Supporting Information

Easy access to 5-cyanotriazoles *via* Pd-catalyzed cyanation of 5-iodotriazoles

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General information

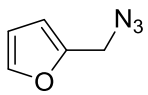
NMR spectra were recorded with Bruker Avance 400 (^{1}H 400 MHz, ^{13}C 100 MHz), and Bruker Avance 600 (^{1}H 600 MHz, ^{13}C 151 MHz) spectrometers at ambient temperature. Chemical shifts are presented in ppm (δ scale) and referenced to tetramethylsilane (TMS, δ = 0 ppm) in the ^{1}H NMR spectra and to the solvent signal in the ^{13}C NMR spectra. MALDI-TOF spectra were recorded with a Bruker Daltonics UltraFlex instrument in a dithranol matrix using PEG 300, PEG 400 or PEG 600 as the internal standard. ESI mass spectra were obtained from Thermo Scientific LTQ Orbitrap and Sciex TripleTOF 5600+ spectrometers. Column chromatography was carried out on Macherey–Nagel silica gel 60 (0.040–0.063 mm).

Experimental procedures and characterization data for compounds

Synthesis of azides S1

General procedure. In a round bottom flask, amine (1 eq), $CuSO_4 \cdot 5H_2O$ (1 mol%), K_2CO_3 (2.9 eq), and 3-azidosulfonyl-3*H*-imidazol-1-ium hydrogen sulfate (1.2 eq) were mixed under an argon atmosphere in MeOH (5 ml per 1 mmol of amine). The reaction mixture was stirred at room temperature overnight (TLC control), then diluted with EtOAc or Et_2O, washed with water. Organic layer was separated, and the aqueous layer was extracted with one of that solvents. The organic layers were combined and dried with anhydrous $MgSO_4$, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography or used without purification.

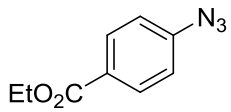
(2-Azidomethyl)furan (S1e)



Prepared from furfurylamine (265 µl, 3 mmol) according to the general procedure. The product was used in the next step without purification. Yield 210.3 mg (57%). Yellowish oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 1.4 Hz, 1H), 6.36 (m, 2H), 4.30 (s, 2H). Spectral data are in accordance with the literature.[1]

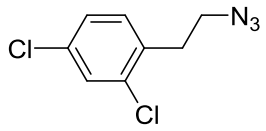
Synthesis of ethyl 4-azidobenzoate (S1h)



To a cooled stirring solution of benzocaine (1.794 g, 10.86 mmol) in aqueous HCl (1:1, 15 ml) and AcOH (10 ml) $NaNO_2$ (1 g, 14.49 mmol) was added. The reaction mixture was maintained at room temperature for 1 h. Then, NaN_3 (1 g, 15.38 mmol) was added to cooled reaction mixture. After the addition of all sodium azide, the reaction was carried out at room temperature for 2 hours, then the reaction mixture was diluted with methylene chloride (100 ml), water (100 ml) and extracted three times in portions of methylene chloride of 100 ml. The organic layers were combined and dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography. Eluent: CH_2Cl_2 – hexanes = 1:2. Yield 2.032 g (98%). Yellowish liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (m, 2H), 7.06 (m, 2H), 4.37 (q, *J* = 7.1 Hz, 2H), 1.39 (t, *J* = 7.1 Hz, 3H). Spectral data are in accordance with the literature.[2]

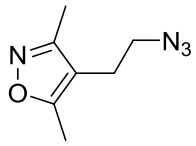
1-(2-Azidoethyl)-2,4-dichlorobenzene (S1n)



Prepared from 1-(2-aminoethyl)-2,4-dichlorobenzene (302 µl, 2 mmol) according to the general procedure. Eluent CH_2Cl_2. Yield 419 mg (97%). Colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (m, 1H), 7.21 (m, 2H), 3.52 (t, *J* = 7.1 Hz, 2H), 2.99 (t, *J* = 7.1 Hz, 2H). Spectral data are in accordance with the literature.[3]

4-(2-Azidoethyl)-3,5-dimethylisoxazole (S1o)



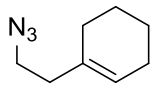
Prepared from 4-(2-aminoethyl)-3,5-dimethylisoxazole (427.1 mg, 3.05 mmol) according to the general procedure. Eluent CH_2Cl_2. Yield 383.6 mg (77%). Pale yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.37 (t, *J* = 7.0 Hz, 2H), 2.57 (t, *J* = 7.0 Hz, 2H), 2.35 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6 (C_q), 159.0 (C_q), 109.7 (C_q), 50.6, 21.9, 10.6, 9.8.

HRMS (ESI-TOF) calcd for $C_7H_{11}N_4O$ $[M+H]^+$ 167.0927; found 167.0930.

1-(2-Azidoethyl)cyclohex-1-ene (S1p)



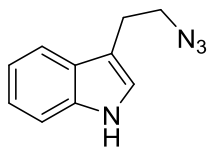
Prepared from 1-(2-aminoethyl)cyclohex-1-ene (278 µl, 2 mmol) according to the general procedure. Eluent CH_2Cl_2. Yield 280.9 mg (93%). Colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.52 (m, 1H), 3.31 (t, *J* = 7.1 Hz, 2H), 2.24 (m, 2H), 2.01 (m, 2H), 1.94 (m, 2H), 1.64 (m, 2H), 1.56 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 133.3 (C_q), 123.6, 49.2, 36.8, 27.7, 24.8, 22.4, 21.8.

HRMS (ESI-TOF) calcd for $C_8H_{14}N$ $[M-N_2+H]^+$ 124.1121; found 124.1123.

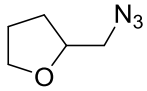
3-(2-Azidoethyl)-1*H*-indole (S1q)



Prepared from tryptamine (1.6 g, 10 mmol) according to the general procedure using 3-azidosulfonyl-3*H*-imidazol-1-ium hydrogen chloride instead of hydrogen sulfate and K_2CO_3 (2.35 g, 17 mmol). Eluent CH_2Cl_2. Yield 1.256 g (67%). Colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (br s, 1H, NH), 7.60 (m, 1H), 7.38 (m, 1H), 7.22 (m, 1H), 7.08 (d *J* = 2.3 Hz, 1H), 3.57 (t, *J* = 7.2 Hz, 2H), 3.07 (t, *J* = 7.2 Hz, 2H). Spectral data are in accordance with the literature.[4]

(2-Azidomethyl)tetrahydrofuran (S1r)



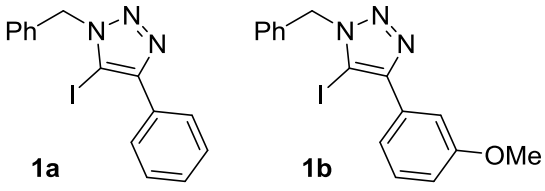
Prepared from tetrahydrofurfurylamine (310 μl, 3 mmol) according to the general procedure. The product was used in the next step without purification. Yield 271 mg (71%). Pale yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.09 (m, 1H), 3.92 (m, 1H), 3.80 (m, 1H), 3.37 (dd, *J* = 12.7, 4.0 Hz, 1H), 3.23 (dd, *J* = 12.7, 5.9 Hz, 1H), 2.06 – 1.85 (m, 3H), 1.68 (m, 1H). Spectral data are in accordance with the literature.[5]

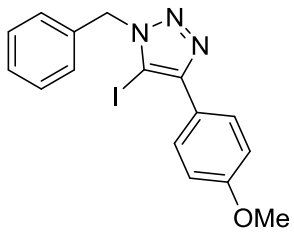
Synthesis of 5-Iodo-1*H*-1,2,3-triazoles 1

General procedure. In a vial with a screw cap, organic azide (0.8 mmol), 1-iodoalkyne (0.96 mmol), CuI (7.6 mg, 0.04 mmol, 5 mol%), and tris[(1-*tert*-butyl-1*H*-1,2,3-triazol-4-yl)methyl]amine (TTTA) (17.1 mg, 0.04 mmol, 5 mol%) were mixed under an argon atmosphere in THF (1.6 ml). The reaction mixture was stirred at 50 °C overnight (TLC control), then diluted with CH_2Cl_2, washed with EDTA solution and water. The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography. Products, that were almost completely insoluble in CH_2Cl_2, were isolated in pure form by filtration.

5-Iodotriazoles **1a**,**b**,**d**,**f**,**g**,**s**,**w**,**x** were prepared as described in literature.[6]



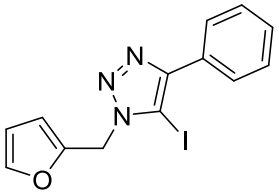
1-Benzyl-5-iodo-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (1c)



Prepared from benzyl azide (100 μl, 0.8 mmol) and (4-methoxyphenyl)iodoacetylene (247.7 mg, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 268.6 mg (86%). White solid; mp 128 – 129 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (m, 2H), 7.38 – 7.33 (m, 5H), 6.99 (m, 2H), 5.65 (s, 2H), 3.84 (s, 3H). Spectral data are in accordance with the literature.[7]

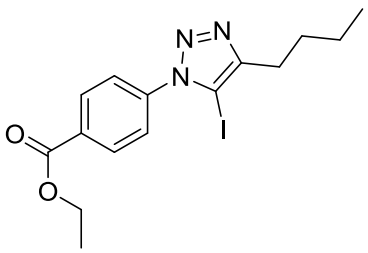
1-(Furan-2-ylmethyl)-5-iodo-4-phenyl-1*H*-1,2,3-triazole (1e)



Prepared from azide **S1e** (98.5 mg, 0.8 mmol) and (iodoethynyl)benzene (121.6 μl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 254.3 mg (91%). White solid; mp 122 – 123 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (m, 2H), 7.44 (m, 4H), 6.46 (m, 1H), 6.37 (dd, *J* = 3.3, 1.9 Hz, 1H), 5.66 (s, 2H). Spectral data are in accordance with the literature.[8]

Ethyl 4-(4-butyl-5-iodo-1H-1,2,3-triazol-1-yl)benzoate (1h)



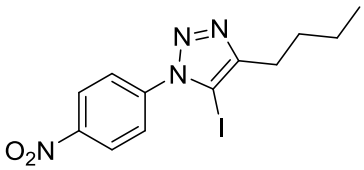
Prepared from azide **S1h** (116 μl, 0.8 mmol) and 1-iodohex-1-yne (131 μl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2, the CH_2Cl_2 – MeOH = 200:1. Yield 267.5 mg (84%). Yellowish solid; mp 108 – 109 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (m, 2H), 7.66 (m, 2H), 4.44 (q, *J* = 7.1 Hz, 2H), 2.76 (t, *J* = 7.7 Hz, 2H), 1.75 (m, 2H), 1.49 – 1.40 (m, 5H), 0.98 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0(C_q, $\underline{C}O_2Et$), 152.7 (C_q), 139.9 (C_q), 131.2 (C_q), 130.2 (2C), 125.3 (2C), 78.1 (C_q, $\underline{C}$-I), 61.1 ($\underline{C}H_2$, Et), 30.7, 25.5, 21.9, 13.9 ($\underline{C}H_3$, Et), 13.4 ($\underline{C}H_3$, Bu).

HRMS (ESI-TOF) calcd for $C_{15}H_{19}IN_3O_2$ $[M+H]^+$ 400.0516; found 400.0520.

4-Butyl-5-iodo-1-(4-nitrophenyl)-1*H*-1,2,3-triazole (1i)



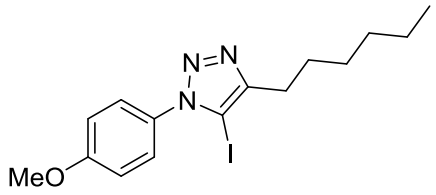
Prepared from 1-azido-4-nitrobenzene (131.3 mg, 0.8 mmol) and 1-iodohex-1-yne (131 μl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 268 mg (90%). Yellowish solid; mp 108 – 109 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (m, 2H), 7.83 (m, 2H), 2.76 (t, *J* = 7.7 Hz, 2H), 1.75 (m, 2H), 1.44 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.3 (C_q), 147.6 (C_q), 141.3 (C_q), 126.1 (2C), 124.4 (2C), 77.8 (C_q, $\underline{C}$-I), 30.6, 25.5, 21.9, 13.4 ($\underline{C}H_3$).

HRMS (ESI-TOF) calcd for $C_{12}H_{14}IN_4O_2$ $[M+H]^+$ 373.0156; found 373.0155.

4-Hexyl-5-iodo-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (1j)



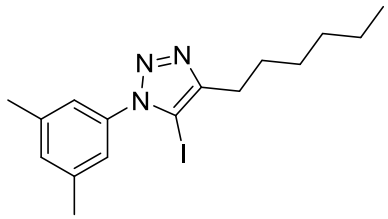
Prepared from 1-azido-4methoxybenzene (680 mg, 4.56 mmol) and 1-iodooct-1-yne (1.183 g, 5.02 mmol) according to the general procedure, heating 40 h; eluent: hexanes – EtOAc = 4:1. Yield 1.024 g (58%). Off-white solid; mp 107 – 108 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (m, 2H), 7.02 (m, 2H), 3.87 (s, 3H), 2.72 (t, *J* = 7.7 Hz, 2H), 1.75 (m, 2H), 1.40 (m, 2H), 1.34 (m, 4H), 0.89 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5 (C_q), 152.3 (C_q), 130.1 (C_q), 127.4 (2C), 114.3 (2C), 79. 8 (C_q, C-I), 55.6, 31.5, 29.0, 28.9, 26.3, 22.5, 14.1.

HRMS (MALDI-TOF) calcd for $C_{15}H_{21}IN_3O$ $[M+H]^+$ 386.0724; found 386.0726.

1-(3,5-Dimethylphenyl)-4-hexyl-5-iodo-1*H*-1,2,3-triazole (1k)



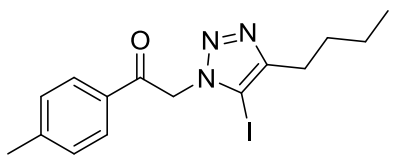
Prepared from 1-azido-3,5-dimethylbenzene (589 mg, 4 mmol) and 1-iodooct-1-yne (1.03 g, 4.4 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 954 mg (62%). Brownish solid; mp 79 – 80 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (s, 1H), 7.11 (s, 2H), 2.73 (t, *J* = 7.7 Hz, 2H), 2.39 (s, 6H), 1.75 (m, 2H), 1.42 – 1.32 (m, 6H), 0.89 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.4 (C_q), 139.1, 136.9 (C_q), 131.4, 123.6 (2C), 79.1 (C_q, C-I), 31.5, 29.0, 28.9, 26.3, 22.6, 21.2, 14.1.

HRMS (MALDI-TOF) calcd for $C_{16}H_{23}IN_3$ $[M+H]^+$ 384.0931; found 384.0929.

2-(4-Butyl-5-iodo-1H-1,2,3-triazol-1-yl)-1-(4-methylphenyl)ethanone (1l)



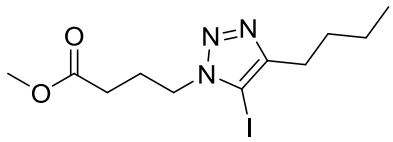
Prepared from 2-azido-1-(4-methylphenyl)ethan-1-one (438 mg, 2.5 mmol) and 1-iodohex-1-yne (624 mg, 3 mmol) according to the general procedure; eluent: CH_2Cl_2 – MeOH = 100:1. Yield 1.057 g (92%). Off-white solid; mp 109 – 110 °C (dec.).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (m, 2H), 7.34 (m, 2H), 5.81 (s, 2H), 2.70 (t, *J* = 7.7 Hz, 2H), 2.45 (s, 3H), 1.72 (m, 2H), 1.40 (m, 2H), 0.95 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 189.1 (C_q, C=O), 152.4 (C_q), 145.6 (C_q), 131.6 (C_q), 129.8 (2C), 128.2 (2C), 80.0 (C_q, C-I), 55.9, 31.1, 25.9, 22.3, 21.8, 13.9.

HRMS (MALDI-TOF) calcd for $C_{15}H_{21}IN_3O$ $[M+H]^+$ 384.0567; found 384.0569.

Methyl 4-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)butanoate (1m)



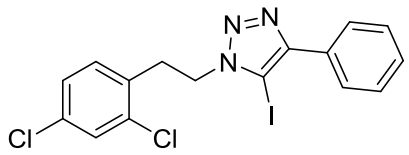
Prepared from methyl 4-azidobutyrate (117 mg, 0.82 mmol) and 1-iodohex-1-yne (131 µl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 256.3 mg (89%). Colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.43 (t, *J* = 6.9 Hz, 2H), 3.69 (s, 3H), 2.65 (m, 2H), 2.39 (t, *J* = 7.3 Hz, 2H), 2.22 (m, 2H), 1.67 (m, 2H), 1.38 (sextet, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3 (C_q, $\underline{C}O_2Me$), 151.6 (C_q), 77.6 (C_q, $\underline{C}$-I), 51.4 ($CO_2\underline{Me}$), 49.2, 30.7, 30.0, 25.4, 24.5, 21.9, 13.4 ($\underline{C}H_3$, Bu).

HRMS (ESI-TOF) calcd for $C_{11}H_{19}IN_3O_2$ $[M+H]^+$ 352.0516; found 352.0522.

1-(2,4-Dichlorophenethyl)-5-iodo-4-phenyl-1*H*-1,2,3-triazole (1n)



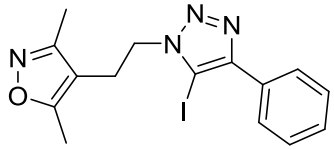
Prepared from azide **S1n** (173 mg, 0.8 mmol) and (iodoethynyl)benzene (121.6 µl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 345.9 mg (97%). White solid; mp 188 – 189 °C.

^{1}H NMR (400 MHz, $CDCl_3$/CD_3OD) δ 7.86 (m, 2H), 7.47 (m, 2H), 7.42 (m, 2H), 7.14 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.98 (d, *J* = 8.2 Hz, 1H), 4.71 (t, *J* = 7.1 Hz, 2H), 3.37 (t, *J* = 7.1 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$/CD_3OD) δ 149.3 (C_q), 134.6 (C_q), 133.5 (C_q), 132.5 (C_q), 131.5, 129.4(C_q), 129.1, 128.3, 128.1 (2C), 127.03 (2C), 126.99, 77.1 ($\underline{C}$-I), 49.3, 33.4.

HRMS (ESI-TOF) calcd for $C_{16}H_{13}Cl_2IN_3$ $[M+H]^+$ 443.9526; found 443.9524.

4-(2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-3,5-dimethylisoxazole (1o)



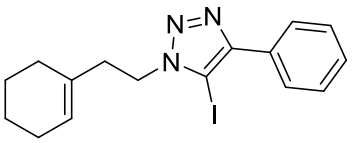
Prepared from azide **S1o** (138.5 mg, 0.833 mmol) and (iodoethynyl)benzene (121.6 µl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 299.8 mg (91%). White solid; mp 166 – 167 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (m, 2H), 7.47 (m, 2H), 7.42 (m, 1H), 4.54 (t, *J* = 7.0 Hz, 2H), 2.98 (t, *J* = 7.0 Hz, 2H), 2.22 (s, 3H), 2.13 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2 (C_q), 159.0 (C_q), 149.5 (C_q), 129.6 (C_q), 128.3, 128.2 (2C), 127.1 (2C), 108.6 (C_q), 76.6 (C_q, $\underline{C}$-I), 49.4, 23.2, 10.2, 9.7.

HRMS (ESI-TOF) calcd for $C_{15}H_{16}IN_4O$ $[M+H]^+$ 395.0363; found 395.0366.

1-(2-(Cyclohex-1-en-1-yl)ethyl)-5-iodo-4-phenyl-1*H*-1,2,3-triazole (1p)



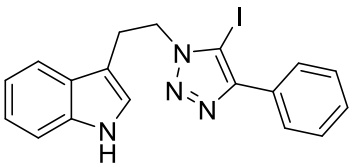
Prepared from azide **S1p** (125.6 mg, 0.83 mmol) and (iodoethynyl)benzene (121.6 μl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2 – MeOH = 100:1. Yield 176.1 mg (56%). White solid; mp 128 – 129 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (m, 2H), 7.47 (m, 2H), 7.40 (m, 1H), 5.43 (m, 1H), 4.51 (m, 2H), 2.56 (m, 2H), 2.03 (m, 2H), 1.95 (m, 2H), 1.65 (m, 2H), 1.56 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.2 (C_q), 132.4 (C_q), 130.0 (C_q), 128.11 (2C), 128.08, 127.1 (2C), 124.5, 75.8 (C_q, C-I), 49.3, 37.9, 27.9, 24.8, 22.3, 21.7.

HRMS (ESI-TOF) calcd for $C_{16}H_{19}IN_3$ $[M+H]^+$ 380.0618; found 380.0619.

3-(2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-indole (1q)



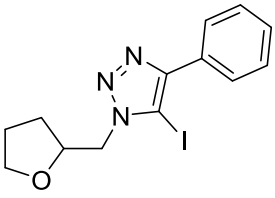
Prepared from azide **S1q** (151.8 mg, 0.815 mmol) and (iodoethynyl)benzene (121.6 μl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2 – MeOH = 50:1. Yield 322 mg (97%). White solid; mp 167 – 168 °C (dec.).

^{1}H NMR (400 MHz, $CDCl_3$/CD_3OD) δ 7.85 (m, 2H), 7.61 (m, 1H), 7.46 (m, 2H), 7.40 (m, 2H), 7.19 (m, 1H), 7.12 (m, 1H), 6.99 (s, 1H), 4.71 (t, *J* = 7.7 Hz, 2H), 3.41 (t, *J* = 7.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$/CD_3OD) δ 149.3 (C_q), 135.9 (C_q), 129.7 (C_q), 128.2, 128.1 (2C), 127.1 (2C), 126.7 (C_q), 122.4, 121.5, 118.9, 117.8, 111.0, 109.9 (C_q), 76.9 (C_q, C-I), 51.2, 26.0.

HRMS (ESI-TOF) calcd for $C_{18}H_{16}IN_4$ $[M+H]^+$ 415.0414; found 415.0410.

5-Iodo-4-phenyl-1-((tetrahydrofuran-2-yl)methyl)-1*H*-1,2,3-triazole (1r)



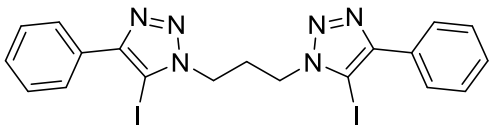
Prepared from azide **S1r** (104.2 mg, 0.82 mmol) and (iodoethynyl)benzene (121.6 μl, 0.96 mmol) according to the general procedure; eluent: CH_2Cl_2 – MeOH = 50:1. Yield 278.2 mg (98%). White solid (foam); mp 91 – 92 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (m, 2H), 7.46 (m, 2H), 7.40 (m, 1H), 4.49 (m, 3H), 3.92 (m, 1H), 3.79 (m, 1H), 2.07 (m, 1H), 1.89 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3 (C_q), 129.9 (C_q), 128.11, 128.09 (2C), 127.2 (2C), 77.1 (C_q), 76.8, 68.1, 53.7, 28.7, 25.1.

HRMS (ESI-TOF) calcd for $C_{13}H_{15}IN_3O$ $[M+H]^+$ 356.0254; found 356.0257.

1,3-Bis(5-iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)propane (1t)



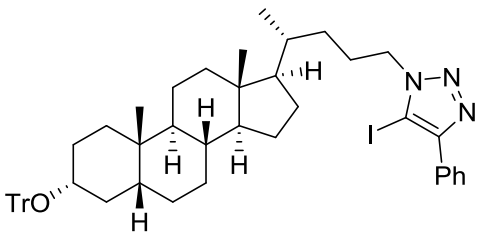
Prepared from 1,3-diazidopropane (106 mg, 0.8 mmol) and (iodoethynyl)benzene (261 µl, 2 mmol) according to the general procedure using 10 mol% of CuI and TTTA; isolated by filtration from suspension in CH_2Cl_2. Yield 464.5 mg (95%). White solid; mp > 250 °C.

^{1}H NMR (400 MHz, $CDCl_3$/TFA) δ 7.76 – 7.51 (m, 10H), 4.90 (t, *J* = 6.8 Hz, 4H), 2.99 (quintet, *J* = 6.8 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$/TFA) δ 146.9 (2C_q), 132.1, 129.3 (4C), 127.5 (4C), 121.4 (2C_q), 82.0 (2C-I), 50.6 (2C), 26.2.

HRMS (ESI-TOF) calcd for $C_{19}H_{17}I_2N_6$ $[M+H]^+$ 582.9599; found 582.9595.

24-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)-3α-trityloxy-5β-cholane (1u)



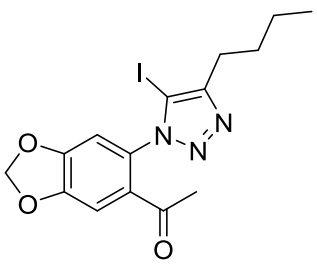
Prepared from 24-azido-3α-trityloxy-5β-cholane[9] (220 mg, 0.35 mmol) and (iodoethynyl)benzene (54.7 µl, 0.42 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 2:1, then CH_2Cl_2. Yield 268.8 mg (95%). White foam; mp 110 – 111 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (m, 2H), 7.51 (m, 8H), 7.40 (m, 1H), 7.25 (m, 9H), 4.39 (m, 2H), 3.41 (tt, *J* = 10.7, 4.3 Hz, 1H), 2.02 (m, 1H), 1.92 – 0.82 (m, 26H), 0.93 (d, *J* = 6.5 Hz, 3H), 0.76 (s, 3H), 0.60 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3 (C_q, triazole C-Ph), 145.2 (3C_q, OTr), 130.0 (C_q), 128.5 (6C), 128.13 (2C), 128.11, 127.2 (6C), 127.1 (2C), 126.4 (3C), 86.2 (C_q, C(Ph_3)), 75.7 (C_q, triazole C-I), 73.9, 56.0, 55.6, 51.0, 42.3, 42.1, 39.9, 39.7, 35.4, 35.3, 34.9, 34.5, 34.0, 32.2, 28.5, 27.9, 26.9, 26.3, 26.0, 23.8, 22.9, 20.4, 18.2, 11.6.

HRMS (ESI-TOF) calcd for $C_{51}H_{60}IN_3NaO$ $[M+Na]^+$ 880.3673; found 880.3673.

1-[6-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-1,3-benzodioxol-5-yl]ethanone (1v)



Prepared from 1-(6-azido-1,3-benzodioxol-5-yl)ethanone (580 mg, 2.83 mmol) and 1-iodohex-1-yne (423 µl, 3.1 mmol) according to the general procedure in 3 ml THF; eluent: hexanes – EtOAc = 3:1. Yield 785.5 mg (67%). Pale-brown solid; mp 110 – 111 °C (dec.).

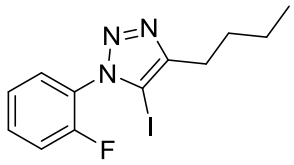
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (s, 1H), 6.74 (s, 1H), 6.16 (s, 2H),

2.73 (t, *J* = 7.7 Hz, 2H), 1.93 (s, 3H), 1.73 (m, 2H), 1.41 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195. 7 (C_q, $CH_3\underline{C}(O)$), 152.6(C_q), 150.6 (C_q), 149.4 (C_q), 131.3 (C_q), 130.5 (C_q), 109.1, 109.05, 103.1, 82.2 (C_q, <u>C</u>-I), 31.1, 28.1, 25.9, 22.2, 13.8 (<u>C</u>H_3, Bu).

HRMS (MALDI-TOF) calcd for $C_{15}H_{17}IN_3O_3$ $[M+H]^+$ 414.0309; found 414.0310.

4-Butyl-1-(2-fluorophenyl)-5-iodo-1*H*-1,2,3-triazole (1y)



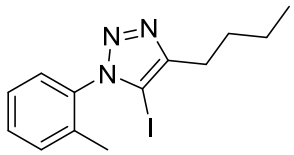
Prepared from 1-azido-2-fluorobenzene (55 mg, 0.4 mmol) and 1-iodohex-1-yne (66 μl, 0.48 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 110.9 mg (80%). White solid; mp 90 – 91 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (m, 1H), 7.45 (m, 1H), 7.37 – 7.28 (m, 2H), 2.76 (m, 2H), 1.77 (m, 2H), 1.45 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7 (d, *J* = 255 Hz, C_q, <u>C</u>-F), 152.5 (C_q), 132.4 (d, *J* = 7.4 Hz), 129.2, 125.3 (d, *J* = 12.5 Hz, C_q), 124.9 (d, *J* = 4.0 Hz), 117.0 (d, *J* = 19.2 Hz), 81.4 (C_q, <u>C</u>-I), 31.2, 26.0, 22.5, 14.0.

HRMS (ESI-TOF) calcd for $C_{12}H_{14}FIN_3$ $[M+H]^+$ 346.0211; found 346.0215.

4-Butyl-5-iodo-1-(*o*-tolyl)-1*H*-1,2,3-triazole (1aa)



Prepared from 1-azido-2-methylbenzene (66.6 mg, 0.5 mmol) and 1-iodohex-1-yne (83 μl, 0.6 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 63.2 mg (37%). Off-white solid; mp 85 – 86 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (m, 1H), 7.39 – 7.33 (m, 2H), 7.22 (m, 1H), 2.76 (m, 2H), 2.02 (s, 3H), 1.77 (m, 2H), 1.43 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0 (C_q), 136.5 (C_q), 135.9 (C_q), 131.2, 130.7, 127.9, 126.8, 81.1 (C_q, <u>C</u>-I), 31.2, 26.0, 22.4, 17.5, 14.0.

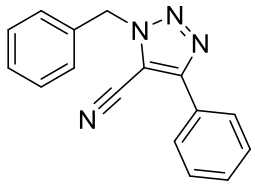
HRMS (ESI-TOF) calcd for $C_{13}H_{17}IN_3$ $[M+H]^+$ 342.0462; found 342.0464.

Synthesis of 5-Cyano-1*H*-1,2,3-triazoles 2

General procedure. In vial with a screw cap, 5-iodotriazole (0.2 mmol), $Pd(dba)_2$ (2.3 mg, 0.004 mmol, 2 mol%), Dpephos (4.3 mg, 0.008 mmol, 4 mol%), and KCN (26 mg, 0.4 mmol, 2 eq) were mixed under an argon atmosphere in dioxane (2 ml). The reaction mixture was stirred at 120 °C for 20 h (TLC control), then diluted with CH_2Cl_2 and washed with water. Organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2. The organic layers were

combined and dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography. (Caution: KCN is highly TOXIC and must be handled with care. All the wastes, particularly the aqueous phase following extraction, should be disposed in accordance with safety regulations and guidelines).

1-Benzyl-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2a)



Prepared from **1a** (72.2 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 1:1. Yield 51 mg (98 %). White solid; mp 105 – 106 °C.

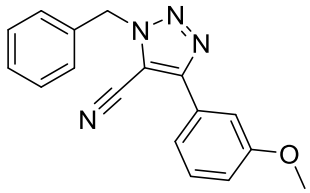
Reaction scaling to 2 mmol (722.4 mg) **7a** in a glass reactor with screw cap was carried out. Yield 504 mg (97%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (m, 2H), 7.54 – 7.34 (m, 8H), 5.70 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2 (C_q), 132.5 (C_q), 129.9, 129.0, 128.9 (2C), 128.8 (2C), 128.1 (2C), 127.3 (C_q), 126.1 (2C), 109.5 (C_q), 106.3 (C_q), 54.0 ($\underline{C}H_2$, Bn).

HRMS (ESI-TOF) calcd for $C_{16}H_{13}N_4$ $[M+H]^+$ 261.1135; found 261.1137.

1-Benzyl-5-cyano-4-(3-methoxyphenyl)-1*H*-1,2,3-triazole (2b)



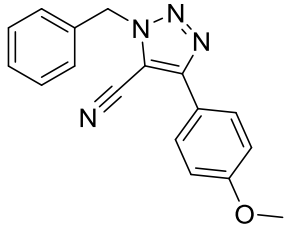
Prepared from **1b** (78.2 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 55.3 mg (95%). White solid; mp 85 – 86 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.54 (m, 2H), 7.49 – 7.32 (m, 6H), 6.99 (m, 1H), 5.69 (s, 2H), 3.85 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7 (C_q, $\underline{C}$-OMe), 152.0 (C_q), 132.5 (C_q), 129.9, 129.0, 128.9 (2C), 128.4 (C_q), 128.1 (2C), 118.4, 116.3, 110.8, 109.5 (C_q), 106.5 (C_q), 55.0, 54.0.

HRMS (MALDI-TOF) calcd for $C_{17}H_{15}N_4O$ $[M+H]^+$ 291.1240; found 291.1233.

1-Benzyl-5-cyano-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (2c)



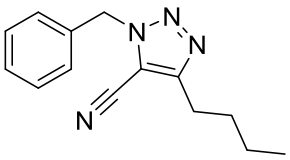
Prepared from **1c** (78.2 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 2:1. Yield 42.2 mg (73%). White solid; mp 96 – 97 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (m, 2H), 7.43 – 7.38 (m, 5H), 6.99 (m, 2H), 5.67 (s, 2H), 3.85 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7 (C_q, C-OMe), 152.2 (C_q), 132.6 (C_q), 128.92, 128.86 (2C), 128.0 (2C), 127.6 (2C), 119.8 (C_q), 114.1 (2C), 109.8 (C_q), 105.3 (C_q), 55.0, 53.9.

HRMS (MALDI-TOF) calcd for $C_{17}H_{15}N_4O$ $[M+H]^+$ 291.1240; found 291.1247.

1-Benzyl-5-cyano-4-butyl-1*H*-1,2,3-triazole (2d)



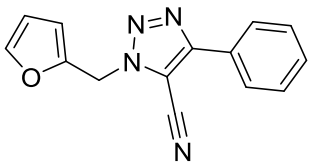
Prepared from **1d** (68.2 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 2:1. Yield 46 mg (96%). Yellowish oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (m, 5H), 5.62 (s, 2H), 2.80 (m, 2H), 1.72 (quintet, *J* = 7.6 Hz, 2H), 1.38 (sextet, *J* = 7.4 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3 (C_q), 132.6 (C_q), 128.9, 128.8 (2C), 128.0 (2C), 108.6 (C_q), 108.4 (C_q), 53.9 (CH_2, Bn), 30.2, 24.8, 21.8, 13.2 (CH_3).

HRMS (MALDI-TOF) calcd for $C_{14}H_{16}KN_4$ $[M+K]^+$ 279.1007; found 279.1005.

1-(Furan-2-ylmethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2e)



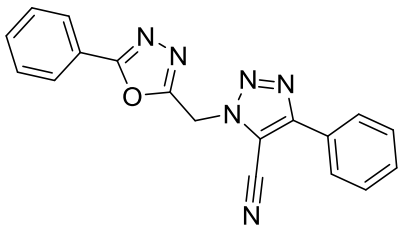
Prepared from **1e** (70.2 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 2:1. Yield 48.7 mg (94%). White solid; mp 152 – 153 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (m, 2H), 7.46 (m, 4H), 6.62 (m, 1H), 6.41 (dd, *J* = 3.4, 1.9 Hz, 1H), 5.72 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2 (C_q), 145.2 (C_q), 143.8, 130.0, 128.8 (2C), 127.2 (C_q), 126.2 (2C), 111.2, 110.6, 109.2 (C_q), 106.4 (C_q), 46.6 (CH_2).

HRMS (ESI-TOF) calcd for $C_{14}H_{11}N_4O$ $[M+H]^+$ 251.0927; found 251.0928.

5-Cyano-4-phenyl-1-((5-phenyl-1,3,4-oxadiazol-2-yl)methyl)-1*H*-1,2,3-triazole (2f)



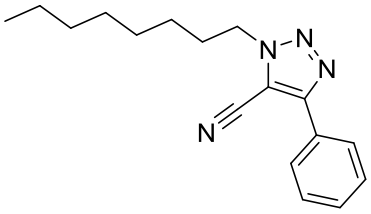
Prepared from **1f** (85.8 mg, 0.2 mmol) according to the general procedure, heating 30 h; eluent: EtOAc – hexanes = 1:2. Yield 42.5 mg (65%). White solid; mp 151 – 152 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 8.03 (m, 4H), 7.61 – 7.44 (m, 6H), 6.08 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1 (C_q), 158.2 (C_q), 152.5 (C_q), 132.1, 130.4, 128.93 (2C), 128.85 (2C), 126.9 (2C), 126.7 (C_q), 126.3 (2C), 122.4 (C_q), 108.8 (C_q), 107.2 (C_q), 44.0 (CH_2).

HRMS (ESI-TOF) calcd for $C_{18}H_{13}N_6O$ $[M+H]^+$ 329.1145; found 329.1150.

1-Octyl-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2g)



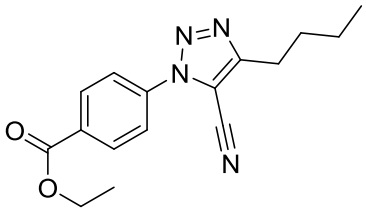
Prepared from **1g** (78.9 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 2:1. Yield 55.3 mg (98%). Yellowish liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (m, 2H), 7.49 (m, 3H), 4.54 (t, *J* = 7.3 Hz, 2H), 2.03 (m, 2H), 1.37 – 1.27 (m, 10H), 0.88 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6 (C_q), 129.8, 128.8 (2C), 127.4 (C_q), 126.1 (2C), 109.6 (C_q), 106.5 (C_q), 50.3, 31.3, 29.5, 28.6, 28.4, 25.9, 22.2, 13.7 ($\underline{C}H_3$).

HRMS (MALDI-TOF) calcd for $C_{17}H_{23}N_4$ $[M+H]^+$ 283.1917; found 283.1921.

Ethyl 4-(4-butyl-5-cyano-1*H*-1,2,3-triazol-1-yl)benzoate (2h)



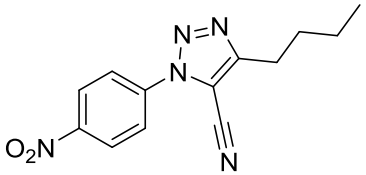
Prepared from **1h** (79.8 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 55.1 mg (92%). Yellowish oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (m, 2H), 7.89 (m, 2H), 4.44 (q, *J* = 7.3 Hz, 2H), 2.94 (m, 2H), 1.83 (m, 2H), 1.51 – 1.41 (m, 5H), 0.99 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.6 (C_q, $\underline{C}O_2Et$), 156.4 (C_q), 138.1 (C_q), 131.8 (C_q), 130.9 (2C), 121.9 (2C), 108.9 (C_q), 108.0 (C_q), 61.2 ($\underline{C}H_2$, Et), 30.2, 24.8, 21.8, 13.9 ($\underline{C}H_3$, Et), 13.2 ($\underline{C}H_3$, Bu).

HRMS (MALDI-TOF) calcd for $C_{16}H_{19}N_4O_2$ $[M+H]^+$ 299.1503; found 299.1503.

4-Butyl-5-cyano-1-(4-nitrophenyl)-1*H*-1,2,3-triazole (2i)



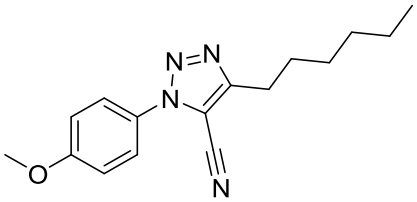
Prepared from **1i** (74 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 2:1. Yield 40.2 mg (74%). Yellowish solid; mp 63 – 64 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (m, 2H), 8.05 (m, 2H), 2.96 (m, 2H), 1.84 (quintet, *J* = 7.6 Hz, 2H), 1.47 (sextet, *J* = 7.4 Hz, 2H), 1.00 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.9 (C_q), 147.9 (C_q), 139.3 (C_q), 125.2 (2C), 122.7 (2C), 108.7 (C_q), 108.0 (C_q), 30.2, 24.8, 21.8, 13.2 ($\underline{C}H_3$, Bu).

HRMS (ESI-TOF) calcd for $C_{13}H_{14}N_5O_2$ $[M+H]^+$ 272.1142; found 272.1144.

5-Cyano-4-hexyl-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (2j)



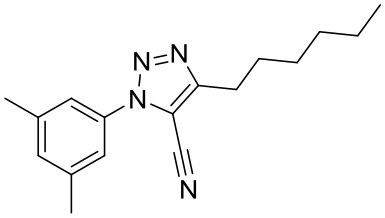
Prepared from **1j** (77.1 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 56.5 mg (99%). Yellowish solid; mp 63 – 64 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (m, 2H), 7.06 (m, 2H), 3.89 (s, 3H), 2.90 (t, *J* = 7.7 Hz, 2H), 1.82 (m, 2H), 1.49 – 1.27 (m, 6H), 0.90 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5 (C_q, C-OMe), 155.6 (C_q), 128.1 (C_q), 124.0 (2C), 114.5 (2C), 109.2 (C_q), 108.3 (C_q), 55.3, 31.0, 28.4, 28.2, 25.1, 22.1, 13.6 (CH_3).

HRMS (MALDI-TOF) calcd for $C_{16}H_{21}N_4O$ $[M+H]^+$ 285.1710; found 285.1716.

5-Cyano-1-(3,5-dimethylphenyl)-4-hexyl-1*H*-1,2,3-triazole (2k)



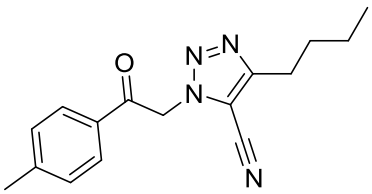
Prepared from **1k** (76.7 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 1:1. Yield 23.6 mg (42%). Colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (s, 2H), 7.18 (s, 1H), 2.91 (t, *J* = 7.7 Hz, 2H), 2.43 (s, 6H), 1.82 (m, 2H), 1.49 – 1.28 (m, 6H), 0.90 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8 (C_q), 139.6 (C_q, 2C, C-Me), 134.9 (C_q), 131.7, 120.2 (2C, C-H_{Ar}), 109.1 (C_q), 108.2 (C_q), 31.0, 28.4, 28.3, 25.1, 22.1, 20.9, 13.6 (CH_3, Hex).

HRMS (MALDI-TOF) calcd for $C_{17}H_{23}N_4$ $[M+H]^+$ 283.1917; found 283.1914.

5-Cyano-4-butyl-1-(2-oxo-2-(*p*-tolyl)ethyl)-1*H*-1,2,3-triazole (2l)



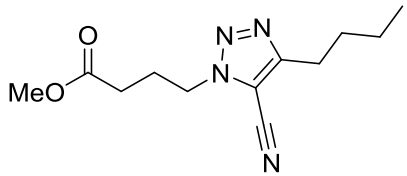
Prepared from **1l** (76.6 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 44 mg (78%). Pale yellow solid; mp 53 – 54 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (m, 2H), 7.35 (m, 2H), 5.94 (s, 2H), 2.89 (t, *J* = 7.7 Hz, 2H), 2.46 (s, 3H), 1.79 (m, 2H), 1.43 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 187.6 (C_q, C=O), 154.8 (C_q), 145.8 (C_q), 130.5 (C_q), 129.5 (2C), 127.9 (2C), 110.5 (C_q), 108.6 (C_q), 55.0 (C(O)CH_2), 30.2, 24.9, 21.8, 21.5, 13.3 (CH_3, Bu).

HRMS (MALDI-TOF) calcd for $C_{16}H_{19}N_4O$ $[M+H]^+$ 283.1553; found 283.1549.

Methyl 4-(4-butyl-5-cyano-1*H*-1,2,3-triazol-1-yl)butanoate (2m)



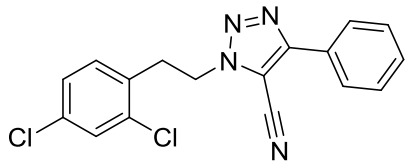
Prepared from **1m** (70.2 mg, 0.2 mmol) according to the general procedure, heating 40 h; eluent: CH_2Cl_2 – MeOH = 50:1. Yield 22.6 mg (45%). Yellowish oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.56 (t, *J* = 6.8 Hz, 2H), 3.70 (s, 3H), 2.84 (m, 2H), 2.41 (m, 2H), 2.31 (m, 2H), 1.75 (m, 2H), 1.40 (sextet, *J* = 7.4 Hz, 2H), 0.96 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8 (C_q, $\underline{C}O_2Me$), 154.8 (C_q), 108.8 (C_q), 108.5 (C_q), 51.6, 49.0, 30.2, 29.9, 24.8, 24.4, 21.8, 13.2 ($\underline{C}H_3$, Bu).

HRMS (ESI-TOF) calcd for $C_{12}H_{19}N_4O_2$ $[M+H]^+$ 251.1503; found 251.1506.

1-(2,4-Dichlorophenethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2n)



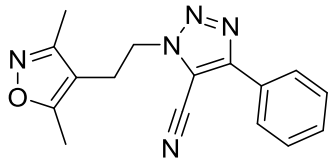
Prepared from **1n** (88.8 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 2:1. Yield 68 mg (99%). Yellowish solid; mp 87 – 88 °C.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.0 (m, 2H), 7.48 (m, 4H), 7.15 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.99 (d, *J* = 8.2 Hz, 1H), 4.80 (t, *J* = 7.1 Hz, 2H), 3.43 (t, *J* = 7.1 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 152.0 (C_q), 135.0 (C_q), 134.5 (C_q), 132.1 (C_q), 131.8, 130.4, 129.9, 129.2 (2C), 127.7, 127.6 (C_q), 126.6 (2C), 109.4 (C_q), 107.3 (C_q), 49.5, 33.8.

HRMS (MALDI-TOF) calcd for $C_{17}H_{13}Cl_2N_4$ $[M+H]^+$ 343.0512; found 343.0505.

4-(2-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-3,5-dimethylisoxazole (2o)



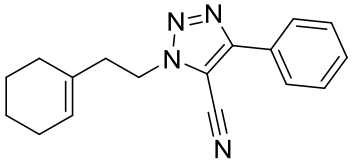
Prepared from **1o** (78.8 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – MeOH = 50:1. Yield 55.1 mg (94%). White solid; mp 116 – 117 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (m, 2H), 7.51 (m, 3H), 4.63 (t, *J* = 7.1 Hz, 2H), 3.05 (t, *J* = 7.1 Hz, 2H), 2.20 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4 (C_q), 158.7 (C_q), 151.6 (C_q), 130.1, 128.9 (2C), 126.9 (C_q), 126.1 (2C), 109.1 (C_q), 107.8 (C_q), 106.9 (C_q), 49.3, 23.0, 10.3, 9.6.

HRMS (MALDI-TOF) calcd for $C_{16}H_{15}N_5NaO$ $[M+Na]^+$ 316.1169; found 316.1162.

1-(2-(Cyclohex-1-en-1-yl)ethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2p)



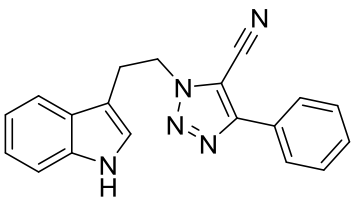
Prepared from **1p** (75.8 mg, 0.2 mmol) according to the general procedure, heating 44 h; eluent: CH_2Cl_2 – hexanes = 2:1. Yield 39.7 mg (71%). White solid; mp 52 – 53 °C.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (m, 2H), 7.50 (m, 2H), 7.46 (m, 1H), 5.36 (m, 1H), 4.61 (t, *J* = 7.1 Hz, 2H), 2.62 (m, 2H), 2.02 (m, 2H), 1.92 (m, 2H), 1.66 (m, 2H), 1.54 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 151.8 (C_q), 132.0 (C_q), 130.2, 129.2 (2C), 127.9 (C_q), 126.5 (2C), 126.0, 110.1 (C_q), 107.2 (C_q), 49.3, 38.4, 27.9, 25.2, 22.6, 21.9.

HRMS (MALDI-TOF) calcd for $C_{17}H_{19}N_2$ $[(M-N_2)+H]^+$ 251.1543; found 251.1539.

3-(2-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-indole (2q)



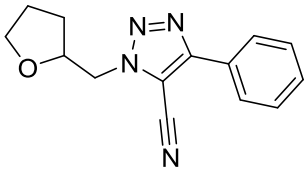
Prepared from **1q** (82.9 mg, 0.2 mmol) according to the general procedure, addition of the catalyst was repeated after 20 h, additional heating for 20 h; eluent: CH_2Cl_2 – MeOH = 100:1. Yield 53.4 mg (85%). Yellowish solid; mp 125 – 126 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (br s, 1H), 7.93 (m, 2H), 7.51 – 7.39 (m, 4H), 7.34 (m, 1H), 7.18 (m, 1H), 7.10 (m, 1H), 6.95 (d, *J* = 2.4 Hz, 1H), 4.77 (t, *J* = 7.3 Hz, 2H), 3.46 (t, *J* = 7.3 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.5 (C_q), 135.8 (C_q), 129.8, 128.8 (2C), 127.4 (C_q), 126.5 (C_q), 126.2 (2C), 122.4, 122.1, 119.6, 117.6, 111.1, 109.7 (C_q), 109.2 (C_q), 107.0 (C_q), 51.1, 26.0.

HRMS (ESI-TOF) calcd for $C_{19}H_{16}N_5$ $[M+H]^+$ 314.1400; found 314.1399.

5-Cyano-4-phenyl-1-((tetrahydrofuran-2-yl)methyl)-1*H*-1,2,3-triazole (2r)



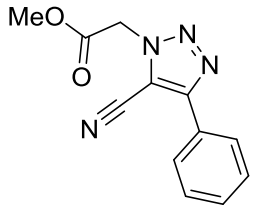
Prepared from **1r** (71 mg, 0.2 mmol) according to the general procedure, addition of the catalyst was repeated after 20 h, additional heating for 20 h; eluent: CH_2Cl_2 – MeOH = 100:1. Yield 36.3 mg (71%). Yellowish solid; mp 83 – 84 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (m, 2H), 7.49 (m, 3H), 4.66 (dd, *J* = 13.6, 3.4 Hz, 1H), 4.47 (dd, *J* = 13.6, 7.6 Hz, 1H), 4.41 (m, 1H), 3.93 (m, 1H), 3.81 (m, 1H), 2.16 (m, 1H), 1.92 (m, 2H), 1.78 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.4 (C_q), 129.7, 128.7 (2C), 127.4 (C_q), 126.2 (2C), 109.8 (C_q), 108.0 (C_q), 76.5, 68.1, 53.8, 28.5, 25.2.

HRMS (ESI-TOF) calcd for $C_{14}H_{15}N_4O$ $[M+H]^+$ 255.1240; found 255.1237.

Methyl 2-(5-cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)acetate (2s)



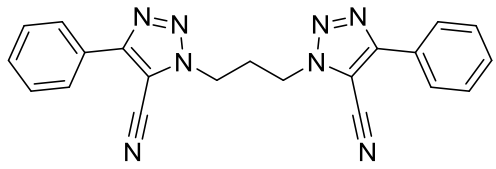
Prepared from methyl **1s** (68.6 mg, 0.2 mmol) according to the general procedure, addition of the catalyst was repeated after 20 h, additional heating for 20 h; eluent: CH_2Cl_2. Yield 19.2 mg (40%). White solid; mp 144 – 145 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (m, 2H), 7.50 (m, 3H), 5.35 (s, 2H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7 (C_q, $\underline{C}O_2Me$), 152.0 (C_q), 130.1, 128.8 (2C), 127.0 (C_q), 126.2 (2C), 109.1 (C_q), 107.8 (C_q), 53.2, 50.1.

HRMS (ESI-TOF) calcd for $C_{12}H_{11}N_4O_2$ $[M+H]^+$ 243.0877; found 243.0878.

1,3-Bis(5-cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)propane (2t)



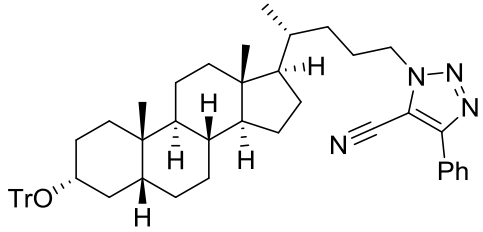
Prepared from **1t** (116.4 mg, 0.2 mmol) according to the general procedure, heating 44 h; eluent: CH_2Cl_2 – MeOH = 100:1. Yield 63.9 mg (84%). White solid; mp 165 – 166 °C.

^{1}H NMR (600 MHz, $CDCl_3$/CD_3OD) δ 8.00 (m, 4H), 7.50 (m, 6H), 4.73 (t, *J* = 6.7 Hz, 4H), 2.89 (quintet, *J* = 6.7 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$/CD_3OD) δ 152.4 (C_q), 130.5, 129.2 (2C), 127.3 (C_q), 126.6 (2C), 109.5 (C_q), 107.4 (C_q), 47.2 (2C), 28.7.

HRMS (ESI-TOF) calcd for $C_{21}H_{17}N_8$ $[M+H]^+$ 381.1571; found 381.1569.

24-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)-3*α*-trityloxy-5β-cholane (2u)



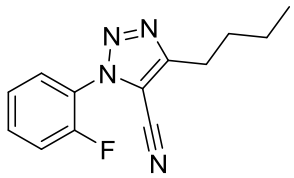
Prepared from **1u** (171.6 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2 – hexanes = 2:1. Yield 141.5 mg (93%). White solid (foam); mp 116 – 117 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (m, 2H), 7.52 (m, 7H), 7.48 (m, 2H), 7.27 (m, 6H), 7.21 (m, 3H), 4.50 (m, 2H), 3.43 (tt, *J* = 10.8, 4.3 Hz, 1H), 2.11 (m, 1H), 1.91 (m, 2H), 1.81 – 0.78 (m, 24H), 0.93 (m, 3H), 0.76 (s, 3H), 0.60 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7 (C_q, triazole $\underline{C}$-Ph), 145.2 ($3C_q$, OTr), 129.8, 128.8 (2C), 128.5 (6C), 127.4 (C_q), 127.2 (6C), 126.4 (3C), 126.2 (2C), 109.7 (C_q), 106.5 (C_q), 86.2 (C_q, $\underline{C}(Ph_3)$), 73.9, 56.0, 55.5, 50.8, 42.3, 42.1, 39.9, 39.7, 35.4, 35.3, 34.8, 34.5, 34.0, 32.1, 28.5, 27.9, 26.9, 26.3, 25.9, 23.8, 22.9, 20.4, 18.1, 11.6.

HRMS (ESI-TOF) calcd for $C_{52}H_{60}N_4NaO$ $[M+Na]^+$ 779.4659; found 779.4667.

4-Butyl-5-cyano-1-(2-fluorophenyl)-1*H*-1,2,3-triazole (2y)

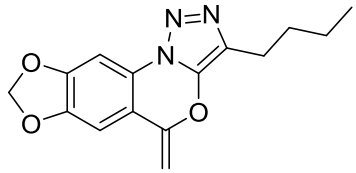


Prepared from **1y** (69 mg, 0.2 mmol) according to the general procedure; eluent: CH_2Cl_2. Yield 12.0 mg (24%). Yellowish oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 2H), 7.43 – 7.35 (m, 2H), 2.94 (m, 2H), 1.84 (m, 2H), 1.46 (m, 2H), 0.99 (t, *J* = 7.4 Hz, 3H).

HRMS (ESI-TOF) calcd for $C_{13}H_{14}FN_4$ $[M+H]^+$ 245.1197; found 245.1197.

3-Butyl-5-methylene-5*H*-[1,3]dioxolo[4,5-*g*][1,2,3]triazolo[1,5-*a*][3,1]benzoxazine (3)



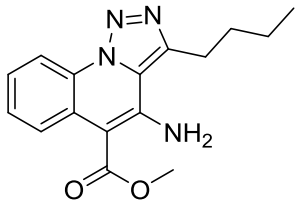
Prepared from **1v** (82.6 mg, 0.2 mmol) according to the general procedure; eluent: EtOAc – hexanes = 1:3. Yield 27.4 mg (48%). Pale yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 6.95 (s, 1H), 6.07 (s, 2H), 4.86 (d, *J* = 3.3 Hz, 2H), 4.82 (d, *J* = 3.3 Hz, 2H), 2.67 (m, 2H), 1.70 (m, 2H), 1.41 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.2 (C_q), 149.8 (C_q), 147.2 (C_q), 141.4 (C_q), 127.5 (C_q), 124.8 (C_q), 109.7 (C_q), 103.1, 101.9, 96.1, 89.3, 30.2, 23.0, 21.9, 13.4 ($\underline{C}H_3$, Bu).

HRMS (ESI-TOF) calcd for $C_{15}H_{16}N_3O_3$ $[M+H]^+$ 286.1186; found 286.1190.

Methyl 4-amino-3-butyl[1,2,3]triazolo[1,5-*a*]quinoline-5-carboxylate (4)



Prepared from **1w** (77.1 mg, 0.2 mmol) according to the general procedure; eluent: PhH – MeCN = 30:1. Yield 24.5 mg (41%). White solid; mp 122 – 123 °C.

The repeated addition of the catalyst after 20 h and an additional heating for 20 h increased the yield to 34.8 mg (58%).

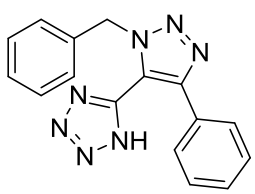
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (m, 1H), 8.46 (m, 1H), 7.44 (m, 2H), 6.83 (br s, 2H), 4.01 (s, 3H), 3.17 (t, *J* = 7.8 Hz, 2H), 1.88 (q, *J* = 7.6 Hz, 2H), 1.50 (m, 2H), 1.00 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5 (C_q, $\underline{C}O_2Me$), 142.7 (C_q), 142.65 (C_q), 142.58 (C_q), 127.0, 126.8 (C_q), 125.8, 124.9, 122.9 (C_q), 122.7 (C_q), 115.7, 96.3 (C_q), 51.4 ($CO_2\underline{Me}$), 31.4, 26.8, 22.0, 13.4 ($\underline{C}H_3$, Bu).

HRMS (MALDI-TOF) calcd for $C_{16}H_{19}N_4O_2$ $[M+H]^+$ 299.1503; found 291.1500.

Modification of 5-cyanotriazoles

Synthesis of 5-(1-benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)-1*H*-tetrazole (5)



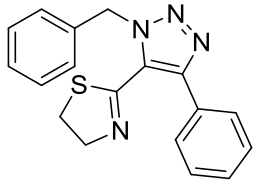
In a vial with a screw cap, **2a** (52.1 mg, 0.2 mmol), NaN_3 (26 mg, 0.4 mmol), and NH_4Cl (21.4 mg, 0.4 mmol) were mixed under an argon atmosphere in DMF (1 ml). The reaction mixture was stirred at 100 °C for 24 h, then diluted with CH_2Cl_2, and washed with aqueous HCl (5%). Organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2. The organic layers were combined and dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography. Eluent: CH_2Cl_2 – MeOH = 5:1. Yield 43.2 mg (72%). White solid; mp 128 – 129 °C (dec.).

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.83 (m, 2H), 7.47 – 7.19 (m, 6H), 7.12 (m, 2H), 5.75 (s, 2H), 5.29 (br s, 1H, N<u>H</u>).

^{13}C NMR (101 MHz, DMSO-d_6) δ 150.2 (C_q), 144.7 (C_q), 136.0 (C_q), 130.8 (C_q), 128.6 (2C), 128.4 (2C), 128.0, 127.9, 127.7 (2C), 127.2 (2C), 125.6 (C_q), 51.8 (<u>C</u>H_2).

HRMS (MALDI-TOF) calcd for $C_{16}H_{14}N_7$ $[M+H]^+$ 304.1305; found 304.1306.

Synthesis 2-(1-benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)-4,5-dihydrothiazole (6)



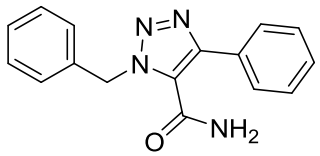
In vial with a screw cap, **2a** (52.1 mg, 0.2 mmol), 2-mercaptoethylamine hydrochloride (34.1 mg, 0.3 mmol) and NaOH (2.3 mg, 0.06 mmol, 20 mol%) were mixed in *t*-BuOH (100 μl). The reaction mixture was stirred at 80 °C for 22 h, then diluted with CH_2Cl_2 and washed with water. Organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2. The organic layers were combined and dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography. Eluent: CH_2Cl_2 – MeOH = 50:1. Yield 43.3 mg (68%). Colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (m, 2H), 7.41 (m, 3H), 7.30 (m, 3H), 7.24 (m, 2H), 5.84 (s, 2H), 4.36 (t, J = 8.5 Hz, 2H), 3.26 (t, J = 8.5 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0 (C_q), 147.8 (C_q), 134.8 (C_q), 129.5 (C_q), 128.6 (2C), 128.5, 128.3 (2C), 127.9 (2C), 127.8, 127.5 (2C), 126.3 (C_q), 64.3, 52.9, 33.8.

HRMS (MALDI-TOF) calcd for $C_{18}H_{17}N_4S$ $[M+H]^+$ 321.1168; found 321.1169.

Synthesis of 1-benzyl-4-phenyl-1*H*-1,2,3-triazole-5-carboxamide (7)



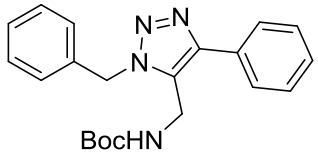
The mixture of **2a** (52.1 mg, 0.2 mmol), 6M solution of NaOH (9 µl, 0.05 mmol), and 30% solution of H_2O_2 (56 µl, 0.39 mmol) in EtOH (95%, 1 ml) was stirred at 50 °C for 1.5 h, then diluted with CH_2Cl_2 and washed with aqueous HCl (5%). Organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2. The organic layers were combined and dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography. Eluent: CH_2Cl_2 – MeOH = 30:1, then CH_2Cl_2 – MeOH = 10:1. Yield 44.7 mg (80%). White solid; mp 192 – 193 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.33 (s, 1H, NH_2), 8.16 (s, 1H, NH_2), 7.76 (m, 2H), 7.46 (m, 2H), 7.41 – 7.26 (m, 6H), 5.67 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.4 (C_q, $\underline{C}$(O)NH_2), 143.6 (C_q), 135.5 (C_q), 130.1 (C_q), 129.9 (C_q), 128.79 (2C), 128.76 (2C), 128.4, 128.2, 127.9 (2C), 126.8 (2C), 52.1 ($\underline{C}H_2$, Bn).

HRMS (MALDI-TOF) calcd for $C_{16}H_{15}N_4O$ $[M+H]^+$ 279.1240; found 279.1234.

Synthesis of *tert*-butyl ((1-benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)methyl)carbamate (8)



The mixture of **2a** (52.1 mg, 0.2 mmol), Boc_2O (87.3 mg, 0.4 mmol), and $NiCl_2 \cdot 6H_2O$ (4.8 mg, 0.02 mmol, 10 mol%) in MeOH (1 ml) was cooled to 0 °C, then $NaBH_4$ (53 mg, 1.4 mmol) was added. Then reaction mixture was maintained at room temperature for 1 h, then diluted with CH_2Cl_2 and washed with water. Organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2. The organic layers were combined and dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography. Eluent: CH_2Cl_2 – MeOH = 50:1. Yield 59.2 mg (81%). White solid; mp 106 – 107 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (m, 2H), 7.43 (m, 2H), 7.44 – 7.27 (m, 6H), 5.63 (s, 2H), 4.80 (br s, 1H), 4.45 (d, J = 5.6 Hz, 2H), 1.41 (s, 9H).

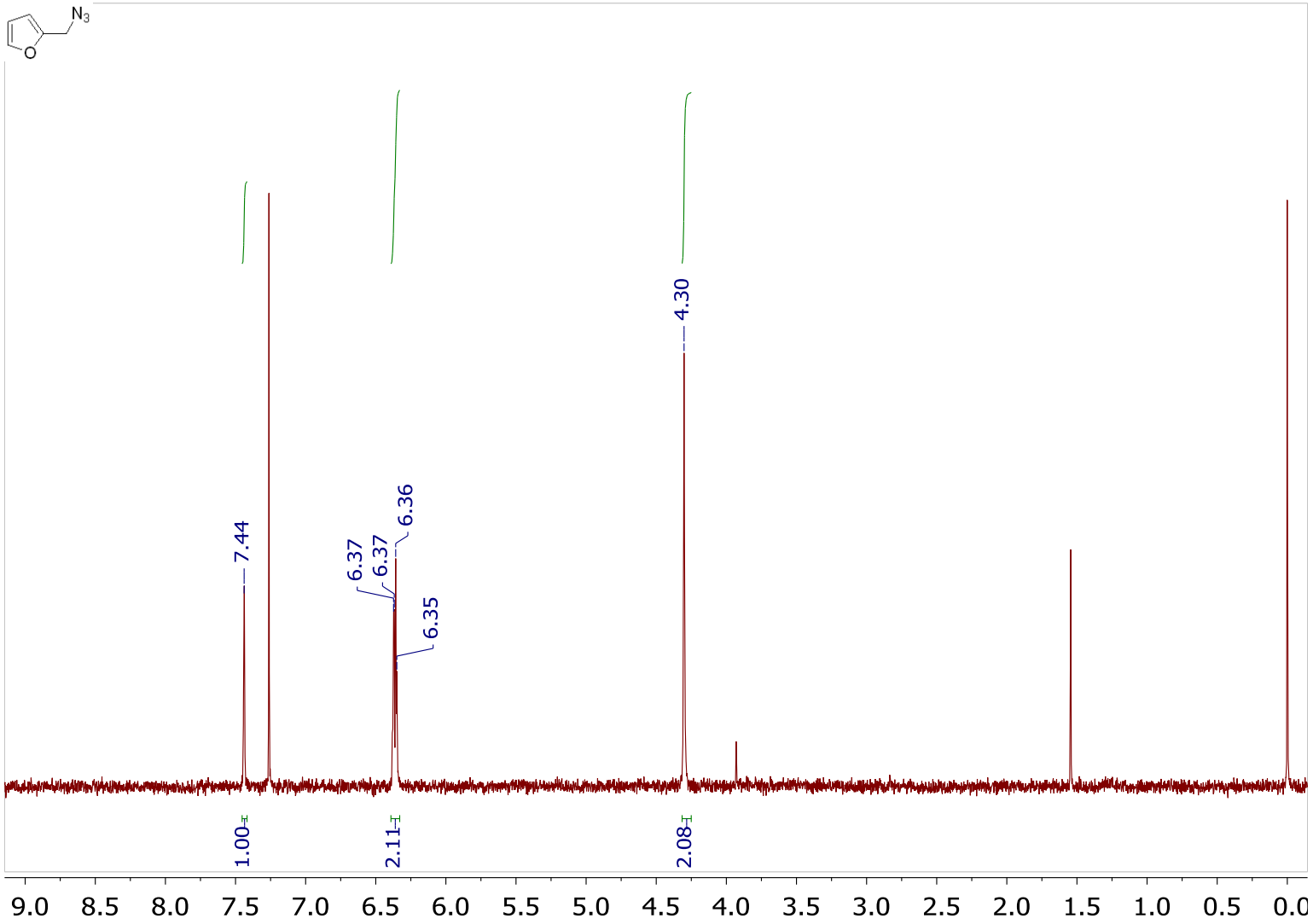
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.0 (C_q, O$\underline{C}$(O)NH), 145.8 (C_q), 134.7 (C_q), 130.3 (C_q), 129.4 (C_q), 128.6 (2C), 128.4 (2C), 128.0, 127.8, 127.1 (2C), 127.0 (2C), 79.9 (C_q, $\underline{C}(CH_3)_3$), 51.8 ($\underline{C}H_2$, Bn), 32.5 ($\underline{C}H_2$NH), 27.9 (3C, C($\underline{C}H_3)_3$).

HRMS (ESI-TOF) calcd for $C_{21}H_{25}N_4O_2$ $[M+H]^+$ 365.1972; found 365.1968.

Copies of ^{1}H and ^{13}C NMR spectra

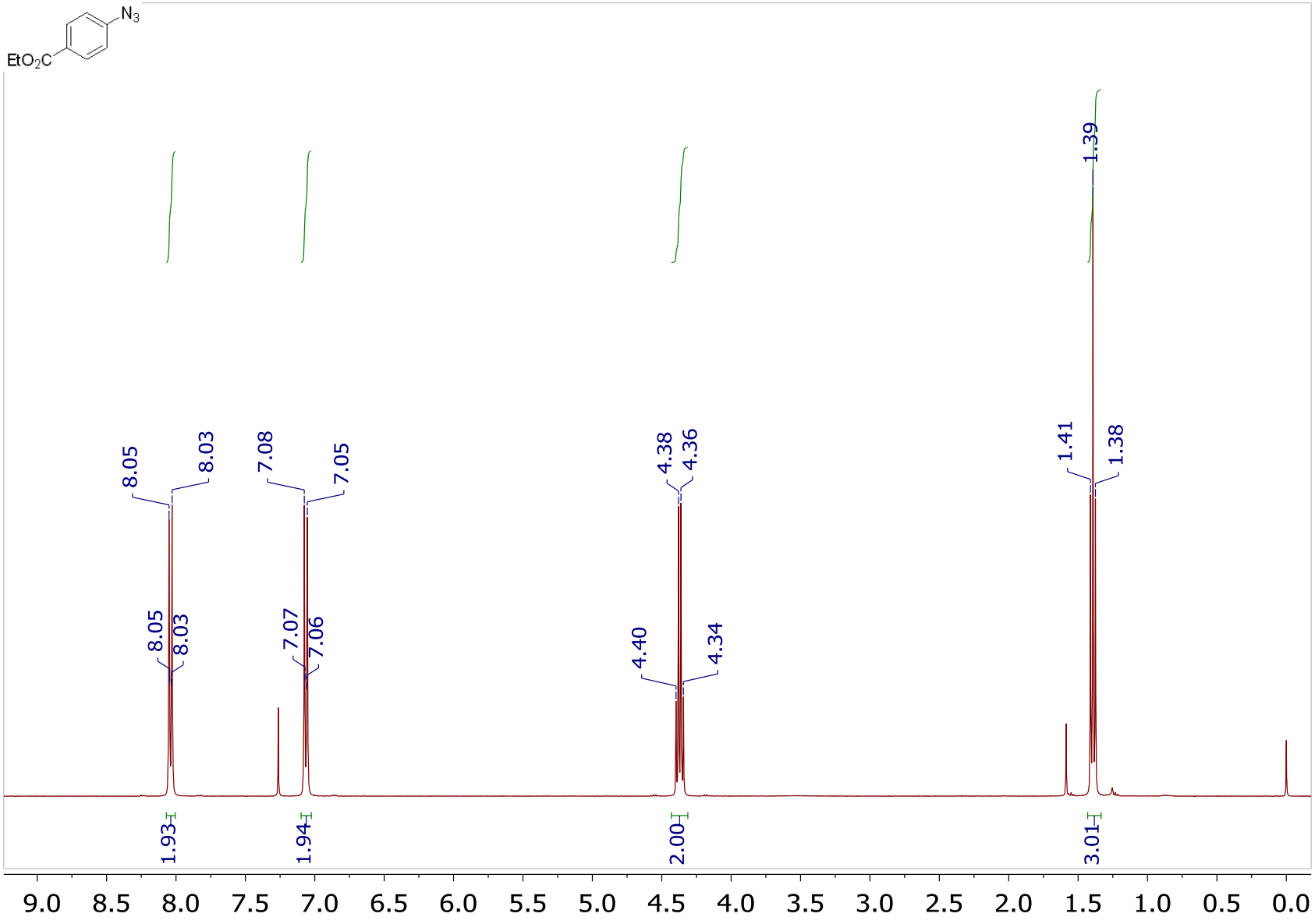
(2-Azidomethyl)furan (S1e)

^{1}H NMR (400 MHz, $CDCl_3$)



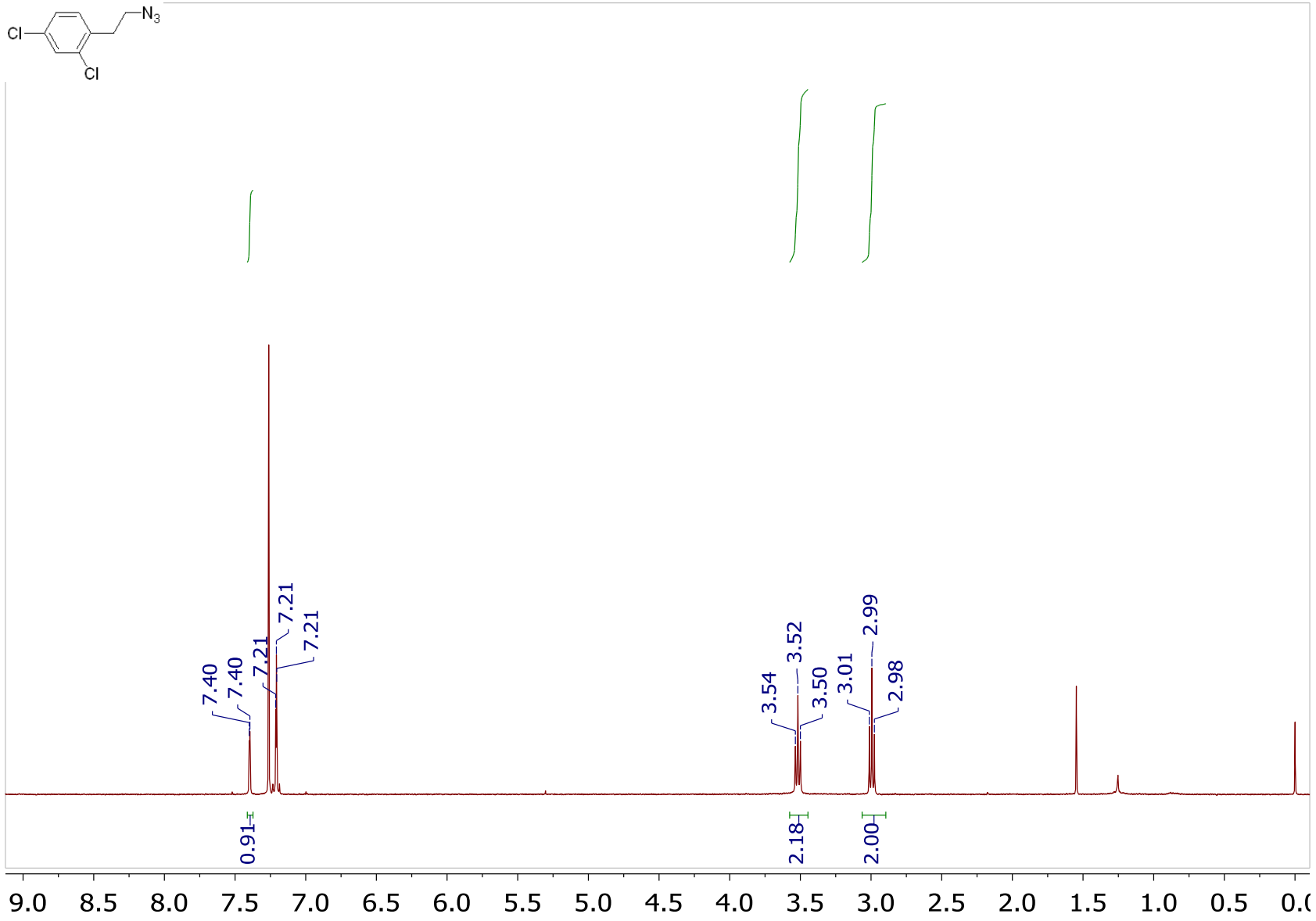
Ethyl (4-azido)benzoate (S1h)

^{1}H NMR (400 MHz, $CDCl_3$)



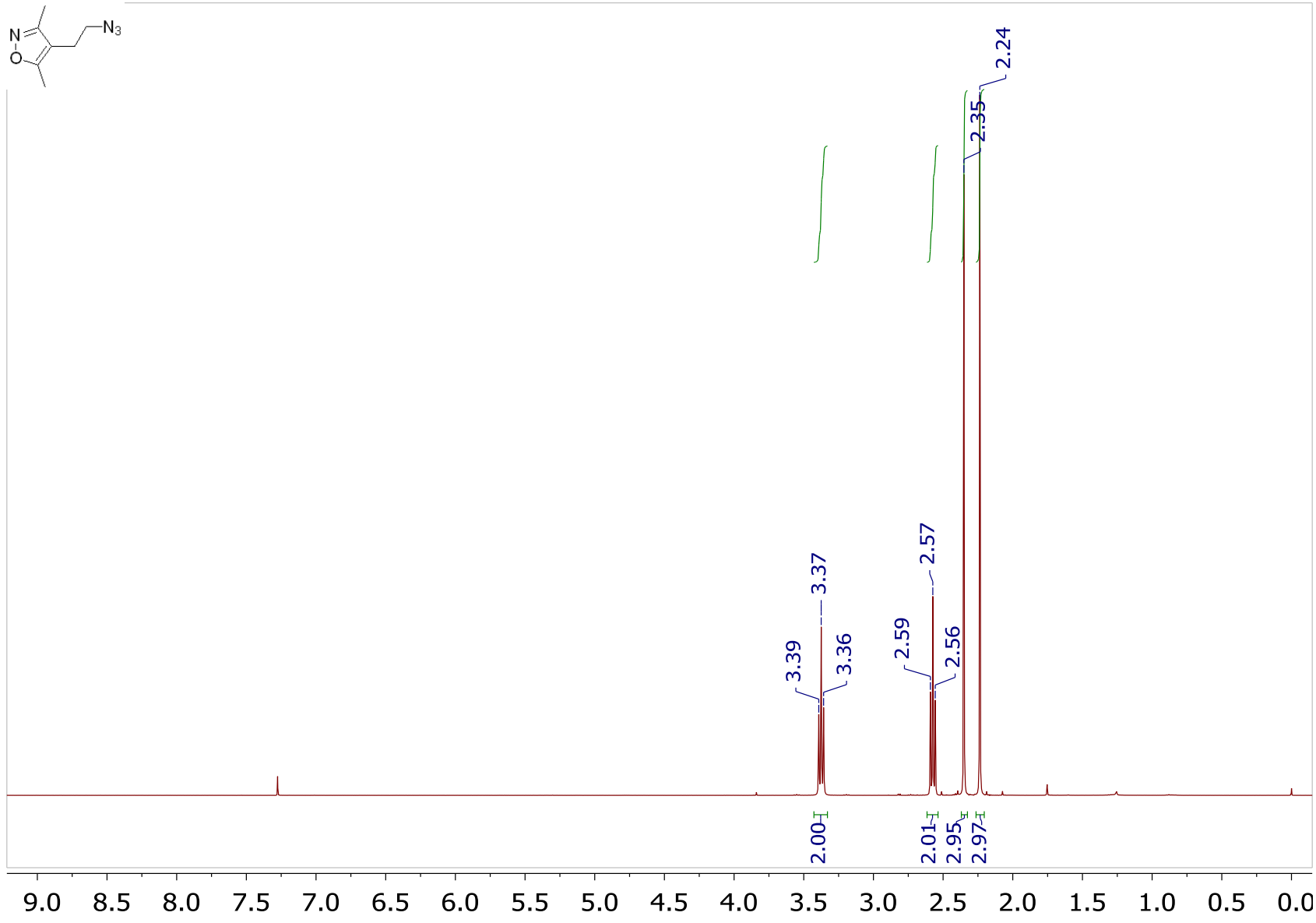
1-(2-Azidoethyl)-2,4-dichlorobenzene (S1n)

^{1}H NMR (400 MHz, $CDCl_3$)



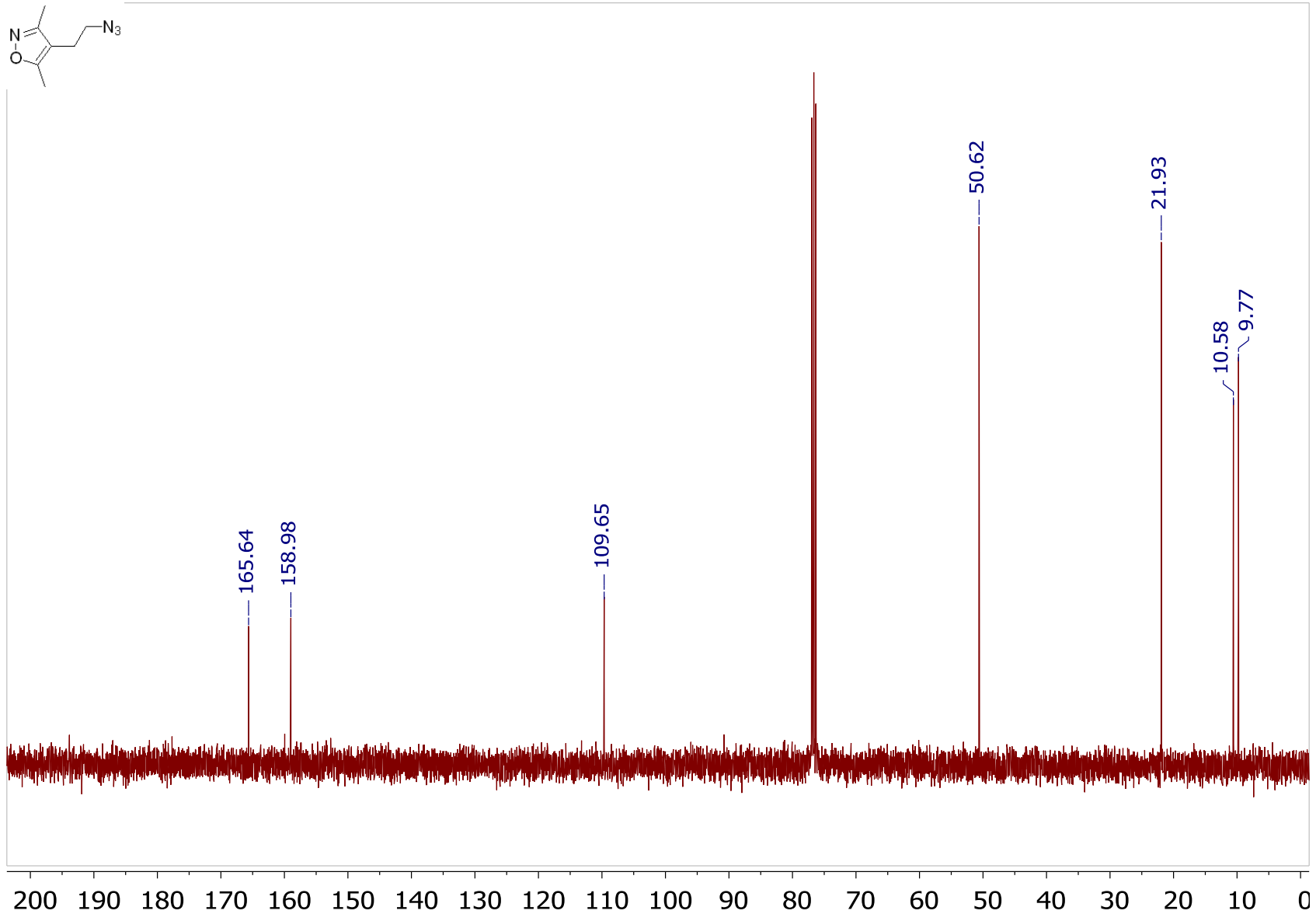
4-(2-Azidoethyl)-3,5-dimethylisoxazole (S1o)

^{1}H NMR (400 MHz, $CDCl_3$)



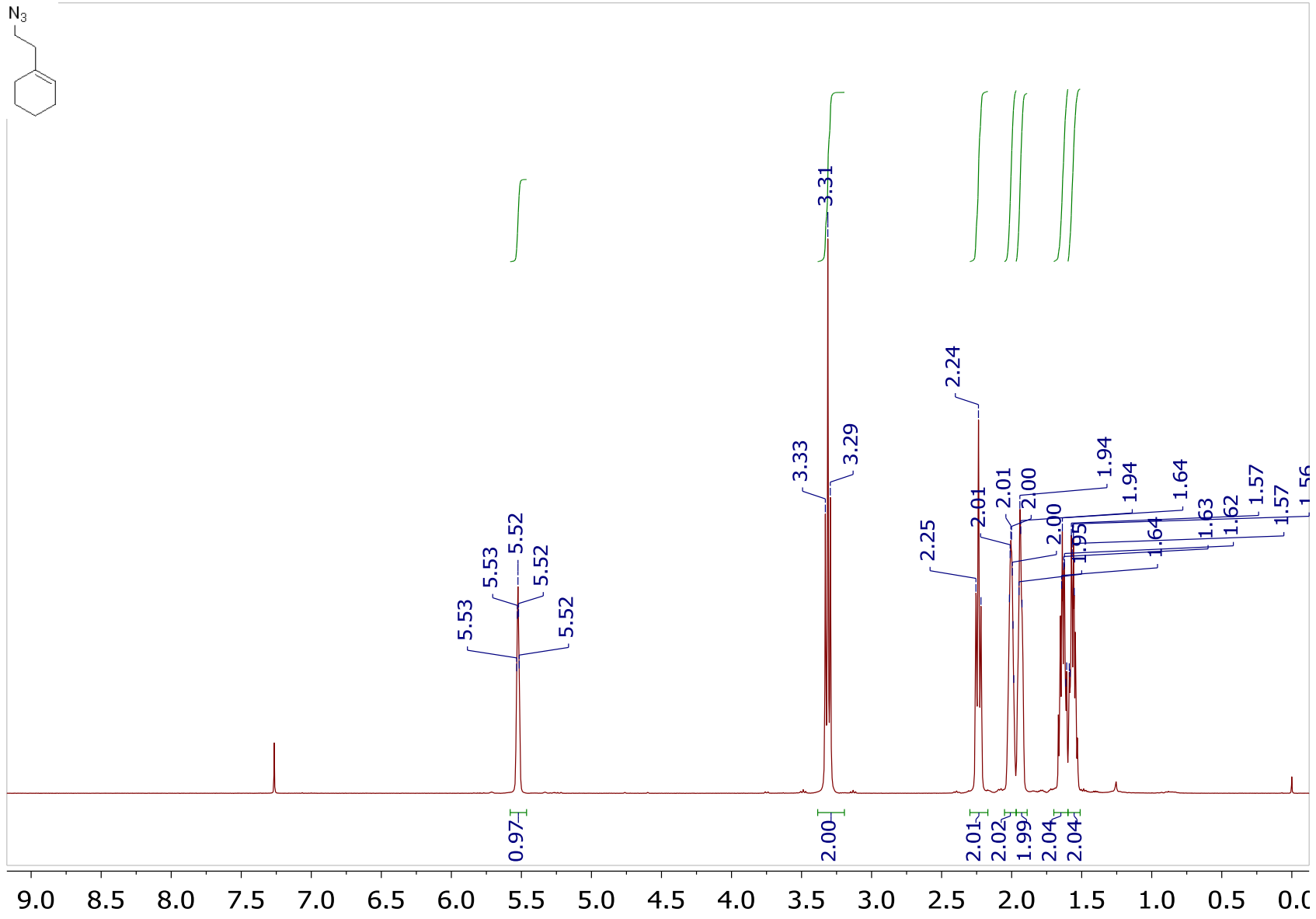
4-(2-Azidoethyl)-3,5-dimethylisoxazole (S1o)

^{13}C NMR (101 MHz, $CDCl_3$)



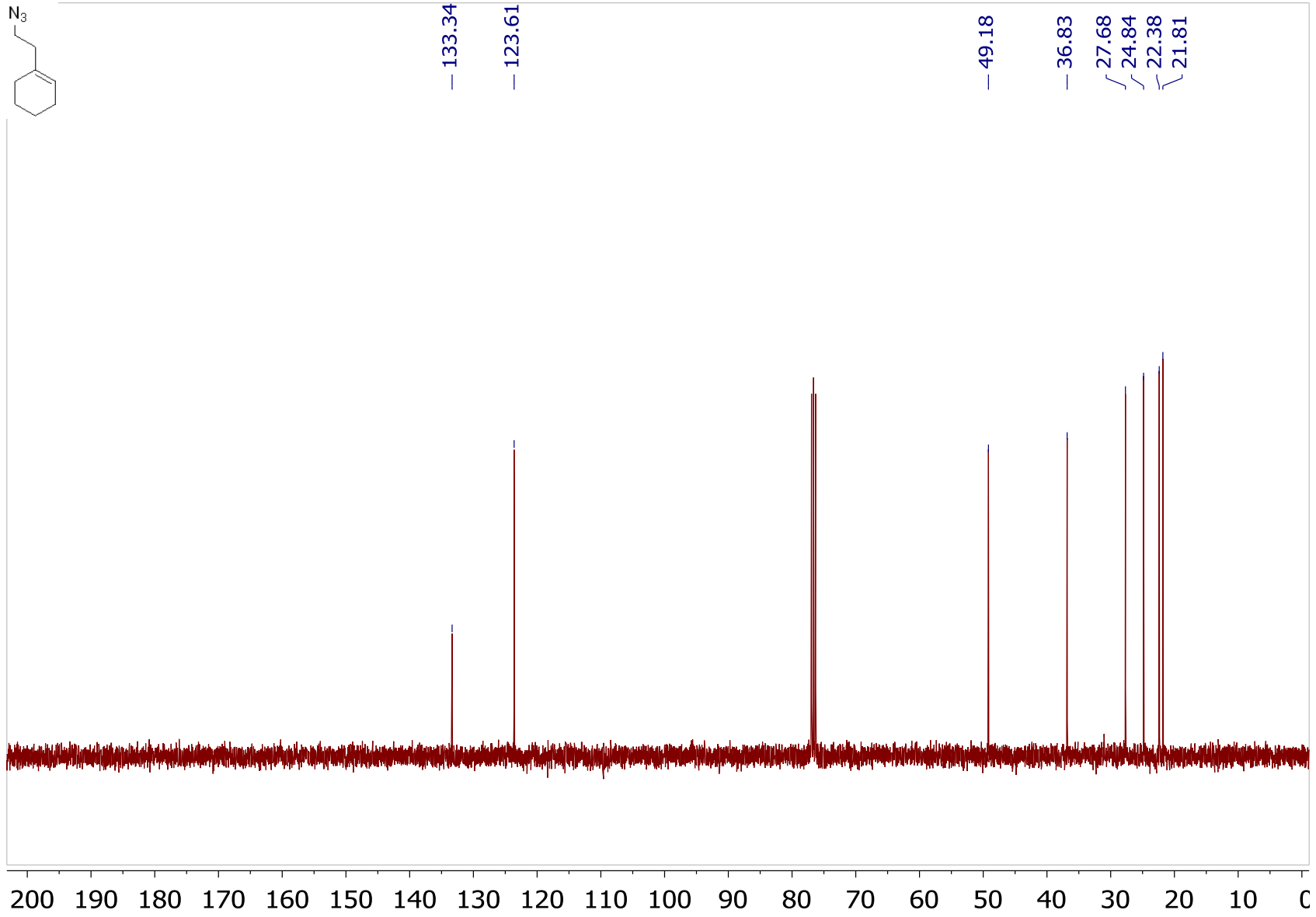
1-(2-Azidoethyl)cyclohex-1-ene (S1p)

^{1}H NMR (400 MHz, $CDCl_3$)



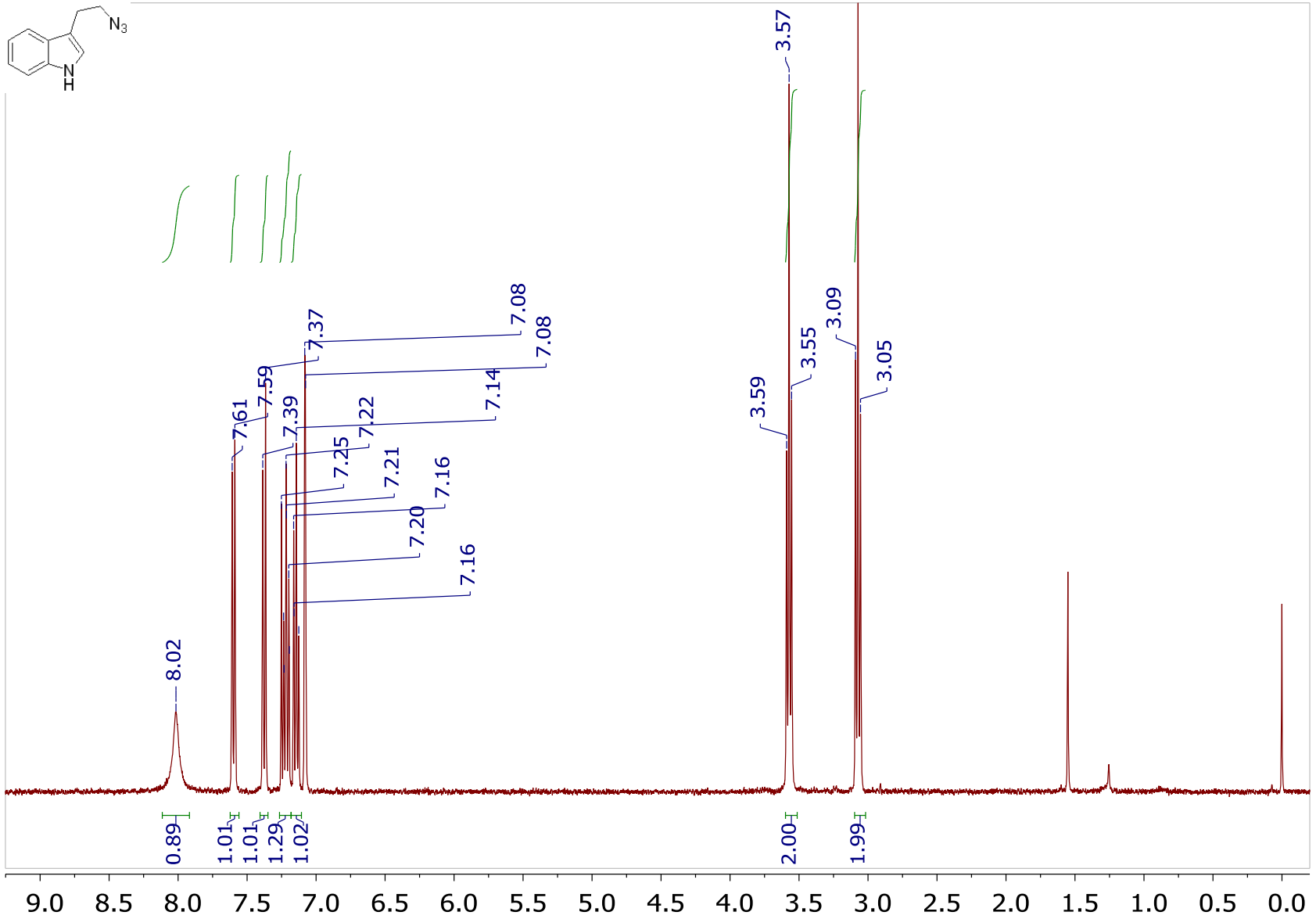
1-(2-Azidoethyl)cyclohex-1-ene (S1p)

^{13}C NMR (101 MHz, $CDCl_3$)



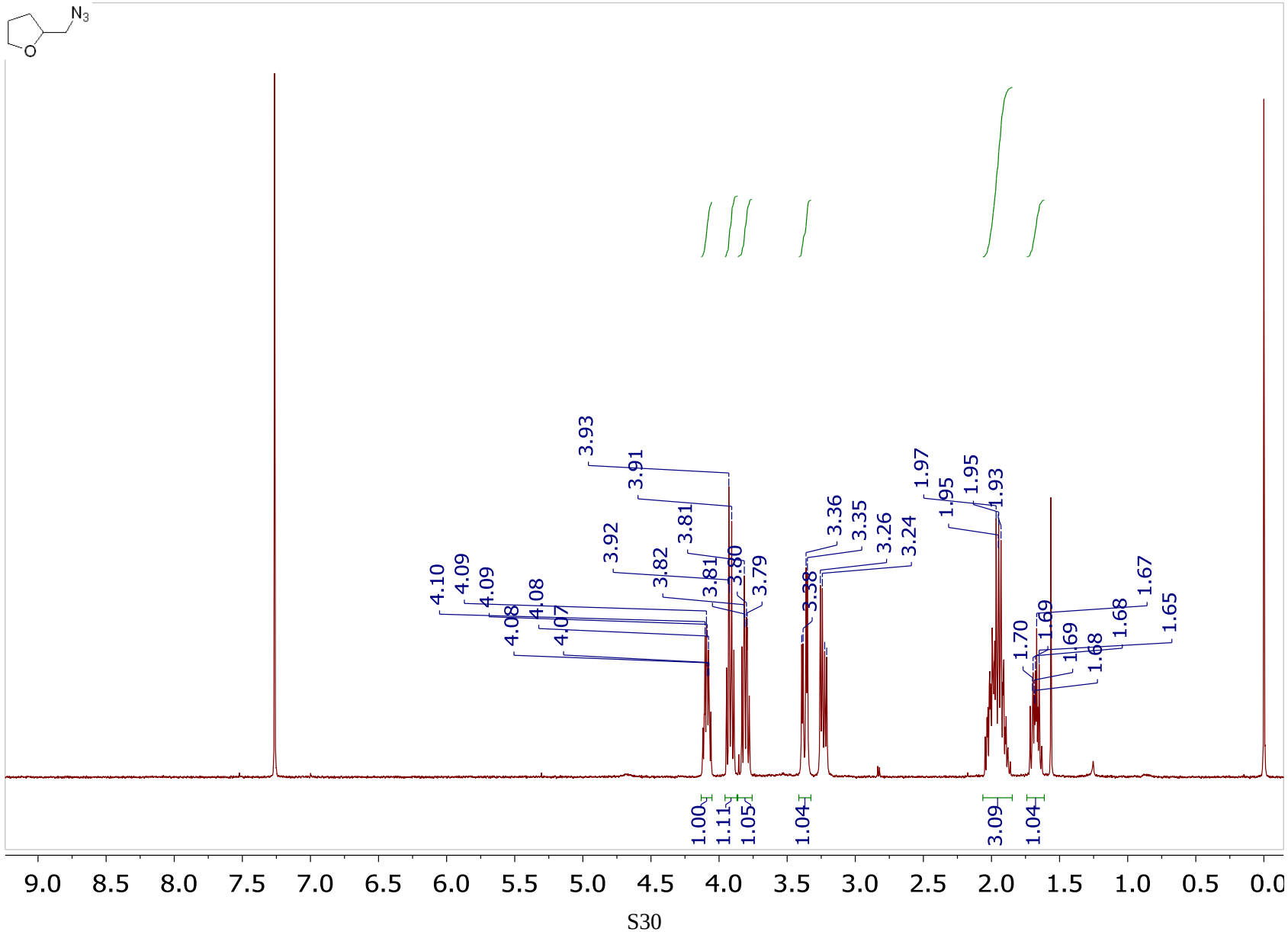
3-(2-Azidoethyl)-1*H*-indole (S1q)

^{1}H NMR (400 MHz, $CDCl_3$)



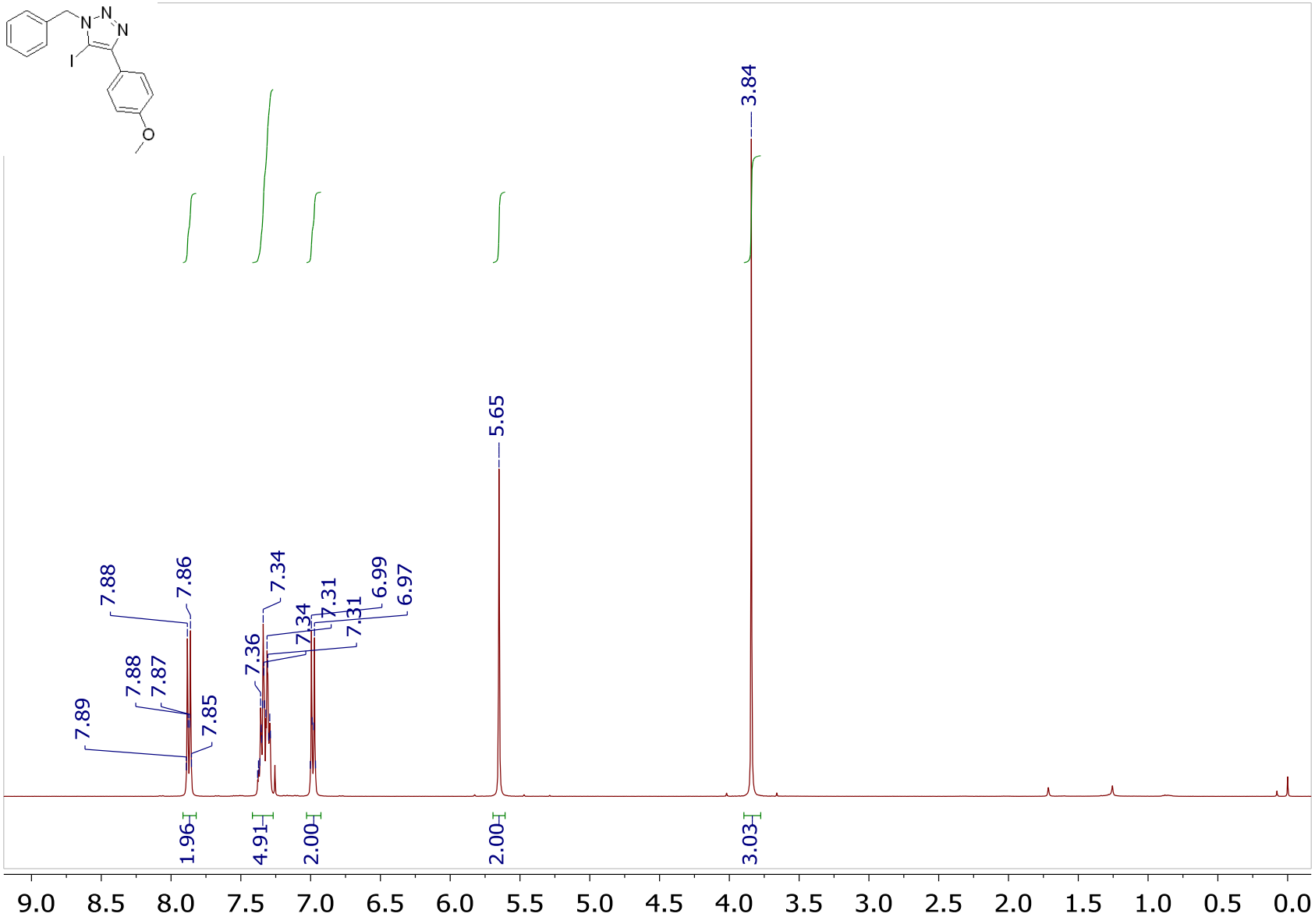
(2-Azidomethyl)tetrahydrofuran (S1q)

^{1}H NMR (400 MHz, $CDCl_3$)



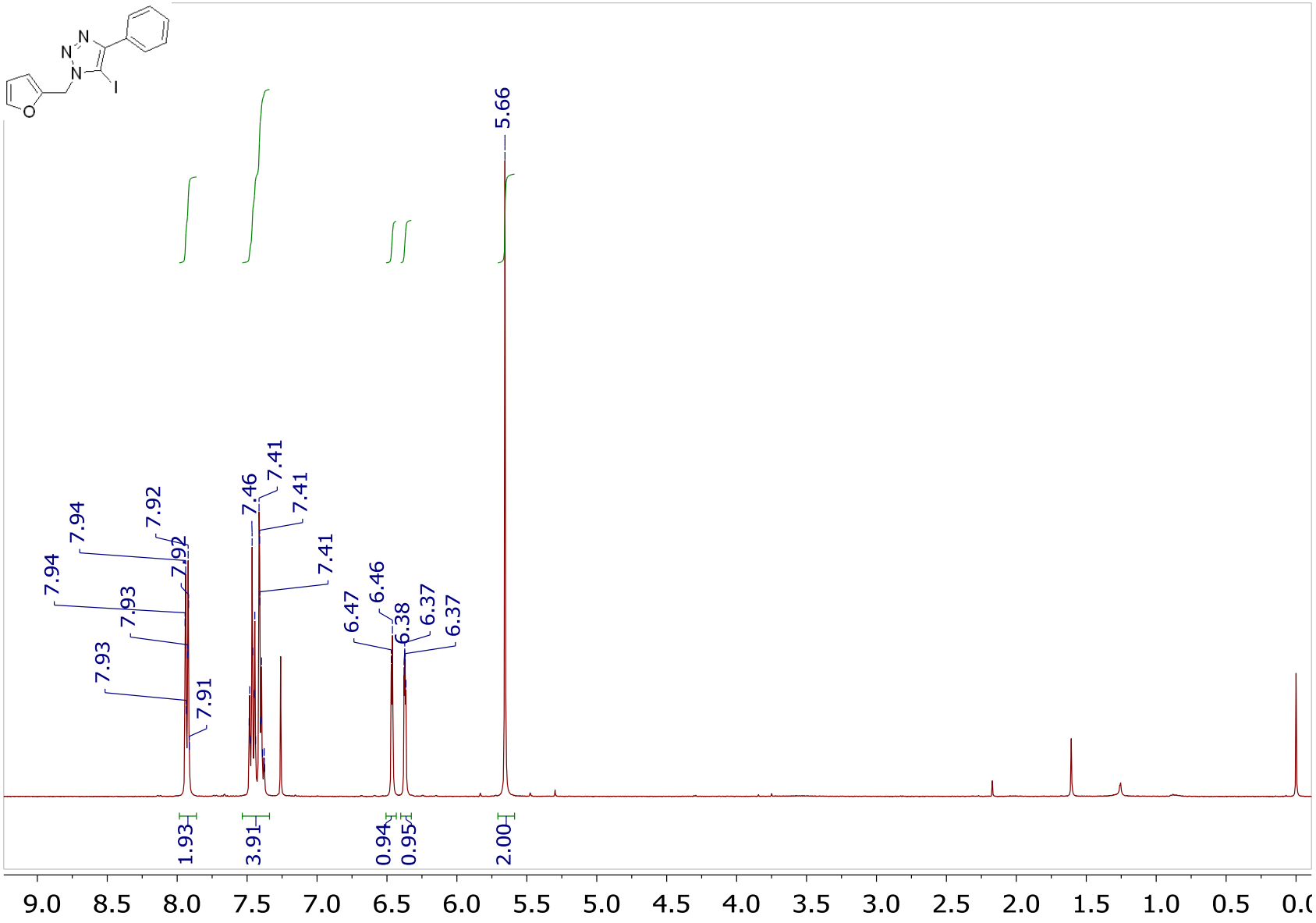
1-Benzyl-5-iodo-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (1c)

^{1}H NMR (400 MHz, $CDCl_3$)



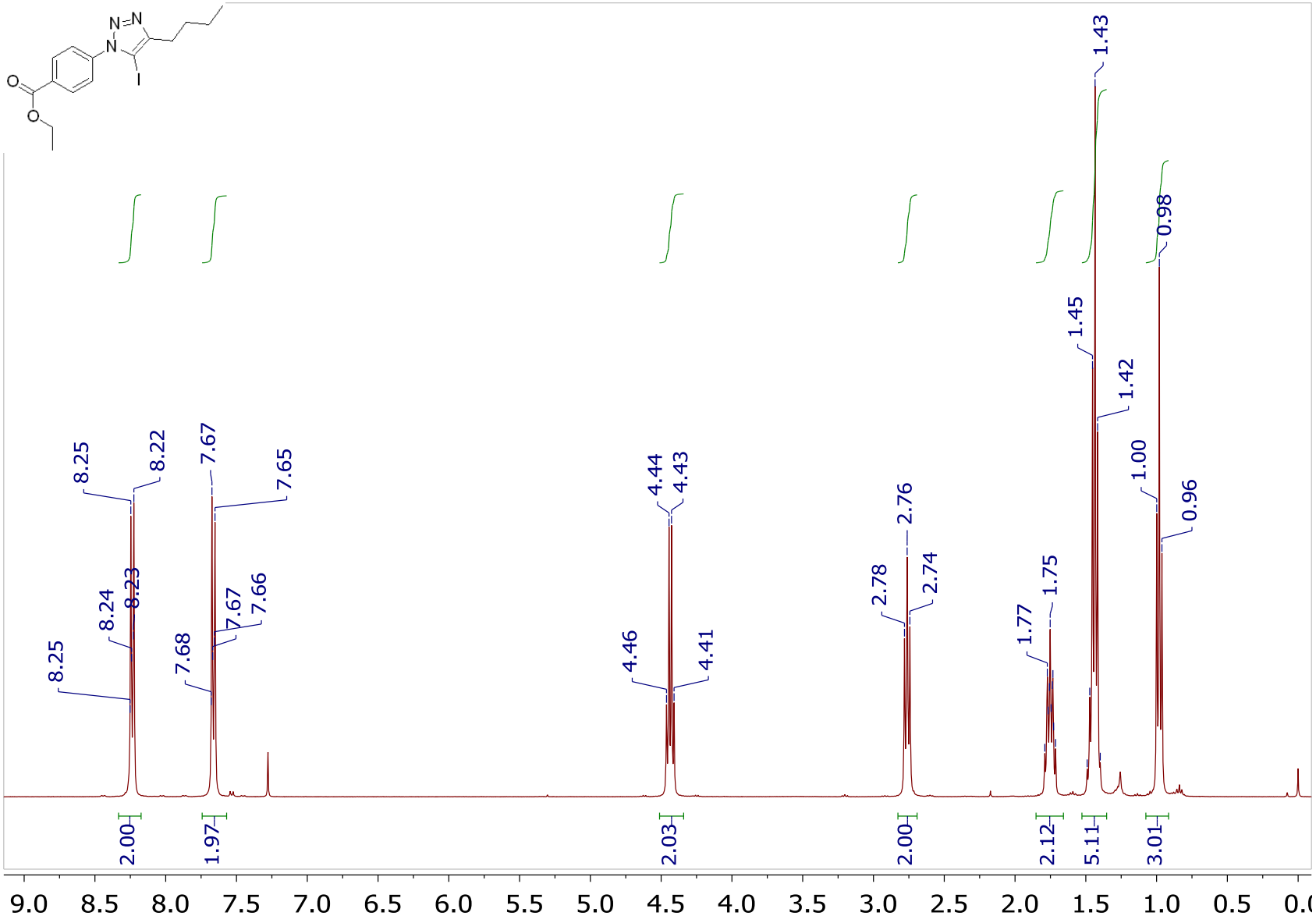
1-(Furan-2-ylmethyl)-5-iodo-4-phenyl-1*H*-1,2,3-triazole (1e)

^{1}H NMR (400 MHz, $CDCl_3$)



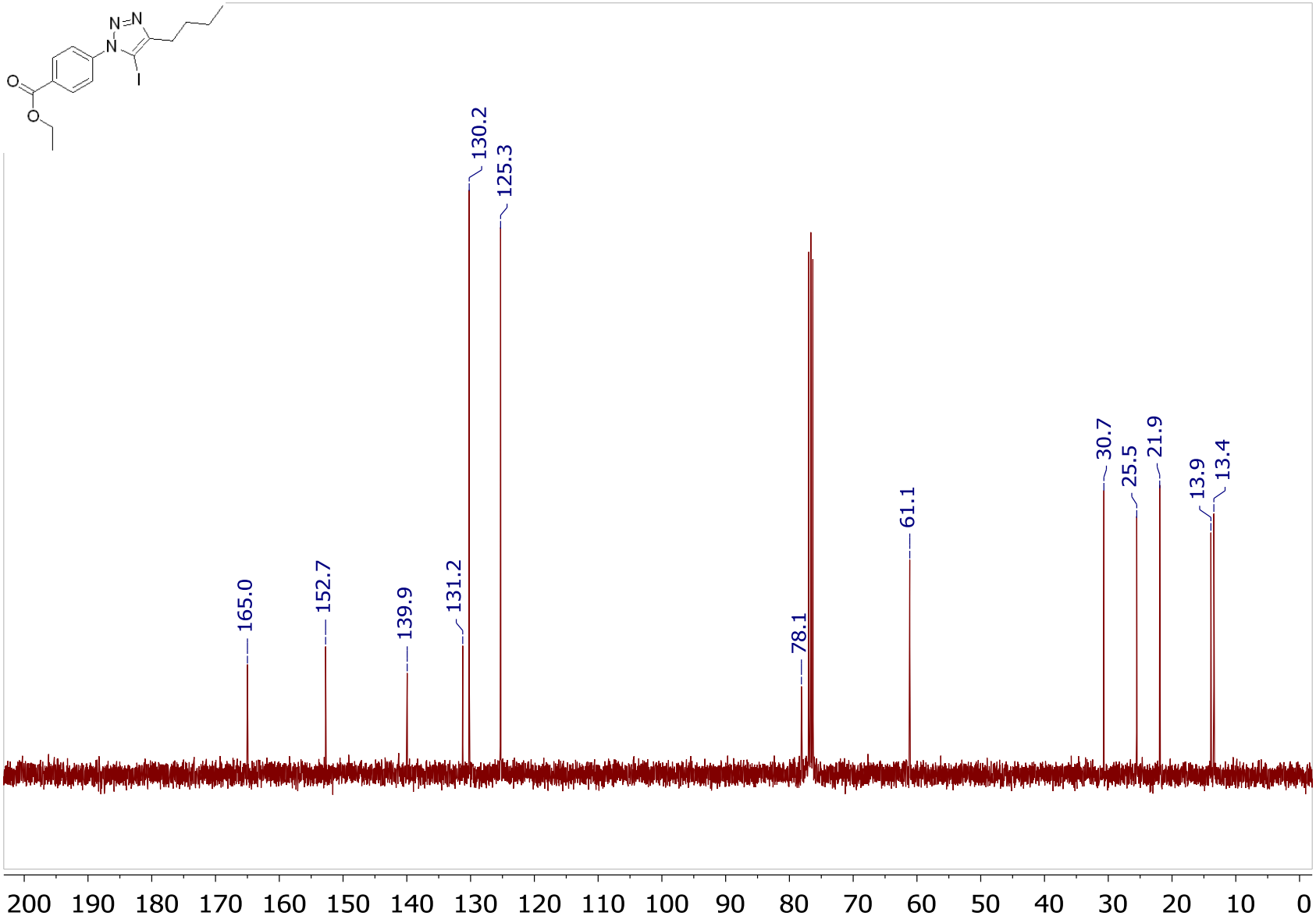
Ethyl 4-(4-butyl-5-iodo-1H-1,2,3-triazol-1-yl)benzoate (1h)

^{1}H NMR (400 MHz, $CDCl_3$)



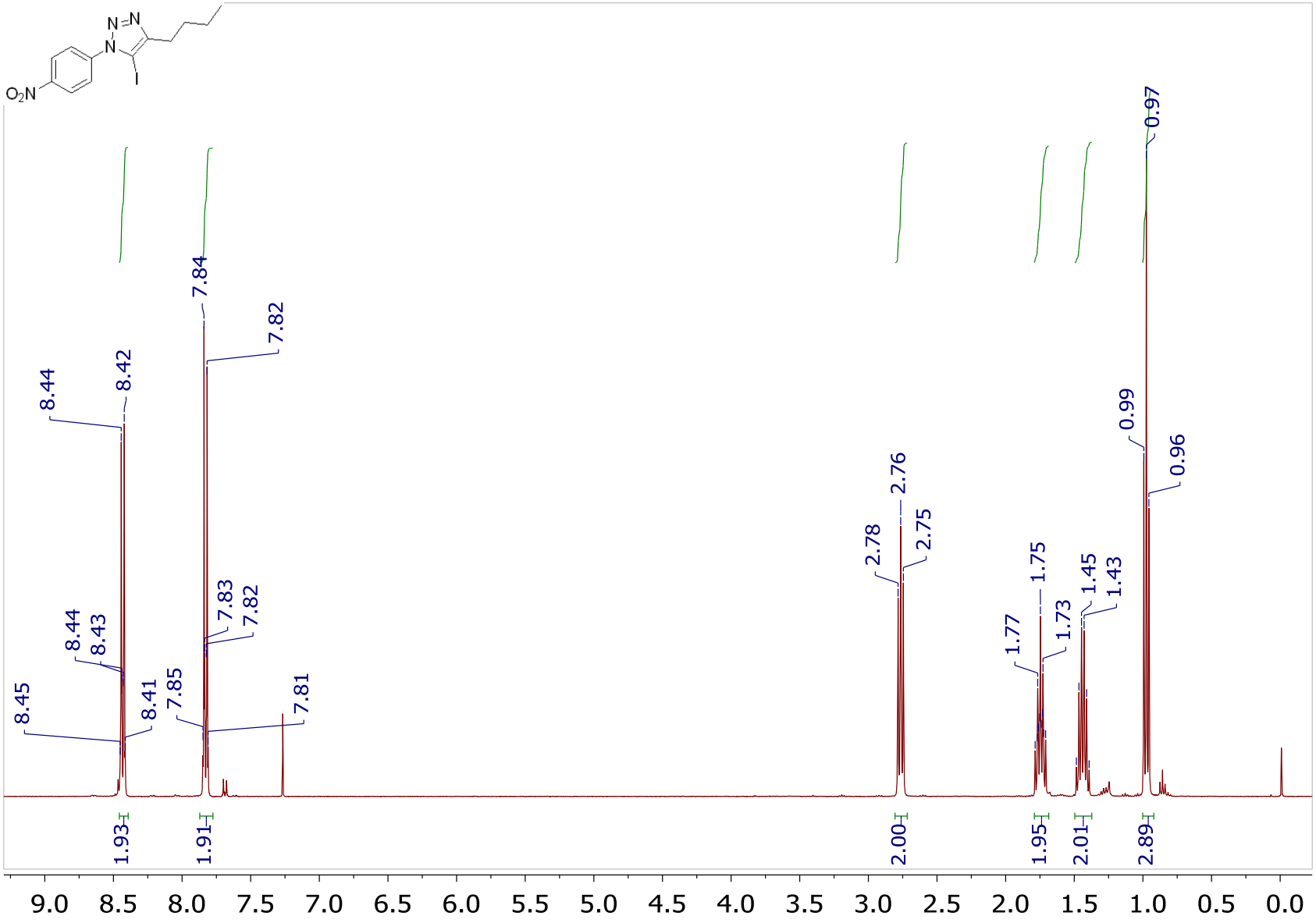
Ethyl 4-(4-butyl-5-iodo-1H-1,2,3-triazol-1-yl)benzoate (1h)

^{13}C NMR (101 MHz, $CDCl_3$)



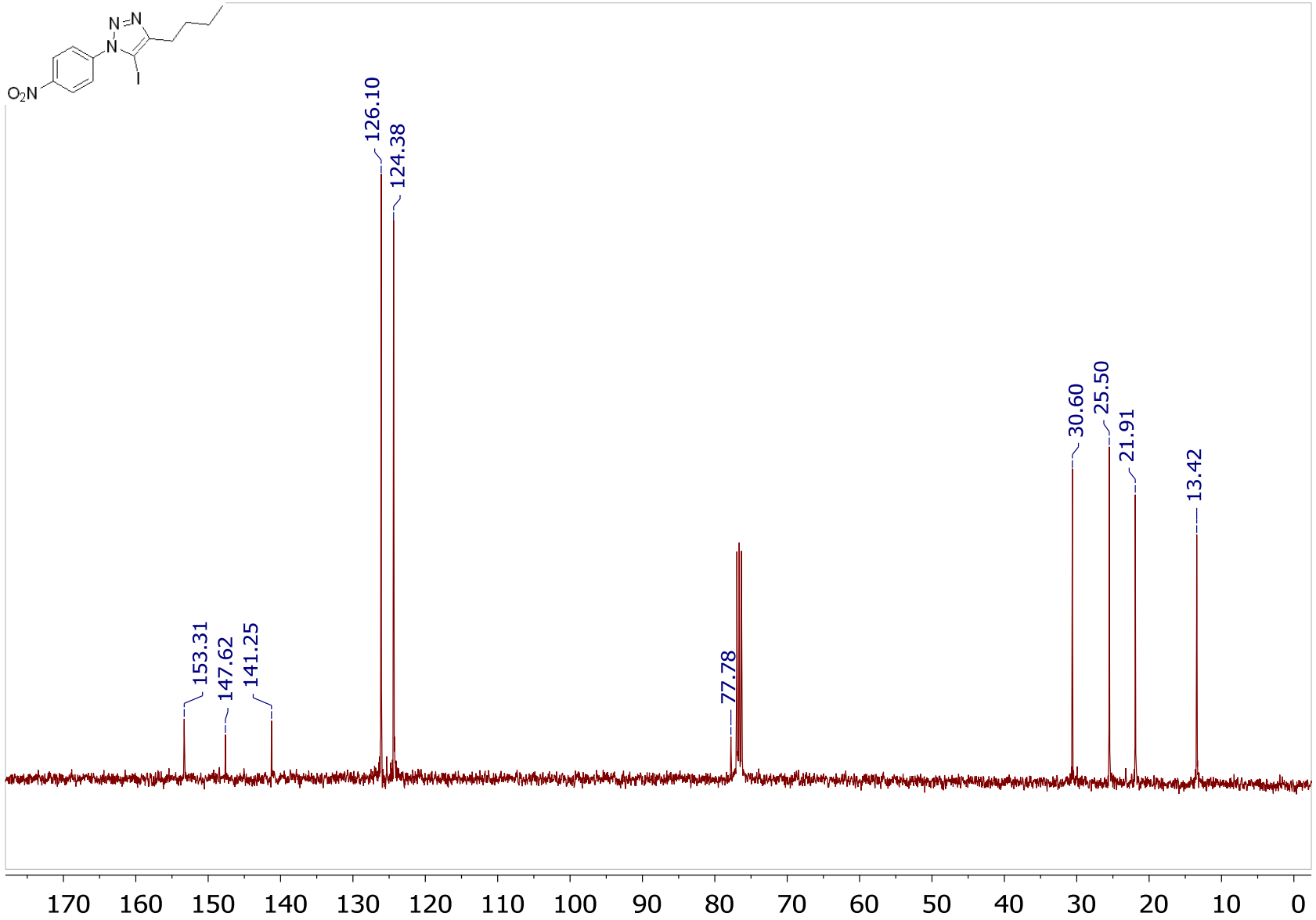
4-Butyl-5-iodo-1-(4-nitrophenyl)-1*H*-1,2,3-triazole (1i)

^{1}H NMR (400 MHz, $CDCl_3$)



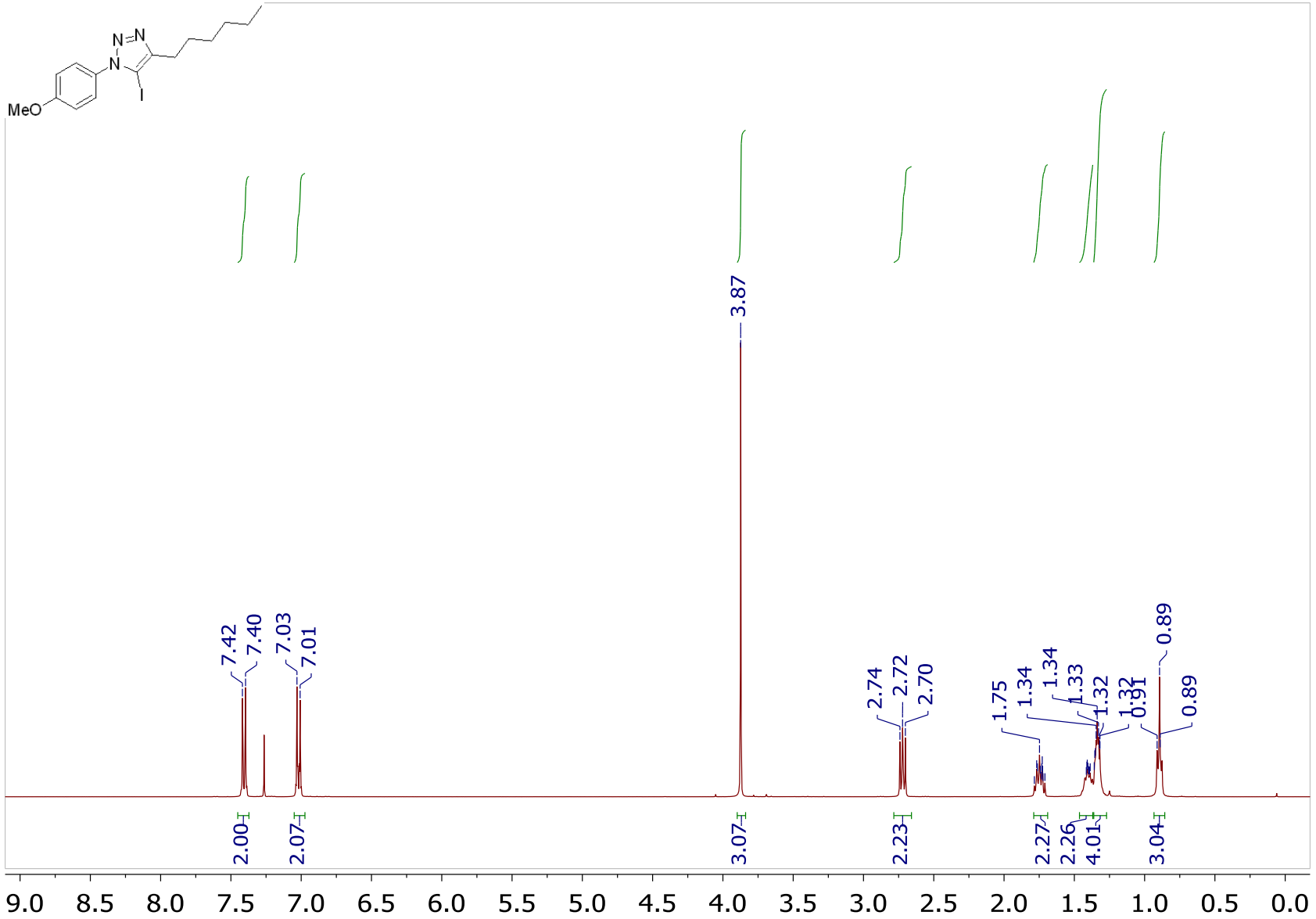
4-Butyl-5-iodo-1-(4-nitrophenyl)-1*H*-1,2,3-triazole (1i)

^{13}C NMR (101 MHz, $CDCl_3$)



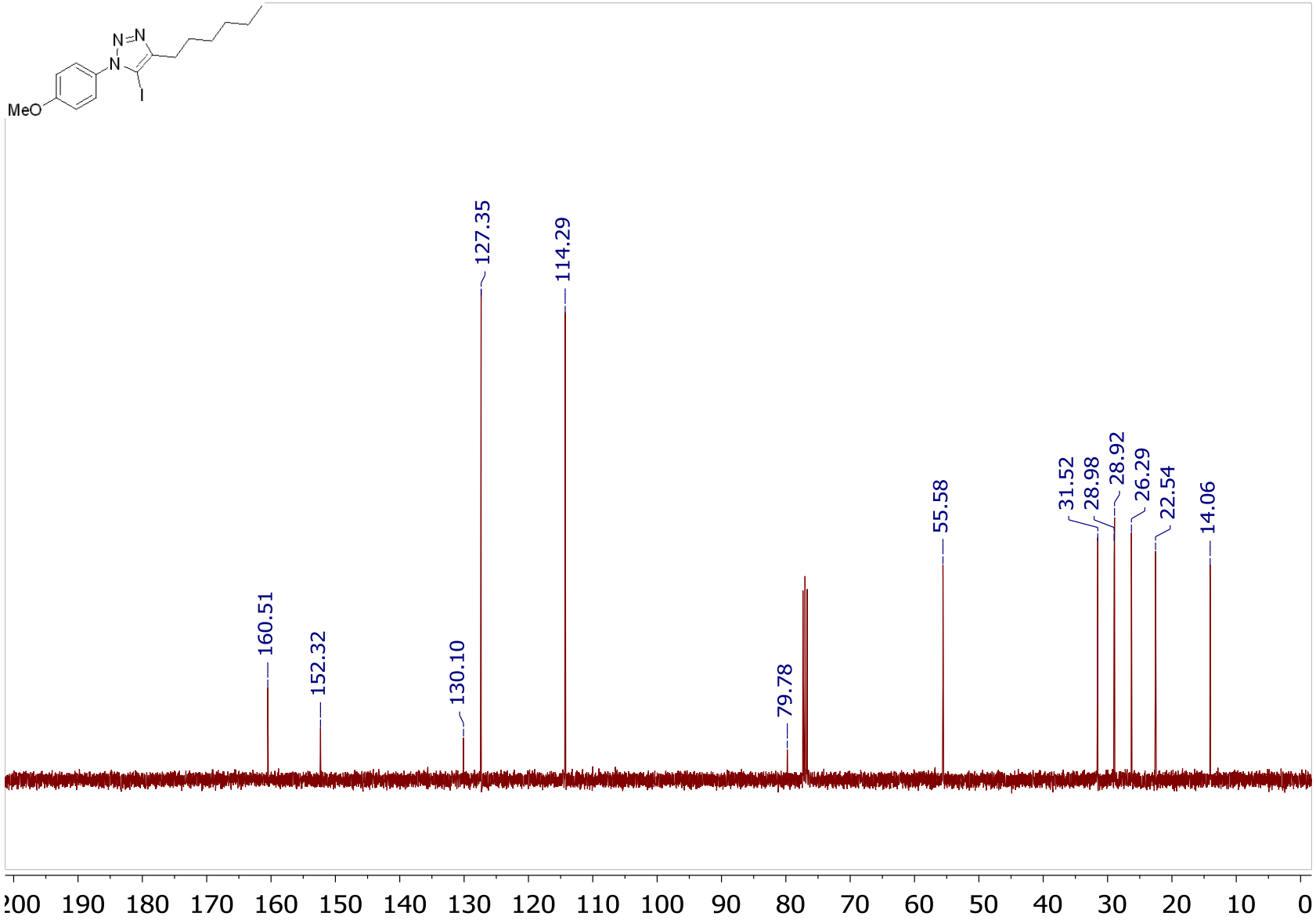
4-Hexyl-5-iodo-1-(4-methoxyphenyl)-1H-1,2,3-triazole (1j)

^{1}H NMR (400 MHz, $CDCl_3$)



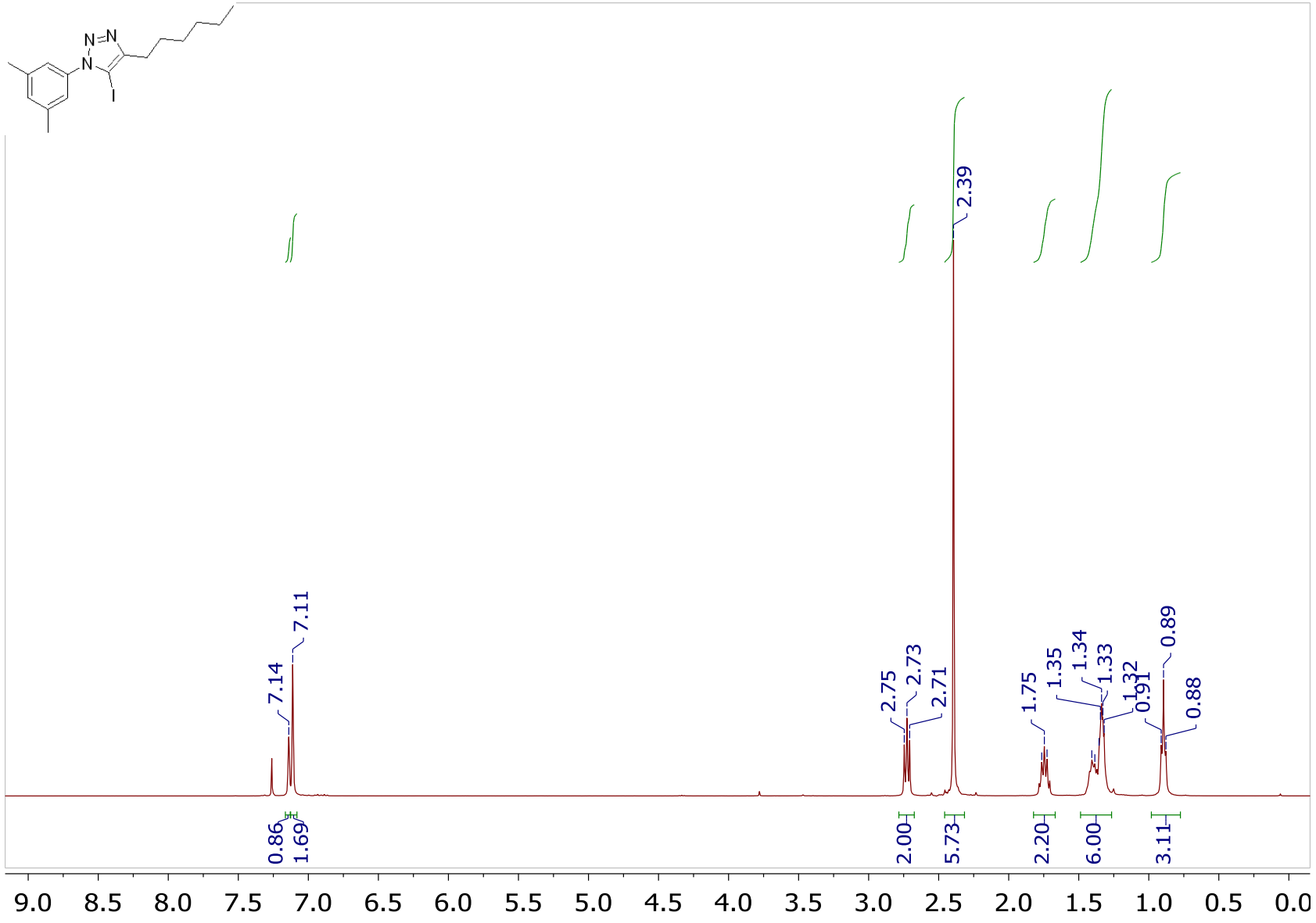
4-Hexyl-5-iodo-1-(4-methoxyphenyl)-1H-1,2,3-triazole (1j)

^{13}C NMR (101 MHz, $CDCl_3$)



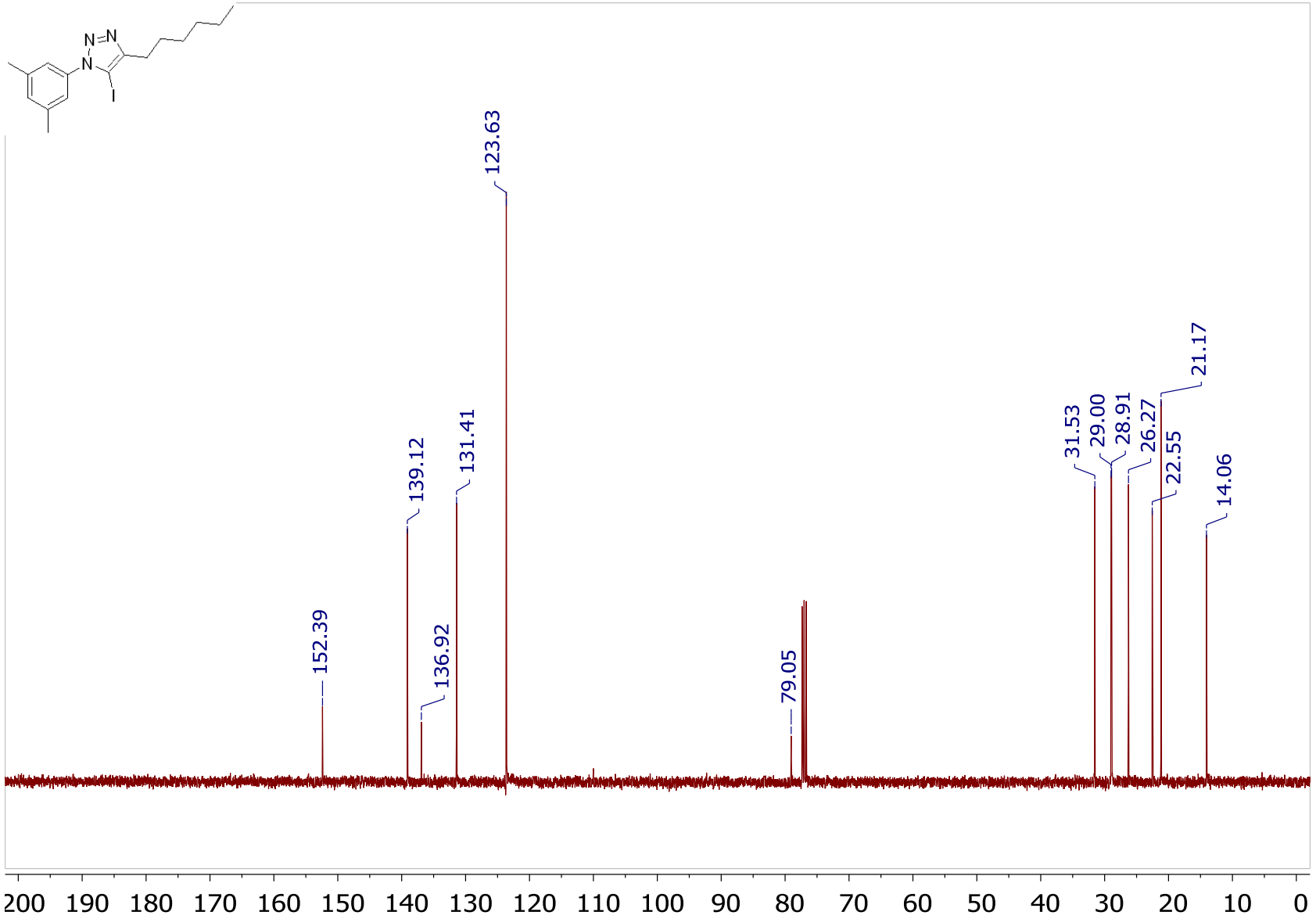
1-(3,5-Dimethylphenyl)-4-hexyl-5-iodo-1*H*-1,2,3-triazole (1k)

^{1}H NMR (400 MHz, $CDCl_3$)



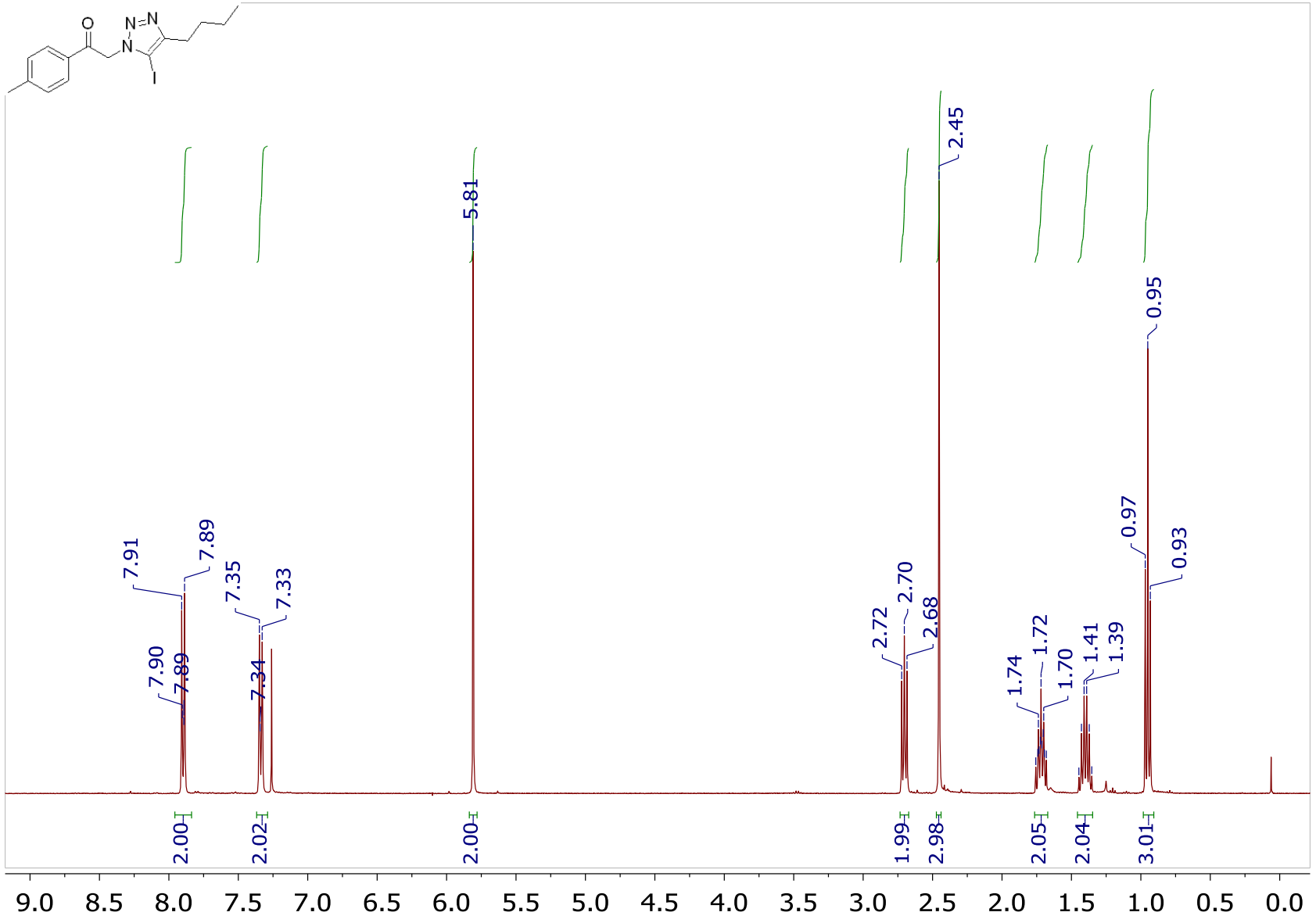
1-(3,5-Dimethylphenyl)-4-hexyl-5-iodo-1*H*-1,2,3-triazole (1k)

^{13}C NMR (101 MHz, $CDCl_3$)



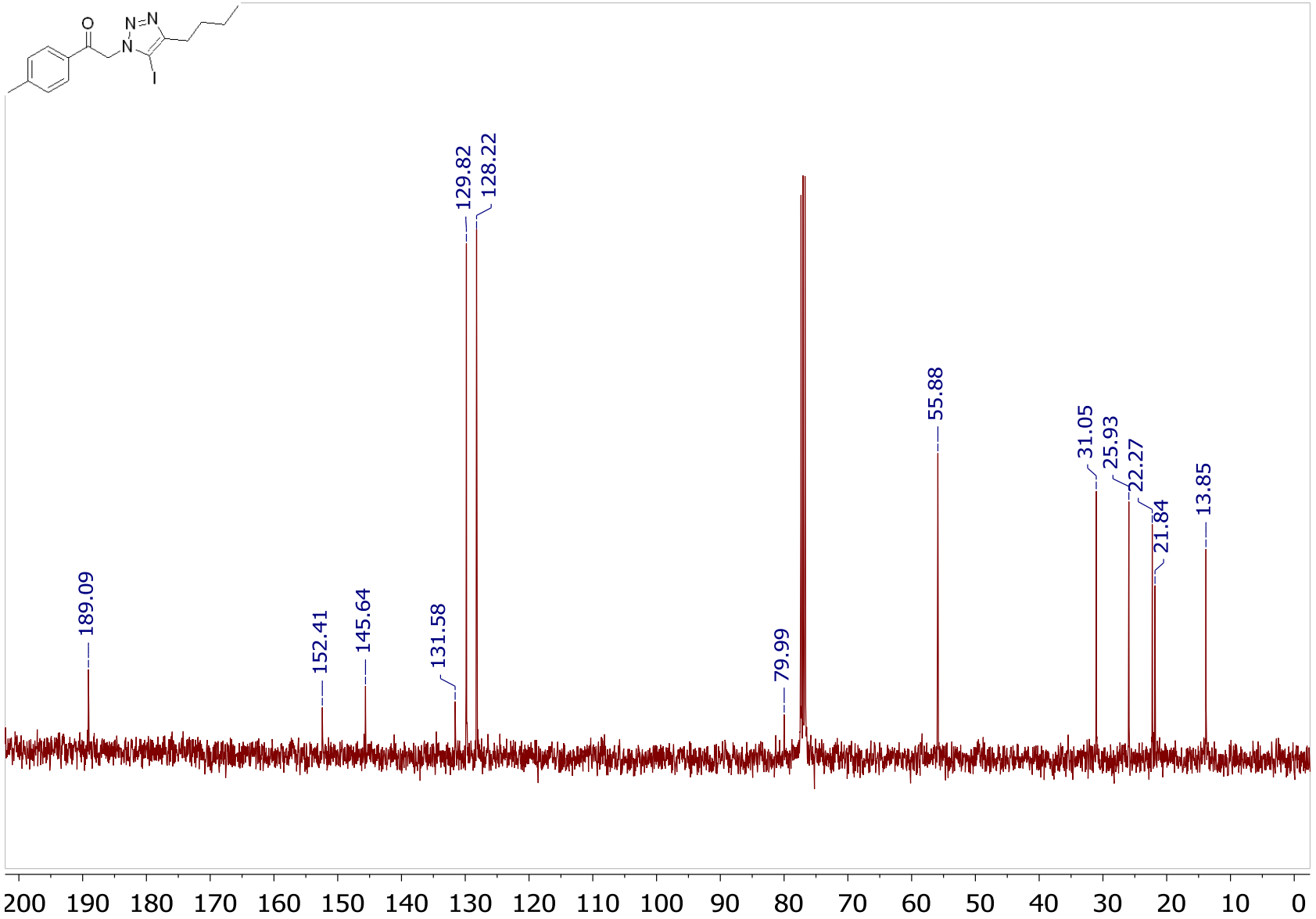
2-(4-Butyl-5-iodo-1H-1,2,3-triazol-1-yl)-1-(4-methylphenyl)ethanone (1l)

^{1}H NMR (400 MHz, $CDCl_3$)



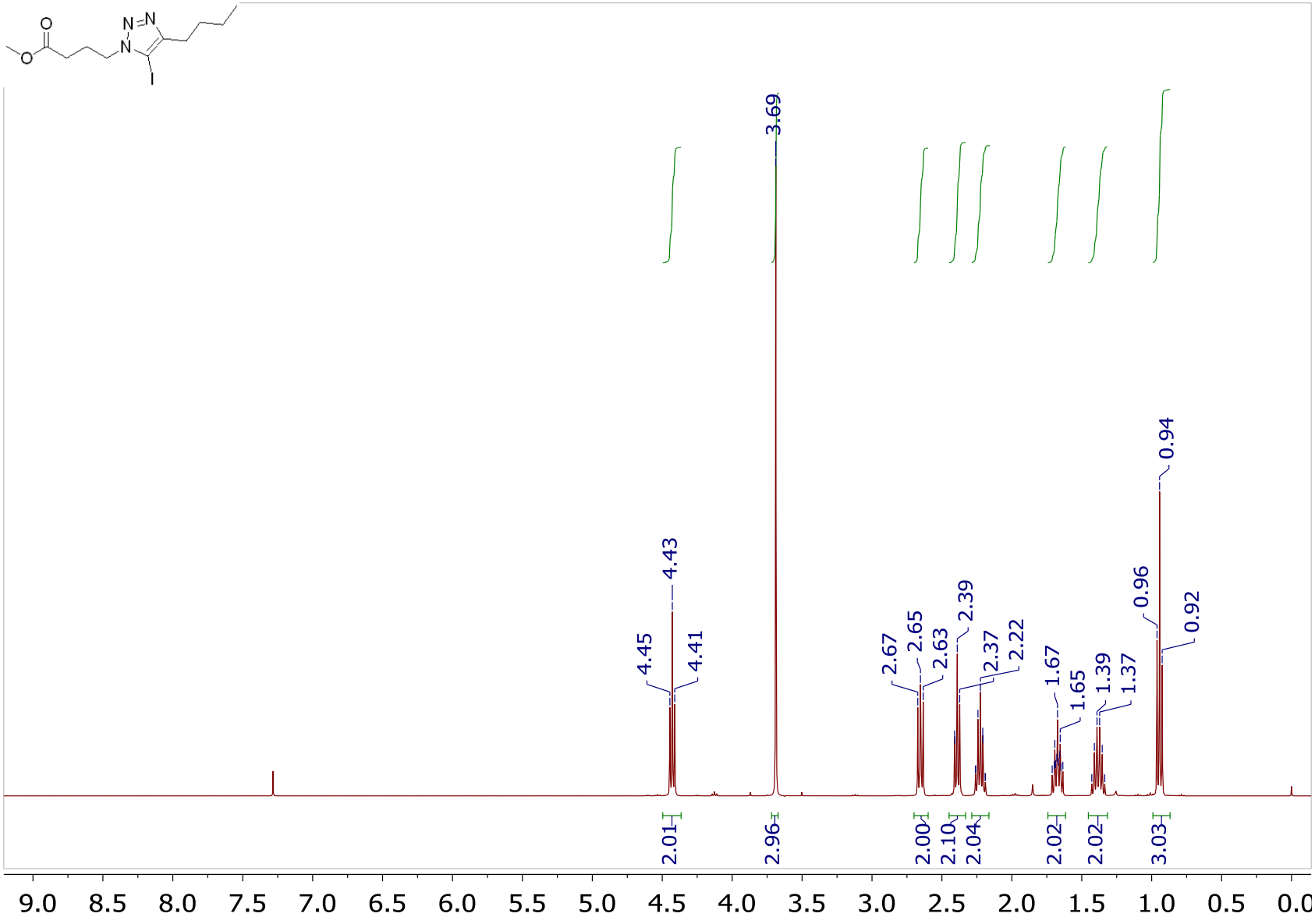
2-(4-Butyl-5-iodo-1H-1,2,3-triazol-1-yl)-1-(4-methylphenyl)ethanone (1l)

^{13}C NMR (101 MHz, $CDCl_3$)



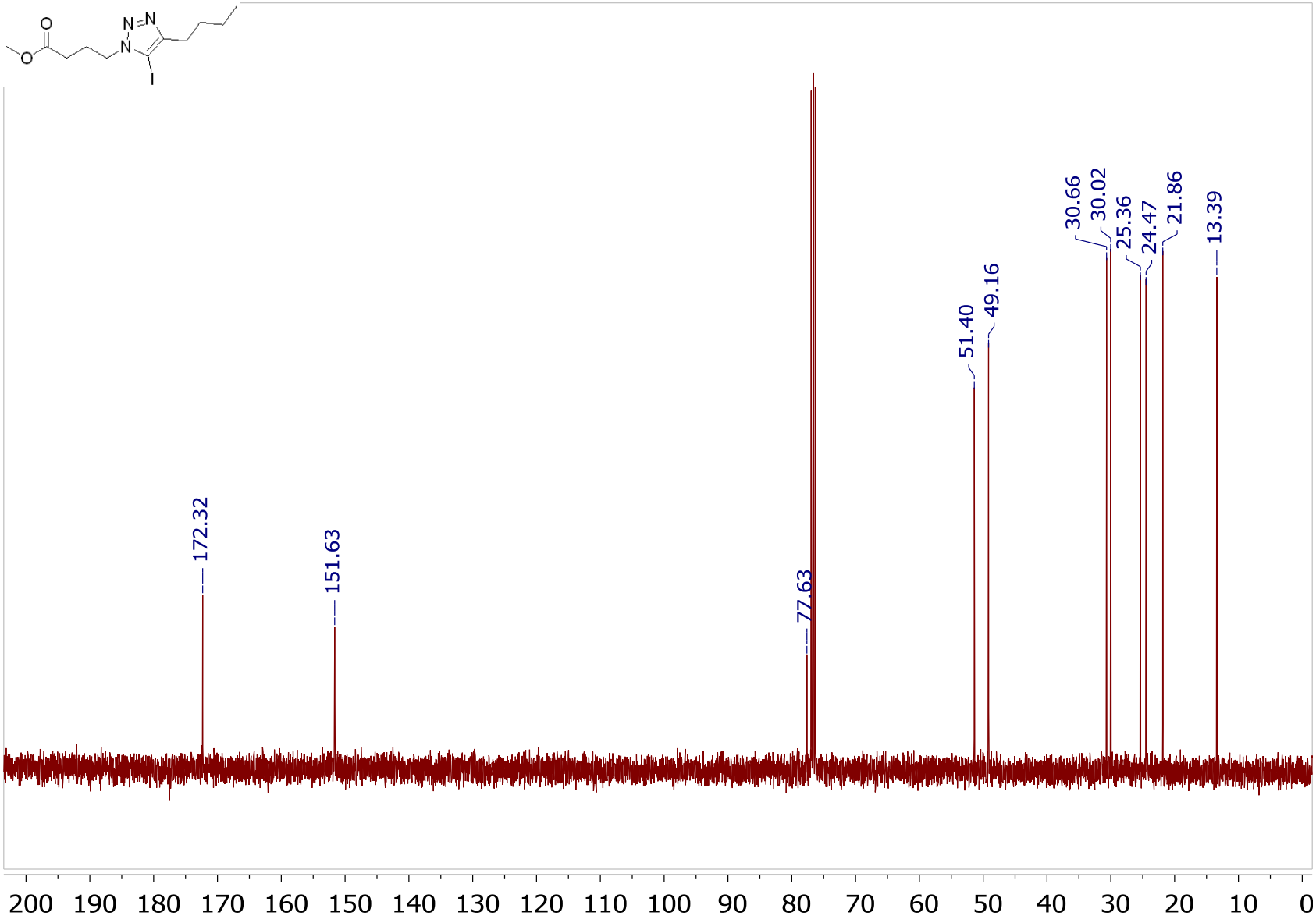
Methyl 4-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)butanoate (1m)

^{1}H NMR (400 MHz, $CDCl_3$)



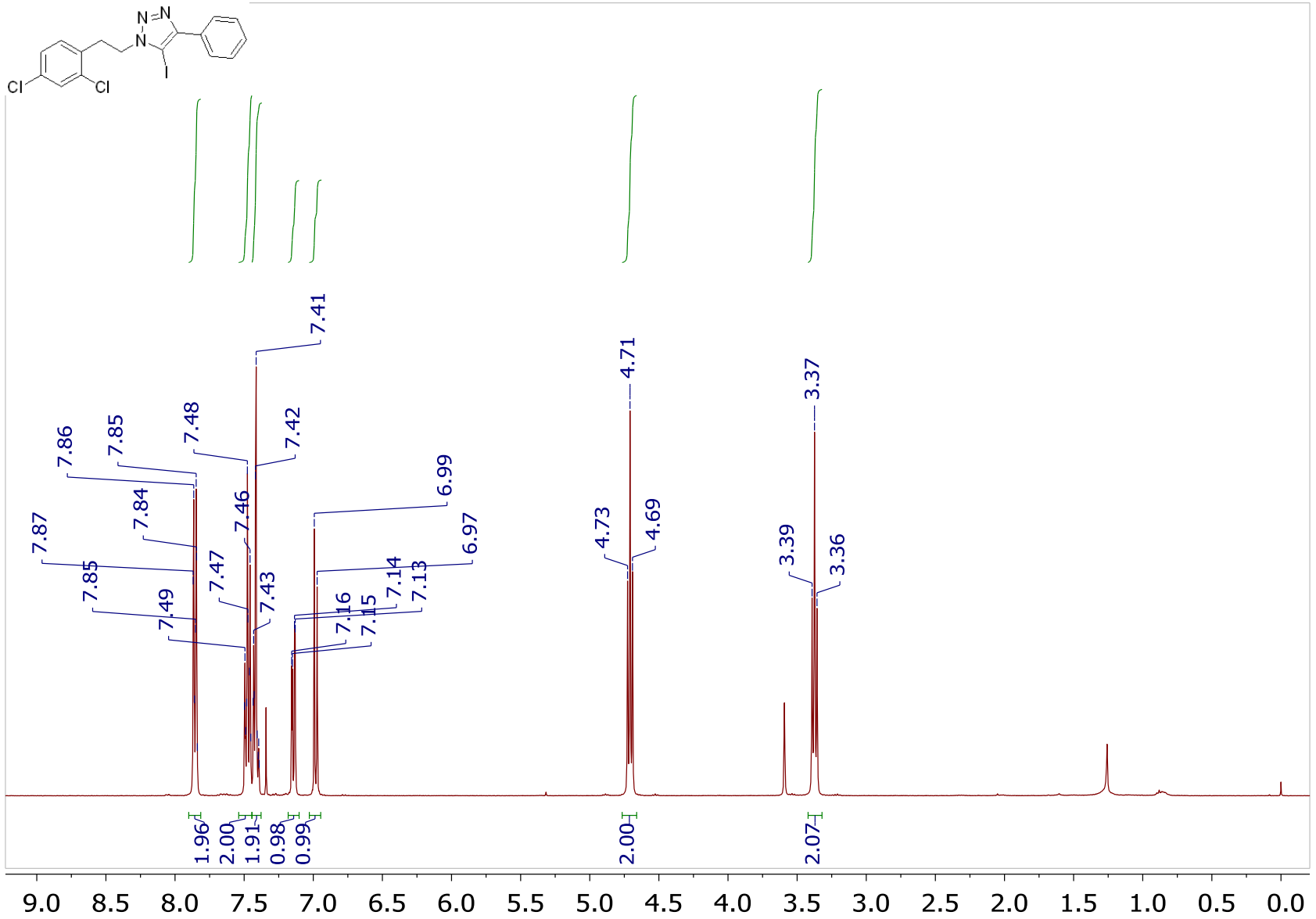
Methyl 4-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)butanoate (1m)

^{13}C NMR (101 MHz, $CDCl_3$)



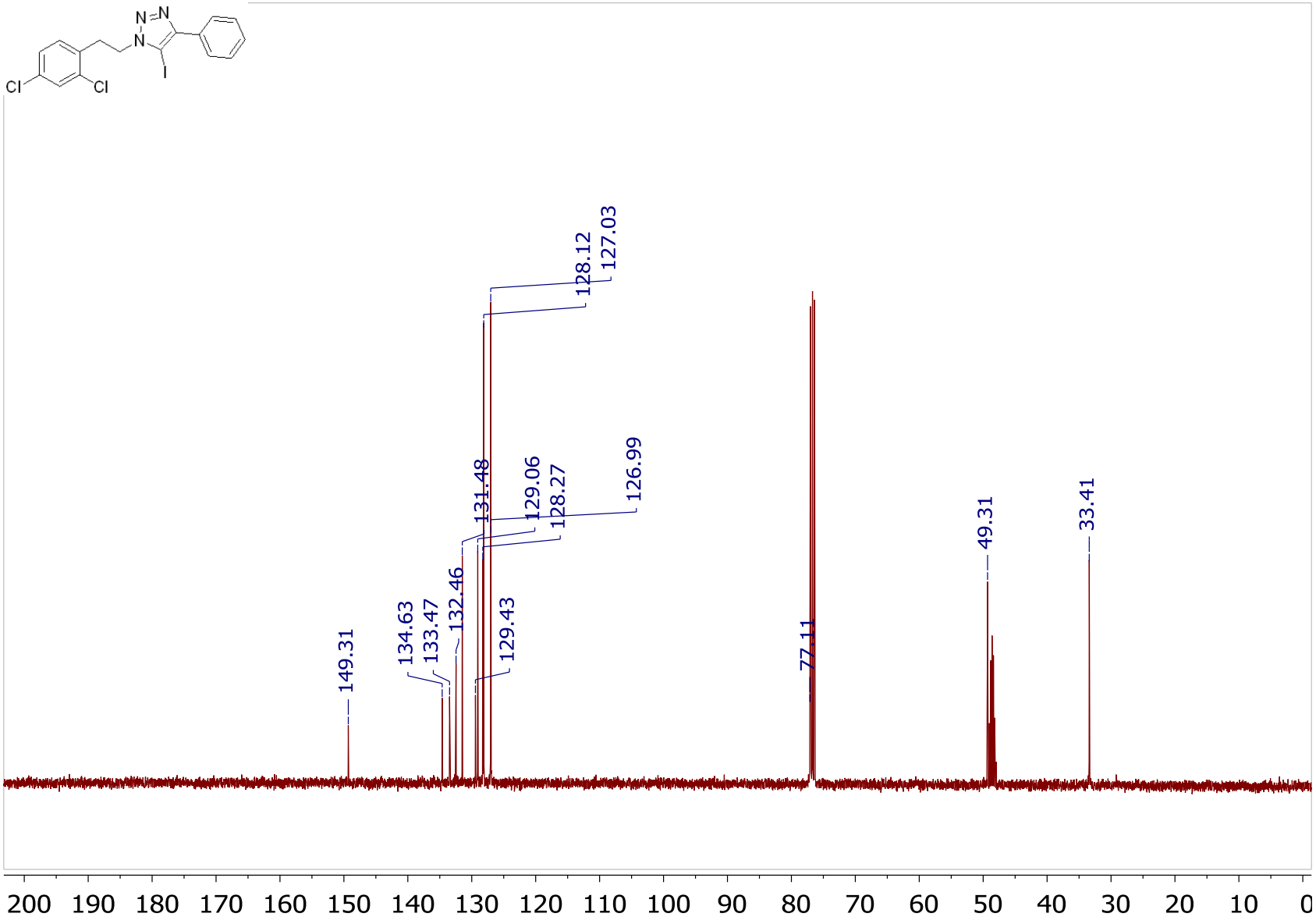
1-(2,4-Dichlorophenethyl)-5-iodo-4-phenyl-1*H*-1,2,3-triazole (1n)

^{1}H NMR (400 MHz, $CDCl_3/CD_3OD$)



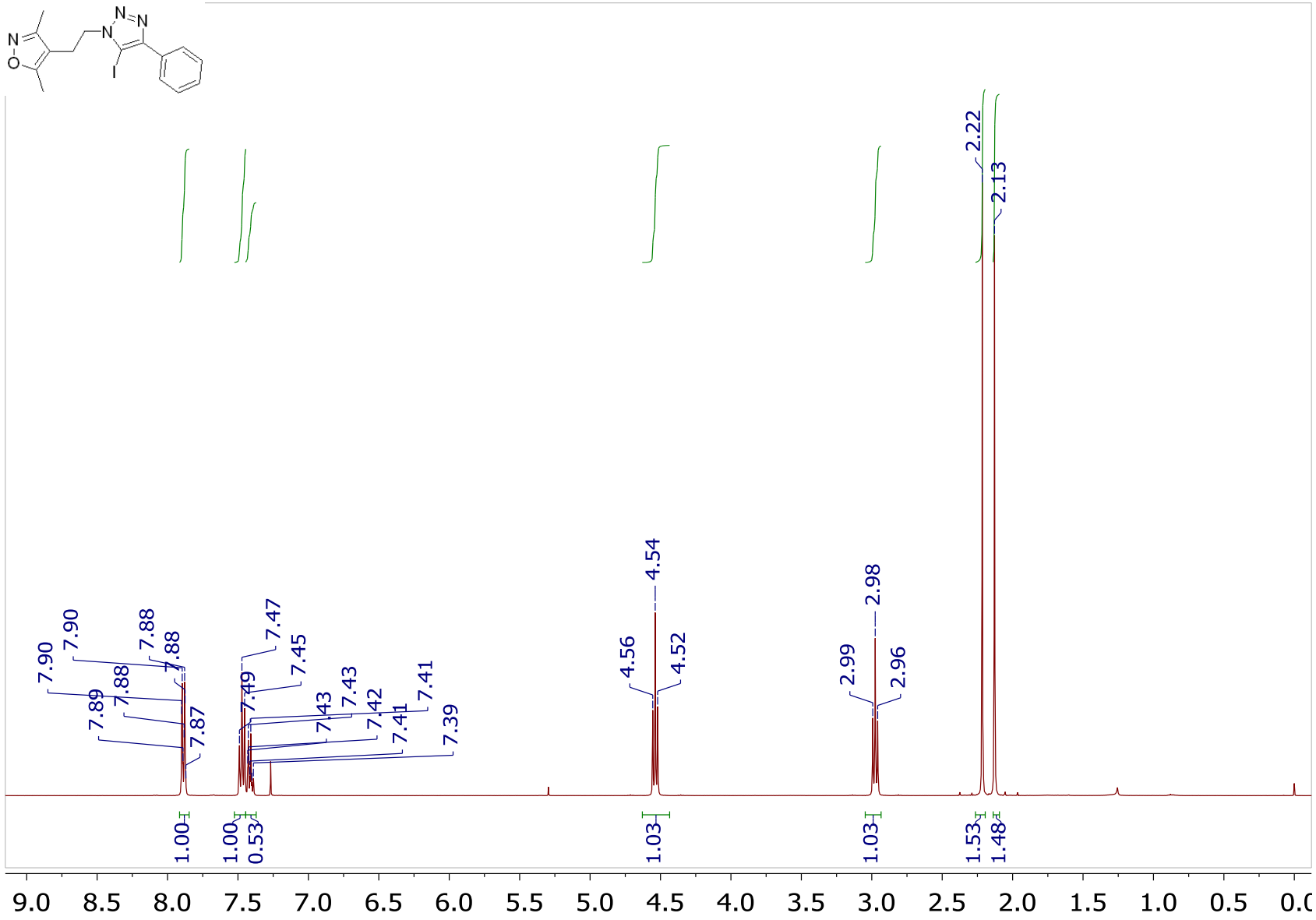
1-(2,4-Dichlorophenethyl)-5-iodo-4-phenyl-1*H*-1,2,3-triazole (1n)

^{13}C NMR (101 MHz, $CDCl_3/CD_3OD$)



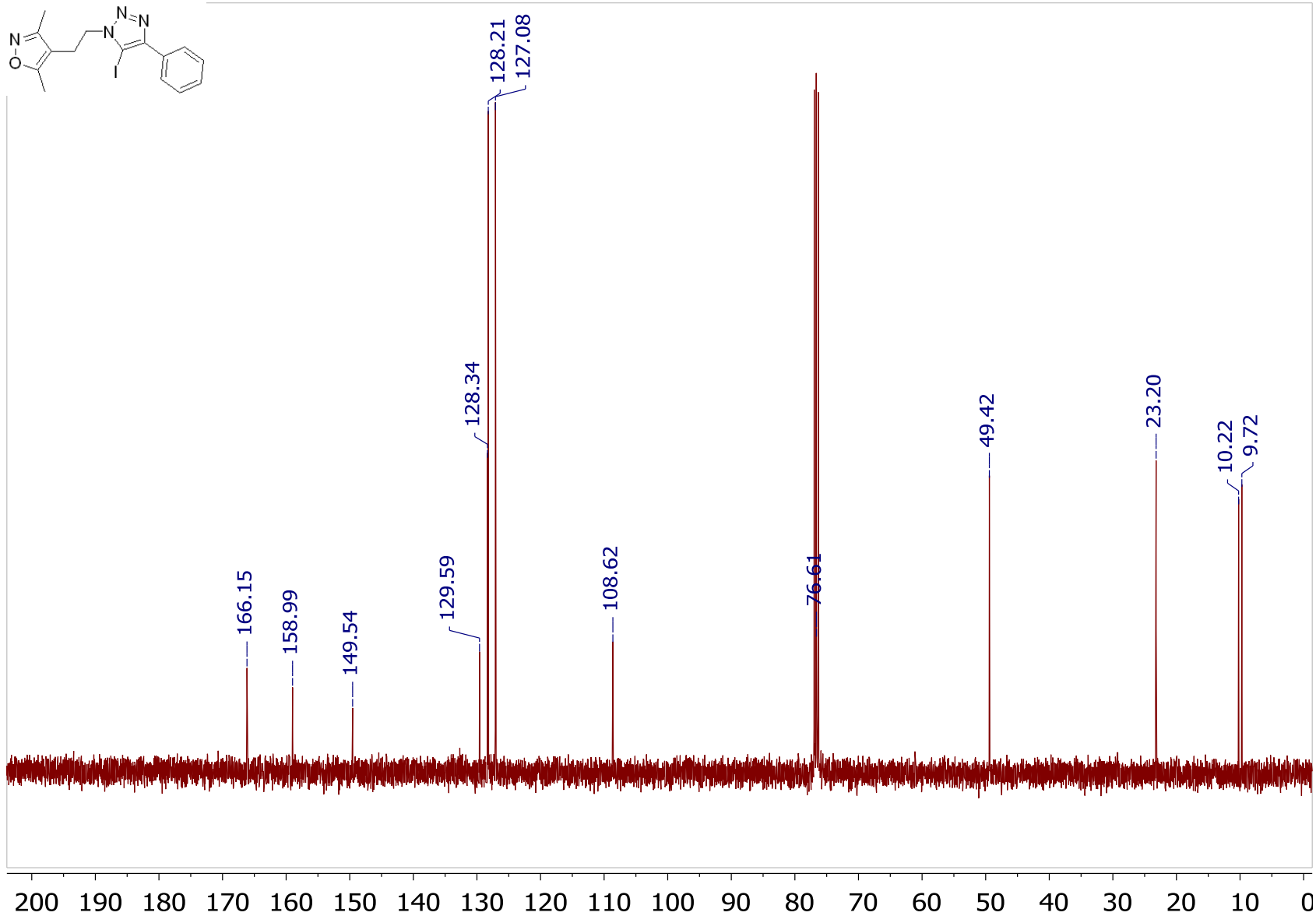
4-(2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-3,5-dimethylisoxazole (1o)

^{1}H NMR (400 MHz, $CDCl_3$)



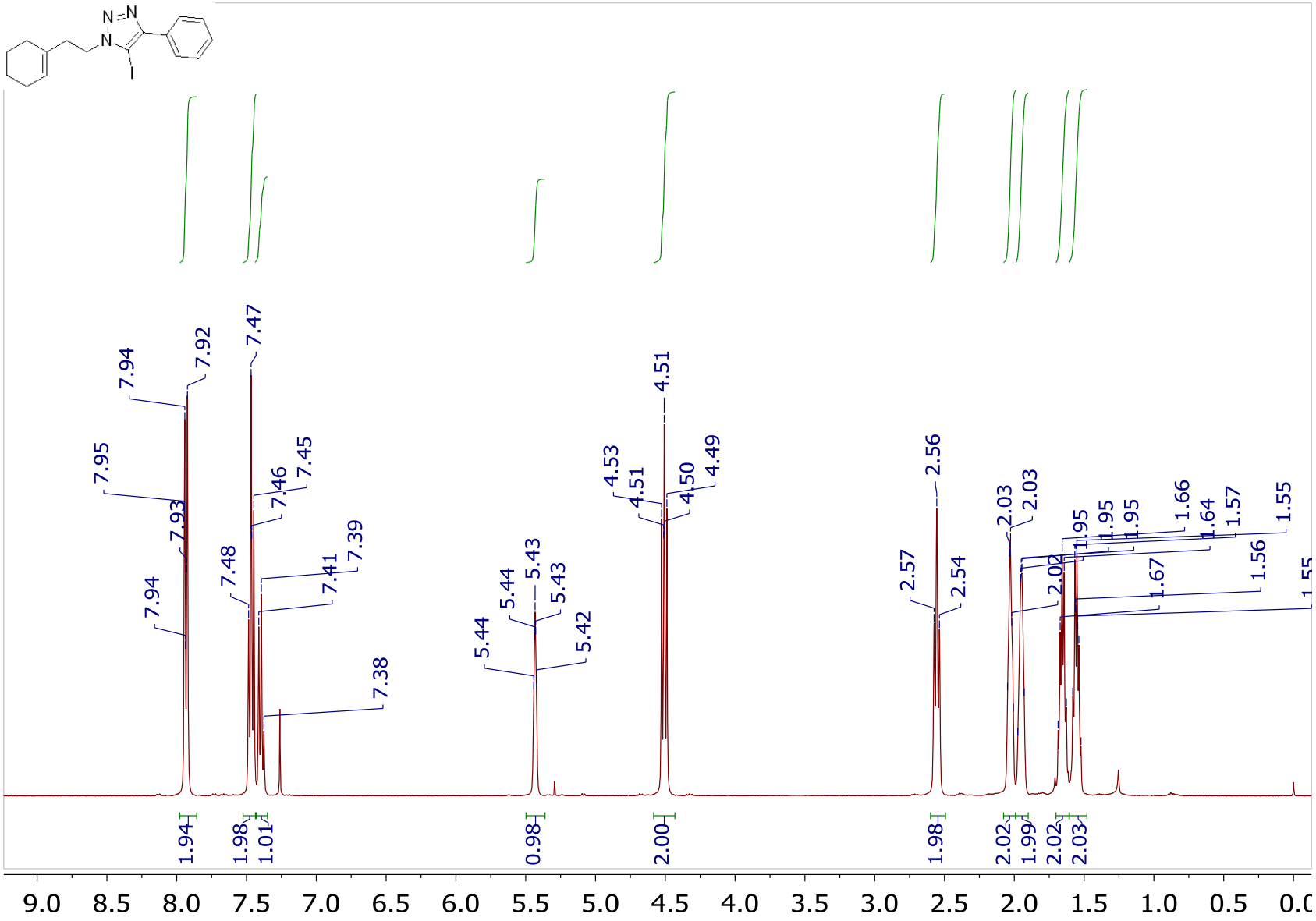
4-(2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-3,5-dimethylisoxazole (1o)

^{13}C NMR (101 MHz, $CDCl_3$)



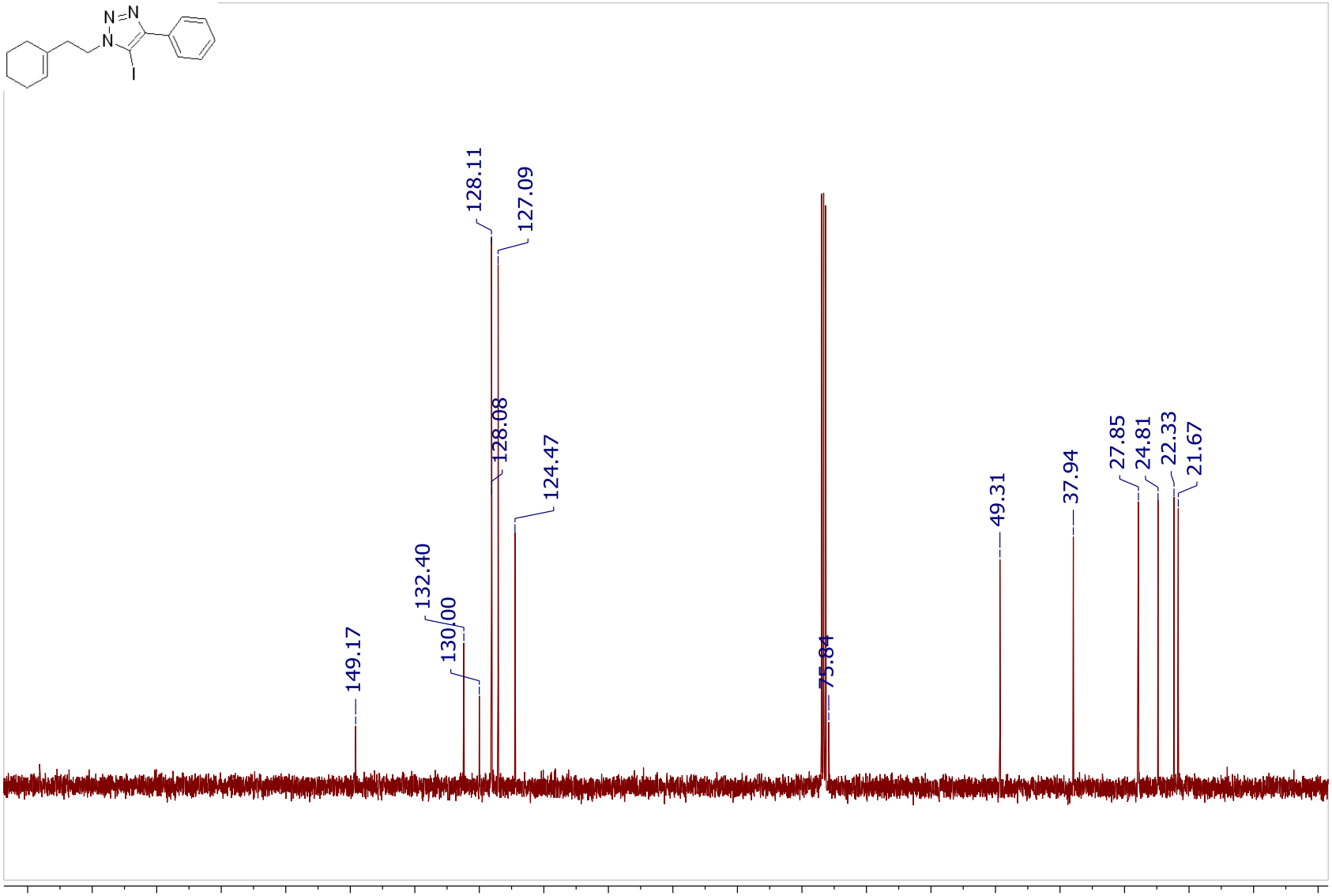
1-(2-(Cyclohex-1-en-1-yl)ethyl)-5-iodo-4-phenyl-1*H*-1,2,3-triazole (1p)

^{1}H NMR (400 MHz, $CDCl_3$)



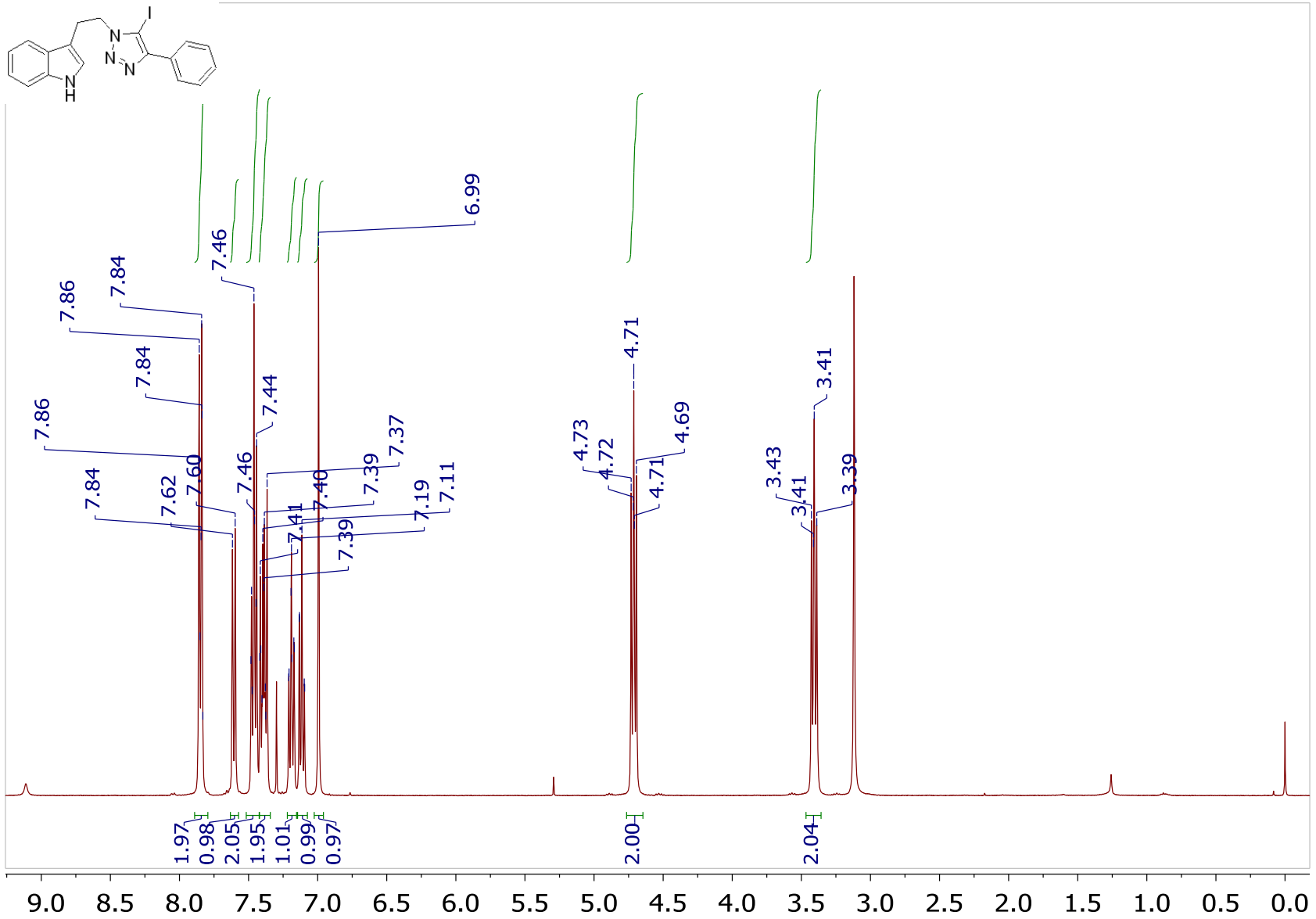
1-(2-(Cyclohex-1-en-1-yl)ethyl)-5-iodo-4-phenyl-1*H*-1,2,3-triazole (1p)

^{13}C NMR (101 MHz, $CDCl_3$)



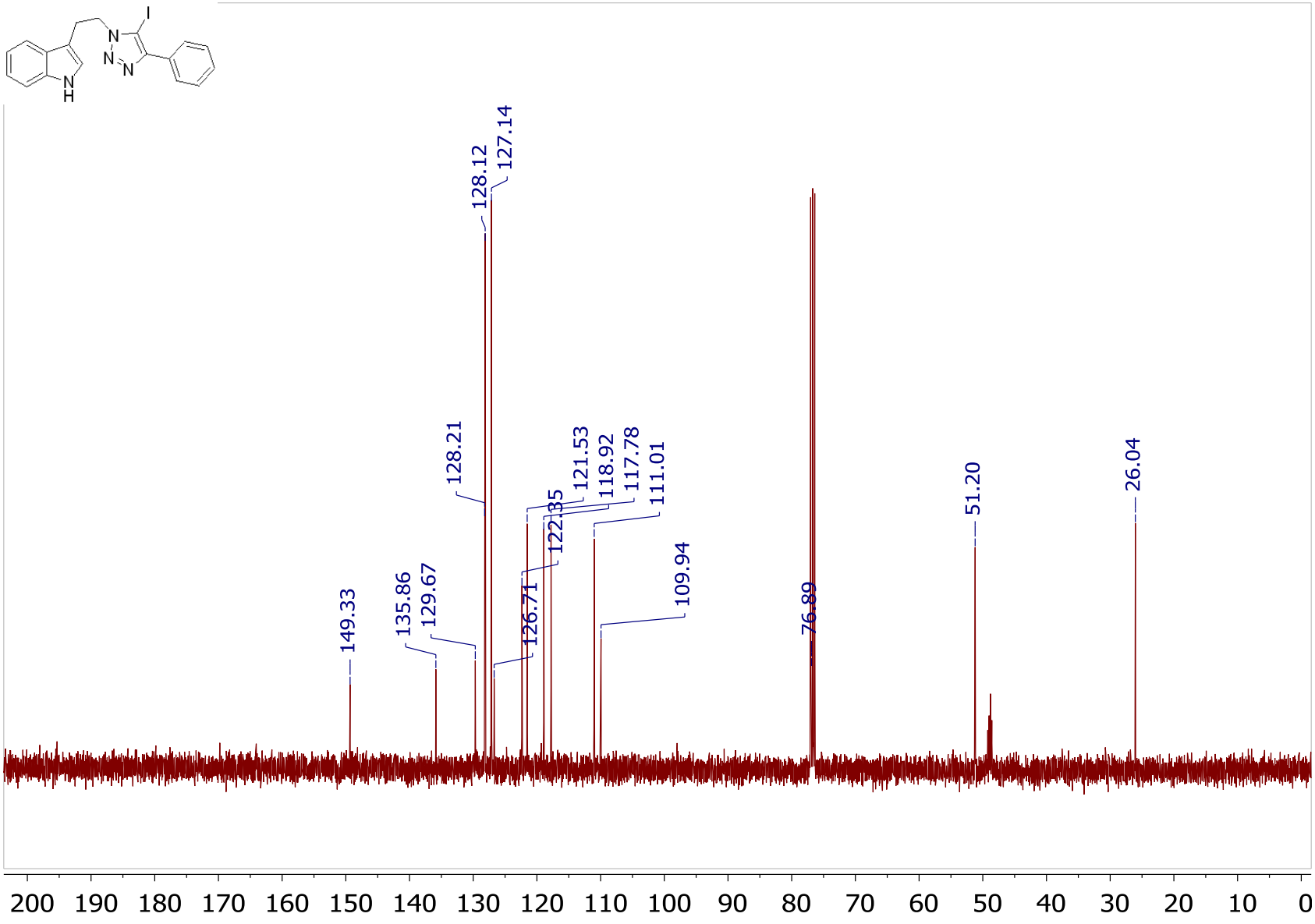
3-(2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-indole (1q)

^{1}H NMR (400 MHz, $CDCl_3$/CD_3OD)



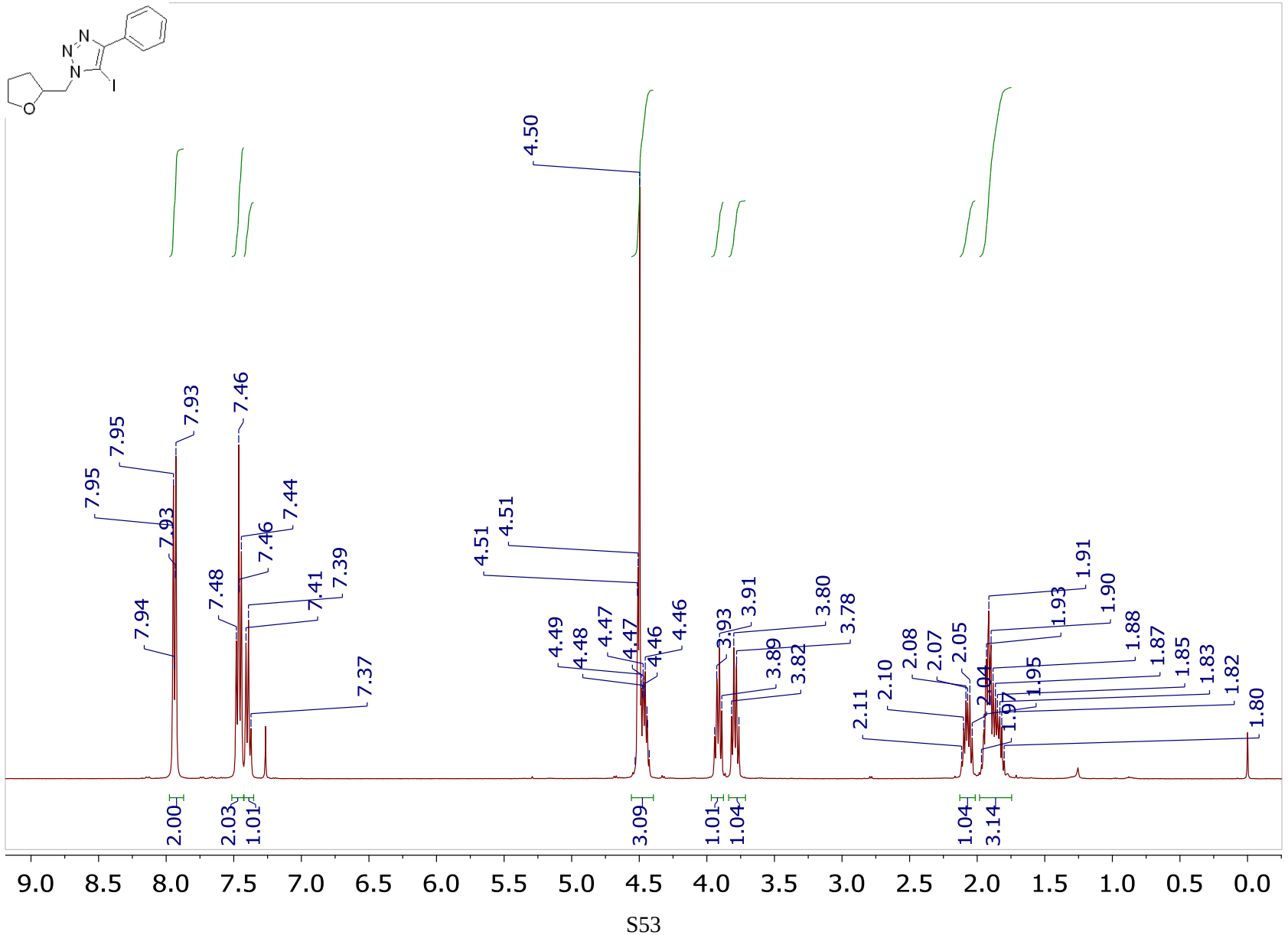
3-(2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-indole (1q)

^{13}C NMR (101 MHz, $CDCl_3/CD_3OD$)



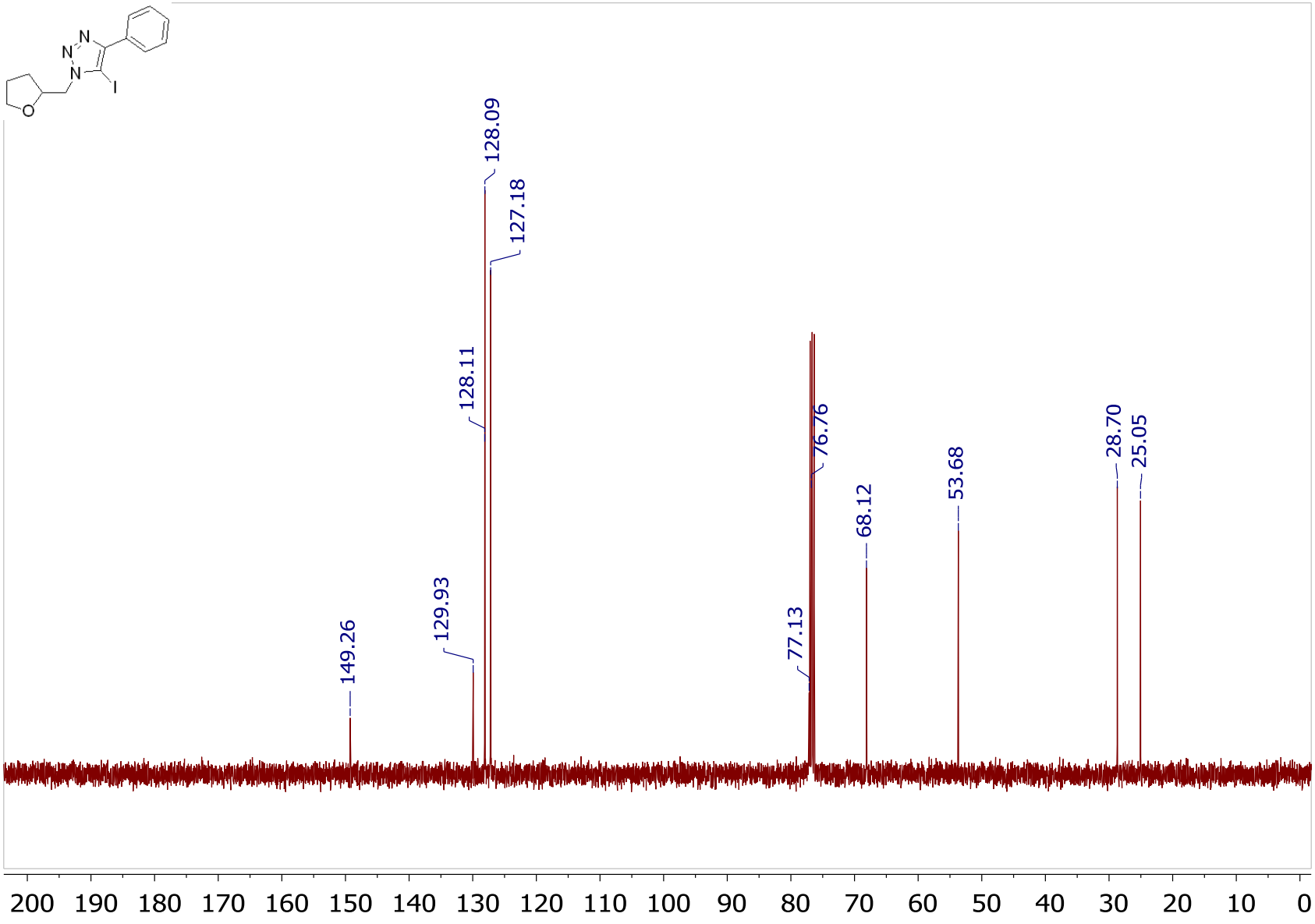
5-Iodo-4-phenyl-1-((tetrahydrofuran-2-yl)methyl)-1*H*-1,2,3-triazole (1r)

^{1}H NMR (400 MHz, $CDCl_3$)



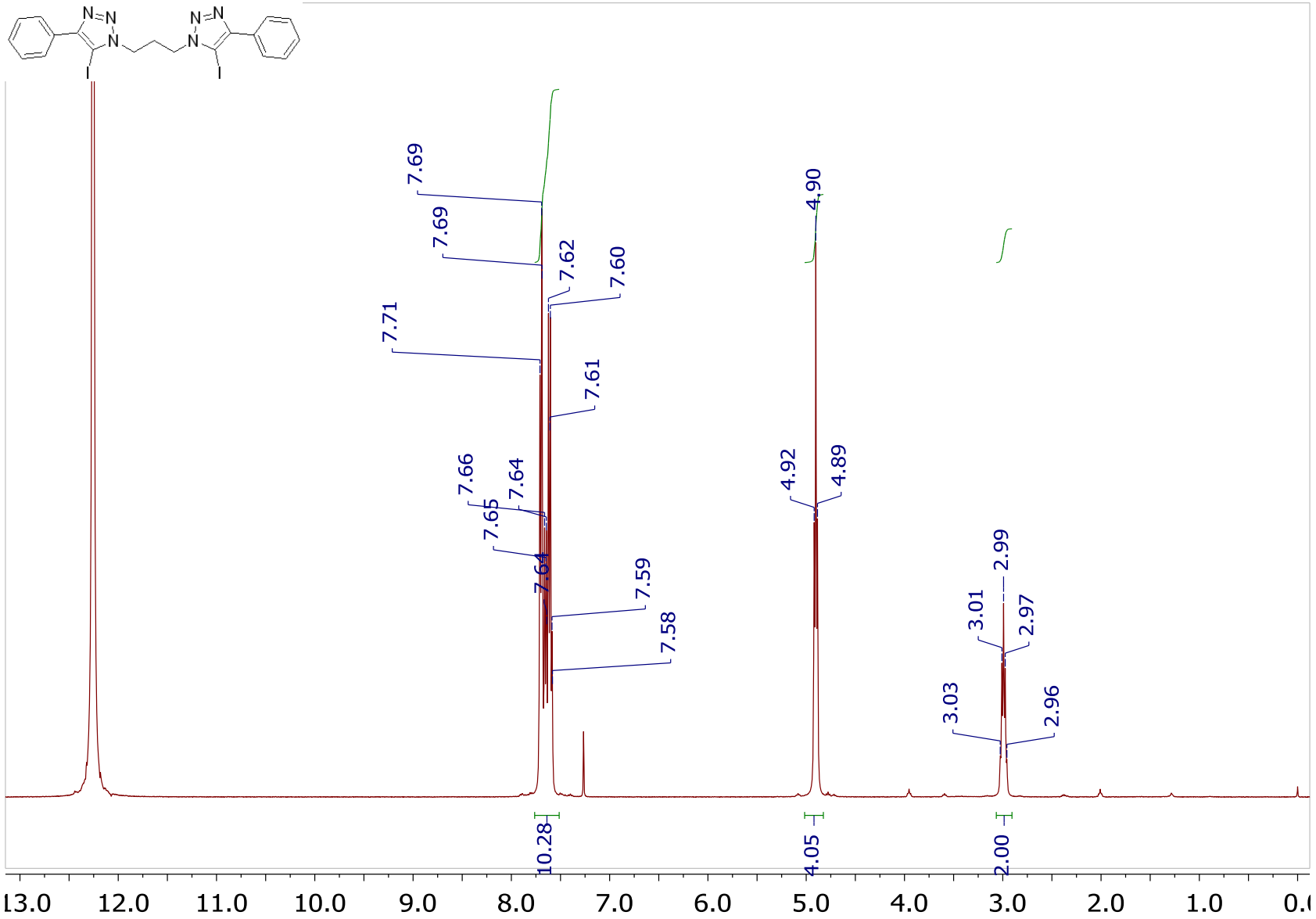
5-Iodo-4-phenyl-1-((tetrahydrofuran-2-yl)methyl)-1*H*-1,2,3-triazole (1r)

^{13}C NMR (101 MHz, $CDCl_3$)



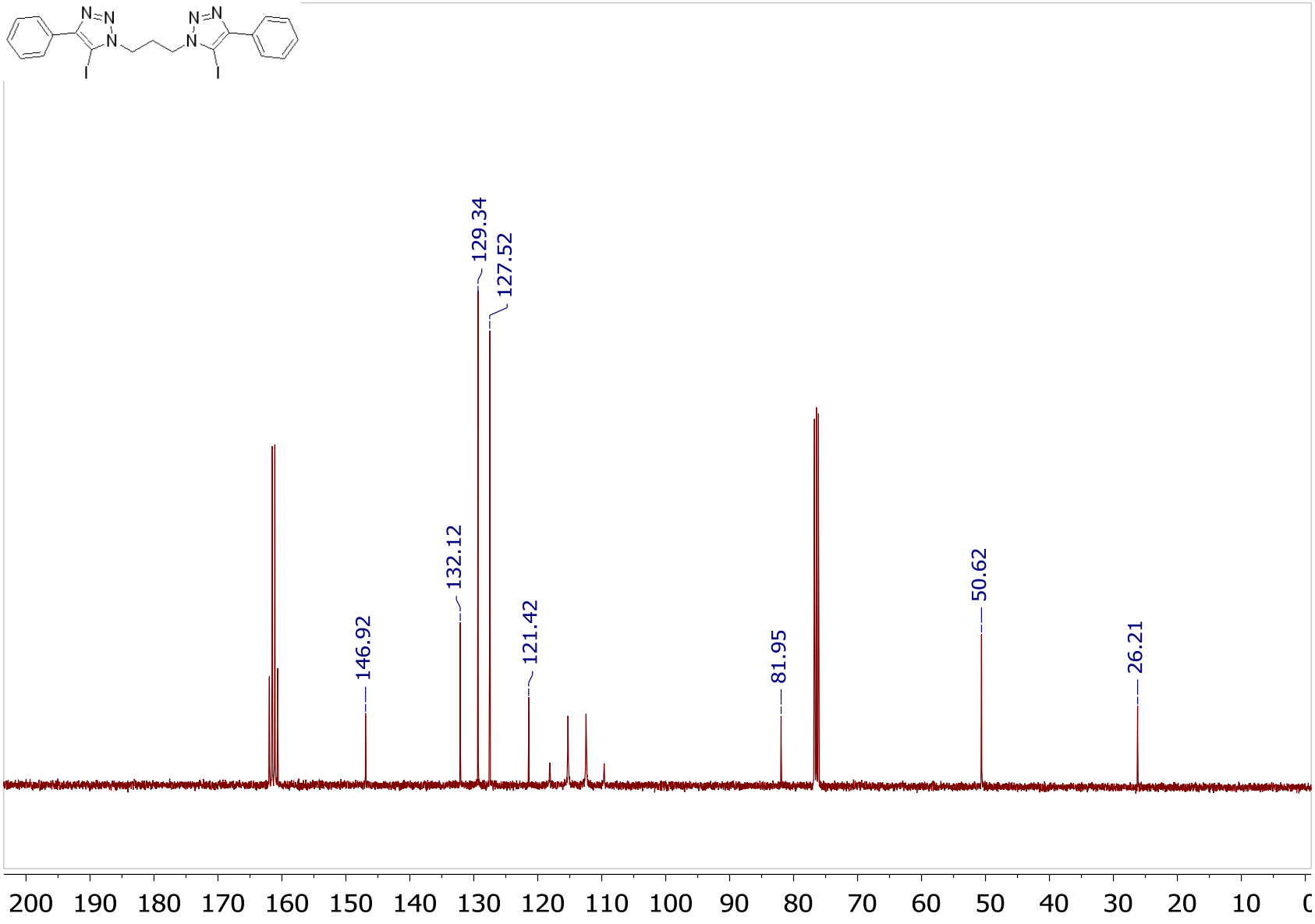
1,3-Bis(5-iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)propane (1t)

^{1}H NMR (400 MHz, $CDCl_3$/TFA)



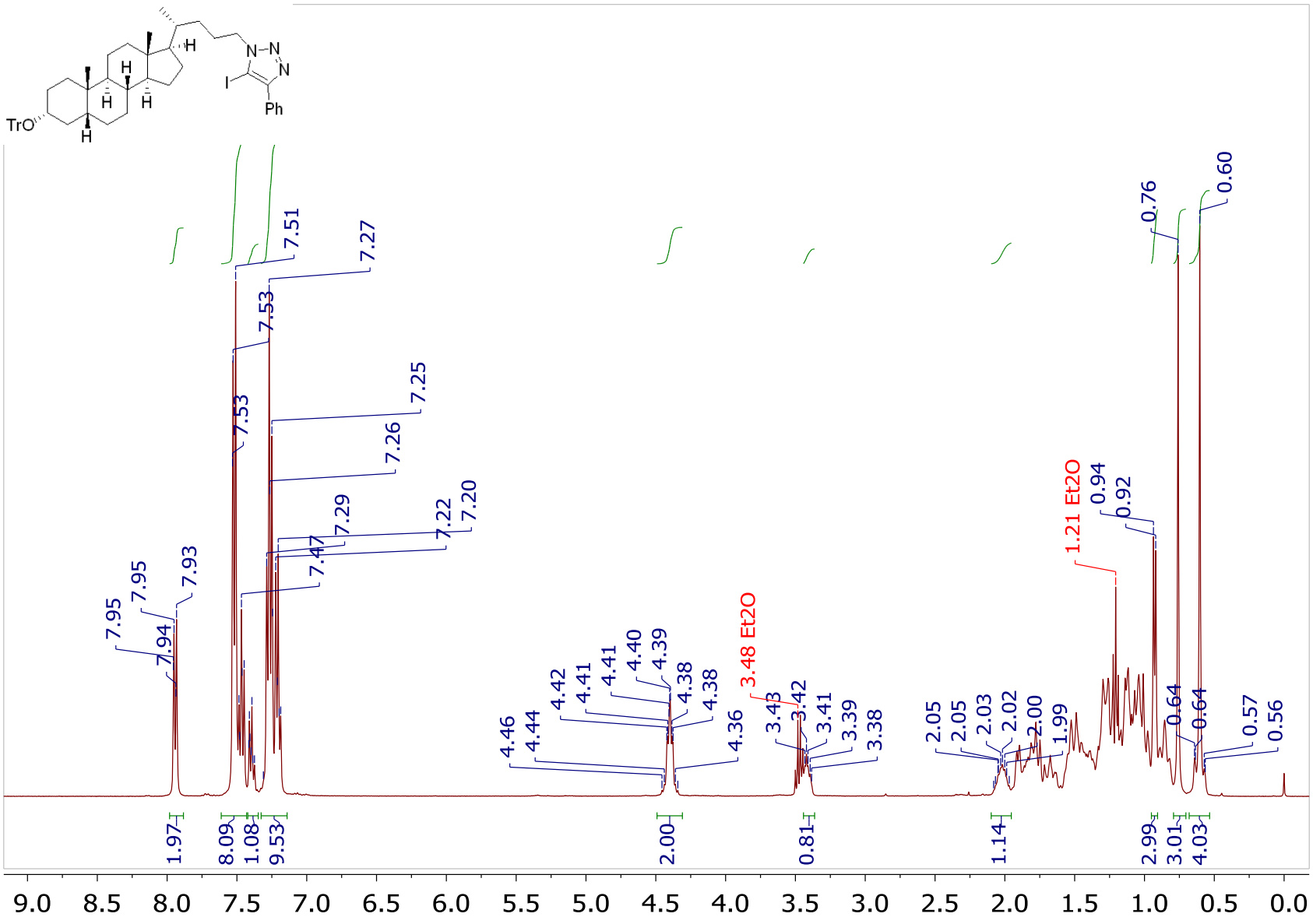
1,3-Bis(5-iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)propane (1t)

^{13}C NMR (101 MHz, $CDCl_3$/TFA)



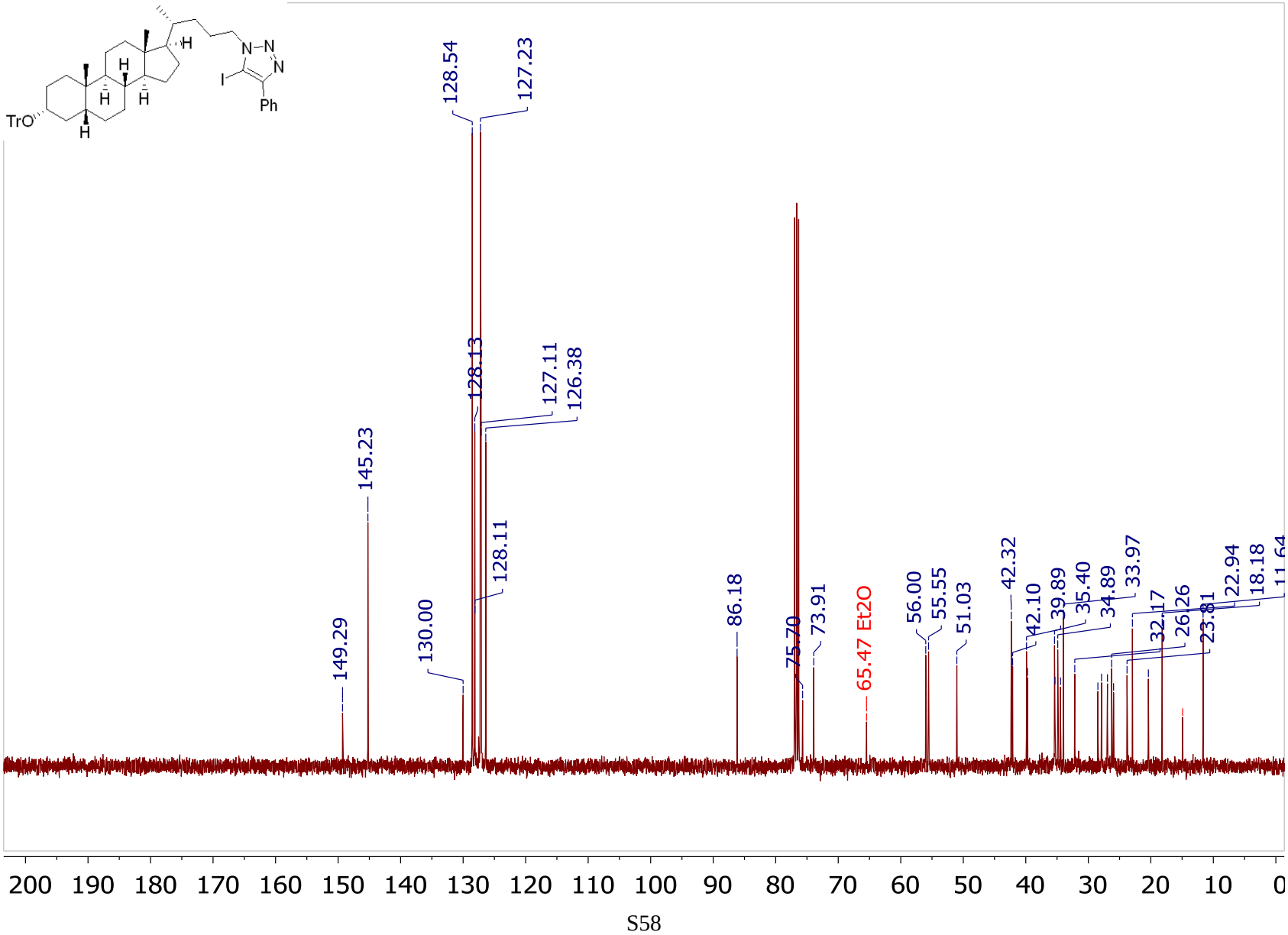
24-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)-3*α*-trityloxy-5β-cholane (1u)

^{1}H NMR (400 MHz, $CDCl_3$)



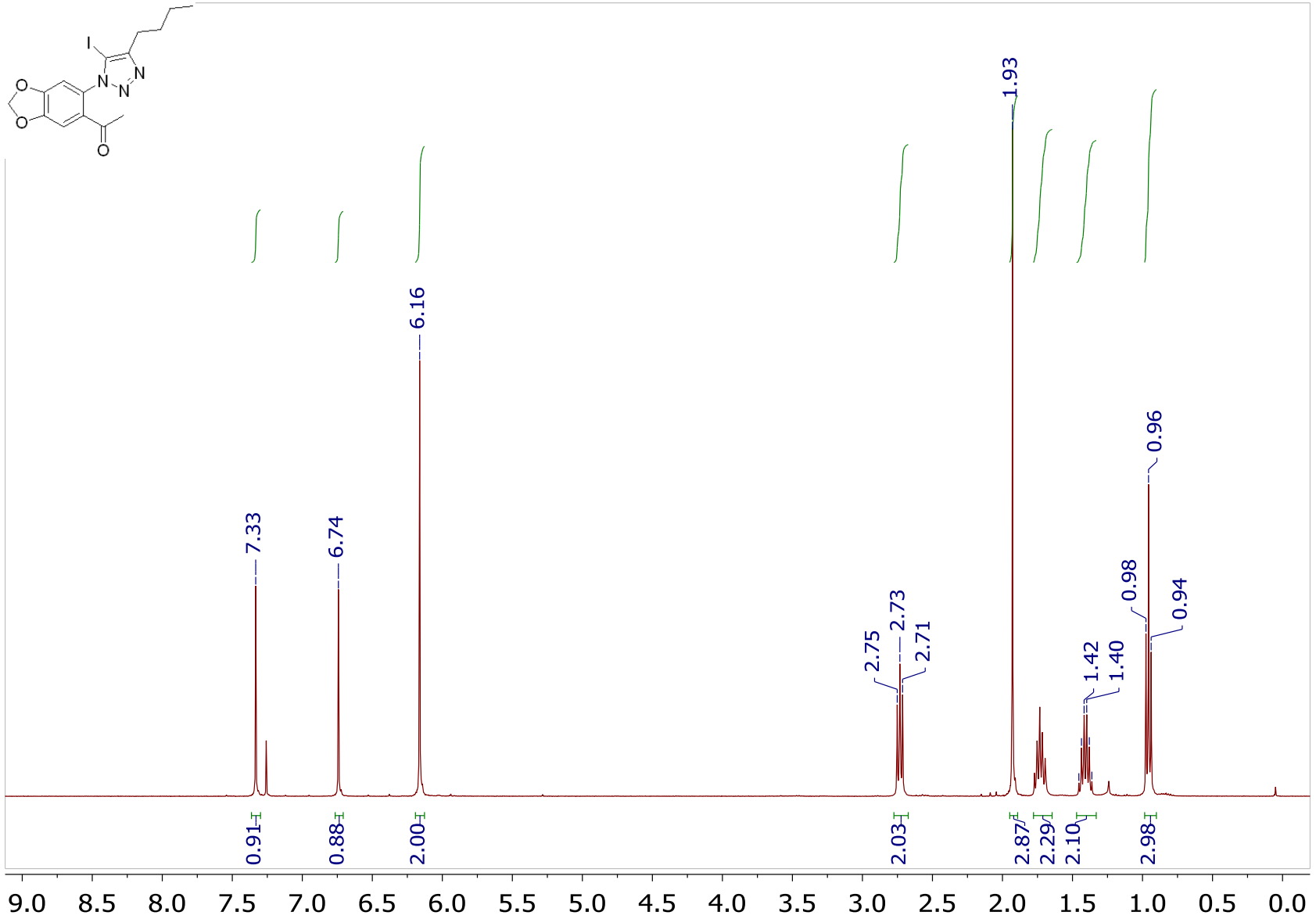
24-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)-3*α*-trityloxy-5β-cholane (1u)

^{13}C NMR (101 MHz, $CDCl_3$)



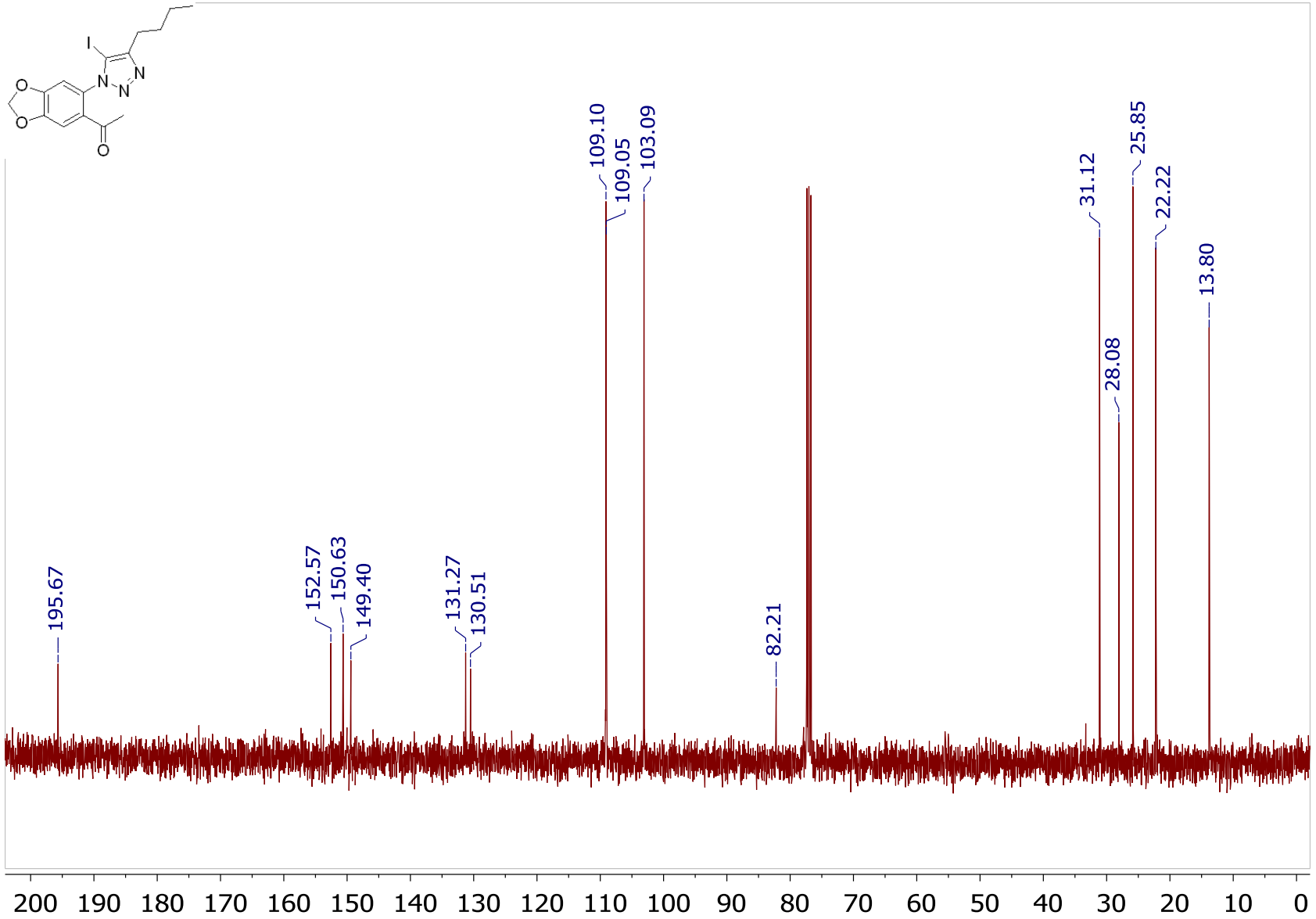
1-[6-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-1,3-benzodioxol-5-yl]ethanone (1v)

^{1}H NMR (400 MHz, $CDCl_3$)



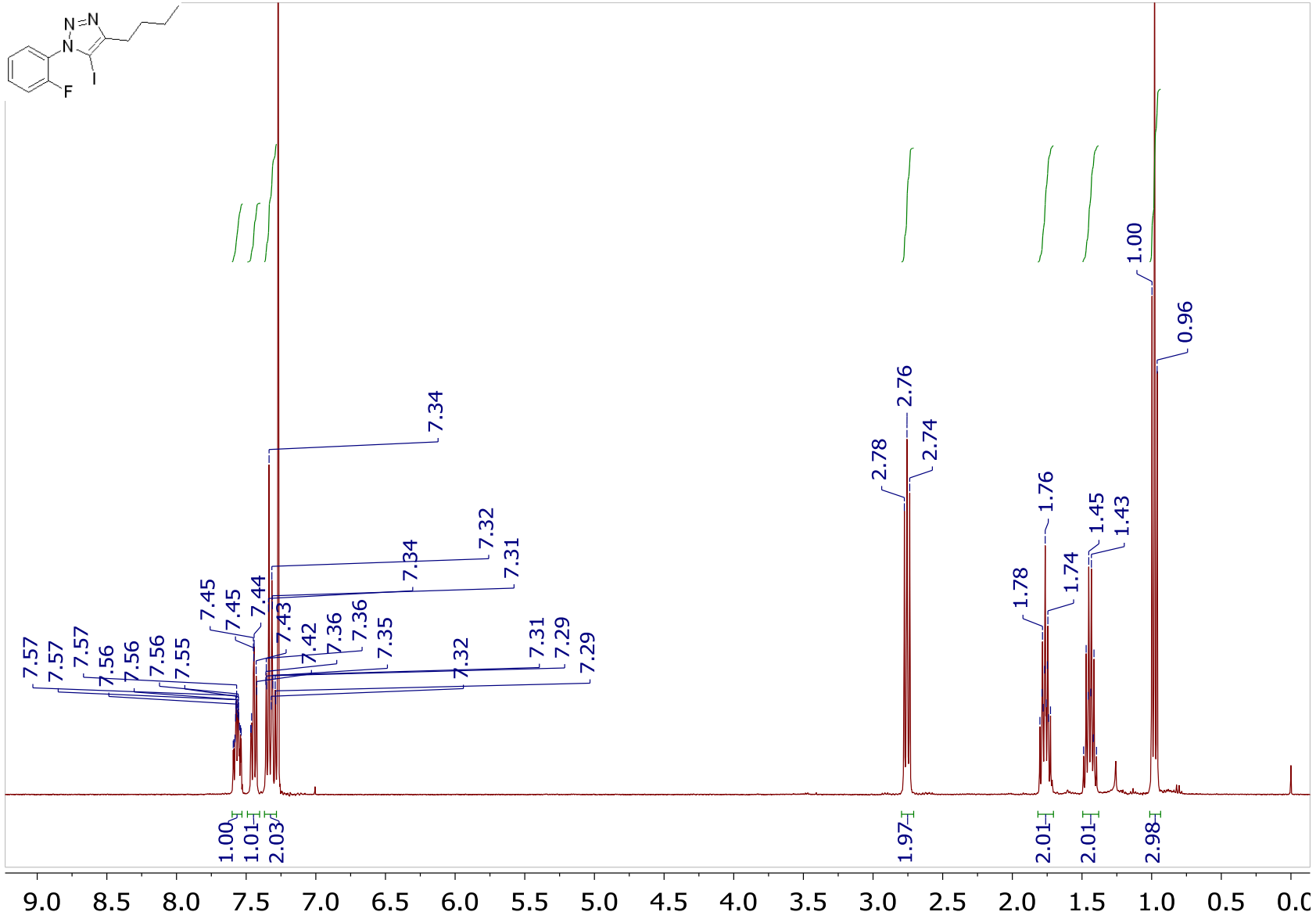
1-[6-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-1,3-benzodioxol-5-yl]ethanone (1v)

^{13}C NMR (101 MHz, $CDCl_3$)



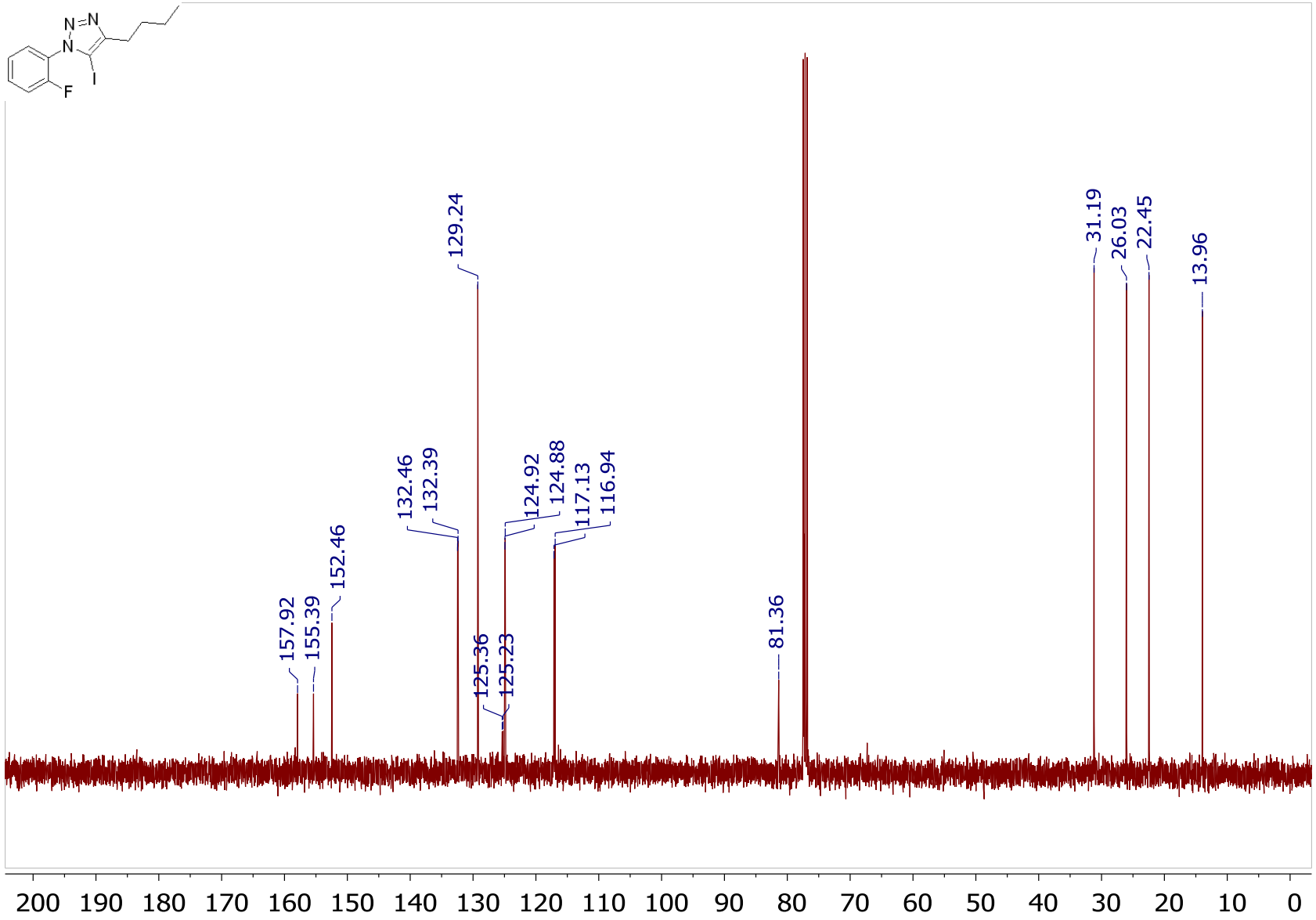
4-Butyl-1-(2-fluorophenyl)-5-iodo-1*H*-1,2,3-triazole (1y)

^{1}H NMR (400 MHz, $CDCl_3$)



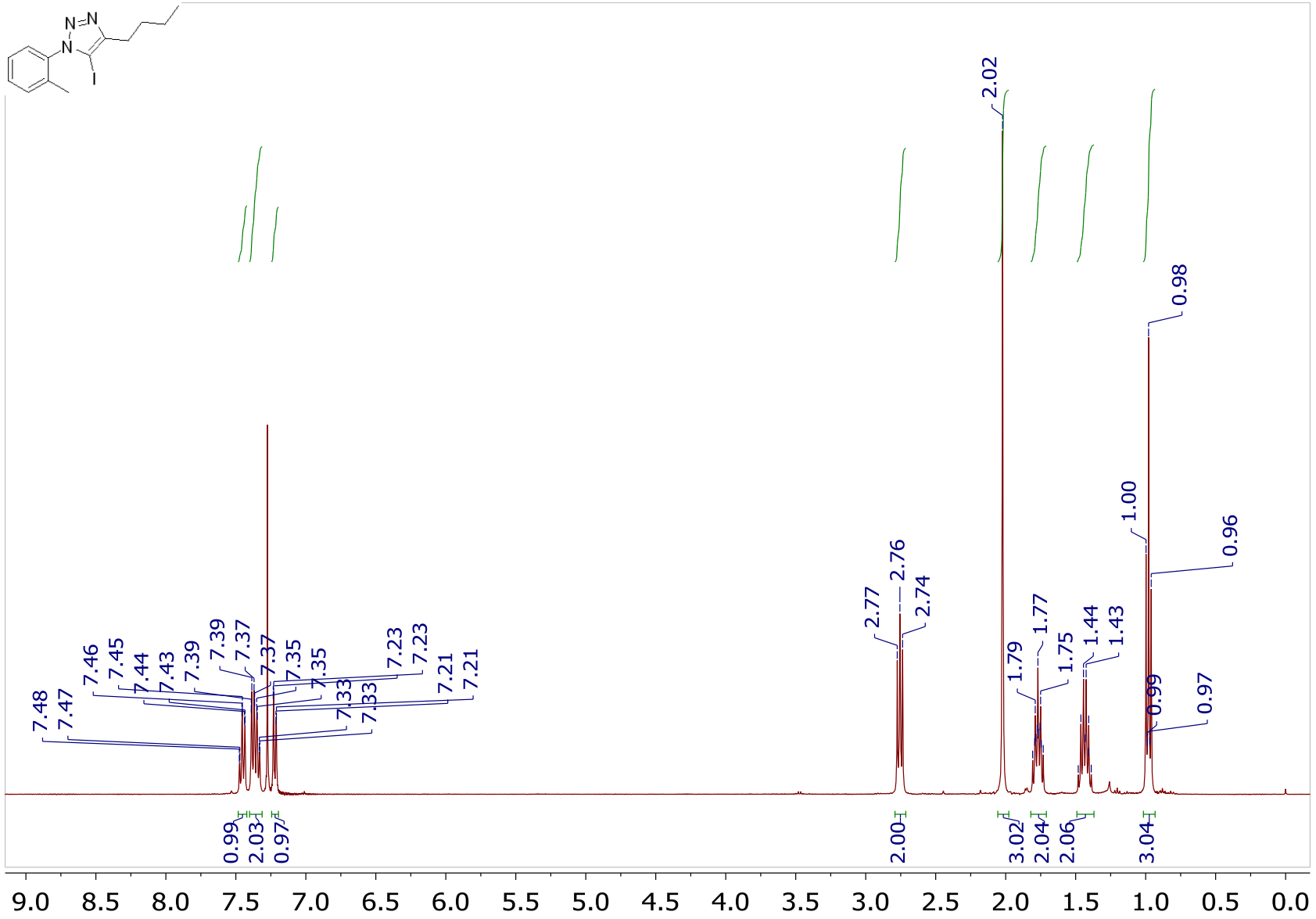
4-Butyl-1-(2-fluorophenyl)-5-iodo-1*H*-1,2,3-triazole (1y)

^{13}C NMR (101 MHz, $CDCl_3$)



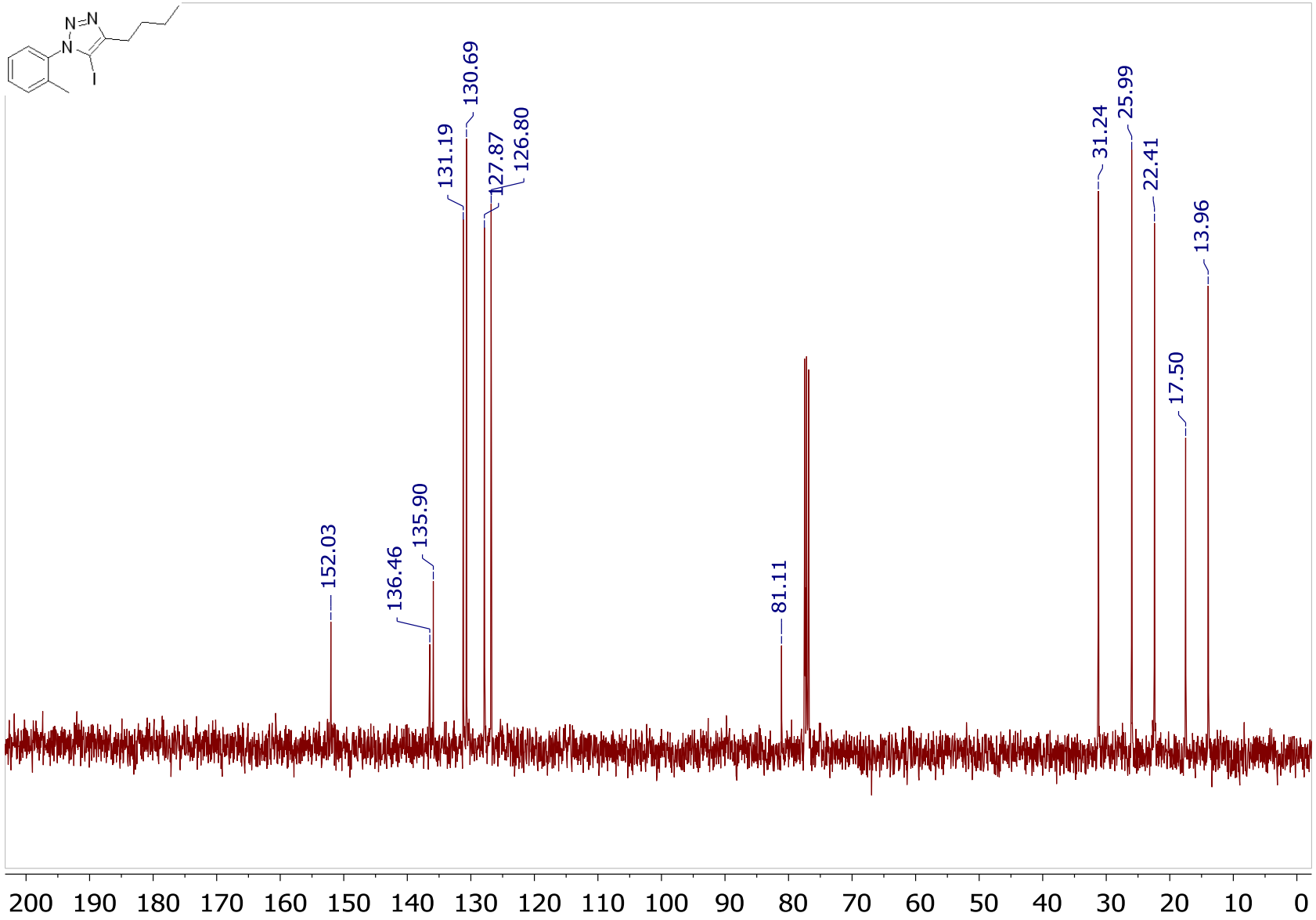
4-Butyl-5-iodo-1-(*o*-tolyl)-1*H*-1,2,3-triazole (1aa)

^{1}H NMR (400 MHz, $CDCl_3$)



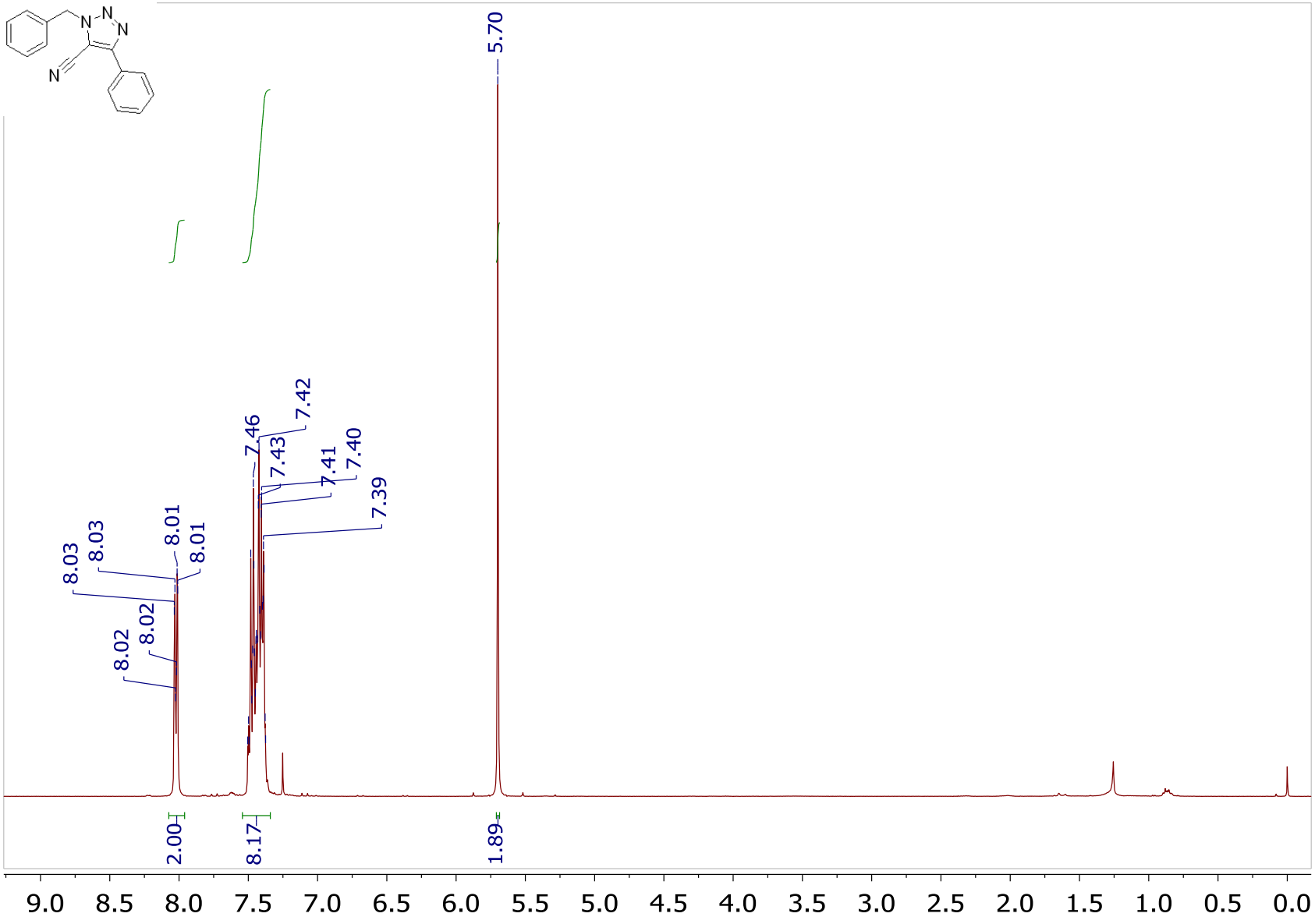
4-Butyl-5-iodo-1-(*o*-tolyl)-1*H*-1,2,3-triazole (1aa)

^{13}C NMR (101 MHz, $CDCl_3$)



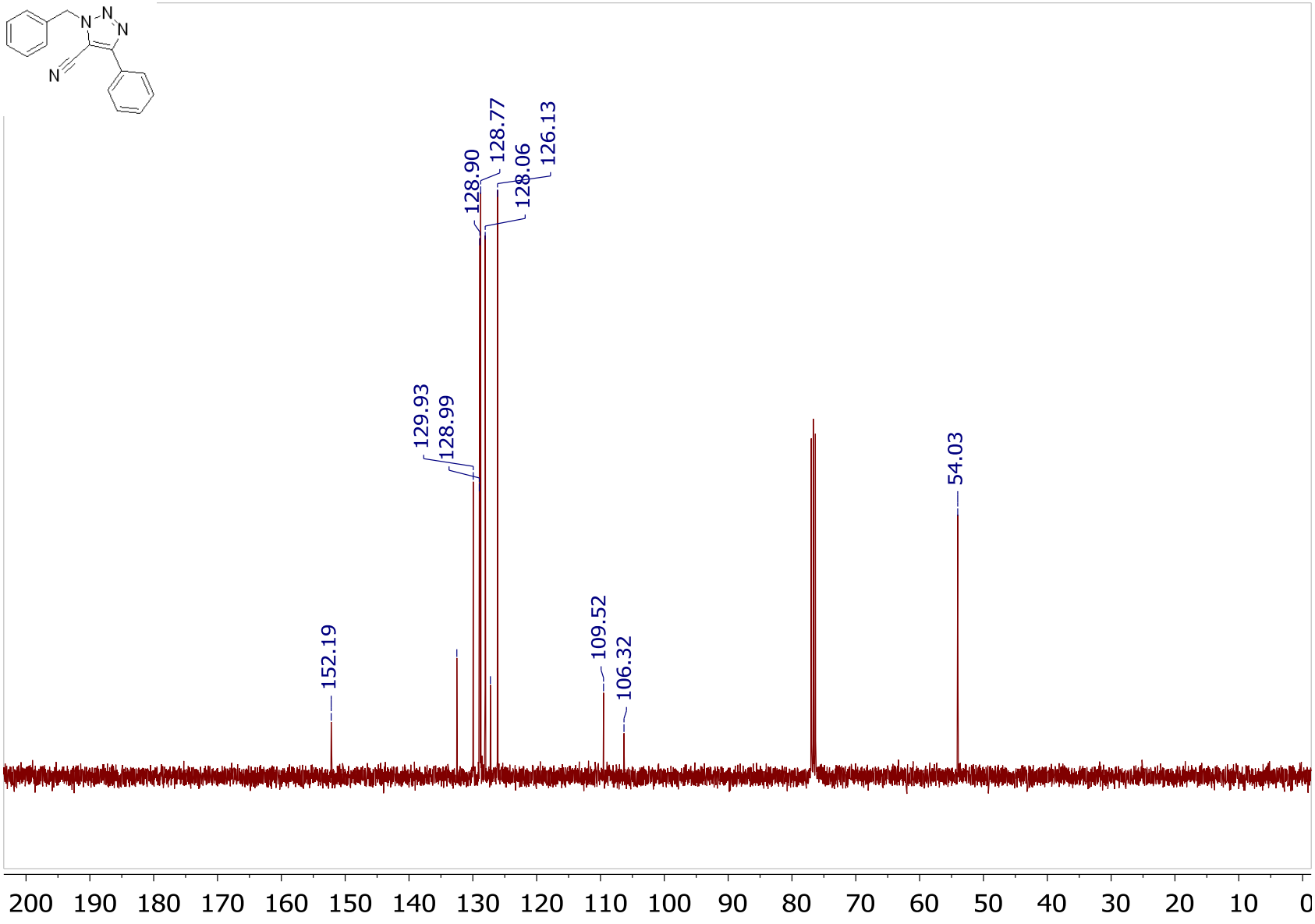
1-Benzyl-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2a)

^{1}H NMR (400 MHz, $CDCl_3$)



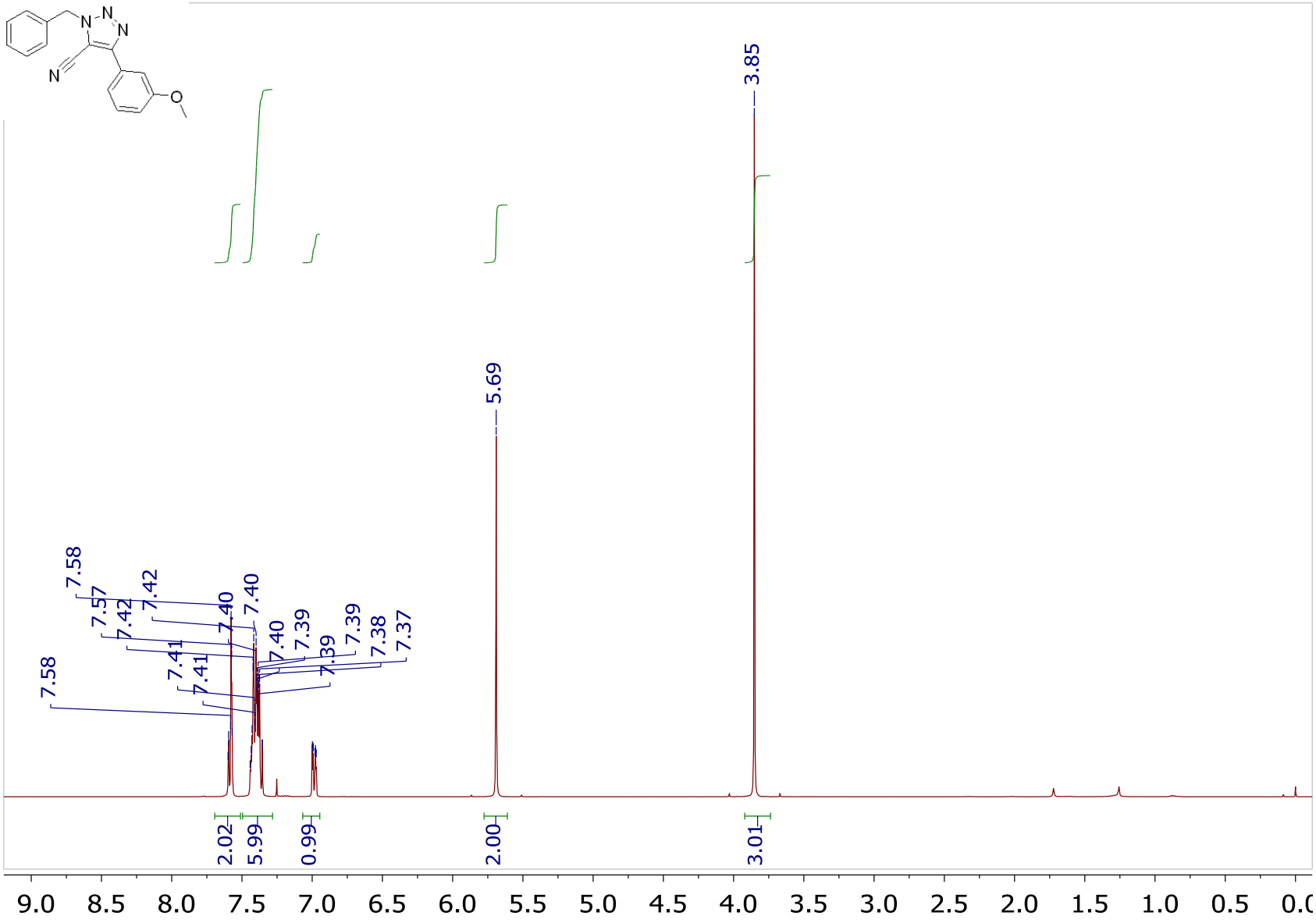
1-Benzyl-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2a)

^{13}C NMR (101 MHz, $CDCl_3$)



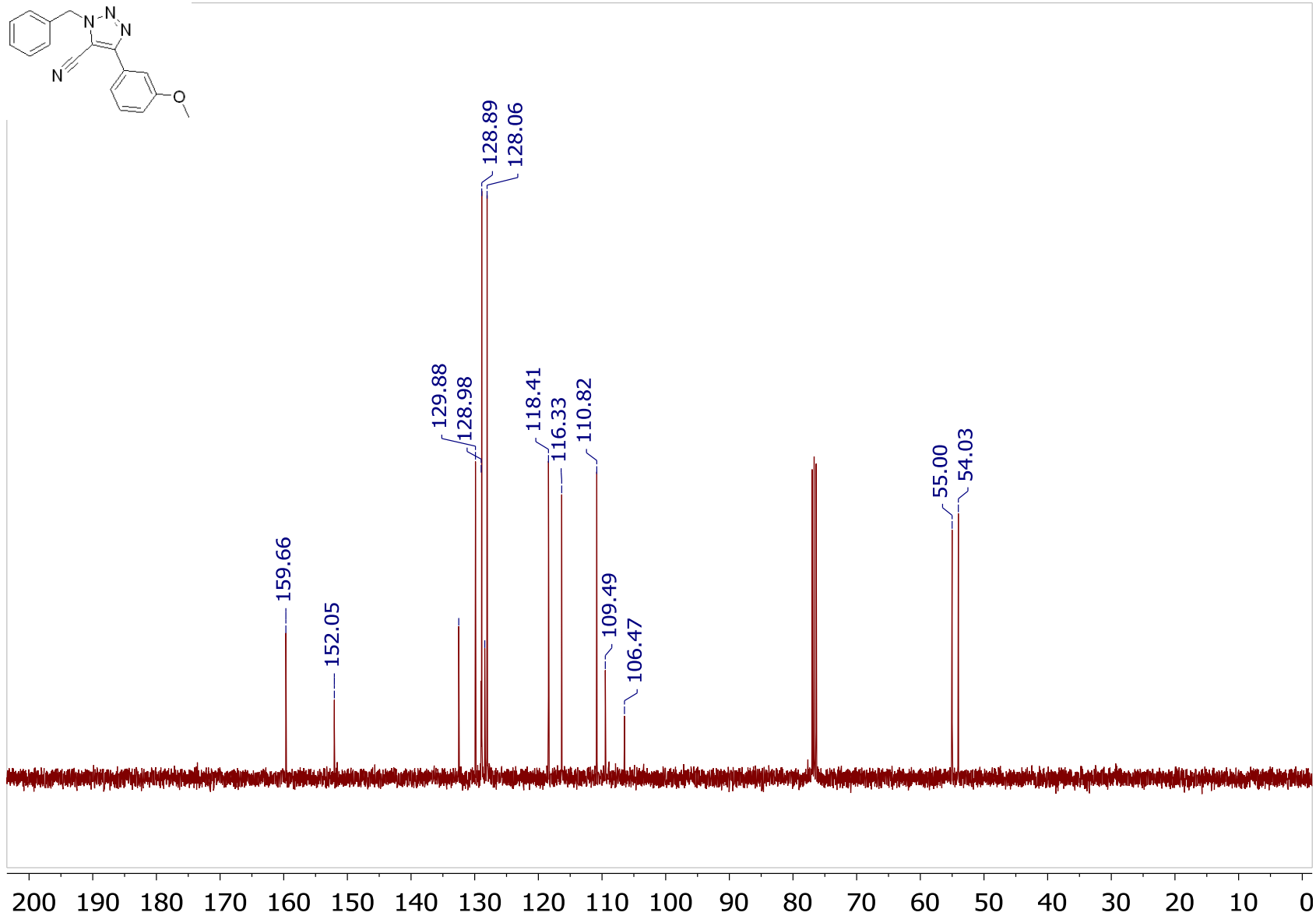
1-Benzyl-5-cyano-4-(3-methoxyphenyl)-1*H*-1,2,3-triazole (2b)

^{1}H NMR (400 MHz, $CDCl_3$)



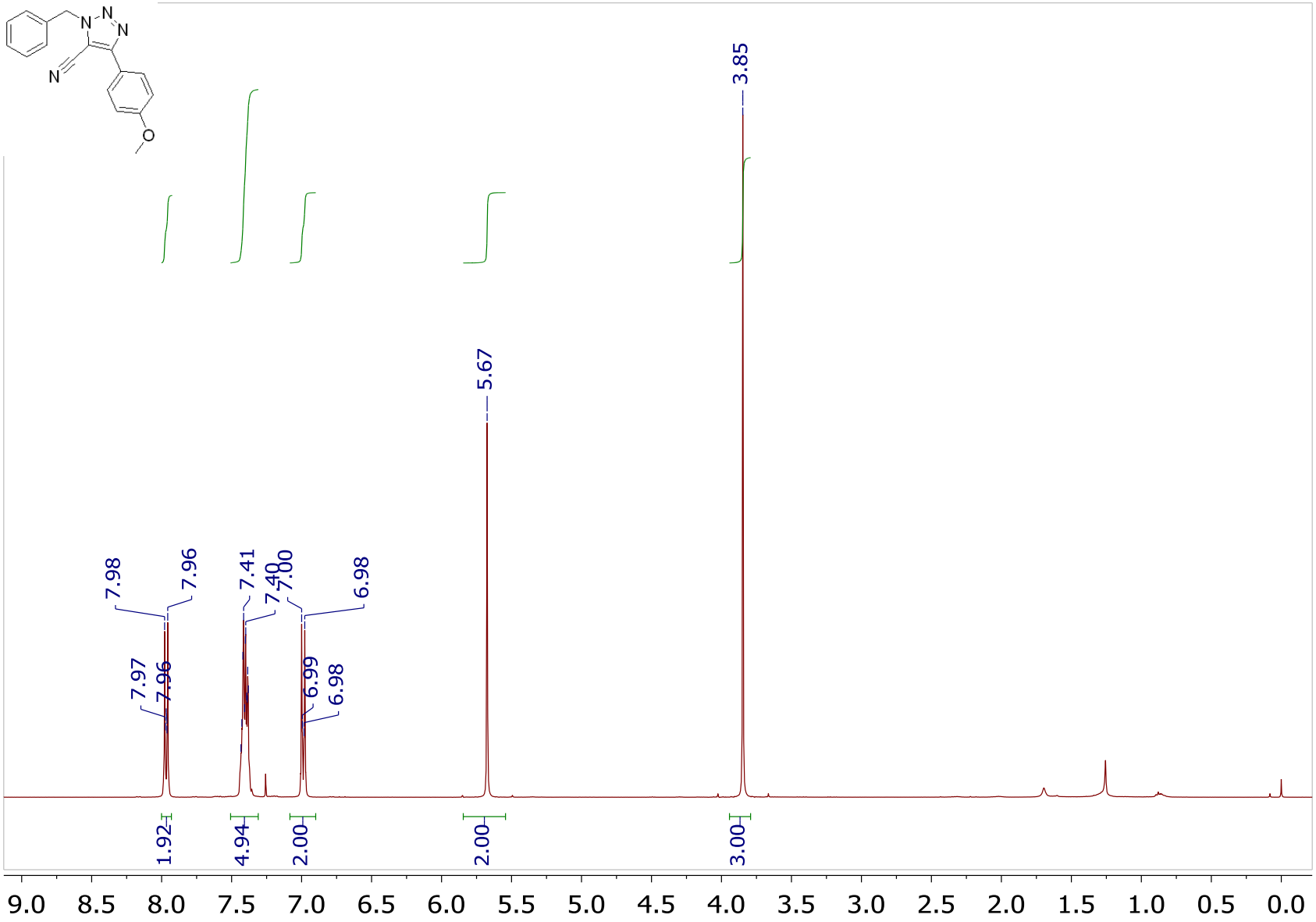
1-Benzyl-5-cyano-4-(3-methoxyphenyl)-1*H*-1,2,3-triazole (2b)

^{13}C NMR (101 MHz, $CDCl_3$)



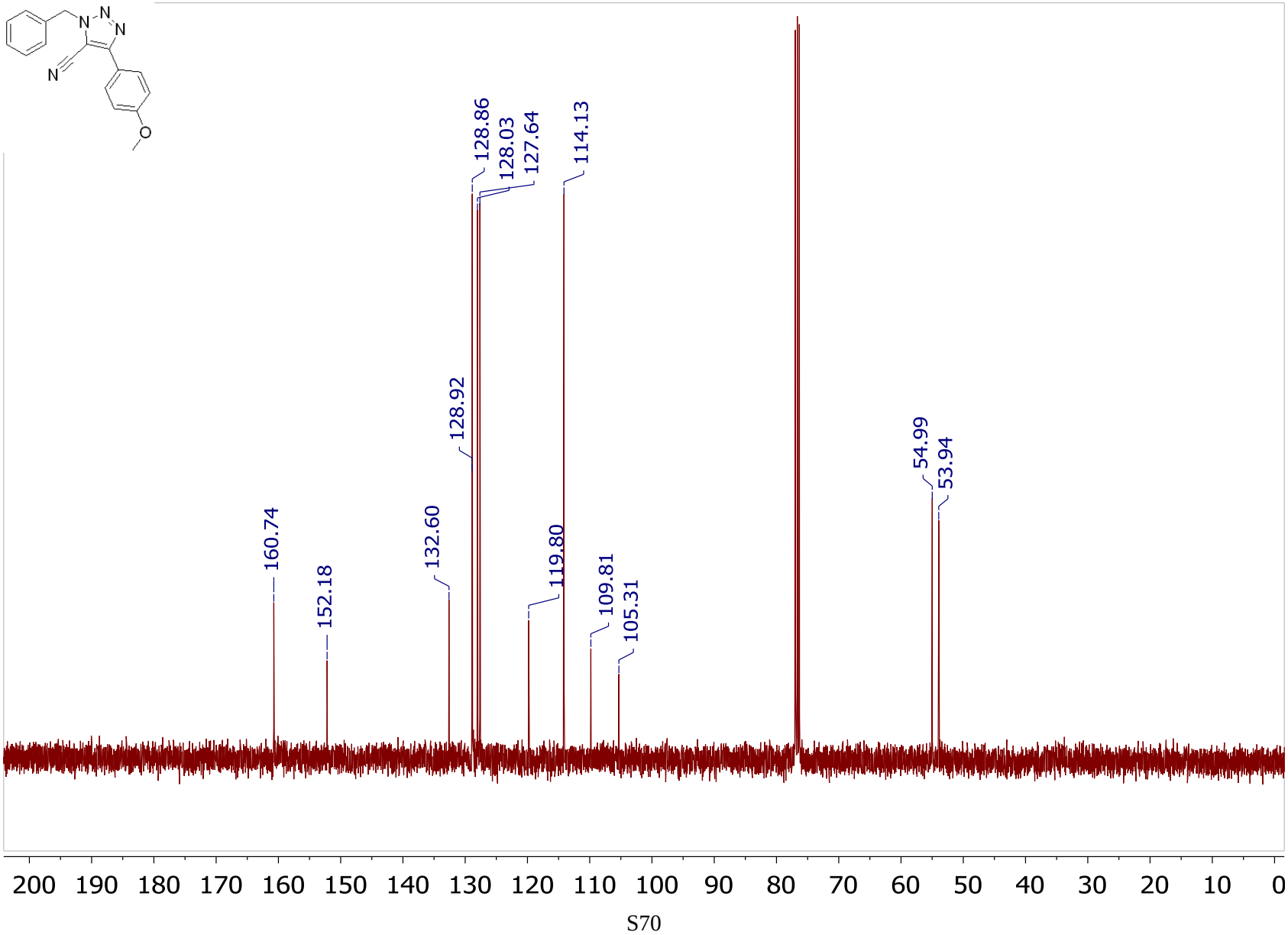
1-Benzyl-5-cyano-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (2c)

^{1}H NMR (400 MHz, $CDCl_3$)



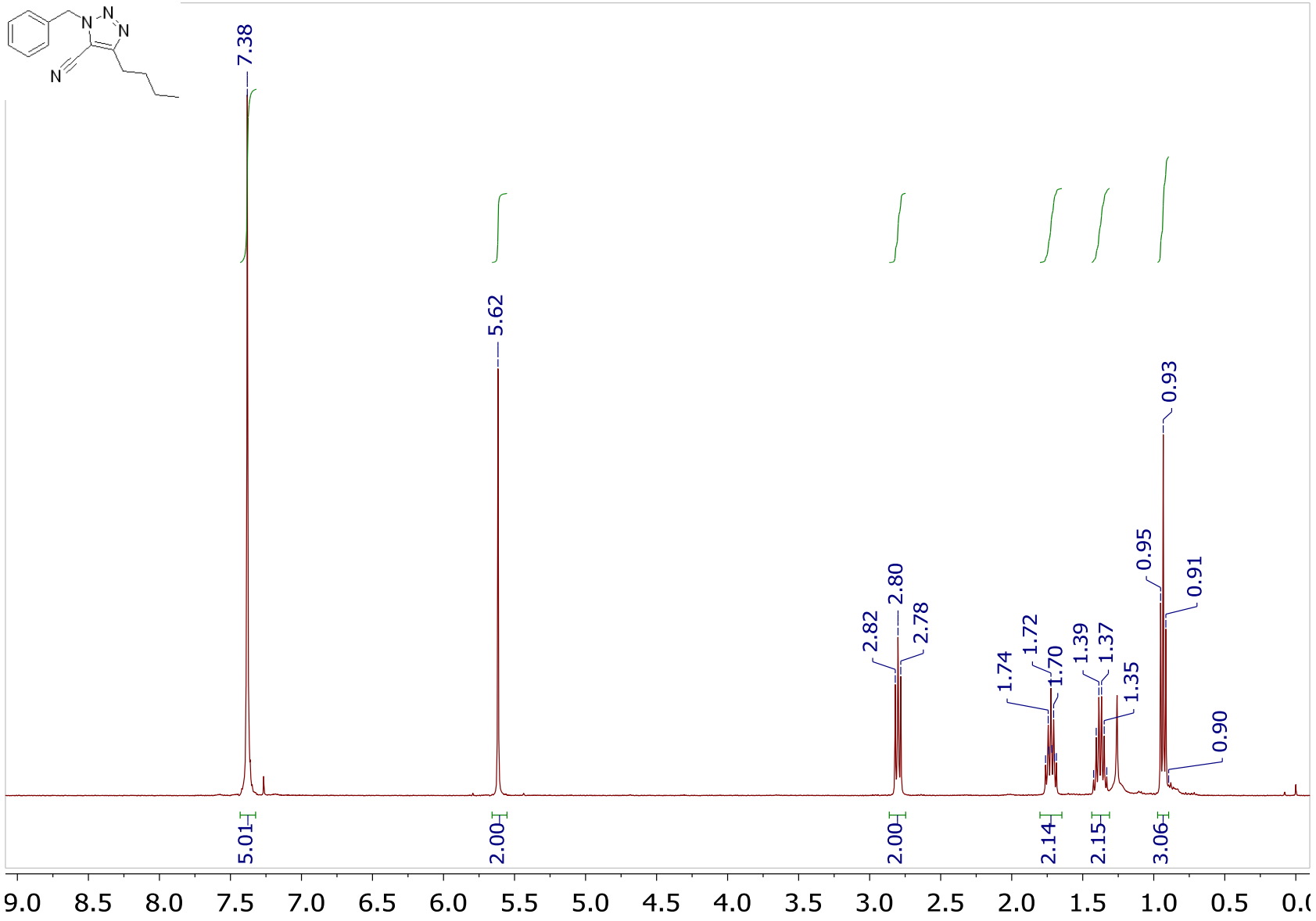
1-Benzyl-5-cyano-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (2c)

^{13}C NMR (101 MHz, $CDCl_3$)



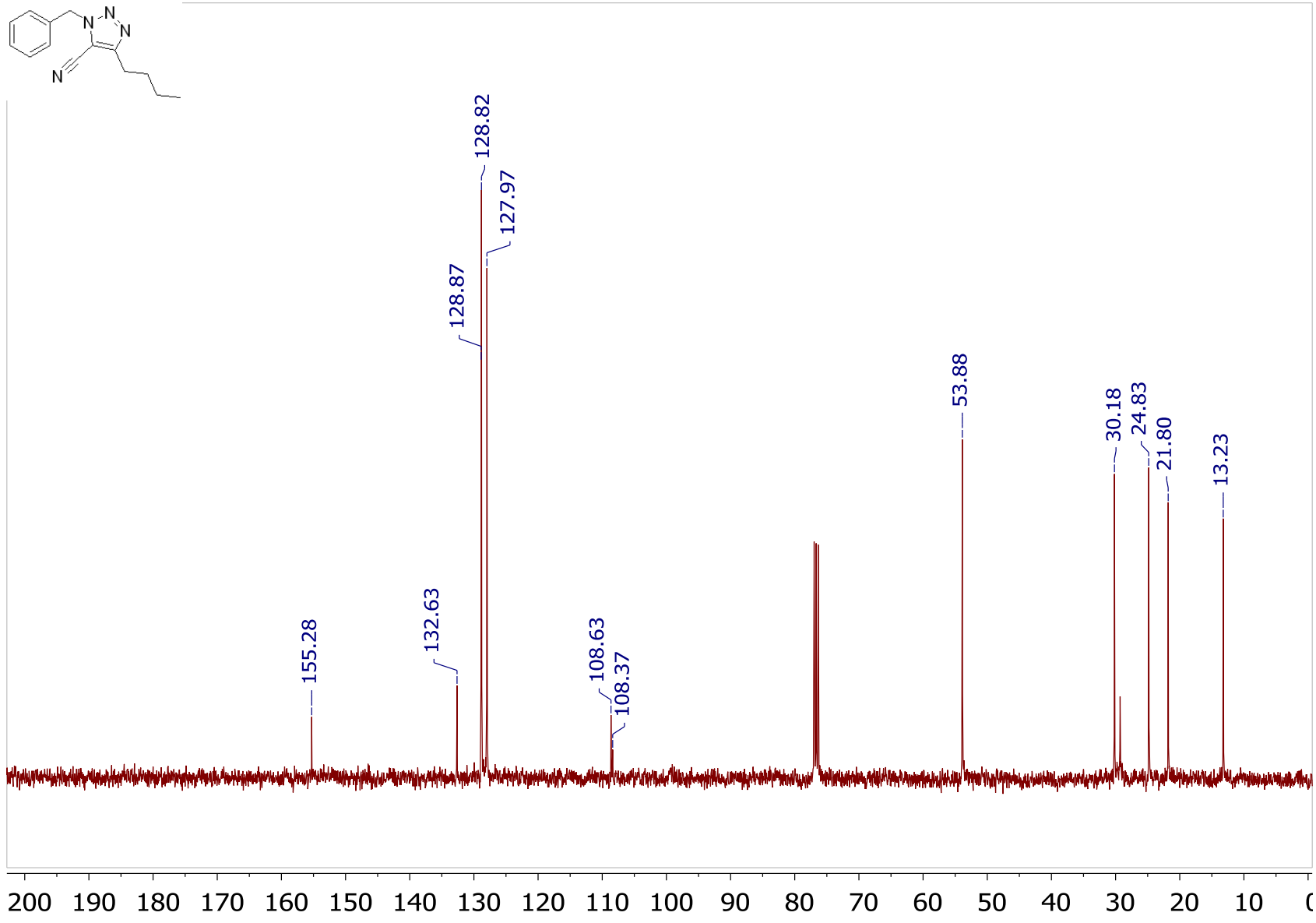
1-Benzyl-5-cyano-4-butyl-1*H*-1,2,3-triazole (2d)

^{1}H NMR (400 MHz, $CDCl_3$)



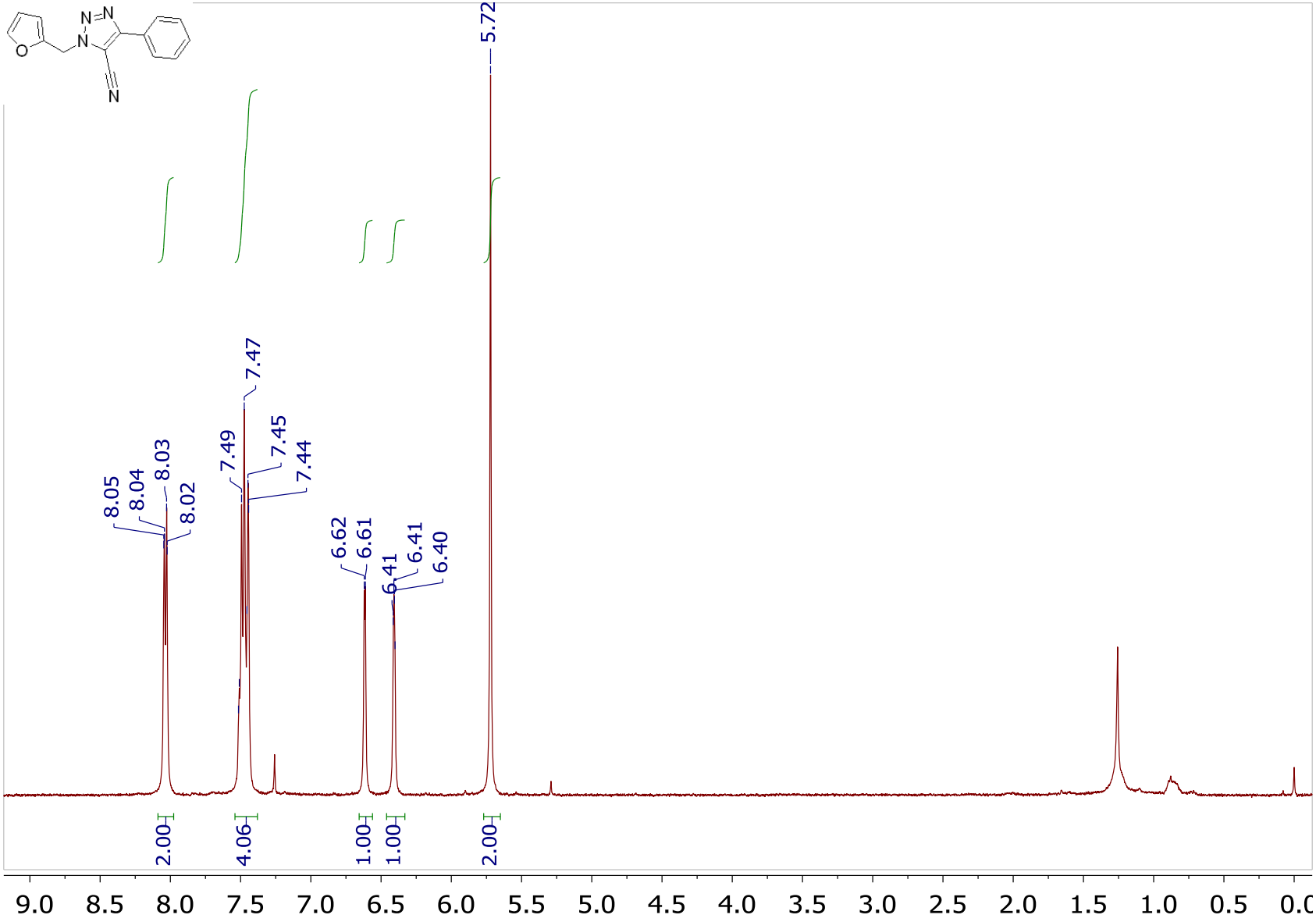
1-Benzyl-5-cyano-4-butyl-1*H*-1,2,3-triazole (2d)

^{13}C NMR (101 MHz, $CDCl_3$)



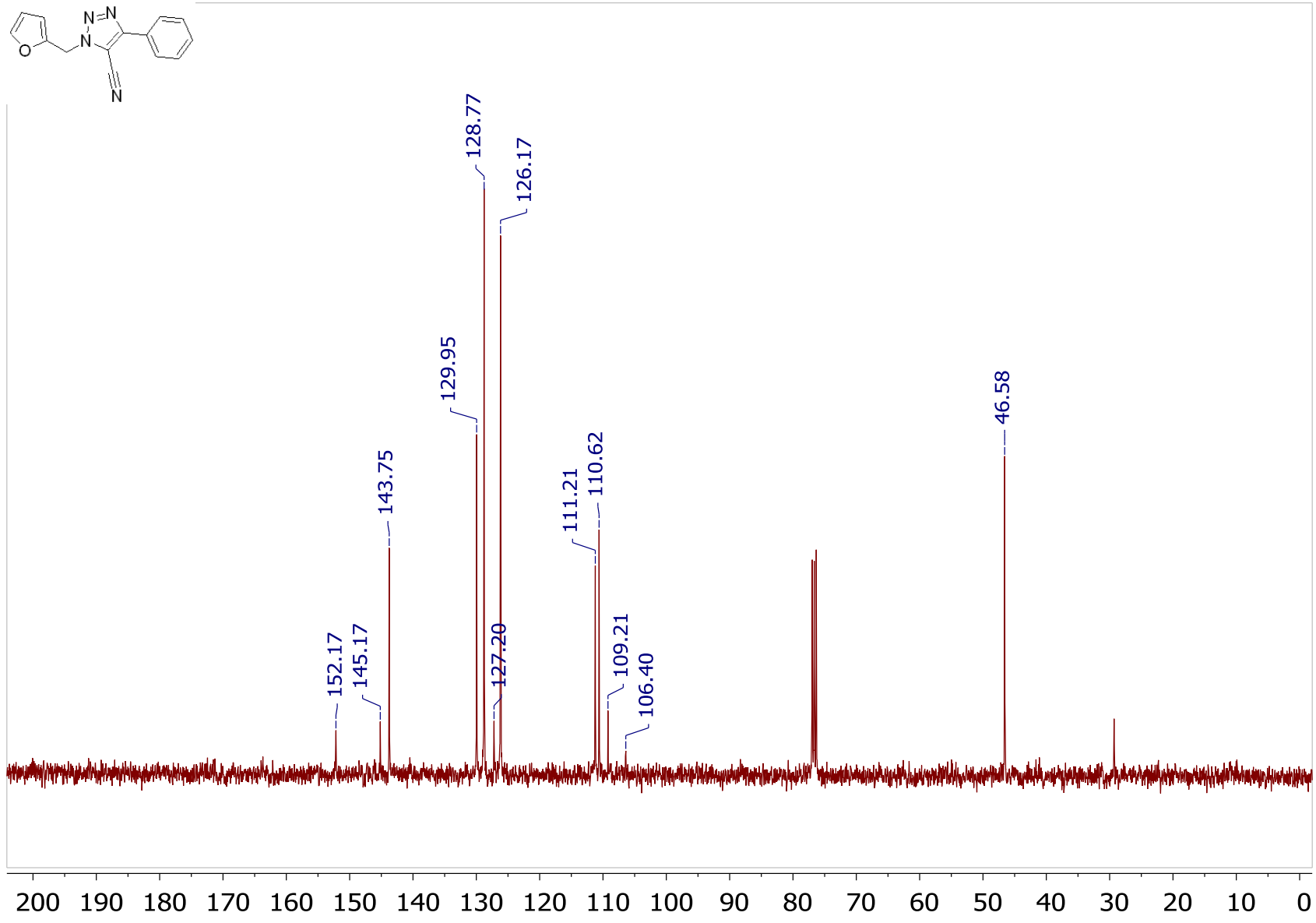
1-(Furan-2-ylmethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2e)

^{1}H NMR (400 MHz, $CDCl_3$)



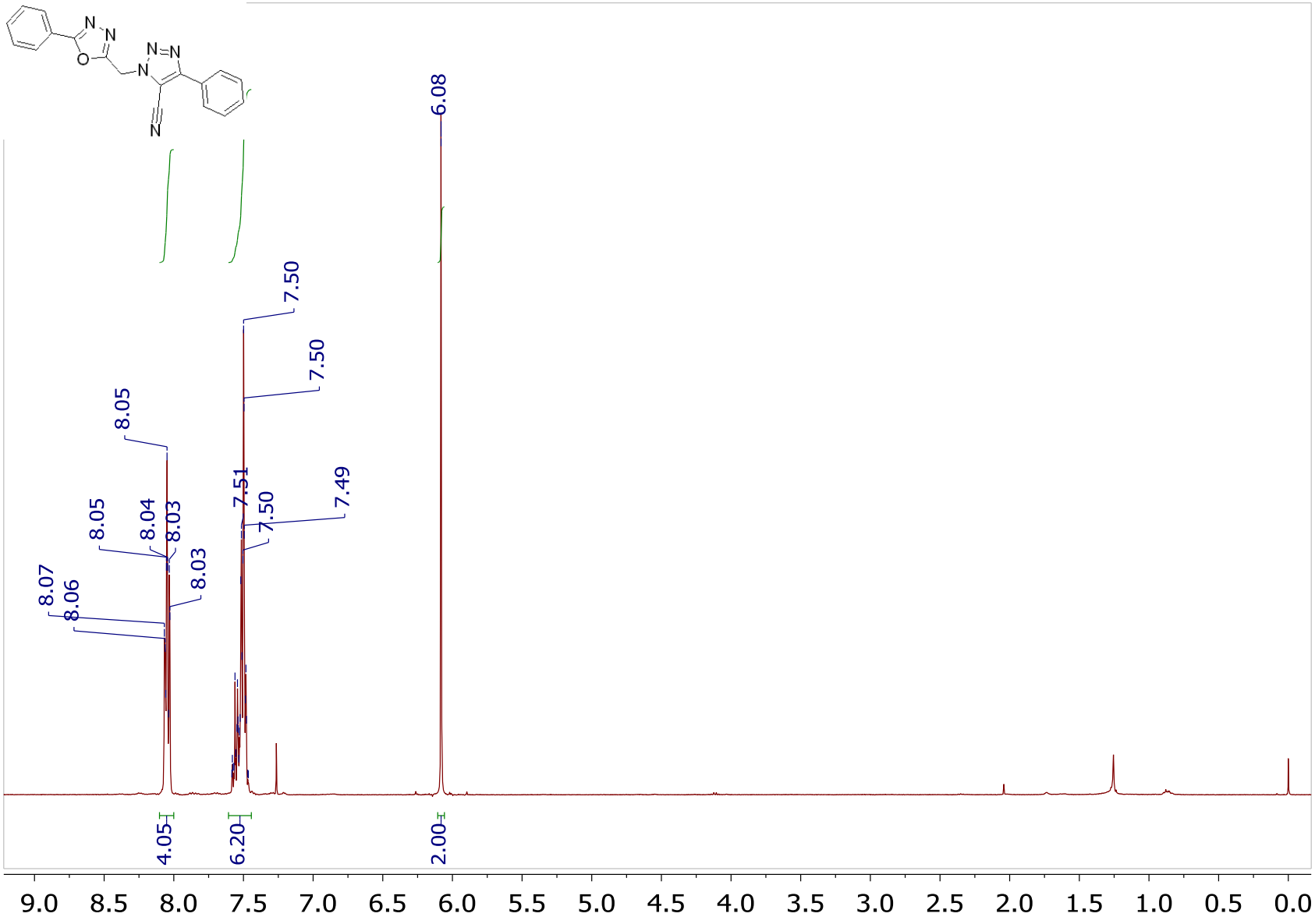
1-(Furan-2-ylmethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2e)

^{13}C NMR (101 MHz, $CDCl_3$)



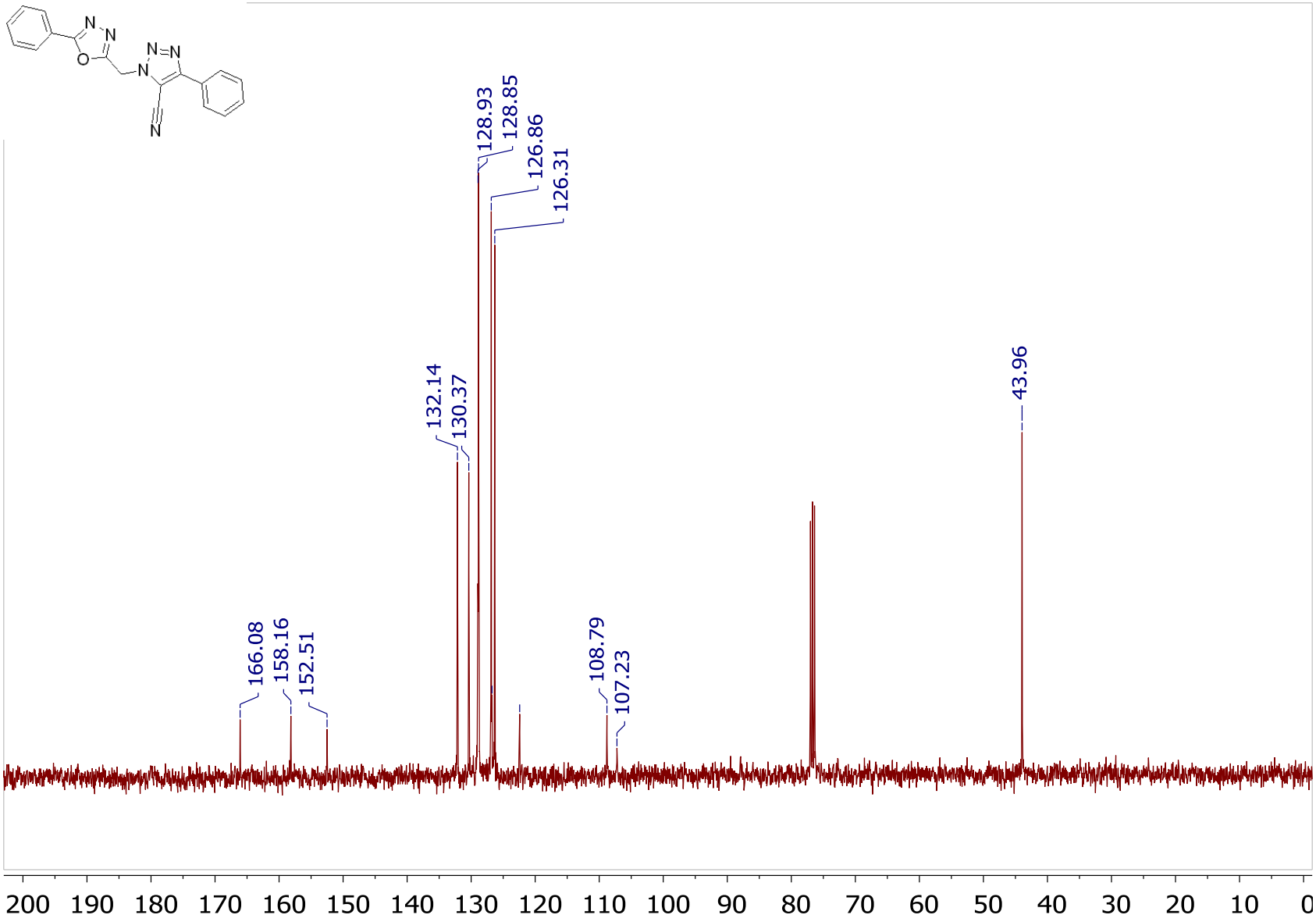
5-Cyano-4-phenyl-1-((5-phenyl-1,3,4-oxadiazol-2-yl)methyl)-1*H*-1,2,3-triazole (2f)

^{1}H NMR (400 MHz, $CDCl_3$)



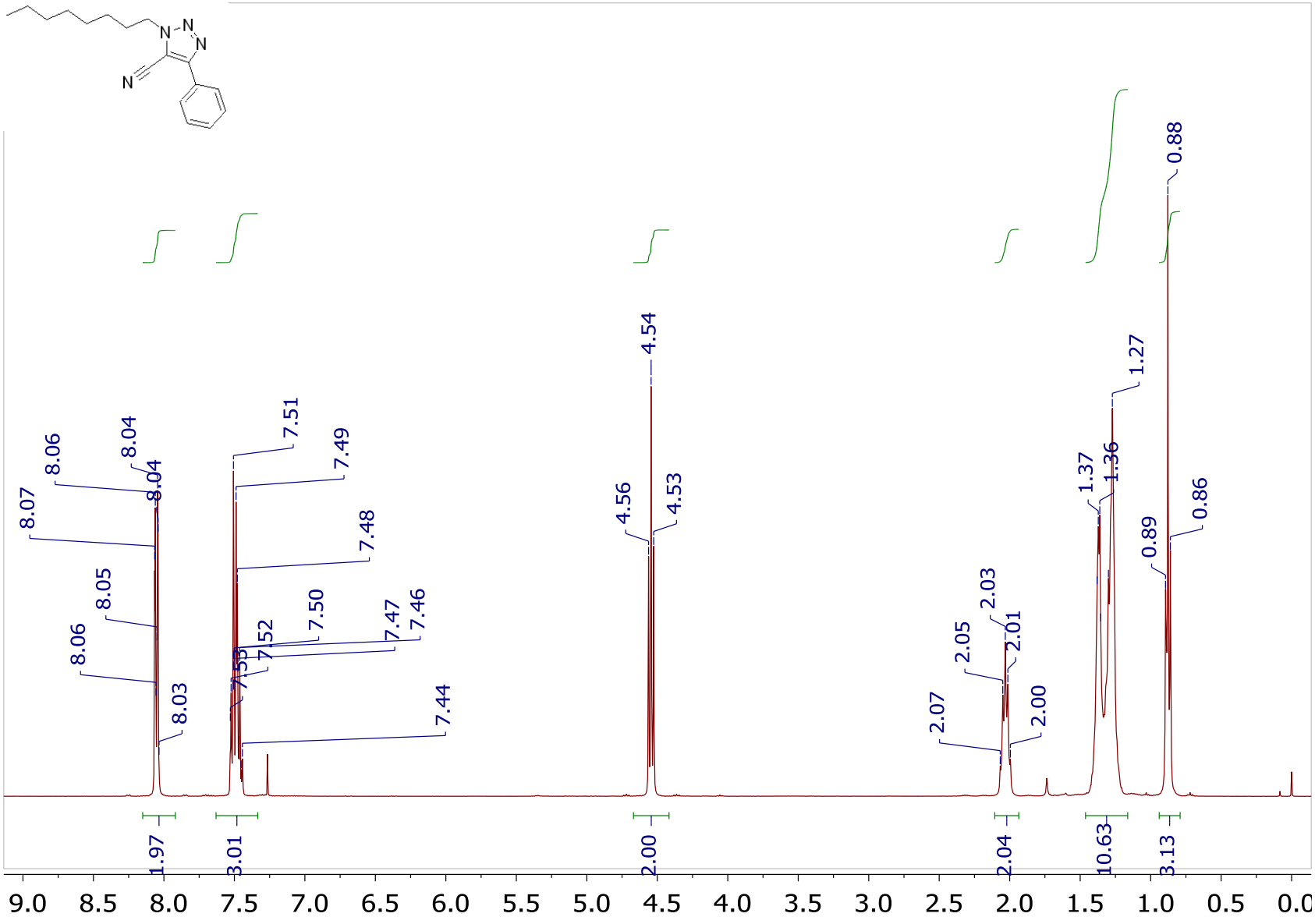
5-Cyano-4-phenyl-1-((5-phenyl-1,3,4-oxadiazol-2-yl)methyl)-1*H*-1,2,3-triazole (2f)

^{13}C NMR (101 MHz, $CDCl_3$)



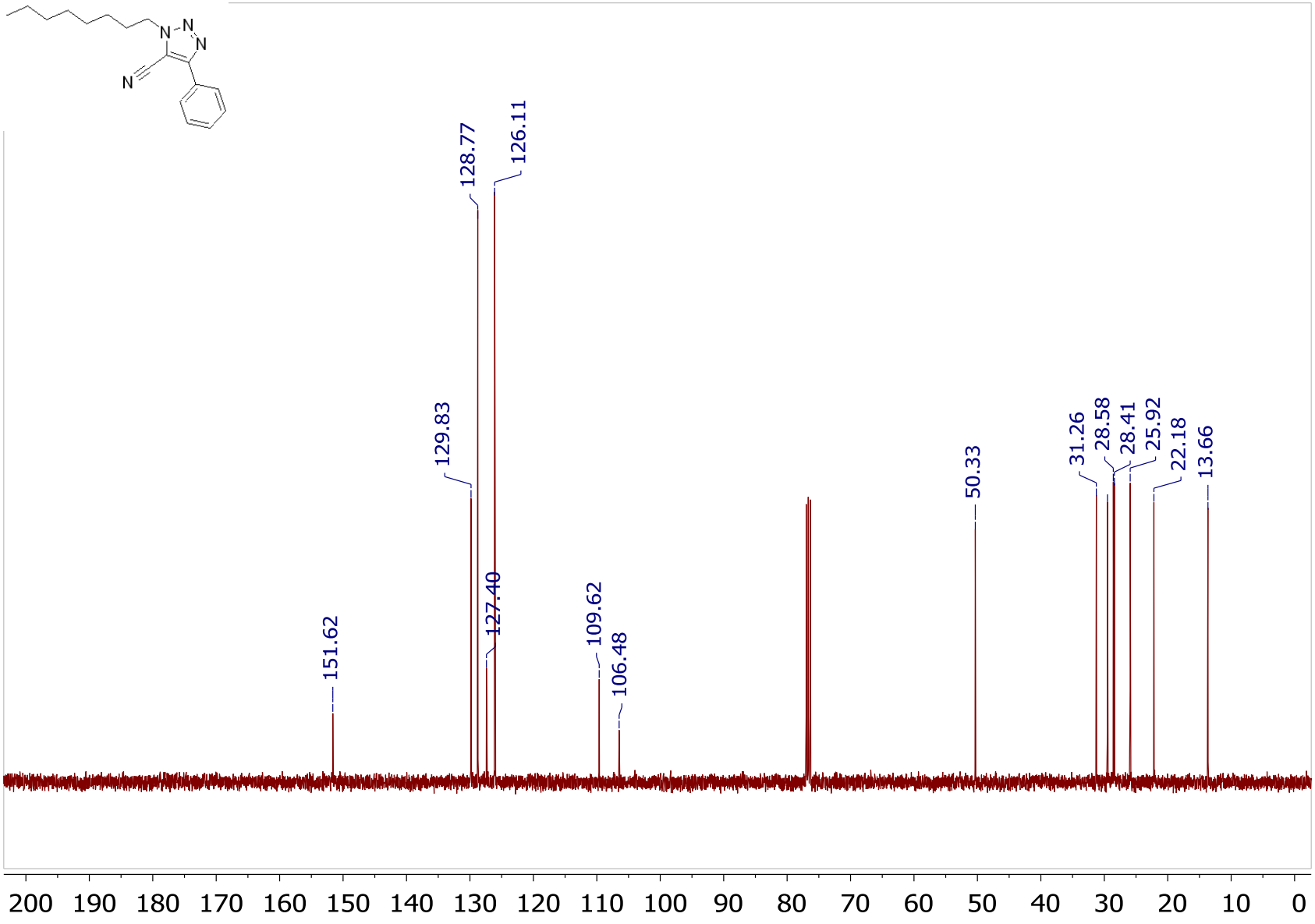
1-Octyl-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2g)

^{1}H NMR (400 MHz, $CDCl_3$)



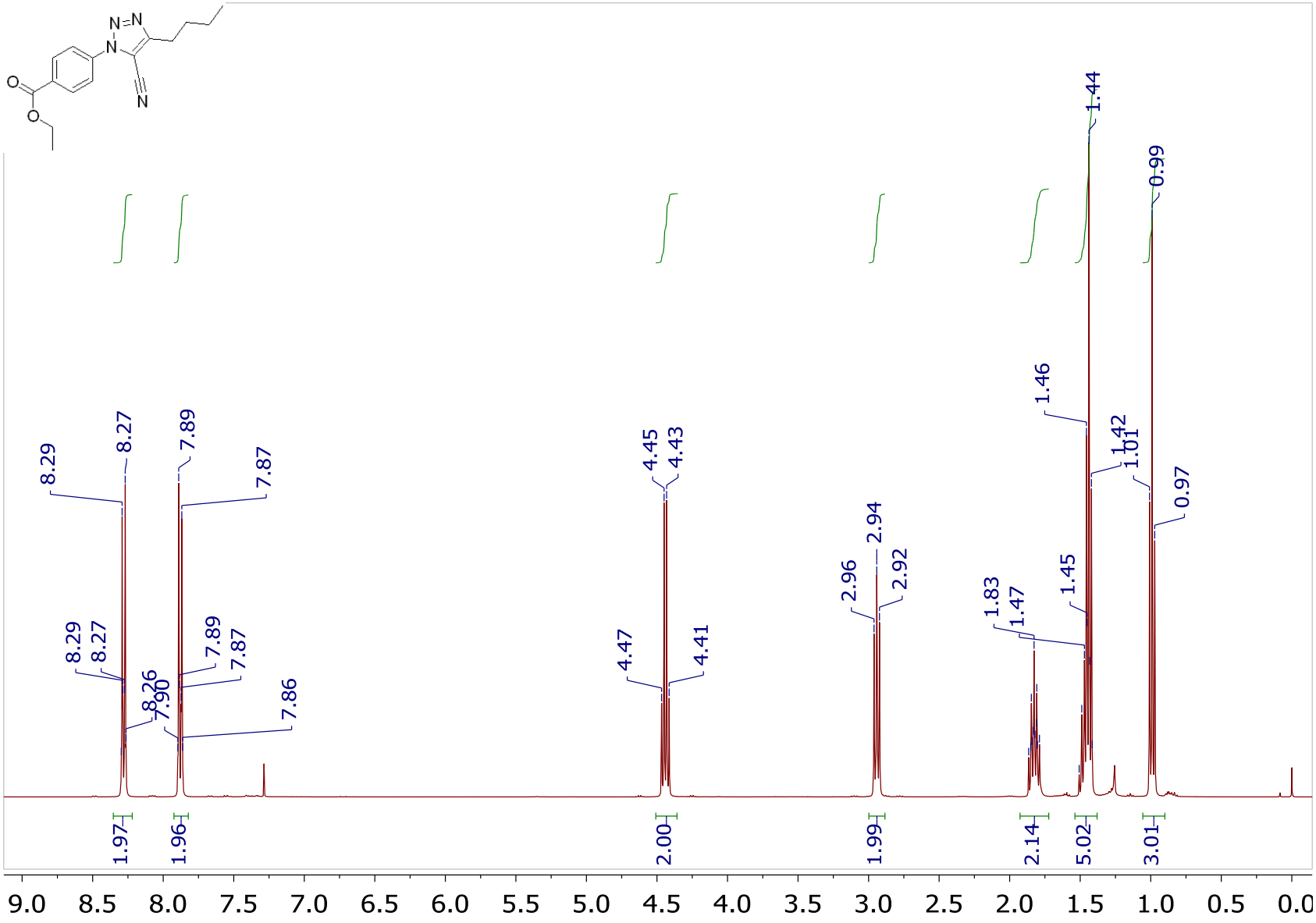
1-Octyl-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2g)

^{13}C NMR (101 MHz, $CDCl_3$)



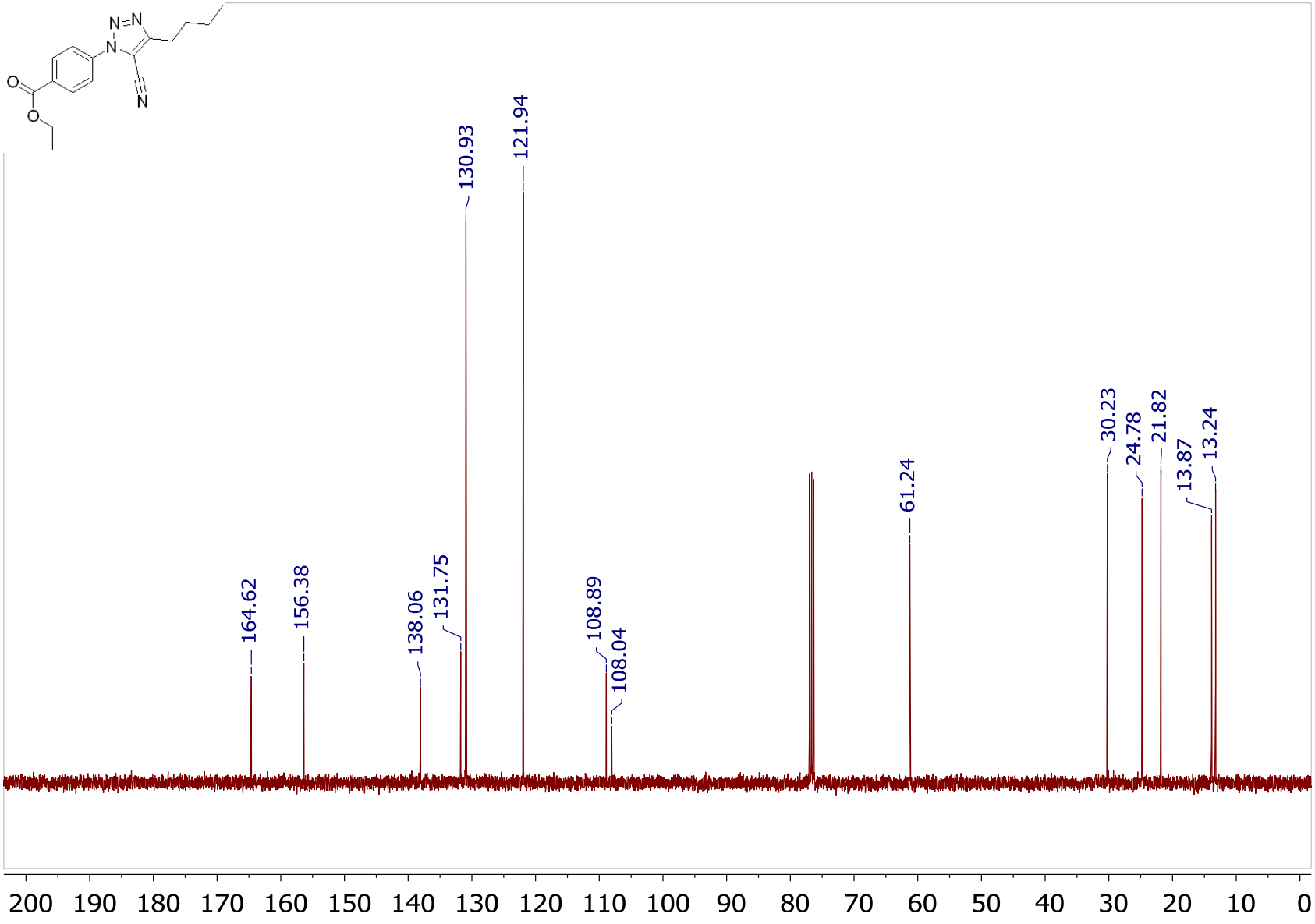
4-Butyl-1-(4-carbethoxyphenyl)-5-cyano-1*H*-1,2,3-triazole (2h)

^{1}H NMR (400 MHz, $CDCl_3$)



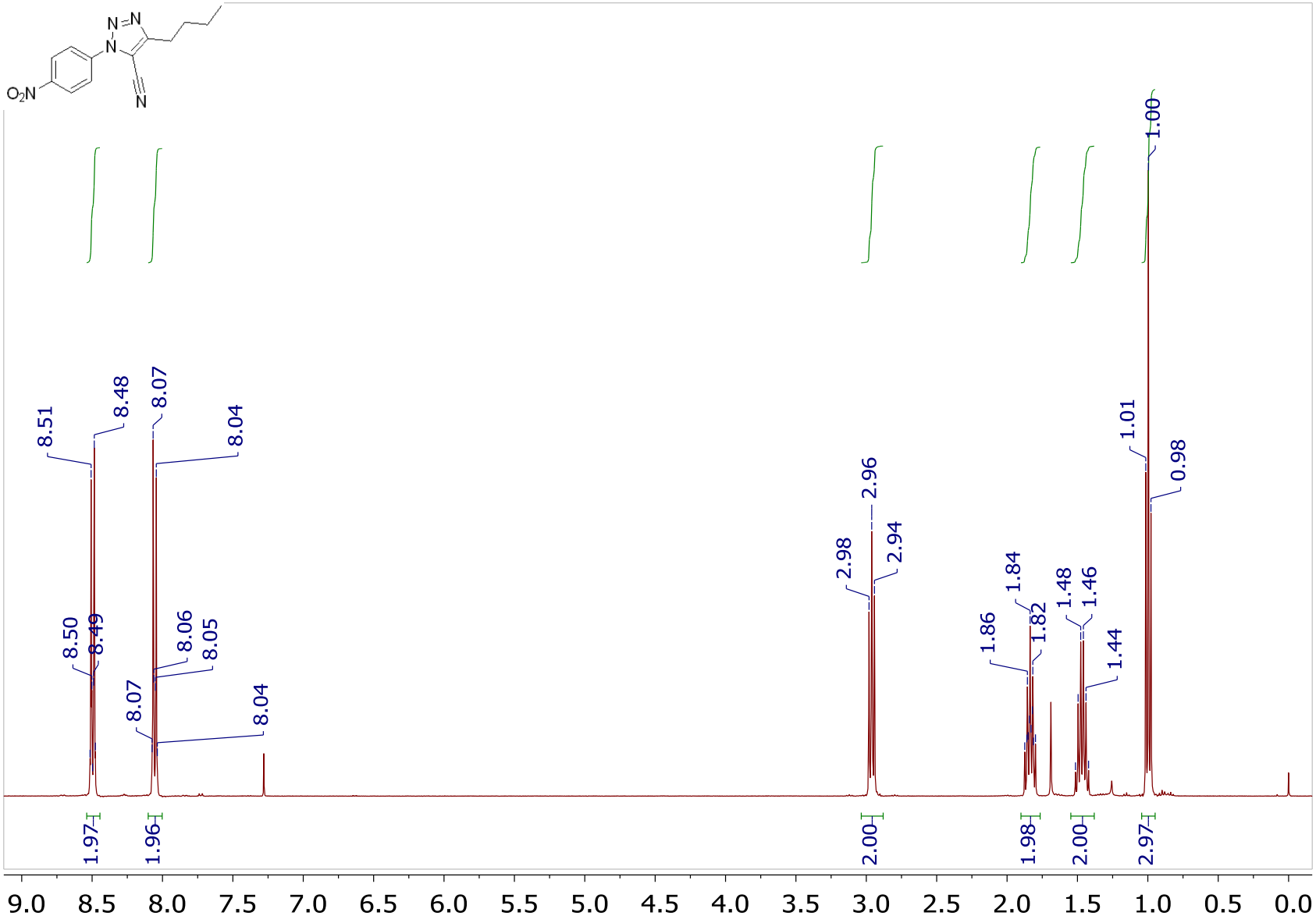
4-Butyl-1-(4-carbethoxyphenyl)-5-cyano-1*H*-1,2,3-triazole (2h)

^{13}C NMR (101 MHz, $CDCl_3$)



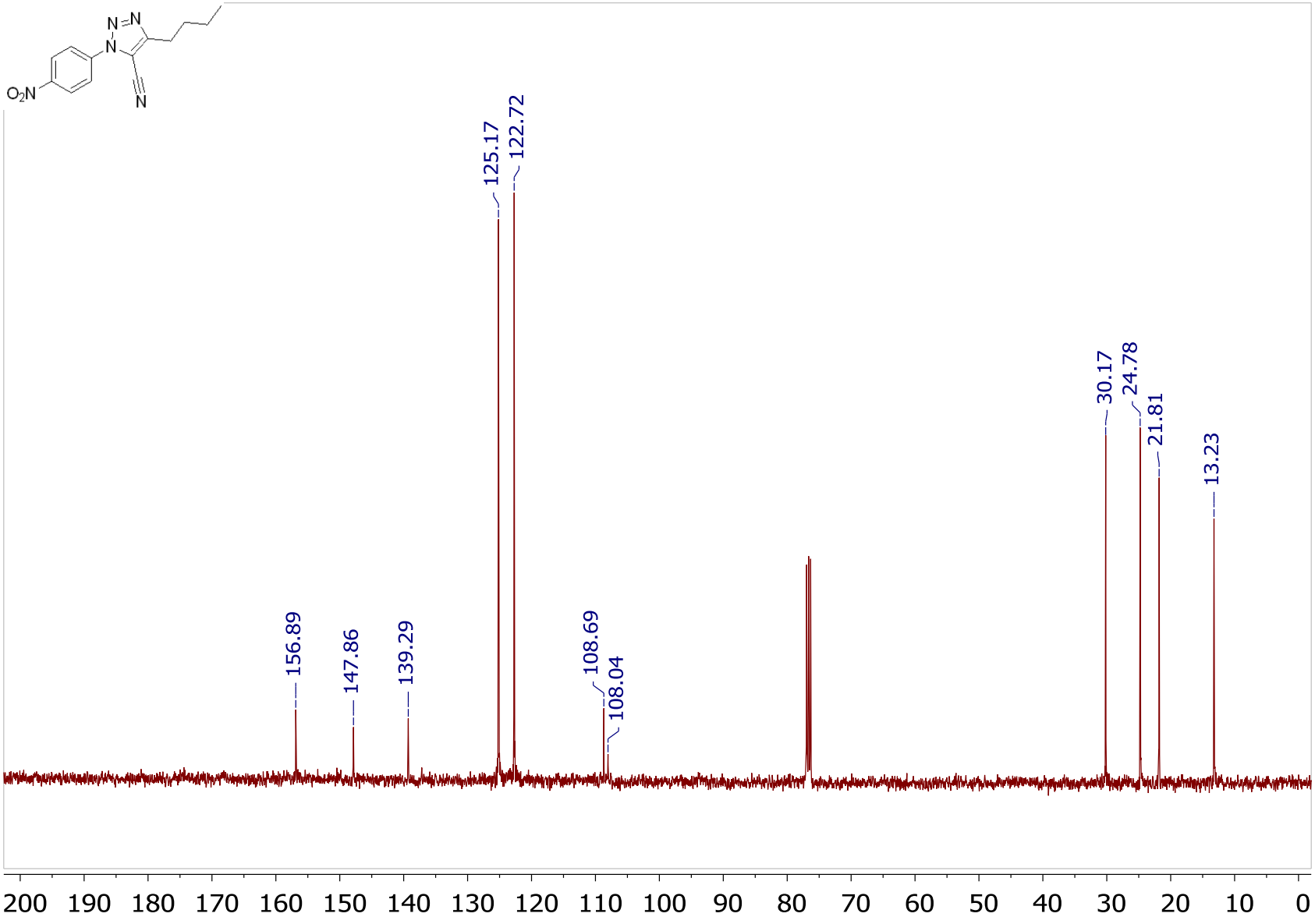
4-Butyl-5-cyano-1-(4-nitrophenyl)-1*H*-1,2,3-triazole (2i)

^{1}H NMR (400 MHz, $CDCl_3$)



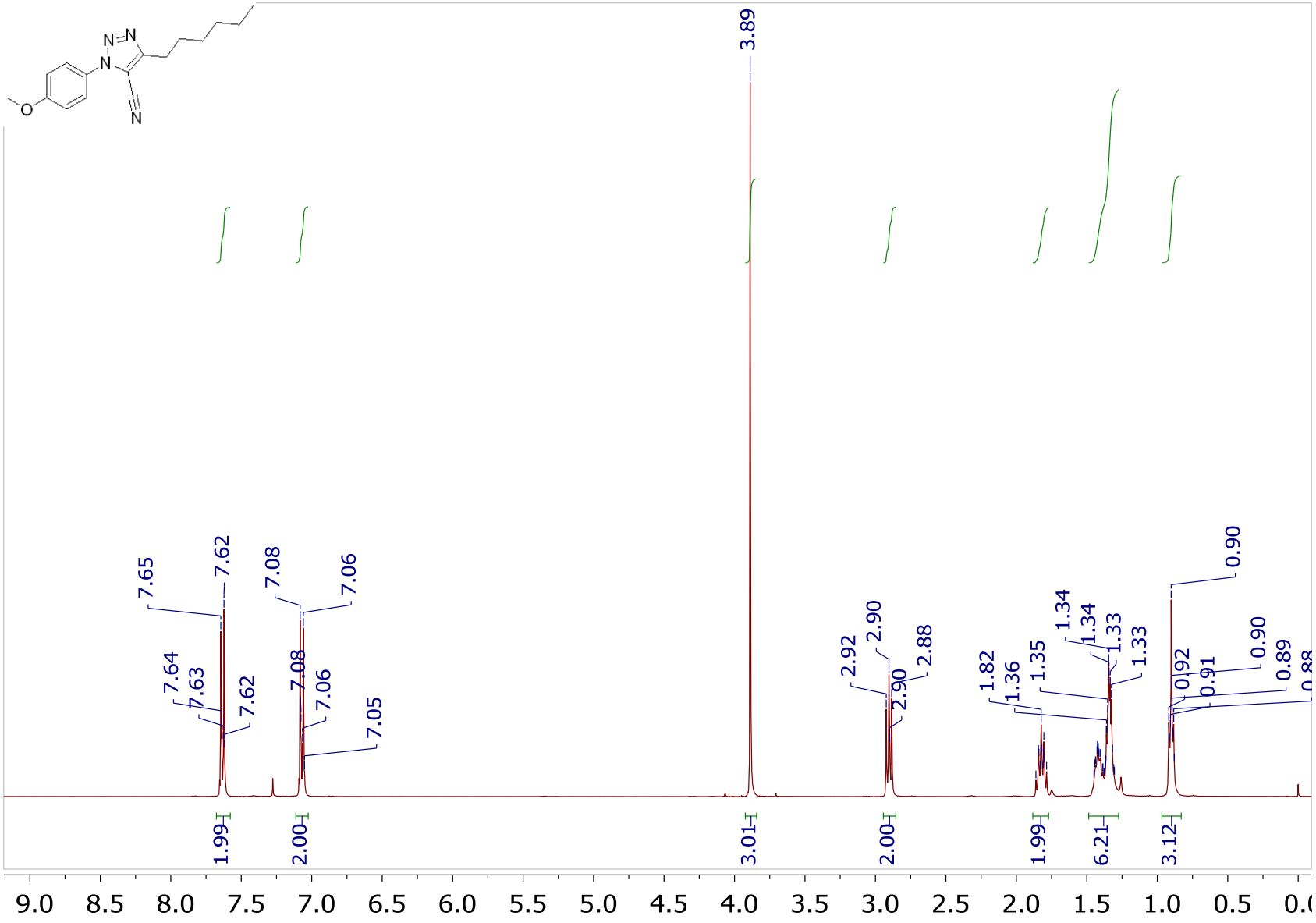
4-Butyl-5-cyano-1-(4-nitrophenyl)-1*H*-1,2,3-triazole (2i)

^{13}C NMR (101 MHz, $CDCl_3$)



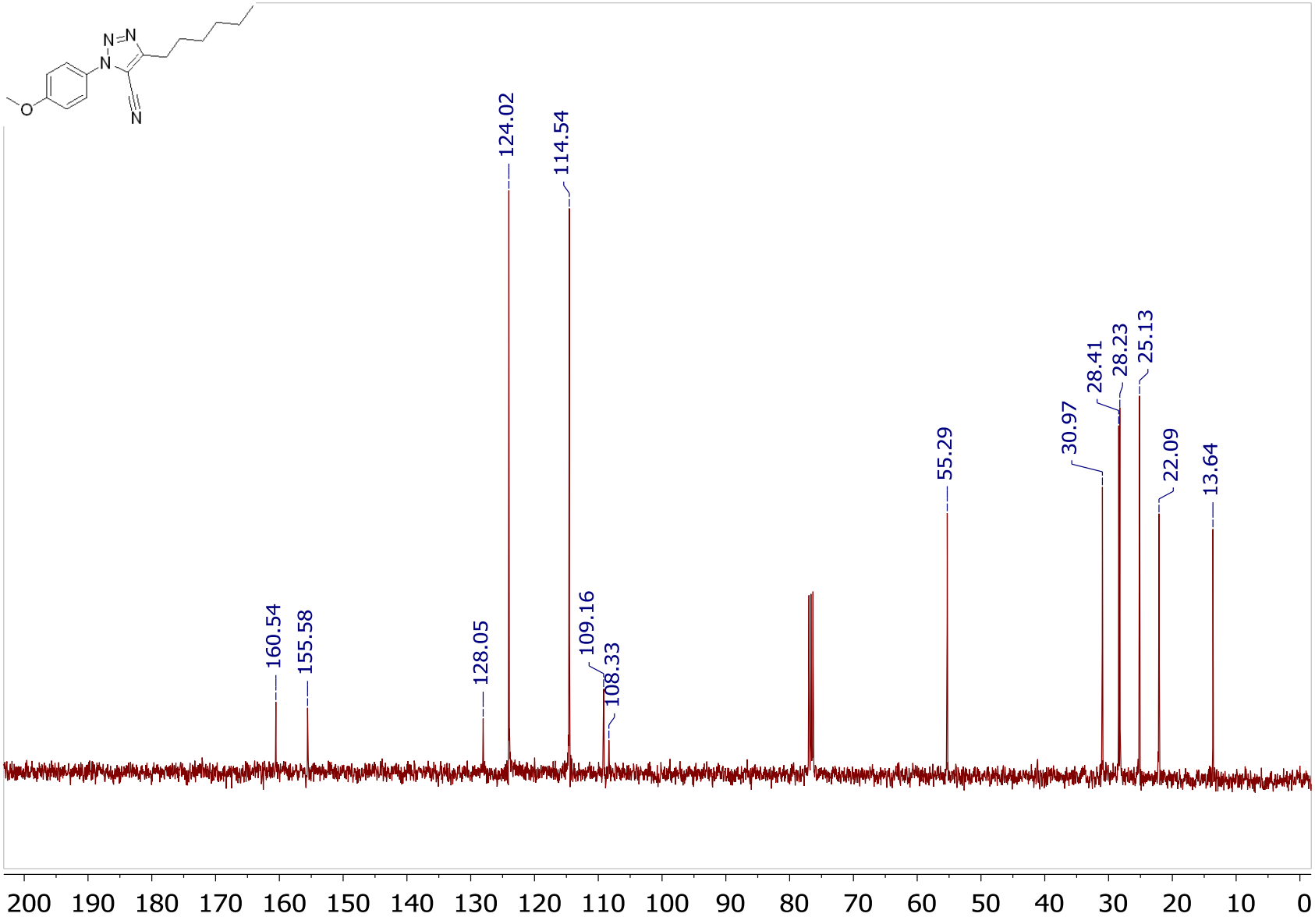
5-Cyano-4-hexyl-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (2j)

^{1}H NMR (400 MHz, $CDCl_3$)



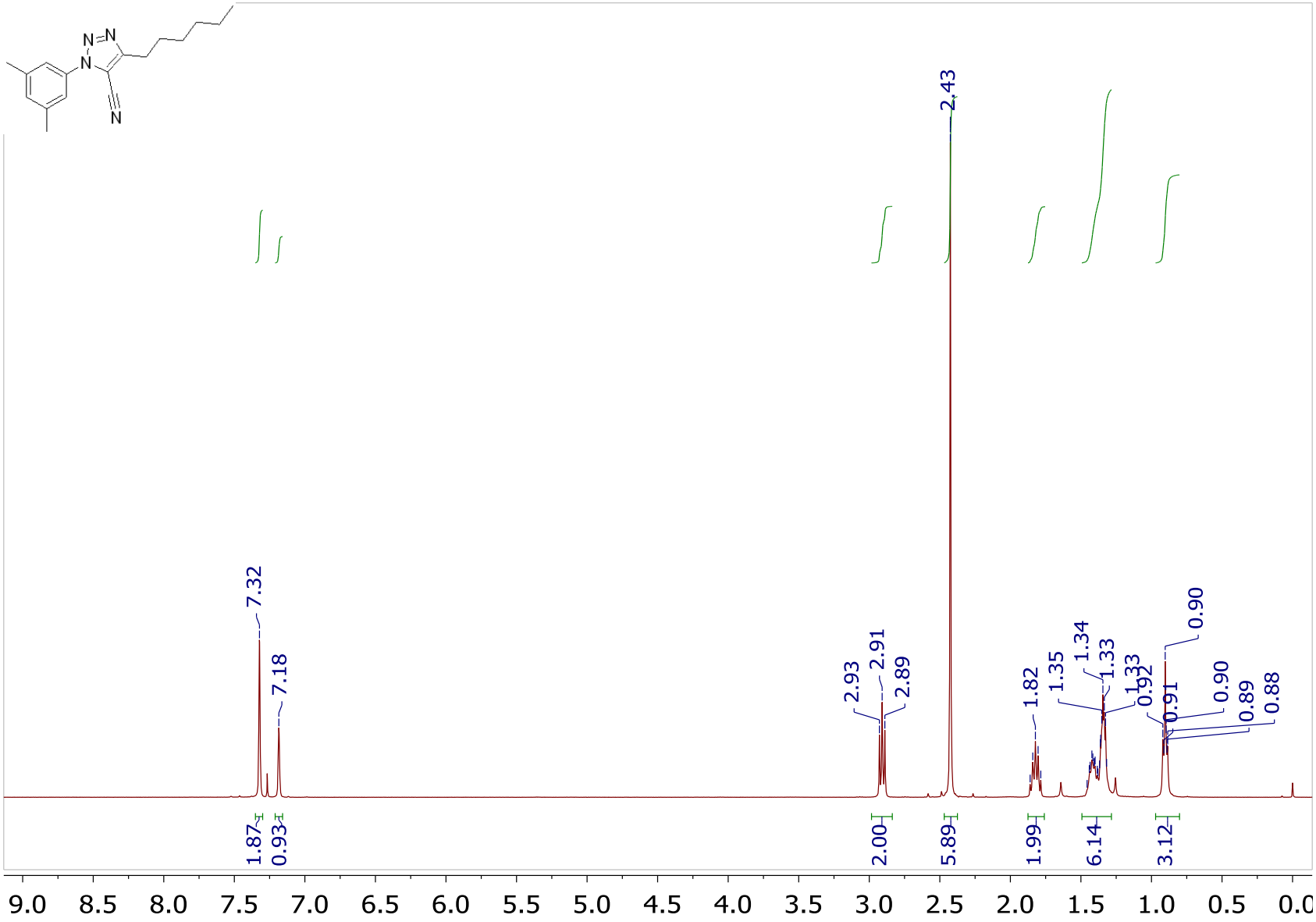
5-Cyano-4-hexyl-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (2j)

^{13}C NMR (101 MHz, $CDCl_3$)



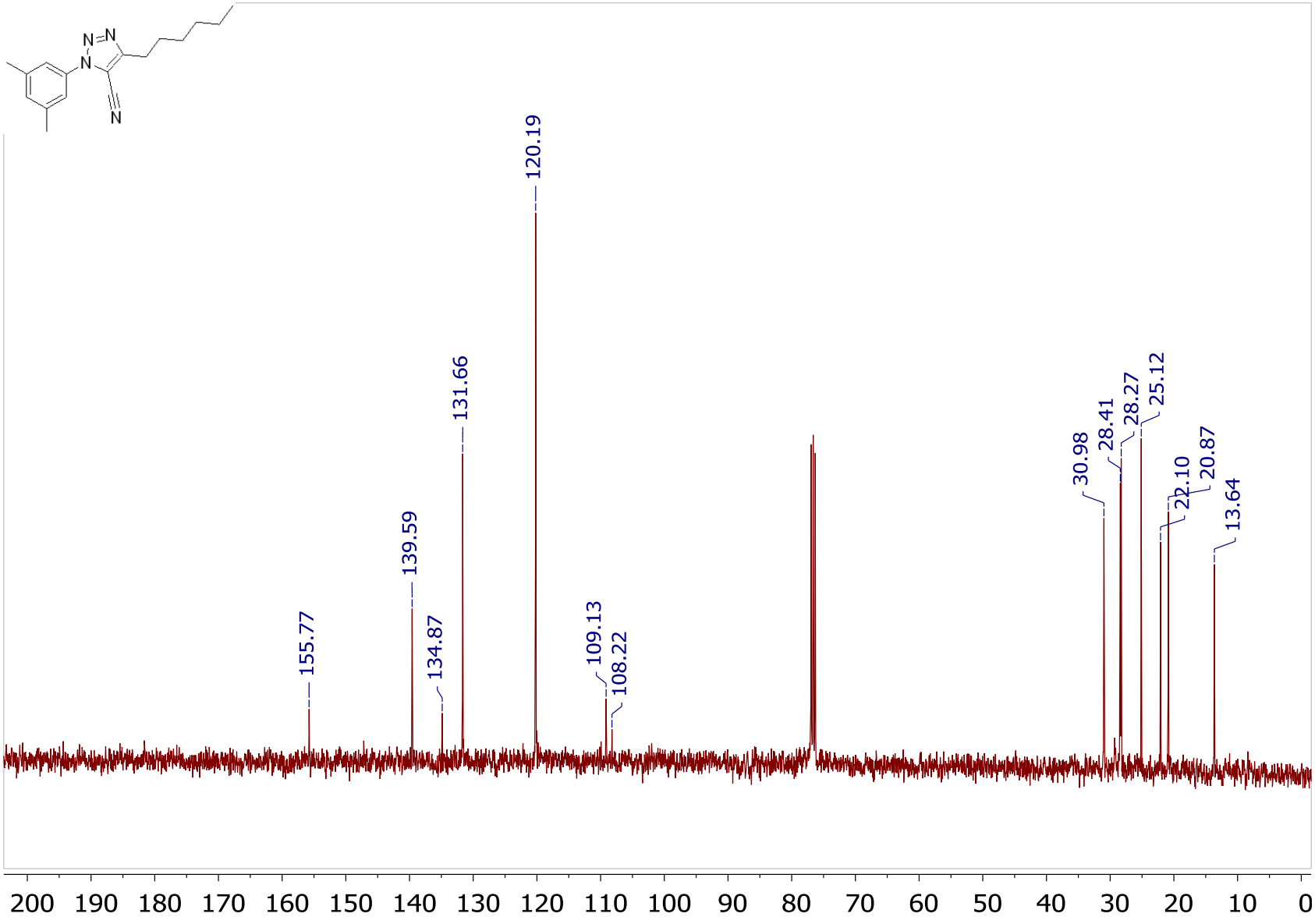
5-Cyano-1-(3,5-dimethylphenyl)-4-hexyl-1*H*-1,2,3-triazole (2k)

^{1}H NMR (400 MHz, $CDCl_3$)



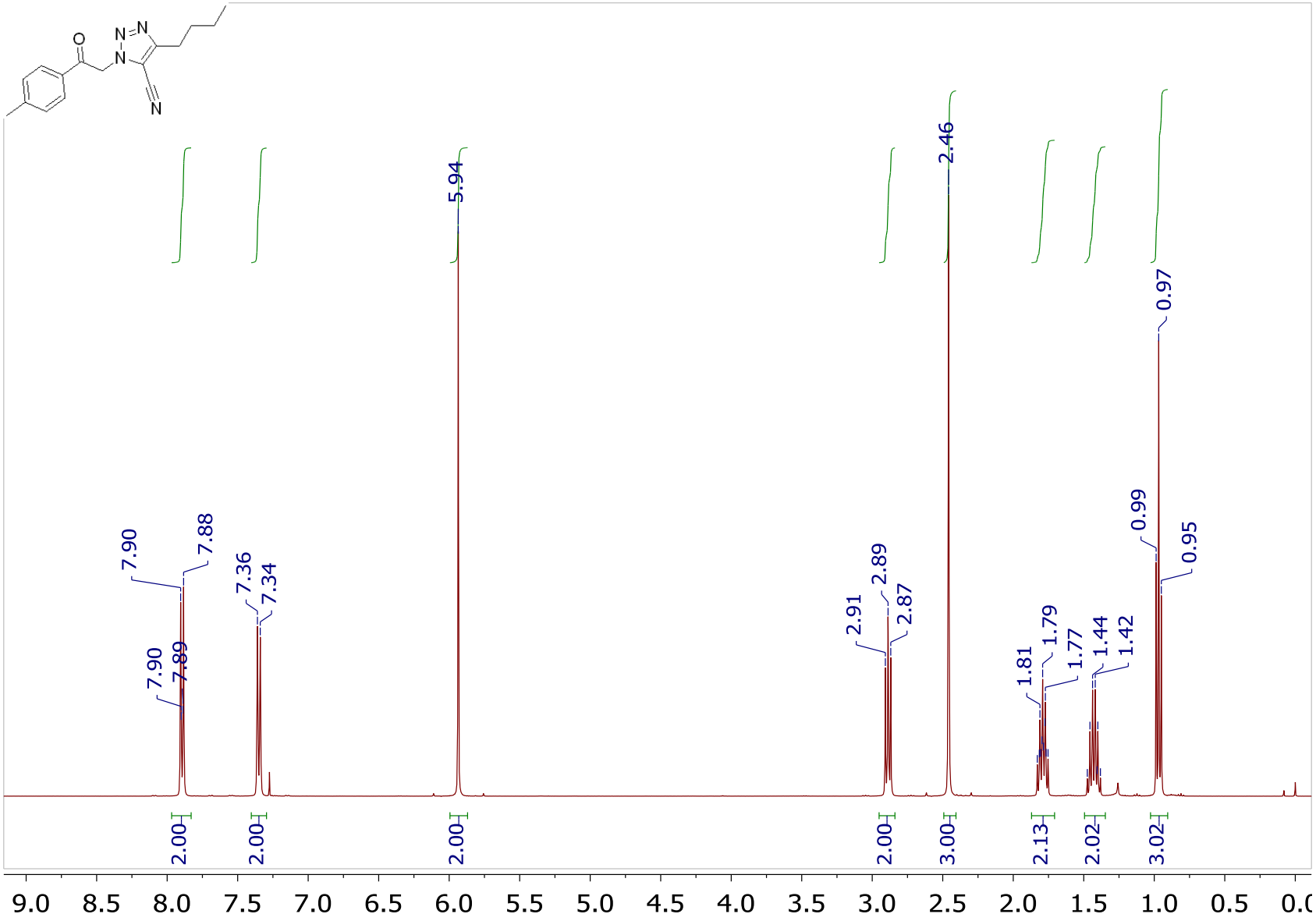
5-Cyano-1-(3,5-dimethylphenyl)-4-hexyl-1*H*-1,2,3-triazole (2k)

^{13}C NMR (101 MHz, $CDCl_3$)



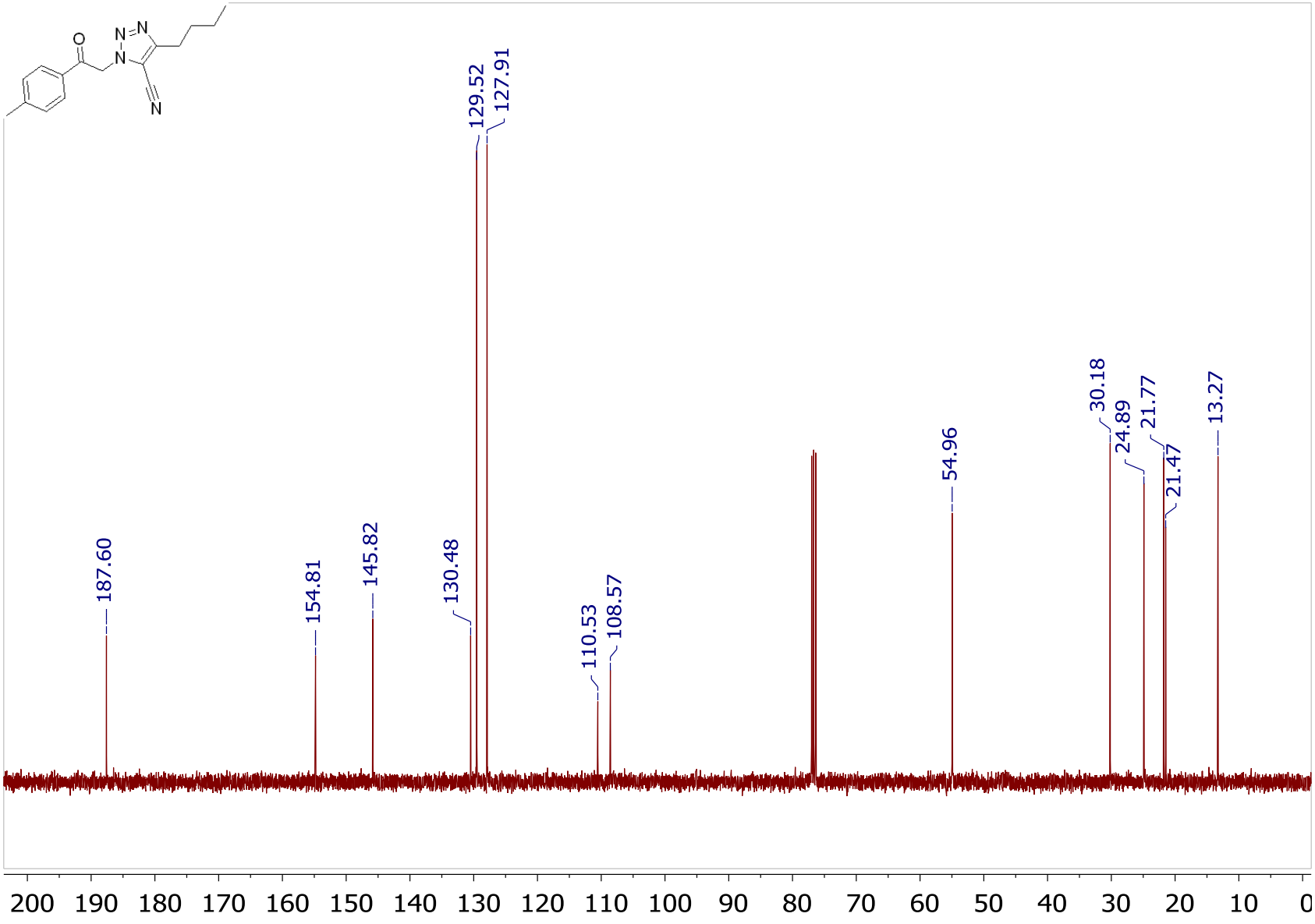
5-Cyano-4-butyl-1-(2-oxo-2-(*p*-tolyl)ethyl)-1*H*-1,2,3-triazole (2l)

^{1}H NMR (400 MHz, $CDCl_3$)



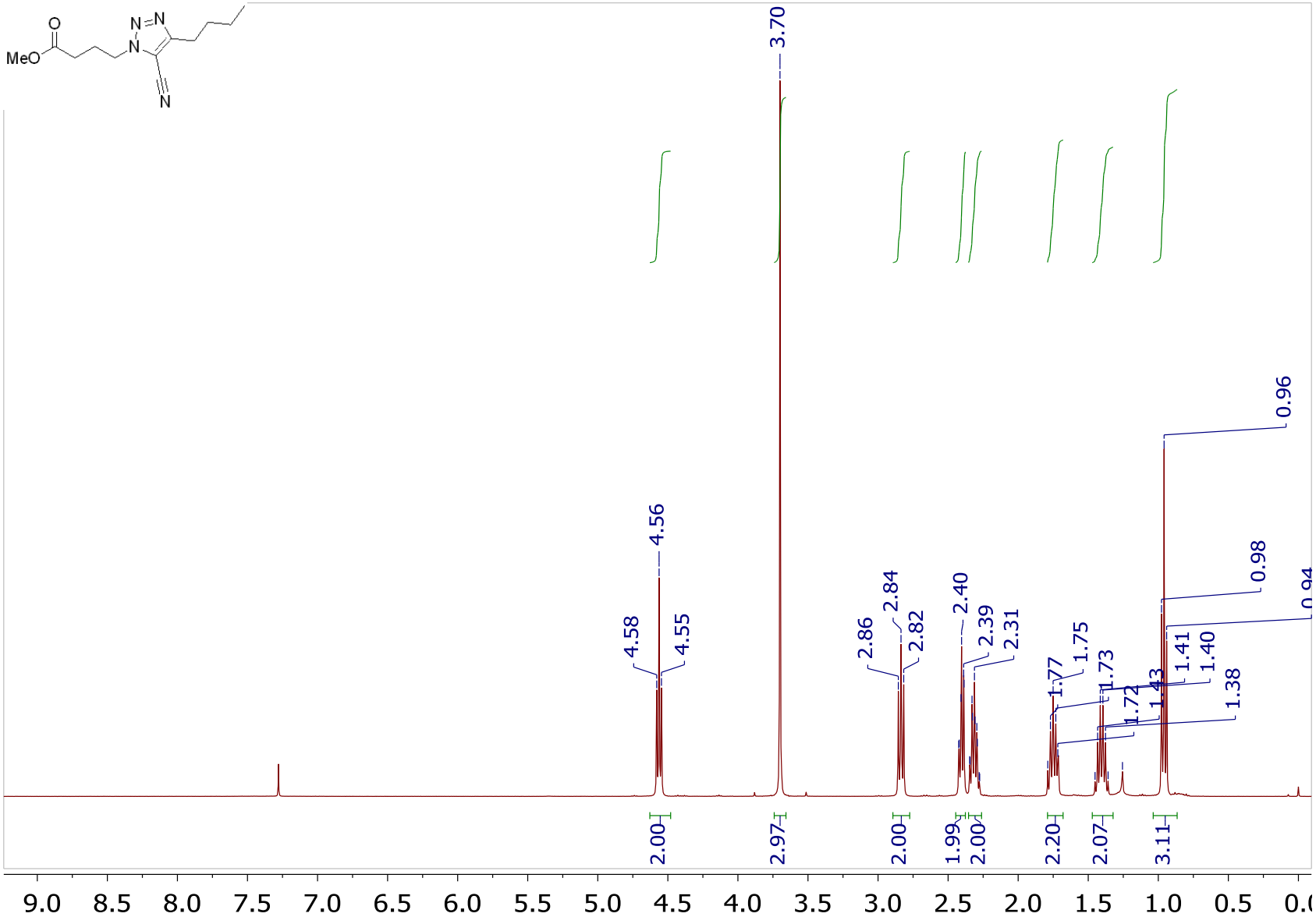
5-Cyano-4-butyl-1-(2-oxo-2-(*p*-tolyl)ethyl)-1*H*-1,2,3-triazole (2l)

^{13}C NMR (101 MHz, $CDCl_3$)



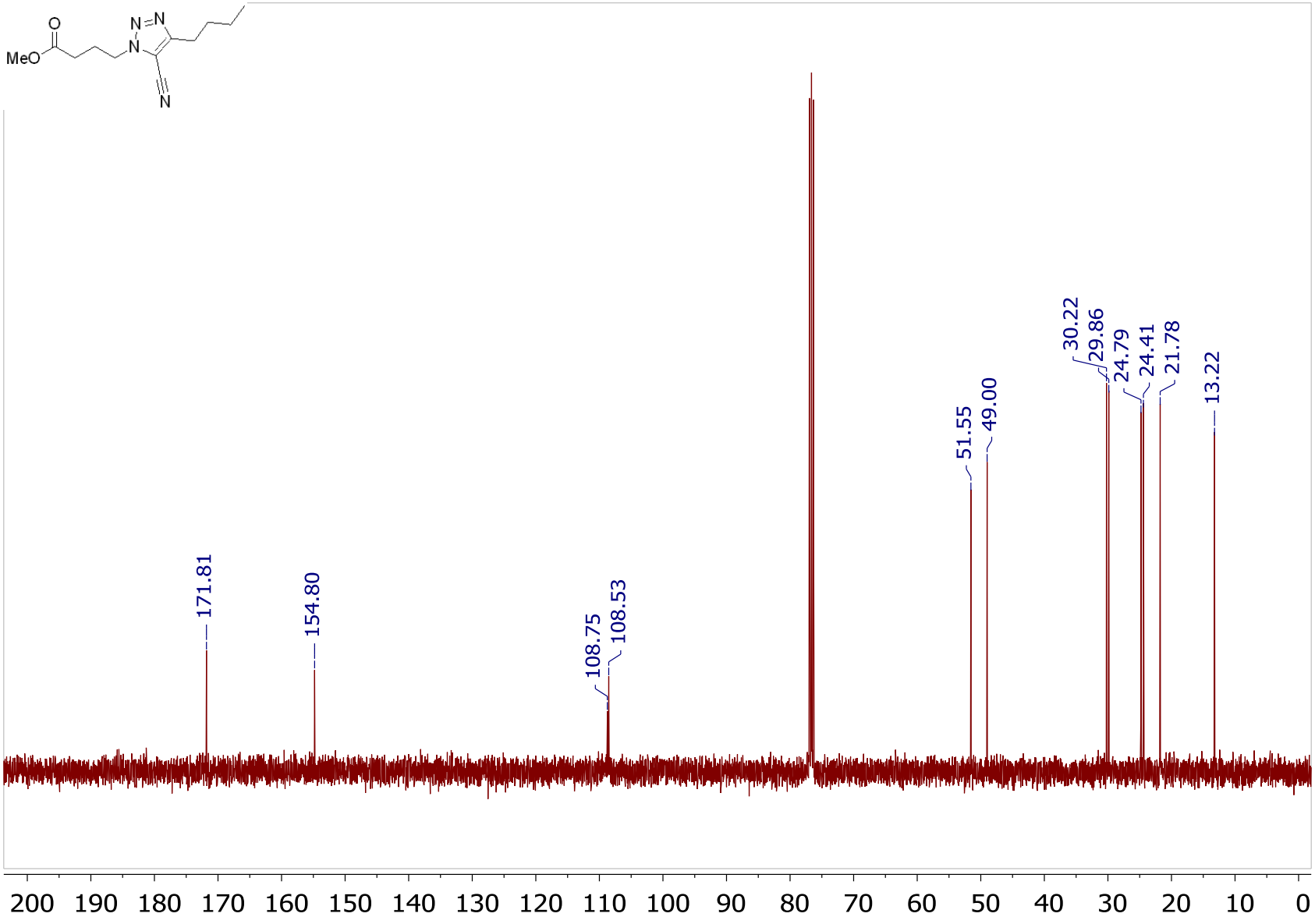
Methyl 4-(4-butyl-5-cyano-1*H*-1,2,3-triazol-1-yl)butanoate (2m)

^{1}H NMR (400 MHz, $CDCl_3$)



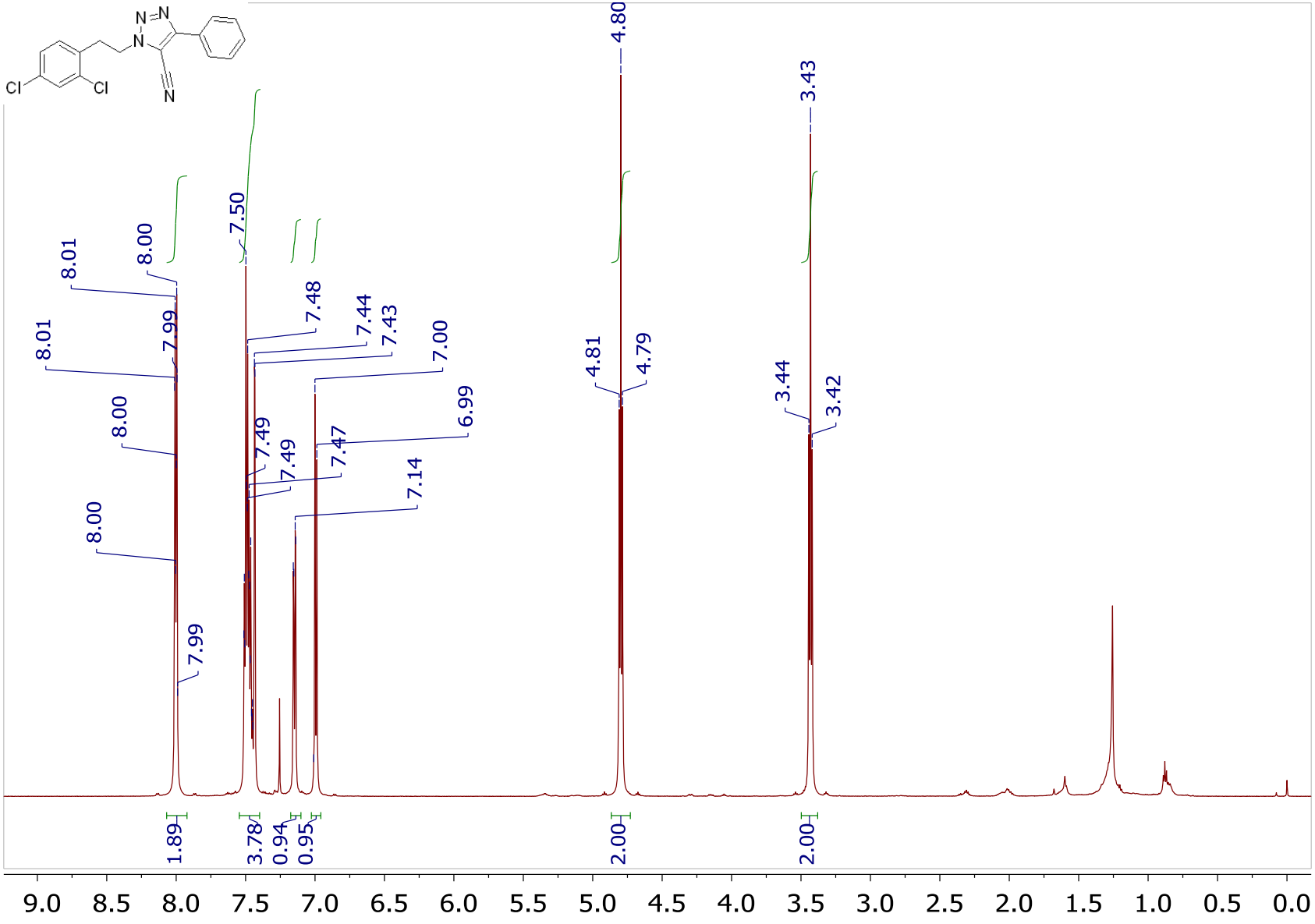
Methyl 4-(4-butyl-5-cyano-1*H*-1,2,3-triazol-1-yl)butanoate (2m)

^{13}C NMR (101 MHz, $CDCl_3$)



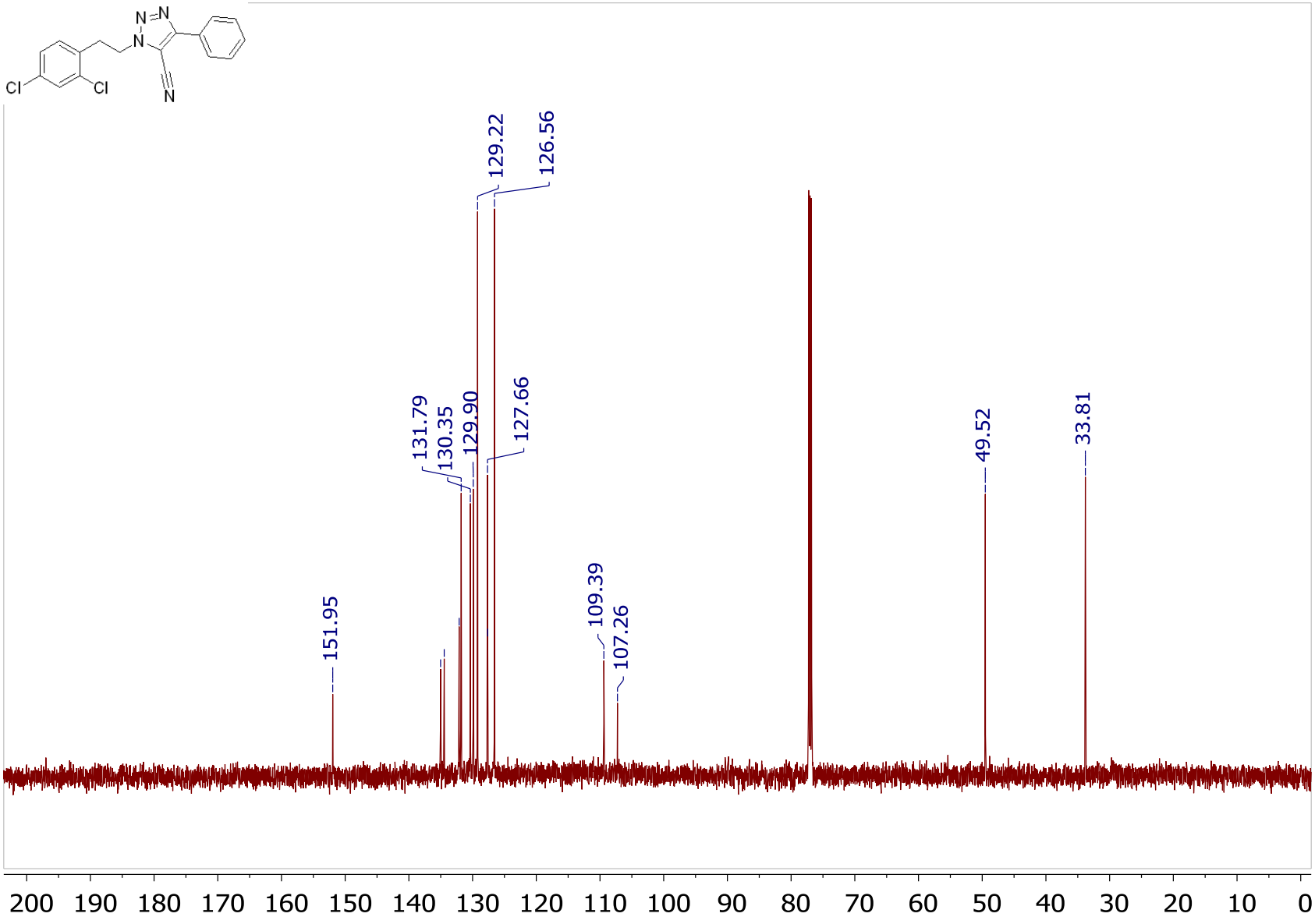
1-(2,4-Dichlorophenethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2n)

^{1}H NMR (600 MHz, $CDCl_3$)



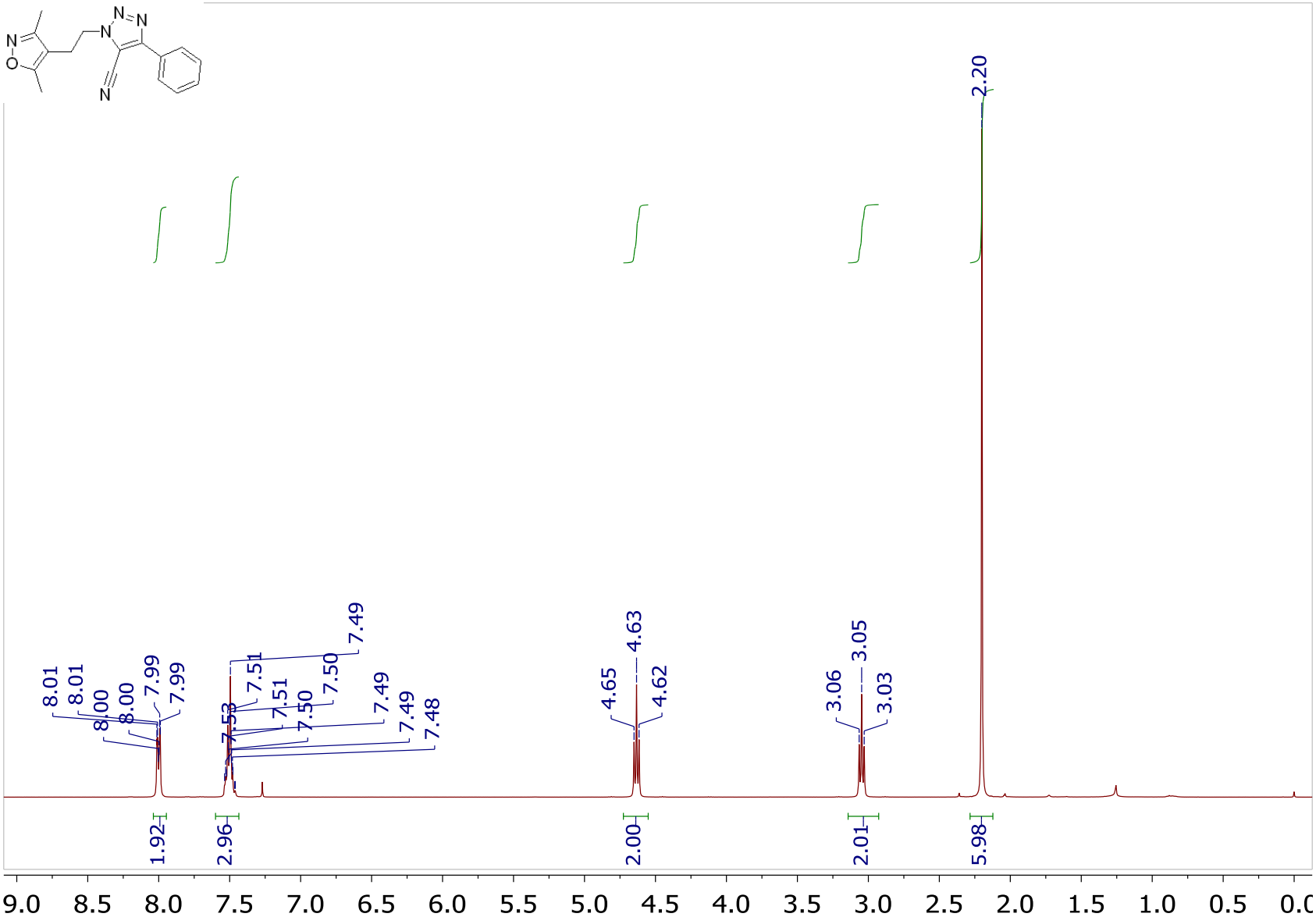
1-(2,4-Dichlorophenethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2n)

^{13}C NMR (151 MHz, $CDCl_3$)



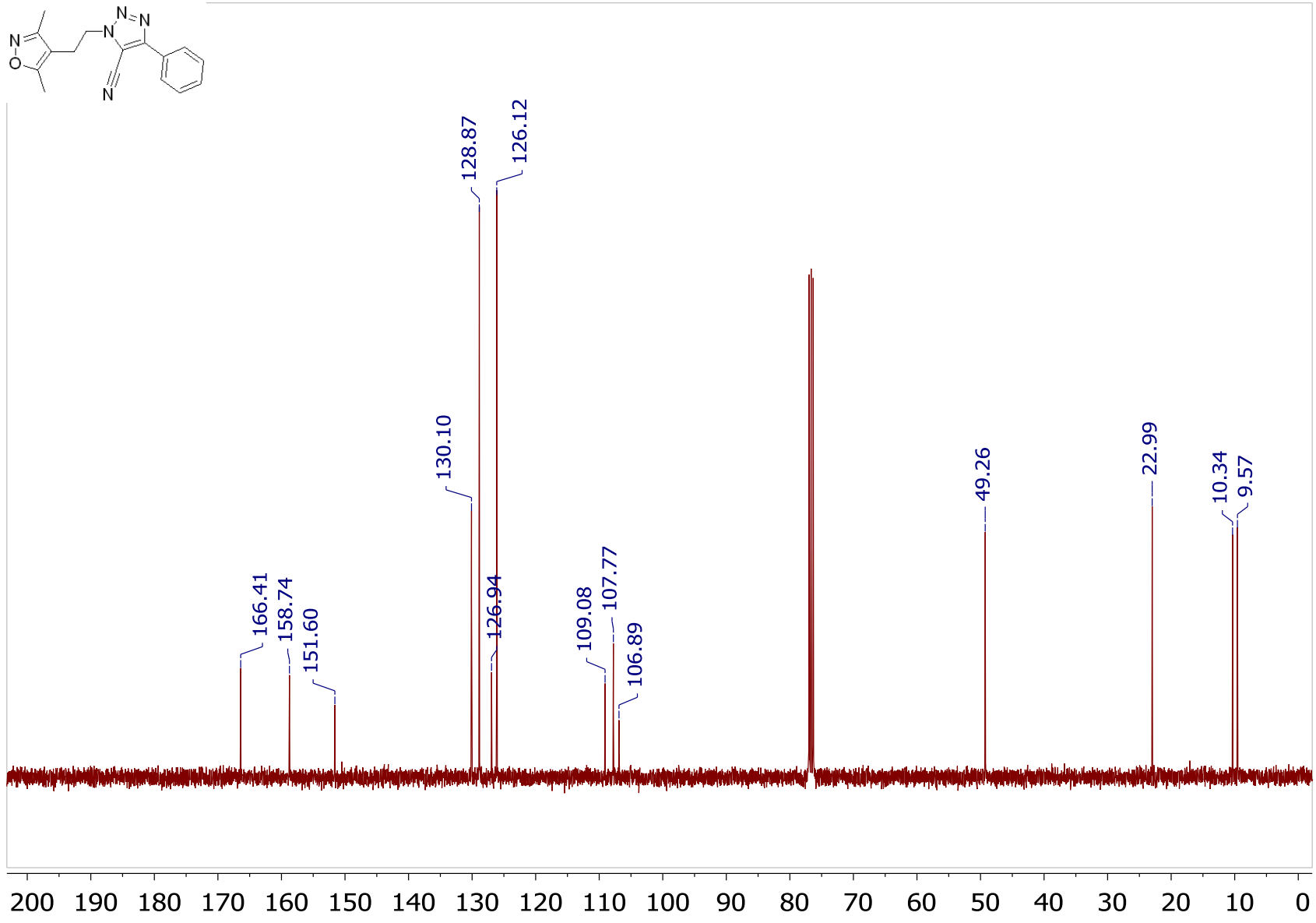
4-(2-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-3,5-dimethylisoxazole (2o)

^{1}H NMR (400 MHz, $CDCl_3$)



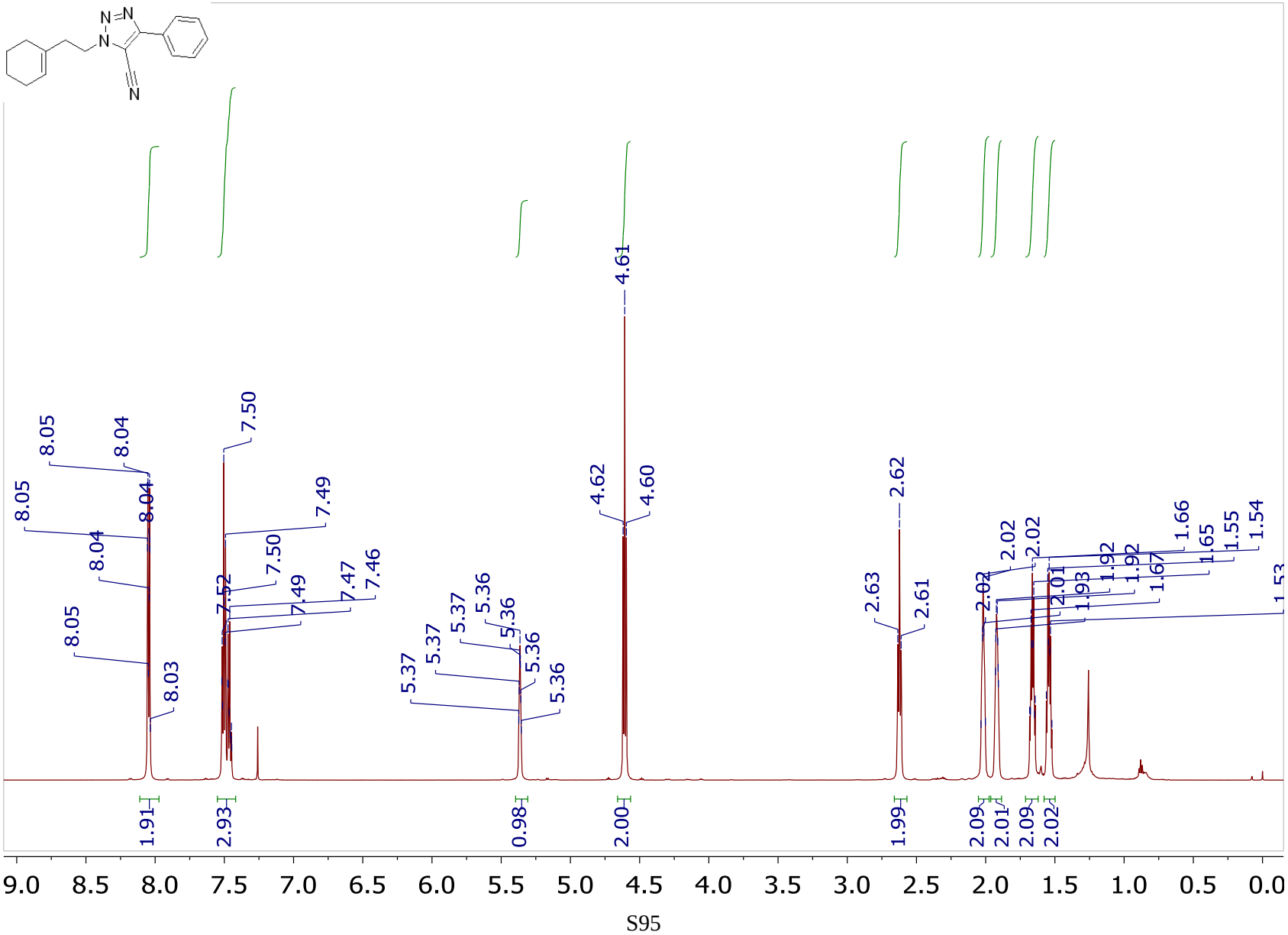
4-(2-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-3,5-dimethylisoxazole (2o)

^{13}C NMR (101 MHz, $CDCl_3$)



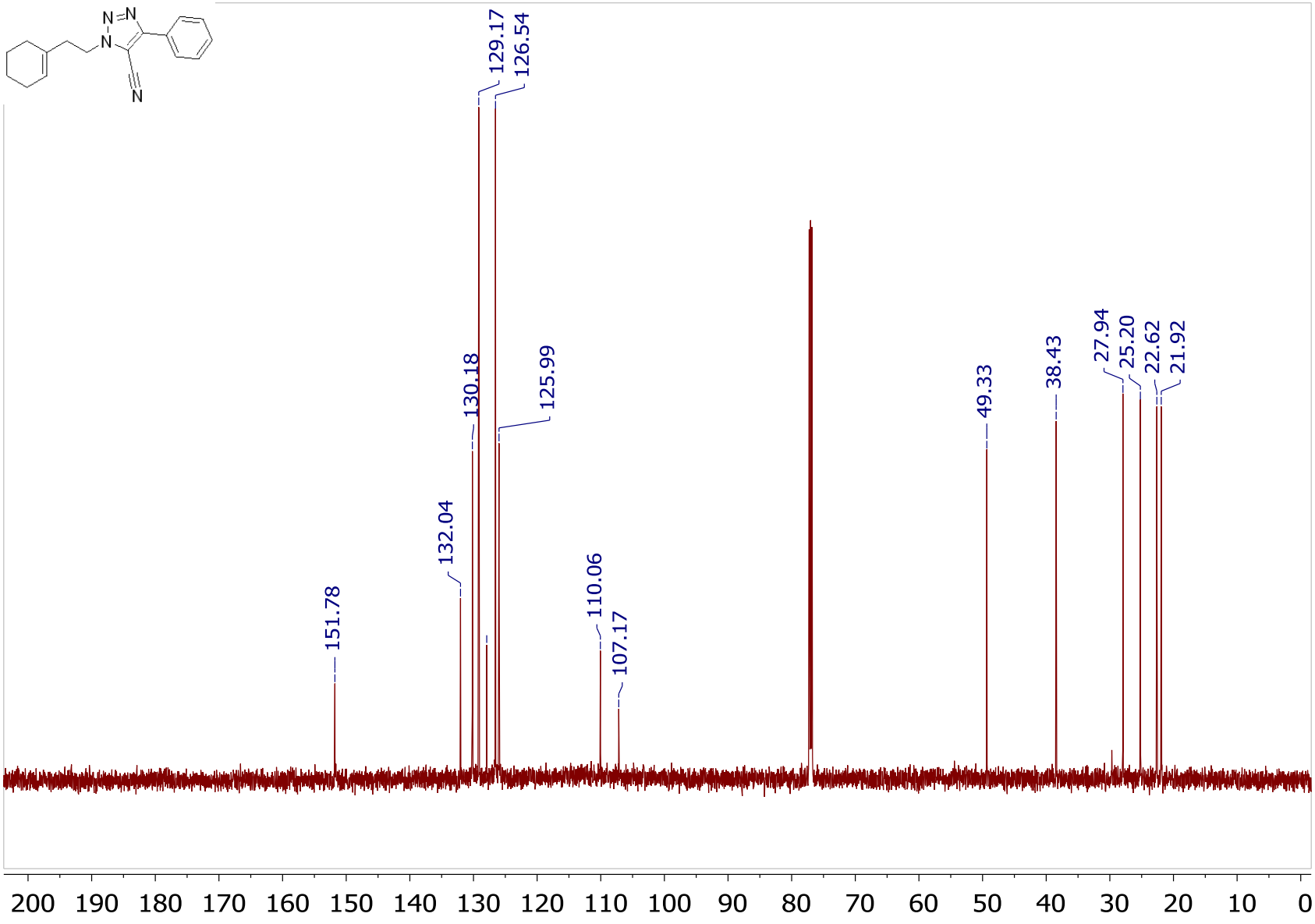
1-(2-(Cyclohex-1-en-1-yl)ethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2p)

^{1}H NMR (600 MHz, $CDCl_3$)



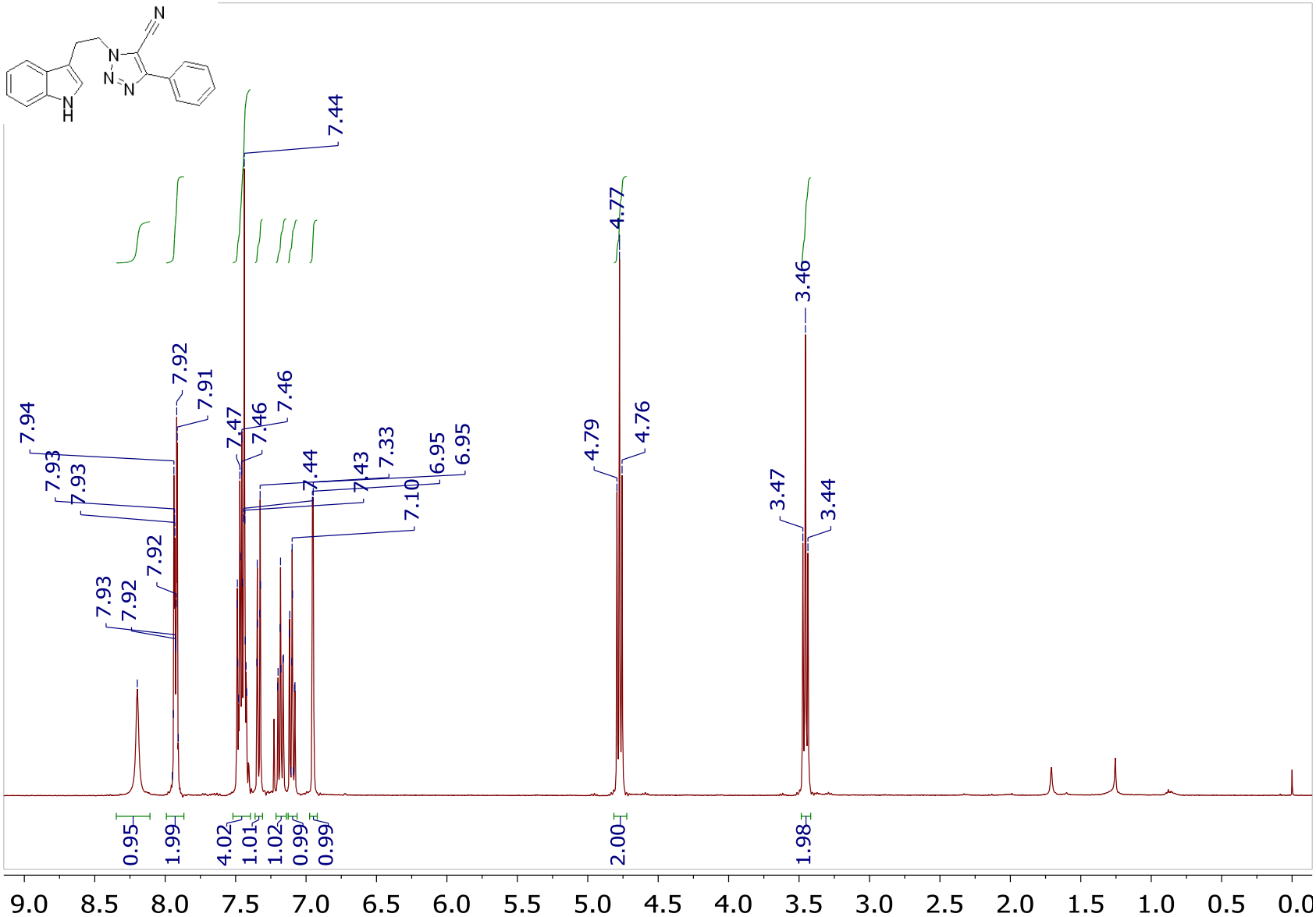
1-(2-(Cyclohex-1-en-1-yl)ethyl)-5-cyano-4-phenyl-1*H*-1,2,3-triazole (2p)

^{13}C NMR (151 MHz, $CDCl_3$)



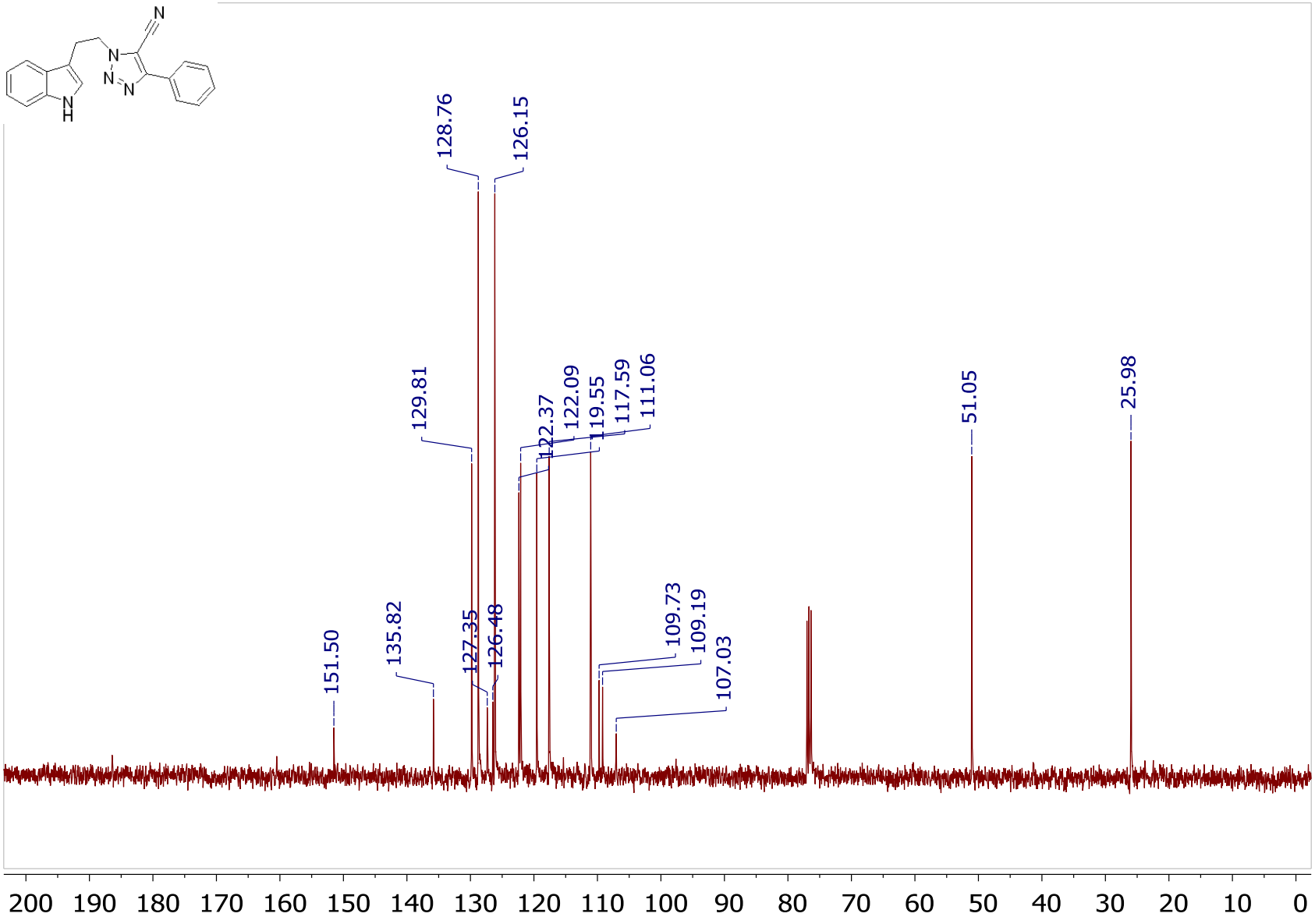
3-(2-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-indole (2q)

^{1}H NMR (400 MHz, $CDCl_3$)



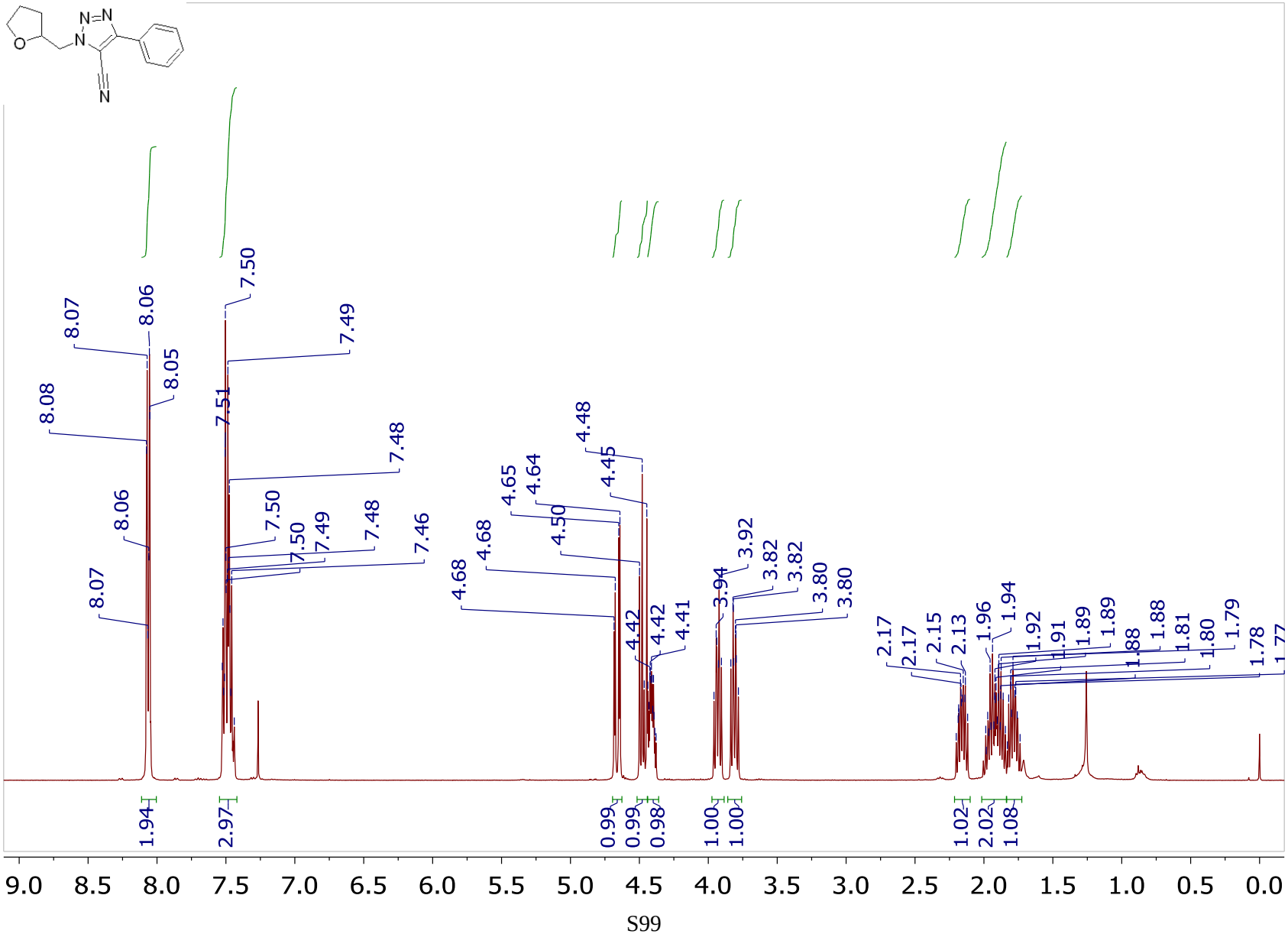
3-(2-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-indole (2q)

^{13}C NMR (101 MHz, $CDCl_3$)



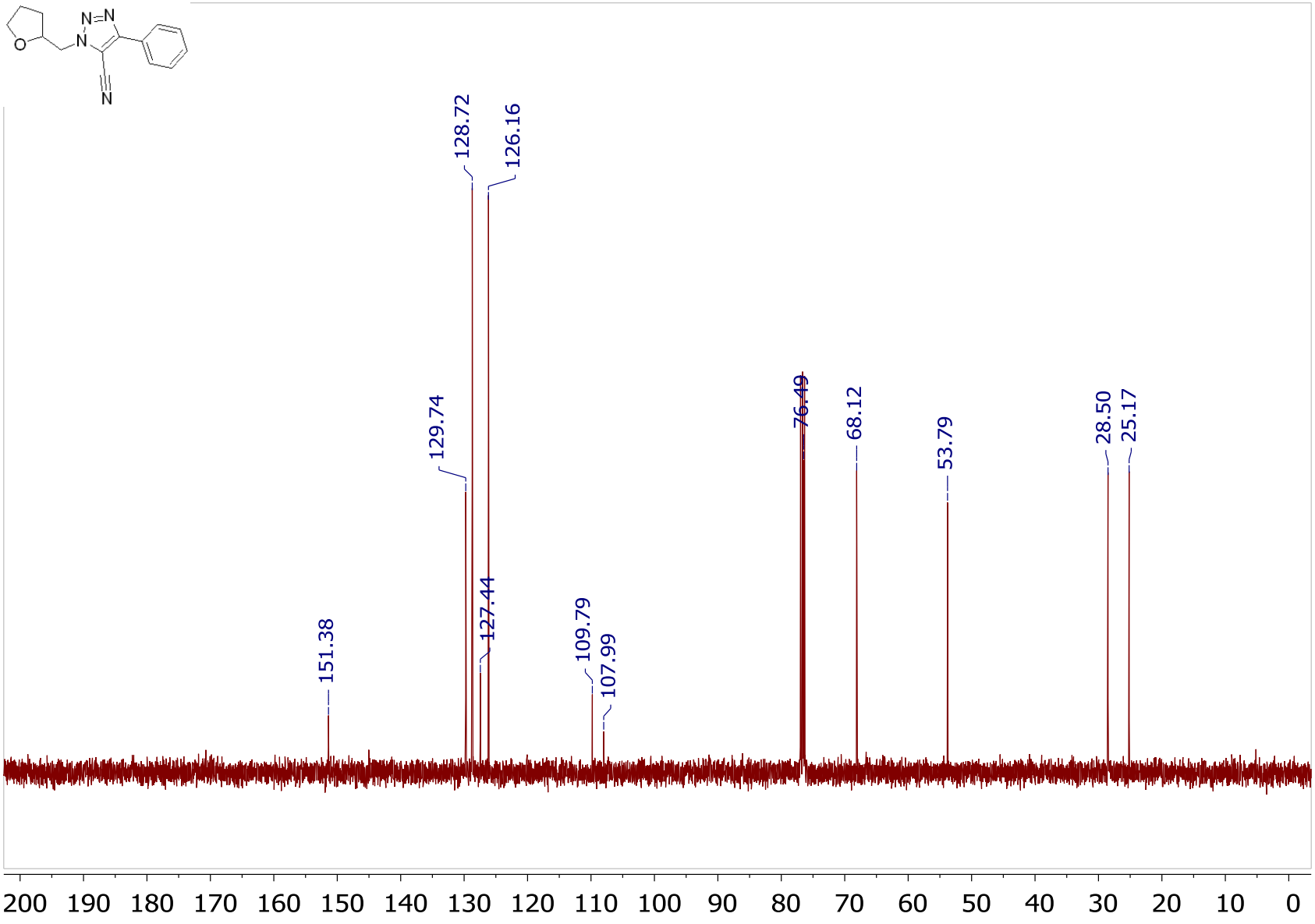
5-Cyano-4-phenyl-1-((tetrahydrofuran-2-yl)methyl)-1*H*-1,2,3-triazole (2r)

^{1}H NMR (400 MHz, $CDCl_3$)



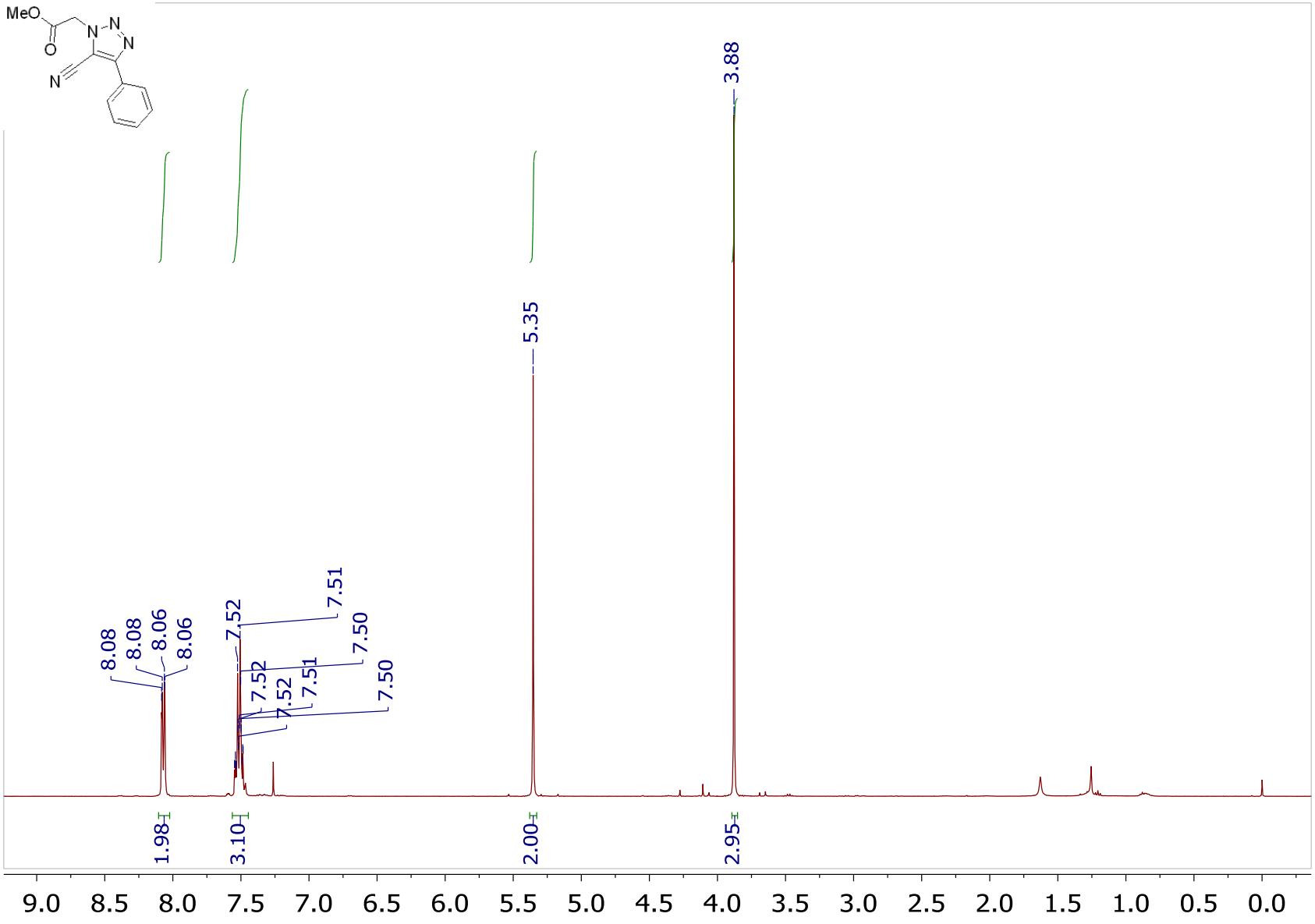
5-Cyano-4-phenyl-1-((tetrahydrofuran-2-yl)methyl)-1*H*-1,2,3-triazole (2r)

^{13}C NMR (101 MHz, $CDCl_3$)



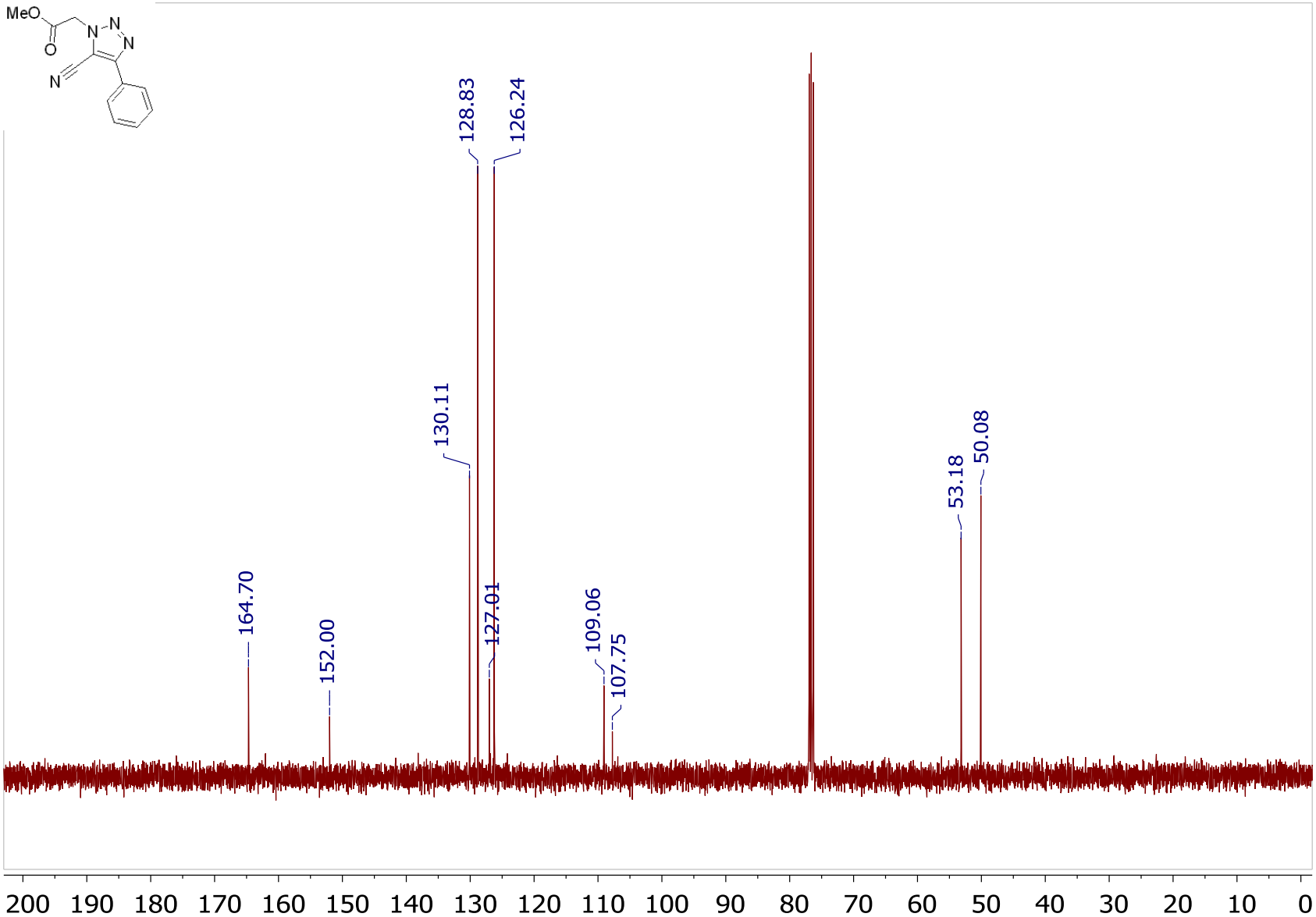
Methyl 2-(5-cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)acetate (2s)

^{1}H NMR (400 MHz, $CDCl_3$)



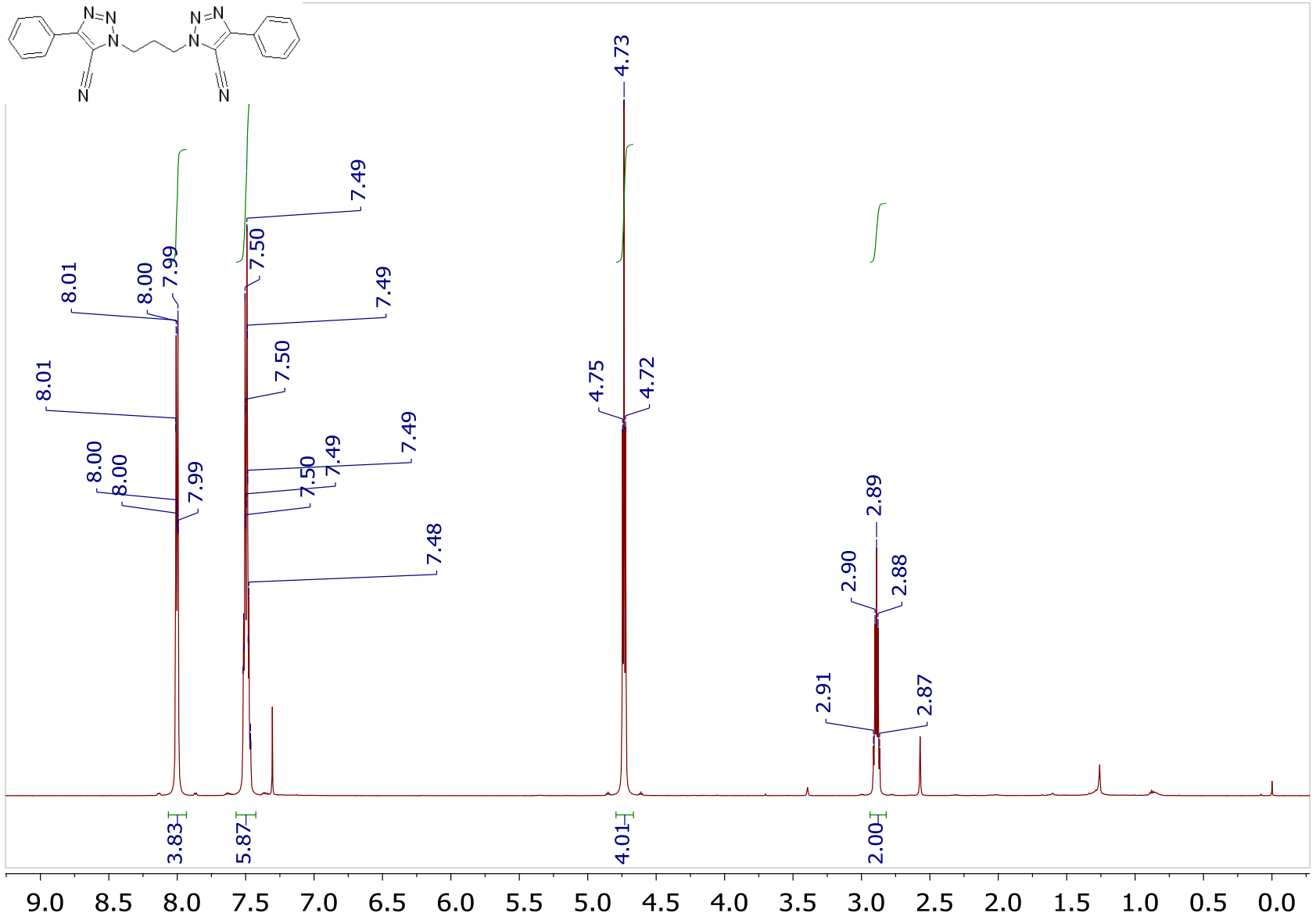
Methyl 2-(5-cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)acetate (2s)

^{13}C NMR (101 MHz, $CDCl_3$)



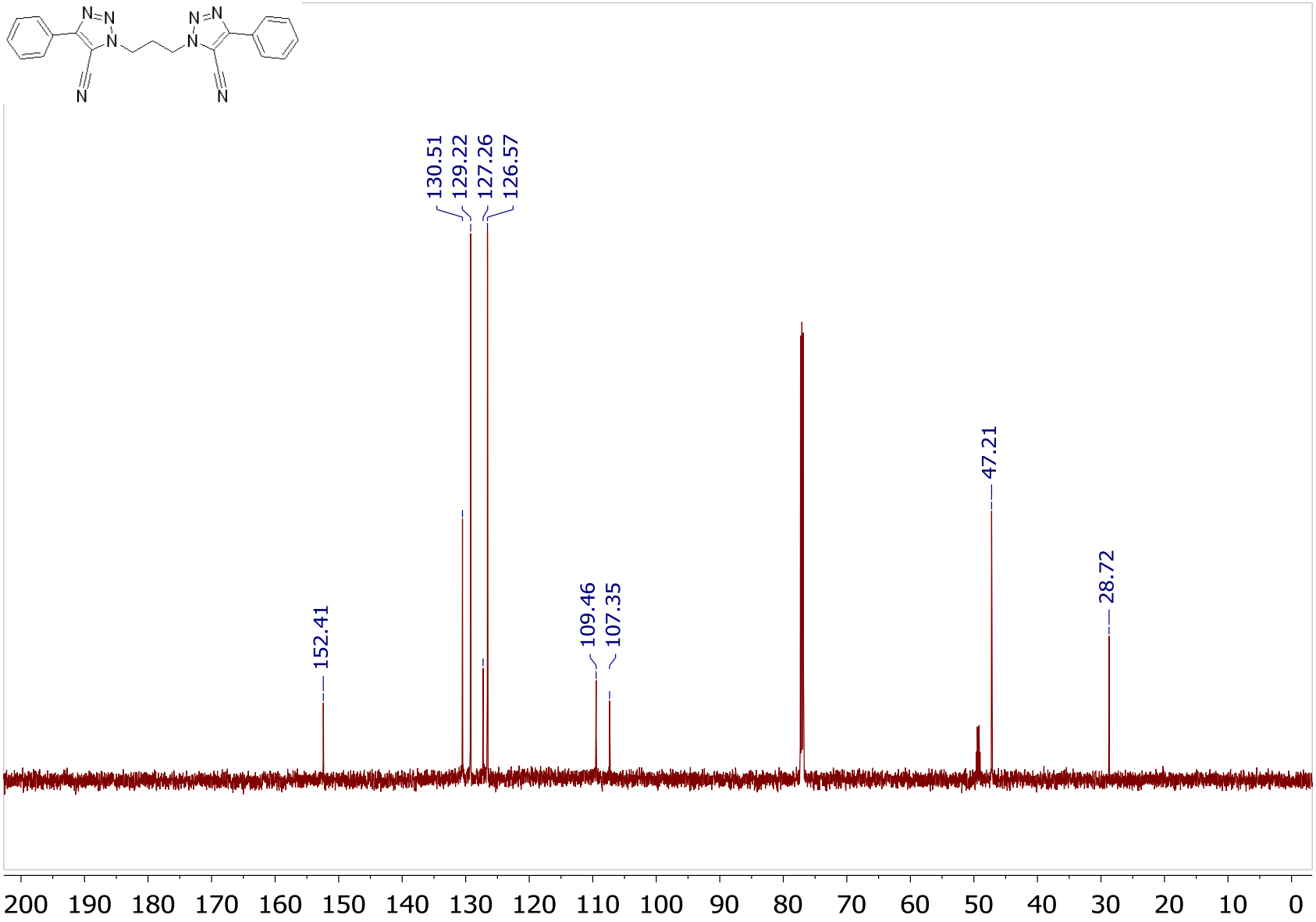
1,3-Bis(5-cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)propane (2t)

^{1}H NMR (600 MHz, $CDCl_3/CD_3OD$)



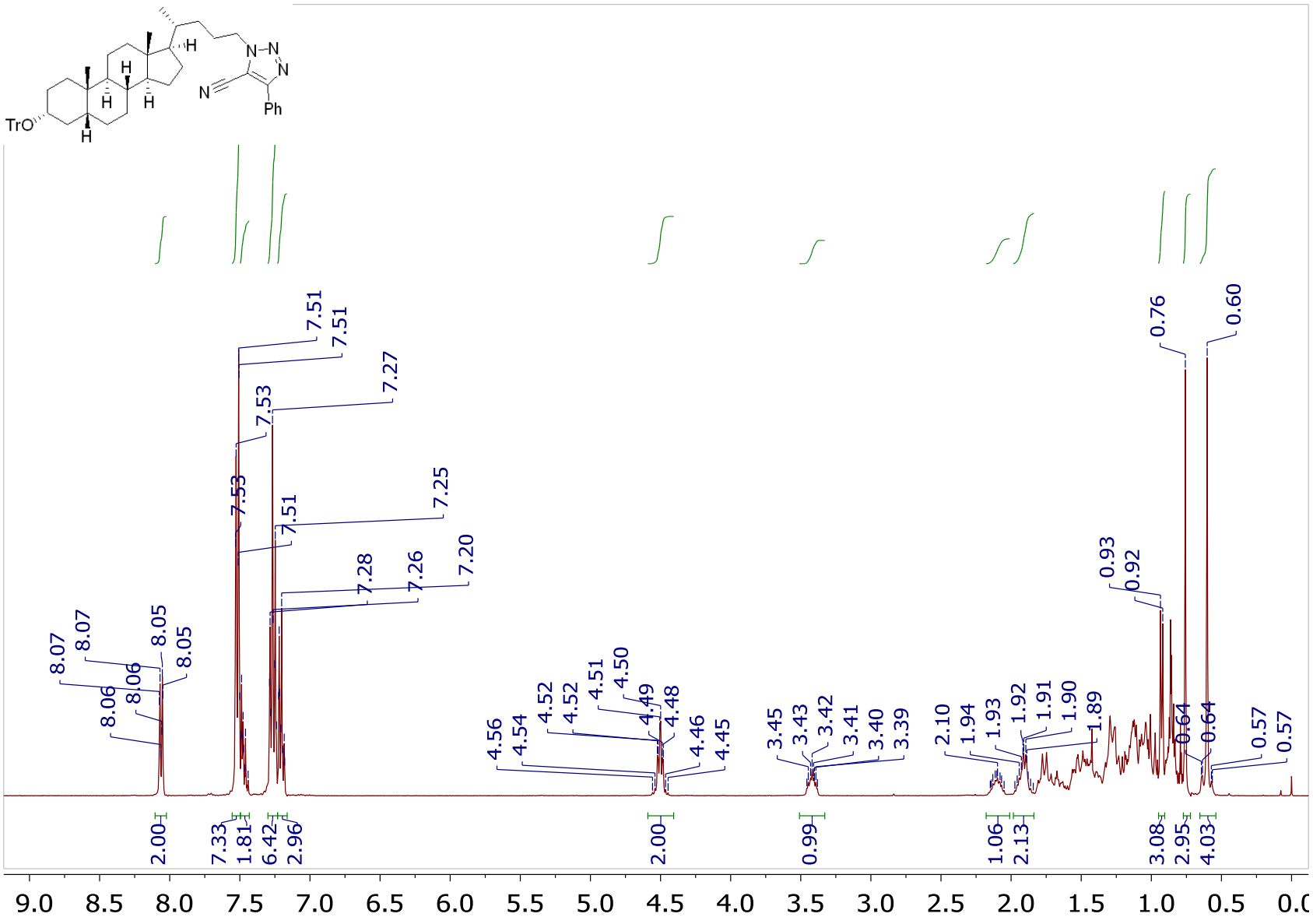
1,3-Bis(5-cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)propane (2t)

^{13}C NMR (151 MHz, $CDCl_3/CD_3OD$)



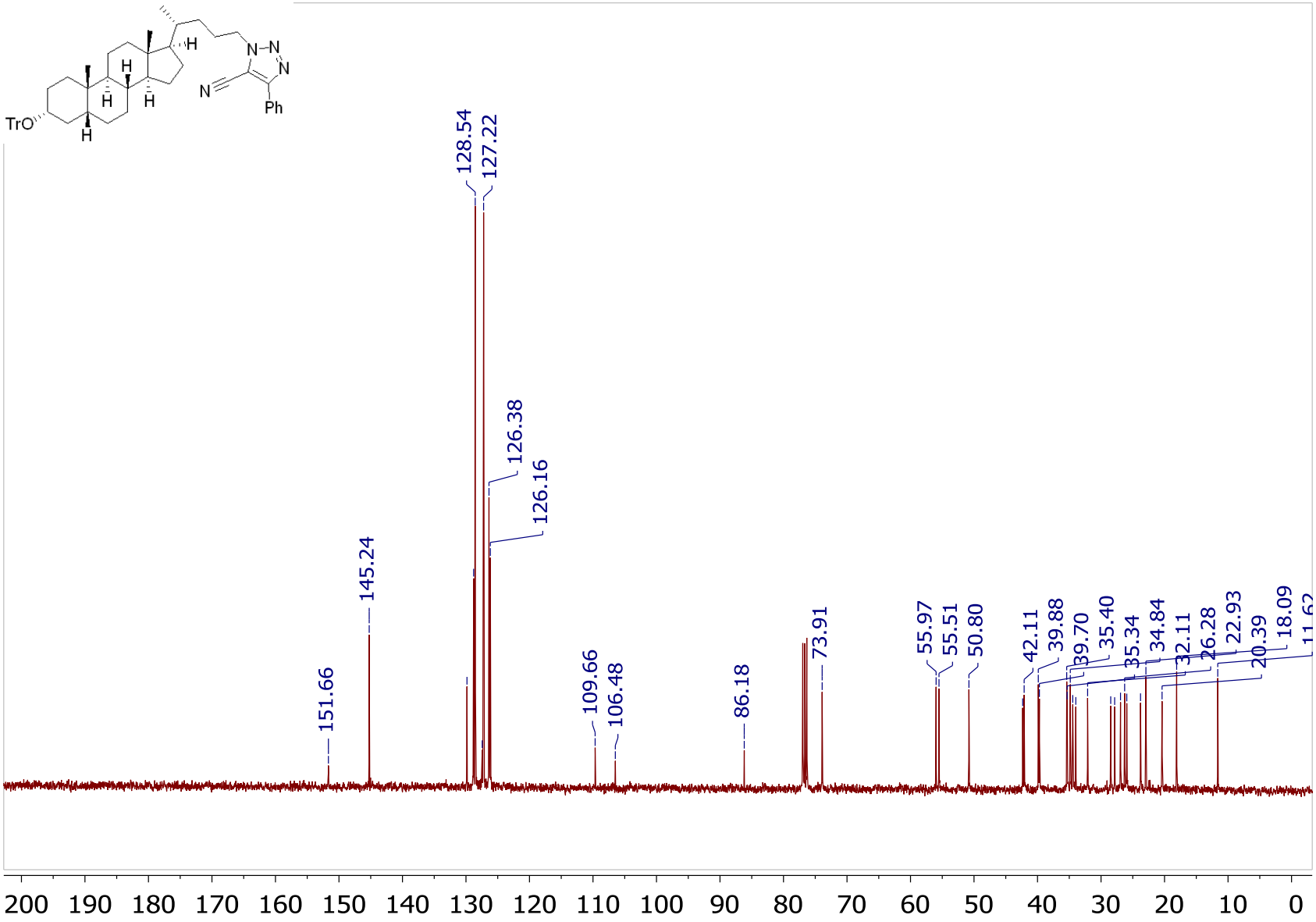
24-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)-3*α*-trityloxy-5β-cholane (2u)

^{1}H NMR (400 MHz, $CDCl_3$)



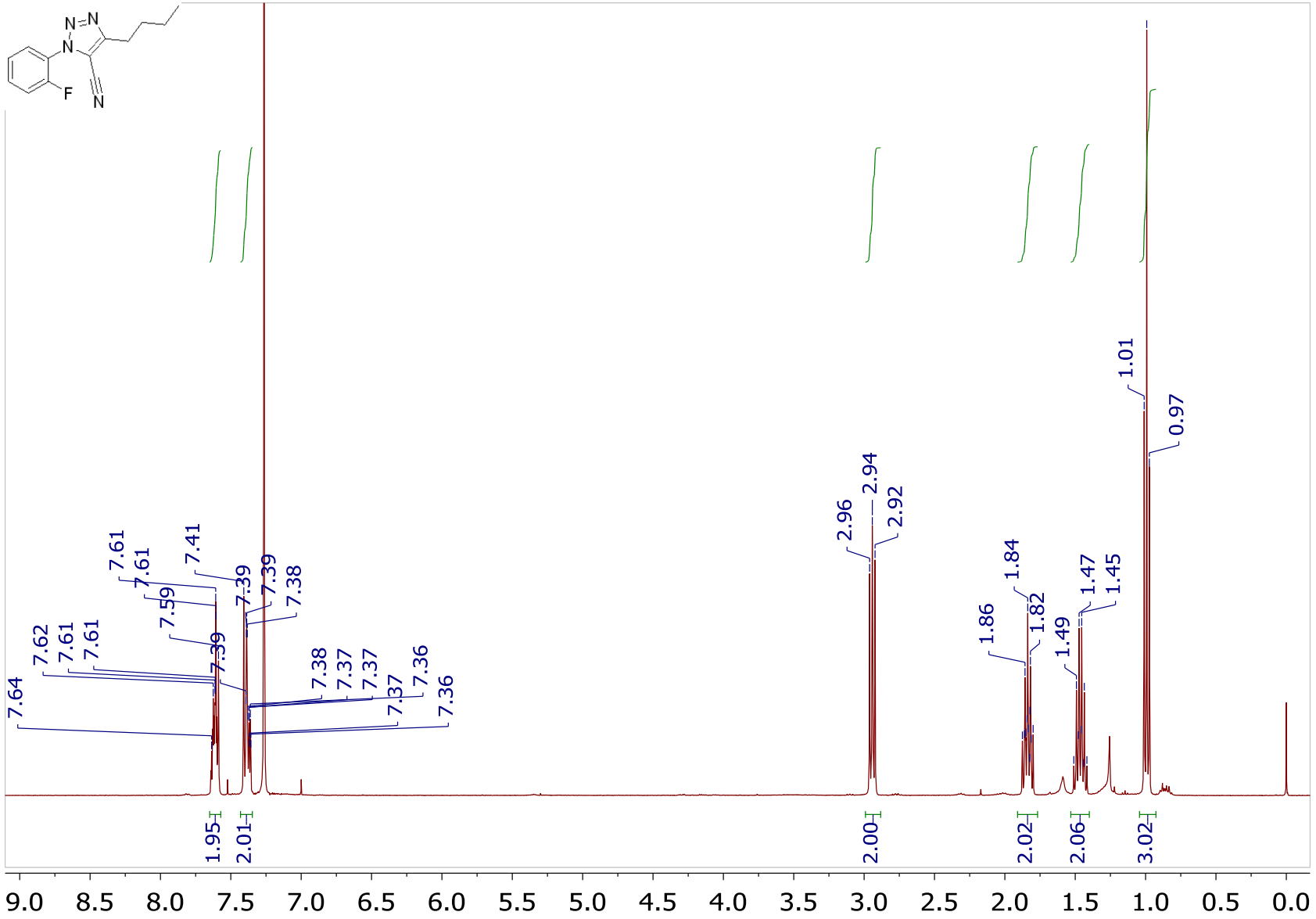
24-(5-Cyano-4-phenyl-1*H*-1,2,3-triazol-1-yl)-3*α*-trityloxy-5β-cholane (2u)

^{13}C NMR (101 MHz, $CDCl_3$)



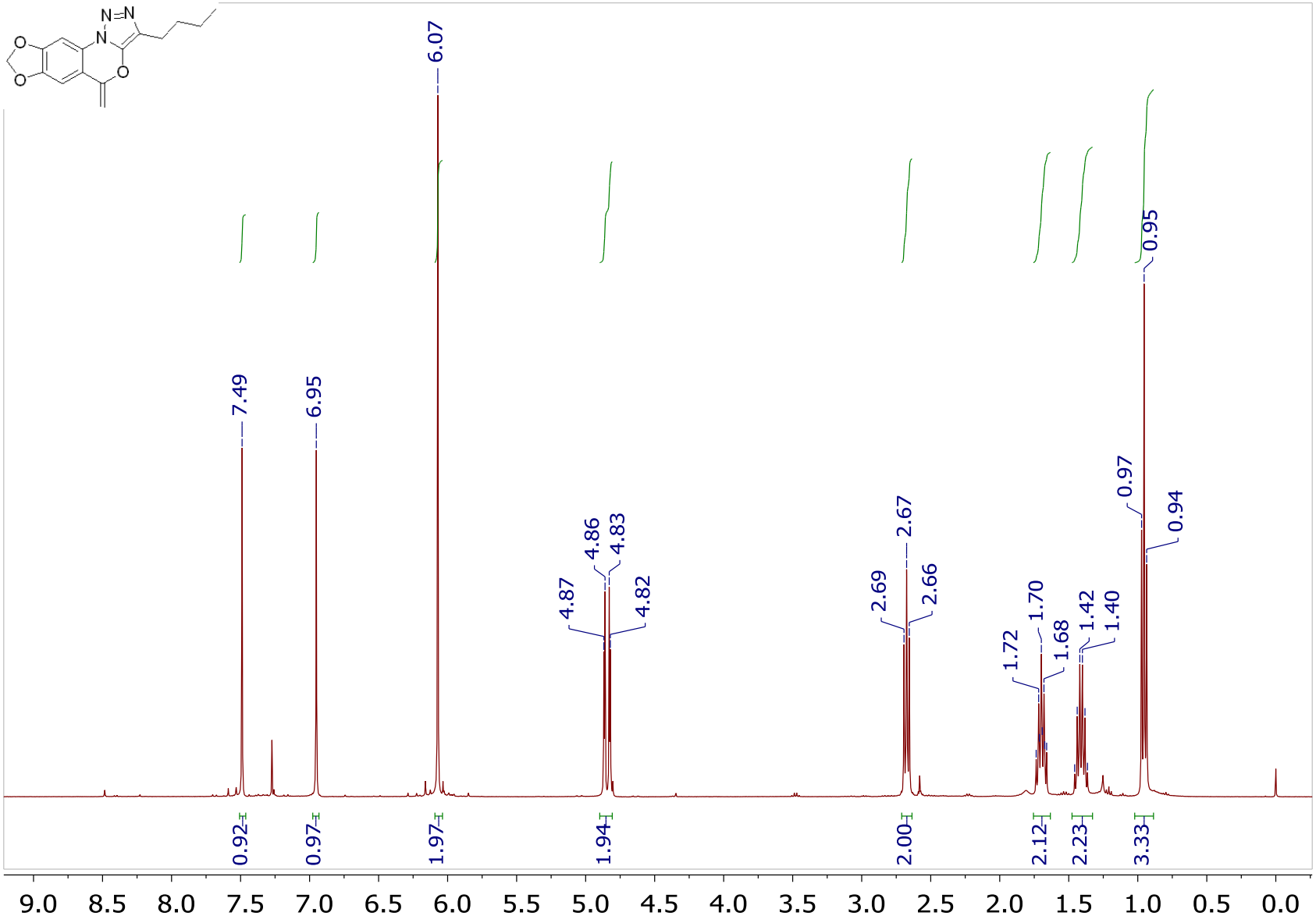
4-Butyl-5-cyano-1-(2-fluorophenyl)-1*H*-1,2,3-triazole (2y)

^{1}H NMR (400 MHz, $CDCl_3$)



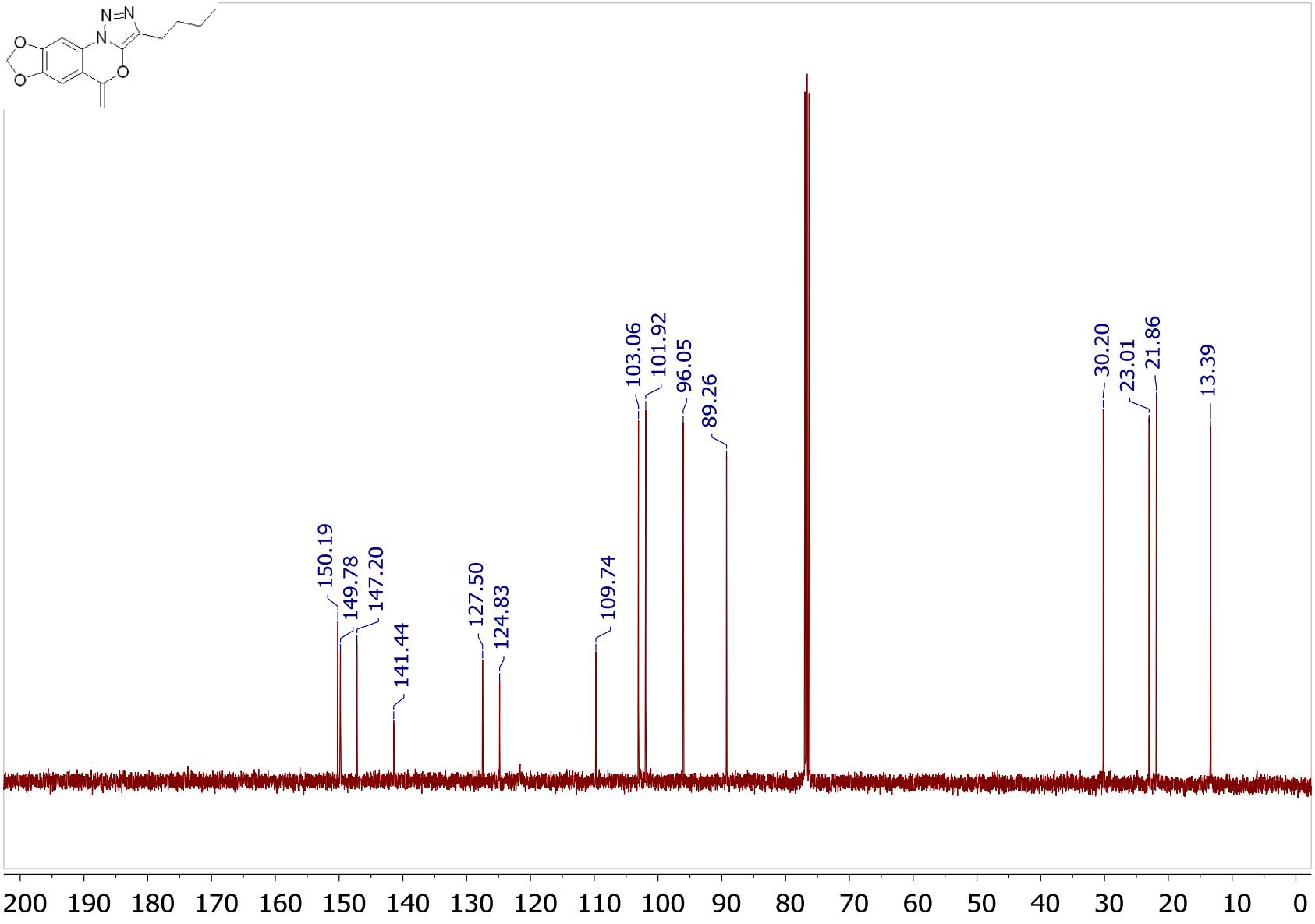
3-Butyl-5-methylene-5*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*d*][1,2,3]triazolo[5,1-*b*][1,3]oxazine (3)

^{1}H NMR (400 MHz, $CDCl_3$)



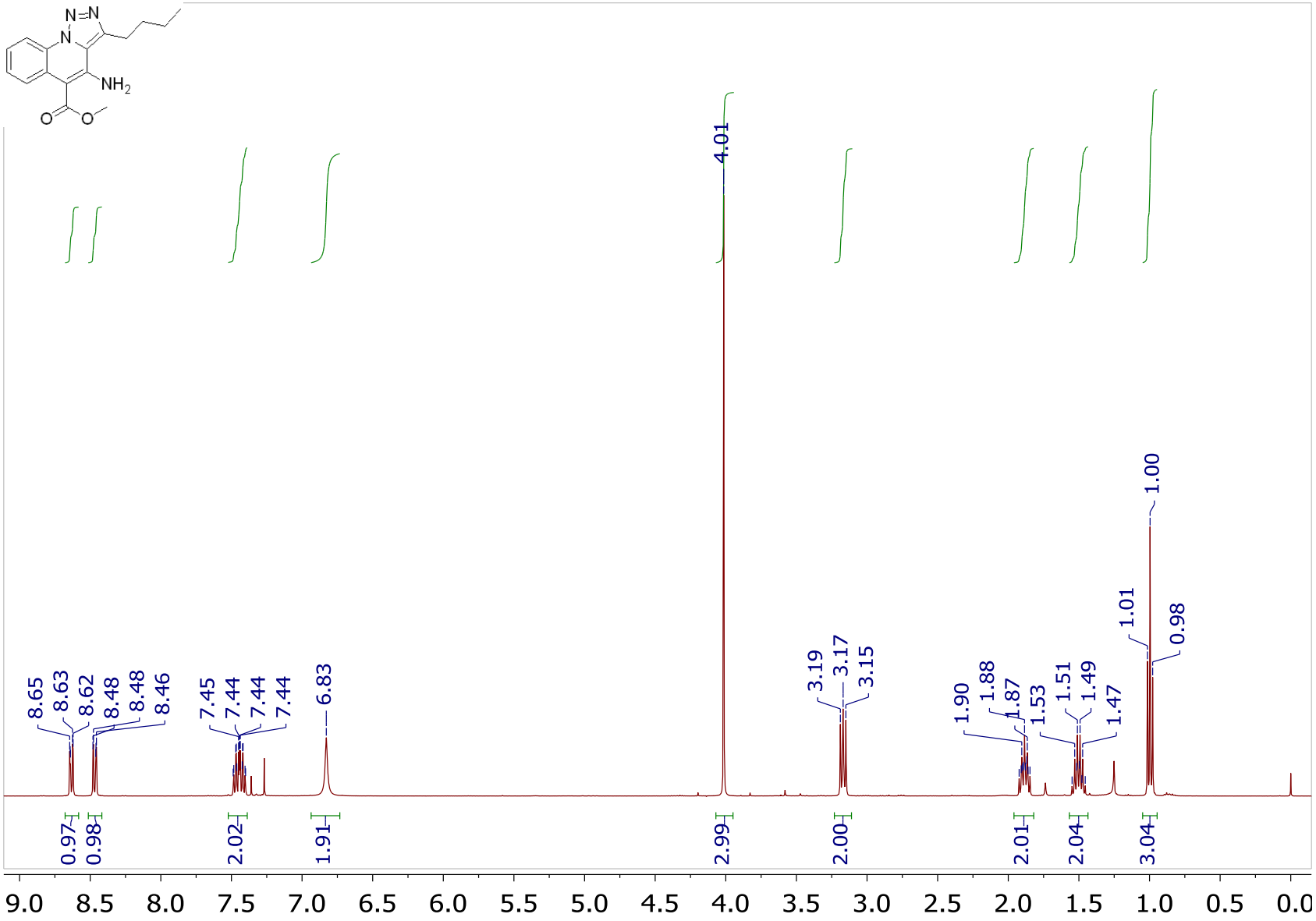
3-Butyl-5-methylene-5*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*d*][1,2,3]triazolo[5,1-*b*][1,3]oxazine (3)

^{13}C NMR (101 MHz, $CDCl_3$)



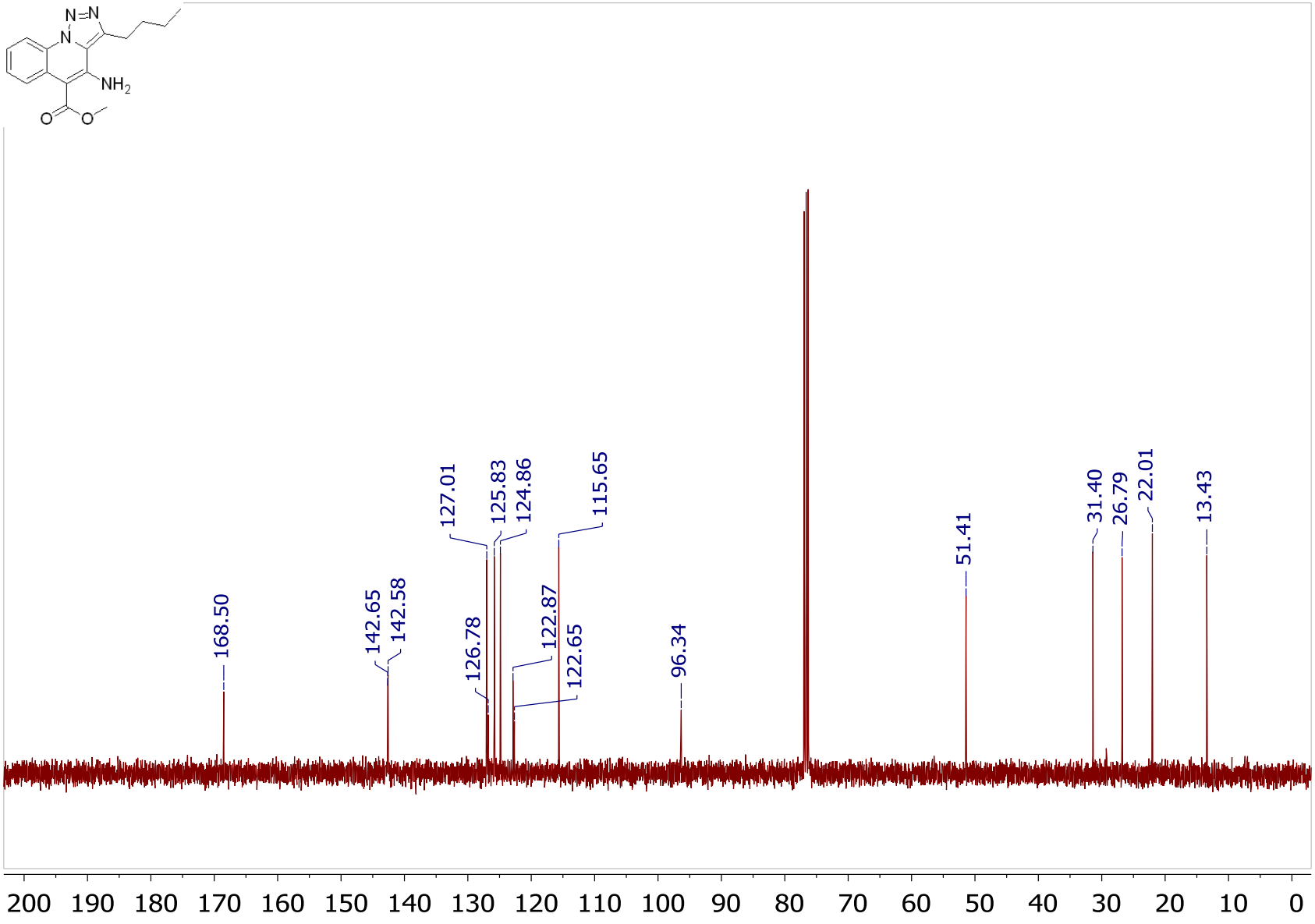
Methyl 4-amino-3-butyl[1,2,3]triazolo[1,5-*a*]quinoline-5-carboxylate (4)

^{1}H NMR (400 MHz, $CDCl_3$)



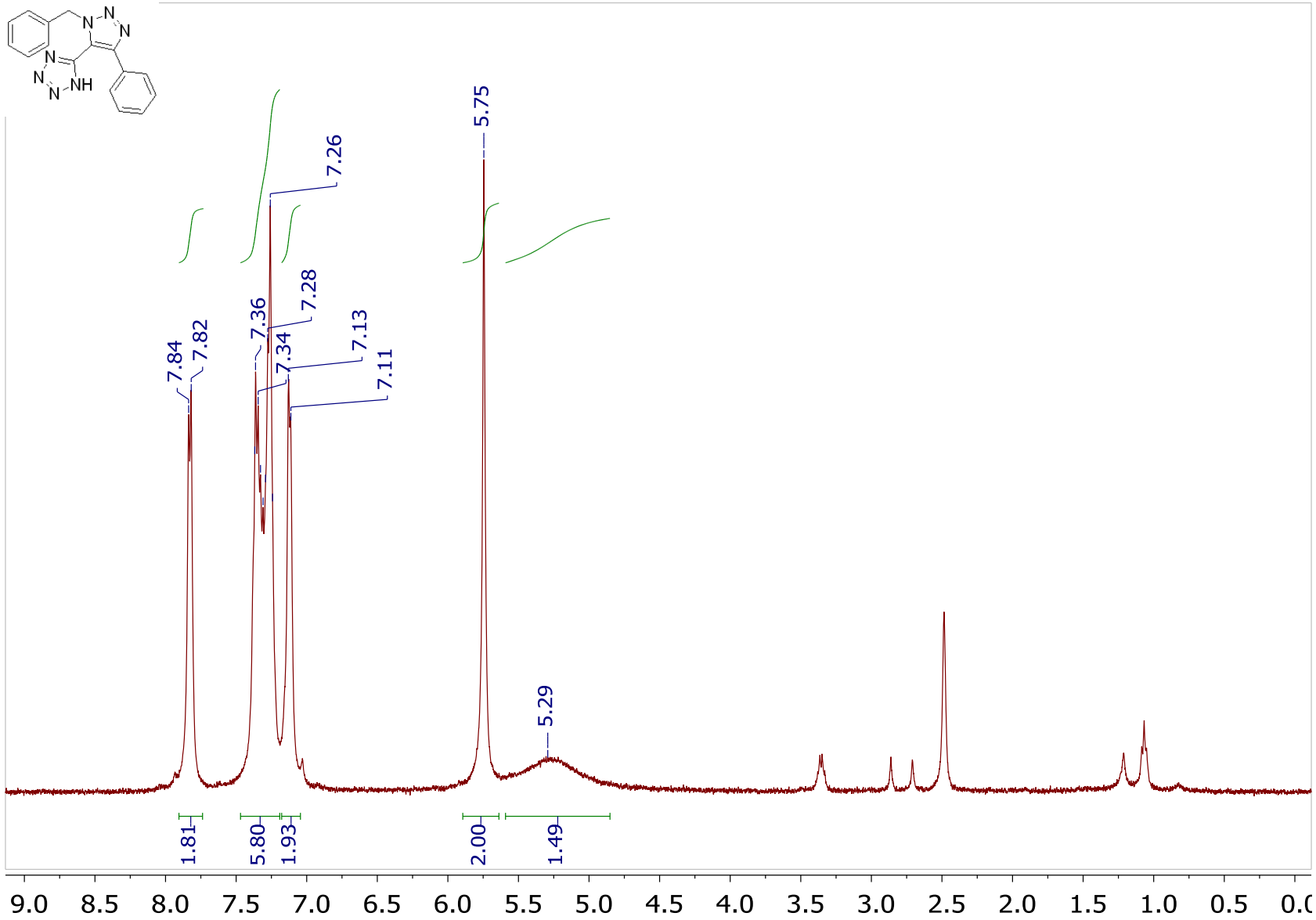
Methyl 4-amino-3-butyl[1,2,3]triazolo[1,5-*a*]quinoline-5-carboxylate (4)

^{13}C NMR (101 MHz, $CDCl_3$)



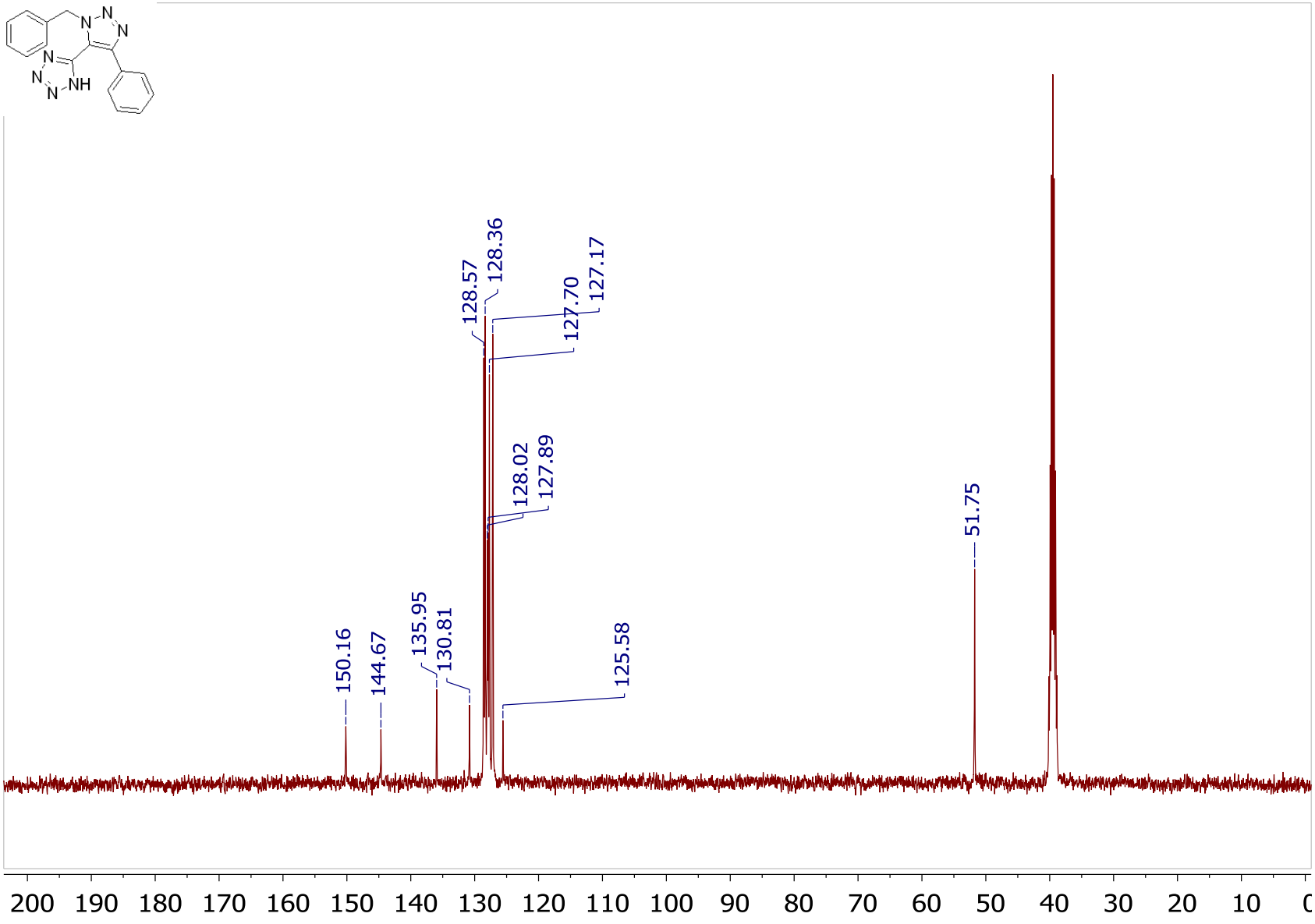
5-(1-Benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)-1*H*-tetrazole (5)

^{1}H NMR (400 MHz, DMSO-d_6)



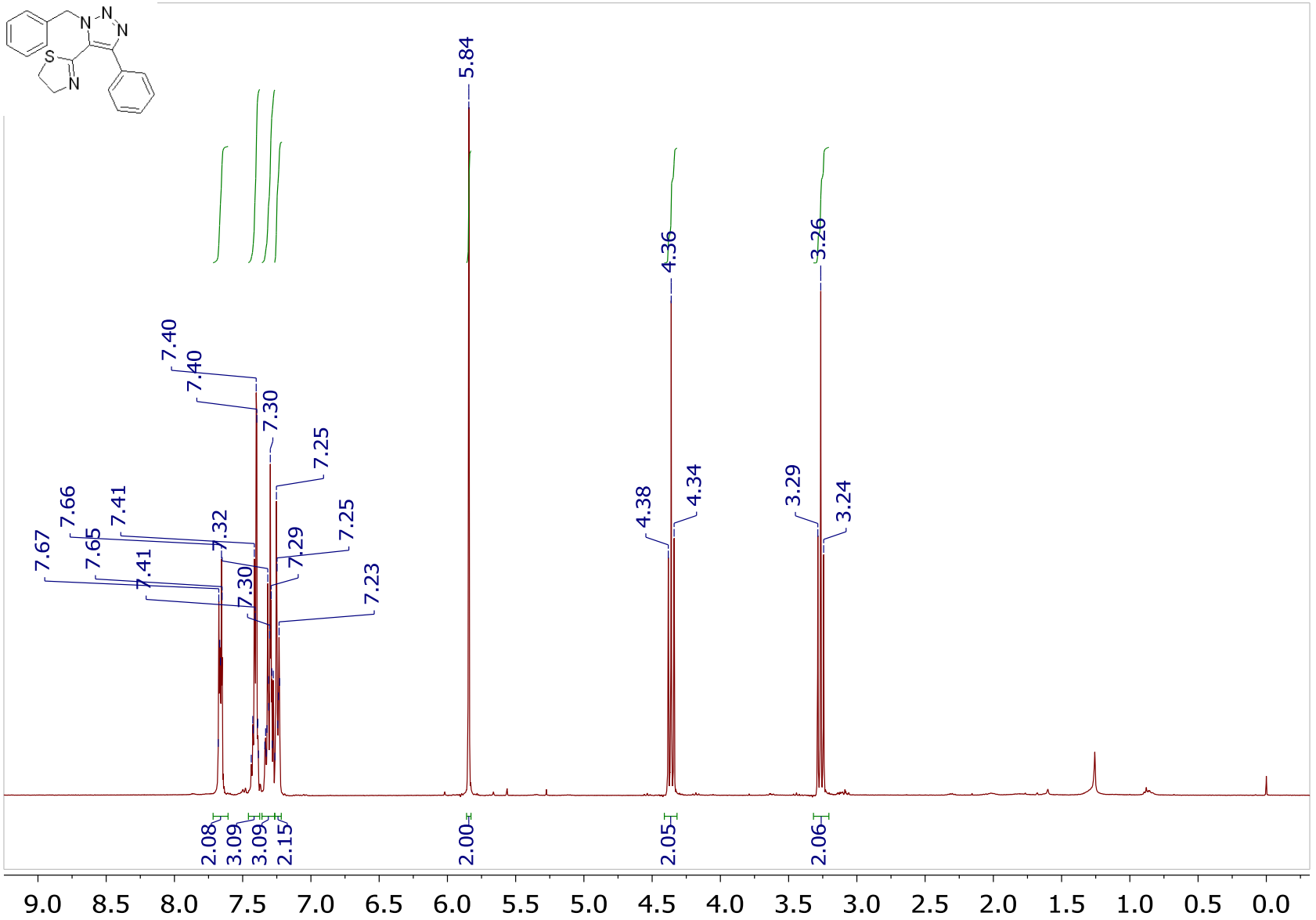
5-(1-Benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)-1*H*-tetrazole (5)

^{13}C NMR (101 MHz, DMSO-d_6)



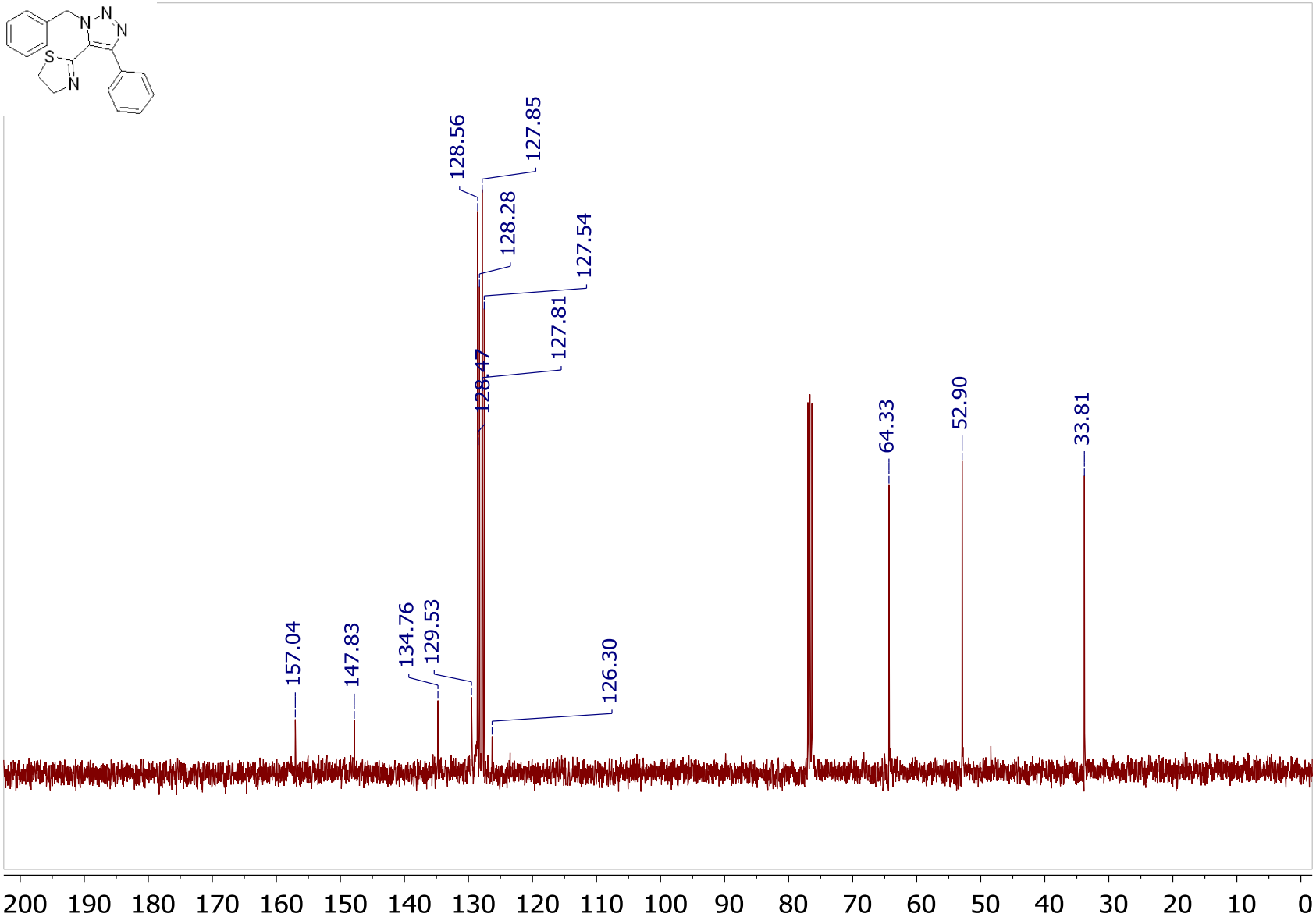
2-(1-Benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)-4,5-dihydrothiazole (6)

^{1}H NMR (400 MHz, $CDCl_3$)



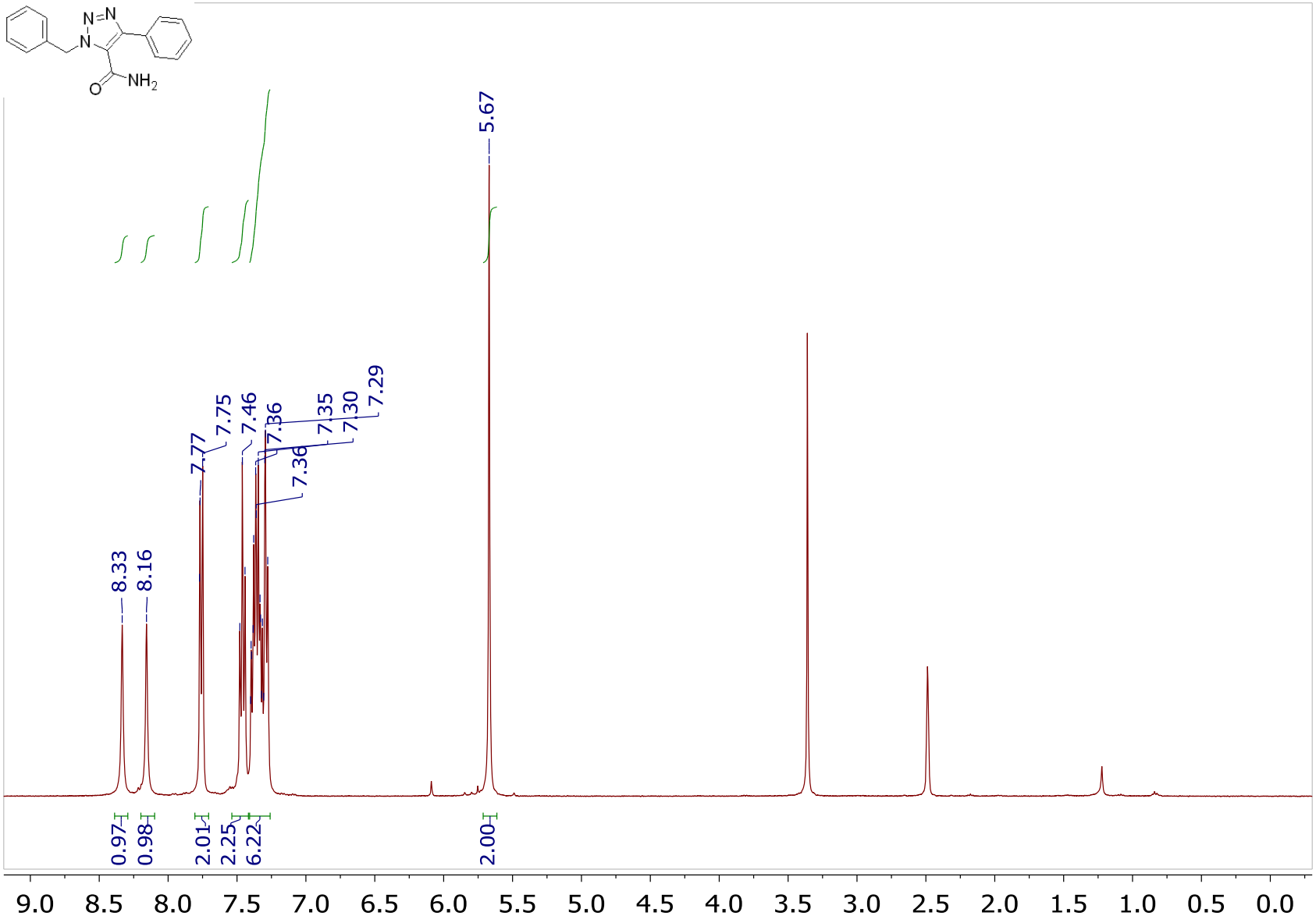
2-(1-Benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)-4,5-dihydrothiazole (6)

^{13}C NMR (101 MHz, $CDCl_3$)



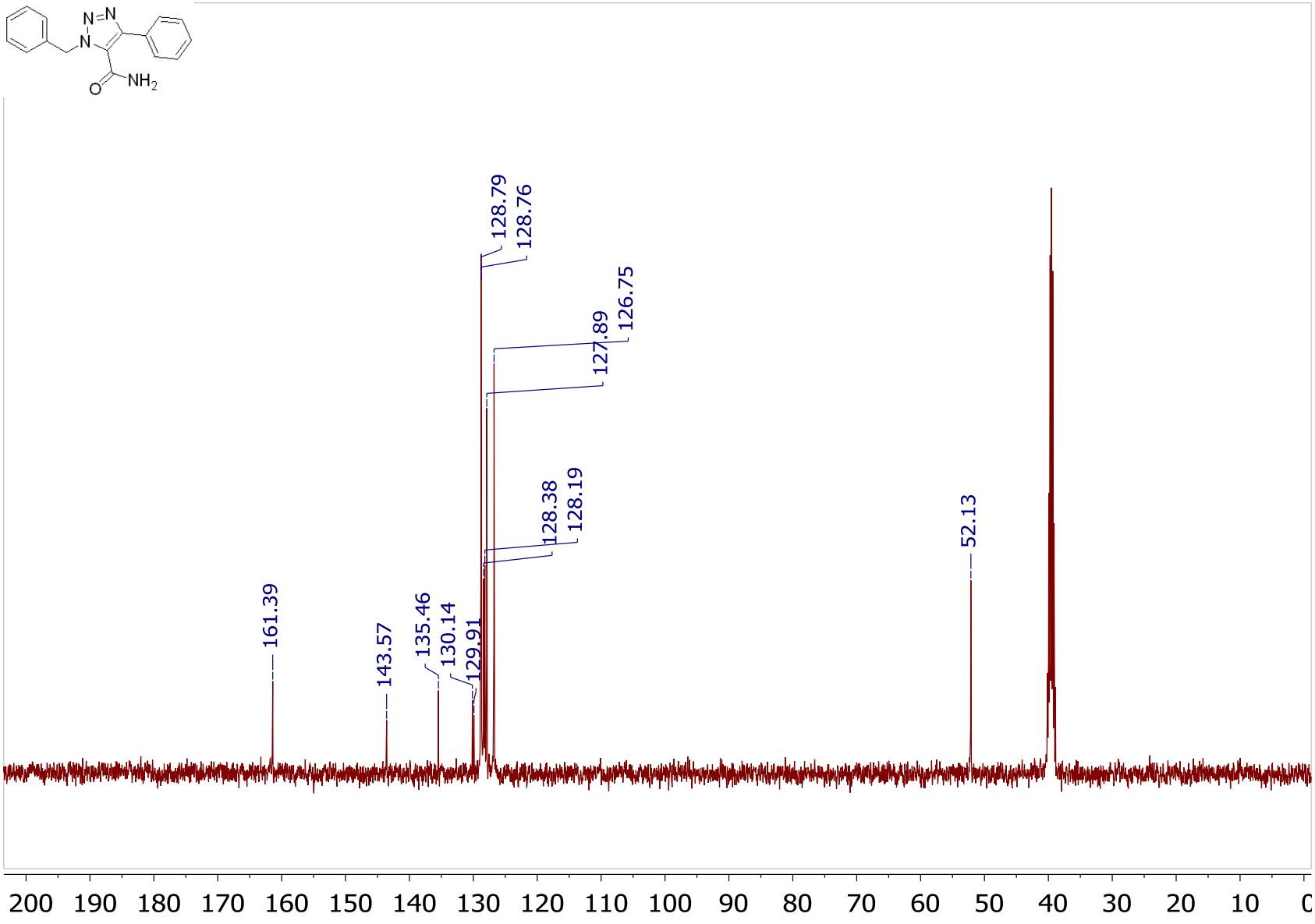
1-Benzyl-4-phenyl-1*H*-1,2,3-triazole-5-carboxamide (7)

^{1}H NMR (400 MHz, DMSO-d_6)



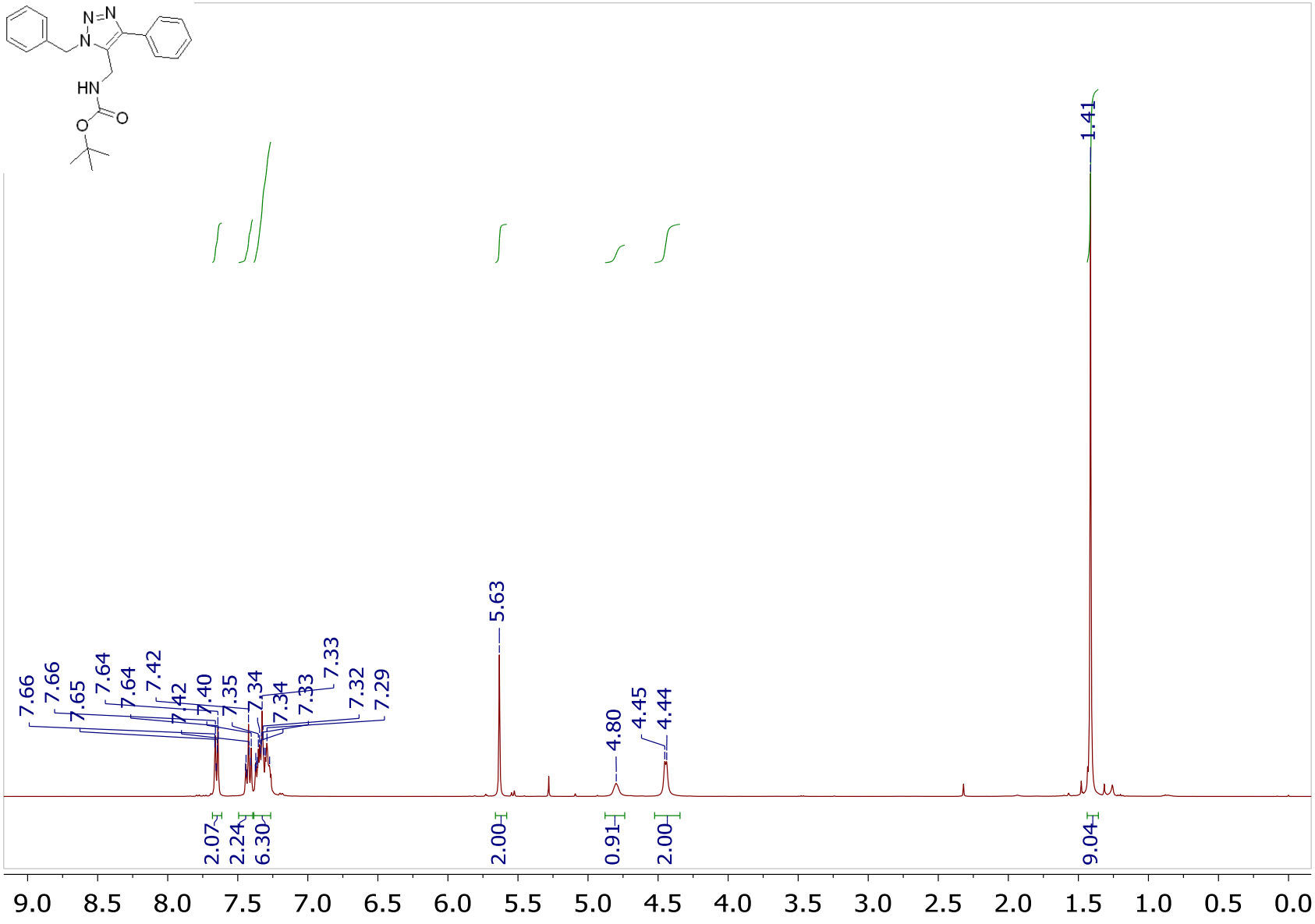
1-Benzyl-4-phenyl-1*H*-1,2,3-triazole-5-carboxamide (7)

^{13}C NMR (101 MHz, DMSO-d_6)



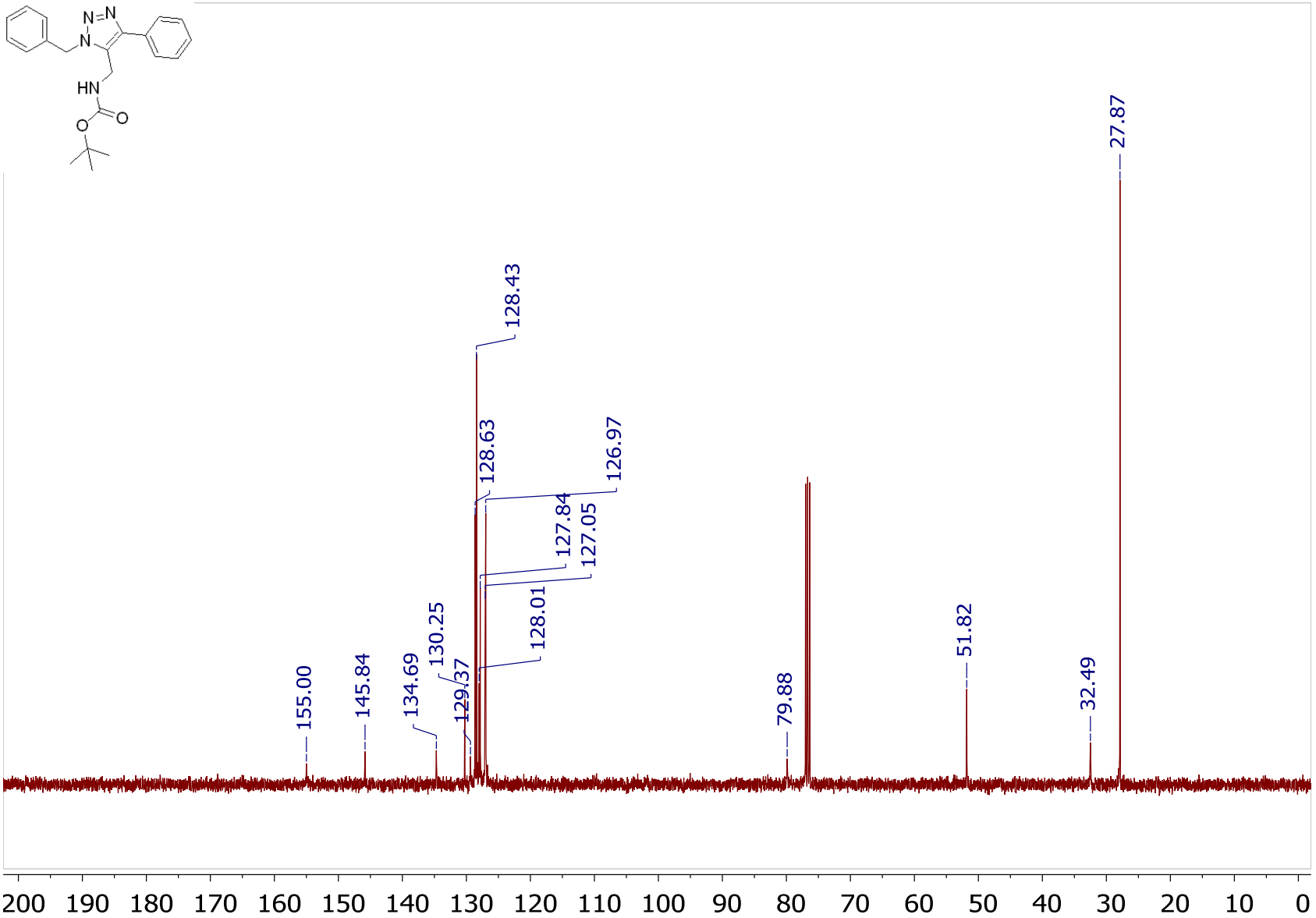
tert-Butyl ((1-benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)methyl)carbamate (8)

^{1}H NMR (400 MHz, $CDCl_3$)



tert-Butyl ((1-benzyl-4-phenyl-1_H_-1,2,3-triazol-5-yl)methyl)carbamate (8)

^{13}C NMR (101 MHz, $CDCl_3$)



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