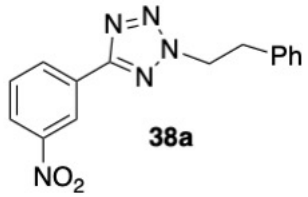
5-(3-bromophenyl)-1-phenethyl-1H-tetrazole - 13C - CDCl3 - 125 MHz



2-phenethyl-5-(3-nitrophenyl)-2H-tetrazole - 1H - CDCl3 - 400 MHz



2-phenethyl-5-(3-nitrophenyl)-2H-tetrazole - 13C - CDCl3 - 100 MHz

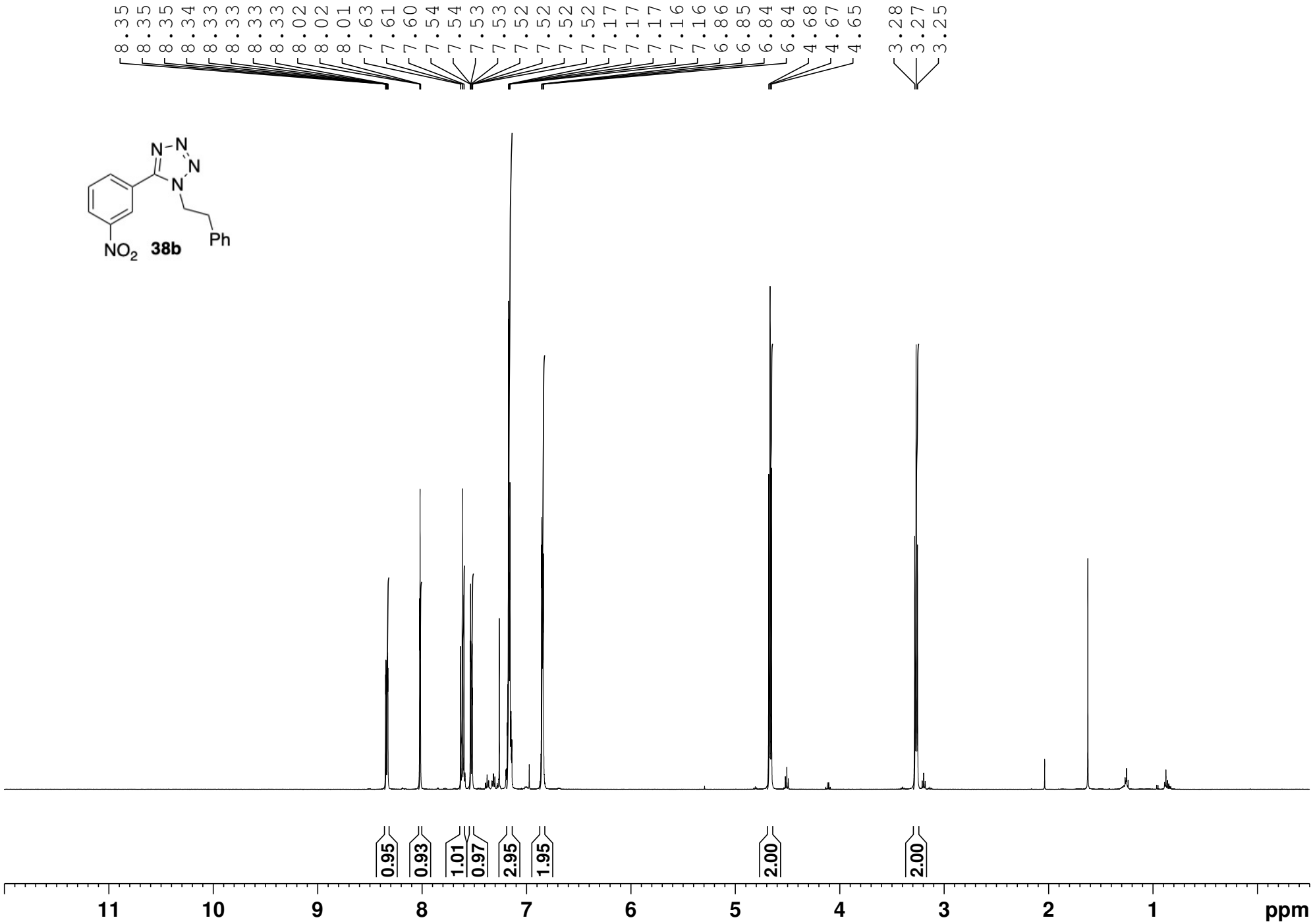


38a

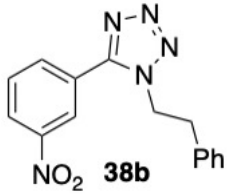
163.353
148.847
136.307
132.593
130.187
129.337
129.047
128.762
127.455
124.952
121.997
54.629
35.814

240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

1-phenethyl-5-(3-nitrophenyl)-1H-tetrazole - 1H - CDCl3 - 500 MHz

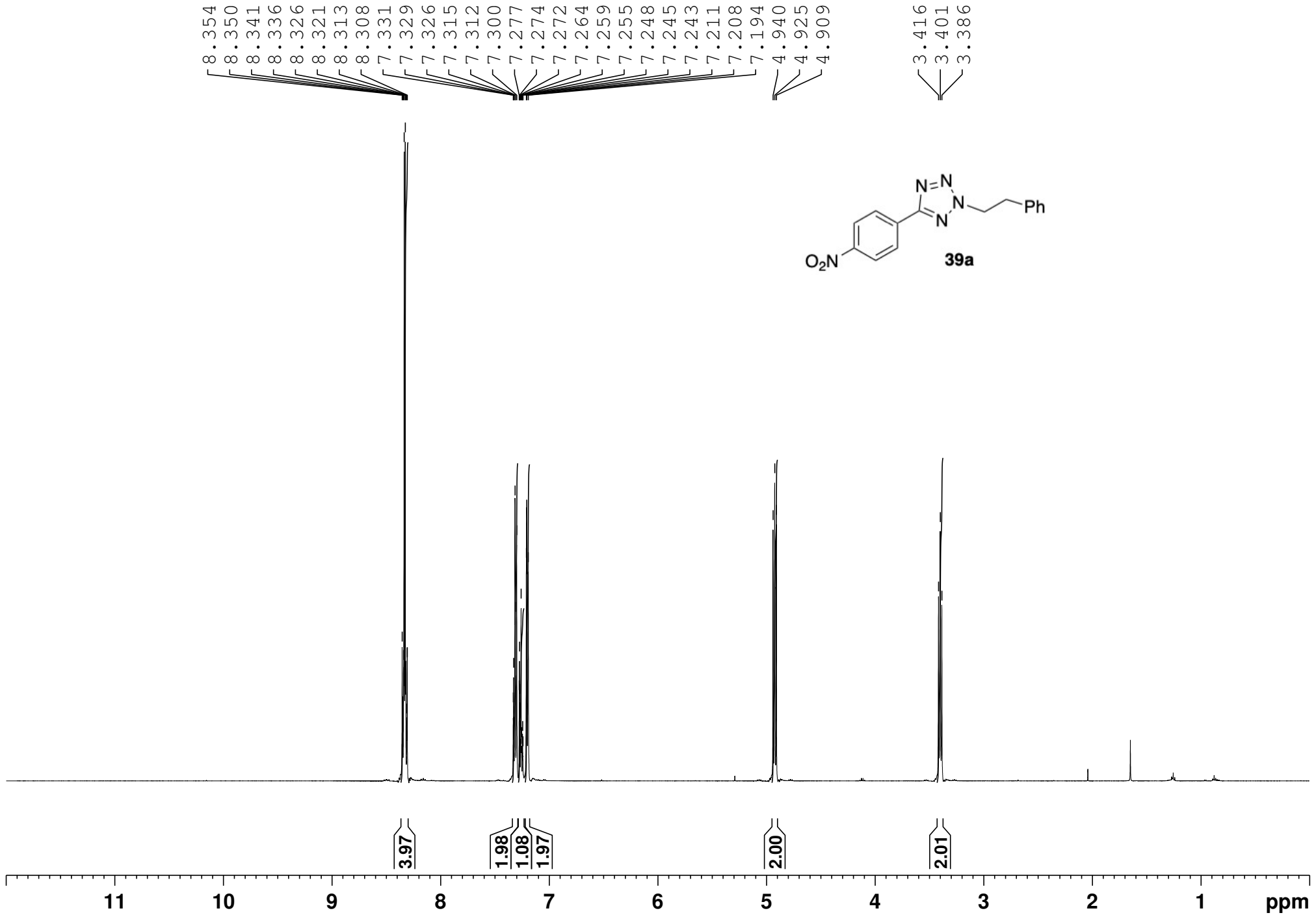


1-phenethyl-5-(3-nitrophenyl)-1H-tetrazole - 13C - CDCl3 - 125 MHz

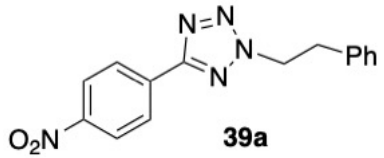


38b

2-phenethyl-5-(4-nitrophenyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz

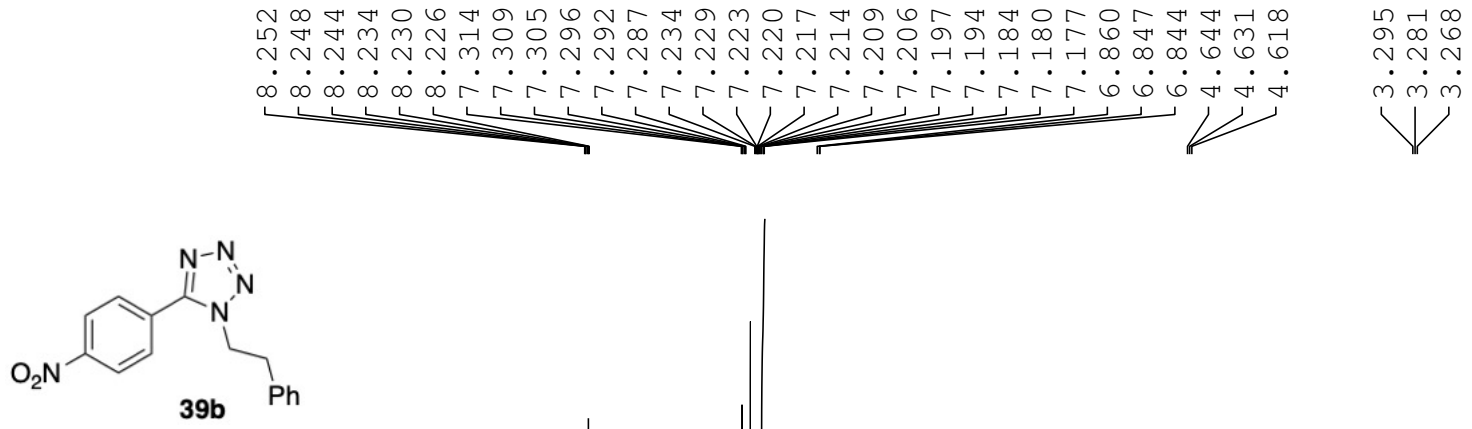


2-phenethyl-5-(4-nitrophenyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz



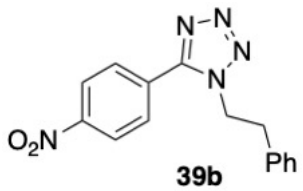
39a

1-phenethyl-5-(4-nitrophenyl)-1H-tetrazole - 1H - CDCl3 - 500 MHz



39b

1-phenethyl-5-(4-nitrophenyl)-1H-tetrazole - 13C - CDCl3 - 125 MHz

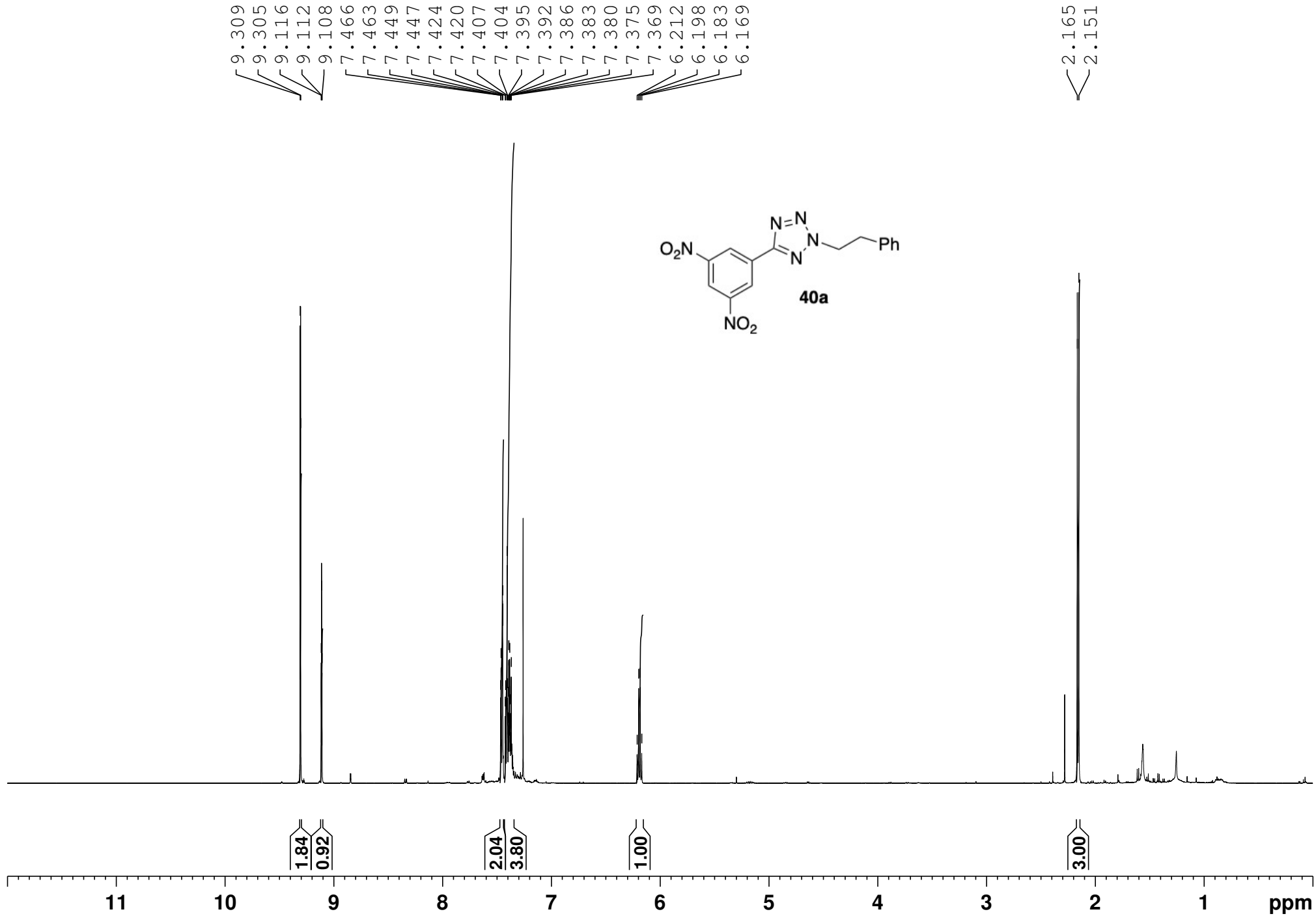


39b

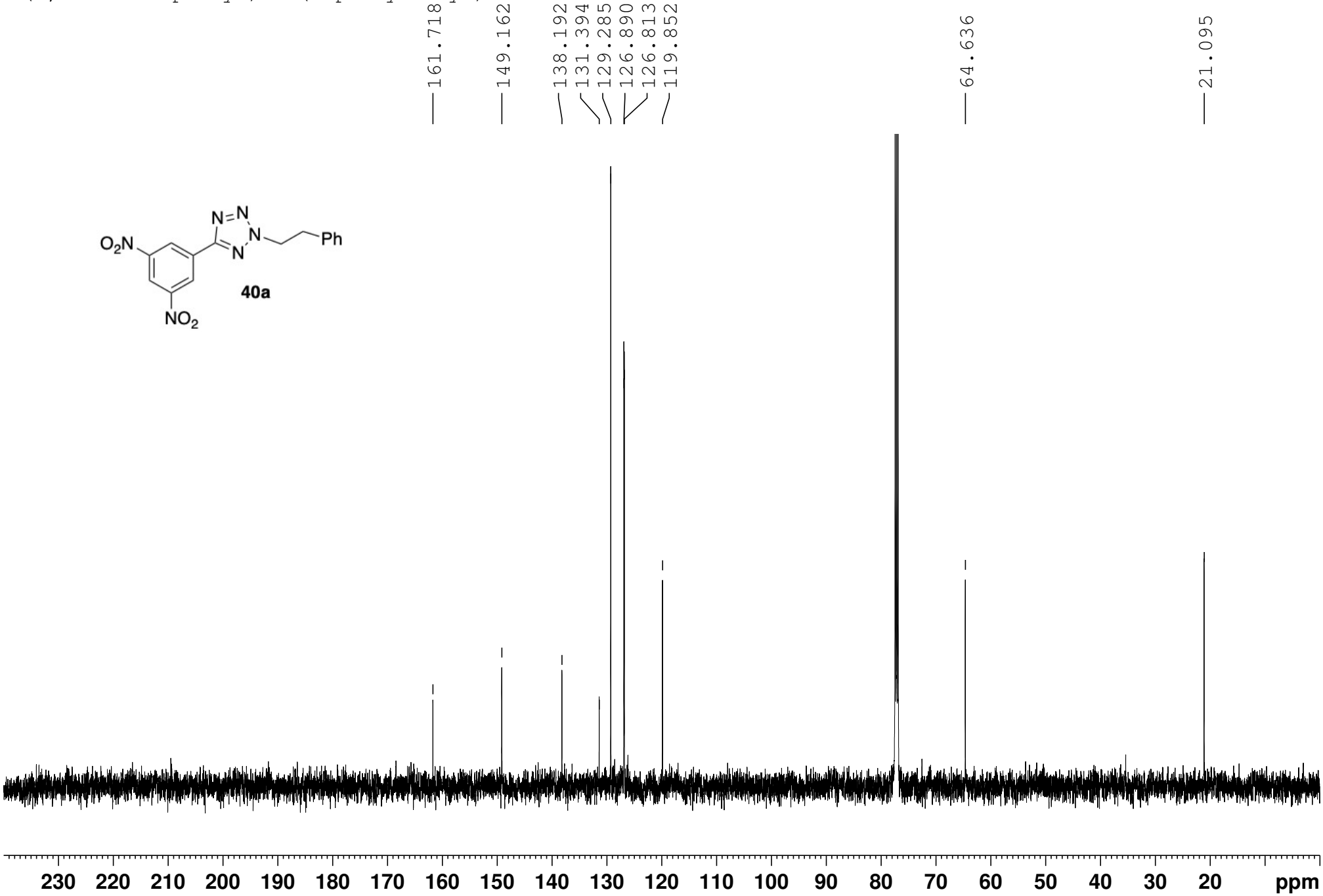
153.469
149.308
135.992
130.056
130.023
129.239
128.830
127.805
124.155
49.828
36.393

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

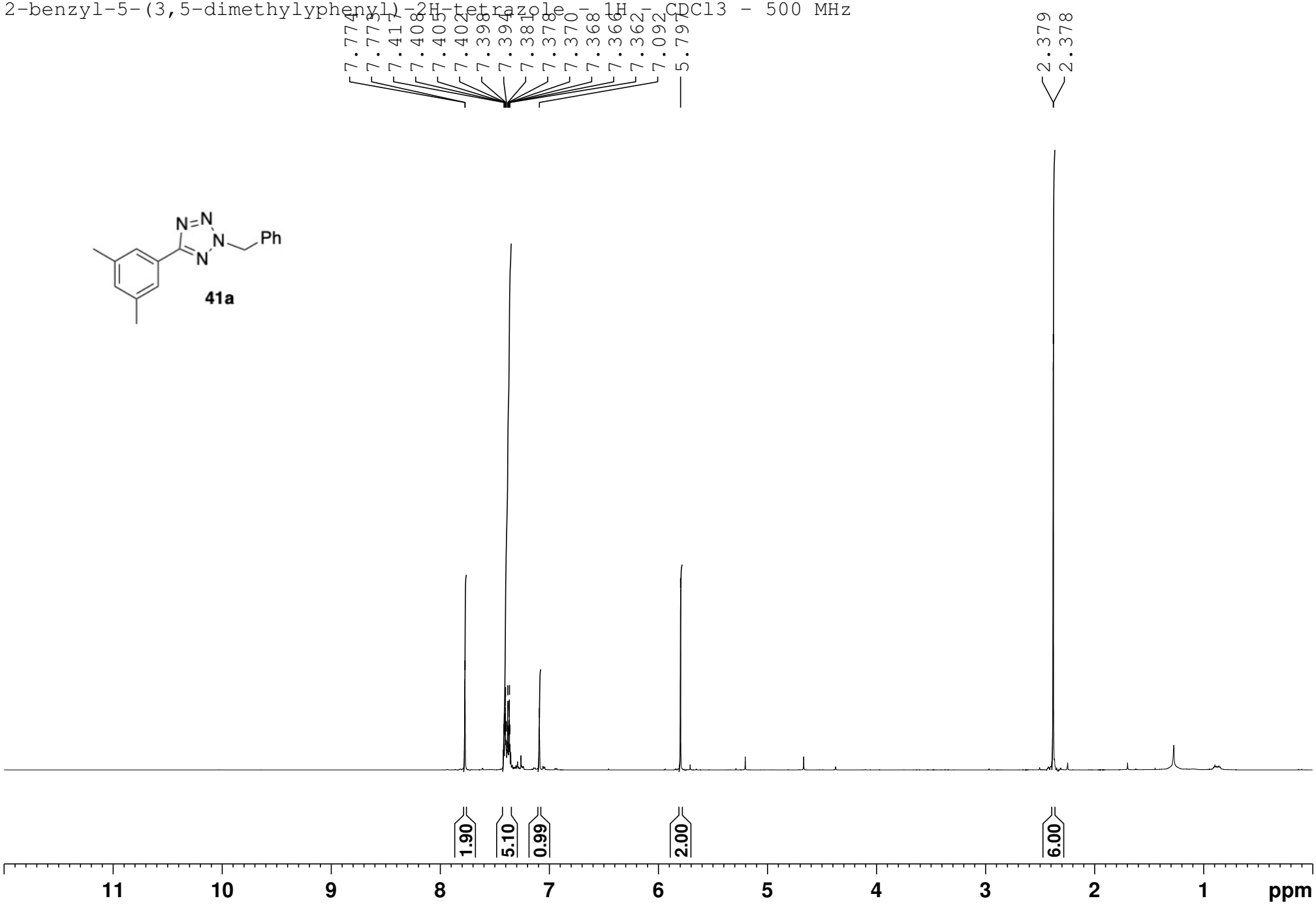
5-(3,5-dinitrophenyl)-2-(1-phenylethyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz



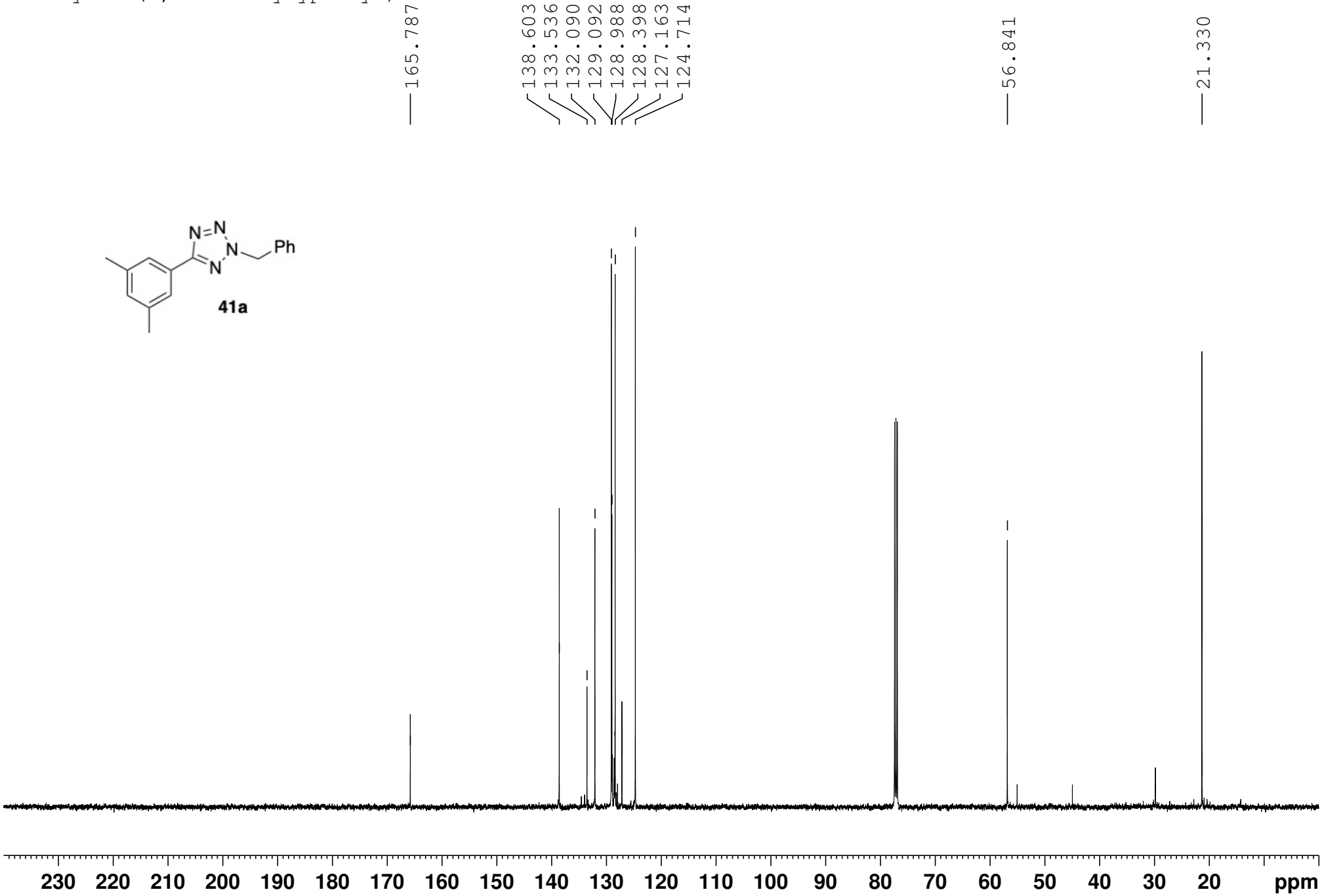
5-(3,5-dinitrophenyl)-2-(1-phenylethyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz



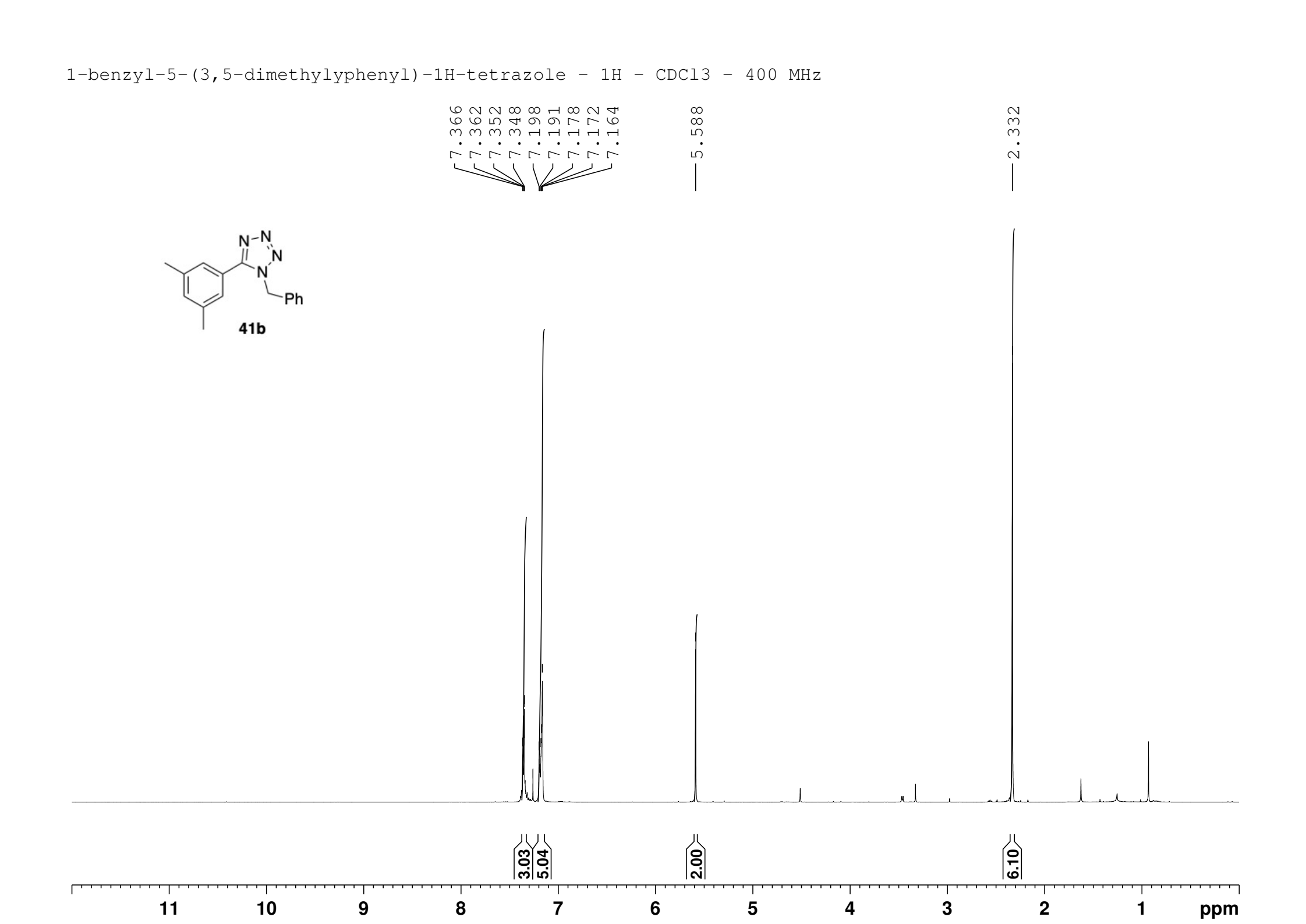
2-benzyl-5-(3,5-dimethylyphenyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz



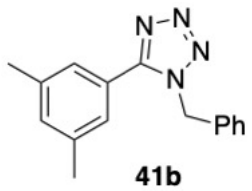
2-benzyl-5-(3,5-dimethylyphenyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz



1-benzyl-5-(3,5-dimethylyphenyl)-1H-tetrazole - 1H - CDCl3 - 400 MHz



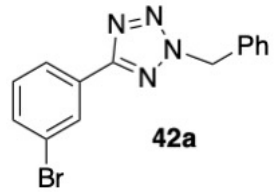
1-benzyl-5-(3,5-dimethylyphenyl)-1H-tetrazole - 13C - CDCl3 - 125 MHz



41b

2-benzyl-5-(3-bromophenyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz

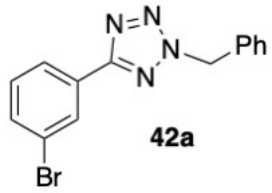
8.298
8.295
8.292
8.085
8.083
8.080
8.070
8.067
8.065
7.586
7.584
7.582
7.580
7.570
7.568
7.566
7.564
7.431
7.426
7.422
7.416
7.414
7.411
7.408
7.407
7.402
7.399
7.398
7.392
7.390
7.387
7.381
7.376
7.373
7.366
7.364
7.354
7.338
7.322
5.802



42a

2-benzyl-5-(3-bromophenyl)-2H-tetrazole - 13C - CDCl3 - 100 MHz

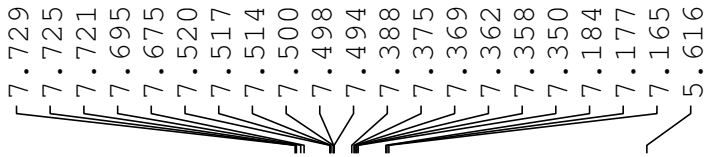
164.322
133.387
133.269
130.542
129.950
129.422
129.190
129.181
128.547
125.528
123.045
57.075

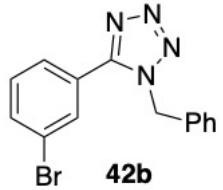


42a

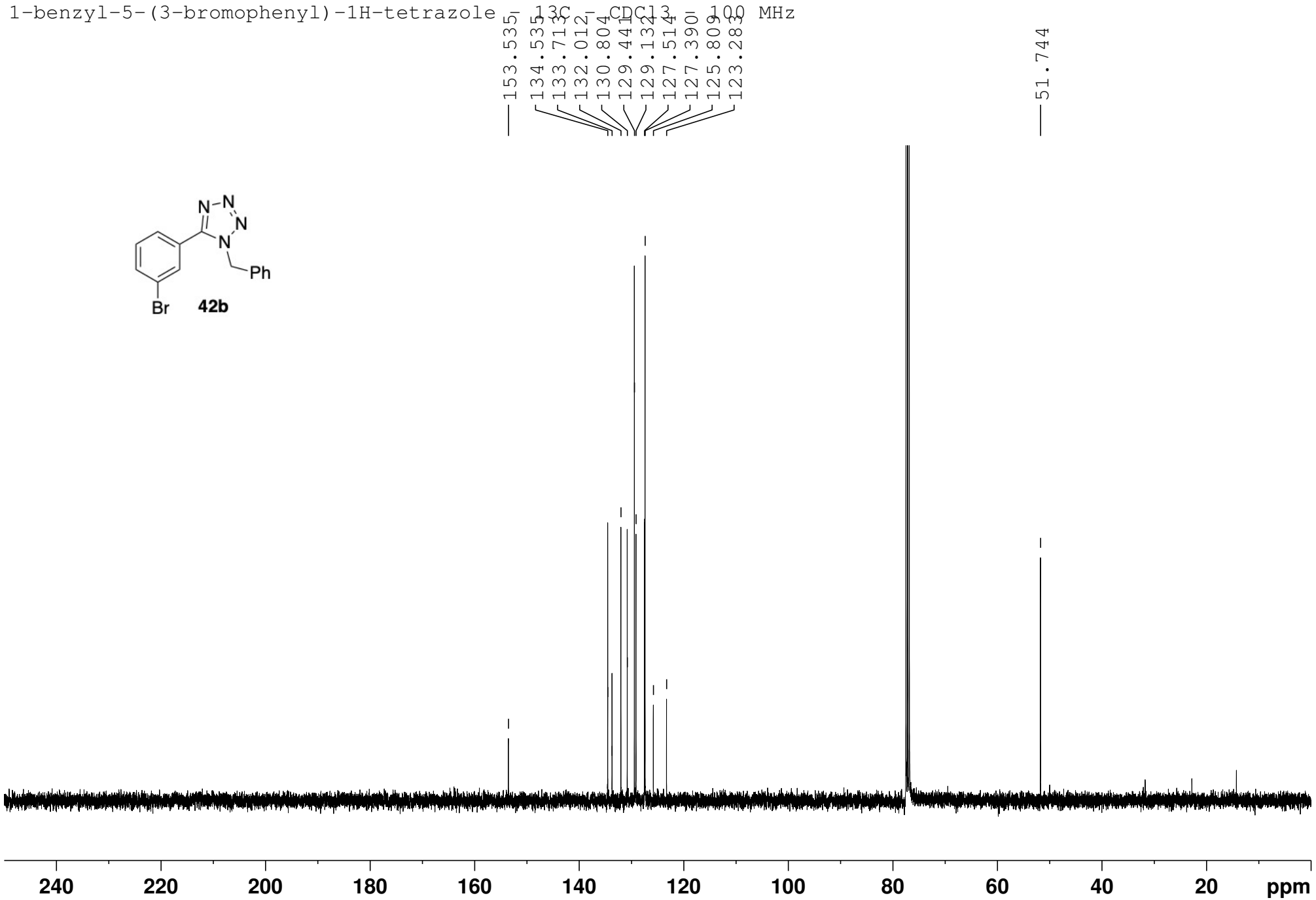
240 220 200 180 160 140 120 100 80 60 40 20 ppm

1-benzyl-5-(3-bromophenyl)-1H-tetrazole - 1H - CDCl3 - 400 MHz



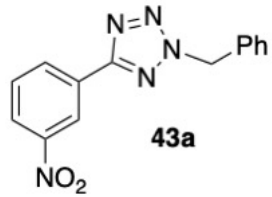


42b


1-benzyl-5-(3-bromophenyl)-1H-tetrazole_ 13C_ CDCl3_ 100 MHz
153.535
134.535
133.713
132.012
130.804
129.441
129.134
127.514
127.390
125.809
123.283
51.744
N
N
N
N
Ph
Br
42b
240
220
200
180
160
140
120
100
80
60
40
20
ppm

2-benzyl-5-(3-nitrophenyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz

8.965
8.962
8.477
8.475
8.474
8.472
8.461
8.459
8.458
8.456
8.304
8.302
8.299
8.297
8.287
8.285
8.283
8.280
7.672
7.671
7.656
7.640
7.639
7.456
7.452
7.448
7.442
7.440
7.437
7.417
7.411
7.401
7.400
7.396
7.389
7.385
7.382
7.380
7.374
7.372
5.834

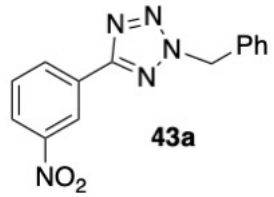


43a

0.93
0.99
0.98
1.00
1.94
2.97
2.00

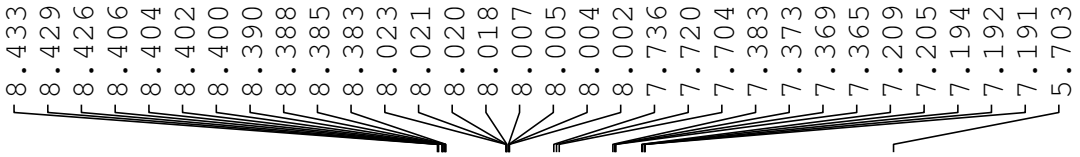
11 10 9 8 7 6 5 4 3 2 1 ppm

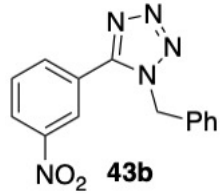
2-benzyl-5-(3-nitrophenyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz



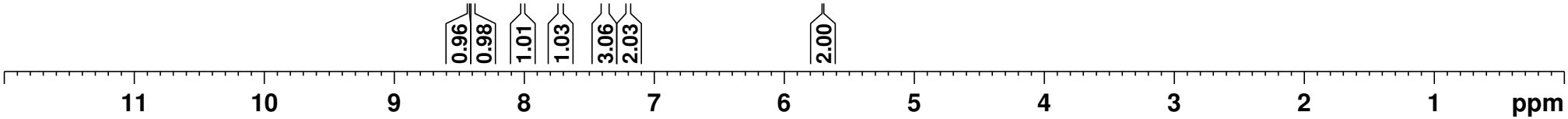
43a

1-benzyl-5-(3-nitrophenyl)-1H-tetrazole - 1H - CDCl3 - 500 MHz

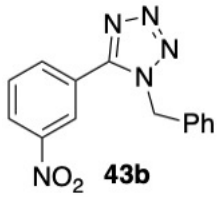




43b



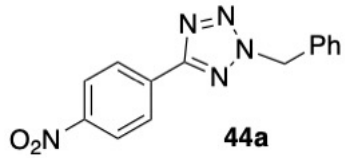
1-benzyl-5-(3-nitrophenyl)-1H-tetrazole - 13C - CDCl3 - 125 MHz



43b

2-benzyl-5-(4-nitrophenyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz

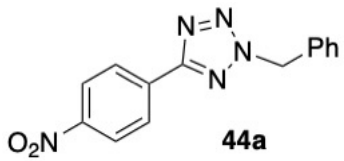
8.313
7.452
7.448
7.444
7.439
7.436
7.433
7.418
7.414
7.407
7.402
7.400
7.397
7.392
7.390
7.387
7.386
7.384
7.377
7.374
5.838



44a

2-benzyl-5-(4-nitrophenyl)-2H-tetrazole 1H CDCl3 125 MHz

163.675
148.951
133.144
132.999
129.305
129.232
128.627
127.732
124.269
57.266

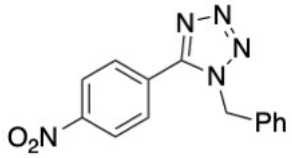


44a

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

1-benzyl-5-(4-nitrophenyl)-1H-tetrazole - 1H - CDCl3 - 500 MHz

8.361
8.352
8.343
8.339
8.334
7.804
7.795
7.785
7.781
7.777
7.381
7.378
7.372
7.367
7.150
7.143
7.135
7.131
5.678

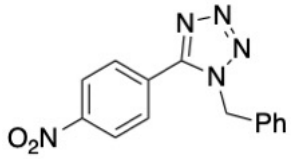


44b

1.96
1.97
2.91
1.98
2.00

11 10 9 8 7 6 5 4 3 2 1 ppm

1-benzyl-5-(4-nitrophenyl)-1H-tetrazole - 13C - CDCl3 - 125 MHz

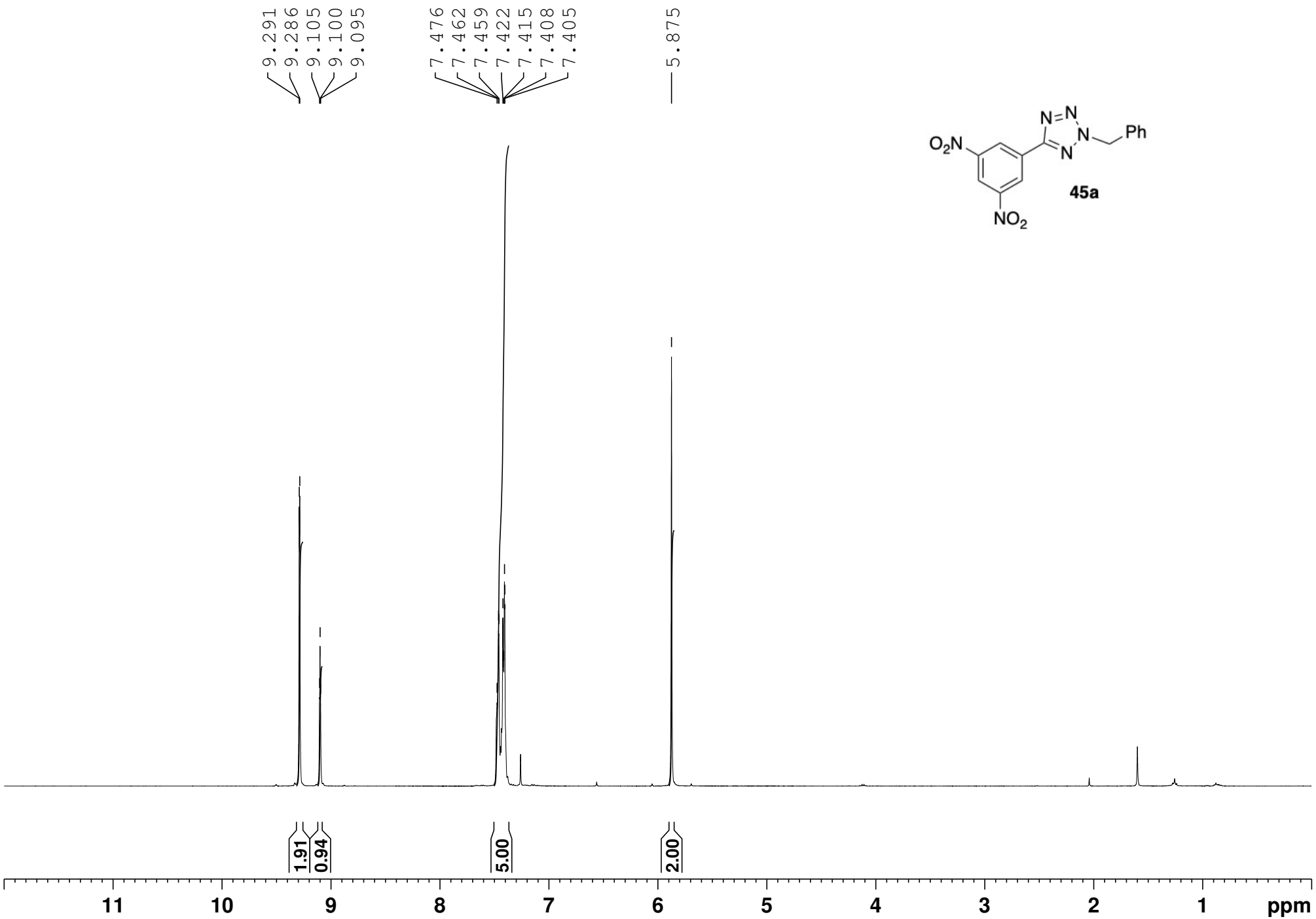


44b

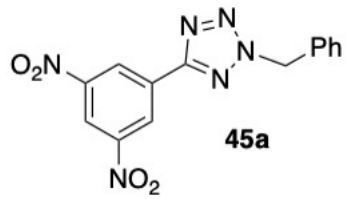
153.070
149.570
133.394
130.176
130.000
129.613
129.344
127.116
124.436
51.974

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

2-benzyl-5-(3,5-dinitrophenyl)-2H-tetrazole - 1H - CDCl3 - 400 MHz

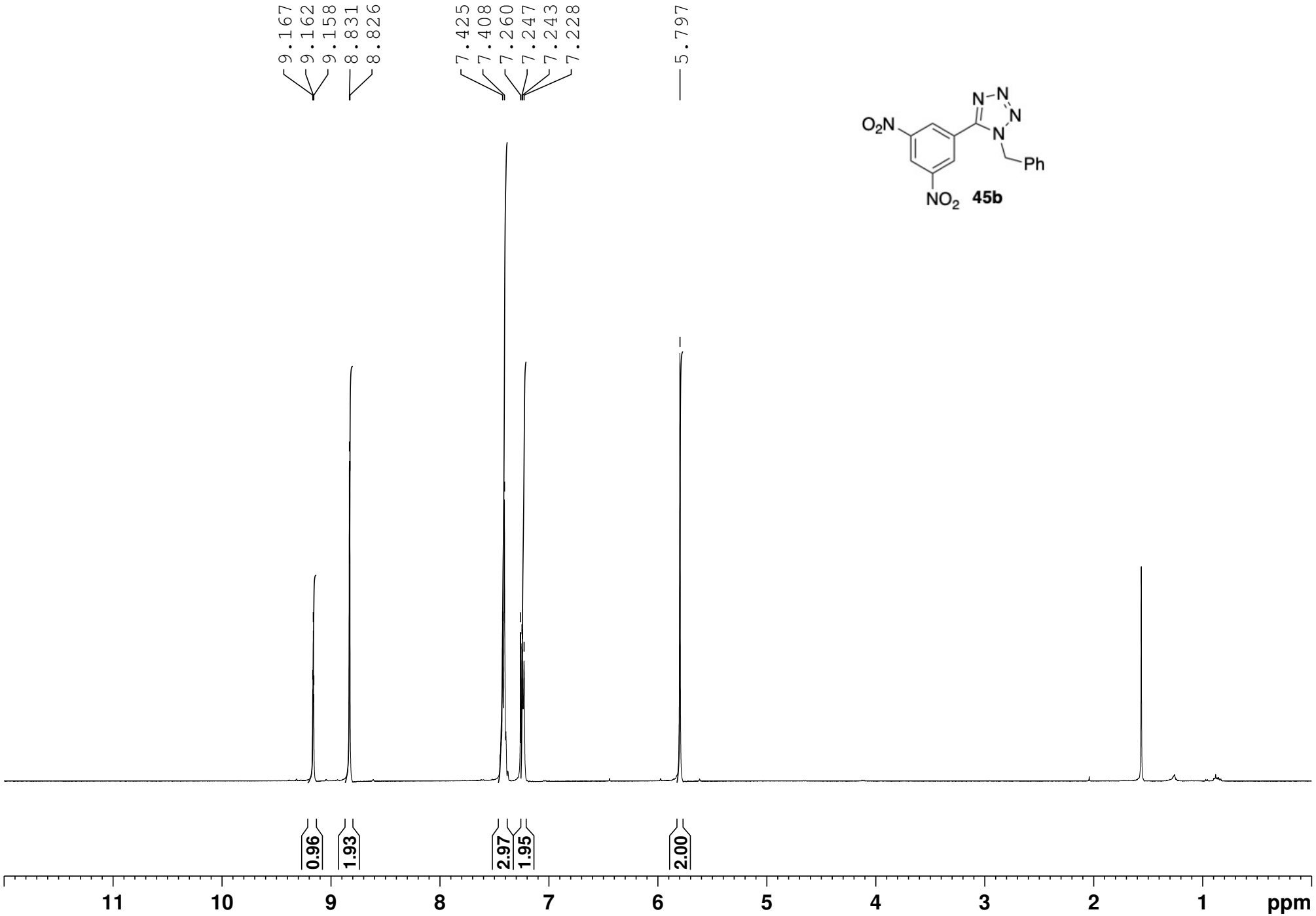


2-benzyl-5-(3,5-dinitrophenyl)-2H-tetrazole - 13C - CDCl3 - 100 MHz

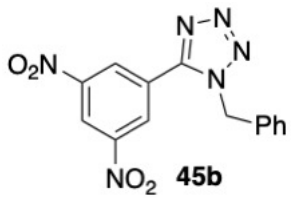


45a

1-benzyl-5-(3,5-dinitrophenyl)-1H-tetrazole - 1H - CDCl3 - 400 MHz



1-benzyl-5-(3,5-dinitrophenyl)-1H-tetrazole - 13C - CDCl3 - 100 MHz

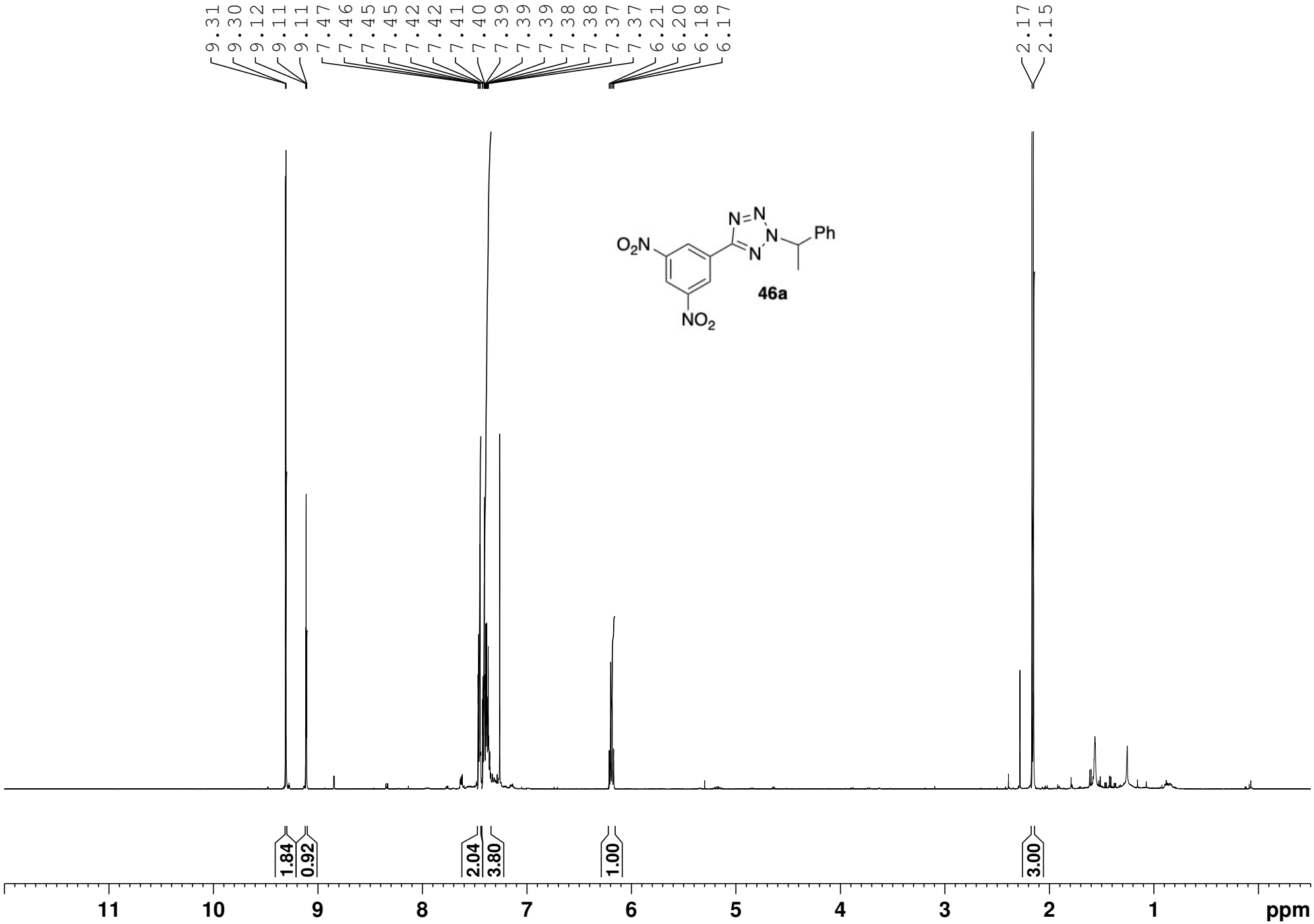


45b

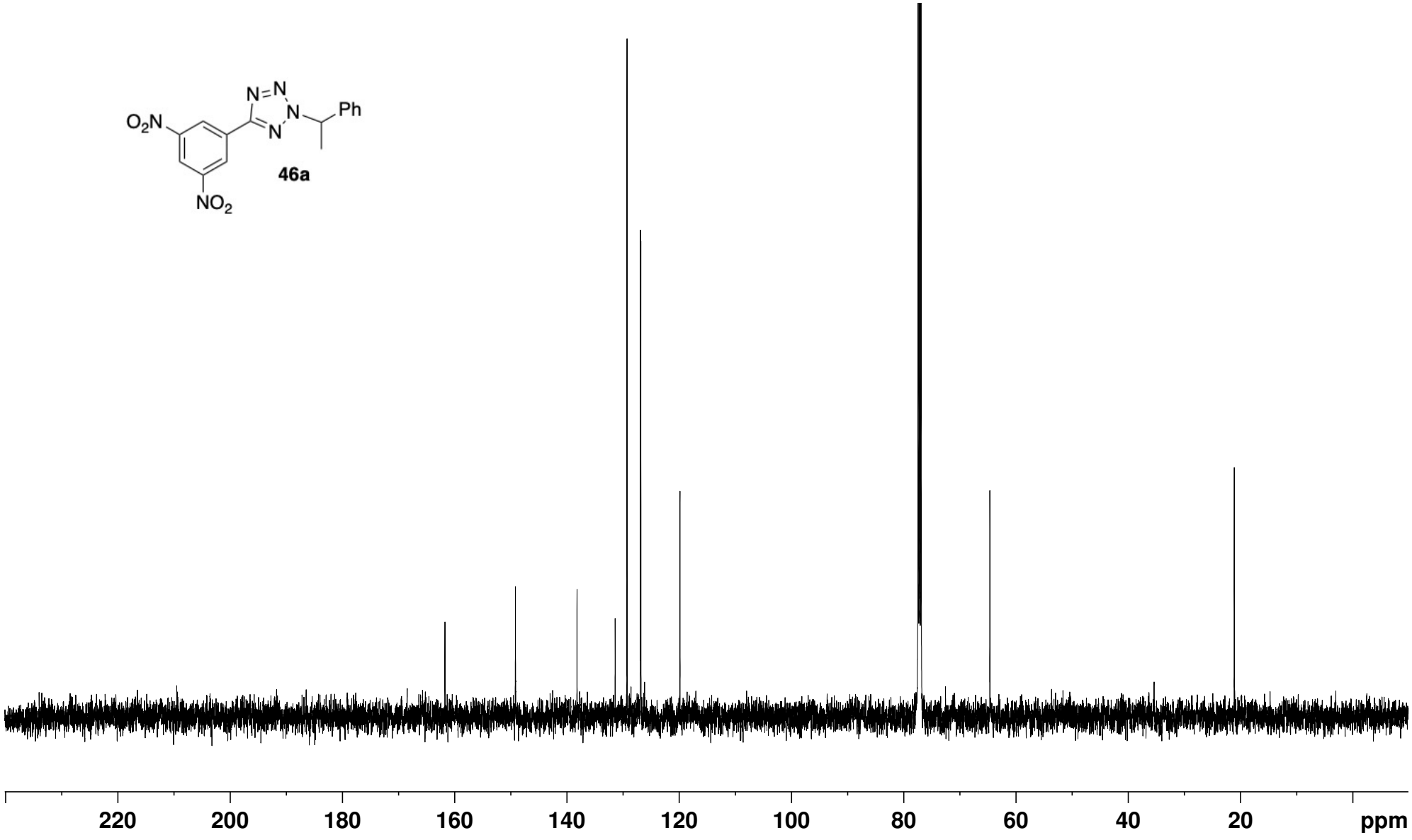
151.120
149.012
132.523
129.932
129.845
128.821
127.481
127.350
121.020
52.695

240 220 200 180 160 140 120 100 80 60 40 20 ppm

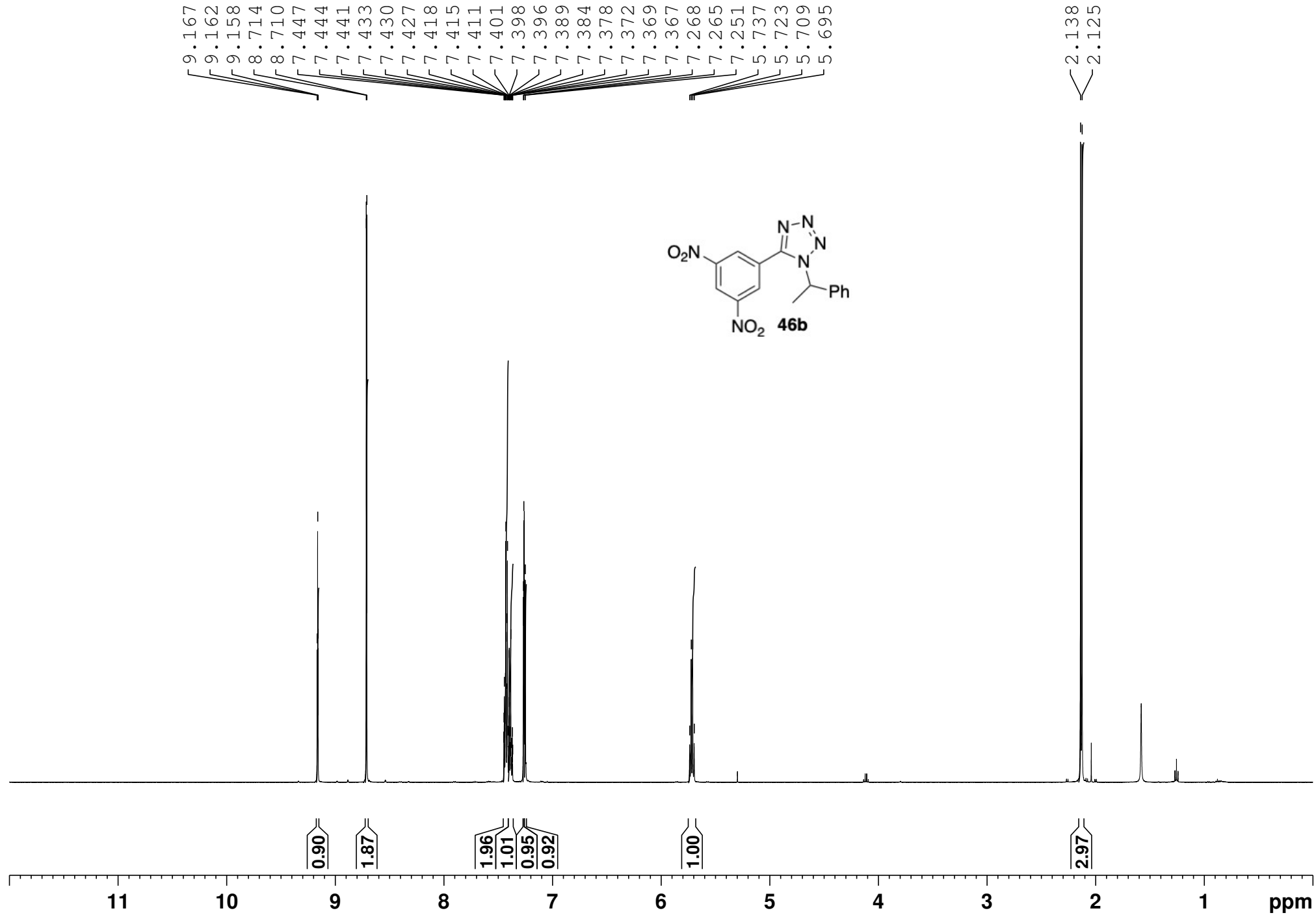
5-(3,5-dinitrophenyl)-2-(1-phenylethyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz



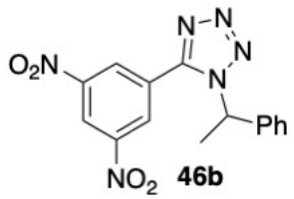
5-(3,5-dinitrophenyl)-2-(1-phenylethyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz



5-(3,5-dinitrophenyl)-1-(1-phenylethyl)-1H-tetrazole - 1H - CDCl3 - 500 MHz

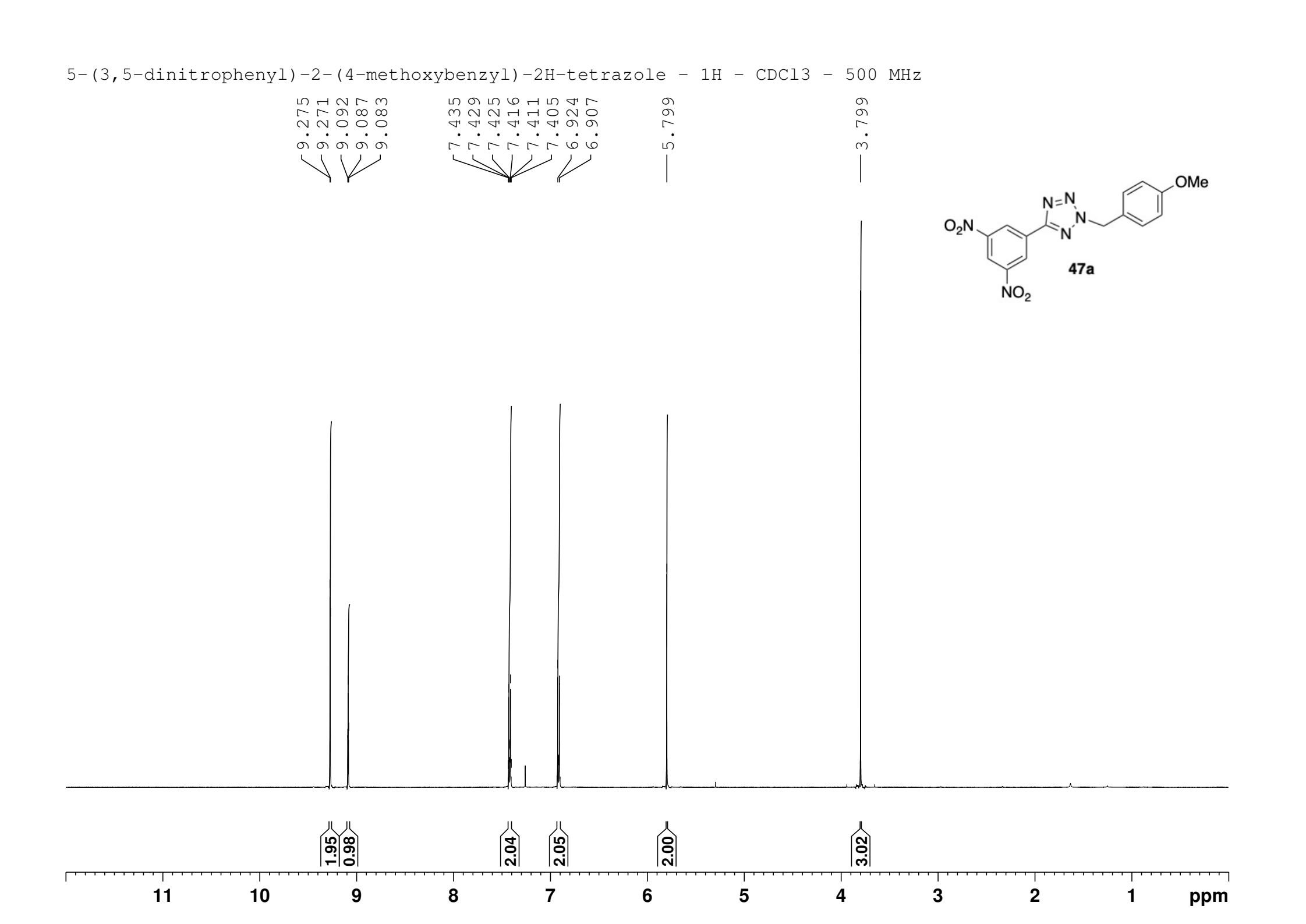


5-(3,5-dinitrophenyl)-1-(1-phenylethyl)-1H-tetrazole - 13C - CDCl3 - 125 MHz

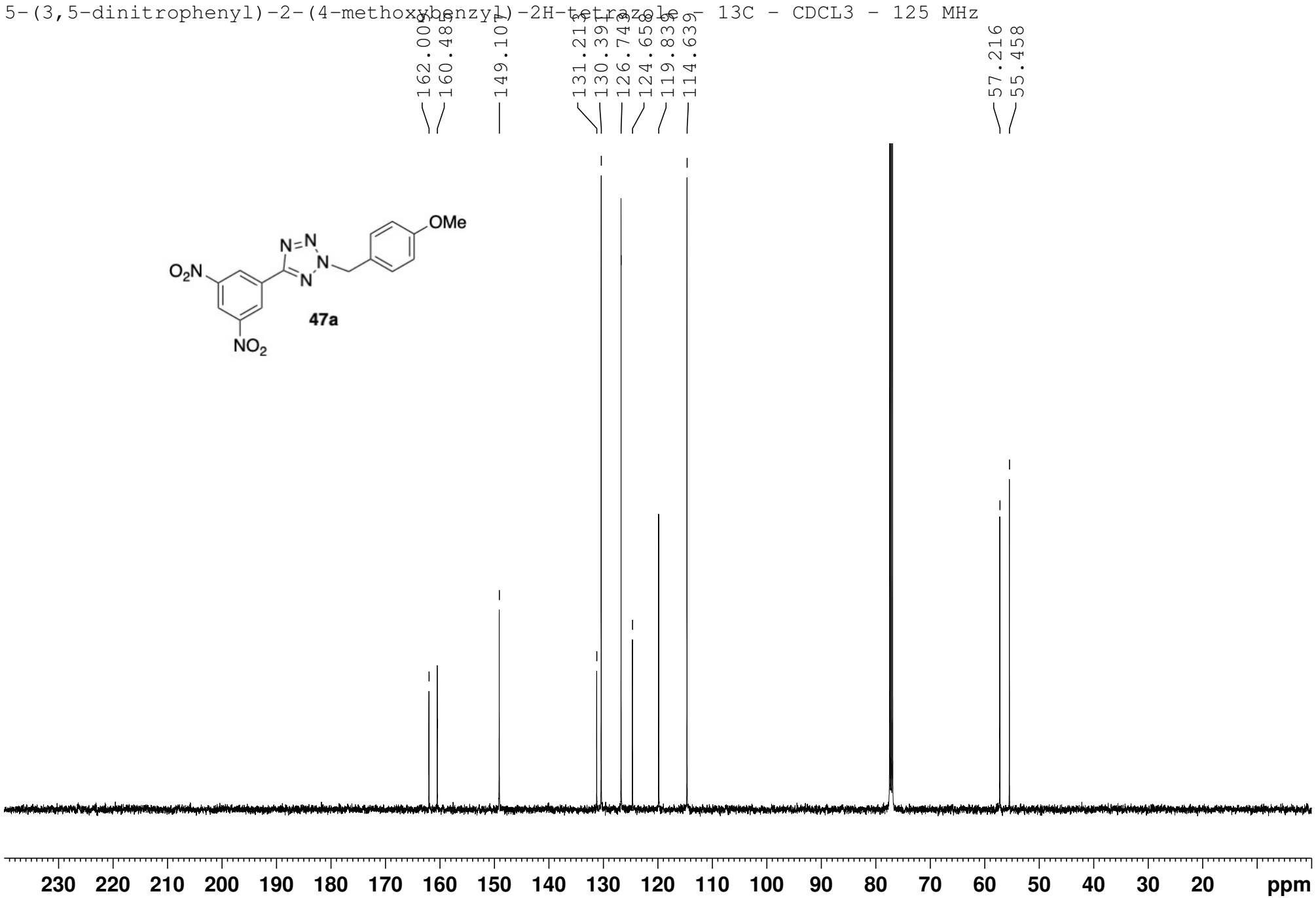


46b

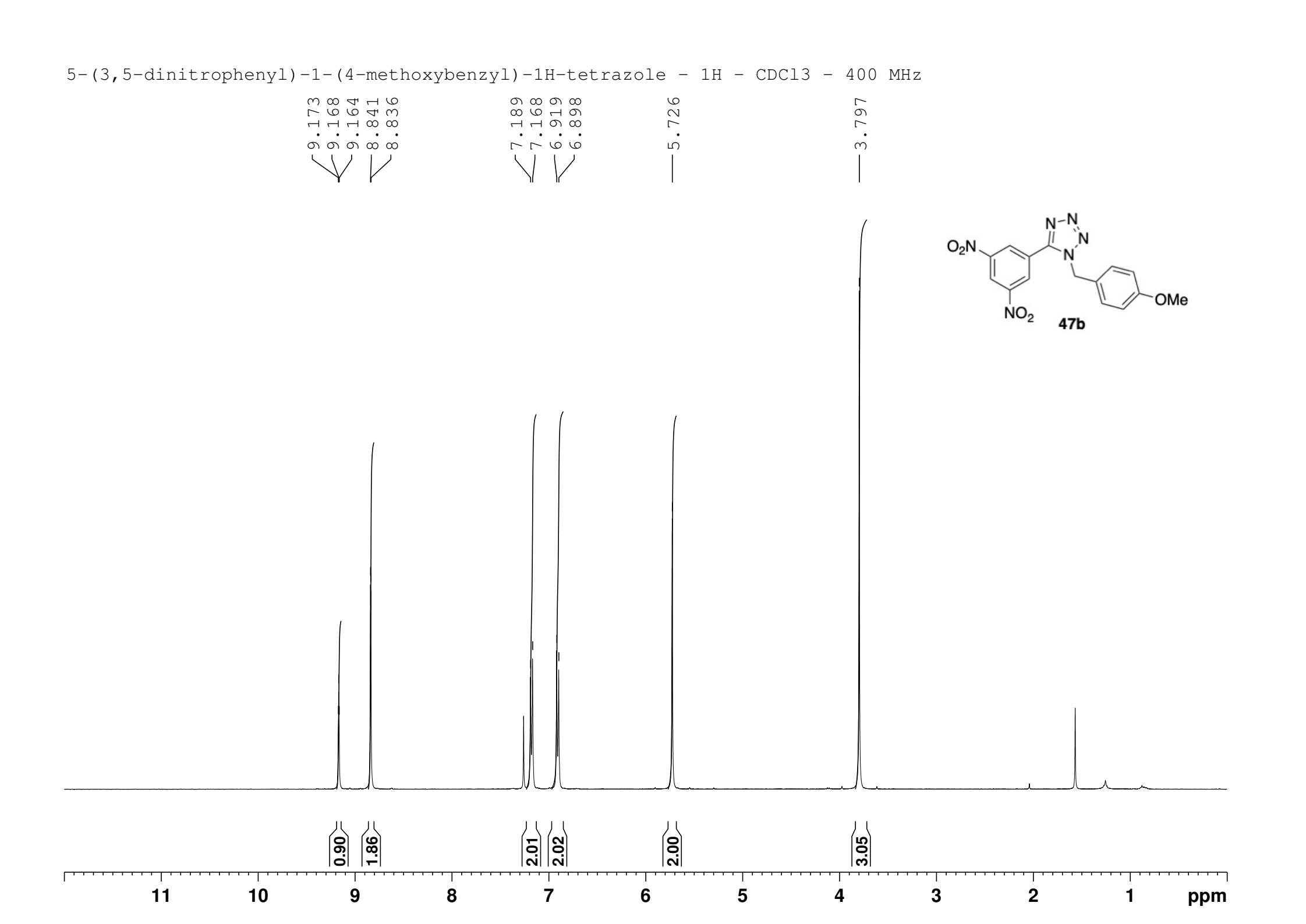
5-(3,5-dinitrophenyl)-2-(4-methoxybenzyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz



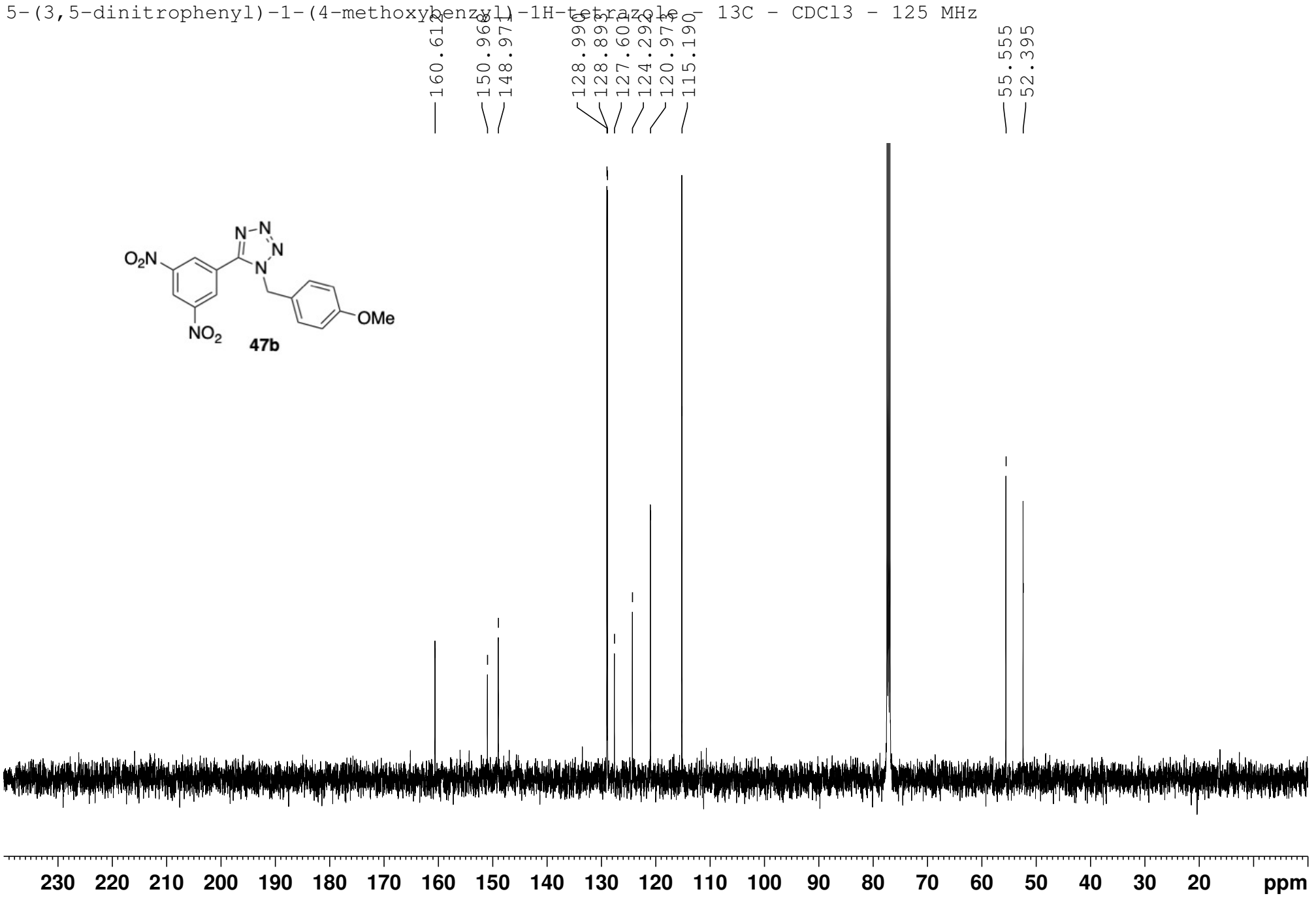
5-(3,5-dinitrophenyl)-2-(4-methoxybenzyl)-2H-tetrazole - 13C - CDCL3 - 125 MHz



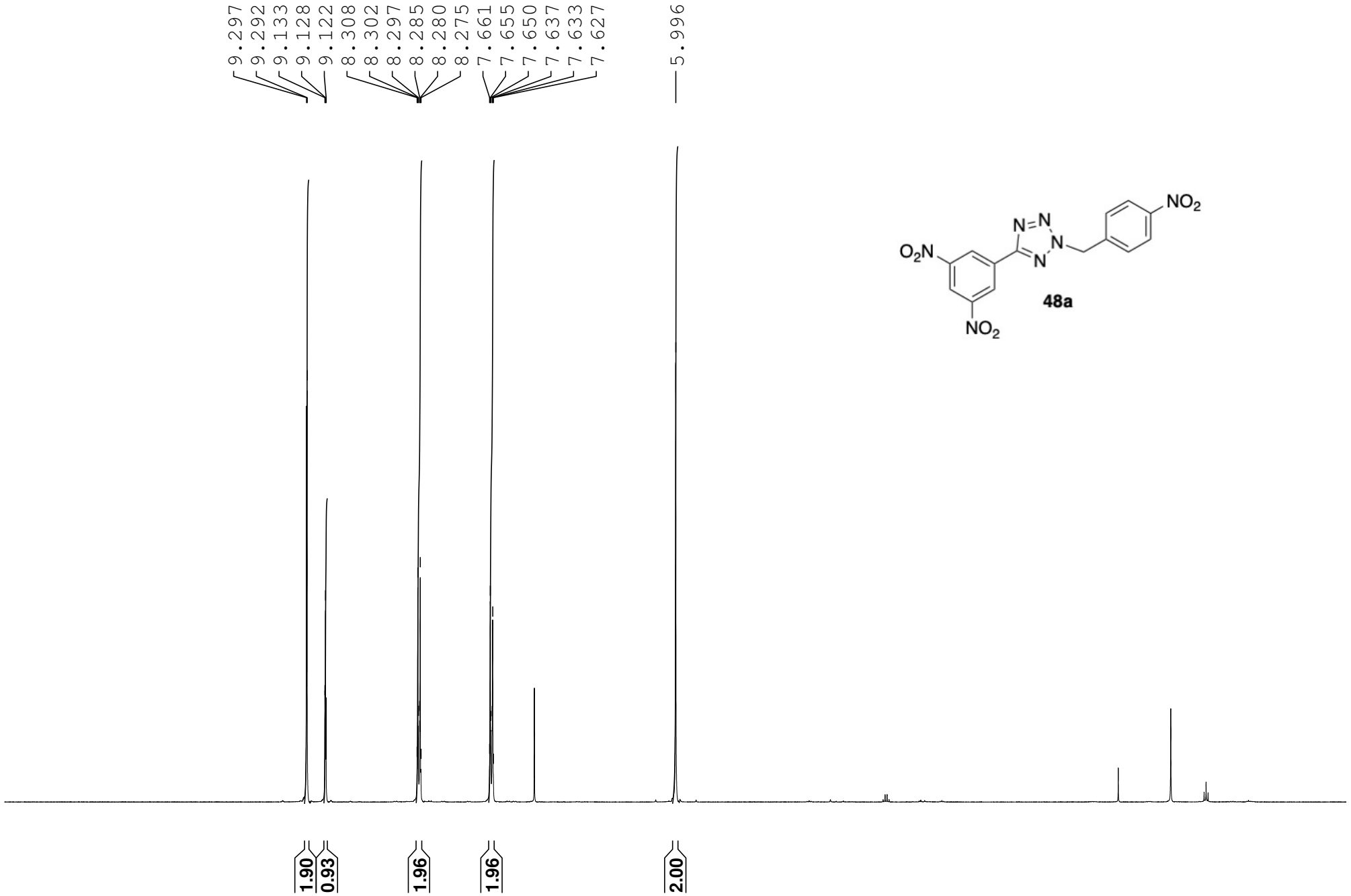
5-(3,5-dinitrophenyl)-1-(4-methoxybenzyl)-1H-tetrazole - 1H - CDCl3 - 400 MHz



5-(3,5-dinitrophenyl)-1-(4-methoxybenzyl)-1H-tetrazole - 13C - CDCl3 - 125 MHz

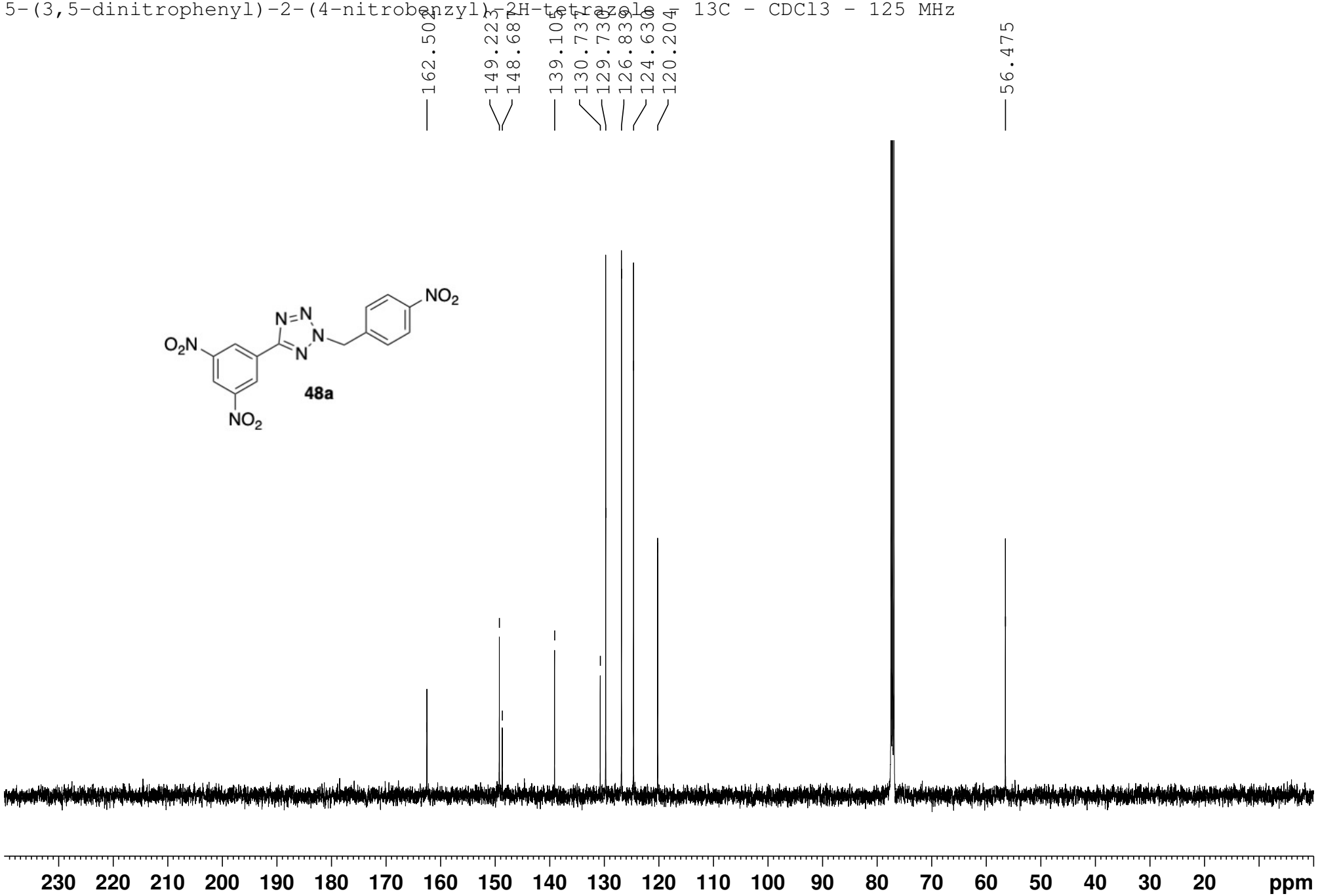


5-(3,5-dinitrophenyl)-2-(4-nitrobenzyl)-2H-tetrazole - 1H - CDCl3 - 400 MHz

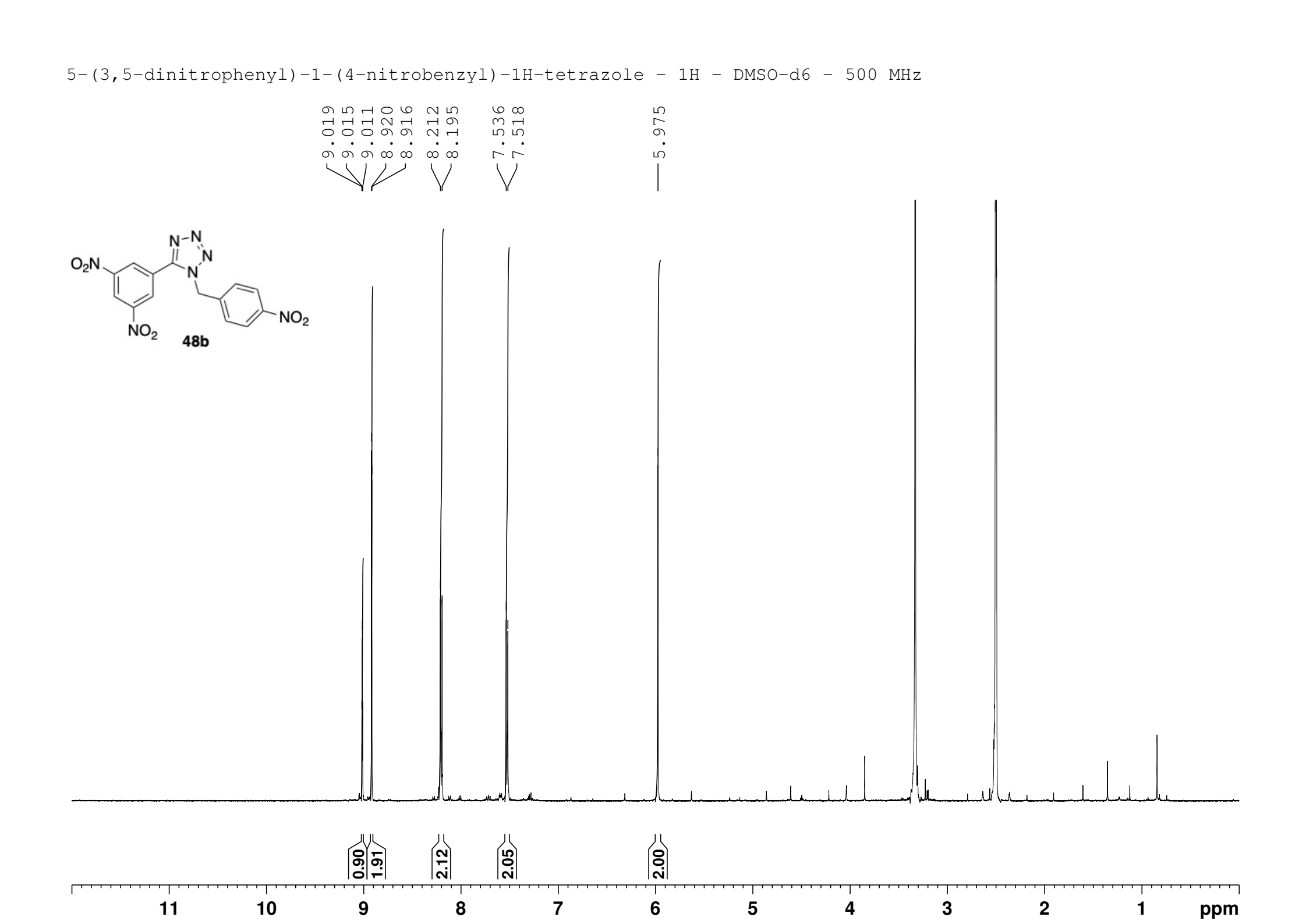


48a

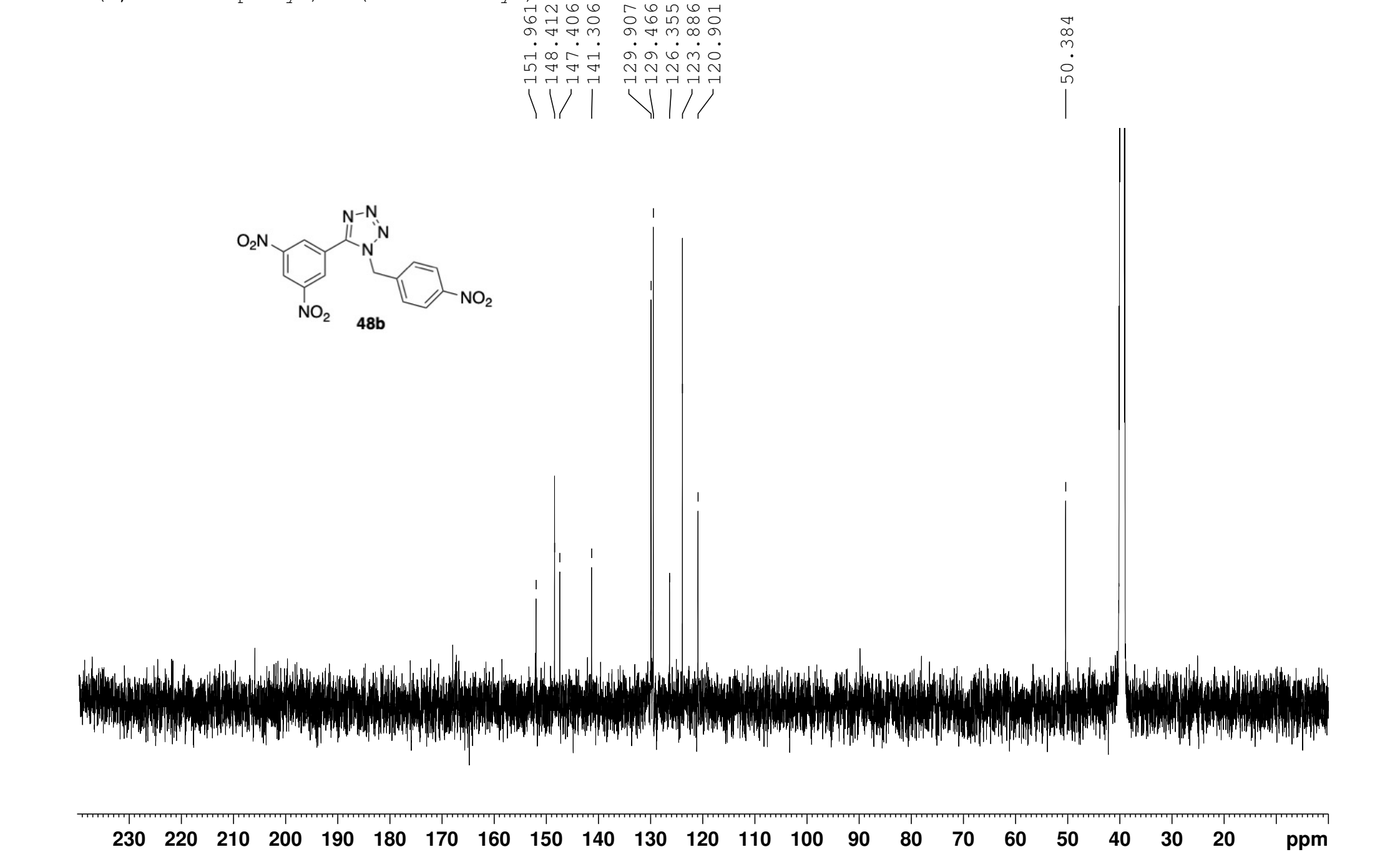
5-(3,5-dinitrophenyl)-2-(4-nitrobenzyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz



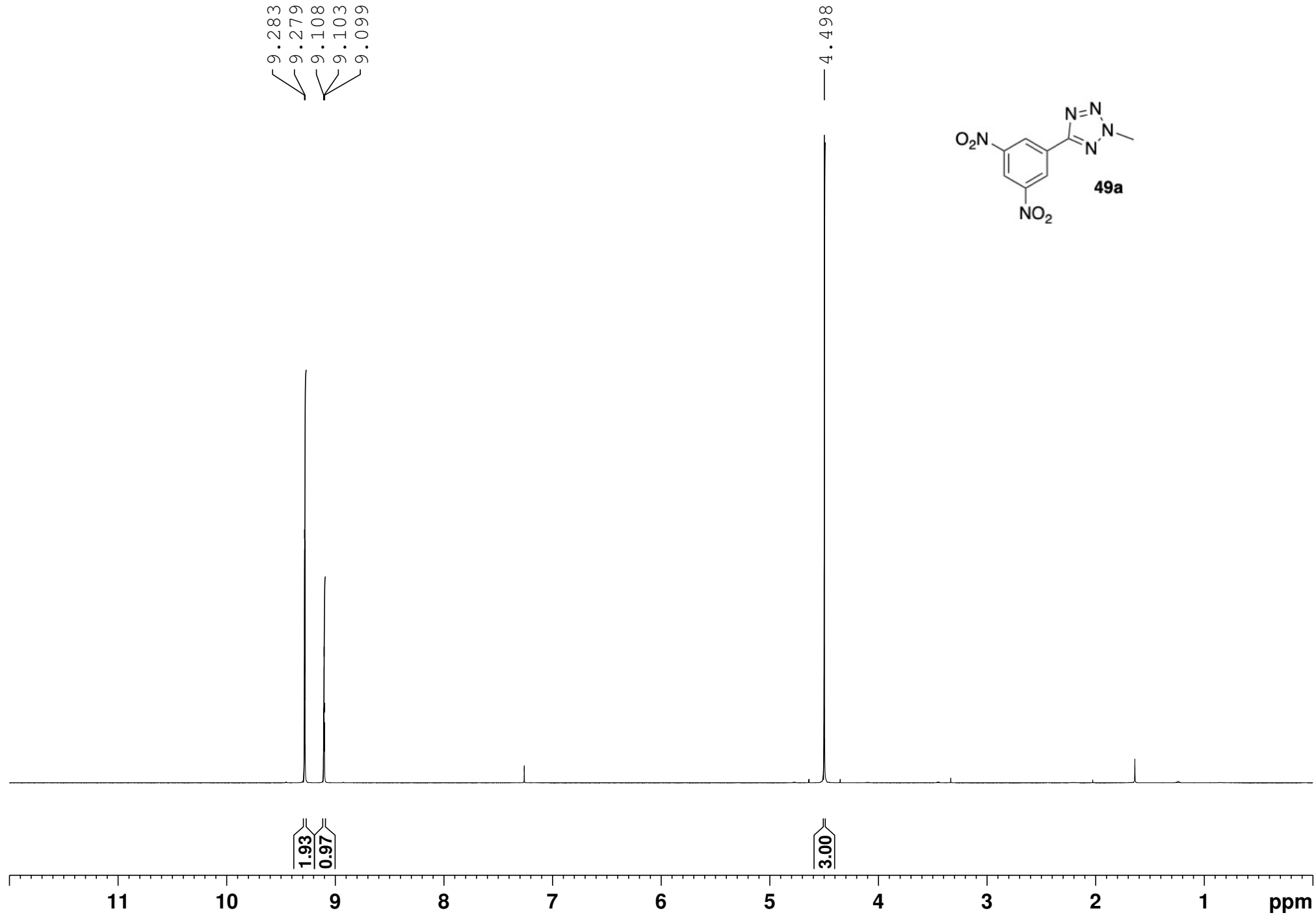
5-(3,5-dinitrophenyl)-1-(4-nitrobenzyl)-1H-tetrazole - 1H - DMSO-d6 - 500 MHz



5-(3,5-dinitrophenyl)-1-(4-nitrobenzyl)-1H-tetrazole - 13C - DMSO-d6 - 125 MHz

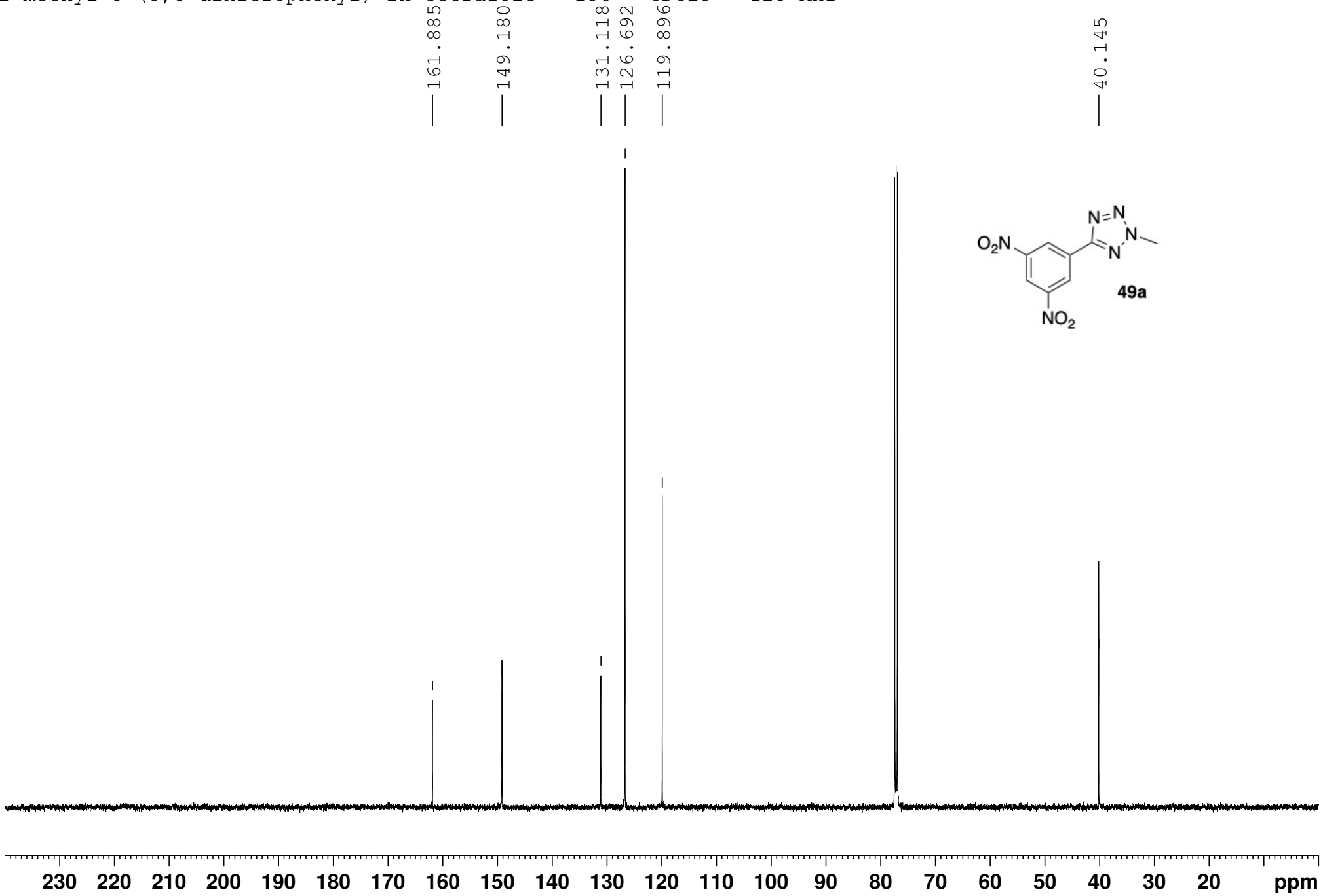


2-methyl-5-(3,5-dinitrophenyl)-2H-tetrazole - 1H - CDCl3 - 500 MHz

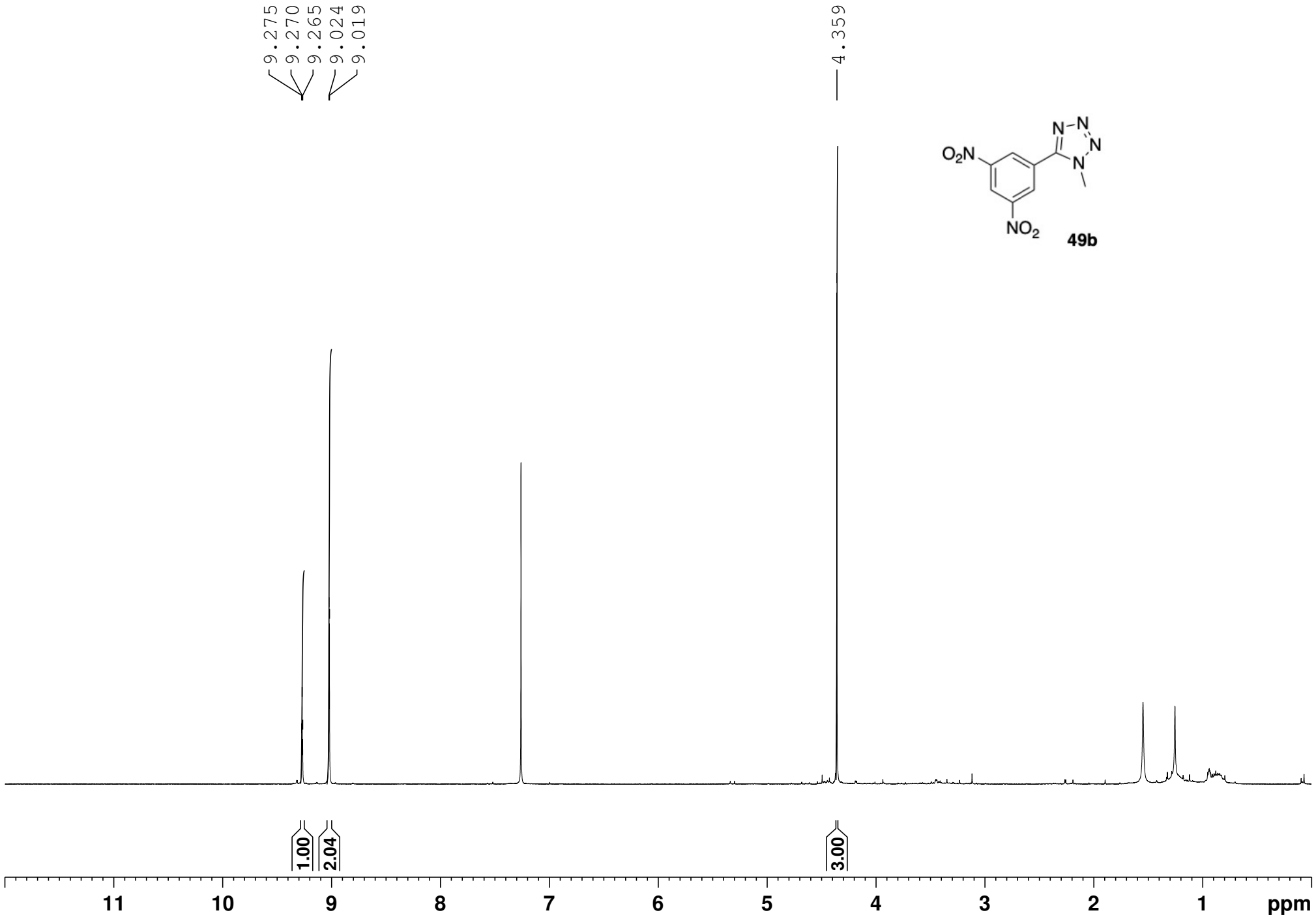


49a

2-methyl-5-(3,5-dinitrophenyl)-2H-tetrazole - 13C - CDCl3 - 125 MHz

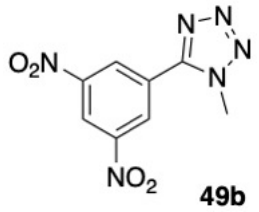


1-methyl-5-(3,5-dinitrophenyl)-1H-tetrazole - 1H - CDCl3 - 400 MHz



49b

1-methyl-5-(3,5-dinitrophenyl)-1H-tetrazole - 13C - CDCl3+MeOD - 125 MHz



49b