Supporting Information

Divergent Cyclization of 2-(5-Iodo-1,2,3-triazolyl)benzamides toward Triazole-Fused Lactams and Cyclic Imidates

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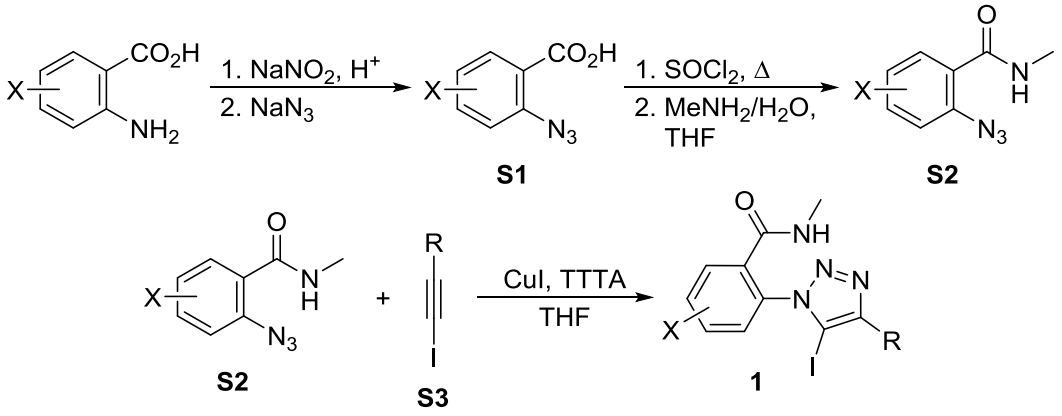
General information

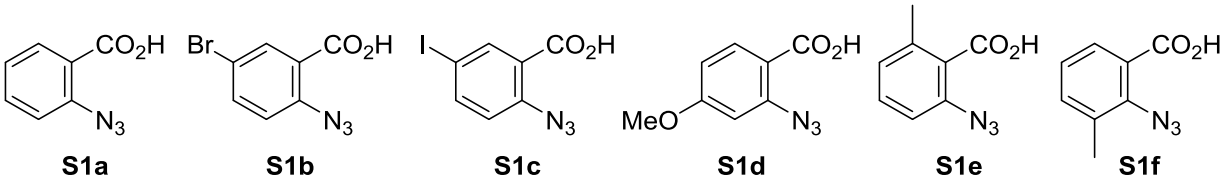
NMR spectra were recorded with Bruker Avance 400, Agilent 400MR (^{1}H 400 MHz, ^{13}C 100 MHz), and Bruker Avance 600 (^{1}H 600 MHz, ^{13}C 151 MHz) spectrometers at ambient temperature. Chemical shifts are presented in ppm (δ scale) and referenced to hexamethyldisiloxane (HMDS, δ = 0.05 ppm) or tetramethylsilane (TMS, δ = 0 ppm) in the ^{1}H NMR spectra and to the solvent signal in the ^{13}C NMR spectra. UV–vis spectra were recorded in solutions using a Hitachi U-2900 UV-vis spectrometer in a quartz cuvette (Hellma, l = 1 cm). Emission spectra were measured using a Horiba Jobin Yvon Fluoromax-2 spectrometer in a quartz cuvette (Hellma, l = 1 cm). IR spectra were recorded with a Thermo Nicolet 200 FT-IR instrument in KBr pellets. IR bands in 2365–2340 cm^{-1} range belong to atmospheric CO_2. 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. Elemental analyses were performed with an Elementar Vario MICRO cube apparatus. Column chromatography was carried out on Macherey–Nagel silica gel 60 (0.040–0.063 mm).

Experimental procedures and characterization data for compounds

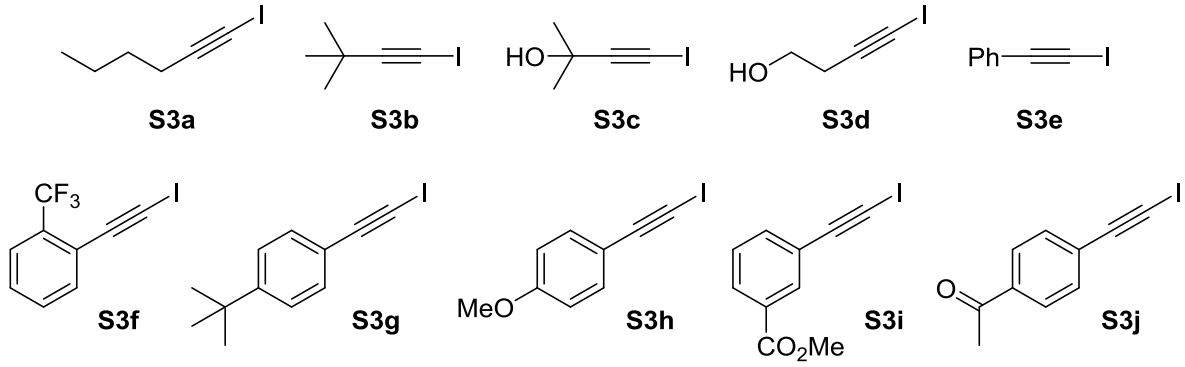
General scheme for the synthesis of starting compounds



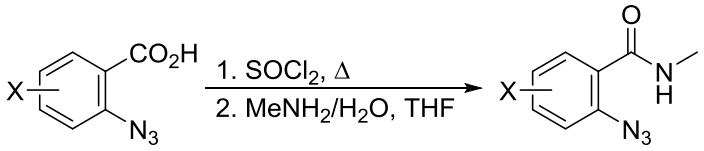
2-Azidobenzoic acids **S1a-f** were prepared from the corresponding commercially available anthranilic acids by the standard diazotization/azidation protocol according to the reported procedures.



1-Iodoalkynes **S3a-i** were prepared from the corresponding terminal acetylenes by a modified literature procedure[1] (treatment with I_2 in the methanol solution in the presence of 3 equiv of MeONa). Iodide **S3j** was prepared using *N*-iodosuccinimide/$AgNO_3$ halogenation system according to a general literature procedure.[2]



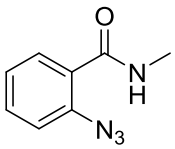
Synthesis of 2-azido-*N*-methylbenzamides S2



S1 **S2**

General procedure 1 (GP1). The mixture of 2-azidobenzoic acid **S1** (6.0 mmol, 1 equiv) and $SOCl_2$ (3 mL) was refluxed for 1 h. Then the excess $SOCl_2$ was evaporated *in vacuo* and the residue was dissolved in THF (12 mL). The obtained mixture was cooled in an ice bath and 40% solution of $MeNH_2$ in water (1.55 mL, 18.0 mmol, 3 equiv) was added dropwise. After stirring at ambient temperature overnight, the mixture was diluted with CH_2Cl_2 (50 mL) and washed with water (60 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The crude product was purified by column chromatography.

2-Azido-*N*-methylbenzamide (S2a)

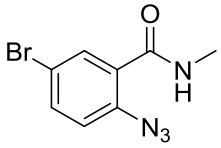


Prepared from **S1a** (2.445 g, 15.0 mmol) according to **GP1**; eluent: CH_2Cl_2–MeOH = 50:1. Yield 2.571 g (97%). White solid; mp 97–98 °C (lit.[3] 95–97 °C).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (dd, J = 7.9, 1.7 Hz, 1H), 7.55–7.40 (m, 2H), 7.23–7.12 (m, 2H), 2.98 (d, J = 4.8 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.2 (C_{quat}), 136.7 (C_{quat}), 132.1, 132.0, 125.04, 124.98 (C_{quat}), 118.3, 26.7.

2-Azido-5-bromo-*N*-methylbenzamide (S2b)



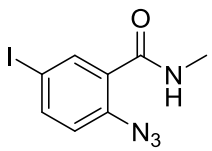
Prepared from **S1b** (363 mg, 1.5 mmol) according to **GP1**; eluent: hexanes–EtOAc = 2:1. Yield 298 mg (78%). Beige solid; mp 130–132 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 2.4 Hz, 1H), 7.58 (dd, J = 8.5, 2.4 Hz, 1H), 7.48 (br s, 1H), 7.06 (d, J = 8.5 Hz, 1H), 3.01 (d, J = 4.8 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 163.8 (C_{quat}), 135.9 (C_{quat}), 134.9 (2C), 126.4 (C_{quat}), 120.0, 118.3 (C_{quat}), 26.9.

HRMS (MALDI-TOF) calcd for $C_8H_8{}^{81}BrN_2O$ $[M–N_2+H]^+$ 228.9794; found 228.9795.

2-Azido-5-iodo-*N*-methylbenzamide (S2c)



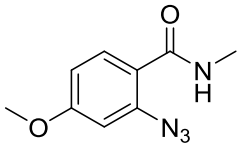
Prepared from **S1c** (578 mg, 2.0 mmol) according to **GP1**; eluent: hexanes–EtOAc = 3:1 and 2:1. Yield 510 mg (84%). Beige solid; mp 106–108 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, J = 2.2 Hz, 1H), 7.78 (dd, J = 8.4, 2.2 Hz, 1H), 7.41 (br s, 1H), 6.95 (d, J = 8.4 Hz, 1H), 3.02 (d, J = 4.8 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 163.7 (C_{quat}), 140.8 (2C), 136.7 (C_{quat}), 126.5 (C_{quat}), 120.2, 88.6 (C_{quat}), 26.9.

HRMS (MALDI-TOF) calcd for $C_8H_8IN_2O$ $[M–N_2+H]^+$ 274.9676; found 274.9680.

2-Azido-4-methoxy-*N*-methylbenzamide (S2d)



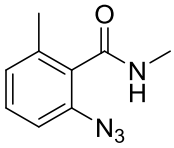
Prepared from **S1d** (57.9 mg, 0.3 mmol) according to **GP1**; eluent: CH_2Cl_2–EtOAc = 1:1. Yield 56.1 mg (91%). Beige solid; mp 91–93 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 8.8 Hz, 1H), 7.48 (br s, 1H), 6.77 (dd, J = 8.8, 2.4 Hz, 1H), 6.66 (d, J = 2.4 Hz, 1H), 3.87 (s, 3H), 3.01 (d, J = 4.8 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 164.9 (C_{quat}), 162.4 (C_{quat}), 138.1 (C_{quat}), 133.9, 117.6 (C_{quat}), 110.2, 104.0, 55.5, 26.6.

HRMS (MALDI-TOF) calcd for $C_9H_{11}N_4O_2$ $[M+H]^+$ 207.0877; found 207.0874.

2-Azido-*N*,6-dimethylbenzamide (S2e)



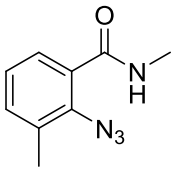
Prepared from **S1e** (200 mg, 1.13 mmol) according to **GP1**; eluent: hexanes–EtOAc = 1:1. Yield 196 mg (91%). Pale yellow solid; mp 153–155 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 1H), 7.01–6.95 (m, 2H), 5.86 (br s, 1H), 2.99 (d, J = 4.9 Hz, 3H), 2.30 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.9 (C_{quat}), 137.2 (C_{quat}), 136.7 (C_{quat}), 129.9, 129.2 (C_{quat}), 126.6, 115.5, 26.5, 19.0.

HRMS (MALDI-TOF) calcd for $C_9H_{11}N_4O$ $[M+H]^+$ 191.0927; found 191.0929.

2-Azido-*N*,3-dimethylbenzamide (S2f)



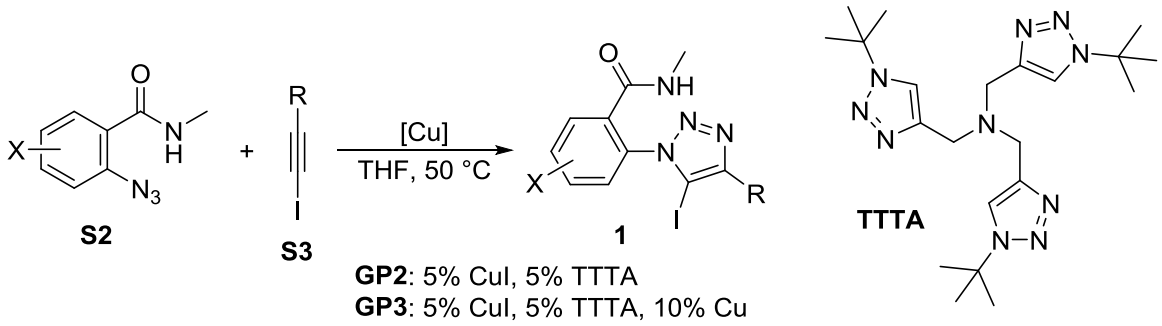
Prepared from **S1f** (354 mg, 2.0 mmol) according to **GP1**; eluent: hexanes–EtOAc = 1:1. Yield 323 mg (85%). Light brown solid; mp 73–75 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 7.52 (m, 1H), 7.24 (m, 1H), 7.11 (m, 1H), 6.81 (br s, 1H), 3.01 (d, J = 4.8 Hz, 3H), 2.37 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 167.1 (C_{quat}), 135.2 (C_{quat}), 133.3, 132.6 (C_{quat}), 129.2 (C_{quat}), 127.7, 125.5, 26.8, 18.1.

HRMS (MALDI-TOF) calcd for $C_9H_{11}N_2O$ $[M–N_2+H]^+$ 163.0866; found 163.0863.

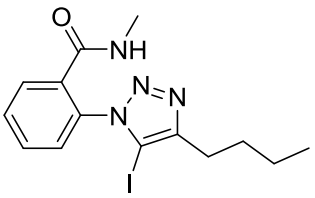
Synthesis of 2-(5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamides 1



General procedure 2 (GP2). 2-Azido-*N*-methylbenzamide **S2** (1.5 mmol, 1 equiv), 1-iodoalkyne **S3** (1.73 mmol, 1.15 equiv), CuI (14.3 mg, 0.075 mmol, 5 mol %), and tris[(1-*tert*-butyl-1*H*-1,2,3-triazol-4-yl)methyl]amine (TTTA) (32.2 mg, 0.075 mmol, 5 mol %) were mixed under an Ar atmosphere in THF (5 mL). The reaction mixture was stirred at 50 °C in a dry block overnight or for several days (TLC control), then diluted with CH_2Cl_2 (50 mL), washed with EDTA solution (50 mL) and water (50 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography.

General procedure 3 (GP3). Synthesis was performed as described for **GP2** with the catalytic system comprising CuI (5 mol %), Cu powder (10 mol %), and TTTA (5 mol %).

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1a)



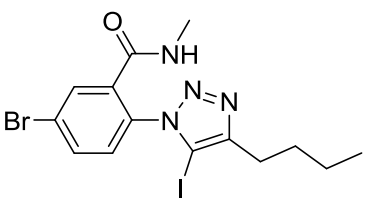
Prepared from azide **S2a** (528.6 mg, 3.0 mmol) and iodoalkyne **S3a** (469 μL, 3.45 mmol) according to **GP2** at room temperature; eluent: CH_2Cl_2–EtOAc = 4:1. Yield 1.116 g (97%). Light brown solid; mp 124–125 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (m, 1H), 7.68–7.60 (m, 2H), 7.34 (m, 1H), 5.80 (m, 1H), 2.75 (m, 2H), 2.72 (d, J = 4.9 Hz, 3H), 1.74 (m, 2H), 1.41 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.8 (C_{quat}), 152.5 (C_{quat}), 134.5 (C_{quat}), 133.9 (C_{quat}), 131.03, 130.97, 129.8, 128.3, 82.5 (C_{quat}), 31.0, 26.8, 25.7, 22.1, 13.8.

HRMS (MALDI-TOF) calcd for $C_{14}H_{18}IN_4O$ $[M+H]^+$ 385.0520; found 385.0523.

5-Bromo-2-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1b)



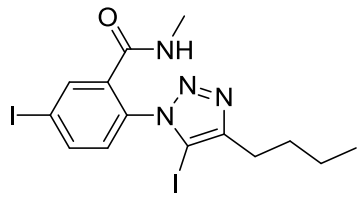
Prepared from azide **S2b** (204.1 mg, 0.8 mmol) and iodoalkyne **S3a** (119 μL, 0.88 mmol, 1.1 equiv) according to **GP3**; eluent: hexanes–EtOAc = 2:1. Yield 165 mg (45%). White solid; mp 155–157 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 2.2 Hz, 1H), 7.74 (dd, J = 8.4, 2.2 Hz, 1H), 7.21 (d, J = 8.4 Hz, 1H), 6.03 (m, 1H), 2.74 (m, 2H), 2.72 (d, J = 4.8 Hz, 3H), 1.73 (m, 2H), 1.40 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 164.4 (C_{quat}), 152.8 (C_{quat}), 136.0 (C_{quat}), 134.1, 132.9, 132.8 (C_{quat}), 129.8, 125.2 (C_{quat}), 82.5 (C_{quat}), 31.0, 26.9, 25.7, 22.1, 13.8.

HRMS (MALDI-TOF) calcd for $C_{14}H_{17}BrIN_4O$ $[M+H]^+$ 462.9625; found 462.9623.

(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-5-iodo-*N*-methylbenzamide (1c)



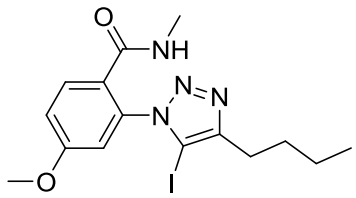
Prepared from azide **S2c** (271.9 mg, 0.9 mmol) and iodoalkyne **S3a** (134 μL, 0.99 mmol, 1.1 equiv) according to **GP3**; eluent: hexanes–EtOAc = 2:1. Yield 262 mg (57%). Beige solid; mp 152–155 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 2.0 Hz, 1H), 7.94 (dd, J = 8.3, 2.0 Hz, 1H), 7.06 (d, J = 8.3 Hz, 1H), 5.98 (m, 1H), 2.73 (m, 2H), 2.71 (d, J = 4.9 Hz, 3H), 1.73 (m, 2H), 1.40 (m, 2H), 0.97 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 164.3 (C_{quat}), 152.8 (C_{quat}), 140.1, 138.8, 135.9 (C_{quat}), 133.5 (C_{quat}), 129.8, 96.9 (C_{quat}), 82.4 (C_{quat}), 31.0, 26.9, 25.7, 22.1, 13.8.

HRMS (MALDI-TOF) calcd for $C_{14}H_{17}I_2N_4O$ $[M+H]^+$ 510.9486; found 510.9485.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-4-methoxy-*N*-methylbenzamide (1d)



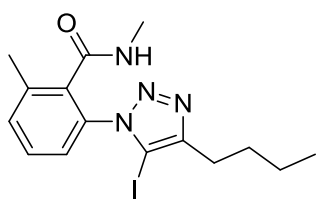
Prepared from azide **S2d** (201.1 mg, 0.975 mmol) and iodoalkyne **S3a** (146 μL, 1.073 mmol, 1.1 equiv) according to **GP2** at room temperature; eluent: hexanes–EtOAc = 1:1. Yield 342 mg (85%). Beige solid; mp 129–131 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.7 Hz, 1H), 7.12 (dd, J = 8.7, 2.5 Hz, 1H), 6.80 (d, J = 2.5 Hz, 1H), 5.72 (m, 1H), 3.88 (s, 3H), 2.74 (m, 2H), 2.68 (d, J = 4.8 Hz, 3H), 1.74 (m, 2H), 1.41 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.6 (C_{quat}), 161.3 (C_{quat}), 152.6 (C_{quat}), 135.1 (C_{quat}), 131.5, 126.4 (C_{quat}), 116.5, 113.6, 82.6 (C_{quat}), 55.8, 31.0, 26.8, 25.7, 22.1, 13.7.

HRMS (MALDI-TOF) calcd for $C_{15}H_{20}IN_4O_2$ $[M+H]^+$ 415.0625; found 415.0626.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*,6-dimethylbenzamide (1e)



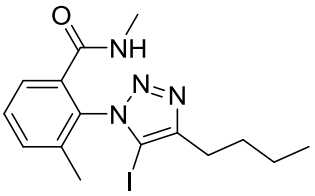
Prepared from azide **S2e** (128.3 mg, 0.675 mmol) and iodoalkyne **S3a** (101 μL, 0.743 mmol, 1.1 equiv) according to **GP2** at room temperature; eluent: hexanes–EtOAc = 1:1. Yield 198 mg (74%). Yellow solid; mp 142–144 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49–7.42 (m, 2H), 7.15 (m, 1H), 5.73 (m, 1H), 2.72 (m, 2H), 2.69 (d, J = 4.9 Hz, 3H), 2.47 (s, 3H), 1.73 (m, 2H), 1.41 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 166.0 (C_{quat}), 152.1 (C_{quat}), 137.7 (C_{quat}), 135.7 (C_{quat}), 133.8 (C_{quat}), 132.7, 129.4, 125.3, 82.1 (C_{quat}), 31.0, 26.3, 25.7, 22.2, 19.5, 13.8.

HRMS (MALDI-TOF) calcd for $C_{15}H_{20}IN_4O$ $[M+H]^+$ 399.0676; found 399.0679.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*,3-dimethylbenzamide (1f)



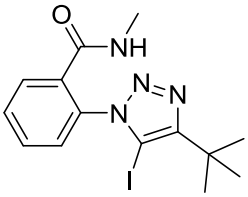
Prepared from azide **S2f** (190.2 mg, 1.0 mmol) and iodoalkyne **S3a** (149 μL, 1.1 mmol, 1.1 equiv) according to **GP3**; eluent: hexanes–EtOAc = 1:1. Yield 200 mg (50%). Pale yellow solid; mp 142–144 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, J = 7.6, 1.5 Hz, 1H), 7.52 (t, J = 7.6 Hz, 1H), 7.46 (m, 1H), 5.83 (m, 1H), 2.76 (m, 2H), 2.67 (d, J = 4.9 Hz, 3H), 1.98 (s, 3H), 1.75 (m, 2H), 1.39 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 166.1 (C_{quat}), 152.6 (C_{quat}), 136.9 (C_{quat}), 135.3 (C_{quat}), 132.8 (C_{quat}), 132.7, 130.9, 127.1, 82.9 (C_{quat}), 31.0, 26.7, 25.7, 22.1, 17.3, 13.8.

HRMS (MALDI-TOF) calcd for $C_{15}H_{20}IN_4O$ $[M+H]^+$ 399.0676; found 399.0669.

2-(4-*tert*-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1g)



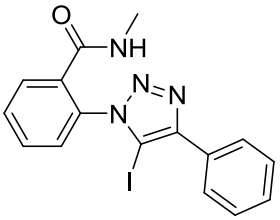
Prepared from azide **S2a** (176.2 mg, 1.0 mmol) and iodoalkyne **S3b** (229 mg, 1.1 mmol, 1.1 equiv) according to **GP2** at room temperature; eluent: hexanes–EtOAc = 1:1. Yield 265 mg (69%). White solid; mp 161–163 °C.

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 7.76 (m, 1H), 7.70–7.64 (m, 2H), 7.41 (m, 1H), 2.72 (s, 3H), 1.53 (s, 9H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$–CD_3OD) δ 166.5 (C_{quat}), 156.5 (C_{quat}), 134.1 (C_{quat}), 134.0 (C_{quat}), 130.6, 130.4, 128.5, 128.4, 78.6 (C_{quat}), 31.3 (C_{quat}), 28.9 (3C), 25.8.

HRMS (MALDI-TOF) calcd for $C_{14}H_{18}IN_4O$ $[M+H]^+$ 385.0520; found 385.0517.

2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1h)



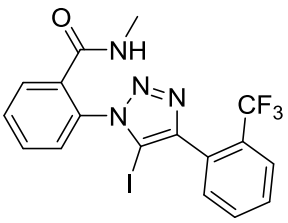
Prepared from azide **S2a** (704.8 mg, 4.0 mmol) and iodoalkyne **S3e** (1.049 g, 4.6 mmol) according to **GP2**; eluent: CH_2Cl_2–MeOH = 20:1. Yield 1.483 g (92%). Pale yellow solid; mp 170–171 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06–8.02 (m, 2H), 7.88 (m, 1H), 7.71–7.64 (m, 2H), 7.54–7.48 (m, 2H), 7.47–7.39 (m, 2H), 5.86 (m, 1H), 2.76 (d, J = 4.9 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.8 (C_{quat}), 149.9 (C_{quat}), 134.7 (C_{quat}), 133.9 (C_{quat}), 131.1, 131.0, 129.7 (C_{quat}), 129.6, 128.8, 128.7, 128.5 (2C), 127.4 (2C), 80.7 (C_{quat}), 26.8.

HRMS (MALDI-TOF) calcd for $C_{16}H_{14}IN_4O$ $[M+H]^+$ 405.0207; found 405.0208.

2-{5-Iodo-4-[2-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-*N*-methylbenzamide (1i)



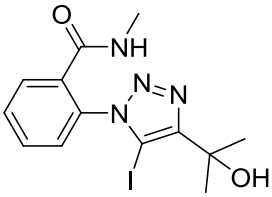
Prepared from azide **S2a** (176.2 mg, 1.0 mmol) and iodoalkyne **S3f** (326 mg, 1.1 mmol, 1.1 equiv) according to **GP2** at room temperature; eluent: hexanes–CH_2Cl_2–EtOAc = 2:2:1. Yield 392 mg (83%). Beige solid; mp 184–186 °C.

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 7.86 (m, 1H), 7.81 (m, 1H), 7.74–7.63 (m, 4H), 7.52 (m, 1H), 7.48 (m, 1H), 2.76 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD) δ 166.4 (C_{quat}), 149.7 (C_{quat}), 134.2 (C_{quat}), 133.6 (C_{quat}), 132.7, 131.5, 130.9 (2C), 129.8 (q, J_{CF} = 30.7 Hz, C_{quat}), 129.5, 129.0, 128.23, 128.16 (q, J_{CF} = 1.9 Hz, C_{quat}), 126.2 (q, J_{CF} = 5.1 Hz), 123.4 (q, J_{CF} = 274 Hz, CF_3), 85.0 (C_{quat}), 26.2.

HRMS (MALDI-TOF) calcd for $C_{17}H_{13}F_3IN_4O$ $[M+H]^+$ 473.0081; found 473.0083.

2-[4-(1-Hydroxy-1-methylethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1j)



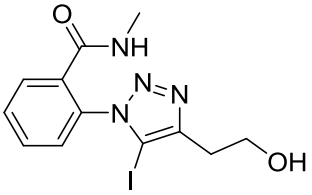
Prepared from azide **S2a** (176.2 mg, 1.0 mmol) and iodoalkyne **S3c** (231 mg, 1.1 mmol, 1.1 equiv) according to **GP2** at room temperature; eluent: CH_2Cl_2–MeOH = 10:1. Yield 370 mg (96%). Beige solid; mp 142–144 °C.

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 7.75 (m, 1H), 7.71–7.61 (m, 3H), 7.43 (m, 1H), 2.754 (d, J = 4.0 Hz, 3H, CH_3NH), 2.749 (s, 3H, CH_3ND), 1.74 (s, 6H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD) δ 166.7 and 166.6 [C(O)NH/D], 155.2 (br, C_{quat}), 134.3 (C_{quat}), 133.7 (C_{quat}), 130.8, 130.5, 128.5, 128.3, 79.4 (br, C_{quat}), 68.2 (C_{quat}), 29.0 (2C), 26.1 and 26.0 (CH_3NH/D).

HRMS (MALDI-TOF) calcd for $C_{13}H_{16}IN_4O_2$ $[M+H]^+$ 387.0312; found 387.0314.

2-[4-(2-Hydroxyethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1k)



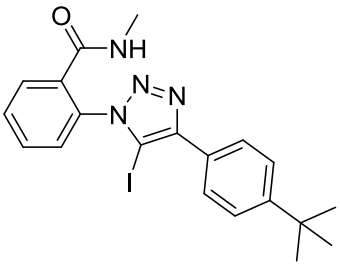
Prepared from azide **S2a** (176.2 mg, 1.0 mmol) and iodoalkyne **S3d** (215.6 mg, 1.1 mmol, 1.1 equiv) according to **GP2** at room temperature; due to a low solubility the precipitated product was isolated by filtration, washed with CH_2Cl_2, and dried *in vacuo*. Yield 329.0 mg (88%). White solid; mp 161–163 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (br q, J = 4.6 Hz, 1H), 7.73–7.64 (m, 3H), 7.45 (m, 1H), 4.78 (br t, J = 5.3 Hz, 1H), 3.67 (br td, J = 7.4, 5.3 Hz, 2H), 2.78 (t, J = 7.4 Hz, 2H), 2.59 (d, J = 4.6 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6) δ 165.5 (C_{quat}), 147.9 (C_{quat}), 134.8 (C_{quat}), 134.3 (C_{quat}), 130.6, 130.3, 128.6, 128.5, 85.9 (C_{quat}), 60.1, 29.9, 26.1.

HRMS (MALDI-TOF) calcd for $C_{12}H_{14}IN_4O_2$ $[M+H]^+$ 373.0156; found 373.0160.

2-[4-(4-*tert*-Butylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1l)



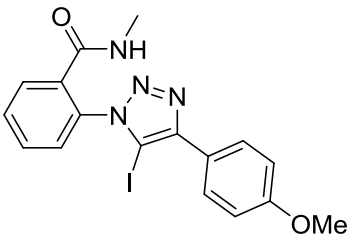
Prepared from azide **S2a** (176.2 mg, 1.0 mmol) and iodoalkyne **S3g** (312.5 mg, 1.1 mmol, 1.1 equiv) according to **GP2** at room temperature; eluent: hexanes–CH_2Cl_2–EtOAc = 1:1:2. Yield 435 mg (94%). Beige solid; mp 180–182 °C.

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 7.95–7.89 (m, 2H), 7.77 (m, 1H), 7.73–7.66 (m, 2H), 7.56–7.50 (m, 2H), 7.48 (m, 1H), 2.76 (s, 3H), 1.38 (s, 9H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$–CD_3OD) δ 166.6 (C_{quat}), 151.4 (C_{quat}), 149.4 (C_{quat}), 134.1 (C_{quat}), 133.8 (C_{quat}), 130.6, 130.4, 128.4, 128.3, 126.7 (2C), 126.4 (C_{quat}), 125.0 (2C), 80.6 (C_{quat}), 34.1 (C_{quat}), 30.5 (3C), 25.8.

HRMS (MALDI-TOF) calcd for $C_{20}H_{22}IN_4O$ $[M+H]^+$ 461.0833; found 461.0832.

2-[5-Iodo-4-(4-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1m)



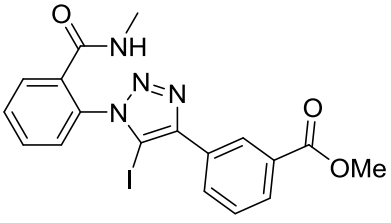
Prepared from azide **S2a** (176.2 mg, 1.0 mmol) and iodoalkyne **S3h** (284 mg, 1.1 mmol, 1.1 equiv) according to **GP2** at room temperature; eluent: hexanes–EtOAc = 1:1. Yield 390 mg (90%). Beige solid; mp 171–173 °C.

^{1}H NMR (400 MHz, $CDCl_3$–DMSO-d_6) δ 8.23 (br s, 1H), 7.99–7.93 (m, 2H), 7.76 (m, 1H), 7.71–7.62 (m, 2H), 7.46 (m, 1H), 7.05–6.98 (m, 2H), 3.85 (s, 3H), 2.70 (d, J = 4.5 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$–DMSO-d_6) δ 164.3 (C_{quat}), 157.9 (C_{quat}), 146.9 (C_{quat}), 133.4 (C_{quat}), 133.1 (C_{quat}), 129.0, 128.8, 127.3 (2C), 126.9 (2C), 121.3 (C_{quat}), 112.3 (2C), 80.4 (C_{quat}), 53.7, 24.8.

HRMS (MALDI-TOF) calcd for $C_{17}H_{16}IN_4O_2$ $[M+H]^+$ 435.0312; found 435.0308.

Methyl 3-(5-iodo-1-{2-[(methylamino)carbonyl]phenyl}-1*H*-1,2,3-triazol-4-yl)benzoate (1n)



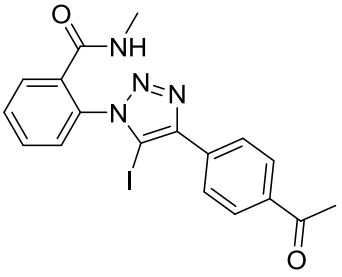
Prepared from azide **S2a** (123.3 mg, 0.7 mmol) and iodoalkyne **S3i** (230.3 mg, 0.105 mmol, 1.15 equiv) according to **GP2**; eluent: CH_2Cl_2–MeOH = 30:1. Yield 317.7 mg (98%). White solid; mp 147–149 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (t, J = 1.8 Hz, 1H), 8.25 (ddd, J = 7.8, 1.8, 1.2 Hz, 1H), 8.10 (ddd, J = 7.8, 1.8, 1.2 Hz, 1H), 7.83 (m, 1H), 7.69–7.63 (m, 2H), 7.58 (t, J = 7.8 Hz, 1H), 7.40 (m, 1H), 6.09 (br q, J = 4.9 Hz, 1H), 3.96 (s, 3H), 2.77 (d, J = 4.9 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 166.7 (C_{quat}), 165.8 (C_{quat}), 149.0 (C_{quat}), 134.7 (C_{quat}), 133.9 (C_{quat}), 131.7, 131.2, 131.1, 130.5 (C_{quat}), 130.1 (C_{quat}), 129.8, 129.4, 128.7 (2C), 128.4, 81.1 (C_{quat}), 52.3, 26.9.

HRMS (MALDI-TOF) calcd for $C_{18}H_{16}IN_4O_3$ $[M+H]^+$ 463.0262; found 463.0254.

2-[4-(4-Acetylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1o)



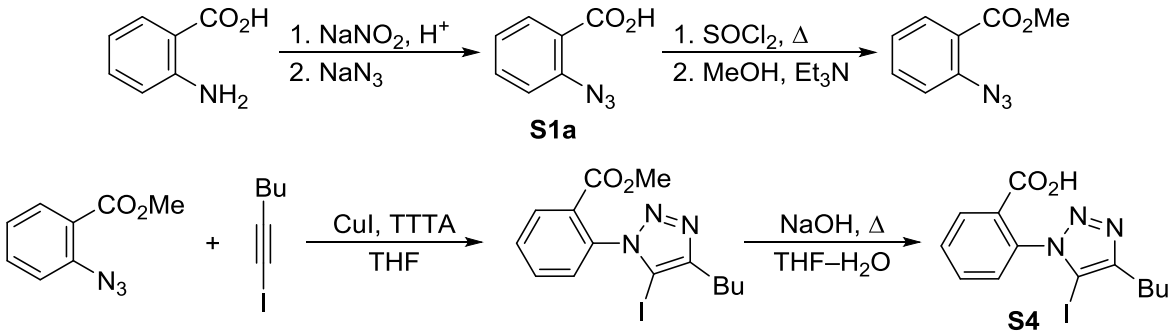
Prepared from azide **S2a** (123.3 mg, 0.7 mmol) and iodoalkyne **S3j** (217.4 mg, 0.105 mmol, 1.15 equiv) according to **GP2**; eluent: hexanes–EtOAc = 1:2. Yield 215.1 mg (69%). Light beige solid; mp 170–173 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 8.21–8.16 (m, 2H), 8.10–8.06 (m, 2H), 7.80 (m, 1H), 7.70–7.63 (m, 2H), 7.41 (m, 1H), 6.39 (br q, J = 4.5 Hz, 1H), 2.76 (d, J = 4.5 Hz, 3H, CH_3NH), 2.75 (s, 3H, CH_3ND), 2.66 (s, 3H).

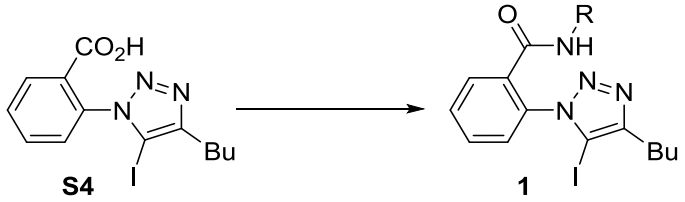
$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 197.8 (C_{quat}), 166.0 and 165.9 [C(O)NH/D], 148.6 (C_{quat}), 136.7 (C_{quat}), 134.63 and 134.59 [C_{Ar}C(O)NH/D], 134.3 (C_{quat}), 133.9 (C_{quat}), 131.2, 131.0, 129.2, 128.7, 128.6 (2C), 127.3 (2C), 81.7 (C_{quat}), 26.8 and 26.64 (CH_3NH/D), 26.62.

HRMS (MALDI-TOF) calcd for $C_{18}H_{16}IN_4O_2$ $[M+H]^+$ 447.0312; found 447.0309.

Scheme for the synthesis of 2-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzoic acid[4] (S4)



Synthesis of 2-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzamides 1



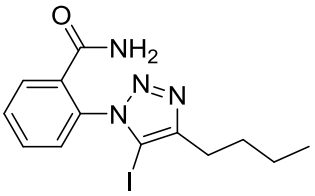
GP4: 1. *i*-BuOC(O)Cl, Et_3N, THF, 0 °C; 2. RNH_2, rt
GP5: RNH_2, HBTU, Et_3N, DMF, rt

General procedure 4 (GP4). The suspension of 2-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzoic acid **S4** (222.7 mg, 0.6 mmol, 1 equiv) in THF (4 mL) was cooled in an ice bath. Then isobutyl

chloroformate (116.7 μL, 0.9 mmol, 1.5 equiv) and Et_3N (167.3 μL, 1.2 mmol, 2 equiv) were added to the reaction mixture. After stirring for 40 min, the corresponding primary amine (1.2 mmol, 2 equiv) was added and the stirring was continued at ambient temperature. Upon completion of the reaction, the mixture was diluted with CH_2Cl_2 (30 mL) and washed with water (30 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The crude product was purified by column chromatography.

General procedure 5 (GP5). 2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzoic acid **S4** (222.7 mg, 0.6 mmol, 1 equiv), 2-(1*H*-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HBTU) (273.1 mg, 0.72 mmol, 1.2 equiv), Et_3N (167.3 μL, 1.2 mmol, 2 equiv), and the corresponding primary amine (0.72 mmol, 1.2 equiv) were mixed under an Ar atmosphere in DMF (6 mL). After stirring at ambient temperature overnight, the solvent was evaporated *in vacuo*. The obtained residue was dissolved in CH_2Cl_2 (30 mL) and washed with water (4×30 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The crude product was purified by column chromatography.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzamide (1p)



Prepared from carboxylic acid **S4** (259.8 mg, 0.7 mmol) and 25% aqueous ammonia (210 μL, 0.28 mmol, 4 equiv) according to **GP4**; eluent: CH_2Cl_2–MeOH = 20:1. Yield 236.9 mg (91%). White solid; mp 114–116 °C.

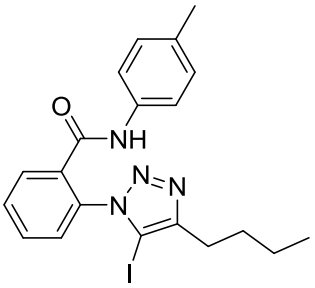
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (m, 1H), 7.68–7.61 (m, 2H), 7.32 (m, 1H), 5.77 (br s, 1H), 5.70 (br s, 1H), 2.73 (m, 2H), 1.73 (m, 2H), 1.40 (m, 2H), 0.96 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 166.9 (C_{quat}), 152.7 (C_{quat}), 134.1 (C_{quat}), 133.5 (C_{quat}), 131.6, 131.0, 130.1, 128.5, 82.6 (C_{quat}), 31.0, 25.8, 22.2, 13.8.

Anal. calcd for $C_{13}H_{15}IN_4O$: C, 42.18; H, 4.08; N, 15.13; found C, 42.44; H, 4.22; N, 14.88.

HRMS (MALDI-TOF) calcd for $C_{13}H_{16}IN_4O$ $[M+H]^+$ 371.0363; found 371.0362.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methylphenyl)benzamide (1q)



Prepared from carboxylic acid **S4** (259.8 mg, 0.7 mmol) and *p*-toluidine (90.0 mg, 0.84 mmol, 1.2 equiv) according to **GP5**; eluent: hexanes–EtOAc = 2:1. Yield 291.8 mg (91%). White solid; mp 148–149 °C.

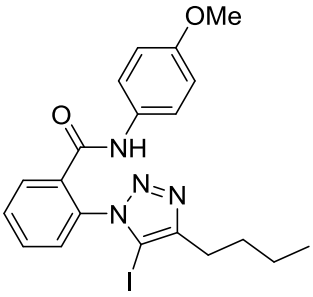
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (m, 1H), 7.69–7.61 (m, 2H), 7.55 (br s, 1H), 7.35 (m, 1H), 7.25–7.19 (m, 2H), 7.05–7.00 (m, 2H), 2.66 (m, 2H), 2.26 (s, 3H), 1.59 (m, 2H), 1.26 (m, 2H), 0.83 (t, J = 7.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 162.8 (C_{quat}), 153.1 (C_{quat}), 134.8 (C_{quat}), 134.7 (C_{quat}), 134.4 (C_{quat}), 133.7 (C_{quat}), 131.5, 131.3, 130.6, 129.4 (2C), 128.5, 119.9 (2C), 82.8 (C_{quat}), 31.0, 25.8, 22.1, 20.8, 13.7.

Anal. calcd for $C_{20}H_{21}IN_4O$: C, 52.19; H, 4.60; N, 12.17; found C, 52.26; H, 4.86; N, 11.89.

HRMS (MALDI-TOF) calcd for $C_{20}H_{22}IN_4O$ $[M+H]^+$ 461.0833; found 461.0835.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methoxyphenyl)benzamide (1r)



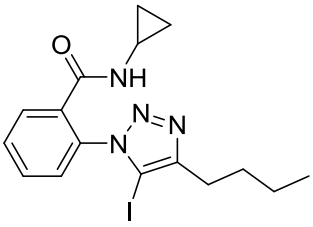
Prepared from carboxylic acid **S4** (259.8 mg, 0.7 mmol) and *p*-anisidine (103.4 mg, 0.84 mmol, 1.2 equiv) according to **GP5**; eluent: CH_2Cl_2–MeOH = 20:1. Yield 311 mg (93%). Beige solid; mp 123–125 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (m, 1H), 7.72–7.64 (m, 2H), 7.51 (br s, 1H), 7.38 (m, 1H), 7.29–7.24 (m, 2H), 6.81–6.76 (m, 2H), 3.76 (s, 3H), 2.69 (m, 2H), 1.62 (m, 2H), 1.29 (m, 2H), 0.86 (t, J = 7.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 162.9 (C_{quat}), 156.4 (C_{quat}), 152.7 (C_{quat}), 134.6 (C_{quat}), 133.7 (C_{quat}), 131.2, 130.9, 130.4 (C_{quat}), 130.1, 128.3, 121.7 (2C), 113.8 (2C), 82.9 (C_{quat}), 55.3, 30.9, 25.7, 22.0, 13.7.

HRMS (MALDI-TOF) calcd for $C_{20}H_{22}IN_4O_2$ $[M+H]^+$ 477.0782; found 477.0778.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-cyclopropylbenzamide (1s)



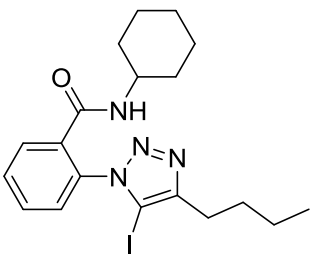
Prepared from carboxylic acid **S4** (222.7 mg, 0.6 mmol) and cyclopropylamine (49.9 μL, 0.72 mmol, 1.2 equiv) according to **GP5**; eluent: hexanes–CH_2Cl_2–EtOAc = 1:1:2. Yield 204 mg (83%). White solid; mp 133–135 °C.

^1H NMR (600 MHz, $CDCl_3$) δ 7.86 (m, 1H), 7.63 (m, 1H), 7.60 (m, 1H), 7.29 (m, 1H), 5.82 (br s, 1H), 2.72 (m, 2H), 2.61 (ttd, J = 7.1, 3.8, 3.2 Hz, 1H), 1.73 (m, 2H), 1.43 (m, 2H), 0.96 (t, J = 7.4 Hz, 3H), 0.70–0.61 (m, 2H), 0.24–0.16 (m, 2H).

$^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 166.4 (C_{quat}), 152.6 (C_{quat}), 134.5 (C_{quat}), 133.9 (C_{quat}), 131.2, 131.1, 130.1, 128.2, 82.6 (C_{quat}), 31.0, 25.8, 22.7, 22.3, 13.8, 6.5 (2C).

HRMS (MALDI-TOF) calcd for $C_{16}H_{20}IN_4O$ $[M+H]^+$ 411.0676; found 411.0675.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-cyclohexylbenzamide (1t)



Prepared from carboxylic acid **S4** (222.7 mg, 0.6 mmol) and cyclohexylamine (136.8 μL, 1.2 mmol, 2 equiv) according to **GP4**; eluent: hexanes–EtOAc = 2:1. Yield 254 mg (94%). White solid; mp 96–98 °C.

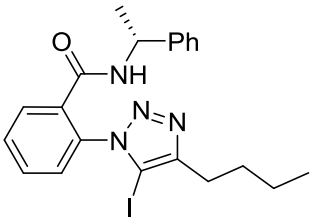
^1H NMR (400 MHz, $CDCl_3$) δ 7.88 (m, 1H), 7.64 (m, 1H), 7.60 (m,

1H), 7.29 (m, 1H), 5.52 (br d, *J* = 7.9 Hz, 1H), 3.69 (tdt, *J* = 10.7, 7.9, 4.0 Hz, 1H), 2.73 (m, 2H), 1.78–1.64 (m, 4H), 1.63–1.50 (m, 2H), 1.44 (m, 2H), 1.33–1.20 (m, 3H), 1.07 (m, 1H), 0.97 (t, *J* = 7.4 Hz, 3H), 0.92–0.81 (m, 2H).

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 164.0 (C_{quat}), 152.6 (C_{quat}), 135.0 (C_{quat}), 133.7 (C_{quat}), 131.1, 131.0, 130.1, 128.3, 82.7 (C_{quat}), 48.5, 32.4 (2C), 31.1, 25.8, 25.2, 24.6 (2C), 22.3, 13.8.

HRMS (MALDI-TOF) calcd for $C_{19}H_{26}IN_4O$ $[M+H]^+$ 453.1146; found 453.1141.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[(1*R*)-1-phenylethyl]benzamide (1u)



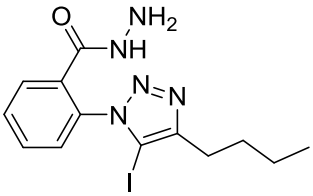
Prepared from carboxylic acid **S4** (276.3 mg, 0.744 mmol) and (*R*)-1-phenylethylamine (116 µL, 0.893 mmol, 1.2 equiv) according to **GP4**; eluent: hexanes–EtOAc = 1:1. Yield 335.8 mg (95%). White solid; mp 85–87 °C.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (m, 1H), 7.62 (m, 1H), 7.60 (m, 1H), 7.30–7.26 (m, 3H), 7.22 (m, 1H), 7.15–7.12 (m, 2H), 5.99 (br d, *J* = 7.6 Hz, 1H), 5.03 (dq, *J* = 7.6, 6.9 Hz, 1H), 2.71–2.62 (m, 2H), 1.71 (m, 2H), 1.43 (m, 2H), 1.27 (d, *J* = 6.9 Hz, 3H), 0.96 (t, *J* = 7.4 Hz, 3H).

$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 164.0 (C_{quat}), 152.7 (C_{quat}), 142.3 (C_{quat}), 134.6 (C_{quat}), 133.8 (C_{quat}), 131.2, 131.1, 130.3, 128.6 (2C), 128.4, 127.4, 126.1 (2C), 82.6 (C_{quat}), 49.4, 31.0, 25.9, 22.4, 21.4, 13.8.

HRMS (MALDI-TOF) calcd for $C_{21}H_{24}IN_4O$ $[M+H]^+$ 475.0989; found 475.0987.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzohydrazide (1v)



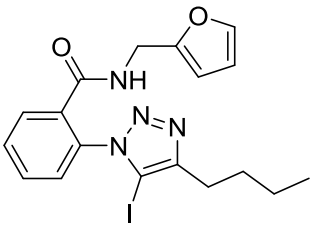
Prepared from carboxylic acid **S4** (111.4 mg, 0.3 mmol) and hydrazine hydrate (67.4 µL, 1.5 mmol, 5 equiv) according to **GP4**; eluent: CH_2Cl_2–MeOH = 20:1. Yield 89.0 mg (77%). Pale yellow solid; mp 94–96 °C.

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 7.72 (m, 1H), 7.66–7.58 (m, 2H), 7.36 (m, 1H), 3.16 (br s, 3H), 2.71 (m, 2H), 1.72 (m, 2H), 1.40 (m, 2H), 0.95 (t, *J* = 7.3 Hz, 3H).

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD) δ 166.2 (C_{quat}), 152.1 (C_{quat}), 134.4 (C_{quat}), 132.3 (C_{quat}), 131.2, 130.7, 129.1, 128.4, 82.2 (C_{quat}), 30.8, 25.6, 22.1, 13.6.

HRMS (MALDI-TOF) calcd for $C_{13}H_{16}IN_4O$ $[M–NH_3+H]^+$ 371.0363; found 371.0358.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(2-furylmethyl)benzamide (1w)



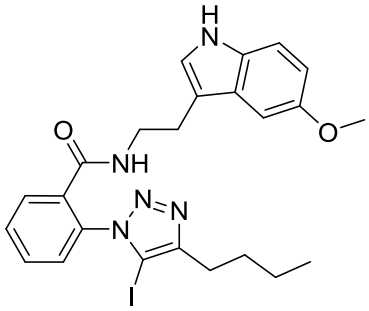
Prepared from carboxylic acid **S4** (297 mg, 0.8 mmol) and (2-furylmethyl)amine (144.3 µL, 1.6 mmol) according to **GP4**; eluent: hexanes–EtOAc = 2:1. Yield 291.3 mg (81%). Beige solid; mp 203–205 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (m, 1H), 7.63–7.56 (m, 2H), 7.32–7.26 (m, 2H), 6.25 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.14 (br t, *J* = 5.6 Hz, 1H), 6.10 (m, 1H), 4.31 (d, *J* = 5.6 Hz, 2H), 2.65 (m, 2H), 1.68 (m, 2H), 1.39 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 164.8 (C_{quat}), 152.4 (C_{quat}), 150.3 (C_{quat}), 142.1, 134.0 (C_{quat}), 133.9 (C_{quat}), 131.2, 130.9, 129.9, 128.5, 110.3, 107.5, 82.4 (C_{quat}), 36.8, 30.9, 25.8, 22.2, 13.8.

HRMS (MALDI-TOF) calcd for $C_{18}H_{20}IN_4O_2$ $[M+H]^+$ 451.0625; found 451.0627.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]benzamide (1x)



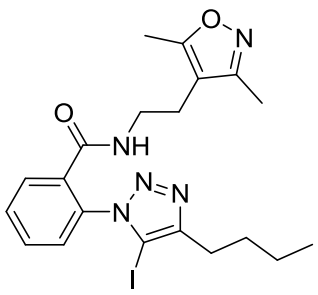
Prepared from carboxylic acid **S4** (297 mg, 0.8 mmol) and [2-(5-methoxy-1*H*-indol-3-yl)ethyl]amine (228.3 mg, 1.2 mmol, 1.5 equiv) according to **GP4**; eluent: CH_2Cl_2–MeOH = 50:1. Yield 370.6 mg (85%). Beige solid; mp 81–83 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (br s, 1H), 7.72 (m, 1H), 7.60–7.53 (m, 2H), 7.29 (m, 1H), 7.19 (d, *J* = 8.8 Hz, 1H), 6.99–6.94 (m, 2H), 6.81 (dd, *J* = 8.8, 2.4 Hz, 1H), 5.87 (br t, *J* = 5.7 Hz, 1H), 3.81 (s, 3H), 3.49 (td, *J* = 6.8, 5.7 Hz, 2H), 2.72 (t, *J* = 6.8 Hz, 2H), 2.64 (m, 2H), 1.69 (m, 2H), 1.38 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.3 (C_{quat}), 153.9 (C_{quat}), 152.5 (C_{quat}), 134.7 (C_{quat}), 134.0 (C_{quat}), 131.5 (C_{quat}), 131.0, 130.9, 129.6, 128.3, 127.4 (C_{quat}), 123.2, 112.3, 112.0, 111.8 (C_{quat}), 100.3, 82.5 (C_{quat}), 55.9, 39.9, 31.1, 25.7, 24.8, 22.3, 13.8.

HRMS (MALDI-TOF) calcd for $C_{24}H_{27}IN_5O_2$ $[M+H]^+$ 544.1204; found 544.1203.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[2-(3,5-dimethylisoxazol-4-yl)ethyl]benzamide (1y)



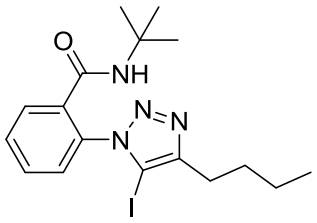
Prepared from carboxylic acid **S4** (297 mg, 0.8 mmol) and [2-(3,5-dimethylisoxazol-4-yl)ethyl]amine (224 mg, 1.6 mmol, 2 equiv) according to **GP4**; eluent: CH_2Cl_2–MeOH = 50:1. Yield 342.2 mg (87%). White solid; mp 166–168 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (m, 1H), 7.64–7.59 (m, 2H), 7.31 (m, 1H), 6.19 (br t, *J* = 5.7 Hz, 1H), 3.18 (m, 2H), 2.71 (m, 2H), 2.33 (m, 2H), 2.27 (s, 3H), 2.16 (s, 3H), 1.70 (m, 2H), 1.40 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.7 (C_{quat}), 165.4 (C_{quat}), 159.5 (C_{quat}), 152.6 (C_{quat}), 134.4 (C_{quat}), 133.9 (C_{quat}), 131.2, 131.0, 129.6, 128.4, 110.2 (C_{quat}), 82.5 (C_{quat}), 39.5, 31.1, 25.8, 22.2, 22.0, 13.8, 10.9, 10.1.

HRMS (MALDI-TOF) calcd for $C_{20}H_{25}IN_5O_2$ $[M+H]^+$ 494.1047; found 494.1049.

_N_-(_tert_-Butyl)-2-(4-butyl-5-iodo-1_H_-1,2,3-triazol-1-yl)benzamide (1z)



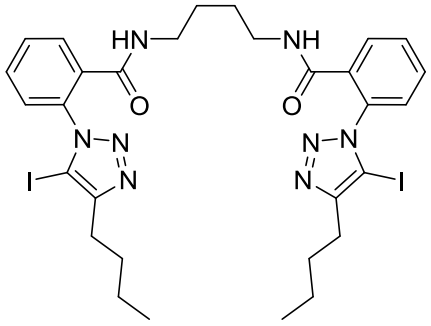
Prepared from carboxylic acid **S4** (222.7 mg, 0.6 mmol) and *tert*-butylamine (126.1 μL, 1.2 mmol, 2 equiv) according to **GP4**; eluent: hexanes–EtOAc = 2:1. Yield 205 mg (80%). White solid; mp 111–113 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (m, 1H), 7.62 (m, 1H), 7.58 (m, 1H), 7.28 (m, 1H), 5.42 (br s, 1H), 2.73 (m, 2H), 1.73 (m, 2H), 1.44 (m, 2H), 1.16 (s, 9H), 0.96 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 164.1 (C_{quat}), 152.6 (C_{quat}), 135.9 (C_{quat}), 133.6 (C_{quat}), 131.1, 130.8, 129.9, 128.1, 82.6 (C_{quat}), 51.6 (C_{quat}), 31.1, 28.2 (3C), 25.8, 22.3, 13.7.

HRMS (MALDI-TOF) calcd for $C_{17}H_{24}IN_4O$ $[M+H]^+$ 427.0989; found 427.0988.

_N_,_N'_-Butane-1,4-diylbis[2-(4-butyl-5-iodo-1_H_-1,2,3-triazol-1-yl)benzamide] (1aa)



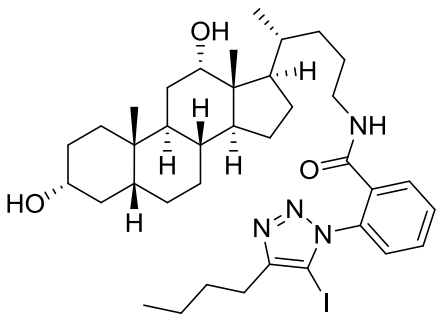
Prepared from carboxylic acid **S4** (267.2 mg, 0.72 mmol, 2.4 equiv) and butane-1,4-diamine (30.1 μL, 0.3 mmol) according to **GP5**; eluent: hexanes–EtOAc = 1:4. Yield 113.0 mg (47%). White solid; mp 135–137 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (m, 2H), 7.58–7.51 (m, 4H), 7.28 (m, 1H), 6.62 (br t, J = 5.5 Hz, 2H), 3.22 (m, 4H), 2.71 (m, 4H), 1.71 (m, 4H), 1.41 (m, 4H), 1.34 (m, 4H), 0.96 (t, J = 7.4 Hz, 6H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.4 (2C_{quat}), 152.1 (2C_{quat}), 134.7 (2C_{quat}), 134.2 (2C_{quat}), 130.6 (4C), 129.1 (2C), 128.2 (2C), 82.5 (2C_{quat}), 39.3 (2C), 31.0 (2C), 26.2 (2C), 25.8 (2C), 22.2 (2C), 13.8 (2C).

HRMS (MALDI-TOF) calcd for $C_{30}H_{37}I_2N_8O_2$ $[M+H]^+$ 795.1123; found 795.1122.

2-(4-Butyl-5-iodo-1_H_-1,2,3-triazol-1-yl)-_N_-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl]-benzamide (1ab)



Prepared from carboxylic acid **S4** (222.7 mg, 0.6 mmol) and (3α,5β,12α)-24-aminocholane-3,12-diol[5] (271.9 mg, 0.72 mmol, 1.2 equiv) according to **GP5**; eluent: CH_2Cl_2–MeOH = 20:1. Yield 284 mg (65%). Pale yellow solid; mp 124–126 °C.

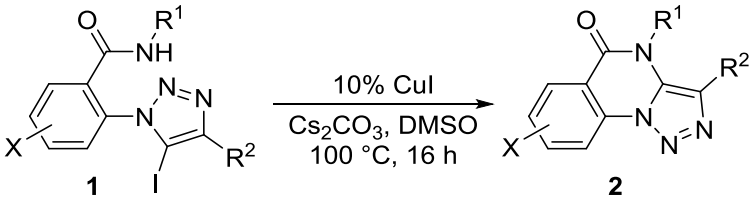
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (m, 1H), 7.65 (m, 1H),

7.62 (m, 1H), 7.32 (m, 1H), 5.96 (br t, J = 5.6 Hz, 1H), 3.96 (m, 1H), 3.59 (tt, J = 11.0, 4.7 Hz, 1H), 3.18–3.03 (m, 2H), 2.74 (m, 2H), 1.99–0.81 (m, 35H), 0.98 (t, J = 7.4 Hz, 3H), 0.90 (s, 3H), 0.66 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 165.1 (C_{quat}), 152.3 (C_{quat}), 134.9 (C_{quat}), 133.7 (C_{quat}), 130.9, 130.7, 129.7, 128.2, 82.7 (C_{quat}), 73.0, 71.5, 47.9, 47.2, 46.3, 42.0, 40.4, 36.3, 35.9, 35.3, 35.2, 34.0, 33.4, 32.7, 31.0, 30.2, 28.3, 27.5, 27.1, 26.0, 26.0, 25.7, 23.6, 23.0, 22.2, 17.4, 13.7, 12.5.

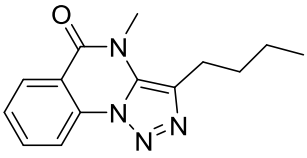
HRMS (MALDI-TOF) calcd for $C_{37}H_{56}IN_4O_3$ $[M+H]^+$ 731.3392; found 731.3396.

Synthesis of [1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-ones 2



General procedure 6 (GP6). In a vial with screw cap, 2-(5-iodotriazolyl)benzamide **1** (0.20 mmol, 1 equiv), CuI (3.8 mg, 0.020 mmol, 10 mol %), and Cs_2CO_3 (130.3 mg, 0.40 mmol, 2 equiv) were mixed under an Ar atmosphere in DMSO (2 mL). The reaction mixture was stirred at 100 °C in a dry block for 16 h, then diluted with CH_2Cl_2 (20 mL), washed with EDTA solution (20 mL) and water (4×20 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was subjected to column chromatography on silica gel to afford pure triazole-fused lactam **2**.

3-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2a)



Prepared from iodotriazole **1a** (76.8 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 4:1. Yield 51.0 mg (99%). White solid; mp 97–98 °C.

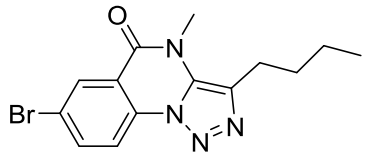
^1H NMR (400 MHz, $CDCl_3$) δ 8.34 (br d, J = 8.3 Hz, 1H), 8.29 (dd, J = 7.9, 1.4 Hz, 1H), 7.81 (ddd, J = 8.3, 7.4, 1.4 Hz, 1H), 7.53 (m, 1H), 3.76 (s, 3H), 3.00 (m, 2H), 1.77 (m, 2H), 1.46 (m, 2H), 0.97 (t, J = 7.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.9 (C_{quat}), 134.9, 134.5 (C_{quat}), 132.5 (C_{quat}), 130.3 (C_{quat}), 129.1, 127.5, 115.9 (C_{quat}), 115.3, 33.1, 30.6, 25.9, 22.3, 13.8.

IR (KBr, cm^{-1}) ν 2954, 2925, 2870, 1670, 1622, 1604, 1574, 1516, 1485, 1469, 1454, 1387, 1334, 1317, 1244, 1136, 1099, 1072, 995, 781, 762, 685.

HRMS (MALDI-TOF) calcd for $C_{14}H_{17}N_4O$ $[M+H]^+$ 257.1397; found 257.1389.

3-Butyl-7-bromo-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2b)



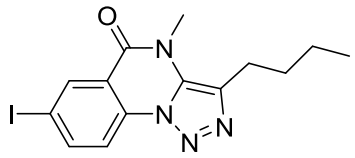
Prepared from iodotriazole **1b** (92.6 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 58 mg (87%). Pale pink solid; mp 150–152 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, J = 2.1 Hz, 1H), 8.23 (d, J = 8.7 Hz, 1H), 7.91 (dd, J = 8.7, 2.1 Hz, 1H), 3.77 (s, 3H), 3.00 (m, 2H), 1.78 (m, 2H), 1.47 (m, 2H), 0.99 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 157.7 (C_{quat}), 137.9, 133.3 (C_{quat}), 132.3 (C_{quat}), 131.8, 130.5 (C_{quat}), 121.1 (C_{quat}), 117.3 (C_{quat}), 117.1, 33.0, 30.7, 25.8, 22.3, 13.8.

HRMS (MALDI-TOF) calcd for $C_{14}H_{16}BrN_4O$ $[M+H]^+$ 335.0502; found 335.0504.

3-Butyl-7-iodo-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2c)



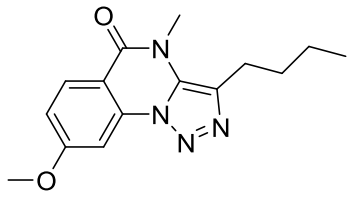
Prepared from iodotriazole **1c** (102.0 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 62 mg (81%). White solid; mp 131–133 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (m, 1H), 8.12–8.06 (m, 2H), 3.76 (s, 3H), 3.00 (m, 2H), 1.78 (m, 2H), 1.47 (m, 2H), 0.98 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 157.5 (C_{quat}), 143.5, 137.8, 133.9 (C_{quat}), 132.3 (C_{quat}), 130.5 (C_{quat}), 117.3 (C_{quat}), 117.0, 91.7 (C_{quat}), 33.0, 30.7, 25.8, 22.3, 13.8.

HRMS (MALDI-TOF) calcd for $C_{14}H_{16}IN_4O$ $[M+H]^+$ 383.0363; found 383.0362.

3-Butyl-8-methoxy-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2d)



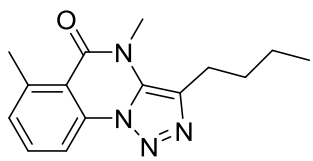
Prepared from iodotriazole **1d** (82.8 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 37.5 mg (65%). Yellow solid; mp 84–86 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 8.9 Hz, 1H), 7.73 (d, J = 2.4 Hz, 1H), 7.04 (dd, J = 8.9, 2.4 Hz, 1H), 3.99 (s, 3H), 3.75 (s, 3H), 3.01 (m, 2H), 1.78 (m, 2H), 1.48 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 164.8 (C_{quat}), 158.7 (C_{quat}), 136.1 (C_{quat}), 132.9 (C_{quat}), 130.8, 130.2 (C_{quat}), 116.3, 108.8 (C_{quat}), 97.7, 56.1, 33.1, 30.3, 25.9, 22.3, 13.8.

HRMS (MALDI-TOF) calcd for $C_{15}H_{19}N_4O_2$ $[M+H]^+$ 287.1503; found 287.1506.

3-Butyl-4,6-dimethyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2e)



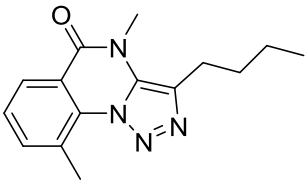
Prepared from iodotriazole **1e** (79.6 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 18 mg (33%). Beige solid; mp 94–96 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (m, 1H), 7.66 (m, 1H), 7.33 (m, 1H), 3.72 (s, 3H), 3.00 (m, 2H), 2.88 (s, 3H), 1.77 (m, 2H), 1.47 (m, 2H), 0.98 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.7 (C_{quat}), 143.4 (C_{quat}), 135.8 (C_{quat}), 134.0, 133.1 (C_{quat}), 132.4 (C_{quat}), 130.9, 129.6 (C_{quat}), 113.5, 33.1, 30.4, 25.9, 23.2, 22.3, 13.8.

HRMS (MALDI-TOF) calcd for $C_{15}H_{19}N_4O$ $[M+H]^+$ 271.1553; found 271.1556.

3-Butyl-4,9-dimethyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2f)



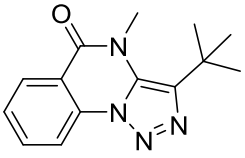
Prepared from iodotriazole **1f** (79.6 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 45 mg (83%). White solid; mp 114–116 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (m, 1H), 7.63 (m, 1H), 7.41 (m, 1H), 3.78 (s, 3H), 3.03 (m, 2H), 2.96 (s, 3H), 1.80 (m, 2H), 1.48 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.2 (C_{quat}), 138.1, 133.6 (C_{quat}), 132.8 (C_{quat}), 128.9 (C_{quat}), 128.6 (C_{quat}), 127.0, 126.8, 117.1 (C_{quat}), 33.0, 30.7, 25.9, 23.4, 22.3, 13.8.

HRMS (MALDI-TOF) calcd for $C_{15}H_{19}N_4O$ $[M+H]^+$ 271.1553; found 271.1555.

3-*tert*-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2g)



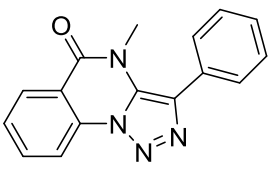
Prepared from iodotriazole **1g** (76.8 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 39 mg (76%). White solid; mp 140–142 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (br d, J = 8.2 Hz, 1H), 8.31 (br d, J = 7.9 Hz, 1H), 7.83 (m, 1H), 7.56 (m, 1H), 3.89 (s, 3H), 1.61 (s, 9H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 160.0 (C_{quat}), 138.0 (C_{quat}), 134.9, 134.8 (C_{quat}), 133.1 (C_{quat}), 128.9, 127.6, 115.5 (2C, CH + C_{quat}), 35.3, 32.2 (3C), 31.8 (C_{quat}).

HRMS (MALDI-TOF) calcd for $C_{14}H_{17}N_4O$ $[M+H]^+$ 257.1397; found 257.1402.

4-Methyl-3-phenyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2h)



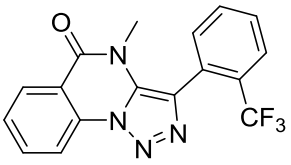
Prepared from iodotriazole **1h** (80.8 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 41.6 mg (75%). The reaction performed with 1.451 g (3.59 mmol) of **1h** afforded 806.1 mg (81%) of **2h**. White solid; mp 195–196 °C (lit.[6] 200 °C (dec.)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (br d, J = 8.2 Hz, 1H), 8.31 (br d, J = 7.9 Hz, 1H), 7.86 (m, 1H), 7.61–7.54 (m, 3H), 7.53–7.44 (m, 3H), 3.41 (s, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.9 (C_{quat}), 135.0, 134.4 (C_{quat}), 132.6 (C_{quat}), 131.0 (C_{quat}), 130.6 (2C), 130.3 (C_{quat}), 129.0, 128.8, 128.3 (2C), 127.8, 115.9 (C_{quat}), 115.3, 32.3.

HRMS (MALDI-TOF) calcd for $C_{16}H_{12}N_4KO$ $[M+K]^+$ 315.0643; found 315.0645.

4-Methyl-3-[2-(trifluoromethyl)phenyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2i)



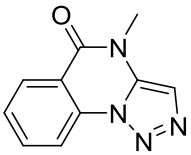
Prepared from iodotriazole **1i** (94.4 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 68.5 mg (99%). White solid; mp 185–187 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (br d, J = 8.2 Hz, 1H), 8.36 (m, 1H), 7.90 (m, 1H), 7.86 (m, 1H), 7.72–7.56 (m, 4H), 3.23 (s, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.8 (C_{quat}), 135.1, 134.4 (C_{quat}), 134.0, 133.5 (C_{quat}), 131.6, 131.2 (q, J_{CF} = 29.3 Hz, C_{quat}), 129.9, 129.2, 128.9 (C_{quat}), 127.9, 126.7 (C_{quat}), 126.3, 123.6 (q, J_{CF} = 273 Hz, CF_3), 116.0 (C_{quat}), 115.4, 31.3.

HRMS (MALDI-TOF) calcd for $C_{17}H_{12}F_3N_4O$ $[M+H]^+$ 345.0958; found 345.0961.

4-Methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2j)



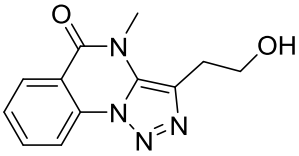
Prepared from iodotriazole **1j** (77.2 mg, 0.2 mmol) according to **GP6**; eluent: CH_2Cl_2–EtOAc = 2:1. Yield 30.0 mg (75%). Off-white solid; mp 215–216 °C.

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 8.39 (br d, J = 8.3 Hz, 1H), 8.36 (m, 1H), 7.91 (m, 1H), 7.63 (m, 1H), 7.53 (s, 1H), 3.66 (s, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$–CD_3OD) δ 158.5 (C_{quat}), 137.0 (C_{quat}), 135.1, 134.2 (C_{quat}), 129.1, 128.0, 116.4, 116.0 (C_{quat}), 115.2, 31.4.

HRMS (ESI-TOF) calcd for $C_{10}H_9N_4O$ $[M+H]^+$ 201.0771; found 201.0775.

3-(2-Hydroxyethyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2k)



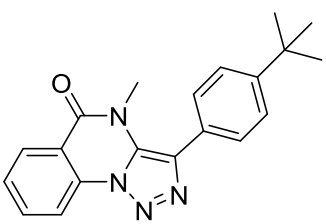
Prepared from iodotriazole **1k** (111.7 mg, 0.3 mmol) according to **GP6**; eluent: CH_2Cl_2–MeOH = 20:1. Yield 57.8 mg (79%). White solid; mp 216–219 °C.

^{1}H NMR (400 MHz, DMSO-d_6–$CDCl_3$ = 3:1 + CD_3OD) δ 8.31 (d, J = 8.2 Hz, 1H), 8.24 (dd, J = 7.9, 1.2 Hz, 1H), 7.92 (m, 1H), 7.62 (m, 1H), 4.76 (br t, J = 5.7 Hz, 0.5H due to H/D exchange), 3.78 (m, 2H), 3.77 (s, 3H), 3.15 (t, J = 6.5 Hz, 2H).

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6–$CDCl_3$ = 3:1 + CD_3OD) δ 158.0 (C_{quat}), 134.8, 134.0 (C_{quat}), 133.6 (C_{quat}), 128.6, 127.39 (C_{quat}), 127.37, 115.6 (C_{quat}), 114.6, 61.2 and 61.1 (CH_2OH/D), 30.2, 29.1 and 29.0 (CH_2CH_2OH/D).

HRMS (MALDI-TOF) calcd for $C_{12}H_{13}N_4O_2$ $[M+H]^+$ 245.1033; found 245.1036.

3-(4-*tert*-Butylphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2l)



Prepared from iodotriazole **1l** (92.1 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 66.1 mg (99%). White solid; mp 183–185 °C.

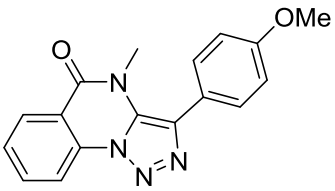
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (br d, J = 8.2 Hz, 1H), 8.31 (br d,

J = 7.8 Hz, 1H), 7.87 (m, 1H), 7.58 (m, 1H), 7.53–7.47 (m, 4H), 3.45 (s, 3H), 1.38 (s, 9H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.0 (C_{quat}), 151.9 (C_{quat}), 135.0, 134.5 (C_{quat}), 132.5 (C_{quat}), 131.1 (C_{quat}), 130.3 (2C), 129.1, 127.7, 127.2 (C_{quat}), 125.3 (2C), 115.9 (C_{quat}), 115.4, 34.7 (C_{quat}), 32.4, 31.3 (3C).

HRMS (MALDI-TOF) calcd for $C_{20}H_{21}N_4O$ $[M+H]^+$ 333.1710; found 333.1701.

3-(4-Methoxyphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2m)



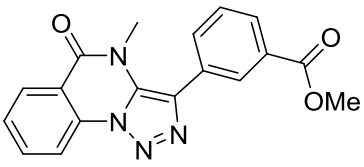
Prepared from iodotriazole **1m** (52.1 mg, 0.12 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 36.1 mg (98%). White solid; mp 204–205 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (br d, *J* = 8.2 Hz, 1H), 8.33 (m, 1H), 7.87 (m, 1H), 7.59 (m, 1H), 7.50–7.45 (m, 2H), 7.04–6.99 (m, 2H), 3.88 (s, 3H), 3.42 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 160.0 (C_{quat}), 159.0 (C_{quat}), 135.0, 134.5 (C_{quat}), 132.5 (C_{quat}), 131.9 (2C), 130.8 (C_{quat}), 129.1, 127.7, 122.4 (C_{quat}), 115.9 (C_{quat}), 115.3, 113.8 (2C), 55.3, 32.1.

HRMS (MALDI-TOF) calcd for $C_{17}H_{15}N_4O_2$ $[M+H]^+$ 307.1190; found 307.1193.

Methyl 3-(4-methyl-5-oxo-4,5-dihydro[1,2,3]triazolo[1,5-*a*]quinazolin-3-yl)benzoate (2n)



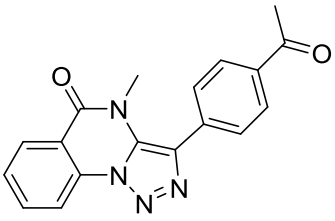
Prepared from iodotriazole **1n** (69.3 mg, 0.15 mmol) according to **GP6**; eluent: hexanes–EtOAc = 1:1. Yield 37.6 mg (75%). White solid; mp 179–181 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 8.44 (br d, *J* = 8.2 Hz, 1H), 8.36 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.24 (m, 1H), 8.16 (m, 1H), 7.90 (ddd, *J* = 8.2, 7.5, 1.4 Hz, 1H), 7.81 (ddd, *J* = 7.6, 1.7, 1.2 Hz, 1H), 7.64–7.57 (m, 2H), 3.95 (s, 3H), 3.43 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 166.4 (C_{quat}), 158.9 (C_{quat}), 135.1, 134.8, 134.4 (C_{quat}), 133.0 (C_{quat}), 131.6, 130.7 (C_{quat}), 130.3 (C_{quat}), 130.0 (C_{quat}), 129.9, 129.2, 128.6, 128.0, 115.9 (C_{quat}), 115.4, 52.3, 32.5.

HRMS (MALDI-TOF) calcd for $C_{18}H_{15}N_4O_3$ $[M+H]^+$ 335.1139; found 335.1138.

3-(4-Acetylphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2o)



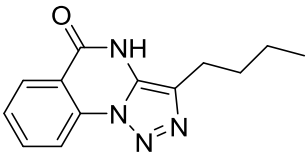
Prepared from iodotriazole **1o** (66.9 mg, 0.15 mmol) according to **GP6**; eluent: hexanes–EtOAc = 1:1. Yield 27.6 mg (58%). White solid; mp 223–224 °C.

^1H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 8.44 (br d, *J* = 8.2 Hz, 1H), 8.36 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.11–8.07 (m, 2H), 7.91 (ddd, *J* = 8.2, 7.5, 1.4 Hz, 1H), 7.72–7.68 (m, 2H), 7.64 (m, 1H), 3.45 (s, 3H), 2.69 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD) δ 197.7 (C_{quat}), 159.0 (C_{quat}), 136.9 (C_{quat}), 135.2, 134.9 (C_{quat}), 134.3 (C_{quat}), 133.0 (C_{quat}), 130.7 (2C), 130.0 (C_{quat}), 129.1, 128.3 (2C), 128.1, 115.9 (C_{quat}), 115.4, 32.7, 26.6.

HRMS (MALDI-TOF) calcd for $C_{18}H_{15}N_4O_2$ $[M+H]^+$ 319.1190; found 319.1184.

3-Butyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2p)



Prepared from iodotriazole **1p** (55.5 mg, 0.15 mmol) according to **GP6**; eluent: CH_2Cl_2–MeOH = 20:1. Yield 24.7 mg (68%). White solid; mp 238–240 °C.

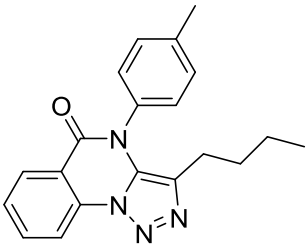
^1H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 8.36 (br d, J = 8.2 Hz, 1H), 8.31 (dd, J = 8.0, 1.2 Hz, 1H), 7.88 (m, 1H), 7.59 (m, 1H), 2.82 (m, 2H), 1.72 (m, 2H), 1.42 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD) δ 159.8 (C_{quat}), 135.2, 135.0 (C_{quat}), 131.0 (C_{quat}), 129.5 (C_{quat}), 128.7, 127.6, 116.3 (C_{quat}), 115.2, 30.9, 23.2, 22.0, 13.4.

IR (KBr, cm^{-1}) ν 2958, 2924, 2873, 2858, 2823, 1670, 1651, 1628, 1614, 1574, 1520, 1483, 1456, 1396, 1383, 1350, 1321, 1238, 1227, 1147, 849, 756, 696, 640, 536.

HRMS (MALDI-TOF) calcd for $C_{13}H_{15}N_4O$ $[M+H]^+$ 243.1240; found 243.1245.

3-Butyl-4-(4-methylphenyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2q)



Prepared from iodotriazole **1q** (46.0 mg, 0.1 mmol) according to **GP6**; eluent: hexanes–EtOAc = 4:1. Yield 23.1 mg (69%). White solid; mp 134–135 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 8.43 (br d, J = 8.2 Hz, 1H), 8.34 (br d, J = 7.9 Hz, 1H), 7.86 (m, 1H), 7.56 (m, 1H), 7.39–7.33 (m, 2H), 7.28–7.22 (m, 2H), 2.45 (s, 3H), 1.89 (m, 2H), 1.30 (m, 2H), 1.04 (m, 2H), 0.70 (t, J = 7.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.2 (C_{quat}), 140.2 (C_{quat}), 135.2, 135.1 (C_{quat}), 132.8 (C_{quat}), 132.5 (C_{quat}), 131.0 (C_{quat}), 130.4 (2C), 129.6, 128.4 (2C), 127.6, 116.3 (C_{quat}), 115.5, 31.9, 24.5, 22.3, 21.3, 13.5.

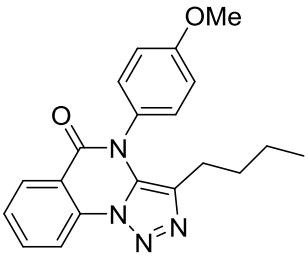
IR (KBr, cm^{-1}) ν 2952, 2925, 2862, 1678, 1618, 1601, 1568, 1512, 1483, 1385, 1319, 1308, 1284, 1171, 1136, 1107, 870, 816, 789, 760, 683.

Anal. calcd for $C_{20}H_{20}N_4O$: C, 72.27; H, 6.06; N, 16.86; found C, 71.92; H, 5.91; N, 16.60.

HRMS (MALDI-TOF) calcd for $C_{20}H_{21}N_4O$ $[M+H]^+$ 333.1710; found 333.1703.

3-Butyl-4-(4-methoxyphenyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2r)

Prepared from iodotriazole **1r** (71.4 mg, 0.15 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 40.1 mg (77%). Beige solid; mp 153–155 °C.

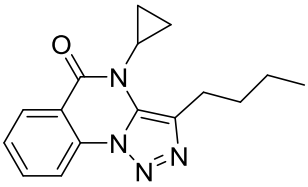


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (br d, J = 8.2 Hz, 1H), 8.35 (dd, J = 8.0, 1.1 Hz, 1H), 7.88 (m, 1H), 7.58 (m, 1H), 7.35–7.29 (m, 2H), 7.11–7.06 (m, 2H), 3.90 (s, 3H), 1.95 (m, 2H), 1.34 (m, 2H), 1.09 (m, 2H), 0.75 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 160.5 (C_{quat}), 159.3 (C_{quat}), 135.2, 135.0 (C_{quat}), 132.6 (C_{quat}), 131.0 (C_{quat}), 129.7 (2C), 129.5, 127.9 (C_{quat}), 127.6, 116.2 (C_{quat}), 115.4, 115.0 (2C), 55.6, 31.9, 24.5, 22.2, 13.6.

HRMS (MALDI-TOF) calcd for $C_{20}H_{21}N_4O_2$ $[M+H]^+$ 349.1659; found 349.1660.

3-Butyl-4-cyclopropyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2s)



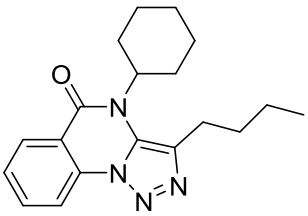
Prepared from iodotriazole **1s** (82.1 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 4:1. Yield 45.6 mg (81%). White solid; mp 125–127 °C.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.34 (br d, J = 8.3 Hz, 1H), 8.27 (dd, J = 7.9, 1.5 Hz, 1H), 7.81 (m, 1H), 7.52 (m, 1H), 3.16 (tt, J = 6.9, 3.8 Hz, 1H), 3.11 (m, 2H), 1.84 (m, 2H), 1.47 (m, 2H), 1.33–1.28 (m, 2H), 1.04–1.01 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 160.0 (C_{quat}), 134.8, 134.6 (C_{quat}), 133.1 (C_{quat}), 131.1 (C_{quat}), 129.0, 127.4, 116.8 (C_{quat}), 115.3, 32.5, 27.1, 25.8, 22.6, 13.9, 10.4 (2C).

HRMS (MALDI-TOF) calcd for $C_{16}H_{19}N_4O$ $[M+H]^+$ 283.1553; found 283.1552.

3-Butyl-4-cyclohexyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2t)



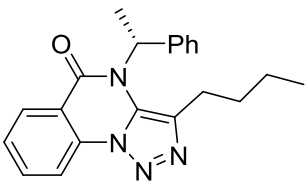
Prepared from iodotriazole **1t** (67.8 mg, 0.15 mmol) according to **GP6**; eluents: hexanes–EtOAc = 10:1 and 4:1. Yield 44.9 mg (92%). White solid; mp 108–110 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (br d, J = 8.1 Hz, 1H), 8.24 (dd, J = 8.0, 1.0 Hz, 1H), 7.78 (m, 1H), 7.51 (m, 1H), 4.10 (tt, J = 12.0, 3.5 Hz, 1H), 2.94 (m, 2H), 2.72 (m, 2H), 1.95 (m, 2H), 1.84 (m, 2H), 1.78–1.67 (m, 3H), 1.48 (m, 2H), 1.39–1.24 (m, 3H), 0.98 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.2 (C_{quat}), 134.6, 134.5 (C_{quat}), 133.0 (C_{quat}), 129.4 (C_{quat}), 128.8, 127.5, 117.6 (C_{quat}), 115.3, 60.9, 32.6, 29.0 (2C), 27.5, 26.4 (2C), 25.0, 22.6, 13.9.

HRMS (MALDI-TOF) calcd for $C_{19}H_{25}N_4O$ $[M+H]^+$ 325.2023; found 325.2030.

3-Butyl-4-[(1*R*)-1-phenylethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2u)



Prepared from iodotriazole **1u** (71.2 mg, 0.15 mmol) according to **GP6**; eluent: hexanes–EtOAc = 4:1. Yield 39.9 mg (77%). White solid; mp 194–195 °C.

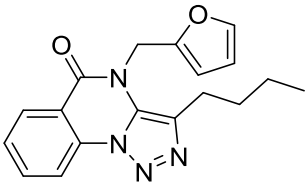
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (br d, J = 8.3 Hz, 1H), 8.24 (br d, J

= 8.0 Hz, 1H), 7.83 (m, 1H), 7.52 (m, 1H), 7.39–7.26 (m, 5H), 5.99 (br s, 1H), 2.87 (m, 1H), 2.75 (m, 1H), 2.06 (d, *J* = 7.0 Hz, 3H), 1.77–1.50 (m, 2H), 1.40–1.27 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.6 (C_{quat}), 139.1 (C_{quat}), 134.9, 134.6 (C_{quat}), 132.5 (C_{quat}), 129.8 (C_{quat}), 129.1, 128.6 (2C), 127.5, 127.4, 125.9 (2C), 116.8 (C_{quat}), 115.3, 55.4 (br), 32.0, 27.0, 22.4, 16.6, 13.7.

HRMS (MALDI-TOF) calcd for $C_{21}H_{23}N_2O$ $[M–N_2+H]^+$ 319.1805; found 319.1808.

3-Butyl-4-(2-furylmethyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2w)



Prepared from iodotriazole **1w** (73.3 mg, 0.163 mmol) according to **GP6**; eluent: hexanes–EtOAc = 4:1. Yield 46.2 mg (88%). White solid; mp 108–109 °C.

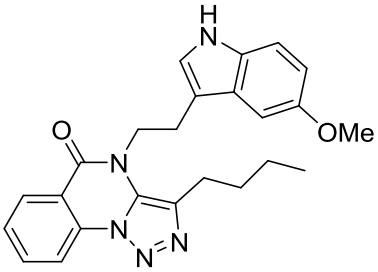
^1H NMR (400 MHz, $CDCl_3$) δ 8.32 (br d, *J* = 8.2 Hz, 1H), 8.24 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.76 (m, 1H), 7.48 (m, 1H), 7.28 (m, 1H), 6.30 (d, *J* = 3.3 Hz, 1H), 6.27 (dd, *J* = 3.3, 1.8 Hz, 1H), 5.33 (s, 2H), 2.95 (m, 2H), 1.70 (m, 2H), 1.40 (m, 2H), 0.90 (t, *J* = 7.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.7 (C_{quat}), 148.6 (C_{quat}), 142.5, 135.1, 134.8 (C_{quat}), 131.9 (C_{quat}), 130.2 (C_{quat}), 129.3, 127.5, 115.8 (C_{quat}), 115.4, 110.7, 108.9, 40.4, 32.4, 25.7, 22.4, 13.8.

IR (KBr, cm^{-1}) *v* 2952, 2922, 2858, 1674, 1620, 1599, 1566, 1510, 1450, 1309, 1240, 1159, 1144, 1068, 1007, 924, 795, 756, 681.

HRMS (MALDI-TOF) calcd for $C_{18}H_{19}N_4O_2$ $[M+H]^+$ 323.1503; found 323.1495.

3-Butyl-4-[2-(5-methoxy-1*H*-indol-3-yl)ethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2x)



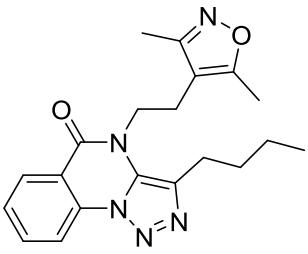
Prepared from iodotriazole **1x** (108.7 mg, 0.2 mmol) according to **GP6**; eluent: CH_2Cl_2–MeOH = 50:1. Yield 67 mg (81%). White solid; mp 239–240 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 8.41 (br d, *J* = 8.3 Hz, 1H), 8.38 (dd, *J* = 8.0, 1.3 Hz, 1H), 8.13 (br s, 1H), 7.85 (m, 1H), 7.58 (m, 1H), 7.26 (d, *J* = 8.9 Hz, 1H), 7.19 (d, *J* = 2.3 Hz, 1H), 7.07 (d, *J* = 1.9 Hz, 1H), 6.86 (dd, *J* = 8.9, 2.3 Hz, 1H), 4.49 (m, 2H), 3.86 (s, 3H), 3.20 (m, 2H), 2.93 (m, 2H), 1.77 (m, 2H), 1.40 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.8 (C_{quat}), 154.2 (C_{quat}), 134.9, 134.7 (C_{quat}), 132.0 (C_{quat}), 131.3 (C_{quat}), 129.4 (C_{quat}), 129.1, 127.63 (C_{quat}), 127.58, 122.4, 116.1 (C_{quat}), 115.4, 112.8, 112.0, 111.3 (C_{quat}), 100.3, 55.8, 44.4, 32.6, 26.0, 24.5, 22.5, 13.8.

HRMS (MALDI-TOF) calcd for $C_{24}H_{26}N_3O_2$ $[M–N_2+H]^+$ 388.2020; found 388.2022.

3-Butyl-4-[2-(3,5-dimethylisoxazol-4-yl)ethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2y)



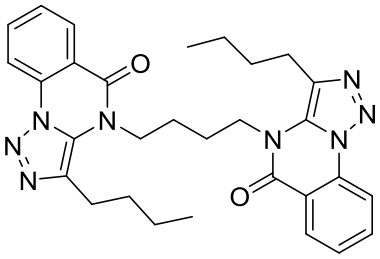
Prepared from iodotriazole **1y** (98.7 mg, 0.2 mmol) according to **GP6**; eluent: hexanes–EtOAc = 2:1. Yield 68 mg (93%). White solid; mp 169–171 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (br d, J = 8.3 Hz, 1H), 8.32 (br d, J = 7.8 Hz, 1H), 7.87 (m, 1H), 7.59 (m, 1H), 4.26 (m, 2H), 2.97 (m, 2H), 2.78 (m, 2H), 2.35 (s, 6H), 1.84 (m, 2H), 1.48 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 166.0 (C_{quat}), 159.4 (C_{quat}), 158.8 (C_{quat}), 135.2, 134.6 (C_{quat}), 131.6 (C_{quat}), 129.05, 128.96 (C_{quat}), 127.7, 115.7 (C_{quat}), 115.4, 109.4 (C_{quat}), 43.2, 32.4, 26.1, 22.5, 21.6, 13.8, 11.0, 10.2.

HRMS (MALDI-TOF) calcd for $C_{20}H_{24}N_5O_2$ $[M+H]^+$ 366.1925; found 366.1927.

4,4'-Butane-1,4-diylbis(3-butyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one) (2aa)



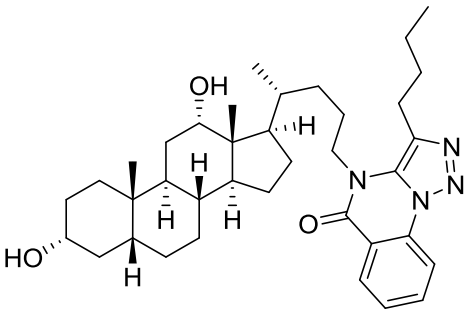
Prepared from iodotriazole **1aa** (79.4 mg, 0.1 mmol) according to **GP6** using CuI (3.8 mg, 20 mol%) and Cs_2CO_3 (130.4 mg, 4 equiv) in DMSO (2 mL); eluent: hexanes–CH_2Cl_2–EtOAc = 2:1:1. Yield 51.0 mg (95%). White solid; mp 191–192 °C.

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 8.29 (br d, J = 8.2 Hz, 2H), 8.20 (br d, J = 7.9 Hz, 2H), 7.78 (m, 2H), 7.49 (m, 2H), 4.20 (m, 4H), 2.79 (m, 4H), 1.84 (m, 4H), 1.69 (m, 4H), 1.35 (m, 4H), 0.87 (t, J = 7.3 Hz, 6H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$–CD_3OD) δ 158.8 (2C_{quat}), 135.1 (2C), 134.4 (2C_{quat}), 131.6 (2C_{quat}), 129.1 (2C_{quat}), 129.0 (2C), 127.7 (2C), 115.7 (2C_{quat}), 115.2 (2C), 42.8 (2C), 32.5 (2C), 25.8 (2C), 25.7 (2C), 22.3 (2C), 13.7 (2C).

HRMS (MALDI-TOF) calcd for $C_{30}H_{35}N_8O_2$ $[M+H]^+$ 539.2877; found 539.2878.

3-Butyl-4-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2ab)



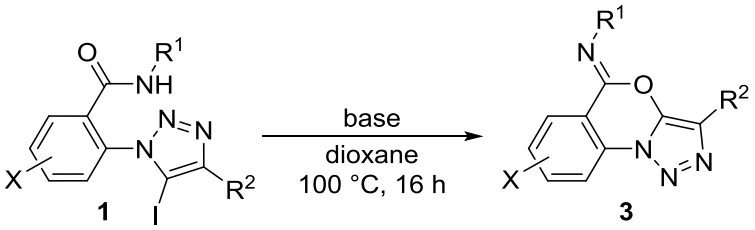
Prepared from iodotriazole **1ab** (109.6 mg, 0.15 mmol) according to **GP6**; eluent: hexanes–EtOAc = 1:2. Yield 79.6 mg (88%). Off-white solid; mp 103–106 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (br d, J = 8.2 Hz, 1H), 8.34 (dd, J = 8.0, 1.2 Hz, 1H), 7.84 (m, 1H), 7.57 (m, 1H), 4.18 (ddd, J = 13.8, 10.7, 5.5 Hz, 1H), 4.09 (ddd, J = 13.8, 10.7, 5.4 Hz, 1H), 3.97 (m, 1H), 3.61 (tt, J = 11.0, 4.7 Hz, 1H), 2.94–2.88 (m, 2H), 1.92–0.85 (m, 32H), 1.00 (d, J = 6.6 Hz, 3H), 1.00 (t, J = 7.4 Hz, 3H), 0.90 (s, 3H), 0.68 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.5 (C_{quat}), 134.8, 134.5 (C_{quat}), 131.8 (C_{quat}), 129.3 (C_{quat}), 129.0, 127.5, 116.0 (C_{quat}), 115.2, 72.9, 71.5, 48.1, 47.0, 46.3, 44.1, 42.0, 36.3, 35.9, 35.3, 35.1, 34.0, 33.5, 32.6, 32.3, 30.3, 28.6, 27.5, 27.0, 26.0, 25.8, 25.2, 23.6, 23.0, 22.5, 17.6, 13.8, 12.6.

HRMS (MALDI-TOF) calcd for $C_{37}H_{55}N_4O_3$ $[M+H]^+$ 603.4269; found 603.4268.

Synthesis of 5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imines 3



GP7 (method **A**): 20% CTAB, K_2CO_3
GP8 (method **B**): Na_2CO_3

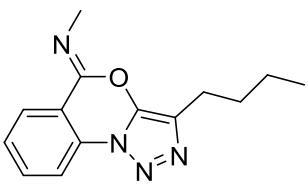
General procedure 7 (GP7, method **A** in the main text**).** In a vial with screw cap, 2-(5-iodotriazolyl)benzamide **1** (0.20 mmol, 1 equiv), cetyltrimethylammonium bromide (CTAB) (14.6 mg, 0.040 mmol, 20 mol %), and K_2CO_3 (55.3 mg, 0.40 mmol, 2 equiv) were mixed under an Ar atmosphere in dioxane (2 mL). The reaction mixture was stirred at 100 °C in a dry block for 16 h, then diluted with CH_2Cl_2 (20 mL), and washed with water (20 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was subjected to column chromatography on deactivated silica gel (*vide infra*) to afford pure triazole-fused cyclic imidate **3**.

Column chromatography on deactivated silica gel

Macherey–Nagel silica gel 60 (0.040–0.063 mm) was suspended in the mixture PhH–MeCN (20:1) containing 2% v/v Et_3N and stored for at least 24 h. Then, the column was filled with deactivated silica gel and washed with 3-fold volume of the corresponding eluent. A concentrated solution of the sample in the eluent (with small amounts of CH_2Cl_2 to increase the solubility) was used for loading on the column.

General procedure 8 (GP8, method **B** in the main text**).** Synthesis was performed as described for **GP7** with Na_2CO_3 (2 equiv) in dioxane without addition of CTAB.

3-Butyl-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3a)



Prepared from iodotriazole **1a** (38.4 mg, 0.1 mmol) according to **GP7**; eluent: PhH–MeCN = 20:1. Yield 25.2 mg (98%). Yellowish oil.

^1H NMR (400 MHz, $CDCl_3$) δ 8.12 (m, 1H), 8.10 (m, 1H), 7.65 (m, 1H), 7.40 (m, 1H), 3.31 (s, 3H), 2.76 (t, J = 7.5 Hz, 2H), 1.74 (m, 2H),

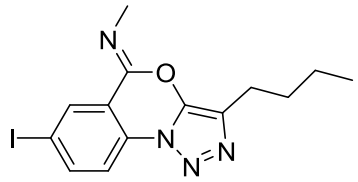
1.42 (m, 2H), 0.96 (t, J = 7.4 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 144.5 (C_{quat}), 142.2 (C_{quat}), 133.3, 132.2 (C_{quat}), 128.5 (C_{quat}), 128.1, 127.9, 114.7, 114.4 (C_{quat}), 33.6, 30.3, 23.4, 22.2, 13.7.

IR (KBr, cm^{-1}) ν 3296, 3078, 2956, 2929, 2871, 2860, 1647, 1601, 1522, 1448, 1408, 1323, 1282, 1240, 1161, 758, 671.

HRMS (MALDI-TOF) calcd for $C_{14}H_{19}N_4O_2$ $[M+H_2O+H]^+$ 275.1503; found 275.1508.

3-Butyl-7-iodo-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3c)



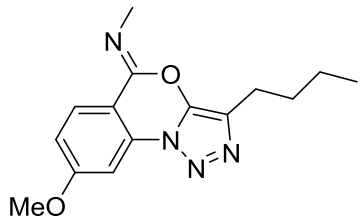
Prepared from iodotriazole **1c** (102.0 mg, 0.2 mmol) according to **GP7**; eluent: PhH–MeCN = 40:1. Yield 61.9 mg (81%). White solid; mp 125–127 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, J = 1.8 Hz, 1H), 7.96 (dd, J = 8.6, 1.8 Hz, 1H), 7.85 (d, J = 8.6 Hz, 1H), 3.33 (s, 3H), 2.76 (t, J = 7.5 Hz, 2H), 1.75 (m, 2H), 1.43 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 142.9 (C_{quat}), 142.0 (2C, CH + C_{quat}), 136.7, 131.6 (C_{quat}), 128.7 (C_{quat}), 116.4, 115.9 (C_{quat}), 92.0 (C_{quat}), 33.8, 30.2, 23.4, 22.2, 13.7.

HRMS (MALDI-TOF) calcd for $C_{14}H_{16}IN_4O$ $[M+H]^+$ 383.0363; found 383.0363.

3-Butyl-8-methoxy-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3d)



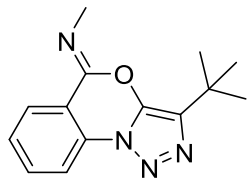
Prepared from iodotriazole **1d** (82.9 mg, 0.2 mmol) according to **GP7**; eluent: PhH–MeCN = 20:1. Yield 52.8 mg (92%). White solid; mp 90–91 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.9 Hz, 1H), 7.54 (d, J = 2.5 Hz, 1H), 6.92 (dd, J = 8.9, 2.5 Hz, 1H), 3.94 (s, 3H), 3.28 (s, 3H), 2.76 (t, J = 7.6 Hz, 2H), 1.76 (m, 2H), 1.44 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 163.5 (C_{quat}), 144.5 (C_{quat}), 142.5 (C_{quat}), 133.4 (C_{quat}), 129.7, 128.5 (C_{quat}), 115.9, 106.8 (C_{quat}), 98.1, 55.9, 33.3, 30.2, 23.4, 22.1, 13.7.

HRMS (MALDI-TOF) calcd for $C_{15}H_{19}N_4O_2$ $[M+H]^+$ 287.1503; found 287.1504.

3-*tert*-Butyl-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3g)



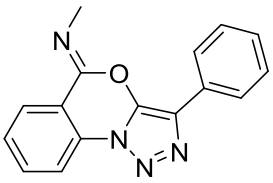
Prepared from iodotriazole **1g** (76.8 mg, 0.2 mmol) according to **GP7**; eluent: PhH–MeCN = 20:1. Yield 49.9 mg (97%). White solid; mp 120–122 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 8.14–8.10 (m, 2H), 7.66 (m, 1H), 7.41 (m, 1H), 3.32 (s, 3H), 1.47 (s, 9H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 144.7 (C_{quat}), 140.9 (C_{quat}), 136.1 (C_{quat}), 133.2, 132.2 (C_{quat}), 127.9 (2C), 114.8, 114.2 (C_{quat}), 33.9, 30.9 (C_{quat}), 29.3 (3C).

HRMS (MALDI-TOF) calcd for $C_{14}H_{16}KN_4O$ $[M+K]^+$ 295.0956; found 295.0952.

_N_-Methyl-3-phenyl-5_H_-[1,2,3]triazolo[1,5-_a_][3,1]benzoxazin-5-imine (3h)



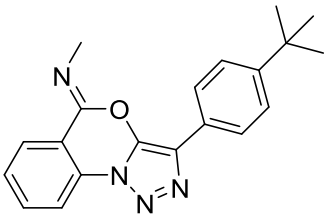
Prepared from iodotriazole **1h** (109.7 mg, 0.271 mmol) according to **GP8**; eluent: hexanes–EtOAc = 1:1. Yield 67 mg (89%). White solid; mp 191–192 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19–8.14 (m, 2H), 8.02–7.97 (m, 2H), 7.69 (m, 1H), 7.50–7.42 (m, 3H), 7.33 (m, 1H), 3.43 (s, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 144.0 (C_{quat}), 141.5 (C_{quat}), 133.5, 132.0 (C_{quat}), 129.2 (C_{quat}), 128.8 (2C), 128.3, 128.2, 127.8, 127.8, 125.1 (2C), 114.9, 114.2 (C_{quat}), 34.1.

HRMS (MALDI-TOF) calcd for $C_{16}H_{12}N_4NaO$ $[M+Na]^+$ 299.0903; found 299.0898.

3-(4-_tert_-Butylphenyl)-_N_-methyl-5_H_-[1,2,3]triazolo[1,5-_a_][3,1]benzoxazin-5-imine (3l)



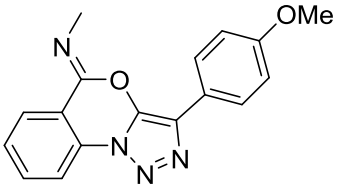
Prepared from iodotriazole **1l** (92.1 mg, 0.2 mmol) according to **GP8**; eluent: PhH–MeCN = 20:1. Yield 65.5 mg (99%). Pale yellow solid; mp 146–148 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (dd, J = 7.9, 1.3 Hz, 1H), 8.10 (m, 1H), 7.93–7.89 (m, 2H), 7.64 (m, 1H), 7.52–7.48 (m, 2H), 7.40 (m, 1H), 3.39 (s, 3H), 1.36 (s, 9H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 150.8 (C_{quat}), 144.0 (C_{quat}), 141.3 (C_{quat}), 133.3, 132.0 (C_{quat}), 128.1, 128.0, 127.8 (C_{quat}), 126.2 (C_{quat}), 125.7 (2C), 124.8 (2C), 114.8, 114.1 (C_{quat}), 34.6 (C_{quat}), 34.0, 31.2 (3C).

HRMS (MALDI-TOF) calcd for $C_{20}H_{21}N_4O$ $[M+H]^+$ 333.1710; found 333.1710.

3-(4-Methoxyphenyl)-_N_-methyl-5_H_-[1,2,3]triazolo[1,5-_a_][3,1]benzoxazin-5-imine (3m)



Prepared from iodotriazole **1m** (86.8 mg, 0.2 mmol) according to **GP8**; eluent: PhH–MeCN = 20:1. Yield 45.3 mg (74%). Beige solid; mp 188–190 °C.

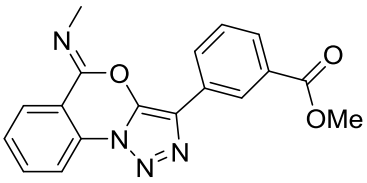
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19–8.15 (m, 2H), 7.95–7.90 (m, 2H), 7.70 (m, 1H), 7.46 (m, 1H), 7.04–6.99 (m, 2H), 3.85 (s, 3H), 3.43 (s, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.1 (C_{quat}), 144.1 (C_{quat}), 140.7 (C_{quat}), 133.3, 132.0 (C_{quat}), 128.1, 128.0, 127.6 (C_{quat}), 126.2 (2C), 121.7 (C_{quat}), 114.8, 114.15 (2C), 114.11 (C_{quat}), 55.2, 34.0.

HRMS (MALDI-TOF) calcd for $C_{17}H_{15}N_4O_2$ $[M+H]^+$ 307.1190; found 307.1193.

Methyl 3-[5-(methylimino)-5_H_-[1,2,3]triazolo[1,5-_a_][3,1]benzoxazin-3-yl]benzoate (3n)

Prepared from iodotriazole **1n** (69.3 mg, 0.15 mmol) according to **GP8** with heating for 38 h; eluent: PhH–MeCN = 20:1. Yield 46.5 mg (93%). White solid; mp 185–187 °C.

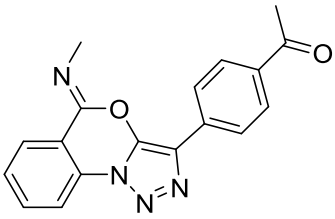


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (br s, 1H), 8.09–7.99 (m, 3H), 7.84 (m, 1H), 7.60 (m, 1H), 7.41 (m, 1H), 7.36 (m, 1H), 3.85 (s, 3H), 3.35 (s, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 166.6 (C_{quat}), 143.6 (C_{quat}), 141.6 (C_{quat}), 133.5, 131.7 (C_{quat}), 130.5 (C_{quat}), 129.3 (C_{quat}), 128.9 (2C), 128.6, 128.4, 128.1, 126.7 (C_{quat}), 125.9, 114.8, 114.0 (C_{quat}), 52.2, 33.9.

HRMS (MALDI-TOF) calcd for $C_{18}H_{15}N_4O_3$ $[M+H]^+$ 335.1139; found 335.1140.

3-(4-Acetylphenyl)-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3o)



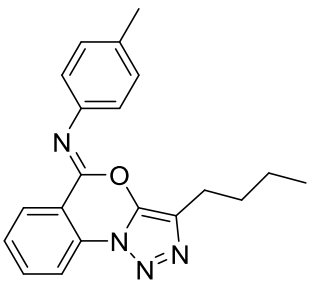
Prepared from iodotriazole **1o** (66.9 mg, 0.15 mmol) according to **GP8** with heating for 34 h; eluent: PhH–MeCN = 20:1. Yield 39.1 g (82%). White solid; mp 192–194 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20–8.14 (m, 2H), 8.10–8.03 (m, 4H), 7.72 (m, 1H), 7.48 (m, 1H), 3.45 (s, 3H), 2.63 (s, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.1 (C_{quat}), 143.3 (C_{quat}), 142.1 (C_{quat}), 135.7 (C_{quat}), 133.5, 131.6 (C_{quat}), 128.9 (2C), 128.4, 128.2 (C_{quat}), 128.1, 126.7 (C_{quat}), 124.6 (2C), 114.8, 114.0 (C_{quat}), 34.1, 26.5.

HRMS (MALDI-TOF) calcd for $C_{18}H_{15}N_4O_2$ $[M+H]^+$ 319.1190; found 319.1188.

3-Butyl-*N*-(4-methylphenyl)-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3q)



Prepared from iodotriazole **1q** (69.0 mg, 0.15 mmol) according to **GP8** with heating for 34 h; eluent: PhH–MeCN = 30:1. Yield 25.0 mg (50%). Beige solid; mp 91–93 °C.

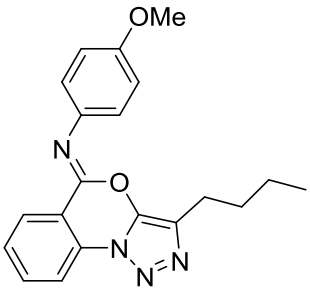
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, J = 8.0 Hz, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.72 (m, 1H), 7.49 (m, 1H), 7.24–7.17 (m, 4H), 2.69 (t, J = 7.6 Hz, 2H), 2.38 (s, 3H), 1.67 (m, 2H), 1.36 (m, 2H), 0.91 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 142.0 (C_{quat}), 141.8 (C_{quat}), 141.1 (C_{quat}), 135.1 (C_{quat}), 133.9, 132.9 (C_{quat}), 129.4 (2C), 129.0, 128.8 (C_{quat}), 128.1, 123.3 (2C), 114.8, 114.5 (C_{quat}), 30.1, 23.5, 22.2, 21.0, 13.7.

HRMS (MALDI-TOF) calcd for $C_{20}H_{21}N_4O$ $[M+H]^+$ 333.1710; found 333.1713.

3-Butyl-*N*-(4-methoxyphenyl)-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3r)

Prepared from iodotriazole **1r** (71.4 mg, 0.15 mmol) according to **GP8** with heating for 48 h; eluent: PhH–MeCN = 20:1. Yield 37.7 mg (72%). Beige solid; mp 126–128 °C.

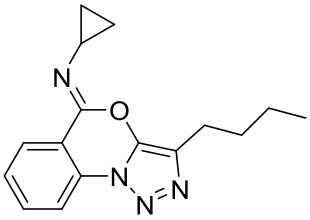


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, J = 7.9, 1.0 Hz, 1H), 8.15 (d, J = 8.1 Hz, 1H), 7.70 (m, 1H), 7.47 (m, 1H), 7.39–7.32 (m, 2H), 6.96–6.89 (m, 2H), 3.85 (s, 3H), 2.72 (t, J = 7.6 Hz, 2H), 1.71 (m, 2H), 1.39 (m, 2H), 0.93 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 157.4 (C_{quat}), 141.8 (C_{quat}), 141.2 (C_{quat}), 136.5 (C_{quat}), 133.6, 132.7 (C_{quat}), 128.9, 128.7 (C_{quat}), 128.1, 125.5 (2C), 114.7 (2C, CH + C_{quat}), 113.9 (2C), 55.4, 30.2, 23.5, 22.2, 13.7.

HRMS (MALDI-TOF) calcd for $C_{20}H_{21}N_4O_2$ $[M+H]^+$ 349.1659; found 349.1664.

3-Butyl-*N*-cyclopropyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3s)



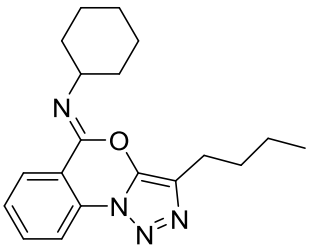
Prepared from iodotriazole **1s** (82.1 mg, 0.2 mmol) according to **GP7**; eluent: PhH–MeCN = 20:1. Yield 49.5 mg (88%). White solid; mp 94–96 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 8.1 Hz, 1H), 8.04 (dd, J = 8.1, 1.1 Hz, 1H), 7.61 (m, 1H), 7.36 (m, 1H), 3.55 (tt, J = 6.8, 3.5 Hz, 1H), 2.77 (t, J = 7.5 Hz, 2H), 1.76 (m, 2H), 1.44 (m, 2H), 1.01–0.92 (m, 4H), 0.97 (t, J = 7.3 Hz, 3H), 0.92–0.86 (m, 4H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 143.6 (C_{quat}), 142.2 (C_{quat}), 132.8, 131.8 (C_{quat}), 128.4 (C_{quat}), 127.8, 127.7, 114.6 (2C, CH + C_{quat}), 30.3, 28.9, 23.4, 22.2, 13.7, 8.8 (2C).

HRMS (MALDI-TOF) calcd for $C_{16}H_{19}N_4O$ $[M+H]^+$ 283.1553; found 283.1555.

3-Butyl-*N*-cyclohexyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3t)



Prepared from iodotriazole **1t** (90.5 mg, 0.2 mmol) according to **GP7** with heating for 36 h; eluent: PhH–MeCN = 20:1. Yield 59.4 mg (92%). White solid; mp 72–74 °C.

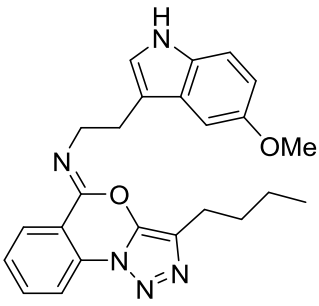
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (dd, J = 8.0, 1.1 Hz, 1H), 8.09 (dd, J = 8.1, 1.0 Hz, 1H), 7.64 (m, 1H), 7.40 (m, 1H), 3.97 (tt, J = 9.5, 3.5 Hz, 1H), 2.77 (t, J = 7.5 Hz, 2H), 1.88–1.79 (m, 4H), 1.76 (m, 2H), 1.68 (m, 1H), 1.55–1.27 (m, 7H), 0.98 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 142.4 (C_{quat}), 141.3 (C_{quat}), 133.0, 132.3 (C_{quat}), 128.5, 128.3 (C_{quat}), 127.8, 114.7 (C_{quat}), 114.6, 54.9, 33.4 (2C), 30.2, 25.7, 24.5 (2C), 23.5, 22.1, 13.7.

HRMS (MALDI-TOF) calcd for $C_{19}H_{27}N_4O_2$ $[M+H_2O+H]^+$ 343.2129; found 343.2128.

3-Butyl-*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3x)

Prepared from iodotriazole **1x** (81.5 mg, 0.15 mmol) according to **GP7** with heating for 20 h; eluent: PhH–MeCN = 15:1. Yield 50.8 mg (82%). Pale yellow solid; mp 144–146 °C.

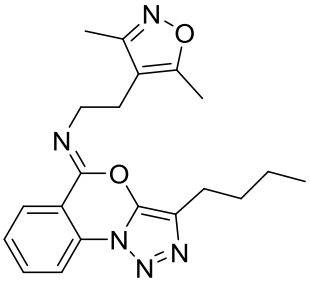


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (dd, J = 8.1, 1.0 Hz, 1H), 8.14 (br s, 1H), 8.06 (d, J = 8.1 Hz, 1H), 7.62 (m, 1H), 7.39 (m, 1H), 7.20 (d, J = 8.8 Hz, 1H), 7.12 (d, J = 2.3 Hz, 1H), 7.05 (d, J = 2.0 Hz, 1H), 6.83 (dd, J = 8.8, 2.3 Hz, 1H), 3.94 (t, J = 7.3 Hz, 2H), 3.84 (s, 3H), 3.14 (t, J = 7.3 Hz, 2H), 2.63 (t, J = 7.6 Hz, 2H), 1.67 (m, 2H), 1.37 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 153.8 (C_{quat}), 143.1 (C_{quat}), 142.1 (C_{quat}), 133.2, 132.2 (C_{quat}), 131.3 (C_{quat}), 128.4 (C_{quat}), 128.3, 127.85 (C_{quat}), 127.83, 122.7, 114.6, 114.4 (C_{quat}), 114.0 (C_{quat}), 111.9, 111.8, 100.7, 55.8, 47.4, 30.3, 26.4, 23.2, 22.1, 13.7.

HRMS (MALDI-TOF) calcd for $C_{24}H_{26}N_5O_2$ $[M+H]^+$ 416.2081; found 416.2077.

3-Butyl-*N*-[2-(3,5-dimethylisoxazol-4-yl)ethyl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3y)



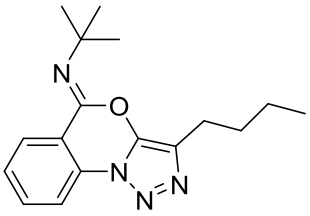
Prepared from iodotriazole **1y** (59.2 mg, 0.12 mmol) according to **GP7** with heating for 20 h; eluent: PhH–MeCN = 20:1. Yield 42.3 mg (96%). White solid; mp 105–107 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, J = 8.2, 1.0 Hz, 1H), 8.11 (dd, J = 8.0, 1.3 Hz, 1H), 7.68 (m, 1H), 7.43 (m, 1H), 3.72 (t, J = 7.0 Hz, 2H), 2.73 (t, J = 7.6 Hz, 2H), 2.72 (t, J = 7.0 Hz, 2H), 2.38 (s, 3H), 2.30 (s, 3H), 1.73 (m, 2H), 1.42 (m, 2H), 0.96 (t, J = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.5 (C_{quat}), 159.7 (C_{quat}), 143.7 (C_{quat}), 141.9 (C_{quat}), 133.5, 132.3 (C_{quat}), 128.4 (C_{quat}), 128.1, 128.0, 114.8, 114.0 (C_{quat}), 111.7 (C_{quat}), 46.3, 30.3, 23.4, 23.3, 22.1, 13.7, 11.1, 10.3.

HRMS (MALDI-TOF) calcd for $C_{20}H_{24}N_5O_2$ $[M+H]^+$ 366.1925; found 366.1928.

3-Butyl-*N*-*tert*-butyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3z)



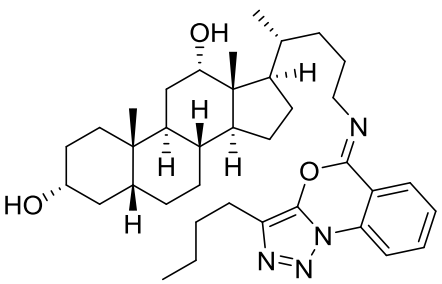
Prepared from iodotriazole **1z** (85.3 mg, 0.2 mmol) according to **GP7** with heating for 57 h; eluent: PhH–MeCN = 20:1. Yield 50.2 mg (84%). White solid; mp 50–51 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, J = 8.0, 1.4 Hz, 1H), 8.09 (dd, J = 8.2, 1.1 Hz, 1H), 7.63 (ddd, J = 8.2, 7.5, 1.4 Hz, 1H), 7.39 (dd, J = 8.0, 7.5, 1.1 Hz, 1H), 2.76 (t, J = 7.5 Hz, 2H), 1.76 (m, 2H), 1.46 (s, 9H), 1.43 (m, 2H), 0.96 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 142.3 (C_{quat}), 139.4 (C_{quat}), 132.9, 132.4 (C_{quat}), 129.1, 128.4 (C_{quat}), 127.7, 115.3 (C_{quat}), 114.6, 54.9 (C_{quat}), 30.7, 29.9 (3C), 23.5, 22.2, 13.7.

HRMS (MALDI-TOF) calcd for $C_{17}H_{23}N_4O$ $[M+H]^+$ 299.1866; found 299.1863.

3-Butyl-*N*-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]-benzoxazin-5-imine (3ab)



Prepared from iodotriazole **1ab** (109.6 mg, 0.15 mmol) according to **GP7**; eluent: PhH–EtOAc = 1:1. Yield 70.2 mg (78%). White solid; mp 85–87 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, J = 8.0, 1.1 Hz, 1H), 8.11 (d, J = 8.1 Hz, 1H), 7.66 (m, 1H), 7.42 (m, 1H), 4.00 (m, 1H), 3.65–3.54 (m, 3H), 2.76 (t, J = 7.6 Hz, 2H), 2.17 (br s, 2H), 1.92–0.81 (m, 30H), 1.03 (d, J = 6.5 Hz, 3H), 0.97 (t, J = 7.4 Hz, 3H), 0.90 (s, 3H), 0.68 (s, 3H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 142.8 (C_{quat}), 142.2 (C_{quat}), 133.2, 132.2 (C_{quat}), 128.4 (C_{quat}), 128.2, 127.9, 114.7, 114.5 (C_{quat}), 73.1, 71.6, 48.2, 47.4, 47.0, 46.4, 42.0, 36.3, 35.9, 35.4, 35.2, 34.0, 33.6, 33.5, 30.4, 30.3, 28.5, 27.5, 27.1, 26.9, 26.1, 23.6, 23.4, 23.1, 22.1, 17.7, 13.7, 12.7.

HRMS (MALDI-TOF) calcd for $C_{37}H_{55}N_4O_3$ $[M+H]^+$ 603.4269; found 603.4268.

Details of X-ray diffraction measurements

Crystallographic data were collected at 100 K on a Bruker SMART APEX II diffractometer equipped with a PHOTON II CMOS detector using graphite monochromatized Mo–Kα radiation (λ = 0.71073 Å) using a ω-scan mode. Absorption correction based on measurements of equivalent reflections was applied.[7] The structure was solved by direct methods and refined by full matrix least-squares on F2 with anisotropic thermal parameters for all non-hydrogen atoms using Olex2 package.[8] Hydrogen atoms were placed in calculated positions and refined using a riding model. Crystallographic details are presented in Table S1. CCDC 2242839 contains the supplementary crystallographic data for the structure. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* **www.ccdc.cam.ac.uk/data_request/cif**.

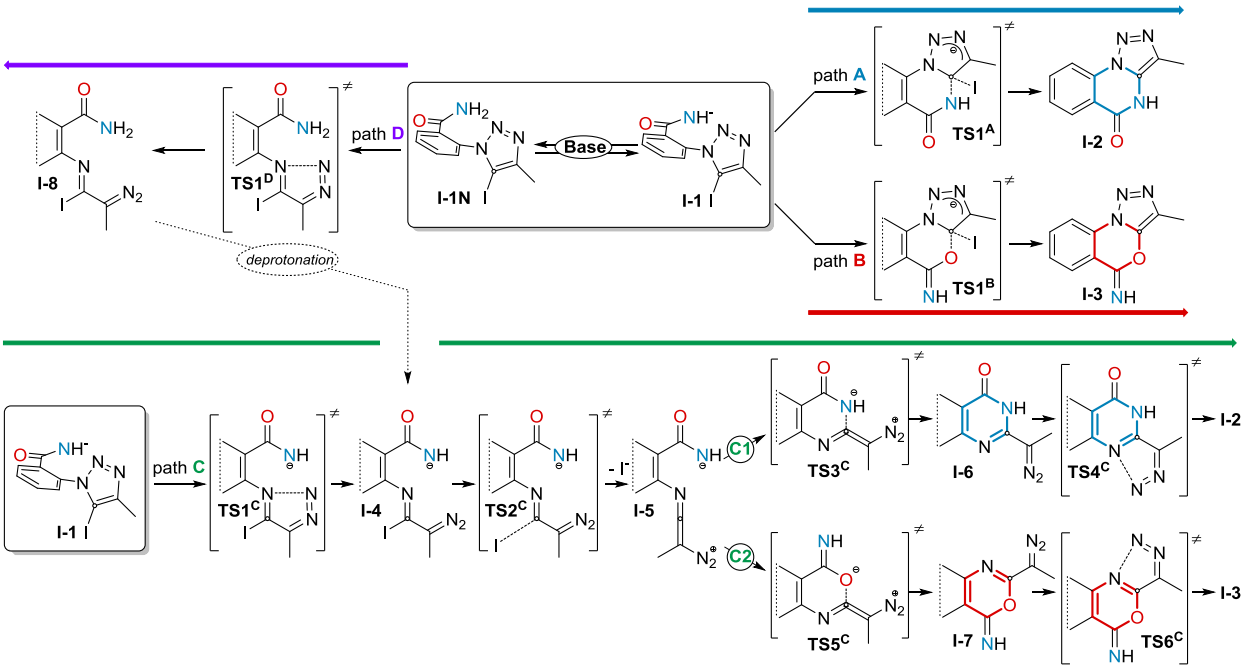
Table S1. Details of the X-ray crystal data collection and structure refinement for compound **3h**.

Empirical formula	$C_{16}H_{12}N_4O$
M_w	276.30
Temperature (K)	100
Size (mm)	0.4 × 0.1 × 0.08
Cryst. system	monoclinic
Space group	P 2_1/c
a (Å)	7.6681(5)
b (Å)	12.2337(8)
c (Å)	13.8648(8)
α (deg)	90
β (deg)	100.657(2)
γ (deg)	90
V (Å^3)	1278.21(14)
Z	4
ρ_{cald} (g·cm^{-3})	1.436
Abs coeff (mm^{-1})	0.095
F(000)	576.0
θ range (deg)	2.24 < *θ* < 31.57
no. of collected/unique rflns	22327 / 4252
Completeness to *θ* (%)	99.5
no. of data/restraints/params	4252/0/238
Goodness of fit on *F*2	1.032
Final *R* indices ($I > 2\sigma(I)$)	R1 = 0.0472, wR2 = 0.1076
R indices (all data)	R1 = 0.0720, wR2 = 0.1194
Largest diff peak/hole (e/Å^3)	0.349 / −0.270

Details of DFT calculations

The calculations were performed using ORCA 5.0.3 program package.[9] DFT calculations were performed at B3LYP[10]/ma-SVP[11] level of theory using PCM[12] solvation model with DMSO as solvent. RIJCOSX approximation was used to speed up the calculations. Thermodynamic properties were calculated for ideal gas at 298.15 K using QRRHO approach[13] for vibrational entropy correction. The nature of optimized intermediates and transition states was verified by frequency analysis. IRC calculations were performed to verify the connectivity of the PES. CYLView[14] was used to visualize structures.

Scheme S1. Non-catalytic pathways for cyclization of 2-(5-iodotriazolyl)benzamides.



Scheme S2. Calculated free energies (ΔG_{298}, kcal/mol) of intermediates for paths **A-D**.

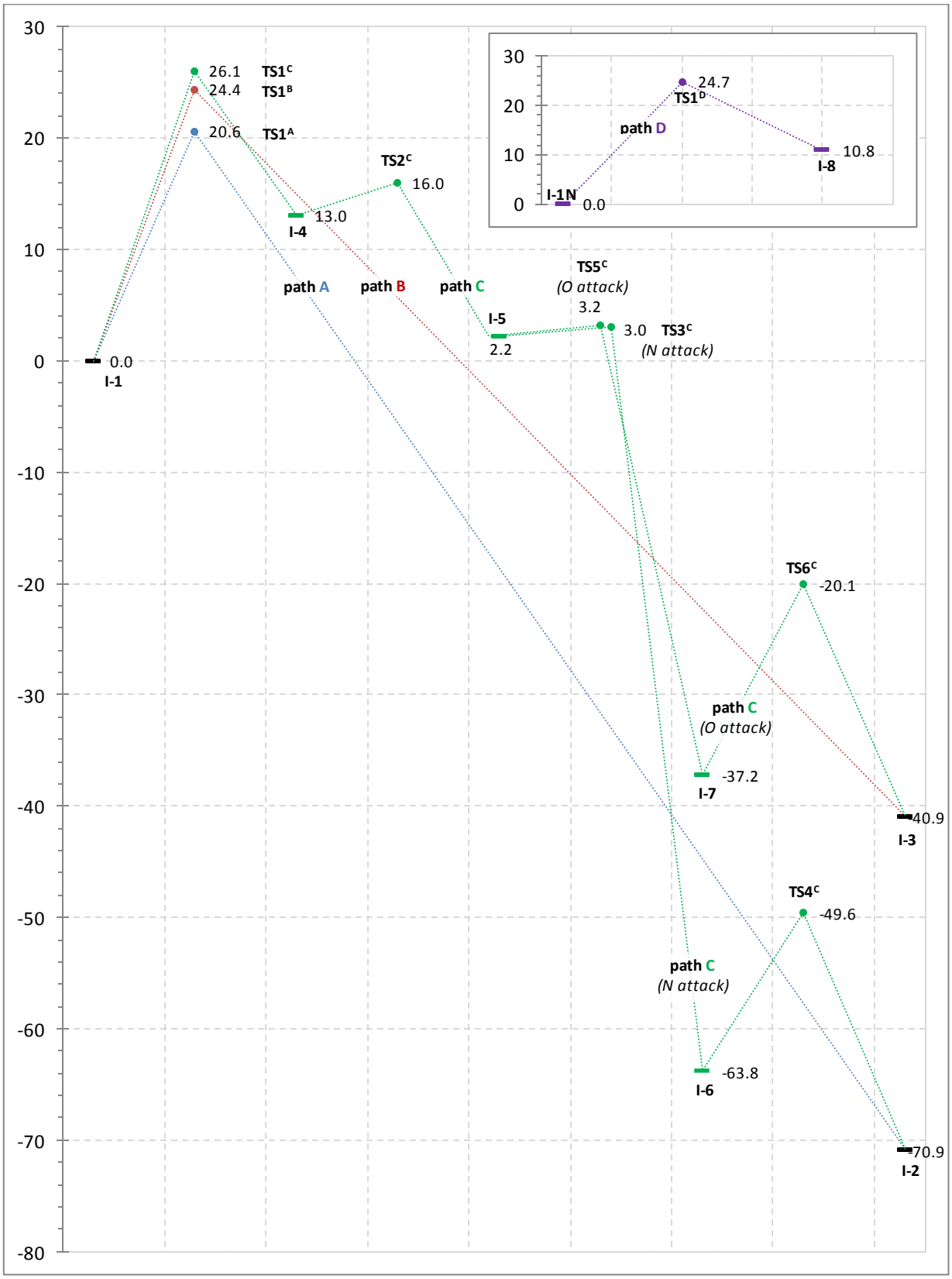


Table S2. Electronic and free energies (kcal/mol) of the reaction paths **A-C**.

Path A

	$I\text{-}1_2$	→	$TS1^A$	→	I-2
E	0.3		21.1		-65.1
ΔG	0.2		20.6		-70.9

	$I\text{-}1_3$	→	$TS1^A$	→	I-2
E	0.8		21.1		-65.1
ΔG	0.6		20.6		-70.9

Path B

	$I\text{-}1_1$	→	$TS1^B$	→	I-3
E	0.6		24.1		-65.1
ΔG	0.6		24.4		-70.9

	$I\text{-}1_4$	→	$TS1^B$	→	I-3
E	0.0		24.1		-65.1
ΔG	0.0		24.4		-70.9

Path C

	$I\text{-}1_1$	→	$TS1^C{}_1$	→	$I\text{-}4_1$	→	$TS2^C{}_1$	→	$I\text{-}5_1$	→	$TS5^C{}_1$	→	I-7	→	$TS6^C$	→	I-3
E	0.0		28.6		16.2		20.0		14.5		14.6		-28.6		-11.9		-34.4
ΔG	0.0		26.1		13.0		16.2		2.3		3.3		-37.2		-20.1		-40.9

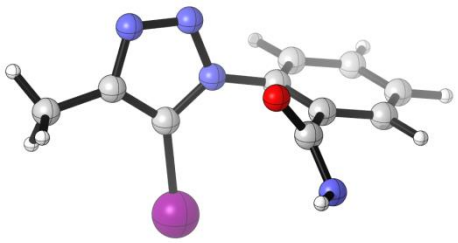
	$I\text{-}1_2$	→	$TS1^C{}_2$	→	$I\text{-}4_2$	→	$TS2^C{}_2$	→	$I\text{-}5_2$	→	$TS5^C{}_2$	→	I-7	→	$TS6^C$	→	I-3
E	0.8		28.9		16.5		20.0		14.4		14.6		-28.6		-11.9		-34.4
ΔG	0.6		26.1		13.0		16.0		2.2		3.2		-37.2		-20.1		-40.9

	$I\text{-}1_3$	→	$TS1^C{}_2$	→	$I\text{-}4_2$	→	$TS2^C{}_3$	→	$I\text{-}5_3$	→	$TS3^C{}_1$	→	I-6	→	$TS4^C$	→	I-2
E	0.3		28.9		16.5		20.0		14.66		14.71		-56.3		-42.2		-65.1
ΔG	0.2		26.1		13.0		16.0		2.5		3.2		-63.8		-49.6		-70.9

	$I\text{-}1_3$	→	$TS1^C{}_1$	→	$I\text{-}4_1$	→	$TS2^C{}_4$	→	$I\text{-}5_4$	→	$TS3^C{}_2$	→	I-6	→	$TS4^C$	→	I-2
E	0.6		28.9		16.2		20.1		14.64		14.66		-56.3		-42.2		-65.1
ΔG	0.6		26.1		13.0		16.1		2.2		3.0		-63.8		-49.6		-70.9

Cartesian coordinates of all intermediates and transition states

$I\text{-}1_4$

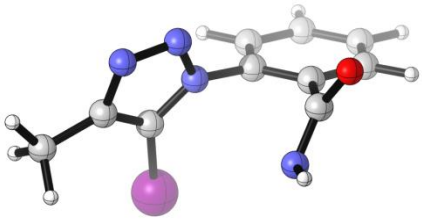


E_{PCM} = -977.0603 E_h
ZPE = 0.1698 E_h
G_{298} = -976.9322 E_h

C	-2.55326350870345	-1.20272165639229	-1.51513024003103
C	-1.18788512085671	-0.89807367572894	-1.36640117300843
C	-0.85029805711785	0.05321178068966	-0.38335088336516
C	-1.82407350990887	0.67567125621000	0.40829337779348
C	-3.17370211206590	0.36602867891498	0.22617069262517
C	-3.53597498427766	-0.57871786562415	-0.74121556821757
H	-2.83962014869778	-1.93998254325748	-2.26781166351322
H	-1.51244540624006	1.39670936471343	1.16739849834761
H	-3.93390167283076	0.85629699749736	0.83955522661248
H	-4.58877609403753	-0.83173019375891	-0.89365663416151
N	0.51857059323073	0.42864596832858	-0.14961012489988
N	0.97307748895402	1.62245859531477	-0.56294827783831

N	2.22769116259884	1.71951904340025	-0.21318443875016
C	2.62015042148525	0.59204450251084	0.44187216505990
C	1.51372310652394	-0.24865004569872	0.49072315381870
I	1.30238107973630	-2.10792336355264	1.40888940244450
C	4.00645791786028	0.39483129044388	0.96185135492705
H	3.99698637763281	-0.04350726100139	1.97175603321741
H	4.53092502578159	1.36009823622284	1.00281620821806
H	4.58608029071743	-0.28174862994249	0.31093281317764
C	-0.15994211024721	-1.54802960701165	-2.29219227825471
O	0.69714035670828	-0.77523217779796	-2.82712931011516
N	-0.30008267537609	-2.84786843226723	-2.45558401107250
H	0.42559357913042	-3.16156726221275	-3.11137132301434

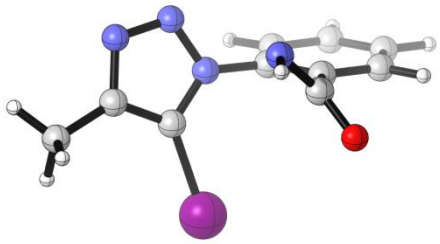
I-1$_3$



E_{PCM} = -977.0607 E_h
ZPE = 0.1697 E_h
G_{298} = -976.9328 E_h

C	-2.61999768464748	-1.30953293695908	-1.43717008488811
C	-1.24039384234151	-1.05333788704687	-1.33684034309480
C	-0.82740153342558	-0.11954319391355	-0.37042926569003
C	-1.74499375564529	0.53384951325626	0.46426562191992
C	-3.10635558203364	0.24380925155812	0.36048786065834
C	-3.54238938810031	-0.68480668003155	-0.59426216538144
H	-2.96659441775291	-2.02259282602407	-2.18966535853895
H	-1.38539413050016	1.27056978785029	1.18637566533008
H	-3.82262191949984	0.74705363274693	1.01479622084838
H	-4.60683310864453	-0.91758388066450	-0.68571774702096
N	0.56260423358619	0.22416433337081	-0.24382752578560
N	1.17588348022091	0.94230764130343	-1.19957936306508
N	2.41910637832847	1.11542958097396	-0.83787495809463
C	2.64534795467229	0.51732013402971	0.36429099702750
C	1.44361518681104	-0.06113017436137	0.75670294643986
I	1.01244647735294	-1.18945559708070	2.45512034737301
C	3.97745615668842	0.52361331611797	1.04003920450308
H	3.89392601680416	0.84598931165709	2.09003777691707
H	4.65674819485261	1.21083094561441	0.51609464045717
H	4.43370937796465	-0.48062749640867	1.03610969111264
C	-0.28321197242485	-1.76903473211322	-2.28592394027556
O	-0.47631009854139	-1.55601072211874	-3.52602189561114
N	0.61099644906249	-2.54622409859982	-1.71522774078544
H	1.17381652721332	-2.98031022315683	-2.45779358435532

I-1$_2$

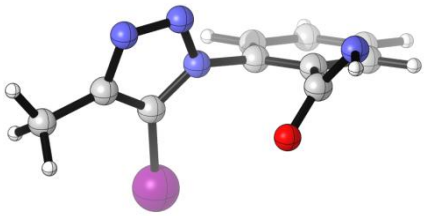


E_{PCM} = -977.0601 E_h
ZPE = 0.1698 E_h
G_{298} = -976.9321 E_h

C	-2.53473756703842	-1.18432280783108	-1.52713440379349
C	-1.17114502382178	-0.86719432837355	-1.38126443143951
C	-0.83652756152401	0.06924465725690	-0.38465934337591
C	-1.81521059049624	0.67488820383831	0.41653752548579
C	-3.16243537843526	0.36141622277932	0.23052561527057
C	-3.52053415201802	-0.57502582890115	-0.74774977077445
H	-2.81676984503934	-1.92167545959793	-2.28219039850163

H	-1.50744861283931	1.38578778882399	1.18673045940719
H	-3.92481766476434	0.83814884655382	0.85177259741829
H	-4.57175956570434	-0.83360323991508	-0.90139488213766
N	0.52943947526017	0.44751949351535	-0.13993939157247
N	0.97891968662688	1.65301602318150	-0.52457221744811
N	2.23033181965102	1.75085712248582	-0.16342860076451
C	2.62607820683072	0.61157728378030	0.46879149556601
C	1.52482465650576	-0.23677482614336	0.49216492569233
I	1.32183075063993	-2.12055055501349	1.36064898014616
C	4.00968015628430	0.41217790312530	0.99513983335600
H	3.99474221688528	-0.03153699934596	2.00273112995234
H	4.53303452052142	1.37760934898341	1.04463183042995
H	4.59338494449892	-0.26071742082335	0.34417006127077
C	-0.16964245186276	-1.56729944369454	-2.29915592589744
O	-0.28821394288640	-2.83261814363778	-2.38021114091128
N	0.67578465198626	-0.78563460658862	-2.93588695795536
H	1.26121624173954	-1.38089231445811	-3.53501168642357

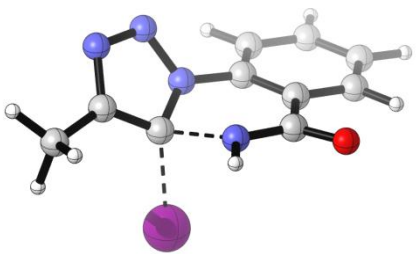
I-1$_1$



E_{PCM} = -977.0613 E_h
ZPE = 0.1698 E_h
G_{298} = -976.9331 E_h

C	-2.62183386610771	-1.27559239715698	-1.46458297887223
C	-1.24430344271578	-1.01268328857753	-1.36612091757975
C	-0.83253784101145	-0.10253541204804	-0.37446258627879
C	-1.74862481861860	0.52663402558249	0.47741329607921
C	-3.11037749382205	0.23367417715487	0.37050684281976
C	-3.54466735786683	-0.67380008795598	-0.60321740519007
H	-2.96622081913355	-1.97529620218753	-2.22955231142644
H	-1.38931853892961	1.24796545889939	1.21500853628150
H	-3.82647078700813	0.71793260786616	1.03921052935472
H	-4.60832675386010	-0.90959829126321	-0.69657565502143
N	0.55705589985804	0.24228614165023	-0.24465898475688
N	1.16543431912194	0.98278069392404	-1.18594861299648
N	2.40976223897893	1.15001846181875	-0.82489493798401
C	2.64168903861759	0.52387050943878	0.36178813221314
C	1.44222568966596	-0.06461459837751	0.74571036545203
I	1.01871908008231	-1.23468851882556	2.41757527202968
C	3.97638583784177	0.51606911289647	1.03244585071486
H	3.89766524914335	0.82424640059116	2.08713238065355
H	4.65592727240811	1.20846845269579	0.51569533759012
H	4.42944171083863	-0.48940223959252	1.01310920227372
C	-0.25434096430492	-1.74296332395293	-2.26964306013749
O	0.67637301910389	-2.38323238445251	-1.68404067972110
N	-0.49565497452577	-1.64518833233022	-3.56019677498037
H	0.21887474924399	-2.19132410879762	-4.05723989051724

TS1^A

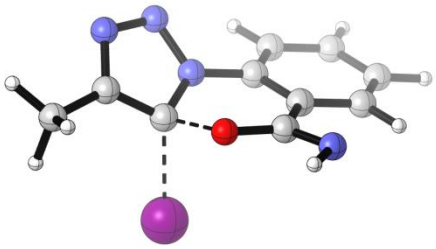


E_{PCM} = -977.0277 E_h
ZPE = 0.1685 E_h
G_{298} = -976.9003 E_h

C	-2.62183386610771	-1.27559239715698	-1.46458297887223
C	-1.24430344271578	-1.01268328857753	-1.36612091757975
C	-0.83253784101145	-0.10253541204804	-0.37446258627879

C	-1.74862481861860	0.52663402558249	0.47741329607921
C	-3.11037749382205	0.23367417715487	0.37050684281976
C	-3.54466735786683	-0.67380008795598	-0.60321740519007
H	-2.96622081913355	-1.97529620218753	-2.22955231142644
H	-1.38931853892961	1.24796545889939	1.21500853628150
H	-3.82647078700813	0.71793260786616	1.03921052935472
H	-4.60832675386010	-0.90959829126321	-0.69657565502143
N	0.55705589985804	0.24228614165023	-0.24465898475688
N	1.16543431912194	0.98278069392404	-1.18594861299648
N	2.40976223897893	1.15001846181875	-0.82489493798401
C	2.64168903861759	0.52387050943878	0.36178813221314
C	1.44222568966596	-0.06461459837751	0.74571036545203
I	1.01871908008231	-1.23468851882556	2.41757527202968
C	3.97638583784177	0.51606911289647	1.03244585071486
H	3.89766524914335	0.82424640059116	2.08713238065355
H	4.65592727240811	1.20846845269579	0.51569533759012
H	4.42944171083863	-0.48940223959252	1.01310920227372
C	-0.25434096430492	-1.74296332395293	-2.26964306013749
O	0.67637301910389	-2.38323238445251	-1.68404067972110
N	-0.49565497452577	-1.64518833233022	-3.56019677498037
H	0.21887474924399	-2.19132410879762	-4.05723989051724

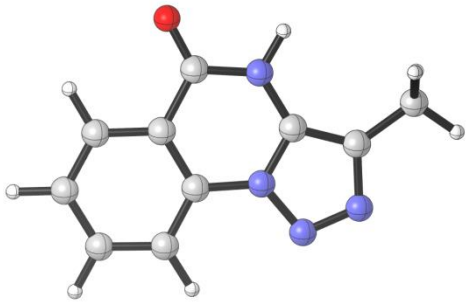
TS1[B]



E_{PCM} = -977.0228 E_h
ZPE = 0.1690 E_h
G_{298} = -976.8943 E_h

C	-2.48311137162639	-1.26880924888389	-1.41568615015243
C	-1.15765367804832	-0.92138736177006	-1.09559491737798
C	-0.96185610012376	0.14907414492022	-0.19656677830799
C	-2.04406103105152	0.86425071147989	0.33628457234416
C	-3.34662055051068	0.50805417746055	-0.01296090460153
C	-3.56677370689365	-0.56878795309536	-0.88419893233795
H	-2.64859237223582	-2.09732336590629	-2.10526195456692
H	-1.85232782634733	1.68617314532767	1.02817429857024
H	-4.19121491991983	1.06179175097376	0.40552714552984
H	-4.58606419603802	-0.86044202906638	-1.14993682942559
N	0.35716849317920	0.50568839477175	0.15349037933017
N	0.80571854587395	1.81825064364467	0.14899457495711
N	2.10192145883827	1.75108184134965	0.24234458693776
C	2.53696003824910	0.46560659841528	0.29524000711811
C	1.39841335446313	-0.36315722002010	0.21917677038823
I	1.27056157951875	-2.20241697060647	1.57176474109312
C	3.97772715186372	0.09162832552427	0.42342020519796
H	4.15260610273080	-0.56033907306783	1.29681883451696
H	4.58730108023472	0.99909299905290	0.54701656260352
H	4.34976942475421	-0.44874350692274	-0.46464611524792
C	-0.00256652775698	-1.64018577583339	-1.75422896412128
O	1.21867484778918	-1.37123705828041	-1.35742725955936
N	-0.26610506173431	-2.47597070915189	-2.71376719087866
H	0.61311726479159	-2.88776046031581	-3.04392168200953

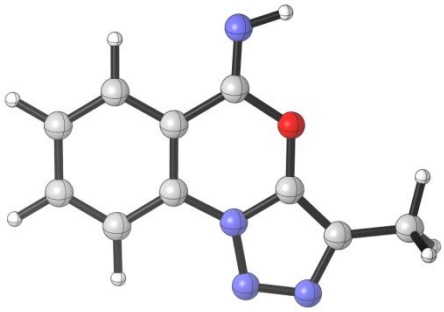
I-2



E_{PCM} = -679.2743 E_h
ZPE = 0.1731 E_h
G_{298} = -679.1386 E_h

C	-3.32939986300302	1.36662620117838	-0.75359091384555
C	-2.13924012013509	1.32127434985787	-0.02859031896748
C	-1.10283615382549	0.49657812627888	-0.48364301805887
C	-1.24505229836171	-0.28180230181069	-1.65464747237059
C	-2.45581527172457	-0.21587059776493	-2.36586235385348
C	-3.49186946062511	0.60093906201534	-1.92110546791527
H	-4.14343410419893	2.00689435317940	-0.40442826776165
H	-2.00670327256199	1.91163456077907	0.87826796681997
H	-2.56319121764700	-0.81852562598330	-3.26969795683442
H	-4.43031635497961	0.64617171859913	-2.47835564277971
N	0.12032201629113	0.39727304421619	0.19512714868292
N	0.46505278196813	1.05113896066522	1.33168553891938
N	1.67694255771948	0.67193833406250	1.62698286492056
C	2.15585037252843	-0.22237641744427	0.71663968155074
C	1.14093200872020	-0.40166069500737	-0.21934087058729
C	-0.14722070070613	-1.16072939722126	-2.13690260265489
O	-0.21882896452038	-1.85388399077570	-3.14865559773678
N	0.99509232995382	-1.15485631588270	-1.35897654835388
C	3.51558352435889	-0.83742206957890	0.79502678539734
H	4.10829386350475	-0.62763050442093	-0.11074557059176
H	3.45965943159196	-1.93288651421532	0.90956703811347
H	4.05435233214198	-0.42842428257515	1.66139921289310
H	1.76612656351025	-1.74849999815148	-1.66105363498583

I-3



E_{PCM} = -679.2254 E_h
ZPE = 0.1719 E_h
G_{298} = -679.0909 E_h

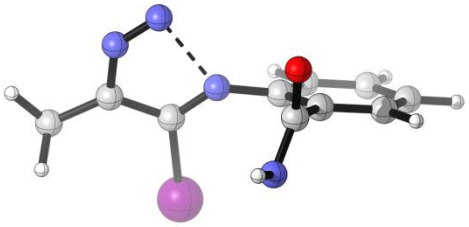
C	-3.13054186130895	1.44191772663685	-0.06188282586618
C	-1.94800863757573	1.38461958730991	0.67639611597198
C	-0.90554160638291	0.57641537130115	0.21342820364020
C	-1.02170952080165	-0.17741084710009	-0.97312124983461
C	-2.22406556551167	-0.10091452373473	-1.69738941566653
C	-3.27032908054861	0.70172196511144	-1.24677974439087
H	-3.95241058619046	2.07006978511812	0.29054176221196
H	-1.82673342529868	1.95393308174649	1.59826170813120
H	-2.32096915904667	-0.68163026944516	-2.61590502511011
H	-4.20030906964924	0.75311750497463	-1.81746685340478
N	0.31607878122954	0.46364681897175	0.89768521168350
N	0.66684941086956	1.08517323512523	2.04562793316395
N	1.88068707783663	0.70079324076974	2.32615630159996
C	2.35525200578021	-0.17069689423713	1.38628337834882
C	1.33503708382878	-0.31941599382673	0.46286226787408
C	0.09149301151975	-1.03120054532874	-1.44628125826893
N	0.05250526998465	-1.73192070106034	-2.50199135848667

O	1.24466456036268	-1.04789042838424	-0.66141491719756
C	3.71588085368698	-0.78362480160174	1.43224451144496
H	3.87008691089917	-1.44873815570111	0.57076105793691
H	3.85169594529549	-1.37523583893213	2.35204627743739
H	4.49869816007255	-0.00823763267137	1.41234274555665
H	0.92465944094860	-2.24863968504181	-2.64897282677536

I^-

E_{PCM} = -297.8907 E_h
G_{298} = -297.9075 E_h

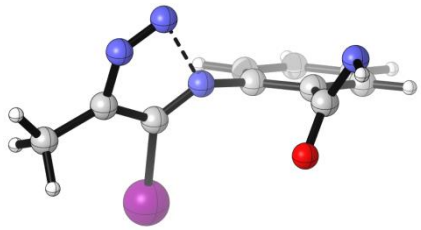
$TS1^C_2$



E_{PCM} = -977.0152 E_h
ZPE = 0.1661 E_h
G_{298} = -976.8916 E_h

C	-2.66232402984632	-1.01531984715356	-1.66406912024625
C	-1.27703983603282	-0.82646896889237	-1.53608238389805
C	-0.79612821002736	-0.13026565906062	-0.40321163570579
C	-1.69995372372933	0.37147165486221	0.55609946861745
C	-3.07329662610043	0.16939147837243	0.40778652738196
C	-3.55840959390086	-0.52950756727586	-0.70563313882265
H	-3.04217542731312	-1.55775650099567	-2.53490941075821
H	-1.31093695505354	0.92781595622825	1.41230315212437
H	-3.76356866466192	0.56129297399340	1.15978728641263
H	-4.63252755413501	-0.69274940199109	-0.82874212852864
N	0.57305860462023	0.12314214661677	-0.26754440781570
N	1.94012903939891	1.46653037927608	-1.26187994872262
N	2.77979963553845	1.14583610775216	-0.50645584564763
C	2.77583637704568	0.30098621019540	0.53163199775101
C	1.44023659953192	-0.24223763519227	0.59930160137658
I	1.04432330185485	-1.67082400016209	2.15519852124471
C	3.98063054458093	0.02839135392009	1.37649157908675
H	3.80375314911090	0.27168114686236	2.43698166377101
H	4.81579074378202	0.64925237513460	1.02242925139398
H	4.29575294242446	-1.02681427470999	1.32099898900080
C	-0.34010960378408	-1.33853312680003	-2.62310393308547
O	-0.23516796962563	-0.59977493620164	-3.65617870410100
N	0.23972305923509	-2.49524588980758	-2.38391210506516
H	0.82883819708695	-2.72963597497096	-3.19361627576410

$TS1^C_1$

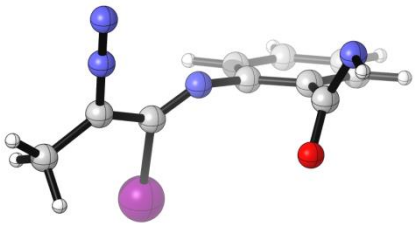


E_{PCM} = -977.0157 E_h
ZPE = 0.1663 E_h
G_{298} = -976.8916 E_h

C	-2.65040894533190	-0.94844416704027	-1.70183853821547
C	-1.26461676714997	-0.77175535044907	-1.56300670809330
C	-0.78630120839906	-0.12457661689596	-0.39836608999168
C	-1.69258333699013	0.34220114922037	0.57525421561584
C	-3.06633565957331	0.14704590308620	0.41693758707007
C	-3.54904281883499	-0.50458645862517	-0.72470922469799
H	-3.02774767395831	-1.44829834035594	-2.59799502706796
H	-1.30564865999662	0.87097317640551	1.44960485063552
H	-3.75757099740328	0.51075419023167	1.18215430130417

H	-4.62308895760880	-0.65992520226898	-0.85854467967146
N	0.57974969951697	0.13403128142031	-0.24961716299608
N	1.93857112955190	1.50183899117329	-1.21888397205934
N	2.77988088931795	1.17394209676082	-0.46778190692395
C	2.78034505387088	0.31006160039226	0.55407738761750
C	1.44748171486424	-0.24237714450613	0.61088418825544
I	1.06046799171001	-1.70476177011752	2.13740388565149
C	3.98477929123323	0.03157844394888	1.39751750617454
H	3.81076444909446	0.27475581834454	2.45867945003667
H	4.82242539757388	0.64864157946654	1.04271075918161
H	4.29466445829847	-1.02496091277812	1.34058531529310
C	-0.31558624624244	-1.31719332901222	-2.62294551974191
O	0.45518988191084	-2.26374572503416	-2.25871232439192
N	-0.41753993606995	-0.76349171315857	-3.81408274977184
H	0.25312116361594	-1.23043857320831	-4.43789765421305

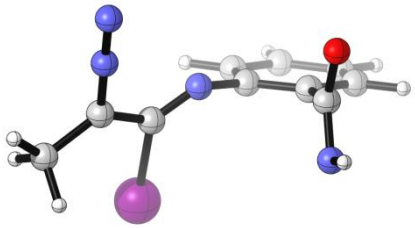
I-4$_1$



E_{PCM} = -977.0355 E_h
ZPE = 0.1665 E_h
G_{298} = -976.9124 E_h

C	-2.73114851568635	-1.03555302552975	-1.67343390119116
C	-1.34686259294781	-0.82591660593055	-1.58532793807264
C	-0.83849859868596	-0.16528055249899	-0.44037809836981
C	-1.71965171832535	0.29369173203623	0.55990140387970
C	-3.09468212364293	0.07247521784607	0.44829659612059
C	-3.60425156236408	-0.60119720275763	-0.66829767467979
H	-3.12945650519925	-1.54887415175920	-2.55296009848620
H	-1.31620102869440	0.84102648579206	1.41461475069670
H	-3.76644978100617	0.43369535557856	1.23195754622976
H	-4.67912274973032	-0.77768678332780	-0.76359771975868
N	0.52435366318897	0.11783743714418	-0.35589108695615
N	3.18568287755452	2.05115194209800	-1.22929464035058
N	2.99240636549354	1.27566831812198	-0.42274845676417
C	2.75960137158034	0.37828705327900	0.50780969060842
C	1.40291851721804	-0.14086418935857	0.49891484631500
I	0.99500594804795	-1.54337372618570	2.22509913299140
C	3.90178895760278	0.00798766335248	1.42443746937151
H	3.67268611503274	0.26007833927339	2.47174357785703
H	4.80456515595786	0.56157050135347	1.12995013372131
H	4.12627069000443	-1.06847814757226	1.36526822213882
C	-0.42005711268961	-1.34678683122093	-2.67599533684187
O	0.35423316358814	-2.30485236721158	-2.35012456432110
N	-0.53882512631583	-0.76057594043961	-3.84990260009634
H	0.12174326431717	-1.21102001874471	-4.49631819613757

I-4$_2$

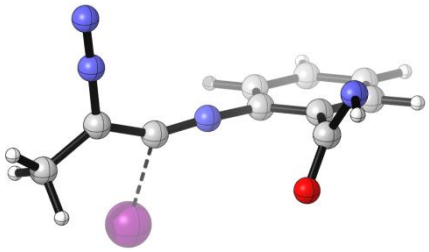


E_{PCM} = -977.0350 E_h
ZPE = 0.1664 E_h
G_{298} = -976.9124 E_h

C	-2.73553128095494	-1.11592938983972	-1.62397819833832
C	-1.35417260448817	-0.88216888490551	-1.55285879187914
C	-0.84722338578319	-0.16818449269224	-0.44189426727543
C	-1.72762195400811	0.32341661879733	0.54381512545061
C	-3.10130173926068	0.08961759265756	0.44413122303710

C	-3.60908138036474	-0.63851735399978	-0.63932905061567
H	-3.13249807900527	-1.67993833422847	-2.47325306160706
H	-1.32486723877297	0.90076382540183	1.37888279823939
H	-3.77379818441493	0.47890047979011	1.21351556247587
H	-4.68266610754332	-0.82905884155647	-0.72148110951628
N	0.51831336707510	0.10970818913952	-0.37121542371082
N	3.19582581004692	1.99042287347844	-1.30105512038500
N	2.99738221522828	1.24071525629164	-0.47190620905381
C	2.75719354776330	0.37167842692447	0.48376968858415
C	1.39649916966052	-0.13584849524407	0.48871614423460
I	0.97623790906113	-1.49054877086307	2.24972893284004
C	3.89480532753405	0.01883630016769	1.41293627743573
H	3.66253534973217	0.29733861780779	2.45284373654476
H	4.80093468152304	0.56159072094980	1.10885849726112
H	4.11527303400656	-1.05964413035635	1.38110061997871
C	-0.43978665113895	-1.35795468005103	-2.67490852971364
O	-0.28350608785434	-0.54477376672034	-3.64360433320674
N	0.07097198765967	-2.56201597666574	-2.52944627637036
H	0.65171139122578	-2.76280472603947	-3.35425238495953

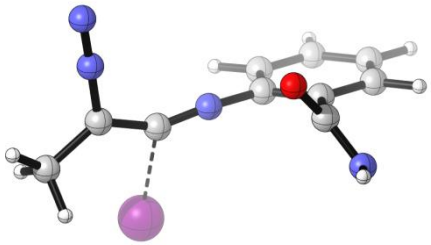
TS2$^{C}_{1}$



E_{PCM} = -977.0295 E_h
ZPE = 0.1660 E_h
G_{298} = -976.9073 E_h

C	-2.74221766716202	-0.97063047169178	-1.75921026356488
C	-1.35219990397865	-0.94929928921367	-1.58110513873503
C	-0.85215973667744	-0.33333084620070	-0.40801423691847
C	-1.71744388432374	0.25212794222143	0.54154480511987
C	-3.09495915964064	0.20833242119819	0.33694537778656
C	-3.60741353008909	-0.40786093821964	-0.81354455648234
H	-3.15019829878266	-1.43871272688938	-2.65828525518952
H	-1.29322026980414	0.73879643220587	1.42170653948193
H	-3.76793753414071	0.65741633773399	1.07171108298844
H	-4.68764857162405	-0.44351753343457	-0.97868243314651
N	0.50717769494160	-0.26661202483068	-0.20269534467959
N	3.17800571148002	2.35609062068568	-0.68144921662207
N	2.99579005905403	1.40814367242048	-0.09540583286598
C	2.80131688458394	0.29591584587126	0.60070297131942
C	1.49523665744720	-0.21967012840621	0.46568844185868
I	1.00980946659087	-1.62631236521539	2.93084614476984
C	3.95691929670725	-0.24787897560158	1.40721799878728
H	3.86264791240807	0.01434165872106	2.47225619440006
H	4.89917051913321	0.16744838990970	1.02182133278486
H	3.99411445981890	-1.34178624830520	1.31434950418451
C	-0.42246655632008	-1.60893444723374	-2.59272662033405
O	0.26421982047419	-2.58966506108010	-2.16180259605791
N	-0.45702933627486	-1.09218753663534	-3.80197307007881
H	0.19329596617881	-1.62260072800968	-4.39534882880626

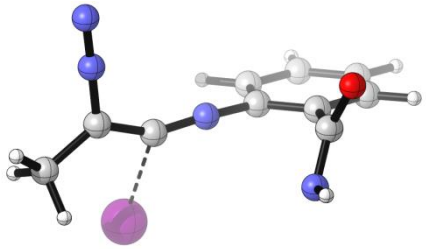
TS2$^{C}_{2}$



E_{PCM} = -977.0294 E_h
ZPE = 0.1659 E_h
G_{298} = -976.9076 E_h

C	-2.69192008997823	-0.98385055893124	-1.85353664970541
C	-1.30358609217901	-0.85306575831434	-1.71149364822946
C	-0.82690301596496	-0.15633437432778	-0.57348954459516
C	-1.71398213824232	0.39765693217302	0.37483724812298
C	-3.08906955669733	0.26426344994686	0.19326910601391
C	-3.57812421796576	-0.42800108439192	-0.92338069731463
H	-3.08085188082360	-1.52608509247370	-2.71838896429161
H	-1.30787403844811	0.92470814129030	1.24034903318592
H	-3.77802946859868	0.69756210737747	0.92271687789119
H	-4.65616049044439	-0.53544544300052	-1.07062249983885
N	0.52563783564161	-0.02133107435746	-0.37259708475968
N	3.08617207640397	2.62091677895778	-1.05649532255242
N	2.95594461098767	1.69851578323435	-0.41727036937296
C	2.82275736405546	0.61989240425320	0.34147077579222
C	1.53306504267322	0.04484826335235	0.26355549721704
I	1.22366010572310	-1.44806751070609	2.66337849737917
C	4.02113833510011	0.16645531147661	1.14097639490723
H	3.91237265017459	0.42030927111350	2.20646277610624
H	4.92473126025677	0.65722979401661	0.75209585804540
H	4.14735167674400	-0.92103294051184	1.04773985490690
C	-0.35114628047114	-1.40407030001172	-2.76642299807107
O	0.46095247136270	-0.56991296100196	-3.28043095823638
N	-0.49621336177929	-2.68399787655899	-3.03649717612722
H	0.18281847446964	-2.93374650660447	-3.76626228747330

TS2$^{C}_{3}$

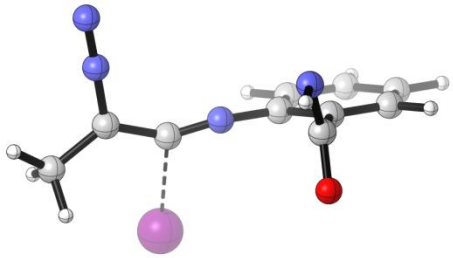


E_{PCM} = -977.0290 E_h
ZPE = 0.1658 E_h
G_{298} = -976.9072 E_h

C	-2.71578535700133	-0.91869999245327	-1.89042119686805
C	-1.32315223256562	-0.83721445311256	-1.74529749871353
C	-0.82143794131331	-0.19165034286401	-0.59039564297169
C	-1.68938330173198	0.35787860743895	0.38017433635964
C	-3.06706669883768	0.25062288573711	0.21090781120863
C	-3.58069821682958	-0.39315236511596	-0.92540115378706
H	-3.12565772362035	-1.40724749309781	-2.77828845664905
H	-1.26568126380005	0.86530759757994	1.24880878265741
H	-3.74133685592018	0.67119488137463	0.96120734029142
H	-4.66204501824914	-0.47998854310101	-1.06147831174645
N	0.53843099166170	-0.06150527167507	-0.41980211944942
N	3.04665799115473	2.71422564654988	-0.91094732279393
N	2.92995397500736	1.74859793813366	-0.33693141670512
C	2.81350897342368	0.61657583581893	0.34404125377695
C	1.53309462548903	0.03400897931382	0.23538183907469
I	1.17026432999009	-1.38434230319480	2.70007437704018
C	4.01751352104513	0.12208762308714	1.11038947997746
H	3.95065560352157	0.38242545367085	2.17808091363477
H	4.92846400376698	0.57344372937271	0.69148305062676
H	4.09455540387041	-0.96960999027360	1.01705560162293

C	-0.40972470558939	-1.39237127425110	-2.83137638872398
O	-0.46485973999535	-0.78867960130631	-3.95057597252928
N	0.30962696933262	-2.43821890536024	-2.49097293053202
H	0.86461758819063	-2.72424108527188	-3.30770798380123

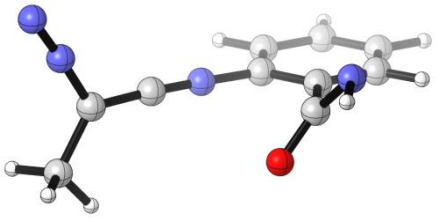
TS2$^{C}_{4}$



E_{PCM} = -977.0293 E_h
ZPE = 0.1658 E_h
G_{298} = -976.9075 E_h

C	-2.66508361103025	-0.93458098841471	-1.89299342951912
C	-1.27814642243695	-0.81007895607025	-1.73366980717226
C	-0.80514409725603	-0.15747339214796	-0.57148861606326
C	-1.69484334820282	0.37167294462566	0.38946236184829
C	-3.06797813638957	0.24075231422712	0.19744048054182
C	-3.55290646874200	-0.41502166979847	-0.94456971091045
H	-3.05355415754887	-1.44081972585434	-2.78088922580581
H	-1.29319832044692	0.87987905028594	1.26809150072093
H	-3.76140137383909	0.64966231629121	0.93652273961700
H	-4.63056444056306	-0.51691414817790	-1.09820767985978
N	0.55168163151863	-0.02560432940262	-0.38297475501850
N	3.11424930938481	2.67699374050861	-0.94553591629695
N	2.97585632859883	1.73364105446454	-0.34087508297426
C	2.83490206670742	0.62708812773096	0.37763825832873
C	1.54903544551042	0.05813349964038	0.26905532560900
I	1.17129607480086	-1.37213536162543	2.73419071630577
C	4.02430105976315	0.14442198894905	1.17377987691156
H	3.92728952662085	0.40511696094317	2.23882856610522
H	4.94012807230827	0.60630528342956	0.77787582905090
H	4.11674728064710	-0.94654203660339	1.08374036736383
C	-0.31825915605249	-1.40811520645202	-2.75476804190614
O	-0.05842794436333	-2.64376176494365	-2.59958773819172
N	0.11420854940240	-0.57749560866530	-3.67578378682397
H	0.74088028260860	-1.09332715694015	-4.30701211386083

I-5$_{1}$

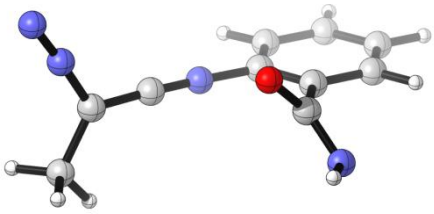


E_{PCM} = -679.1476 E_h
ZPE = 0.1663 E_h
G_{298} = -679.0220 E_h

C	-2.66735589935017	-1.09956382181542	-1.72838677909551
C	-1.29888175990424	-0.87027800928012	-1.52681780514920
C	-0.93848701310266	-0.13590908565076	-0.37054928080132
C	-1.89721676648176	0.35139920158281	0.54038823166003
C	-3.24604191570653	0.09370558373343	0.31282581096621
C	-3.62748998003929	-0.63509219121877	-0.82312824200572
H	-2.97799386937578	-1.65923453639592	-2.61296676039073
H	-1.56623416885418	0.92516032393875	1.40849401127853
H	-3.99771415834108	0.46077808626577	1.01550310762481
H	-4.68547804972046	-0.84075290906005	-1.00671792464121
N	0.38666828858211	0.14331749575999	-0.11912636325885
N	3.94689785487795	2.53019026344222	-0.62363511940514
N	3.42467859209688	1.62155911999651	-0.21615044509542
C	2.87272551277452	0.52340932631111	0.29354636908129
C	1.52167082806450	0.34805413516009	0.04515652683025
C	3.73254867874807	-0.43466290283340	1.09761368330400

H	4.12861008770913	0.05743888019305	1.99923027160567
H	4.56780157938579	-0.81298283115031	0.48862748606154
H	3.10868792867415	-1.28467188495512	1.40488054248260
C	-0.25199508040631	-1.42856293802162	-2.48585615552918
O	0.69561222096737	-2.08976059330679	-1.95470075563387
N	-0.46873370793241	-1.16521490994052	-3.75559036626200
H	0.28834379733454	-1.59246680275495	-4.30317004362680

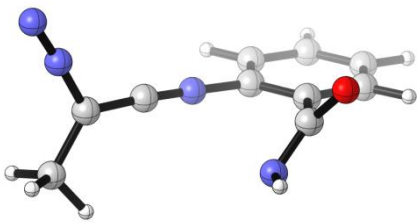
I-5$_2$



E_{PCM} = -679.1476 E_h
ZPE = 0.1663 E_h
G_{298} = -679.0221 E_h

C	-2.61421357628201	-1.11082405469309	-1.80499523520586
C	-1.26203830495794	-0.78889896556086	-1.62157251182974
C	-0.94587719595187	0.02895437447403	-0.50893523813740
C	-1.92991755509421	0.49883776643890	0.38344057787076
C	-3.26379964290614	0.16733901806834	0.16250548488611
C	-3.60254256875104	-0.63659069129506	-0.93565273266341
H	-2.88969196286806	-1.74306572600559	-2.65166538342663
H	-1.62963568202086	1.11359131585017	1.23450178943072
H	-4.03650896631927	0.53106058683804	0.84376192488160
H	-4.64865482472675	-0.89954745886963	-1.11419546417711
N	0.36537547063691	0.36907428816815	-0.25858146409164
N	3.80187182351994	2.86574364702465	-0.98998870365894
N	3.33633754897589	1.94720181388303	-0.53866919768235
C	2.85343960146188	0.84280645918743	0.02572329550642
C	1.50141650385679	0.60861804884212	-0.15755900692982
C	3.79299293802305	-0.07224543743554	0.78965033415090
H	4.34345726065767	0.49261784017591	1.55704103307170
H	4.50832640391895	-0.55905159534919	0.10864162354238
H	3.19459443710569	-0.84752029513215	1.28681756789964
C	-0.19356936315973	-1.25981870528159	-2.60342134077043
O	0.57562216225174	-0.35865216051439	-3.06562584778530
N	-0.20771078528419	-2.54892692376399	-2.86013347447586
H	0.54458227791358	-2.74873114504972	-3.53076003040571

I-5$_3$

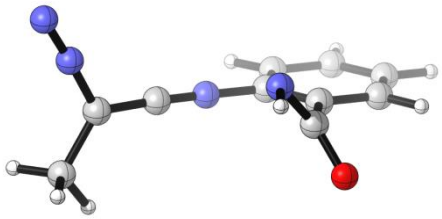


E_{PCM} = -679.1472 E_h
ZPE = 0.1663 E_h
G_{298} = -679.0216 E_h

C	-2.66127869169254	-1.05513872443471	-1.83807128618804
C	-1.29538426874244	-0.78359495545672	-1.66731014422001
C	-0.93537531313327	-0.00823874113530	-0.53858035571944
C	-1.89252200477054	0.46821173452713	0.38222086661898
C	-3.23529392359643	0.16109494221675	0.18983672842959
C	-3.61647899377142	-0.60524632577702	-0.92256269899414
H	-2.97263351323988	-1.63723263736463	-2.70841907688399
H	-1.56324898853060	1.07375130230641	1.22918156458488
H	-3.98434034195762	0.52011880635795	0.89945584727720
H	-4.67062688507385	-0.84950644600161	-1.07861619098737
N	0.38289849646934	0.32359712019129	-0.31958873730163
N	3.81849756664006	2.87354093576514	-0.88890883628966
N	3.34975362027120	1.93535221436936	-0.48310524728870
C	2.86385214333856	0.80167063687786	0.01494385386173
C	1.51212406681016	0.57627246260326	-0.18731629770689

C	3.78391313176884	-0.12445083674057	0.78948383347365
H	3.97907099935453	0.26497652190900	1.80125441333899
H	4.73764612033580	-0.24687539479625	0.25494862861008
H	3.30092178662803	-1.10747904497556	0.87247628365025
C	-0.28898889892089	-1.28834531009128	-2.69683722730731
O	-0.55935406797363	-1.00894824840997	-3.90723648016489
N	0.72414114160925	-1.96833941527855	-2.20881990471456
H	1.31218081817734	-2.27405959666182	-2.99398953607870

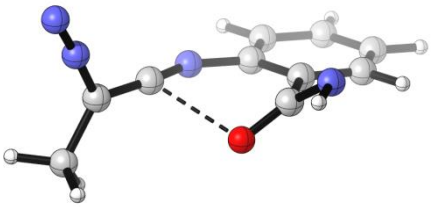
I-5$_4$



E_{PCM} = -679.1473E_h
ZPE = 0.1662 E_h
G_{298} = -679.0221 E_h

C	-2.60902570897201	-1.07814310493151	-1.82277718552058
C	-1.25634113636807	-0.75081934065584	-1.64434132080693
C	-0.93416903426282	0.03635703349971	-0.51255632195724
C	-1.91592517020107	0.48032432899191	0.39818375950142
C	-3.24917233155614	0.15159753761114	0.17713617480513
C	-3.59307987132640	-0.62699239344471	-0.93895235159423
H	-2.88765815636328	-1.69730316675380	-2.67860618219626
H	-1.61216014319729	1.07313820764517	1.26346593604989
H	-4.01860468997547	0.49504118242288	0.87250524696197
H	-4.63959597742386	-0.88810257097376	-1.11752856897114
N	0.37582147535501	0.37621313619613	-0.25792370815616
N	3.81255261382392	2.87857866935245	-0.97118028841346
N	3.34555830414546	1.96021855903416	-0.52092547031586
C	2.86042238176445	0.85685218422803	0.04334195546149
C	1.51030297957360	0.61906075127312	-0.14961667348052
C	3.79578268453083	-0.05207761774358	0.81956810120090
H	4.33815127657331	0.51772374453032	1.58910005588854
H	4.51840672091525	-0.54036363627582	0.14731231837594
H	3.19520882643580	-0.82654183546349	1.31541333530297
C	-0.21405878406727	-1.27407185871878	-2.62825743959699
O	-0.24090971660620	-2.52821913618143	-2.83458493732951
N	0.57216096728694	-0.36270903122709	-3.15541887728750
H	1.20809008491531	-0.82983281041523	-3.81361618792187

TS5$^C_1$

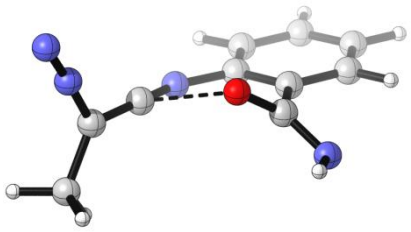


E_{PCM} = -679.1473 E_h
ZPE = 0.1662 E_h
G_{298} = -679.0203 E_h

C	-2.40629159271811	-0.91739443333621	-2.06756784799352
C	-1.11002717889840	-0.52688347941750	-1.69877774448467
C	-0.94589363759476	-0.04222923432035	-0.37690477065563
C	-2.02229014786913	0.06204261240843	0.52242847772495
C	-3.29299401658441	-0.34548163698093	0.12385132926912
C	-3.48050724359639	-0.83797440801789	-1.17506365925590
H	-2.56383749606786	-1.29311912785919	-3.08004371202155
H	-1.84052588179146	0.45926228277688	1.52325066618136
H	-4.13278681668546	-0.27709710564412	0.81932833261125
H	-4.47434947347095	-1.15967261835641	-1.49775557687486
N	0.30129043788875	0.36988682621109	0.07572575837143
N	3.76833022546615	2.67181845473137	-0.97284687792666
N	3.31253536259533	1.73374731889021	-0.55530422894211
C	2.83692707346560	0.60111565919124	-0.03639329024135

C	1.46771117722481	0.45025182506423	-0.07422272394608
C	3.81122226168725	-0.45051566567450	0.45831161069870
H	4.60307959534503	0.01842738106220	1.06110843640416
H	4.26670086232170	-0.99424659290816	-0.38434283843537
H	3.26486717889083	-1.16394525870884	1.09022026830888
C	0.05278342175560	-0.65436863426778	-2.67789735774921
O	1.16780652283562	-1.04210549141790	-2.19320505865061
N	-0.23240246972167	-0.35721904545398	-3.92510009260223
H	0.61994620752379	-0.48220593604024	-4.48414101963946

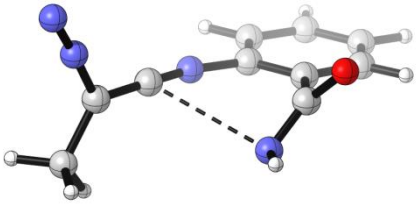
TS5$^{C}_{2}$



E_{PCM} = -679.1474 E_h
ZPE = 0.1661 E_h
G_{298} = -679.0205 E_h

C	-2.47314880978930	-1.07337557599485	-1.78826570260264
C	-1.16546911967100	-0.68905005238465	-1.45535450958342
C	-1.01725472353112	0.12169930512599	-0.30187641597422
C	-2.11504638016710	0.51612179181579	0.48361844703458
C	-3.39949765563521	0.12090337678367	0.11767969759256
C	-3.57451193186619	-0.67371220786119	-1.02365418727151
H	-2.61946938916337	-1.69886909098746	-2.67065604870571
H	-1.93967097591669	1.12963318133331	1.36980566967614
H	-4.25873516433724	0.42896470517646	0.71802754379994
H	-4.57878128412020	-0.98860702997094	-1.31968716424408
N	0.24107887393786	0.54940009150180	0.10274661764386
N	3.73869736317724	2.57900684554743	-1.42866840894153
N	3.26630688646180	1.75651448362778	-0.82741723736910
C	2.77157967549445	0.76097600841948	-0.09041571669199
C	1.39959743250727	0.63850086609549	-0.09759690311939
C	3.72951458642038	-0.18717144274169	0.60617539025351
H	4.47549472700162	0.37792770933098	1.18464131110138
H	4.24365282883699	-0.83483964382736	-0.12130944347192
H	3.15322652513545	-0.81655644967847	1.29778884223571
C	0.01812664820127	-1.10043108103587	-2.32663963662109
O	0.92359179908407	-0.22043821550852	-2.51147711474704
N	-0.03418646661018	-2.32401440019420	-2.80084942507773
H	0.80876055454924	-2.48061117457299	-3.36628760491618

TS3$^{C}_{1}$

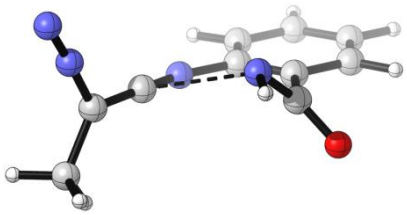


E_{PCM} = -679.1471 E_h
ZPE = 0.1662 E_h
G_{298} = -679.0205 E_h

C	-2.59234657088034	-1.03660389601581	-1.85228016958427
C	-1.25092347180708	-0.70886346377160	-1.60382854557668
C	-0.98704487946625	0.04643224787370	-0.43419889141520
C	-2.01170381417384	0.45142627724083	0.44488213454522
C	-3.32747496093239	0.08764320888675	0.17601634358235
C	-3.61406491487804	-0.66119992261880	-0.97530462224229
H	-2.82995630884797	-1.60271124942896	-2.75573627461974
H	-1.75462624353464	1.04657269599510	1.32359662047512
H	-4.12778764166674	0.39011399966418	0.85535197853983
H	-4.64578706650257	-0.94933608302266	-1.19395665547701
N	0.30289135364063	0.42968244072777	-0.13012289683973
N	3.83882326778783	2.66531983749140	-1.16823291996233

N	3.34544307720905	1.79479794983490	-0.65640937584054
C	2.82957562068178	0.74342265611239	-0.02169272524739
C	1.46149527446107	0.58046478524028	-0.13026851277702
C	3.75675265467621	-0.19691449832682	0.72589487616289
H	4.38134314327833	0.36274408046737	1.43834534198048
H	4.40302619697789	-0.75049854392673	0.02711416914968
H	3.14368136756467	-0.91596165464905	1.28553185116528
C	-0.17748146786949	-1.13437845526058	-2.60185401541949
O	-0.43417909975086	-0.88202694747180	-3.82077772003017
N	0.87491786260741	-1.72926918949122	-2.08450343661900
H	1.50490062142534	-1.98972527555047	-2.85312655394991

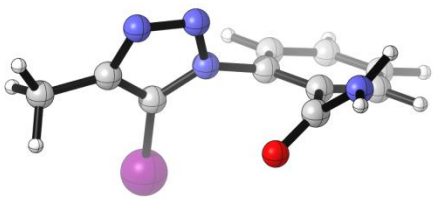
TS3$^{C}_{2}$



E_{PCM} = -679.1472 E_h
ZPE = 0.1661 E_h
G_{298} = -679.0208 E_h

C	-2.52764535586911	-1.06142934907479	-1.81308399301220
C	-1.20277777912583	-0.68811213103301	-1.54075477103436
C	-0.99152513373419	0.10141718187427	-0.38219807943360
C	-2.05004432182594	0.49666275452056	0.45897397862850
C	-3.35314051546878	0.12218956042920	0.14476847584132
C	-3.58865448118844	-0.65645996854647	-0.99767527159313
H	-2.72065413681554	-1.68379074926245	-2.68957361423864
H	-1.82853816648203	1.09198507734346	1.34721890621322
H	-4.18084378844729	0.43024749206476	0.78783257891616
H	-4.60899181347829	-0.95597623458277	-1.25163976316386
N	0.28392653502384	0.50026690091610	-0.02818707205312
N	3.77006665176102	2.72182169807319	-1.25255577368551
N	3.30167767260577	1.85600568638111	-0.71095089563033
C	2.81287218406829	0.80910227928722	-0.04690782491346
C	1.44415676923706	0.64235834088710	-0.11136501834296
C	3.77092588739748	-0.12866266214130	0.66400309385078
H	4.44595089684635	0.43823877453595	1.32250684107981
H	4.36557634627941	-0.70852049264264	-0.05914967294797
H	3.18379828156976	-0.82393992242504	1.27915700055221
C	-0.08610156149322	-1.16975133693394	-2.46483244511136
O	-0.14409352752389	-2.39242330194343	-2.80509971796623
N	0.79408423855180	-0.25713495179522	-2.81722719132593
H	1.47173271311177	-0.69416581393189	-3.45351840062929

I-1N$_{1}$

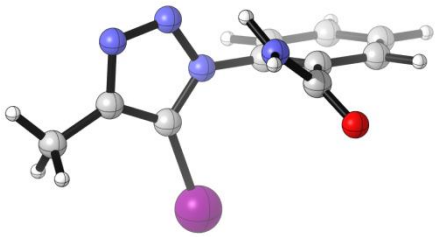


E_{PCM} = -977.5527 E_h
ZPE = 0.1826 E_h
G_{298} = -977.4122 E_h

C	-1.37664549394048	1.19873286701053	0.38116241691485
C	-0.01914742172963	1.30346858334817	0.69903491690537
C	0.83698463556045	0.22709377796408	0.45020620623719
C	0.35372753440245	-0.97581702557252	-0.10007164607288
C	-1.01635017030290	-1.06951481739450	-0.39294536683334
C	-1.87431700037487	0.01131218330360	-0.16395641879824
H	-2.04398263772278	2.04304036334646	0.57039197724862
H	0.37997558909599	2.21390176736343	1.15096968831629
H	-1.41121737730118	-1.99074387566303	-0.82808950156190
H	-2.93476764503173	-0.07765359240219	-0.41252421472815
N	2.21626328878903	0.34495620401962	0.82241162971887

N	2.70717747048811	-0.39575699396310	1.83332383422924
N	3.96977617770450	-0.09913981054358	1.96960166566400
C	4.33451190896322	0.84161891471982	1.05445303453024
C	3.20044566738426	1.13634385359051	0.30594925265588
I	2.98584098735864	2.42821754455753	-1.31435325524095
C	1.28817573080525	-2.11350276426014	-0.44366101857204
O	2.32063453023297	-1.91481360001803	-1.08884095336423
N	0.89998028964652	-3.34035788169283	-0.03955764893871
H	0.08846038802043	-3.48861668220738	0.55065706691158
H	1.47543535542692	-4.14486273915312	-0.27385120949937
C	5.72182504693169	1.38544577650009	0.95406802335727
H	5.74220832574908	2.47106214920352	1.14443512307601
H	6.14751681333402	1.21588862068079	-0.04834669710769
H	6.36747800651002	0.89163717726229	1.69375809495208

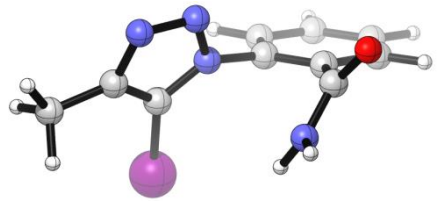
I-1N$_2$



E_{PCM} = -977.5517 E_h
ZPE = 0.1826 E_h
G_{298} = -977.4112 E_h

C	-1.49203209554152	1.16171226127029	0.50956438646389
C	-0.15074411747170	1.21749441032617	0.89522981534624
C	0.72290058837908	0.18744933698300	0.52996378335722
C	0.27746621259489	-0.91139703306655	-0.23088016191030
C	-1.07003534328510	-0.93585671367052	-0.62728709530737
C	-1.95025744311860	0.08218253464456	-0.25397154639685
H	-2.17458707668080	1.96394021995191	0.80032893613493
H	0.23316775558142	2.06009699775010	1.47417699461863
H	-1.42467745001824	-1.77434297370520	-1.23018321750432
H	-2.99732275371174	0.03373795719540	-0.56316801354034
N	2.09597452802592	0.29683791590986	0.94067510483445
N	2.49503961366935	-0.18835262601387	2.13263651279644
N	3.77101433797960	0.05463146415076	2.25448830830957
C	4.23528857498401	0.70628686303584	1.15288609587826
C	3.15239909550456	0.86984425707536	0.29521889284136
I	3.05482757150085	1.78393738168331	-1.57324231914238
C	1.15555418554366	-2.05300075909487	-0.69862098699645
O	1.07451690533685	-2.45220725157082	-1.86395323568877
N	1.97941052743838	-2.61545652186504	0.20726515922326
H	2.01057991162782	-2.32223902759188	1.17882329100021
H	2.57339630845495	-3.38852630795896	-0.08061941352977
C	5.66158644361542	1.11653059614525	0.98851460957829
H	5.74458030924309	2.18645594227731	0.73936385920831
H	6.15012826912538	0.54772756936340	0.17989445140497
H	6.21130214122248	0.93116550677523	1.92187578902051

I-1N$_3$

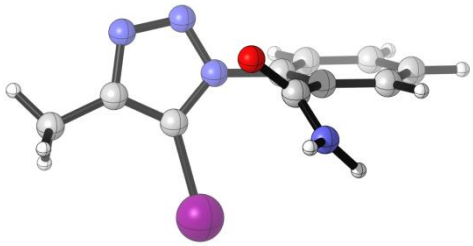


E_{PCM} = -977.5516 E_h
ZPE = 0.1825 E_h
G_{298} = -977.4112 E_h

C	-1.25169417262543	1.22123686829358	0.60841936374323
C	-1.04658235588457	0.19365758592523	1.53143995473385
C	-0.22258478723409	-0.88749438138619	1.19700092150666
C	0.39048143094718	-0.96897772220779	-0.06701075423985
C	0.14673428246176	0.05853183270304	-0.99263268819667
C	-0.65475265717586	1.15211790772218	-0.65593951865109

H	-1.89126426109971	2.06676215940868	0.87323339431879
H	-1.53374737432187	0.21572137309436	2.50835876369886
H	0.60611187738042	-0.00083743138464	-1.98199634271722
H	-0.81861736759876	1.94936383258758	-1.38521168513488
N	-0.06891262969379	-1.95324035317913	2.14431770688326
N	-0.55975797703318	-3.17749013352404	1.86698829262722
N	-0.31200973605889	-3.94776463344637	2.88841590210587
C	0.34109409469974	-3.25021590266424	3.85951098011527
C	0.50134710324572	-1.95301061365909	3.38579066204162
I	1.46612639856459	-0.33493431408419	4.27667782729081
C	1.26898283621496	-2.12231373809407	-0.50367731099751
O	1.00399716198538	-2.75189944355885	-1.53052823114185
N	2.34596770321298	-2.38711039482770	0.26237448877150
H	2.61109981191376	-1.80552028682141	1.04984097722313
H	2.97125385178787	-3.14304353887297	-0.00457705630198
C	0.76054278051939	-3.85955298008141	5.15674283118811
H	0.27050503587550	-3.36229778386220	6.00982152945196
H	1.84959742848025	-3.77737860305031	5.30494967046888
H	0.48696716943668	-4.92384557803005	5.17158867921203

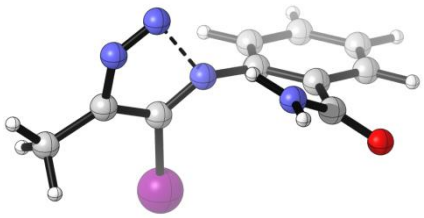
I-1N$_4$



E_{PCM} = -977.5516 E_h
ZPE = 0.1827 E_h
G_{298} = -977.4109 E_h

C	-1.55618611091073	1.10418503255594	0.60091600238504
C	-0.21032286238111	1.18816550630060	0.97043203963243
C	0.69602507773017	0.22118622420291	0.52745163344360
C	0.28152909867813	-0.84278568445496	-0.29945375527999
C	-1.07165495590455	-0.89876359128095	-0.67274466480884
C	-1.98522188943282	0.05990389858035	-0.22275433681008
H	-2.26416145761630	1.85772596645025	0.95443527436023
H	0.14868705261388	2.00547926857290	1.59920709620052
H	-1.42217360975011	-1.72060312474172	-1.30127928001199
H	-3.03540707089081	-0.01438712659127	-0.51558743799632
N	2.06367247119373	0.34911403964227	0.94315539636415
N	2.41425457826762	0.06148322651704	2.20901311844424
N	3.69654603226374	0.26954674543481	2.32572843371433
C	4.21414878559131	0.70129332896792	1.14180980605253
C	3.15891496048244	0.75880332785280	0.23906877245688
I	3.14363737871143	1.39466197505090	-1.74543618982312
C	1.23308984990188	-1.93960903616273	-0.72086455228075
O	2.03501717117955	-2.43293942290703	0.07621452349215
N	1.12217008072942	-2.35973062987027	-1.99865610235796
H	0.52493236720078	-1.89753902604840	-2.67543037724422
H	1.71840322416967	-3.11564132878298	-2.32400534184579
C	5.66030856447314	1.02377863829481	0.95482539595731
H	5.79525856089706	2.03467492985754	0.53785070810427
H	6.14356772054591	0.31229124901908	0.26467798841800
H	6.17962178125656	0.97282644854020	1.92205737043338

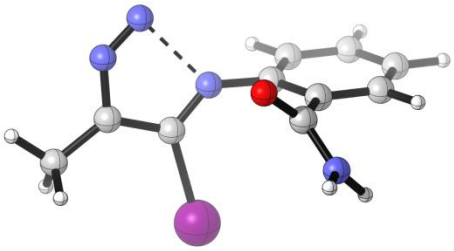
TS1$^{D}_{1}$



E_{PCM} = -977.5099 E_h
ZPE = 0.1794 E_h
G_{298} = -977.3728 E_h

C	-2.90889646315150	1.71106455277891	-0.86419169620280
C	-1.63781285474781	1.58332741279313	-0.30631222932563
C	-0.88490527261400	0.40353483277122	-0.47900011599920
C	-1.43119999926142	-0.67036794384543	-1.23041470259632
C	-2.70995482549541	-0.50806046450603	-1.79409231152111
C	-3.45183809467672	0.65878377806798	-1.61204796322248
H	-3.47536294129709	2.63396195037612	-0.71351036208157
H	-1.20566634662393	2.39721328892969	0.27989431750487
H	-3.11711182928819	-1.33074855327613	-2.38466476299290
H	-4.44821748987789	0.74750558598000	-2.05178042398327
N	0.36725677232360	0.32504131598598	0.13678413321636
N	1.02546629875612	-0.46075776267440	1.99279124147733
N	2.08467940106261	0.02217186384564	1.82697271534987
C	2.56159798026454	0.77744372228516	0.82748106037176
C	1.48190474876922	0.91756429697865	-0.11337901911284
I	1.83152289153463	2.08017388274905	-1.87150289621660
C	-0.74108993749310	-1.98445655820205	-1.52108291886327
O	-1.03595696725178	-2.62788110207193	-2.53655480452693
N	0.16114566987097	-2.44330673790972	-0.63000723806384
H	0.42188660934782	-1.91740348933483	0.19779512291528
H	0.62912998472616	-3.32492083331155	-0.81885008505369
C	3.95817010392342	1.31210300121503	0.78980426700284
H	3.97379262958558	2.41323974530673	0.74439227781268
H	4.52200830444539	0.93003464733838	-0.07705852679743
H	4.48776062716876	1.00248556773041	1.70158892090890

TS1$^{D}_{2}$

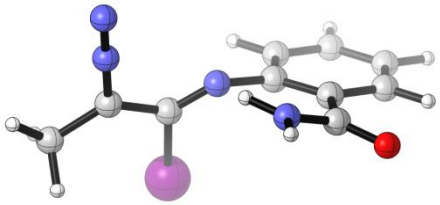


E_{PCM} = -977.5081 E_h
ZPE = 0.1791 E_h
G_{298} = -977.3715 E_h

C	-3.17612026051979	1.62431972608771	-0.74050651002063
C	-1.90565651910728	1.60873298877426	-0.16238000089226
C	-1.02172146191940	0.53746657153859	-0.39299783000353
C	-1.43545355889001	-0.54223864563407	-1.21606661335077
C	-2.71633098200827	-0.50178185210504	-1.79384771882556
C	-3.58654535150718	0.56626850592608	-1.55937451053030
H	-3.84648806867149	2.46643348356160	-0.54908650127986
H	-1.57327174825573	2.43105079634987	0.47486877361810
H	-3.04564016675200	-1.33485133747605	-2.41993898340883
H	-4.58223312901992	0.56707361605423	-2.00948601073909
N	0.22287951291417	0.56574033816457	0.23255276407966
N	0.84044339400829	0.19648683379573	2.24711847035502
N	1.95401423045687	0.39411797066424	1.93225088434140
C	2.50446049062439	0.71111066804219	0.75281006448467
C	1.41237270623033	0.79182019675164	-0.18473828339912
I	1.87883934762410	1.32811600579208	-2.20726989327147
C	-0.56621195709251	-1.75828230851802	-1.42342889171516
O	0.00309721319726	-2.31896225905314	-0.48231000419226
N	-0.48859909446826	-2.21892661812026	-2.69215553946762

H	-0.87761019253567	-1.71140638533101	-3.47913301437457
H	0.05543780911229	-3.05582001351940	-2.88274582909487
C	3.97133706007343	0.93125572088900	0.55789477278535
H	4.19074146926402	1.94927778425457	0.19611000216764
H	4.40400587644785	0.21696196521638	-0.16190152920701
H	4.48656238079452	0.79645024789423	1.51930393194108

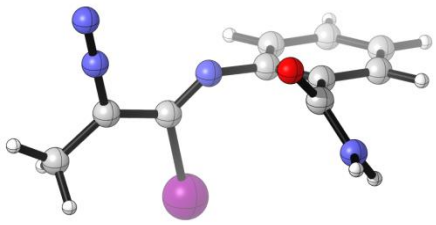
I-8$_1$



E_{PCM} = -977.5315 E_h
ZPE = 0.1797 E_h
G_{298} = -977.3350 E_h

C	-2.84711241333727	1.73712474438414	-0.97067273170601
C	-1.59320093034638	1.56048485475856	-0.38793965697445
C	-0.88912612516151	0.34533672909696	-0.52880870113729
C	-1.48244739412674	-0.72145963921827	-1.26077934724712
C	-2.74076120109272	-0.50648635914140	-1.85153603036282
C	-3.42592697682735	0.70029275073876	-1.71333240039576
H	-3.37337003520578	2.68688676490144	-0.84148897686464
H	-1.14354812340937	2.36098493295157	0.20252508000488
H	-3.17918456132534	-1.32508944970629	-2.42474796468116
H	-4.40771243045081	0.82931402860308	-2.17545164547722
N	0.33819552320869	0.19876559504510	0.11240867643113
N	2.11089691870117	-0.69018292554242	2.86467616247116
N	2.31099273169841	-0.02984055676597	1.96548834460174
C	2.53780582125899	0.74100800298525	0.92181974406535
C	1.40667842028574	0.87118917958222	0.02870703400635
I	1.72767889863137	2.36769523627913	-1.58721697308712
C	-0.87622994623149	-2.09092448261297	-1.47267791951311
O	-1.35104143467020	-2.86154935206179	-2.31858775964920
N	0.16706943882589	-2.45314044302094	-0.69763690795527
H	0.56102604760730	-1.81556218268647	-0.01038543356483
H	0.57140876755797	-3.37684219110191	-0.81931488945848
C	3.90677095605321	1.37003255877342	0.80471747439415
H	3.84927916720112	2.46808052828204	0.86835473404686
H	4.38700056883521	1.09728003161564	-0.14769160015793
H	4.54688531231989	1.01369764386108	1.62388668821082

I-8$_2$

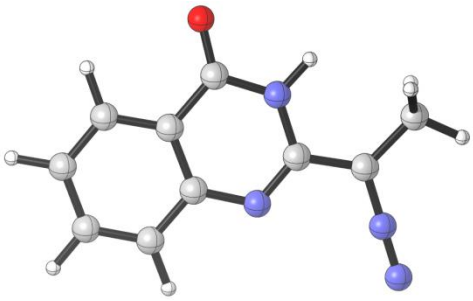


E_{PCM} = -977.5287 E_h
ZPE = 0.1794 E_h
G_{298} = -977.3322 E_h

C	-1.32948322866160	1.85391617173024	-0.31304169505561
C	-0.05153097405676	1.73553883457875	0.23667232532728
C	0.68858247849870	0.54687117608675	0.08371599522340
C	0.12174401752205	-0.53705017707569	-0.63151335412174
C	-1.15876695241156	-0.39099169224630	-1.19081265185618
C	-1.88925740792758	0.79006946775314	-1.02997753300578
H	-1.88894785942850	2.78391455929349	-0.18003270065474
H	0.39055602381693	2.56272916000316	0.79636178944187
H	-1.59609023916714	-1.22527326170155	-1.74560836178601
H	-2.89032906982233	0.87606111777818	-1.45950471143100
N	1.94434825830141	0.44243069622091	0.67326657405830
N	4.00974183869784	-0.45210118184898	3.20757970336167
N	4.14424919711883	0.12224439389534	2.23826978720713
C	4.28799468458273	0.78570225538207	1.11308842253333

C	3.06235166973771	0.91296184974785	0.34530286581231
I	3.32292315096087	2.04546779758167	-1.56882104656356
C	0.85151118729828	-1.85125085363694	-0.76393027845027
O	1.29242953531335	-2.45376104105607	0.21981093324460
N	0.95497036696831	-2.34145953746006	-2.01905772520151
H	0.65390625397686	-1.81503190013151	-2.83195783277023
H	1.40055358752638	-3.24287148763875	-2.16754007730501
C	5.66351710175956	1.31265998082945	0.77855226310374
H	5.65402250755984	2.40848323216814	0.67058217930045
H	6.04483592066272	0.87170059120879	-0.15598339693983
H	6.36308395117309	1.05648484853790	1.58663952652737

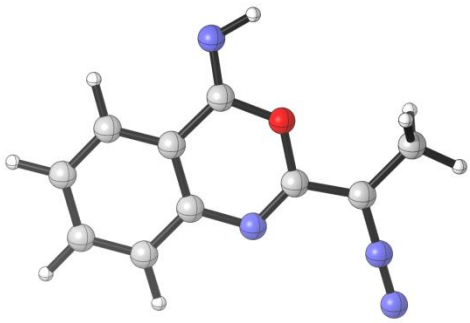
I-6



E_{PCM} = -679.2602 E_h
ZPE = 0.1708 E_h
G_{298} = -679.1273 E_h

C	-3.41326182127683	1.32256070997539	-0.87922758672705
C	-2.26164672774949	1.31974778101138	-0.10342641711472
C	-1.15193269375239	0.51722543562494	-0.46745697321508
C	-1.25184462955901	-0.28142450264977	-1.64217488646695
C	-2.42846405965111	-0.26695920814969	-2.41797516463729
C	-3.50382513182686	0.52837832095550	-2.04327405028125
H	-4.26032045363219	1.94833240220488	-0.58447892332461
H	-2.18743266183459	1.93287452982094	0.79760338290655
H	-2.47719955912599	-0.88894222630379	-3.31449726113428
H	-4.41609574140848	0.54059542648905	-2.64459533053550
N	-0.02263801885679	0.53746789062705	0.32146136717676
N	2.24539125510891	1.20004374324253	2.73478415830962
N	2.23239072586211	0.53480014018575	1.81323097382397
C	2.22116102255472	-0.23147084231191	0.75397020091568
C	0.99522860685780	-0.20635045880789	-0.02929637423358
C	-0.10646379831881	-1.11126581791967	-2.02226597160775
O	-0.04374671747631	-1.85127738125219	-3.00495374544697
N	0.97319364060023	-1.00672114259372	-1.15354336307281
C	3.44745618168651	-1.05448278867852	0.43446884567100
H	3.87312337642395	-0.77240563211922	-0.54338744831056
H	3.20947775380801	-2.13145673541231	0.41548710259152
H	4.22113102478926	-0.89457293481054	1.19736695322550
H	1.78741842677734	-1.56949670912822	-1.39361948851220

I-7

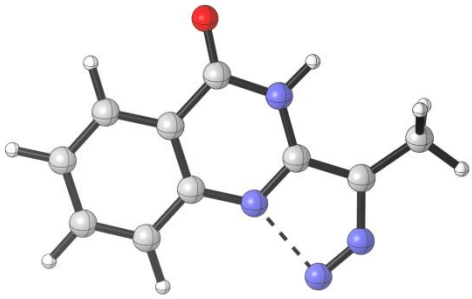


E_{PCM} = -679.2162 E_h
ZPE = 0.1695 E_h
G_{298} = -679.0849 E_h

C	-3.51788453022309	1.30378146987168	-0.97516779870367
C	-2.39017458723828	1.33906653891820	-0.15988048366448
C	-1.25772225012425	0.55941098443245	-0.47728386088152
C	-1.28902064631405	-0.25829497576367	-1.63543183236590
C	-2.43521007532718	-0.28461791293444	-2.45018477795749

C	-3.54473737371542	0.49165432520680	-2.12489113996611
H	-4.38899531057103	1.91316404636878	-0.71936569246732
H	-2.35912470290369	1.96653886551187	0.73368057540224
H	-2.44148799910296	-0.91952384063369	-3.33823991315248
H	-4.43347677555315	0.46957677722064	-2.76020019063970
N	-0.14317739818934	0.61227159910185	0.34729574982962
N	2.17579277517334	1.27820388519890	2.78715043659782
N	2.14243672436652	0.61829222124777	1.86308661558067
C	2.11187345487893	-0.14377257115730	0.79948559338546
C	0.88322381559201	-0.10718614348948	0.03448968432363
C	-0.10307014390673	-1.06157147582883	-1.94860459183491
N	0.02364519010033	-1.84326584820370	-2.94465945486599
O	0.95205478114812	-0.92709797455642	-1.05349463479430
C	3.32050915014634	-0.98000927176231	0.45174355792047
H	3.71840217526954	-0.70099740513835	-0.53673148211486
H	3.06127184797336	-2.05021355102307	0.42873017754124
H	4.11171734855421	-0.83094440598947	1.19893566852817
H	0.94285452996644	-2.29486533659822	-2.95146220570056

TS4[c]



E_{PCM} = -679.2378 E_h
ZPE = 0.1702 E_h
G_{298} = -679.1046 E_h

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C	-2.08691001232811	1.35836142537192	0.01102400602557
C	-1.03764348592974	0.51222934095809	-0.40808956912302
C	-1.21346340094535	-0.29225688591871	-1.56753646777119
C	-2.42471658204030	-0.23700062755173	-2.28292947882596
C	-3.45044184610336	0.60133141175143	-1.86110434448055
H	-4.08227772619161	2.05623108878899	-0.37969904427641
H	-1.94612462491147	1.97331433969080	0.90221414045907
H	-2.53971625241132	-0.86271786176777	-3.17079193382276
H	-4.38967610977943	0.64368991599483	-2.41754300599219
N	0.14628719490916	0.46229821662409	0.29388765109725
N	1.13086444876415	1.23255084240773	1.93828865871676
N	2.08725825146101	0.58094779974016	1.69906970885532
C	2.32419982566792	-0.28713265587570	0.71330354097822
C	1.13309157158111	-0.32030477764517	-0.09224308578294
C	-0.11957362439298	-1.17578187367509	-2.00288579286731
O	-0.15331678607942	-1.92054915591837	-2.98042057683014
N	1.01725317493025	-1.11947893636053	-1.20319592838027
C	3.59651792967551	-1.05176406065639	0.53028280971479
H	4.06716812485601	-0.83743073558112	-0.44461898498490
H	3.43447246552218	-2.14181913012045	0.59111117669283
H	4.31148288311903	-0.77339521507619	1.31663501603981
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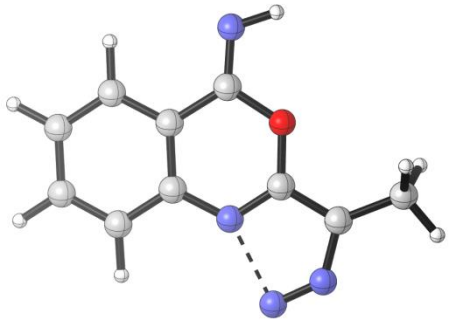
TS6^{C}



E_{PCM} = -679.1895 E_h
ZPE = 0.1690 E_h
G_{298} = -679.0576 E_h

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C	-2.10780435370336	1.35463058502483	0.02221069679882
C	-1.05428266139485	0.52299551860884	-0.39920525739767
C	-1.20436630451024	-0.27246472376958	-1.56329425618986
C	-2.40801762805866	-0.21917743591550	-2.28810261232268
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H	-1.97756576686822	1.96036266629031	0.92121657108514
H	-2.51311252017427	-0.83520472218160	-3.18322870215165
H	-4.37948774930297	0.64509430247247	-2.43408960330015
N	0.13532751594161	0.46791910702427	0.30661777327017
N	1.11862278719495	1.20726597851644	1.92173812734163
N	2.08610291906164	0.56352100685899	1.69077710891416
C	2.30785582825125	-0.29713576355102	0.68937424207344
C	1.11221993202445	-0.30510694614559	-0.09073402126415
C	-0.09414721369761	-1.13978430012038	-1.98559333042670
N	-0.10230622268336	-1.90328438712696	-2.99968201116330
O	1.05039497865330	-1.09749216115315	-1.18136025593365
C	3.56670942474588	-1.07315172008899	0.47423267801134
H	4.01159833270098	-0.85854452913083	-0.51133239343177
H	3.39051406256697	-2.16020140355243	0.53167606321452
H	4.30203580909326	-0.80565381400428	1.24562059264511
H	0.78027237514705	-2.41343108418434	-3.09858237887110

UV-vis and fluorescence spectra

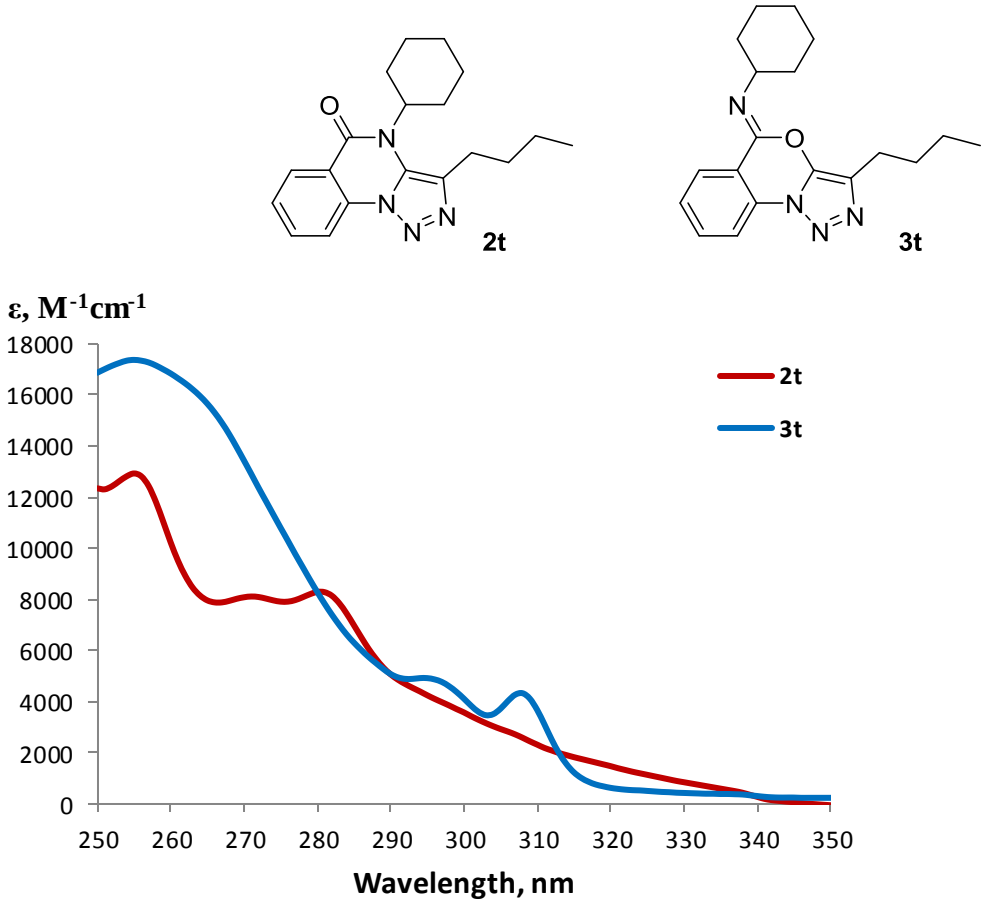


Figure S1. UV-vis spectra for compounds **2t** and **3t** in CH_2Cl_2 (C = 10^{-5} M).

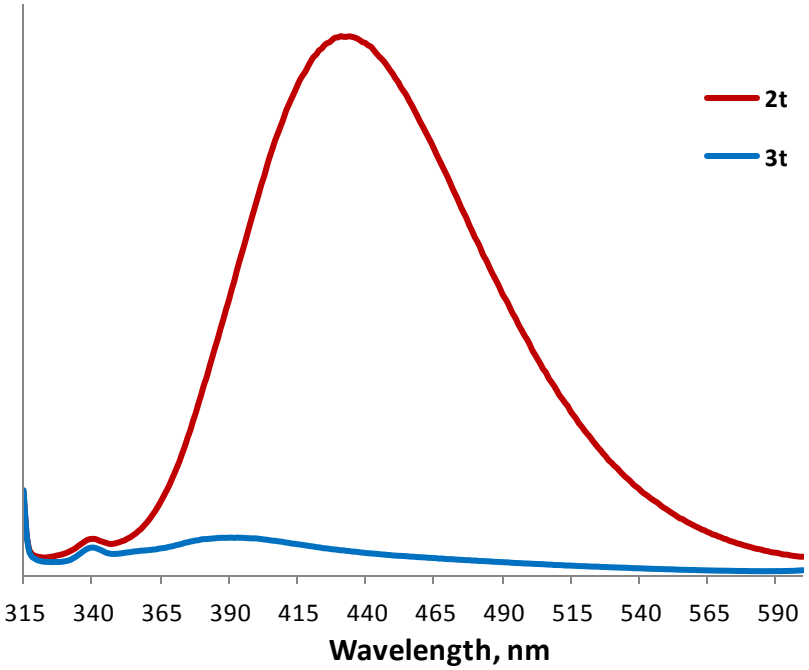
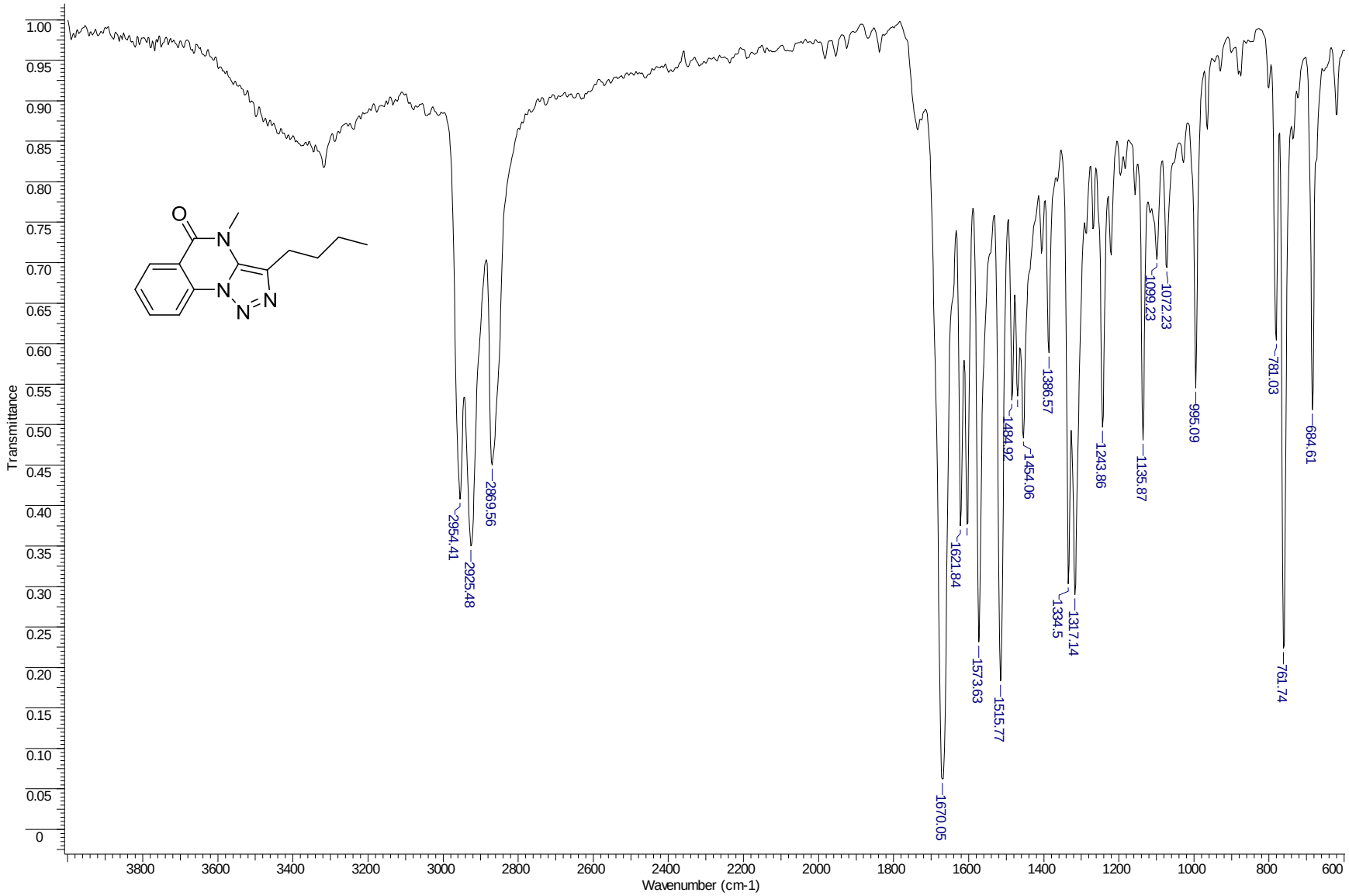


Figure S2. Fluorescence spectra for compounds **2t** and **3t** in CH_2Cl_2 (C = 10^{-5} M, λ_{ex} = 308 nm).

Copies of IR spectra

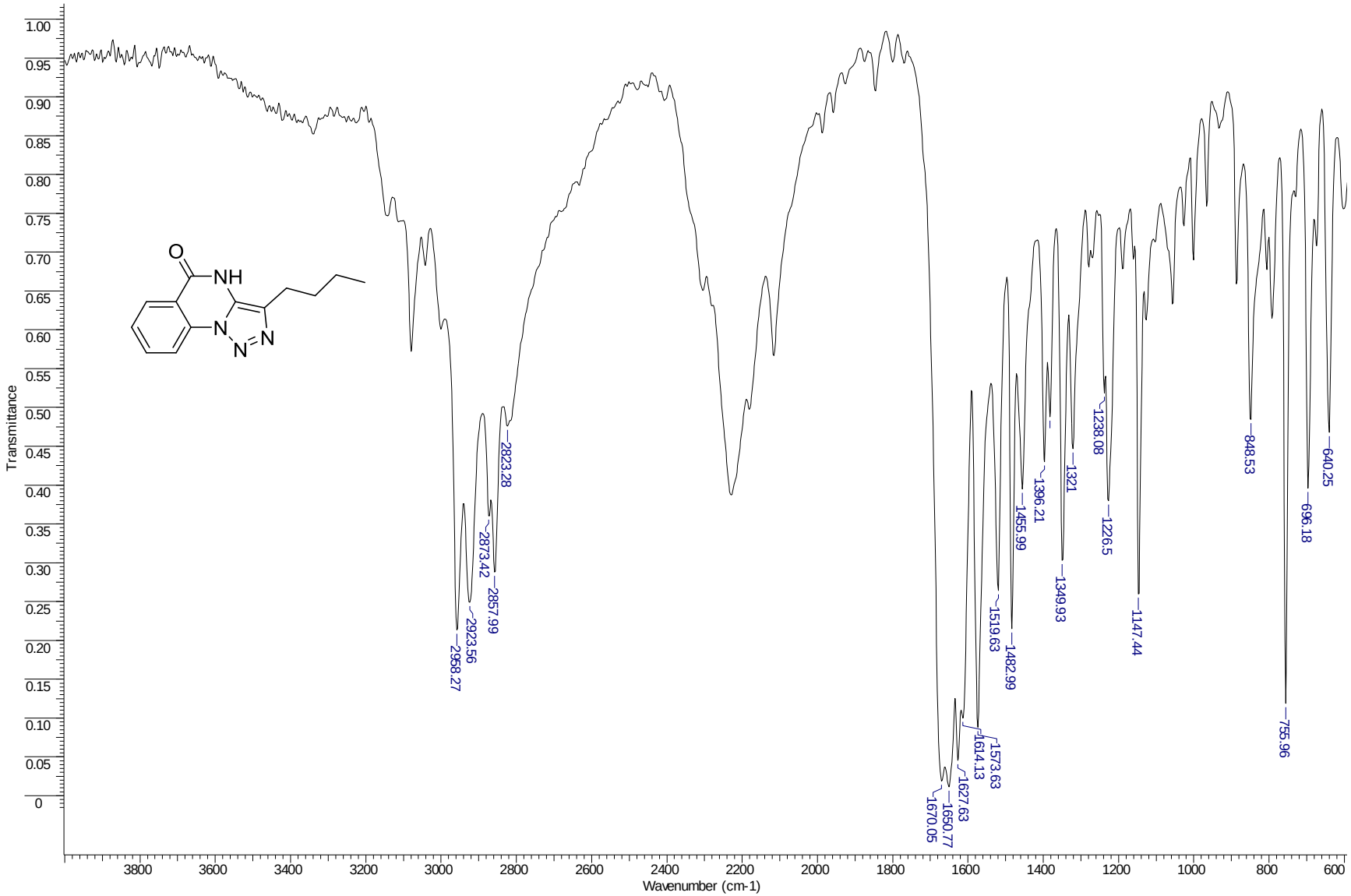
3-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2a)

IR (KBr)



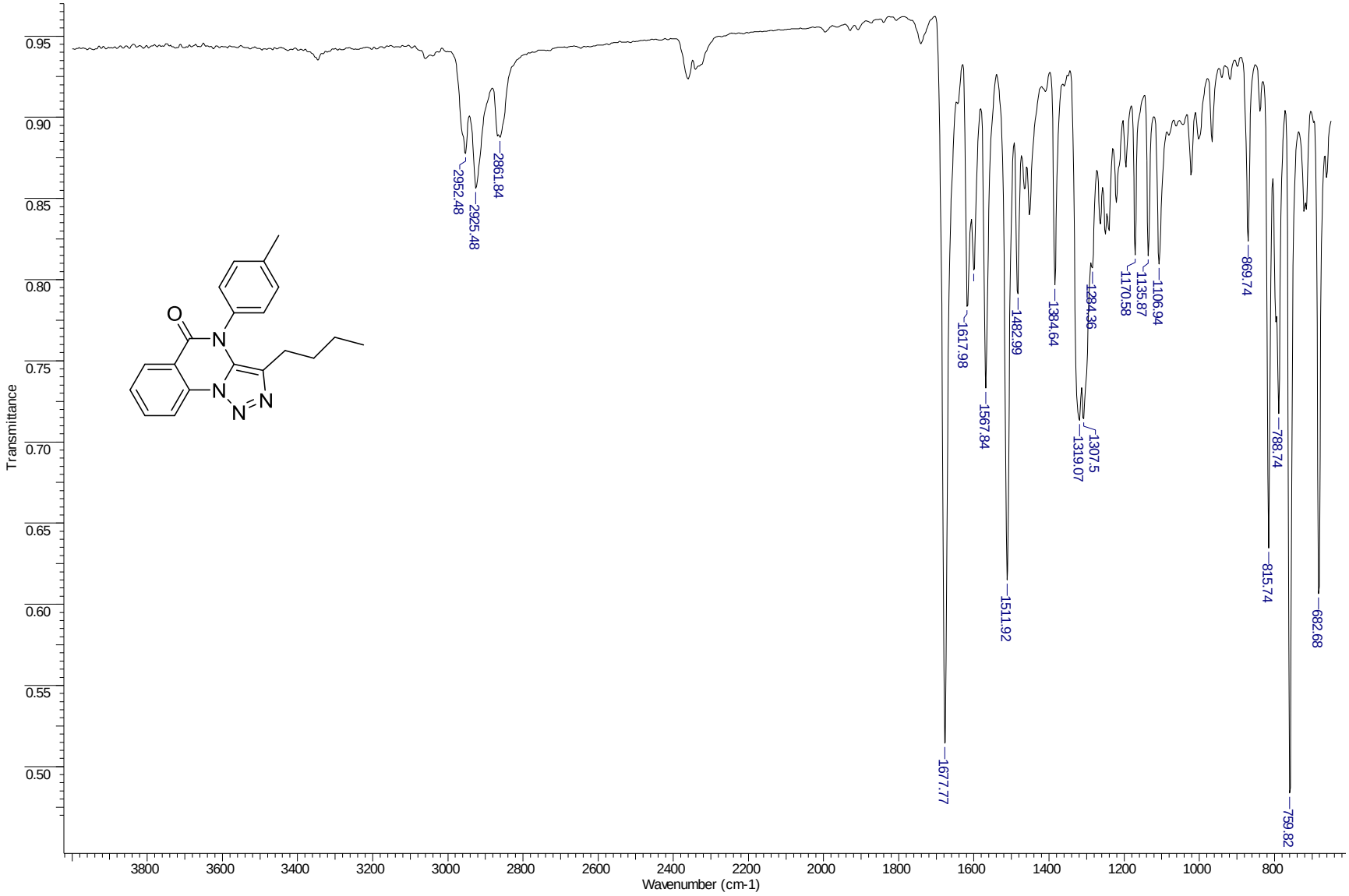
3-Butyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2p)

IR (KBr)



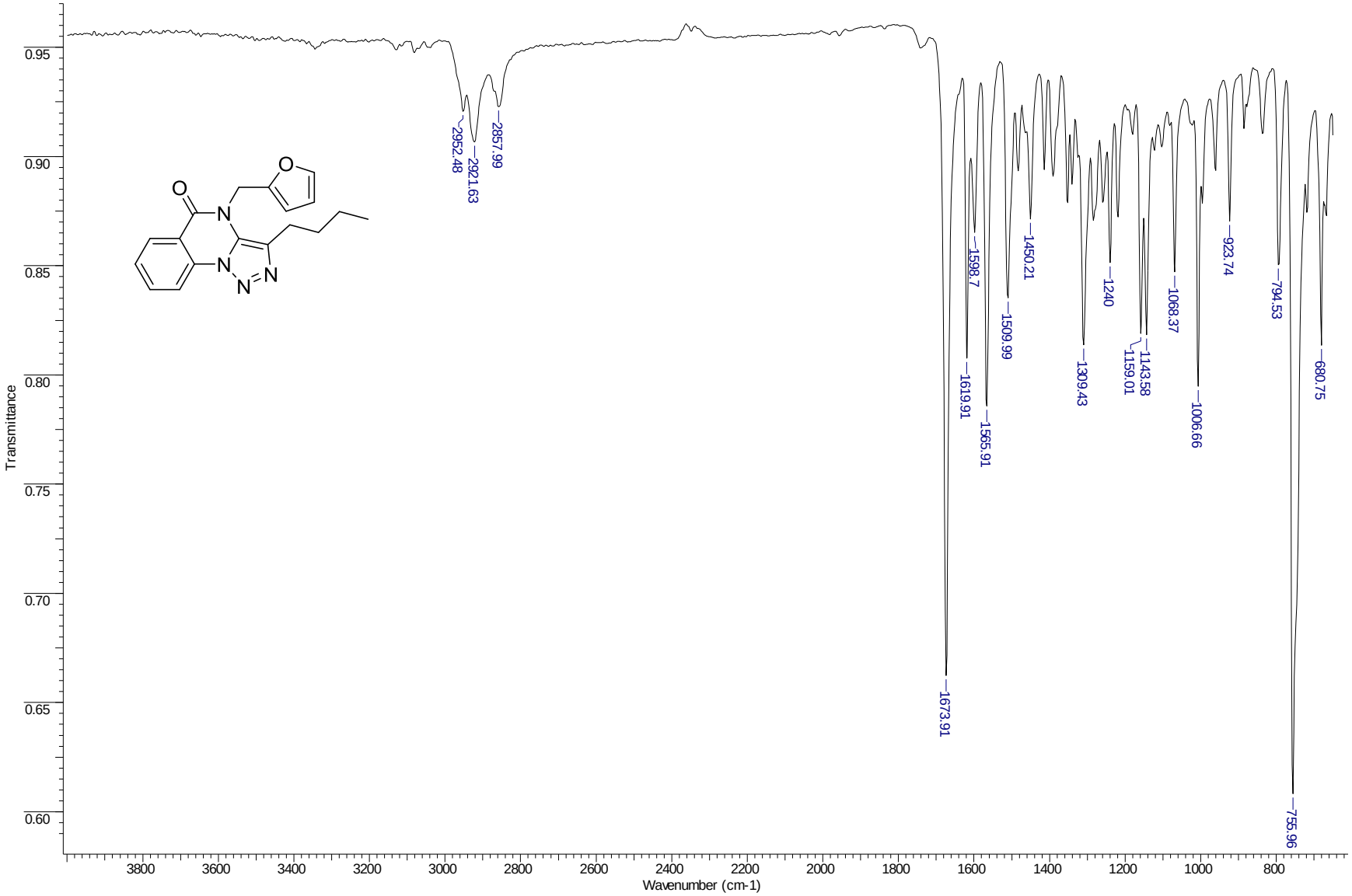
3-Butyl-4-(4-methylphenyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2q)

IR (KBr)



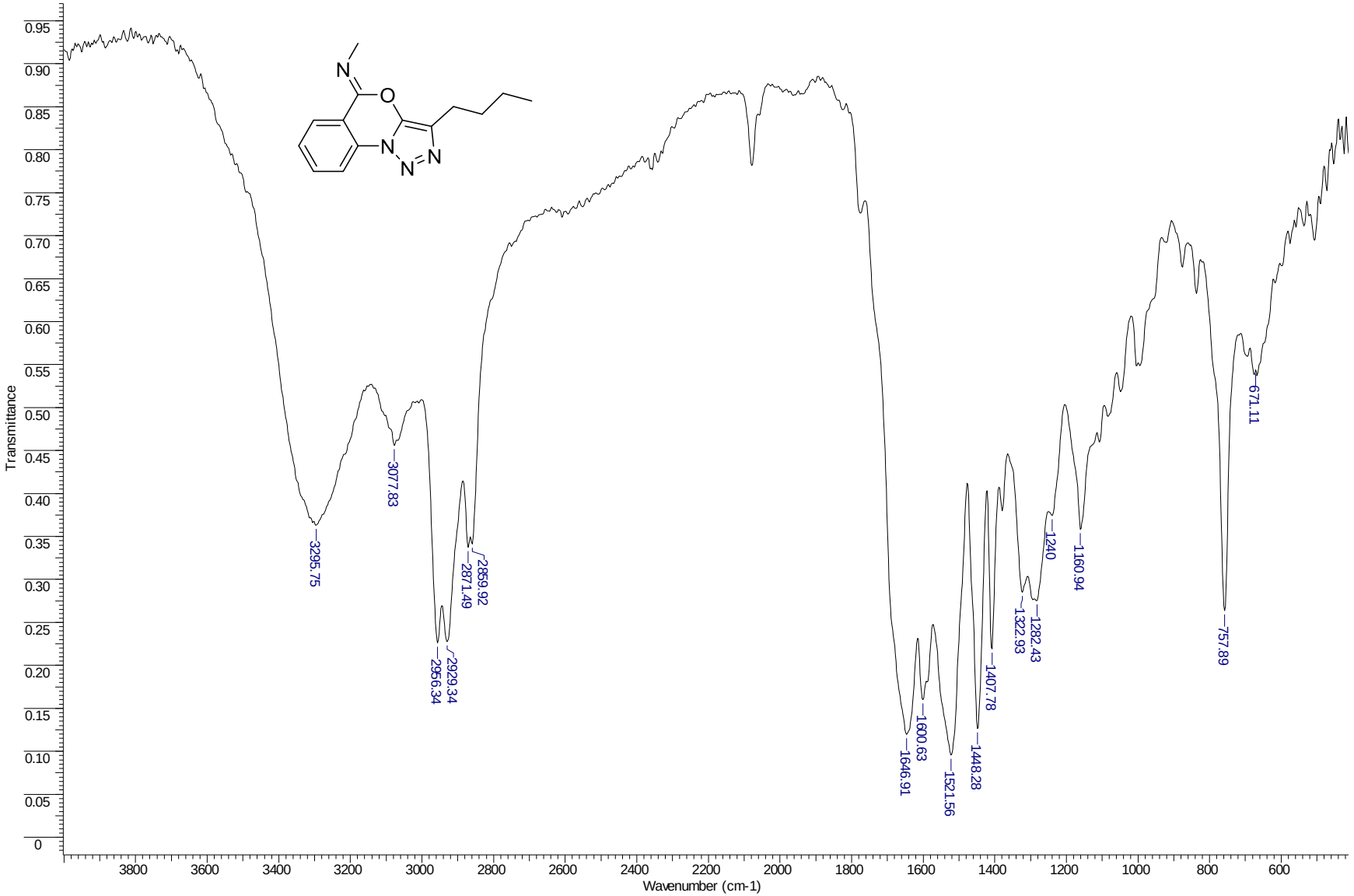
3-Butyl-4-(2-furylmethyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2w)

IR (KBr)



3-Butyl-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3a)

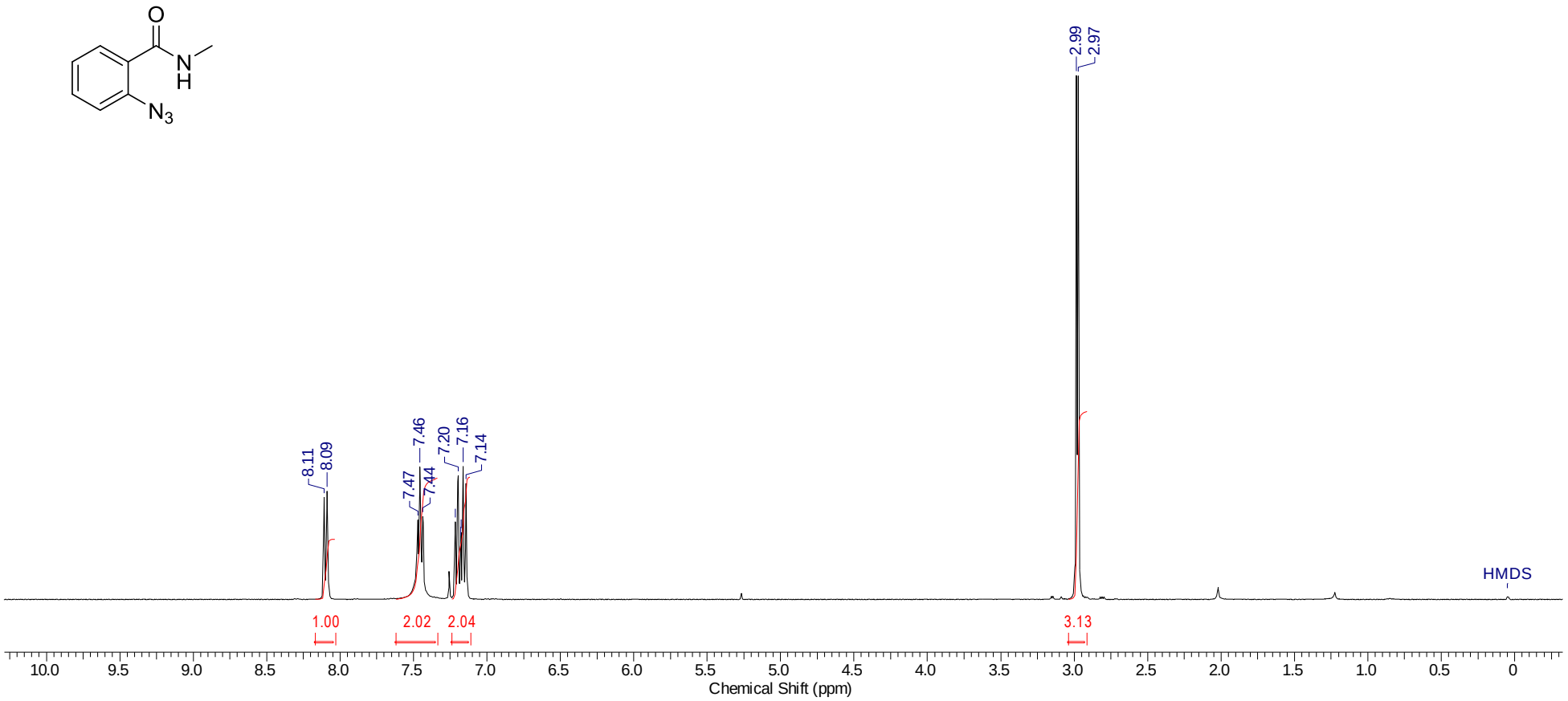
IR (KBr)



Copies of NMR spectra

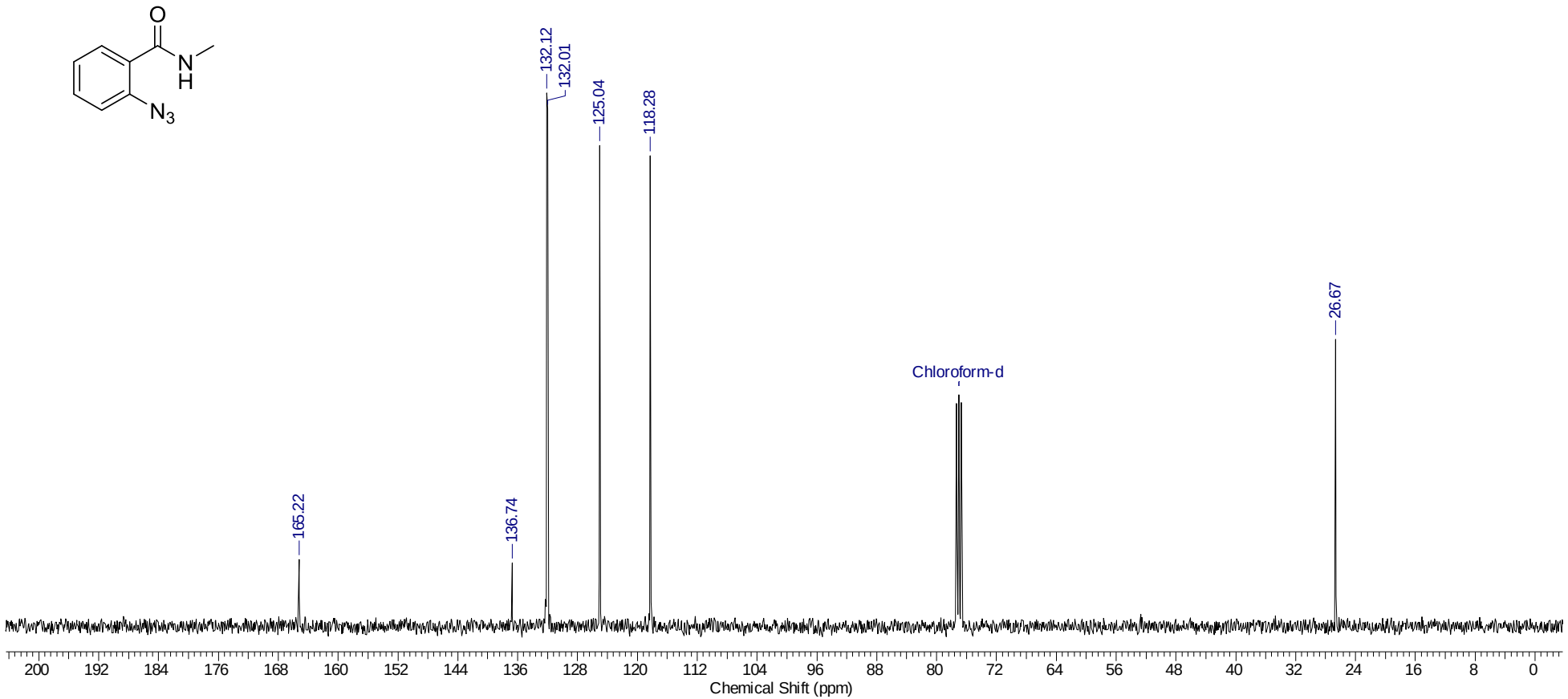
2-Azido-*N*-methylbenzamide (S2a)

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



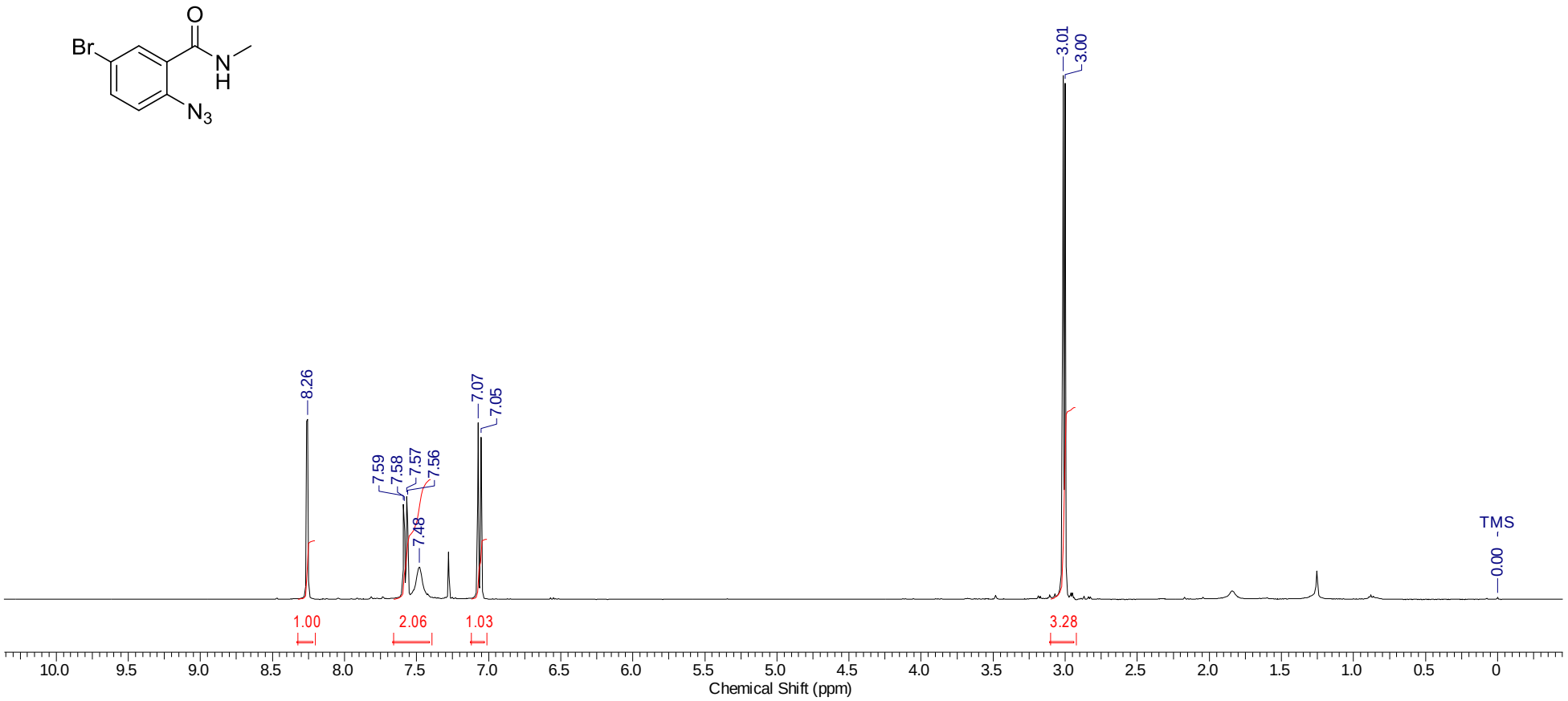
2-Azido-*N*-methylbenzamide (S2a)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



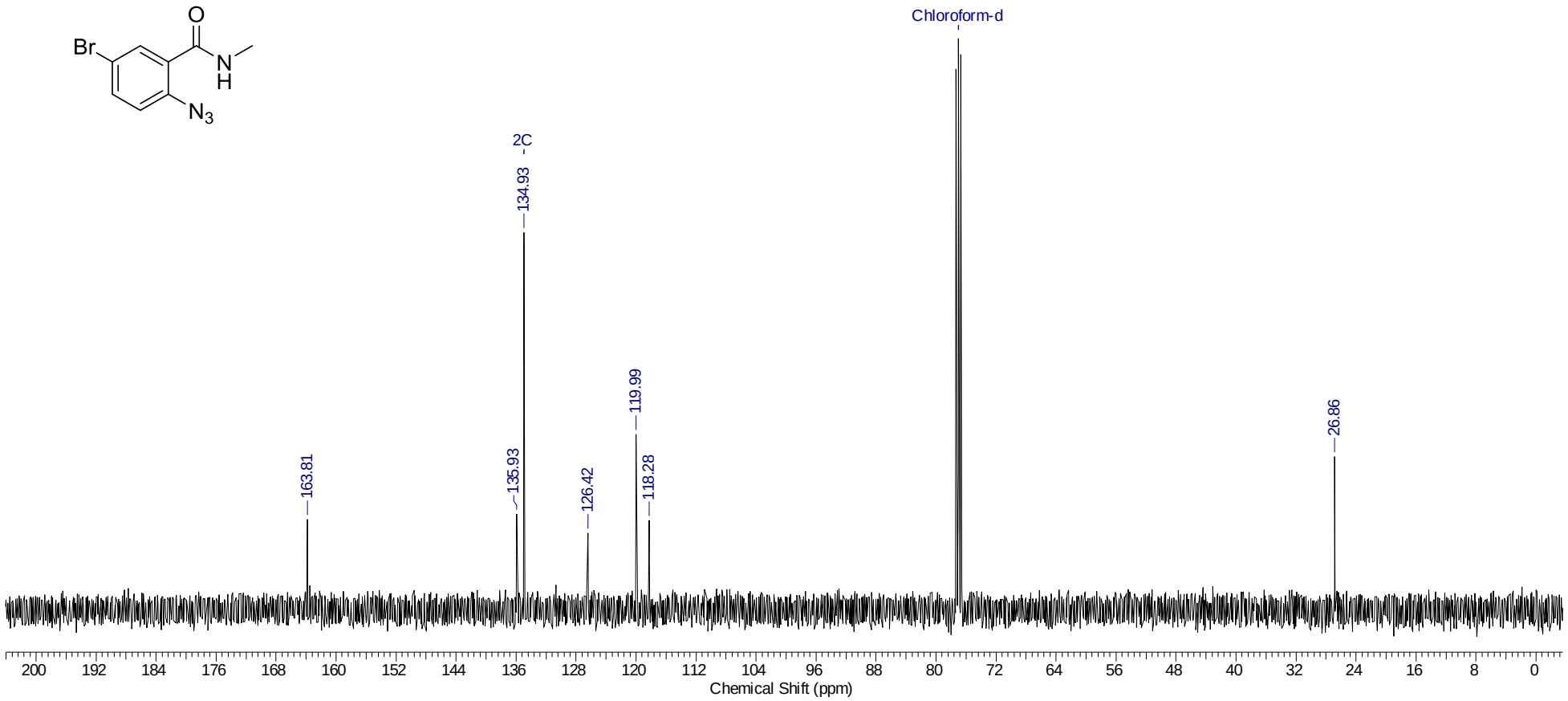
2-Azido-5-bromo-*N*-methylbenzamide (S2b)

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



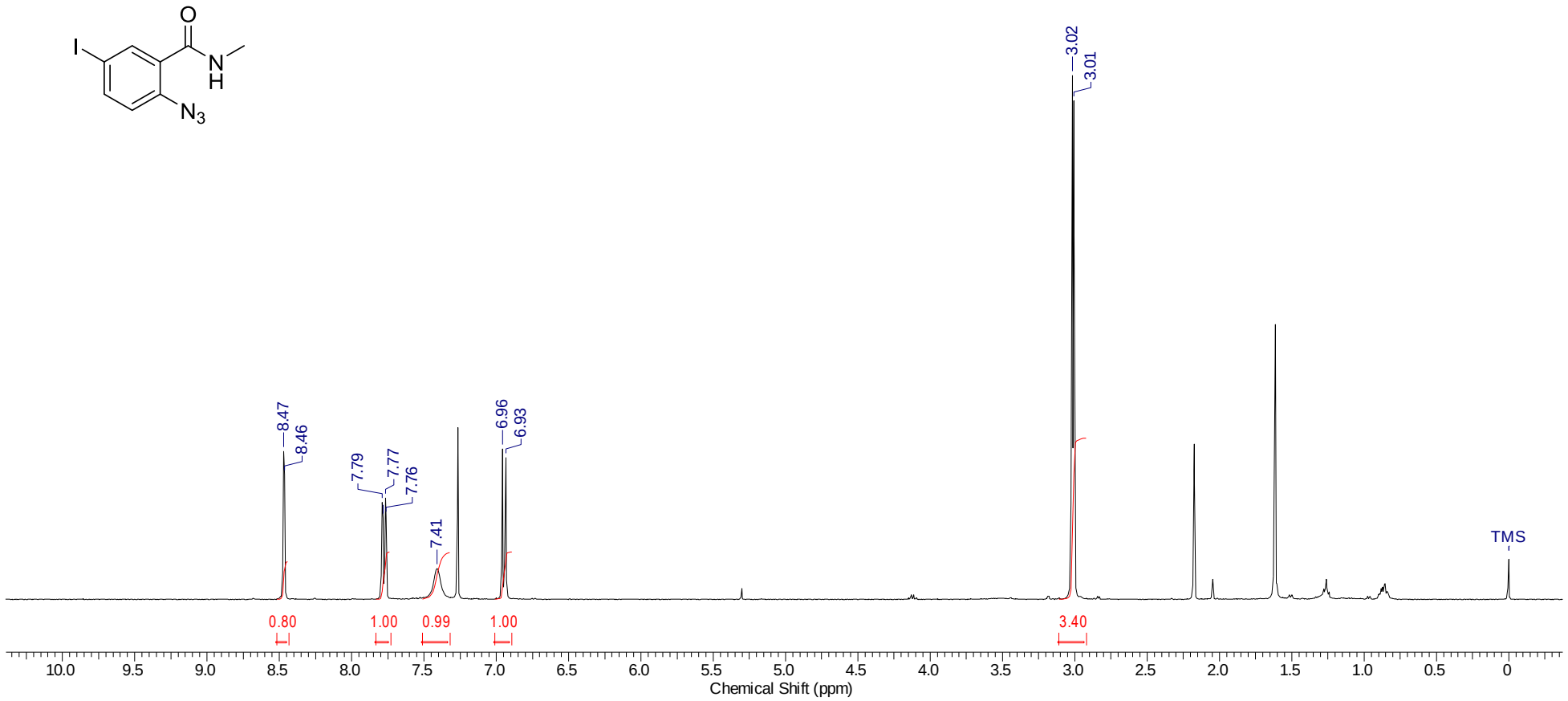
2-Azido-5-bromo-*N*-methylbenzamide (S2b)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



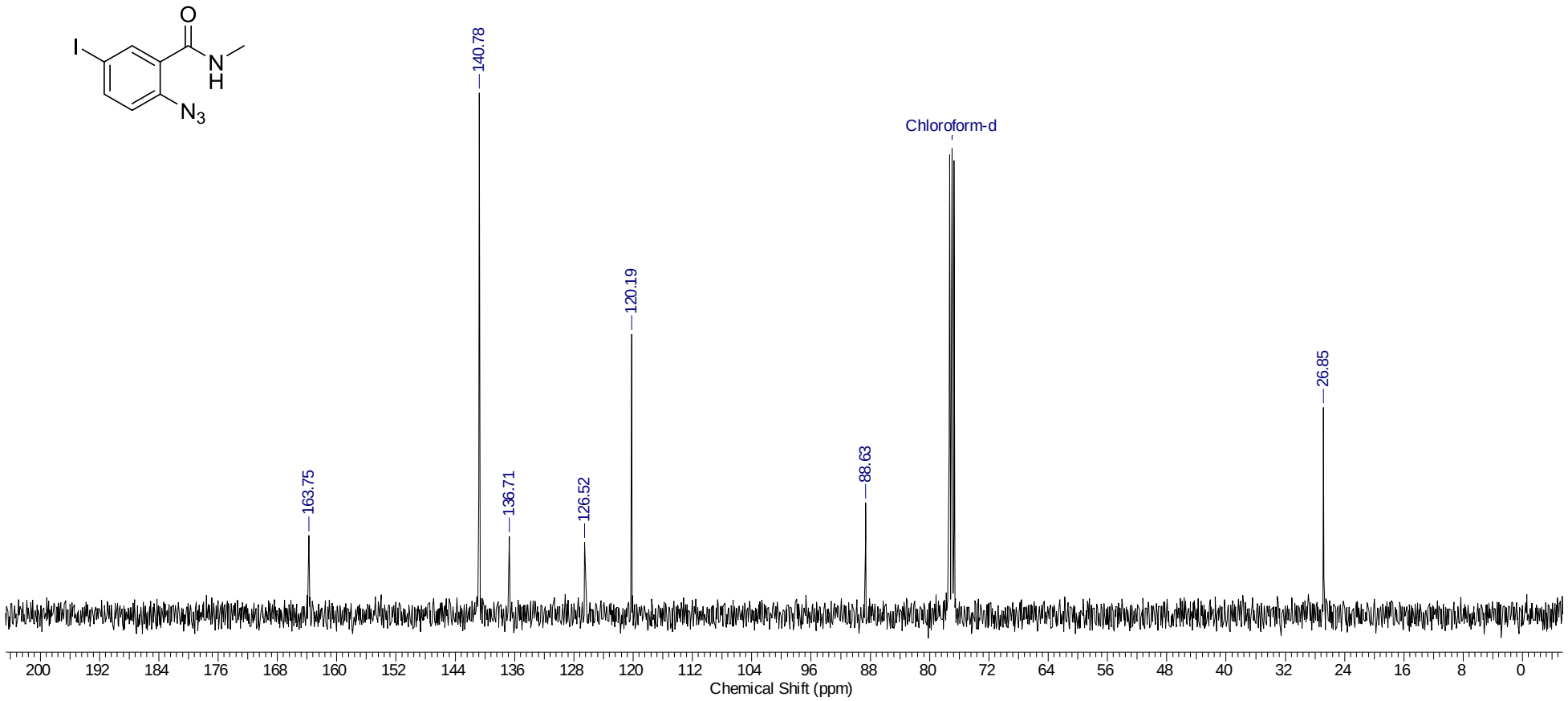
2-Azido-5-iodo-*N*-methylbenzamide (S2c)

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



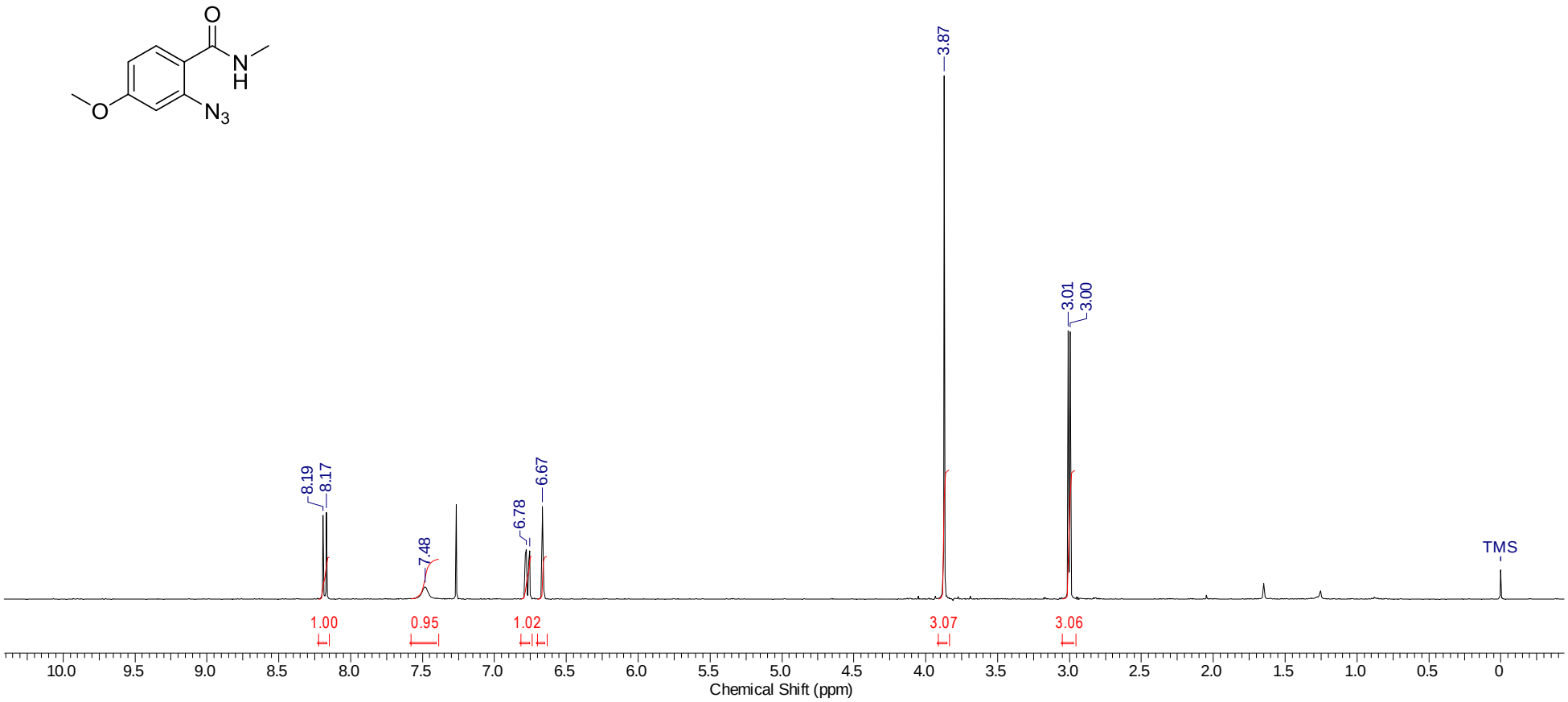
2-Azido-5-iodo-*N*-methylbenzamide (S2c)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



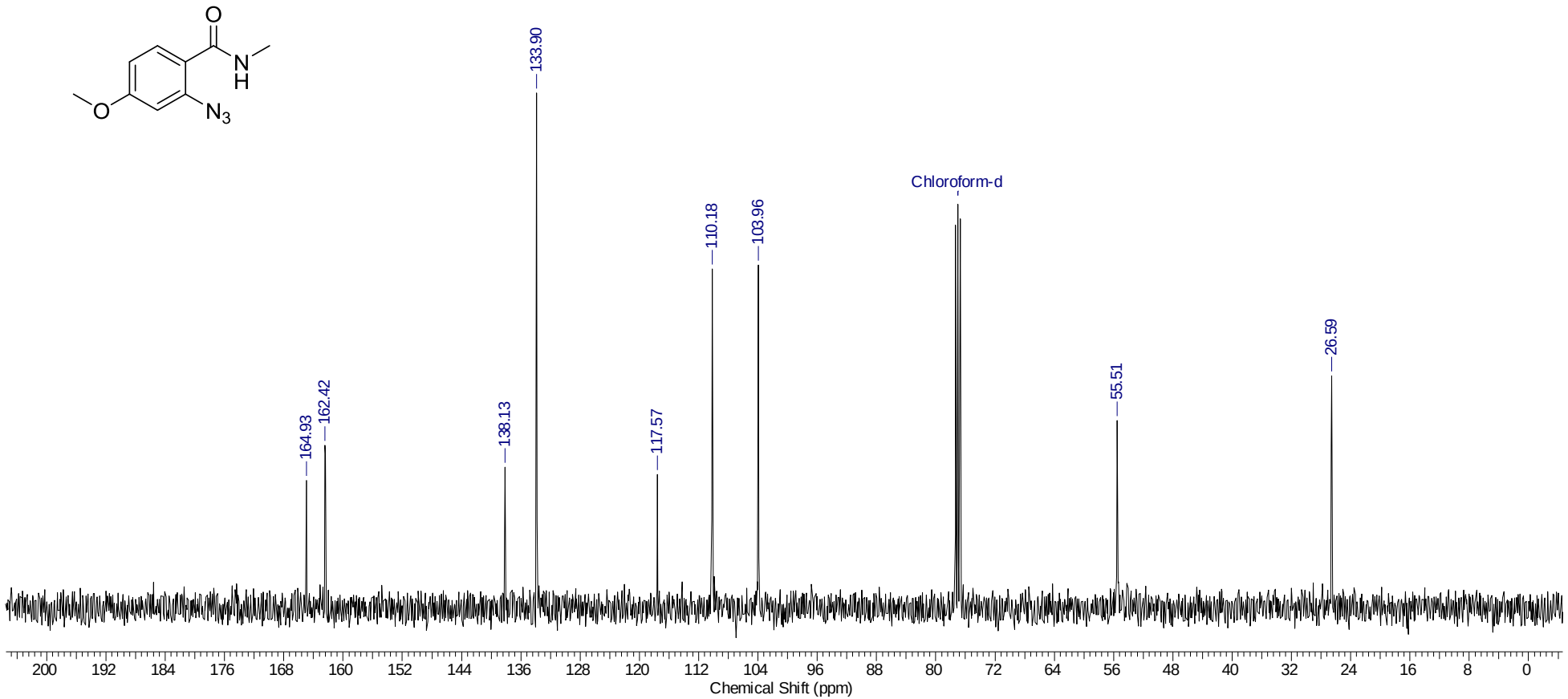
2-Azido-4-methoxy-*N*-methylbenzamide (S2d)

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



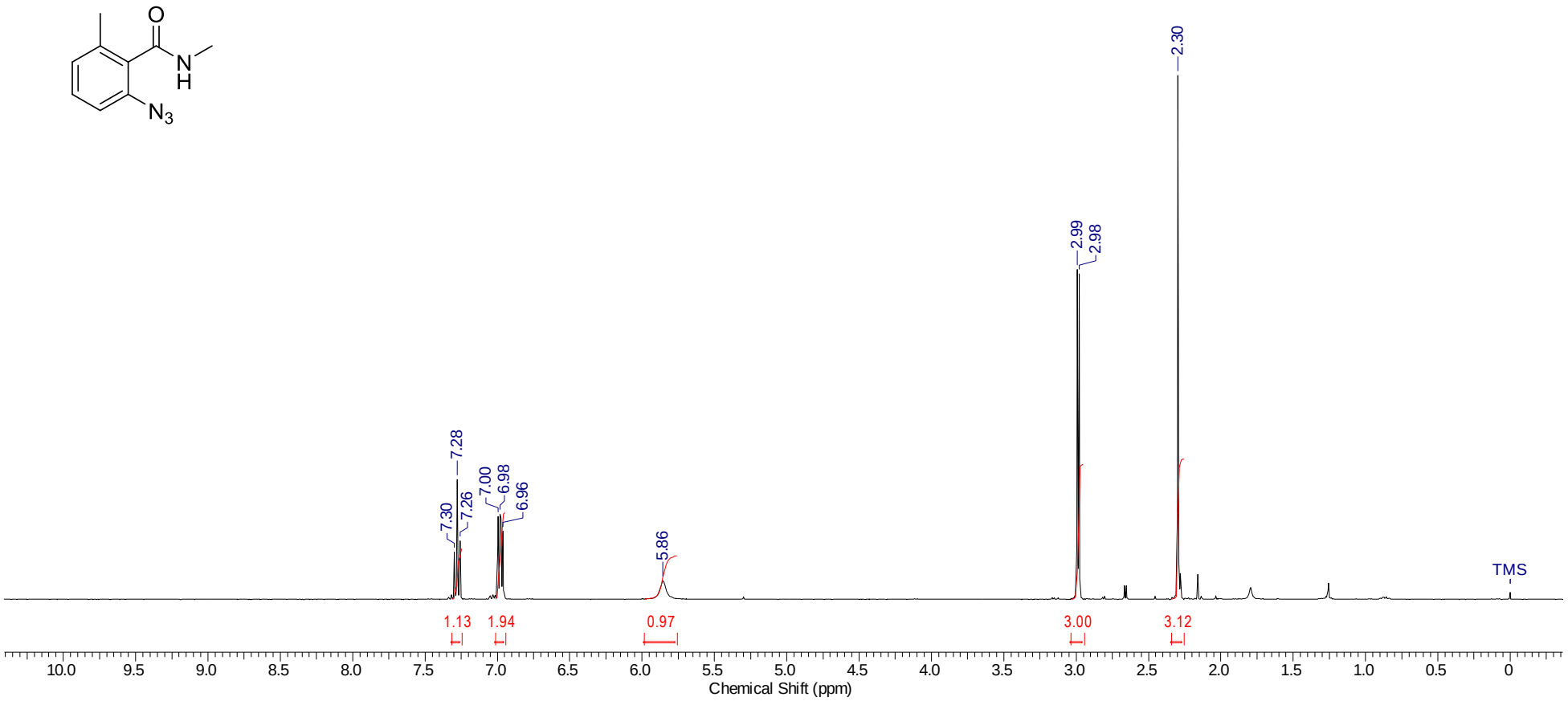
2-Azido-4-methoxy-*N*-methylbenzamide (S2d)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



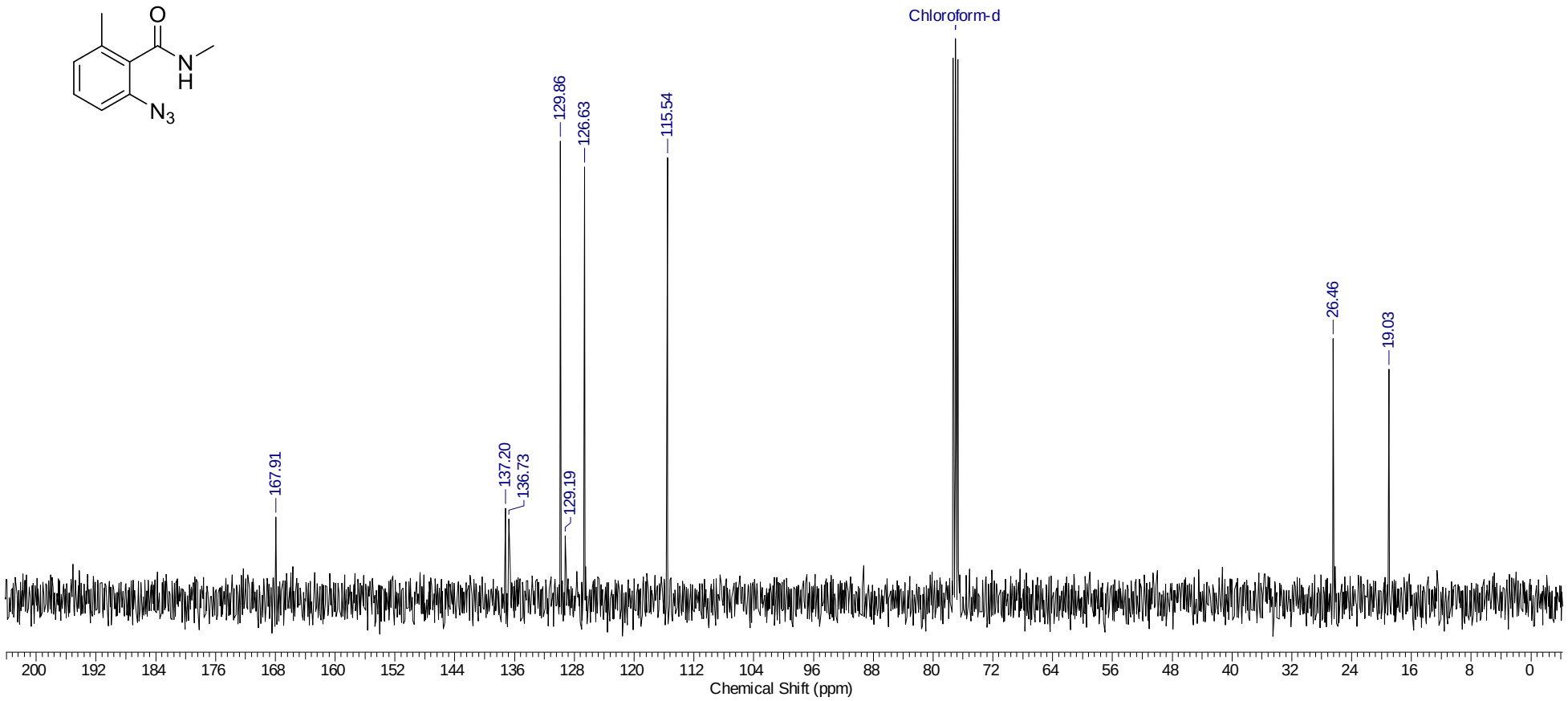
2-Azido-*N*,6-dimethylbenzamide (S2e)

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



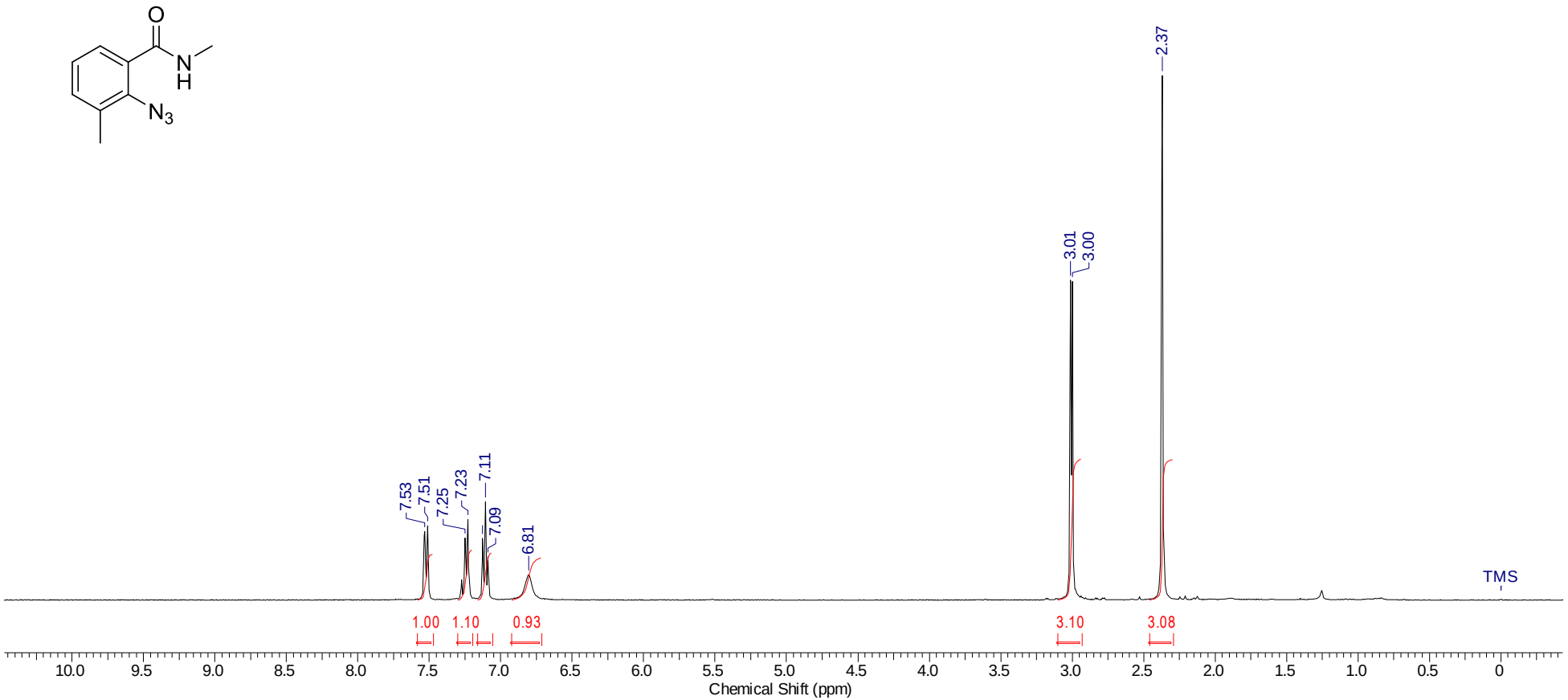
2-Azido-*N*,6-dimethylbenzamide (S2e)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



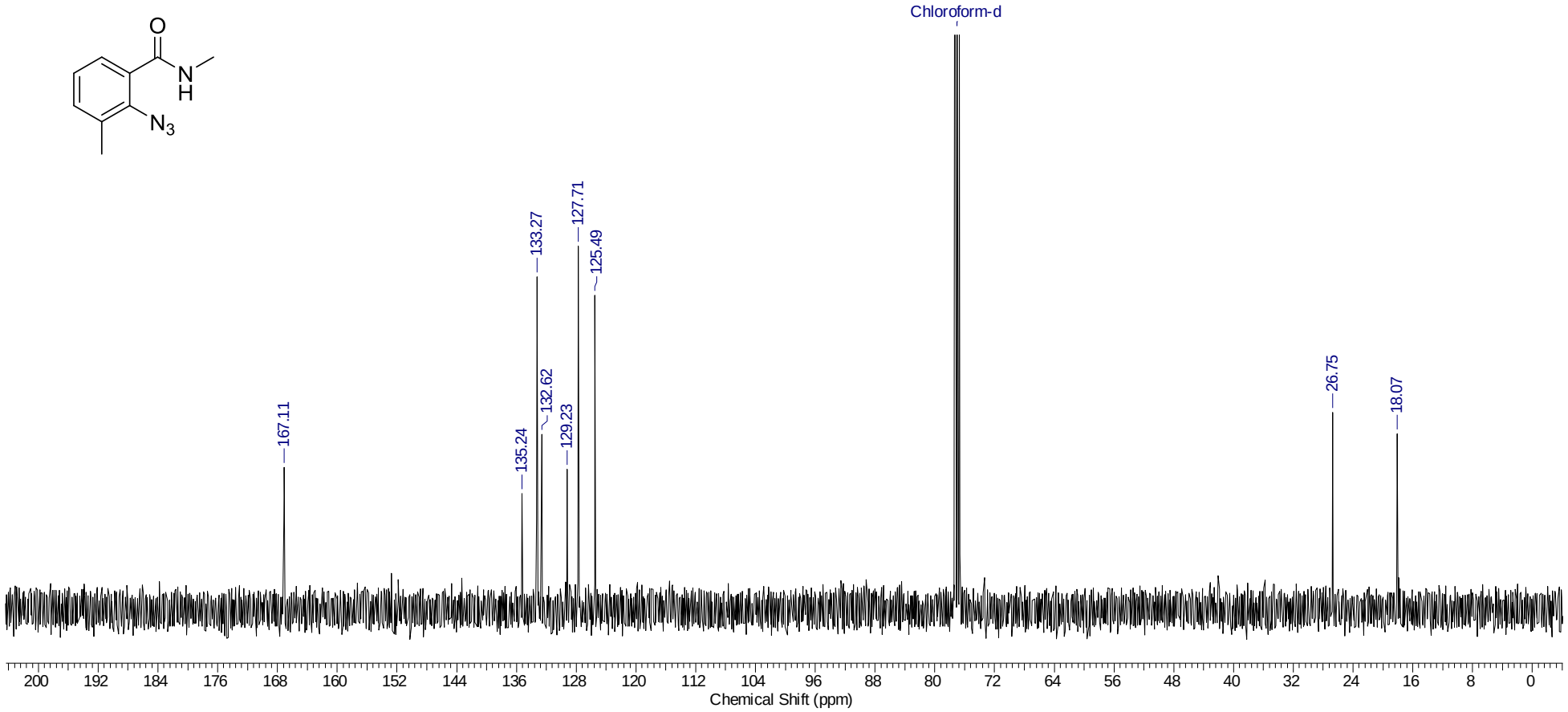
2-Azido-*N*,3-dimethylbenzamide (S2f)

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



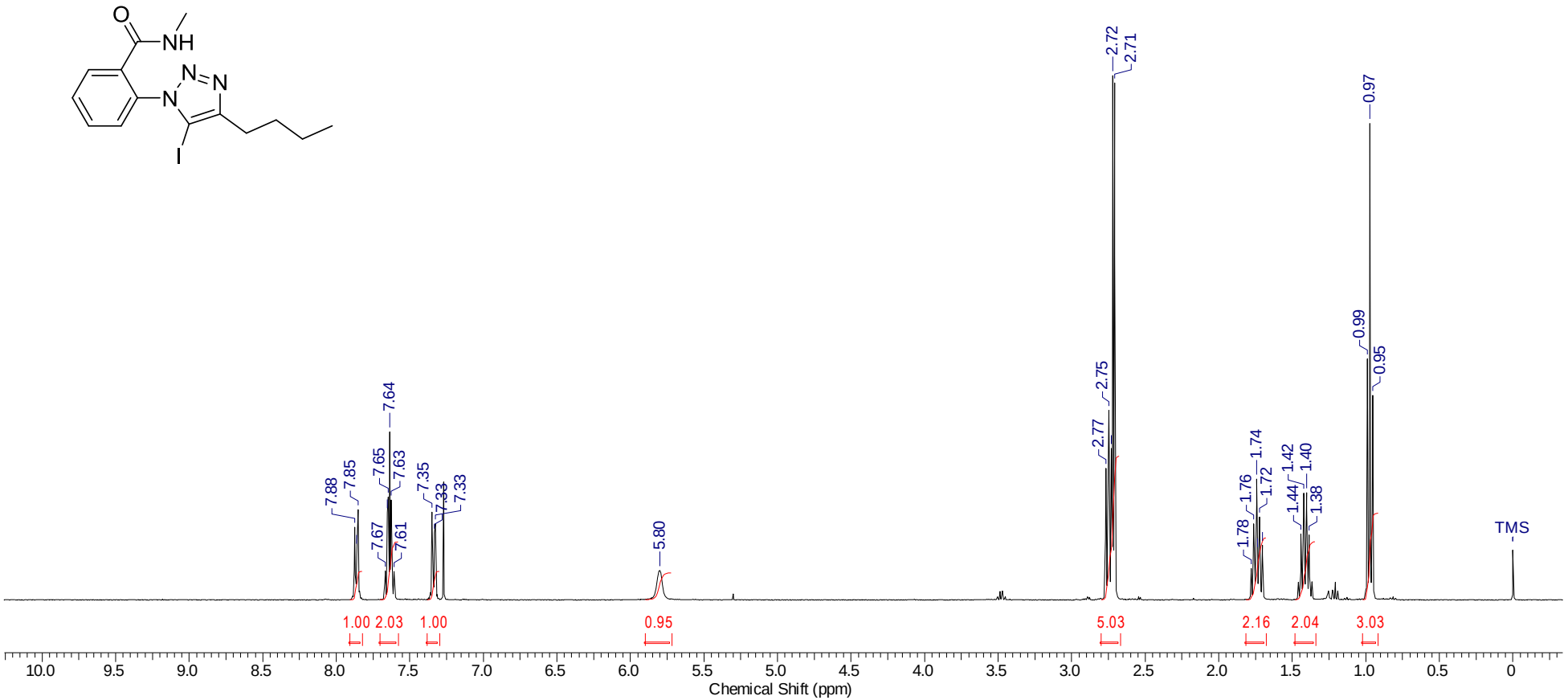
2-Azido-*N*,3-dimethylbenzamide (S2f)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



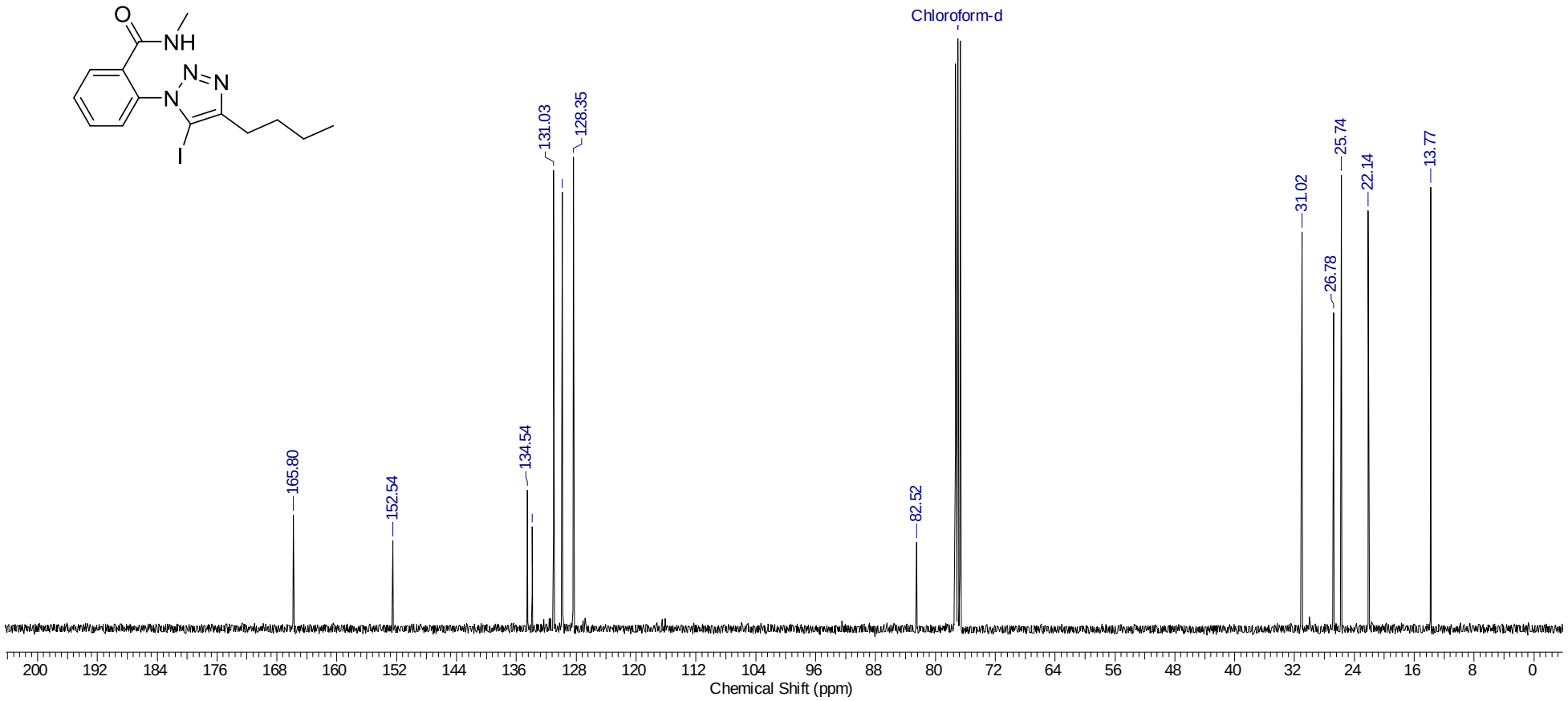
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1a)

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



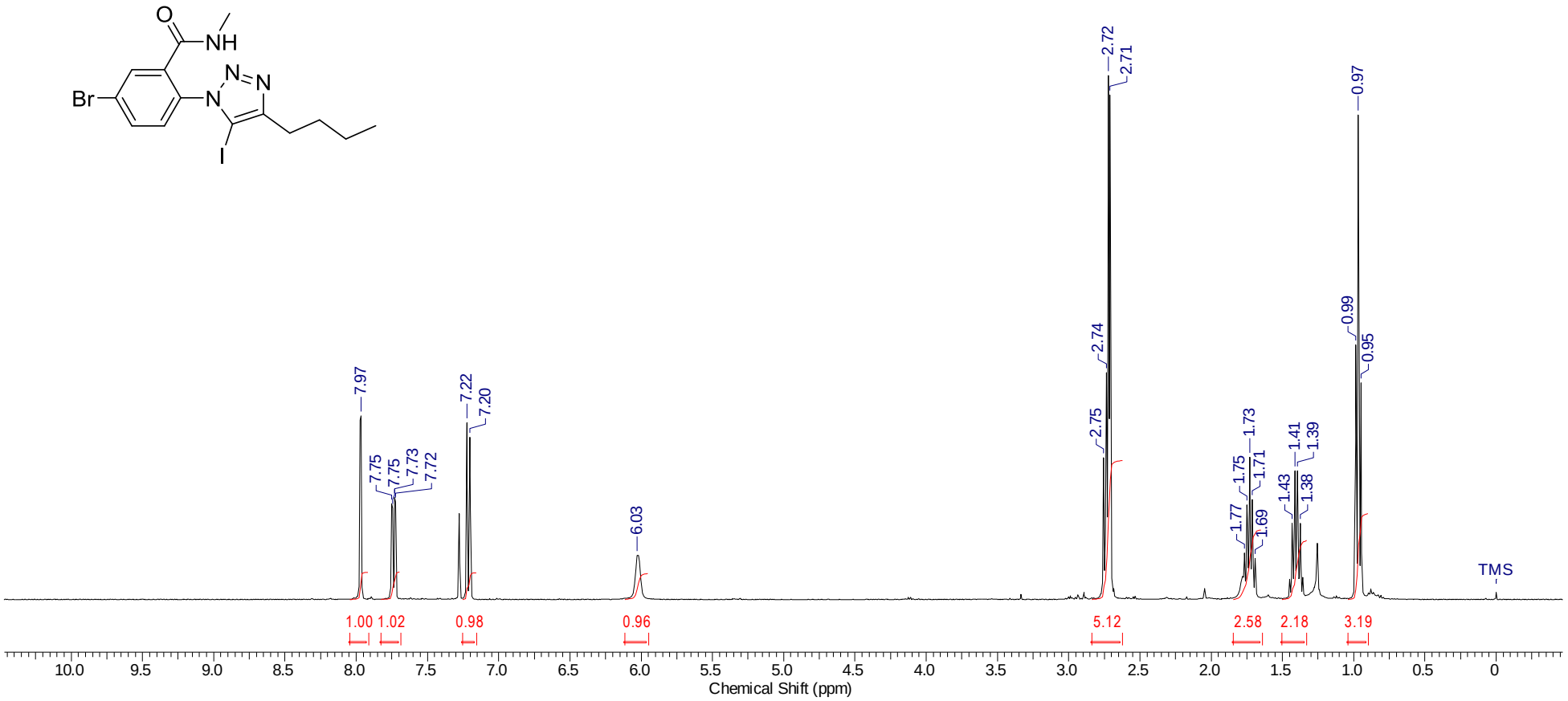
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1a)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



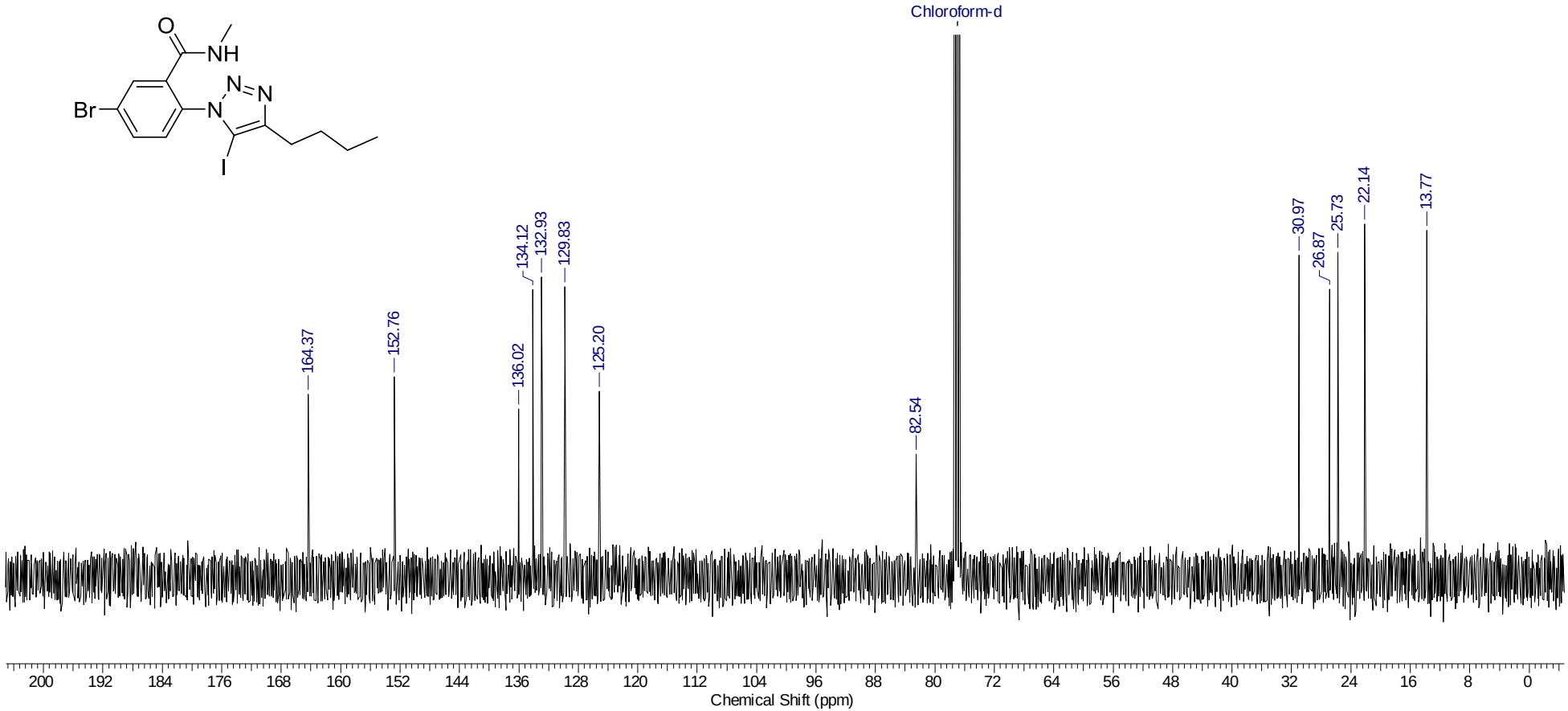
5-Bromo-2-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1b)

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



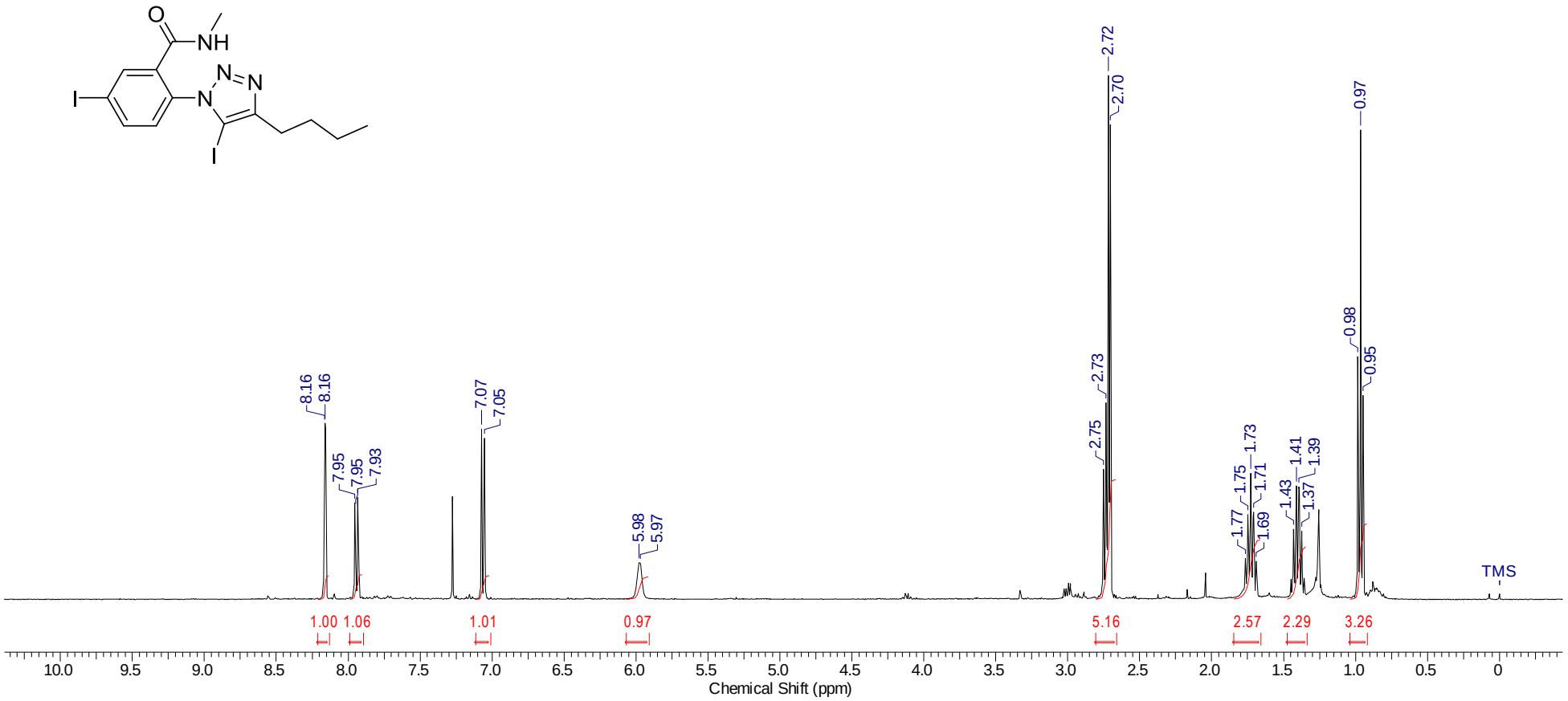
5-Bromo-2-(4-butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1b)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



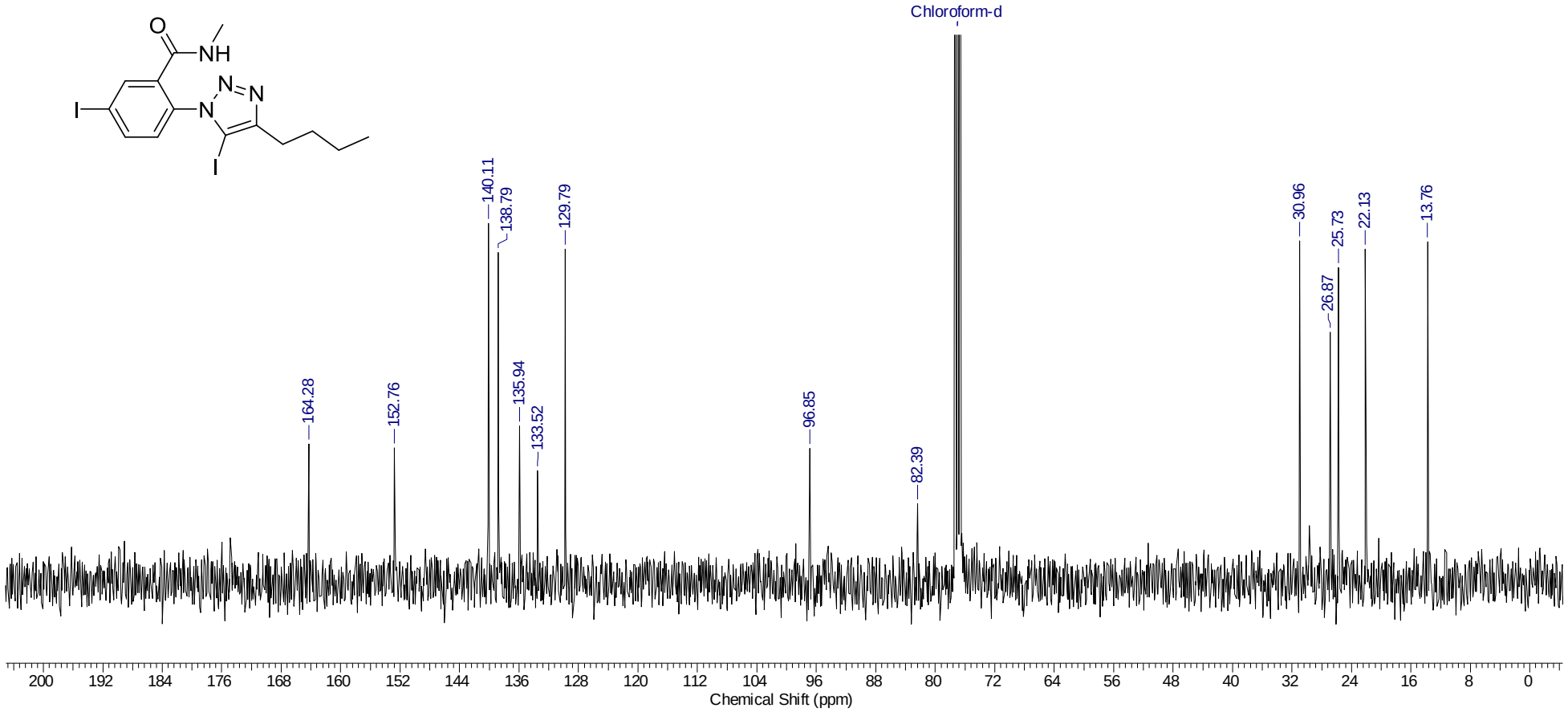
(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-5-iodo-*N*-methylbenzamide (1c)

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



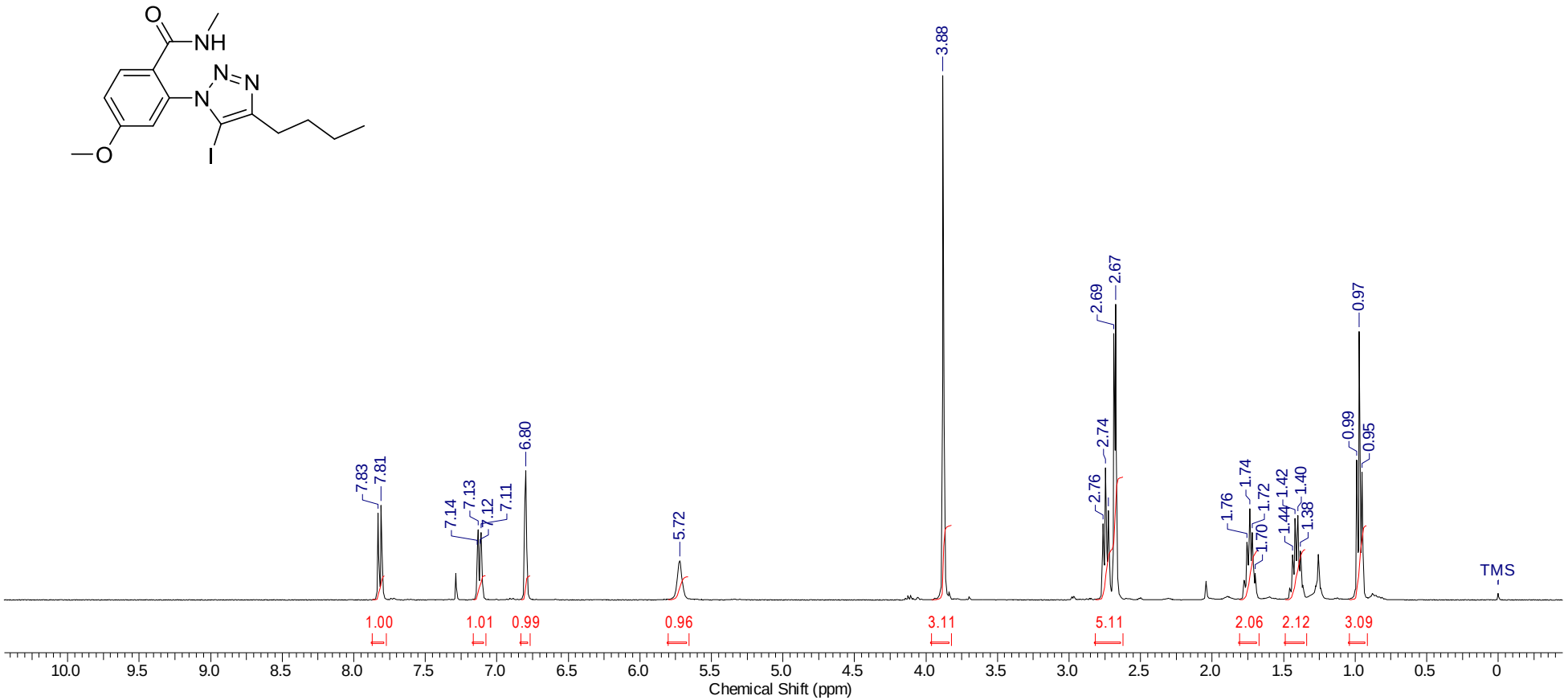
(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-5-iodo-*N*-methylbenzamide (1c)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



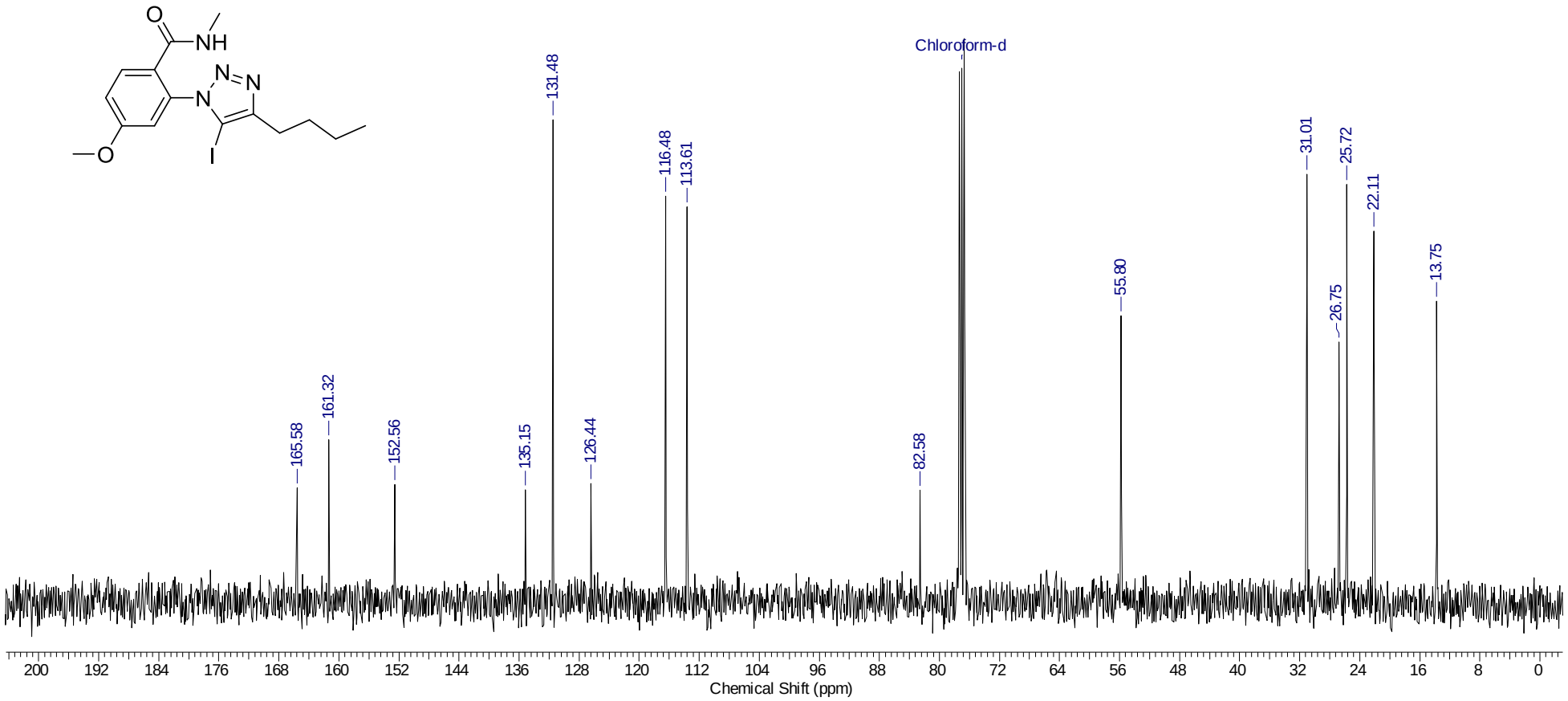
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-4-methoxy-*N*-methylbenzamide (1d)

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



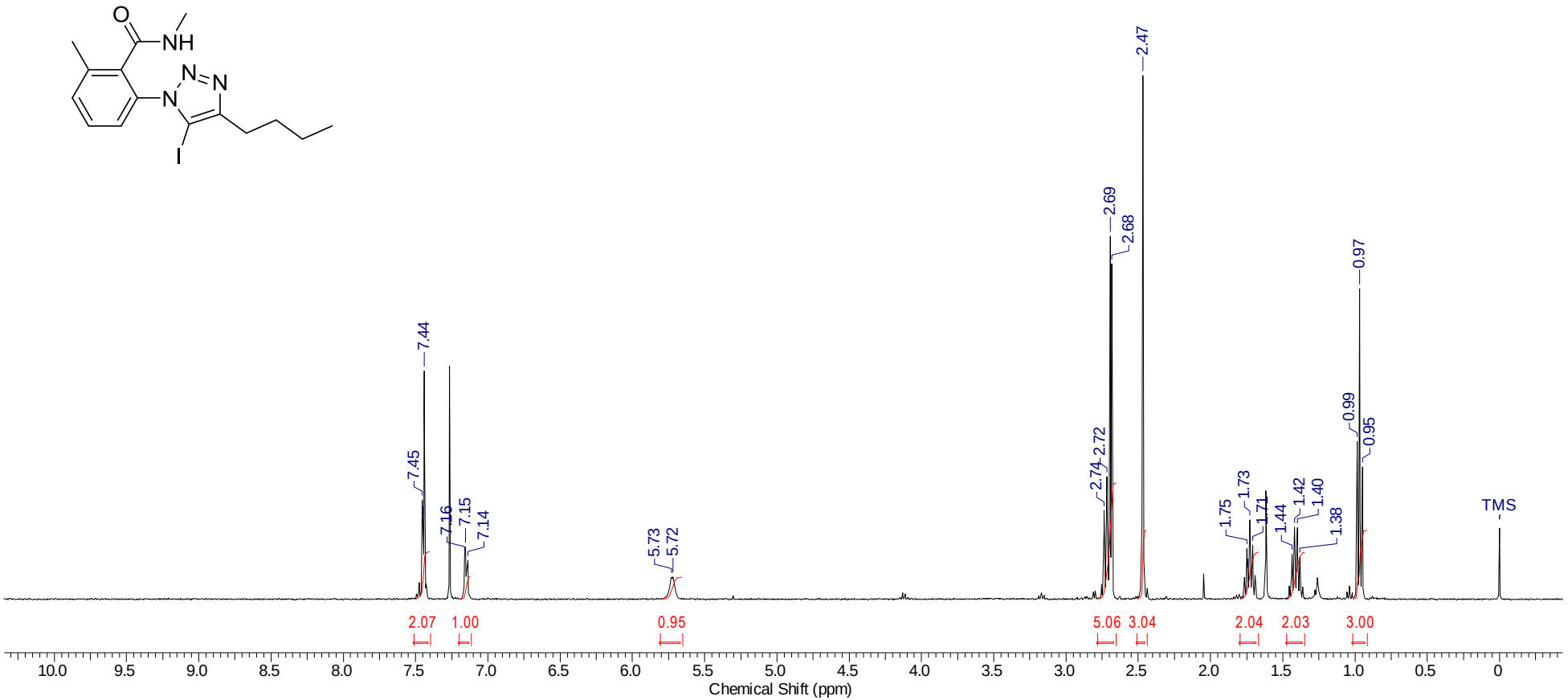
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-4-methoxy-*N*-methylbenzamide (1d)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



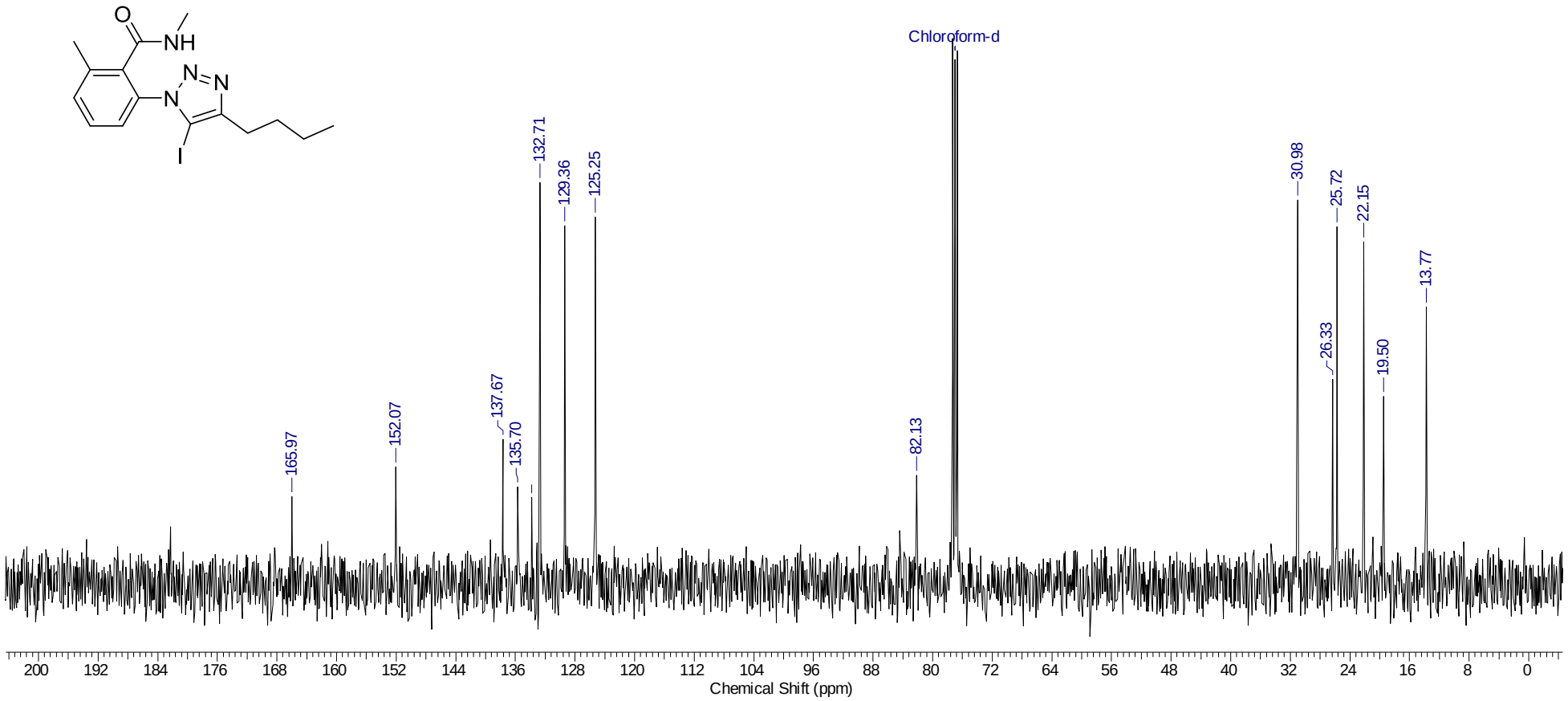
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*,6-dimethylbenzamide (1e)

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



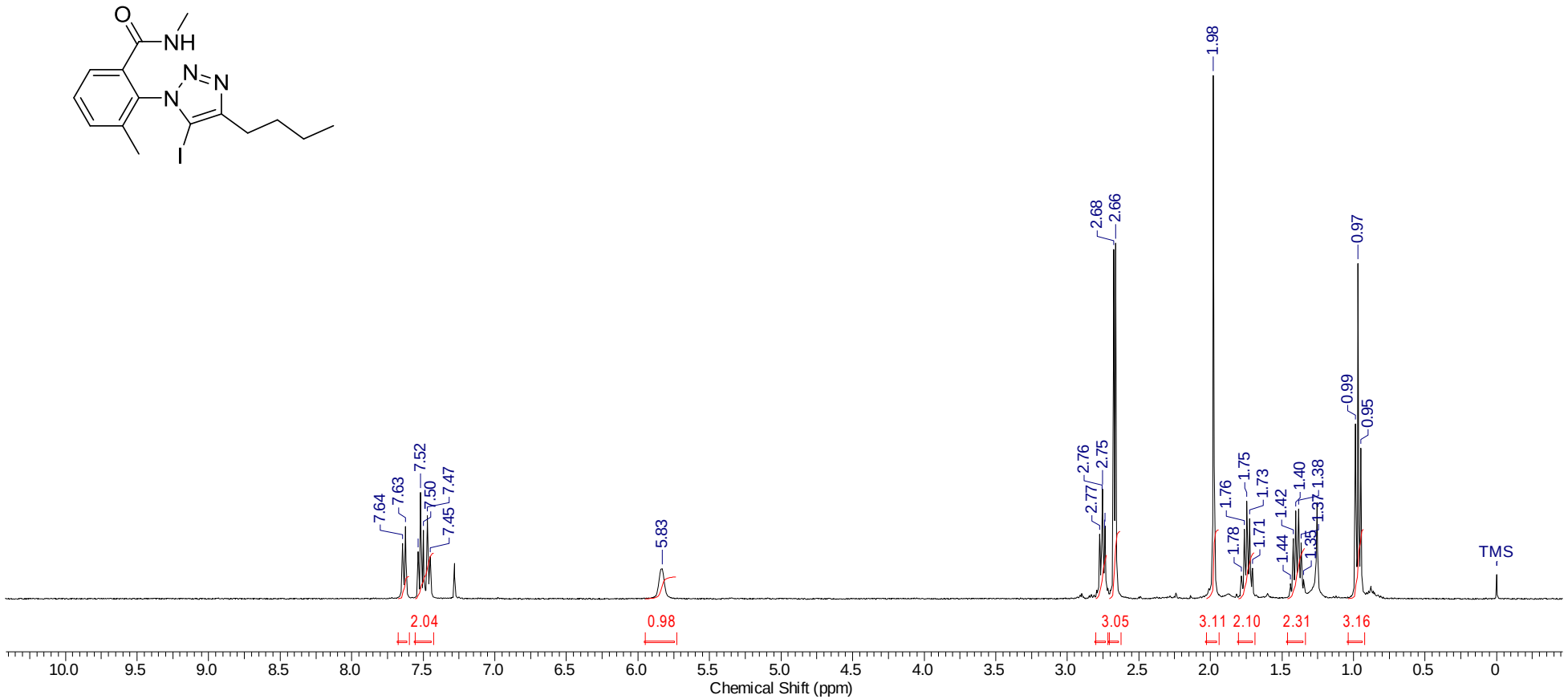
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*,6-dimethylbenzamide (1e)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



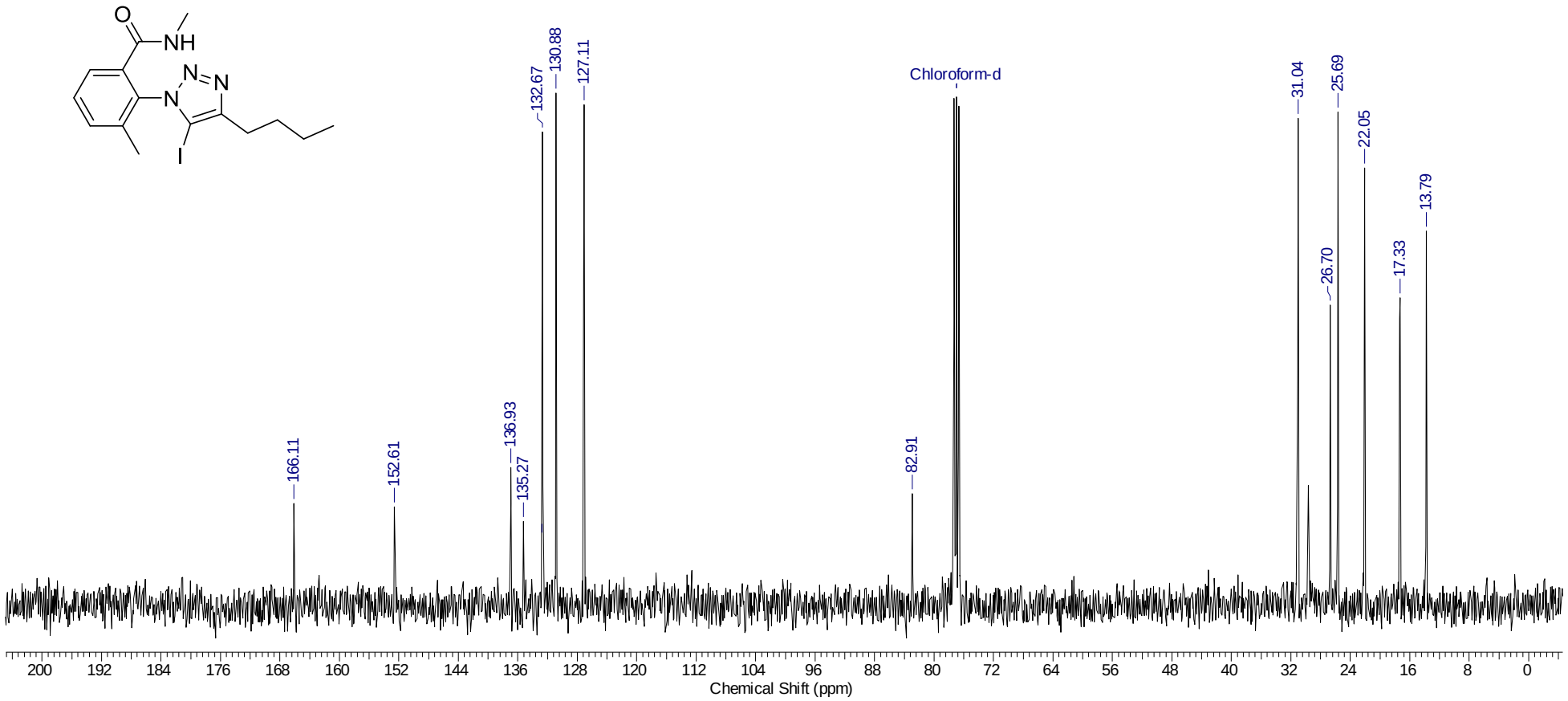
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*,3-dimethylbenzamide (1f)

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



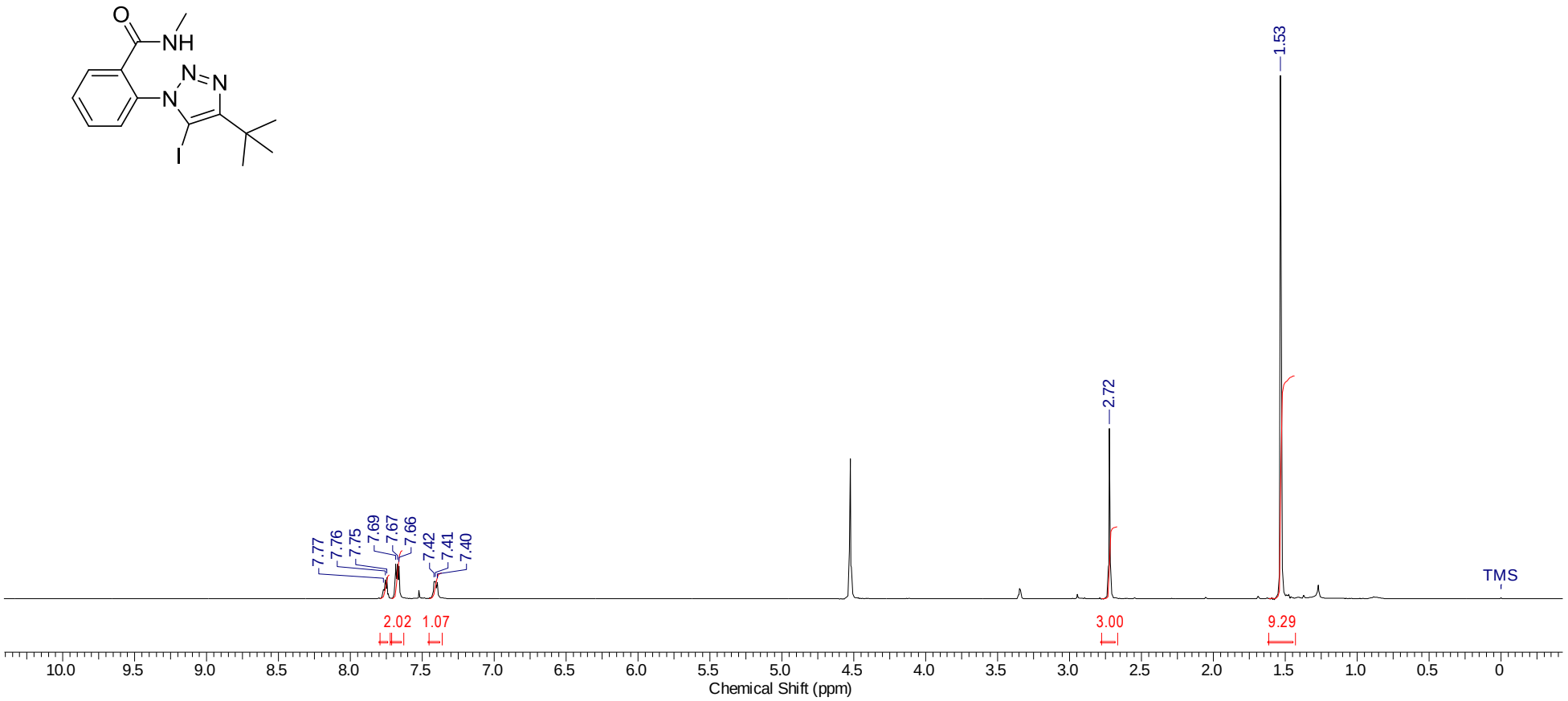
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*,3-dimethylbenzamide (1f)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



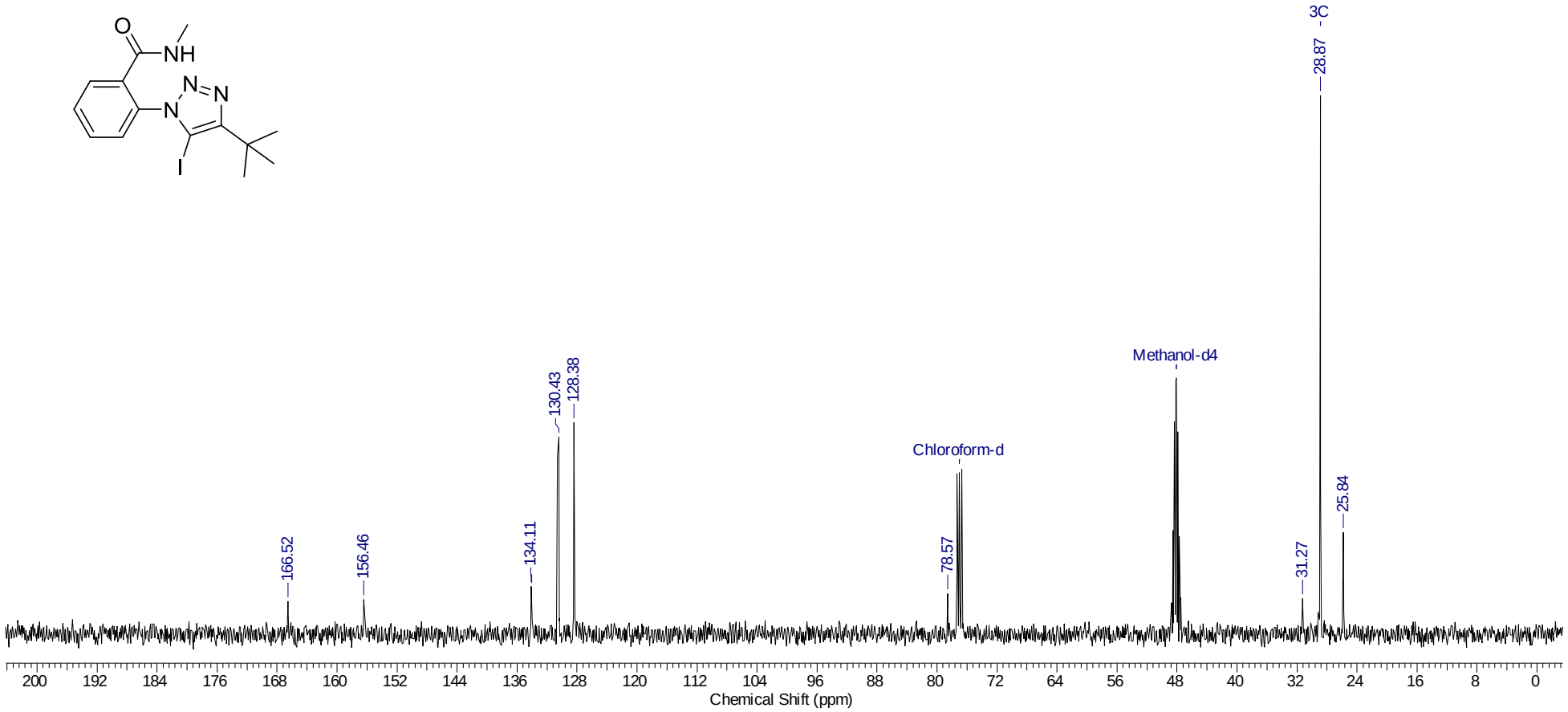
2-(4-*tert*-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1g)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



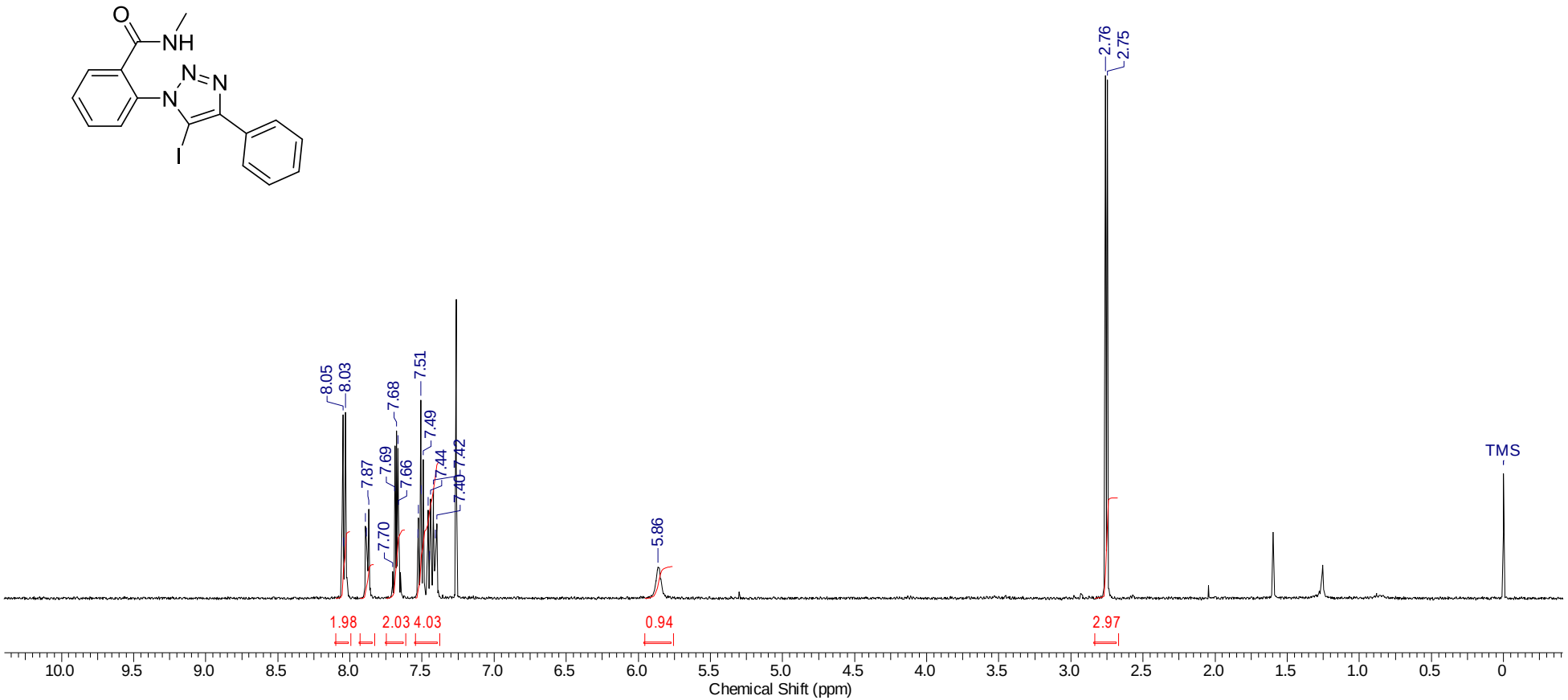
2-(4-*tert*-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1g)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



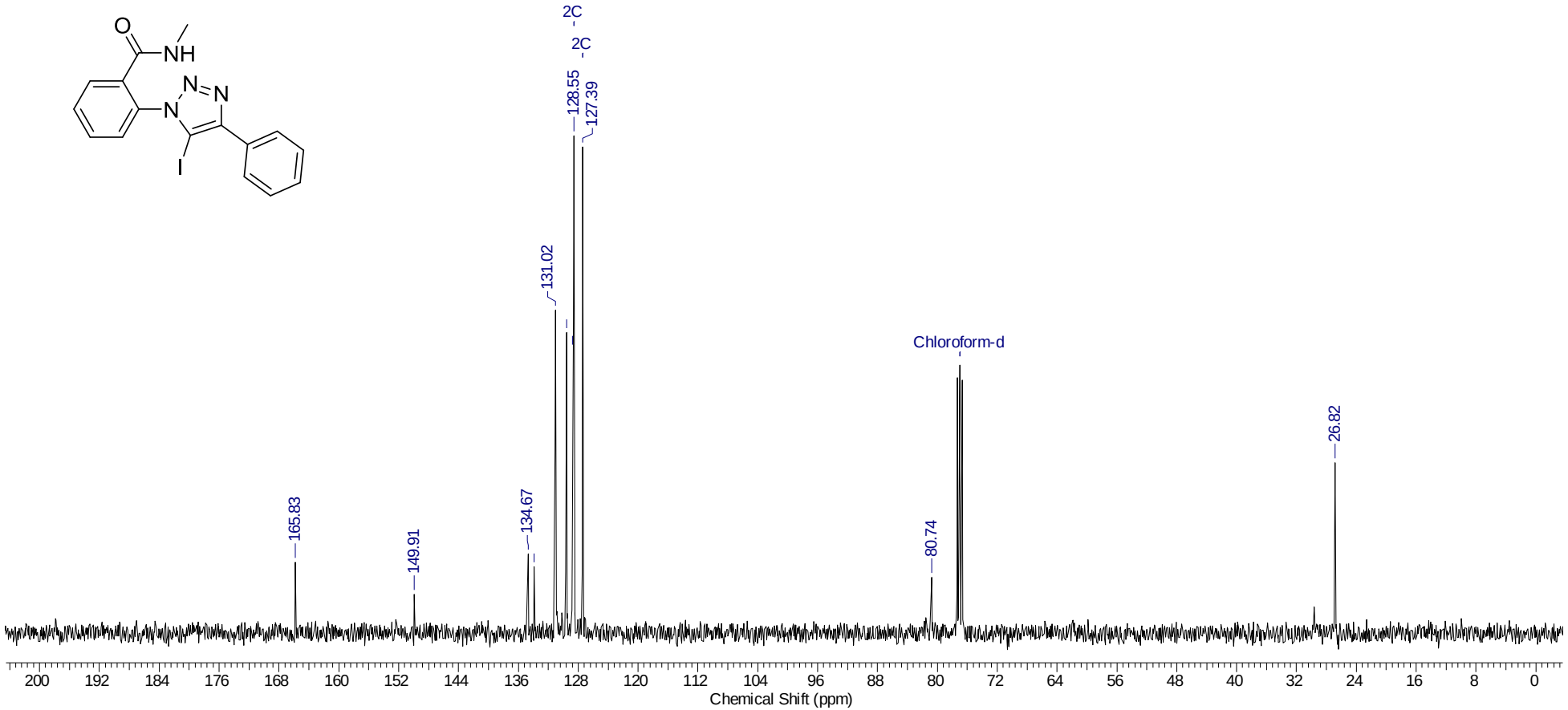
2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1h)

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



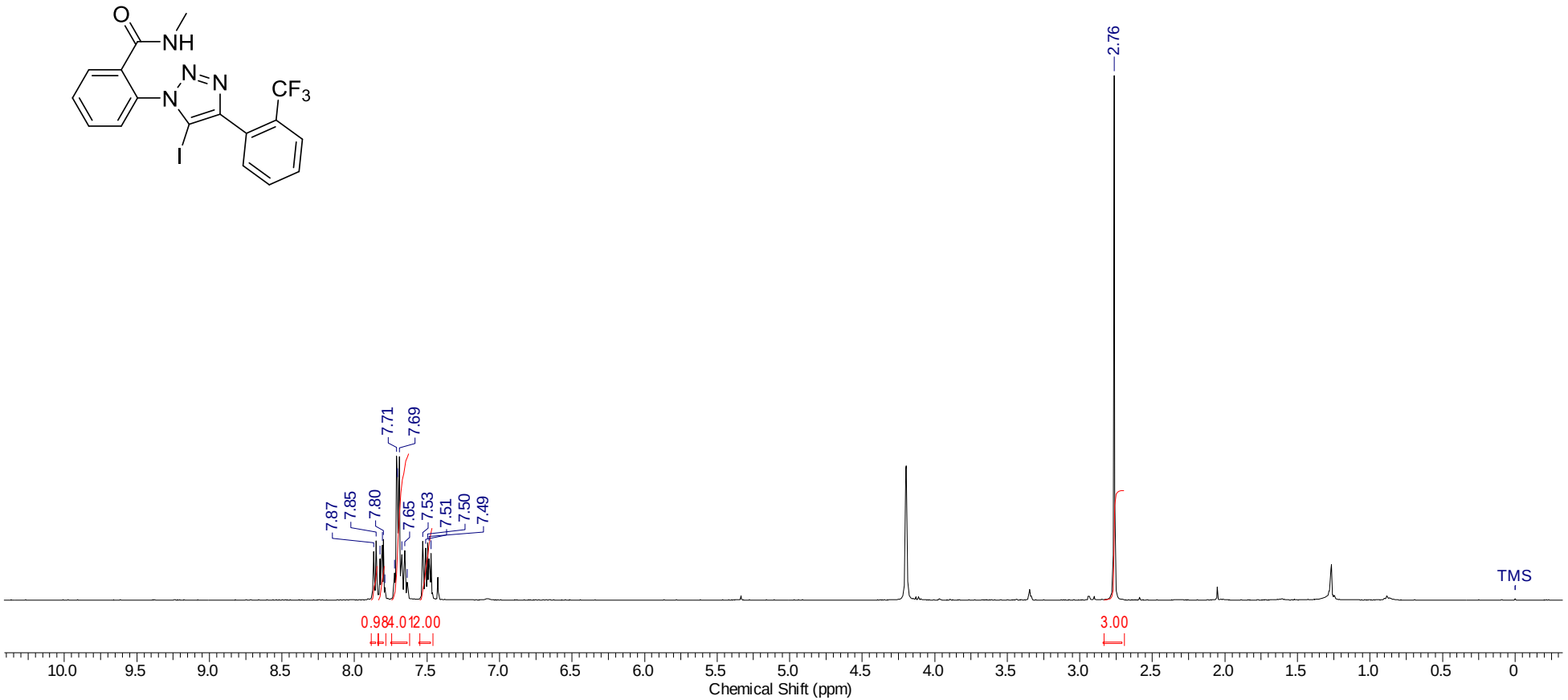
2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)-*N*-methylbenzamide (1h)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



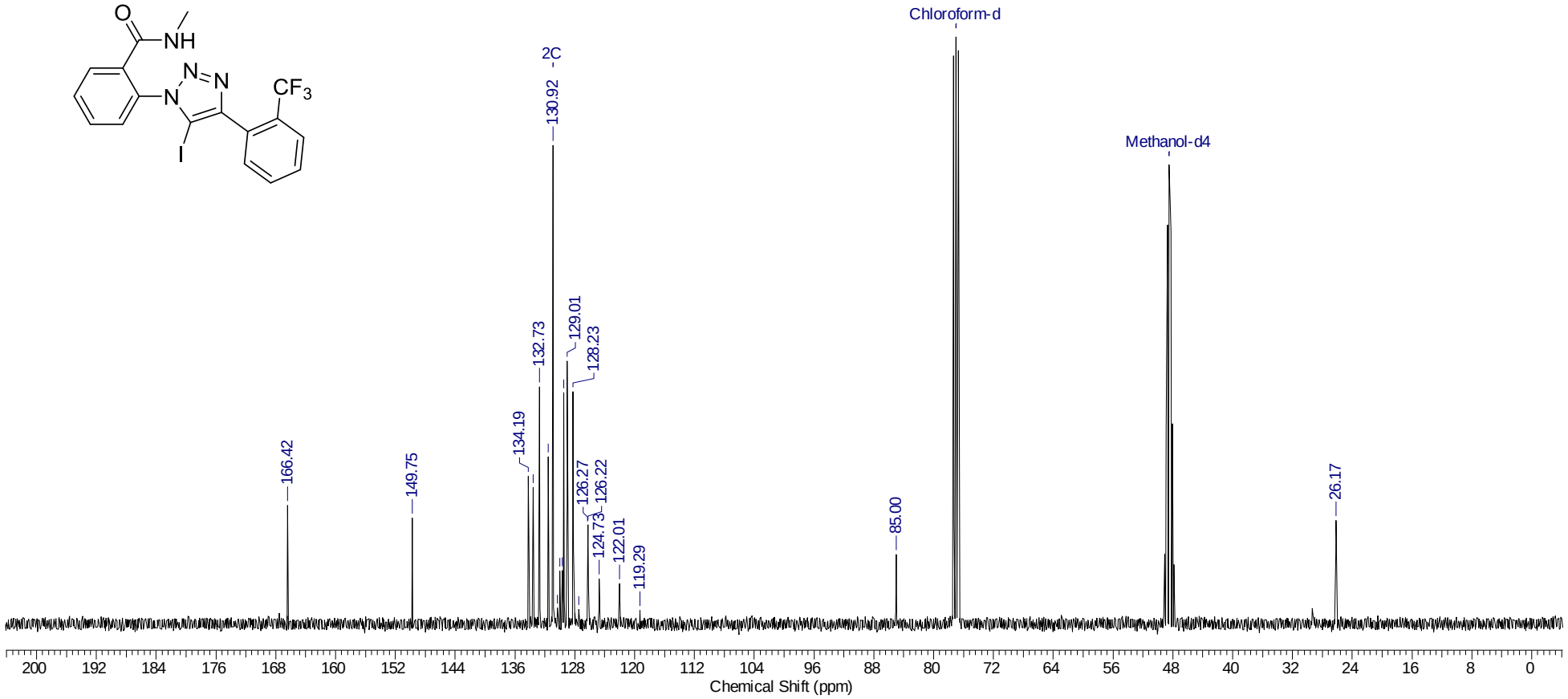
2-{5-Iodo-4-[2-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-*N*-methylbenzamide (1i)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



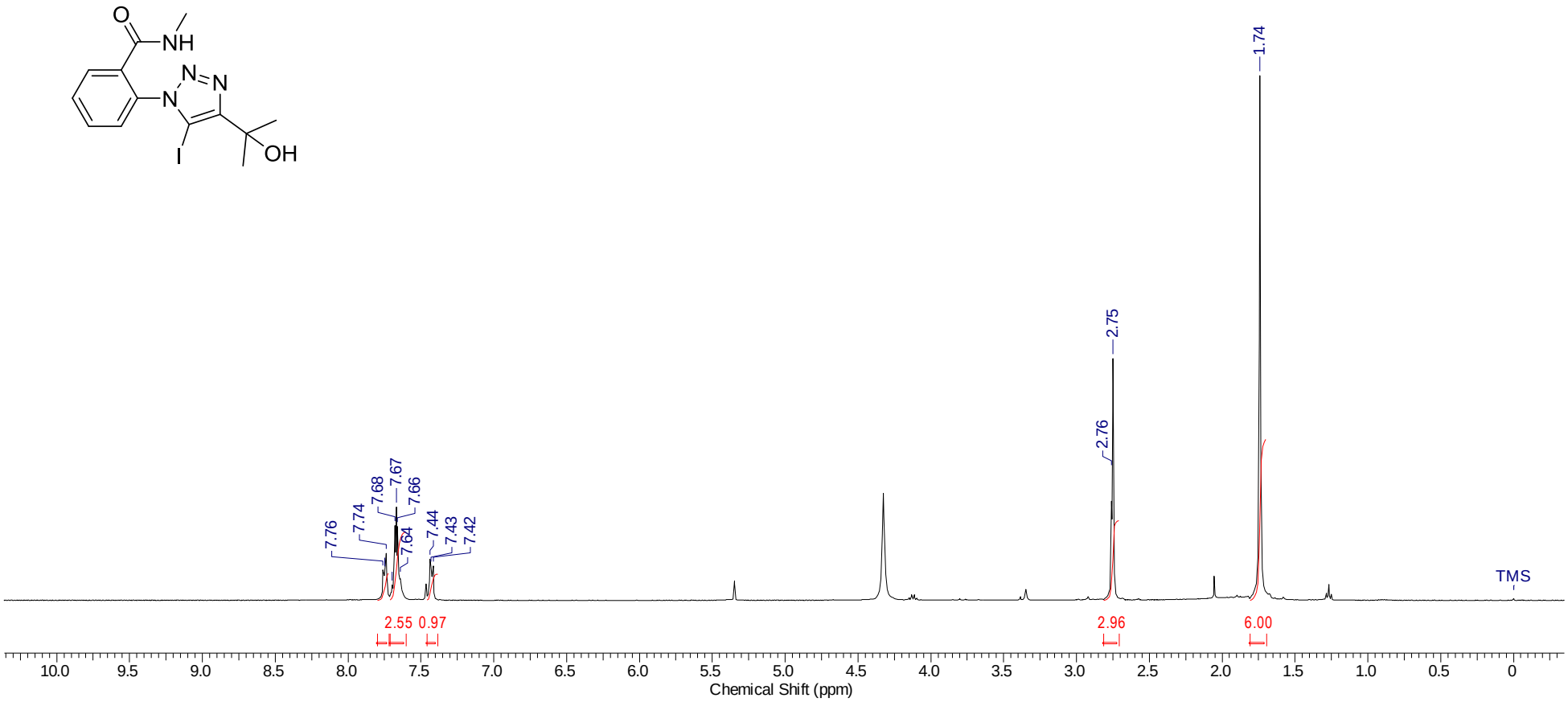
2-{5-Iodo-4-[2-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-*N*-methylbenzamide (1i)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



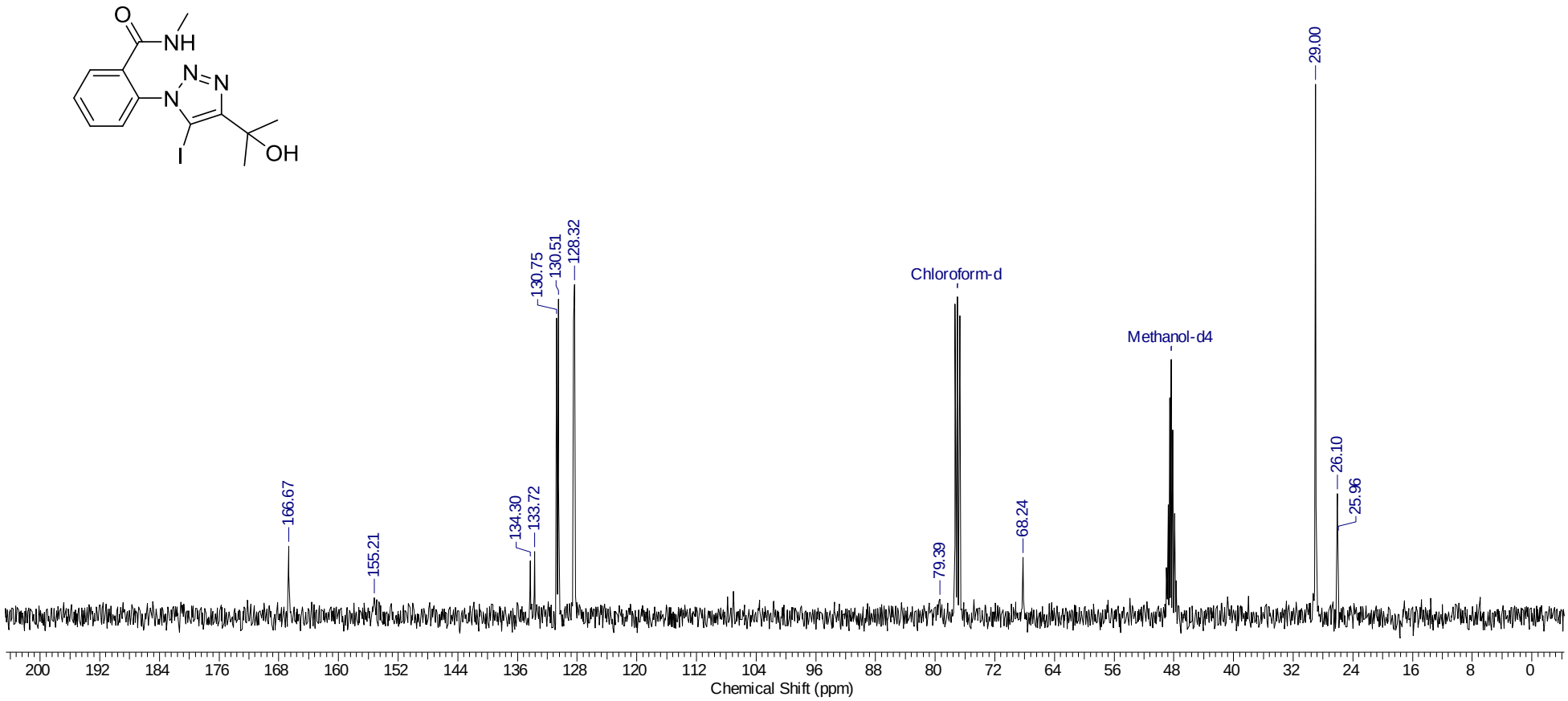
2-[4-(1-Hydroxy-1-methylethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1j)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



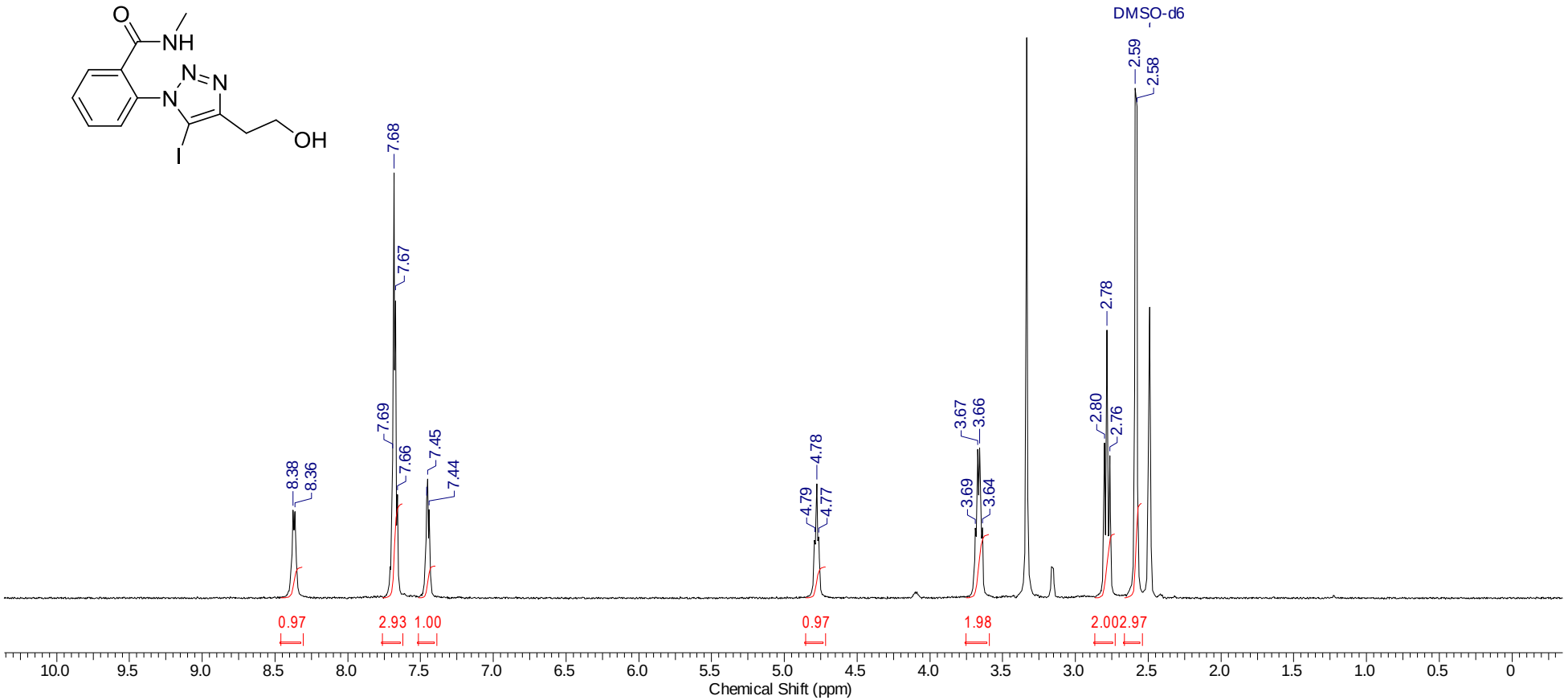
2-[4-(1-Hydroxy-1-methylethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1j)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



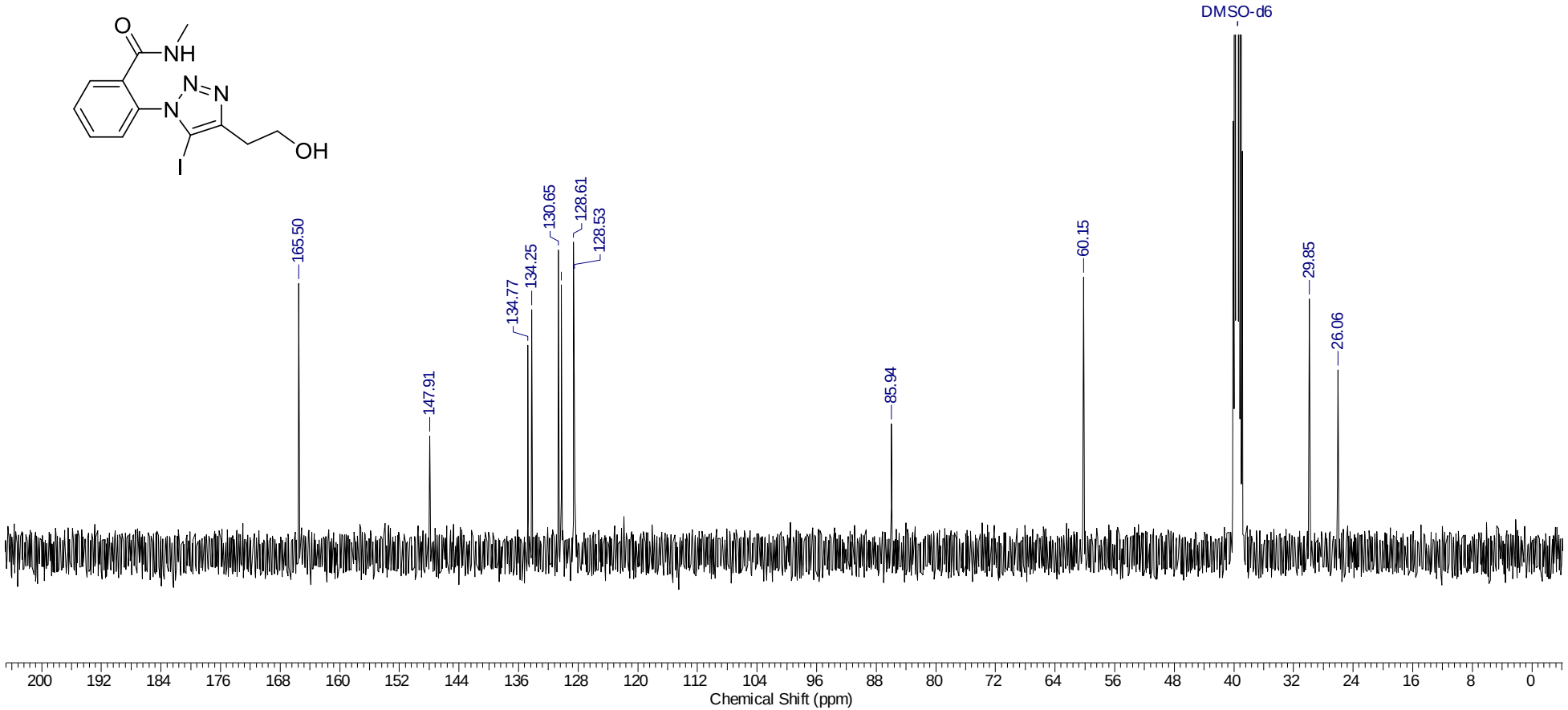
2-[4-(2-Hydroxyethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1k)

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



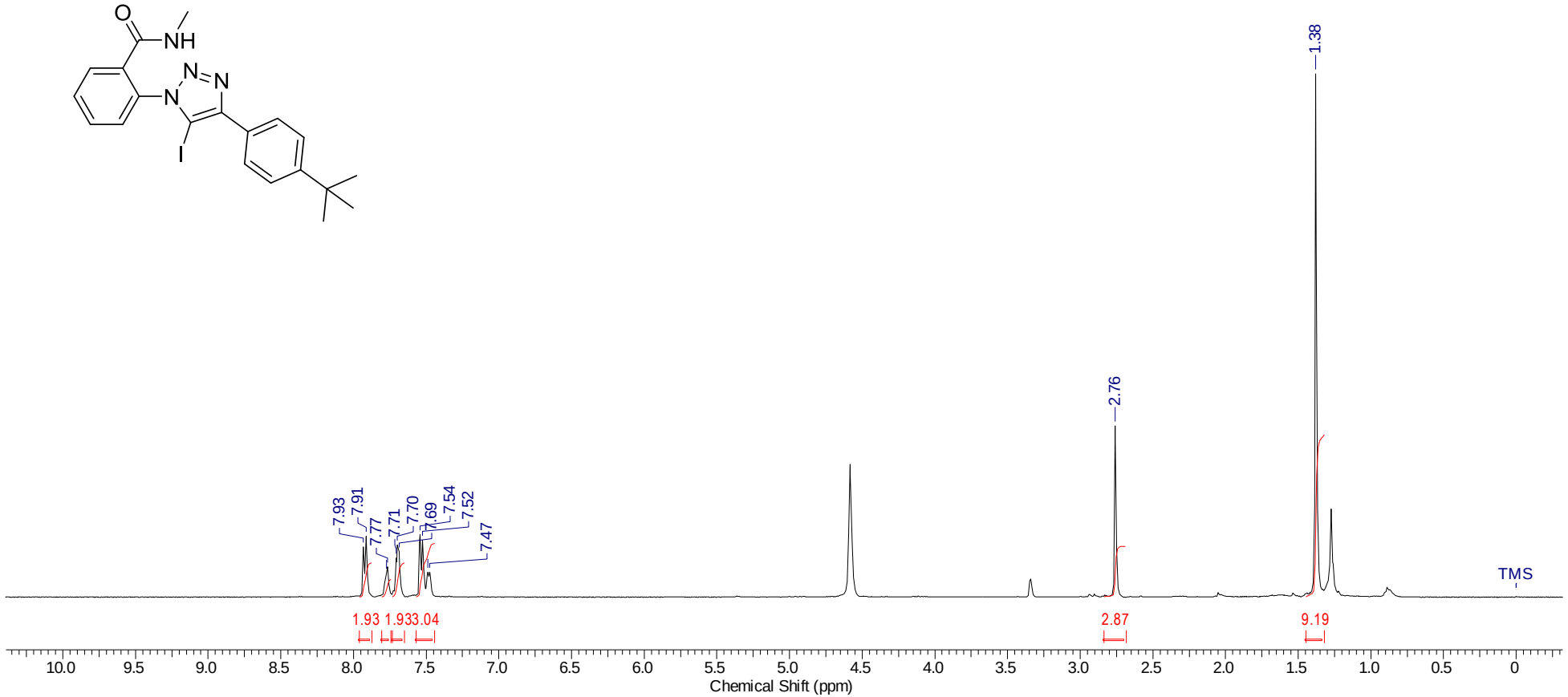
2-[4-(2-Hydroxyethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1k)

$^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6)



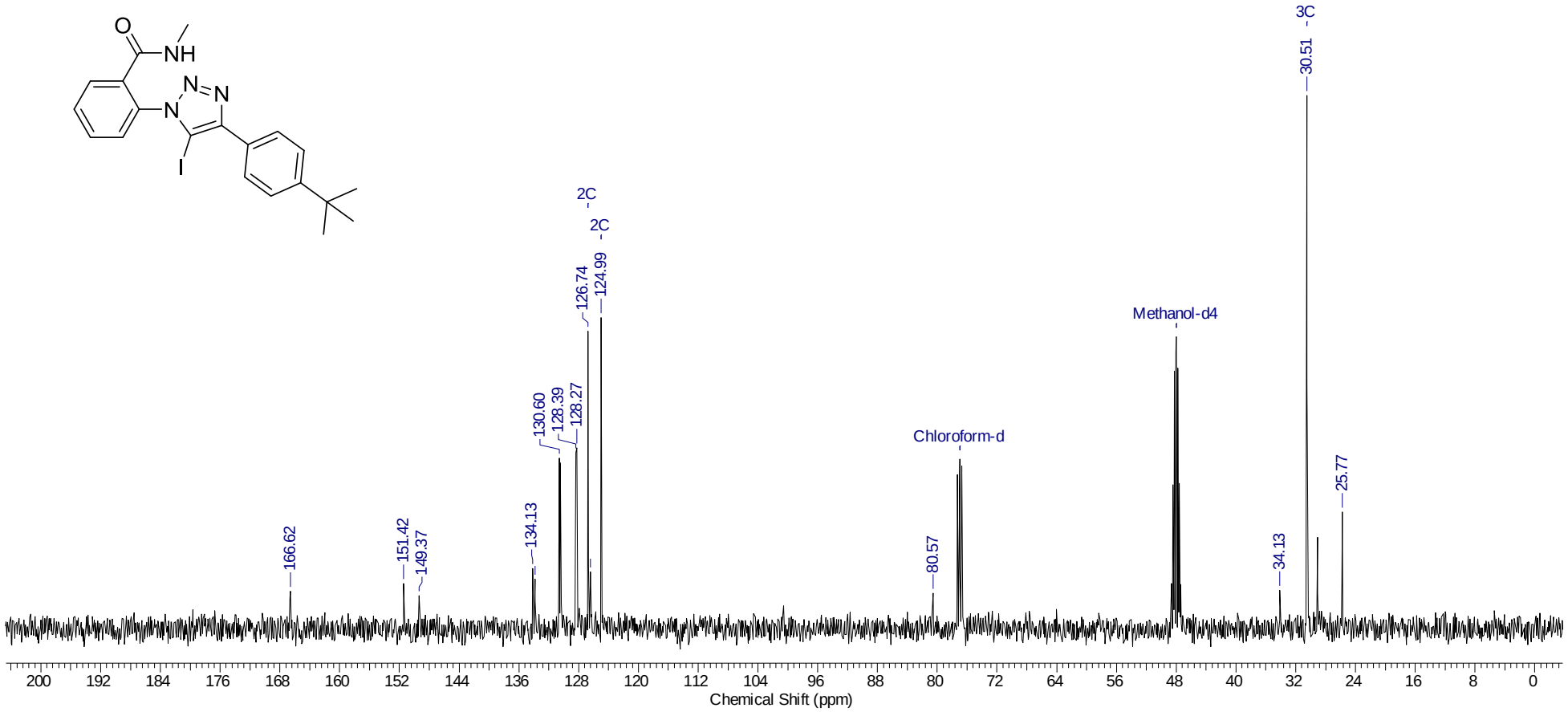
2-[4-(4-*tert*-Butylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1l)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



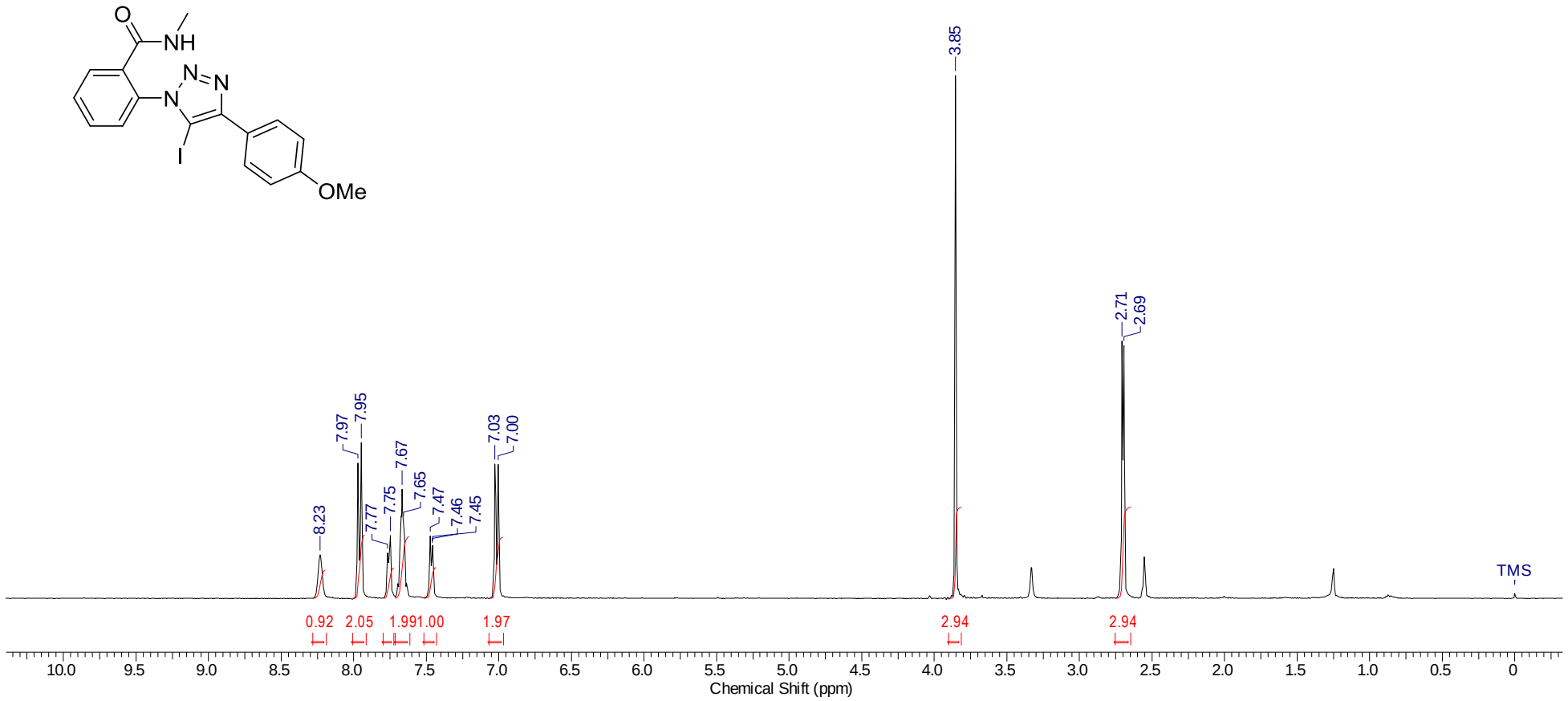
2-[4-(4-*tert*-Butylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1l)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



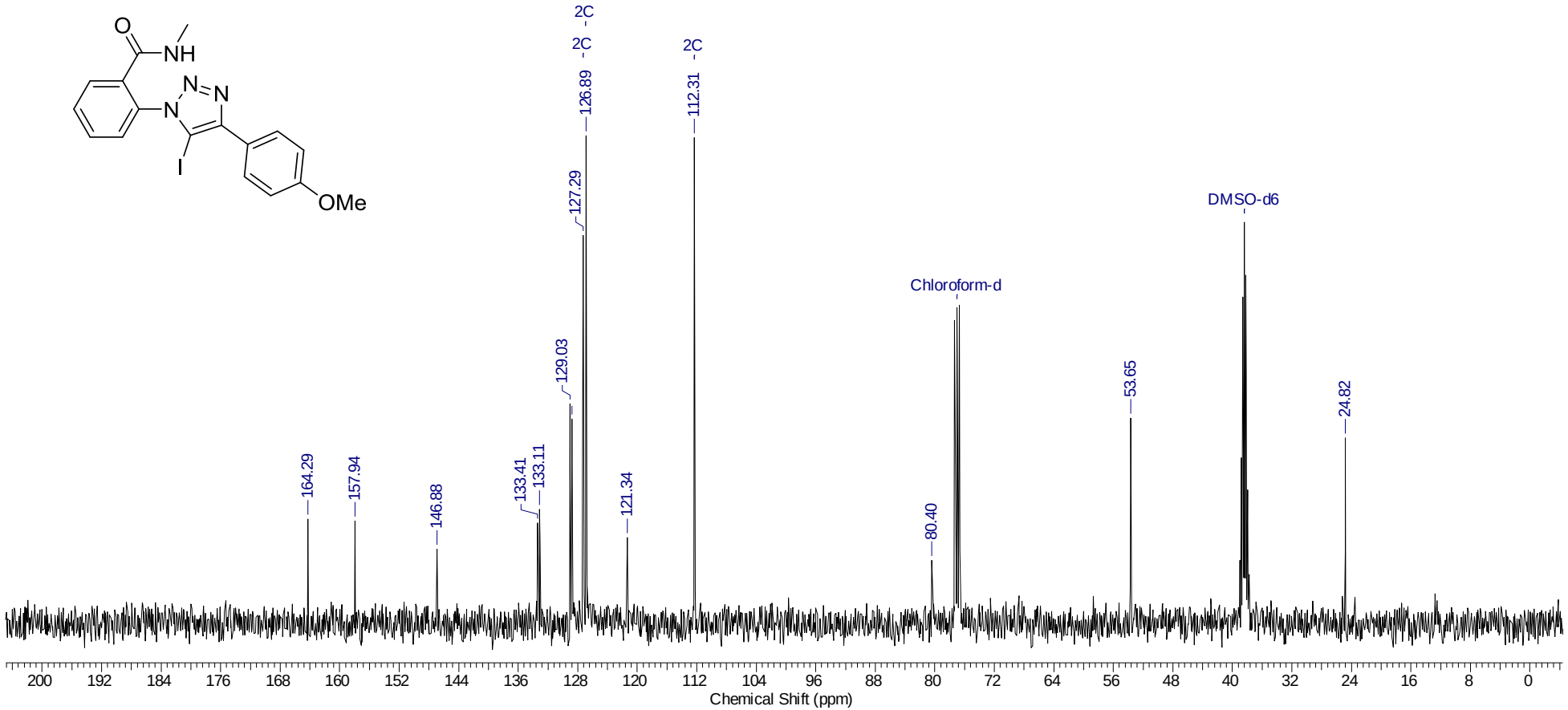
2-[5-Iodo-4-(4-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1m)

^{1}H NMR (400 MHz, $CDCl_3$–DMSO-d_6)



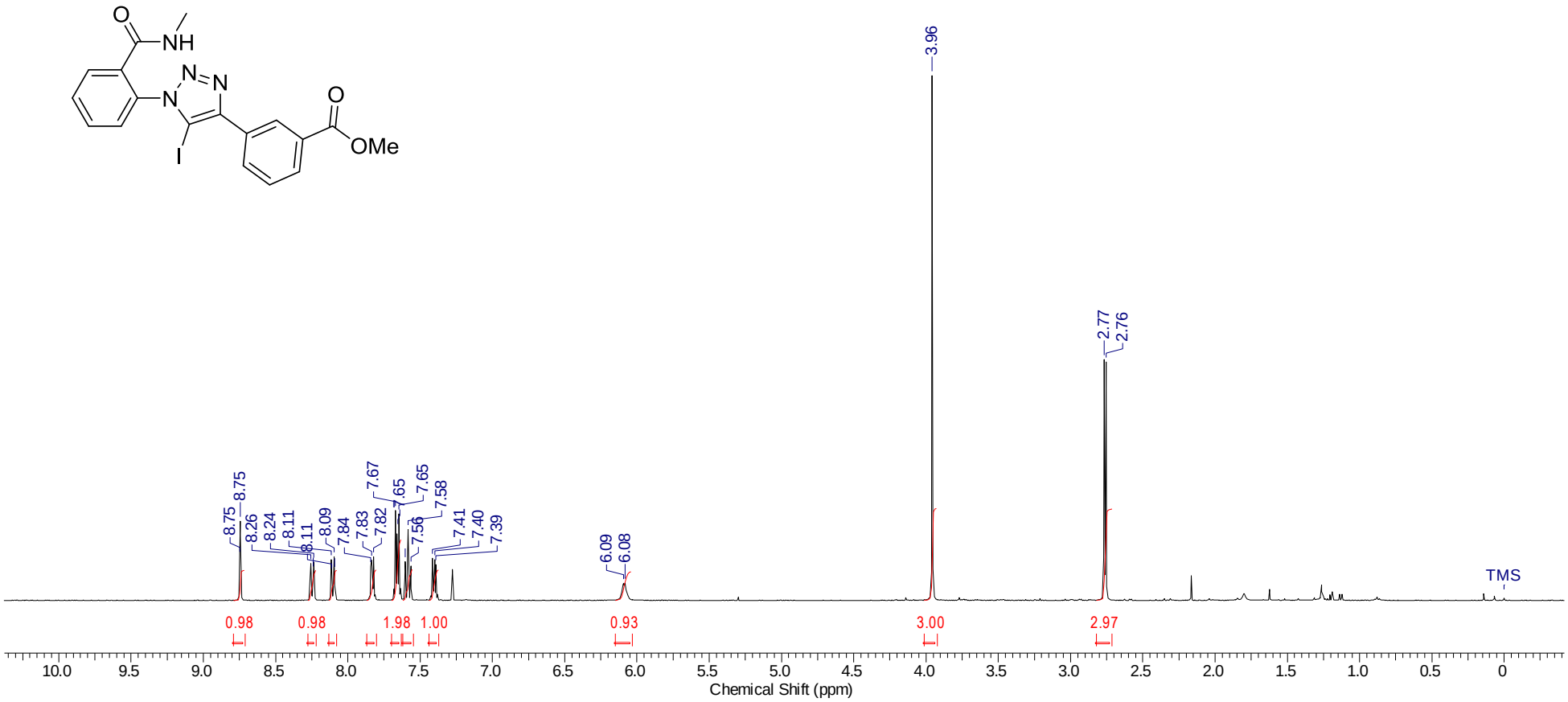
2-[5-Iodo-4-(4-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1m)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–DMSO-d_6)



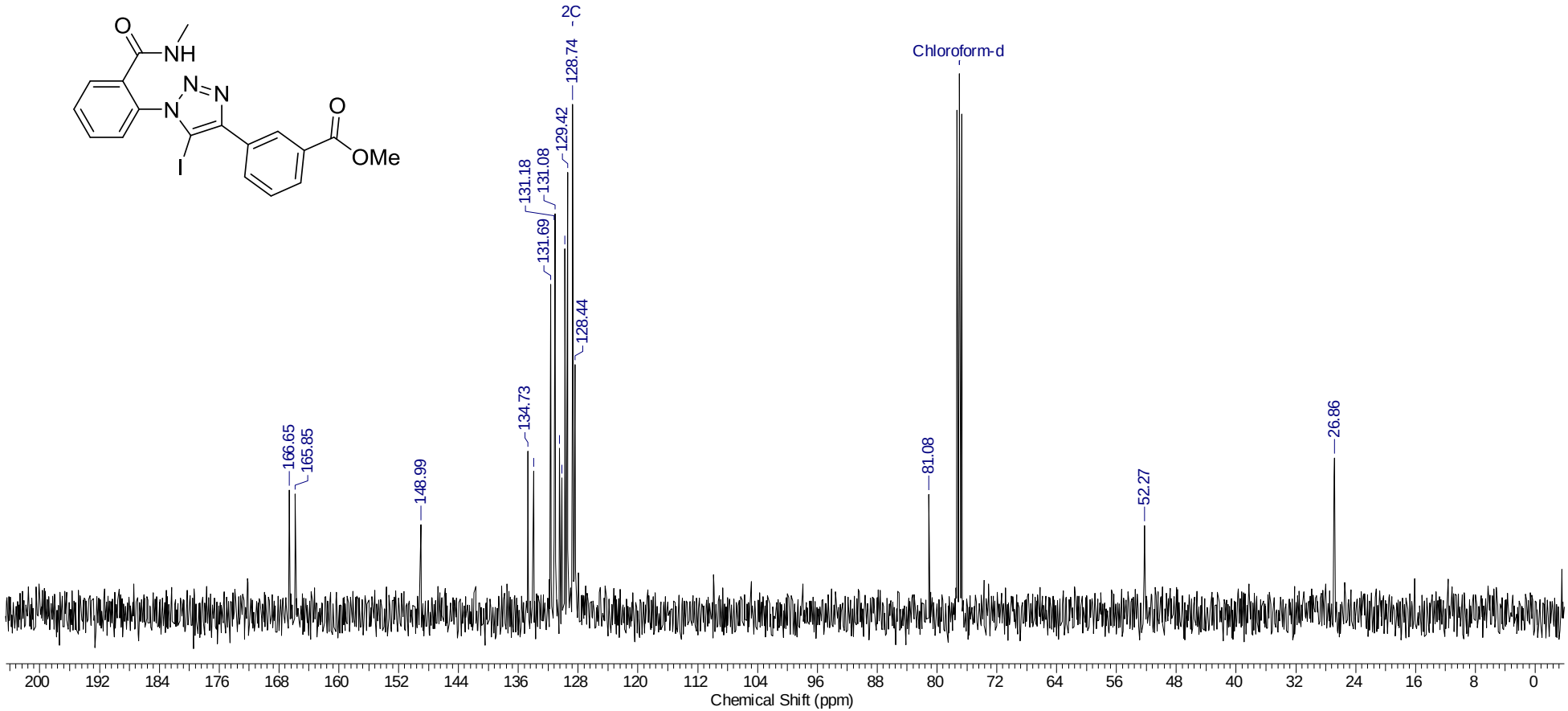
Methyl 3-(5-iodo-1-{2-[(methylamino)carbonyl]phenyl}-1*H*-1,2,3-triazol-4-yl)benzoate (1n)

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



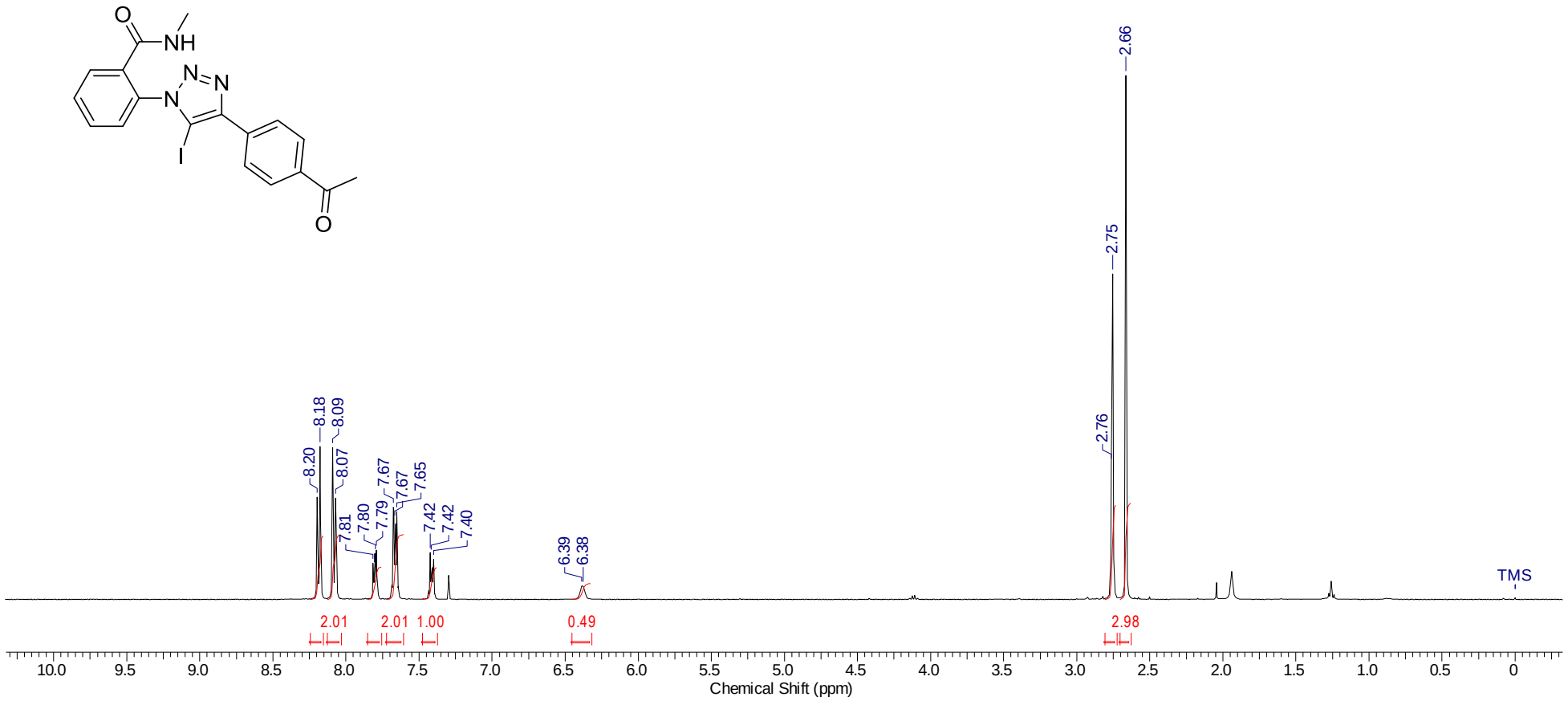
Methyl 3-(5-iodo-1-{2-[(methylamino)carbonyl]phenyl}-1*H*-1,2,3-triazol-4-yl)benzoate (1n)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



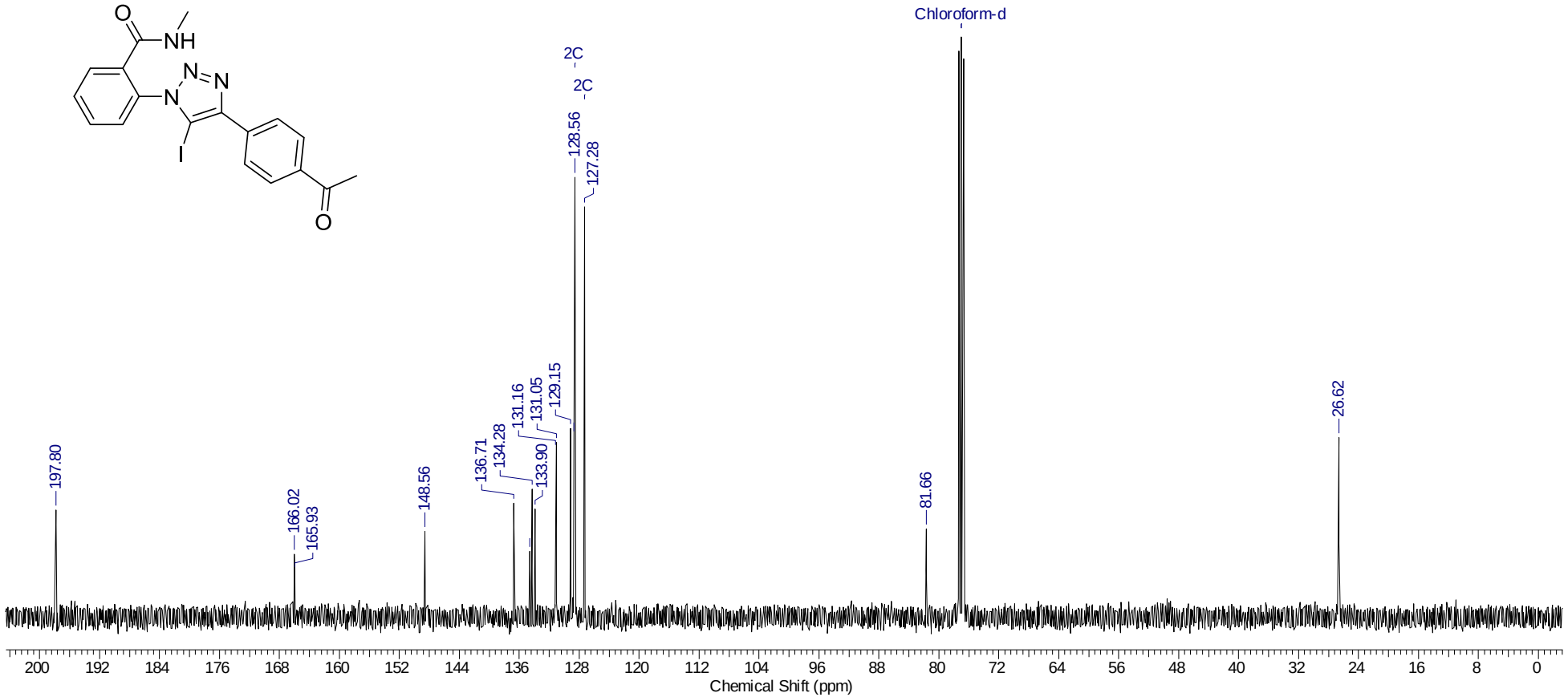
2-[4-(4-Acetylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1o)

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



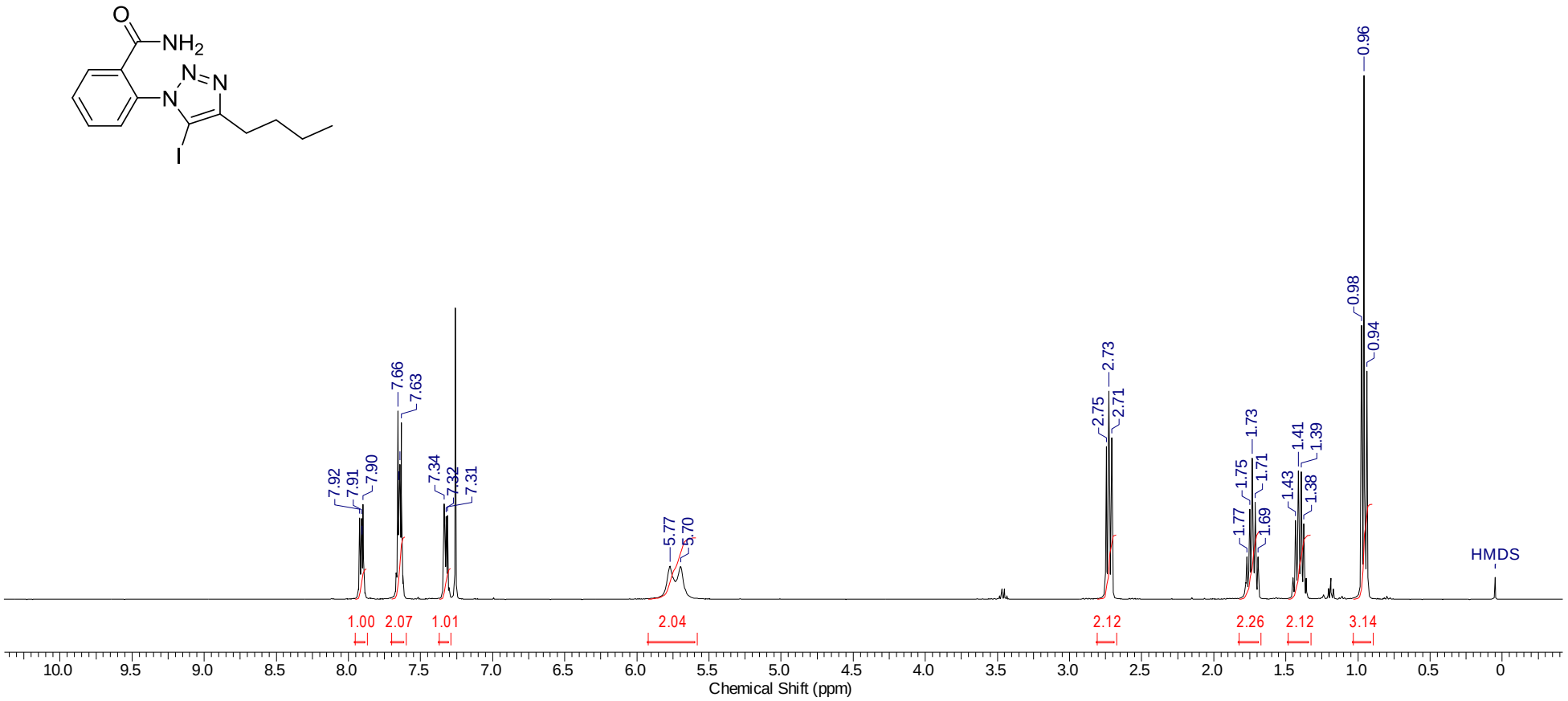
2-[4-(4-Acetylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]-*N*-methylbenzamide (1o)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



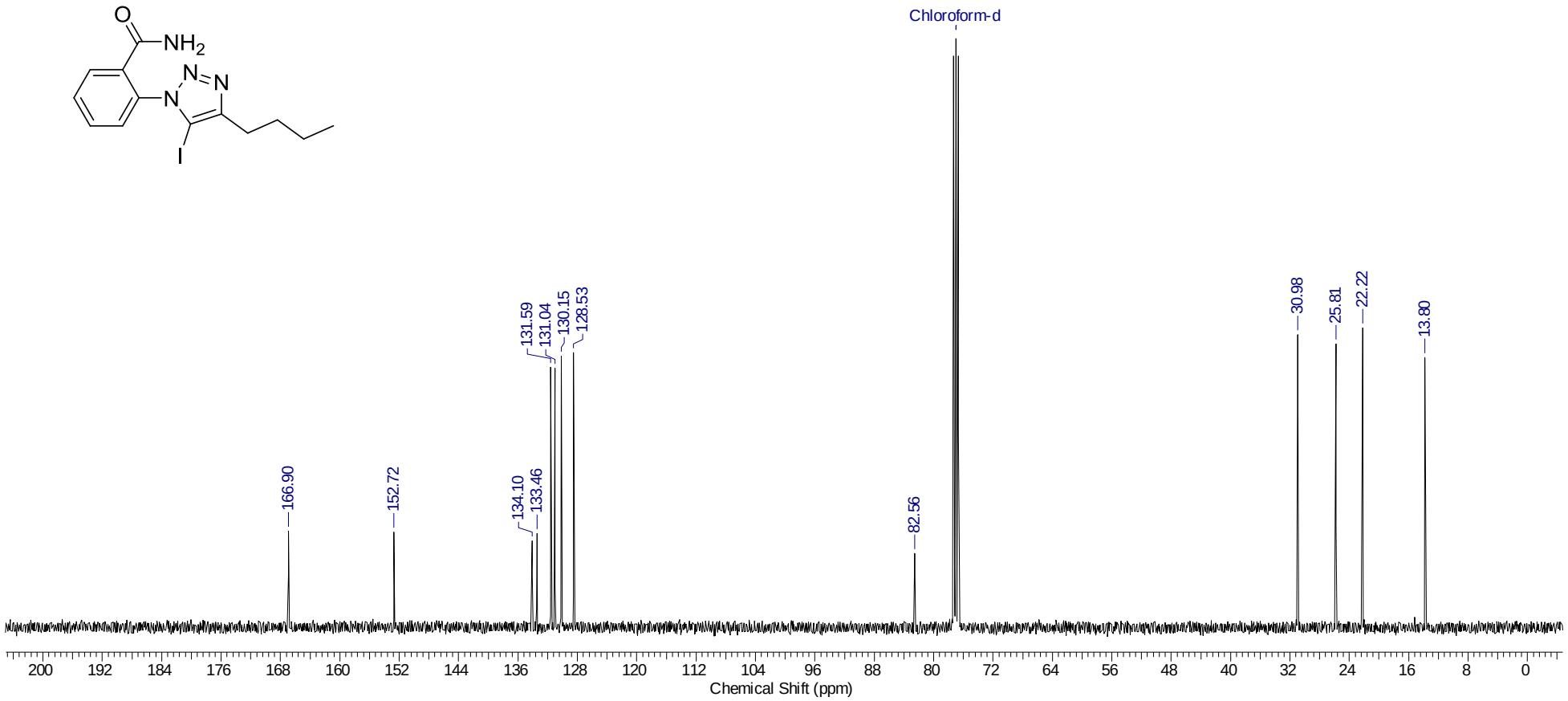
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzamide (1p)

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



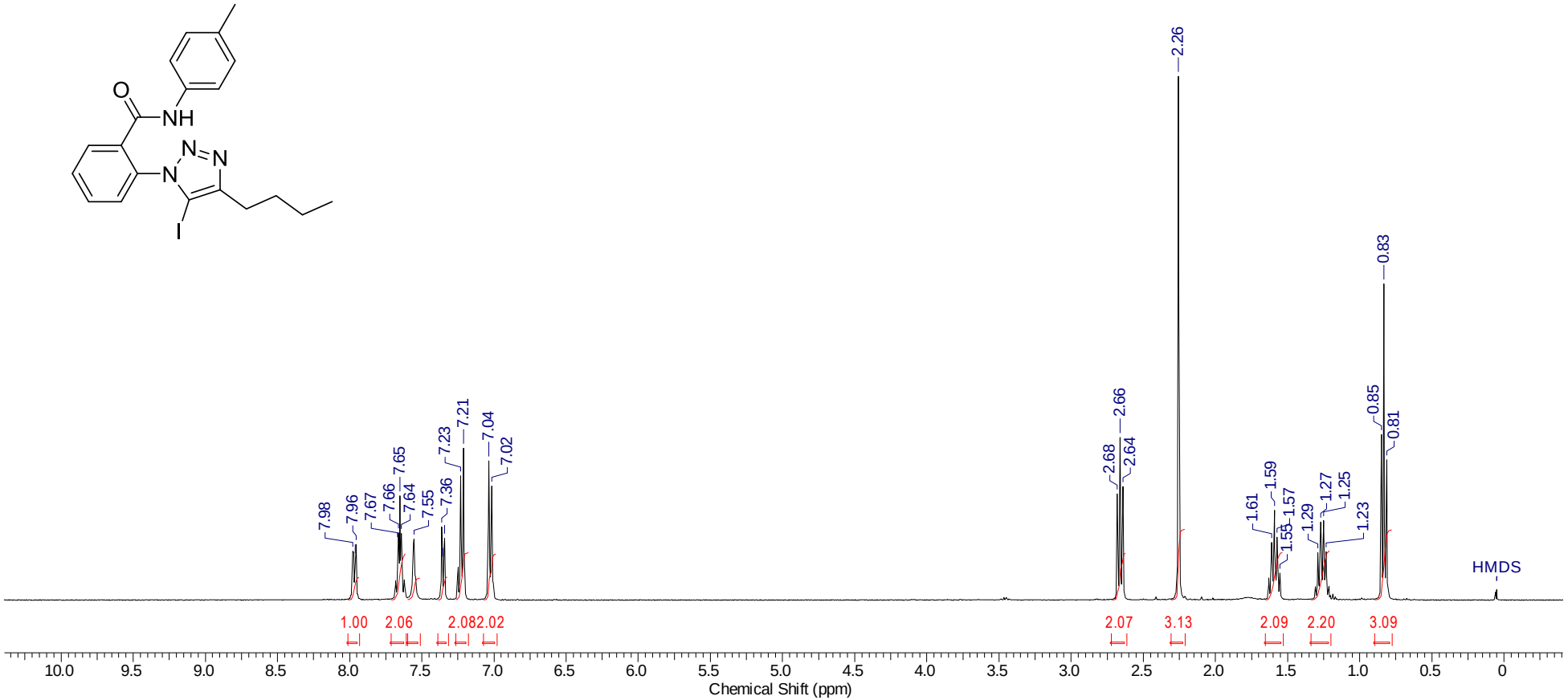
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzamide (1p)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



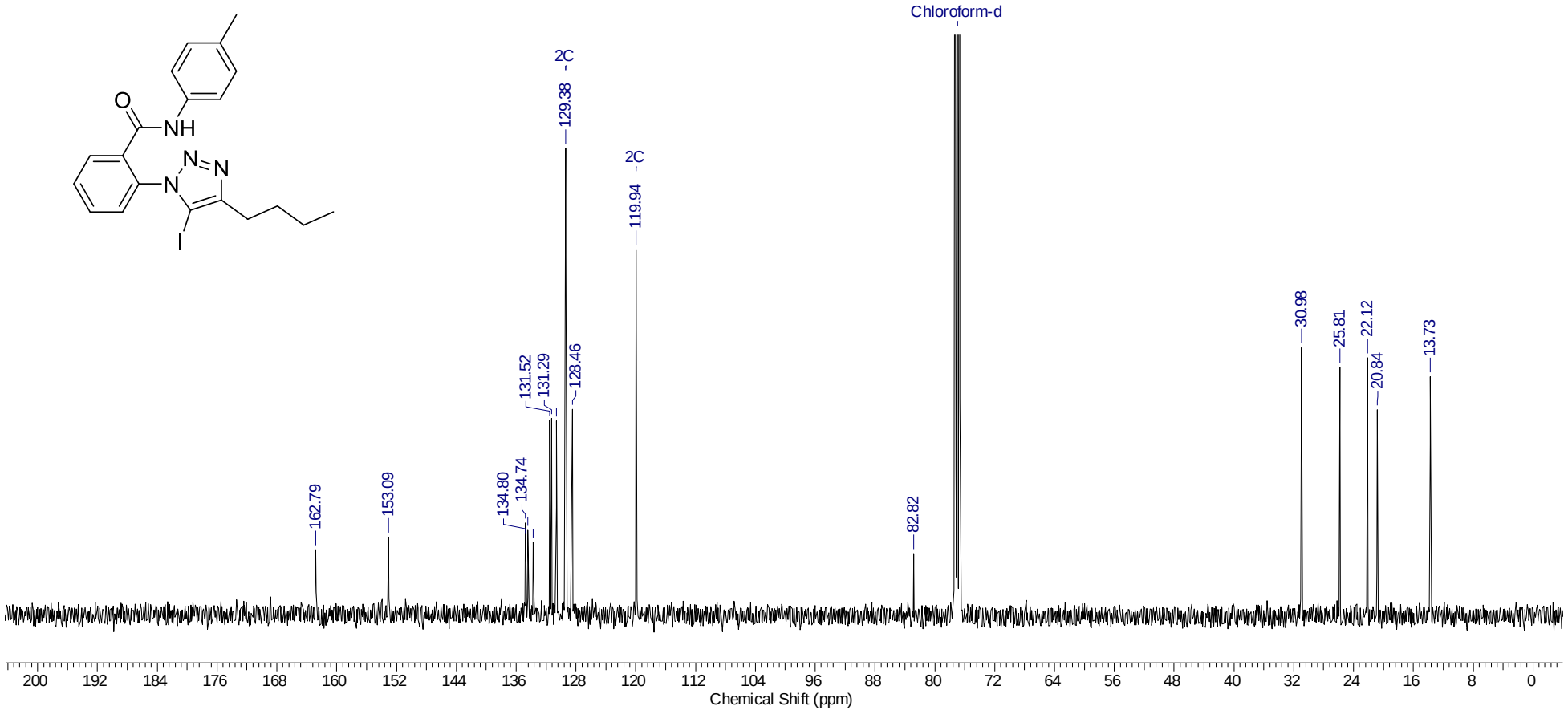
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methylphenyl)benzamide (1q)

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



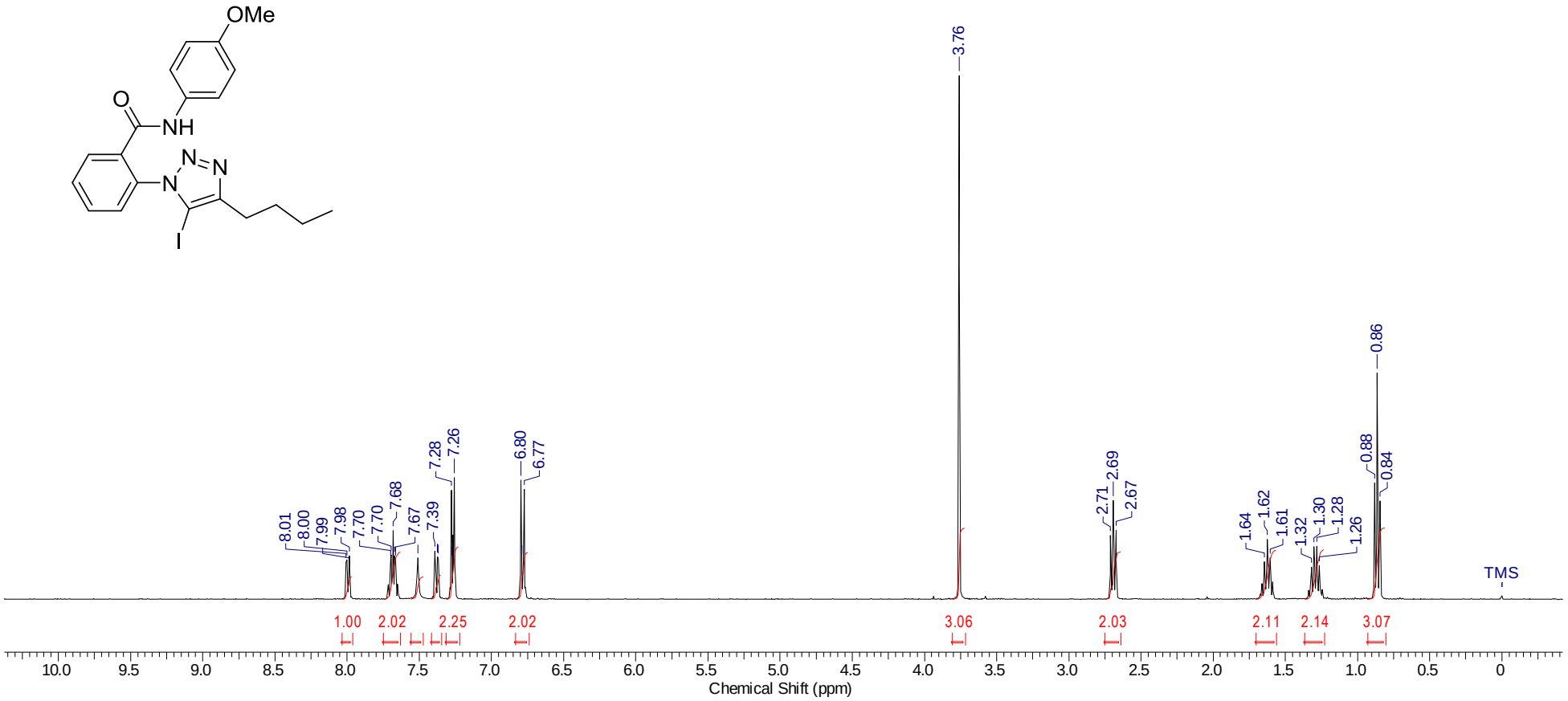
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methylphenyl)benzamide (1q)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



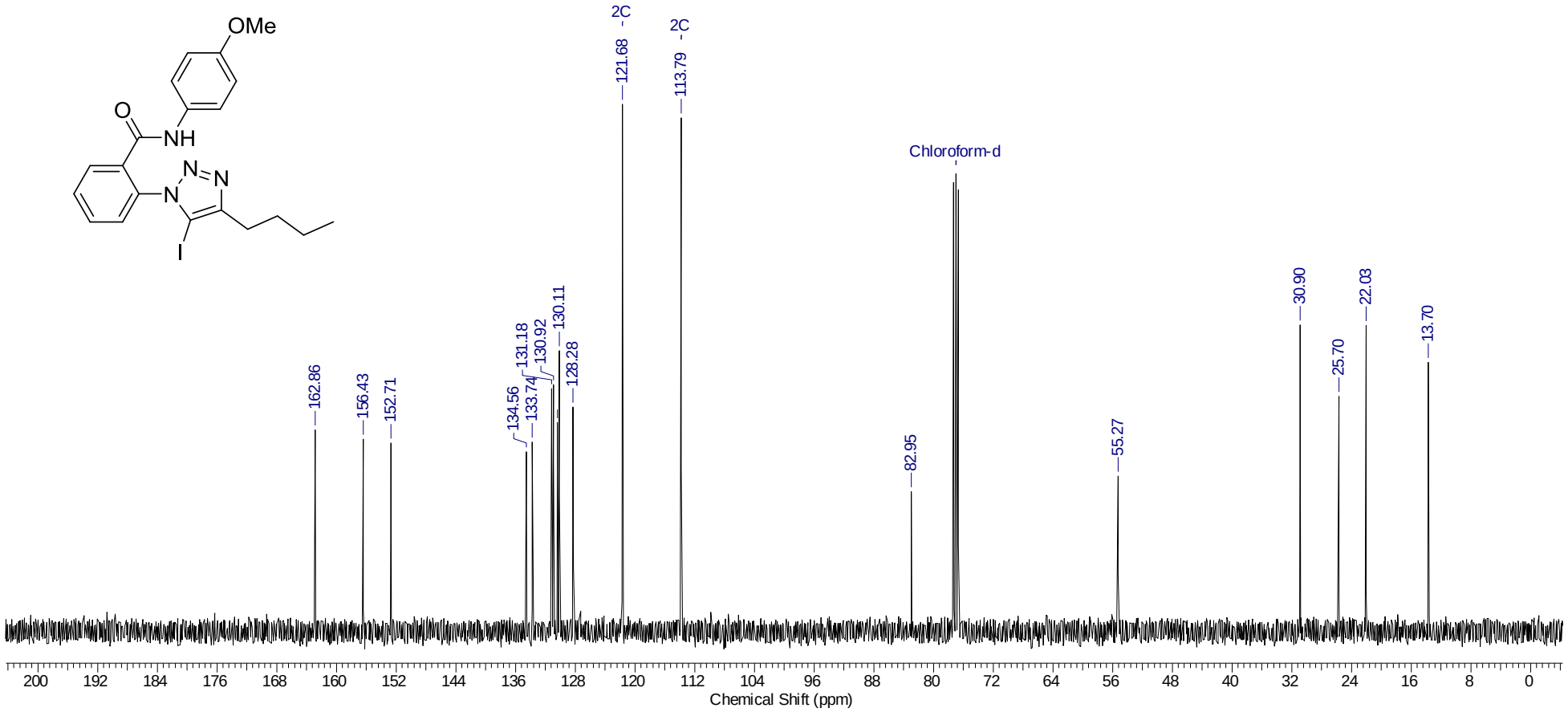
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methoxyphenyl)benzamide (1r)

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



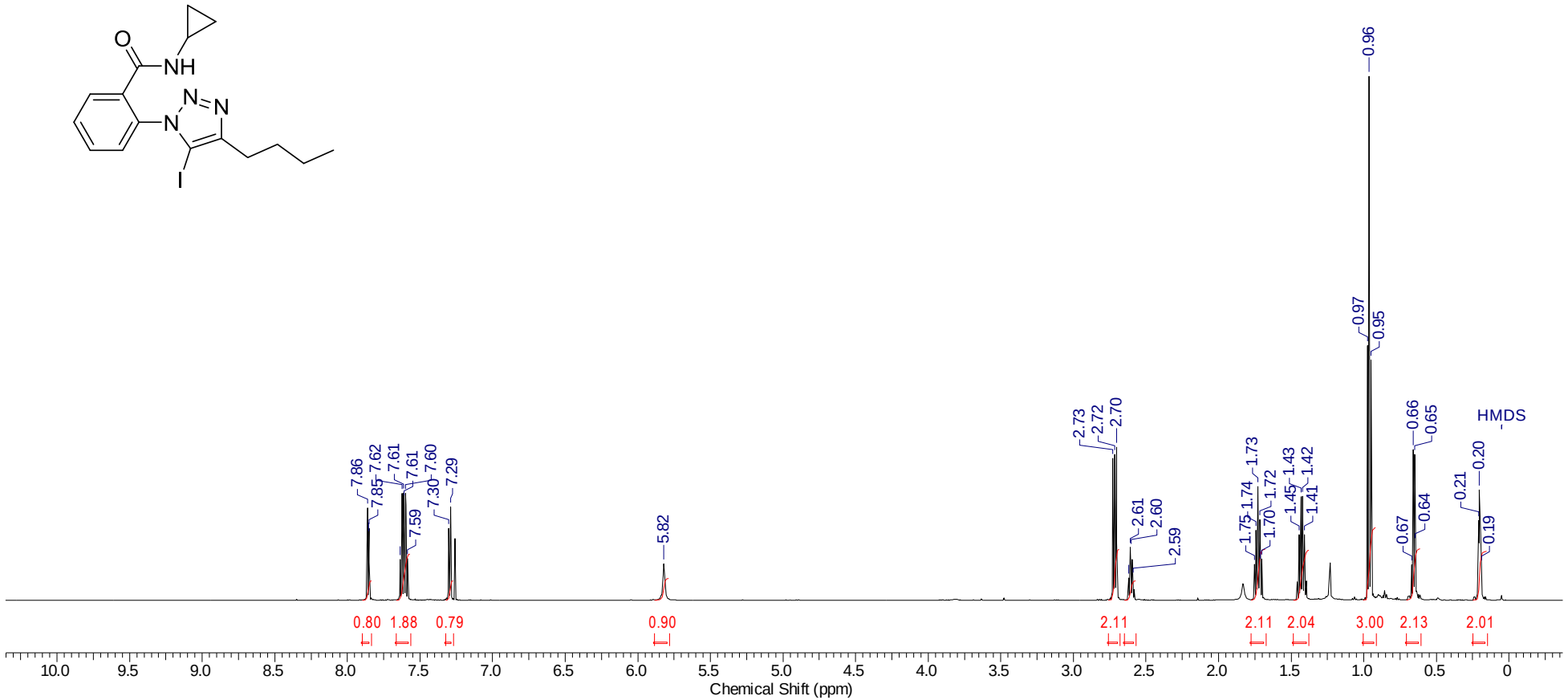
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methoxyphenyl)benzamide (1r)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



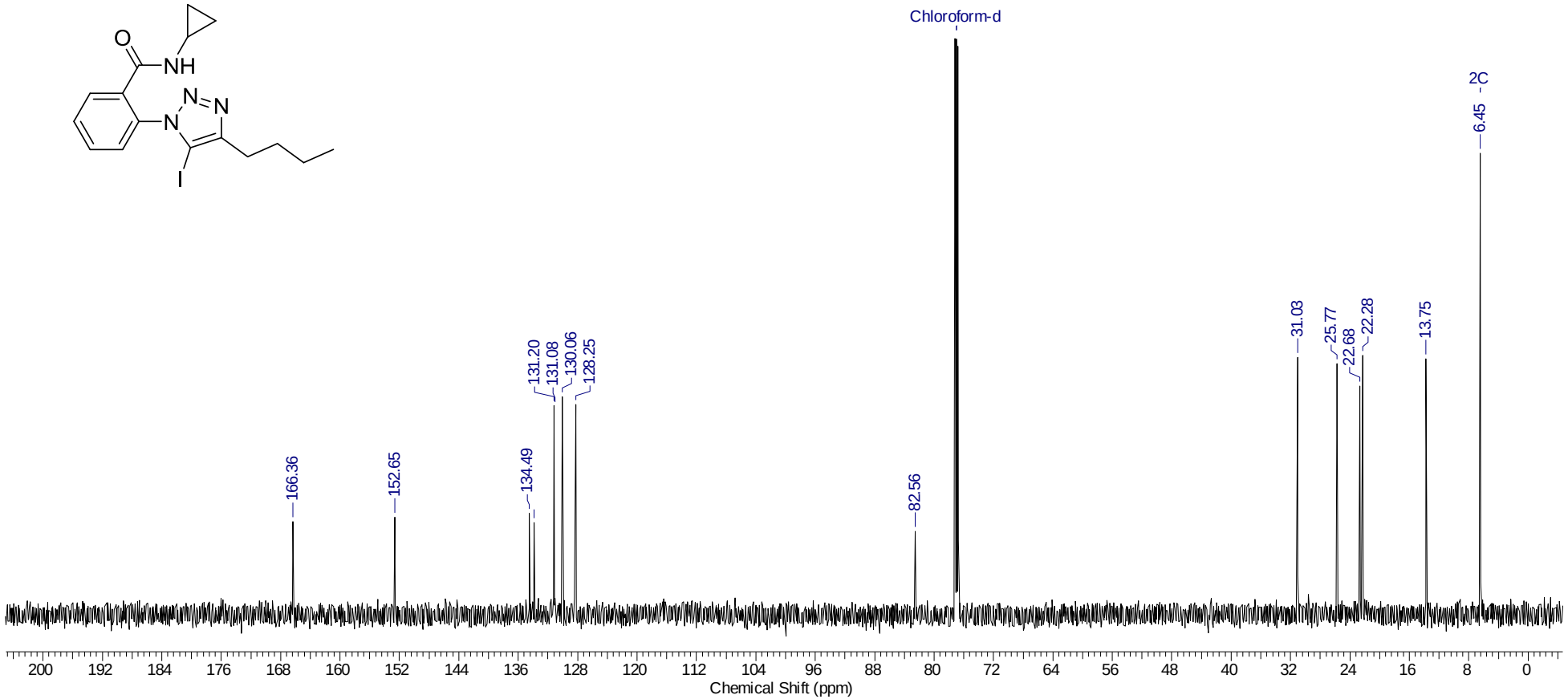
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-cyclopropylbenzamide (1s)

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



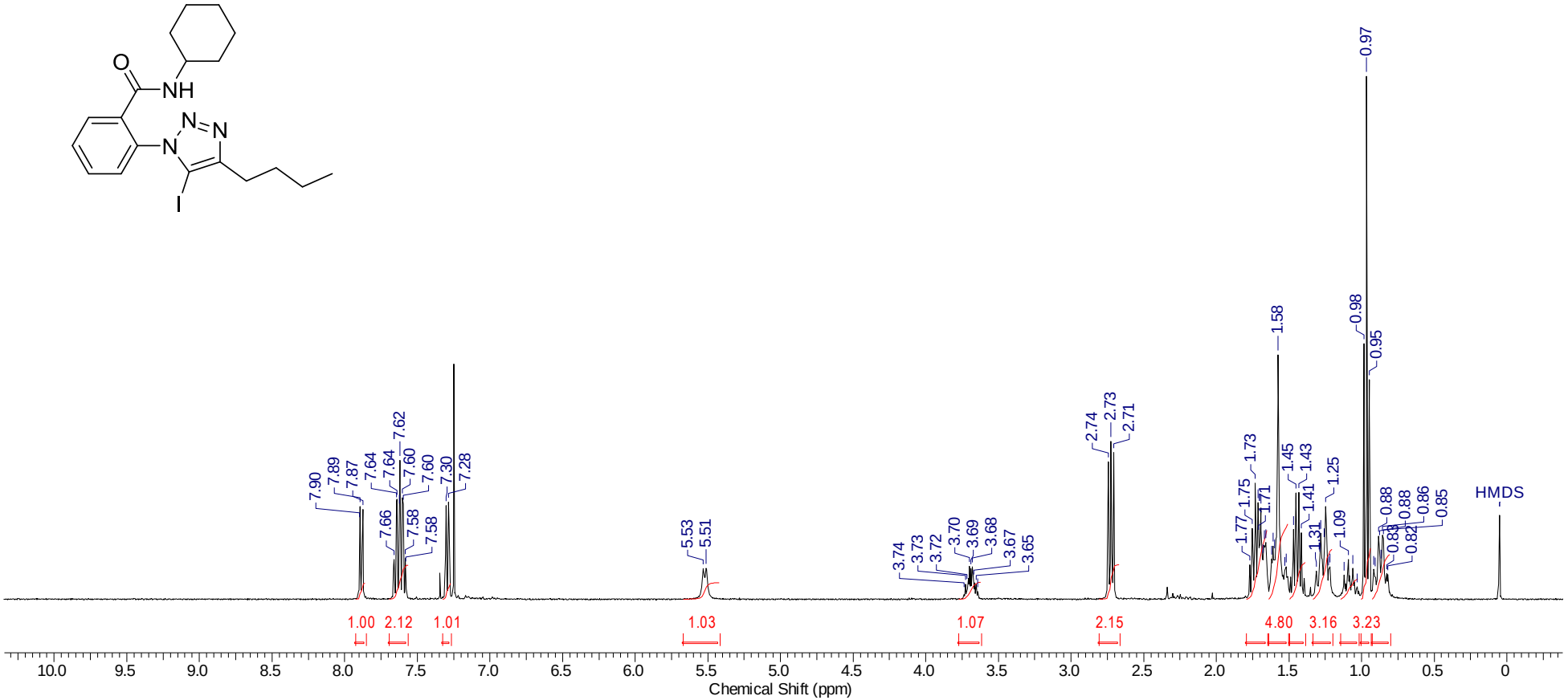
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-cyclopropylbenzamide (1s)

$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$)



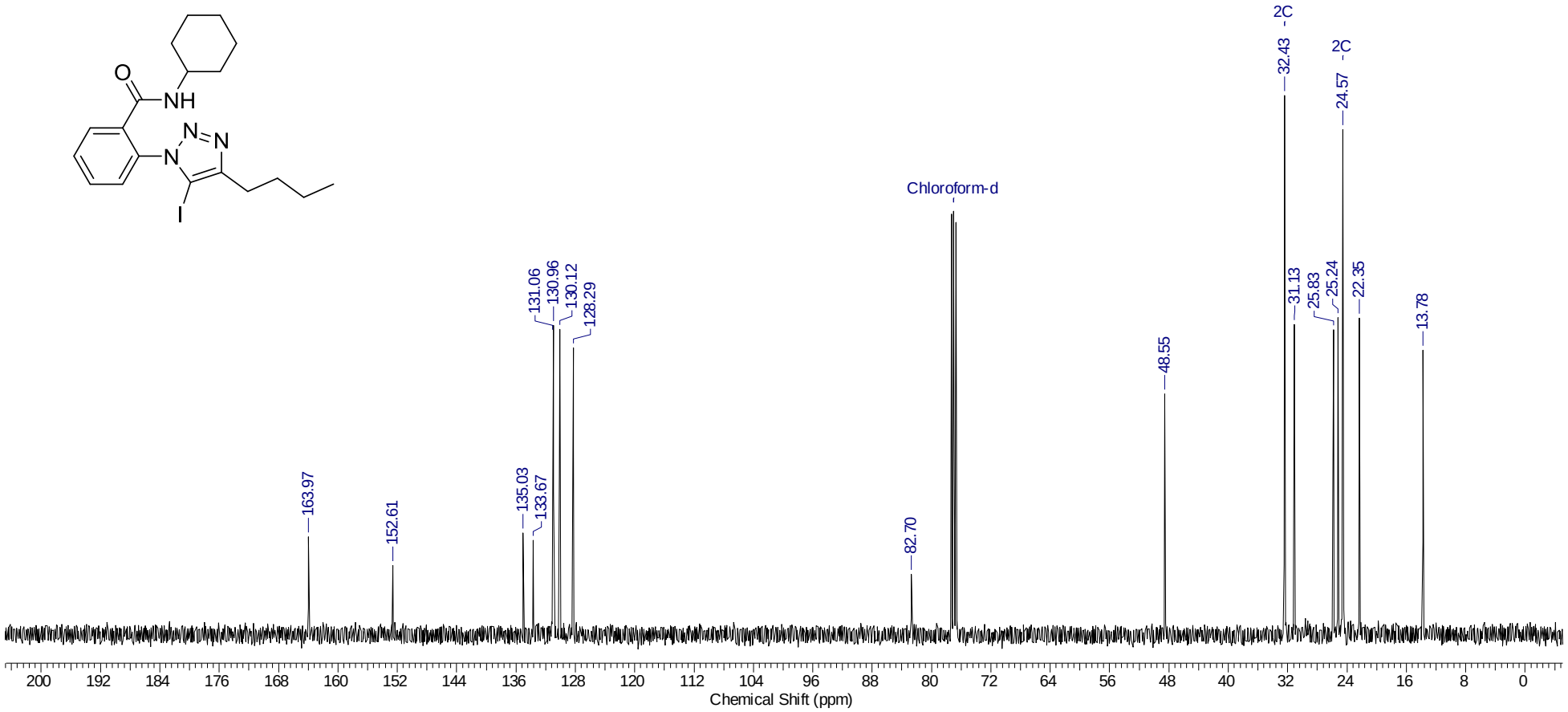
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-cyclohexylbenzamide (1t)

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



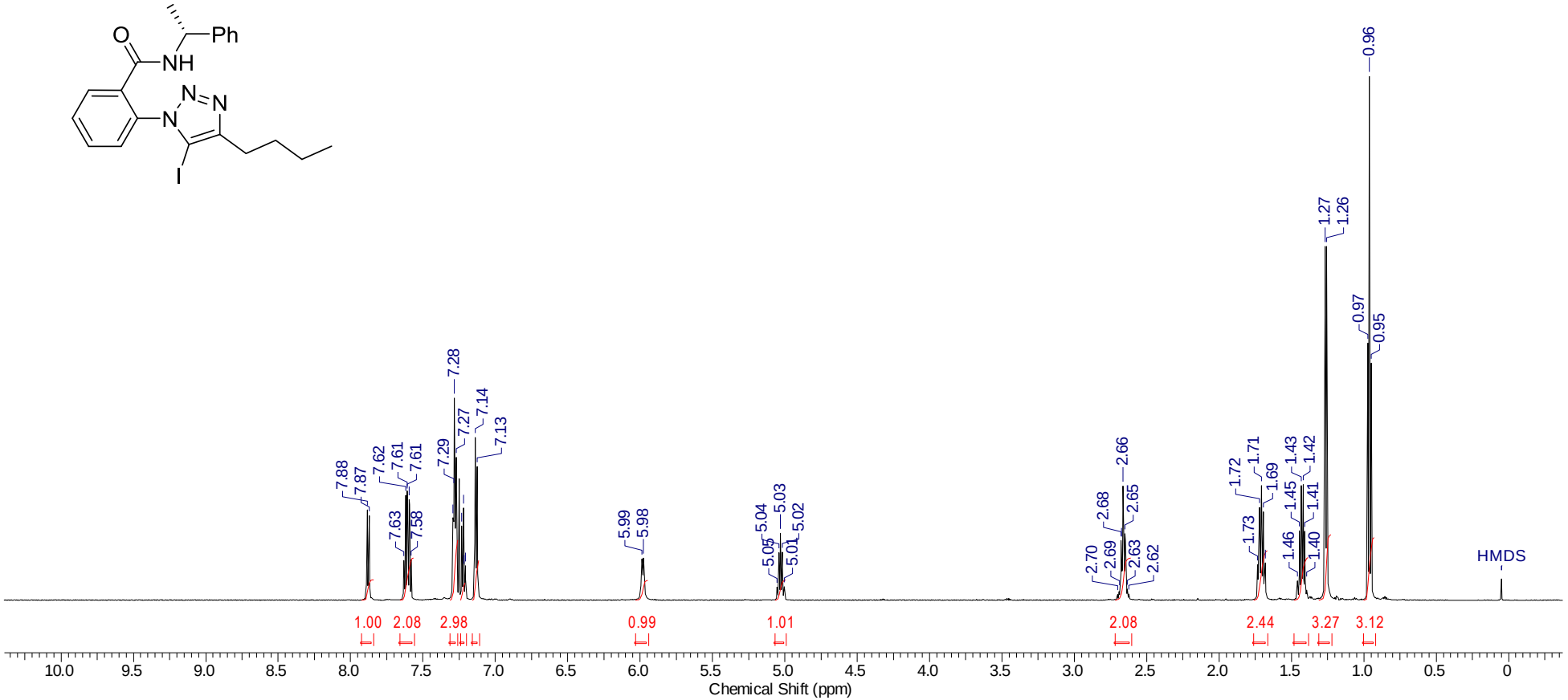
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-cyclohexylbenzamide (1t)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



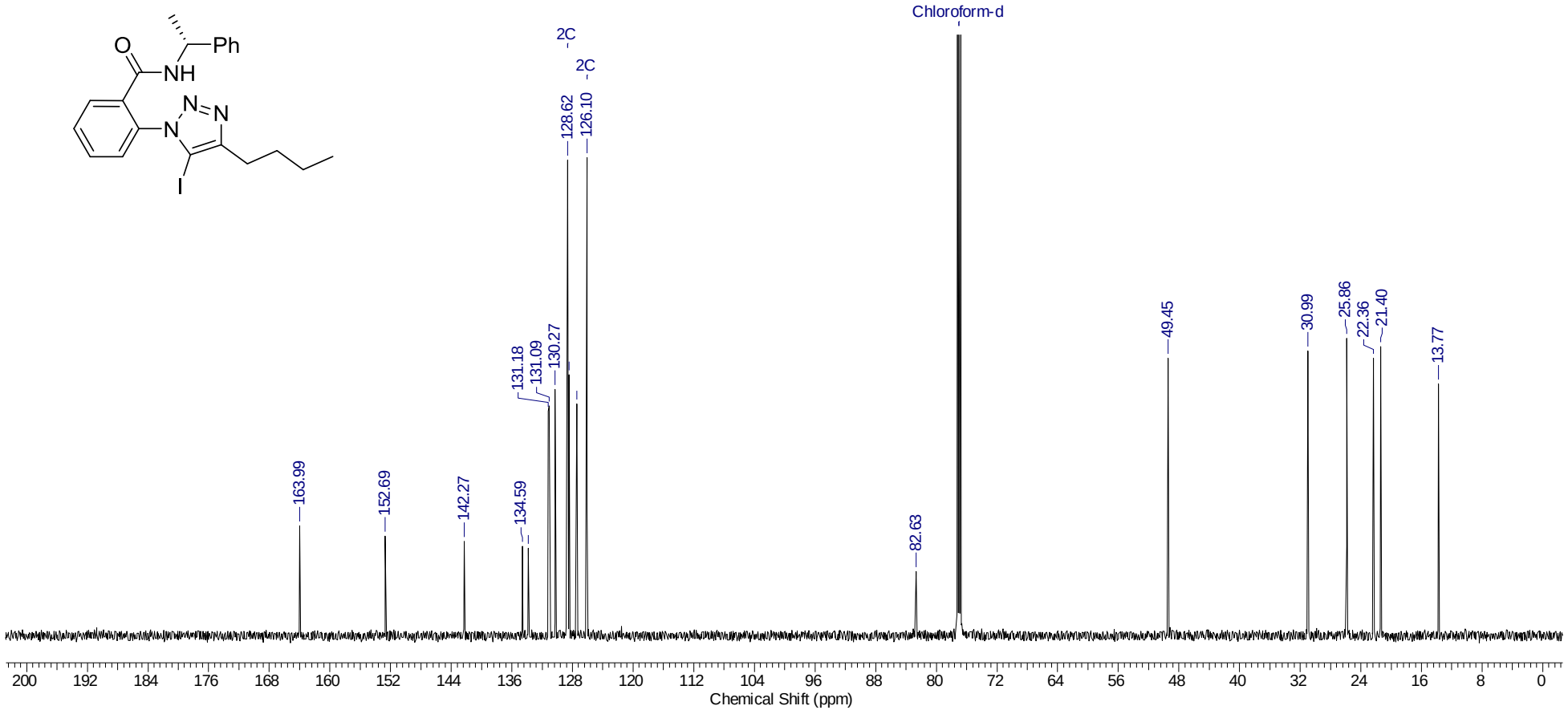
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[(1*R*)-1-phenylethyl]benzamide (1u)

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



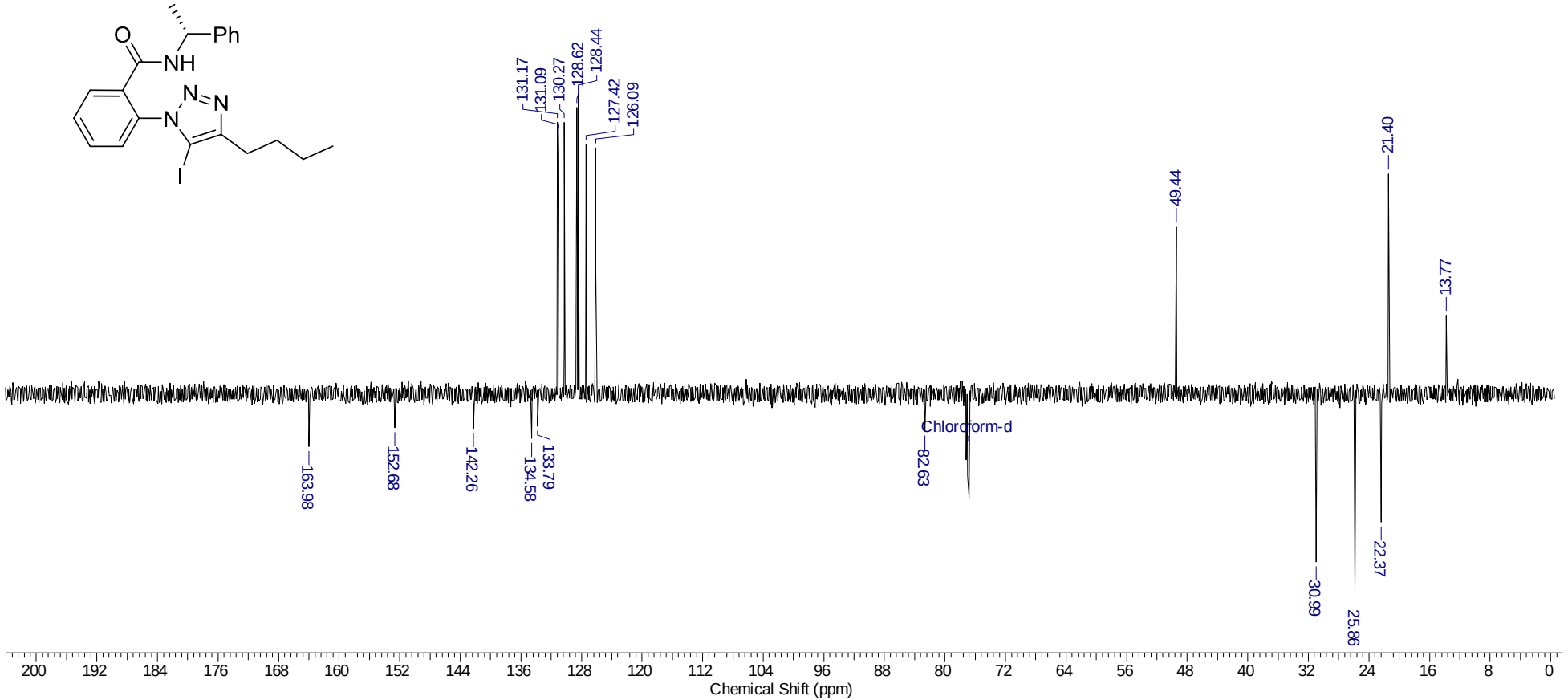
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[(1*R*)-1-phenylethyl]benzamide (1u)

$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$)



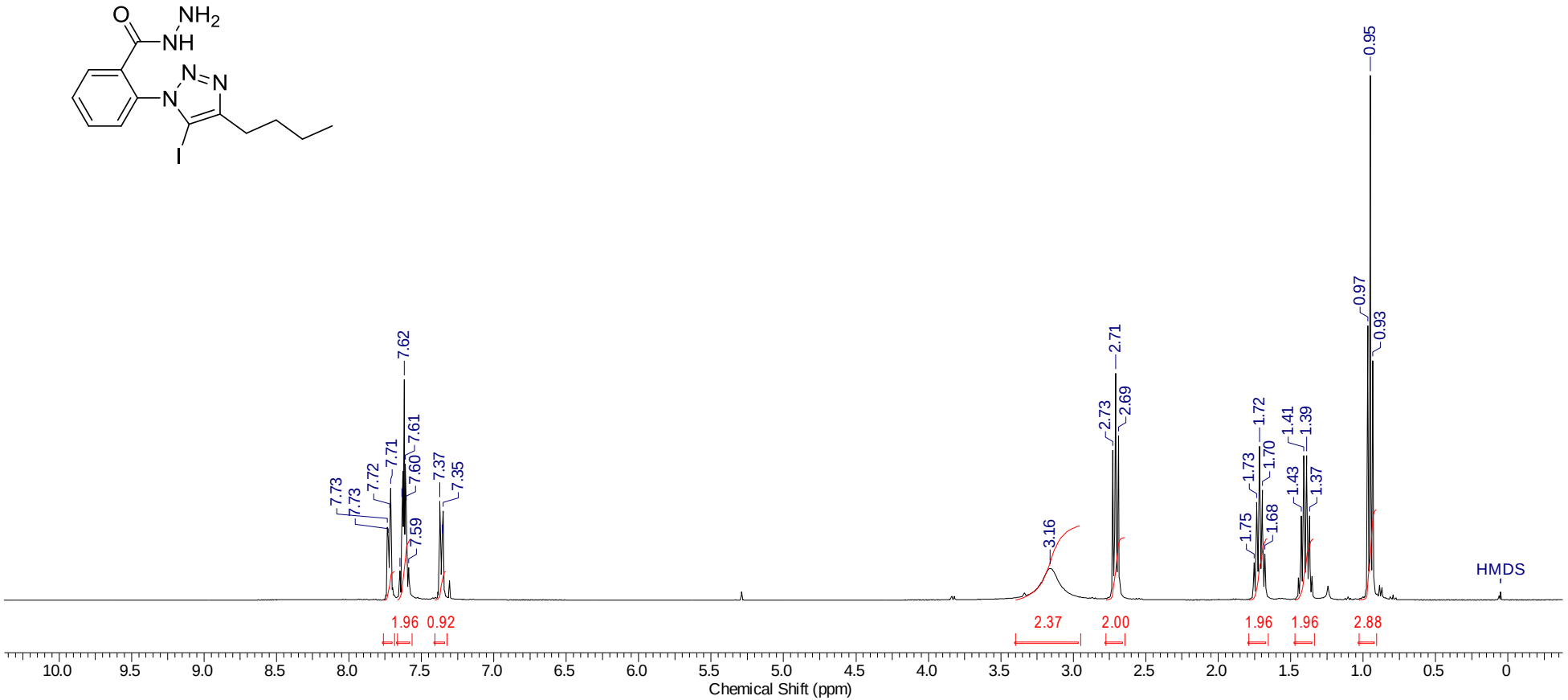
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[(1*R*)-1-phenylethyl]benzamide (1u)

APT (151 MHz, $CDCl_3$)



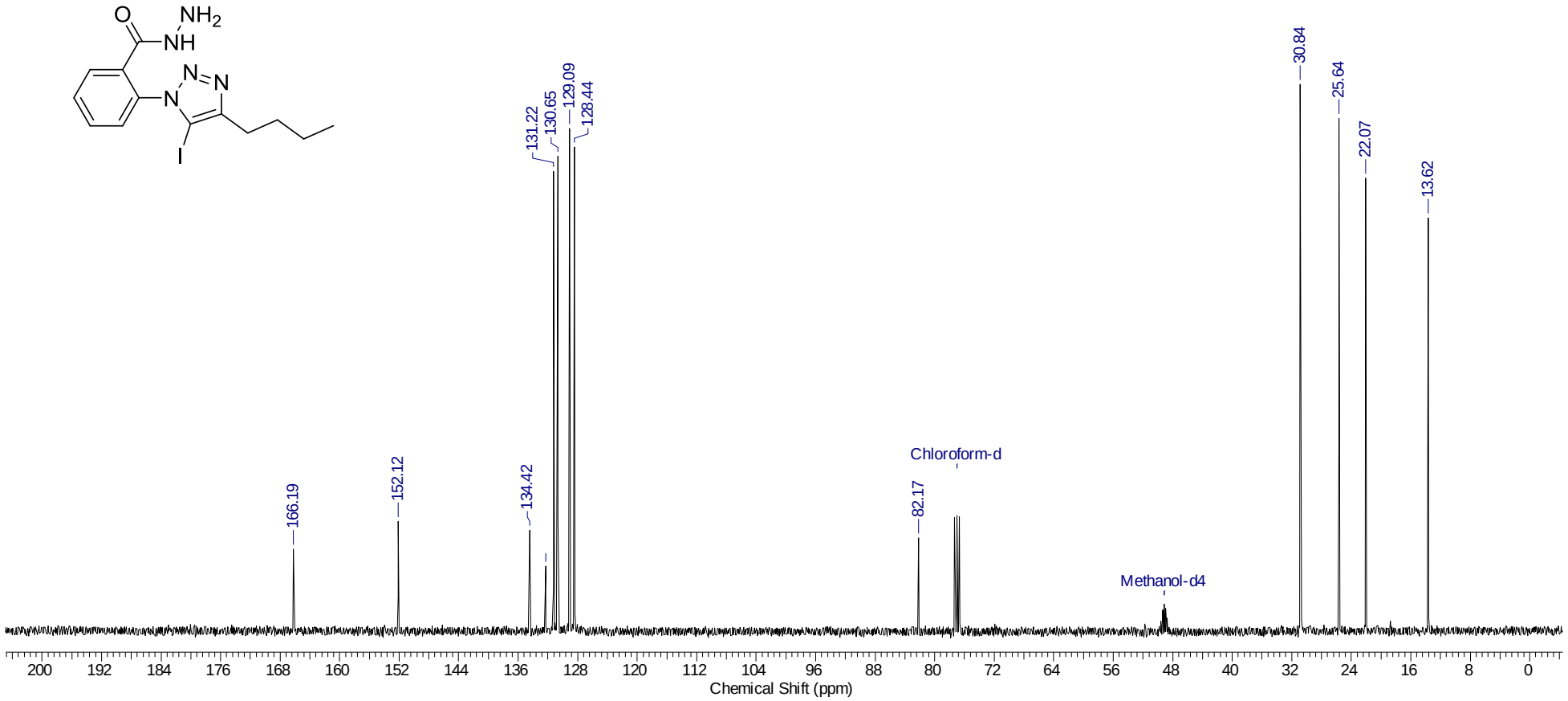
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzohydrazide (1v)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



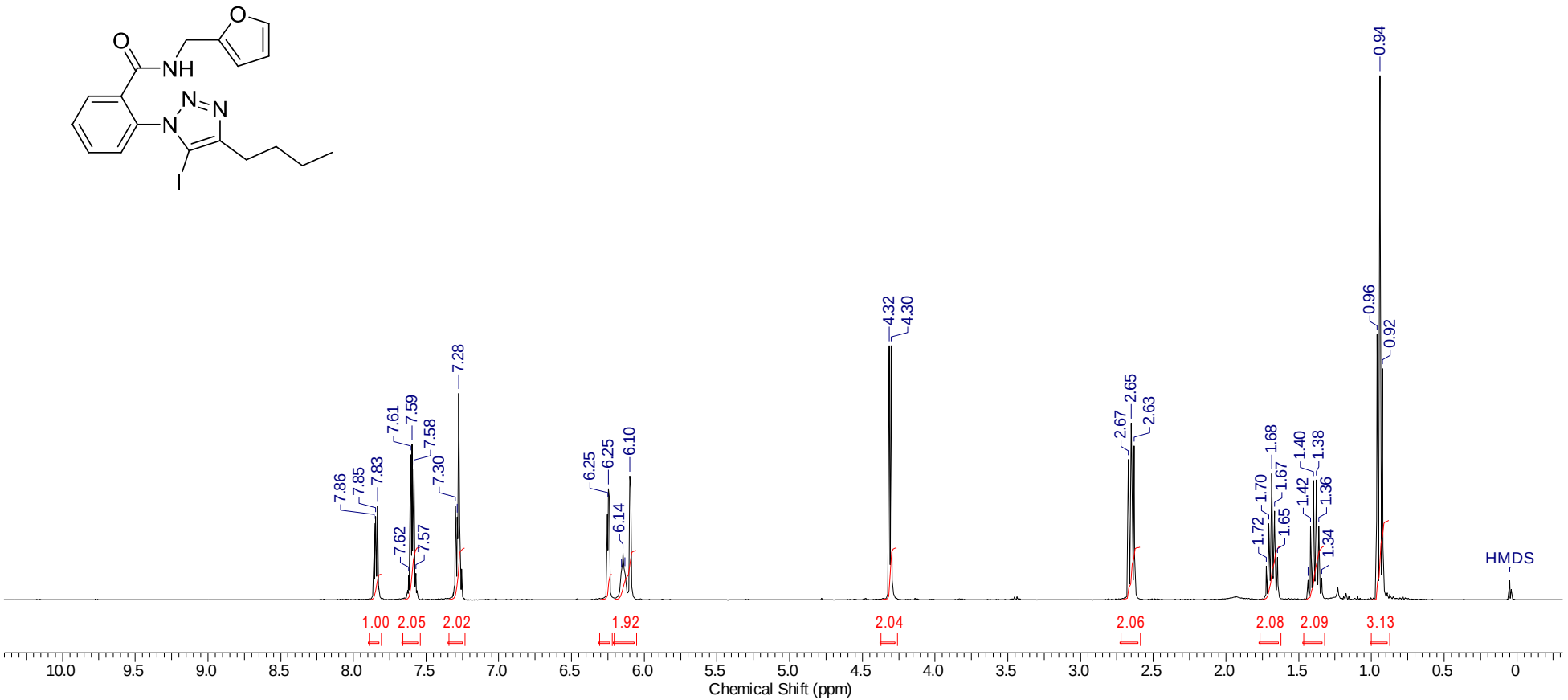
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzohydrazide (1v)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



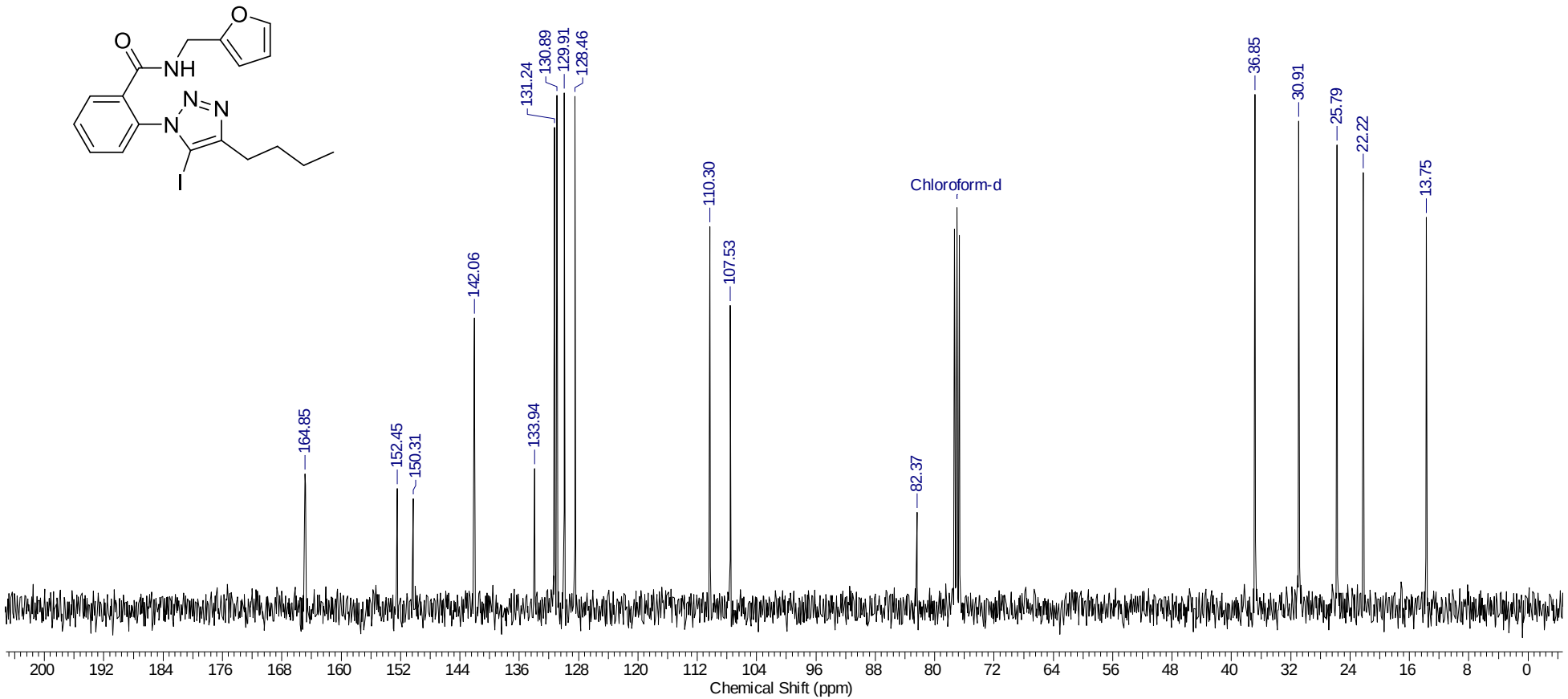
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(2-furylmethyl)benzamide (1w)

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



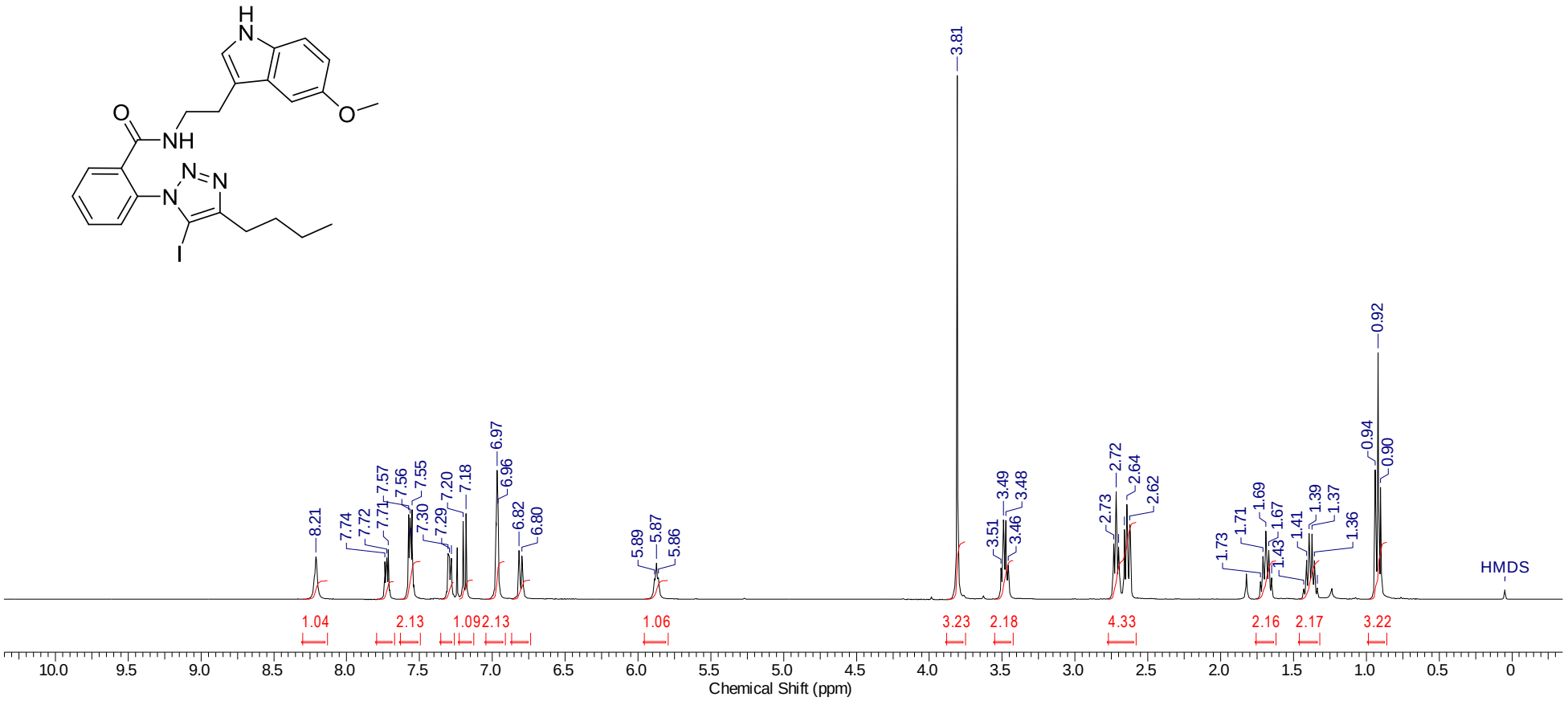
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(2-furylmethyl)benzamide (1w)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



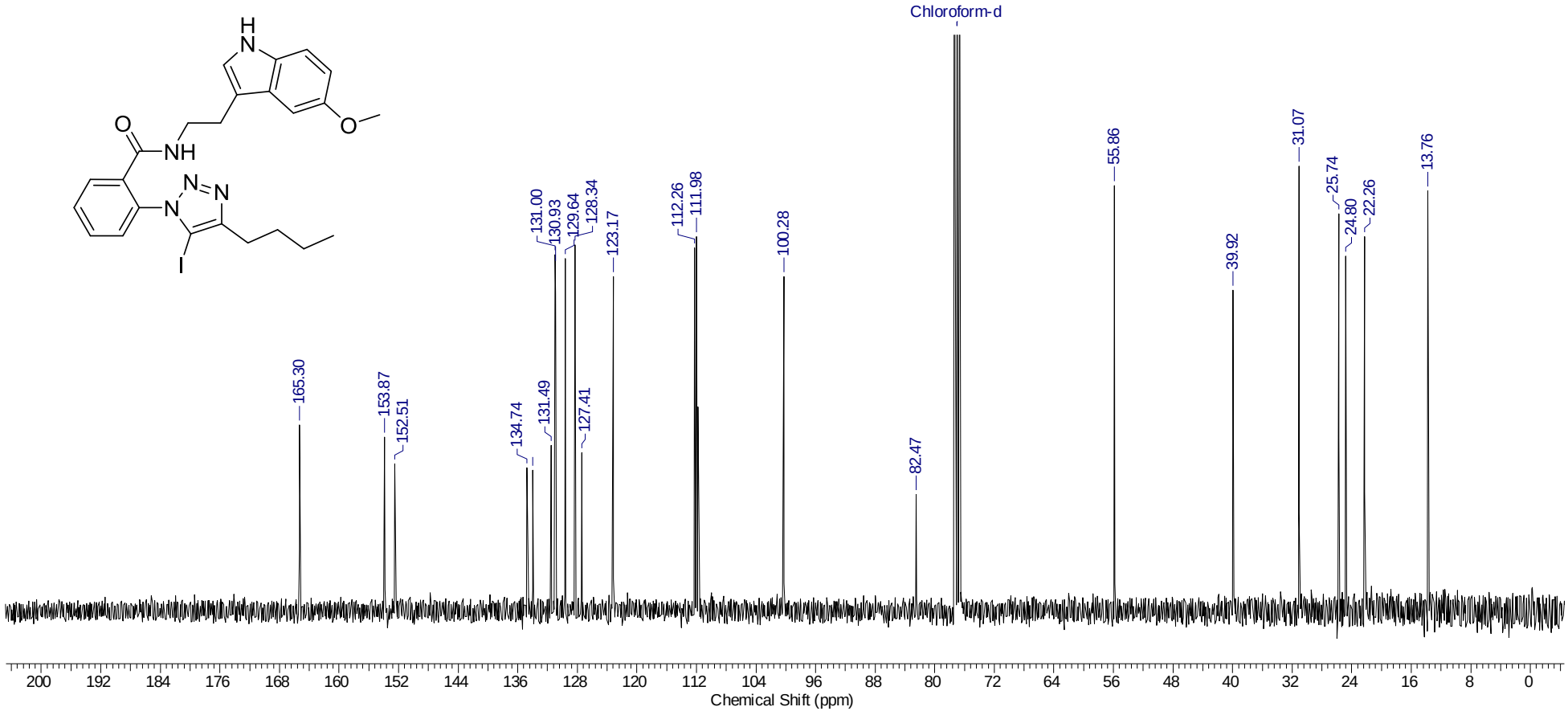
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]benzamide (1x)

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



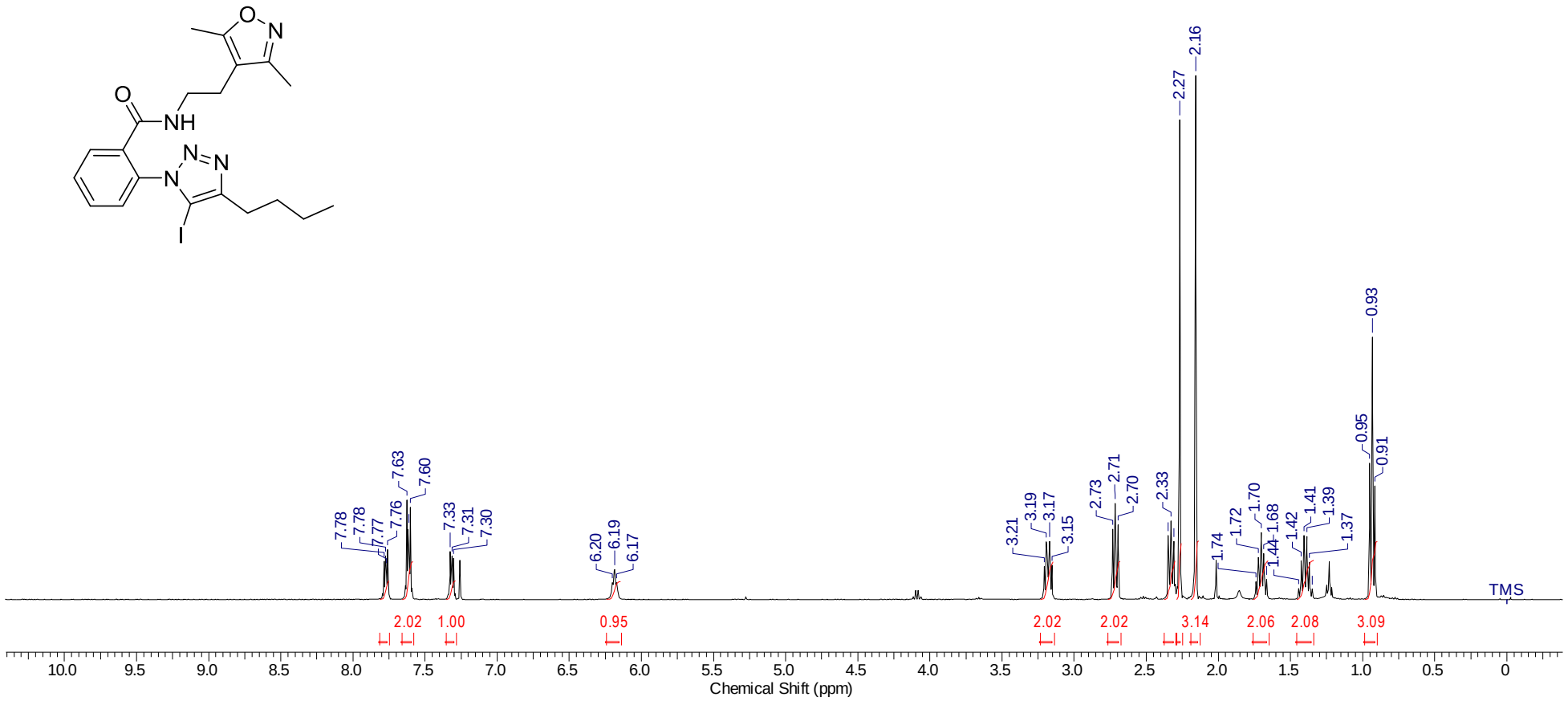
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]benzamide (1x)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



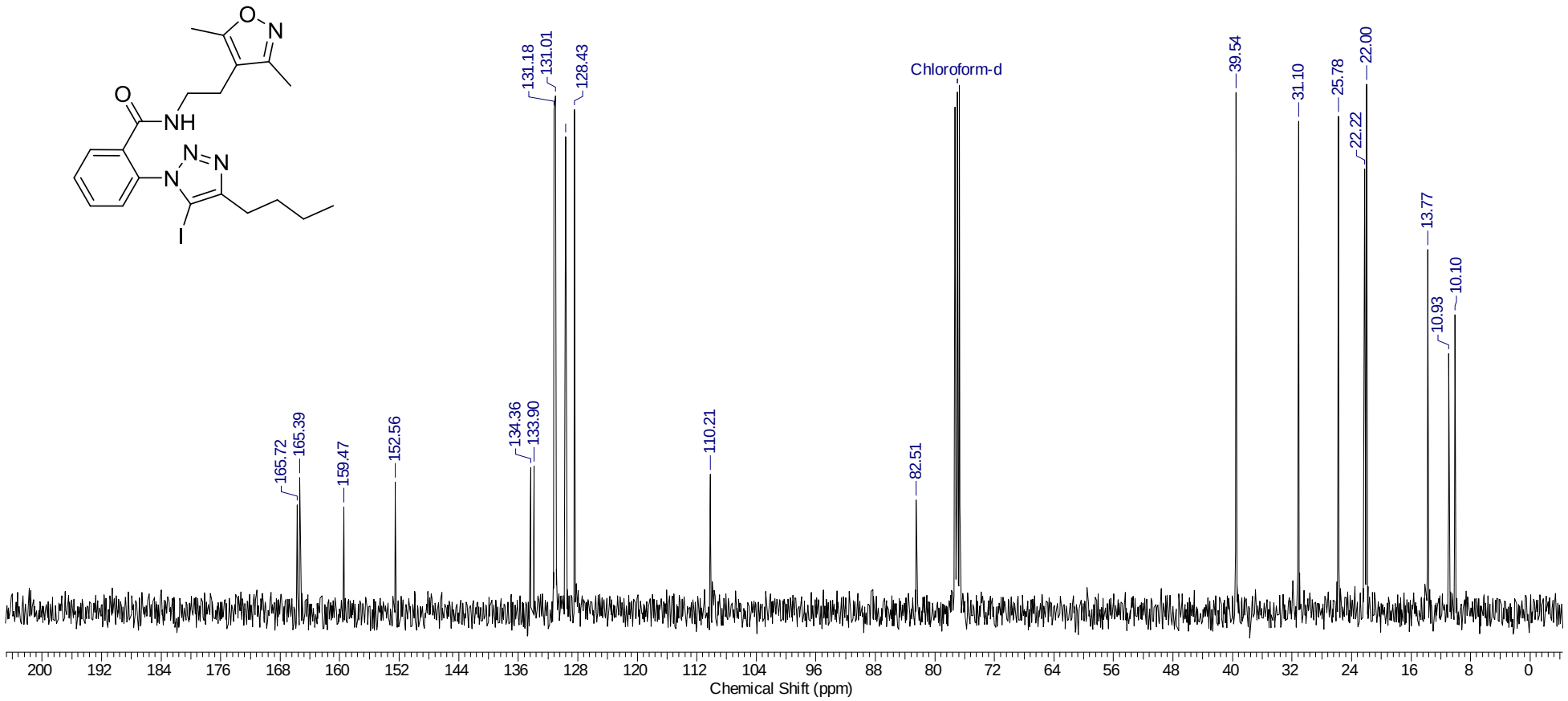
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[2-(3,5-dimethylisoxazol-4-yl)ethyl]benzamide (1y)

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



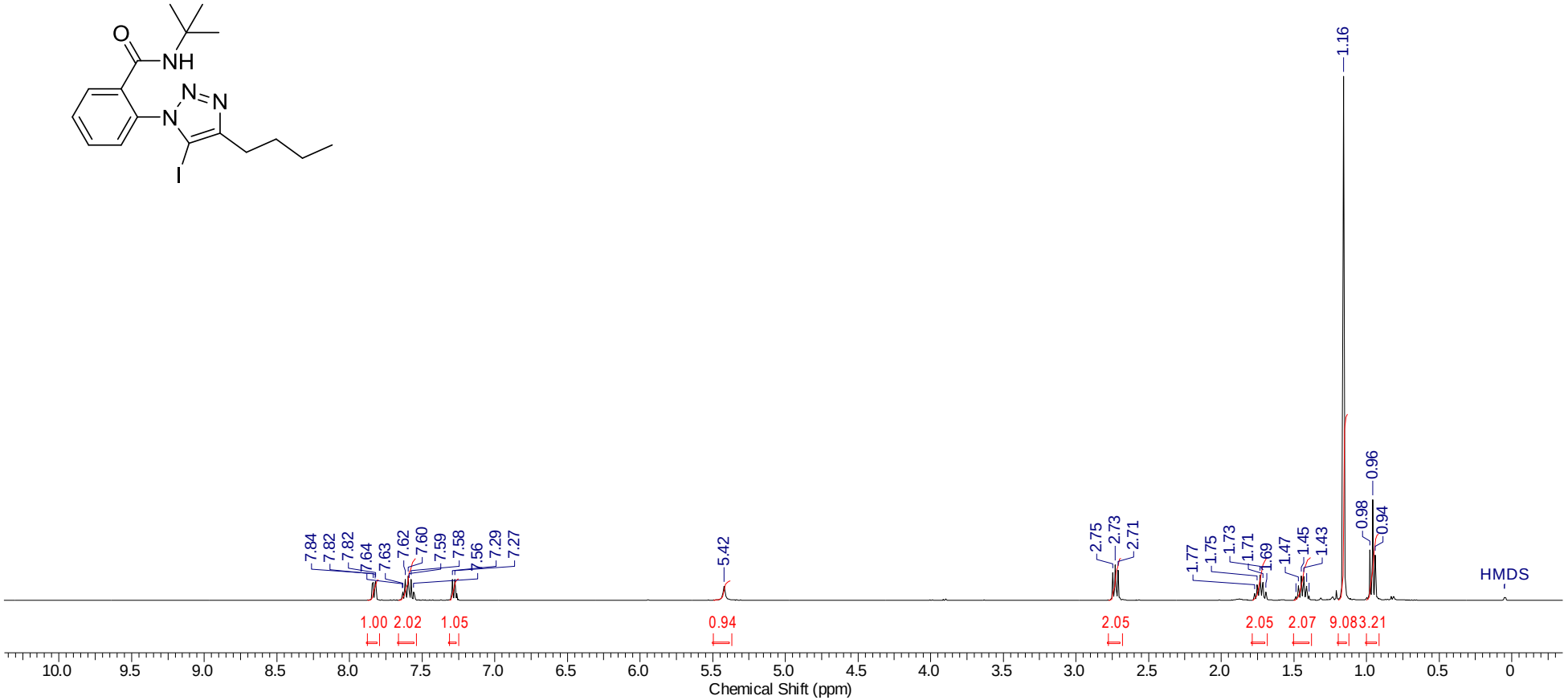
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[2-(3,5-dimethylisoxazol-4-yl)ethyl]benzamide (1y)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



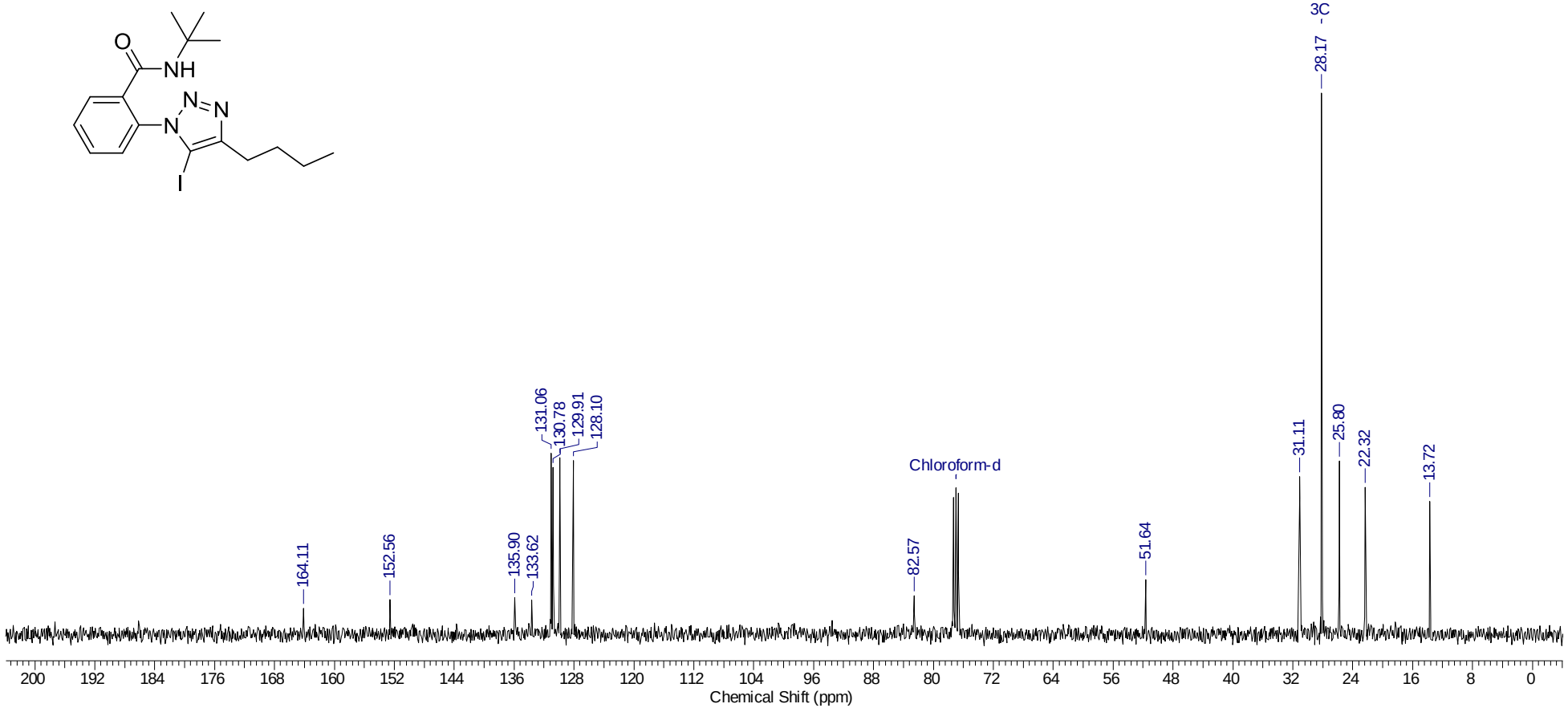
_N_-(_tert_-Butyl)-2-(4-butyl-5-iodo-1_H_-1,2,3-triazol-1-yl)benzamide (1z)

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



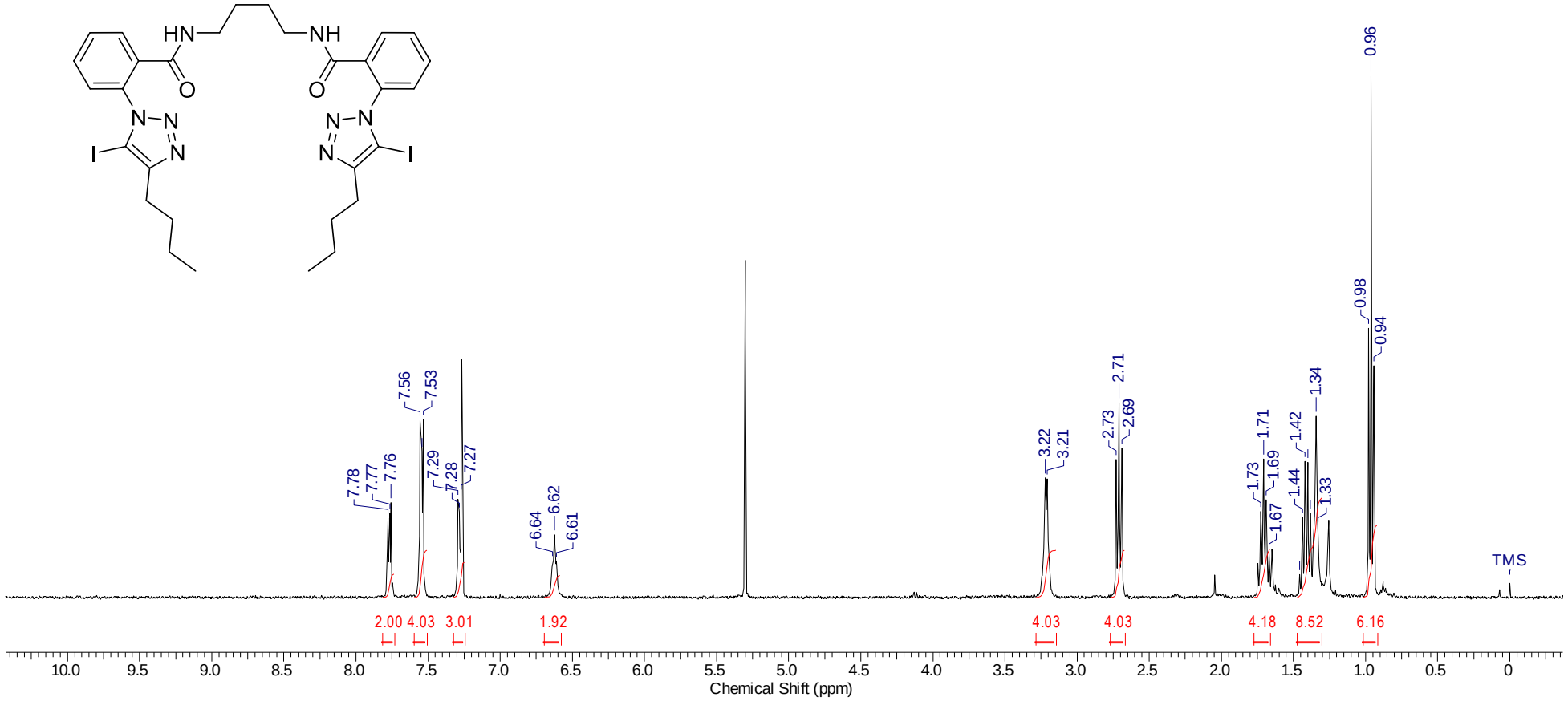
_N_-(_tert_-Butyl)-2-(4-butyl-5-iodo-1_H_-1,2,3-triazol-1-yl)benzamide (1z)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



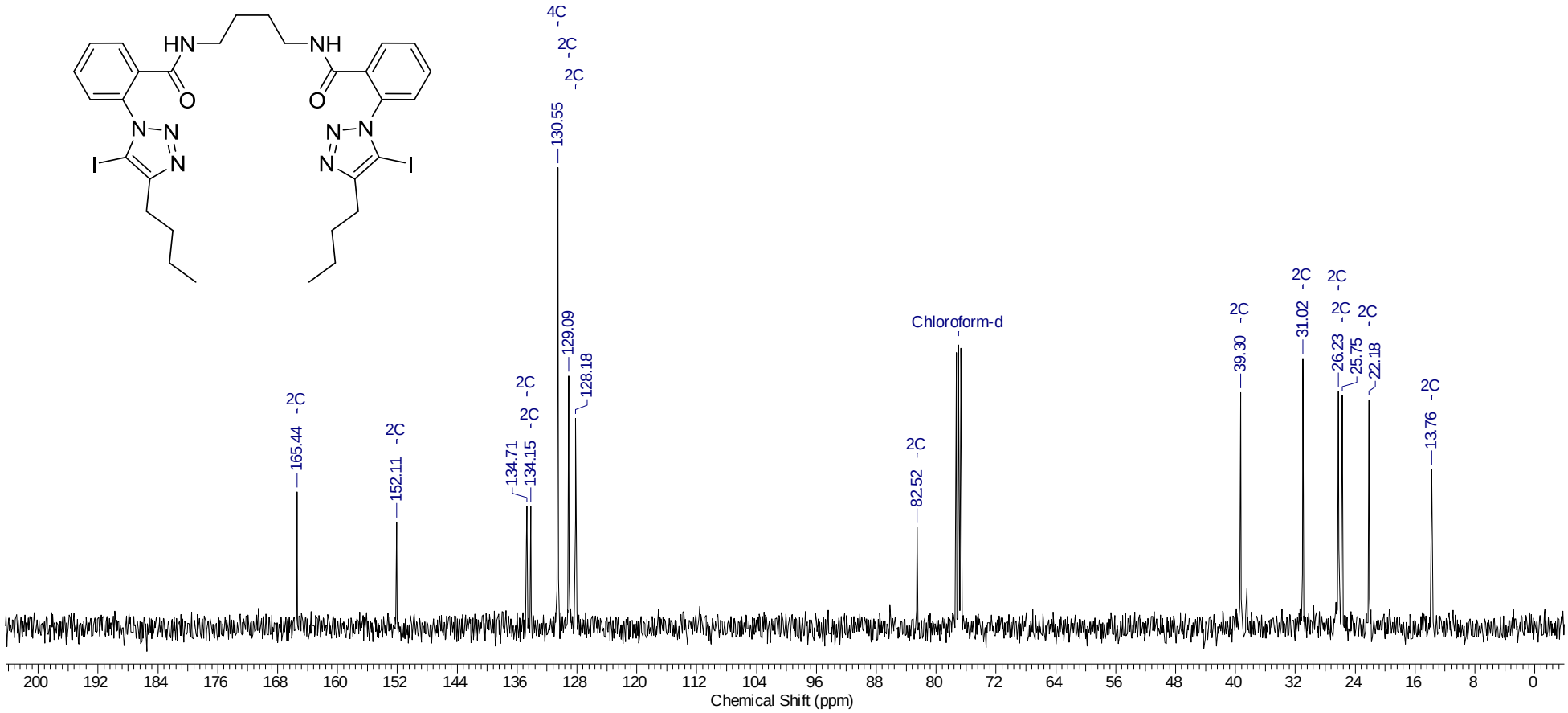
_N_,_N'_-Butane-1,4-diylbis[2-(4-butyl-5-iodo-1_H_-1,2,3-triazol-1-yl)benzamide] (1aa)

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



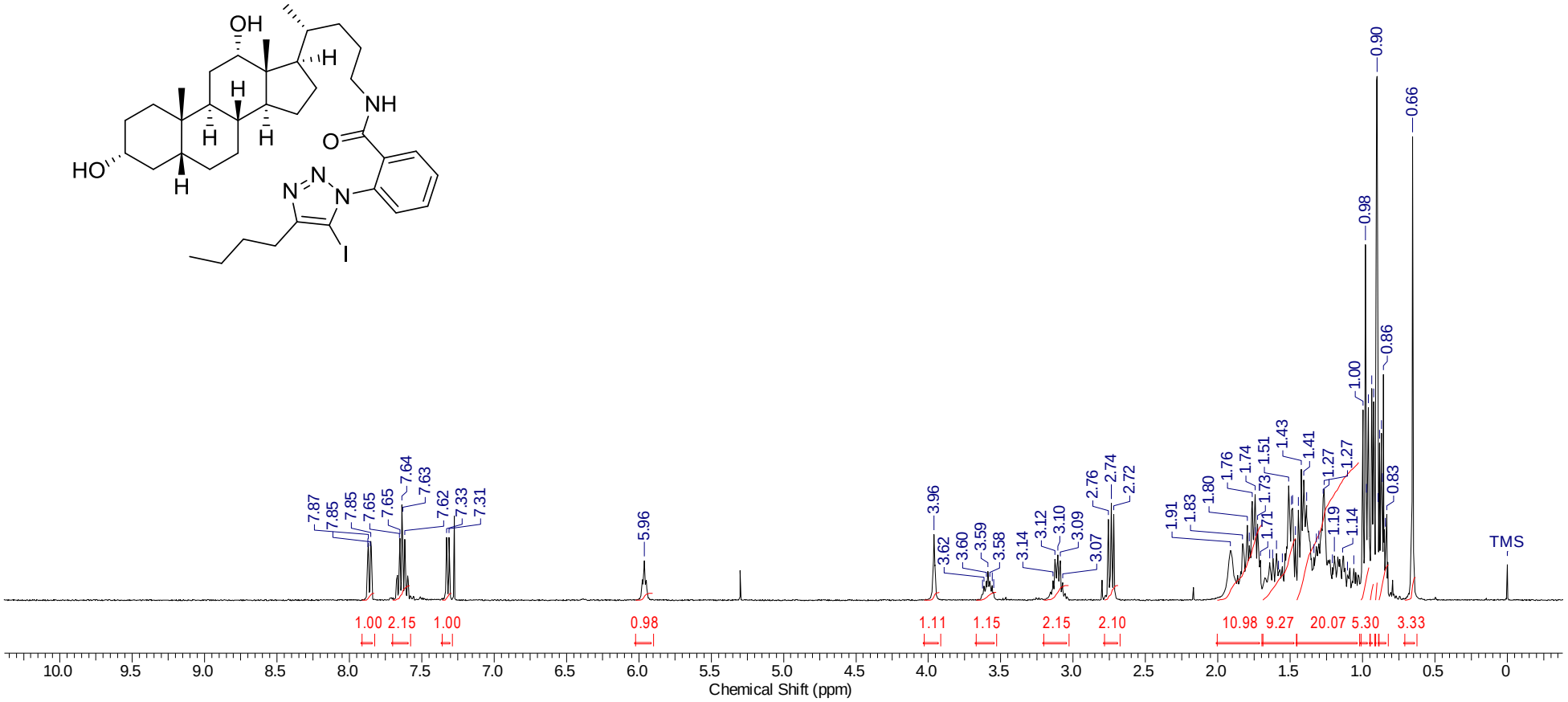
_N_,_N'_-Butane-1,4-diylbis[2-(4-butyl-5-iodo-1_H_-1,2,3-triazol-1-yl)benzamide] (1aa)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



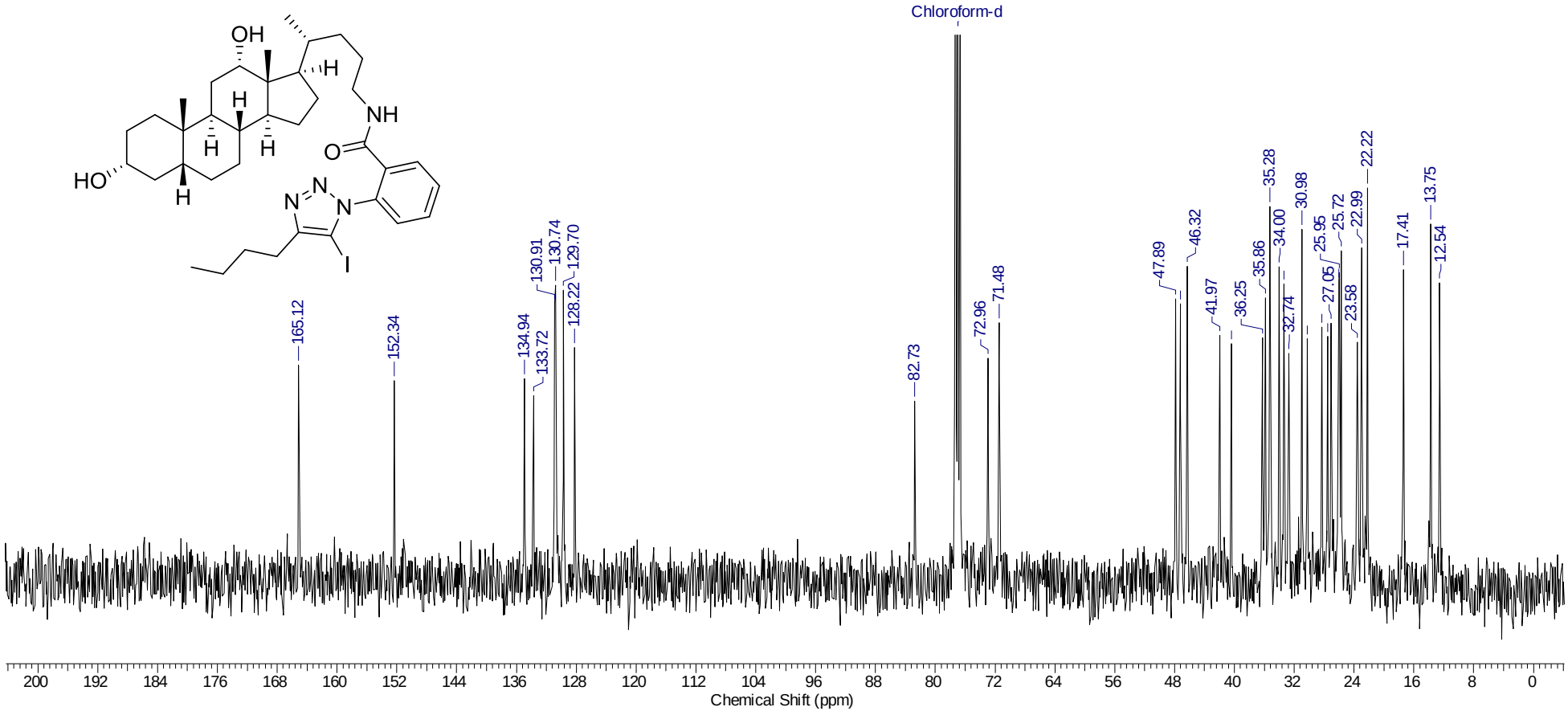
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl]benzamide (1ab)

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



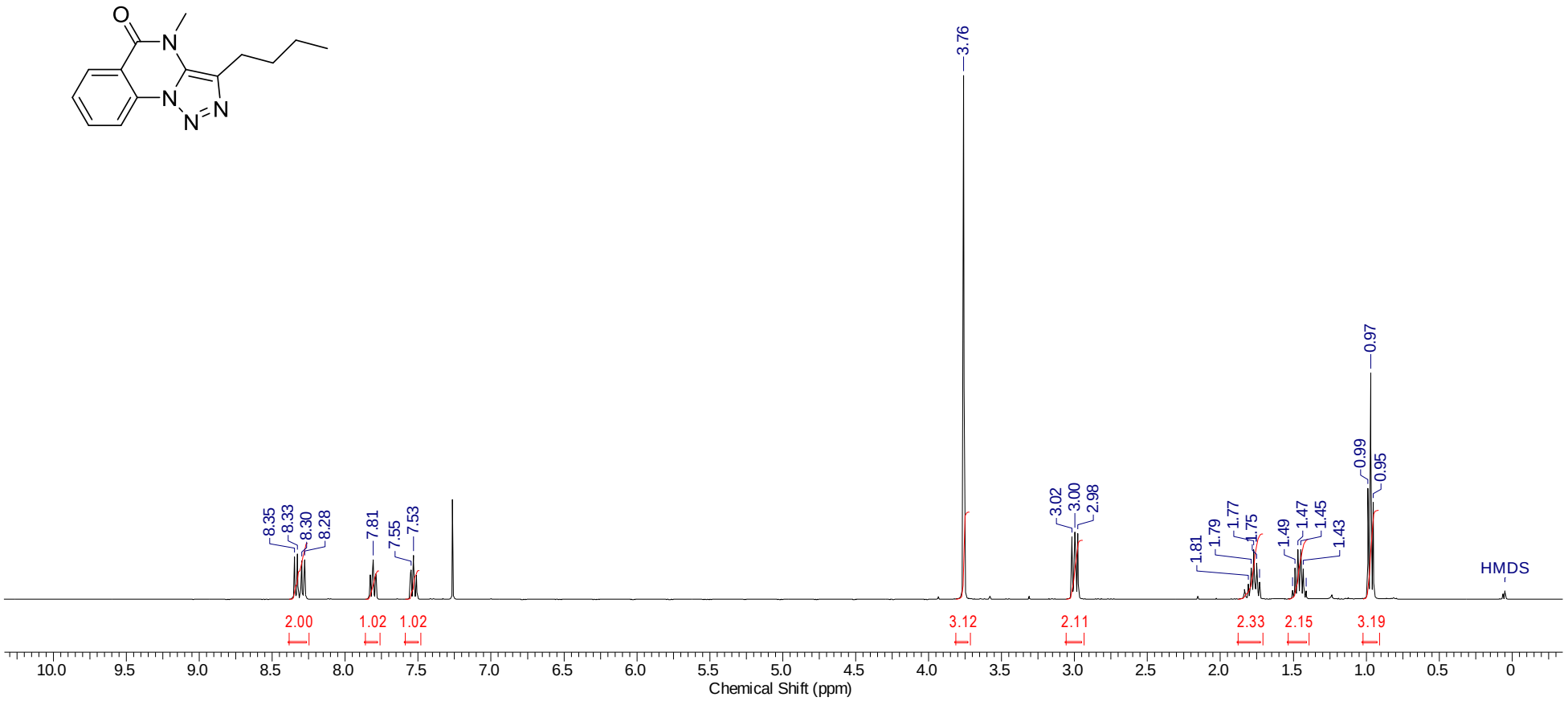
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-*N*-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl]benzamide (1ab)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



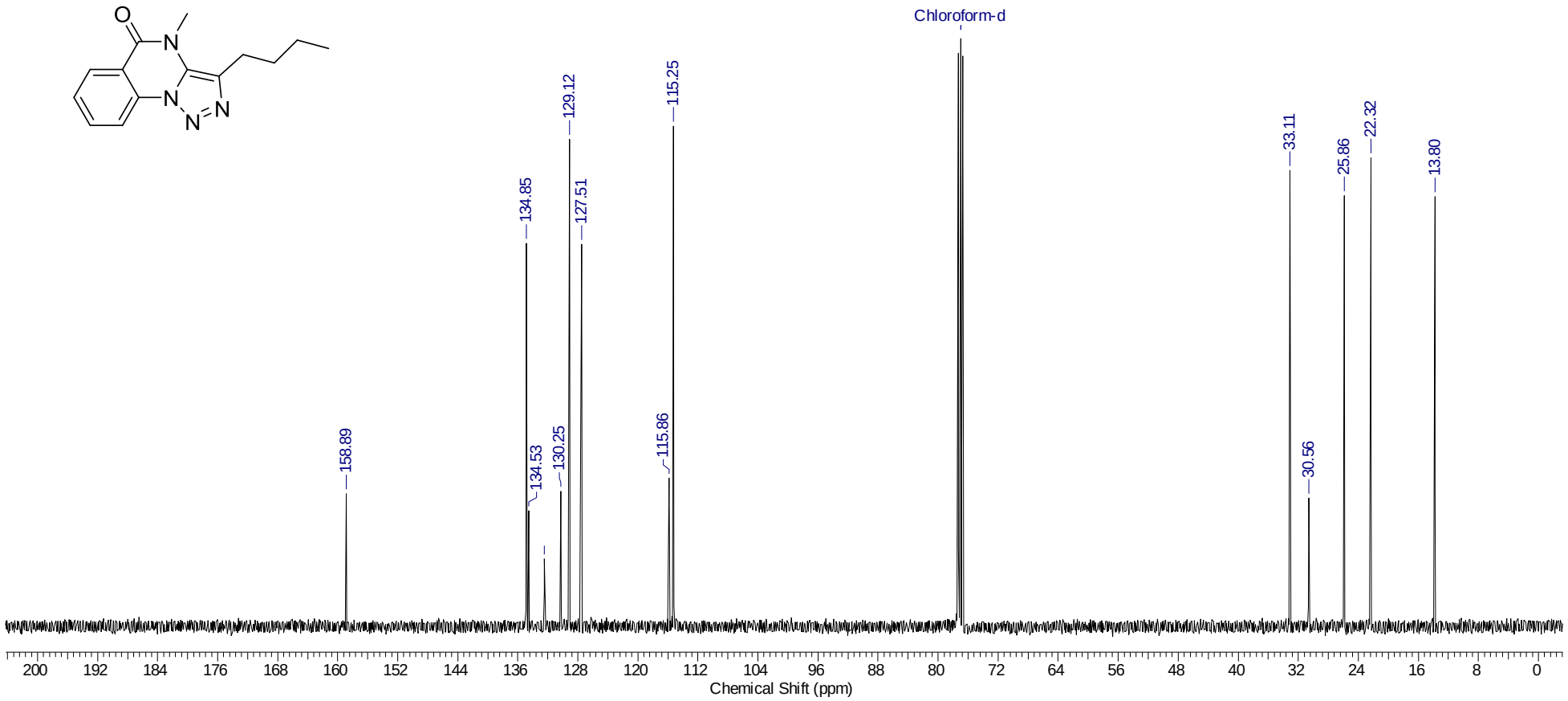
3-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2a)

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



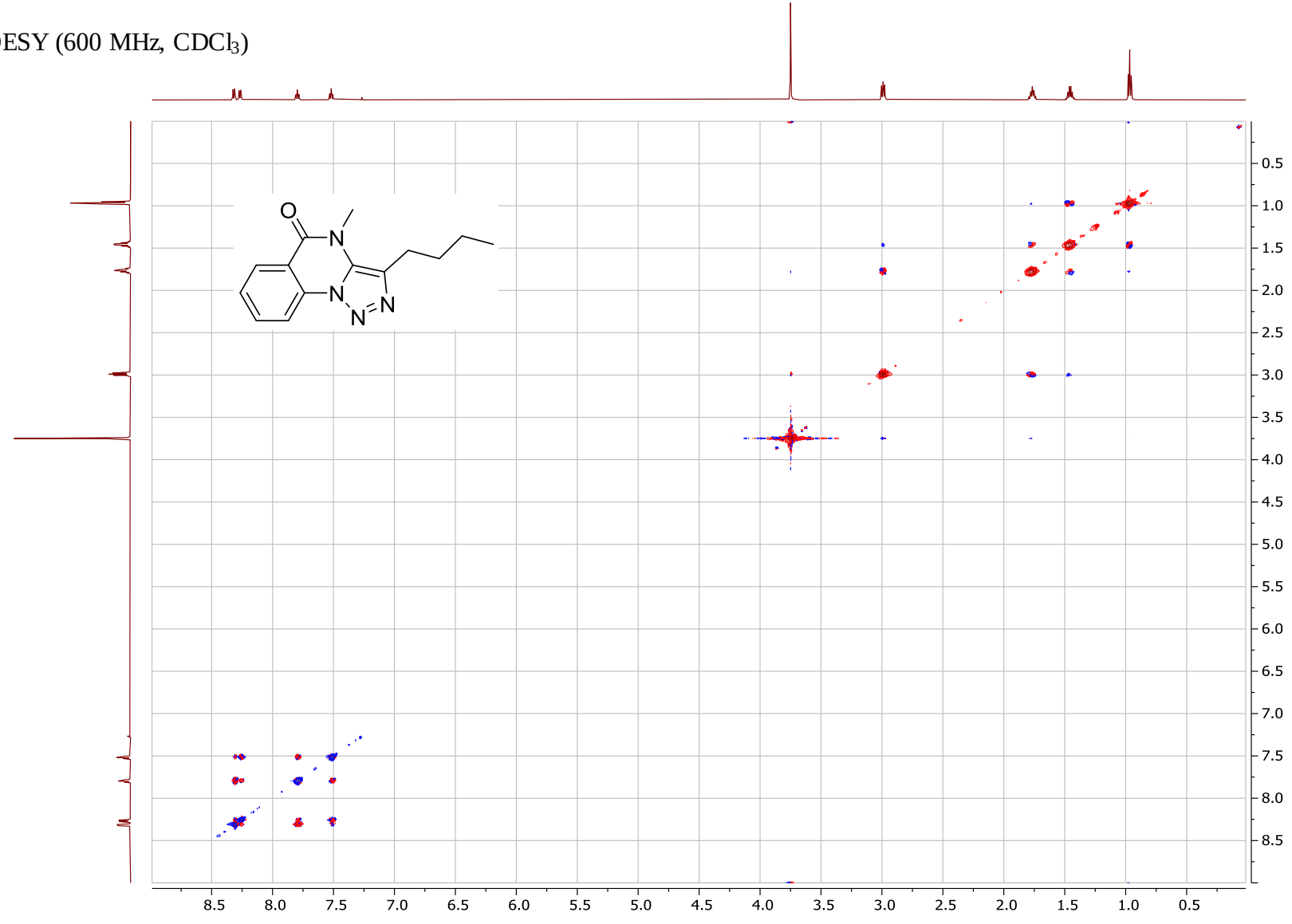
3-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2a)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



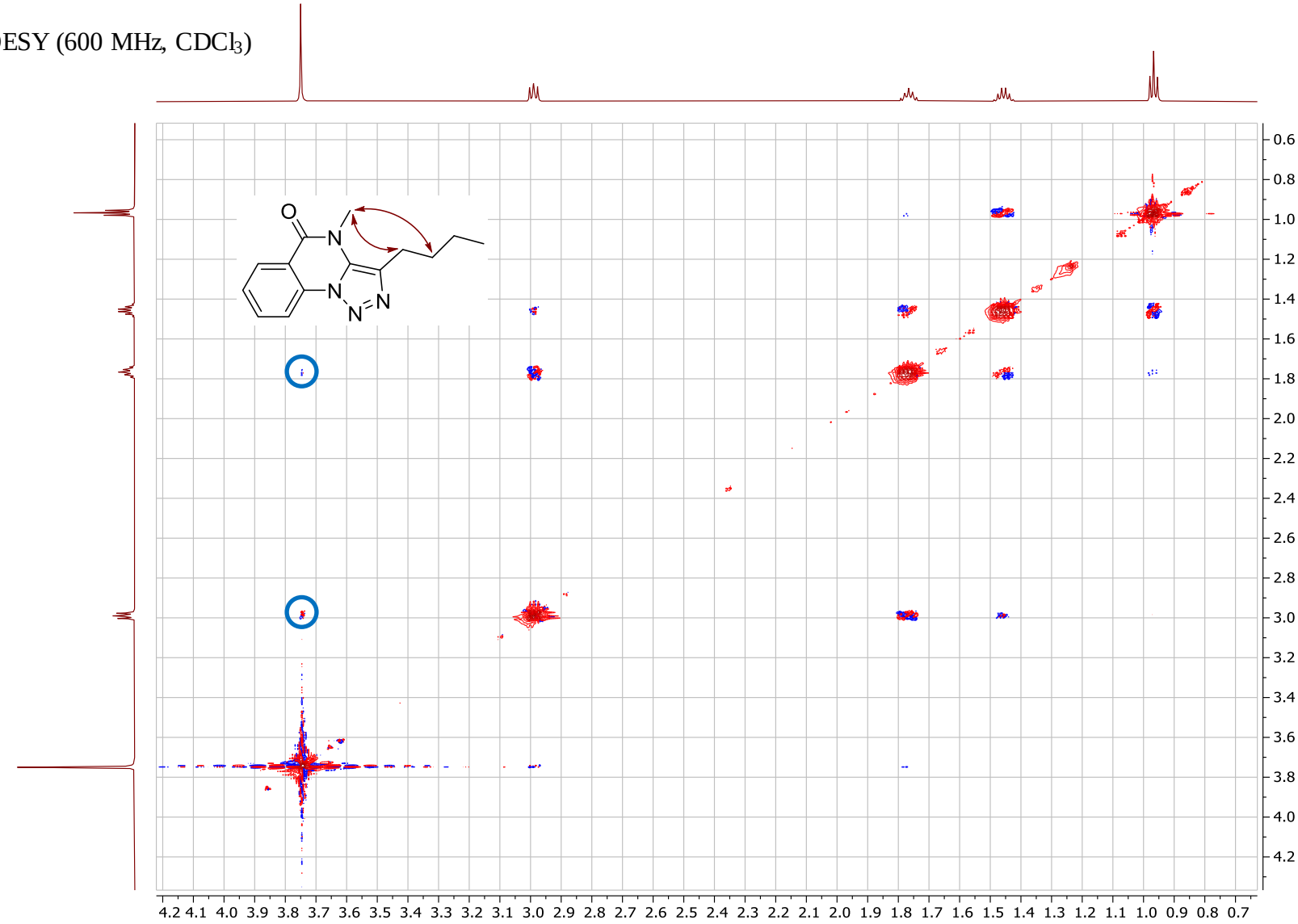
3-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2a)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)



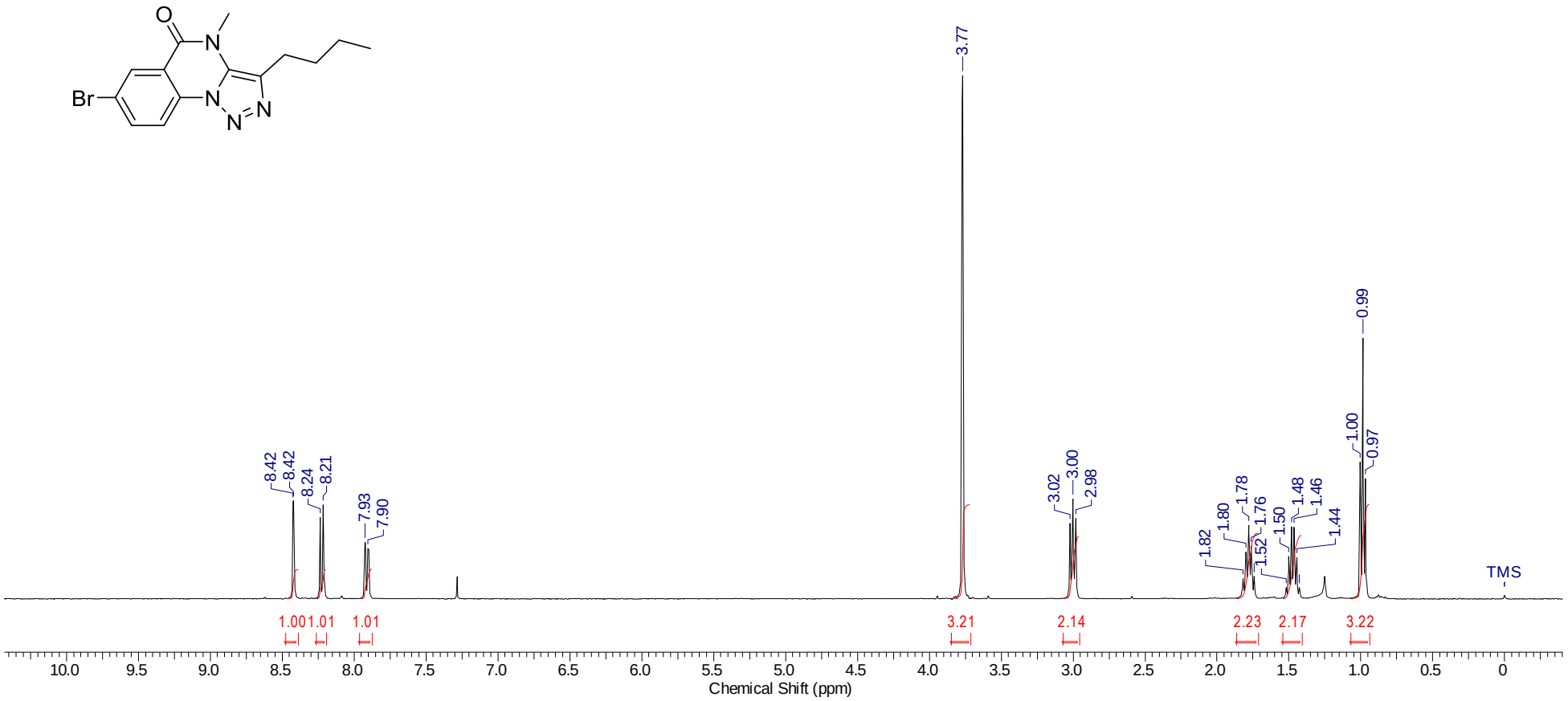
3-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2a)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)



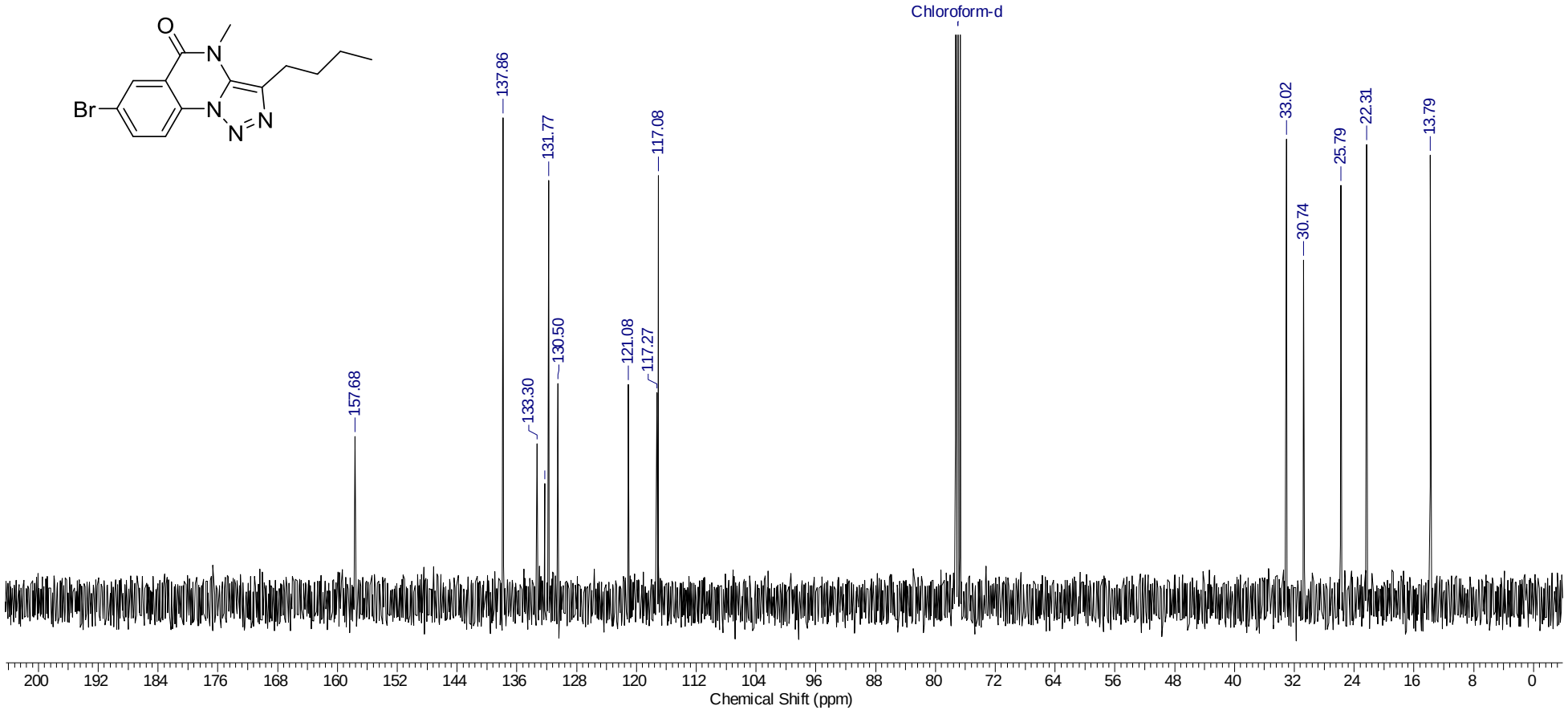
3-Butyl-7-bromo-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2b)

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



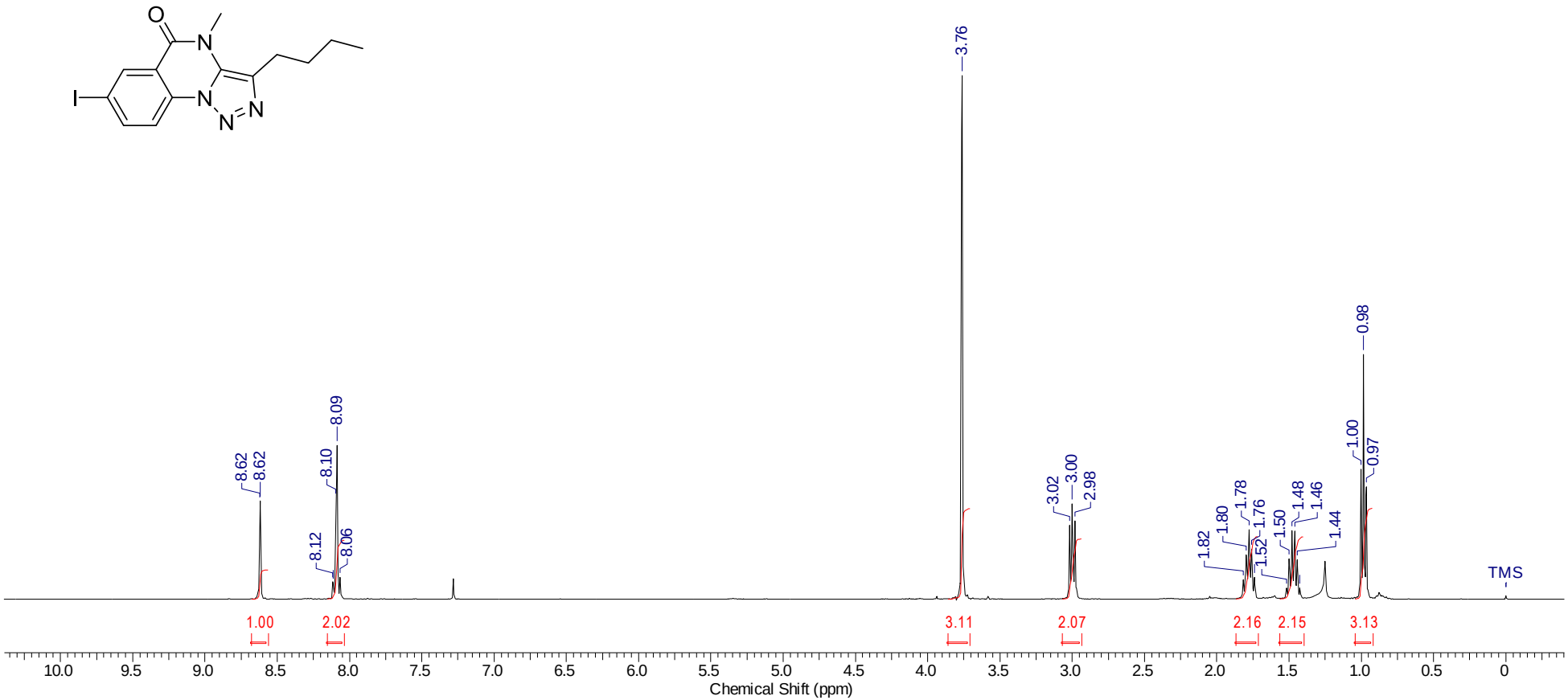
3-Butyl-7-bromo-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2b)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



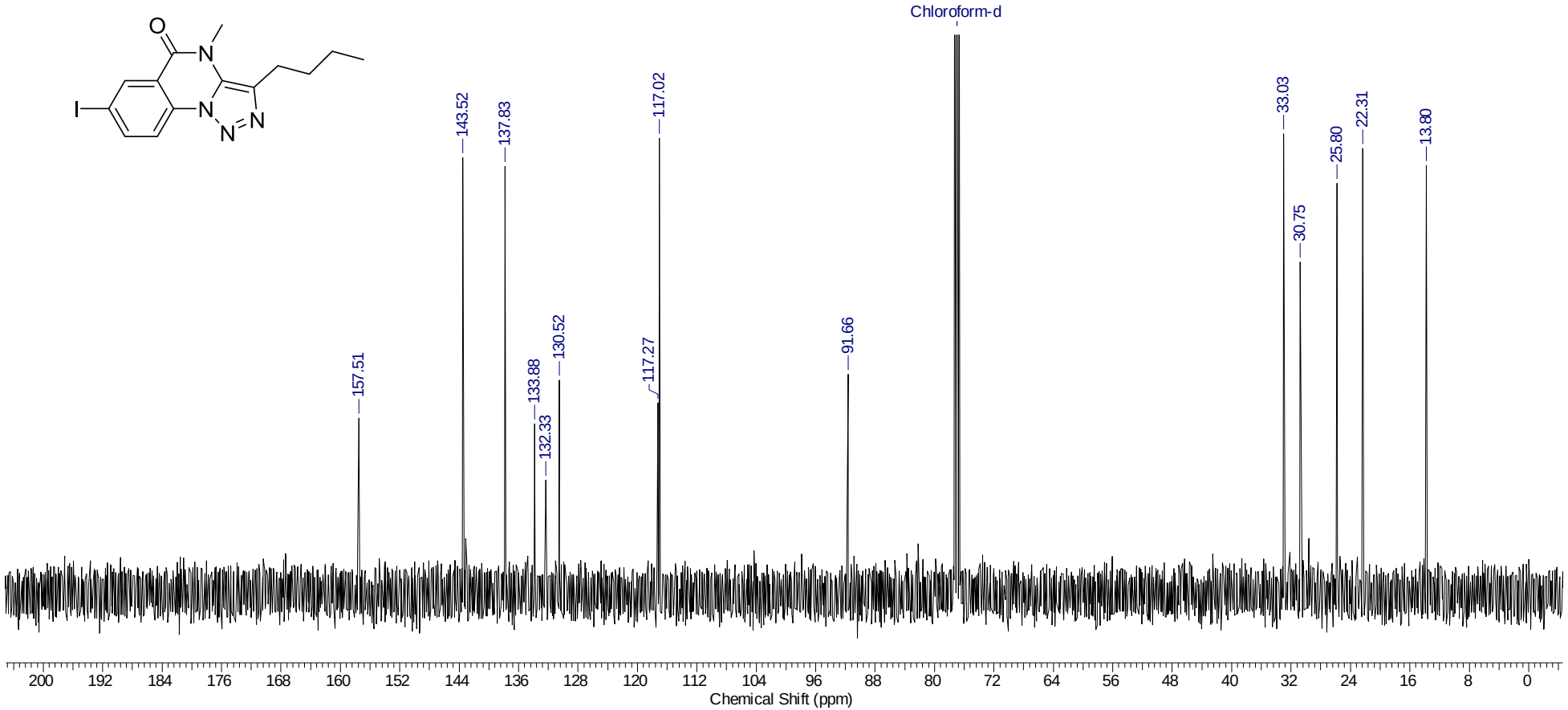
3-Butyl-7-iodo-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2c)

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



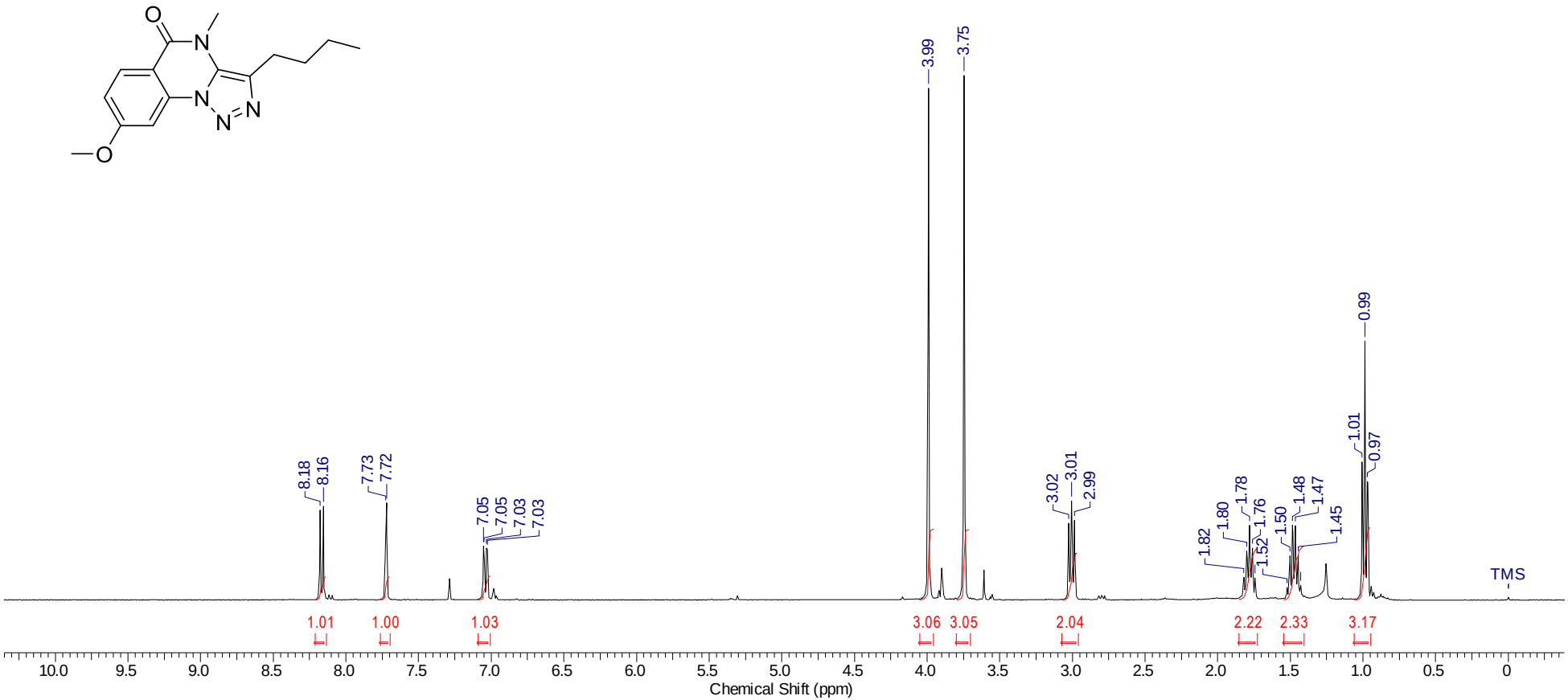
3-Butyl-7-iodo-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2c)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



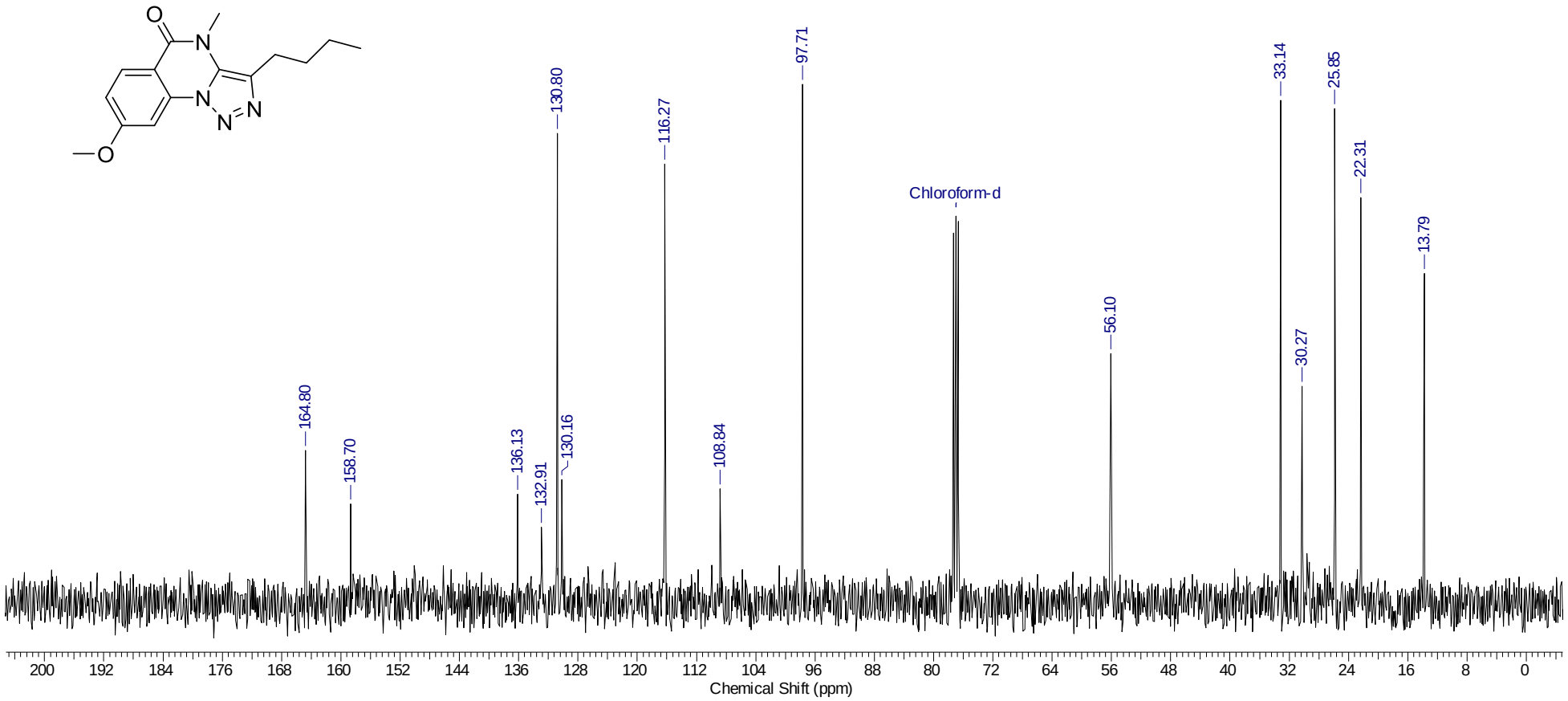
3-Butyl-8-methoxy-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2d)

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



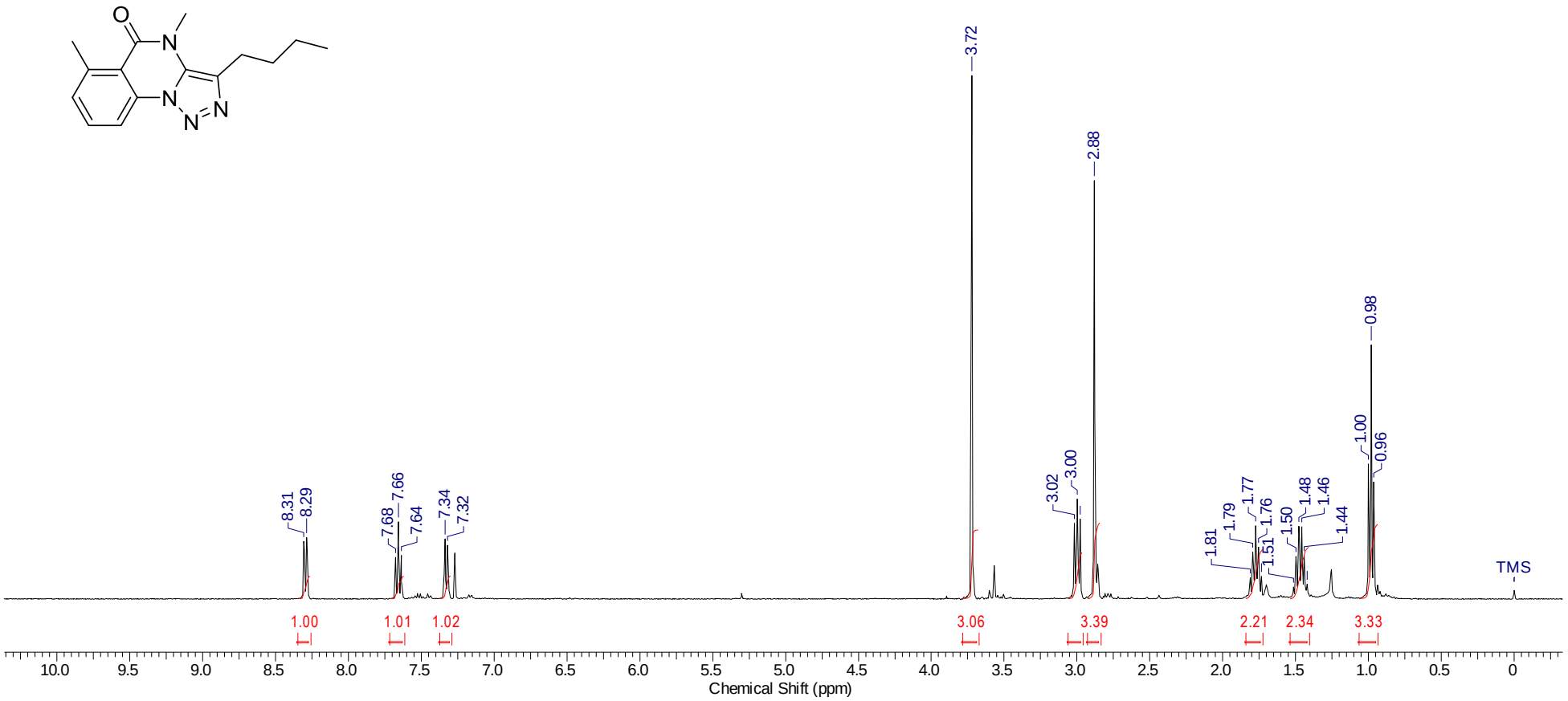
3-Butyl-8-methoxy-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2d)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



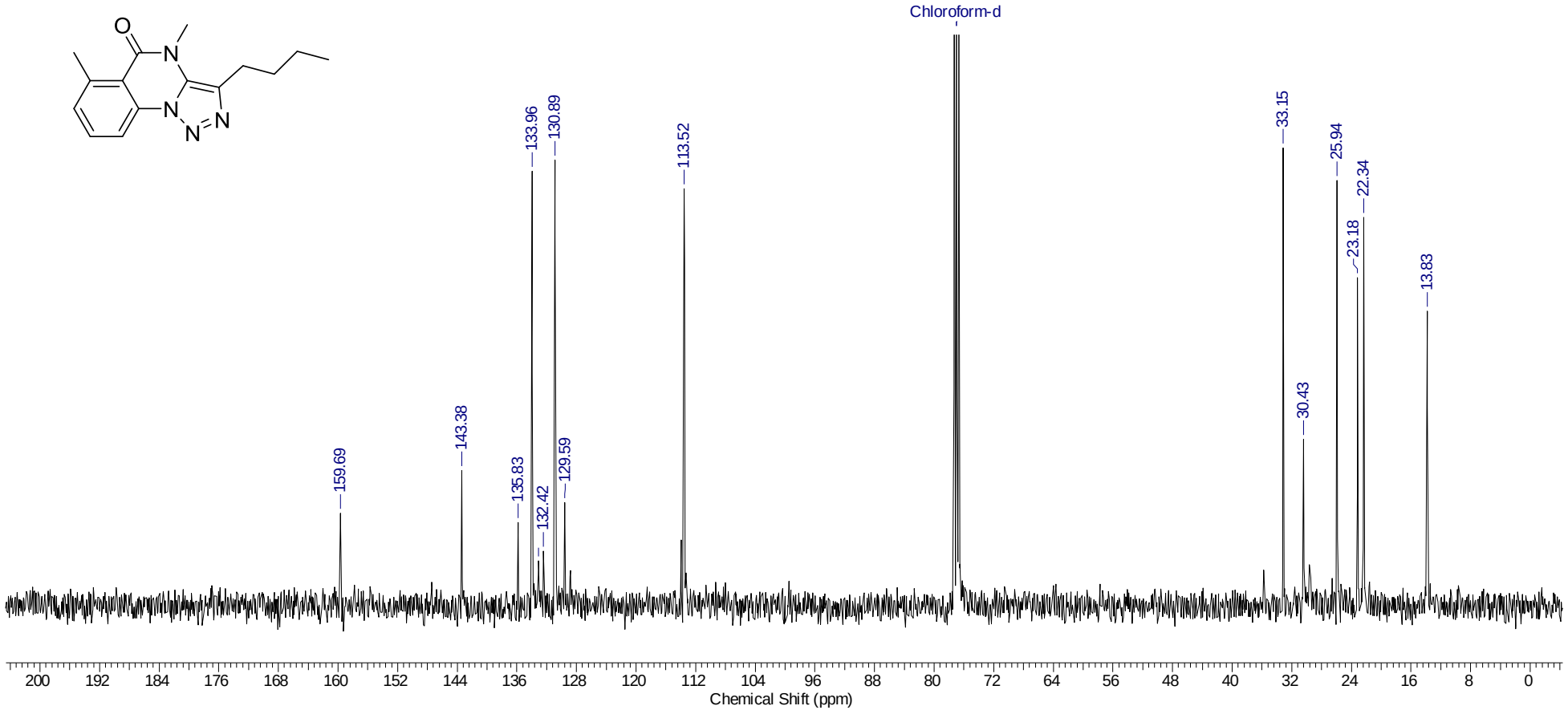
3-Butyl-4,6-dimethyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2e)

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



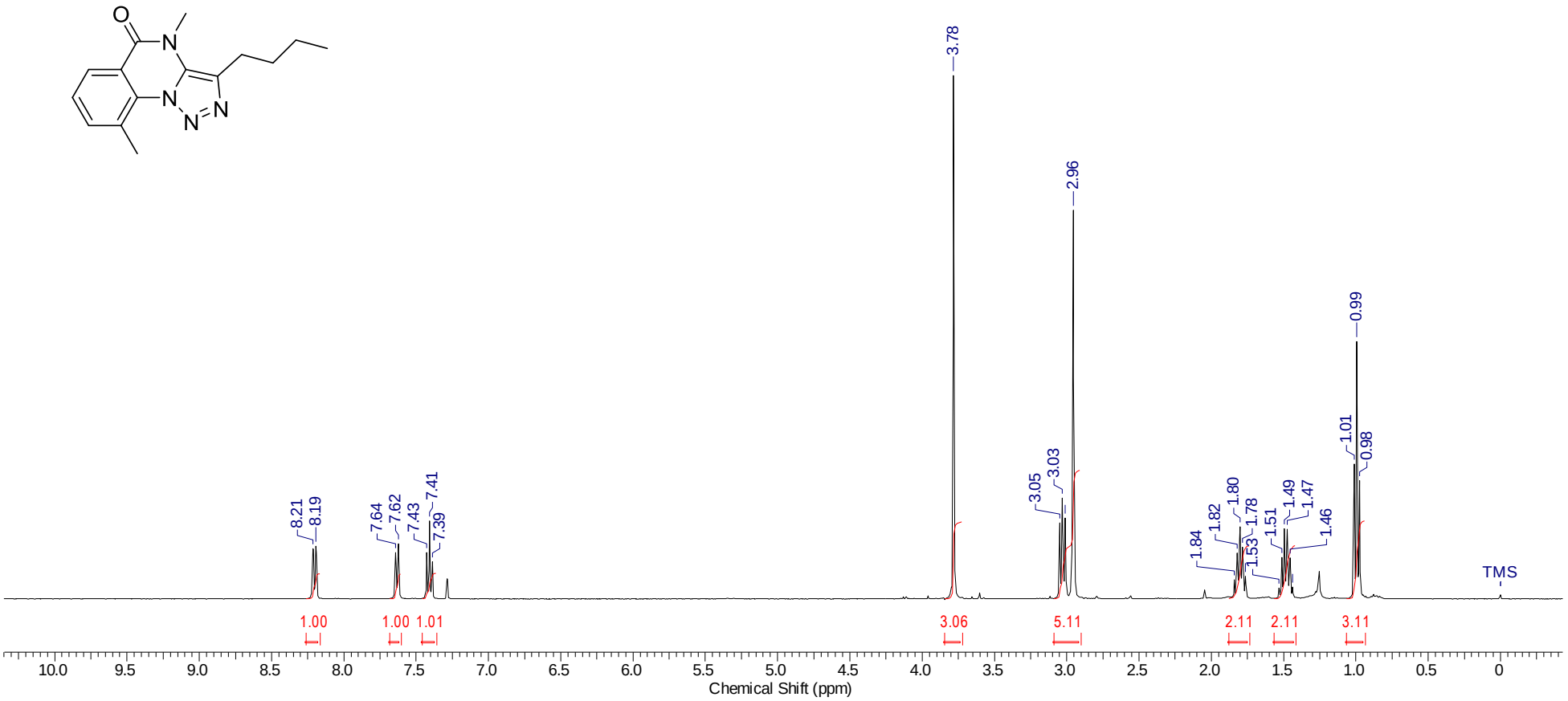
3-Butyl-4,6-dimethyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2e)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



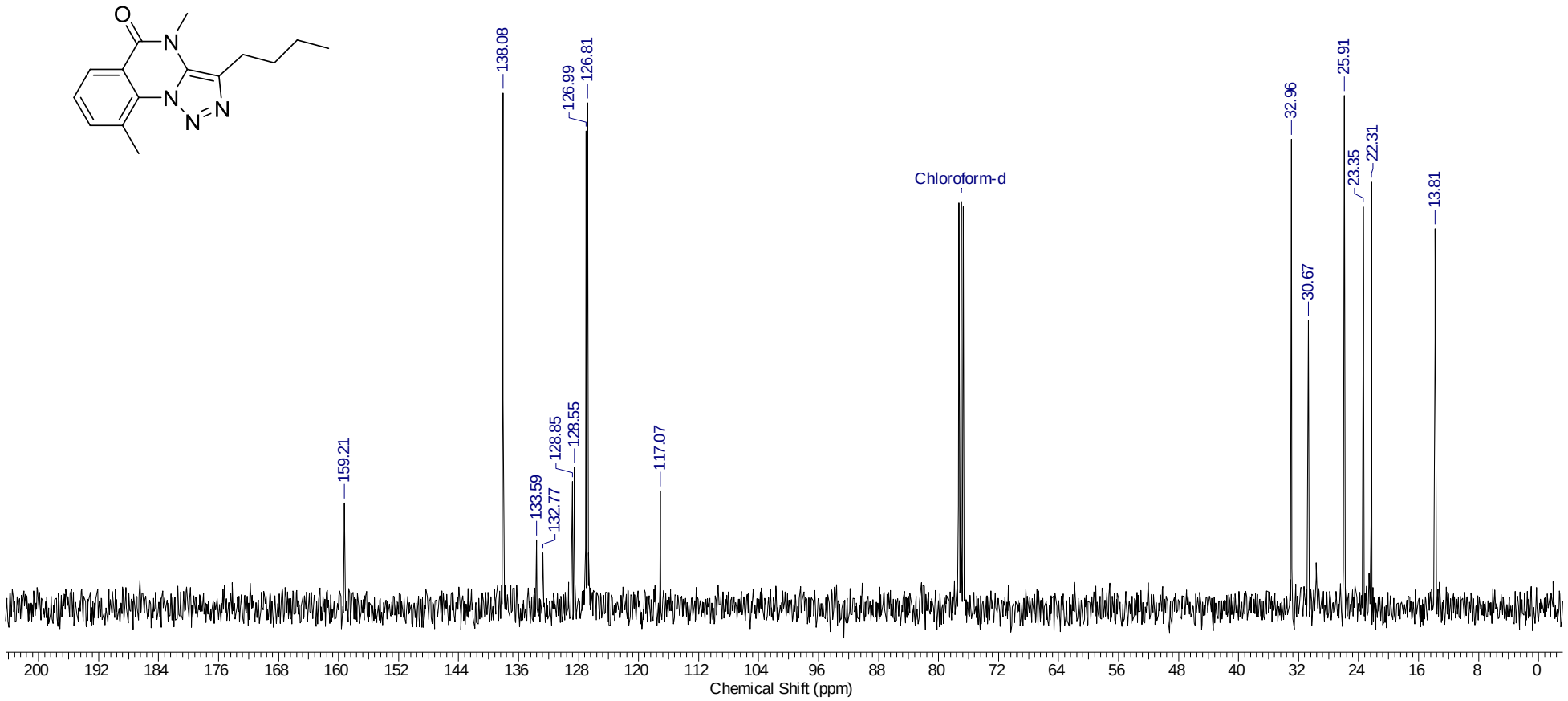
3-Butyl-4,9-dimethyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2f)

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



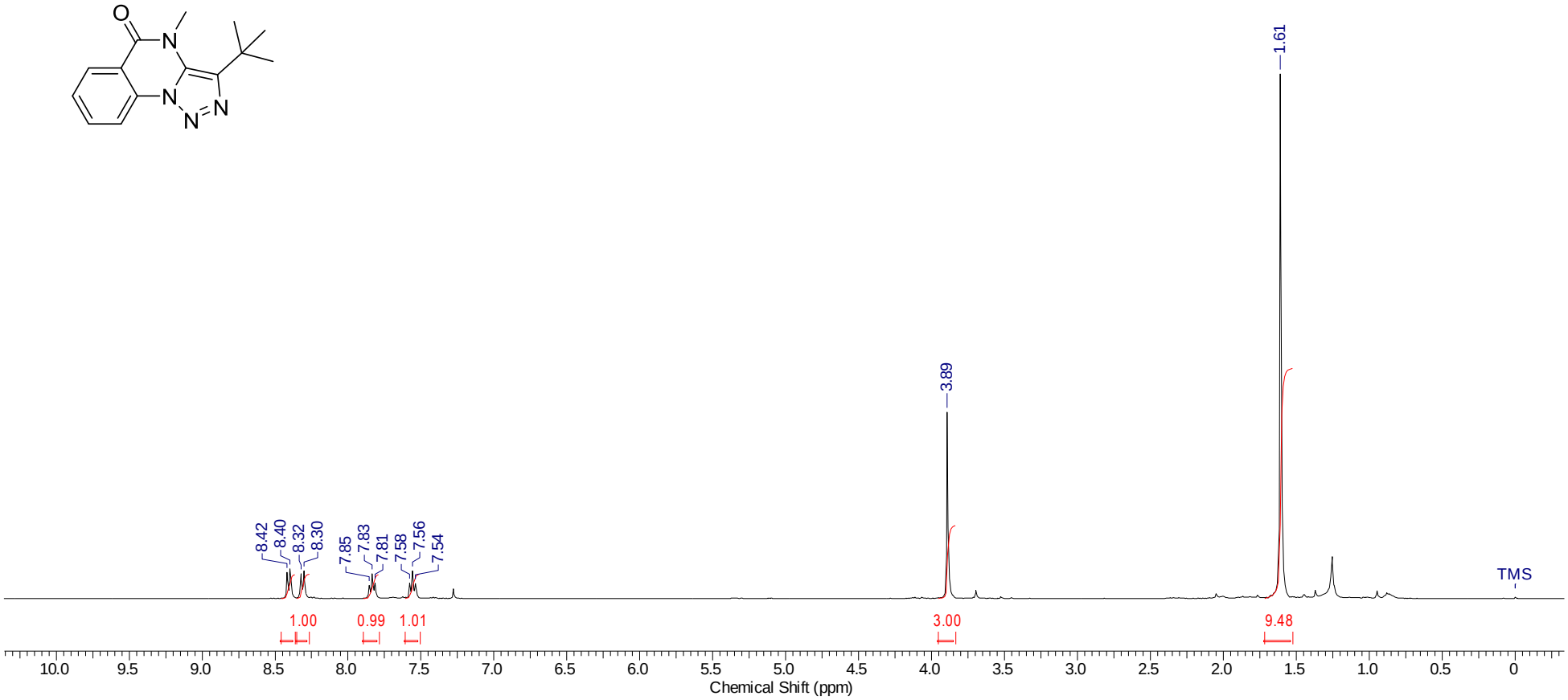
3-Butyl-4,9-dimethyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2f)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



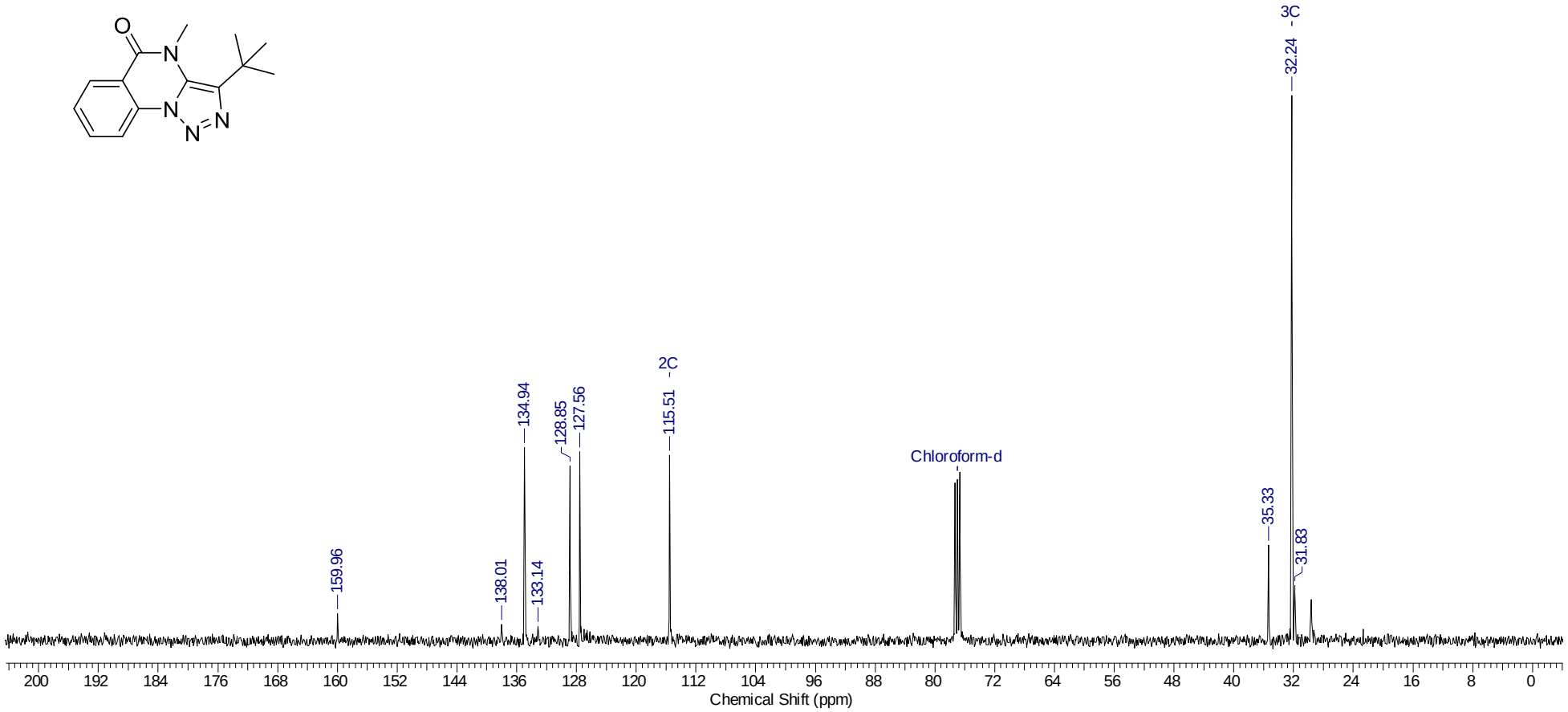
3-*tert*-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2g)

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



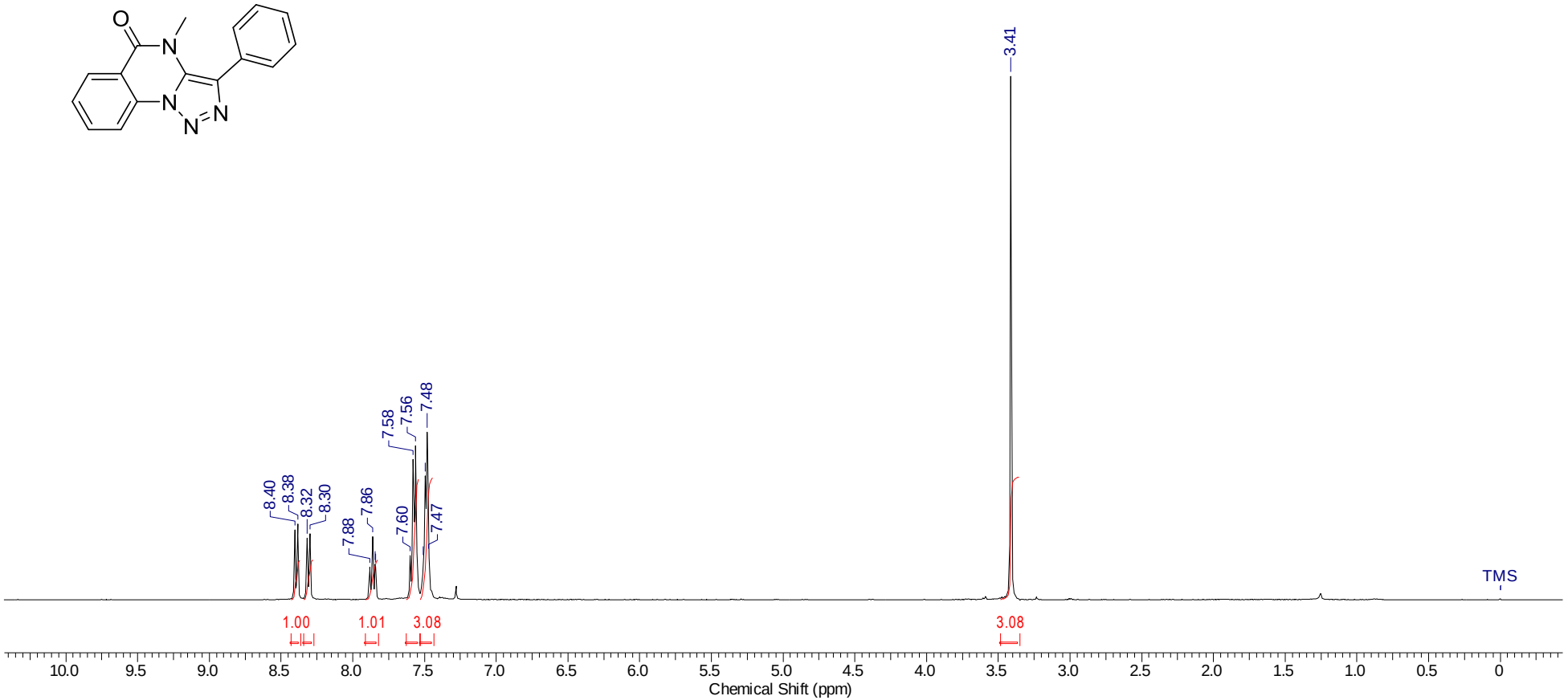
3-*tert*-Butyl-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2g)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



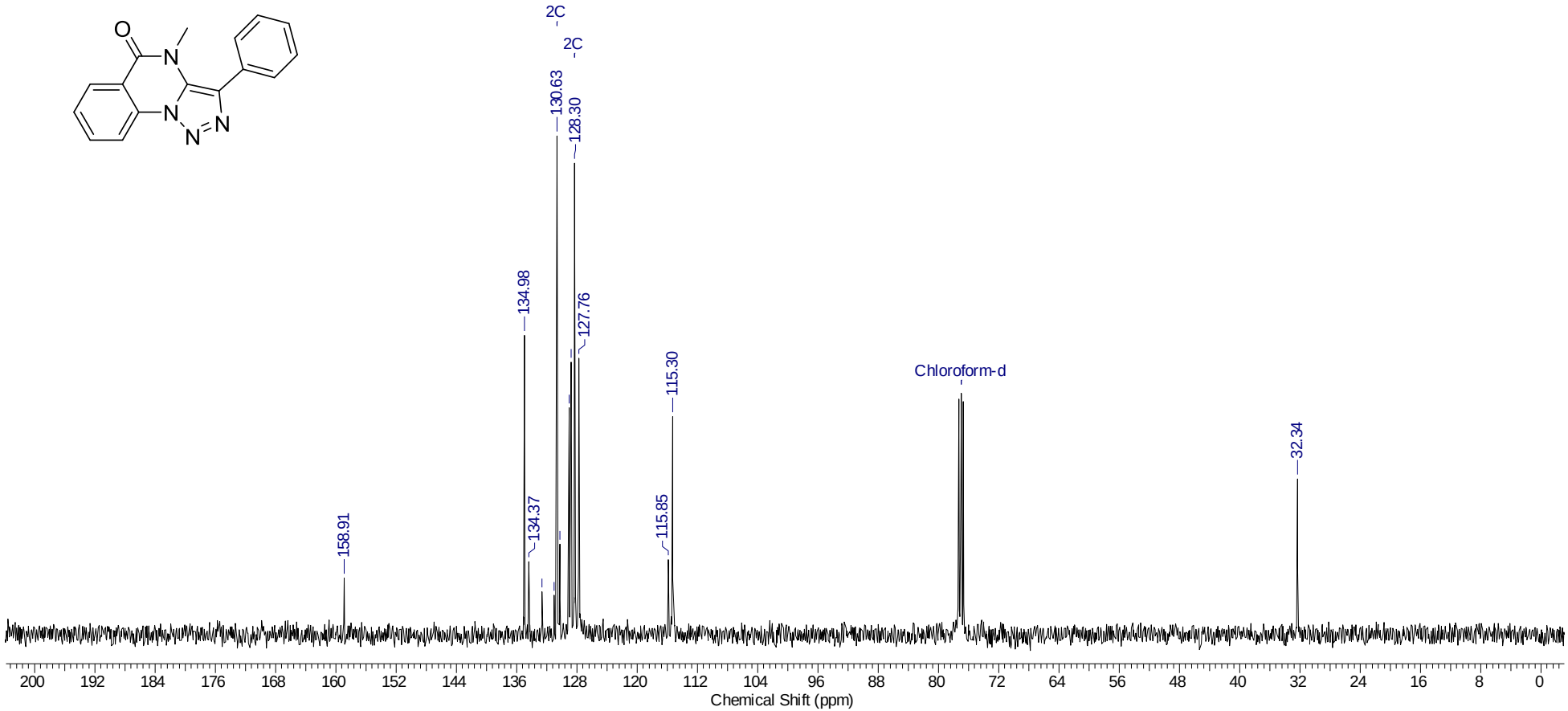
4-Methyl-3-phenyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2h)

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



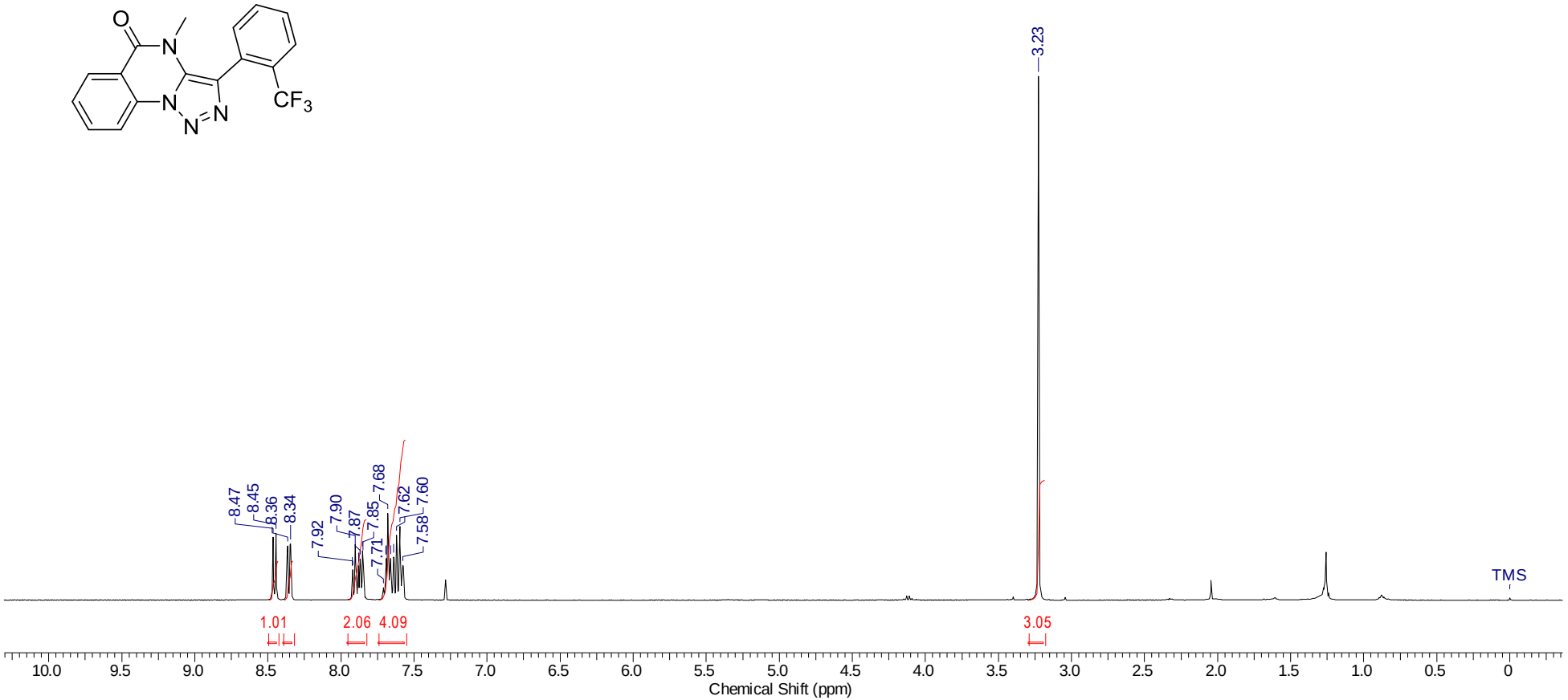
4-Methyl-3-phenyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2h)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



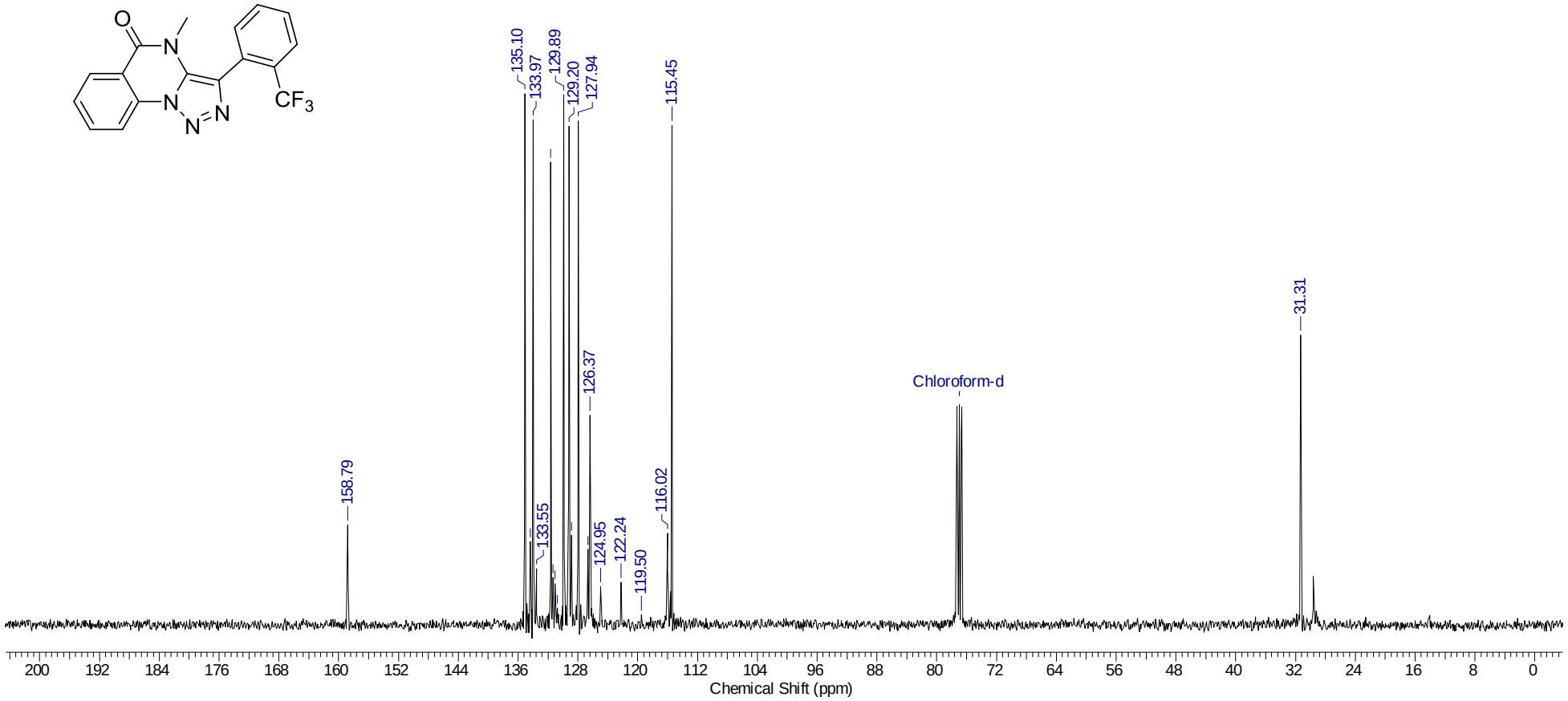
4-Methyl-3-[2-(trifluoromethyl)phenyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2i)

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



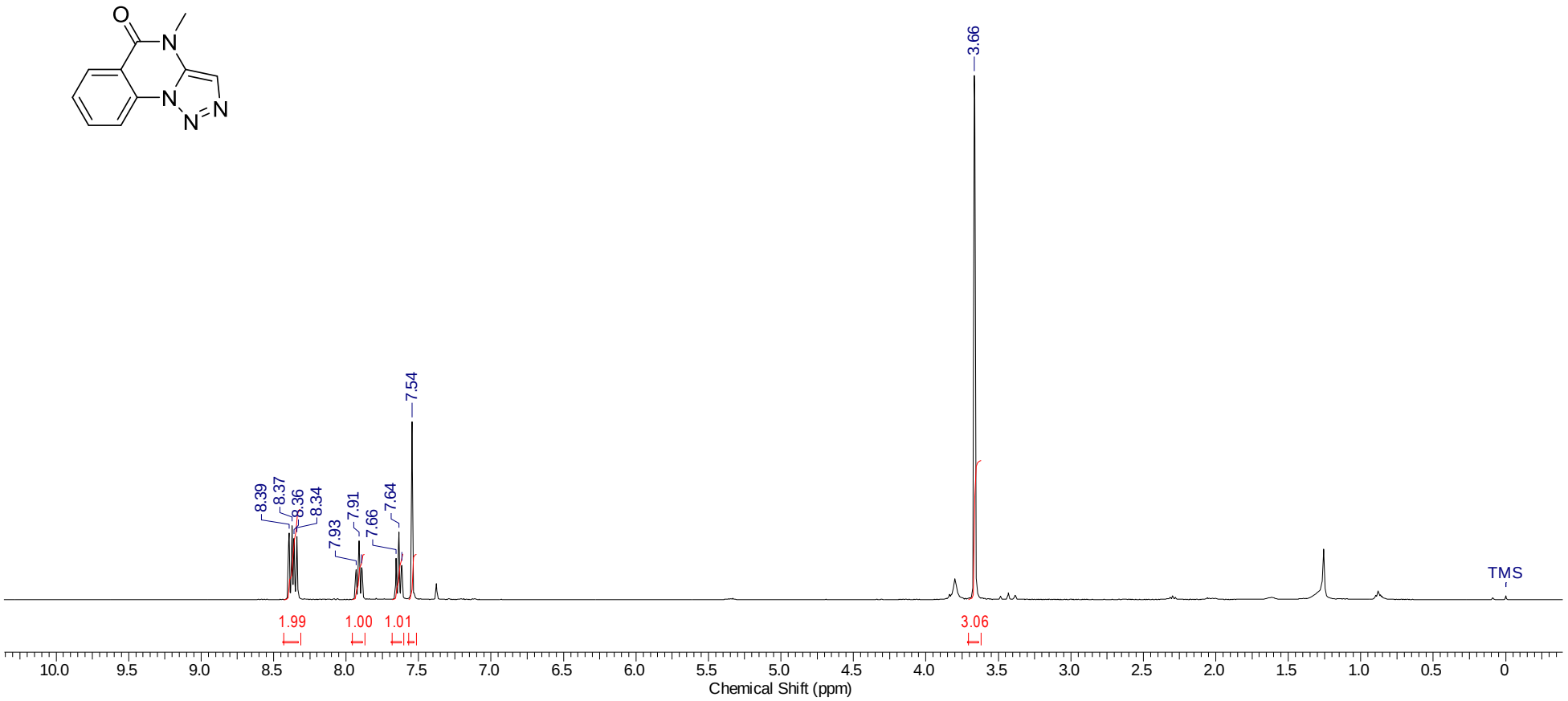
4-Methyl-3-[2-(trifluoromethyl)phenyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2i)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



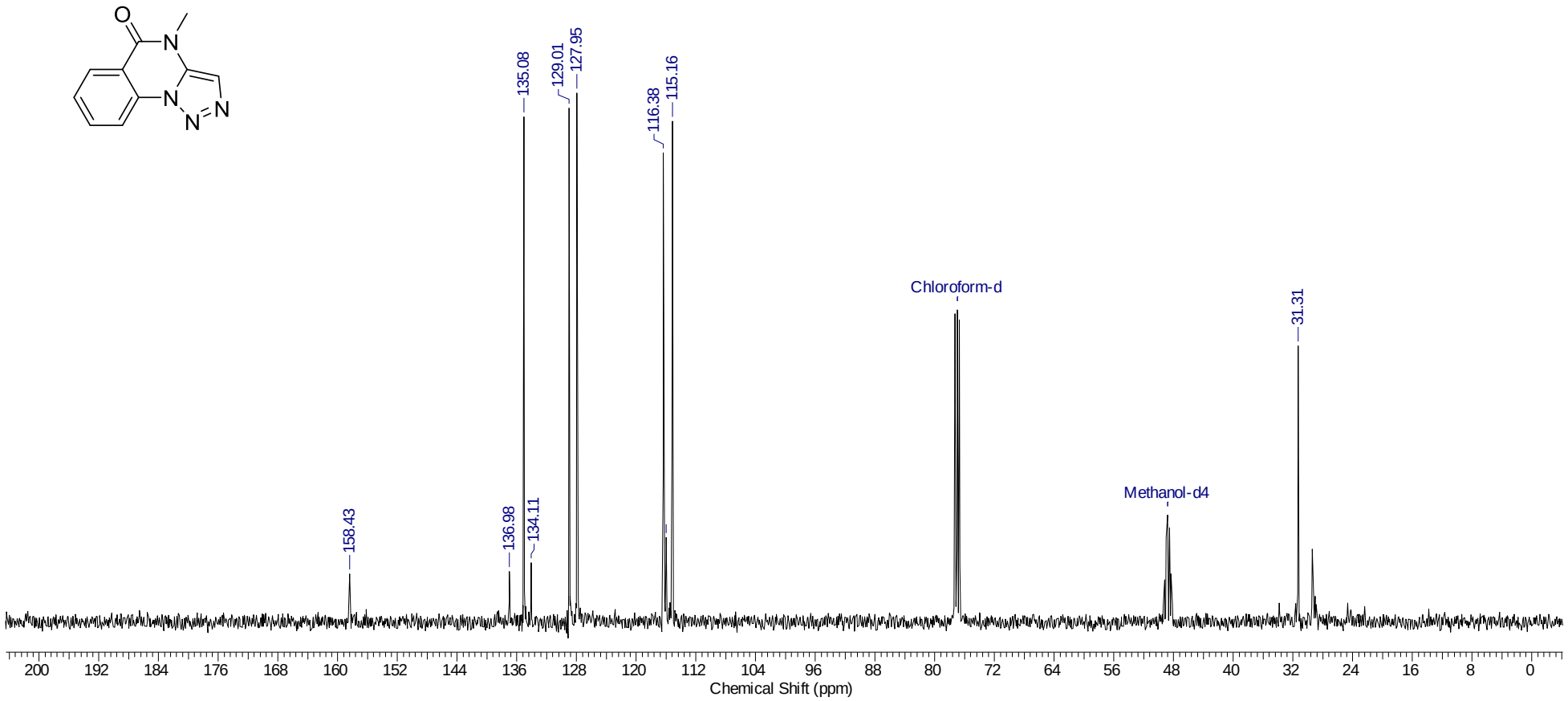
4-Methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2j)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



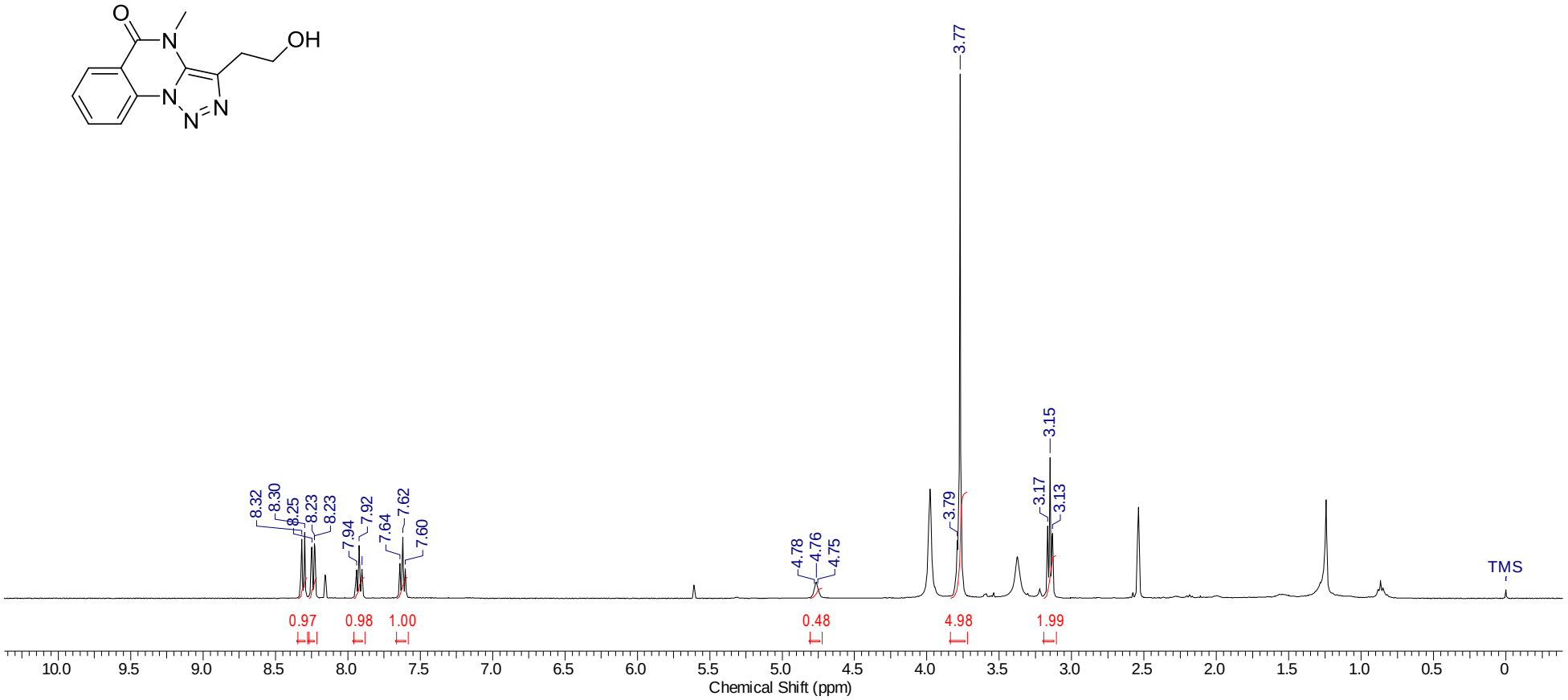
4-Methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2j)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



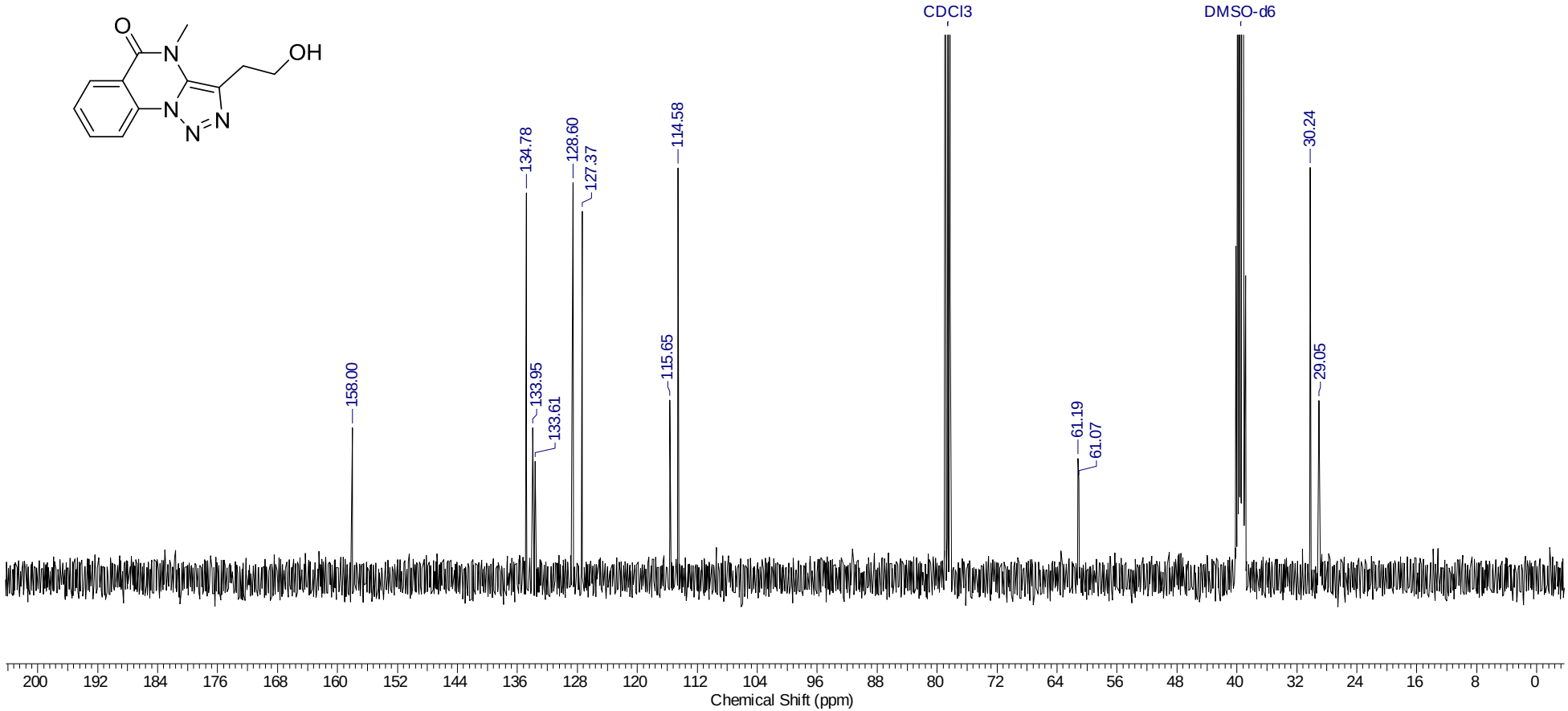
3-(2-Hydroxyethyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2k)

^{1}H NMR (400 MHz, DMSO-d_6–$CDCl_3$ = 3:1 + CD_3OD)



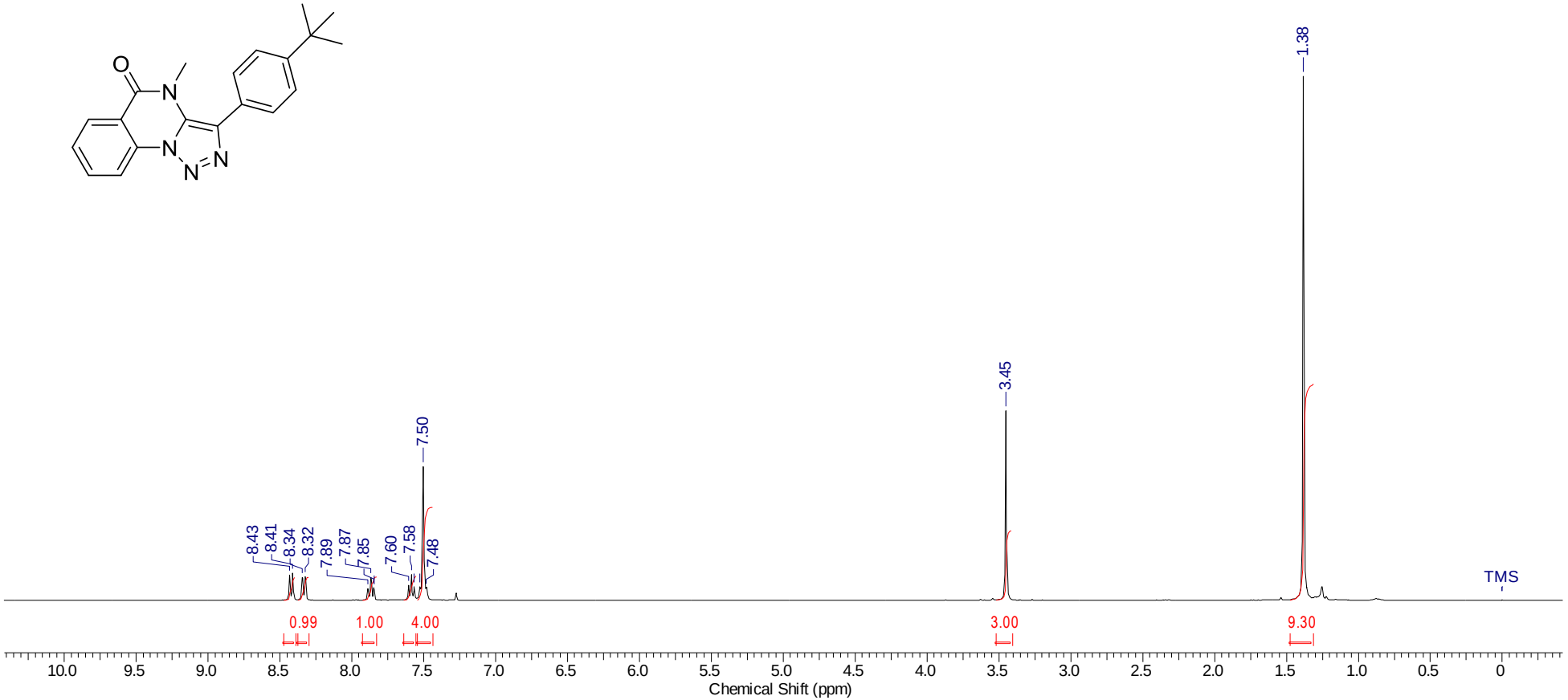
3-(2-Hydroxyethyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2k)

$^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6–$CDCl_3$ = 3:1 + CD_3OD)



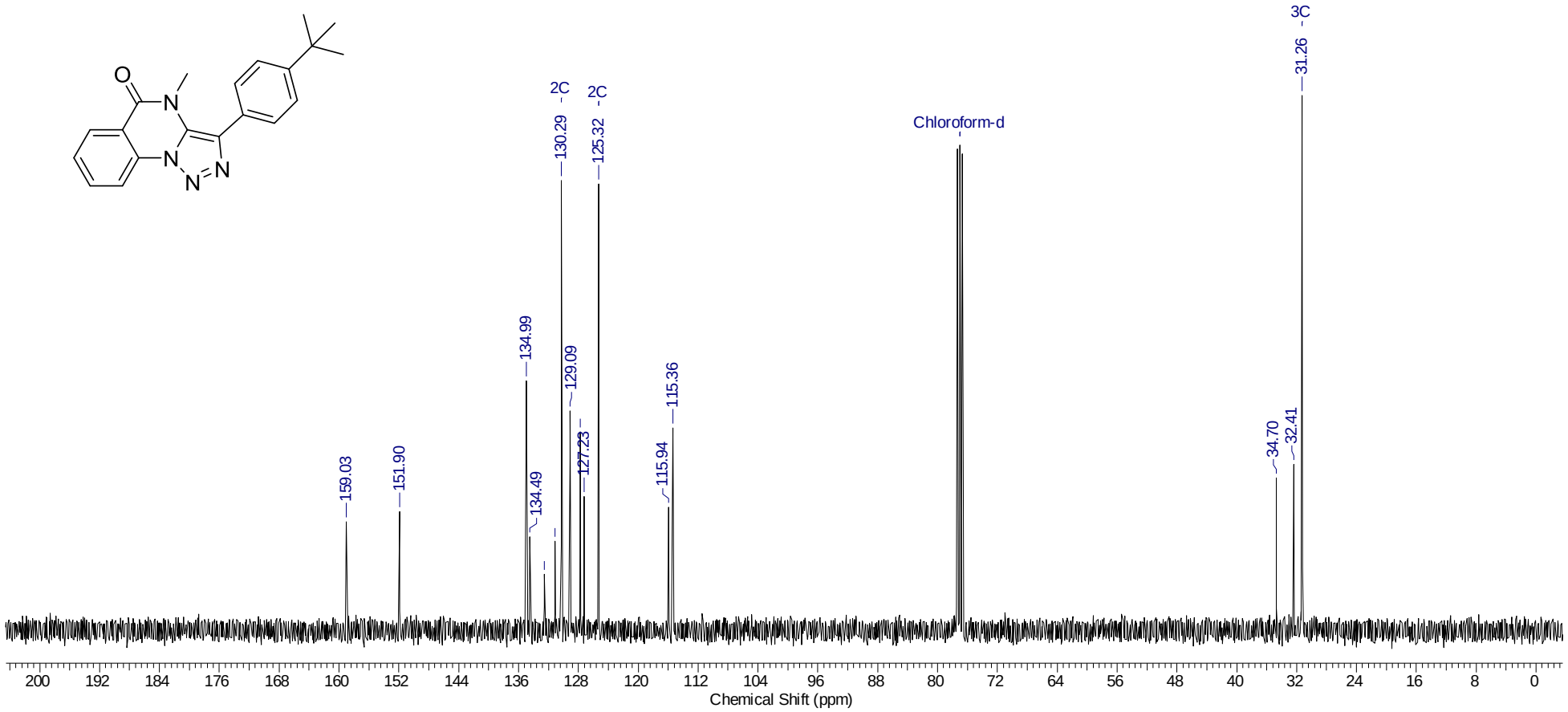
3-(4-*tert*-Butylphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2l)

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



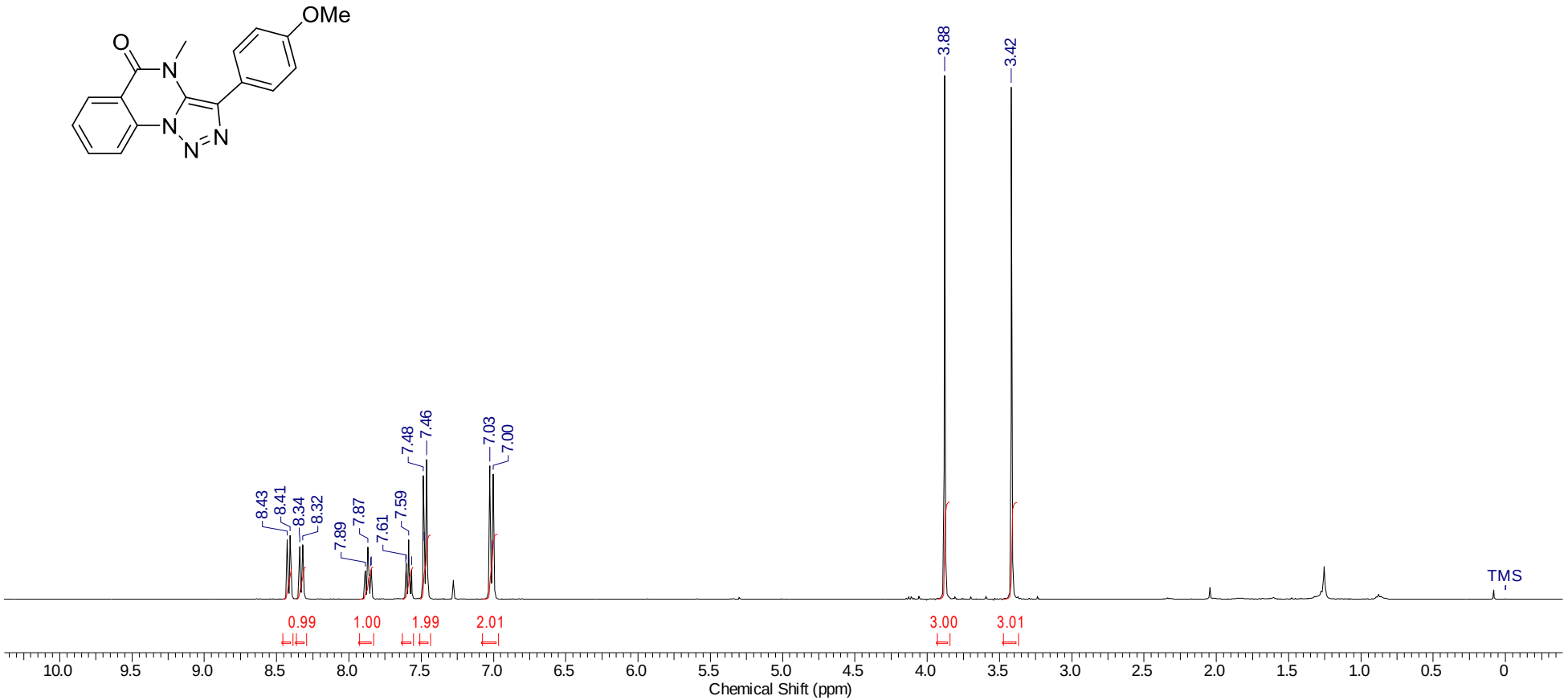
3-(4-*tert*-Butylphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2l)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



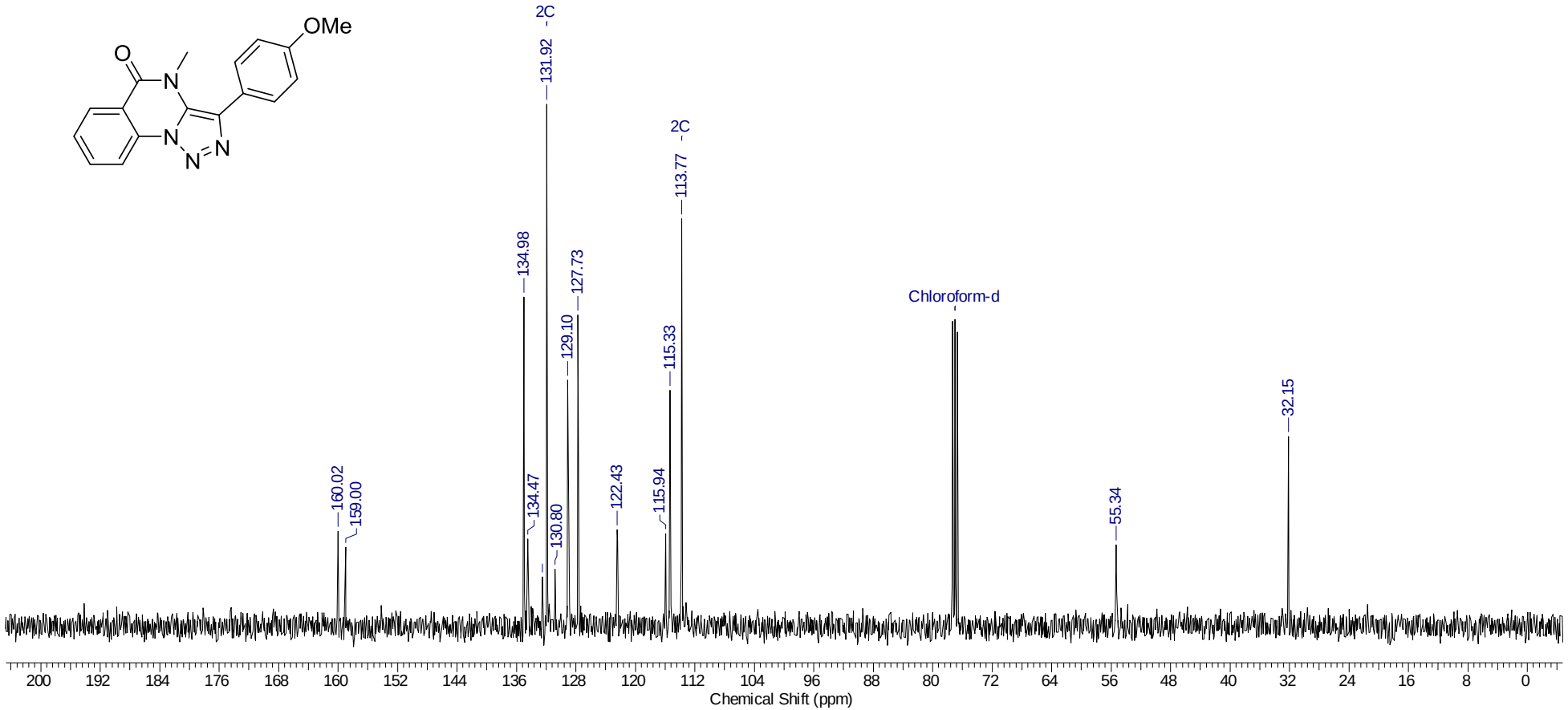
3-(4-Methoxyphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2m)

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



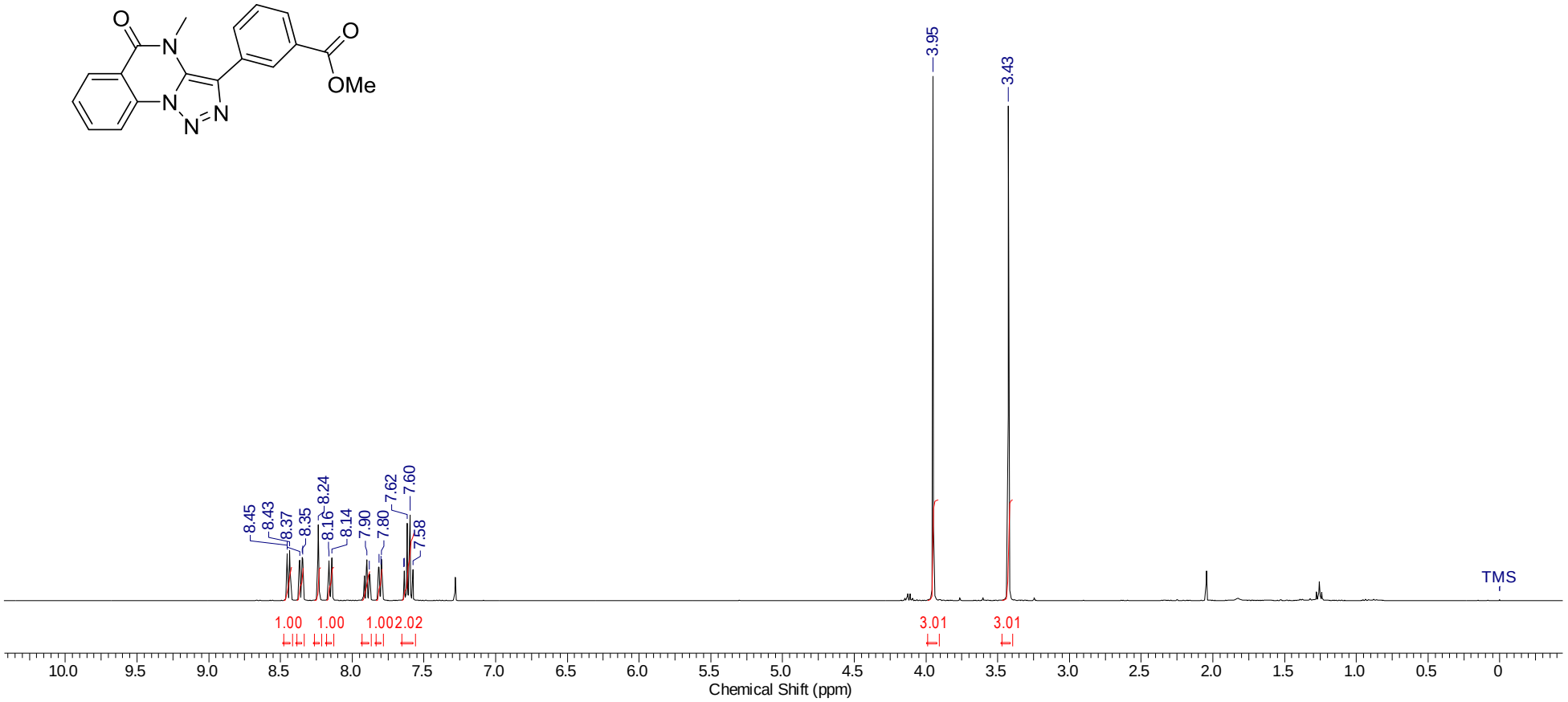
3-(4-Methoxyphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2m)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



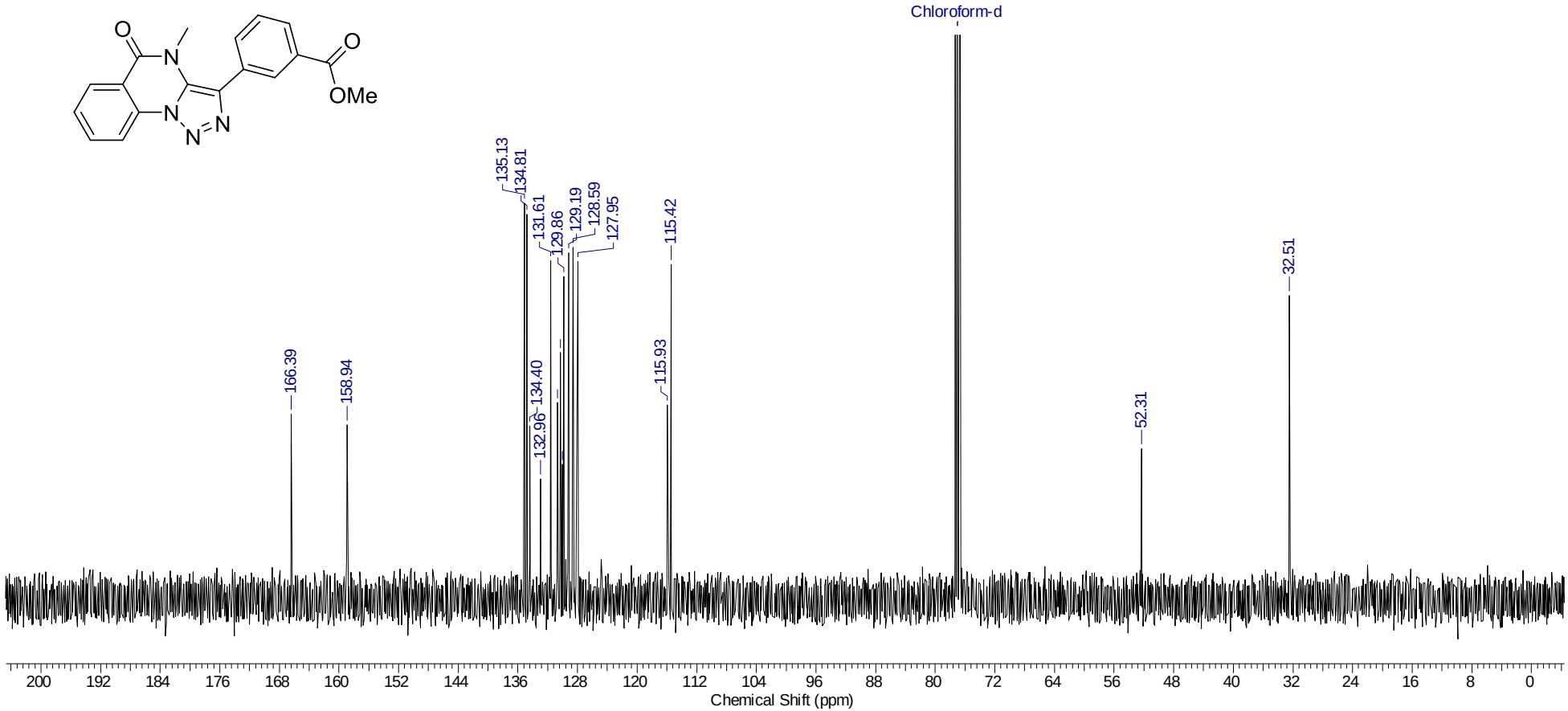
Methyl 3-(4-methyl-5-oxo-4,5-dihydro[1,2,3]triazolo[1,5-*a*]quinazolin-3-yl)benzoate (2n)

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



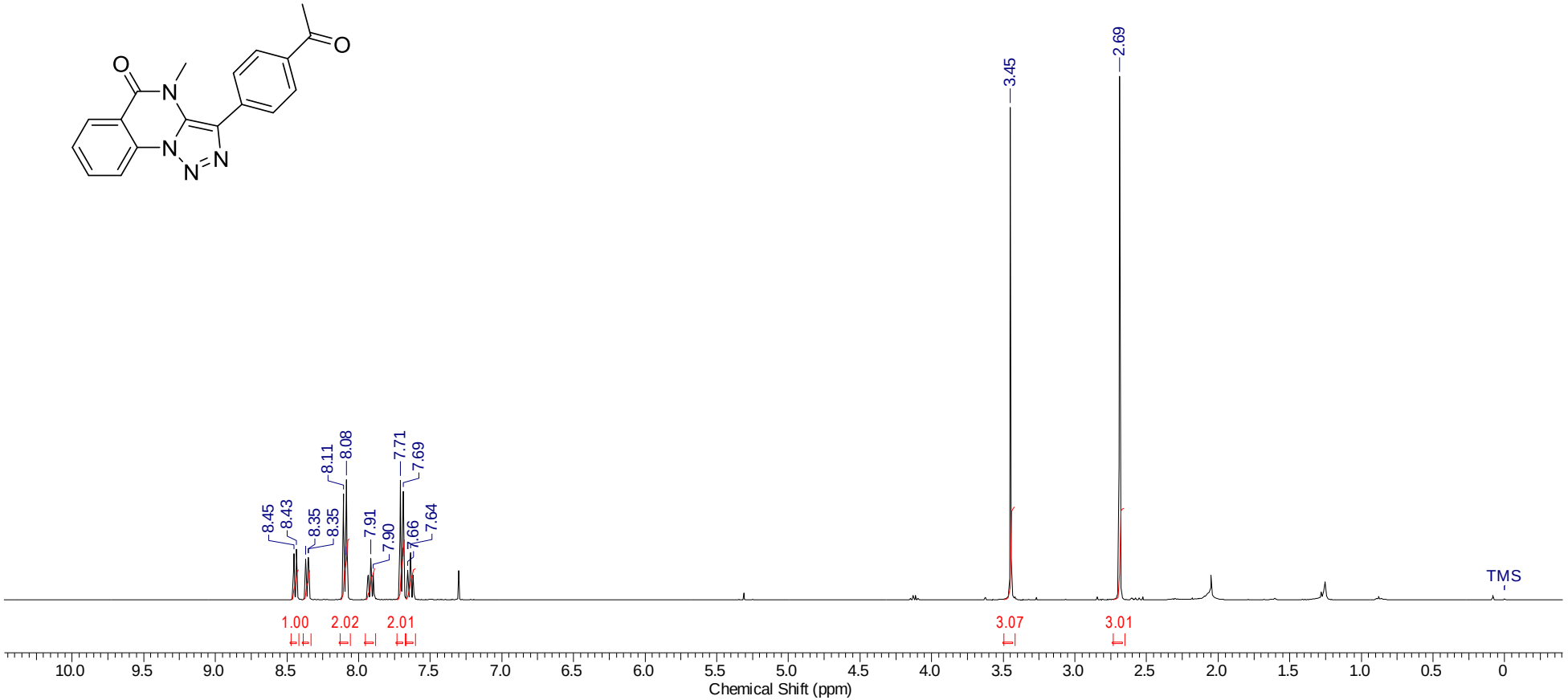
Methyl 3-(4-methyl-5-oxo-4,5-dihydro[1,2,3]triazolo[1,5-*a*]quinazolin-3-yl)benzoate (2n)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



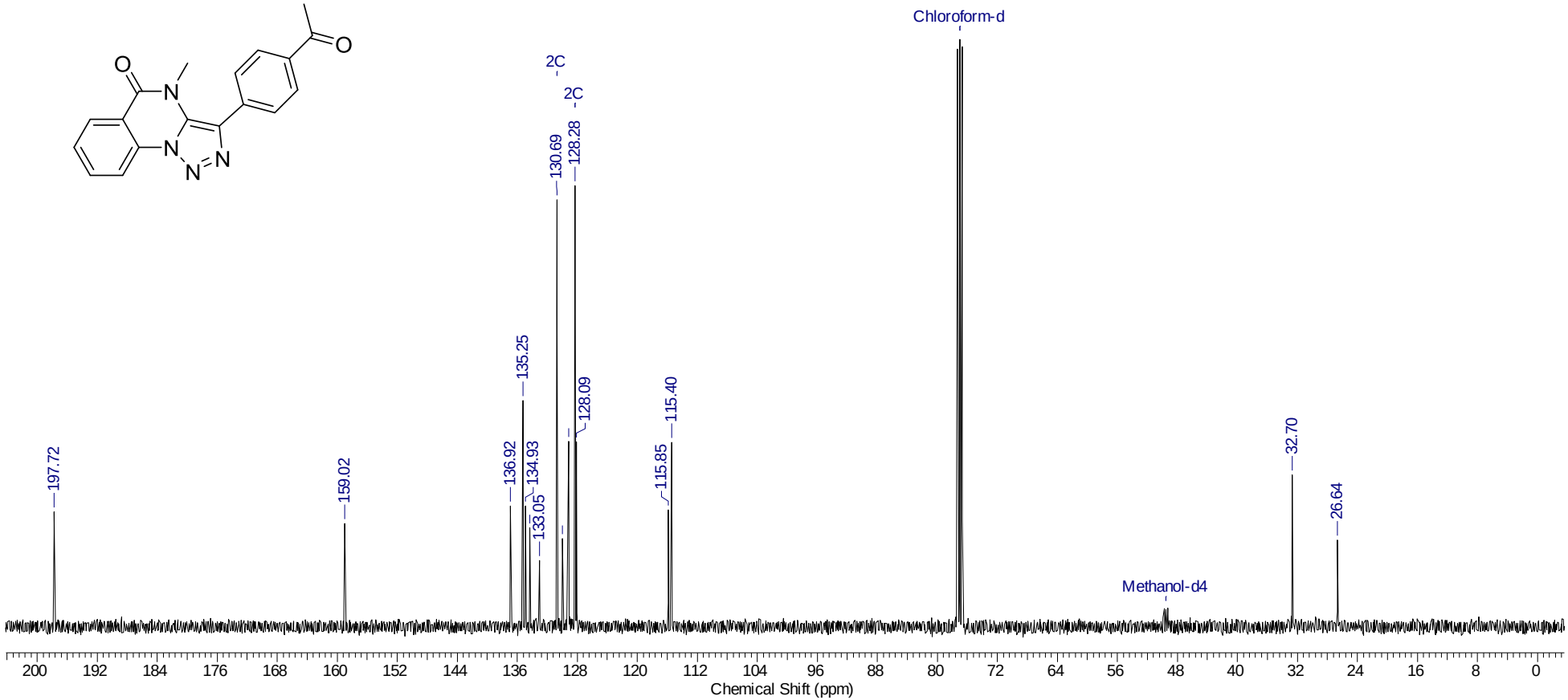
3-(4-Acetylphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2o)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



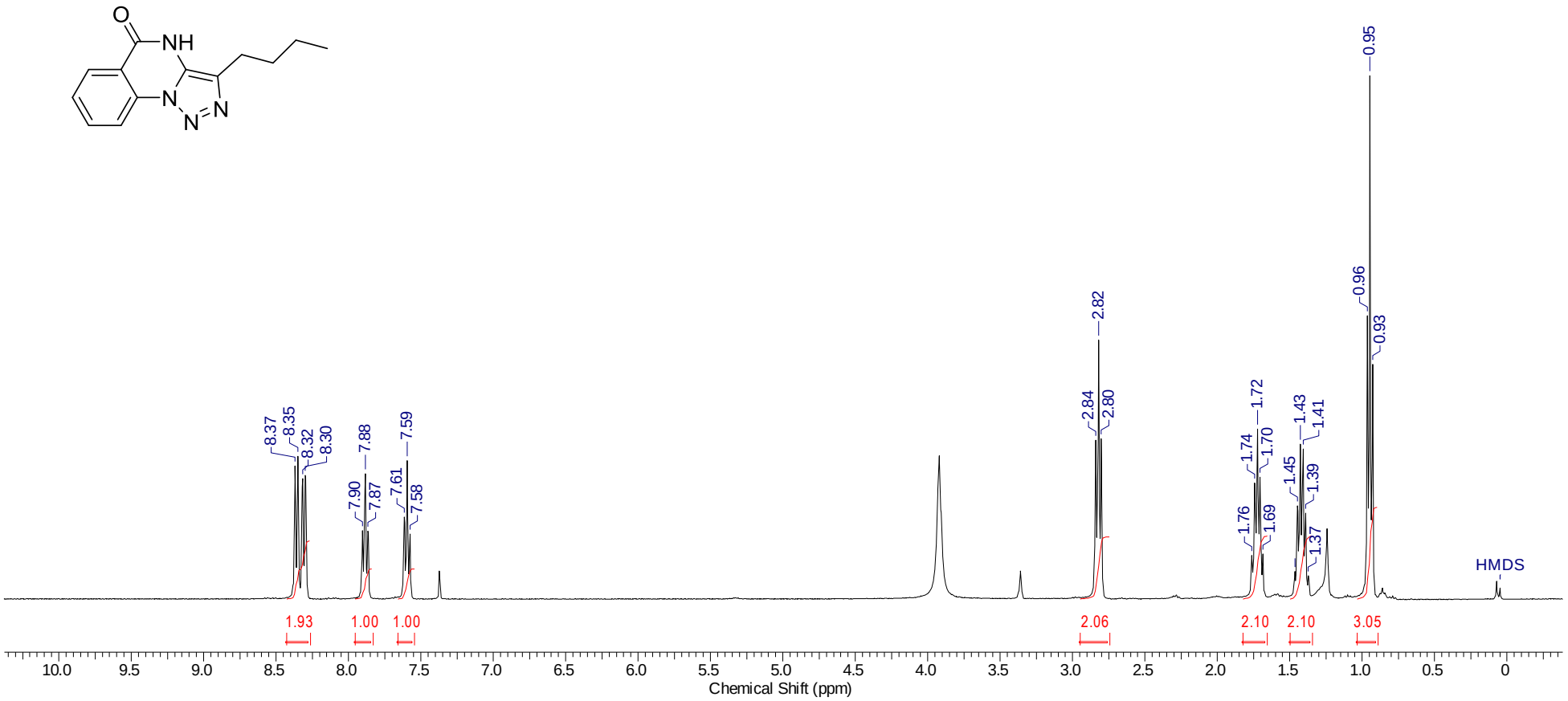
3-(4-Acetylphenyl)-4-methyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2o)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



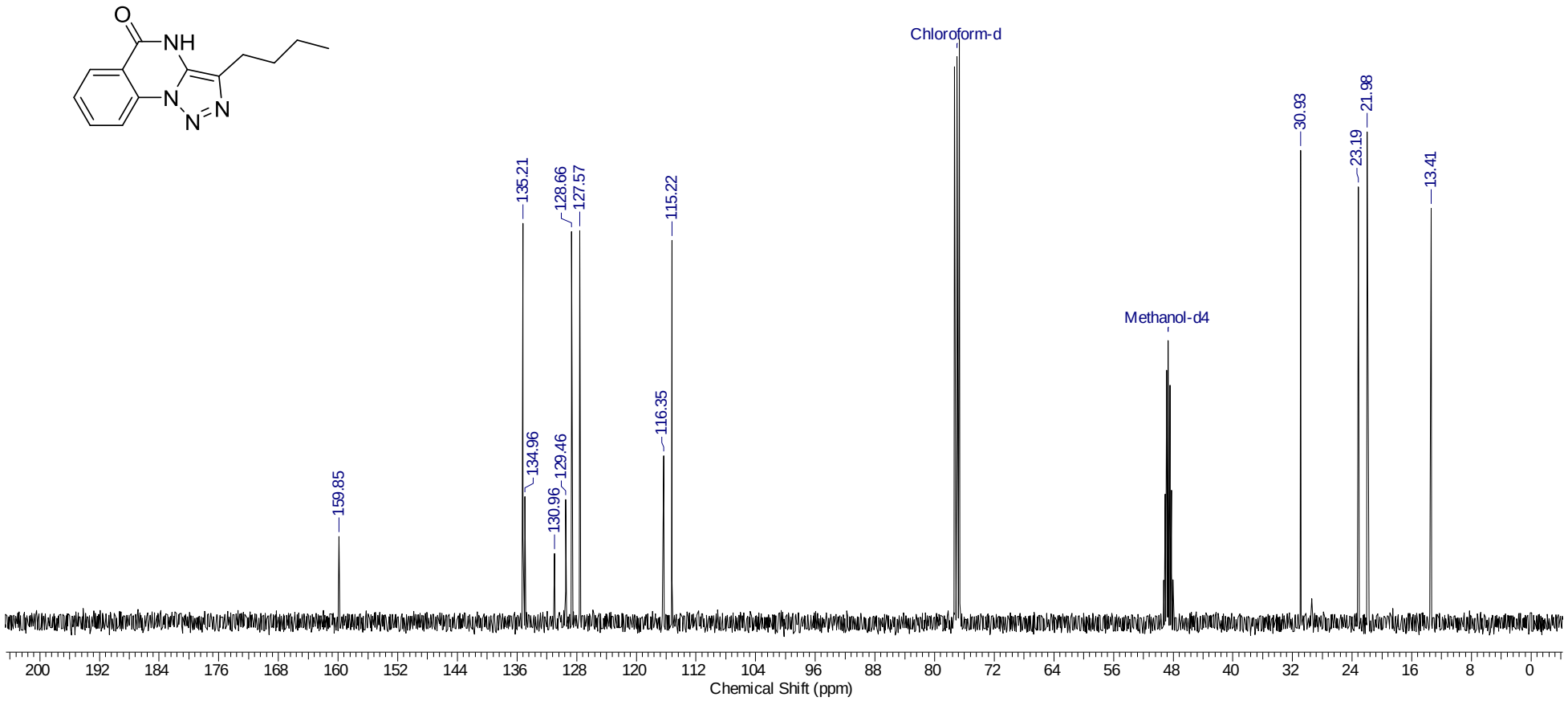
3-Butyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2p)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



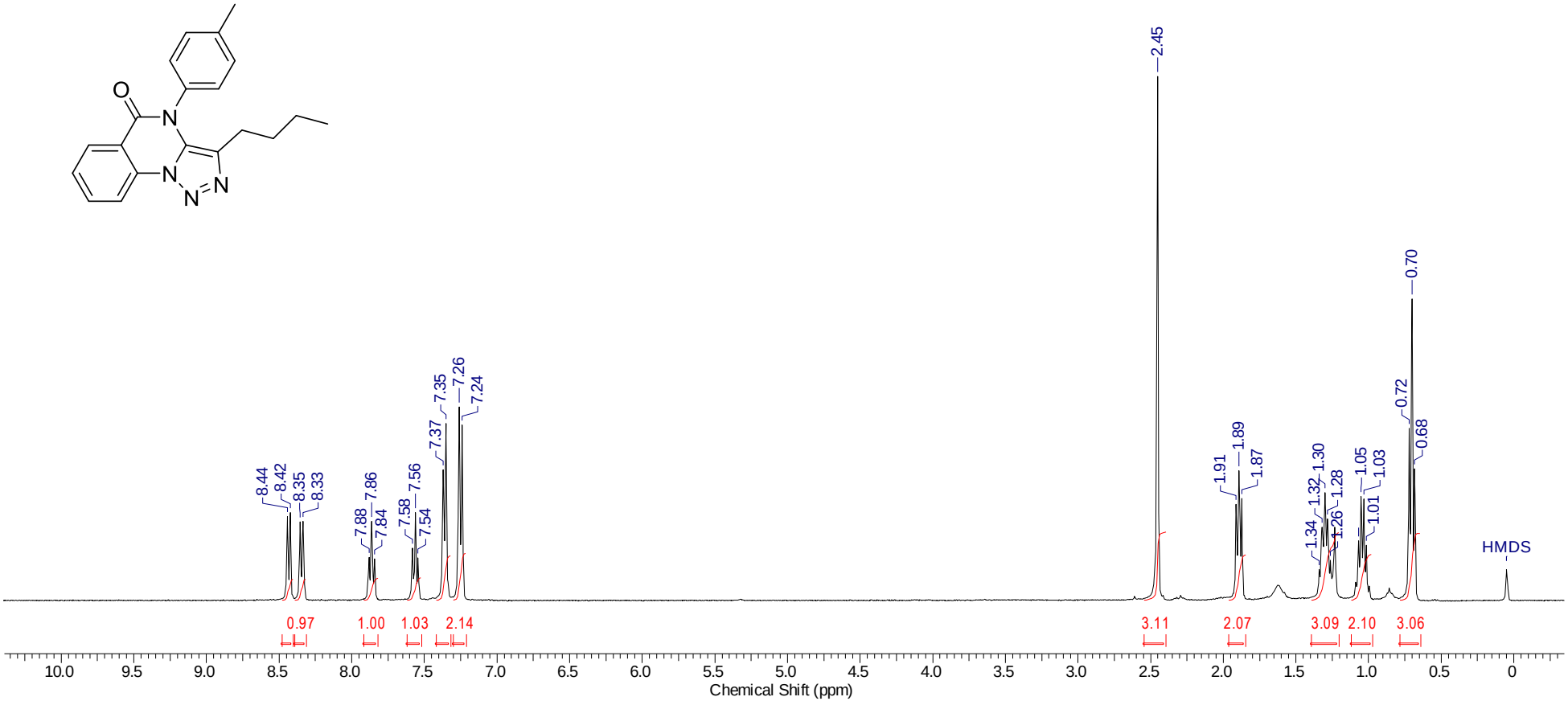
3-Butyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2p)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



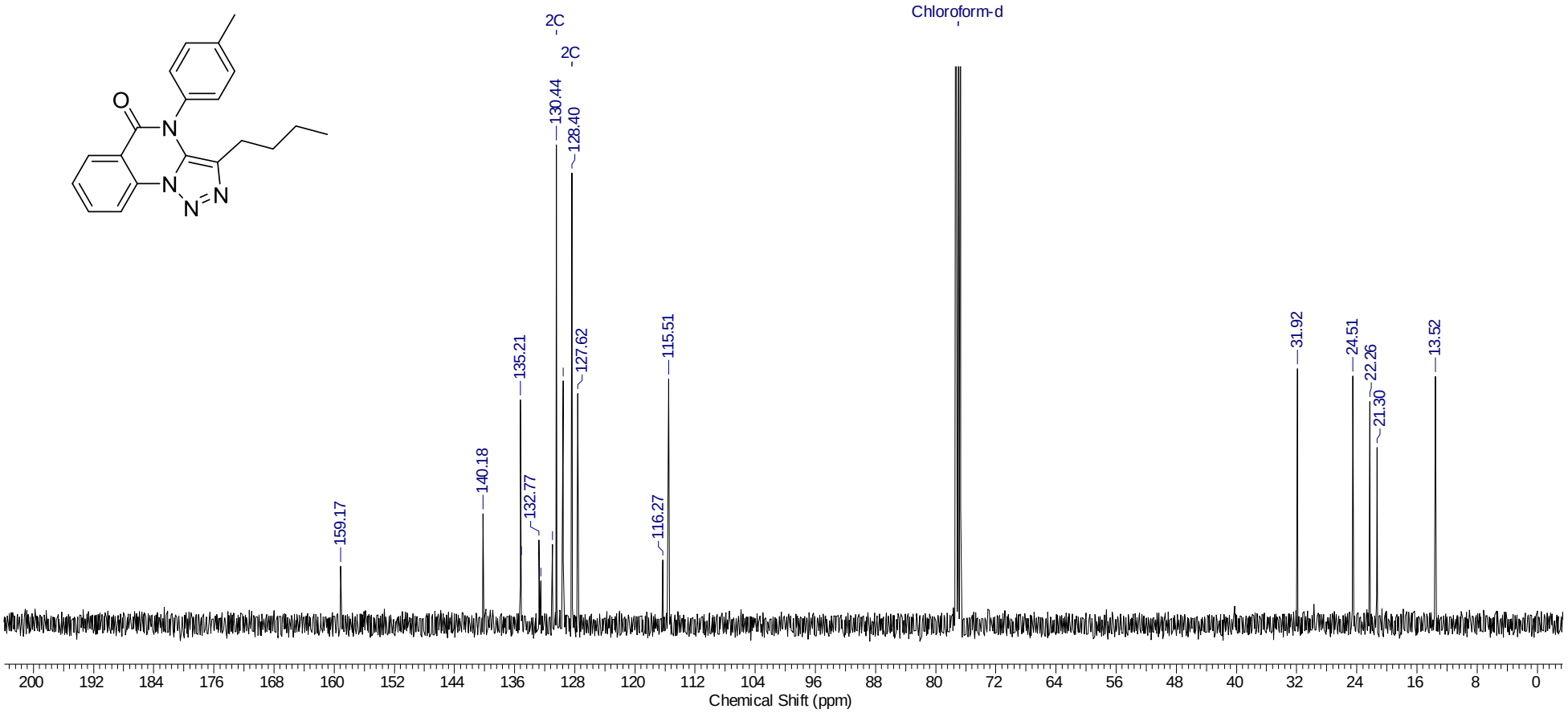
3-Butyl-4-(4-methylphenyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2q)

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



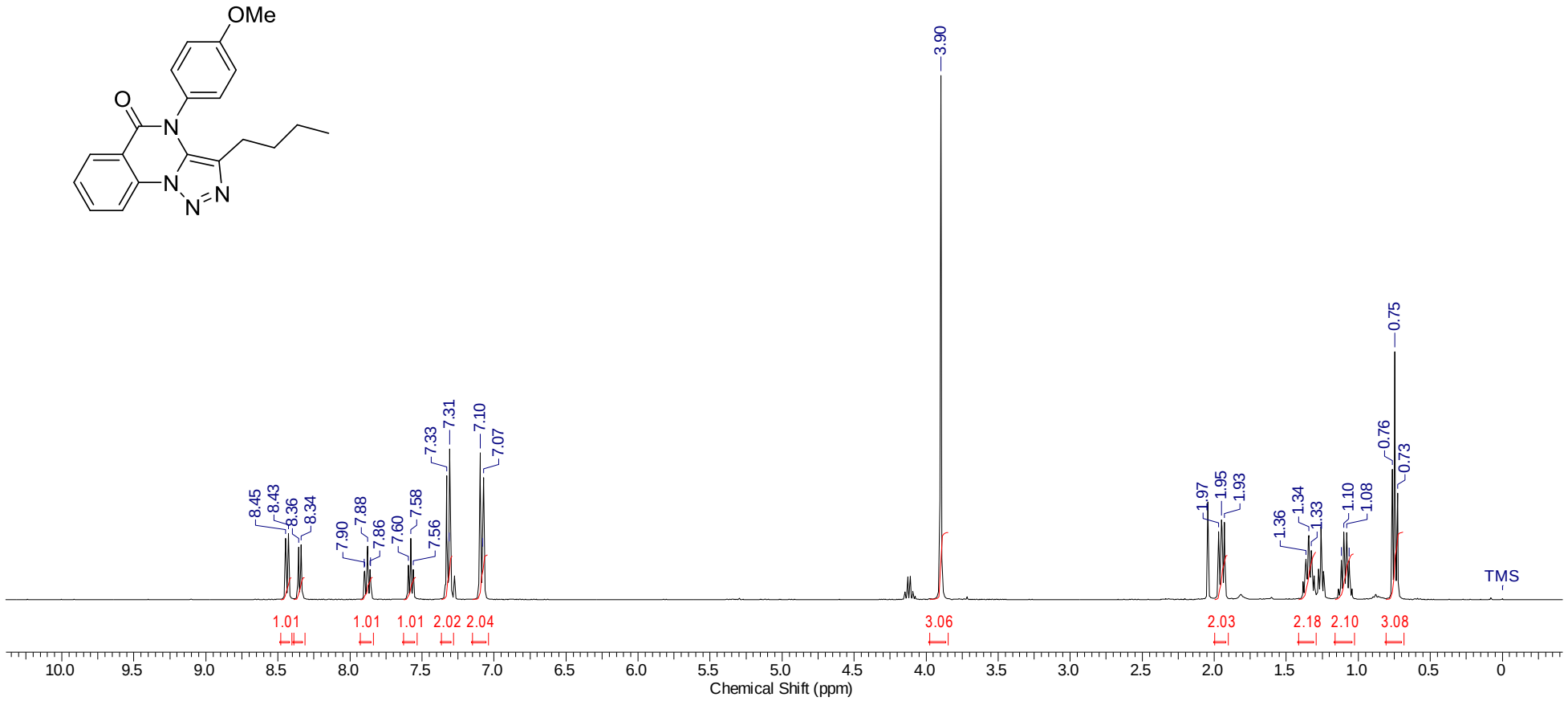
3-Butyl-4-(4-methylphenyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2q)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



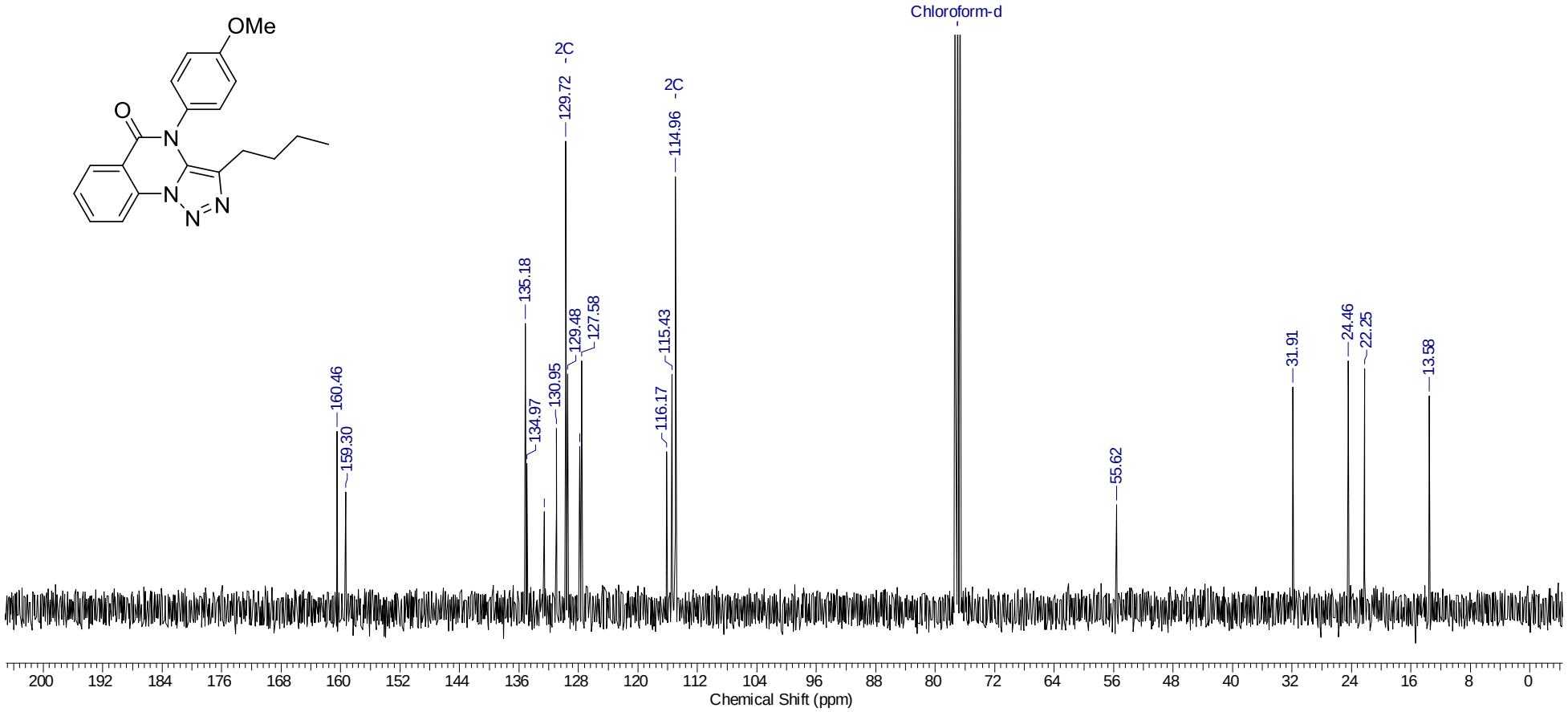
3-Butyl-4-(4-methoxyphenyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2r)

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



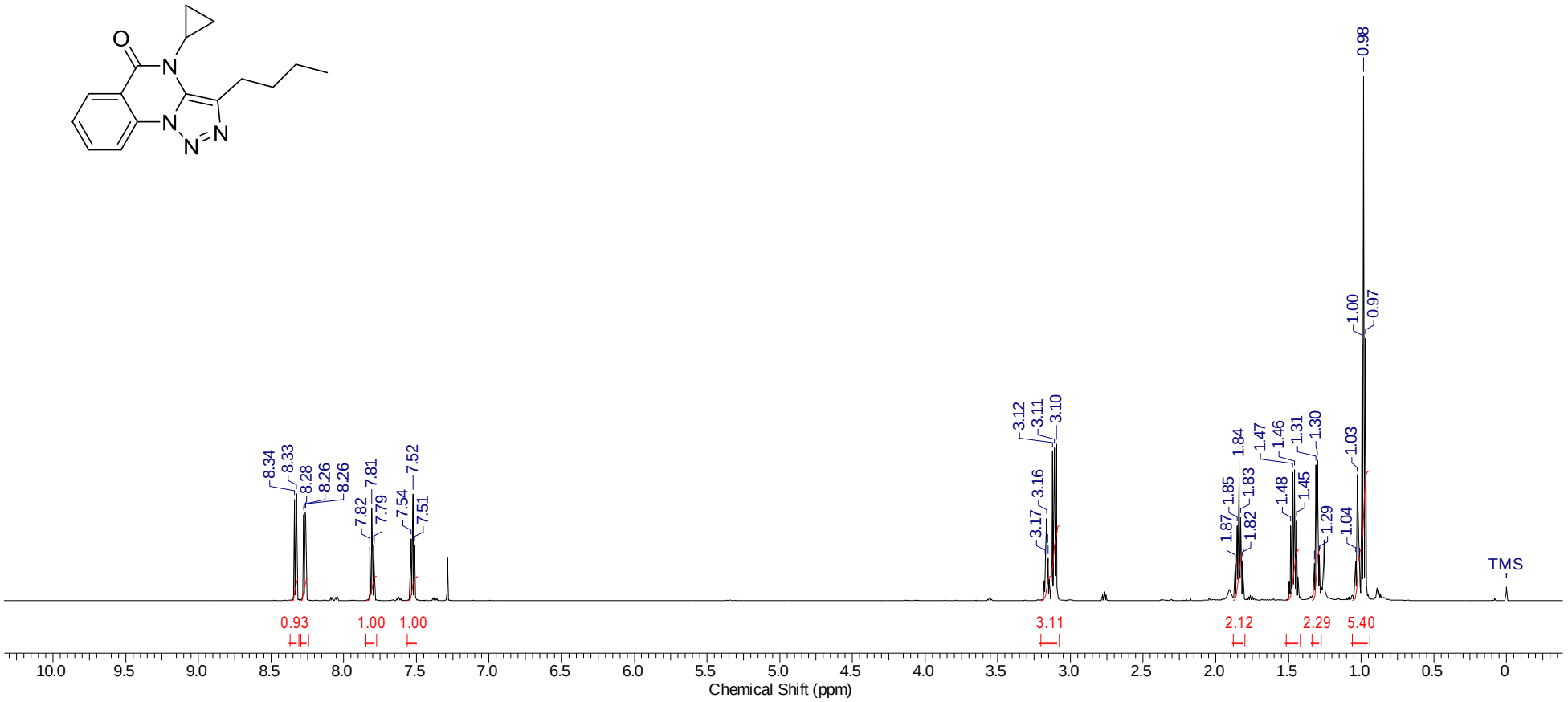
3-Butyl-4-(4-methoxyphenyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2r)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



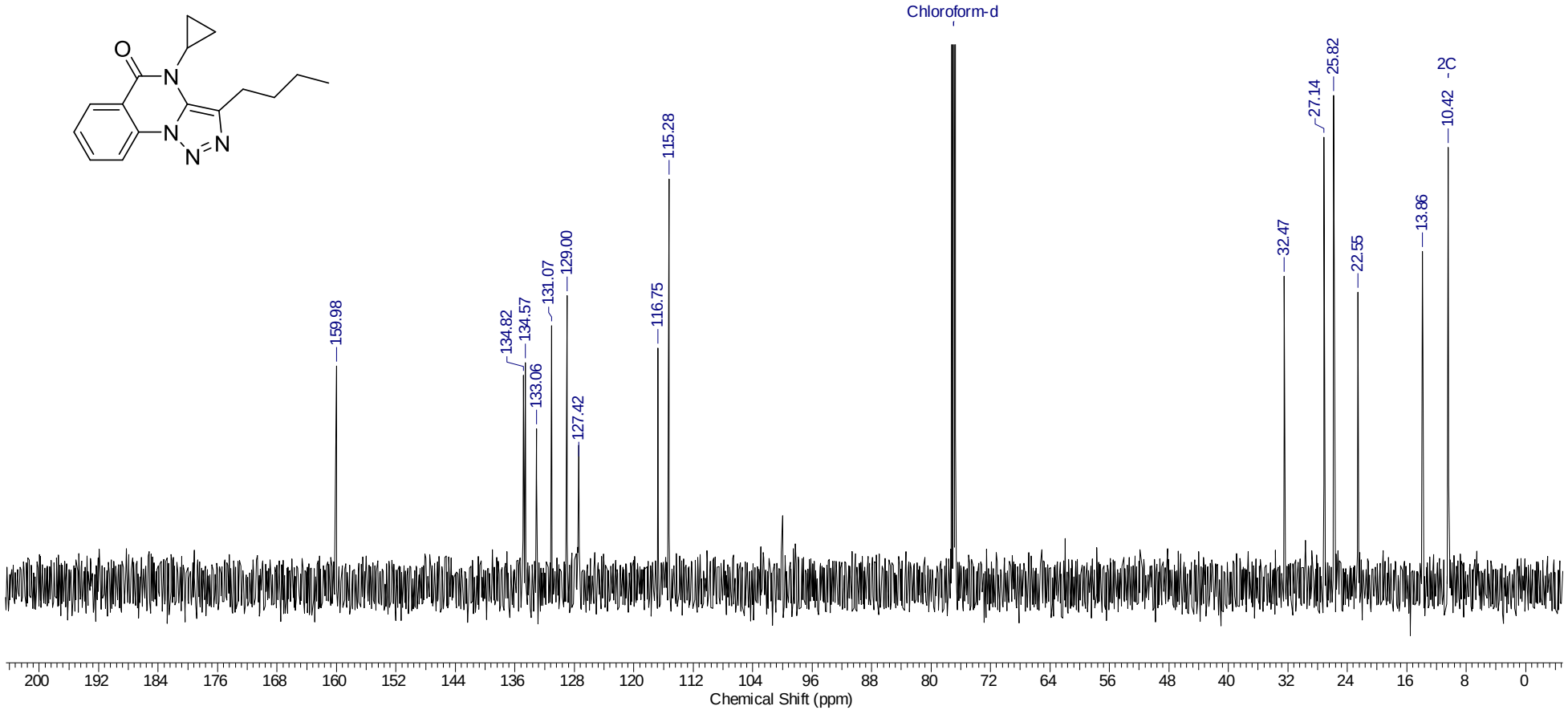
3-Butyl-4-cyclopropyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2s)

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



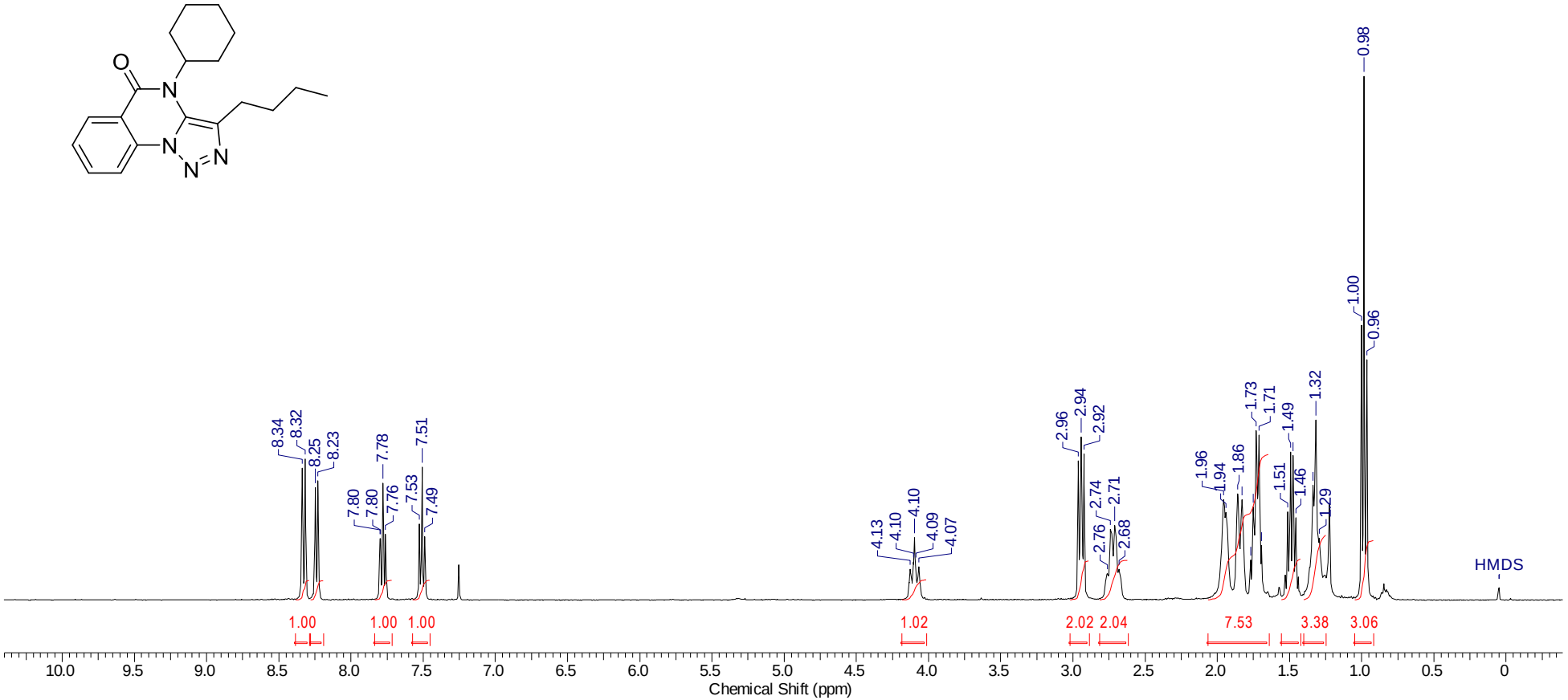
3-Butyl-4-cyclopropyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2s)

$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$)



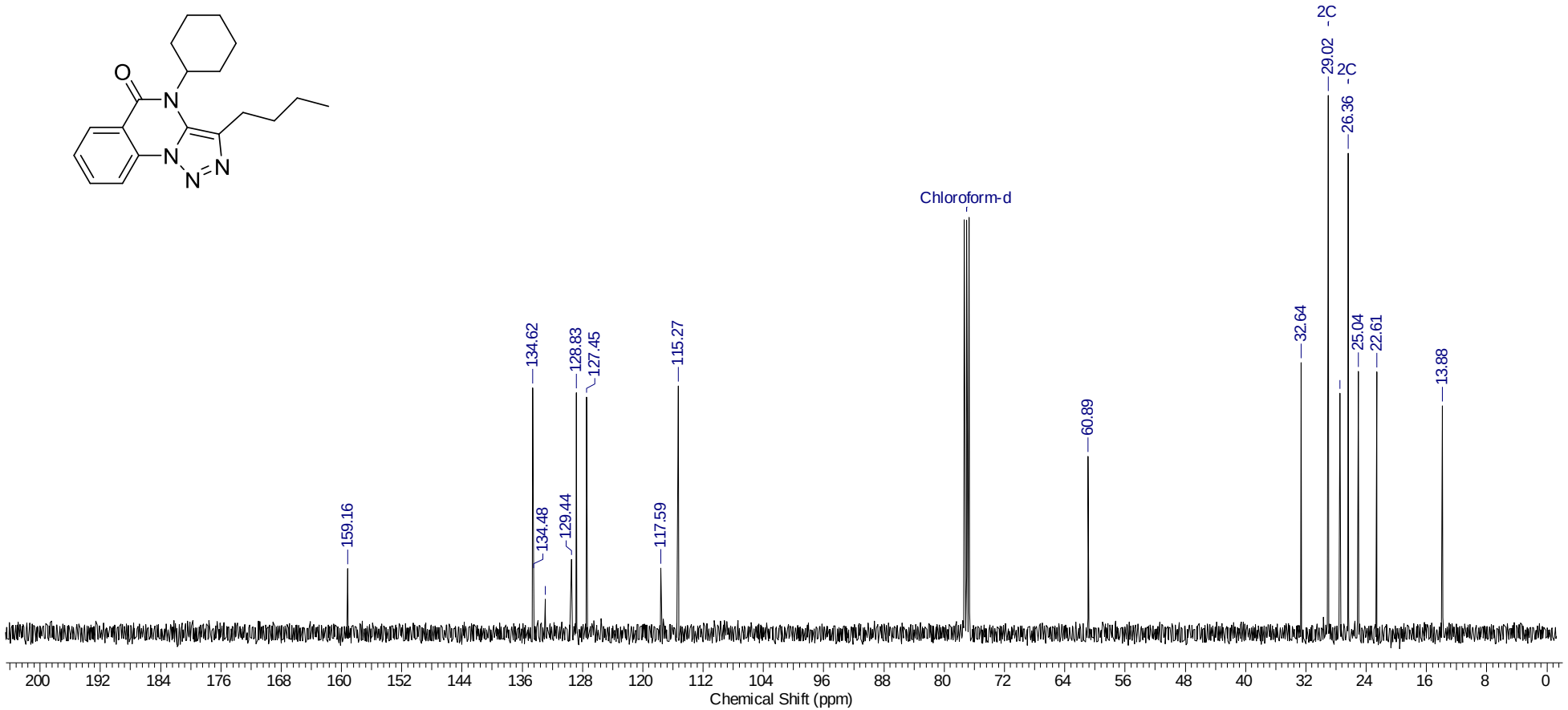
3-Butyl-4-cyclohexyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2t)

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



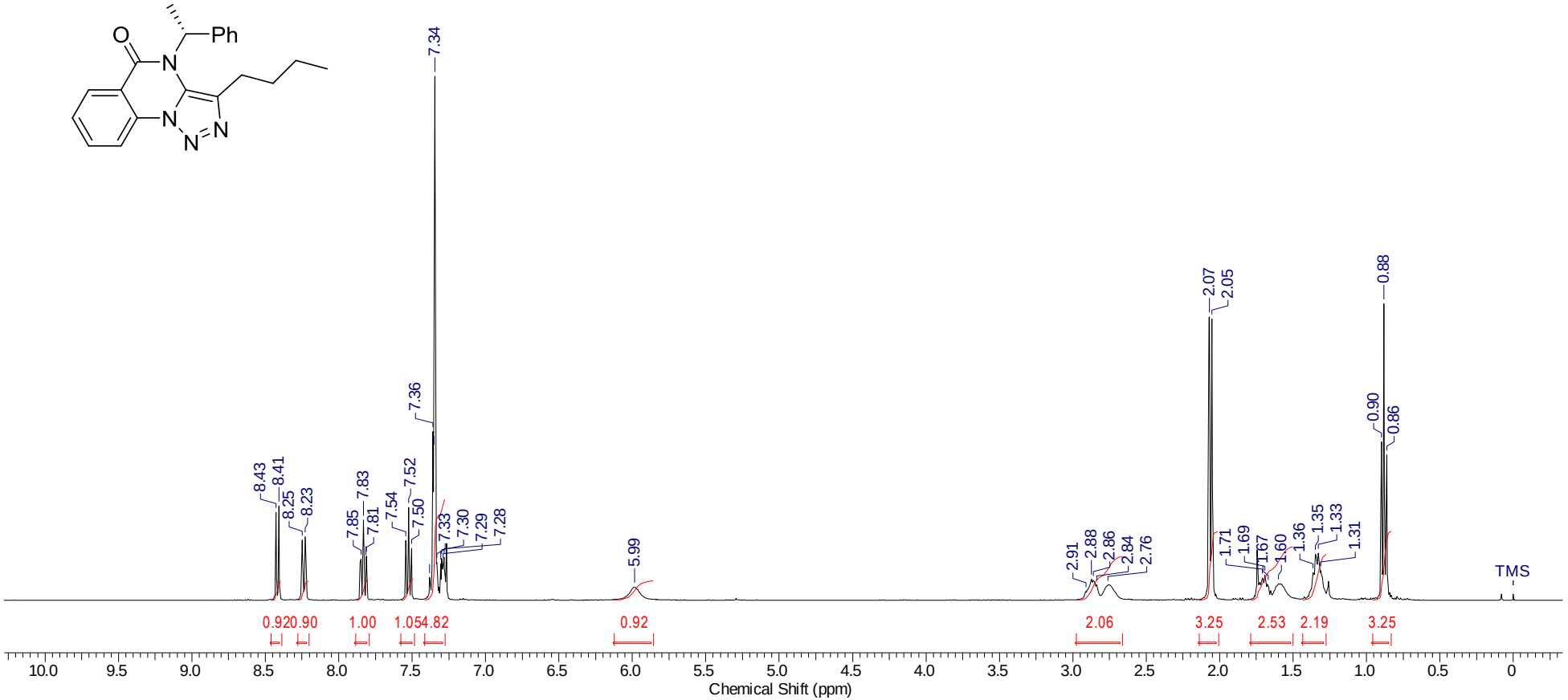
3-Butyl-4-cyclohexyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2t)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



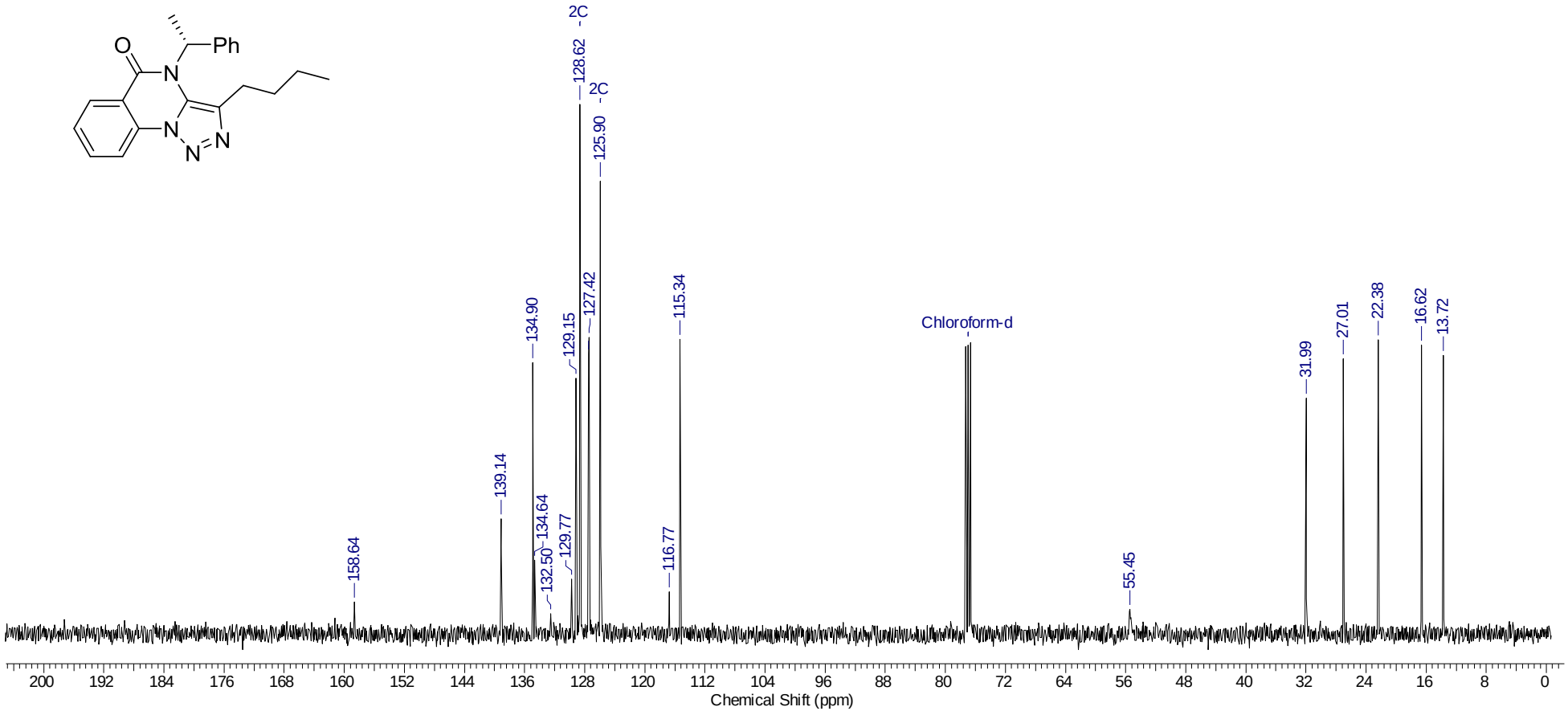
3-Butyl-4-[(1*R*)-1-phenylethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2u)

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



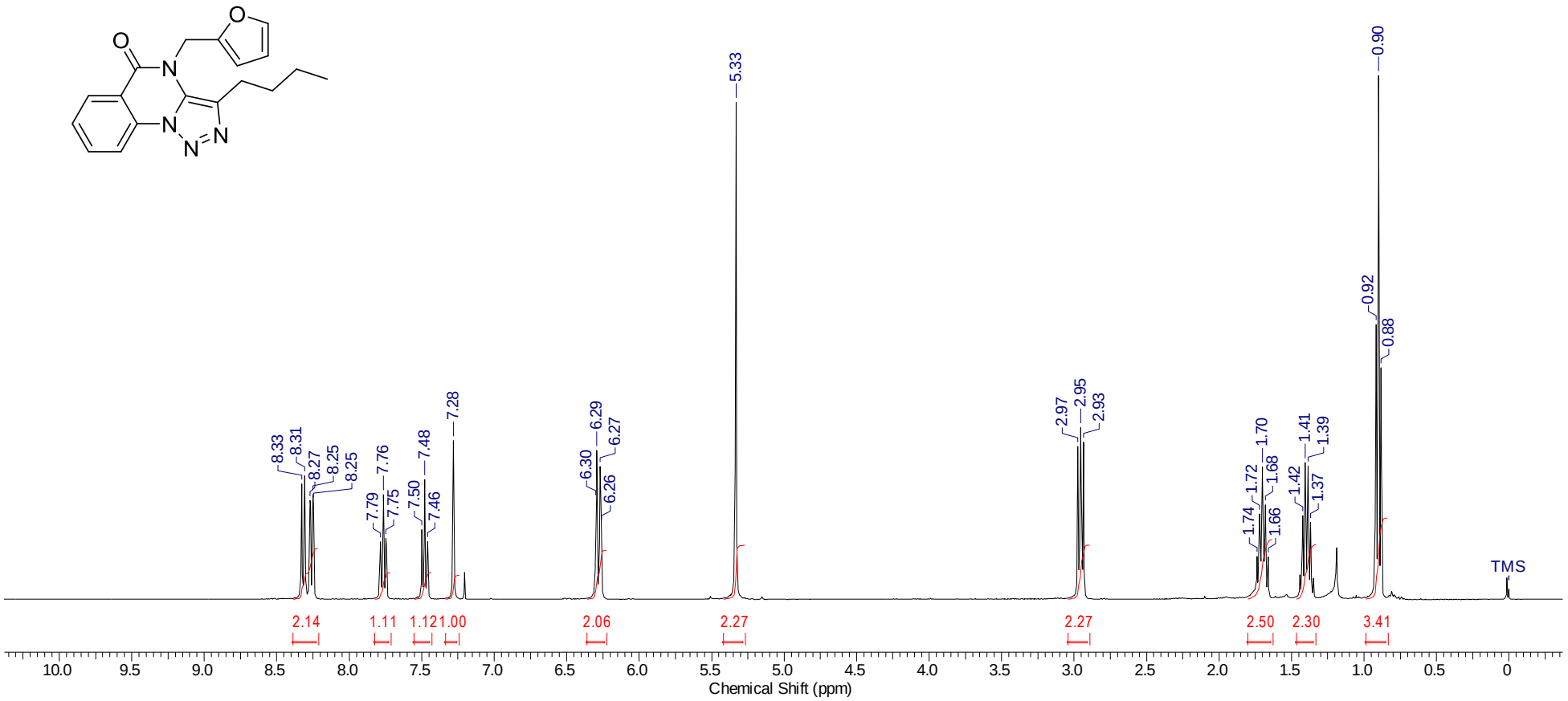
3-Butyl-4-[(1*R*)-1-phenylethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2u)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



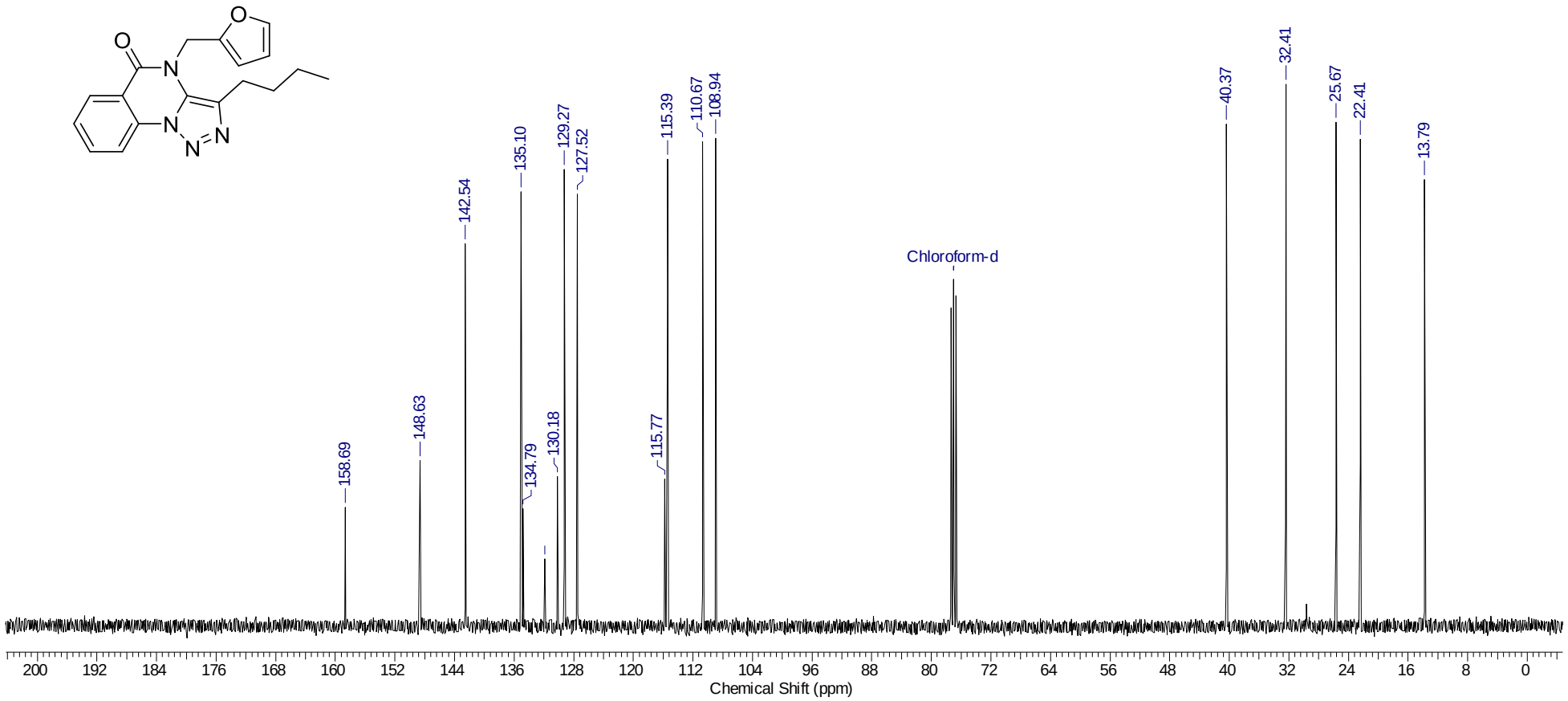
3-Butyl-4-(2-furylmethyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2w)

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



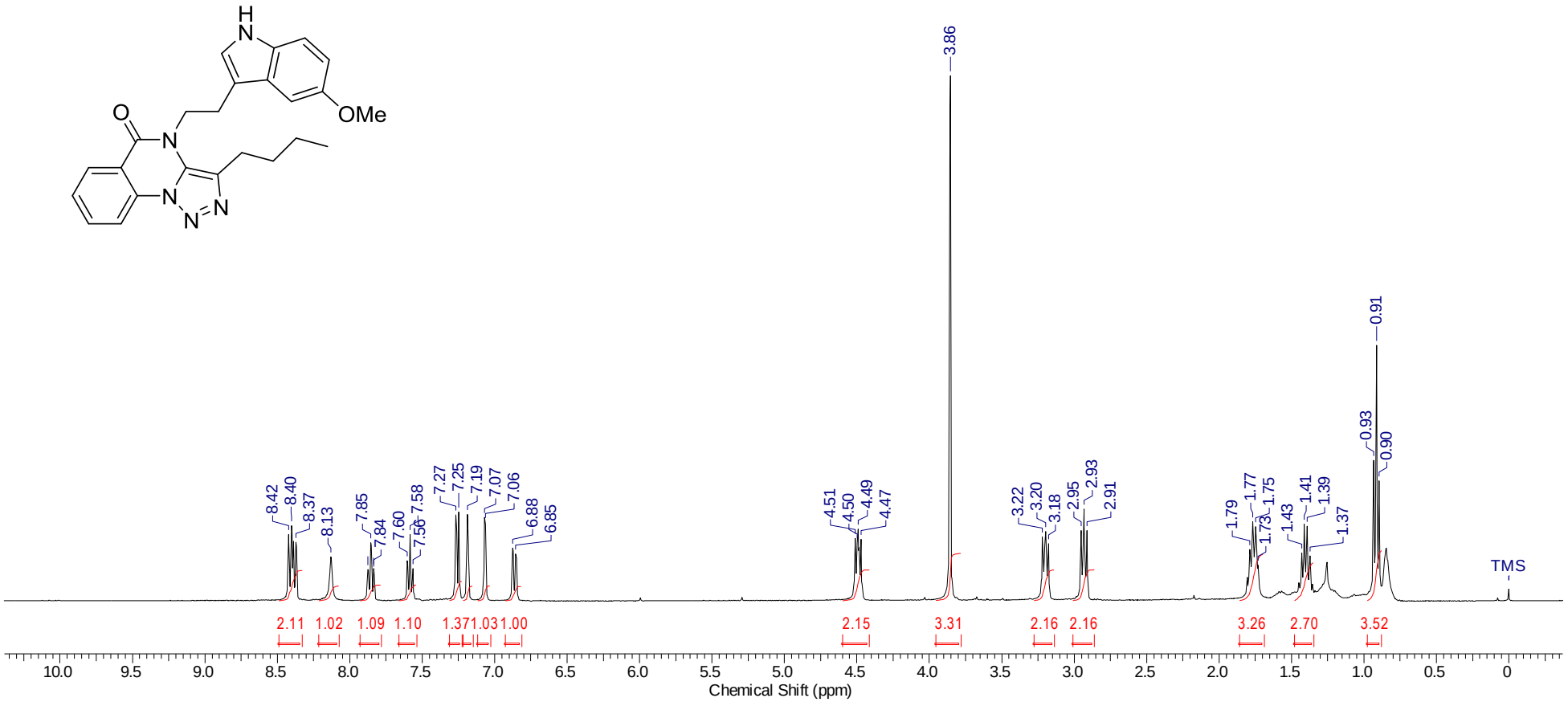
3-Butyl-4-(2-furylmethyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2w)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



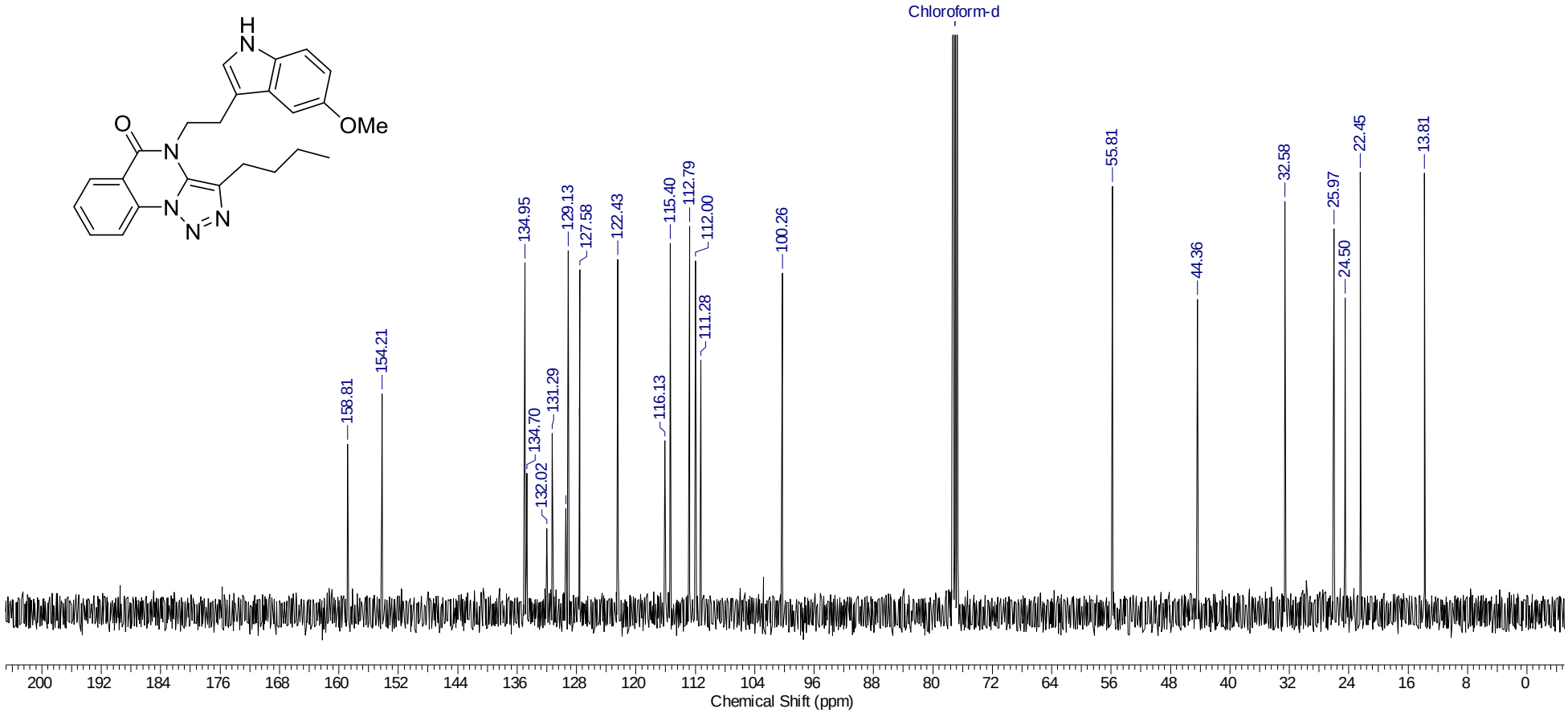
3-Butyl-4-[2-(5-methoxy-1*H*-indol-3-yl)ethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2x)

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



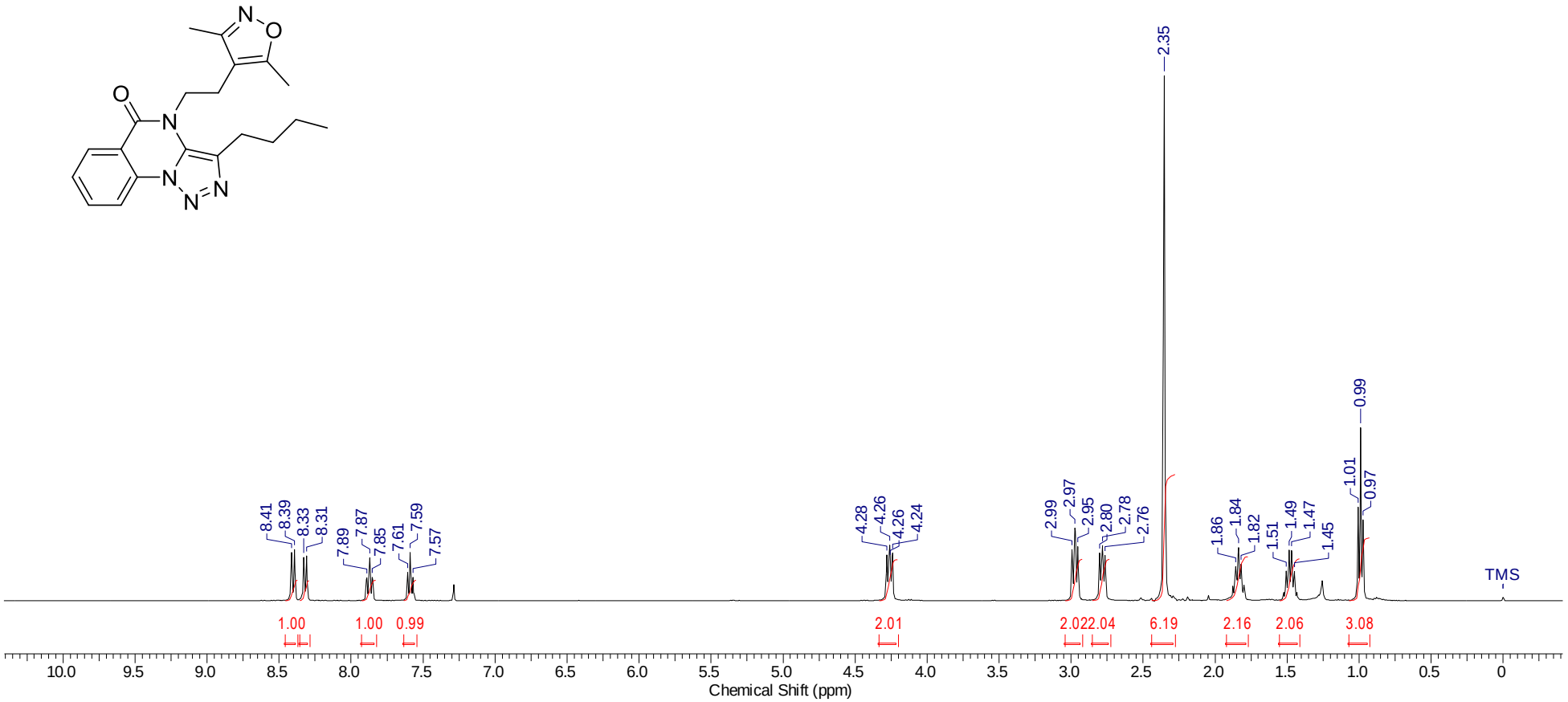
3-Butyl-4-[2-(5-methoxy-1*H*-indol-3-yl)ethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2x)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



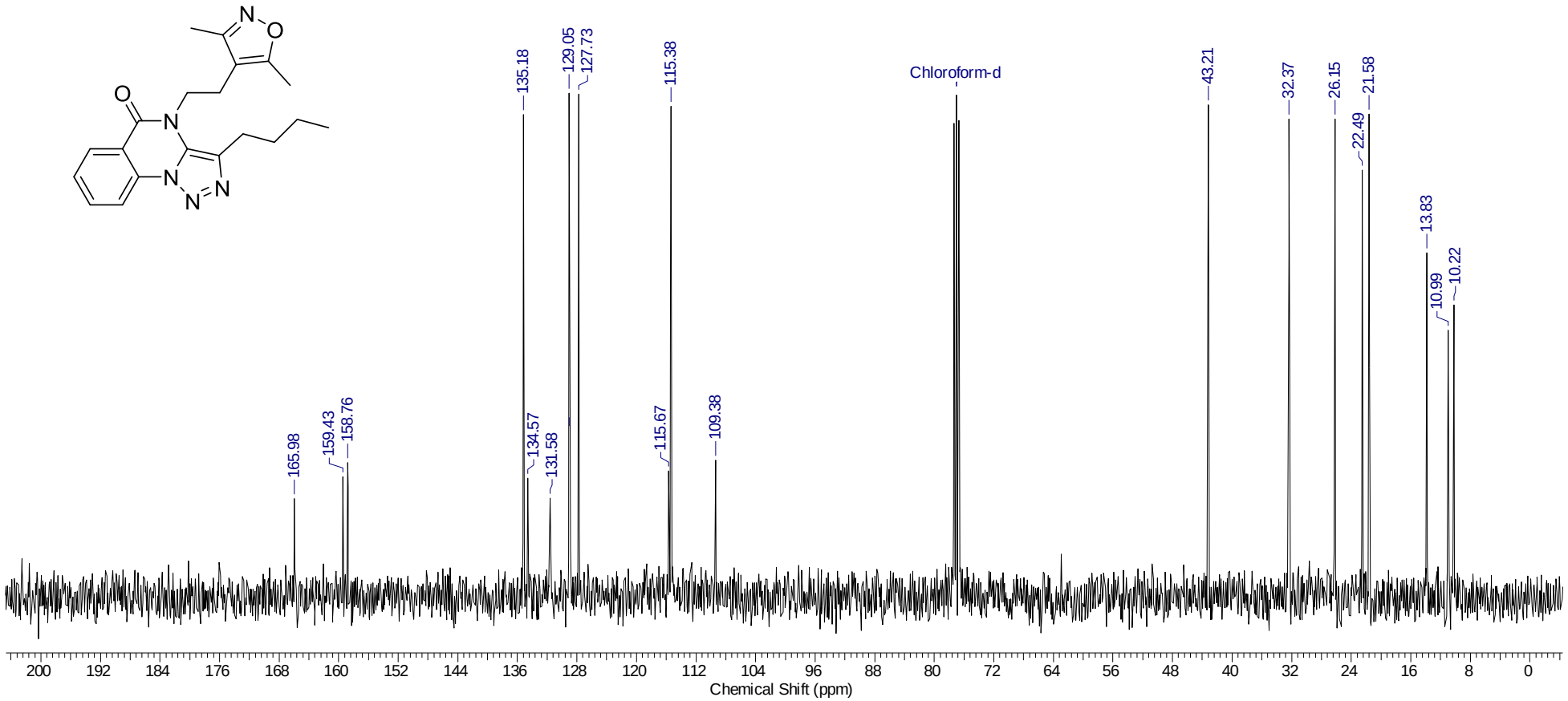
3-Butyl-4-[2-(3,5-dimethylisoxazol-4-yl)ethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2y)

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



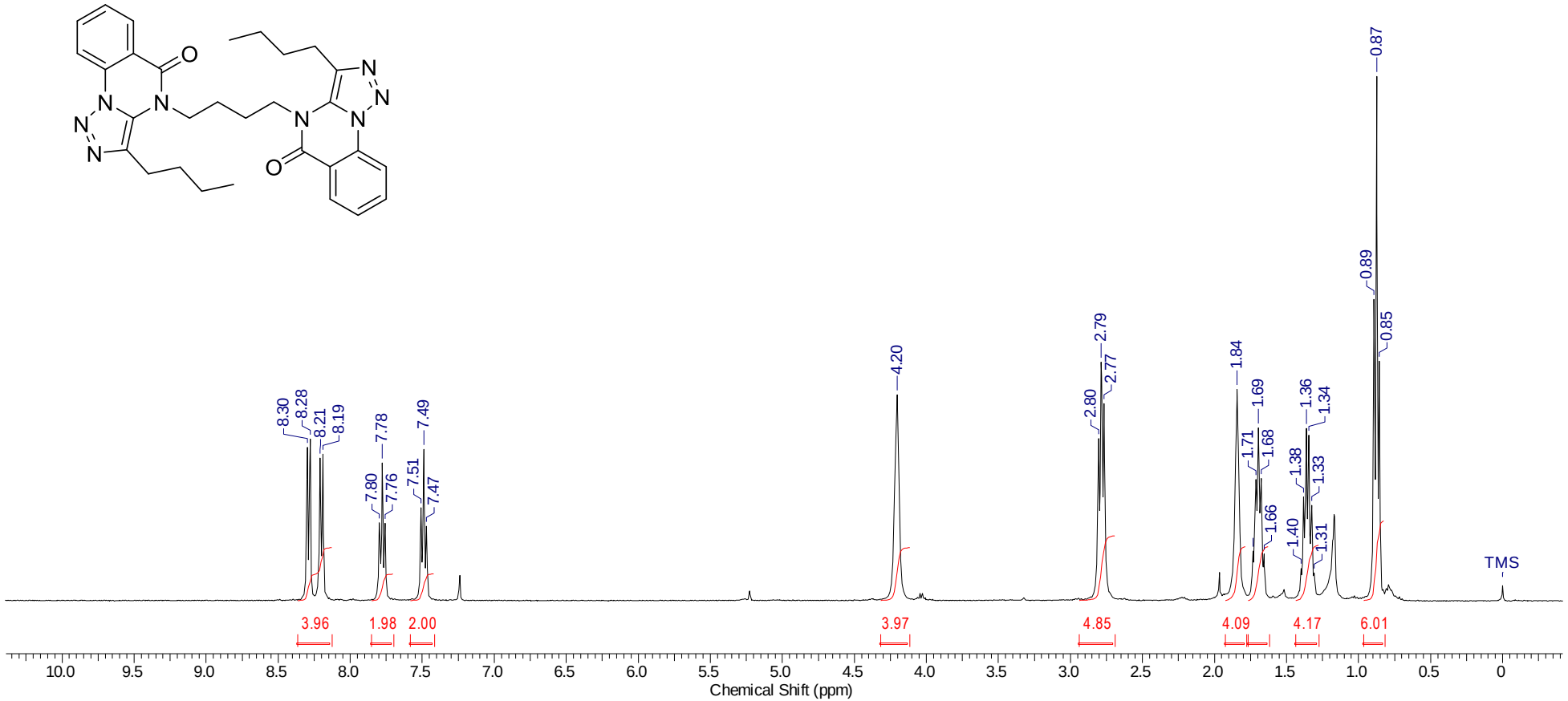
3-Butyl-4-[2-(3,5-dimethylisoxazol-4-yl)ethyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2y)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



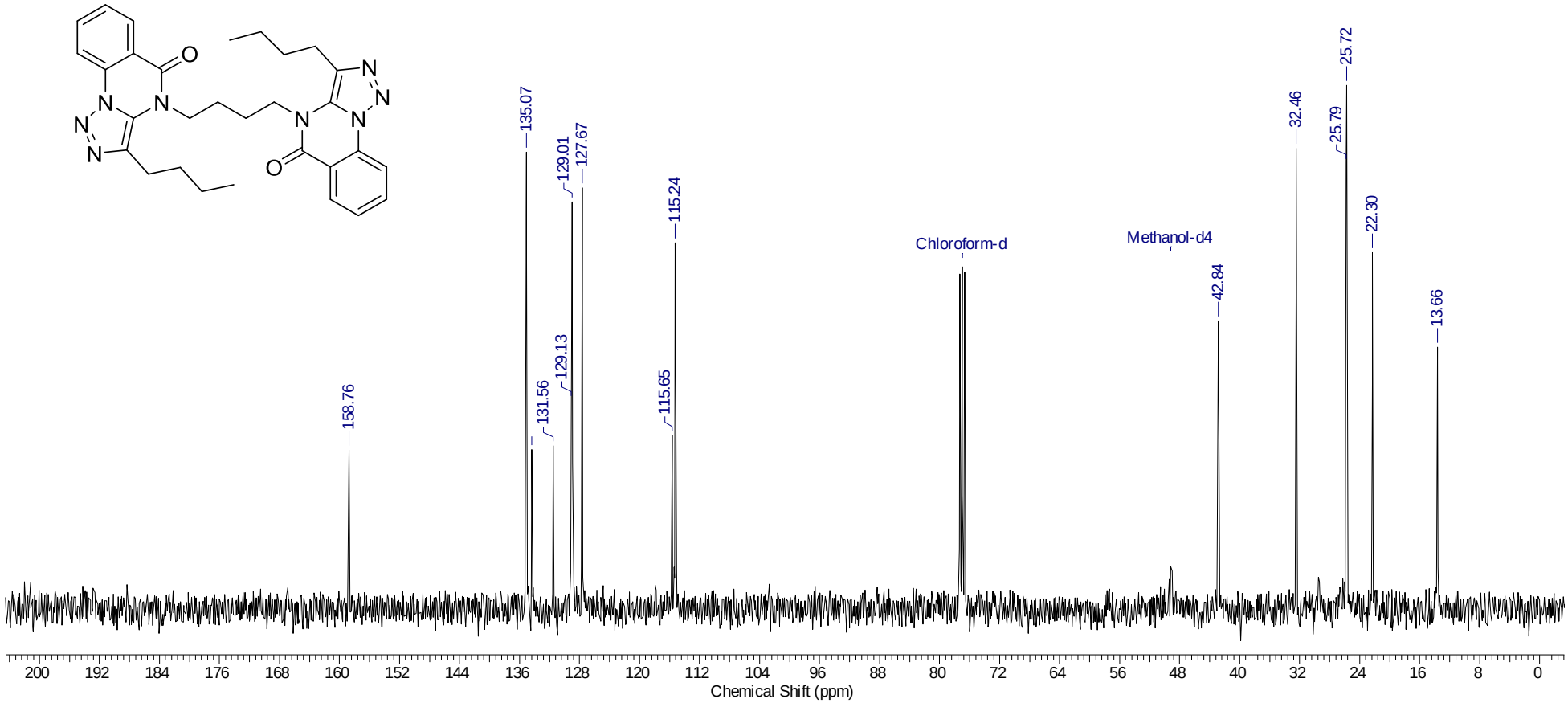
4,4'-Butane-1,4-diylbis(3-butyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one) (2aa)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



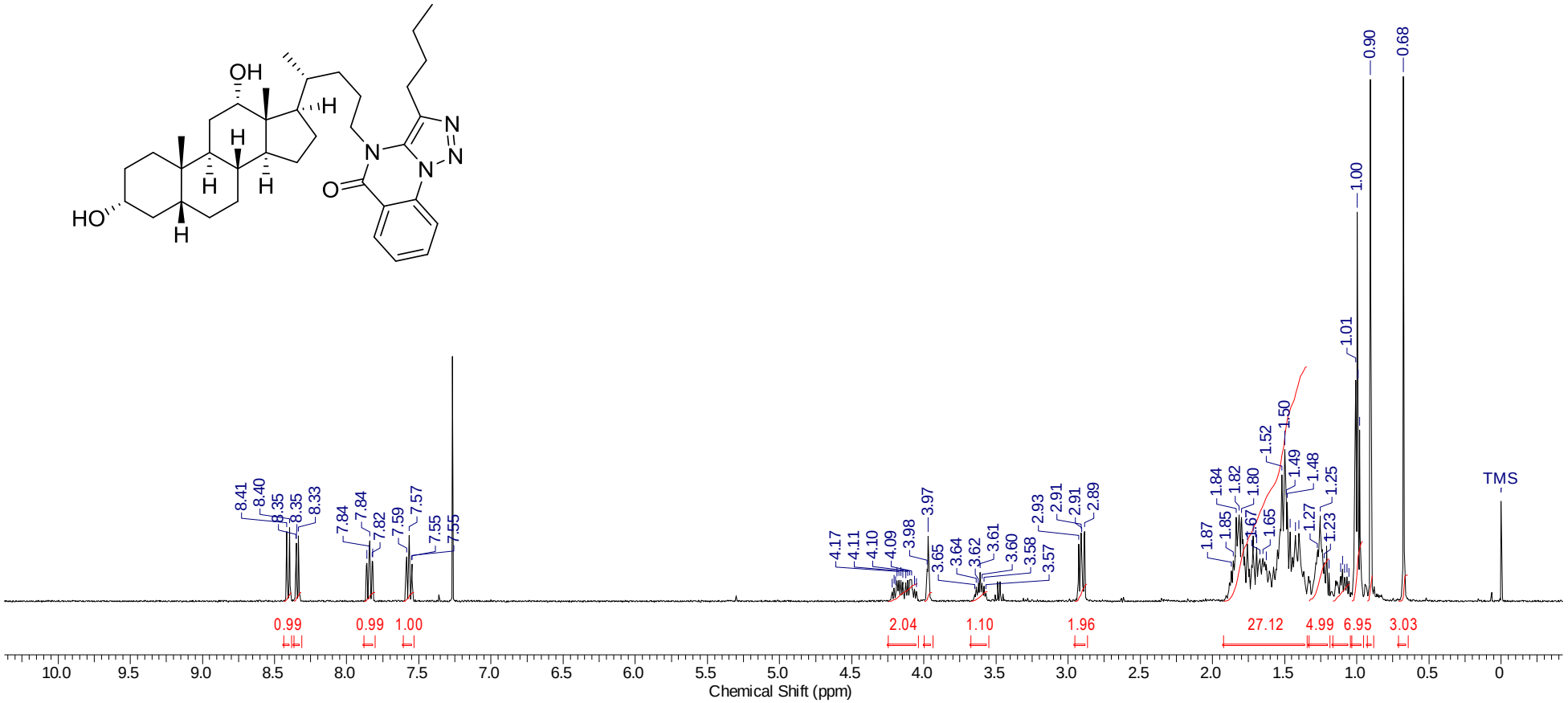
4,4'-Butane-1,4-diylbis(3-butyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one) (2aa)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$–CD_3OD)



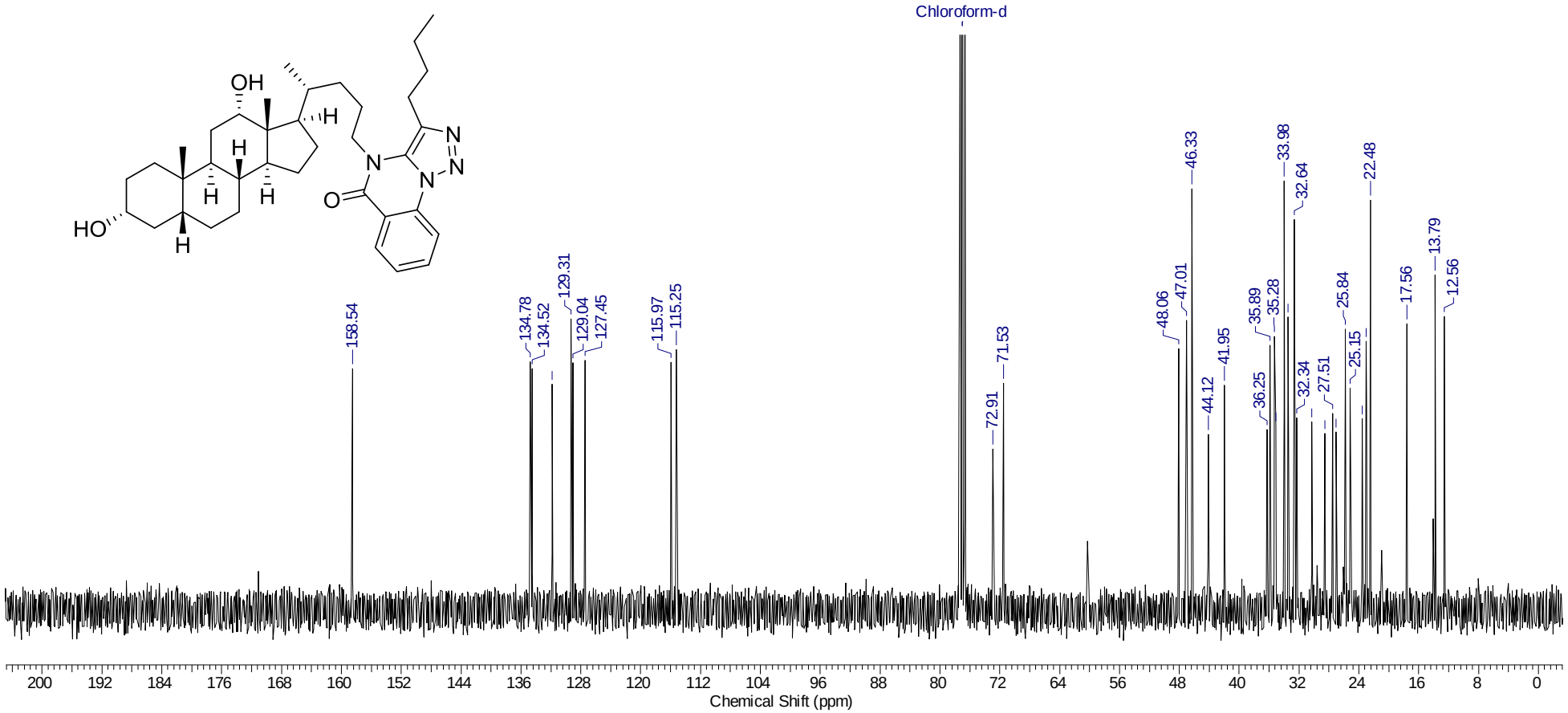
3-Butyl-4-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2ab)

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



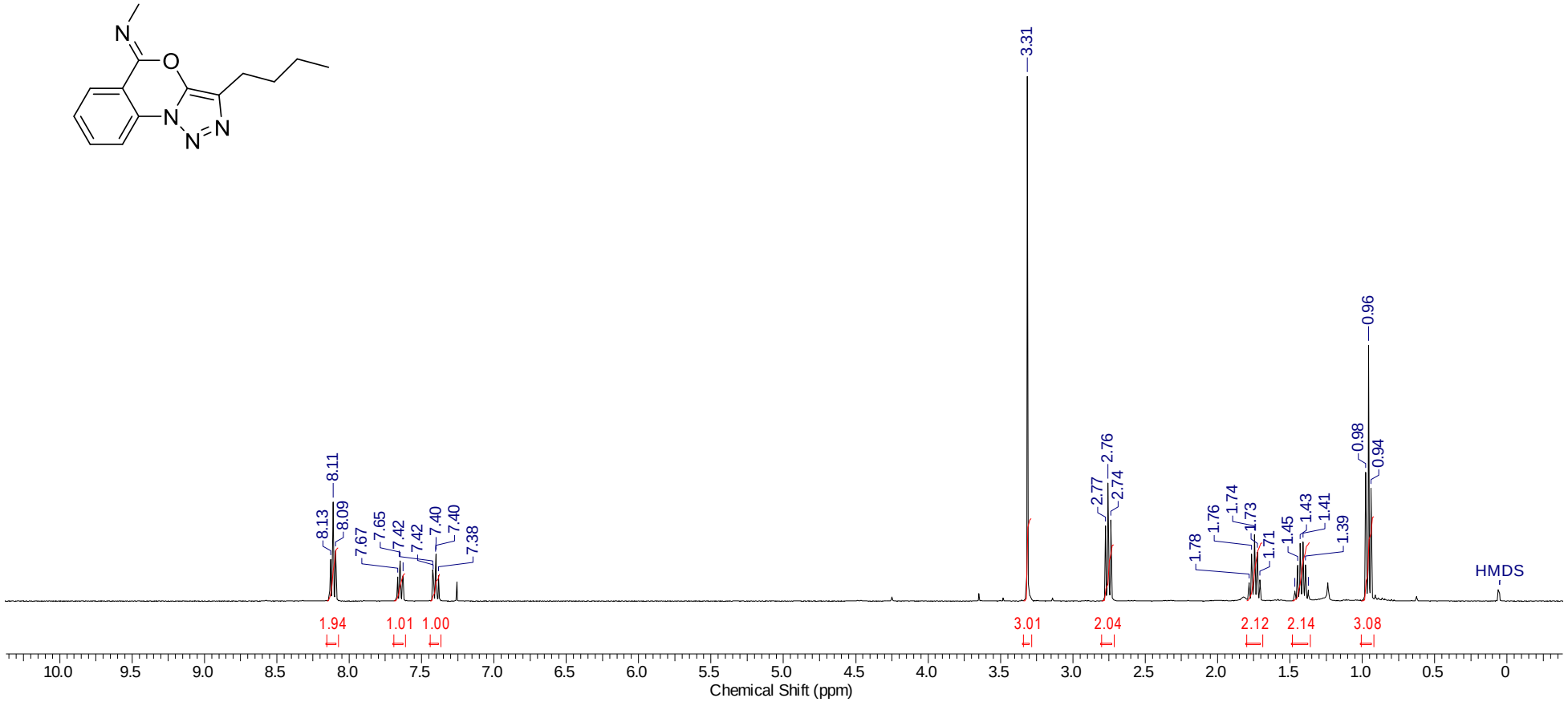
3-Butyl-4-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (2ab)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



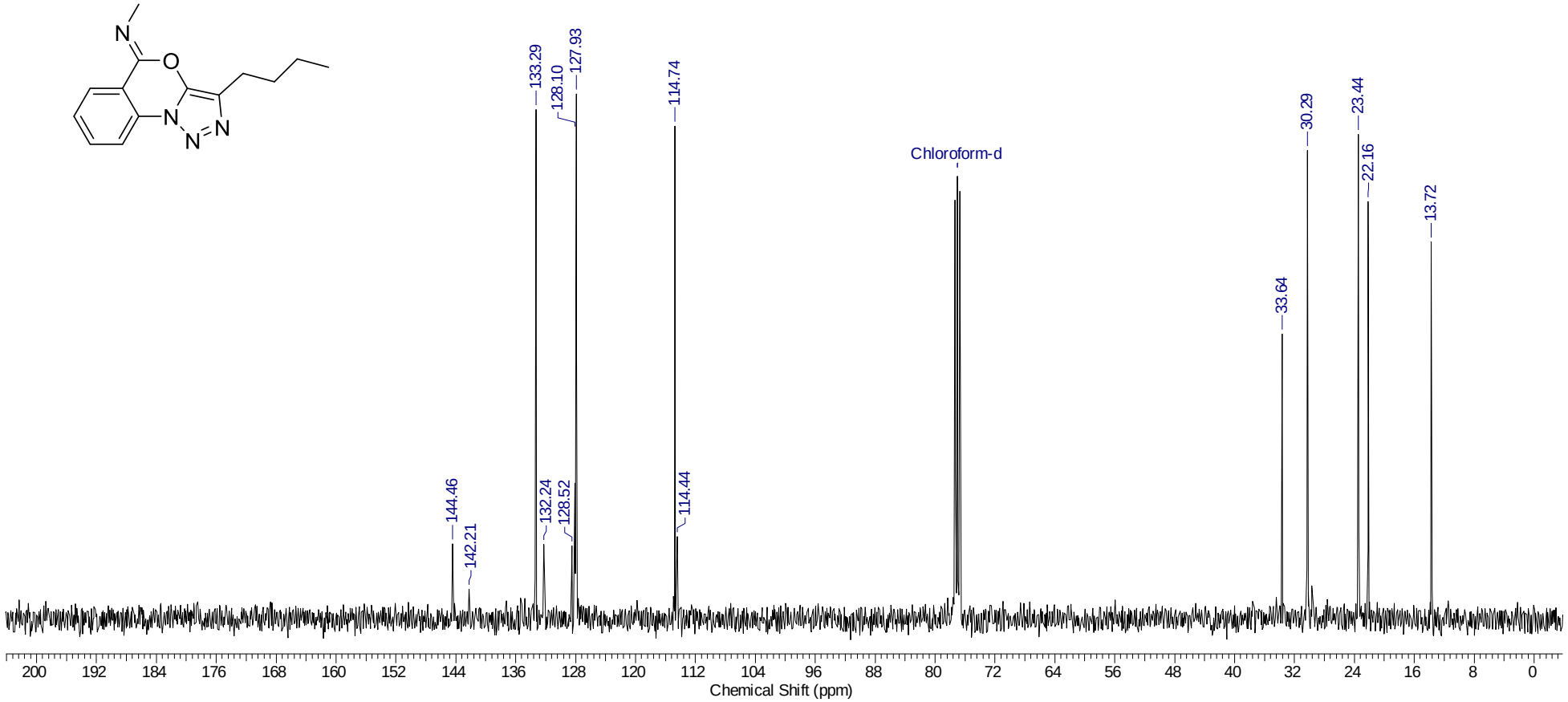
3-Butyl-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3a)

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



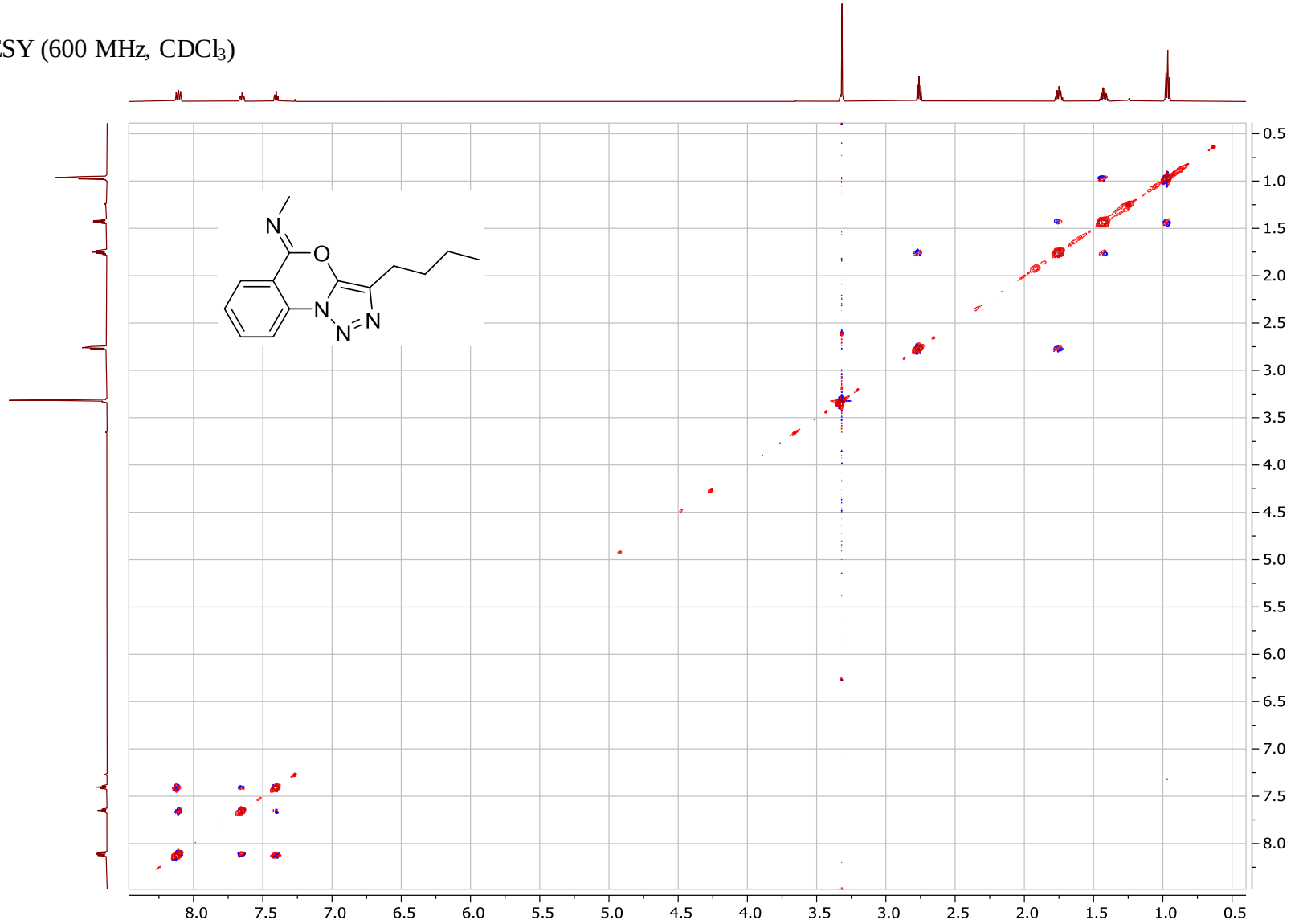
3-Butyl-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3a)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



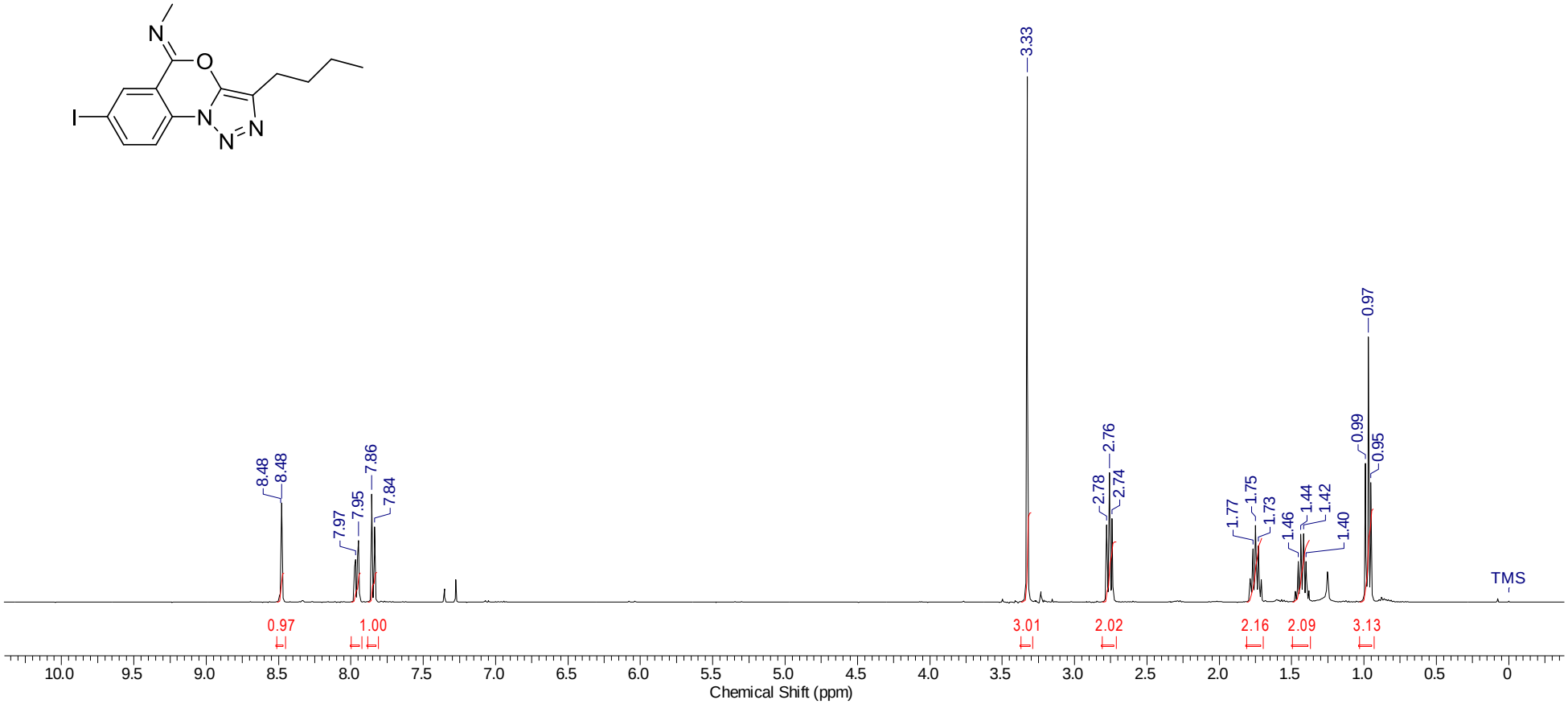
3-Butyl-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3a)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)



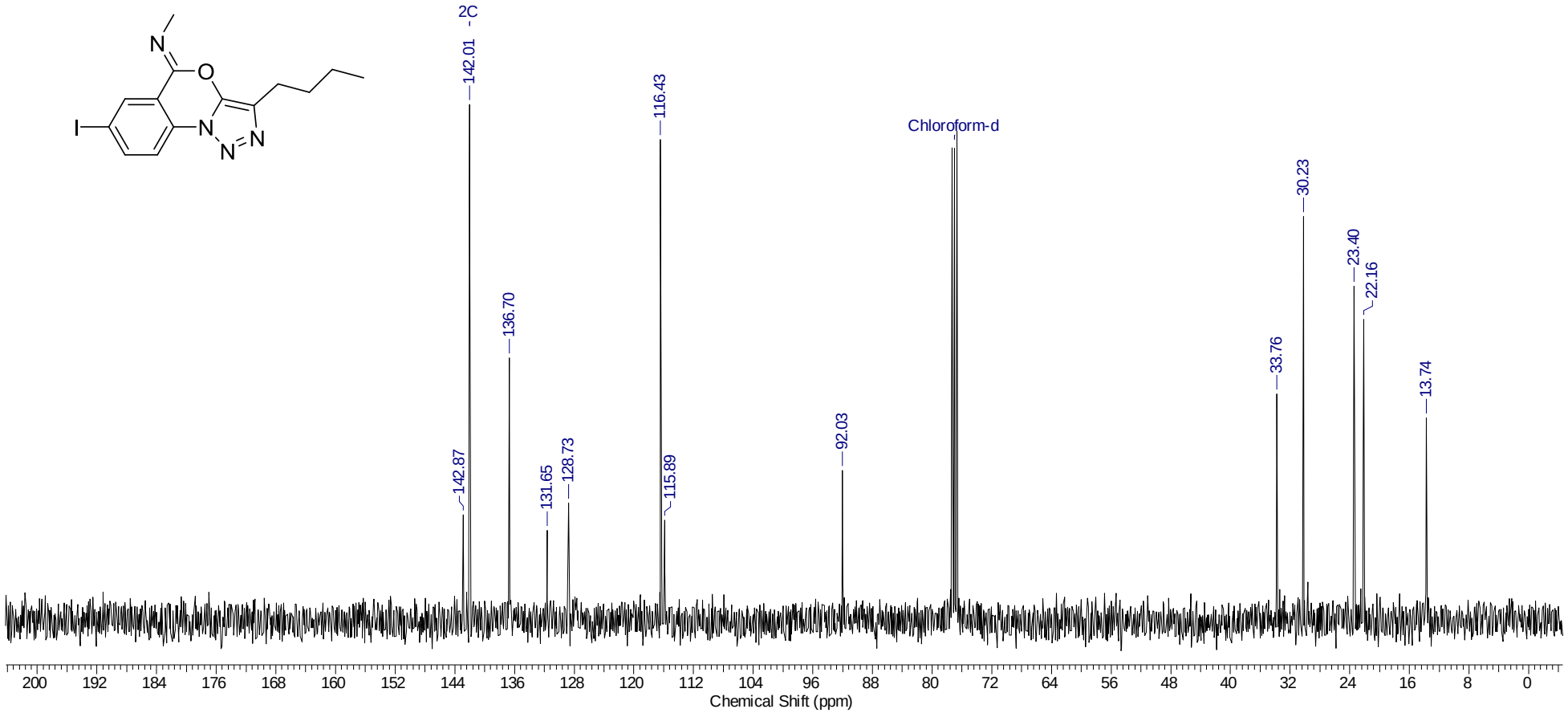
3-Butyl-7-iodo-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3c)

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



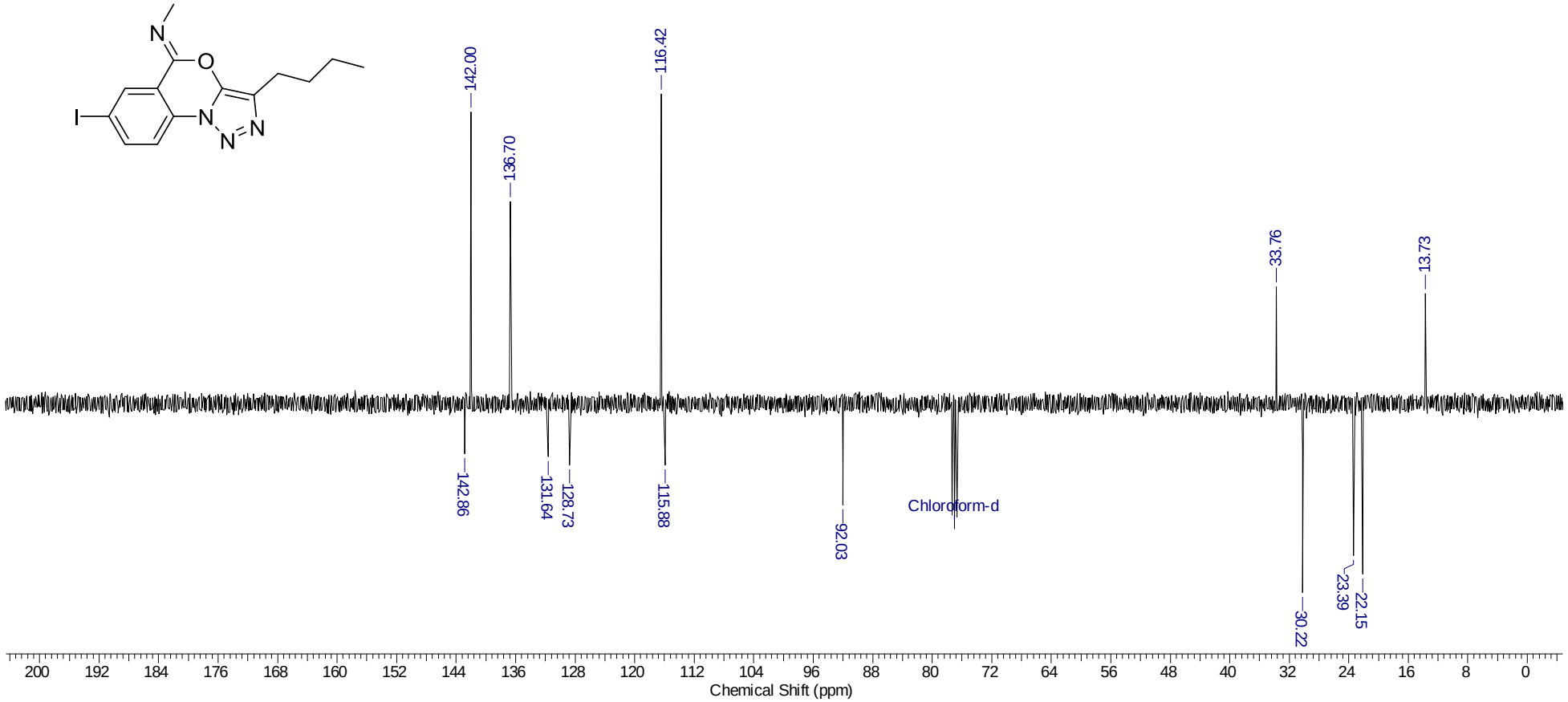
3-Butyl-7-iodo-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3c)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



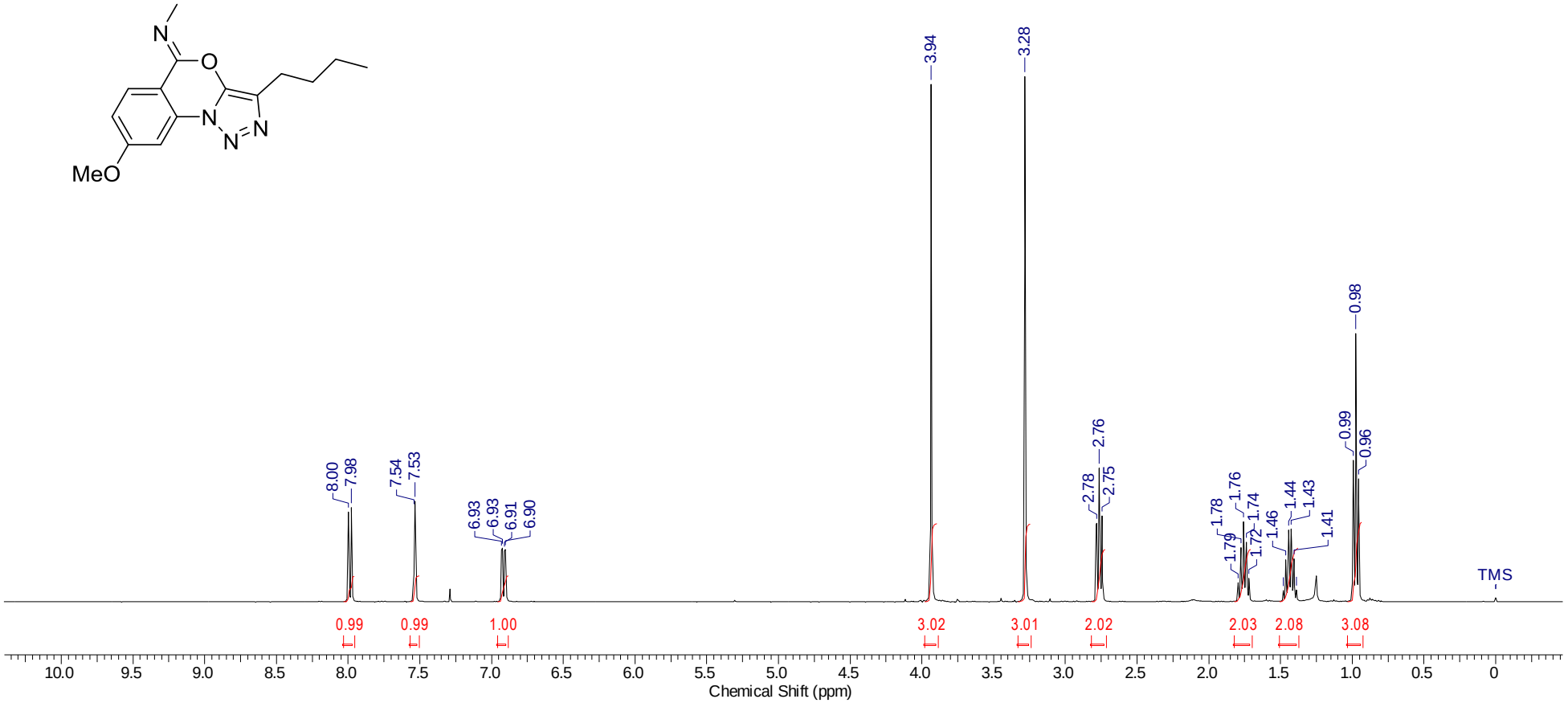
3-Butyl-7-iodo-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3c)

APT (100 MHz, $CDCl_3$)



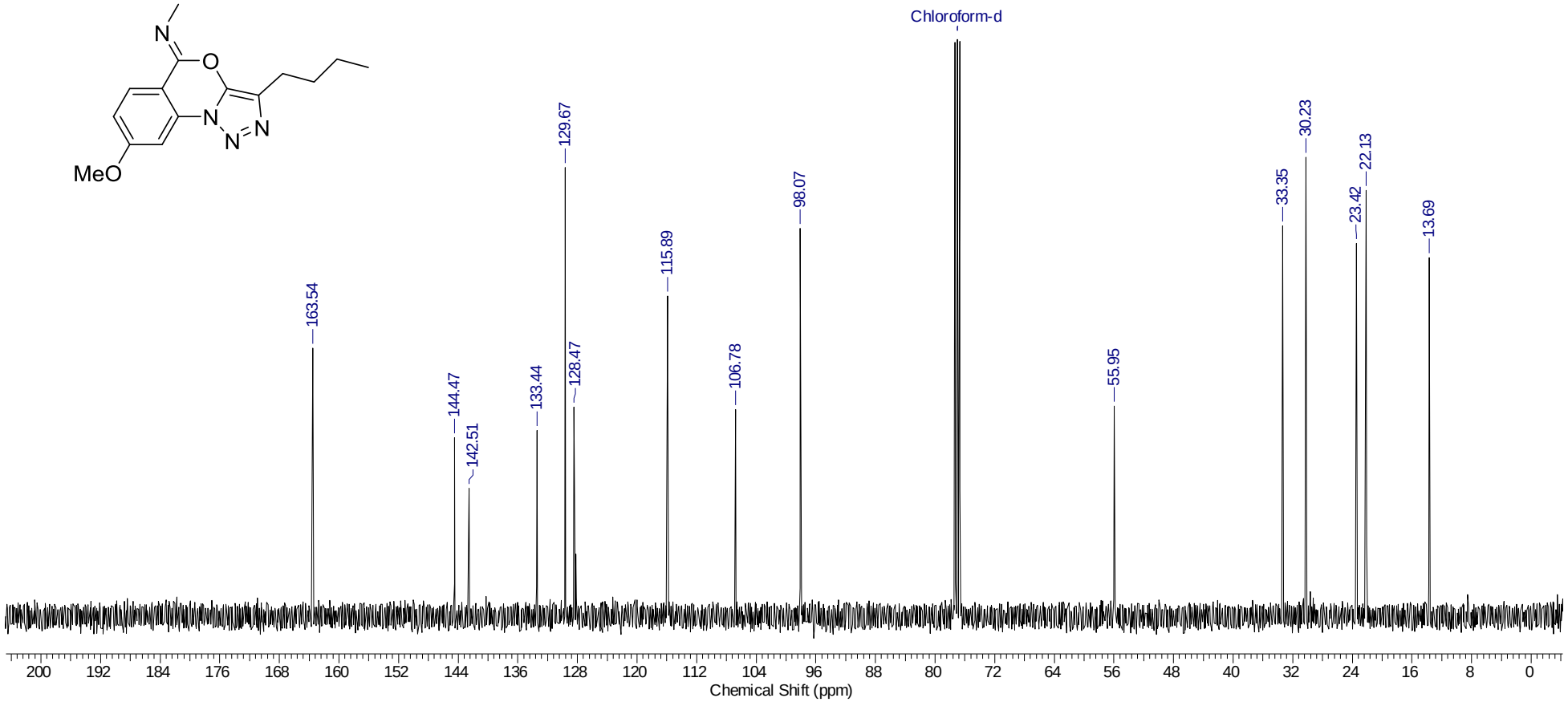
3-Butyl-8-methoxy-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3d)

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



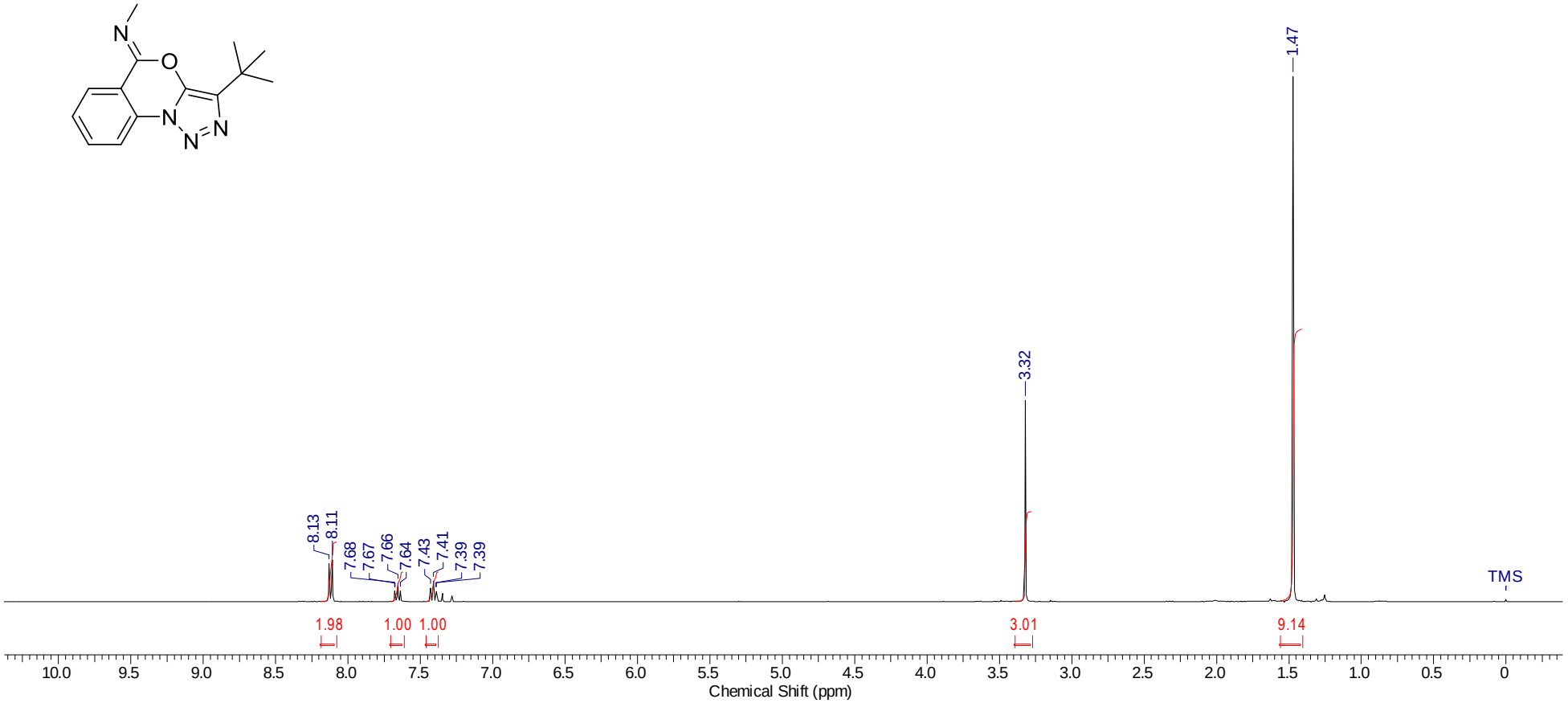
3-Butyl-8-methoxy-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3d)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



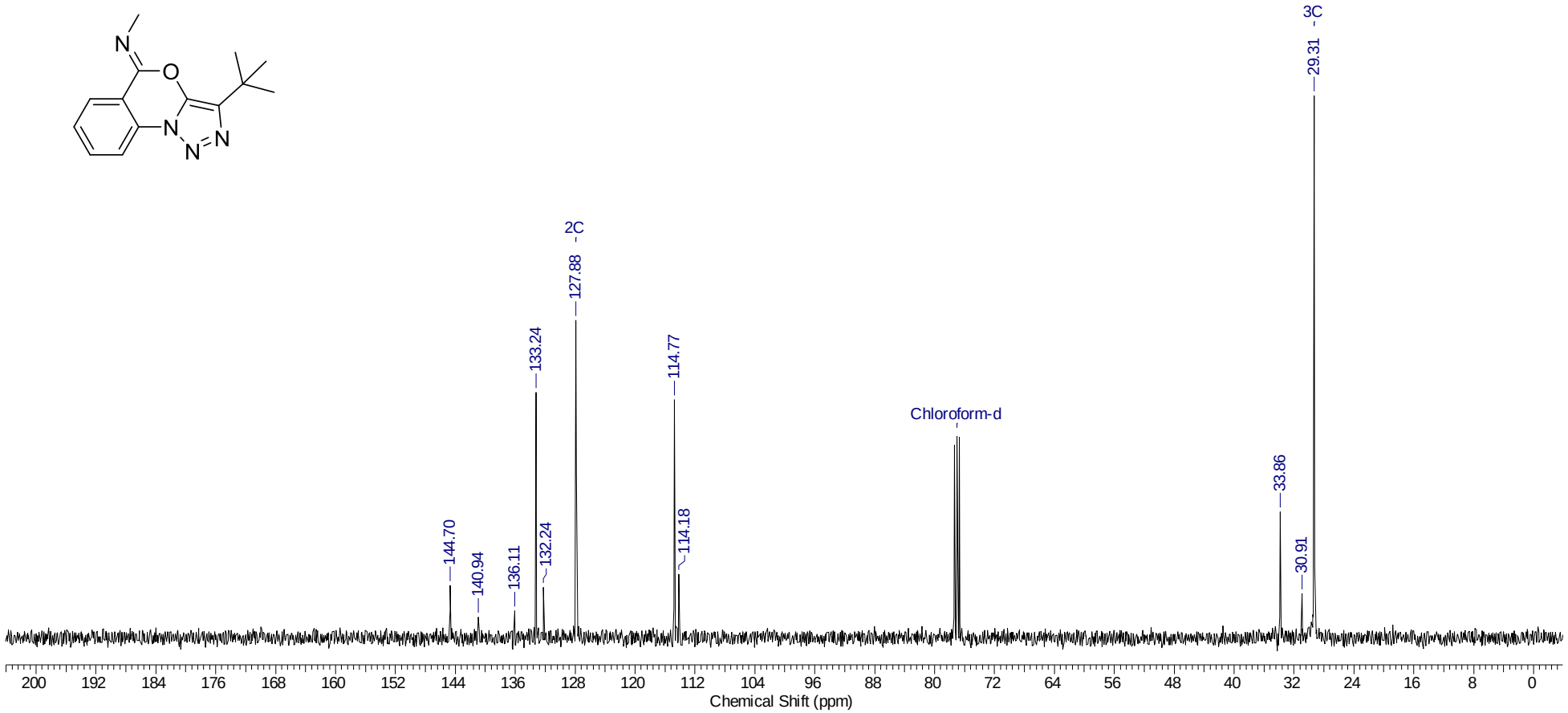
3-*tert*-Butyl-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3g)

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



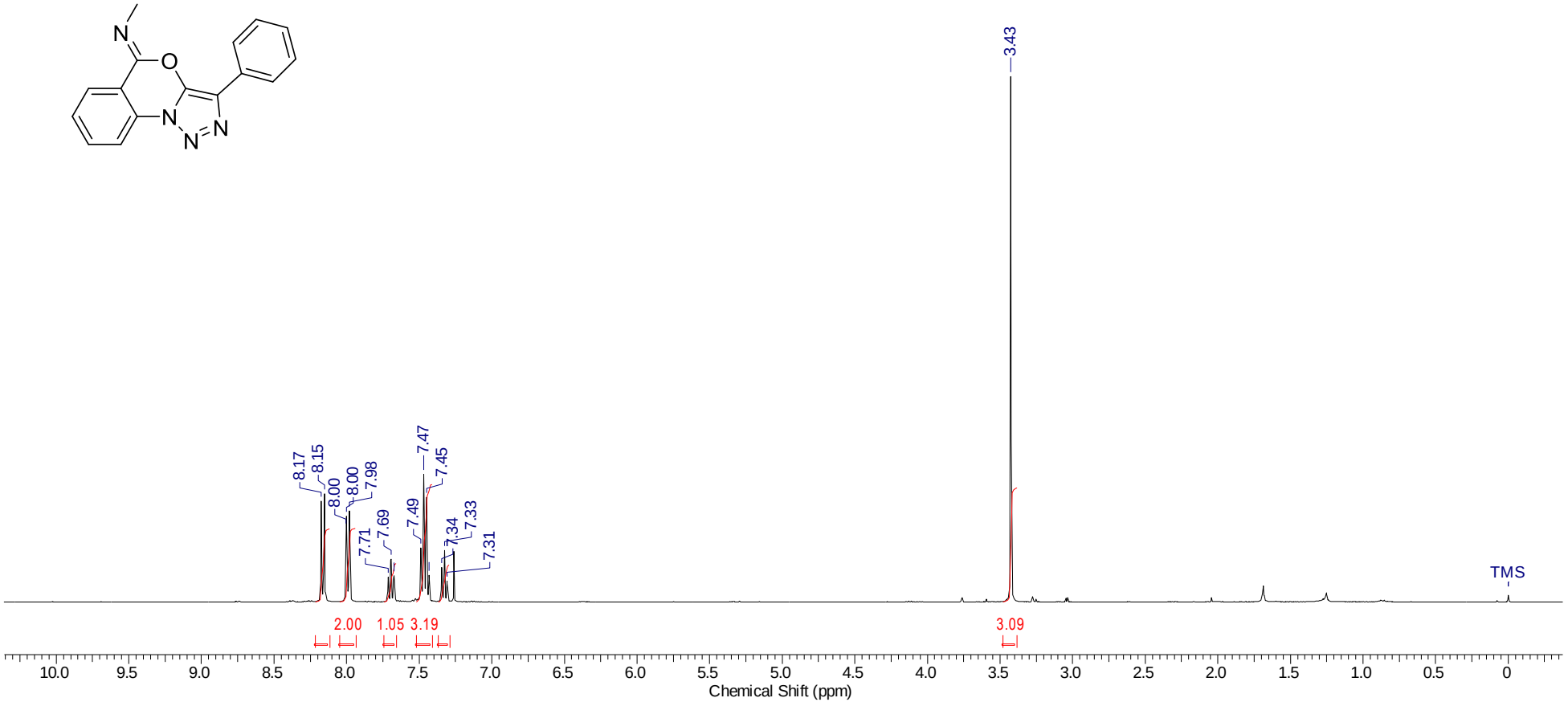
3-*tert*-Butyl-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3g)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



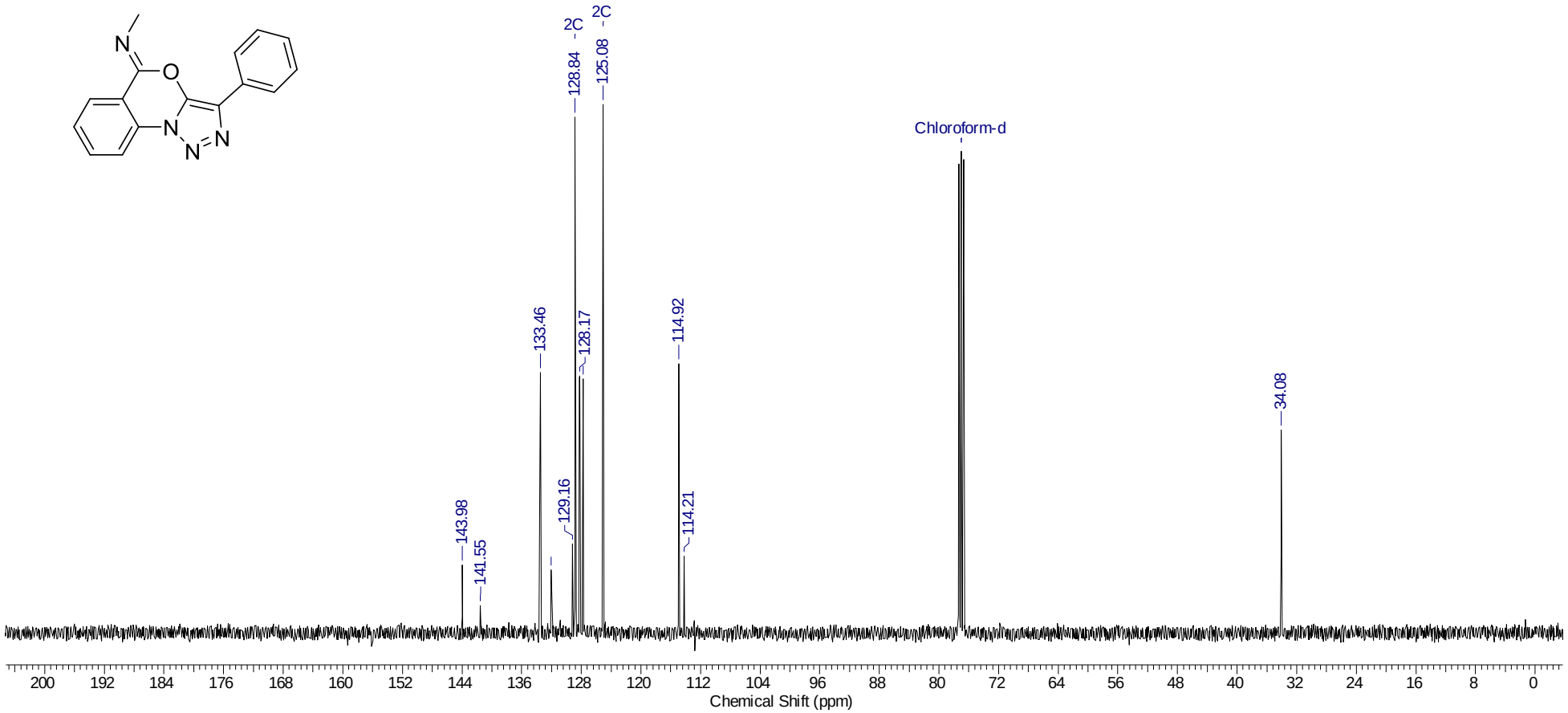
_N_-Methyl-3-phenyl-5_H_-[1,2,3]triazolo[1,5-_a_][3,1]benzoxazin-5-imine (3h)

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



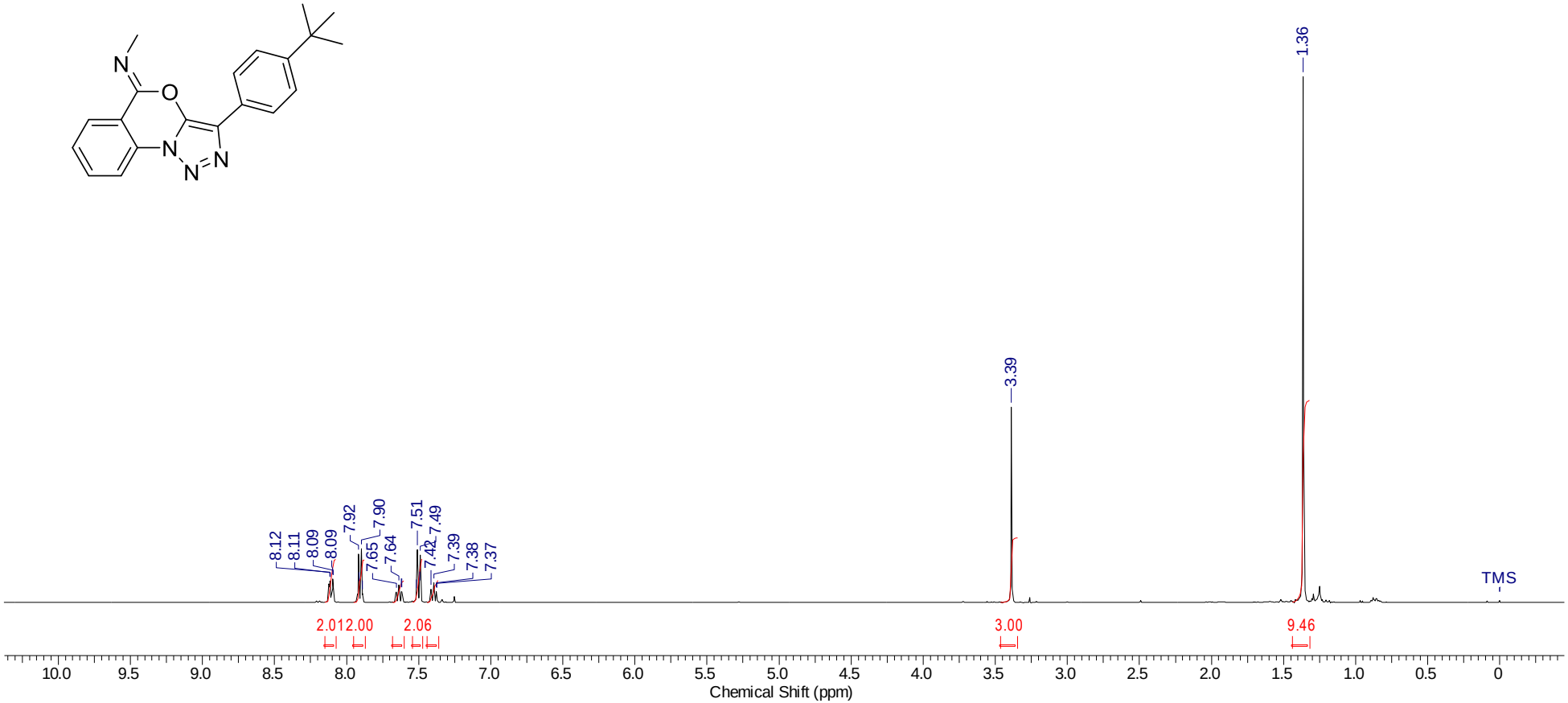
_N_-Methyl-3-phenyl-5_H_-[1,2,3]triazolo[1,5-_a_][3,1]benzoxazin-5-imine (3h)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



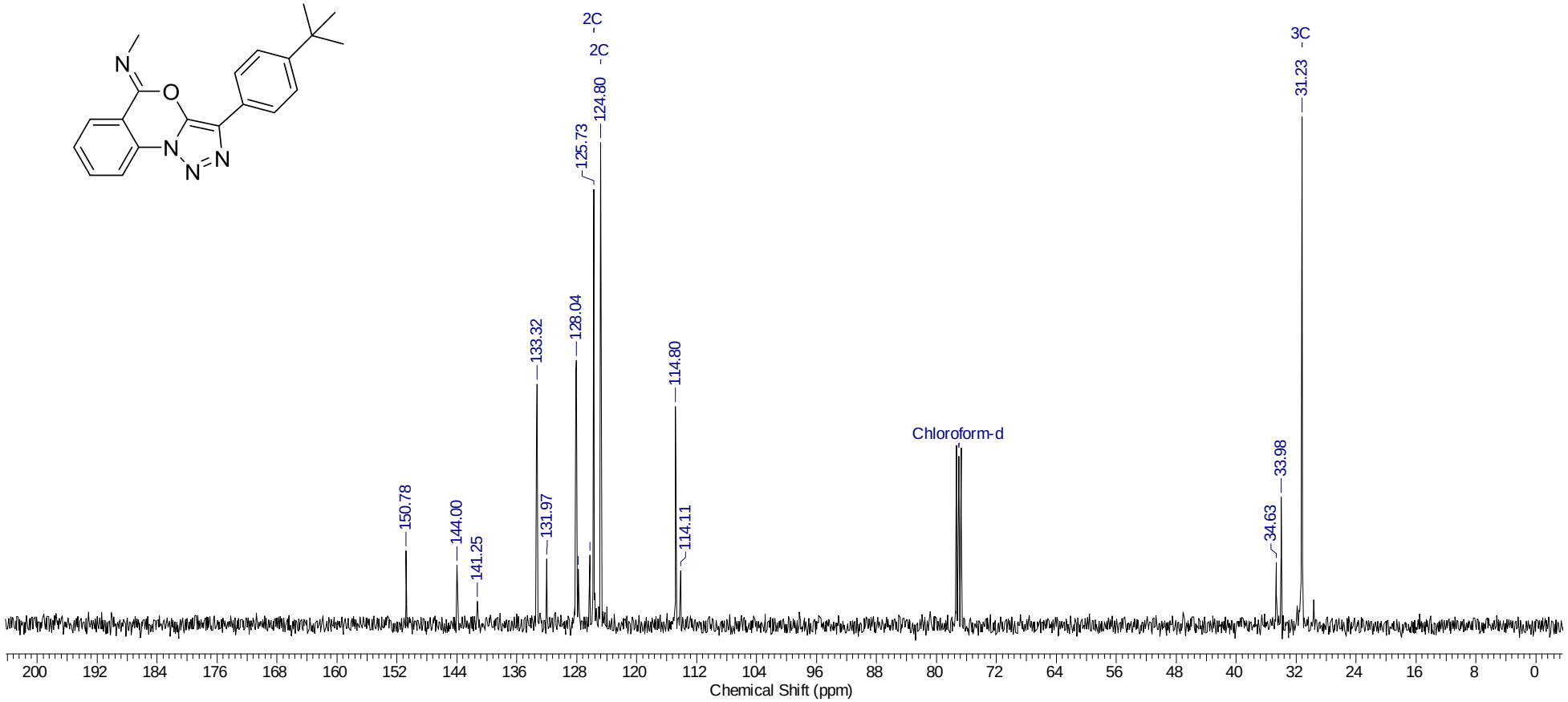
3-(4-*tert*-Butylphenyl)-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3l)

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



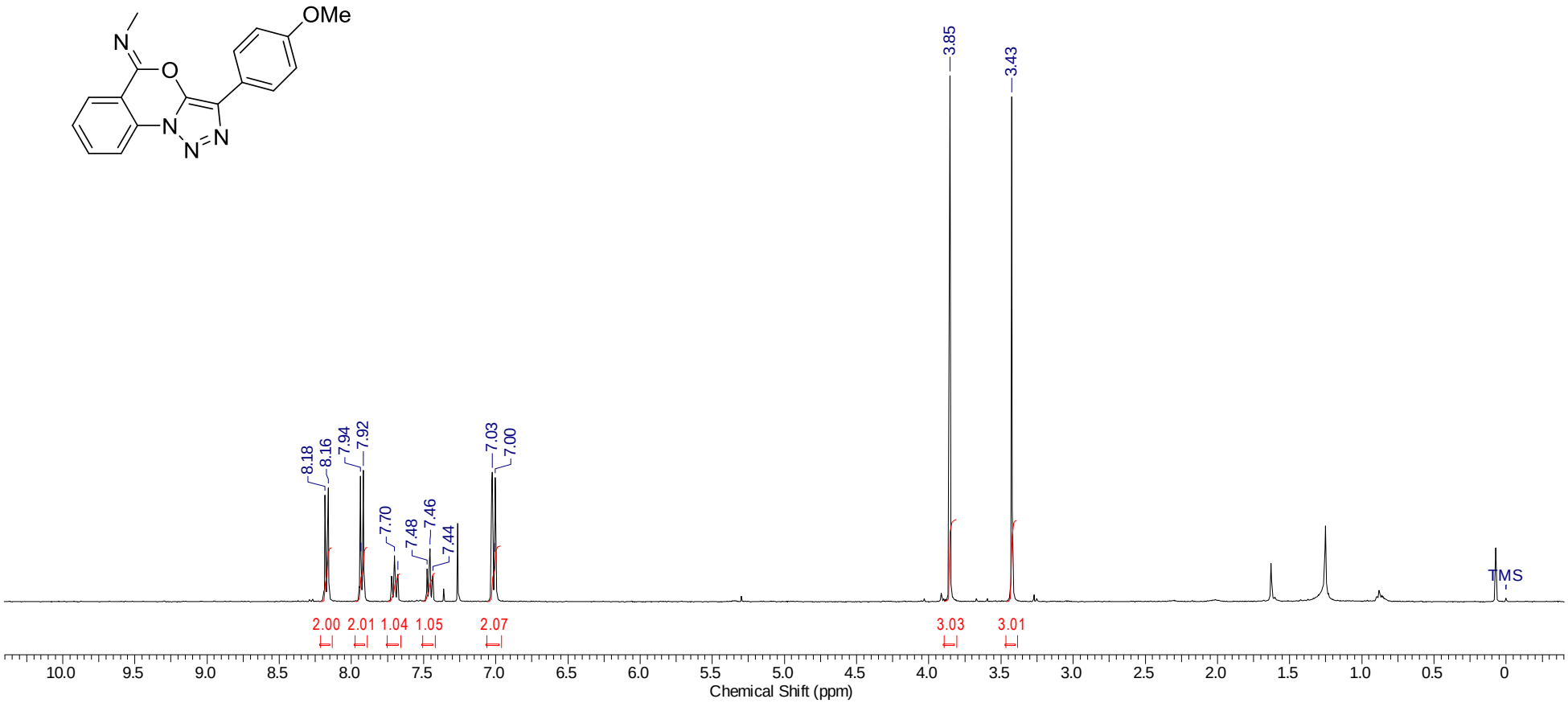
3-(4-*tert*-Butylphenyl)-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3l)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



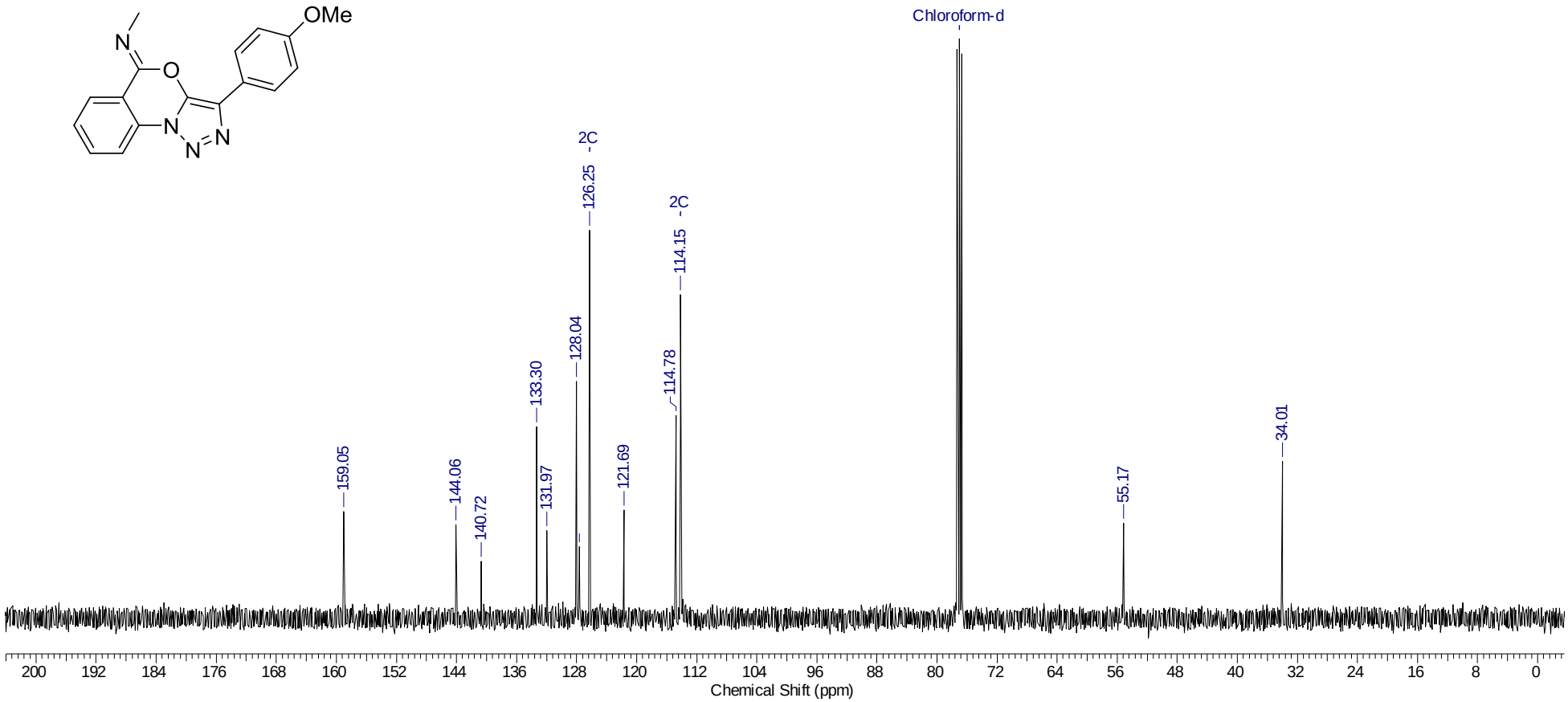
3-(4-Methoxyphenyl)-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3m)

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



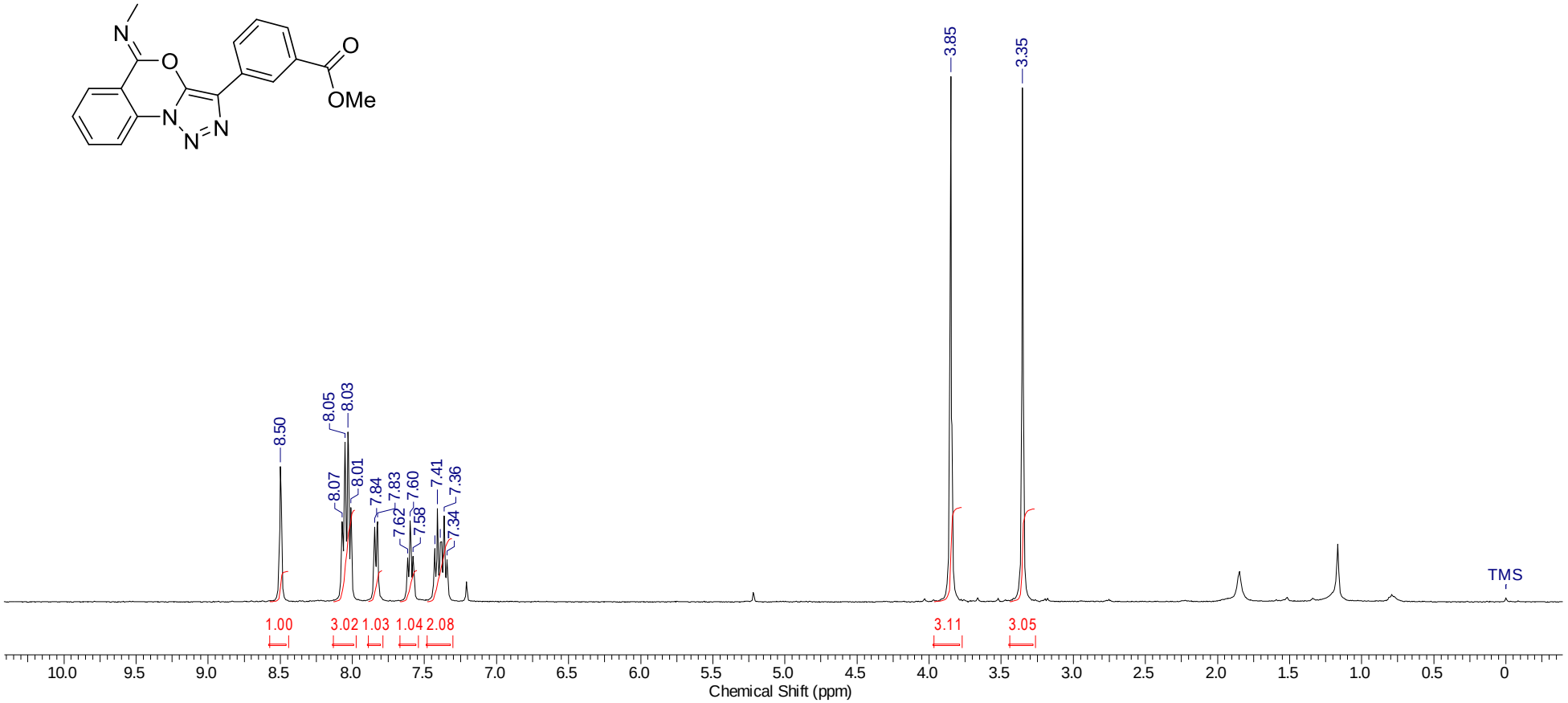
3-(4-Methoxyphenyl)-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3m)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



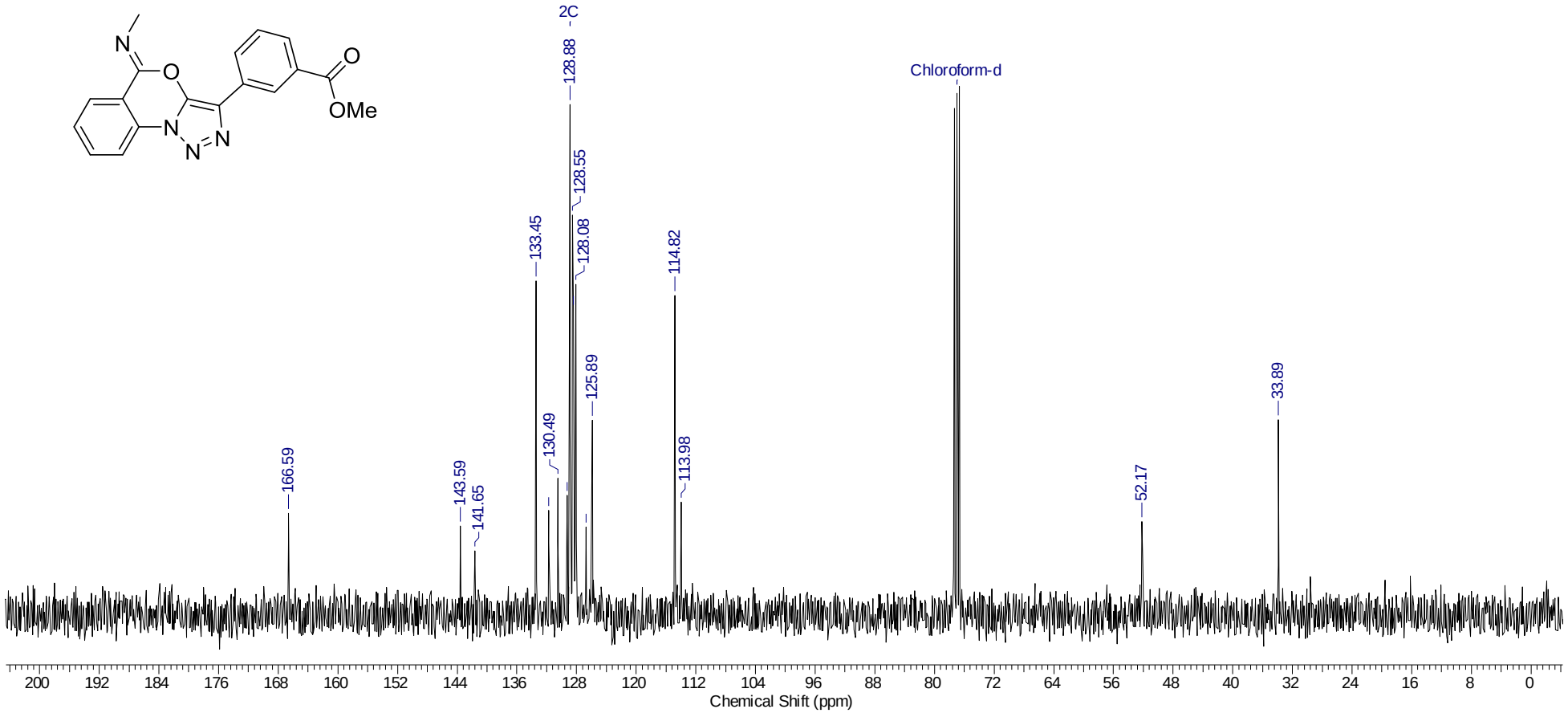
Methyl 3-[5-(methylimino)-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-3-yl]benzoate (3n)

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



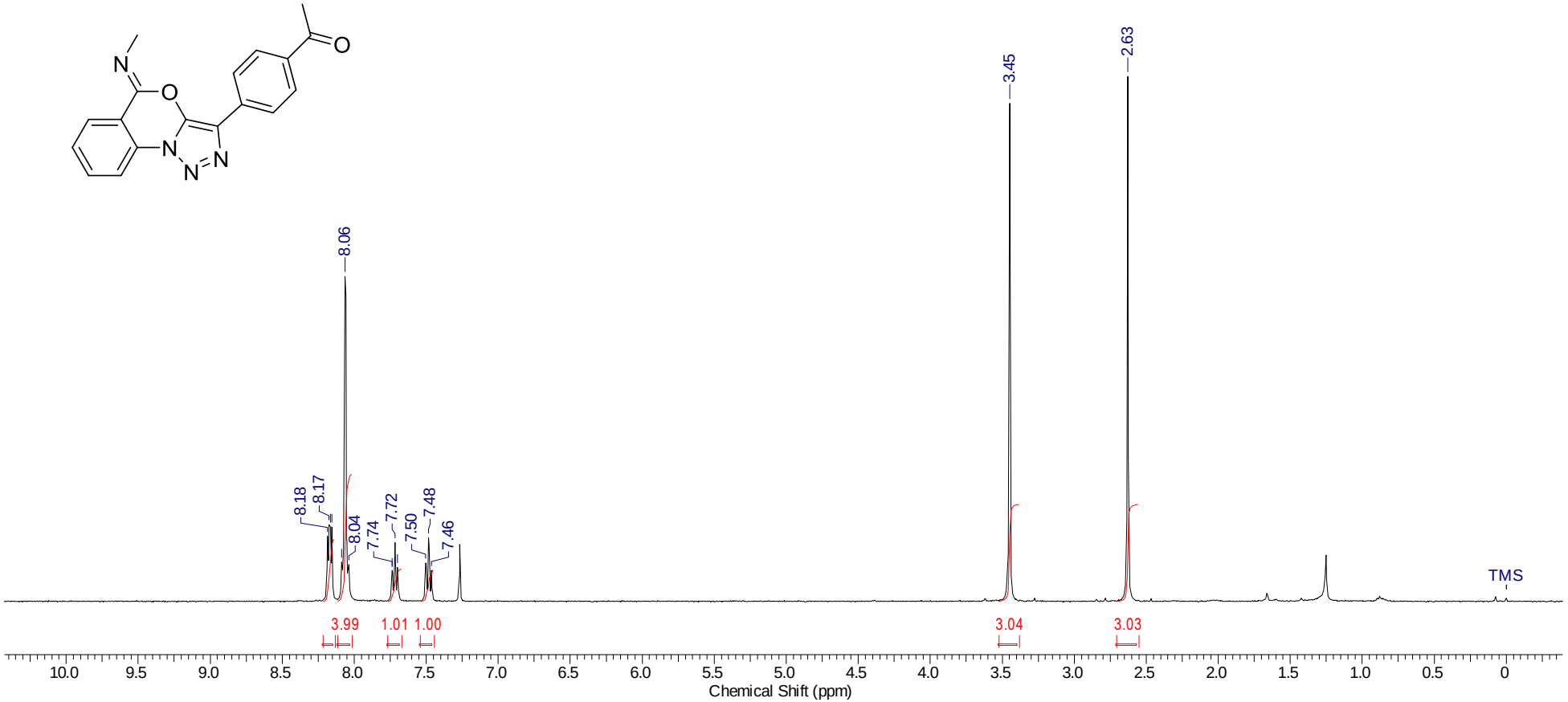
Methyl 3-[5-(methylimino)-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-3-yl]benzoate (3n)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



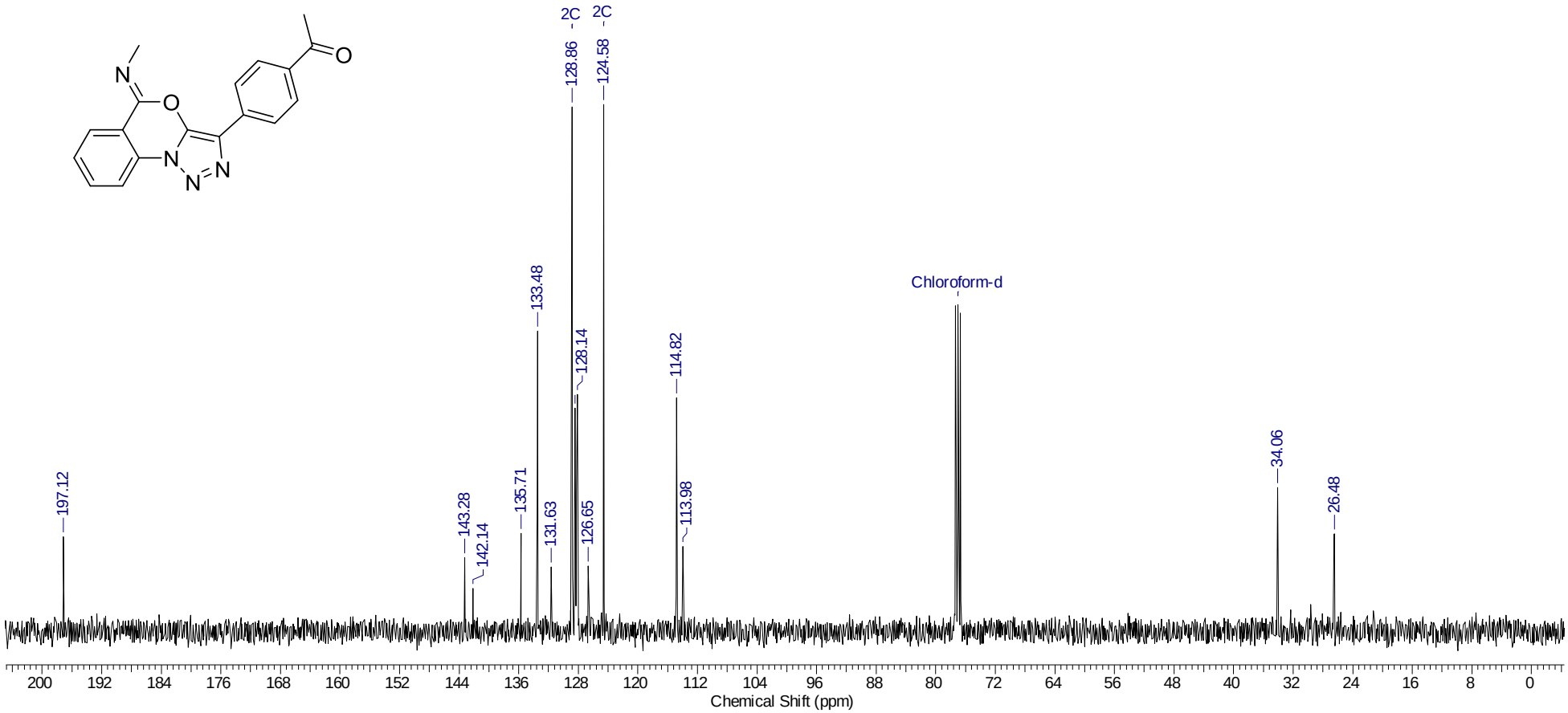
3-(4-Acetylphenyl)-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3o)

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



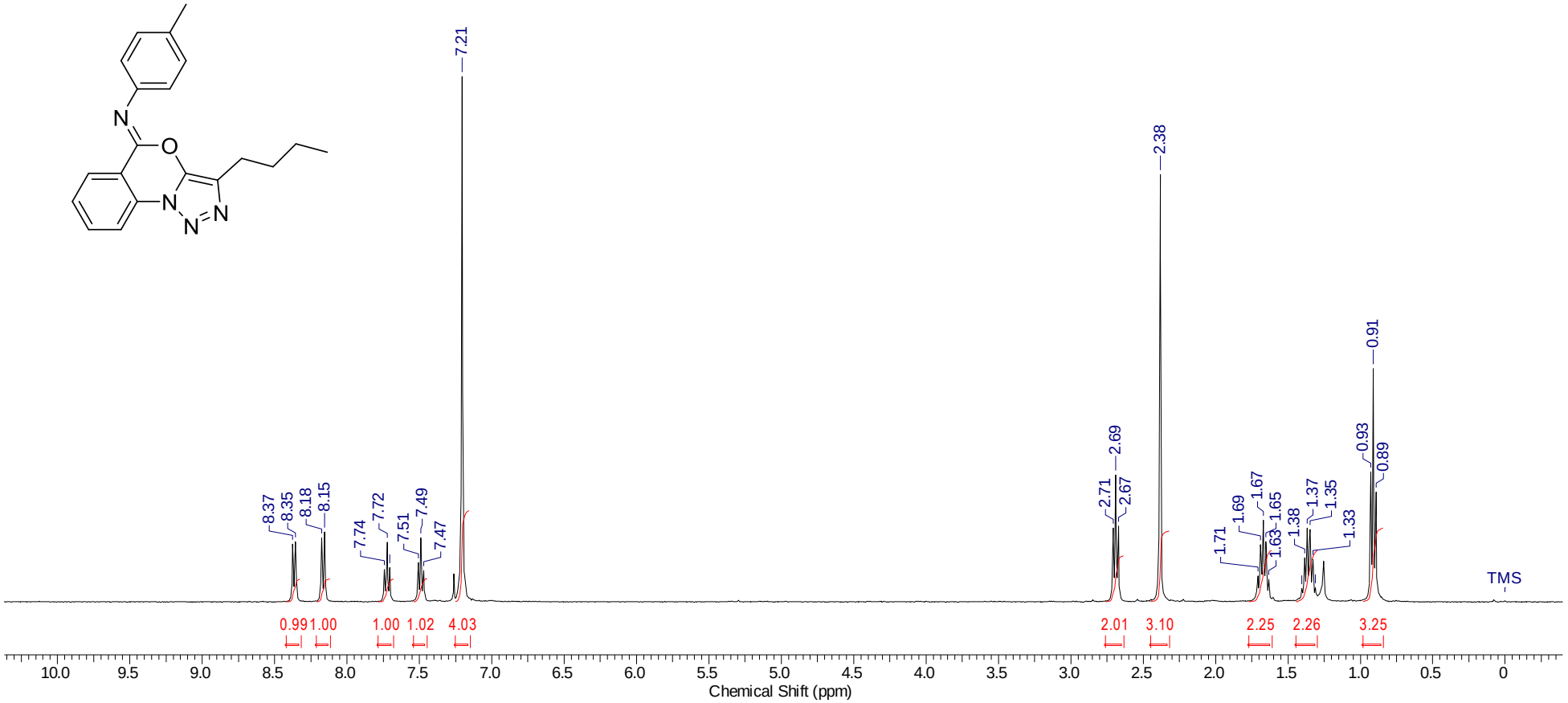
3-(4-Acetylphenyl)-*N*-methyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3o)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



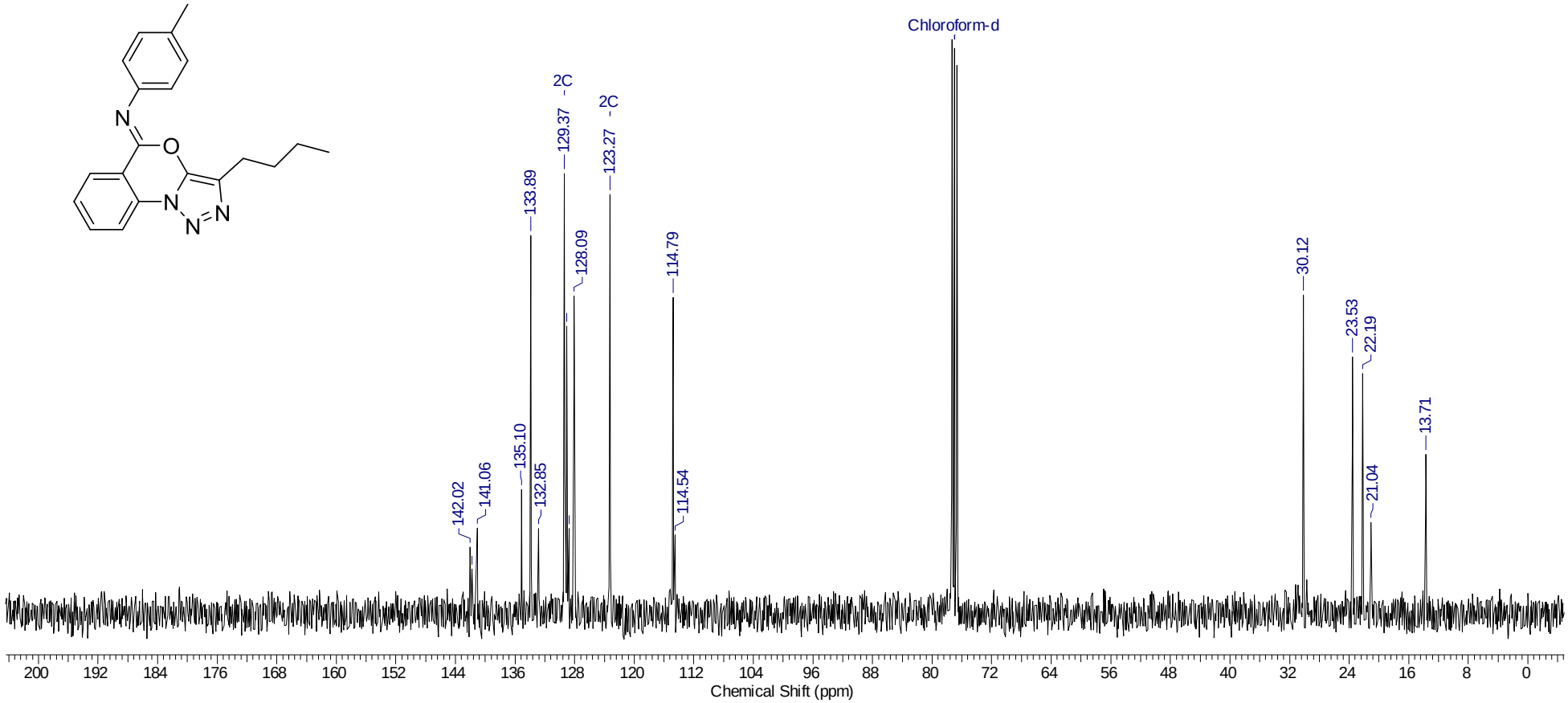
3-Butyl-*N*-(4-methylphenyl)-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3q)

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



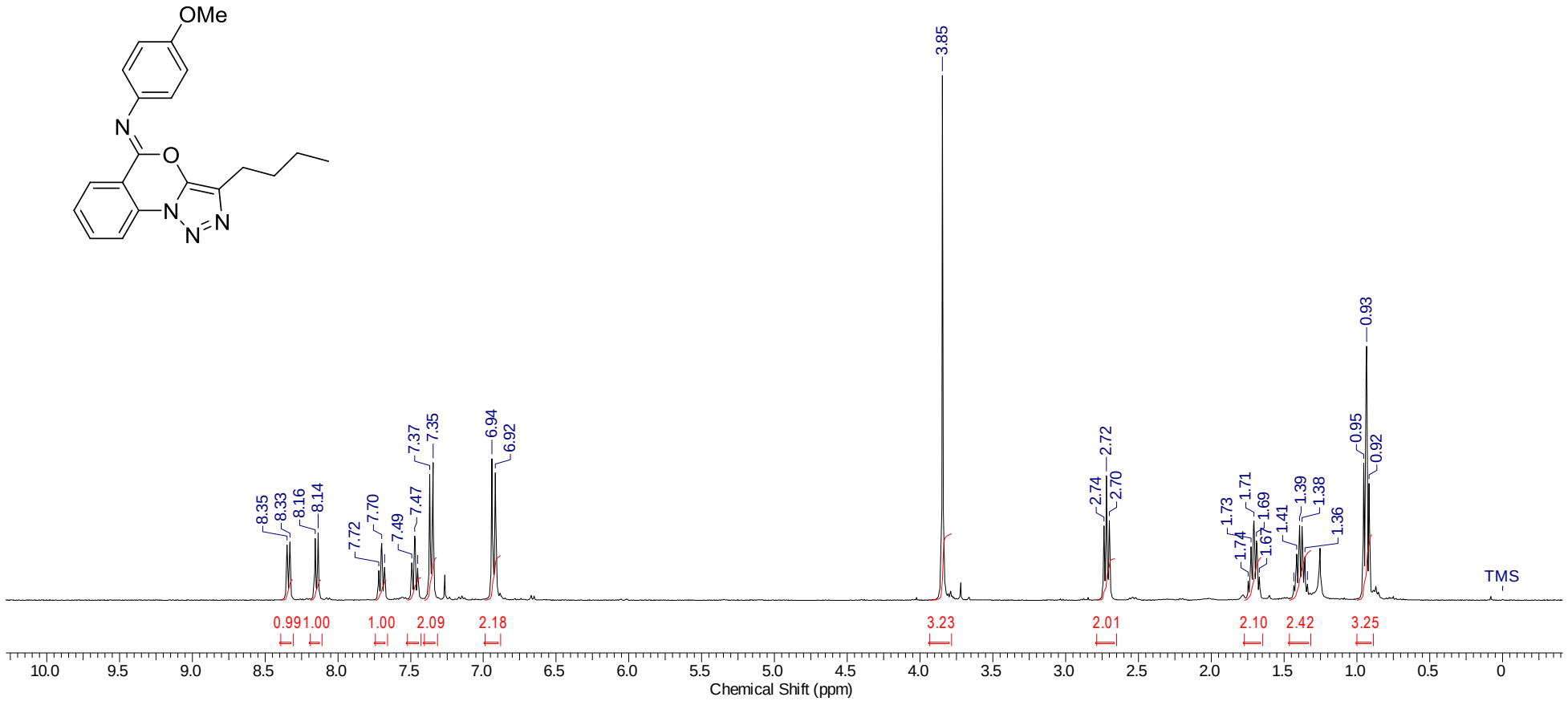
3-Butyl-*N*-(4-methylphenyl)-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3q)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



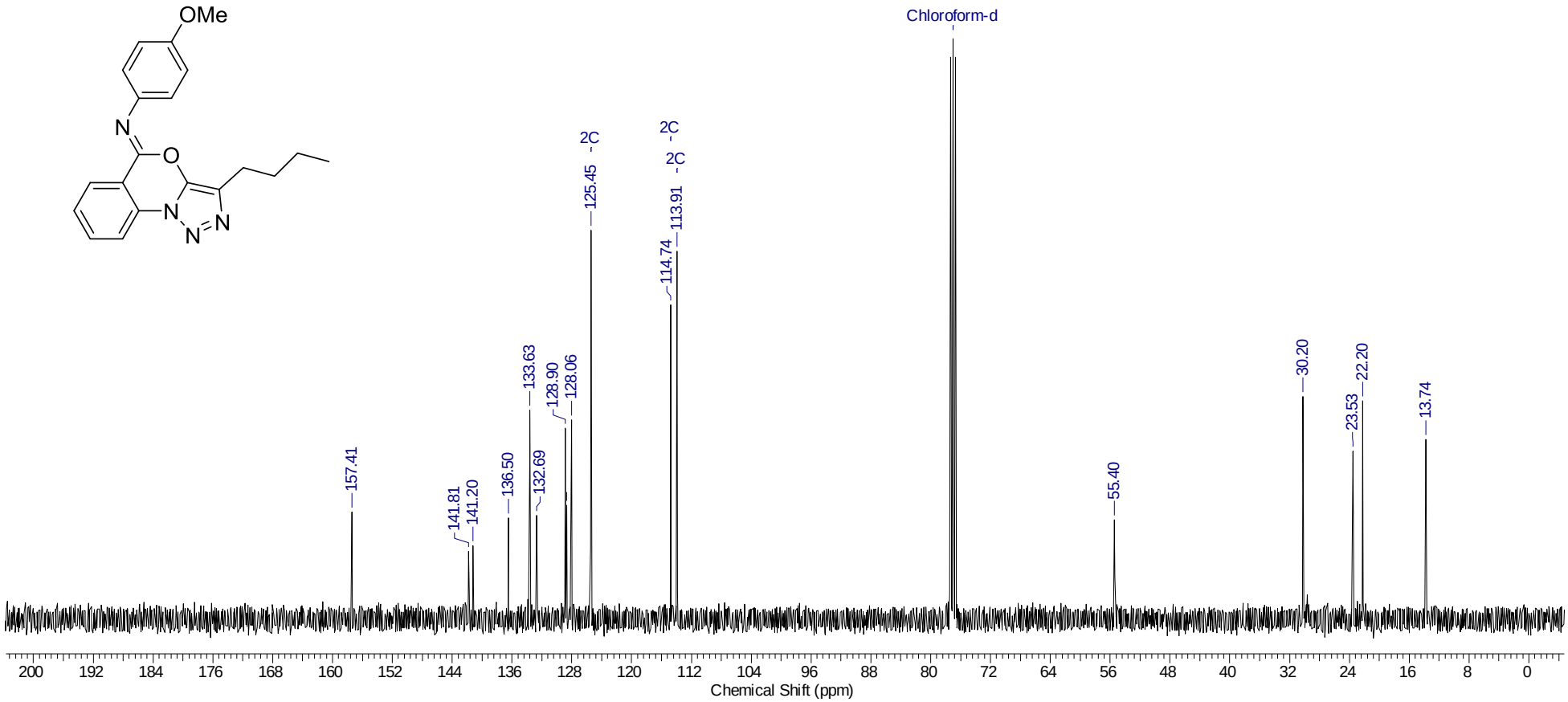
3-Butyl-*N*-(4-methoxyphenyl)-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3r)

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



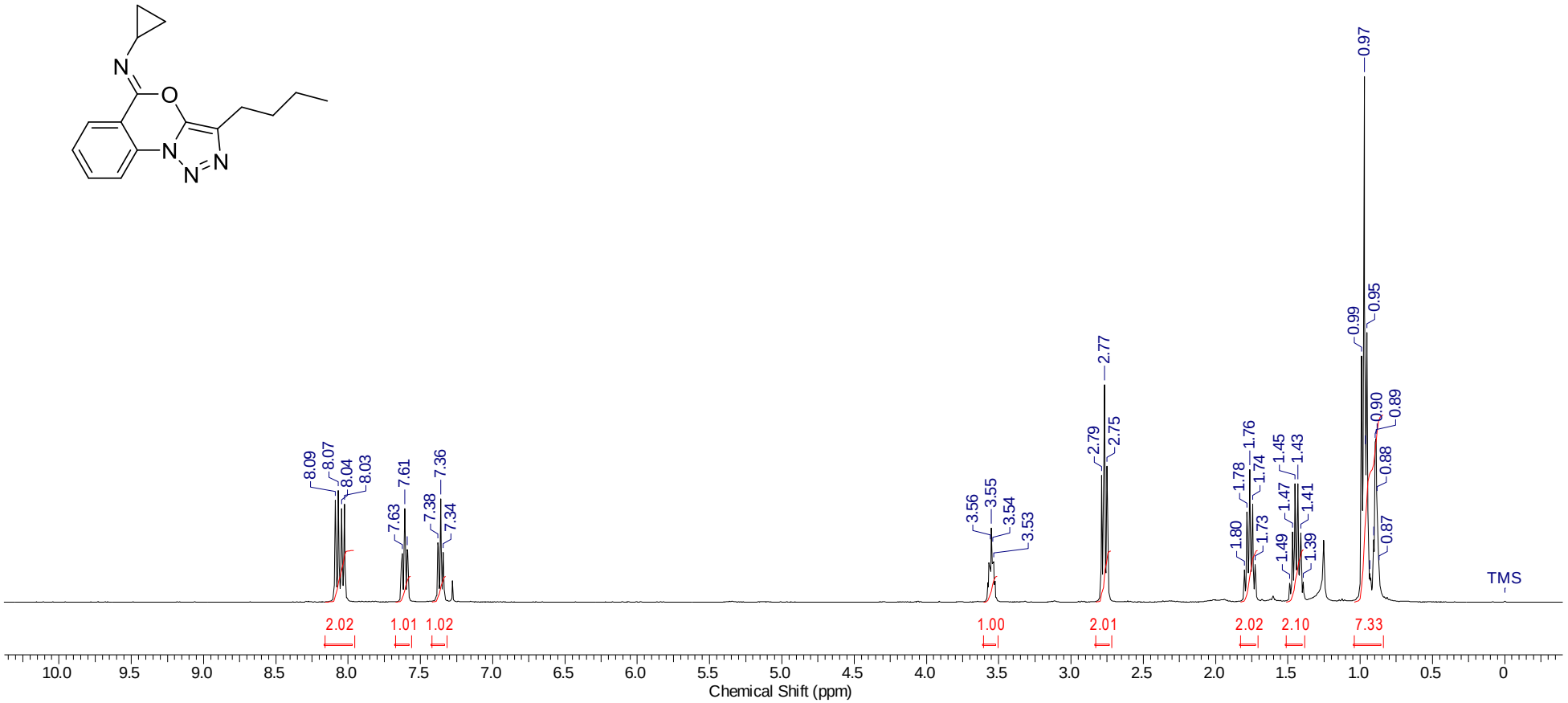
3-Butyl-*N*-(4-methoxyphenyl)-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3r)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



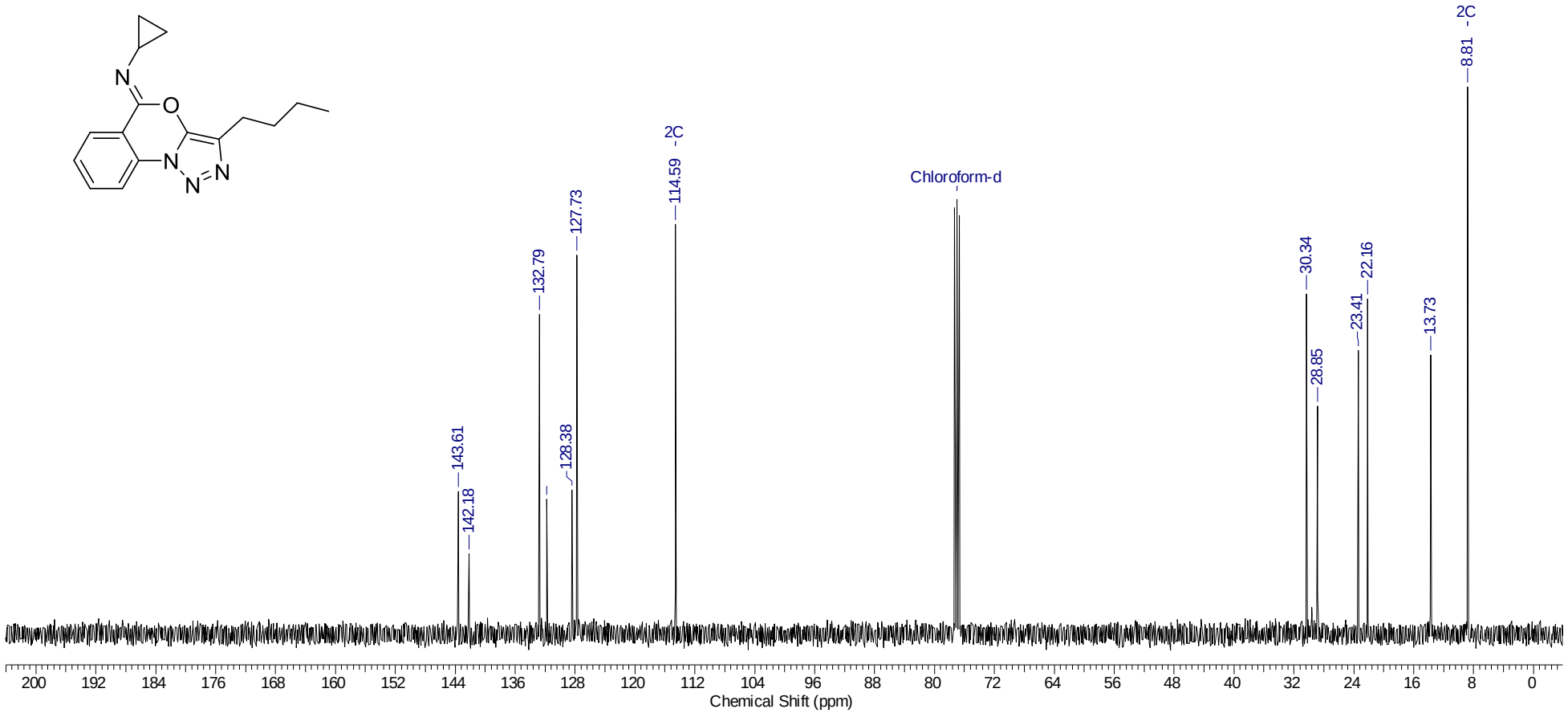
3-Butyl-*N*-cyclopropyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3s)

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



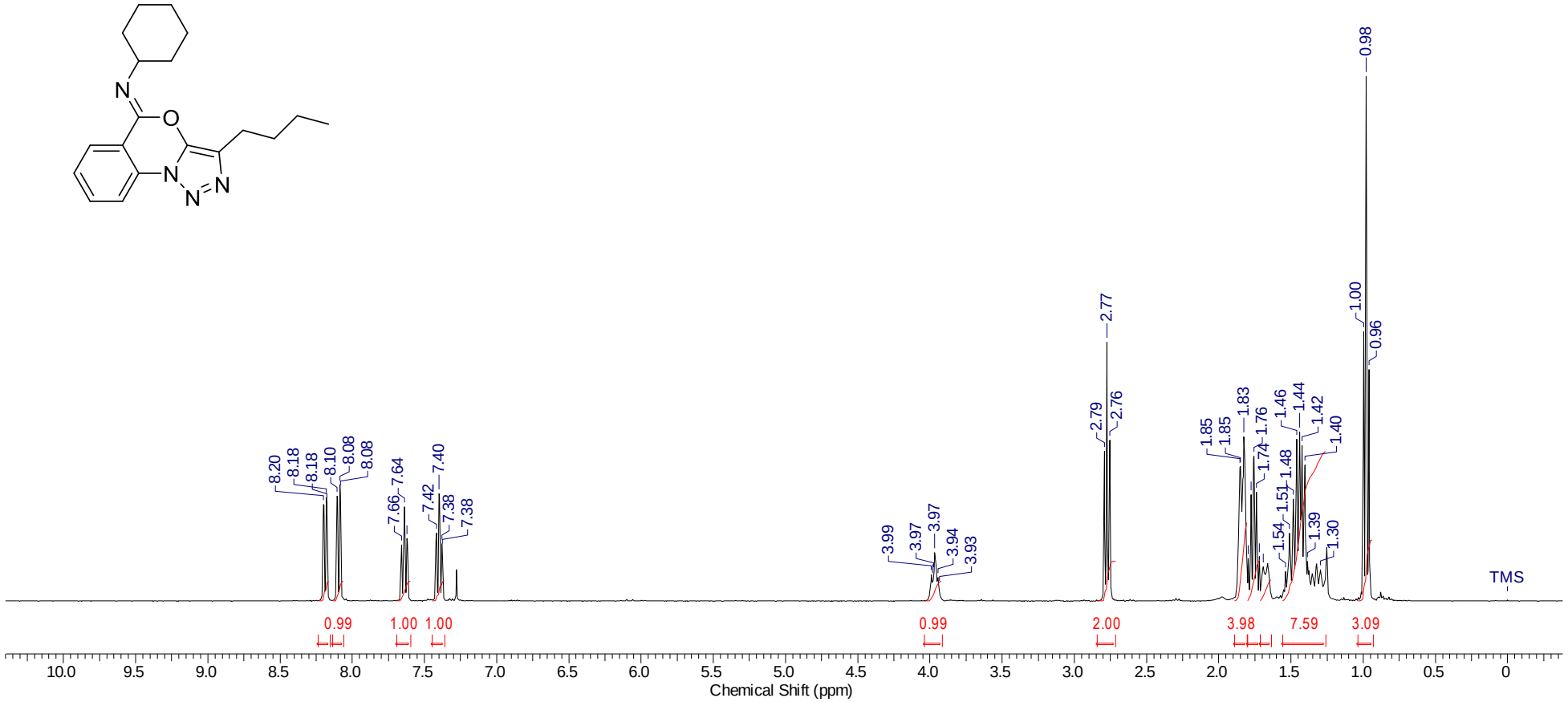
3-Butyl-*N*-cyclopropyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3s)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



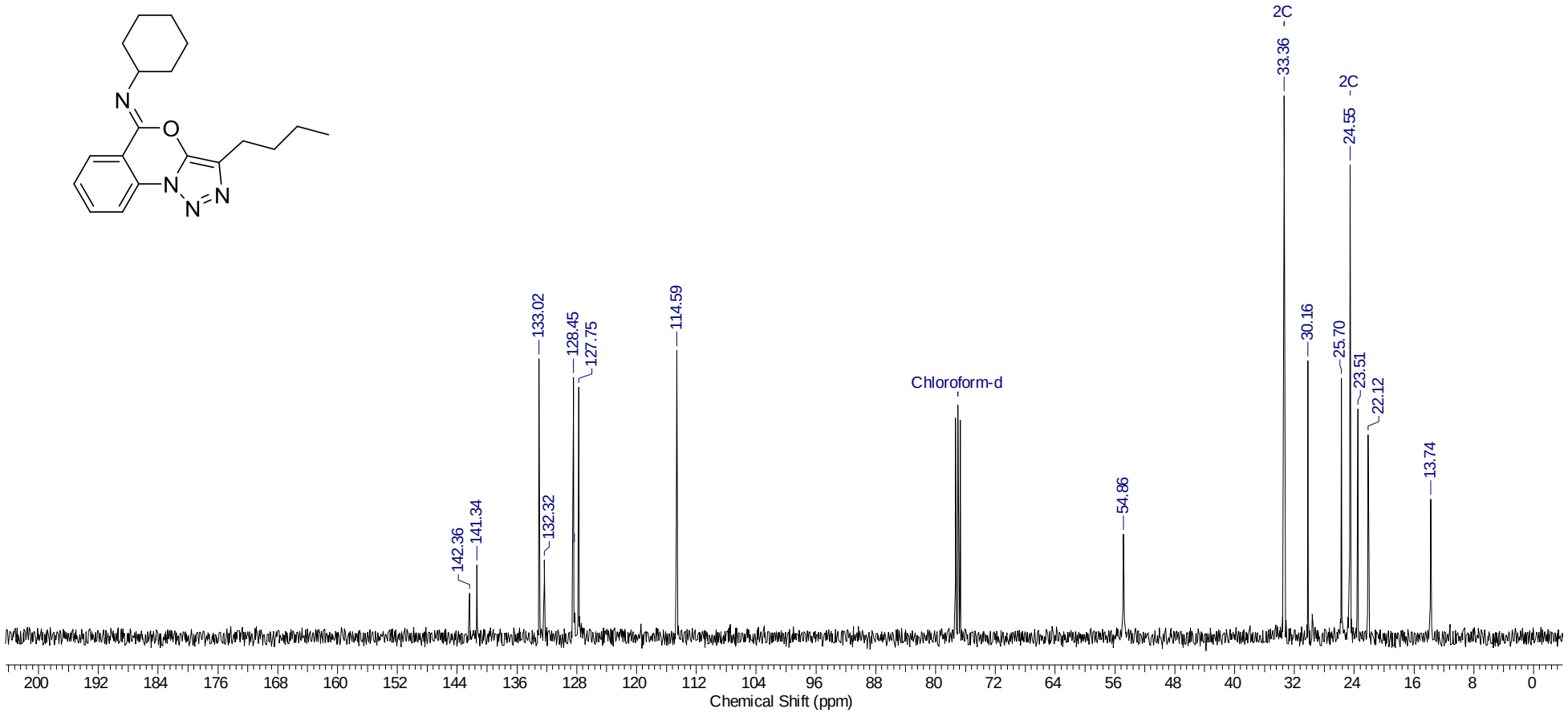
3-Butyl-*N*-cyclohexyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3t)

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



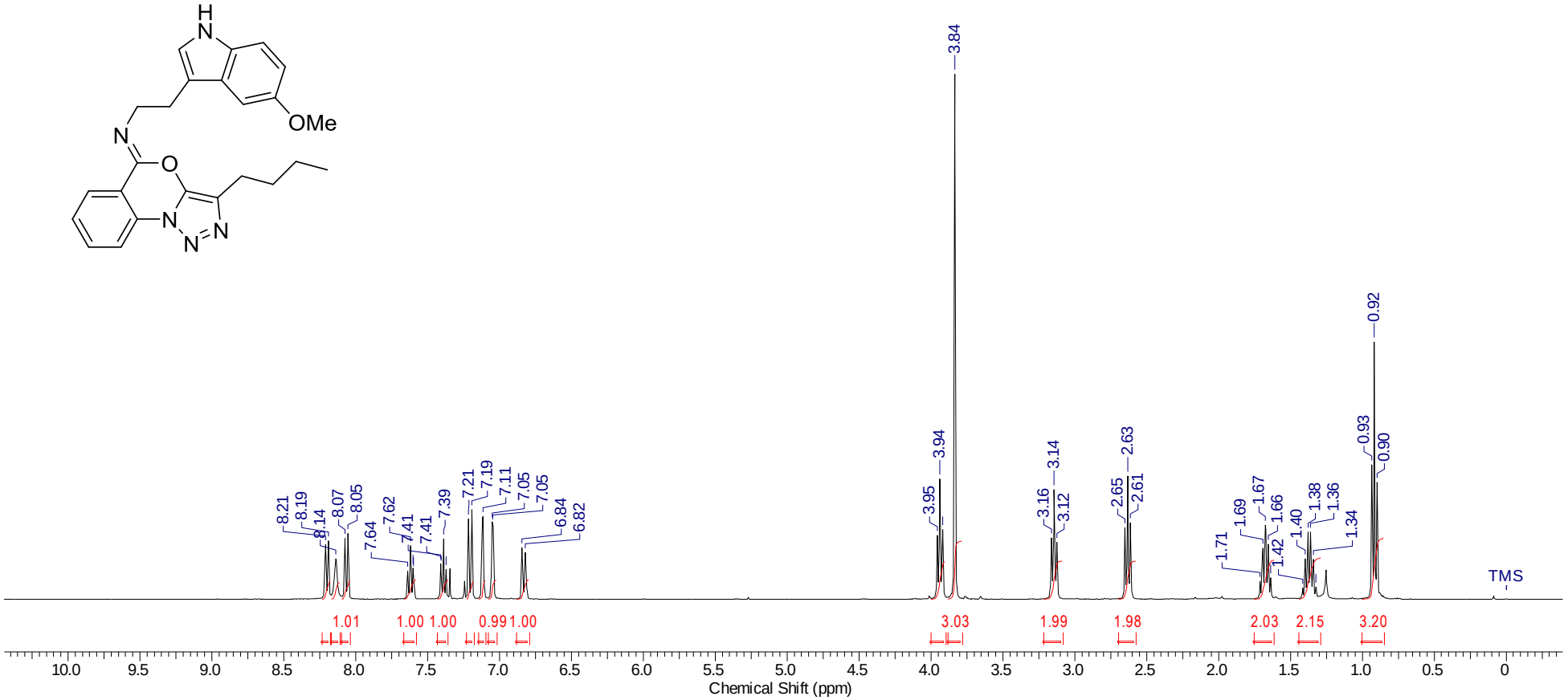
3-Butyl-*N*-cyclohexyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3t)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



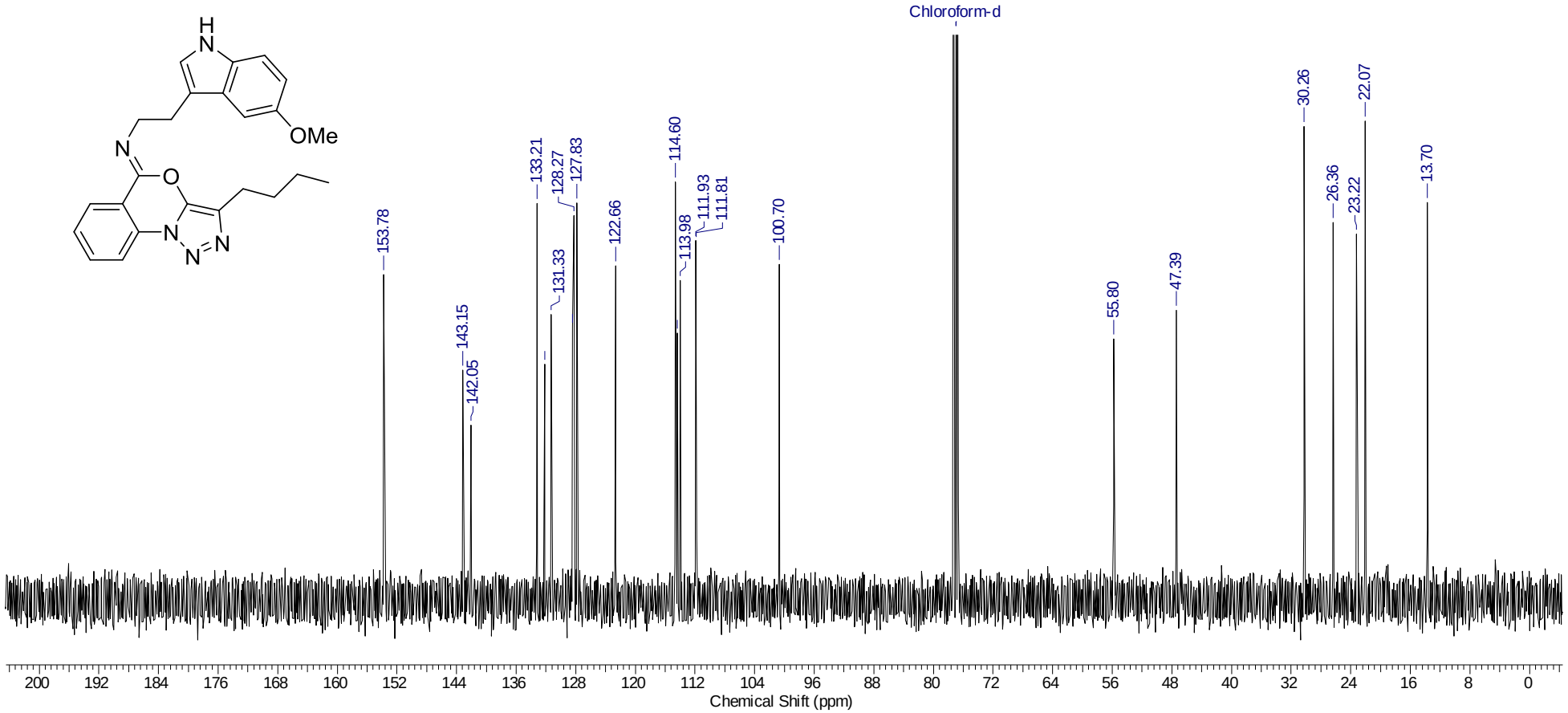
3-Butyl-*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3x)

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



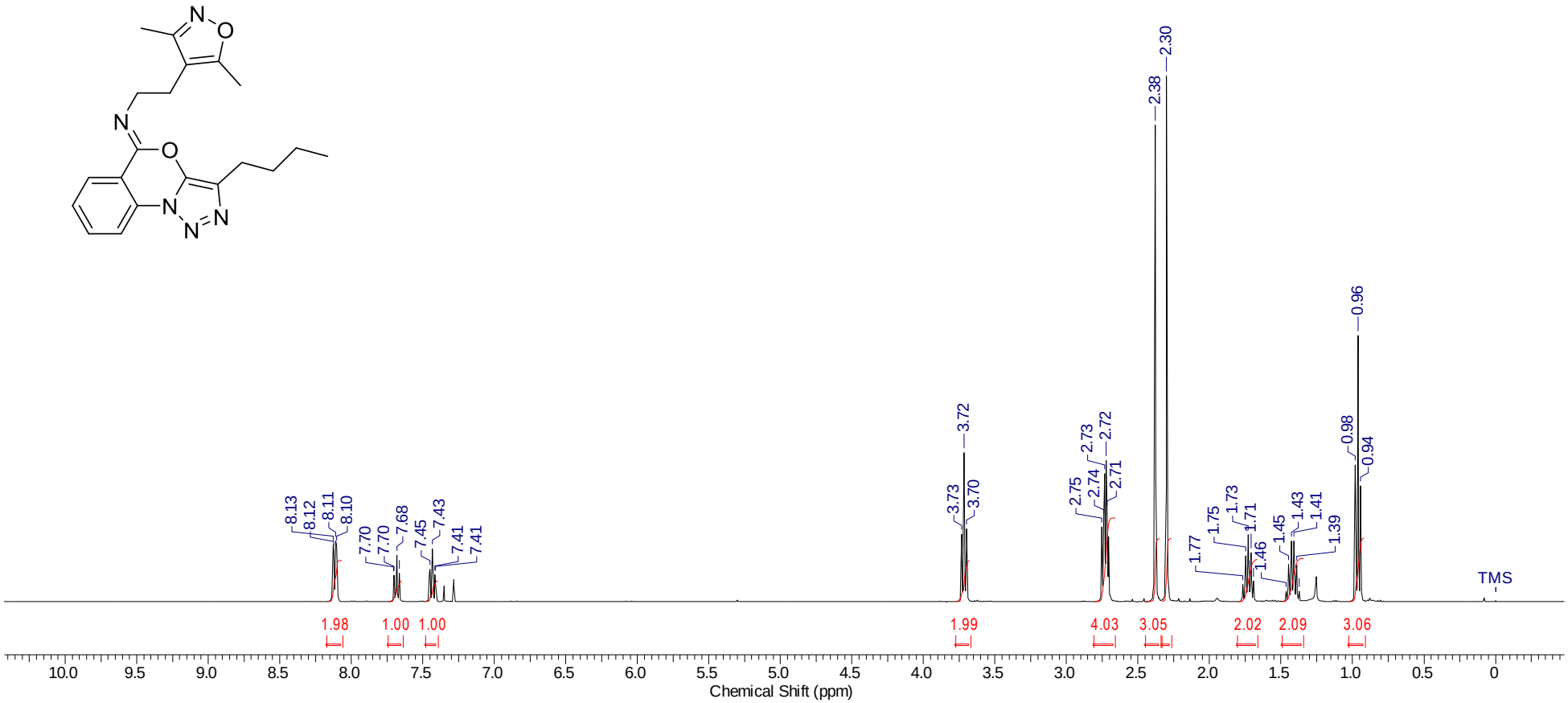
3-Butyl-*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3x)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



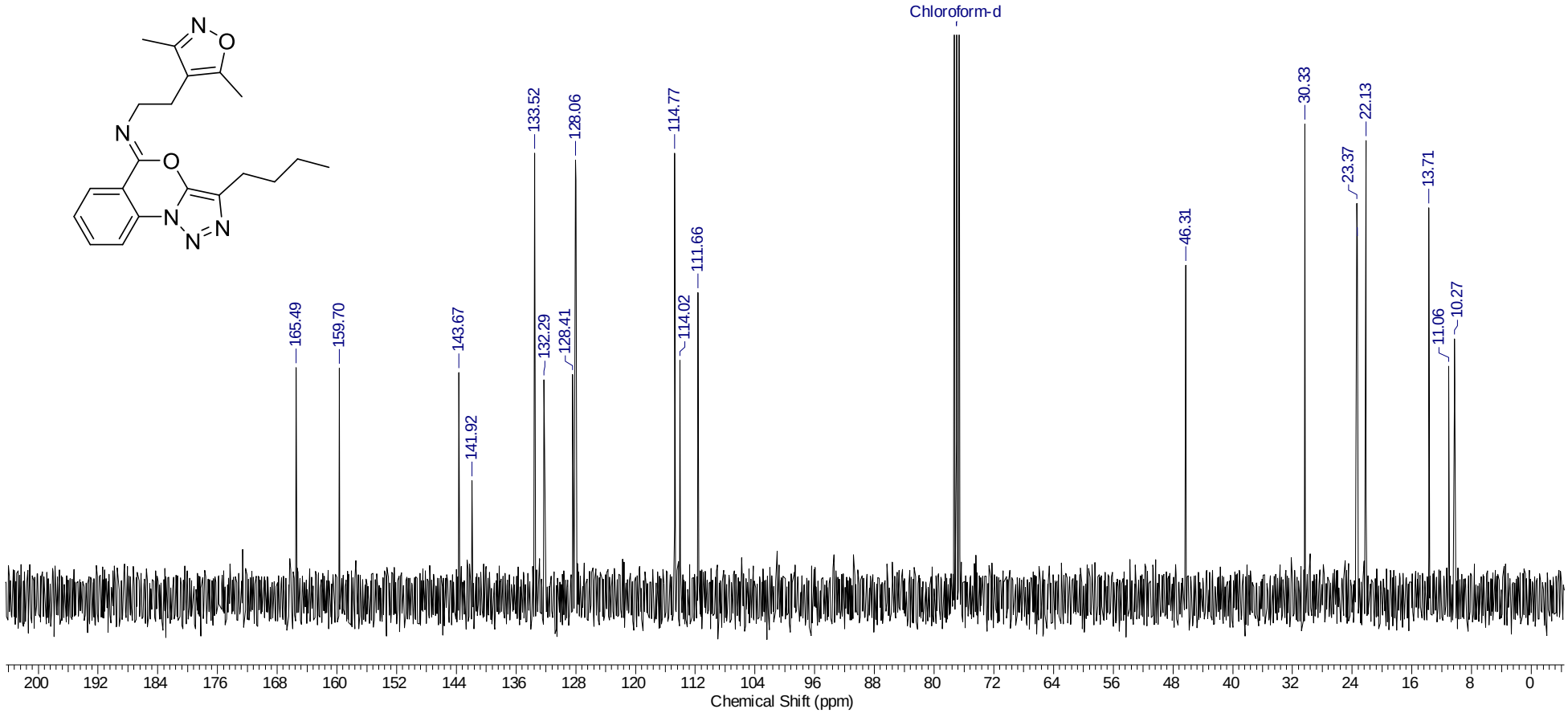
3-Butyl-*N*-[2-(3,5-dimethylisoxazol-4-yl)ethyl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3y)

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



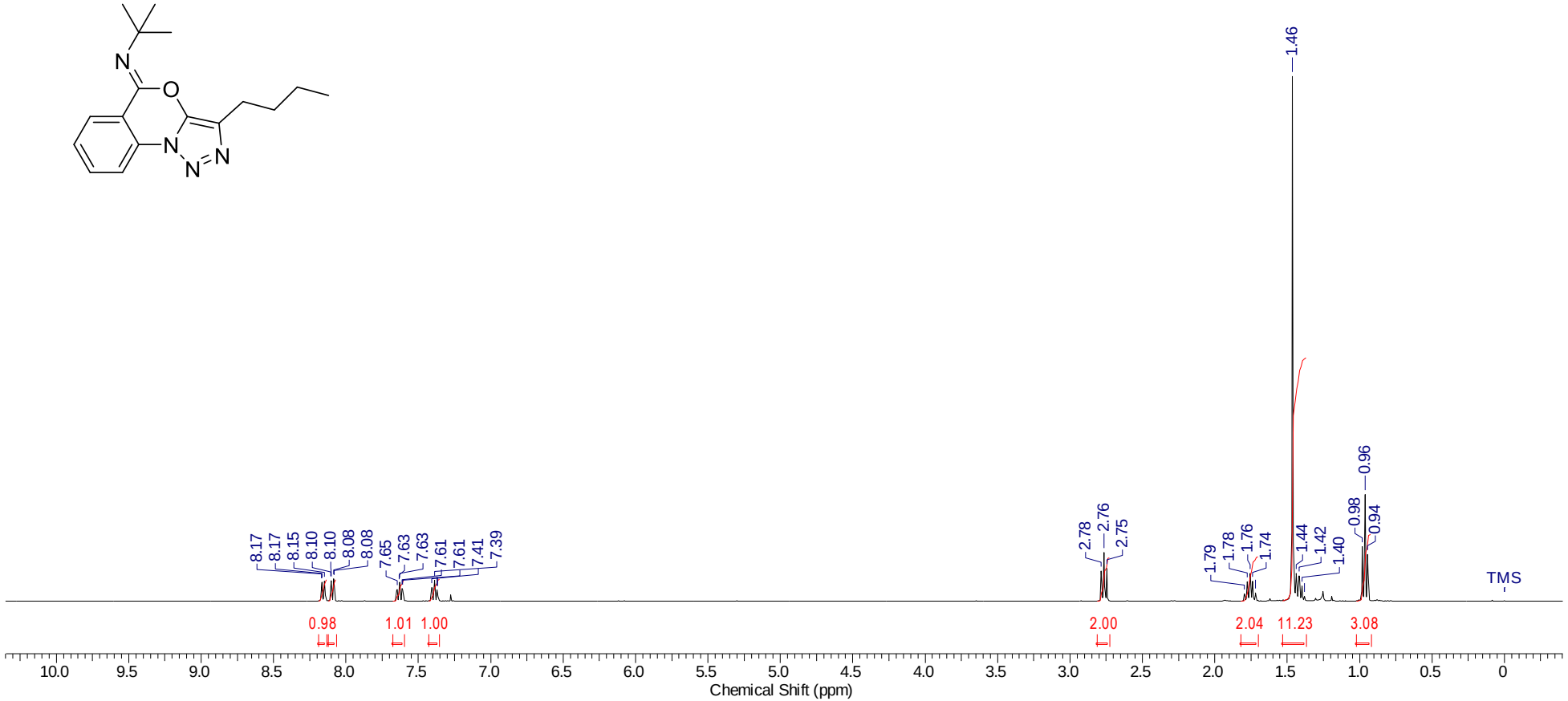
3-Butyl-*N*-[2-(3,5-dimethylisoxazol-4-yl)ethyl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3y)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



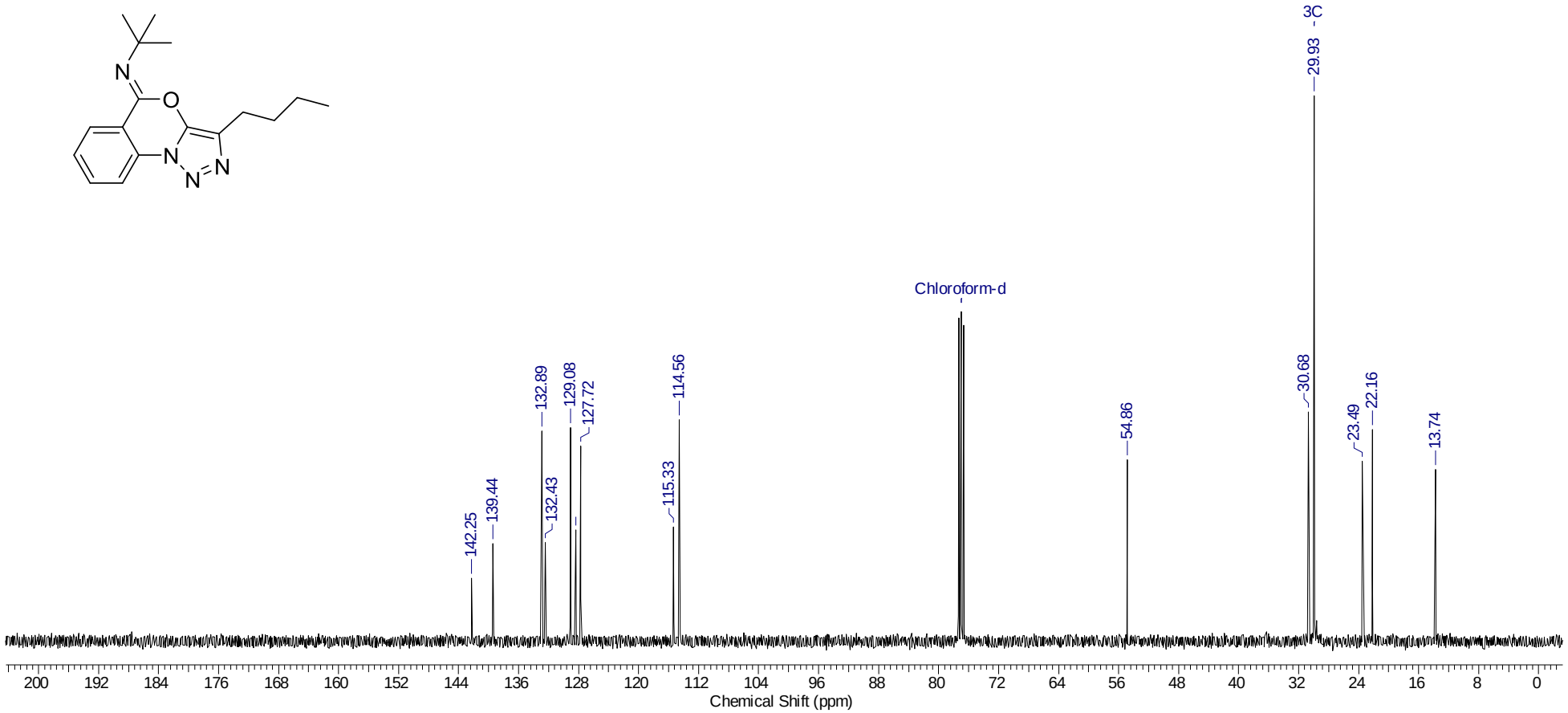
3-Butyl-*N*-*tert*-butyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3z)

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



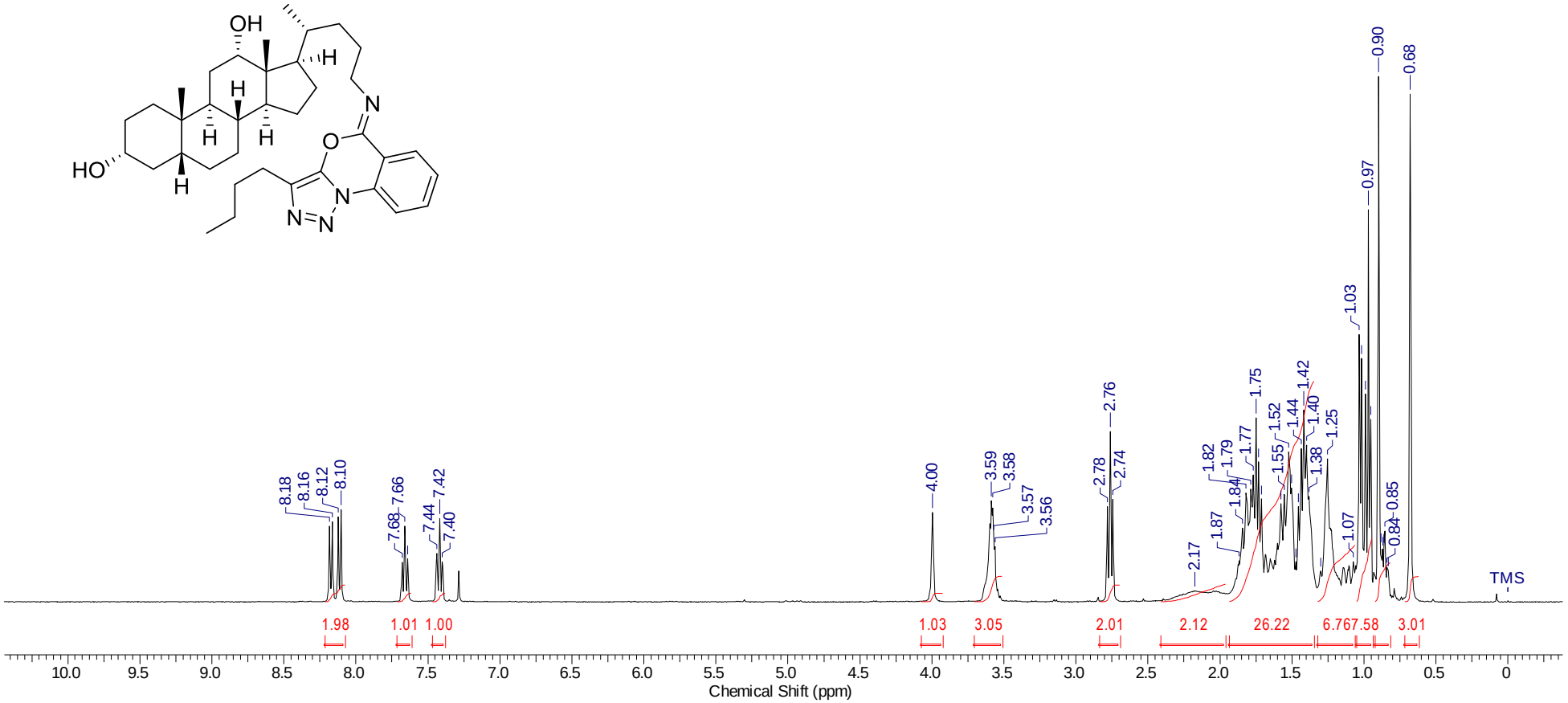
3-Butyl-*N*-*tert*-butyl-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3z)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



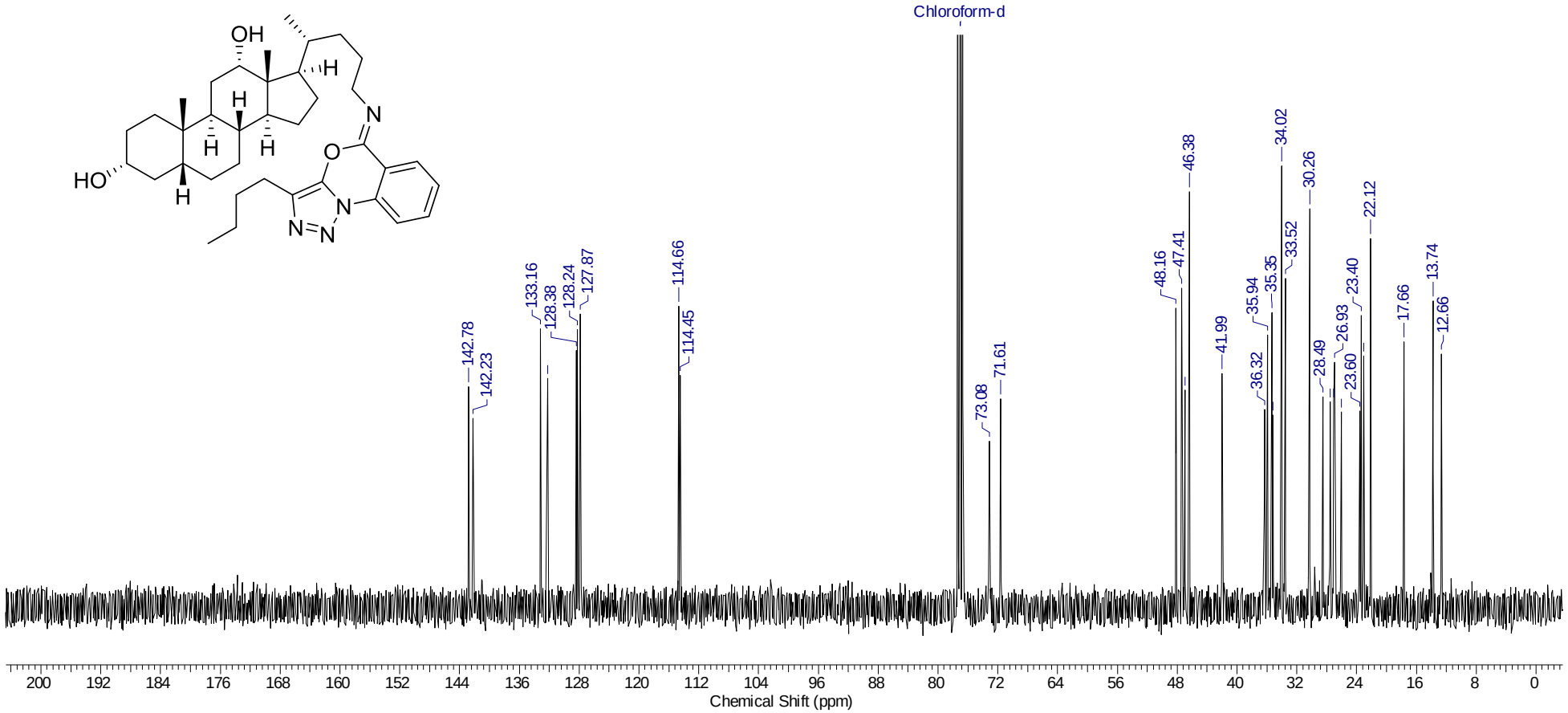
3-Butyl-*N*-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3ab)

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



3-Butyl-*N*-[(3α,5β,12α)-3,12-dihydroxycholan-24-yl]-5*H*-[1,2,3]triazolo[1,5-*a*][3,1]benzoxazin-5-imine (3ab)

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



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