Supporting information

Divergent Assembly of Fused Polycyclic Scaffolds from Iodotriazole-Tethered Benzaldehydes

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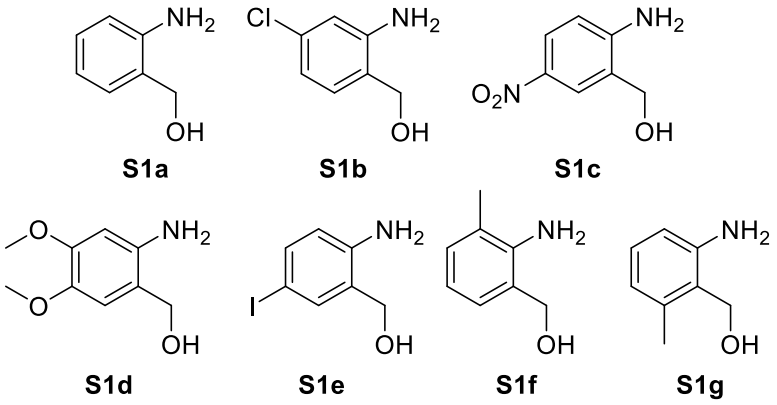
General information

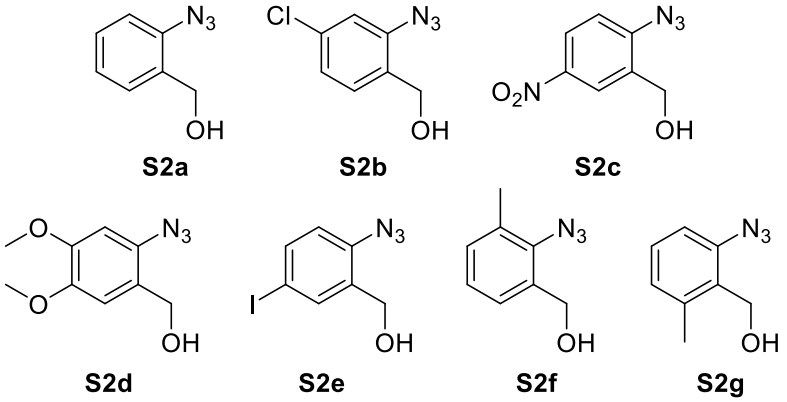
NMR spectra were recorded with Bruker Avance 400 (^{1}H 400 MHz, ^{13}C 100.6 MHz) and Bruker Avance 600 (^{1}H 600 MHz, ^{13}C 150 MHz) spectrometers at ambient temperature. Chemical shifts are presented in ppm (δ scale) and referenced to tetramethylsilane (δ = 0 ppm) in the ^{1}H NMR spectra and to the solvent signal in the ^{13}C NMR spectra. For compounds with low solubility in $CDCl_3$, small amounts of CD_3OD were added to the NMR samples. 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-TOF spectra were recorded with a Thermo Scientific Orbitrap Elite instrument. Column chromatography was carried out on Macherey–Nagel silica gel 60 (0.040–0.063 mm). All reactions were performed under Ar atmosphere, except the oxidation with DDQ in the synthesis of amides **6**.

Experimental procedures and characterization data for compounds

2-Aminobenzyl alcohol **S1a** was commercially available. 2-Aminobenzyl alcohols **S1b-g** were prepared by reduction of the corresponding commercially available anthranilic acids with $BH_3 \cdot SMe_2$ in THF according to the reported general procedure.[1]

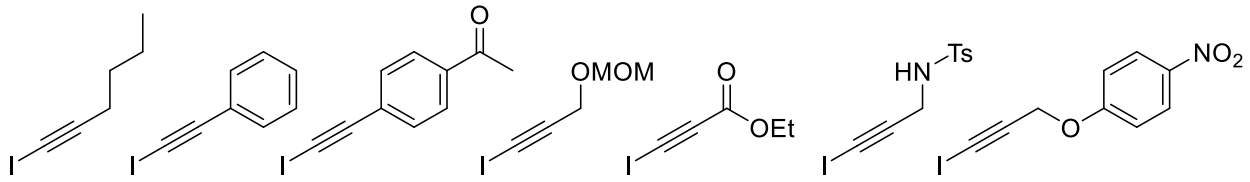


Azides **S2a-g** were prepared from the corresponding alcohols **S1a-g** according to the general literature procedure using diazotization reaction followed by NaN_3 addition.[2]

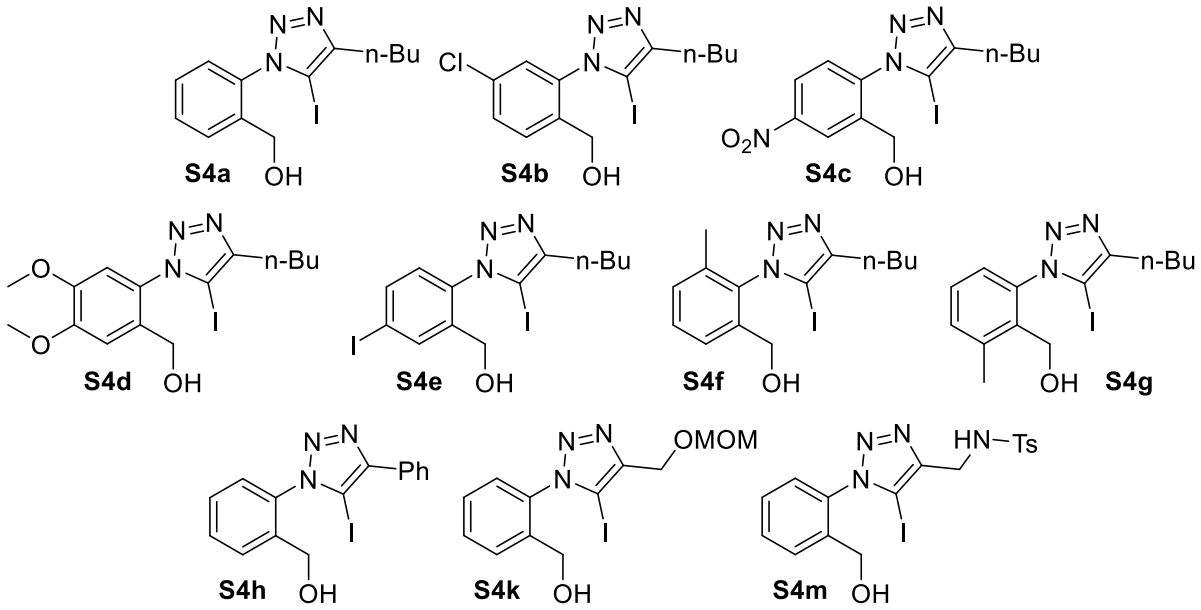


1-Iodoalkynes **S3a**,**b** were prepared from the corresponding terminal acetylenes by a modified literature procedure[3] (treatment with I_2 in the methanol solution in the presence of 3 equiv of MeONa). 1-Iodoalkynes **S3c**,**e**,**g** were prepared by treatment with NIS in the acetone solution in

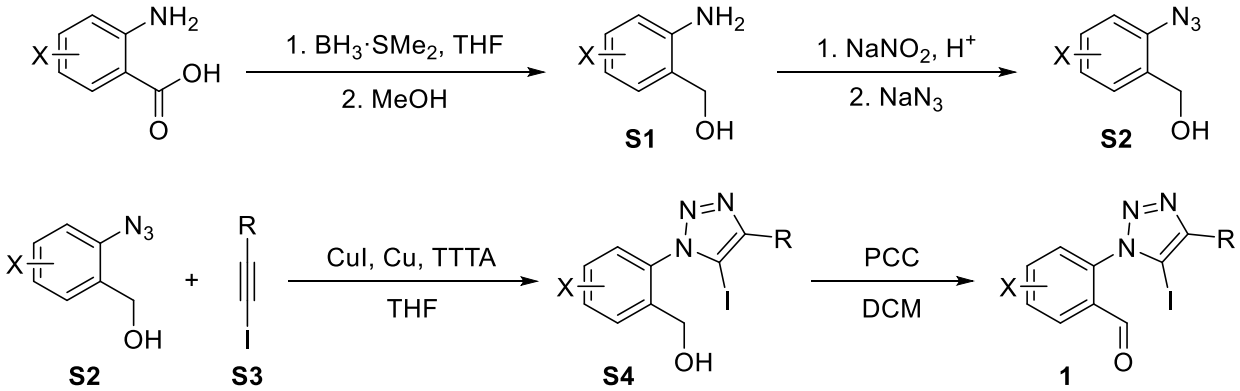
the presence of 5 mol% $AgNO_3$.[4] 1-Iodoalkynes **S3d**[5] and **S3f**[6] were prepared according to the literature.



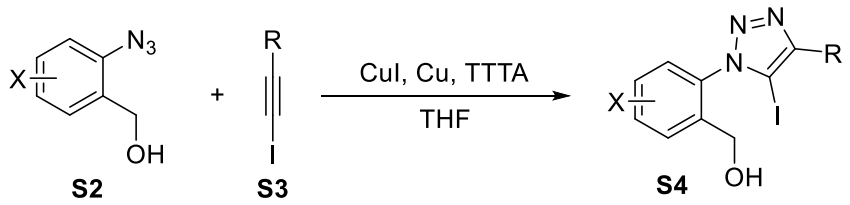
(5-Iodotriazolyl)alcohols **S4a-h,k,m** were obtained by Cu-catalyzed (3+2)-cycloaddition reaction with 1-iodoalkynes according to the literature.[7]



General scheme for the synthesis of starting compounds

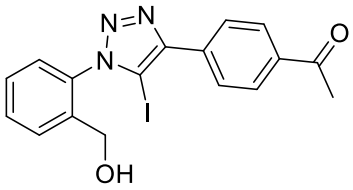


Synthesis of 5-iodotriazoles S4



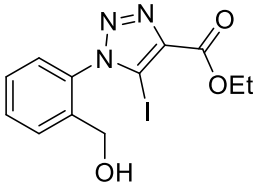
General procedure. Azidobenzyl alcohol **S2** (2 mmol, 1 equiv), 1-iodoalkyne (2.2 mmol, 1.1 equiv), CuI (0.1 mmol, 5 mol %), Cu (0.2 mmol, 10 mol %) and tris[(1-*tert*-butyl-1*H*-1,2,3-triazol-4-yl)methyl]amine (TTTA) (0.1 mmol, 5 mol %) were mixed under Ar atmosphere in THF (5 mL). The reaction mixture was stirred at 50 °C in a dry block overnight or for several days (TLC control), then diluted with CH_2Cl_2 and washed with EDTA solution. The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was purified by column chromatography.

1-(4-{1-[2-(Hydroxymethyl)phenyl]-5-iodo-1*H*-1,2,3-triazol-4-yl}phenyl)ethanone (S4i)



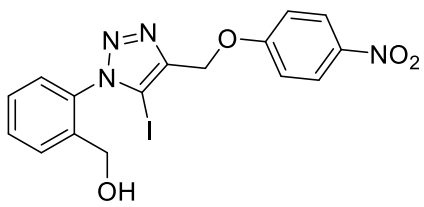
Prepared from azide **S2a** (119 mg, 0.8 mmol) and iodoalkyne **S3c** (238 mg, 0.88 mmol) according to the general procedure; eluent: CH_2Cl_2:MeOH = 50:1 (30:1). Yield 308 mg (92%). Yellowish solid; mp >180 °C. **^{1}H NMR** (400 MHz, $CDCl_3/CD_3OD$) δ 8.21-8.17 (m, 2H), 8.14-8.10 (m, 2H), 7.81 (d, J = 7.7 Hz, 1H, $C_{Ar}\underline{H}$), 7.70-7.64 (m, 1H, $C_{Ar}\underline{H}$), 7.56-7.50 (m, 1H, $C_{Ar}\underline{H}$), 7.34 (m, 1H, $C_{Ar}\underline{H}$), 4.40 (s, 2H, $C\underline{H}_2OH$), 4.25 (br s, 1H, O$\underline{H}$), 2.69 (s, 3H, $C\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3/CD_3OD$) δ 198.4 ($\underline{C}$=O), 148.3 ($\underline{C}_{quat}$), 138.5 ($\underline{C}_{quat}$), 136.4 ($\underline{C}_{quat}$), 134.3 ($\underline{C}_{quat}$), 134.0 ($\underline{C}_{quat}$), 131.0 ($\underline{C}_{Ar}$H), 128.5 (2C), 128.4 ($\underline{C}_{Ar}$H), 127.9 ($\underline{C}_{Ar}$H), 127.6 ($\underline{C}_{Ar}$H), 127.2 (2C), 81.4 ($\underline{C}$–I), 59.5 ($\underline{C}H_2OH$), 26.3 ($\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{17}H_{15}IN_3O_2$ $[M+H]^+$ 420.0203; found 420.0203.

Ethyl 1-[2-(hydroxymethyl)phenyl]-5-iodo-1*H*-1,2,3-triazole-4-carboxylate (S4l)



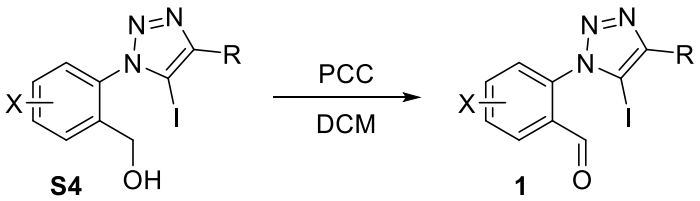
Prepared from azide **S2a** (119 mg, 0.8 mmol) and iodoalkyne **S3e** (197 mg, 0.88 mmol) according to the general procedure; eluent: CH_2Cl_2:MeOH = 50:1. Yield 208 mg (70%). Brownish solid; mp 134-136 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74-7.72 (m, 1H, $C_{Ar}\underline{H}$), 7.66-7.62 (m, 1H, $C_{Ar}\underline{H}$), 7.55-7.50 (m, 1H, $C_{Ar}\underline{H}$), 7.32-7.28 (m, 1H, $C_{Ar}\underline{H}$), 4.49 (q, J = 7.1 Hz, 2H, $C\underline{H}_2CH_3$), 4.36 (br s, J = 6.3 Hz, 2H, $C\underline{H}_2OH$), 2.51 (br s, $CH_2O\underline{H}$), 1.47 (t, J = 7.1 Hz, 3H, $CH_2C\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 160.1 ($\underline{C}$=O), 142.0 ($\underline{C}_{quat}$), 138.1 ($\underline{C}_{quat}$), 134.3 ($\underline{C}_{quat}$), 131.5 ($\underline{C}_{Ar}$H), 129.8 ($\underline{C}_{Ar}$H), 128.5 ($\underline{C}_{Ar}$H), 127.9 ($\underline{C}_{Ar}$H), 87.8 ($\underline{C}$–I), 61.8, 60.8, 14.2 ($\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{12}H_{13}IN_3O_3$ $[M+H]^+$ 373.9996; found 373.9993.

(2-{5-Iodo-4-[(4-nitrophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenyl)methanol (S4n)



Prepared from azide **S2a** (273 mg, 1.8 mmol) and iodoalkyne **S3g** (613 mg, 2 mmol) according to the general procedure; eluent: hexanes:EtOAc = 1:1. Yield 736 mg (87%). White solid; mp 173-175 °C (dec.). **^{1}H NMR** (400 MHz, $CDCl_3/CD_3OD$) δ 8.27-8.24 (m, 2H), 7.79-7.78 (m, 1H), 7.68-7.64 (m, 1H), 7.53-7.49 (m, 1H), 7.32-7.29 (m, 1H), 7.23-7.19 (m, 2H), 5.33 (s, 2H, C$\underline{H}_2$O), 4.35 (s, 2H, C$\underline{H}_2$OH). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3/CD_3OD$) δ 162.9 ($\underline{C}_{quat}$), 146.1 ($\underline{C}_{quat}$), 141.5 ($\underline{C}_{quat}$), 138.3 ($\underline{C}_{quat}$), 133.7 ($\underline{C}_{quat}$), 130.9 ($\underline{C}_{Ar}$H), 128.2 ($\underline{C}_{Ar}$H), 127.7 ($\underline{C}_{Ar}$H), 127.2 ($\underline{C}_{Ar}$H), 125.5 (2C), 114.6 (2C), 85.3 ($\underline{C}$–I), 61.8, 59.2. **HRMS** (MALDI-TOF) calcd for $C_{16}H_{14}IN_4O_4$ $[M+H]^+$ 453.0053; found 453.0054.

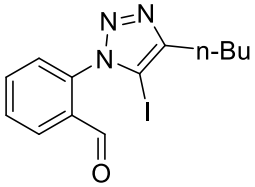
Synthesis of benzaldehydes 1



Procedure A. PCC (2.1 mmol, 1.6 equiv) was added by portions to solution of (5-iodotriazolyl)alcohol **S4** (1.3 mmol, 1 equiv) in CH_2Cl_2 (15 mL) under Ar atmosphere keeping the temperature less than 5 °C and then stirred at room temperature for 20 h. The precipitate was filtered off, the filtrate was diluted with CH_2Cl_2 and washed with water. The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was purified by column chromatography.

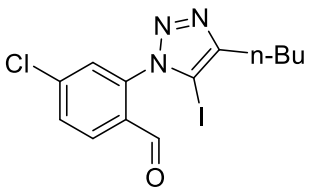
Procedure B. (5-Iodotriazolyl)alcohol **S4** (0.4 mmol, 1 equiv), DMP (0.48 mmol, 1.2 equiv), and $NaHCO_3$ (0.8 mmol, 2 equiv) were mixed under Ar atmosphere in CH_2Cl_2 (5 mL). The reaction mixture was stirred at room temperature for 2 h, then diluted with CH_2Cl_2 and washed with Na_2SO_3 solution. The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was purified by column chromatography.

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



Prepared from alcohol **S4a** (884 mg, 2.5 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 100:1. Yield 827 mg (90%). Yellowish solid; mp 123-125 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.55 (s, 1H, C(O)H), 8.13 (dd, J = 7.6, 1.5 Hz, 1H, $C_{Ar}H$), 7.82 (td, J = 7.6, 1.6 Hz, 1H, $C_{Ar}H$), 7.74 (t, J = 7.5 Hz, 1H, $C_{Ar}H$), 7.48 (dd, J = 7.8, 1.0 Hz, 1H, $C_{Ar}H$), 2.78 (t, J = 7.8 Hz, 2H, CH_2Pr), 1.82-1.74 (m, 2H, CH_2Et), 1.50-1.40 (m, 2H, CH_2CH_3), 0.99 (t, J = 7.3 Hz, 3H, CH_2CH_3). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 187.7 (C=O), 152.7 (C_{quat}), 138.3 (C_{quat}), 134.6, 131.9 (C_{quat}), 131.0 ($C_{Ar}H$), 129.3 ($C_{Ar}H$), 128.5 ($C_{Ar}H$), 82.0 (C–I), 31.0, 25.9, 22.3, 13.8 (CH_2CH_3). **HRMS** (MALDI-TOF) calcd for $C_{13}H_{14}IN_3NaO$ $[M+Na]^+$ 378.0074; found 378.0076.

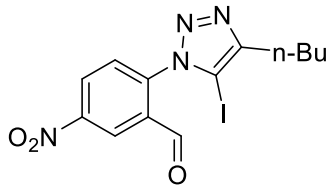
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-4-chlorobenzaldehyde (1b)



Prepared from alcohol **S4b** (516 mg, 1.3 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 100:1. Yield 339 mg (66%). Yellowish solid; mp 115-117 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.50 (s, 1H, C(O)H), 8.08 (d, J = 8.4 Hz, 1H, $C_{Ar}H$), 7.71 (dd, J = 8.4, 1.9 Hz, 1H, $C_{Ar}H$), 7.51 (d, J = 1.9 Hz, 1H, $C_{Ar}H$), 2.78 (t, J = 7.6 Hz, 2H, CH_2Pr), 1.81-1.73 (m, 2H, CH_2Et), 1.49-1.40 (m, 2H, CH_2CH_3), 0.99 (t, J = 7.3 Hz, 3H, CH_2CH_3). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 186.5 (C=O), 152.9 (C_{quat}), 140.8 (C_{quat}), 139.0 (C_{quat}), 131.4 ($C_{Ar}H$),

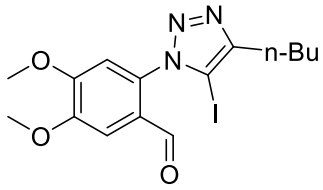
130.3 ($\underline{C}_{Ar}H$), 130.2 ($\underline{C}_{quat}$), 128.6 ($\underline{C}_{Ar}H$), 81.8 ($\underline{C}$–I), 31.0, 25.8, 22.3, 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{13}H_{14}ClIN_3O$ $[M+H]^+$ 389.9865; found 389.9862.

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



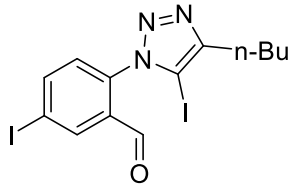
Prepared from alcohol **S4c** (755 mg, 1.9 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 100:1. Yield 654 mg (87%). Yellow solid; mp 128-130 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.63 (s, 1H, C(O)$\underline{H}$), 8.95 (d, J = 2.6 Hz, 1H, $C_{Ar}\underline{H}$), 8.64 (dd, J = 8.7, 2.6 Hz, 1H, $C_{Ar}\underline{H}$), 7.76 (d, J = 8.6 Hz, 1H, $C_{Ar}\underline{H}$), 2.80 (t, J = 7.6 Hz, 2H, $C\underline{H}_2$Pr), 1.82-1.75 (m, 2H, $C\underline{H}_2$Et), 1.50-1.41 (m, 2H, $C\underline{H}_2CH_3$), 1.00 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 185.5 ($\underline{C}$=O), 153.7 ($\underline{C}_{quat}$), 148.8 ($\underline{C}_{quat}$), 142.2 ($\underline{C}_{quat}$), 132.7 ($\underline{C}_{quat}$), 129.8 ($\underline{C}_{Ar}H$), 128.6 ($\underline{C}_{Ar}H$), 124.5 ($\underline{C}_{Ar}H$), 81.2 ($\underline{C}$–I), 30.9, 25.8, 22.3, 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{13}H_{14}IN_4O_3$ $[M+H]^+$ 401.0105; found 401.0107.

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



Prepared from alcohol **S4d** (303 mg, 0.7 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 100:1. Yield 277 mg (91%). Yellowish solid; mp 129-191 °C (dec.). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.34 (s, 1H, C(O)$\underline{H}$), 7.55 (s, 1H, $C_{Ar}\underline{H}$), 6.86 (s, 1H, $C_{Ar}\underline{H}$), 4.04 (s, 3H, $C\underline{H}_3O$), 4.00 (s, 3H, $C\underline{H}_3O$), 2.77 (t, J = 7.6 Hz, 2H, $C\underline{H}_2$Pr), 1.81-1.73 (m, 2H, $C\underline{H}_2$Et), 1.49-1.40 (m, 2H, $C\underline{H}_2CH_3$), 0.99 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 186.6 ($\underline{C}$=O), 153.8 ($\underline{C}_{quat}$), 152.4 ($\underline{C}_{quat}$), 150.6 ($\underline{C}_{quat}$), 133.3 ($\underline{C}_{quat}$), 125.2 ($\underline{C}_{quat}$), 110.4 ($\underline{C}_{Ar}H$), 108.8 ($\underline{C}_{Ar}H$), 82.9 ($\underline{C}$–I), 56.7 ($\underline{C}H_3O$), 56.4 ($\underline{C}H_3O$), 31.0, 25.8, 22.2, 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{19}IN_3O_3$ $[M+H]^+$ 416.0466; found 416.0470.

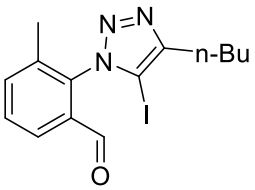
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-5-iodobenzaldehyde (1e)



Prepared from alcohol **S4e** (766 mg, 1.6 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 200:1. Yield 689 mg (90%). White solid; mp 152-154 °C (dec.). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.46 (s, 1H, C(O)$\underline{H}$), 8.43 (d, J = 2.0 Hz, 1H, $C_{Ar}\underline{H}$), 8.13 (dd, J = 8.3, 2.0 Hz, 1H, $C_{Ar}\underline{H}$), 7.22 (d, J = 8.3 Hz, 1H, $C_{Ar}\underline{H}$), 2.77 (t, J = 7.4 Hz, 2H, $C\underline{H}_2$Pr), 1.80-1.73 (m, 2H, $C\underline{H}_2$Et), 1.48-1.39 (m, 2H, $C\underline{H}_2CH_3$), 0.98 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 186.3 ($\underline{C}$=O), 153.0 ($\underline{C}_{quat}$), 143.3 ($\underline{C}_{Ar}H$), 138.2 ($\underline{C}_{Ar}H$), 137.8 ($\underline{C}_{quat}$), 132.7 ($\underline{C}_{quat}$), 129.8 ($\underline{C}_{Ar}H$), 96.8 ($\underline{C}_{Ar}$–I), 81.8 ($\underline{C}$–I), 31.0, 25.8, 22.3, 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{13}H_{14}I_2N_3O$ $[M+H]^+$ 481.9221; found 481.9227.

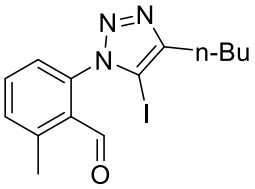
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-3-methylbenzaldehyde (1f)

Prepared from alcohol **S4f** (559 mg, 1.5 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 200:1. Yield 508 mg (91%). White solid; mp 108-110 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.36



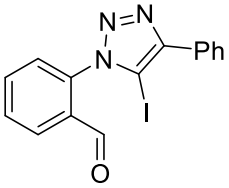
(s, 1H, C(O)H), 7.94-7.92 (m, 1H, $C_{Ar}H$), 7.68-7.62 (m, 2H, $C_{Ar}H$), 2.79 (t, J = 7.6 Hz, 2H, CH_2Pr), 2.04 (s, 3H, CH_3C_{Ar}), 1.783-1.75 (m, 2H, CH_2Et), 1.48-1.39 (m, 2H, CH_2CH_3), 0.99 (t, J = 7.3 Hz, 3H, CH_2CH_3). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, $CDCl_3$) δ 187.9 (C=O), 152.5 (C_{quat}), 137.5 (C_{quat}), 137.2 (C_{quat}), 136.5 ($C_{Ar}H$), 132.6 (C_{quat}), 131.0 ($C_{Ar}H$), 127.1 ($C_{Ar}H$), 82.3 (C–I), 31.0, 25.7, 22.2, 16.9 (CH_3C_{Ar}), 13.8 (CH_2CH_3). **HRMS** (MALDI-TOF) calcd for $C_{14}H_{17}IN_3O$ $[M+Na]^+$ 370.0411; found 370.0415.

2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-6-methylbenzaldehyde (1g)



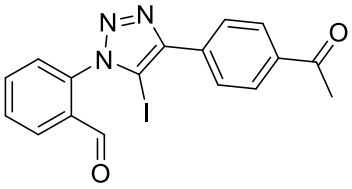
Prepared from alcohol **S4g** (483 mg, 1.3 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 100:1. Yield 434 mg (90%). Yellow solid; mp 106-108 °C. **^1H NMR** (400 MHz, $CDCl_3$) δ 9.56 (s, 1H, C(O)H), 7.64 (t, J = 7.6 Hz, 1H, $C_{Ar}H$), 7.51 (d, J = 7.6 Hz, 1H, $C_{Ar}H$), 7.28 (d, J = 7.3 Hz, 1H, $C_{Ar}H$), 2.77 (t, J = 7.5 Hz, 2H, CH_2Pr), 2.72 (s, 3H, CH_3C_{Ar}), 1.81-1.73 (m, 2H, CH_2Et), 1.49-1.40 (m, 2H, CH_2CH_3), 0.99 (t, J = 7.3 Hz, 3H, CH_2CH_3). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, $CDCl_3$) δ 189.5 (C=O), 152.5 (C_{quat}), 142.1(C_{quat}), 139.5 (C_{quat}), 134.3 ($C_{Ar}H$), 133.2 ($C_{Ar}H$), 130.2 (C_{quat}), 126.3 ($C_{Ar}H$), 82.2 (C–I), 31.0, 25.8, 22.2, 20.9 (CH_3C_{Ar}), 13.8 (CH_2CH_3). **HRMS** (MALDI-TOF) calcd for $C_{14}H_{17}IN_3O$ $[M+H]^+$ 370.0411; found 370.0408.

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



Prepared from alcohol **S4h** (905 mg, 2.4 mmol) according to procedure **A**; eluent: hexanes:CH_2Cl_2:EtOAc = 2:1:1. Yield 751 mg (83%). White solid; mp 172-174 °C (dec.). **^1H NMR** (400 MHz, $CDCl_3$/TFA) δ 9.95 (s, 1H, C(O)H), 8.29-8.27 (m, 1H, $C_{Ar}H$), 8.13-8.06 (m, 2H, $C_{Ar}H$), 7.84-7.82 (m, 2H, $C_{Ph}H$), 7.72-7.62 (m, 4H, $C_{Ar}H$, $C_{Ph}H$). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, $CDCl_3$/TFA) δ 192.0 (C=O), 147.3 (C_{quat}), 136.7 ($C_{Ar}H$), 136.2 ($C_{Ar}H$), 134.3 ($C_{Ar}H$), 133.3 (C_{quat}), 132.6 ($C_{Ar}H$), 130.5 (C_{quat}), 129.9 (2C, $C_{Ph}H$), 129.4 ($C_{Ph}H$), 128.3 (2C, $C_{Ph}H$), 122.3 (C_{quat}), 85.3 (C–I). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{11}IN_3O$ $[M+H]^+$ 375.9941; found 375.9944.

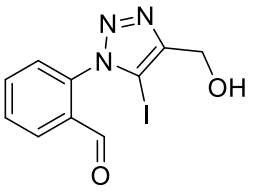
2-[4-(4-Acetylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]benzaldehyde (1i)



Prepared from alcohol **S4i** (251 mg, 0.6 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 100:1. Yield 201 mg (80%). Yellowish solid; mp 178-182 °C (dec.). **^1H NMR** (400 MHz, $CDCl_3$) δ 9.69 (s, 1H, C(O)H), 8.23-8.20 (m, 2H), 8.18 (dd, J = 7.6, 1.6 Hz, 1H, $C_{Ar}H$), 8.13-8.10 (m, 2H), 7.88 (td, J = 7.6, 1.6 Hz, 1H, $C_{Ar}H$), 7.84-7.79 (m, 1H, $C_{Ar}H$), 7.54 (dd, J = 7.7, 1.0 Hz, 1H, $C_{Ar}H$), 2.68 (s, 3H, CH_3). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, $CDCl_3$/CD_3OD) δ 198.3 (HC=O), 187.9 (CH_3C=O), 148.9 (C_{quat}), 137.2 (C_{quat}), 136.7 (C_{quat}), 134.7 ($C_{Ar}H$), 134.0 (C_{quat}), 131.7 (C_{quat}), 131.5 ($C_{Ar}H$), 130.3 ($C_{Ar}H$), 128.8 ($C_{Ar}H$), 128.6 (2C),

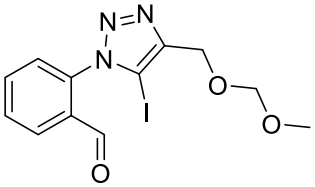
127.3 (2C), 81.7 (C–I), 26.5 (CH_3). **HRMS** (MALDI-TOF) calcd for $C_{17}H_{13}IN_3O_2$ $[M+H]^+$ 418.0047; found 418.0046.

2-[4-(Hydroxymethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]benzaldehyde (1j)



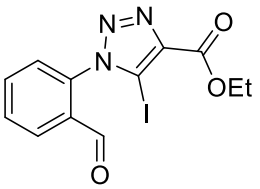
MOM-protected benzaldehyde **1k** (93 mg, 0.25 mmol) was mixed with conc. HCl (660 μL) and EtOH (3 mL) under Ar atmosphere. The reaction mixture was stirred at room temperature for 24 h, then diluted with CH_2Cl_2, and washed with solution of Na_2CO_3. The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was purified by column chromatography (eluent: hexanes:EtOAc:CH_2Cl_2 = 1:1:1). Yield 36 mg (44%). White solid. **^{1}H NMR** (400 MHz, $CDCl_3$/CD_3OD) δ 9.62 (s, 1H, C(O)H), 8.15 (dd, J = 7.6, 1.6 Hz, 1H, $C_{Ar}H$), 7.84 (td, J = 7.6, 1.6 Hz, 1H, $C_{Ar}H$), 7.80-7.76 (m, 1H, $C_{Ar}H$), 7.48 (dd, J = 7.8, 1.1 Hz, 1H, $C_{Ar}H$), 4.87 (d, J = 6.0 Hz, 2H, CH_2), 2.25 (t, J = 6.0 Hz, 1H, OH). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$/CD_3OD) δ 187.9 (C=O), 151.3 (C_{quat}), 137.3 (C_{quat}), 134.7 ($C_{Ar}H$), 131.6 (C_{quat}), 131.3 ($C_{Ar}H$), 130.0 ($C_{Ar}H$), 128.5 ($C_{Ar}H$), 83.3 (C–I), 55.7 (CH_2).

2-{5-Iodo-4-[(methoxymethoxy)methyl]-1*H*-1,2,3-triazol-1-yl}benzaldehyde (1k)



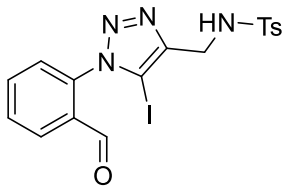
Prepared from alcohol **S4k** (946 mg, 2.5 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 200:1. Yield 648 mg (69%). Yellowish solid; mp 115-117 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.61 (s, 1H, C(O)H), 8.14 (dd, J = 7.6, 1.6 Hz, 1H, $C_{Ar}H$), 7.84 (td, J = 7.6, 1.6 Hz, 1H, $C_{Ar}H$), 7.79-7.76 (m, 1H, $C_{Ar}H$), 7.48 (dd, J = 7.8, 1.1 Hz, 1H, $C_{Ar}H$), 4.80 (s, 2H, CH_2), 4.77 (s, 2H, CH_2), 3.48 (s, 3H, CH_3). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 187.6 (C=O), 148.8 (C_{quat}), 137.7 (C_{quat}), 134.6 ($C_{Ar}H$), 131.7 (C_{quat}), 131.3 ($C_{Ar}H$), 129.7 ($C_{Ar}H$), 128.5 ($C_{Ar}H$), 96.0 (OCH_2O), 84.2 (C–I), 60.3 (CH_3), 55.6 (CH_2O). **HRMS** (MALDI-TOF) calcd for $C_{12}H_{13}IN_3O_3$ $[M+H]^+$ 373.9996; found 373.9995.

Ethyl 1-(2-formylphenyl)-5-iodo-1*H*-1,2,3-triazole-4-carboxylate (1l)



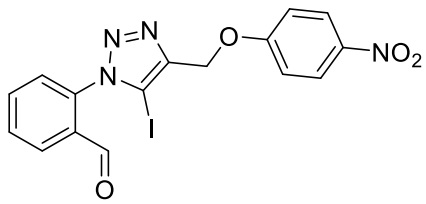
Prepared from alcohol **S4l** (149 mg, 0.4 mmol) according to procedure **B**; eluent: hexanes:CH_2Cl_2:EtOAc = 3:1:1. Yield 105 mg (71%). White solid; mp 140-142 °C (dec.). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.66 (s, 1H, C(O)H), 8.16-8.13 (m, 1H, $C_{Ar}H$), 7.89-7.80 (m, 2H, $C_{Ar}H$), 7.49-7.45 (m, 1H, $C_{Ar}H$), 4.52 (q, J = 7.1 Hz, 2H, CH_2CH_3), 1.49 (t, J = 7.1 Hz, 3H, CH_2CH_3). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 187.4 (HC=O), 160.0 (C=O), 142.3 (C_{quat}), 136.6 (C_{quat}), 134.7 ($C_{Ar}H$), 131.8 (2C, $C_{Ar}H$, C_{quat}), 130.9 ($C_{Ar}H$), 129.0 ($C_{Ar}H$), 88.4 (C–I), 61.9 (CH_2CH_3), 14.3 (CH_3). **HRMS** (MALDI-TOF) calcd for $C_{12}H_{11}IN_3O_3$ $[M+H]^+$ 371.9840; found 371.9840.

***N*-{[1-(2-Formylphenyl)-5-iodo-1*H*-1,2,3-triazol-4-yl]methyl}-4-methylbenzenesulfonamide (1m)**



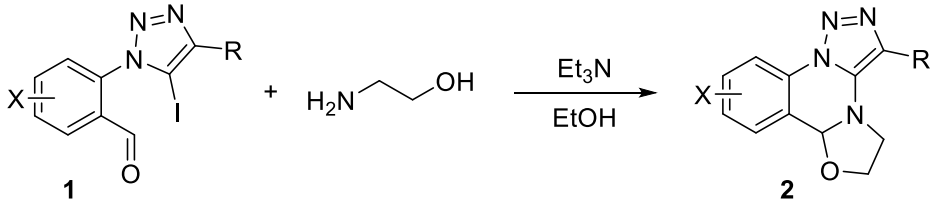
Prepared from alcohol **S4m** (695 mg, 1.5 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 100:1. Yield 647 mg (93%). Yellowish solid; mp 78-80 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.40 (s, 1H, C(O)H), 8.10 (d, J = 7.3 Hz, 1H, $C_{Ar}H$), 7.82-7.74 (m, 4H, $C_{Ar}H$, $C_{Ts}H$), 7.33 (d, J = 7.4 Hz, 1H, $C_{Ar}H$), 7.30-7.27 (m, 2H, $C_{Ts}H$), 5.69 (br s, 1H, NH), 4.36 (s, 2H, CH_2), 2.41 (s, 3H, CH_3). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 187.5 (C=O), 147.5 (C_{quat}), 143.6 (C_{quat}), 137.2 (C_{quat}), 136.6 (C_{quat}), 134.6 ($C_{Ar}H$), 131.5 (C_{quat}), 131.4 ($C_{Ar}H$), 129.9 ($C_{Ar}H$), 129.6 (2C, $C_{Ts}H$), 128.3 ($C_{Ar}H$), 127.3 (2C, $C_{Ts}H$), 82.9 (C–I), 38.8 (CH_2), 21.5 (CH_3). **HRMS** (ESI-TOF) calcd for $C_{17}H_{16}IN_4O_3S$ $[M+H]^+$ 482.9982; found 482.9985.

2-{5-Iodo-4-[(4-nitrophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}benzaldehyde (1n)



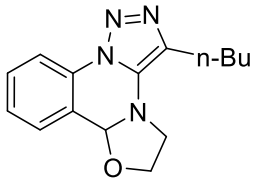
Prepared from alcohol **S4n** (695 mg, 1.5 mmol) according to procedure **A**; eluent: CH_2Cl_2:MeOH = 100:1. Yield 647 mg (93%). White solid; mp 174-176 °C (dec.). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.64 (s, 1H, C(O)H), 8.27-8.25 (m, 2H), 8.17-8.15 (m, $C_{Ar}H$), 8.00-7.96 (m, 1H, $C_{Ar}H$), 7.94-7.90 (m, 1H, $C_{Ar}H$), 7.73 (d, J = 7.7 Hz, 1H, $C_{Ar}H$), 7.37-7.35 (m, 2H), 5.38 (s, 2H, CH_2). **^{13}C{^{1}H} NMR** (100.6 MHz, DMSO-d_6) δ 189.4 (C=O), 163.3 (C_{quat}), 146.4 (C_{quat}), 141.3 (C_{quat}), 136.4 (C_{quat}), 135.2 ($C_{Ar}H$), 131.7 ($C_{Ar}H$), 131.4 (C_{quat}), 131.2 ($C_{Ar}H$), 129.1 ($C_{Ar}H$), 125.9 (2C), 115.5 (2C), 90.2 (C–I), 62.5 (CH_2). **HRMS** (MALDI-TOF) calcd for $C_{16}H_{12}IN_4O_4$ $[M+H]^+$ 450.9899; found 450.9898.

Synthesis of quinazolines 2



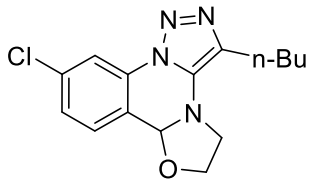
General procedure. (5-Iodotriazolyl)benzaldehyde **1** (0.15 mmol, 1 equiv), 2-aminoethanol (0.225 mmol, 1.5 equiv), and Et_3N (0.3 mmol, 2 equiv) were mixed under Ar atmosphere in EtOH (1.5 mL). The reaction mixture was stirred at 100 °C in a dry block for 2 h, then diluted with CH_2Cl_2, and washed with water. The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was purified by column chromatography.

3-Butyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2a)



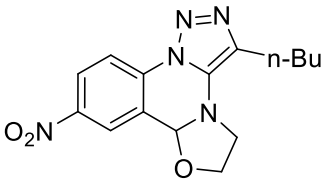
Prepared from benzaldehyde **1a** (35.5 mg, 0.1 mmol) according to the general procedure; eluent: CH_2Cl_2:MeOH = 200:1. Yield 26.8 mg (99%). Yellowish solid; mp 119-121°C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.14 (dd, J = 8.1, 1.1 Hz, 1H, $C_{Ar}\underline{H}$), 7.56–7.50 (m, 2H, $C_{Ar}\underline{H}$), 7.35 (td, J = 7.5, 1.2 Hz, 1H, $C_{Ar}\underline{H}$), 5.70 (s, 1H, C$\underline{H}$), 3.96-3.80 (m, 4H, C$\underline{H}_2$), 2.84-2.70 (m, 2H, C$\underline{H}_2$Pr), 1.81-1.66 (m, 2H, C$\underline{H}_2$Et), 1.49-1.39 (m, 2H, C$\underline{H}_2$CH$_3$), 0.96 (t, J = 7.4 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 136.0 ($\underline{C}_{quat}$), 131.1 ($\underline{C}_{quat}$), 130.9 ($\underline{C}_{Ar}$H), 130.6 ($\underline{C}_{quat}$), 128.4 ($\underline{C}_{Ar}$H), 127.0 ($\underline{C}_{Ar}$H), 118.9 ($\underline{C}_{quat}$), 115.3 ($\underline{C}_{Ar}$H), 87.2 (C$\underline{H}$), 62.4 (O$\underline{C}$H$_2$), 50.9 (N$\underline{C}$H$_2$), 31.5, 25.2, 22.4, 13.9 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{19}N_4O$ $[M+H]^+$ 271.1553; found 271.1552.

3-Butyl-10-chloro-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2b)



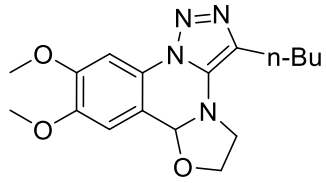
Prepared from benzaldehyde **1b** (58.4 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 44.8 mg (98%). White solid; mp 105-107 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.12 (d, J = 2.0 Hz, 1H, $C_{Ar}\underline{H}$), 7.44 (d, J = 8.3 Hz, 1H, $C_{Ar}\underline{H}$), 7.32 (dd, J = 8.3, 2.0 Hz, 1H, $C_{Ar}\underline{H}$), 5.67 (s, 1H, C$\underline{H}$), 3.97-3.78 (m, 4H, C$\underline{H}_2$), 2.82-2.68 (m, 2H, C$\underline{H}_2$Pr), 1.80-1.64 (m, 2H, C$\underline{H}_2$Et), 1.48-1.39 (m, 2H, C$\underline{H}_2$CH$_3$), 0.96 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 136.9 ($\underline{C}_{quat}$), 136.0 ($\underline{C}_{quat}$), 131.8 ($\underline{C}_{quat}$), 130.6 ($\underline{C}_{quat}$), 129.7 ($\underline{C}_{Ar}$H), 127.1 ($\underline{C}_{Ar}$H), 117.3 ($\underline{C}_{quat}$), 115.5 ($\underline{C}_{Ar}$H), 86.7 (C$\underline{H}$), 62.5 (O$\underline{C}$H$_2$), 50.8 (N$\underline{C}$H$_2$), 31.4, 25.1, 22.4, 13.8 (CH$_2\underline{C}$H$_3$). **HRMS** (ESI-TOF) calcd for $C_{15}H_{18}ClN_4O$ $[M+H]^+$ 305.1164; found 305.1167.

3-Butyl-9-nitro-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2c)



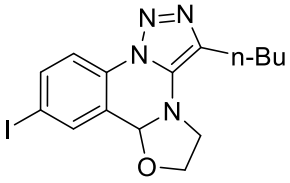
Prepared from benzaldehyde **1c** (60.0 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 3:1. Yield 44.0 mg (93%). Yellow solid; mp 121-123 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.45–8.44 (m, 1H, $C_{Ar}\underline{H}$), 8.41 (dd, J = 8.8, 2.4 Hz, 1H, $C_{Ar}\underline{H}$), 8.27 (d, J = 8.8 Hz, 1H, $C_{Ar}\underline{H}$), 5.81 (s, 1H, C$\underline{H}$), 4.06-3.93 (m, 2H, OC$\underline{H}_2$), 3.89-3.85 (m, 2H, NC$\underline{H}_2$), 2.84-2.71 (m, 2H, C$\underline{H}_2$Pr), 1.83-1.66 (m, 2H, C$\underline{H}_2$Et), 1.49-1.40 (m, 2H, C$\underline{H}_2$CH$_3$), 0.97 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 145.8 ($\underline{C}_{quat}$), 136.3 ($\underline{C}_{quat}$), 135.2 ($\underline{C}_{quat}$), 131.0 ($\underline{C}_{quat}$), 126.4 ($\underline{C}_{Ar}$H), 124.7 ($\underline{C}_{Ar}$H), 120.0 ($\underline{C}_{quat}$), 116.2 ($\underline{C}_{Ar}$H), 86.3 (C$\underline{H}$), 63.0 (O$\underline{C}$H$_2$), 50.7 (N$\underline{C}$H$_2$), 31.4, 25.0, 22.4, 13.8 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{18}N_5O_3$ $[M+H]^+$ 316.1404; found 316.1396.

3-Butyl-9,10-dimethoxy-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2d)



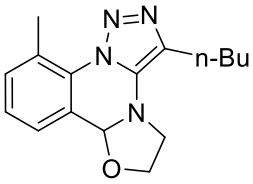
Prepared from benzaldehyde **1d** (62.3 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 1:2. Yield 33.0 mg (67%). Yellowish solid; mp 115-118 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.65 (s, 1H, $C_{Ar}\underline{H}$), 6.95 (s, 1H, $C_{Ar}\underline{H}$), 5.67 (s, 1H, C$\underline{H}$), 4.00 (s, 3H, C$\underline{H}_3$O), 3.96-3.79 (m, 4H, C$\underline{H}_2$), 3.94 (s, 3H, C$\underline{H}_3$O), 2.84-2.70 (m, 2H, C$\underline{H}_2$Pr), 1.80-1.68 (m, 2H, C$\underline{H}_2$Et), 1.48-1.39 (m, 2H, C$\underline{H}_2$CH$_3$), 0.96 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 151.0 ($\underline{C}_{quat}$), 148.1 ($\underline{C}_{quat}$), 135.6 ($\underline{C}_{quat}$), 130.6 ($\underline{C}_{quat}$), 125.2 ($\underline{C}_{quat}$), 110.4 ($\underline{C}_{quat}$), 109.8 ($\underline{C}_{Ar}$H), 98.7 ($\underline{C}_{Ar}$H), 87.3 (C$\underline{H}$), 62.2 (O$\underline{C}$H$_2$), 56.4 (C$\underline{H}_3$O), 56.2 (C$\underline{H}_3$O), 50.9 (N$\underline{C}$H$_2$), 31.5, 25.2, 22.4, 13.8 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{17}H_{23}N_4O_3$ $[M+H]^+$ 331.1765; found 331.1766.

3-Butyl-9-iodo-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2e)



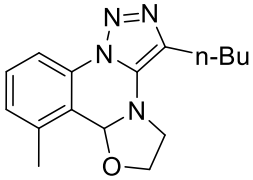
Prepared from benzaldehyde **1e** (72.2 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 53.0 mg (89%). White solid; mp 122-124 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87-7.81 (m, 3H, $C_{Ar}\underline{H}$), 5.64 (s, 1H, C$\underline{H}$), 3.98-3.84 (m, 2H, C$\underline{H}_2$), 3.87-3.77 (m, 2H, C$\underline{H}_2$), 2.82-2.68 (m, 2H, C$\underline{H}_2$Pr), 1.79-1.64 (m, 2H, C$\underline{H}_2$Et), 1.48-1.39 (m, 2H, C$\underline{H}_2$CH$_3$), 0.96 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 139.7 ($\underline{C}_{Ar}$H), 137.1 ($\underline{C}_{Ar}$H), 135.7 ($\underline{C}_{quat}$), 130.8 ($\underline{C}_{quat}$), 130.7 ($\underline{C}_{quat}$), 120.9 ($\underline{C}_{quat}$), 117.1 ($\underline{C}_{Ar}$H), 90.7 ($\underline{C}$–I), 86.2 (C$\underline{H}$), 62.7 (O$\underline{C}$H$_2$), 50.8 (N$\underline{C}$H$_2$), 31.4, 25.1, 22.4, 13.8 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{18}IN_4O$ $[M+H]^+$ 397.0520; found 397.0523.

3-Butyl-11-methyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2f)



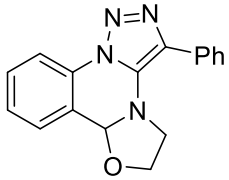
Prepared from benzaldehyde **1f** (55.4 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 36.0 mg (84%). White solid; mp 106-108 °C. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.50-7.46 (m, 2H, $C_{Ar}\underline{H}$), 7.34 (t, J = 7.5 Hz, 1H, $C_{Ar}\underline{H}$), 5.64 (s, 1H, C$\underline{H}$), 4.00-3.95 (m, 1H, C$\underline{H}_2$), 3.86-3.75 (m, 2H, C$\underline{H}_2$), 3.71-3.66 (m, 1H, C$\underline{H}_2$), 2.77-2.73 (m, 5H, C$\underline{H}_2$Pr, C$\underline{H}_3$), 1.70-1.61 (m, 2H, C$\underline{H}_2$Et), 1.43-1.34 (m, 2H, C$\underline{H}_2$CH$_3$), 0.93 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, DMSO-d_6) δ 136.9 ($\underline{C}_{quat}$), 134.4 ($\underline{C}_{Ar}$H), 129.6 ($\underline{C}_{quat}$), 128.6 ($\underline{C}_{quat}$), 127.1 ($\underline{C}_{Ar}$H), 126.9 ($\underline{C}_{quat}$), 126.6 ($\underline{C}_{Ar}$H), 120.4 ($\underline{C}_{quat}$), 87.0 (C$\underline{H}$), 61.6 (O$\underline{C}$H$_2$), 50.5 (N$\underline{C}$H$_2$), 30.8, 24.6, 22.7, 21.8 (C$\underline{H}_3$), 13.7 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{16}H_{21}N_4O$ $[M+H]^+$ 285.1710; found 285.1707.

3-Butyl-8-methyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2g)



Prepared from benzaldehyde **1g** (55.4 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 39.4 mg (92%). White solid; mp 107-109 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.1 Hz, 1H, $C_{Ar}\underline{H}$), 7.41 (t, J = 8.0 Hz, 1H, $C_{Ar}\underline{H}$), 7.17-7.16 (m, 1H, $C_{Ar}\underline{H}$), 5.71 (s, 1H, C$\underline{H}$), 3.99-3.76 (m, 4H, C$\underline{H}_2$), 2.85-2.71 (m, 2H, C$\underline{H}_2$Pr), 2.47 (s, 3H, C$\underline{H}_3$), 1.82-1.64 (m, 2H, C$\underline{H}_2$Et), 1.48-1.39 (m, 2H, C$\underline{H}_2$CH$_3$), 0.96 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 138.2 ($\underline{C}_{quat}$), 135.8 ($\underline{C}_{quat}$), 131.3 ($\underline{C}_{quat}$), 130.5 ($\underline{C}_{Ar}$H), 130.1 ($\underline{C}_{quat}$), 128.7 ($\underline{C}_{Ar}$H), 117.1 ($\underline{C}_{quat}$), 113.0 ($\underline{C}_{Ar}$H), 85.3 (C$\underline{H}$), 61.7 (O$\underline{C}$H$_2$), 50.6 (N$\underline{C}$H$_2$), 31.5, 25.4, 22.4, 18.6 (C$\underline{H}_3$), 13.9 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{16}H_{21}N_4O$ $[M+H]^+$ 285.1710; found 285.1712.

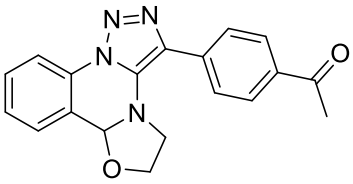
3-Phenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2h)



Prepared from benzaldehyde **1h** (56.3 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 38.0 mg (87%). White solid; mp 131-133 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.20 (d, J = 8.1 Hz, 1H, $C_{Ar}\underline{H}$), 7.77-7.75 (m, 2H), 7.60–7.54 (m, 2H), 7.48-7.32 (m, 4H), 5.80 (s, 1H, C$\underline{H}$), 3.91-3.84 (m, 1H, C$\underline{H}_2$), 3.78-3.68 (m, 2H, C$\underline{H}_2$), 3.63-3.57 (m, 1H, C$\underline{H}_2$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 136.2 ($\underline{C}_{quat}$), 131.1 ($\underline{C}_{quat}$), 131.0 (2C, $\underline{C}_{Ar}$H, C_{quat}), 130.7 ($\underline{C}_{quat}$), 128.5 (3C), 127.4 (3C), 127.3, 119.0 ($\underline{C}_{quat}$), 115.4 ($\underline{C}_{Ar}$H), 87.0 (C$\underline{H}$), 62.3 (O$\underline{C}$H$_2$), 51.9 (N$\underline{C}$H$_2$). **HRMS** (MALDI-TOF) calcd for $C_{17}H_{15}N_4O$ $[M+H]^+$ 291.1240; found 291.1242.

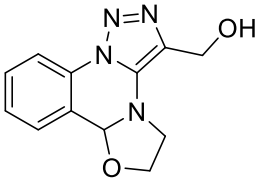
1-[4-(5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-yl)phenyl]ethanone (2i)

Prepared from benzaldehyde **1i** (62.6 mg, 0.15 mmol) according to the general procedure; eluent: CH_2Cl_2:MeOH = 100:1. Yield 43.0 mg (86%). White solid; mp 158-160 °C. **^{1}H NMR** (400



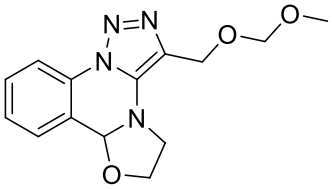
MHz, $CDCl_3$) δ 8.18 (d, J = 8.1 Hz, 1H, $C_{Ar}\underline{H}$), 8.07-8.02 (m, 2H), 7.89-7.84 (m, 2H), 7.61-7.54 (m, 2H, $C_{Ar}\underline{H}$), 7.45-7.40 (m, 1H, $C_{Ar}\underline{H}$), 5.84 (s, 1H, C$\underline{H}$), 3.95-3.88 (m, 1H, C$\underline{H_2}$), 3.85-3.74 (m, 2H, C$\underline{H_2}$), 3.55-3.48 (m, 1H, C$\underline{H_2}$), 2.63 (s, 3H, C$\underline{H_3}$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 197.5 (C$\underline{}$=O), 137.1 ($\underline{C}_{quat}$), 135.7 ($\underline{C}_{quat}$), 135.5 ($\underline{C}_{quat}$), 131.0 ($\underline{C}_{Ar}$H), 130.8 ($\underline{C}_{quat}$), 129.7 ($\underline{C}_{quat}$), 128.6 (2C), 128.5 ($\underline{C}_{Ar}$H), 127.5 ($\underline{C}_{Ar}$H), 126.9 (2C), 118.8 ($\underline{C}_{quat}$), 115.4 ($\underline{C}_{Ar}$H), 86.9 (C$\underline{H}$), 62.3 (O$\underline{C}H_2$), 52.1 (N$\underline{C}H_2$), 26.6 ($\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{19}H_{17}N_4O_2$ $[M+H]^+$ 333.1346; found 333.1345.

5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-ylmethanol (2j)



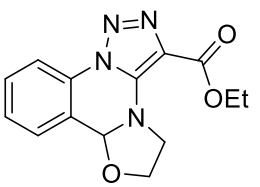
Prepared from benzaldehyde **1k** (32.9 mg, 0.1 mmol) according to the general procedure after removing MOM-protective group; eluent: CH_2Cl_2:MeOH = 10:1. Yield 24.0 mg (98%). Brownish solid; mp 88-92 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09-8.06 (m, 1H, $C_{Ar}\underline{H}$), 7.54-7.49 (m, 2H, $C_{Ar}\underline{H}$), 7.39-7.35 (m, 1H, $C_{Ar}\underline{H}$), 5.68 (s, 1H, C$\underline{H}$), 4.93 (d, J = 13.3 Hz, 1H, C$\underline{H_2}$OH), 4.68 (d, J = 13.3 Hz, 1H, C$\underline{H_2}$OH), 4.38-4.31 (m, 1H, C$\underline{H_2}$), 3.96-3.81 (m, 3H, C$\underline{H_2}$), 3.47 (s, 1H, O$\underline{H}$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 138.0 ($\underline{C}_{quat}$), 131.0 ($\underline{C}_{Ar}$H), 130.6 ($\underline{C}_{quat}$), 129.8 ($\underline{C}_{quat}$), 128.7 ($\underline{C}_{Ar}$H), 127.3 ($\underline{C}_{Ar}$H), 118.7 ($\underline{C}_{quat}$), 115.2 ($\underline{C}_{Ar}$H), 86.7 (C$\underline{H}$), 62.3 (O$\underline{C}H_2$), 55.5 (N$\underline{C}H_2$), 51.4 ($\underline{C}H_2$OH). **HRMS** (MALDI-TOF) calcd for $C_{12}H_{13}N_4O_2$ $[M+H]^+$ 245.1033; found 245.1032.

3-[(Methoxymethoxy)methyl]-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2k)



Prepared from benzaldehyde **1k** (55.9 mg, 0.15 mmol) according to the general procedure; eluent: CH_2Cl_2:MeOH = 50:1. Yield 38.3 mg (89%). White solid; mp 144-146 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.1 Hz, 1H, $C_{Ar}\underline{H}$), 7.58-7.52 (m, 2H, $C_{Ar}\underline{H}$), 7.39 (dd, J = 7.6, 1.1 Hz, 1H, $C_{Ar}\underline{H}$), 5.70 (s, 1H, C$\underline{H}$), 4.85 (d, J = 6.5 Hz, 1H), 4.78 (d, J = 6.5 Hz, 1H), 4.72-4.68 (m, 2H), 4.22-4.18 (m, 1H), 3.97-3.82 (m, 3H), 3.44 (s, 3H, C$\underline{H_3}$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 138.4 ($\underline{C}_{quat}$), 131.0 ($\underline{C}_{Ar}$H), 130.7 ($\underline{C}_{quat}$), 128.6 ($\underline{C}_{Ar}$H), 127.3 ($\underline{C}_{Ar}$H), 126.5 ($\underline{C}_{quat}$), 118.5 ($\underline{C}_{quat}$), 115.3 ($\underline{C}_{Ar}$H), 95.4 (O$\underline{C}H_2$O), 86.8 (C$\underline{H}$), 62.3, 59.9, 55.6, 51.1. **HRMS** (MALDI-TOF) calcd for $C_{14}H_{17}N_4O_3$ $[M+H]^+$ 289.1295; found 289.1294.

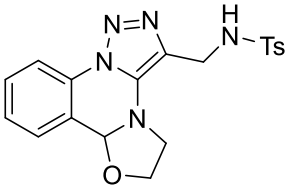
Ethyl 5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline-3-carboxylate (2l)



Prepared from benzaldehyde **1l** (55.7 mg, 0.15 mmol) according to the general procedure; eluent: CH_2Cl_2:MeOH = 100:1. Yield 38.0 mg (89%). White solid; mp 142-144 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.15 (d, J =

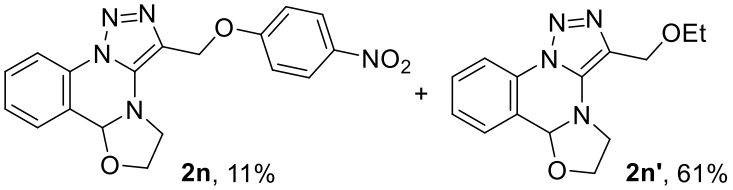
8.2 Hz, 1H, $C_{Ar}\underline{H}$), 7.59-7.53 (m, 2H, $C_{Ar}\underline{H}$), 7.42 (td, *J* = 7.6, 1.0 Hz, 1H, $C_{Ar}\underline{H}$), 5.90 (s, 1H, C<u>H</u>), 4.43 (q, *J* = 7.1 Hz, 2H, $C\underline{H}_2CH_3$), 4.22-4.12 (m, 2H, $C\underline{H}_2$), 4.04-3.95 (m, 2H, $C\underline{H}_2$), 1.45 (t, *J* = 7.1 Hz, 3H, $C\underline{H}_3$). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, $CDCl_3$) δ 161.2 (<u>C</u>=O), 141.4 ($\underline{C}_{quat}$), 130.9 ($\underline{C}_{Ar}H$), 130.0 ($\underline{C}_{quat}$), 128.0 ($\underline{C}_{Ar}H$), 127.8 ($\underline{C}_{Ar}H$), 122.2 ($\underline{C}_{quat}$), 118.3 ($\underline{C}_{quat}$), 115.4 ($\underline{C}_{Ar}H$), 86.0 (<u>C</u>H), 63.0, 60.9, 51.9 ($N\underline{C}H_2$), 14.4 ($\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{14}H_{15}N_4O_3$ $[M+H]^+$ 287.1139; found 287.1140.

***N*-(5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-ylmethyl)-4-methylbenzenesulfonamide (2m)**



Prepared from benzaldehyde **1m** (72.3 mg, 0.10 mmol) according to the general procedure; eluent: hexanes:EtOAc = 1:1. Yield 56.3 mg (95%). White solid; mp 108-112 °C. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.04-8.01 (m, 1H, $C_{Ar}\underline{H}$), 7.98-7.95 (m, 1H, $C_{Ar}\underline{H}$), 7.67-7.63 (m, 4H, $C_{Ar}\underline{H}$, $C_{Ts}\underline{H}$, N<u>H</u>), 7.49-7.45 (m, 1H, $C_{Ar}\underline{H}$), 7.31-7.29 (m, 2H, $C_{Ts}\underline{H}$), 5.66 (s, 1H, C<u>H</u>), 4.19 (dd, *J* = 14.5, 6.2 Hz, 1H, $C\underline{H}_2NH$), 4.06 (dd, *J* = 14.5, 5.3 Hz, 1H, $C\underline{H}_2NH$), 3.95-3.89 (m, 1H, $C\underline{H}_2$), 3.85-3.79 (m, 1H, $C\underline{H}_2$), 3.75-3.67 (m, 2H, $C\underline{H}_2$), 2.24 (s, 3H, $C\underline{H}_3$). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, DMSO-d_6) δ 142.6 ($\underline{C}_{quat}$), 137.3 ($\underline{C}_{quat}$), 137.2 ($\underline{C}_{quat}$), 131.2 ($\underline{C}_{Ar}H$), 130.1 ($\underline{C}_{quat}$), 129.4 ($\underline{C}_{Ar}H$), 129.3 (2C, $\underline{C}_{Ts}H$), 127.4 ($\underline{C}_{Ar}H$), 126.6 (2C, $\underline{C}_{Ts}H$), 125.2 ($\underline{C}_{quat}$), 118.7 ($\underline{C}_{quat}$), 114.3 ($\underline{C}_{Ar}H$), 85.6 (<u>C</u>H), 61.6 ($O\underline{C}H_2$), 50.0 ($N\underline{C}H_2$), 38.1 ($\underline{C}H_2NH$), 20.8 ($\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{19}H_{20}N_5O_3S$ $[M+H]^+$ 398.1281; found 398.1287.

3-(4-Nitrophenoxy)-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2n) and 3-(ethoxymethyl)-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2n')

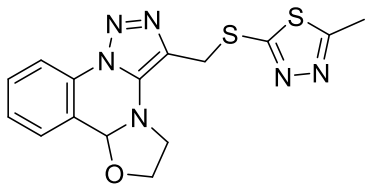


Inseparable mixture of **2n** and **2n'** was obtained from benzaldehyde **1n** (67.5 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 2:1. Yield 31 mg (**2n**, 11%; **2n'**, 61%).

2n: **^{1}H NMR** (400 MHz, DMSO-d_6), selected signals: δ 8.22 (m, 2H), 7.31 (m, 2H), 5.77 (s, 1H, C<u>H</u>), 5.49 (d, *J* = 12.7 Hz, 1H, $C\underline{H}_2OAr$), 5.37 (d, *J* = 12.7 Hz, 1H, $C\underline{H}_2OAr$).

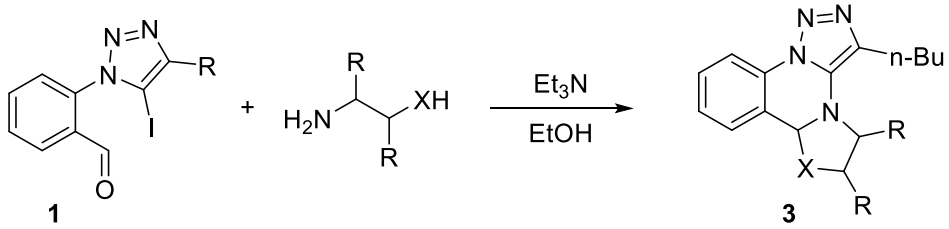
2n': **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.05-8.00 (m, 1H, $C_{Ar}\underline{H}$), 7.69-7.62 (m, 2H, $C_{Ar}\underline{H}$), 7.50-7.44 (m, 1H, $C_{Ar}\underline{H}$), 5.72 (s, 1H, C<u>H</u>), 4.59 (d, *J* = 12.4 Hz, 1H, $C\underline{H}_2OEt$), 4.54 (d, *J* = 12.4 Hz, 1H, $C\underline{H}_2OEt$), 4.13 (m, 1H), 3.88-3.76 (m, 2H), 3.69 (m, 1H), 3.50 (q, *J* = 7.1 Hz, 2H, $C\underline{H}_2Me$), 3.50 (t, *J* = 7.1 Hz, 3H, $C\underline{H}_3$). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, DMSO-d_6) δ 138.2 ($\underline{C}_{quat}$), 131.4 ($\underline{C}_{Ar}H$), 130.2 ($\underline{C}_{quat}$), 129.6 ($\underline{C}_{Ar}H$), 127.5 ($\underline{C}_{Ar}H$), 125.9 ($\underline{C}_{quat}$), 118.7 ($\underline{C}_{quat}$), 114.4 ($\underline{C}_{Ar}H$), 85.7 (<u>C</u>H), 64.4, 62.5, 61.6, 50.4, 15.0 ($\underline{C}H_3$).

3-{[(5-Methyl-1,3,4-thiadiazol-2-yl)thio]methyl}-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2o)



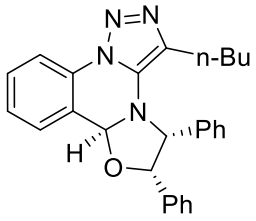
Benzaldehyde **1n** (45.0 mg, 0.10 mmol), 5-methyl-1,3,4-thiadiazole-2-thiol (19.8 mg, 0.15 mmol), 2-aminoethanol (9.1 μL, 0.15 mmol), and Et_3N (48.7 μL, 0.35 mmol) were mixed under Ar atmosphere with dioxane (0.8 mL) and water (0.2 mL). The reaction mixture was stirred at 100 °C in a dry block for 2 h, then diluted with CH_2Cl_2, and washed with water. The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was purified by column chromatography (eluent: hexanes:EtOAc = 1:1). Yield 19.2 mg (54%). Yellowish solid; mp >180 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.1 Hz, 1H, $C_{Ar}\underline{H}$), 7.58-7.52 (m, 2H, $C_{Ar}\underline{H}$), 7.40 (td, J = 7.6, 1.1 Hz, 1H, $C_{Ar}\underline{H}$), 5.74 (s, 1H, C$\underline{H}$), 4.85 (d, J = 13.8 Hz, 1H, C$\underline{H}_2$S), 4.76 (d, J = 13.8 Hz, 1H, C$\underline{H}_2$S), 4.15-4.06 (m, 1H), 3.98-3.93 (m, 3H), 2.74 (s, 3H, C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 165.5 ($\underline{C}_{quat}$), 164.3 ($\underline{C}_{quat}$), 137.4 ($\underline{C}_{quat}$), 131.0 ($\underline{C}_{Ar}$H), 130.6 ($\underline{C}_{quat}$), 128.5 ($\underline{C}_{Ar}$H), 127.5 ($\underline{C}_{Ar}$H), 123.8 ($\underline{C}_{quat}$), 118.6 ($\underline{C}_{quat}$), 115.3 ($\underline{C}_{Ar}$H), 86.8 (C$\underline{H}$), 62.6 (O$\underline{C}H_2$), 50.6 (N$\underline{C}H_2$), 29.2 (C$\underline{H}_2$S), 15.7 (C$\underline{H}_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{15}N_6OS_2$ $[M+H]^+$ 359.0743; found 359.0738.

Synthesis of quinazolines 3



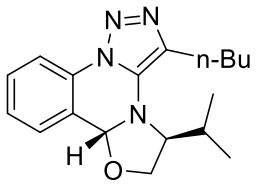
General procedure. (5-Iodotriazolyl)benzaldehyde **1** (0.2 mmol, 1 equiv), the corresponding amine (0.3 mmol, 1.5 equiv), and Et_3N (0.4 mmol, 2 equiv) were mixed under Ar atmosphere in EtOH (2 mL). The reaction mixture was stirred at 100 °C in a dry block for 2 h, then diluted with CH_2Cl_2, and washed with water. The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was purified by column chromatography.

(5*R*,6*S*,7a*S*)-3-Butyl-5,6-diphenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3a)



Prepared from benzaldehyde **1a** (71.0 mg, 0.2 mmol) and (1*S*,2*R*)-2-amino-1,2-diphenylethan-1-ol (63.9 mg, 0.3 mmol) according to the general procedure; eluent: hexanes:EtOAc = 5:1. Yield 56.0 mg (66%, dr = 95:5). Yellowish solid; mp 69-71 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.11-8.10 (m, 1H, $C_{Ar}\underline{H}$), 7.63-7.62 (m, 1H, $C_{Ar}\underline{H}$), 7.53-7.50 (m, 1H, $C_{Ar}\underline{H}$), 7.39 (td, *J* = 7.6, 0.9 Hz, 1H, $C_{Ar}\underline{H}$), 7.15-7.07 (m, 6H, $C_{Ar}\underline{H}$, $C_{Ph}\underline{H}$), 7.01-6.97 (m, 4H, $C_{Ph}\underline{H}$), 6.71 (s, 1H, C$\underline{H}$), 5.23 (d, *J* = 6.1 Hz, 1H, OC$\underline{H}$), 4.79 (d, *J* = 6.1 Hz, 1H, NC$\underline{H}$), 2.25 (t, *J* = 8.0 Hz, 2H, C$\underline{H}_2$Pr), 1.44-1.29 (m, 2H, C$\underline{H}_2$Et), 1.03-0.96 (m, 2H, C$\underline{H}_2$CH$_3$), 0.65 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 137.6 ($\underline{C}_{quat}$), 135.5 ($\underline{C}_{quat}$), 134.7 ($\underline{C}_{quat}$), 134.3 ($\underline{C}_{quat}$), 132.0 ($\underline{C}_{quat}$), 130.1, 127.9, 127.76, 127.74 (2C), 127.71 (2C), 127.5, 127.3 (2C, $\underline{C}_{Ph}$H), 126.8 (2C, $\underline{C}_{Ph}$H), 126.0, 121.7 ($\underline{C}_{quat}$), 115.4, 87.1 (C$\underline{H}$), 82.8 (OC$\underline{H}$), 71.8 (NC$\underline{H}$), 31.6, 24.3, 22.2, 13.5 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{27}H_{27}N_4O$ $[M+H]^+$ 423.2179; found 423.2175.

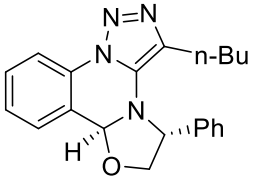
(5*S*,7a*R*)-3-Butyl-5-isopropyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3b)



Prepared from benzaldehyde **1a** (35.5 mg, 0.1 mmol) and (*S*)-valinol (15.5 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 6:1. Yield 28.0 mg (90%, dr = 95:5). Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ major diastereomer (5*S*,7a*R*)-**3b**: 8.16 (d, *J* = 8.1 Hz, 1H, $C_{Ar}\underline{H}$), 7.57-7.7.53 (m, 1H, $C_{Ar}\underline{H}$), 7.51-7.7.49 (m, 1H, $C_{Ar}\underline{H}$), 7.36 (td, *J* = 7.6, 1.0 Hz, 1H, $C_{Ar}\underline{H}$), 5.62 (s, 1H, C$\underline{H}$), 3.93-3.88 (m, 1H, OC$\underline{H}_2$), 3.83-3.73 (m, 2H, OC$\underline{H}_2$, NC$\underline{H}$), 2.84-2.71 (m, 2H, C$\underline{H}_2$Pr), 2.15-2.07 (m, 1H, C$\underline{H}$(CH$_3$)$_2$), 1.85-1.66 (m, 2H, C$\underline{H}_2$Et), 1.51-1.42

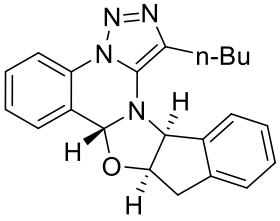
(m, 2H, C$\underline{H}_2$CH$_3$), 1.14 (d, *J* = 6.9 Hz, 3H, CH(C$\underline{H}_3$)$_2$), 1.07 (d, *J* = 6.7 Hz, 3H, CH(C$\underline{H}_3$)$_2$), 0.98 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$); minor diastereomer (5*S*,7a*S*)-**3b** (selected signals): 8.02 (d, *J* = 7.9 Hz, 1H, C$_{Ar}\underline{H}$), 7.47-7.7.45 (m, 2H, C$_{Ar}\underline{H}$), 7.36-7.7.34 (m, 1H, C$_{Ar}\underline{H}$), 7.36 (td, *J* = 7.6, 1.0 Hz, 1H, C$_{Ar}\underline{H}$), 6.06 (s, 1H, C$\underline{H}$), 4.24-4.23 (m, 1H), 4.15-4.13 (m, 1H), 2.79-2.71 (m, 2H, C$\underline{H}_2$Pr), 0.91 (d, *J* = 7.0 Hz, 3H, CH(C$\underline{H}_3$)$_2$), 0.48 (d, *J* = 6.8 Hz, 3H, CH(C$\underline{H}_3$)$_2$). **^{13}C{^{1}H} NMR** (100.6 MHz, CDCl$_3$) *δ* major diastereomer (5*S*,7a*R*)-**3b**: 136.3 (C$_{quat}$), 131.4 (C$_{quat}$), 131.0 (C$_{Ar}$H), 130.2 (C$_{quat}$), 128.6 (C$_{Ar}$H), 126.8 (C$_{Ar}$H), 118.7 (C$_{quat}$), 115.3 (C$_{Ar}$H), 86.2 (CH), 68.9 (OCH$_2$), 64.7 (NCH), 32.2, 31.0, 25.6, 22.6, 20.0 (CH(CH$_3$)$_2$), 17.8 (CH(CH$_3$)$_2$), 13.9 (CH$_2$CH$_3$). **HRMS** (MALDI-TOF) calcd for C$_{18}$H$_{25}$N$_4$O [M+H]$^+$ 313.2023; found 313.2024.

(5*R*,7a*S*)-3-Butyl-5-phenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3c)



Prepared from benzaldehyde **1a** (71.0 mg, 0.2 mmol) and (*R*)-2-phenylglycinol (41.2 mg, 0.3 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 66.0 mg (95%, dr = 90:10). Yellow solid; mp 63-65 °C. **^{1}H NMR** (400 MHz, CDCl$_3$) *δ* major diastereomer (5*R*,7a*S*)-**3c**: 8.17 (d, *J* = 8.0 Hz, 1H, C$_{Ar}\underline{H}$), 7.54–7.52 (m, 2H, C$_{Ar}\underline{H}$), 7.45-7.35 (m, 6H, C$_{Ar}\underline{H}$, C$_{Ph}\underline{H}$), 5.98 (s, 1H, C$\underline{H}$), 4.98 (m, 1H), 4.42 (m, 1H), 3.72 (dd, *J* = 8.7, 7.0 Hz, 1H, OC$\underline{H}_2$), 2.43-2.28 (m, 2H, C$\underline{H}_2$Pr), 1.46-1.39 (m, 2H, C$\underline{H}_2$Et), 1.14-1.00 (m, 2H, C$\underline{H}_2$CH$_3$), 0.70 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$); minor diastereomer (5*R*,7a*R*)-**3c**: 8.06 (d, *J* = 8.0 Hz, 1H, C$_{Ar}\underline{H}$), 7.56–7.54 (m, 2H, C$_{Ar}\underline{H}$), 7.18-7.16 (m, 3H), 7.02-7.00 (m, 2H), 6.19 (s, 1H, C$\underline{H}$), 5.07-5.05 (m, 1H, NC$\underline{H}$), 4.53-4.49 (m, 1H, OC$\underline{H}_2$), 4.07-4.04 (m, 1H, OC$\underline{H}_2$), 2.43-2.28 (m, 2H, C$\underline{H}_2$Pr), 1.46-1.39 (m, 2H, C$\underline{H}_2$Et), 1.14-1.00 (m, 2H, C$\underline{H}_2$CH$_3$), 0.85 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, CDCl$_3$) *δ* major diastereomer (5*R*,7a*S*)-**3c**: 140.1 (C$_{quat}$), 136.4 (C$_{quat}$), 131.3 (C$_{quat}$), 131.2 (C$_{quat}$), 130.9, 129.1 (2C, C$_{Ph}$H), 128.4 (C$_{Ar}$H), 128.0 (C$_{Ar}$H), 127.0 (C$_{Ar}$H), 125.5 (2C, C$_{Ph}$H), 118.7 (C$_{quat}$), 115.2 (C$_{Ar}$H), 88.1 (OCH), 71.2 (OCH$_2$), 67.2 (NCH), 32.1, 24.8, 22.2, 13.6 (CH$_2$CH$_3$). **HRMS** (MALDI-TOF) calcd for C$_{21}$H$_{23}$N$_4$O [M+H]$^+$ 347.1866; found 347.1867.

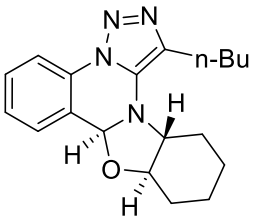
(8b*R*,9a*R*,14b*S*)-1-Butyl-10,14b-dihydro-8b*H*,9a*H*-indeno[1',2':4,5][1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3d)



Prepared from benzaldehyde **1a** (35.5 mg, 0.1 mmol) and (1*S*,2*R*)-2-amino-2,3-dihydro-1*H*-inden-2-ol (22.4 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 34.0 mg (95%, dr > 99:1). Yellowish solid; mp 119-121 °C. **^{1}H NMR** (400 MHz, CDCl$_3$) *δ* 8.18 (d, *J* = 7.9 Hz, 1H, C$_{Ar}\underline{H}$), 7.58-7.52 (m, 2H), 7.42-7.29 (m, 5H), 5.84 (d, *J* = 5.7 Hz, 1H), 5.36 (s, 1H), 4.68-4.65 (m, 1H), 3.33 (d, *J* = 3.4 Hz, 2H, CHC$\underline{H}_2$), 3.03-2.91 (m, 2H, C$\underline{H}_2$Pr), 1.98-1.79 (m, 2H, C$\underline{H}_2$Et), 1.55-1.46 (m, 2H, C$\underline{H}_2$CH$_3$), 1.00 (t, *J* = 7.3 Hz,

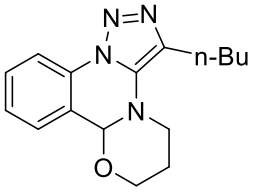
3H, $CH_2C\underline{H}_3$). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, $CDCl_3$) δ 142.6 ($\underline{C}_{quat}$), 137.6 ($\underline{C}_{quat}$), 135.5 ($\underline{C}_{quat}$), 131.3 ($\underline{C}_{quat}$), 131.1 ($\underline{C}_{Ar}H$), 130.5 ($\underline{C}_{quat}$), 129.5, 128.9, 127.8, 126.8, 125.6, 125.2, 118.6 ($\underline{C}_{quat}$), 115.4, 86.0, 76.1, 72.1, 38.9, 31.5, 26.0, 22.5, 13.9 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{22}H_{23}N_4O$ $[M+H]^+$ 359.1866; found 359.1865.

(8b*S*,9a*R*,13a*R*)-1-Butyl-9a,10,11,12,13,13a-hexahydro-8b*H*-[1,3]benzoxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3e)



Prepared from benzaldehyde **1a** (53.3 mg, 0.15 mmol) and (1*R*,2*R*)-2-aminocyclohexanol hydrochloride (34.1 mg, 0.225 mmol) according to the general procedure; eluent: hexanes:EtOAc = 3:1. Yield 48.0 mg (99%, dr = 88:12). Yellowish solid; mp 65-67 °C. **^1H NMR** (400 MHz, $CDCl_3$) δ major diastereomer (8b*S*,9a*R*,13a*R*)-**3e**: 8.05-8.03 (m, 1H, $C_{Ar}\underline{H}$), 7.53-7.51 (m, 1H, $C_{Ar}\underline{H}$), 7.47-7.43 (m, 1H, $C_{Ar}\underline{H}$), 7.37-7.34 (m, 1H, $C_{Ar}\underline{H}$), 6.04 (s, 1H, C$\underline{H}$), 3.74-3.67 (m, 1H), 2.79-2.71 (m, 1H), 2.71-2.66 (m, 2H), 2.27-2.16 (m, 2H), 1.89-1.68 (m, 5H), 1.62-1.52 (m, 1H), 1.50-1.37 (m, 4H), 0.96 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$); minor diastereomer (8b*R*,9a*R*,13a*R*)-**3e** (selected signals): 8.02-8.00 (m, 1H, $C_{Ar}\underline{H}$), 7.53-7.51 (m, 1H, $C_{Ar}\underline{H}$), 7.47-7.43 (m, 1H, $C_{Ar}\underline{H}$), 7.37-7.34 (m, 1H, $C_{Ar}\underline{H}$), 6.20 (s, 1H, C$\underline{H}$), 3.21-3.15 (m, 1H), 3.04-2.98 (m, 1H). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, $CDCl_3$) δ major diastereomer (8b*S*,9a*R*,13a*R*)-**3e**: 136.9 ($\underline{C}_{quat}$), 134.5 ($\underline{C}_{quat}$), 129.7 ($\underline{C}_{Ar}H$), 128.5 ($\underline{C}_{quat}$), 127.6 ($\underline{C}_{Ar}H$), 127.4 ($\underline{C}_{Ar}H$), 127.1 ($\underline{C}_{quat}$), 123.4 ($\underline{C}_{quat}$), 115.2 ($\underline{C}_{Ar}H$), 86.5, 82.5, 68.3, 31.1, 29.4 (2C), 24.8, 24.0, 23.5, 22.5 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{19}H_{25}N_4O$ $[M+H]^+$ 325.2023; found 325.2022.

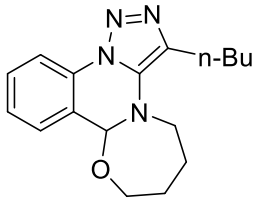
3-Butyl-6,7-dihydro-5*H*,8a*H*-[1,3]oxazino[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3f)



Prepared from benzaldehyde **1a** (71.0 mg, 0.2 mmol) and 3-aminopropanol (18.4 μL, 0.24 mmol) according to the general procedure; eluent: CH_2Cl_2:MeOH = 30:1. Yield 56.2 mg (99%). White solid; mp 79-81 °C. **^1H NMR** (400 MHz, $CDCl_3$) δ 8.09-8.07 (m, 1H, $C_{Ar}\underline{H}$), 7.52-7.48 (m, 1H, $C_{Ar}\underline{H}$), 7.41 (dd, J = 7.7, 1.4 Hz, 1H, $C_{Ar}\underline{H}$), 7.32 (td, J = 7.5, 1.1 Hz, 1H, $C_{Ar}\underline{H}$), 5.66 (s, 1H, C$\underline{H}$), 4.22-4.06 (m, 3H), 3.63-3.55 (m, 1H), 2.92 (dt, J = 15.1, 7.9 Hz, 1H, C$\underline{H}_2$Pr), 2.72 (dt, J = 15.1, 7.5 Hz, 1H, C$\underline{H}_2$Pr), 2.24-2.12 (m, 1H), 1.76-1.68 (m, 2H, CH_2Et), 1.55-1.52 (m, 1H), 1.49-1.40 (m, 2H, C$\underline{H}_2CH_3$), 0.96 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$). **$^{13}C\{^1H\}$ NMR** (100.6 MHz, $CDCl_3$) δ 134.7 ($\underline{C}_{quat}$), 131.3 ($\underline{C}_{quat}$), 130.6 ($\underline{C}_{Ar}H$), 128.5 ($\underline{C}_{quat}$), 127.7 ($\underline{C}_{Ar}H$), 126.8 ($\underline{C}_{Ar}H$), 120.5 ($\underline{C}_{quat}$), 115.2 ($\underline{C}_{Ar}H$), 86.3 (C$\underline{H}$), 68.2 (O$\underline{C}H_2$), 46.5 (N$\underline{C}H_2$), 32.2, 26.2, 24.3, 22.3, 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{16}H_{21}N_4O$ $[M+H]^+$ 285.1710; found 285.1709.

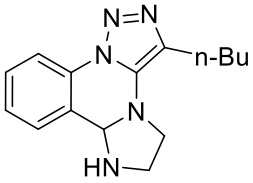
3-Butyl-5,6,7,8-tetrahydro-9a*H*-[1,3]oxazepino[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3g)

Prepared from benzaldehyde **1a** (35.5 mg, 0.1 mmol) and 4-aminobutanol (13.8 μL, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 24.2 mg (81%).



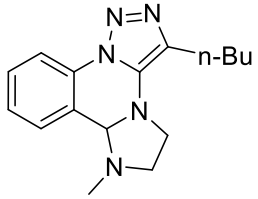
Yellowish oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.12-8.09 (m, 1H, $C_{Ar}\underline{H}$), 7.51-7.47 (m, 1H, $C_{Ar}\underline{H}$), 7.45-7.43 (m, 1H, $C_{Ar}\underline{H}$), 7.34 (td, *J* = 7.5, 1.1 Hz, 1H, $C_{Ar}\underline{H}$), 5.77 (s, 1H, C$\underline{H}$), 4.00 (dt, *J* = 14.9, 4.6 Hz, 1H), 3.81 (ddd, *J* = 12.4, 6.5, 3.1 Hz, 1H), 3.68 (ddd, *J* = 12.4, 7.9, 2.9 Hz, 1H), 3.53-3.45 (m, 1H), 2.93-2.85 (m, 1H, C$\underline{H}_2$), 2.72-2.64 (m, 1H, C$\underline{H}_2$), 2.02-1.70 (m, 6H), 1.49-1.40 (m, 2H, C$\underline{H}_2$CH$_3$), 0.96 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 134.5 ($\underline{C}_{quat}$), 131.1 ($\underline{C}_{quat}$), 130.1 ($\underline{C}_{Ar}$H), 127.6 ($\underline{C}_{Ar}$H), 127.0 ($\underline{C}_{quat}$), 126.7 ($\underline{C}_{Ar}$H), 121.6 ($\underline{C}_{quat}$), 115.2 ($\underline{C}_{Ar}$H), 86.7 (C$\underline{H}$), 67.6 (O$\underline{C}$H$_2$), 48.3 (N$\underline{C}$H$_2$), 32.9, 28.8, 27.7, 26.0, 22.5, 13.9 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{17}H_{23}N_4O$ $[M+H]^+$ 299.1866; found 299.1865.

3-Butyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3h)



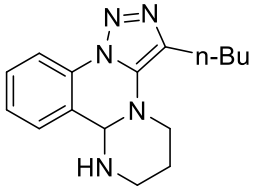
Prepared from benzaldehyde **1a** (71.0 mg, 0.2 mmol) and ethane-1,2-diamine (20.1 μL, 0.3 mmol) according to the general procedure without purification. Yield 48.0 mg (89%). Yellowish solid; mp 70-72 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.00-7.98 (m, 1H, $C_{Ar}\underline{H}$), 7.50 (d, *J* = 7.6 Hz, 1H, $C_{Ar}\underline{H}$), 7.42 (td, *J* = 7.6, 1.0 Hz, 1H, $C_{Ar}\underline{H}$), 7.32-7.28 (m, 1H, $C_{Ar}\underline{H}$), 5.37 (s, 1H, C$\underline{H}$), 3.69-3.69-3.63 (m, 1H, NC$\underline{H}_2$), 3.44-3.38 (m, 1H, NC$\underline{H}_2$), 3.34-3.18 (m, 2H, NC$\underline{H}_2$), 2.74-2.63 (m, 2H, C$\underline{H}_2$Pr), 2.26 (br s., 1H, N$\underline{H}$), 1.77-1.61 (m, 2H, C$\underline{H}_2$Et), 1.46-1.37 (m, 2H, C$\underline{H}_2$CH$_3$), 0.95 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 136.6 ($\underline{C}_{quat}$), 131.4 ($\underline{C}_{quat}$), 130.4 ($\underline{C}_{quat}$), 129.6 ($\underline{C}_{Ar}$H), 127.02 ($\underline{C}_{Ar}$H), 126.96 ($\underline{C}_{Ar}$H), 121.2 ($\underline{C}_{quat}$), 115.3 ($\underline{C}_{Ar}$H), 74.1 (C$\underline{H}$), 50.5 (N$\underline{C}$H$_2$), 45.0 (N$\underline{C}$H$_2$), 32.0, 24.8, 22.4, 13.9 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{20}N_5$ $[M+H]^+$ 270.1713; found 270.1712.

3-Butyl-7-methyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3i)



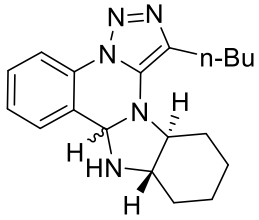
Prepared from benzaldehyde **1a** (53.3 mg, 0.15 mmol) and *N*-methylethane-1,2-diamine (19.6 μL, 0.225 mmol) according to the general procedure; eluent: hexanes:EtOAc = 1:3. Yield 27.0 mg (64%). Yellowish oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.1 Hz, 1H, $C_{Ar}\underline{H}$), 7.49-7.44 (m, 1H, $C_{Ar}\underline{H}$), 7.40-7.36 (m, 1H, $C_{Ar}\underline{H}$), 7.33-7.28 (m, 1H, $C_{Ar}\underline{H}$), 4.77 (s, 1H, C$\underline{H}$), 3.76-3.70 (m, 1H, NC$\underline{H}_2$), 3.64-3.57 (m, 1H, NC$\underline{H}_2$), 3.21-3.16 (m, 1H, NC$\underline{H}_2$), 2.81-2.68 (m, 3H, NC$\underline{H}_2$, C$\underline{H}_2$Pr), 2.30 (s, 3H, NC$\underline{H}_3$), 1.79-1.63 (m, 2H, C$\underline{H}_2$Et), 1.47-1.38 (m, 2H, C$\underline{H}_2$CH$_3$), 0.95 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 138.4 ($\underline{C}_{quat}$), 132.0 ($\underline{C}_{quat}$), 130.2 ($\underline{C}_{quat}$), 129.9 ($\underline{C}_{Ar}$H), 127.9 ($\underline{C}_{Ar}$H), 126.5 ($\underline{C}_{Ar}$H), 120.0 ($\underline{C}_{quat}$), 115.5 ($\underline{C}_{Ar}$H), 79.3 (C$\underline{H}$), 52.5 (N$\underline{C}$H$_2$), 49.1 (N$\underline{C}$H$_2$), 37.9 (N$\underline{C}$H$_3$), 31.7, 25.1, 22.4, 13.9 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{16}H_{22}N_5$ $[M+H]^+$ 284.1870; found 284.1871.

3-Butyl-6,7,8,8a-tetrahydro-5*H*-pyrimido[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3j)



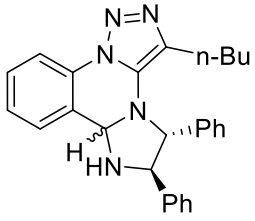
Prepared from benzaldehyde **1a** (35.5 mg, 0.1 mmol) and propane-1,3-diamine (12.6 μL, 0.15 mmol) according to the general procedure without purification. Yield 21.6 mg (76%). White solid; mp 129-131 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.0 Hz, 1H, $C_{Ar}\underline{H}$), 7.48-7.41 (m, 2H, $C_{Ar}\underline{H}$), 7.29 (t, J = 7.5 Hz, 1H, $C_{Ar}\underline{H}$), 5.18 (s, 1H, C$\underline{H}$), 4.13-4.09 (m, 1H), 3.42 (td, J = 13.1, 2.7 Hz, 1H, NC$\underline{H}_2$), 3.30-3.27 (m, 1H), 3.13 (td, J = 13.1, 2.7 Hz, 1H, NC$\underline{H}_2$), 2.90-2.70 (m, 2H), 1.92-1.61 (m, 5H), 1.47-1.38 (m, 2H, C$\underline{H}_2$CH$_3$), 0.95 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 135.9 ($\underline{C}_{quat}$), 131.5 ($\underline{C}_{quat}$), 129.6 ($\underline{C}_{Ar}$H), 129.0 ($\underline{C}_{quat}$), 126.9 ($\underline{C}_{Ar}$H), 126.7 ($\underline{C}_{Ar}$H), 123.3 ($\underline{C}_{quat}$), 115.3 ($\underline{C}_{Ar}$H), 72.1 (C$\underline{H}$), 47.5 (N$\underline{C}$H$_2$), 45.1 (N$\underline{C}$H$_2$), 32.7, 26.3, 25.5, 22.4, 13.9 (CH$_2\underline{C}$H$_3$). **HRMS** (ESI-TOF) calcd for $C_{16}H_{22}N_5$ $[M+H]^+$ 284.1870; found 284.1873.

(8b*RS*,9a*S*,13a*S*)-1-Butyl-8b,9,9a,10,11,12,13,13a-octahydrobenzimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3k)



Prepared from benzaldehyde **1a** (35.5 mg, 0.1 mmol) and (1*S*,2*S*)-1,2-diaminocyclohexane (17.1 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 3:1. Yield 30.2 mg (93%, dr = 70:30). Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ major diastereomer: 8.03-8.01 (m, 1H, $C_{Ar}\underline{H}$), 7.51–7.49 (m, 1H, $C_{Ar}\underline{H}$), 7.42-7.38 (m, 1H, $C_{Ar}\underline{H}$), 7.35-7.31 (m, 1H, $C_{Ar}\underline{H}$), 5.63 (s, 1H, C$\underline{H}$), 2.96-2.88 (m, 1H, C$\underline{H}$), 2.77-2.57 (m, 3H), 2.21-2.08 (m, 2H), 1.88-1.71 (m, 4H), 1.54-1.17 (m, 6H), 0.96 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$); minor diastereomer (selected signals): 7.97-7.95 (m, 1H, $C_{Ar}\underline{H}$), 7.63–7.61 (m, 1H, $C_{Ar}\underline{H}$), 7.42-7.38 (m, 1H, $C_{Ar}\underline{H}$), 7.35-7.31 (m, 1H, $C_{Ar}\underline{H}$), 5.63 (s, 1H, C$\underline{H}$), 2.96-2.88 (m, 1H, C$\underline{H}$), 2.77-2.57 (m, 3H), 2.21-2.08 (m, 2H), 1.88-1.71 (m, 4H), 1.54-1.17 (m, 6H), 0.96 (t, J = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 136.9 ($\underline{C}_{quat}$), 135.1 ($\underline{C}_{quat}$), 130.5 ($\underline{C}_{quat}$), 129.0 ($\underline{C}_{Ar}$H), 127.6 ($\underline{C}_{Ar}$H), 127.1 ($\underline{C}_{Ar}$H), 115.5 ($\underline{C}_{quat}$), 115.3 ($\underline{C}_{Ar}$H), 73.5 (C$\underline{H}$), 72.4, 69.6, 63.4, 31.2, 30.2, 25.0, 24.4, 24.3, 22.6, 13.8 (CH$_2\underline{C}$H$_3$). **HRMS** (MALDI-TOF) calcd for $C_{19}H_{26}N_5$ $[M+H]^+$ 324.2183; found 324.2185.

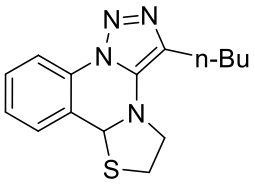
(5*R*,6*R*,7a*RS*)-3-Butyl-5,6-diphenyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3l)



Prepared from benzaldehyde **1a** (35.5 mg, 0.1 mmol) and (1*R*,2*R*)-1,2-diphenylethane-1,2-diamine (31.8 mg, 0.15 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 33.8 mg (80%, dr = 55:45). White solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ major diastereomer: 8.09 (dd, J = 8.1, 0.9 Hz, 1H, $C_{Ar}\underline{H}$), 7.70-7.68 (m, 1H, $C_{Ar}\underline{H}$), 7.56-7.51 (m, 1H,

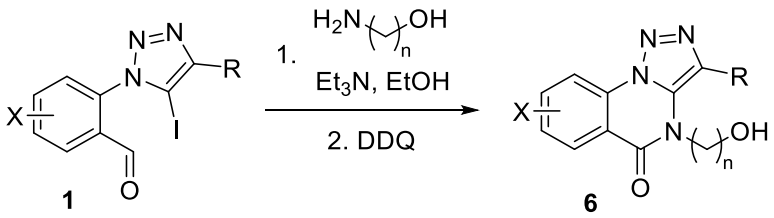
$C_{Ar}\underline{H}$), 7.45-7.32 (m, 6H, $C_{Ar}\underline{H}$, $C_{Ph}\underline{H}$), 7.22-7.18 (m, 3H, $C_{Ph}\underline{H}$), 6.95-6.92 (m, 2H, $C_{Ph}\underline{H}$), 5.80 (s, 1H, C$\underline{H}$), 4.96 (d, *J* = 5.1 Hz, 1H, NC$\underline{H}$), 4.31 (d, *J* = 5.1 Hz, 1H, NC$\underline{H}$), 3.18 (br s, 1H, N$\underline{H}$), 2.21-2.17 (m, 2H, C$\underline{H}_2$Pr), 1.46-1.35 (m, 1H, C$\underline{H}_2$Et), 1.21-1.10 (m, 2H, C$\underline{H}_2$CH$_3$), 1.04-0.93 (m, 1H, C$\underline{H}_2$Et), 0.78 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$); minor diastereomer: 8.15 (dd, *J* = 8.2, 0.9 Hz, 1H, $C_{Ar}\underline{H}$), 7.55-7.53 (m, 1H, $C_{Ar}\underline{H}$), 7.51-7.46 (m, 1H, $C_{Ar}\underline{H}$), 7.40-7.30 (m, 6H, $C_{Ar}\underline{H}$, $C_{Ph}\underline{H}$), 7.27-7.22 (m, 5H, $C_{Ph}\underline{H}$), 5.93 (s, 1H, C$\underline{H}$), 4.78 (d, *J* = 7.2 Hz, 1H, NC$\underline{H}$), 4.26 (d, *J* = 7.2 Hz, 1H, NC$\underline{H}$), 2.77 (br s, 1H, N$\underline{H}$), 2.22-2.18 (m, 2H, C$\underline{H}_2$Pr), 1.33-1.23 (m, 2H, C$\underline{H}_2$Et), 1.04-0.91 (m, 2H, C$\underline{H}_2$CH$_3$), 0.65 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ major diastereomer: 139.6 ($\underline{C}_{quat}$), 139.3 ($\underline{C}_{quat}$), 134.4 ($\underline{C}_{quat}$), 132.3 ($\underline{C}_{quat}$), 131.6 ($\underline{C}_{quat}$), 129.6, 128.94 (2C, $\underline{C}_{Ph}$H), 128.90 (2C, $\underline{C}_{Ph}$H), 128.1, 128.0, 127.7, 126.62 (2C, $\underline{C}_{Ph}$H), 126.58 (2C, $\underline{C}_{Ph}$H), 124.8, 123.9 ($\underline{C}_{quat}$), 116.2 ($\underline{C}_{Ar}$H), 74.3 (C$\underline{H}$), 71.7 (NC$\underline{H}$), 71.0 (NC$\underline{H}$), 31.5, 24.6, 22.5, 13.8 (CH$_2$C$\underline{H}_3$). **HRMS** (MALDI-TOF) calcd for $C_{27}H_{28}N_5$ $[M+H]^+$ 422.2339; found 422.2338.

3-Butyl-5,6-dihydro-7a*H*-[1,3]thiazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3m)



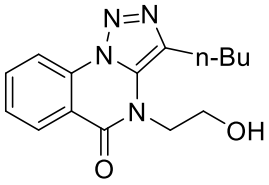
Prepared from benzaldehyde **1a** (53.3 mg, 0.15 mmol) and 2-aminoethanethiol hydrochloride (25.5 mg, 0.225 mmol) according to the general procedure without purification. Yield 39.0 mg (91%, purity 95%). Yellow solid; mp 103-105 °C. **^{1}H NMR** (400 MHz, $CDCl_3$/CD_3OD) δ 8.07 (d, *J* = 8.1 Hz, 1H, $C_{Ar}\underline{H}$), 7.50-7.47 (m, 1H, $C_{Ar}\underline{H}$), 7.38-7.30 (m, 2H, $C_{Ar}\underline{H}$), 5.95 (s, 1H, C$\underline{H}$), 4.57 (dd, *J* = 13.0, 6.1 Hz, 1H), 3.37 (ddd, *J* = 12.9, 10.8, 6.8 Hz, 1H), 3.22 (dd, *J* = 9.8, 6.8 Hz, 1H), 3.01-2.95 (m, 1H), 2.90-2.72 (m, 3H), 1.78-1.65 (m, 2H, C$\underline{H}_2$Et), 1.49-1.40 (m, 2H, C$\underline{H}_2$CH$_3$), 0.98 (t, *J* = 7.3 Hz, 3H, CH$_2$C$\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$/CD_3OD) δ 134.2 ($\underline{C}_{quat}$), 130.3 ($\underline{C}_{quat}$), 129.9 ($\underline{C}_{Ar}$H), 127.2 ($\underline{C}_{Ar}$H), 126.6 ($\underline{C}_{Ar}$H), 121.0 ($\underline{C}_{quat}$), 115.5 ($\underline{C}_{Ar}$H), 115.2 ($\underline{C}_{quat}$), 67.7 (C$\underline{H}$), 54.1 (N$\underline{C}$H$_2$), 31.5, 31.1, 25.9, 22.1, 13.5 (CH$_2$C$\underline{H}_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{19}N_4S$ $[M+H]^+$ 287.1325; found 287.1312.

Oxidative annulation



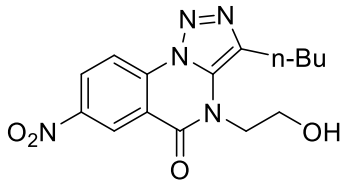
General procedure. (5-Iodotriazolyl)benzaldehyde **1** (0.15 mmol, 1 equiv), aminoalcohol (0.225 mmol, 1.5 equiv), and Et_3N (0.3 mmol, 2 equiv) were mixed under Ar atmosphere in EtOH (1.5 mL). The reaction mixture was stirred at 100 °C in a dry block for 2 h. DDQ (0.3 mmol, 2 equiv) was then added and the obtained mixture was stirred at 60 °C for 2-8 h. After completion of the reaction, the mixture was diluted with CH_2Cl_2 and washed with water. The organic layer was dried with anhydrous Na_2SO_4, and the solvent was evaporated *in vacuo*. The residue was purified by column chromatography.

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



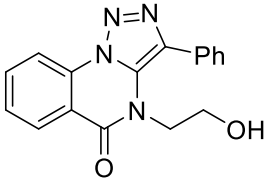
Prepared from benzaldehyde **1a** (53.3 mg, 0.15 mmol) and 2-aminoethanol (13.6 μL, 0.225 mmol) according to the general procedure; eluent: hexanes:EtOAc = 1:1. Yield 33.2 mg (77%). Pinkish solid; mp 141-143 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.18-8.15 (m, 2H, $C_{Ar}\underline{H}$), 7.74-7.70 (m, 1H, $C_{Ar}\underline{H}$), 7.46-7.42 (m, 1H, $C_{Ar}\underline{H}$), 4.36 (t, J = 5.4 Hz, 2H, $NC\underline{H}_2$), 4.08-4.02 (m, 2H, $C\underline{H}_2OH$), 3.37 (br s, 1H, O$\underline{H}$), 2.94 (t, J = 7.7 Hz, 2H, $C\underline{H}_2Pr$), 1.79-1.71 (m, 2H, $C\underline{H}_2Et$), 1.50-1.41 (m, 2H, $C\underline{H}_2CH_3$), 0.98 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 159.6 ($\underline{C}$=O), 134.9 ($\underline{C}_{Ar}H$), 134.3 ($\underline{C}_{quat}$), 132.1 ($\underline{C}_{quat}$), 129.9 ($\underline{C}_{quat}$), 128.8 ($\underline{C}_{Ar}H$), 127.5 ($\underline{C}_{Ar}H$), 115.7 ($\underline{C}_{quat}$), 115.2 ($\underline{C}_{Ar}H$), 60.5, 46.4, 32.2, 26.0, 22.4, 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{19}N_4O_2$ $[M+H]^+$ 287.1503; found 287.1506.

3-Butyl-4-(2-hydroxyethyl)-7-nitro[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6c)



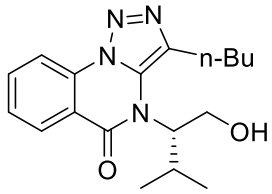
Prepared from benzaldehyde **1c** (60.0 mg, 0.15 mmol) and 2-aminoethanol (13.6 μL, 0.225 mmol) according to the general procedure; eluent: CH_2Cl_2:MeOH = 200:1. Yield 35.4 mg (71%). Brownish solid; mp >185 °C. **^{1}H NMR** (400 MHz, $CDCl_3$/CD_3OD) δ 9.18 (d, J = 2.5 Hz, 1H, $C_{Ar}\underline{H}$), 8.70 (dd, J = 9.0, 2.5 Hz, 1H, $C_{Ar}\underline{H}$), 8.58 (d, J = 9.0 Hz, 1H, $C_{Ar}\underline{H}$), 4.40 (t, J = 5.8 Hz, 2H, $C\underline{H}_2$), 3.96 (t, J = 5.8 Hz, 2H, $C\underline{H}_2$), 3.03 (t, J = 7.7 Hz, 2H, $C\underline{H}_2Pr$), 1.84-1.76 (m, 2H, $C\underline{H}_2Et$), 1.54-1.44 (m, 2H, $C\underline{H}_2CH_3$), 1.00 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$/CD_3OD) δ 158.0 ($\underline{C}$=O), 146.4 ($\underline{C}_{quat}$), 137.9 ($\underline{C}_{quat}$), 132.9 ($\underline{C}_{quat}$), 130.6 ($\underline{C}_{quat}$), 129.6 ($\underline{C}_{Ar}H$), 125.4 ($\underline{C}_{Ar}H$), 117.0 ($\underline{C}_{Ar}H$), 116.6 ($\underline{C}_{quat}$), 59.1, 46.2, 32.0, 25.7, 22.2, 13.7 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{15}H_{18}N_5O_4$ $[M+H]^+$ 332.1353; found 332.1361.

4-(2-Hydroxyethyl)-3-phenyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6h)



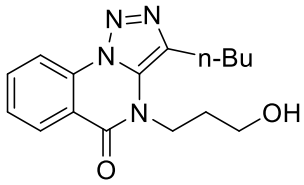
Prepared from benzaldehyde **1h** (56.3 mg, 0.15 mmol) and 2-aminoethanol (13.6 μL, 0.225 mmol) according to the general procedure; eluent: hexanes:EtOAc = 1:1. Yield 32.3 mg (70%). Pink solid; mp 177-179 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.42 (d, J = 8.3 Hz, 1H, $C_{Ar}\underline{H}$), 8.31 (d, J = 8.0 Hz, 1H, $C_{Ar}\underline{H}$), 7.89-7.85 (m, 1H, $C_{Ar}\underline{H}$), 7.60-7.57 (m, 1H, $C_{Ar}\underline{H}$), 7.55–7.47 (m, 5H, $C_{Ph}\underline{H}$), 4.20 (t, J = 5.2 Hz, 2H, $NC\underline{H}_2$), 3.61 (t, J = 5.2 Hz, 2H, $C\underline{H}_2OH$), 2.38 (br s, 1H, O$\underline{H}$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 160.0 ($\underline{C}$=O), 135.3 ($\underline{C}_{Ar}H$), 134.5 ($\underline{C}_{quat}$), 132.3 ($\underline{C}_{quat}$), 130.8 (2C, $\underline{C}_{Ph}H$), 130.6 ($\underline{C}_{quat}$), 130.4 ($\underline{C}_{quat}$), 129.24, 129.18, 128.6 (2C, $\underline{C}_{Ph}H$), 127.9 ($\underline{C}_{Ar}H$), 115.9 ($\underline{C}_{quat}$), 115.5 ($\underline{C}_{Ar}H$), 60.3 ($N\underline{C}H_2$), 46.4 ($\underline{C}H_2OH$). **HRMS** (MALDI-TOF) calcd for $C_{17}H_{15}N_4O_2$ $[M+H]^+$ 307.1190; found 307.1192.

3-Butyl-4-[(1*S*)-1-(hydroxymethyl)-2-methylpropyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6j)



Prepared from benzaldehyde **1a** (53.3 mg, 0.15 mmol) and (*S*)-valinol (23.2 mg, 0.225 mmol) according to the general procedure; eluent: hexanes:EtOAc = 4:1. Yield 26.7 mg (54%). Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.31 (d, J = 8.2 Hz, 1H, $C_{Ar}\underline{H}$), 8.22 (d, J = 7.8 Hz, 1H, $C_{Ar}\underline{H}$), 7.81 (t, J = 8.0 Hz, 1H, $C_{Ar}\underline{H}$), 7.49 (t, J = 7.6 Hz, 1H, $C_{Ar}\underline{H}$), 4.43-4.37 (m, 1H, NC$\underline{H}$), 4.09-4.03 (m, 2H, $C\underline{H}_2OH$), 3.96 (br s, 1H, O$\underline{H}$), 3.06-2.87 (m, 3H, $C\underline{H}_2Pr$, $C\underline{H}(CH_3)_2$), 1.82-1.73 (m, 2H, $C\underline{H}_2Et$), 1.53-1.44 (m, 2H, $C\underline{H}_2CH_3$), 1.15 (d, J = 6.5 Hz, 3H, $CH(C\underline{H}_3)_2$), 1.00 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$), 0.78 (d, J = 6.7 Hz, 3H, $CH(C\underline{H}_3)_2$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 160.2 ($\underline{C}$=O), 135.2 ($\underline{C}_{Ar}H$), 134.5 ($\underline{C}_{quat}$), 133.4 ($\underline{C}_{quat}$), 129.9 ($\underline{C}_{quat}$), 128.8 ($\underline{C}_{Ar}H$), 127.6 ($\underline{C}_{Ar}H$), 116.3 ($\underline{C}_{quat}$), 115.4 ($\underline{C}_{Ar}H$), 69.3, 62.2, 31.6, 27.4, 25.7, 22.4, 20.1, 19.7, 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{18}H_{25}N_4O_2$ $[M+H]^+$ 329.1972; found 329.1979.

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



Prepared from benzaldehyde **1a** (53.3 mg, 0.15 mmol) and 3-aminopropanol (18.8 μL, 0.225 mmol) according to the general procedure; eluent: hexanes:EtOAc = 2:1. Yield 32.7 mg (72%). White solid; mp 152-154 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.40 (d, J = 8.2 Hz, 1H, $C_{Ar}\underline{H}$), 8.33 (dd, J = 8.0, 0.9 Hz, 1H, $C_{Ar}\underline{H}$), 7.89-7.85 (m, 1H, $C_{Ar}\underline{H}$), 7.61-7.56 (m, 1H, $C_{Ar}\underline{H}$), 4.41 (t, J = 6.5 Hz, 2H, $NC\underline{H}_2$), 3.70-3.65 (m, 2H, $C\underline{H}_2OH$), 3.21 (br s, 1H, O$\underline{H}$), 2.98 (t, J = 7.7 Hz, 2H, $C\underline{H}_2Pr$), 2.03-1.97 (m, 2H, $C\underline{H}_2$), 1.86-1.78 (m, 2H, $C\underline{H}_2Et$), 1.53-1.44 (m, 2H, $C\underline{H}_2CH_3$), 0.99 (t, J = 7.3 Hz, 3H, $CH_2C\underline{H}_3$). **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$) δ 159.8 ($\underline{C}$=O), 135.2 ($\underline{C}_{Ar}H$), 134.7 ($\underline{C}_{quat}$), 131.5 ($\underline{C}_{quat}$), 129.8 ($\underline{C}_{quat}$), 129.2 ($\underline{C}_{Ar}H$), 127.7 ($\underline{C}_{Ar}H$), 115.5 ($\underline{C}_{quat}$),

115.3 ($\underline{C}_{Ar}H$), 58.4 ($N\underline{C}H_2$), 40.4 ($\underline{C}H_2OH$), 32.7, 31.6, 25.8, 22.4, 13.8 ($CH_2\underline{C}H_3$). **HRMS** (MALDI-TOF) calcd for $C_{16}H_{21}N_4O_2$ $[M+H]^+$ 301.1659; found 301.1671.

Details of DFT calculations

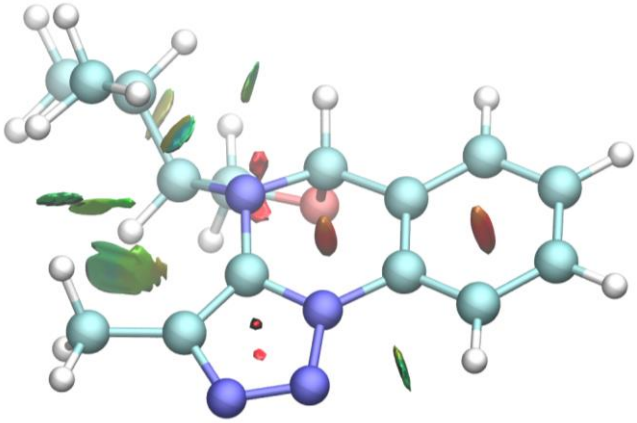
The calculations were performed using ORCA 6.1.0 program package.[8] DFT calculations were performed at PW6B95[9]-D4[10]/def2-TZVP(-f)[11] level of theory using PCM[12] solvation model with EtOH as solvent. RIJCOSX[13] approximation was used to speed up the calculations. The initial structures were prepared in Gabedit.[14] The conformational space of all intermediates was sampled with CREST.[15] Only the energies of the most stable conformers are presented below for clarity. Thermodynamic properties were calculated for ideal gas at 298.15 K using QRRHO approach[16] for vibrational entropy correction. The nature of optimized intermediates was verified by frequency analysis. CYLView[17] was used to visualize structures. Non-covalent interactions map was generated by NCIPLOT[18] and visualized with VMD.[19]

Table S1. Energies of all intermediates.

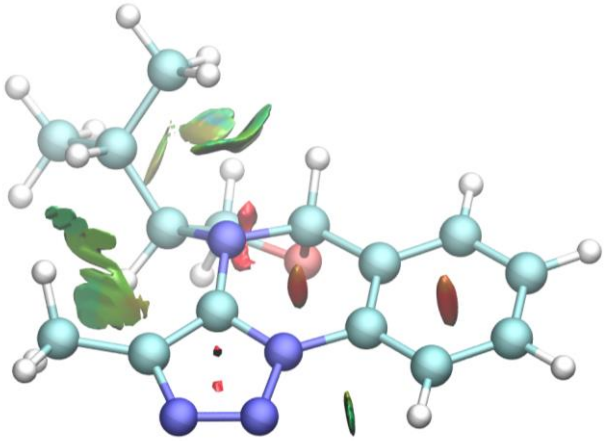
	E_{el} E_h	ZPE E_h	ΔG, 298 K E_h	ΔG_{rel}, 298 K kcal/mol	Amount in equilibrium at 298K, %
			I-3b (calcd. 84.1% in equilibrium)		
I-3b-1	-878.1035	0.3189	-877.8270	0.0	48.2
I-3b-2	-878.1035	0.3192	-877.8266	0.3	28.8
I-3b-3	-878.1011	0.3187	-877.8248	1.4	4.7
I-3b-4	-878.1018	0.3197	-877.8242	1.8	2.4
I-3b-5	-878.0948	0.3186	-877.8186	5.3	0.0
I-3b-6	-878.0949	0.3190	-877.8181	5.6	0.0
			I-3b' (calcd. 15.9% in equilibrium)		
I-3b'-1	-878.1020	0.3185	-877.8260	0.7	15.3
I-3b'-2	-878.0977	0.3185	-877.8217	3.3	0.2
I-3b'-3	-878.0983	0.3186	-877.8223	3.0	0.3
I-3b'-4	-878.0971	0.3184	-877.8213	3.6	0.1
I-3b'-5	-878.0949	0.3191	-877.8177	5.9	0.0
I-3b'-6	-878.0935	0.3186	-877.8174	6.1	0.0
			I-3c (calcd. 84.7% in equilibrium)		
I-3c-1	-991.4133	0.3154	-991.1418	0.0	71.6
I-3c-2	-991.4108	0.3149	-991.1400	1.1	10.9
I-3c-3	-991.4111	0.3159	-991.1385	2.1	2.2
			I-3c' (calcd. 15.3% in equilibrium)		
I-3c'-1	-991.4129	0.3160	-991.1400	1.1	11.4
I-3c'-2	-991.4112	0.3154	-991.1390	1.7	3.9

Fig. S1. NCI plots of most abundant conformers of **I-3b/I-3b'** and **I-3c/I-3c'**.

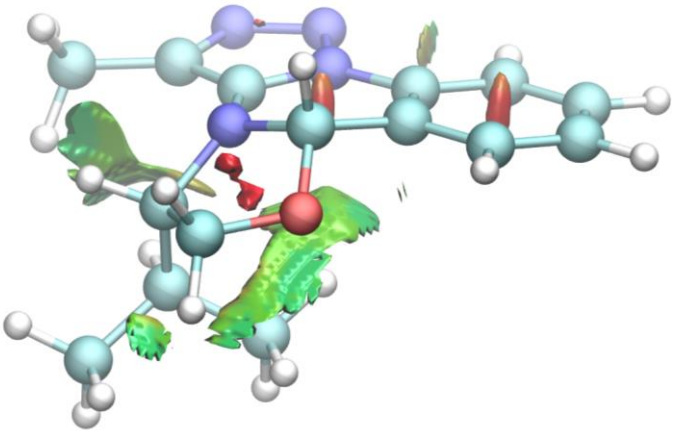
(A) I-3b and **I-3b'**



I-3b-1 (5*S*,7*aR*) (calcd. 48% in equilibrium)

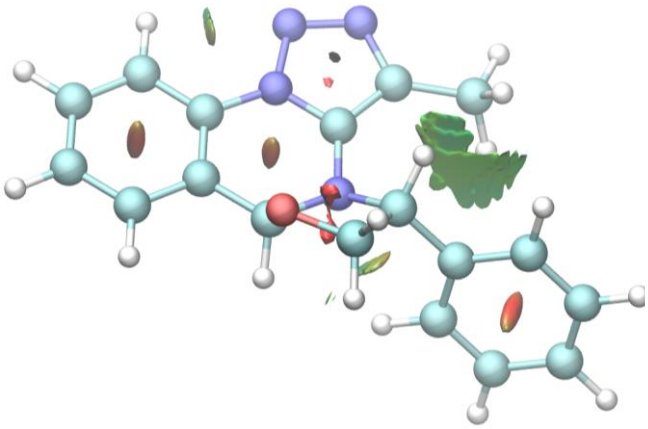


I-3b-2 (5*S*,7*aR*) (calcd. 29% in equilibrium)

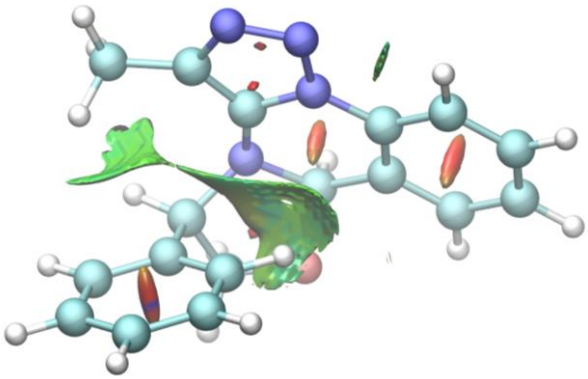


I-3b'-1 (5*S*,7*aS*) (calcd. 15% in equilibrium)

(B) I-3c and **I-3c'**



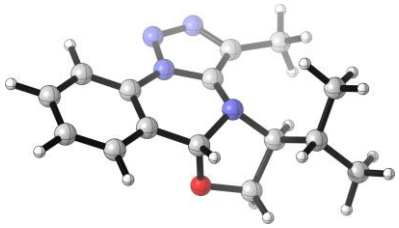
I-3c-1 *(5R,7aS)* (calcd. 72% in equilibrium)



I-3c'-1 (5*R*,7*aR*) (calcd. 11% in equilibrium)

Cartesian coordinates of all intermediates and transition states

I-3b-1



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ZPE = 0.3189 E_h
G_{298} = -877.8270 E_h

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C	2.04418807153688	0.54586388380420	0.33411849150123
N	0.75630842739745	0.17565606002025	-0.28035679978047
C	0.24473553380155	-1.06712116309074	0.02205455956735
N	-1.08905679121906	-1.25948455460605	0.10847054462960
C	-2.04262466531009	-0.25536511139263	-0.05188171624845
C	-1.56067954955777	1.04014436479403	-0.13269977996573
C	-0.10662322777078	1.29836778852257	0.03981320316906
C	-2.45567942285409	2.07739507378053	-0.32353003593188
C	-3.81055679457545	1.82060658761297	-0.41614098441425
C	-4.27401963165143	0.51679036727329	-0.32533533097123
C	-3.39405139015650	-0.53317165408362	-0.15023952054586
H	-3.73875902955625	-1.55132722210903	-0.09283850206560
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H	0.20531829730045	2.14298792624086	-0.57580238589761
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C	1.61307460658946	1.51367495050559	1.46565006105371
H	1.88737909693142	1.16202428265311	2.45328383819340
H	2.03982487320542	2.50217915399201	1.29884767283212
C	2.99071754780693	1.19882234101958	-0.66482421490957
H	2.51031318460797	2.11361850761584	-1.01901587760434
C	3.26404373113771	0.29904425248263	-1.85583518600775
H	2.34091570368347	-0.02776474321735	-2.32578357027769
H	3.82270174988955	-0.58312179760755	-1.54730736250788
H	3.86033440141891	0.82449580162300	-2.59786864045145
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H	4.78766333361610	0.67580451063990	0.40183010178190
H	4.13385144255337	2.24295867399368	0.87004406628970
H	4.96582709663971	2.06272256869704	-0.66669282252326
H	2.51143981672620	-0.34196189437250	0.74323121913200
N	-1.38176518377674	-2.55667992813601	0.31441713974744
N	-0.25281414581341	-3.18046542159881	0.36733384977350
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I-3b-2

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ZPE = 0.3192 E_h
G_{298} = -877.8266 E_h

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C	2.06794928862434	0.38349533951175	0.38504111312121

N	0.78250218940713	0.06409762034312	-0.27155687910291
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C	-1.51681341431438	1.00205227994387	-0.17129651324313
C	-0.05131128479096	1.23681096531330	-0.05660703949396
C	-2.38570713095964	2.06060764914709	-0.36964755315125
C	-3.75012350327815	1.84643214702931	-0.41263667225150
C	-4.25193448177892	0.56217397373320	-0.26436488775747
C	-3.40026223696468	-0.50903914614992	-0.08087567396742
H	-3.77478261655729	-1.51297825217741	0.02223083142965
H	-5.31586869826567	0.39101949185036	-0.30148250755343
H	-4.42153038140607	2.67554769014637	-0.56603699284467
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H	0.26315237085531	2.00497356782478	-0.76407222298597
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C	1.70568369202858	1.59693115096526	1.26850641173847
H	2.02822741275260	1.47482162669772	2.29505328391119
H	2.12912320525524	2.51559030141611	0.86334000052897
C	3.20506628418253	0.63151710533007	-0.59892033136470
H	3.37440915190213	-0.31293501052026	-1.11579198928251
C	4.47106357182716	0.98484777369694	0.16654152245702
H	4.36424679263127	1.93772312319088	0.68289782600892
H	5.31387423152374	1.07299776691687	-0.51389609699502
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H	2.71499124644597	2.65922025830666	-1.20626793518431
H	1.99330282302295	1.40684800171448	-2.21772425979384
H	3.70883517098386	1.77135504311778	-2.34751416364005
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N	-0.32748424237422	-3.24686102037944	0.40608675708508
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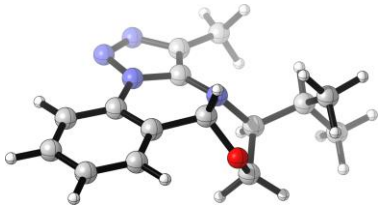
I-3b-3



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C	-3.72042964942351	1.85035736247850	0.09536385366739
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H	0.61213331378101	1.61706030227059	1.92727035789390
H	1.99671467005477	2.54586505704599	1.31021908788032
C	3.20606328951588	0.61213563562249	-0.13259497401191
H	3.39363655408556	-0.35636345562667	-0.59570494921105
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H	4.16345688238947	1.82711658034951	1.38360363069803
H	5.27518106170791	0.88046407719021	0.40874512251177
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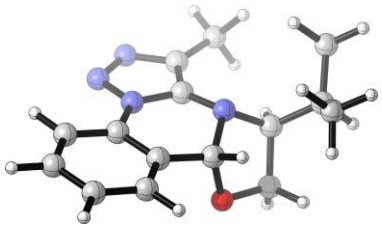
I-3b-4



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C	-1.96581105687139	-0.28325259351157	-0.09748195671811
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C	-2.37236815279097	2.03397404039143	-0.47906583145364
C	-3.71826062530265	1.76495884584769	-0.64081422209271
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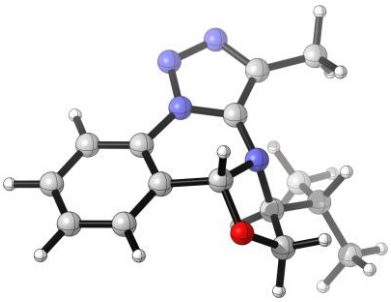
H	-4.40586115456416	2.56601477028942	-0.85827218904110
H	-2.00023293252279	3.04299065437107	-0.56771958954526
H	2.83153313237406	-2.53641304125797	-0.34673542080028
H	0.28462508879705	2.10278908696863	-0.59360613761964
O	0.17865077840916	1.64977198503460	1.40036512180685
C	1.59320727118087	1.60080517221444	1.54119179002962
H	1.82041965668255	1.32560725850006	2.56437680349945
H	2.02466520039613	2.57751694362241	1.32480316172860
C	3.18900915430336	1.06956617489447	-0.39999263254566
H	3.94417374057695	1.48721193171853	0.26936940957108
C	2.73541584409673	2.16996789192424	-1.34612901966972
H	3.58244727425629	2.51899107720096	-1.93111522580220
H	2.32062790634657	3.02786312546349	-0.82291220130363
H	1.98609063529598	1.79341552677837	-2.04042979671018
C	3.82526464140736	-0.06331007296728	-1.18578899712226
H	4.59668662271830	0.31956879374717	-1.84929541382861
H	3.07888959620904	-0.56957371727254	-1.79649362426997
H	4.28051282134414	-0.79644393912473	-0.52509528761203

H	2.47160286809837	-0.31758202843937	1.04971482555273
N	-1.32376403150222	-2.55630793582776	0.41166594360249
N	-0.20162068720093	-3.17379871453438	0.56749787967245
H	2.21021183994965	-3.91309317288127	0.55403914224892
H	2.74767513888227	-2.47489860053399	1.40668655067638

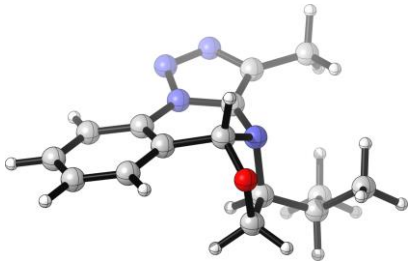
I-3b-5



N_{imag} = 0
E_{El} = -878.0948 E_h
ZPE = 0.3186 E_h
G_{298} = -877.8186 E_h

C	0.91322309930364	-2.33185922355712	-0.59647862817071
C	2.28213290896233	-2.71921442008768	-1.00271370563100
C	1.49785505254889	0.98759698967338	0.24504614008448
N	0.80135961849744	0.19496266348983	-0.79204370914182
C	0.35354454463106	-1.08300704204156	-0.50921147656374
N	-0.91473085227397	-1.30635575628321	-0.09573957685762
C	-1.84569735263924	-0.27932071743003	0.12039267178636
C	-1.51924827806211	0.95867498608539	-0.41636497300331
C	-0.26693963068602	1.07785293725716	-1.25637477600053
C	-2.37412794559235	2.02018936539126	-0.19268014374849
C	-3.53923686476400	1.83882849440989	0.53313844723648
C	-3.85108489494334	0.59166942746874	1.04957445650067
C	-2.99748104764744	-0.47832705674720	0.85597134872690
H	-3.21019450536920	-1.44894971119383	1.27144064599090
H	-4.75705851388951	0.45181247584463	1.61704723860552
H	-4.20444720885616	2.67152742517279	0.69645778282746
H	-2.12273534891930	2.98860236896684	-0.59405816690818
H	2.26887798811218	-3.69385549620411	-1.48024315899863
H	-0.50086702977670	0.83847962998273	-2.29480580286279
O	0.27804828706375	2.37076140024397	-1.18389239655185
C	1.52997824827721	2.30462949388456	-0.49659791032415
H	1.60907074682585	3.16345823840312	0.16028997171158
H	2.34233382042428	2.31940281035180	-1.22235593527387
C	2.85144714121978	0.42918371361029	0.66239110731551
H	3.28573798764708	-0.05196458651173	-0.21431831417250
C	2.71021669059449	-0.58631478149871	1.78827661024169
H	2.37474823151800	-0.08288975690393	2.69384338227648
H	3.66915019224508	-1.05261981901314	2.00052233266920
H	1.99461430549176	-1.36978828685789	1.56311324706399
C	3.78295319431855	1.54554776528746	1.11894933682547
H	3.34117109900953	2.09567267364979	1.94848410932860
H	4.00491568597106	2.24947859385078	0.32169313239839
H	4.72350800130052	1.12431774686710	1.46482961410109
H	0.86296311279012	1.09409980015354	1.13118144983557
N	-1.14485694977358	-2.60903102009393	0.06108367888251
N	-0.03733050960700	-3.22384859459422	-0.22855796775197
H	2.95451789778799	-2.77035418436840	-0.14873617143873
H	2.68755907825928	-1.99118854665837	-1.69974389100898

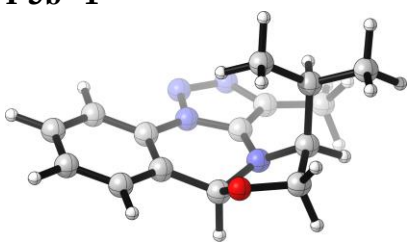
I-3b-6



N_{imag} = 0
E_{El} = -878.0949 E_h
ZPE = 0.3190 E_h
G_{298} = -877.8181 E_h

C	0.89493641255703	-2.40701511731656	-0.27090254332572
C	2.21498078256703	-2.89889808393953	-0.72603376496528
C	1.35142193410405	1.00606588089809	0.50113358935022
N	0.84782772370003	0.12730290427780	-0.59065128130850
C	0.38056950466640	-1.13549706352191	-0.24133952549246
N	-0.89555574699806	-1.30210579195844	0.18771808760921
C	-1.82964423737987	-0.25859057294427	0.24682406599630
C	-1.49811749379333	0.88779177197659	-0.46050937944175
C	-0.19920373301606	0.92551917537085	-1.24285789375201
C	-2.37198048207444	1.95767752820240	-0.42838132046190
C	-3.55731166214483	1.87156784691746	0.28093819763243
C	-3.87245481843391	0.71231759435029	0.97188871790088
C	-3.00394402180217	-0.36265234598542	0.96692910827902
H	-3.22480655424188	-1.26573105309635	1.51066950080002
H	-4.79496098398919	0.64663059110590	1.52602141299511
H	-4.23554008320802	2.70955931424949	0.29700454914932
H	-2.11550108448856	2.85832551953710	-0.96340257753595
H	2.80939733874371	-3.27954843821200	0.10123322702143
H	-0.35098249740944	0.58250635859228	-2.26417899255626
O	0.34548679305138	2.20546360089224	-1.28011324120652
C	0.91978064636973	2.39732478111792	0.01191189465356
H	0.18360162684932	2.83197675557864	0.68519533908552
H	1.75417038491474	3.08032797034862	-0.09869383335467
C	2.85381399959820	0.92543014135451	0.75267179635978
H	3.07414826286054	1.80596410443838	1.36025980036447
C	3.65825532301756	1.02216437573355	-0.53150597757312
H	4.71677839610726	1.12678373288665	-0.30725172359667
H	3.35543802049899	1.87629343556091	-1.13391471390168
H	3.52488404632649	0.12804379146906	-1.13406178843809
C	3.24383812475249	-0.29295647748275	1.57052332725401
H	4.29653652619917	-0.24775240536203	1.83980734854117
H	3.08870297316016	-1.21035053910523	1.01305503657122
H	2.66124729070328	-0.35141303769111	2.48753490963676
H	0.82939869249818	0.77469356534782	1.43054785624651
N	-1.16384425013991	-2.58419989521063	0.41668270775566
N	-0.08032780556504	-3.24799532284462	0.15415735788074
H	2.77122618286006	-2.10098636168459	-1.20619145504799
H	2.08375446857884	-3.70729823385112	-1.44009781912479

I-3b'-1

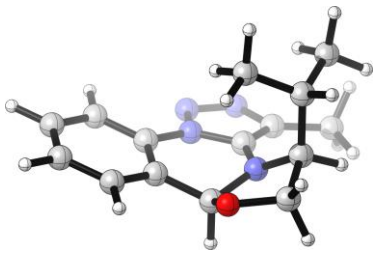


N_{imag} = 0
E_{El} = -878.1020 E_h
ZPE = 0.3185 E_h
G_{298} = -877.8260 E_h

C	1.34667291938174	2.20502796724832	-0.25305402512965
C	2.78406699846946	2.40322910503092	-0.55115035922976
C	1.97532715258359	-0.95691129048269	-0.44481359141085
N	0.81214259428091	-0.17474713535604	-0.86995057396158

C	0.56864760008308	1.07898993534458	-0.41449647509806
N	-0.66644545980475	1.45766468983246	-0.02890105940628
C	-1.75638062624144	0.58614189144393	0.03907944795462
C	-1.58723297325355	-0.68035960410304	-0.50267197069758
C	-0.30685461487903	-1.05615503533528	-1.19154192524843
C	-2.63338071032866	-1.58205191318576	-0.42146683104661
C	-3.82520422207209	-1.22300823701121	0.18005900751885
C	-3.97693271172467	0.04845071839444	0.71030807643591
C	-2.94123558850579	0.95912539731829	0.64873711918125
H	-3.03578281116034	1.94534841999643	1.07008670746833
H	-4.90486368104103	0.33197580686689	1.18040711199444
H	-4.63562236334263	-1.93190141529942	0.23258911070410
H	-2.50878575845581	-2.56928149673398	-0.83725154413722
H	3.01246353197733	2.12170505051158	-1.57684391455738
H	-0.45600594389923	-1.06493847528685	-2.27668450011451
O	0.11795468396658	-2.32919071592601	-0.77725146537469
C	1.53368109973545	-2.33535926623481	-0.92013185289897
H	1.80619915011885	-2.49365254398515	-1.96346773287667
H	1.92525578767042	-3.14255754747903	-0.31303627239926
C	2.27103728199268	-0.86300222658631	1.05322302789561
H	2.39453208049320	0.19624688762720	1.27863892199670
C	3.58722591754994	-1.55714591938804	1.36218797116813
H	3.51937759610592	-2.62820900020109	1.17796258957171
H	3.85281740061866	-1.41940177962180	2.40703708774648
H	4.39564594714559	-1.16003627699604	0.75177509888486
C	1.14594830082203	-1.39381179074203	1.92476141162751
H	0.20065573740431	-0.90055114781275	1.70876576803737
H	1.37982950908245	-1.22611289200130	2.97315614039063
H	1.00617274595757	-2.46296667042426	1.77862084580749
H	2.85831089267375	-0.63525519925802	-0.99475108096930
N	-0.67911468158453	2.75319780110565	0.34293271233919
N	0.53571070263083	3.18193774773025	0.21430445699628
H	3.42425308959702	1.81050053297504	0.09966668496870
H	3.04174342595215	3.44873562802496	-0.41730412413133

I-3b'-2

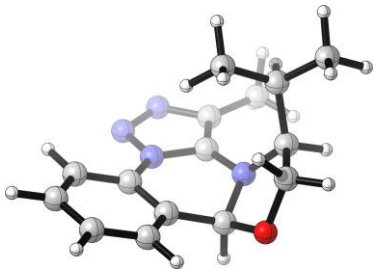


N_{imag} = 0
E_{El} = -878.0977 E_h
ZPE = 0.3185 E_h
G_{298} = -877.8217 E_h

C	1.37455234968553	2.21821296416101	-0.30638750548855
C	2.80954941784068	2.45658967674946	-0.58800627321422
C	1.56242184290839	-0.62343648050468	-2.08746115363003
N	0.54585142995634	0.40227216633696	-1.87184952106729
C	0.49358731412762	1.32324345622614	-0.87533519309984
N	-0.68019332977228	1.55806068506969	-0.24160816303194
C	-1.84593852536799	0.81806790405350	-0.46420809869876
C	-1.86861889244622	0.01085292371758	-1.59280050786678
C	-0.70350979672957	0.04956652108181	-2.53921337327054
C	-2.97752945026062	-0.78001636354352	-1.82587717097272
C	-4.05266640166574	-0.74907595188890	-0.95556375694954
C	-4.01767379303600	0.07148240367885	0.16058411599229
C	-2.90887535458577	0.85377994407383	0.41989815630245
H	-2.85526541387327	1.47790769007706	1.29576483959918
H	-4.85380929032231	0.09557818482591	0.84091261422218
H	-4.91779098926312	-1.36283782566696	-1.14834331722679
H	-2.99640564837025	-1.41685388613300	-2.69564325518869
H	3.44283497246432	2.10040386401710	0.22180318029935

H	-0.89887531718410	0.77394364017654	-3.33936374398618
O	-0.46779546304712	-1.21340420048224	-3.09236438939134
C	0.93851252189945	-1.31476792637618	-3.29330221261975
H	1.22087795731132	-0.81152511616552	-4.21792471540285
H	1.18995006049223	-2.36696954941223	-3.35427925485967
C	1.83314437212442	-1.57321304303085	-0.91311853316103
H	2.40358643819511	-2.39244955167718	-1.35531166980938
C	0.56684299317762	-2.14487958702443	-0.29962292787407
H	0.82199846213084	-2.86823104789995	0.47115324136240
H	-0.05997769650925	-2.63657005458221	-1.03728330201996
H	-0.01981421359323	-1.35678331408560	0.17061320597030
C	2.70777938310685	-0.94171734062640	0.15836298585881
H	3.02813847511904	-1.69873866097474	0.87055914593607
H	2.16732512476533	-0.17885252734690	0.71285622319250
H	3.59668135319347	-0.48707106782466	-0.27333860017042
H	2.50202575084111	-0.15939532898126	-2.38141207756111
N	-0.55185249527194	2.54307968480080	0.66431542145731
N	0.68608862088042	2.91850515233204	0.62454744397942
H	2.99750332166084	3.51934171613780	-0.71485208297846
H	3.11300393041786	1.94885418071132	-1.49761953763227

I-3b'-3

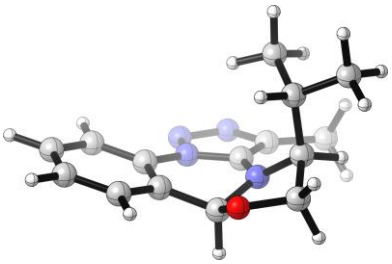


N_{imag} = 0
E_{El} = -878.0983 E_h
ZPE = 0.3186 E_h
G_{298} = -877.8223 E_h

C	1.36860039692851	2.24256377148003	-0.29825904952929
C	2.81218741019261	2.46650612235438	-0.54461036679115
C	1.82703024797838	-1.09629695874358	-0.36425436898456
N	0.86647471479733	-0.14970002212122	-0.95766631789356
C	0.61871941842234	1.10557978272816	-0.48700424660789
N	-0.63653540448056	1.46036218913752	-0.11807833274276
C	-1.68011919592508	0.53714161461488	0.01688025994139
C	-1.49447595648418	-0.69418444168005	-0.59900785613861
C	-0.28571958954378	-0.87554503837751	-1.48477813490080
C	-2.45012424898037	-1.67637178561914	-0.42550945949798
C	-3.58132335609219	-1.42325005133350	0.33087656646537
C	-3.75818988788866	-0.18219560670968	0.92164694792050
C	-2.80184056304155	0.80534307516007	0.77920864287567
H	-2.91007467872817	1.76373355239325	1.25814715275789
H	-4.63990791333312	0.01577337466842	1.50979747050998
H	-4.32722608981429	-2.19164782442388	0.45596953045355
H	-2.30591495023355	-2.63663490093316	-0.89464898890414
H	3.37254458290650	2.53637483192375	0.38551387385169
H	-0.51976954481206	-0.53200779822243	-2.49313369563965
O	0.15733922201756	-2.19429245611925	-1.58845778338427
C	1.06076881473970	-2.40755697136160	-0.50749036435660
H	1.69517515464606	-3.24513333268488	-0.76892496886778
H	0.50605045291377	-2.64056587347985	0.39987980357788
C	2.27623370463154	-0.78586846670427	1.06064705853982
H	2.75660779362841	0.19134206302056	1.03608636127629
C	3.32661803572175	-1.80860962289236	1.47119867911060
H	4.14829626631489	-1.84115124691810	0.75934440028618
H	2.89038432726255	-2.80489716076859	1.53212501371307
H	3.73266560746678	-1.56472701140784	2.44924244209388
C	1.15355220113815	-0.73412719912743	2.08575461648148
H	0.72186872104104	-1.71688029986390	2.25814524443783

H	0.35202308326922	-0.06135913620558	1.79782419862243
H	1.54954342951357	-0.38297077989734	3.03538505359166
H	2.71662685508848	-1.12586583985384	-0.99286716036634
N	-0.67697164544105	2.74544614855063	0.26681359357855
N	0.53112710941946	3.20138987139508	0.16302708137910
H	2.96844111777801	3.38765834278159	-1.09896981488618
H	3.22497435698197	1.64368508524070	-1.12137308197326

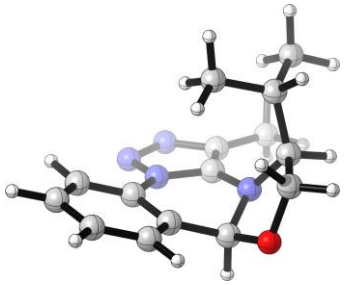
I-3b'-4



N_{imag} = 0
E_{El} = -878.0971 E_h
ZPE = 0.3184 E_h
G_{298} = -877.8213 E_h

C	1.38827527171766	2.18826266571854	-0.29877977936841
C	2.84583331329202	2.34116004082084	-0.51012110404501
C	1.85890893329323	-1.12361850080374	-0.31791725855440
N	0.79651518600789	-0.22834205726208	-0.75499190566263
C	0.59793716831581	1.06654068126081	-0.41747577503208
N	-0.65193785009307	1.49420340547017	-0.12903940197289
C	-1.74572024776491	0.63112891600897	0.00774602208434
C	-1.59817491025313	-0.65616975555926	-0.49572246434698
C	-0.34459818465384	-0.98573402258238	-1.25166284671070
C	-2.62693916877824	-1.56254335842995	-0.32615979001212
C	-3.79214298156594	-1.18332643343801	0.31699681705687
C	-3.92852165450211	0.10800759457770	0.80008682376811
C	-2.90149071441203	1.02155435560737	0.65868739345016
H	-2.98167990973408	2.02049214007740	1.05263573771680
H	-4.83563802640403	0.40487879040022	1.30164881983223
H	-4.59435066154513	-1.89336563291501	0.43788378708787
H	-2.51415731260376	-2.56452377415732	-0.70816827382428
H	3.10216522893775	3.39543962893148	-0.52964962332274
H	-0.48603531322143	-0.76565261281010	-2.31695042438299
O	0.03568039505065	-2.32294866202514	-1.09023659483855
C	1.46329174421674	-2.33270792420183	-1.15389999999939
H	1.79489269202394	-2.22704407979369	-2.18644481297904
H	1.80392470217635	-3.27576445243506	-0.74654962224964
C	1.88412064183538	-1.47281598575702	1.17577111216107
H	1.04651177471449	-2.14832700275793	1.35743683161066
C	1.73181609994037	-0.27576188316719	2.09774267355278
H	0.75033553220180	0.18190394344829	2.01781747765292
H	2.48341382080682	0.48305916065009	1.88753343690798
H	1.86273418925363	-0.59266032021202	3.12996874106258
C	3.18234190785343	-2.20581847418160	1.48018577927498
H	4.03222604593836	-1.53830484947248	1.34273556372957
H	3.32757931287942	-3.06923591452344	0.83515561966761
H	3.19149208342011	-2.55286309813802	2.51010392559627
H	2.82600192716874	-0.72561627987387	-0.62175515716435
N	-0.65626907854576	2.81294832202607	0.14747631085827
N	0.57313485163299	3.20993687703478	0.05075699846049
H	3.15271172257320	1.89412596573293	-1.45279009199554
H	3.42498146882666	1.86652258673152	0.28018505493018

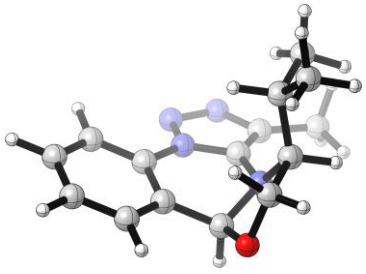
I-3b'-5



N_{imag} = 0
E_{El} = -878.0949 E_h
ZPE = 0.3191 E_h
G_{298} = -877.8177 E_h

C	1.44020625836127	2.17112612343875	-0.27947627007930
C	2.86594309560209	2.40780266768981	-0.60309775757869
C	1.76469379387941	-1.26101326632320	-0.35512041497801
N	0.90691068925599	-0.21822612317822	-0.94895662896608
C	0.68790829870557	1.03241343257440	-0.44006807987109
N	-0.55529274562069	1.38733572663155	-0.02990918700473
C	-1.61286009655467	0.47554558252957	0.07628180862006
C	-1.46920213156058	-0.70954439726806	-0.63473441912929
C	-0.27368562183597	-0.83845324681594	-1.54724988425730
C	-2.43461034989801	-1.68739225801810	-0.50188895976628
C	-3.53584480012770	-1.47251643966856	0.30973677649329
C	-3.67177299368134	-0.27599023511404	0.99517164196061
C	-2.70316393012970	0.70540383542659	0.89289000749028
H	-2.77940154402581	1.62775783613864	1.44366429838080
H	-4.53008293197463	-0.10920684624376	1.62604854180472
H	-4.29023208089896	-2.23695610853948	0.40499481974086
H	-2.32177799597528	-2.61371608253428	-1.04259163726305
H	3.30695609500559	1.51070430202306	-1.02711457210074
H	-0.49473373646597	-0.36749129603354	-2.50573289083203
O	0.11984227710757	-2.14999315166534	-1.80009094750105
C	0.98177665821338	-2.52024331014231	-0.73063463614218
H	1.62120944958094	-3.32176092834166	-1.07990490648626
H	0.39380422118112	-2.87074858116842	0.11743614018102
C	2.04773927750266	-1.22924134466758	1.15101556465317
H	2.40093383081738	-2.24270574006599	1.35751552602239
C	0.82198911226572	-0.98135516905478	2.01677415079685
H	0.54274982455527	0.06890587420183	2.00811676015689
H	1.04299409122540	-1.24762191045335	3.04733182423972
H	-0.03868127393580	-1.56467542158268	1.70089205315946
C	3.17431723460835	-0.28304711122645	1.53364002321418
H	4.03654062164054	-0.40952896792223	0.88254741788182
H	3.49114512199591	-0.47515401609689	2.55612487174395
H	2.85490542101586	0.75328313867569	1.48052112219632
H	2.72211330169865	-1.25390081144968	-0.87443506064838
N	-0.58302670055395	2.66623966092891	0.36493050457640
N	0.62139574788421	3.12555364600787	0.22203348946558
H	3.43704513554645	2.67662454036572	0.28227799608960
H	2.96707937558976	3.21472639694213	-1.32445908626353

I-3b'-6

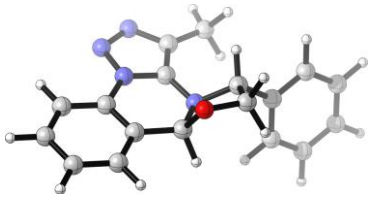


N_{imag} = 0
E_{El} = -878.0935 E_h
ZPE = 0.3186 E_h
G_{298} = -877.8174 E_h

C	1.43900518825121	2.21948428428986	-0.40213933000329
C	2.86779684944047	2.41352449577321	-0.73268659796552
C	1.61993078445344	-1.25393096081293	-0.17595587637393

N	0.90327305913032	-0.20178226307296	-0.93987586783266
C	0.68565363494690	1.07419116524894	-0.47711523811946
N	-0.54043258973847	1.44859567225810	-0.03848686733776
C	-1.61845566061201	0.56028102257462	0.07104216873318
C	-1.49900979998981	-0.62694061361408	-0.63979773636452
C	-0.29135849958498	-0.80437342679600	-1.53404652006282
C	-2.50171510787590	-1.57023826492506	-0.52927032490993
C	-3.61046468093690	-1.31945444252348	0.26097618713837
C	-3.71822154045445	-0.12142508638579	0.94923968920435
C	-2.71536055473208	0.82655554964840	0.86770484497682
H	-2.77242563934168	1.75248522281726	1.41492937578215
H	-4.58257073260164	0.07293678248150	1.56373349356477
H	-4.39261970247788	-2.05752939877286	0.33857013748328
H	-2.41018320388096	-2.49880906597921	-1.07034430725417
H	3.46837919935761	2.54291693078761	0.16527578226176
H	-0.48420723297857	-0.36064422195448	-2.51014333033853
O	0.06870412219160	-2.13478960125005	-1.72660276632884
C	0.79755726428693	-2.49012304750950	-0.55914656317419
H	1.40168557709463	-3.35785558022683	-0.79125083547812
H	0.10086369337727	-2.73325432640017	0.24463733410206
C	1.71256015103267	-1.11679164904191	1.34358207625871
H	0.69850156208767	-0.98500019184174	1.72812795566632
C	2.58920154433148	0.03673512310704	1.81285098504891
H	3.51767248522361	0.06768847264883	1.24396869908525
H	2.84682451797187	-0.10263402207016	2.86021120449986
H	2.10424592515220	1.00037372203605	1.72309793219683
C	2.28480296572409	-2.41820750334080	1.89905865734308
H	1.67224171986276	-3.28278671283129	1.65976465947225
H	2.36713801134297	-2.35659556082131	2.98072196704059
H	3.28321391223643	-2.58907662118140	1.49772083761666
H	2.63221411455922	-1.33123845521698	-0.57225240587125
N	-0.56122758757001	2.74436546550741	0.28296641921996
N	0.63832939372406	3.19929146998823	0.07584667010461
H	3.00401458641555	3.29242155761804	-1.35652321504961
H	3.24594227058039	1.54596407978394	-1.26552929433514

I-3c-1

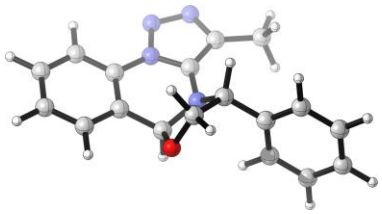


N_{imag} = 0
E_{El} = -991.4133 E_h
ZPE = 0.3154 E_h
G_{298} = -991.1418 E_h

C	0.11419853237234	-2.34965707284622	0.36722374581353
C	1.52258716104054	-2.80526503765804	0.46725947007909
C	1.30412627760877	0.48352288991078	0.84403860446298
N	0.15493956221379	0.14507124852467	-0.01503446493023
C	-0.40919169003501	-1.08963046852368	0.16697113548296
N	-1.74083056344832	-1.27909145039872	0.10361046395711
C	-2.66821127155698	-0.26211268090813	-0.12036530410701
C	-2.16919877381132	1.02634518616275	-0.21781244746846
C	-0.71927599737587	1.31388714990107	-0.02564582153615
C	-3.04980773772636	2.06521373736981	-0.46646147339517
C	-4.40269832103209	1.82055287662241	-0.59985272269739
C	-4.88294560669090	0.52408345843517	-0.49222398429714
C	-4.01957611034366	-0.52691515659215	-0.25727687071193
H	-4.37573732066669	-1.53981825301152	-0.18043192265716
H	-5.93774346617728	0.32820028252165	-0.59980233825866
H	-5.08127035208164	2.63541757313768	-0.79288537401338
H	-2.66504280268289	3.06959732849809	-0.55326376918264
H	1.54458679645636	-3.89013190632917	0.45805231847358
H	-0.36422735256213	1.99305105689992	-0.80424648590385

O	-0.49119422158419	1.93868222258531	1.22793761888545
C	0.91886686452216	1.88895547471030	1.34457888578953
H	1.19540026115449	2.05138070629197	2.37851207419859
H	1.37469417893972	2.65091886657422	0.71060072134237
H	1.32181929941383	-0.19935366514531	1.68891158564883
N	-2.05128375234616	-2.58247964632897	0.24661206767546
N	-0.93226215677308	-3.20764265204516	0.41168178786117
H	2.00586466452322	-2.46377265486390	1.37958770079222
H	2.11315204915502	-2.44175193871548	-0.37036013635174
C	2.63007264268902	0.45623346542857	0.14686592314450
C	3.77078692121636	0.11549459326659	0.85673170914483
C	2.74399776440005	0.81766425773856	-1.18700137303931
C	5.01217848294670	0.13867505302216	0.24435006452003
C	3.98276086381815	0.83805876972901	-1.80221585402813
C	5.12078176820746	0.50052381043454	-1.08737392518433
H	3.68283130132935	-0.18044071491758	1.89204269618765
H	1.85593666368167	1.07090053944510	-1.74580233517195
H	5.89259289702901	-0.13341026780810	0.80533072848247
H	4.06060418332211	1.11575012118855	-2.84187695542719
H	6.08624836085448	0.51372289769324	-1.56833574358055

I-3c-2

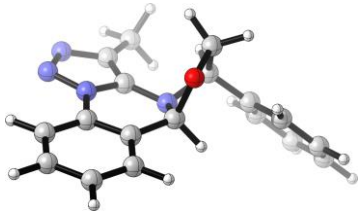


N_{imag} = 0
E_{El} = -991.4108 E_h
ZPE = 0.3149 E_h
G_{298} = -991.1400 E_h

C	0.01745452105833	-2.53268443260008	0.03220337274184
C	1.40646319954332	-3.04224168383966	0.11273251406382
C	1.14735718250160	0.40714784981385	0.79644757283849
N	0.17936188750432	-0.02811184659988	-0.21315044927611
C	-0.43758508426987	-1.24045219493738	-0.10140056501126
N	-1.78145870030913	-1.35021904488160	-0.12839778039022
C	-2.64479412368501	-0.25082572181923	-0.08982023237129
C	-2.07250046831855	0.99694741556637	-0.28829696606921
C	-0.61490022908092	1.11878293027850	-0.66165847555007
C	-2.87869469599515	2.11712694189995	-0.19544250669516
C	-4.22888620469501	1.98956875533019	0.07463937651423
C	-4.78322858421563	0.73242640720608	0.25760575467321
C	-3.99244418425836	-0.39730294681438	0.18542463428888
H	-4.40076576927682	-1.38003678245915	0.34907776107804
H	-5.83576493358592	0.63026200865456	0.46794067171247
H	-4.84951445569933	2.86877196296462	0.13870885371297
H	-2.44026758044419	3.09150017880566	-0.34164088445042
H	2.01189144470246	-2.65656007112316	-0.70461308282730
H	-0.52152517030506	1.24770506835249	-1.74013423865818
O	0.01524842472151	2.22528145645812	-0.07205576649487
C	0.56021496382313	1.76831780227737	1.15994613809979
H	-0.22378713629818	1.65664884996359	1.90881384135112
H	1.29662746387295	2.48966414697249	1.49035934851546
H	1.11293939989248	-0.25971457103594	1.65323302328162
N	-2.16015404198414	-2.63672182611040	-0.03739792411668
N	-1.07273719375051	-3.33344058567893	0.06696616507281
H	1.39936815426764	-4.12573292986867	0.05693858468442
H	1.89039701916347	-2.75179832537961	1.04302709198535
C	2.55400655693829	0.49377176544143	0.27385509424141
C	3.61655466914131	0.38621408495067	1.15951293040751
C	2.81343720965299	0.72103001040331	-1.06838444439918
C	4.91992367072965	0.51098856045203	0.71258355891575
C	4.11679989081499	0.84902535794749	-1.51770606062684

C	5.17329062099977	0.74540207640490	-0.62893846019670
H	3.42051142310422	0.19762150650287	2.20512794882631
H	1.99231568603413	0.78543665966383	-1.76529066537516
H	5.73788463170223	0.41851380151705	1.41001012267033
H	4.30735272678986	1.02579963581656	-2.56491709797050
H	6.18883780921308	0.83943772950409	-0.98036875919666

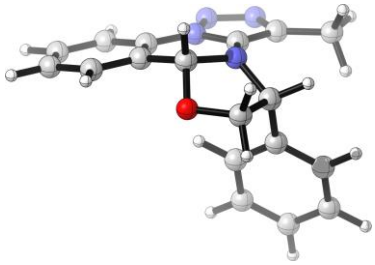
I-3c-3



N_{imag} = 0
E_{El} = -991.4111 E_h
ZPE = 0.3159 E_h
G_{298} = -991.1385 E_h

C	-0.27472367429852	-2.72873002997541	0.61514019259723
C	0.98865351357784	-3.48567621306358	0.79163605312193
C	1.49670547082480	-0.16017528391676	0.86121824153992
N	0.30359115505848	-0.33114319607750	0.00156740573250
C	-0.50836728753364	-1.40520781185339	0.30696416002463
N	-1.85136745205073	-1.30576901957322	0.23340086883422
C	-2.53321159599971	-0.14885828900394	-0.14423694992564
C	-1.76555075343877	0.99466574657043	-0.28975223968402
C	-0.31807534115824	0.97536283605296	0.06018544269324
C	-2.37944026570562	2.16219469914404	-0.70631788727205
C	-3.73932743838632	2.18634753369912	-0.95316921441747
C	-4.49136109687156	1.03299218161456	-0.79083079962268
C	-3.89337579033903	-0.14680394249111	-0.39304499490433
H	-4.46140500102855	-1.05422541591412	-0.28034693654057
H	-5.55155794088298	1.04838316210487	-0.98648286790872
H	-4.21244591690622	3.09956345172788	-1.27566167977495
H	-1.78376049192279	3.05311496325947	-0.83253659963144
H	0.77776283482077	-4.54734130982501	0.71443838109795
H	0.23536438594213	1.64092924150592	-0.59891909551511
O	-0.13005925305740	1.43699577726788	1.41090346899918
C	0.91454682528417	0.66514988841613	2.00300679009545
H	0.49075795866372	0.01338105857135	2.76391820432320
H	1.64303427972631	1.32748930792994	2.45925602159657
H	1.83197196542201	-1.12833026978169	1.20632647413381
N	-2.43800384942285	-2.49123460295525	0.47442161417860
N	-1.48427672903132	-3.33020756448547	0.71013692368554
H	1.44613893336372	-3.30478269250204	1.76236239045010
H	1.71543532078185	-3.22461563213653	0.02678148535344
C	2.60502416552416	0.50163064814305	0.08825017550408
C	2.76385074655694	1.87954551451611	0.06070569516240
C	3.48204988431237	-0.29143768902350	-0.63902414887751
C	3.77809784767158	2.45473510352735	-0.68648777930375
C	4.49844600106306	0.27956898752789	-1.38214480676311
C	4.64750197454180	1.65673149563447	-1.40872119570707
H	2.09252599620957	2.51054591255386	0.62364109199543
H	3.36738063517278	-1.36506923588218	-0.61714413994095
H	3.88962243226059	3.52757243352397	-0.70069739914162
H	5.17668692616186	-0.34947960266261	-1.93715407201800
H	5.44087062509371	2.10460785783202	-1.98628827417043

I-3c'-1



N_{imag} = 0
E_{El} = -991.4129 E_h
ZPE = 0.3160 E_h
G_{298} = -991.1400 E_h

C	0.80947490230372	2.17854940981989	-0.94942170539270
C	2.11745312000034	2.35363390225857	-1.62202940820318
C	1.34736576115886	-0.94495442014261	-1.29690660829412
N	0.09547104511013	-0.19140024910312	-1.39330445528386
C	-0.00308904831020	1.06855648914445	-0.89099288055496
N	-1.07356928068417	1.46213952425967	-0.17536266773070
C	-2.11199428470237	0.60819989628361	0.20216724713732
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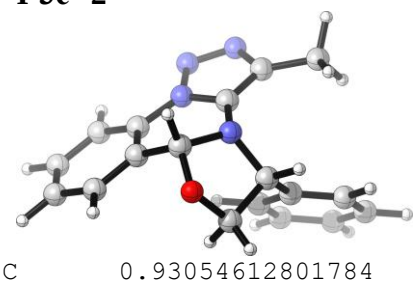
I-3c'-2



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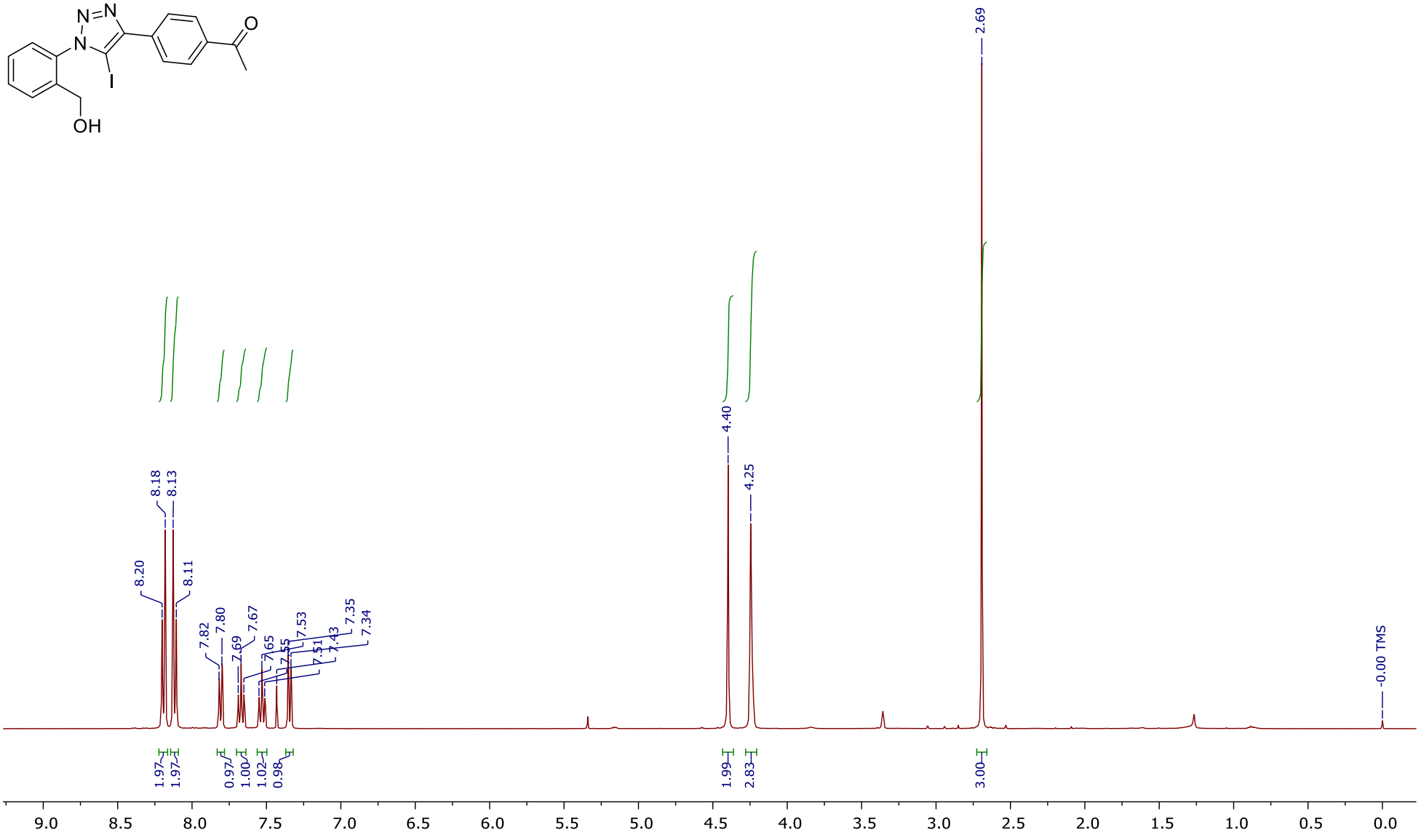
Copies of NMR spectra

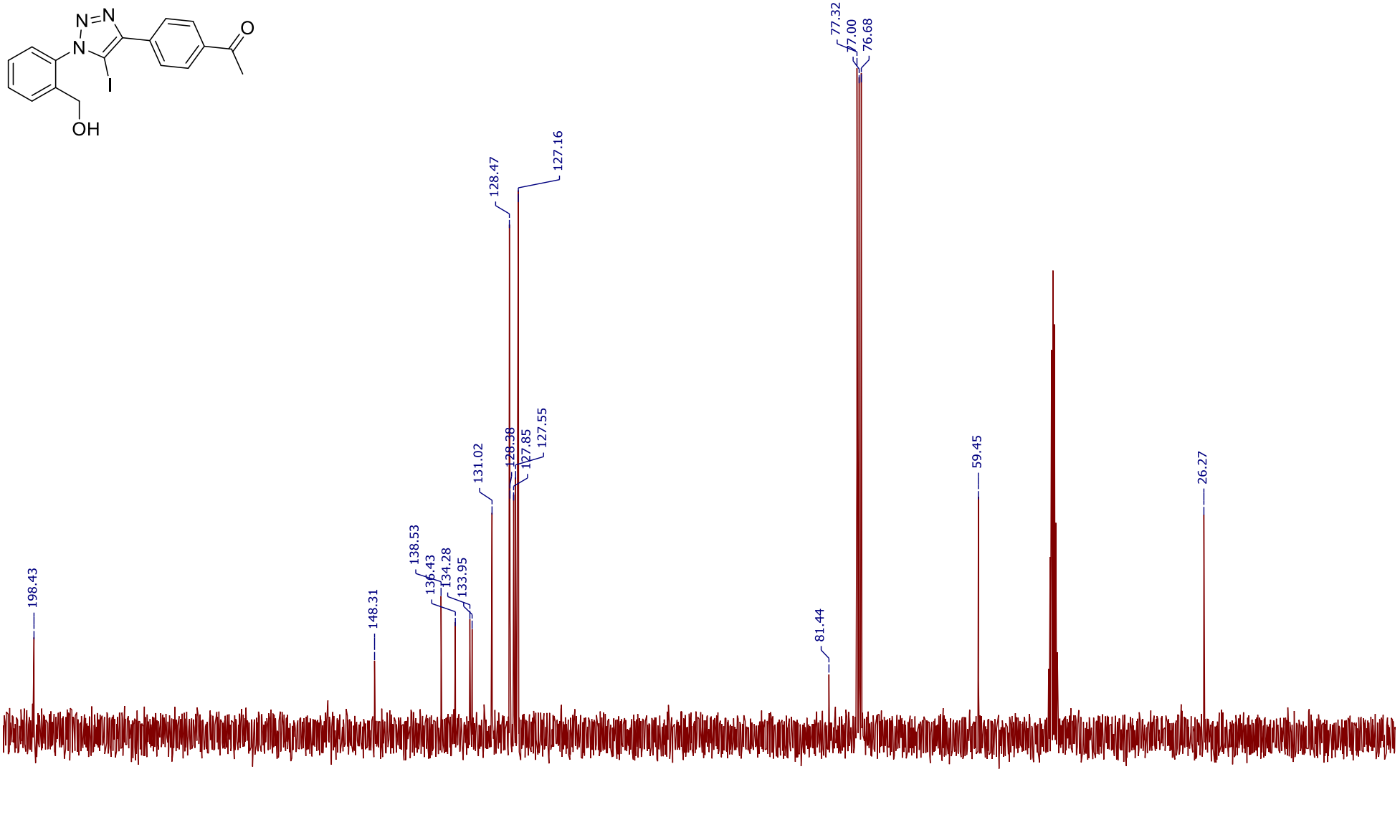
1-(4-{1-[2-(Hydroxymethyl)phenyl]-5-iodo-1*H*-1,2,3-triazol-4-yl}phenyl)ethanone (S4i)

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



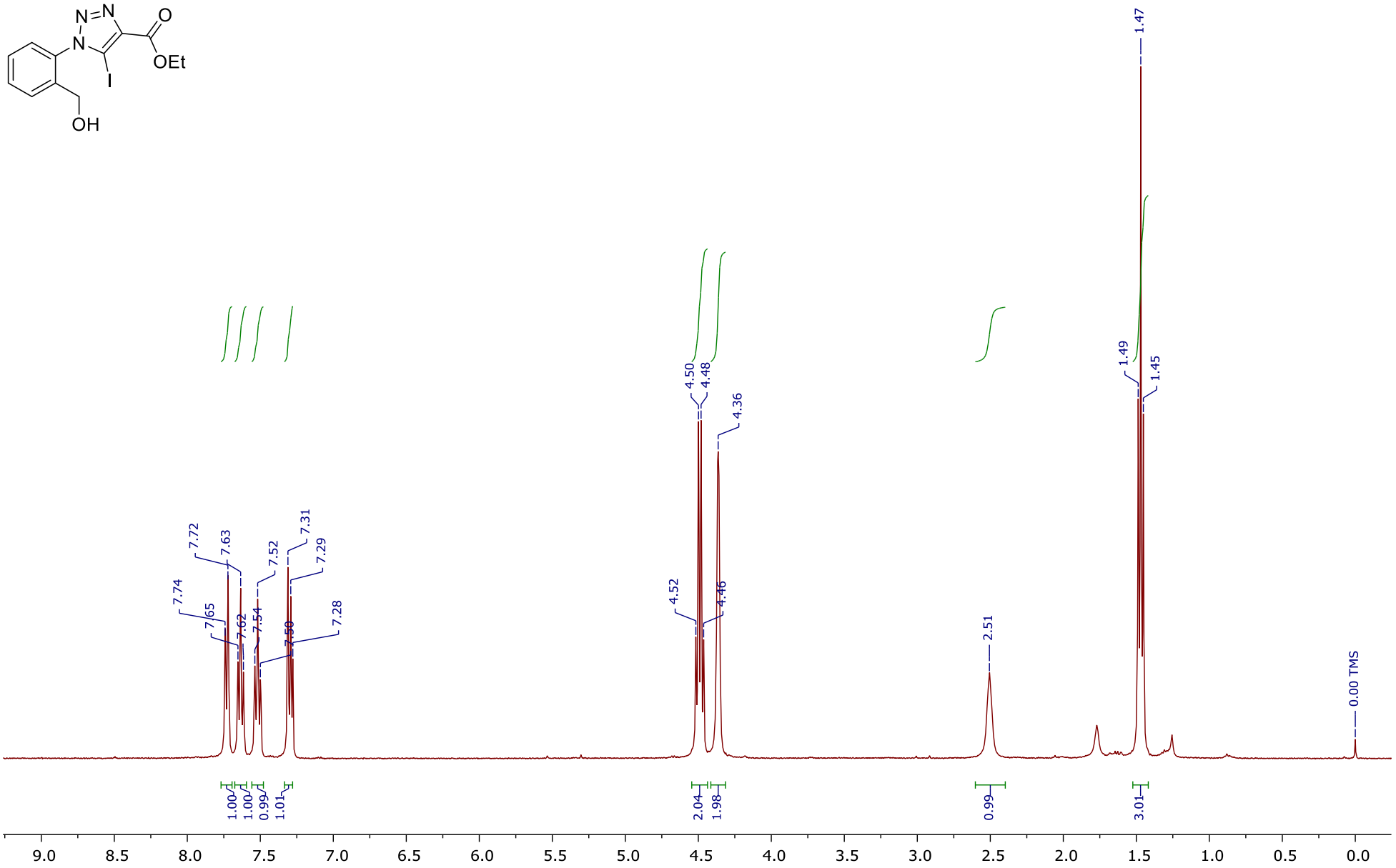
1-(4-{1-[2-(Hydroxymethyl)phenyl]-5-iodo-1*H*-1,2,3-triazol-4-yl}phenyl)ethanone (S4i)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3/CD_3OD$)



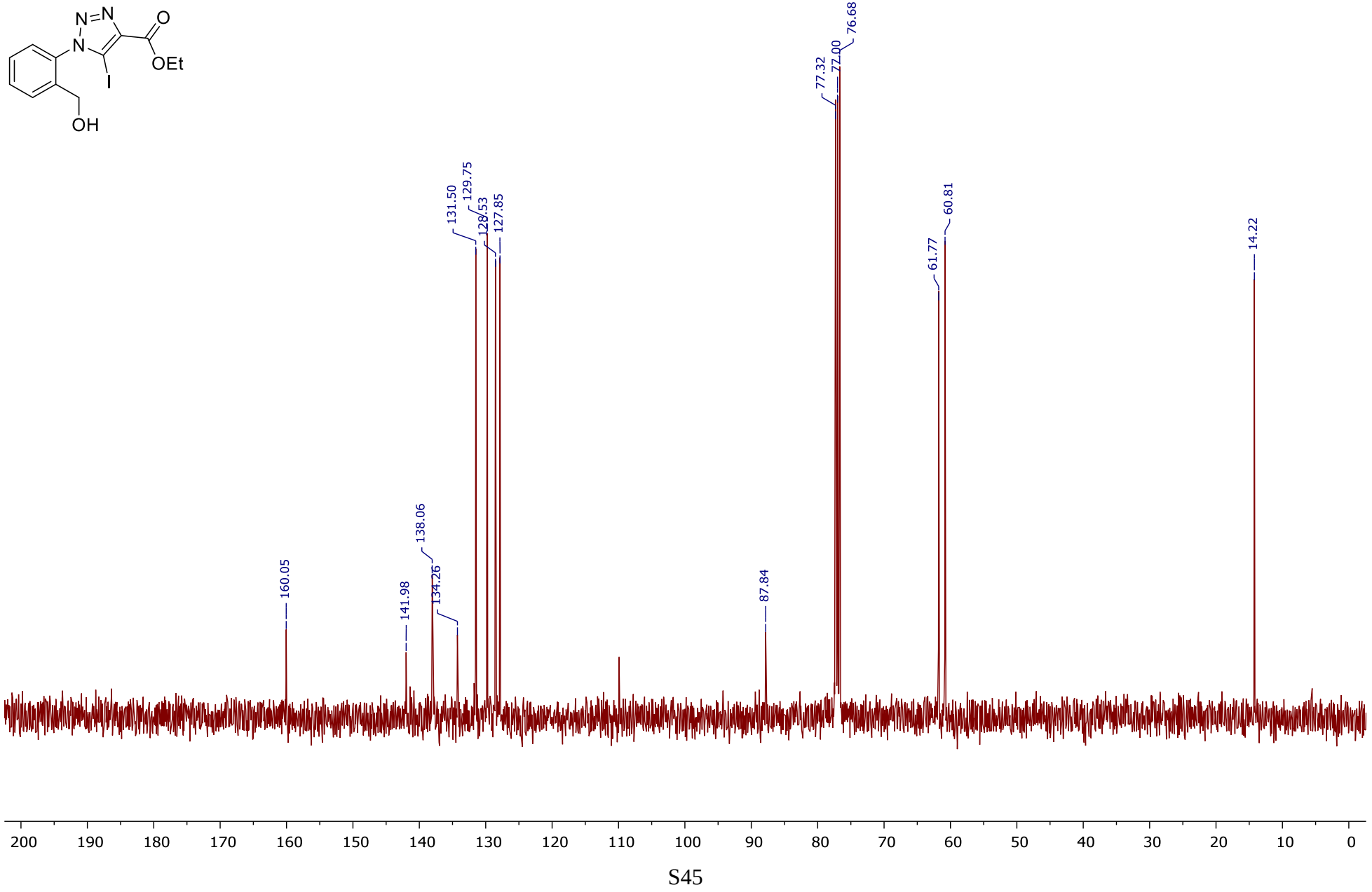
Ethyl 1-[2-(hydroxymethyl)phenyl]-5-iodo-1*H*-1,2,3-triazole-4-carboxylate (S4l)

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



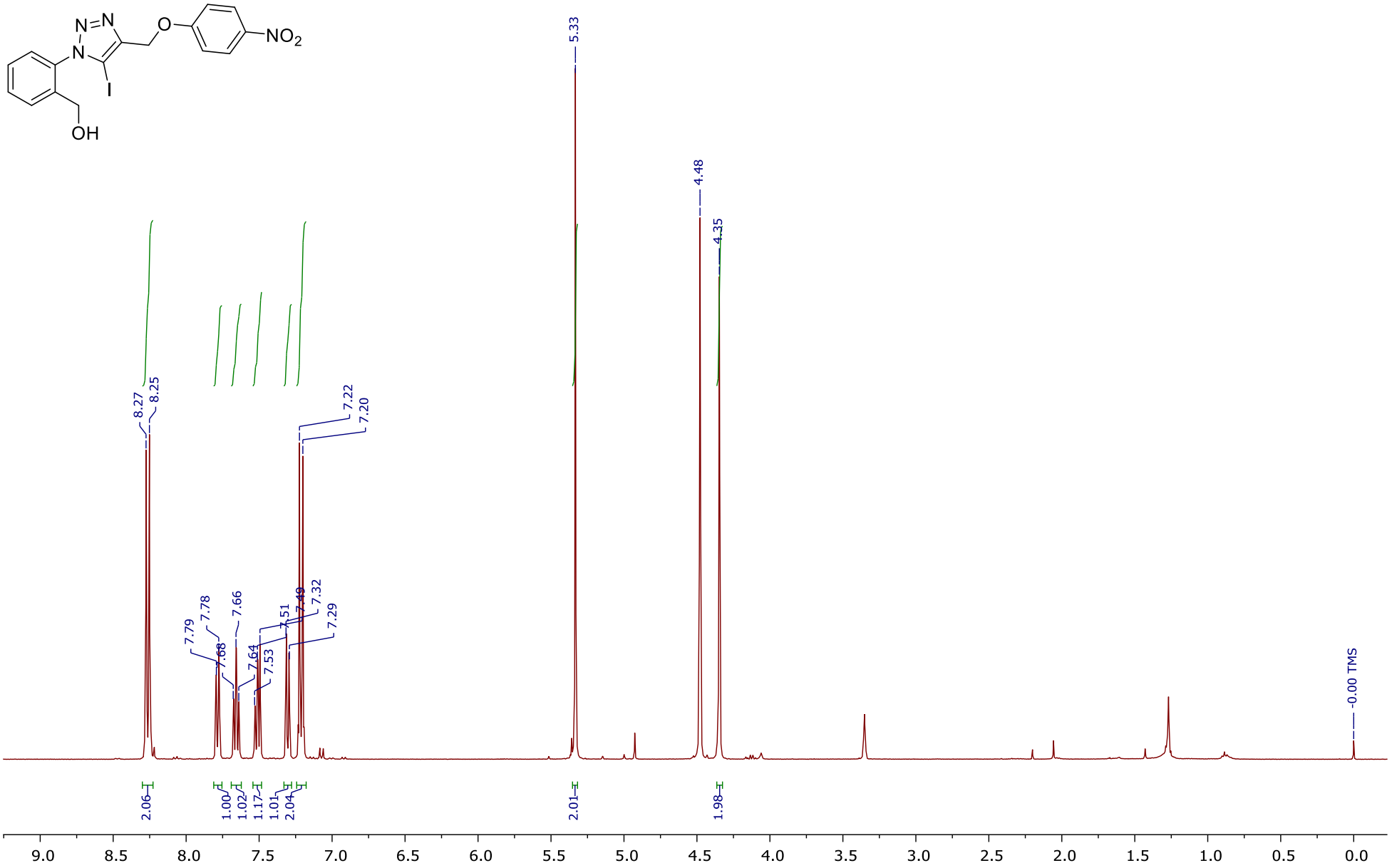
Ethyl 1-[2-(hydroxymethyl)phenyl]-5-iodo-1*H*-1,2,3-triazole-4-carboxylate (S4l)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



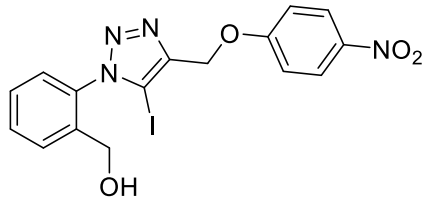
(2-{5-Iodo-4-[(4-nitrophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenyl)methanol (S4n)

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



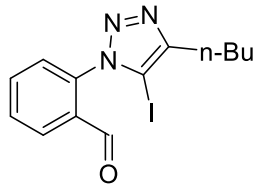
(2-{5-Iodo-4-[(4-nitrophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}phenyl)methanol (S4n)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3/CD_3OD$)



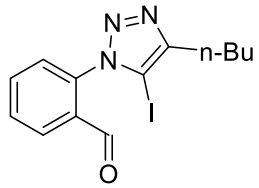
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)benzaldehyde (1a)

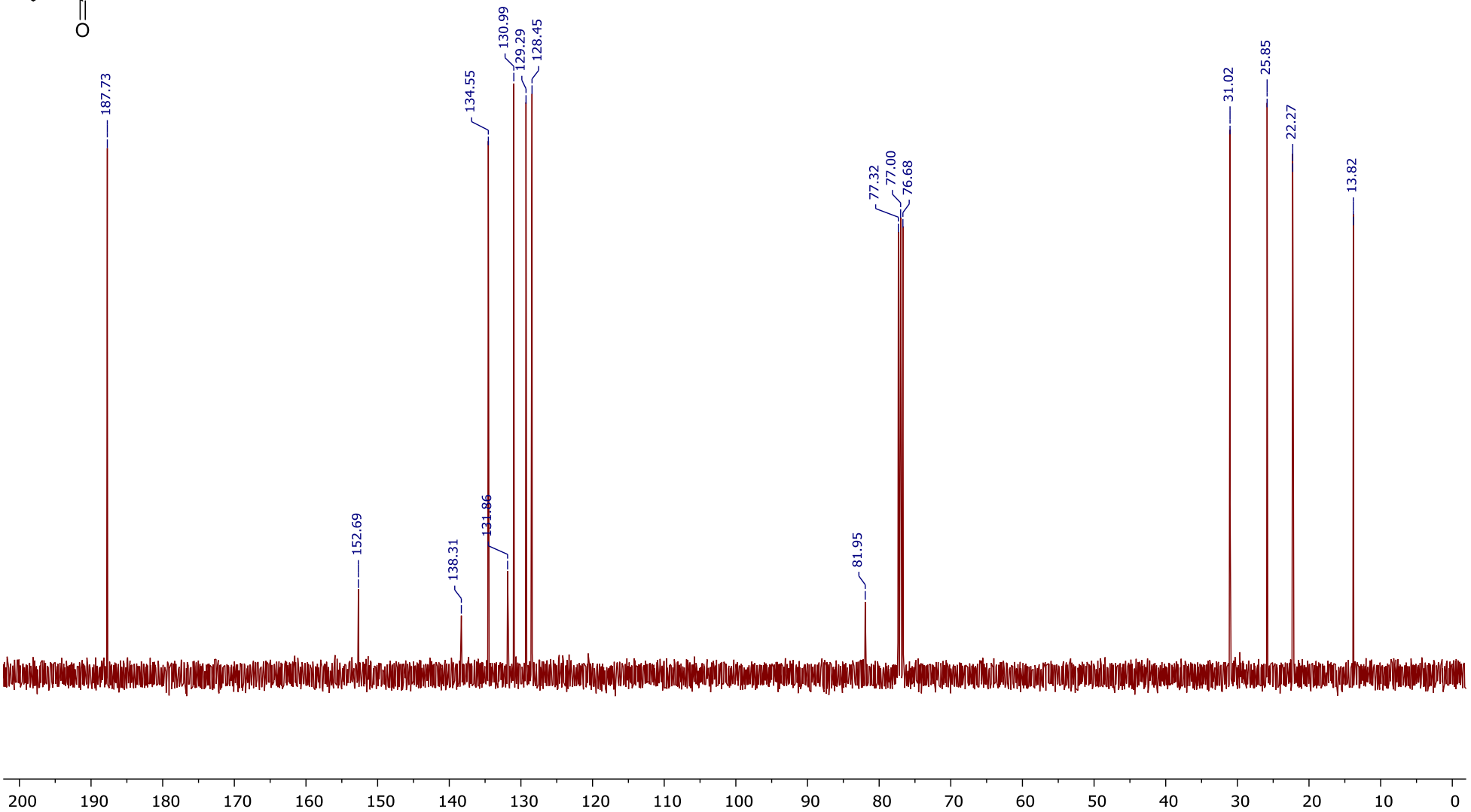
^{1}H NMR (400 MHz, $CDCl_3$)



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

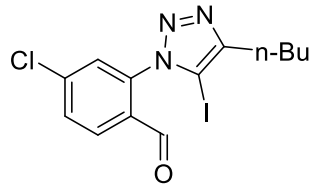
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)





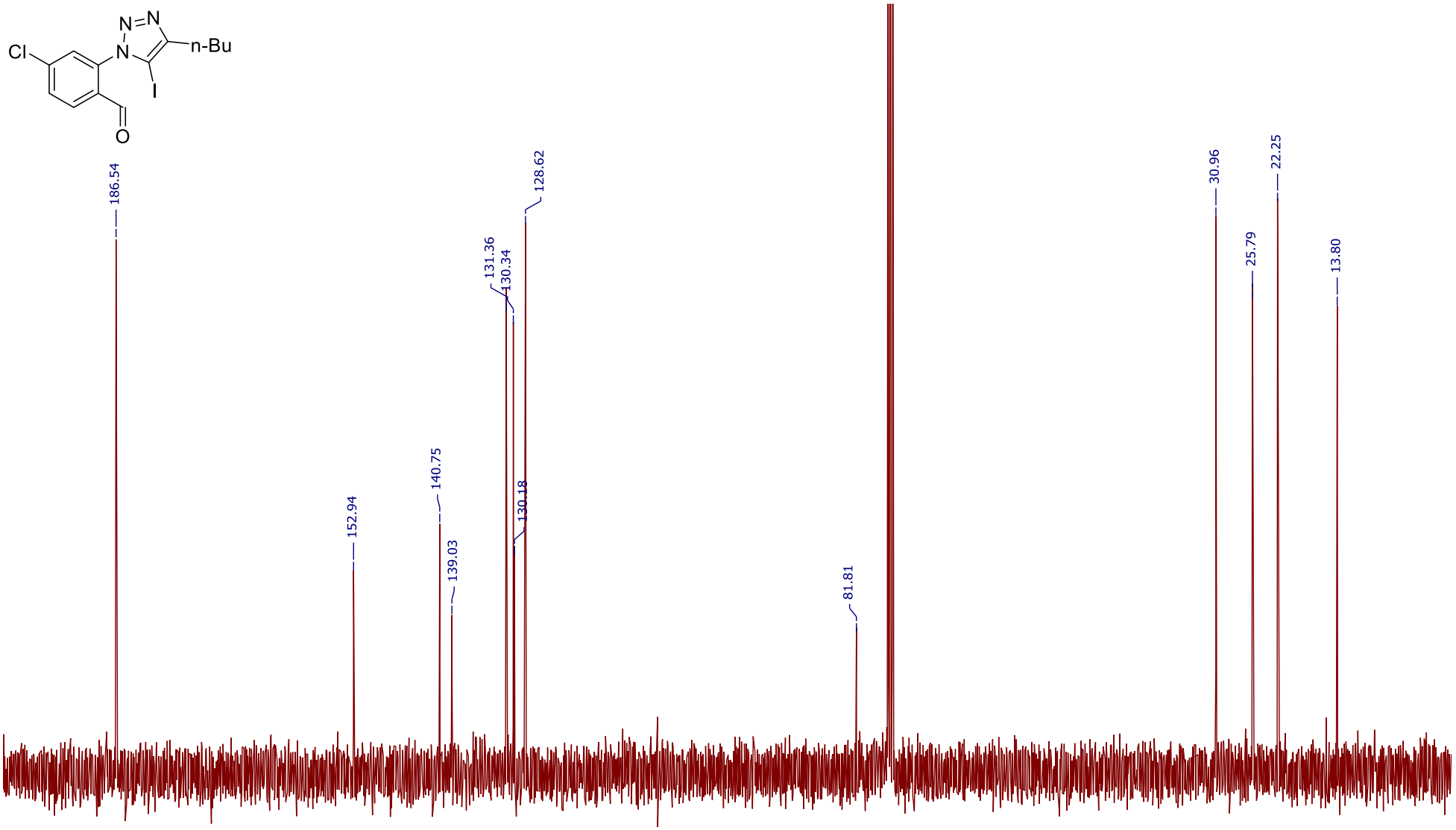
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-4-chlorobenzaldehyde (1b)

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



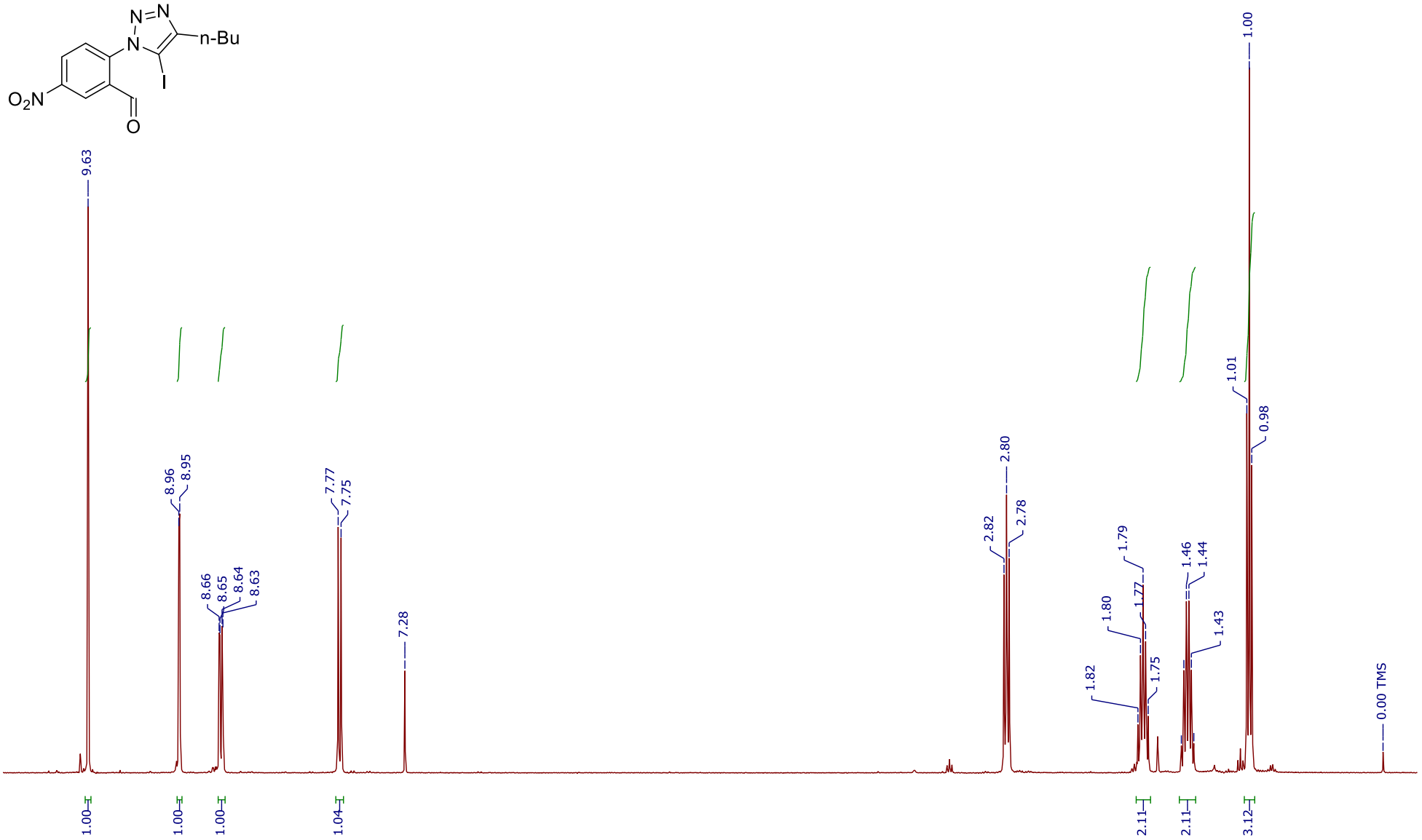
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-4-chlorobenzaldehyde (1b)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



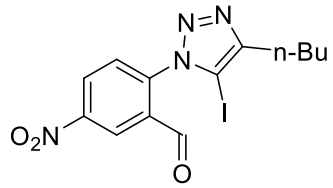
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-5-nitrobenzaldehyde (1c)

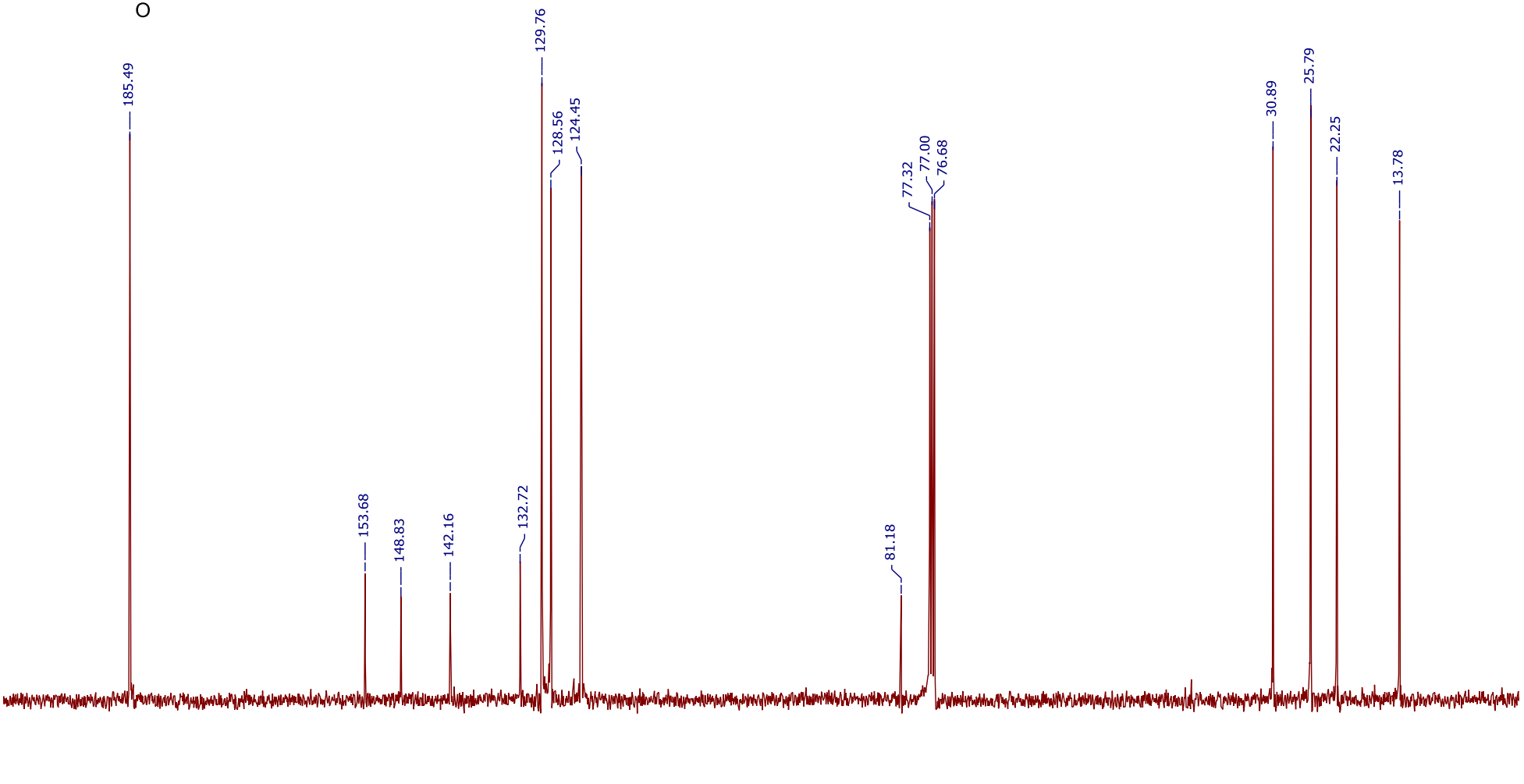
^{1}H NMR (400 MHz, $CDCl_3$)



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

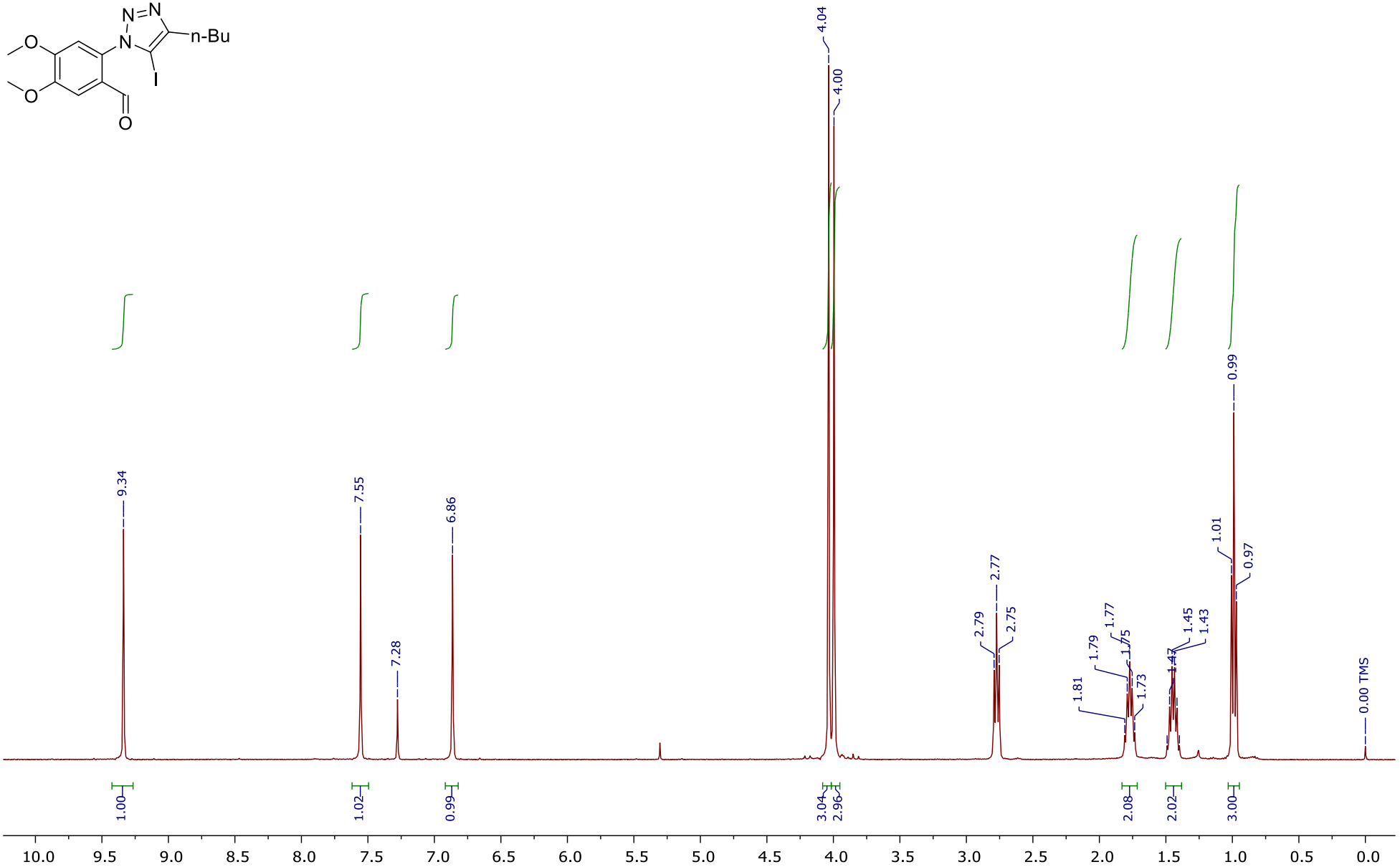
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)





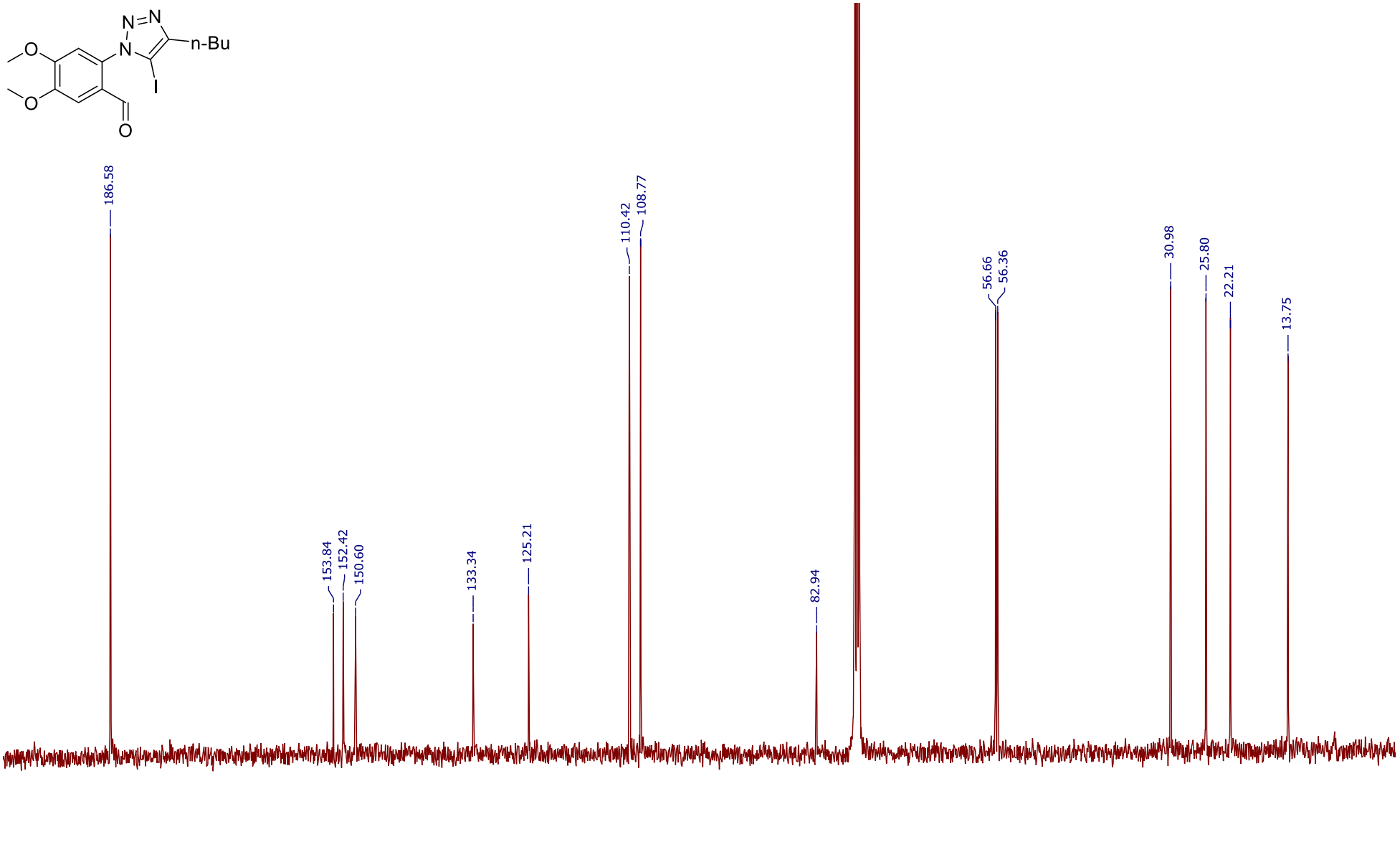
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-4,5-dimethoxybenzaldehyde (1d)

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



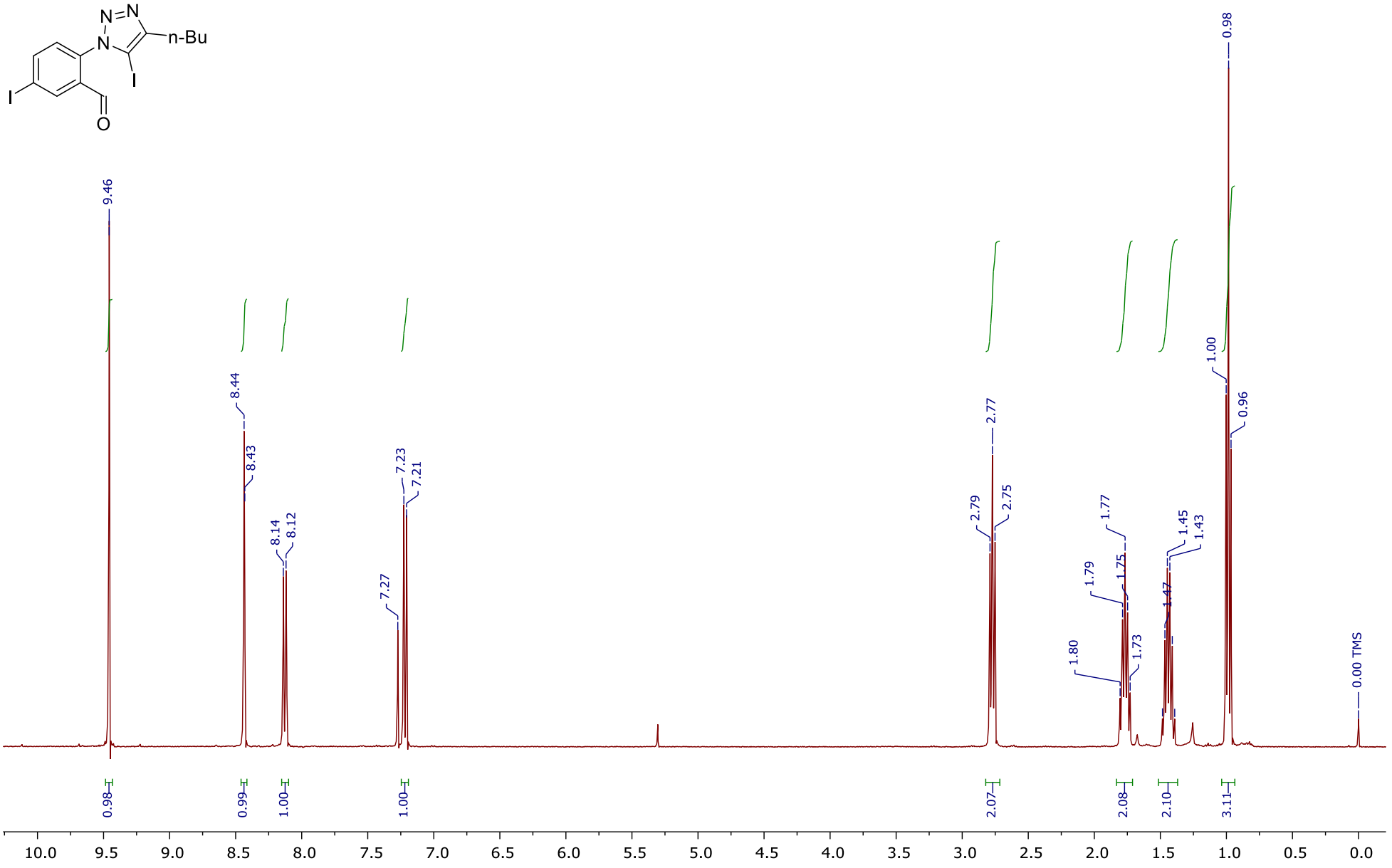
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-4,5-dimethoxybenzaldehyde (1d)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



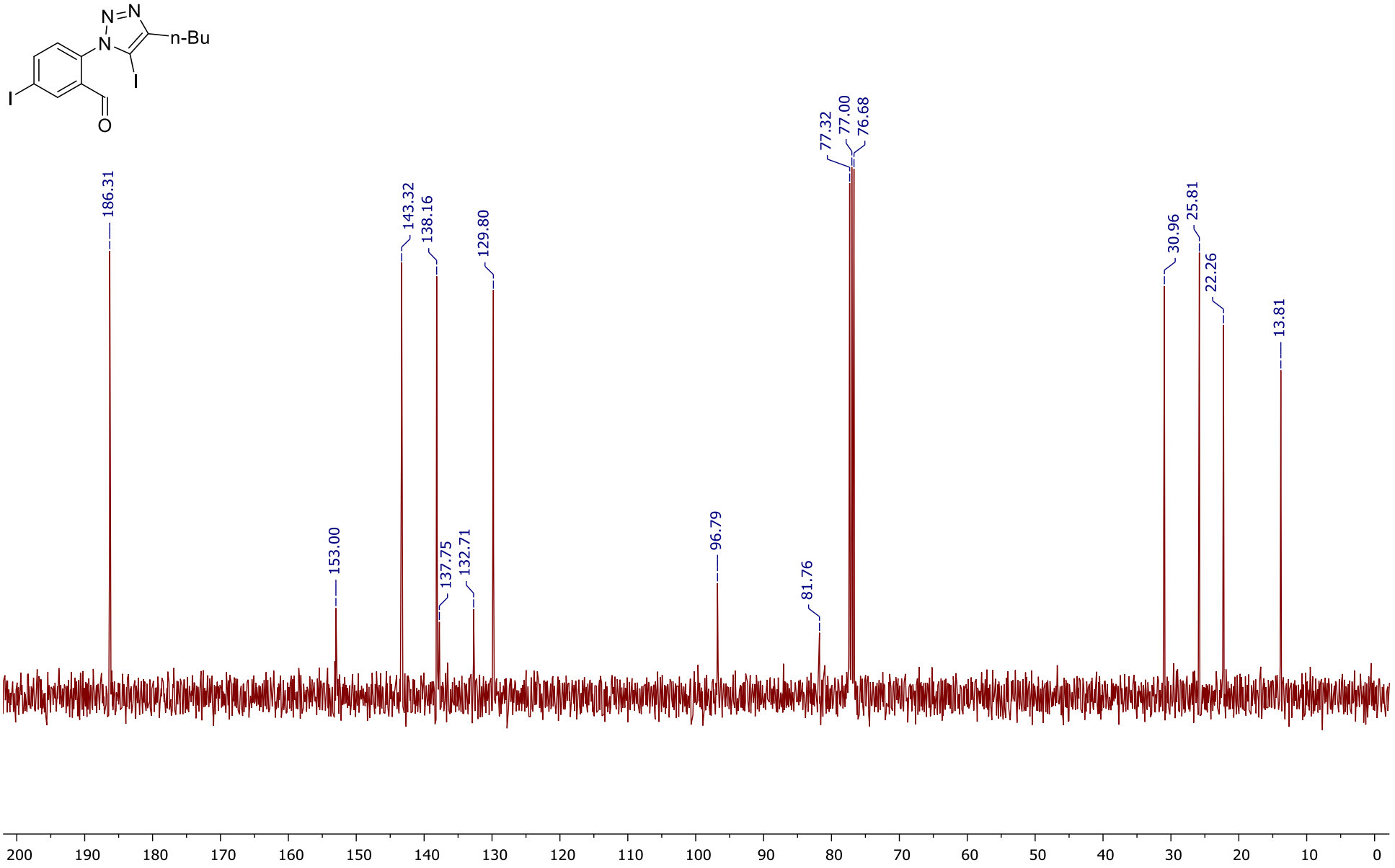
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-5-iodobenzaldehyde (1e)

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



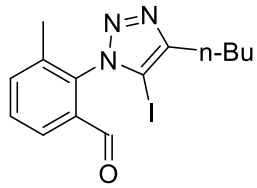
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-5-iodobenzaldehyde (1e)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



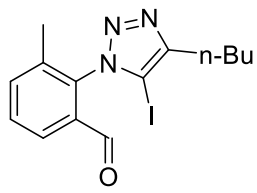
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-3-methylbenzaldehyde (1f)

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



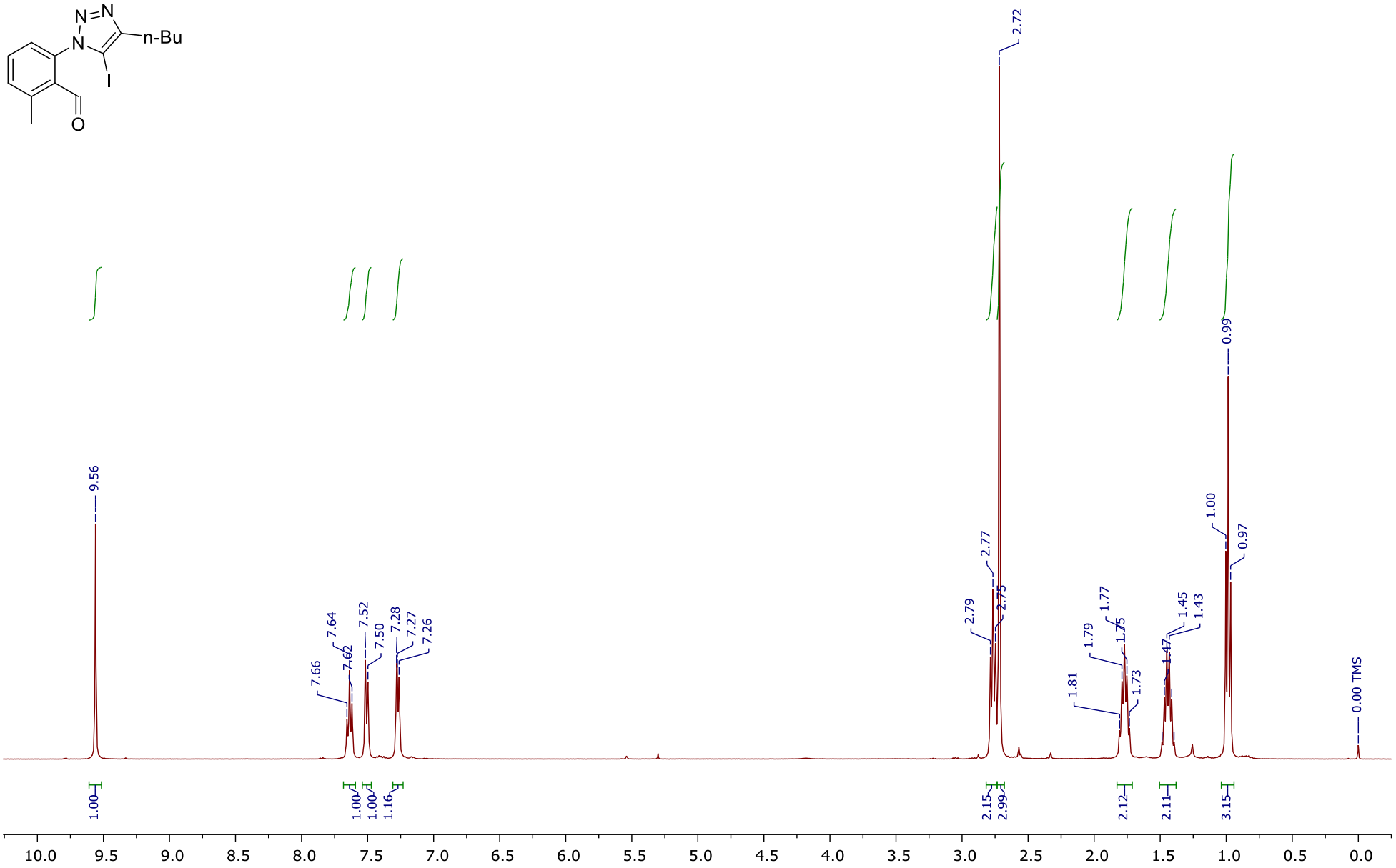
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-3-methylbenzaldehyde (1f)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



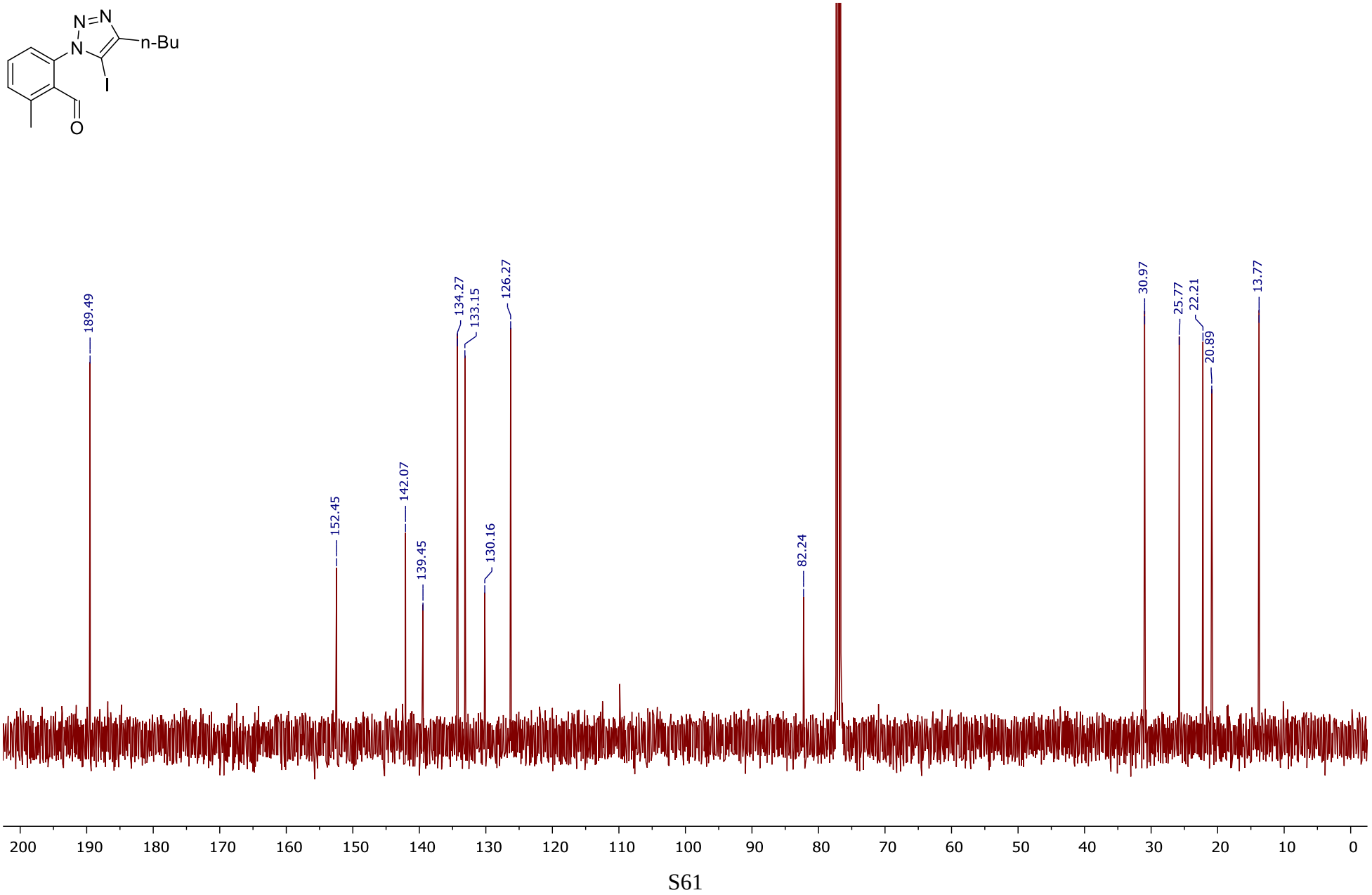
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-6-methylbenzaldehyde (1g)

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



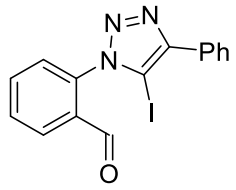
2-(4-Butyl-5-iodo-1*H*-1,2,3-triazol-1-yl)-6-methylbenzaldehyde (1g)

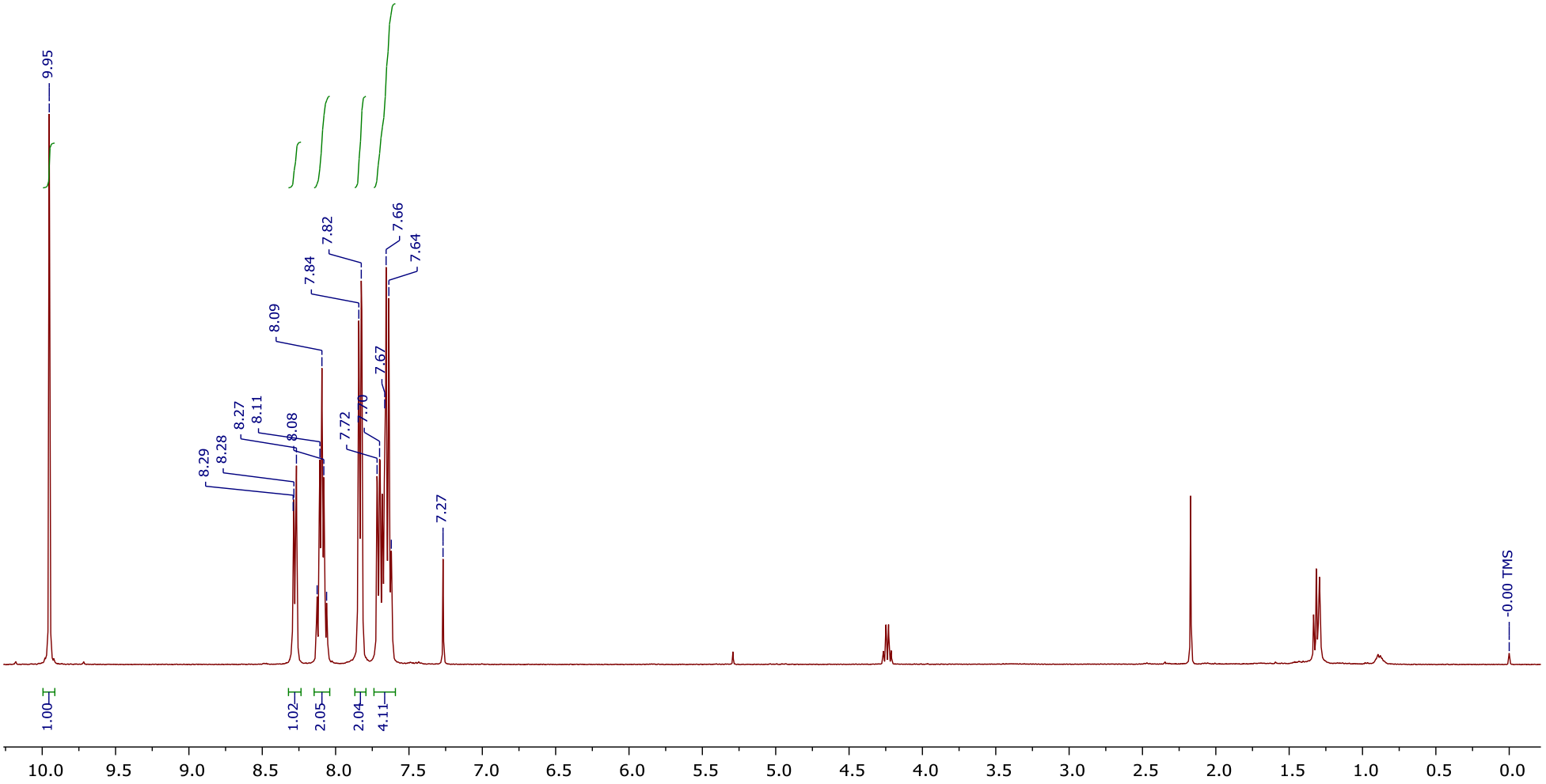
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



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

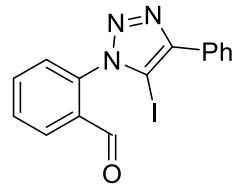
^{1}H NMR (400 MHz, $CDCl_3$/TFA)





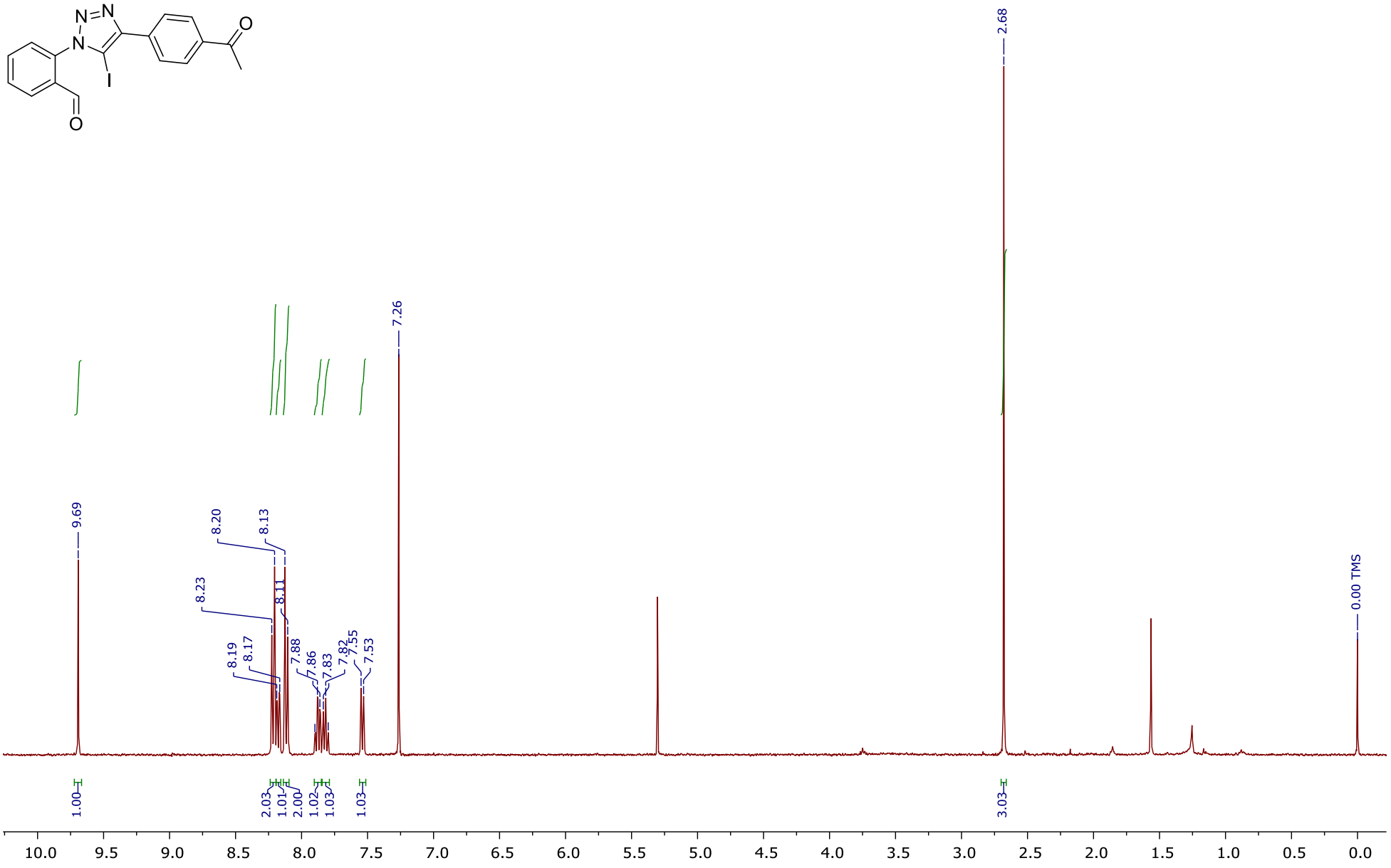
2-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)benzaldehyde (1h)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$/TFA)



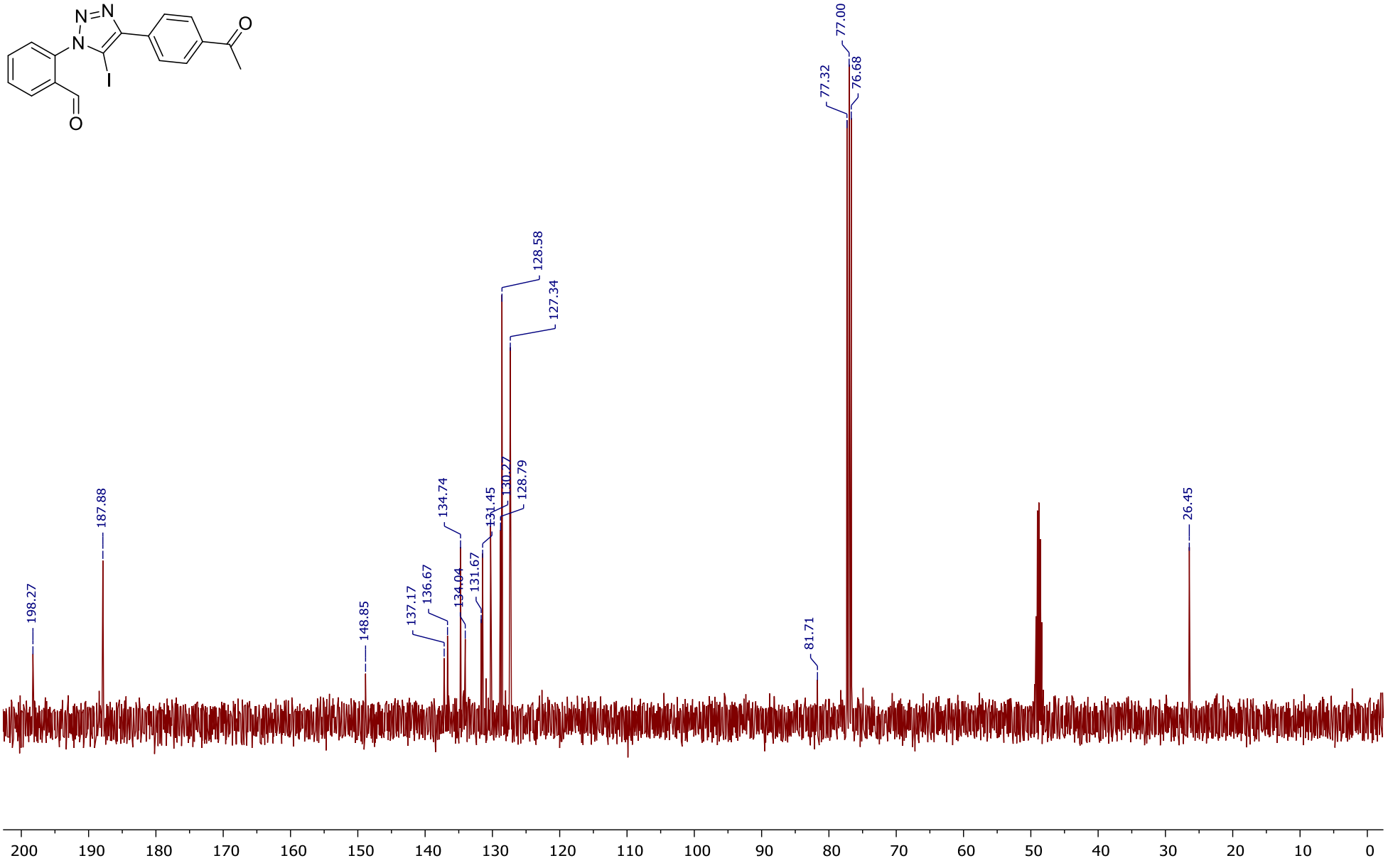
2-[4-(4-Acetylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]benzaldehyde (1i)

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



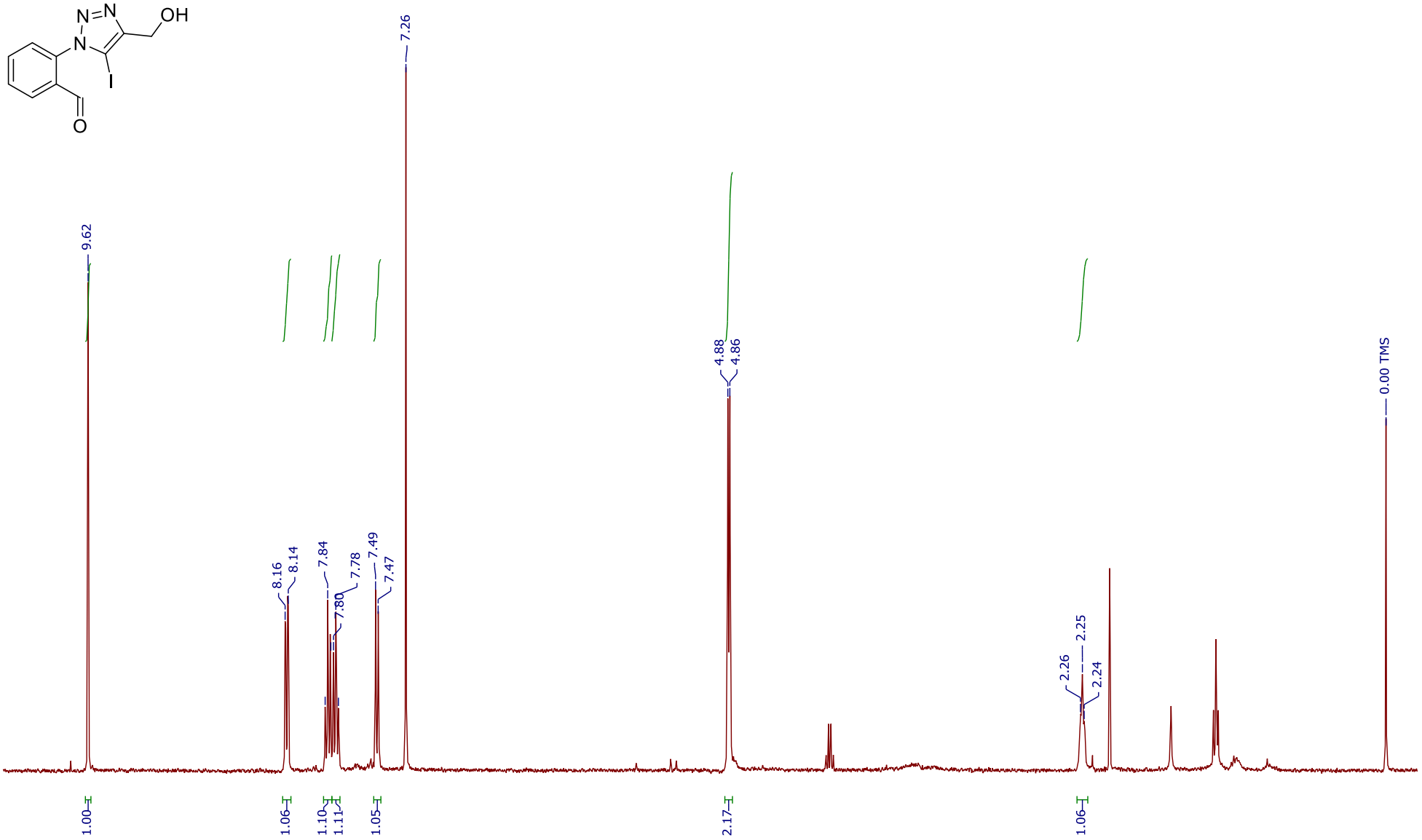
2-[4-(4-Acetylphenyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]benzaldehyde (1i)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3/CD_3OD$)



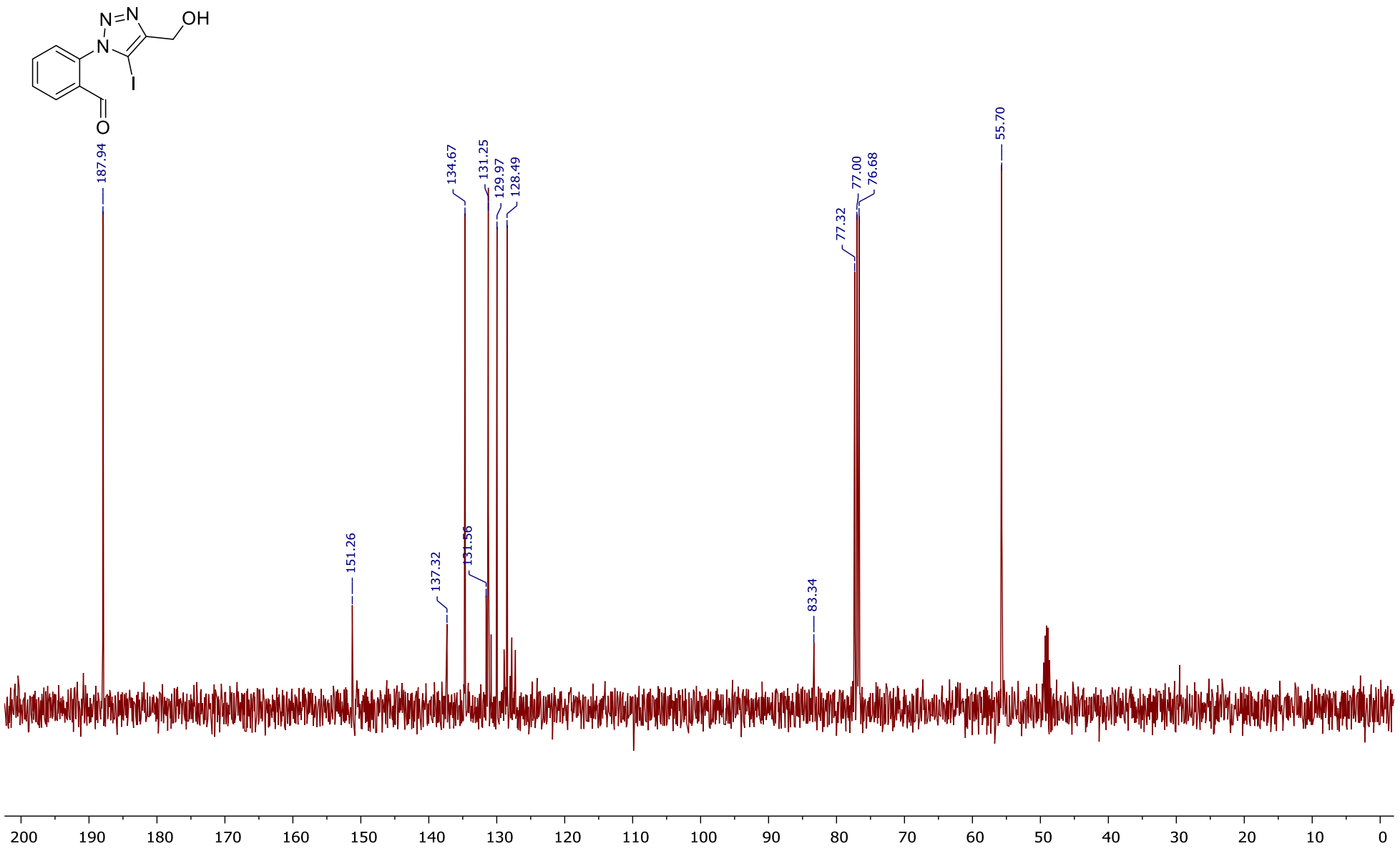
2-[4-(Hydroxymethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]benzaldehyde (1j)

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



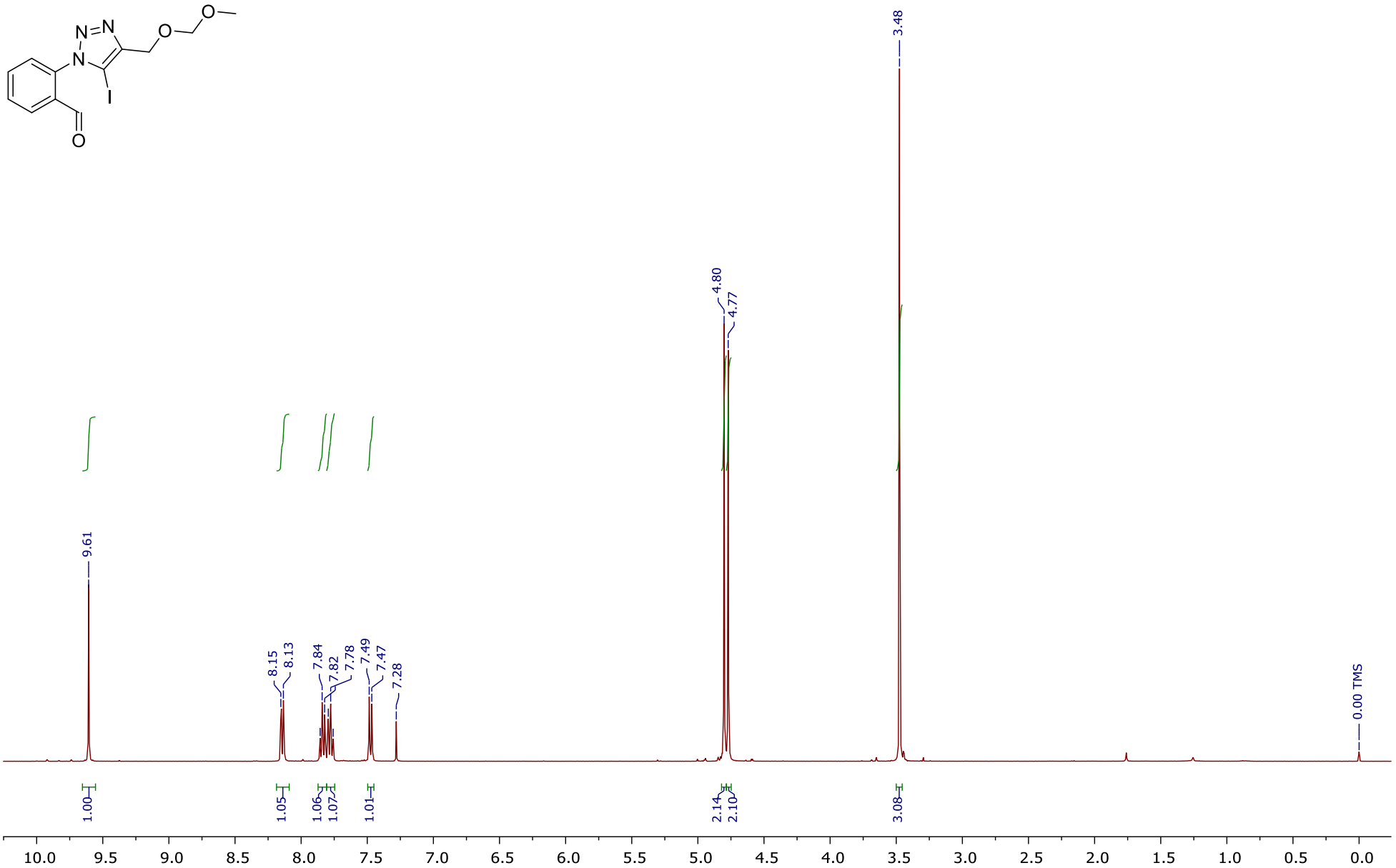
2-[4-(Hydroxymethyl)-5-iodo-1*H*-1,2,3-triazol-1-yl]benzaldehyde (1j)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3/CD_3OD$)



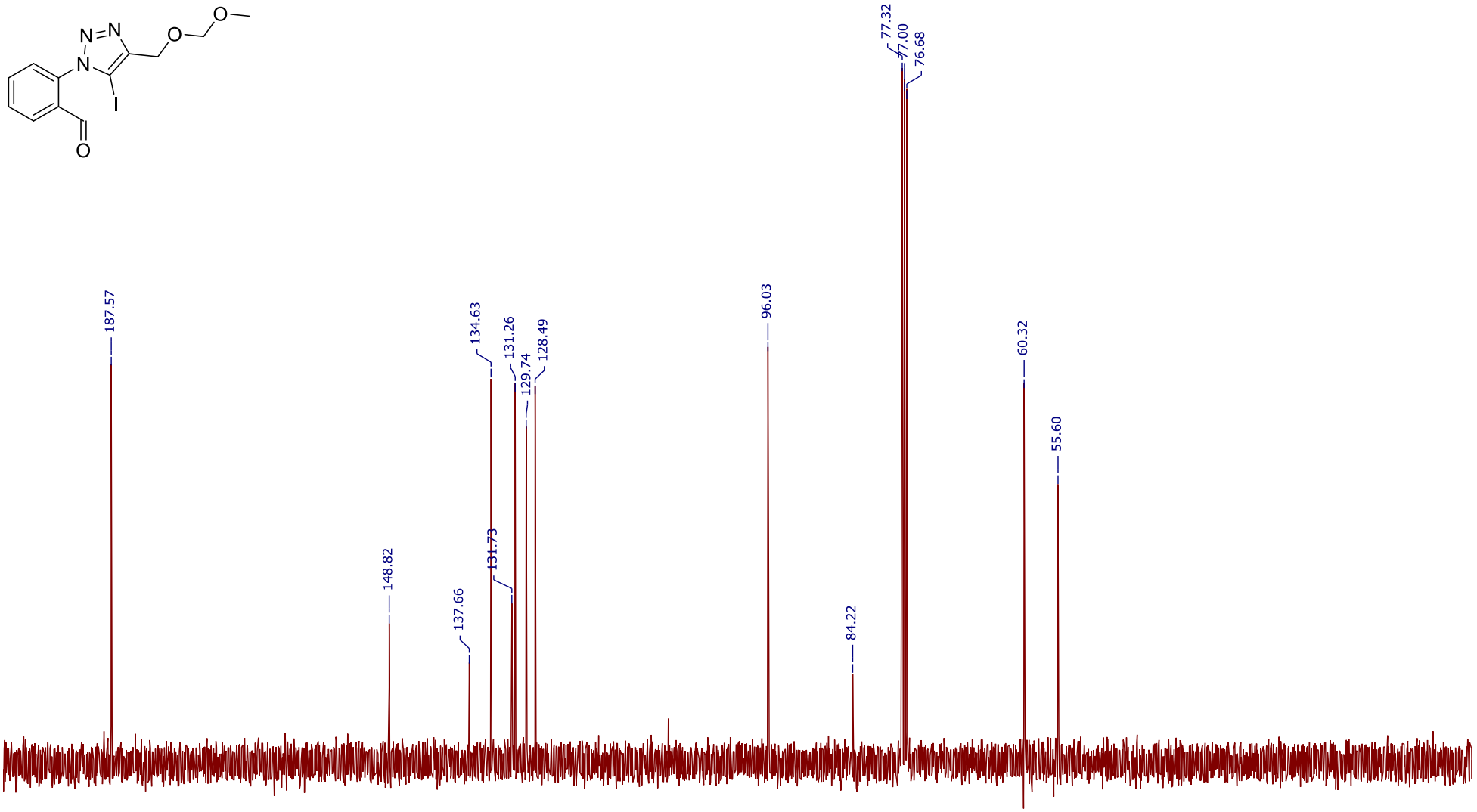
2-{5-Iodo-4-[(methoxymethoxy)methyl]-1*H*-1,2,3-triazol-1-yl}benzaldehyde (1k)

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



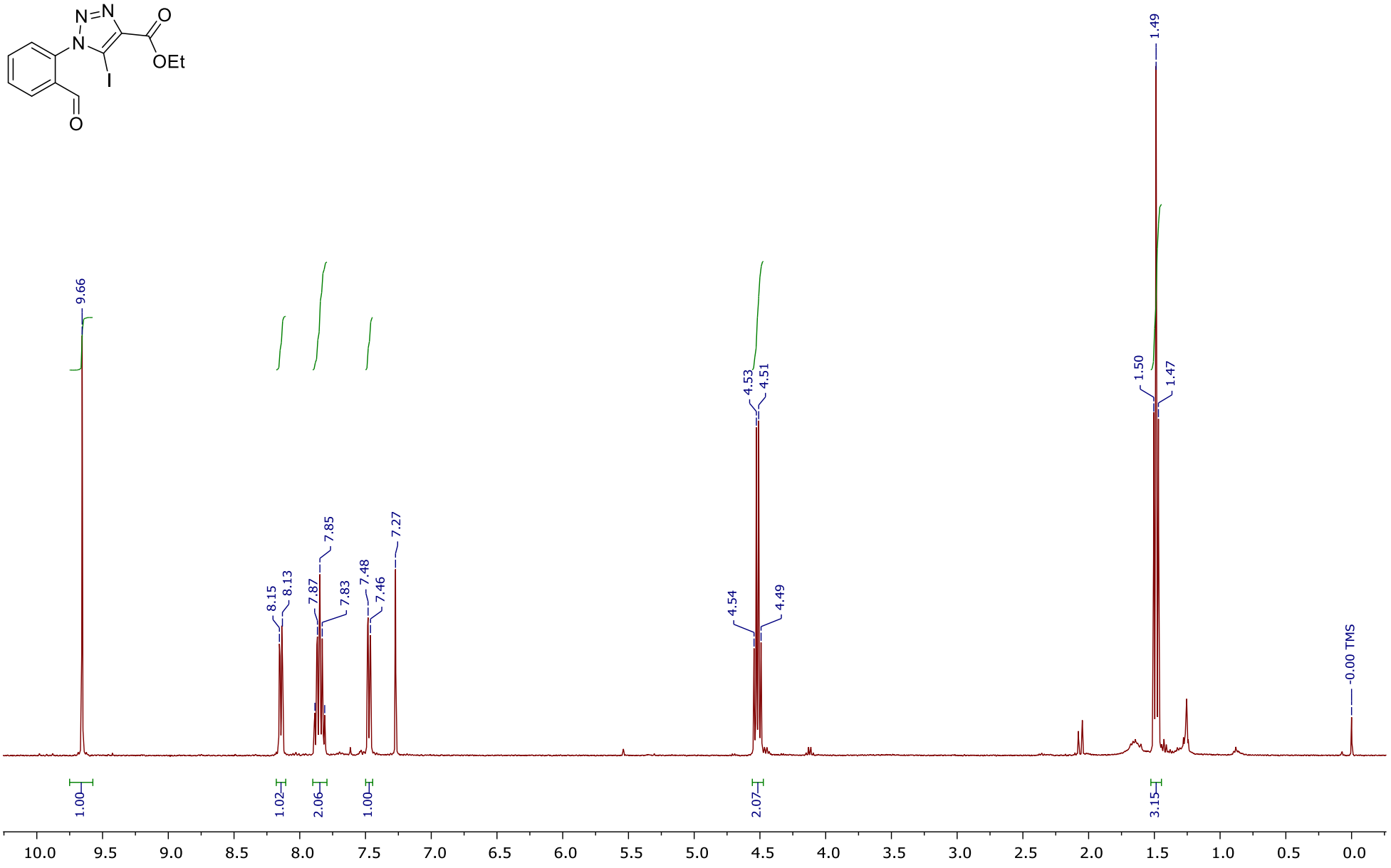
2-{5-Iodo-4-[(methoxymethoxy)methyl]-1*H*-1,2,3-triazol-1-yl}benzaldehyde (1k)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



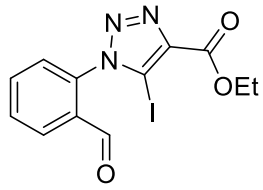
Ethyl 1-(2-formylphenyl)-5-iodo-1*H*-1,2,3-triazole-4-carboxylate (1l)

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



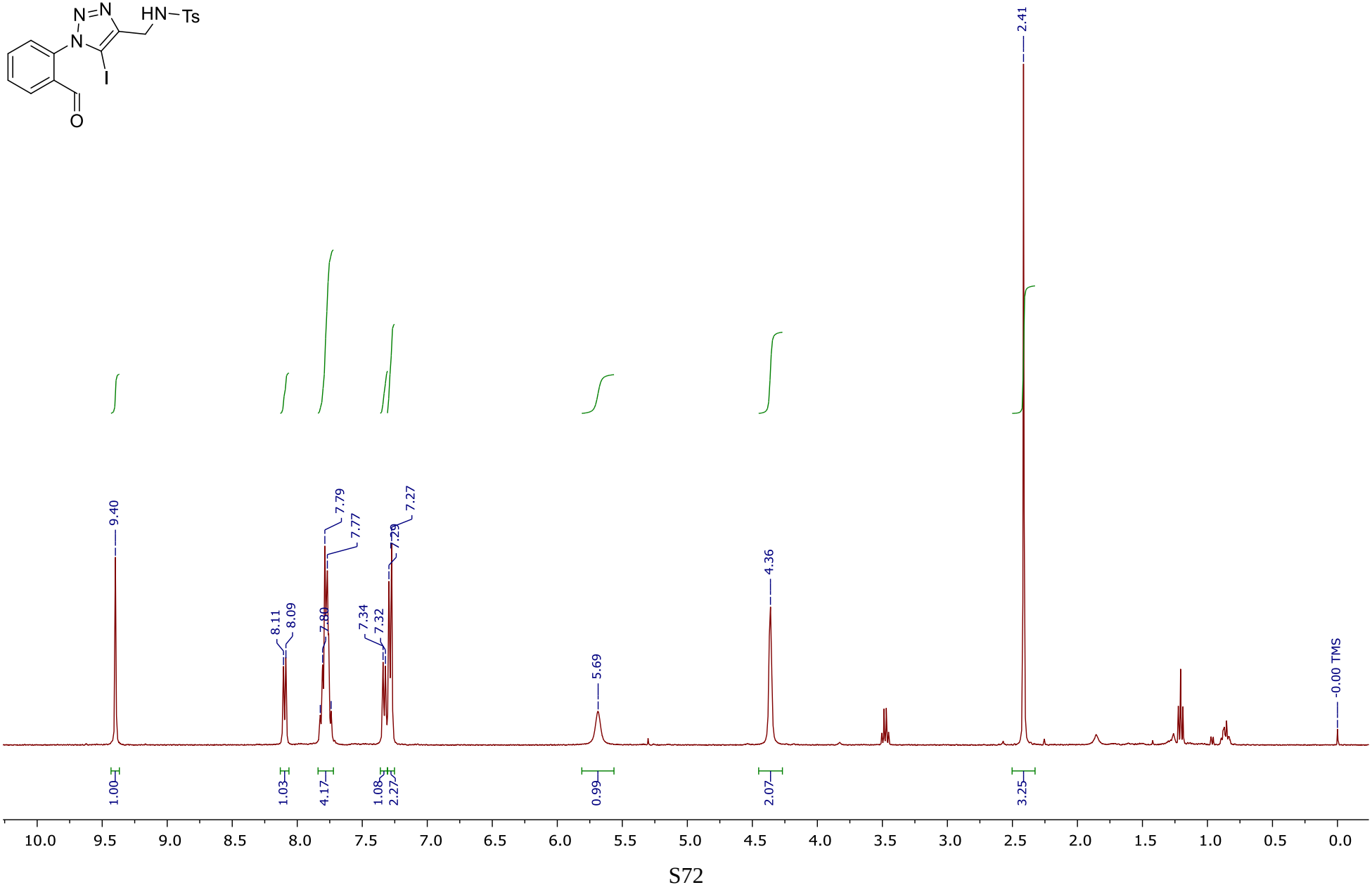
Ethyl 1-(2-formylphenyl)-5-iodo-1*H*-1,2,3-triazole-4-carboxylate (1l)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



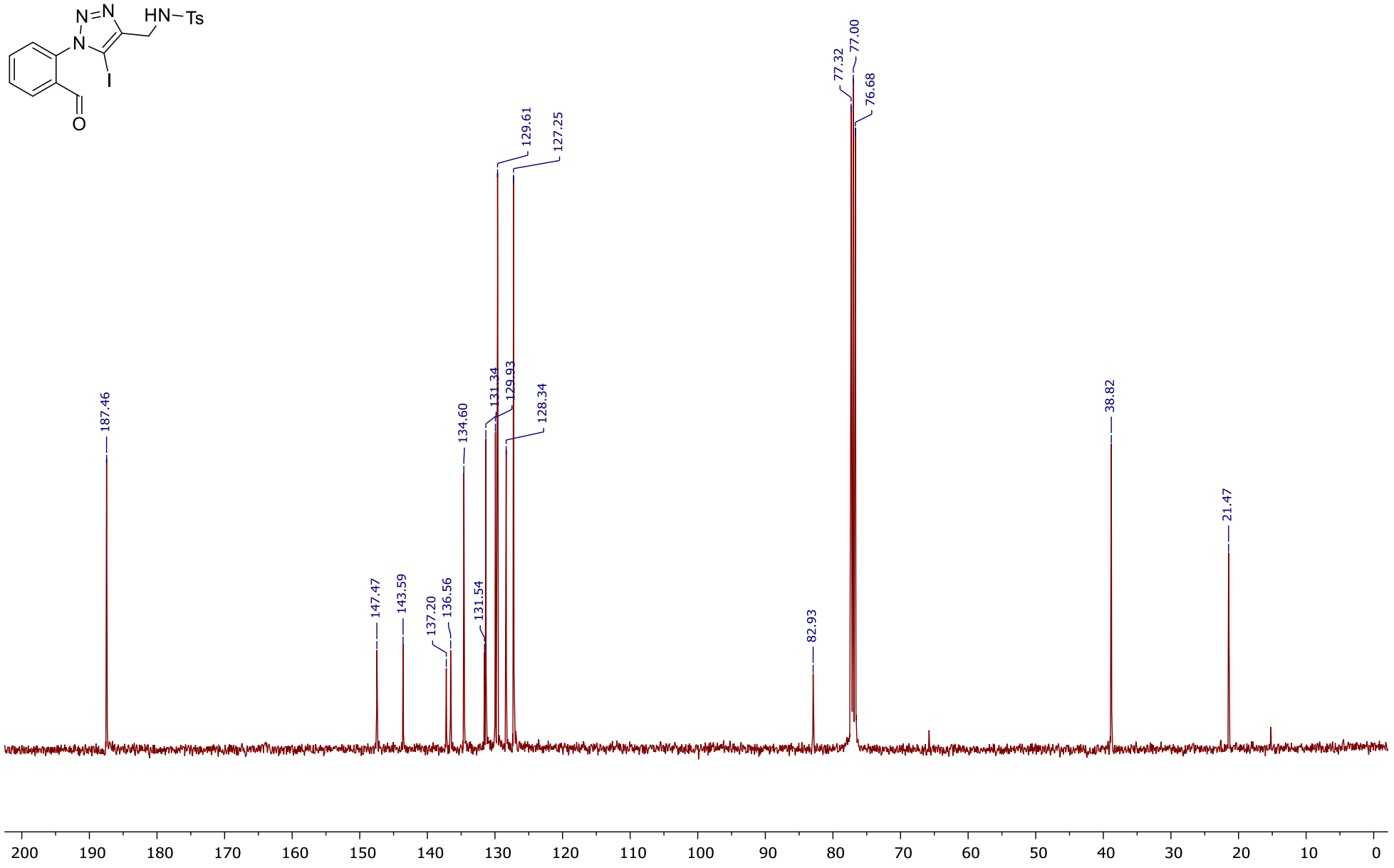
***N*-{[1-(2-Formylphenyl)-5-iodo-1*H*-1,2,3-triazol-4-yl]methyl}-4-methylbenzenesulfonamide (1m)**

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



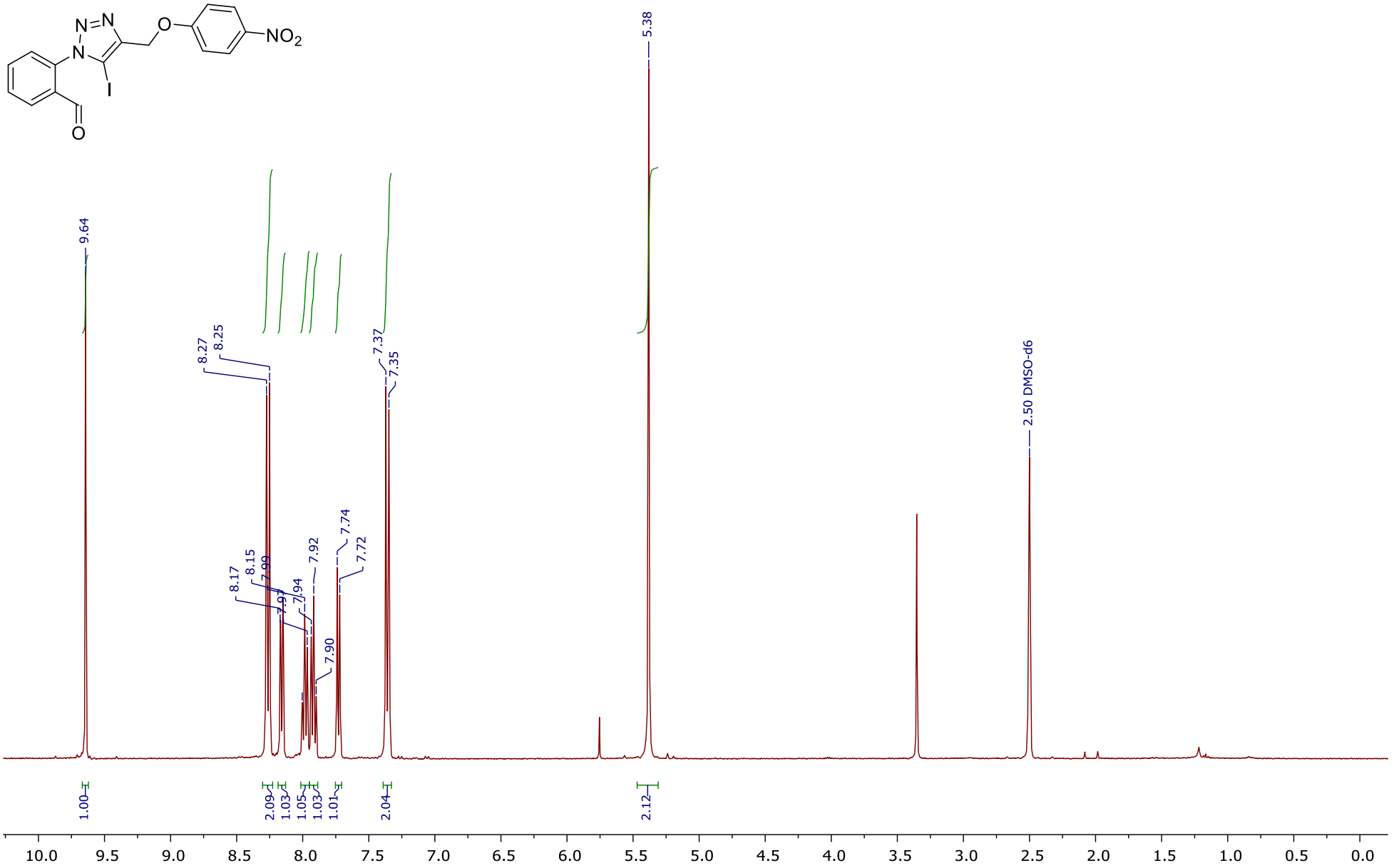
***N*-{[1-(2-Formylphenyl)-5-iodo-1*H*-1,2,3-triazol-4-yl]methyl}-4-methylbenzenesulfonamide (1m)**

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



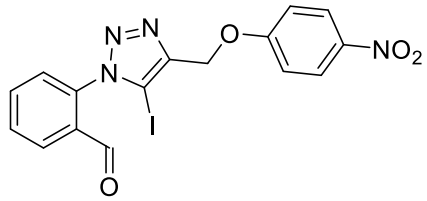
2-{5-Iodo-4-[(4-nitrophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}benzaldehyde (1n)

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



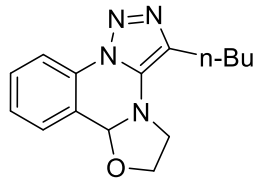
2-{5-Iodo-4-[(4-nitrophenoxy)methyl]-1*H*-1,2,3-triazol-1-yl}benzaldehyde (1n)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, DMSO-d_6)



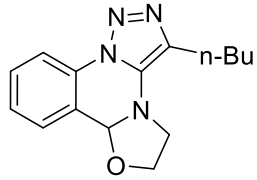
3-Butyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2a)

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



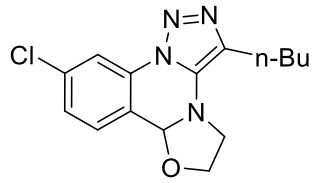
3-Butyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2a)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



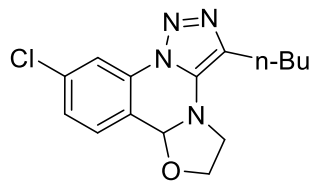
3-Butyl-10-chloro-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2b)

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



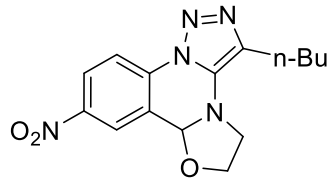
3-Butyl-10-chloro-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2b)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



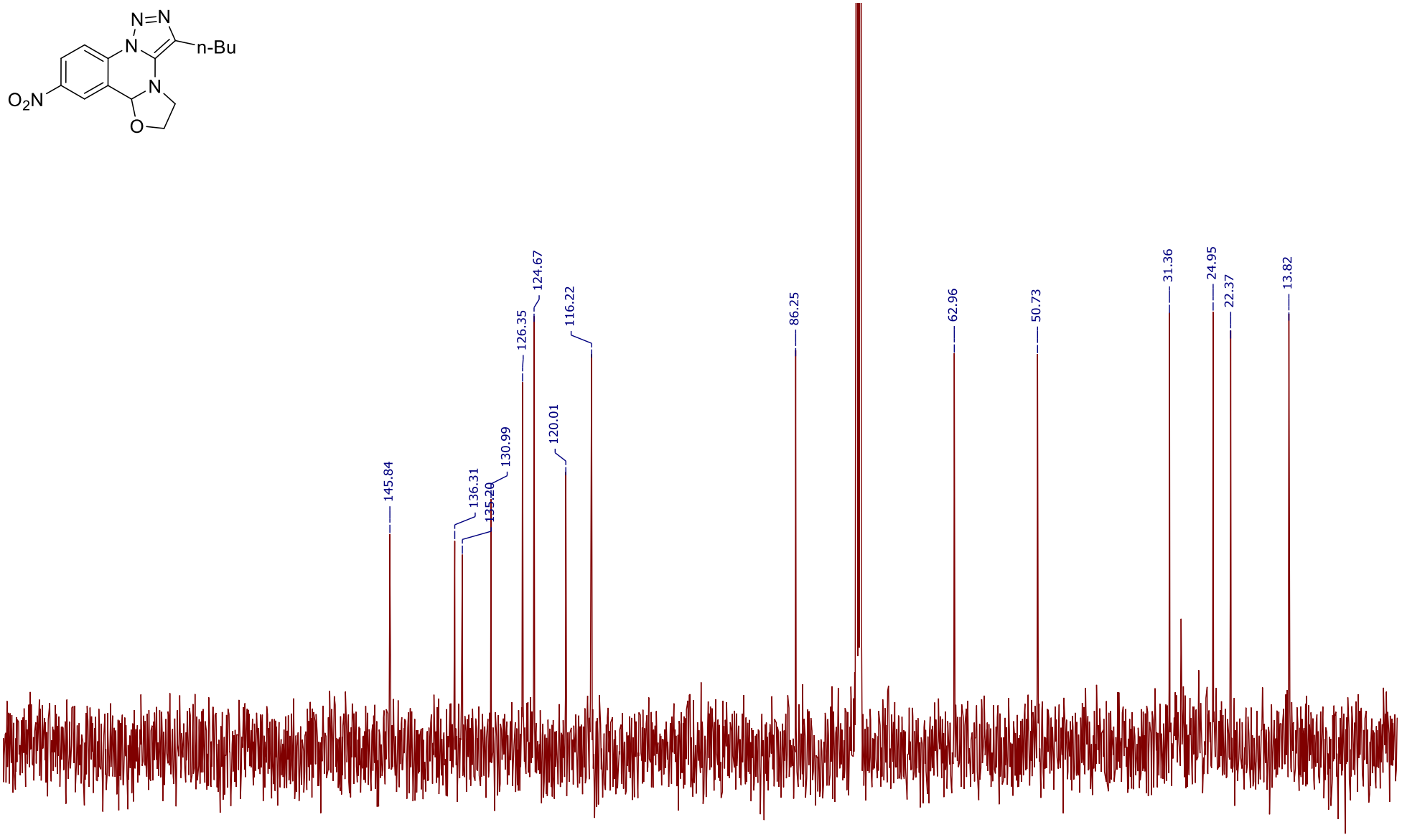
3-Butyl-9-nitro-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2c)

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



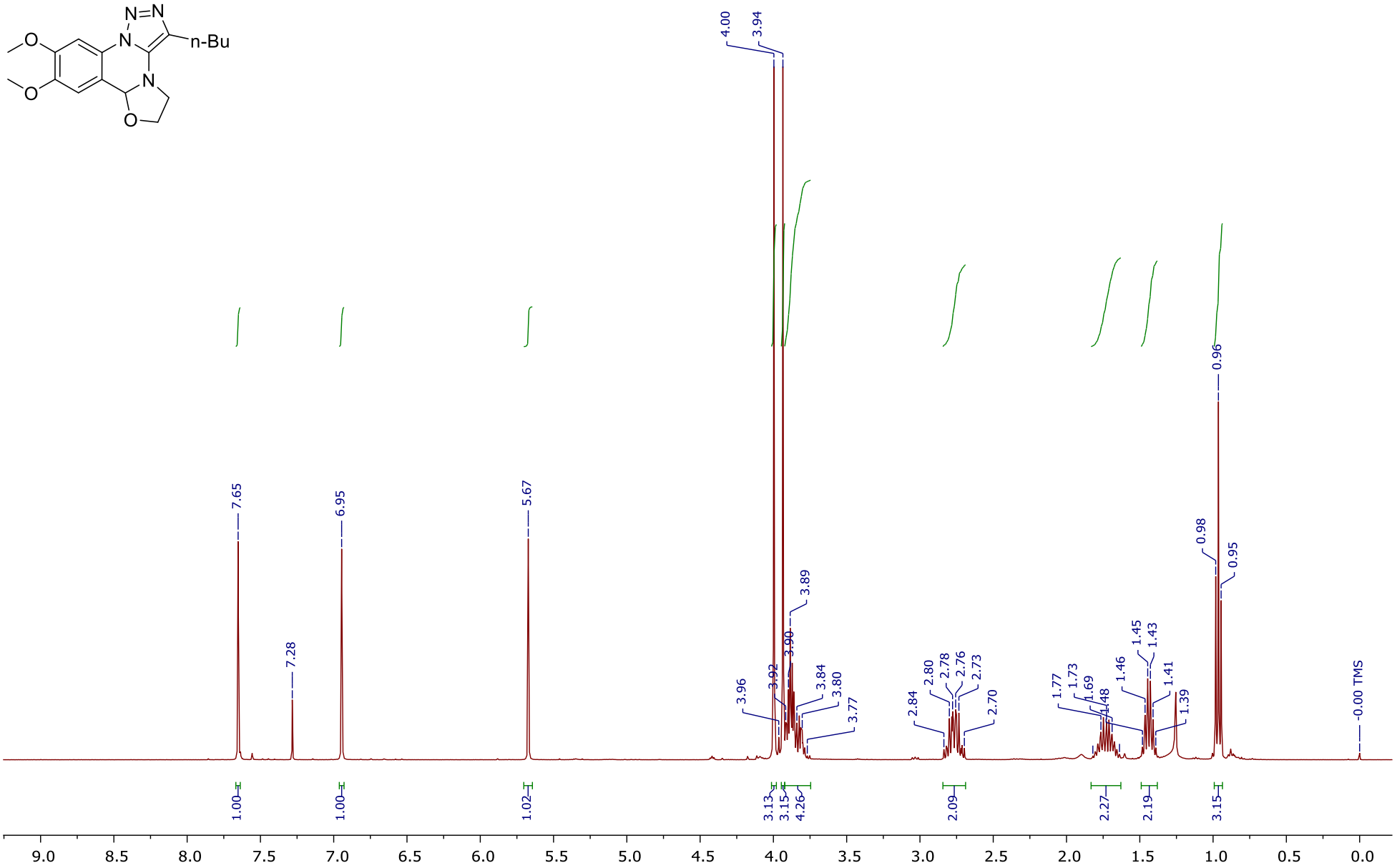
3-Butyl-9-nitro-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2c)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



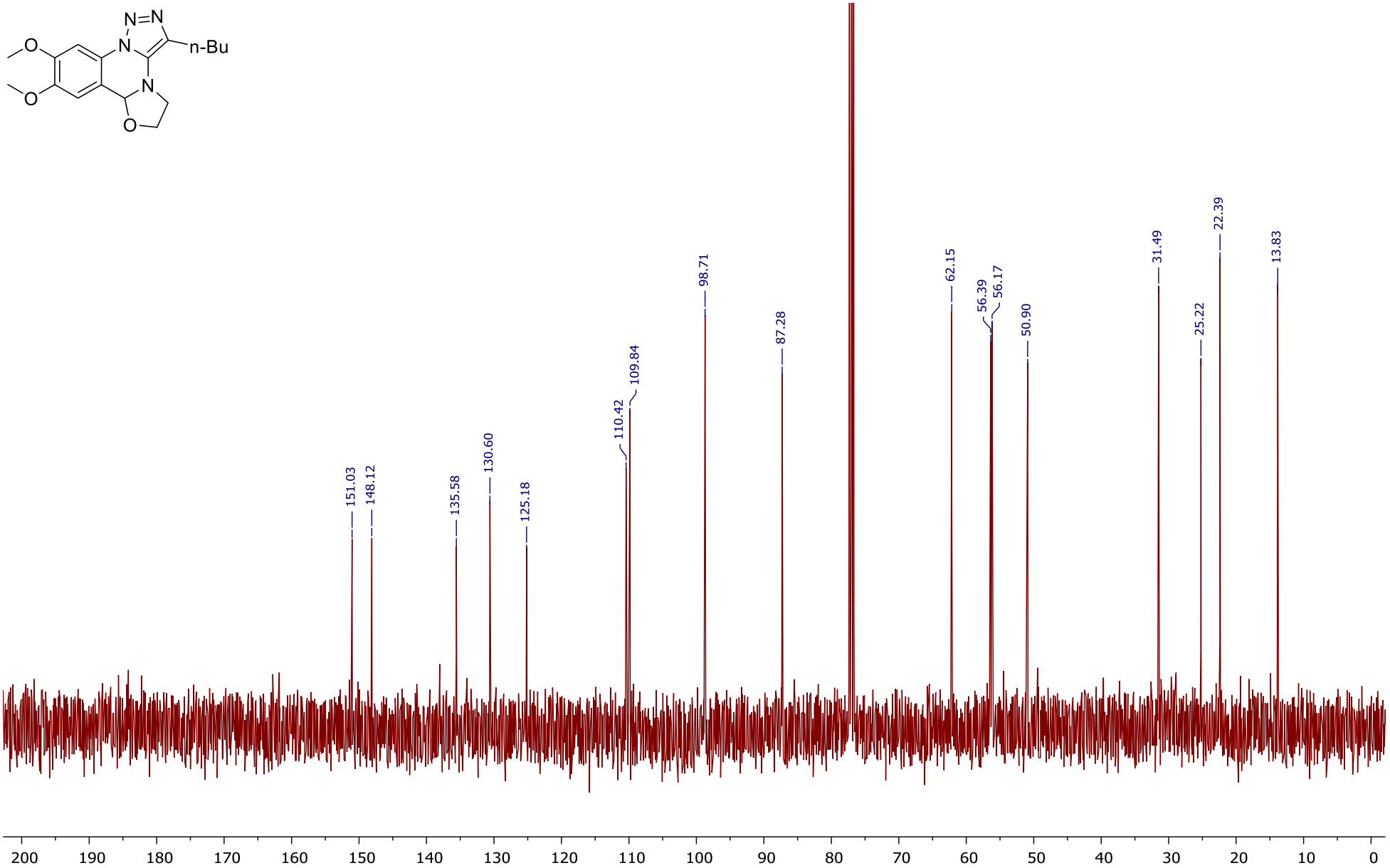
3-Butyl-9,10-dimethoxy-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2d)

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



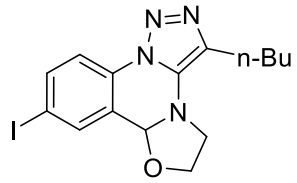
3-Butyl-9,10-dimethoxy-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2d)

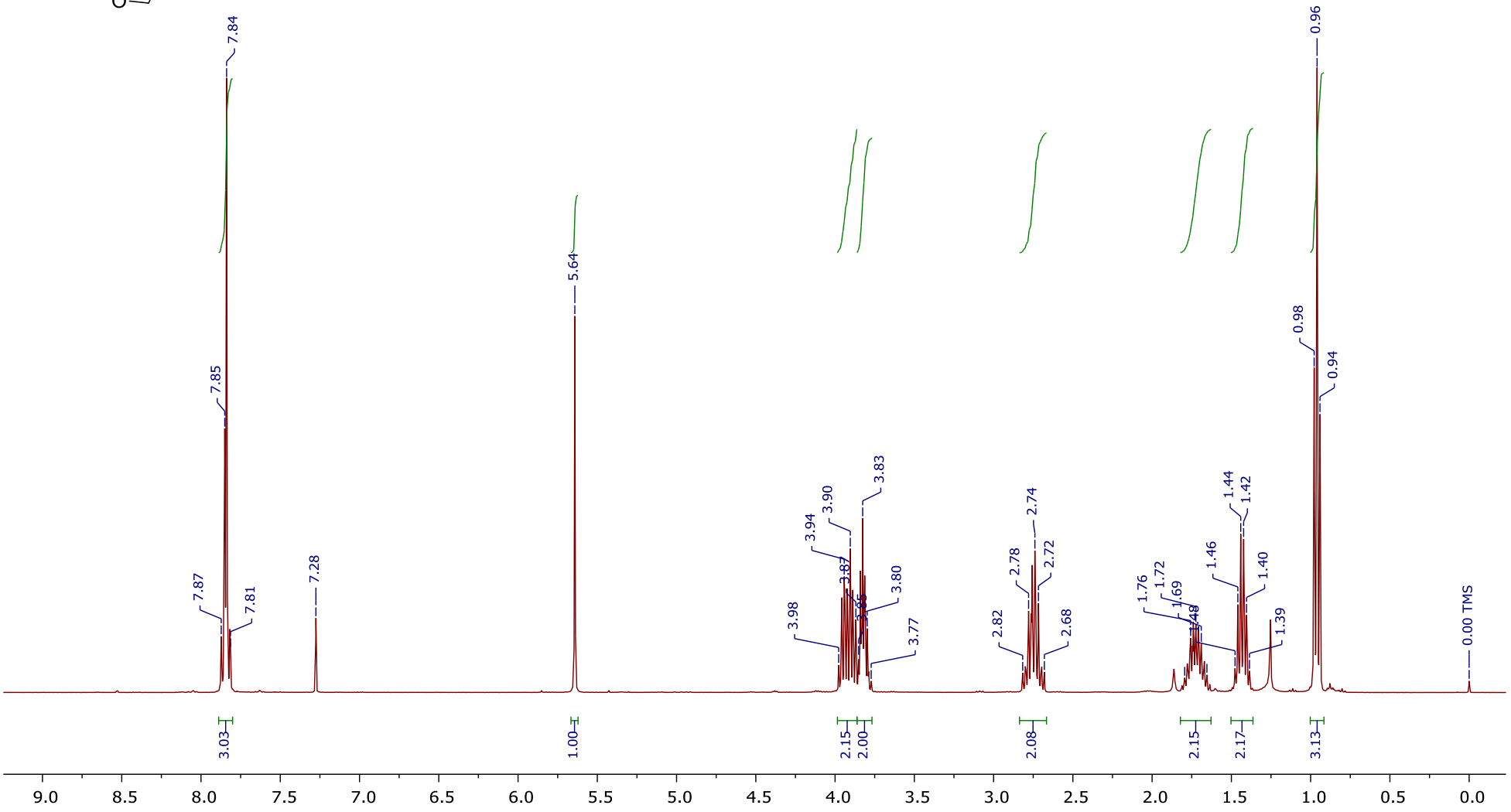
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



3-Butyl-9-iodo-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2e)

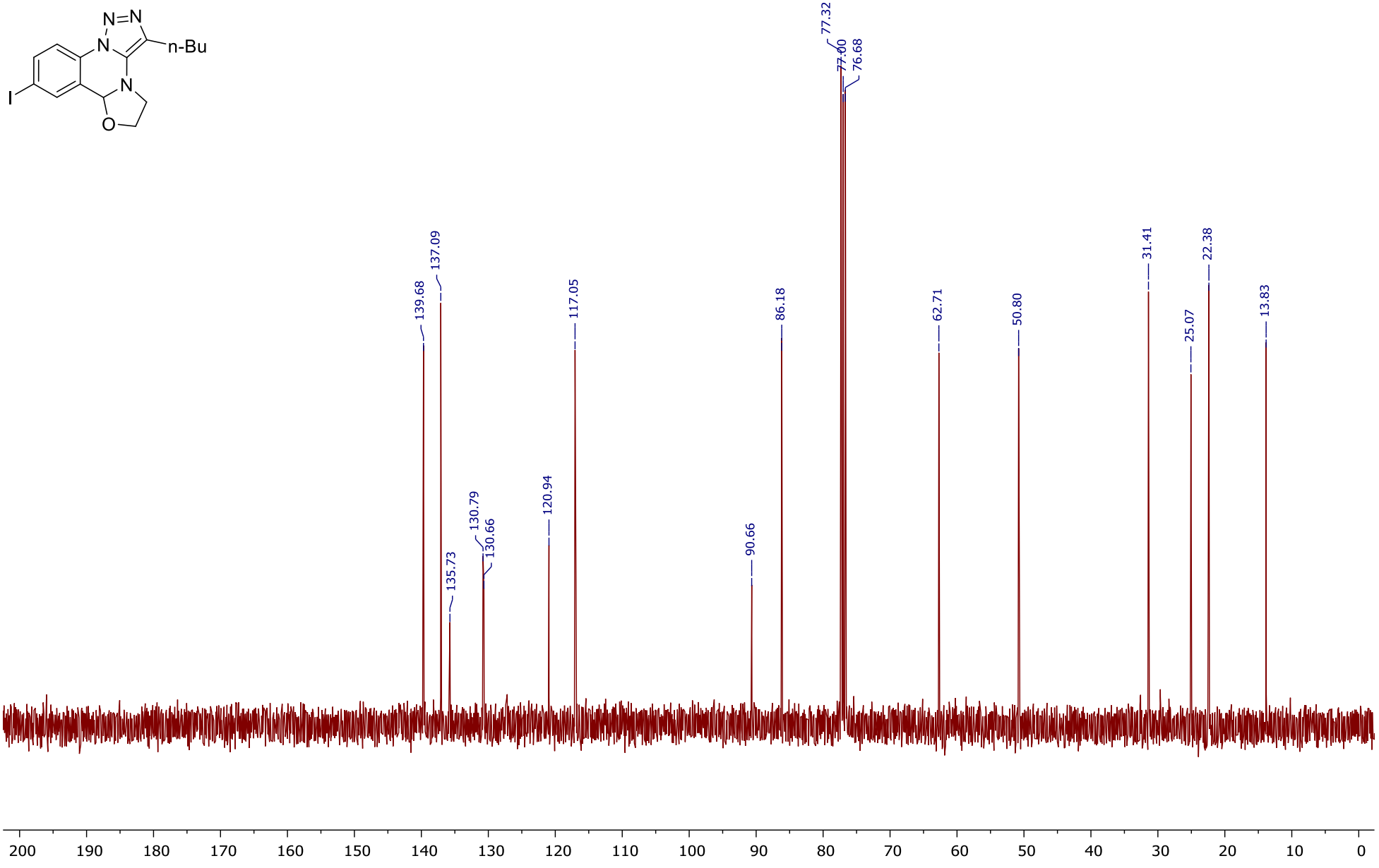
^{1}H NMR (400 MHz, $CDCl_3$)





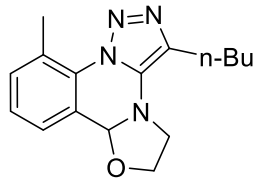
3-Butyl-9-iodo-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2e)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



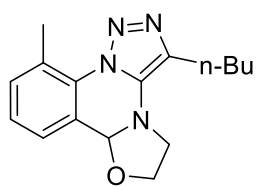
3-Butyl-11-methyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2f)

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



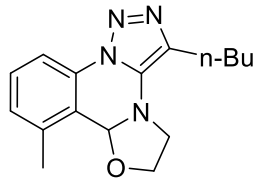
3-Butyl-11-methyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2f)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, DMSO-d_6)



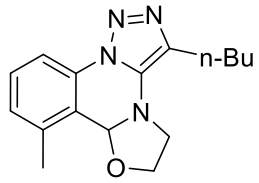
3-Butyl-8-methyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2g)

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



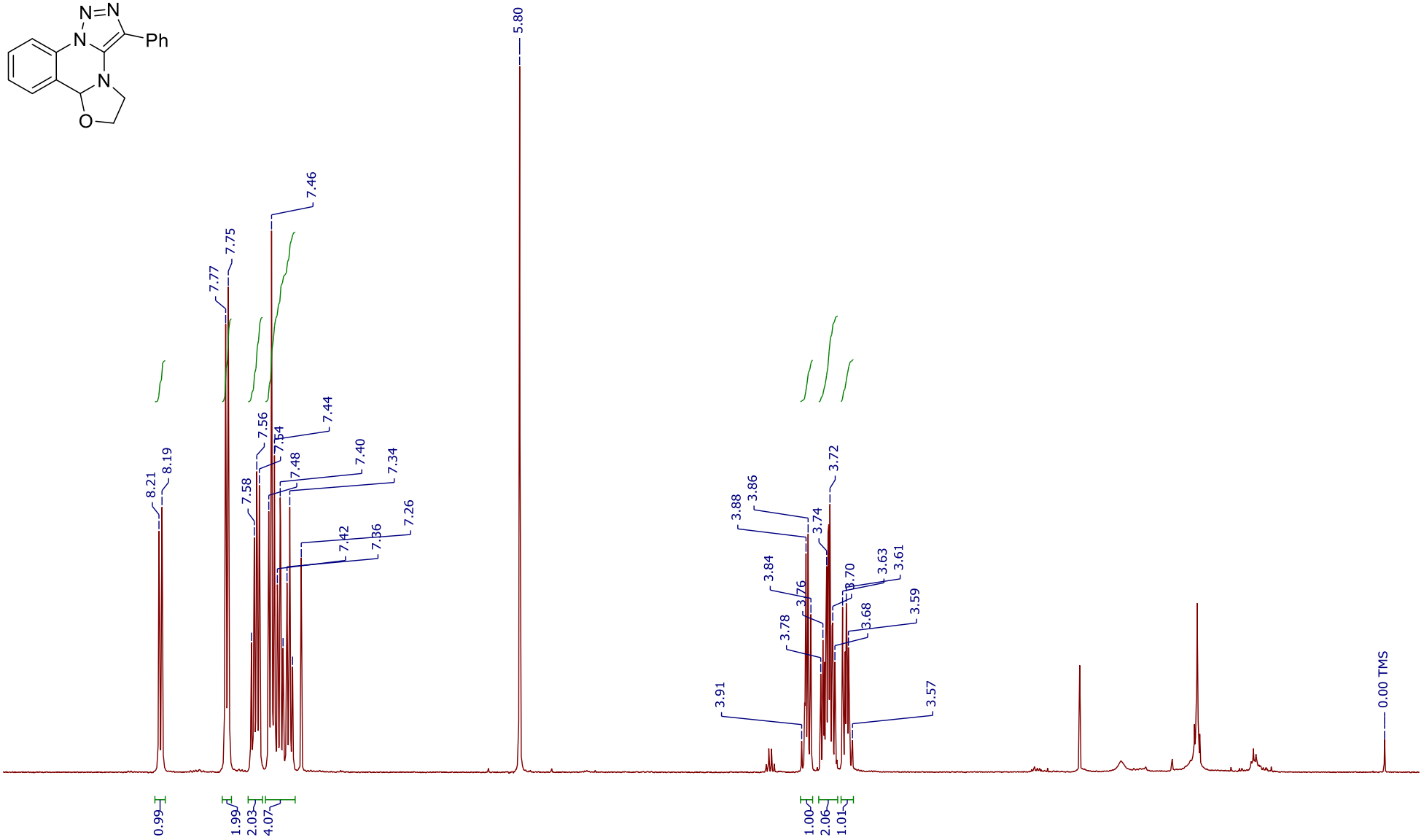
3-Butyl-8-methyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2g)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



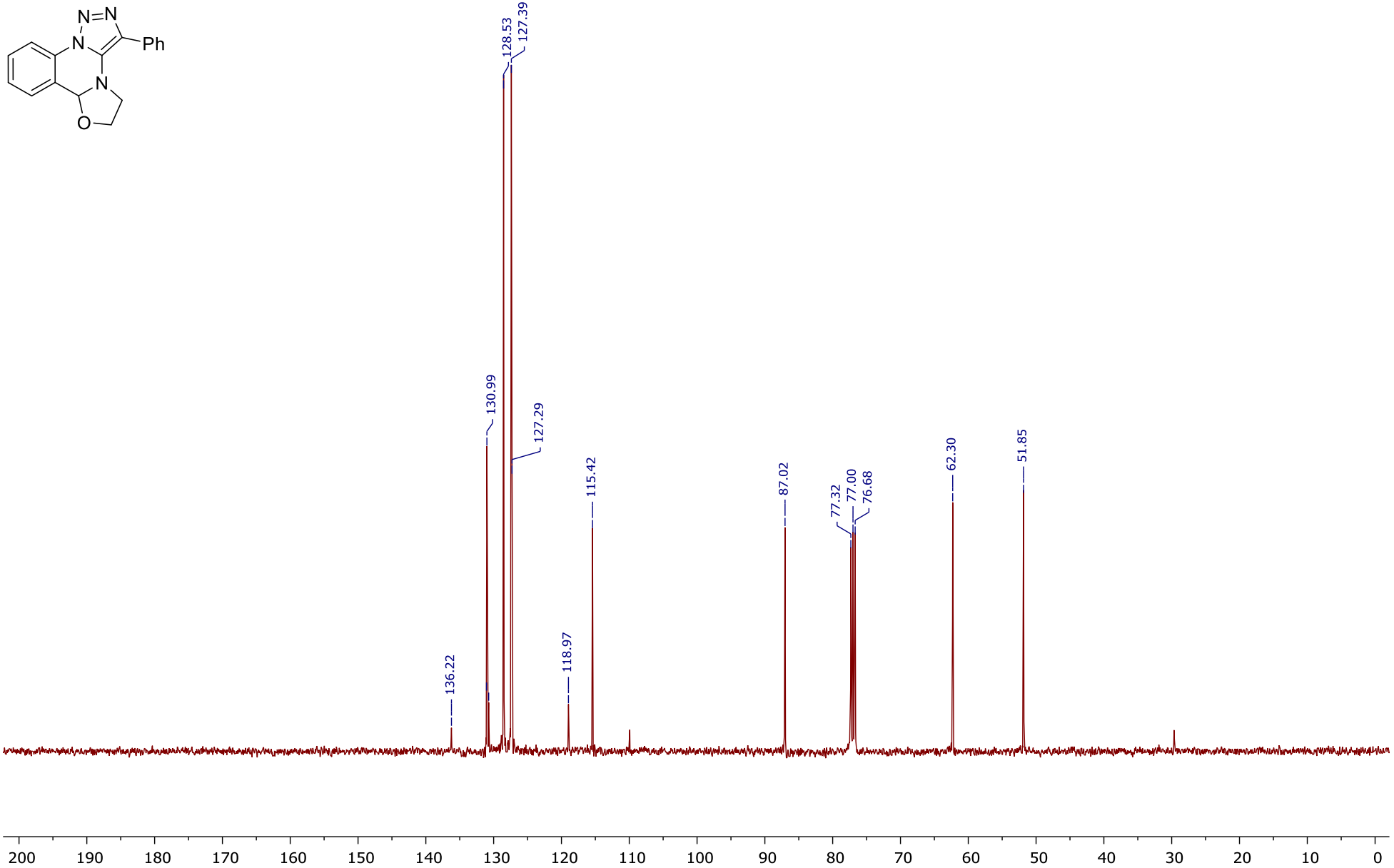
3-Phenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2h)

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



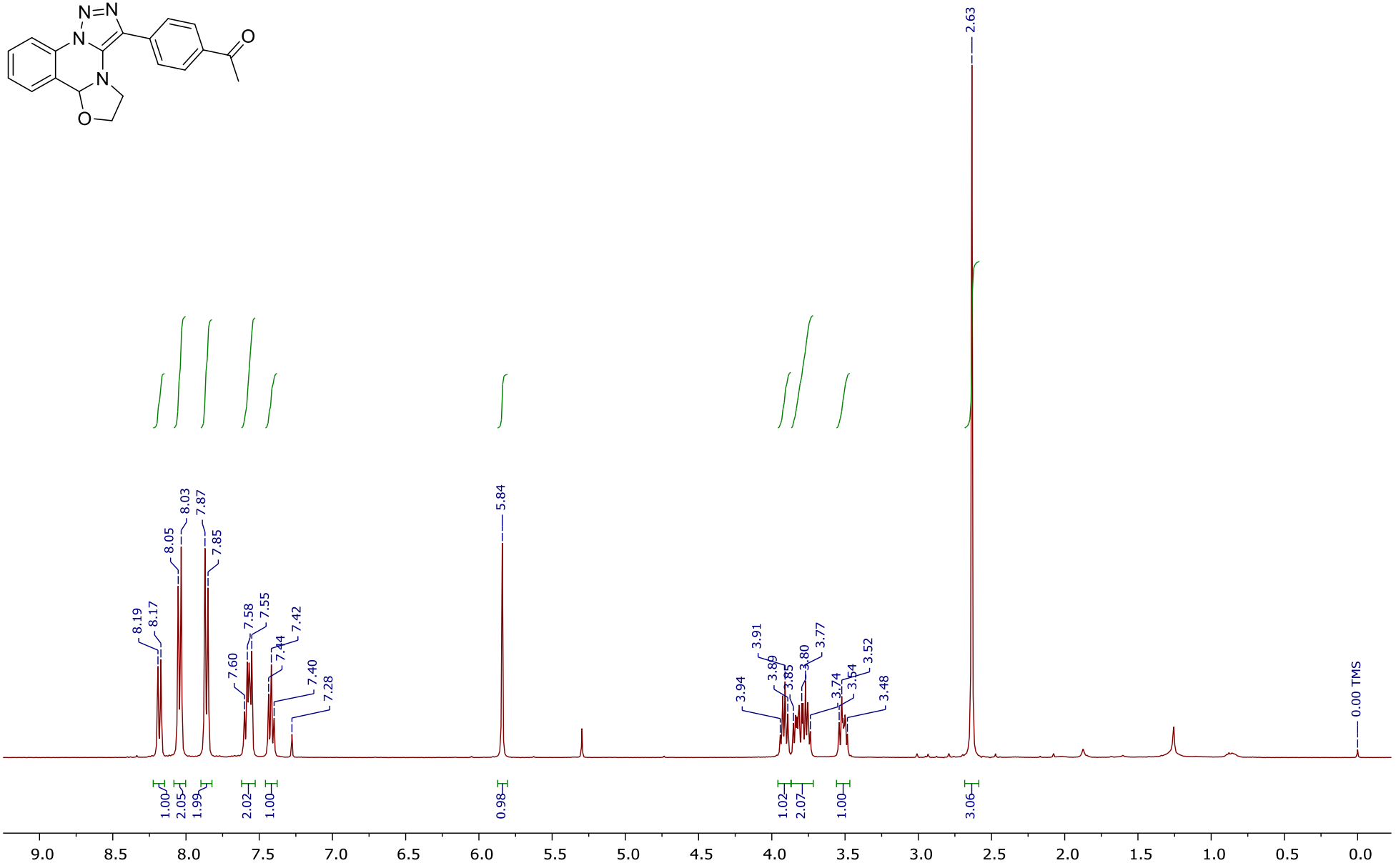
3-Phenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2h)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



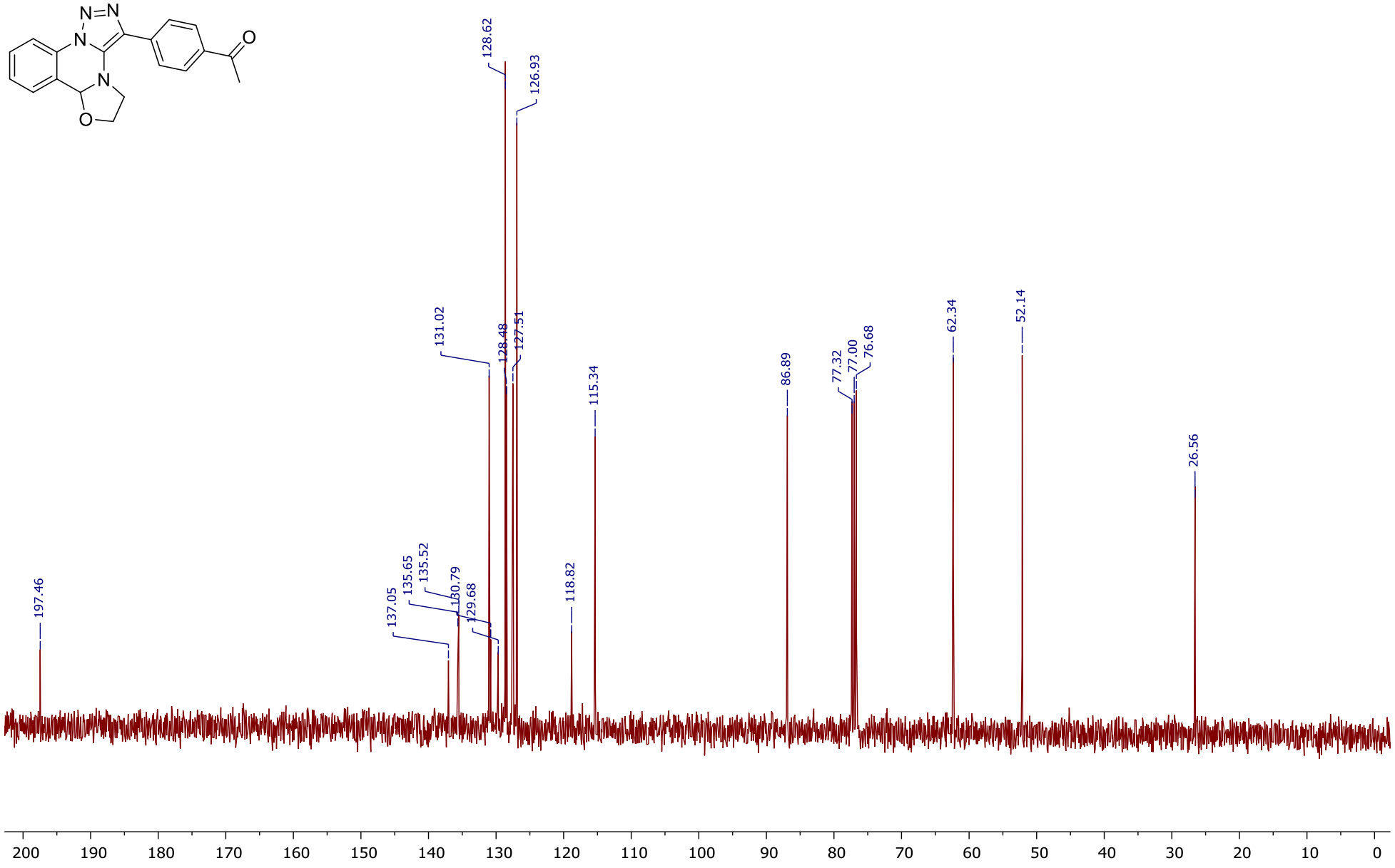
1-[4-(5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-yl)phenyl]ethanone (2i)

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



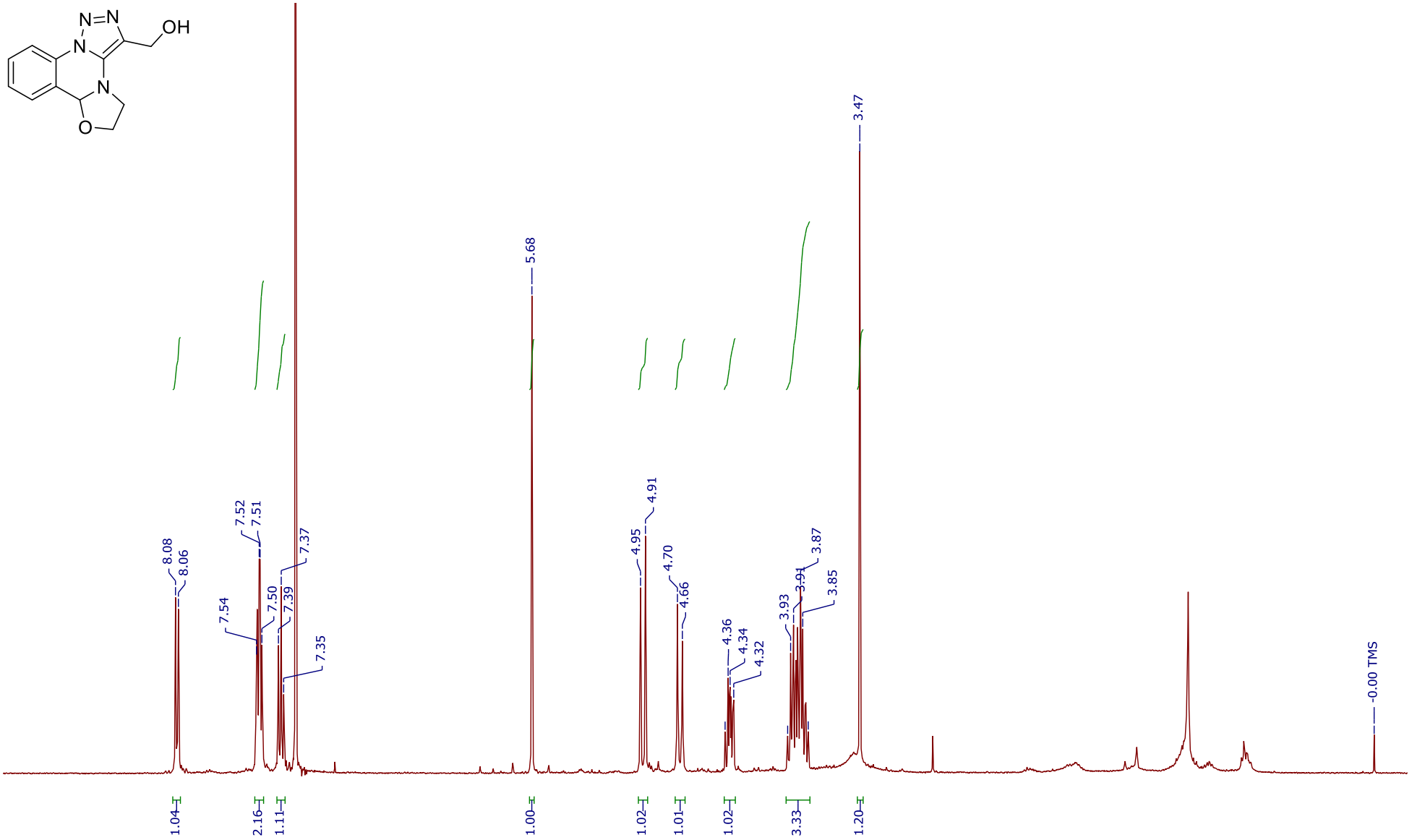
1-[4-(5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-yl)phenyl]ethanone (2i)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



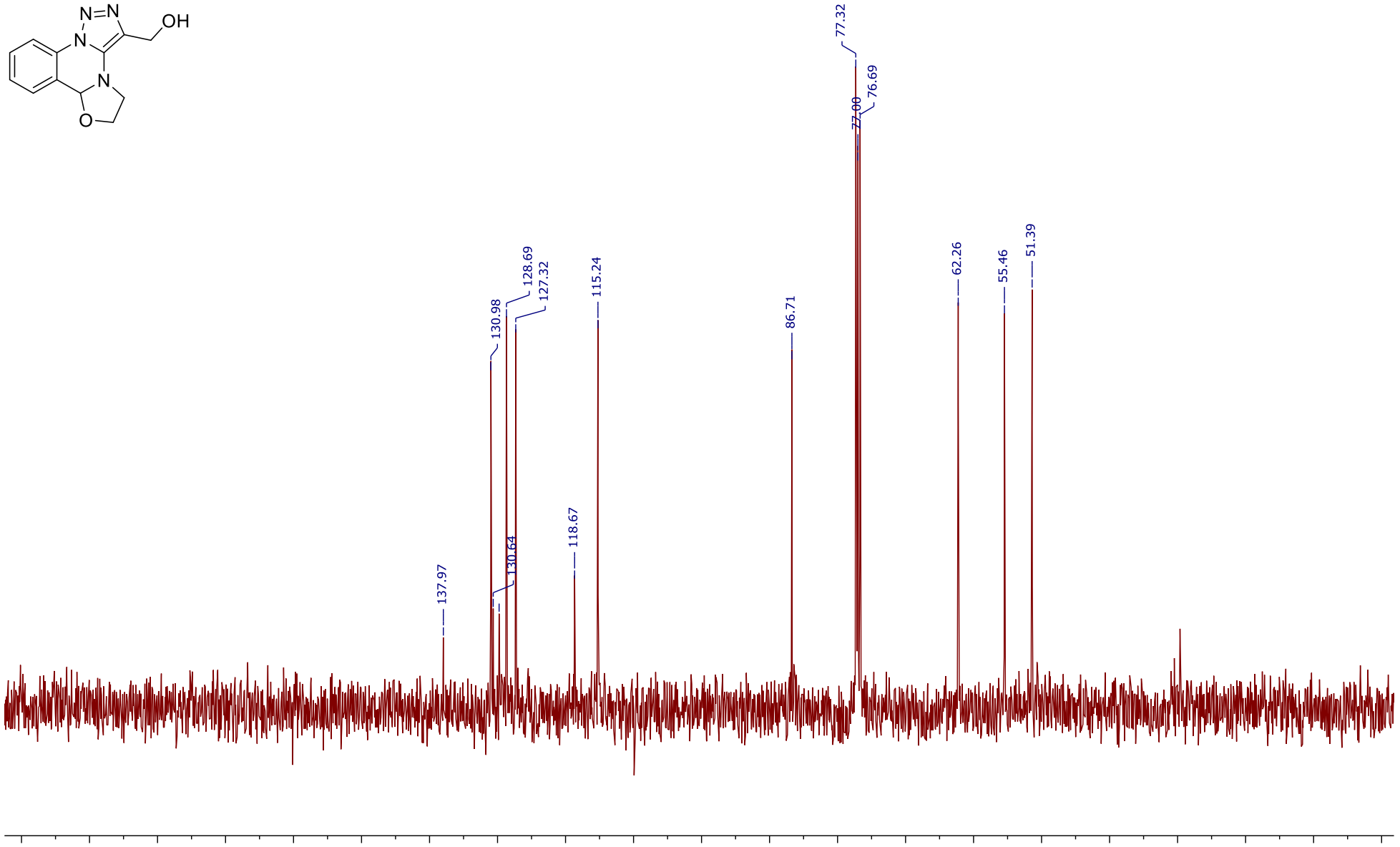
5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-ylmethanol (2j)

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



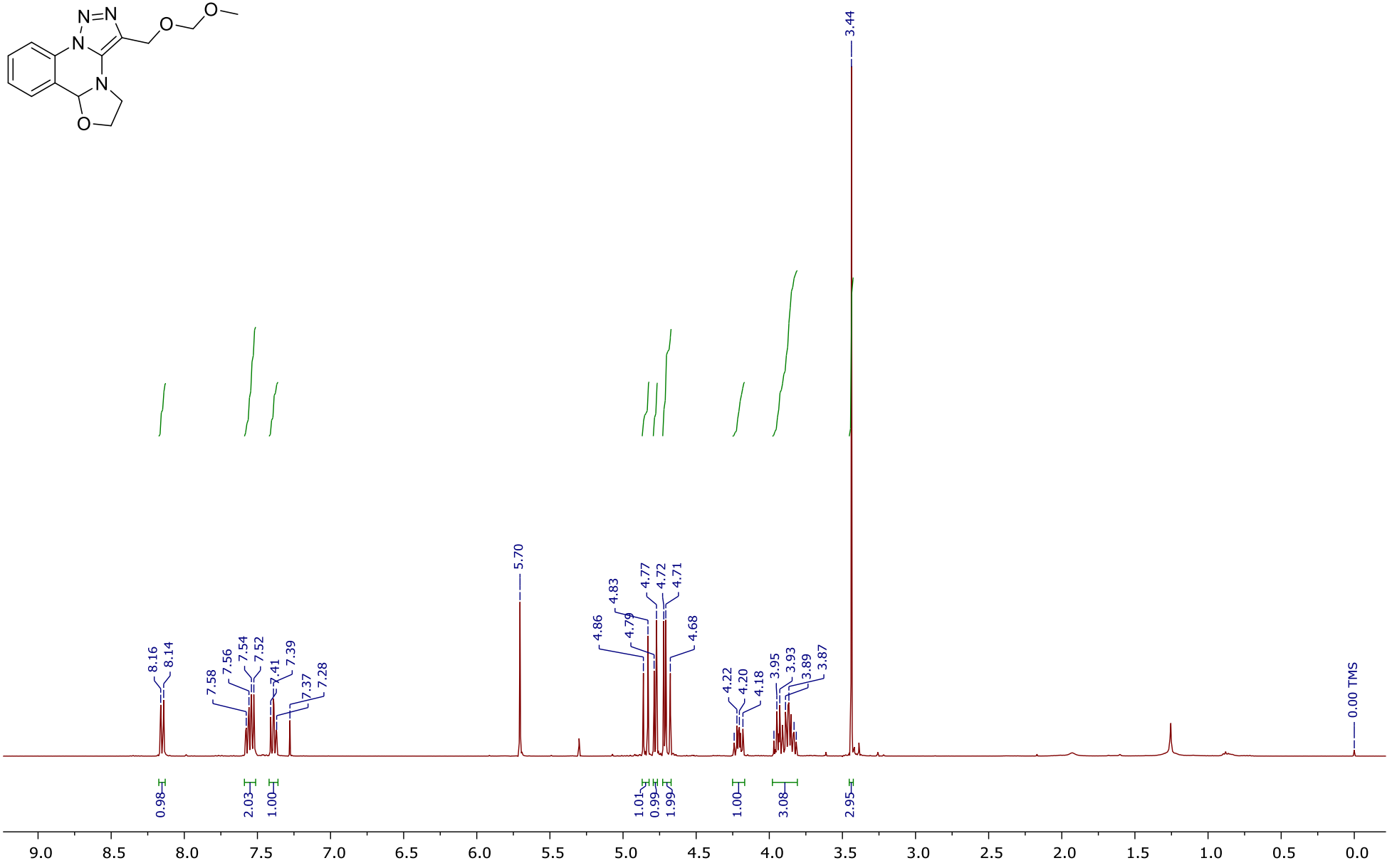
5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-ylmethanol (2j)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



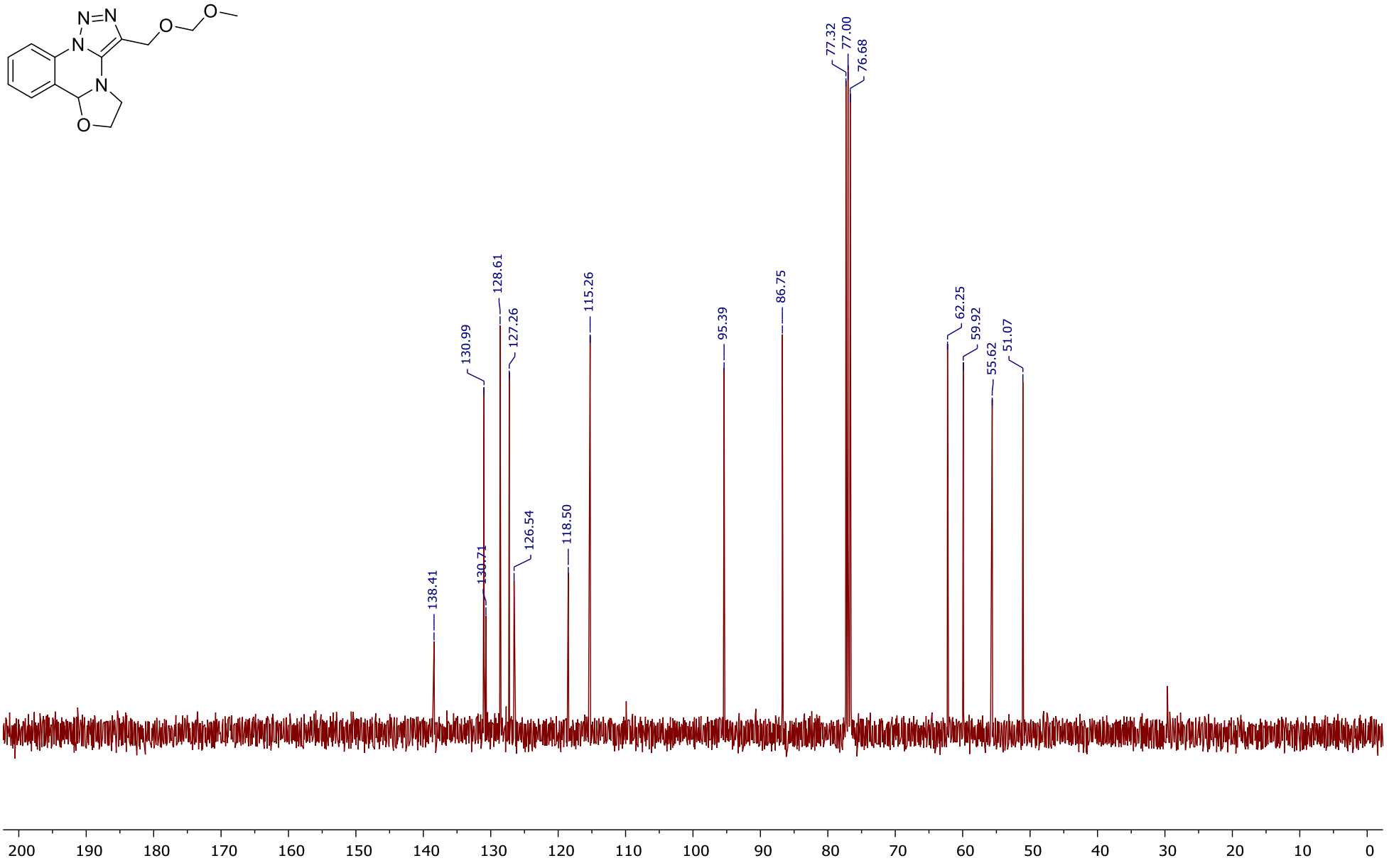
3-[(Methoxymethoxy)methyl]-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2k)

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



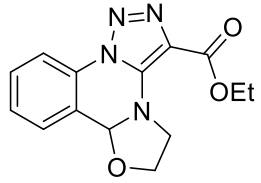
3-[(Methoxymethoxy)methyl]-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2k)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



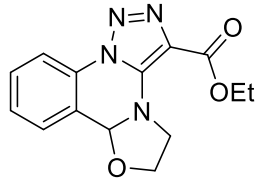
Ethyl 5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline-3-carboxylate (2l)

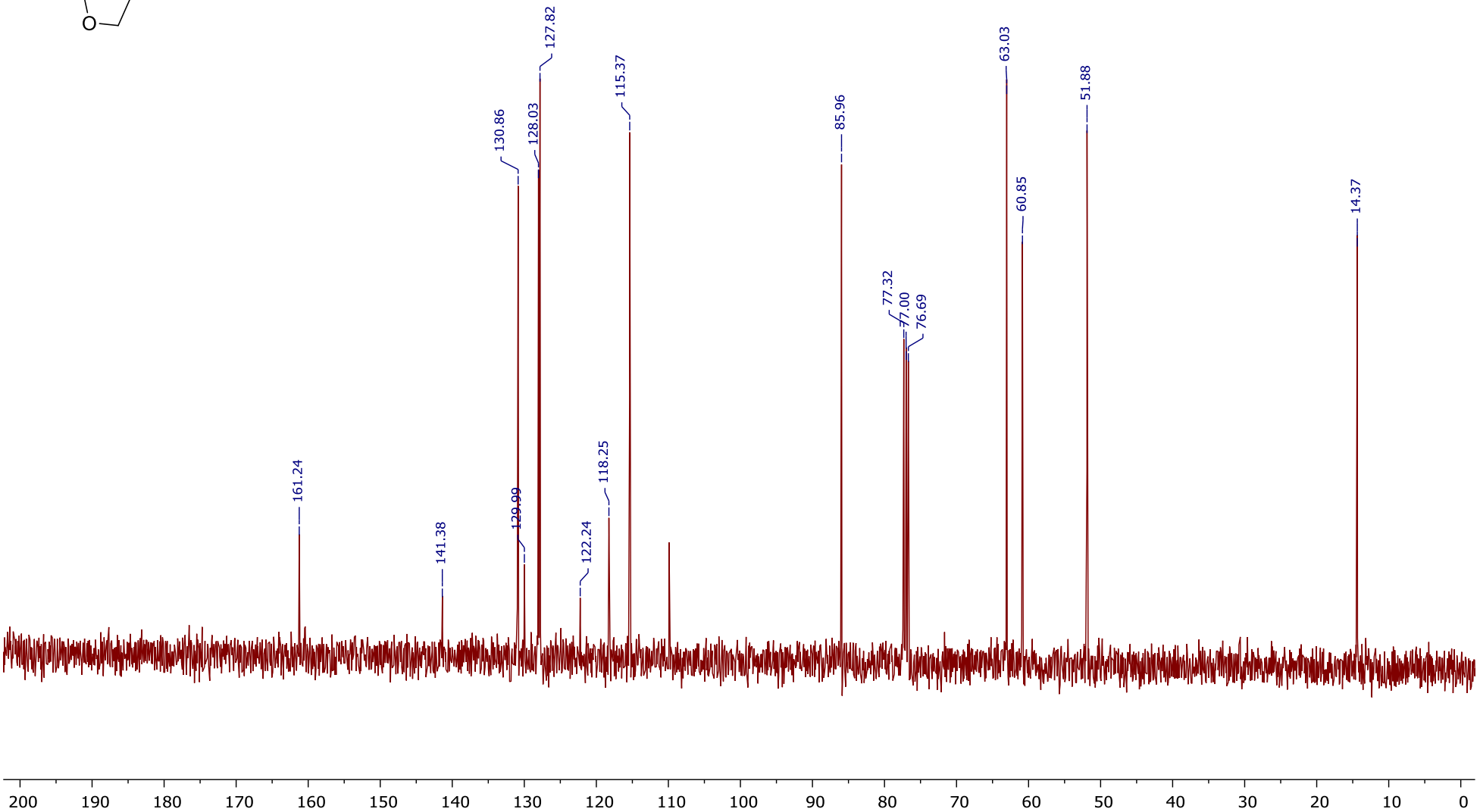
^{1}H NMR (400 MHz, $CDCl_3$)



Ethyl 5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline-3-carboxylate (2l)

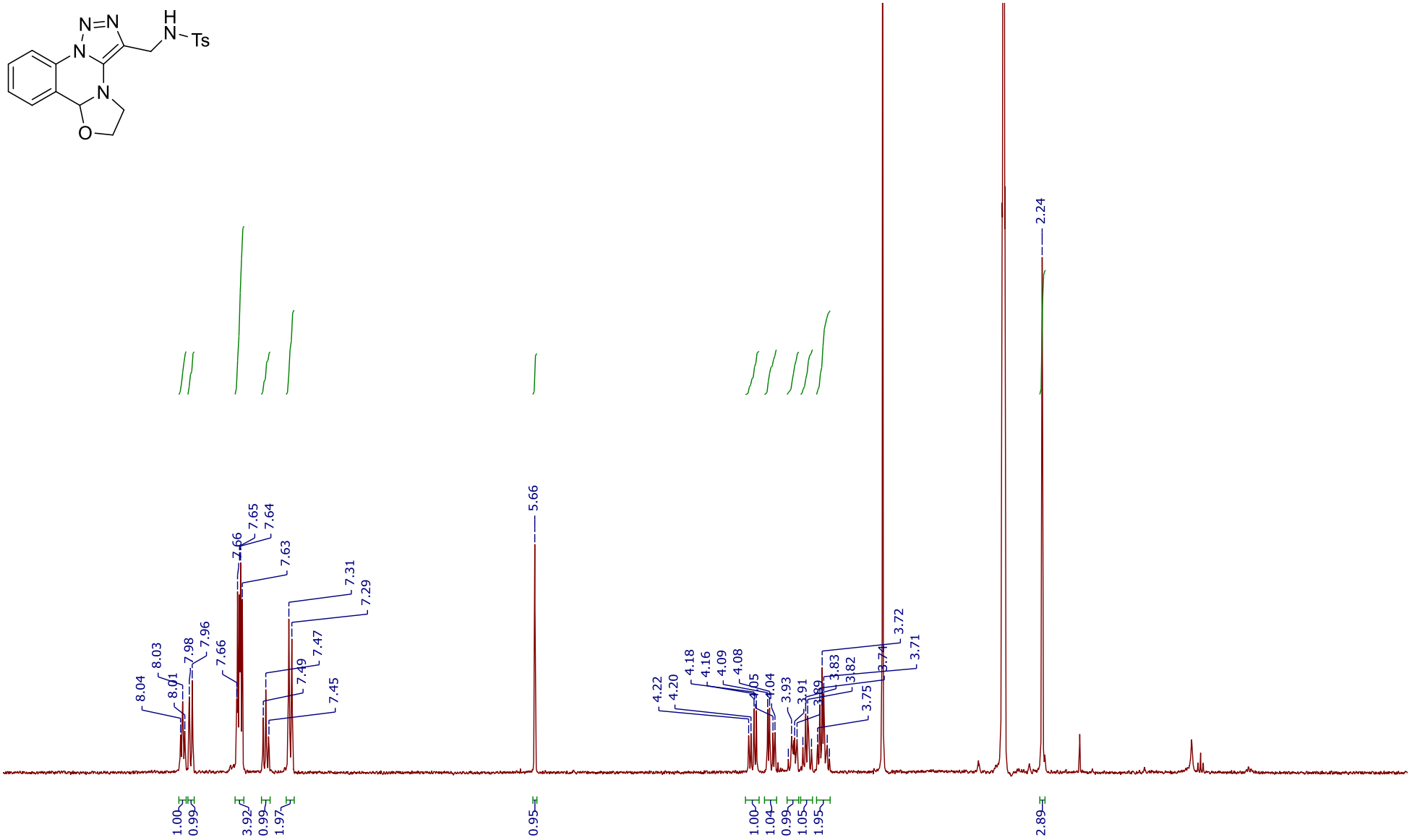
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)





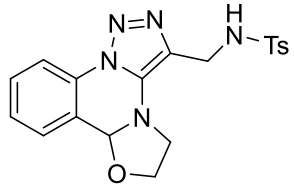
***N*-(5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-ylmethyl)-4-methylbenzenesulfonamide (2m)**

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



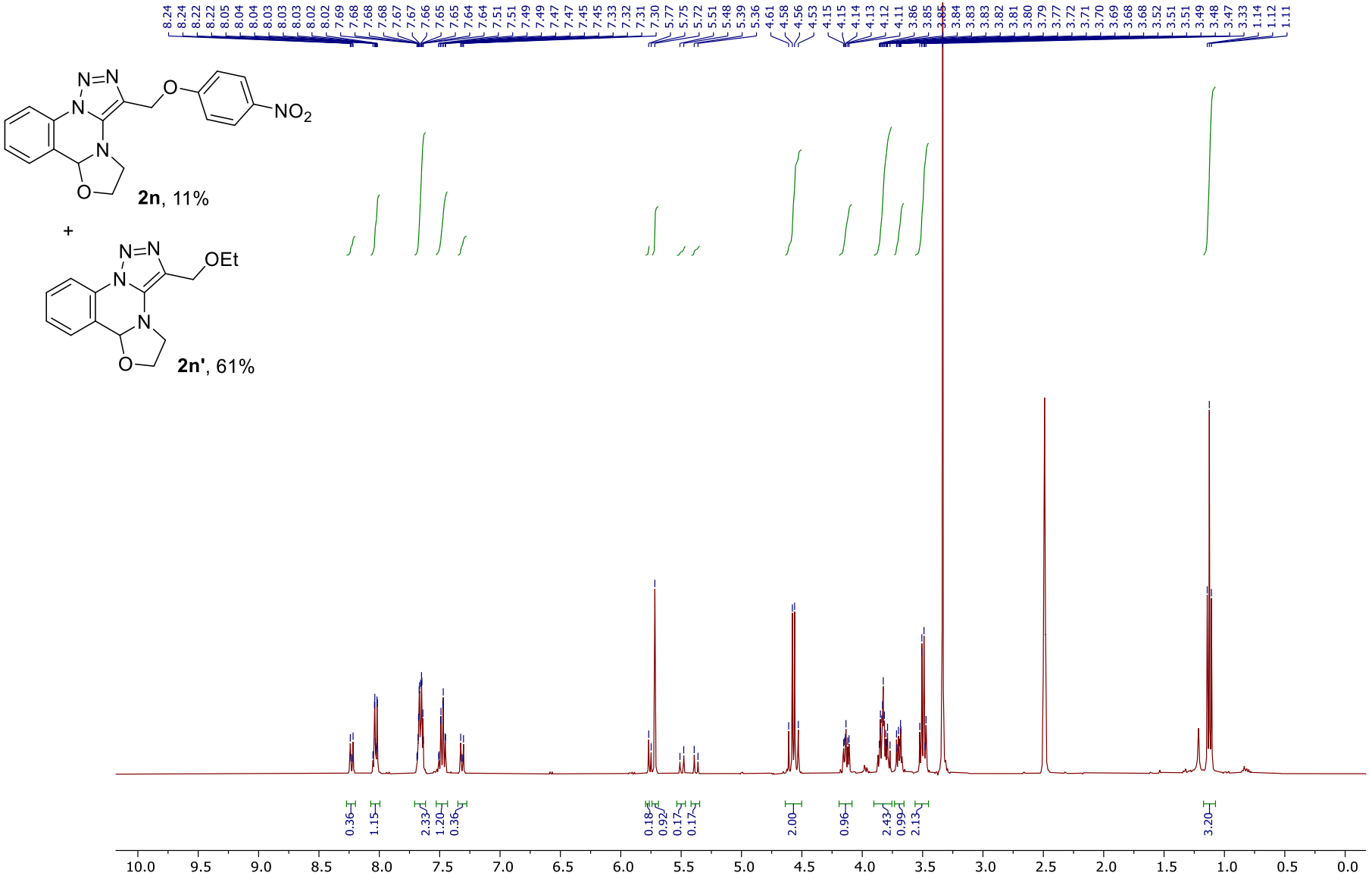
***N*-(5,6-Dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolin-3-ylmethyl)-4-methylbenzenesulfonamide (2m)**

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, DMSO-d_6)



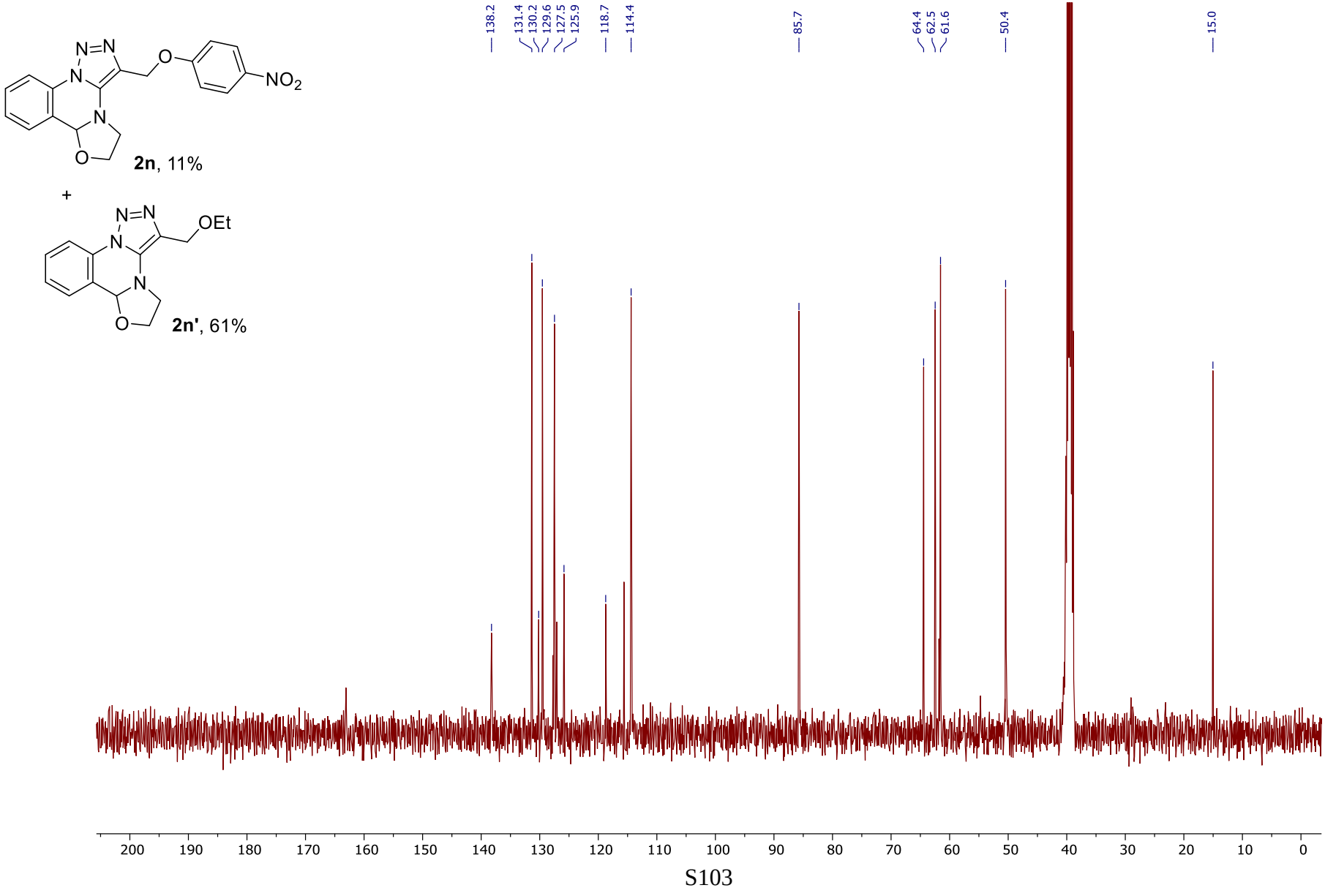
3-(4-Nitrophenoxy)-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2n) and 3-(ethoxymethyl)-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2n')

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



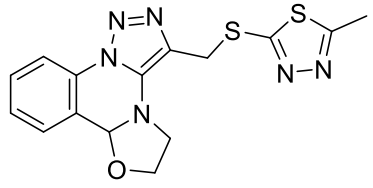
3-(4-Nitrophenoxy)-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2n) and 3-(ethoxymethyl)-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2n')

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, DMSO-d_6)



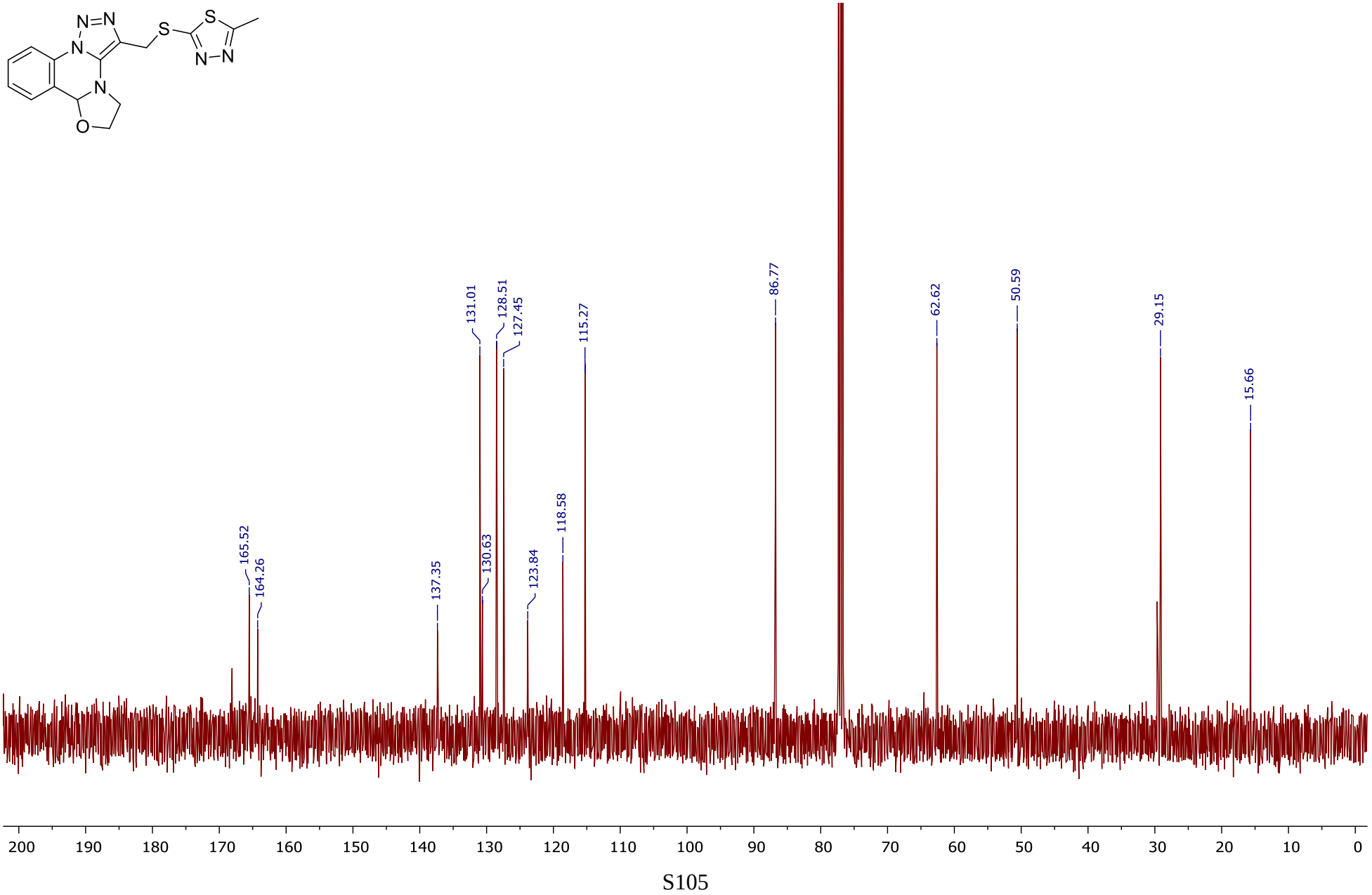
3-{[(5-Methyl-1,3,4-thiadiazol-2-yl)thio]methyl}-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2o)

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



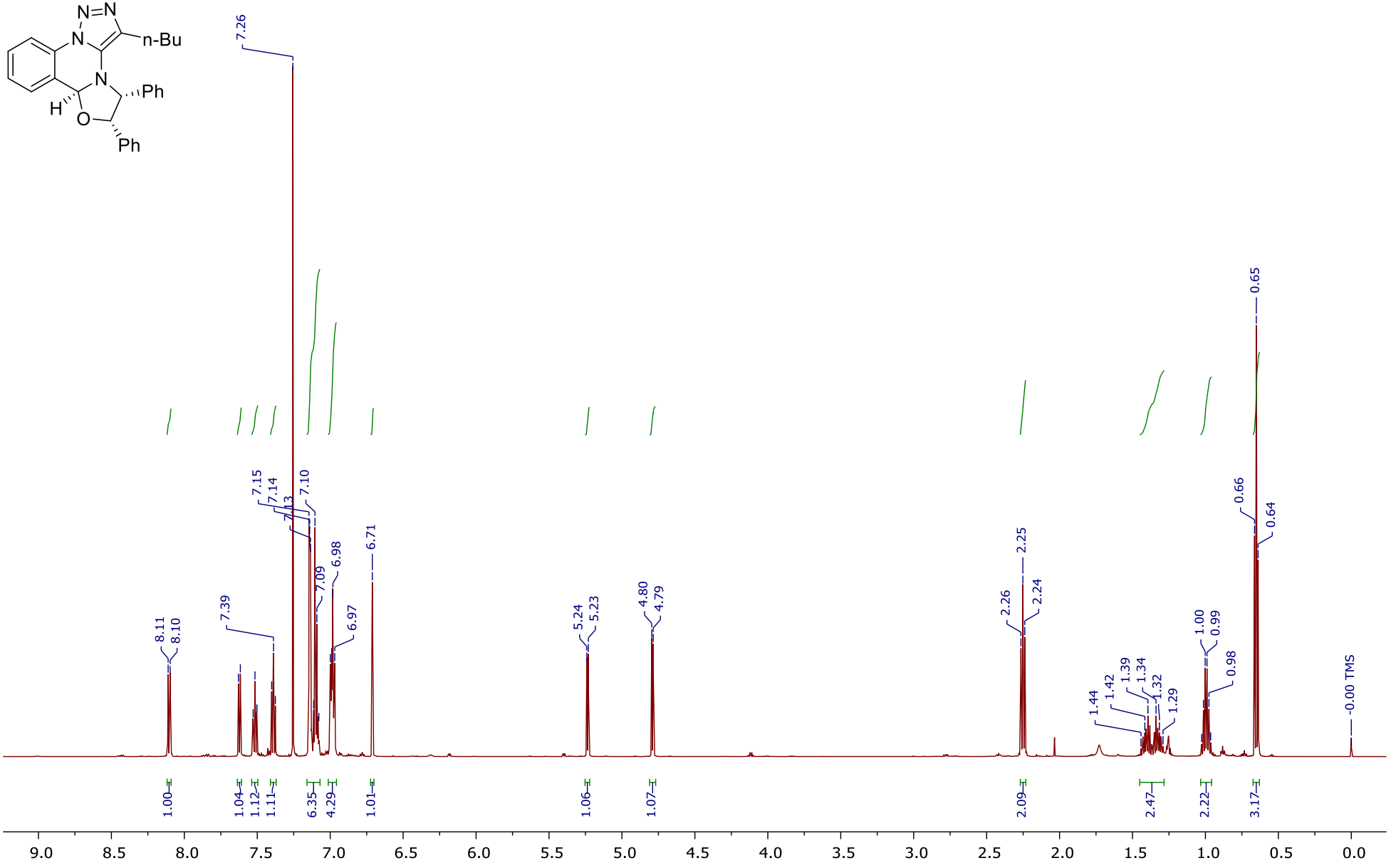
3-{[(5-Methyl-1,3,4-thiadiazol-2-yl)thio]methyl}-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (2o)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



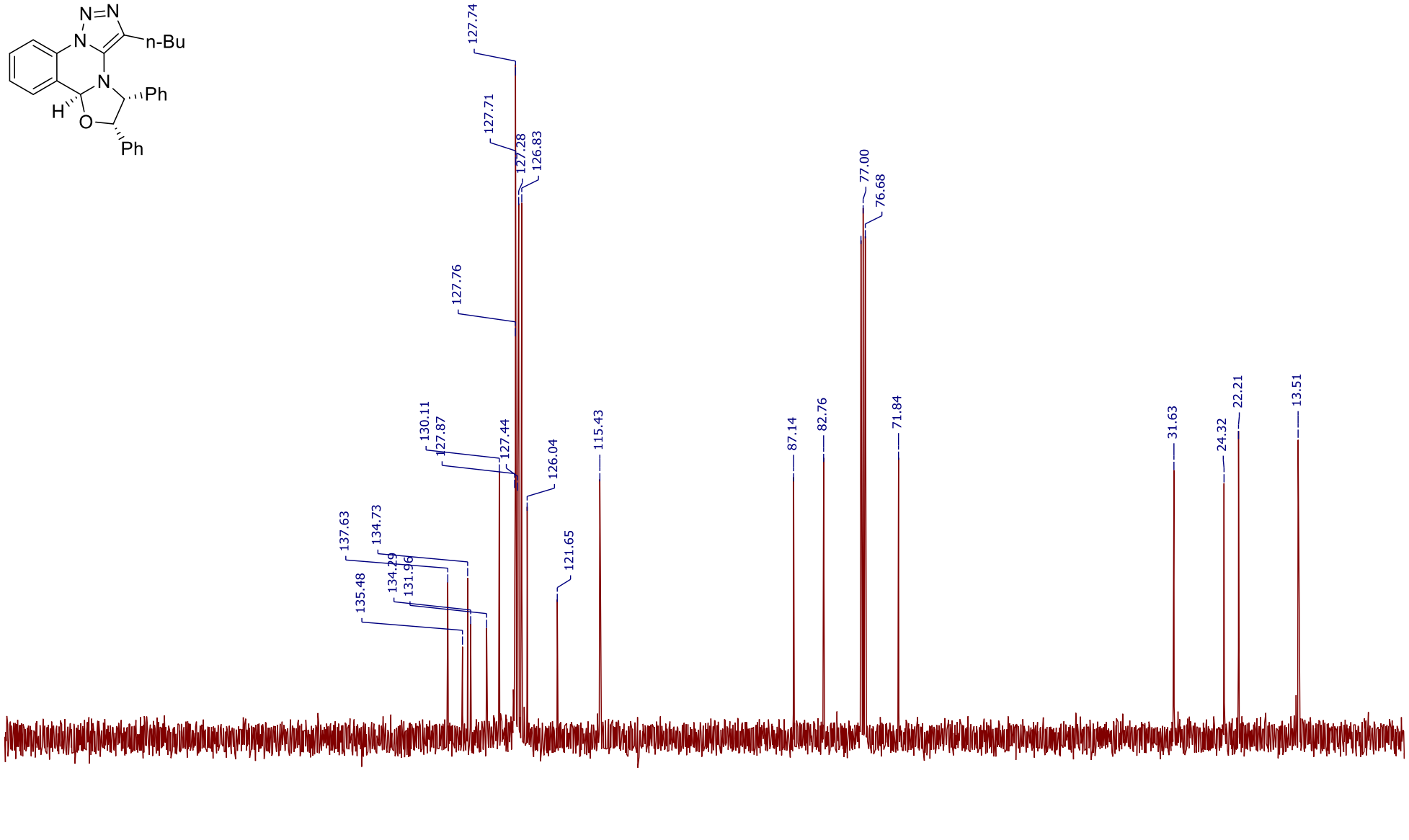
(5*R*,6*S*,7a*S*)-3-Butyl-5,6-diphenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3a)

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



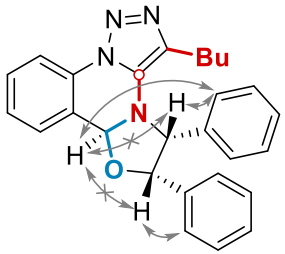
(5*R*,6*S*,7a*S*)-3-Butyl-5,6-diphenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3a)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)

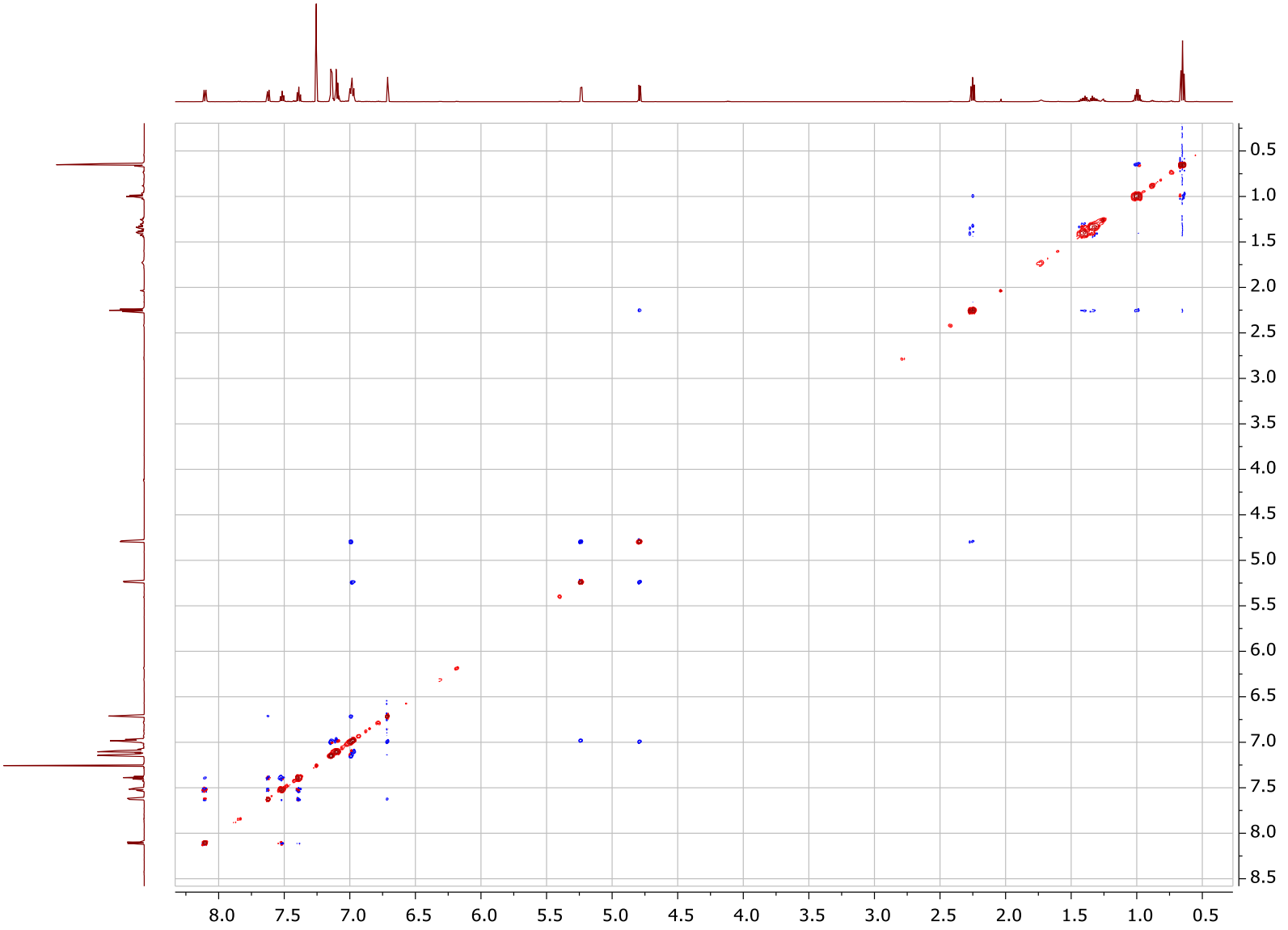


(5*R*,6*S*,7a*S*)-3-Butyl-5,6-diphenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3a)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)

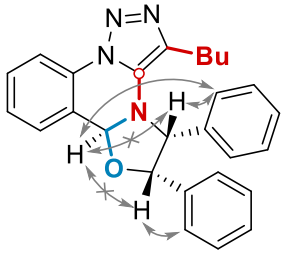


3a, major

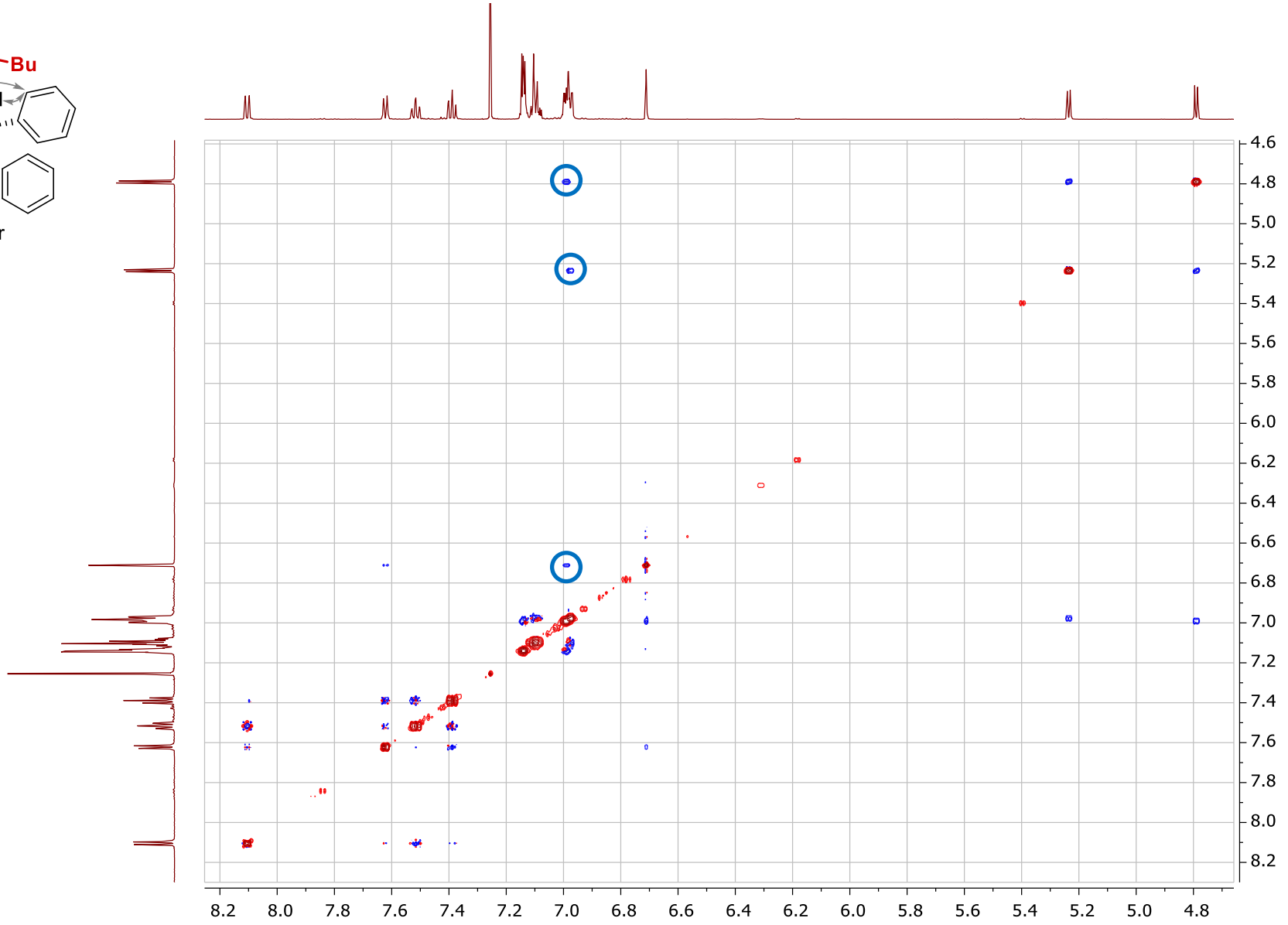


(5*R*,6*S*,7a*S*)-3-Butyl-5,6-diphenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3a)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)

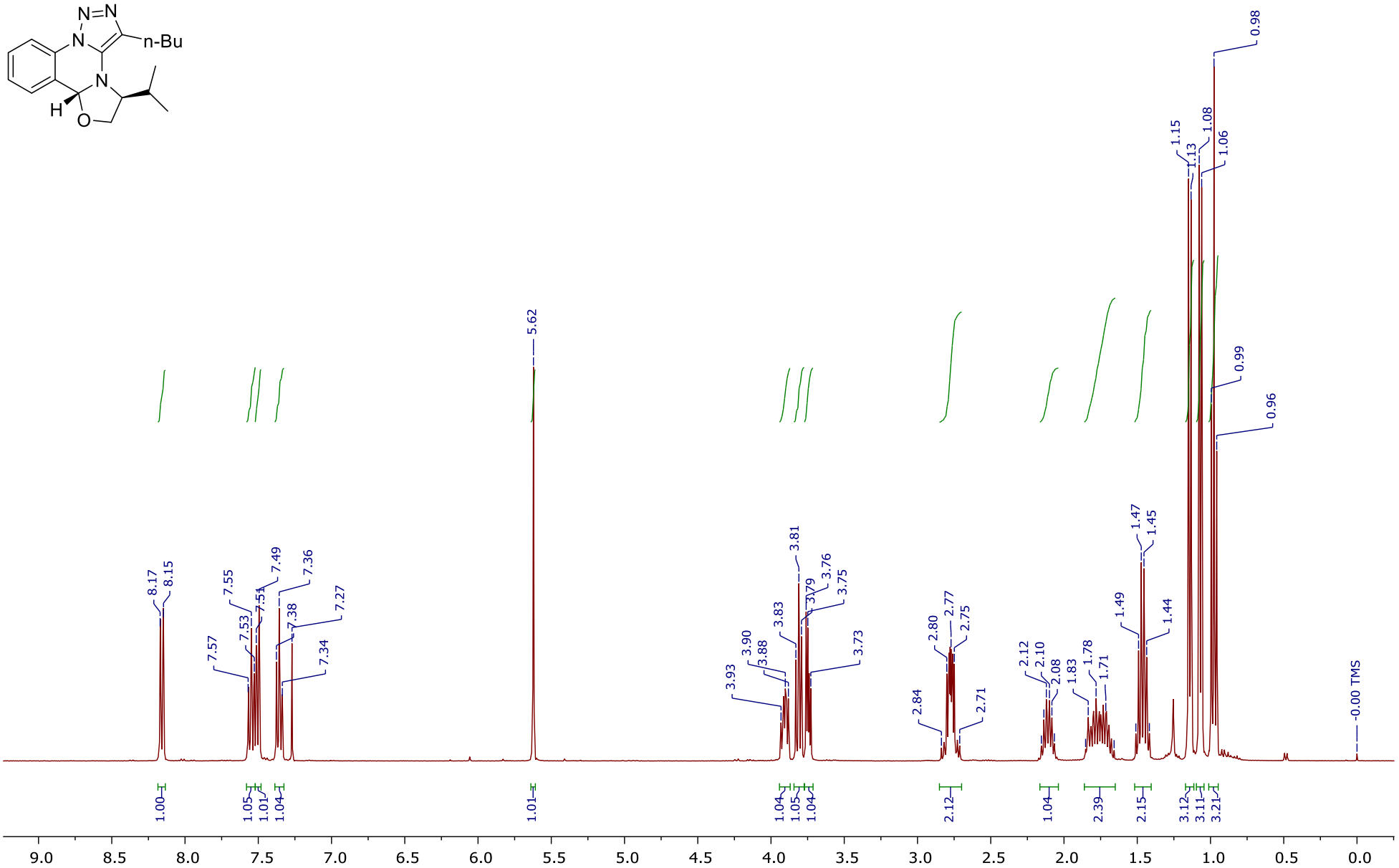


3a, major



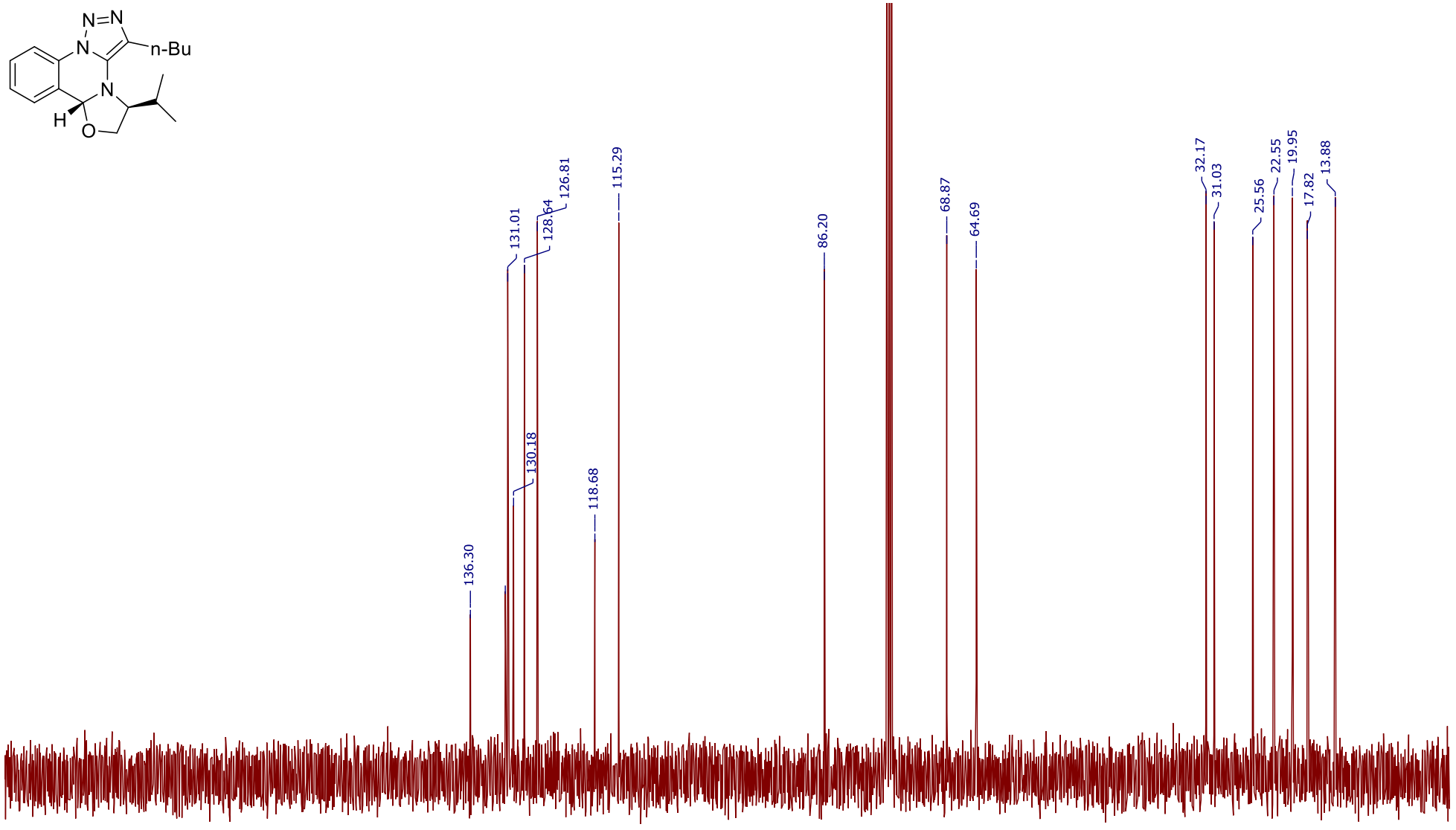
(5*S*,7a*R*)-3-Butyl-5-isopropyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3b)

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



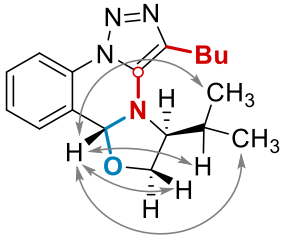
(5*S*,7a*R*)-3-Butyl-5-isopropyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3b)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)

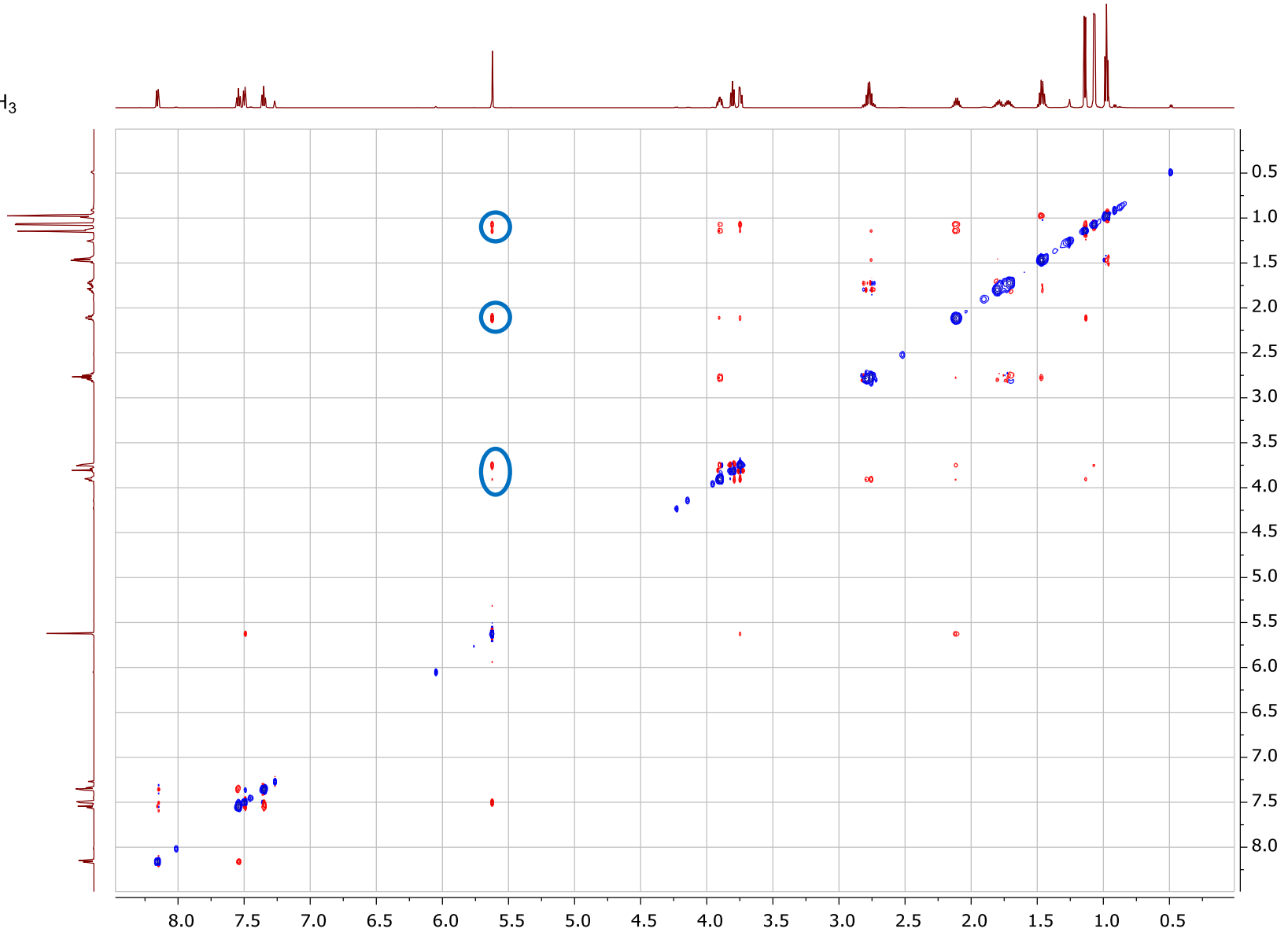


(5*S*,7a*R*)-3-Butyl-5-isopropyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3b)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)

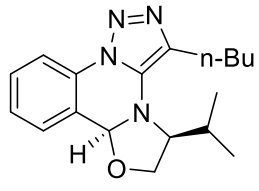


3b, major



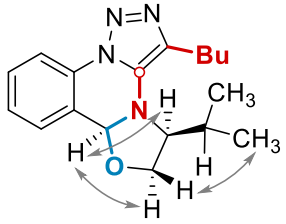
(5*S*,7a*S*)-3-Butyl-5-isopropyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3b')

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

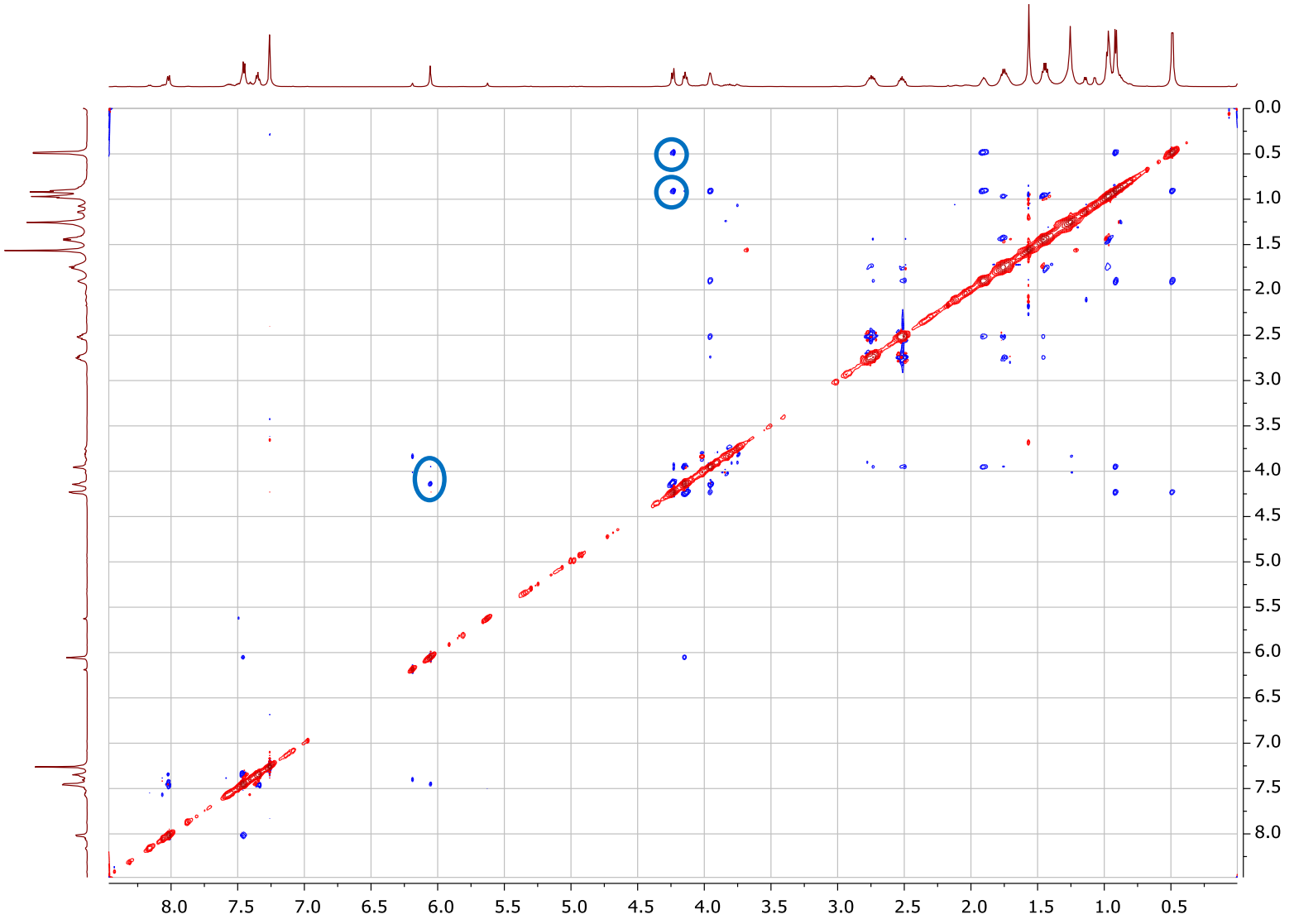


(5*S*,7a*S*)-3-Butyl-5-isopropyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3b')

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)

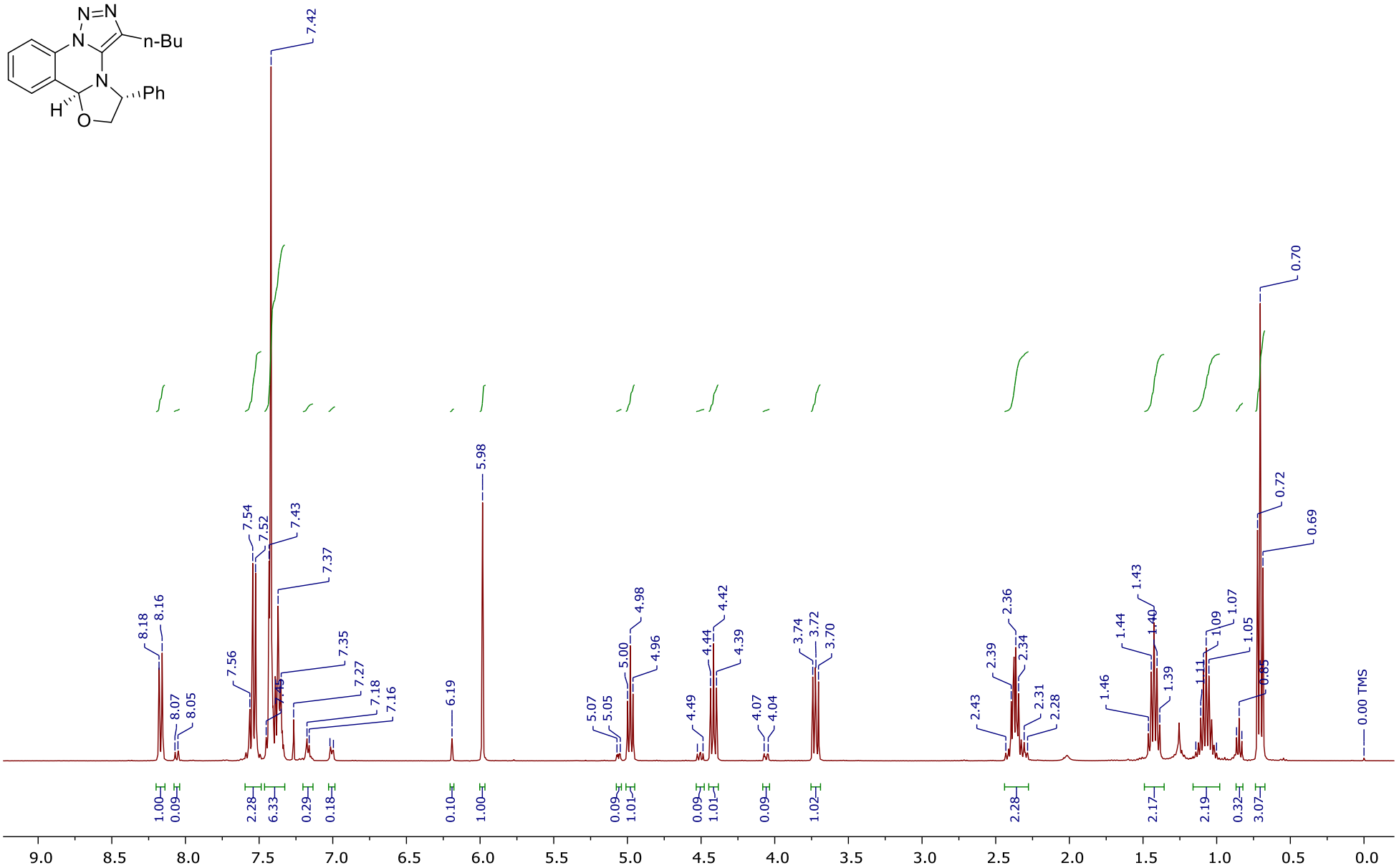


3b', minor



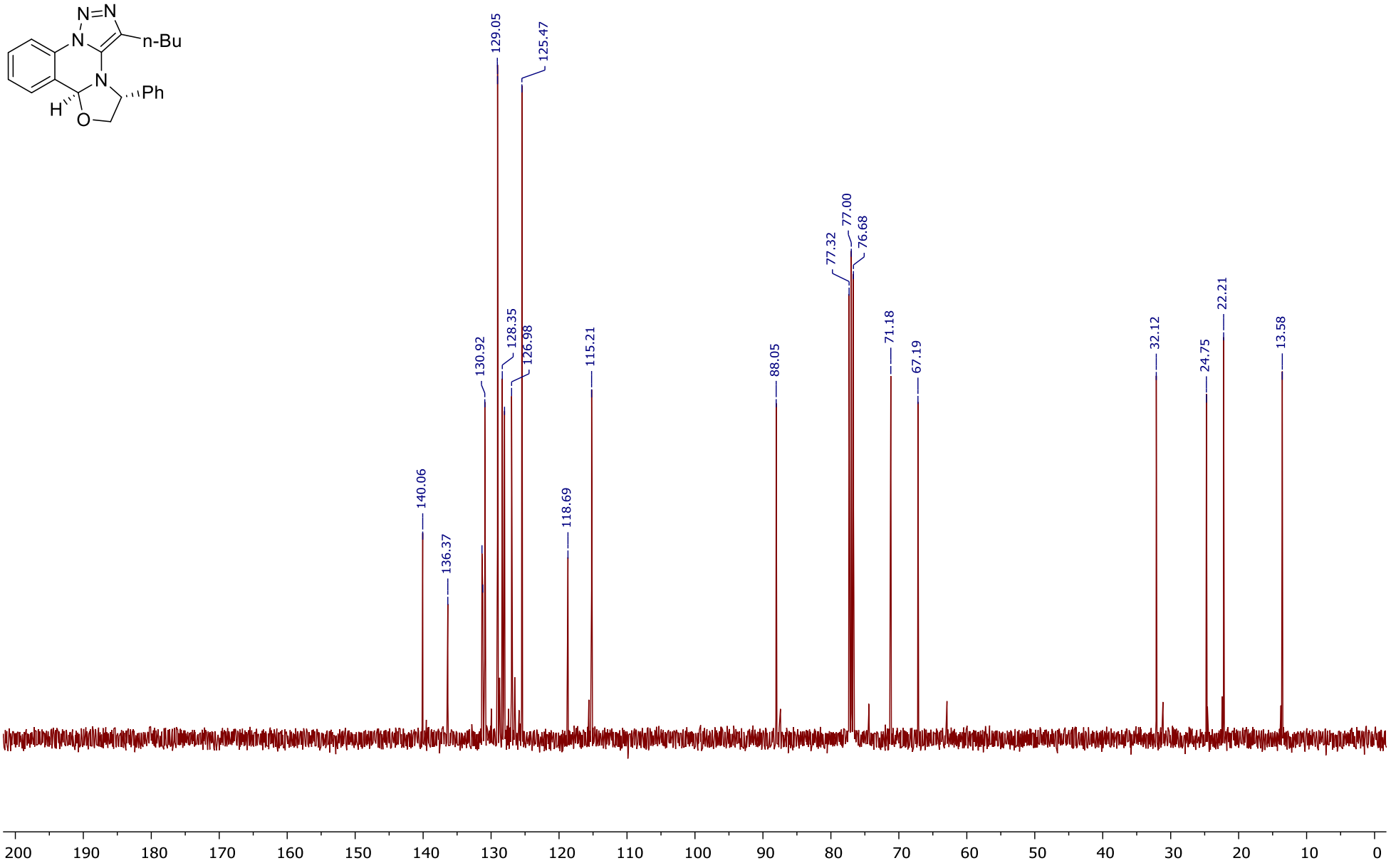
(5*R*,7a*S*)-3-Butyl-5-phenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3c)

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



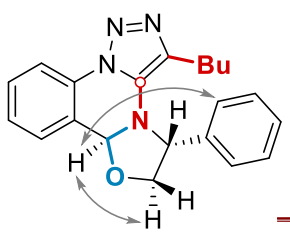
(5*R*,7a*S*)-3-Butyl-5-phenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3c)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)

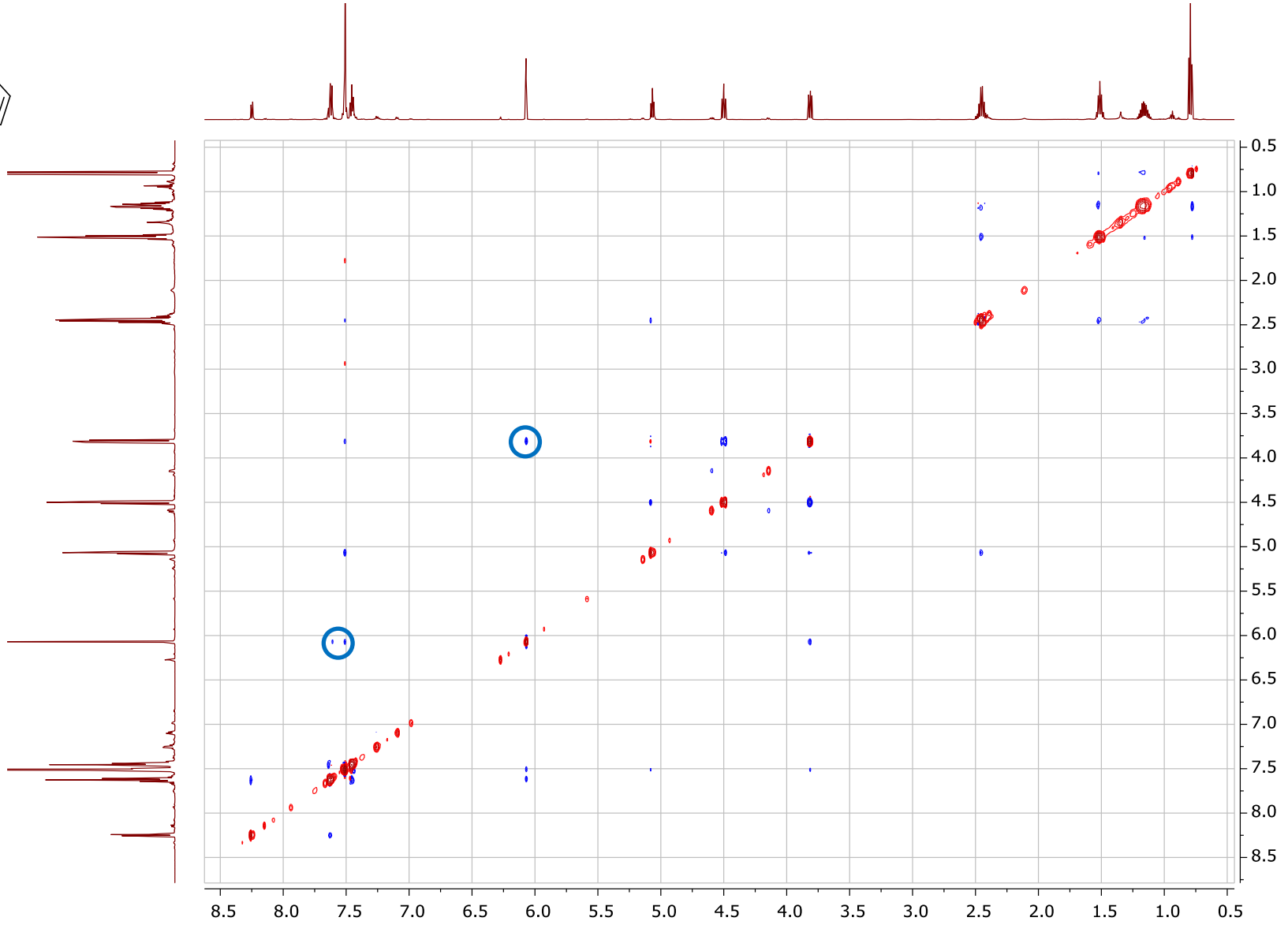


(5*R*,7a*S*)-3-Butyl-5-phenyl-5,6-dihydro-7a*H*-[1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3c)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)

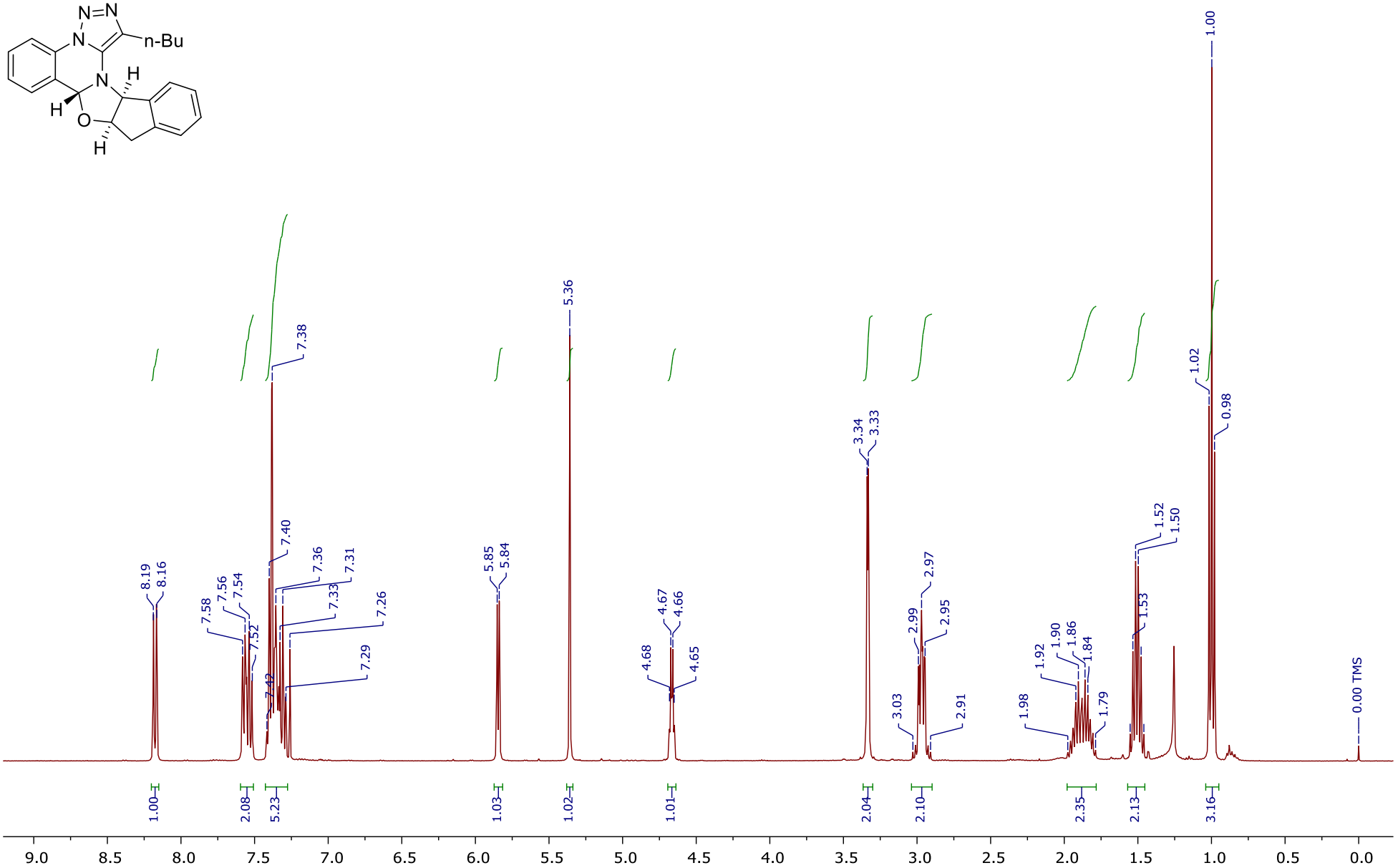


3c, major



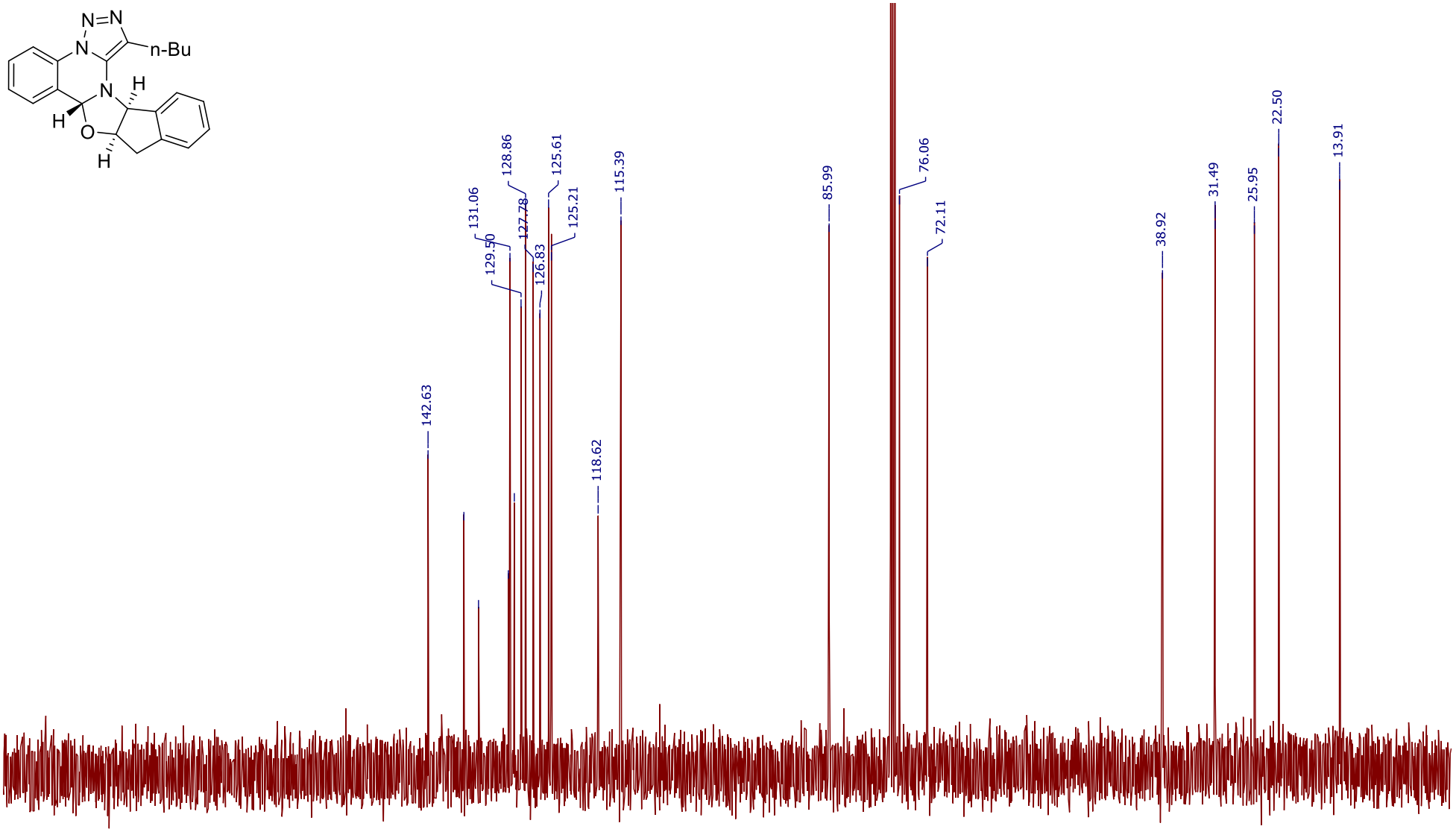
(8b*R*,9a*R*,14b*S*)-1-Butyl-10,14b-dihydro-8b*H*,9a*H*-indeno[1',2':4,5][1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3d)

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



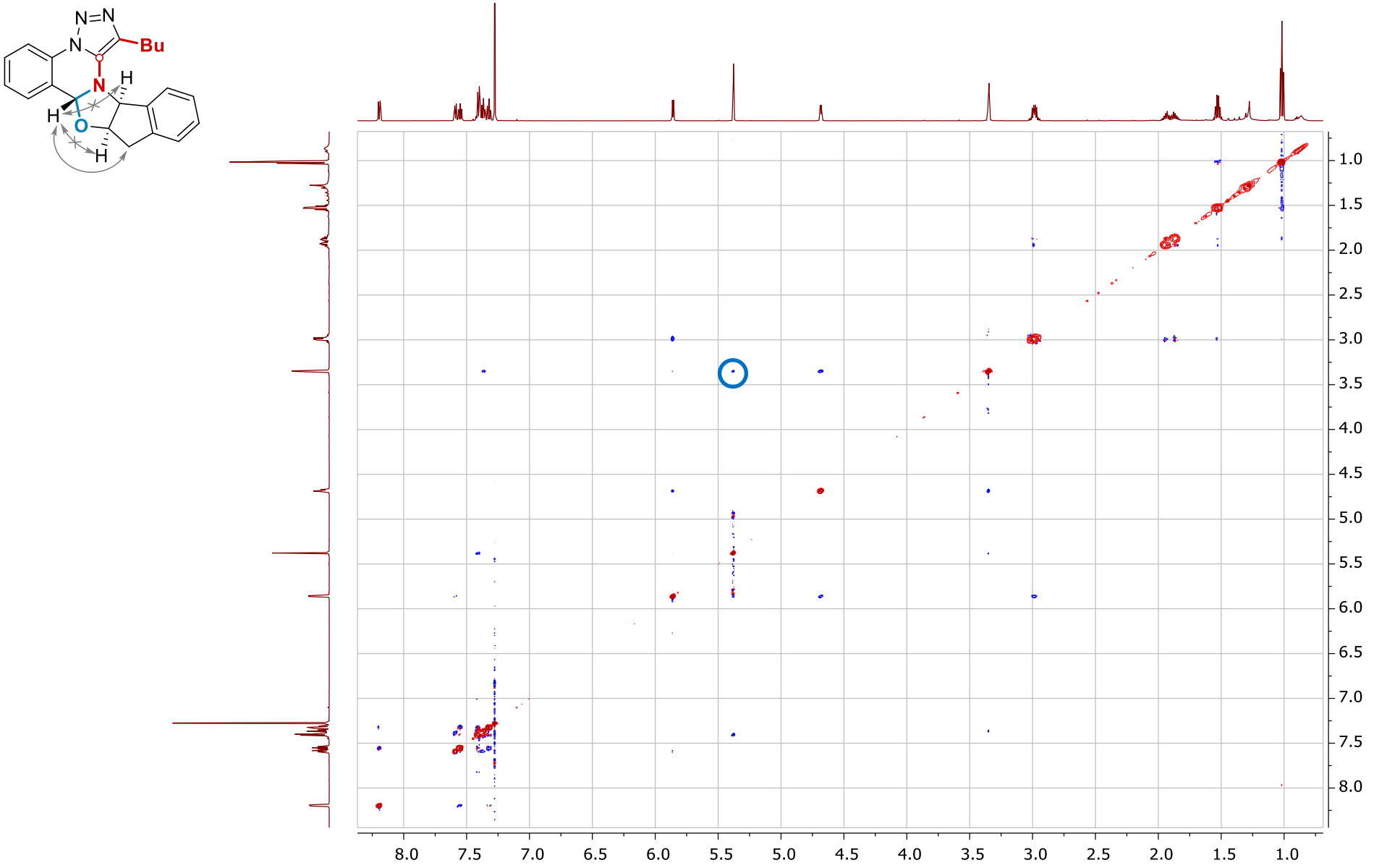
(8b*R*,9a*R*,14b*S*)-1-Butyl-10,14b-dihydro-8b*H*,9a*H*-indeno[1',2':4,5][1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3d)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



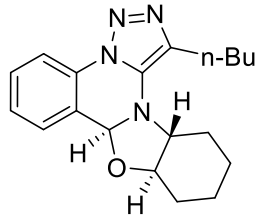
(8b*R*,9a*R*,14b*S*)-1-Butyl-10,14b-dihydro-8b*H*,9a*H*-indeno[1',2':4,5][1,3]oxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3d)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)



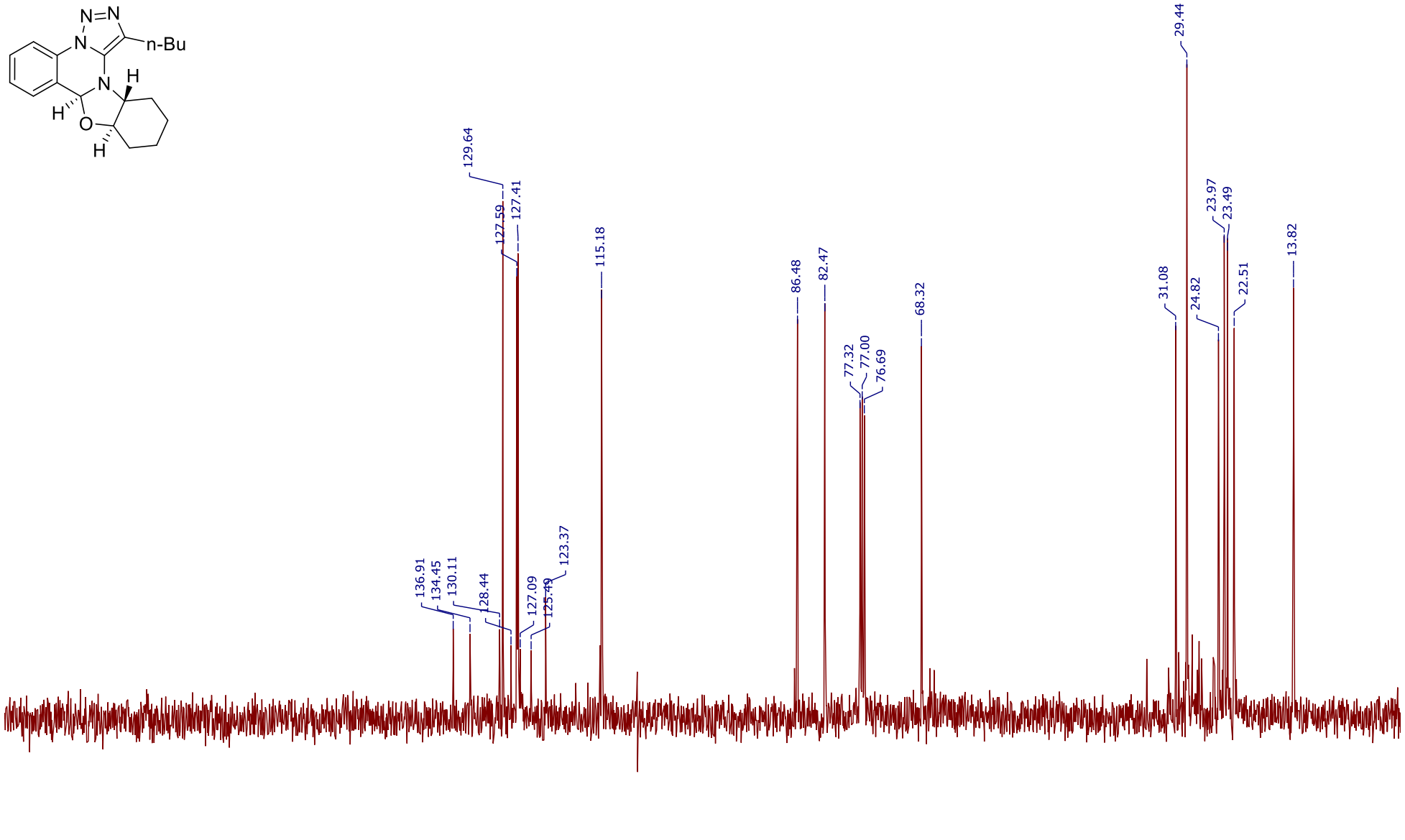
(8b*S*,9a*R*,13a*R*)-1-Butyl-9a,10,11,12,13,13a-hexahydro-8b*H*-[1,3]benzoxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3e)

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



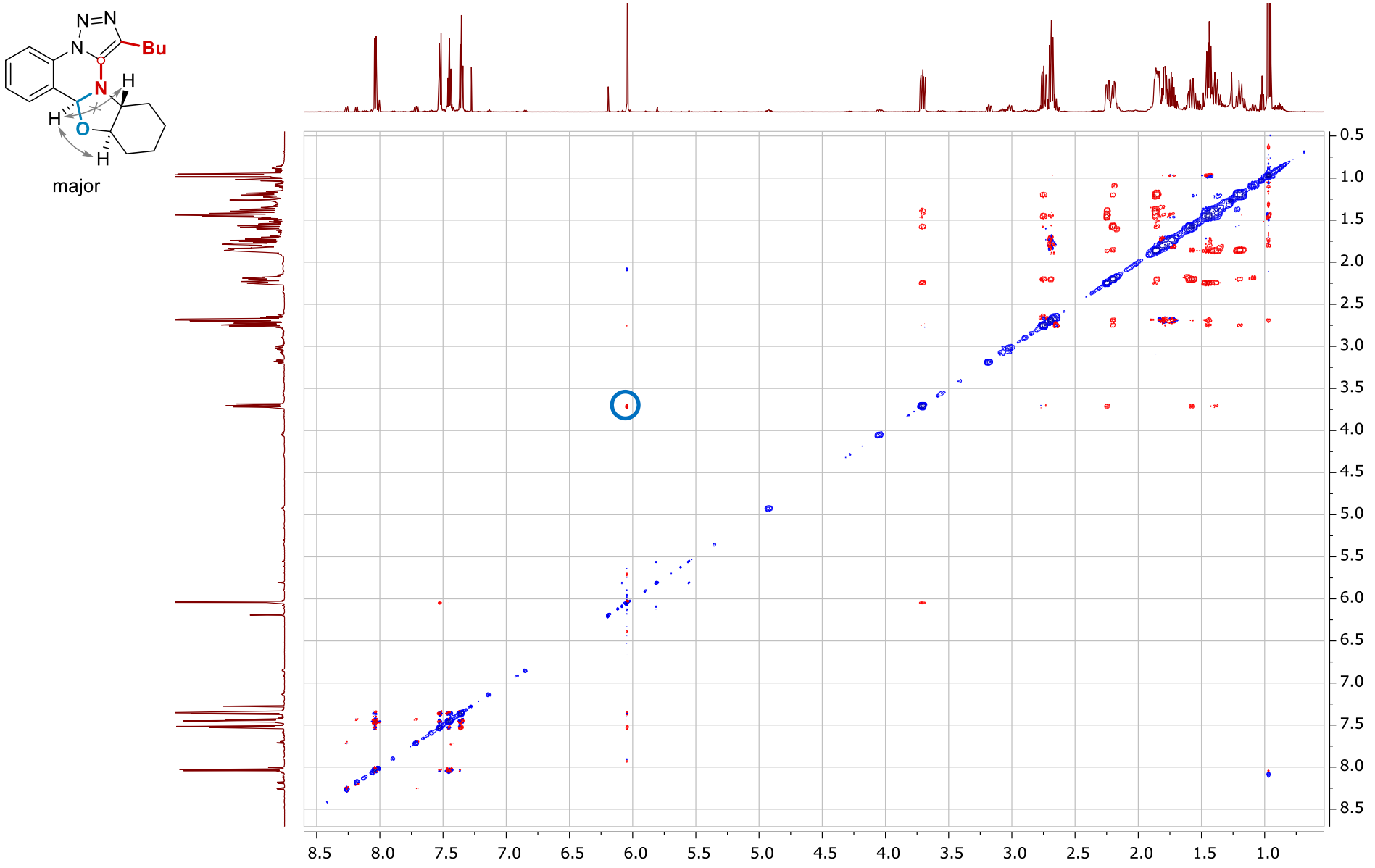
(8b*S*,9a*R*,13a*R*)-1-Butyl-9a,10,11,12,13,13a-hexahydro-8b*H*-[1,3]benzoxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3e)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



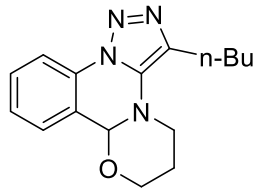
(8b*S*,9a*R*,13a*R*)-1-Butyl-9a,10,11,12,13,13a-hexahydro-8b*H*-[1,3]benzoxazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3e)

^{1}H–^{1}H NOESY (600 MHz, $CDCl_3$)



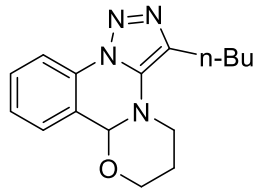
3-Butyl-6,7-dihydro-5*H*,8a*H*-[1,3]oxazino[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3f)

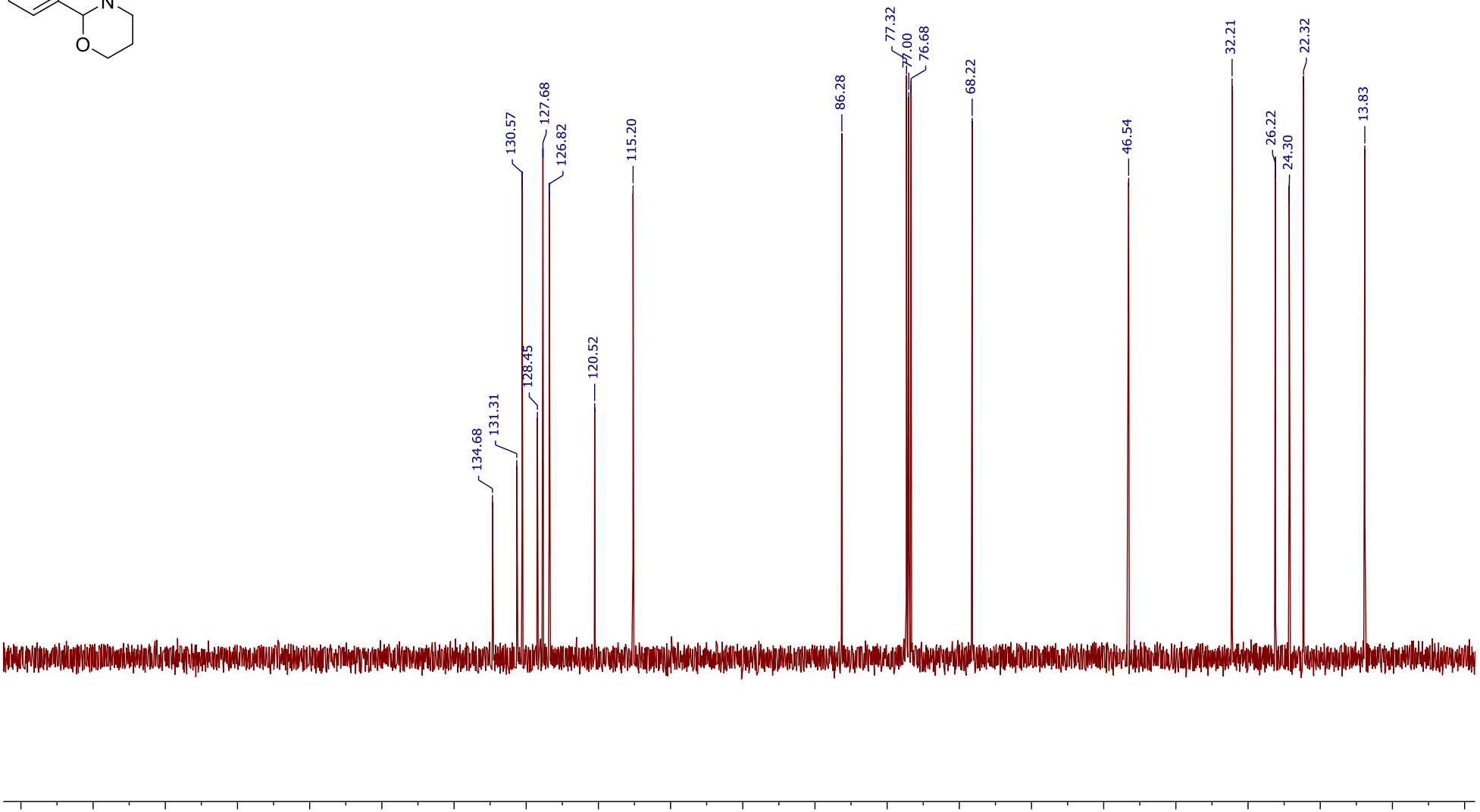
^{1}H NMR (400 MHz, $CDCl_3$)



3-Butyl-6,7-dihydro-5*H*,8a*H*-[1,3]oxazino[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3f)

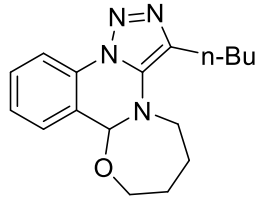
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)





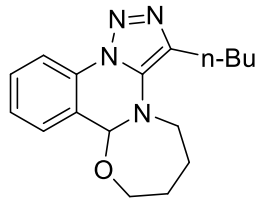
3-Butyl-5,6,7,8-tetrahydro-9a*H*-[1,3]oxazepino[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3g)

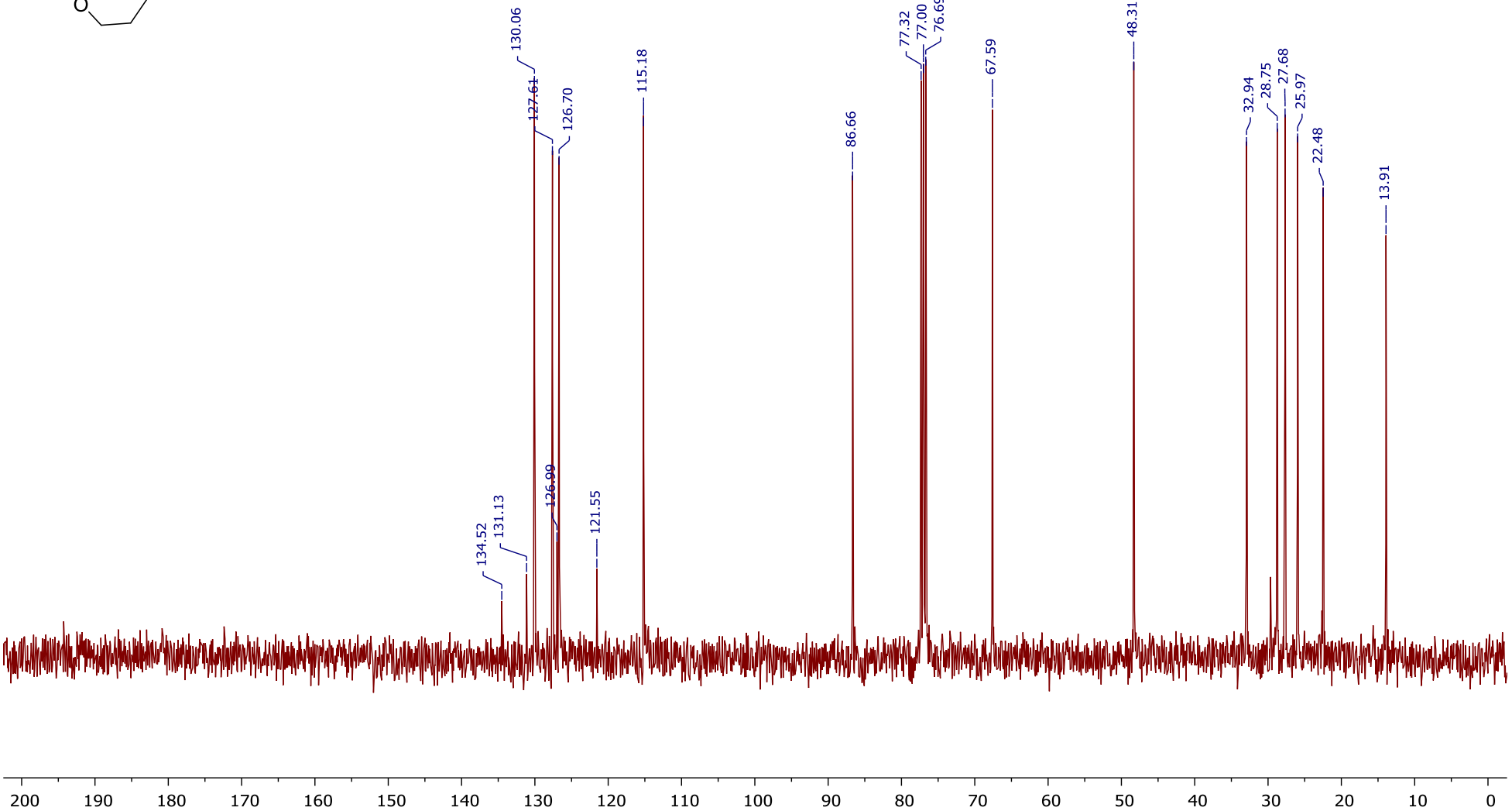
^{1}H NMR (400 MHz, $CDCl_3$)



3-Butyl-5,6,7,8-tetrahydro-9a*H*-[1,3]oxazepino[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3g)

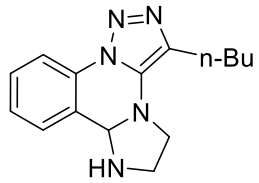
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)





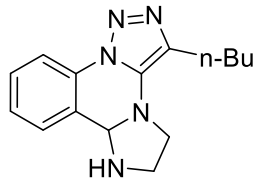
3-Butyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3h)

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



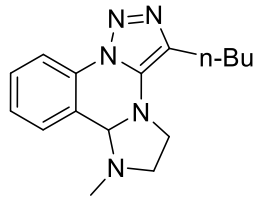
3-Butyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3h)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



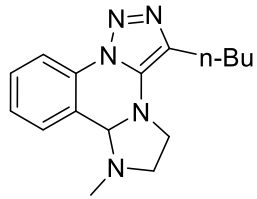
3-Butyl-7-methyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3i)

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



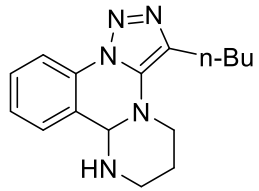
3-Butyl-7-methyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3i)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



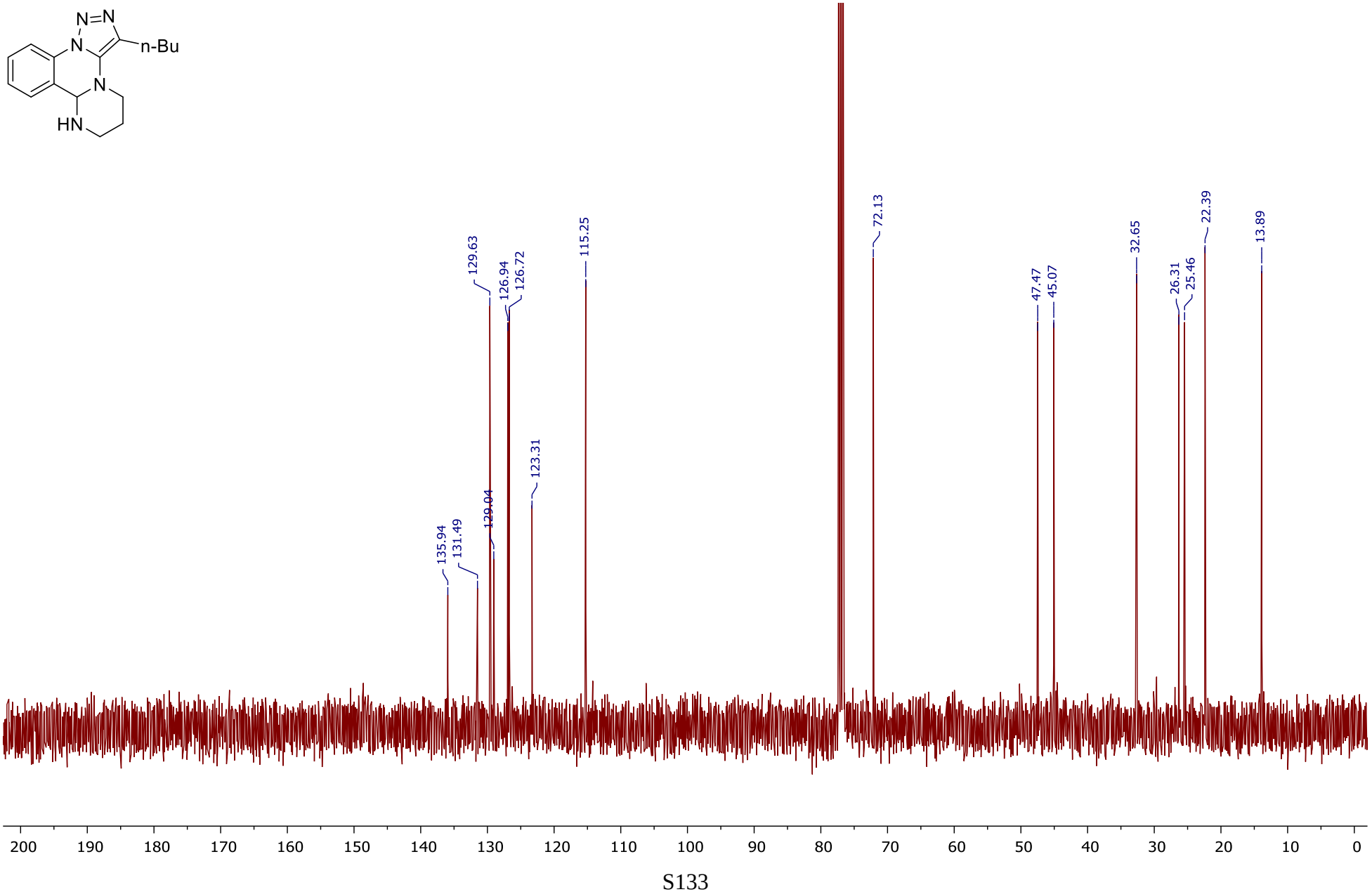
3-Butyl-6,7,8,8a-tetrahydro-5*H*-pyrimido[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3j)

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



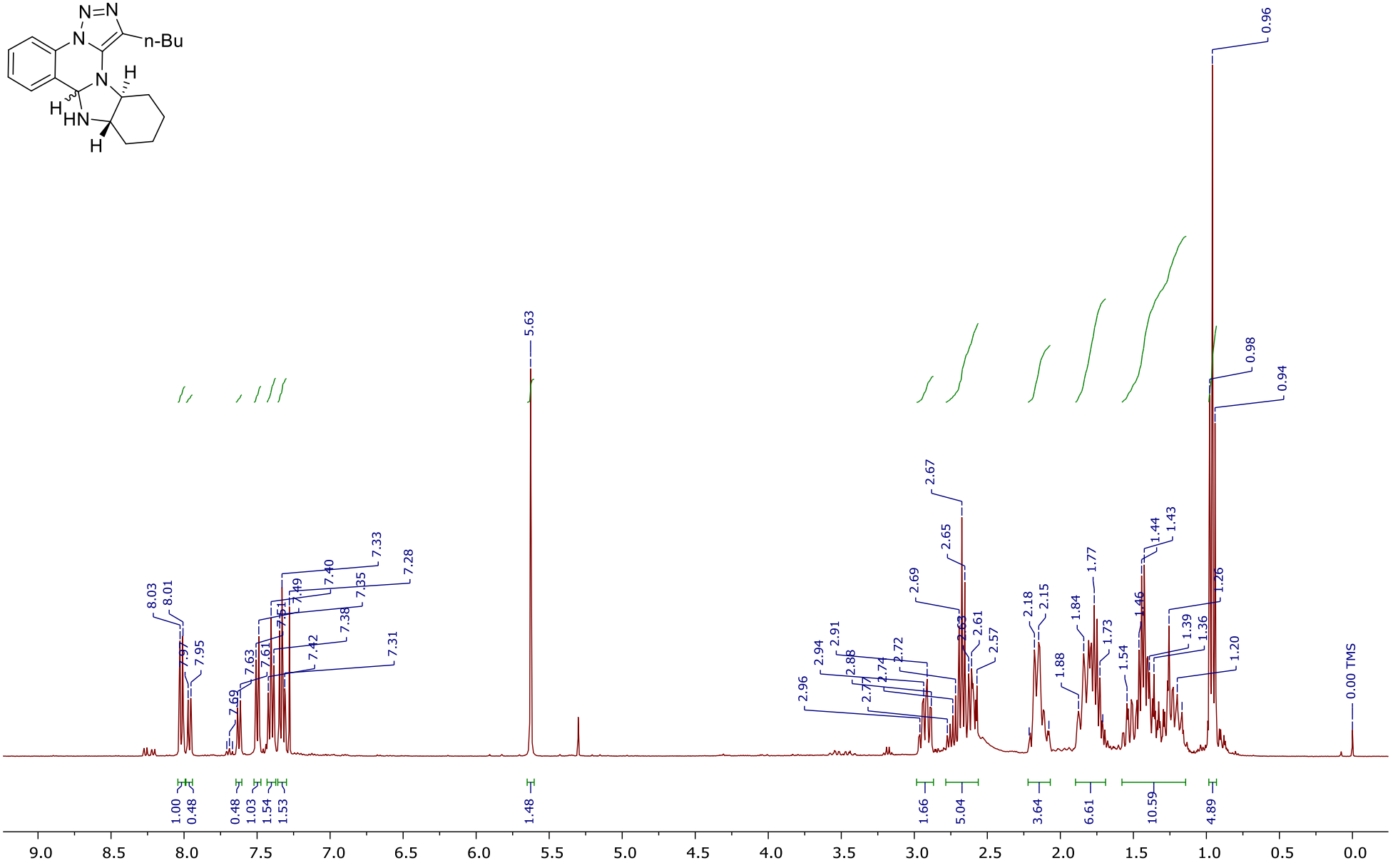
3-Butyl-6,7,8,8a-tetrahydro-5*H*-pyrimido[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3j)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



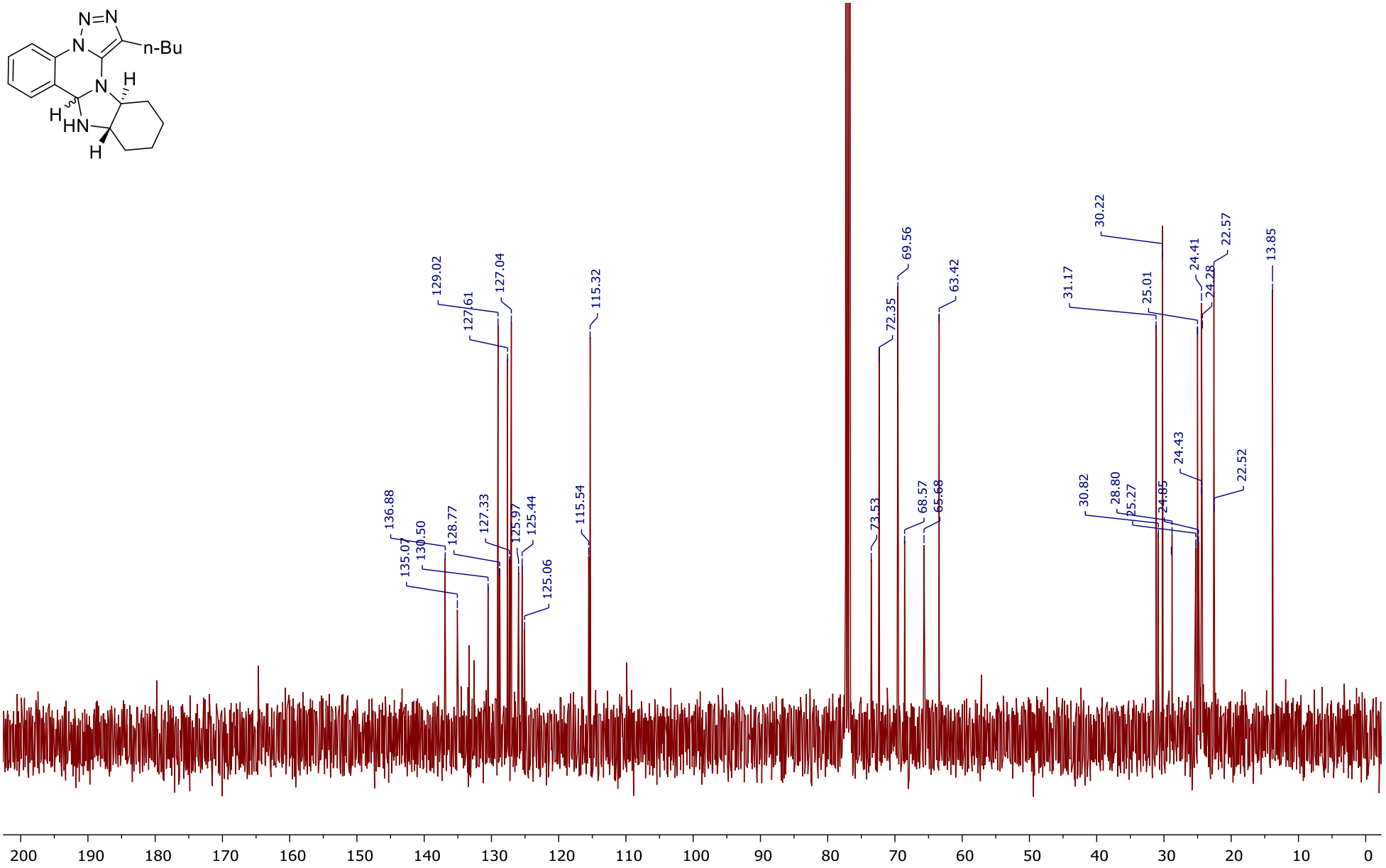
(8b*RS*,9a*S*,13a*S*)-1-Butyl-8b,9,9a,10,11,12,13,13a-octahydrobenzimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3k)

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



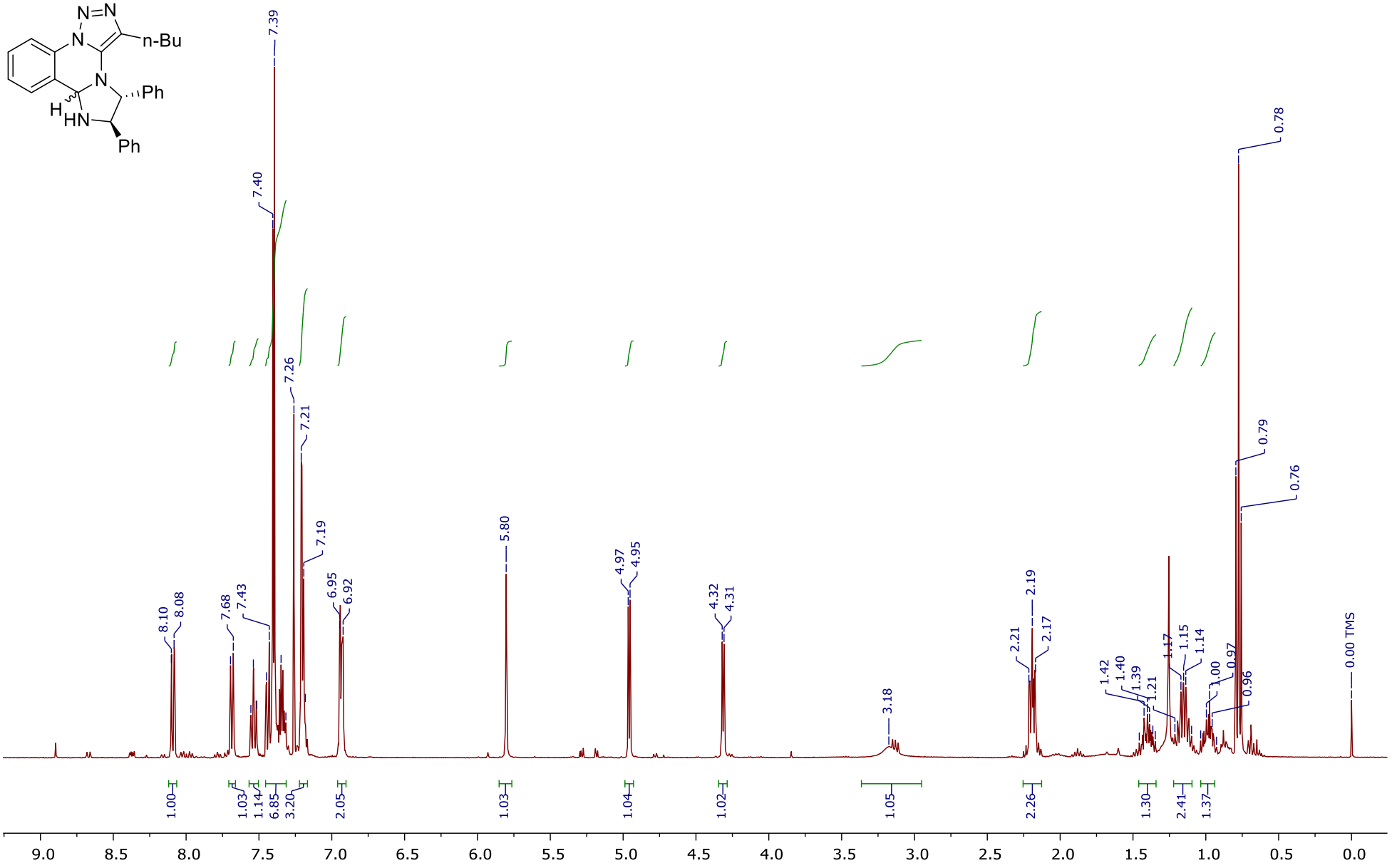
(8b*RS*,9a*S*,13a*S*)-1-Butyl-8b,9,9a,10,11,12,13,13a-octahydrobenzimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3k)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



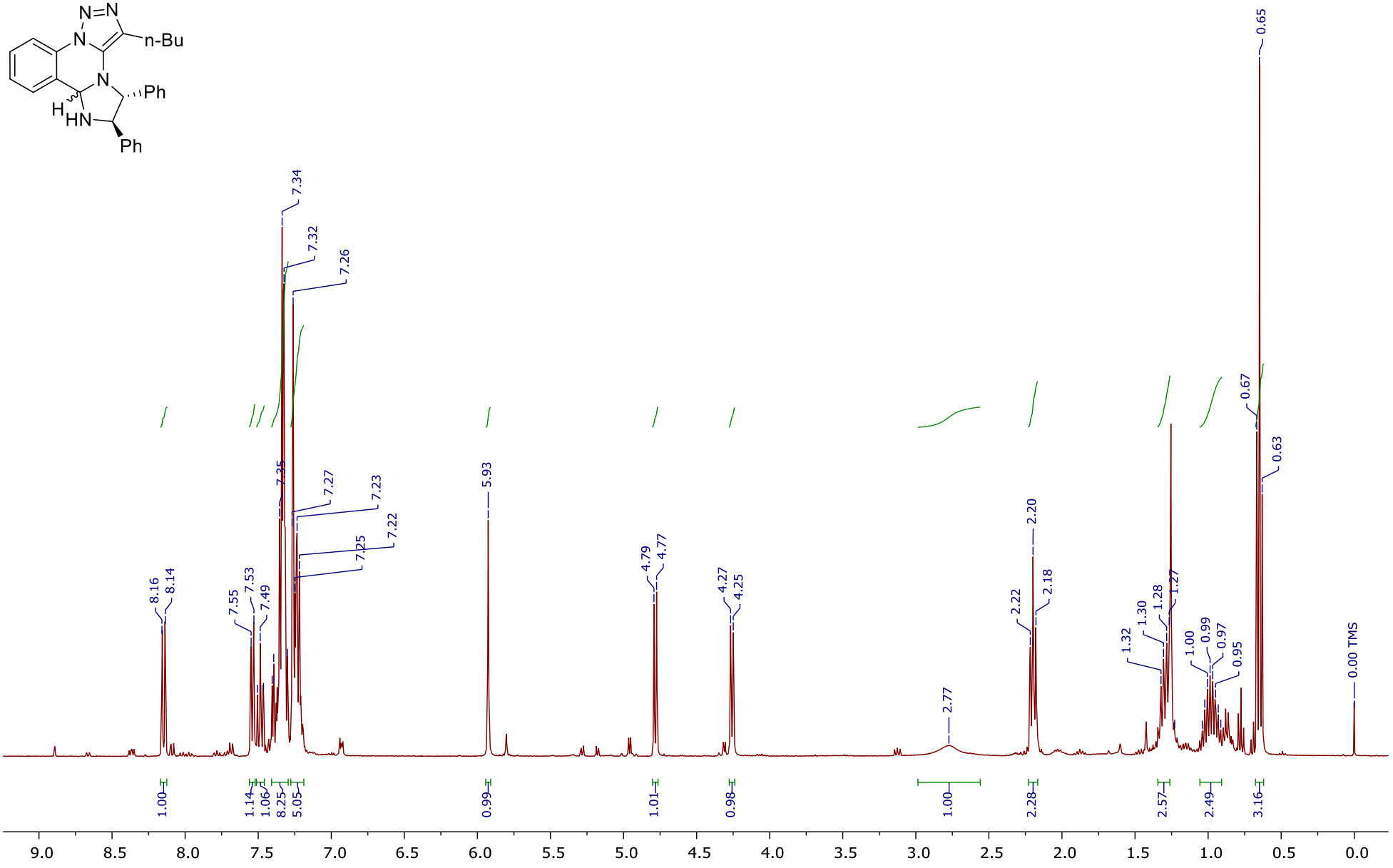
(5*R*,6*R*)-3-Butyl-5,6-diphenyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3l, major)

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



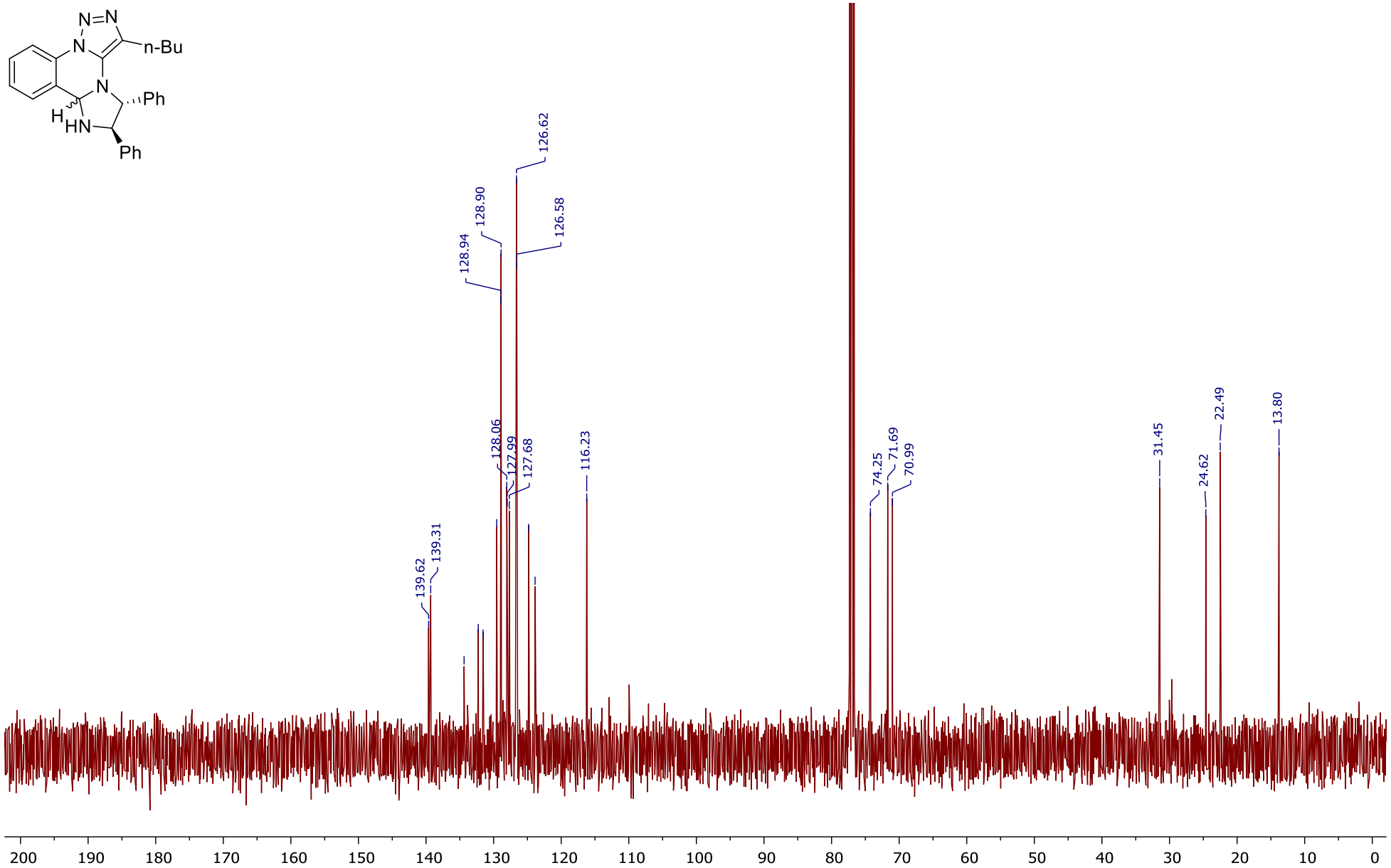
(5*R*,6*R*)-3-Butyl-5,6-diphenyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3l', minor)

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



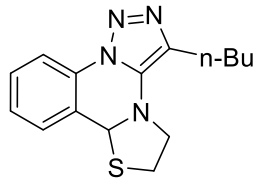
(5*R*,6*R*)-3-Butyl-5,6-diphenyl-5,6,7,7a-tetrahydroimidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3l, major)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



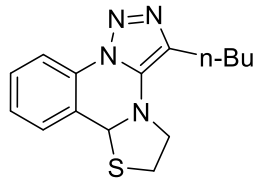
3-Butyl-5,6-dihydro-7a*H*-[1,3]thiazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3m)

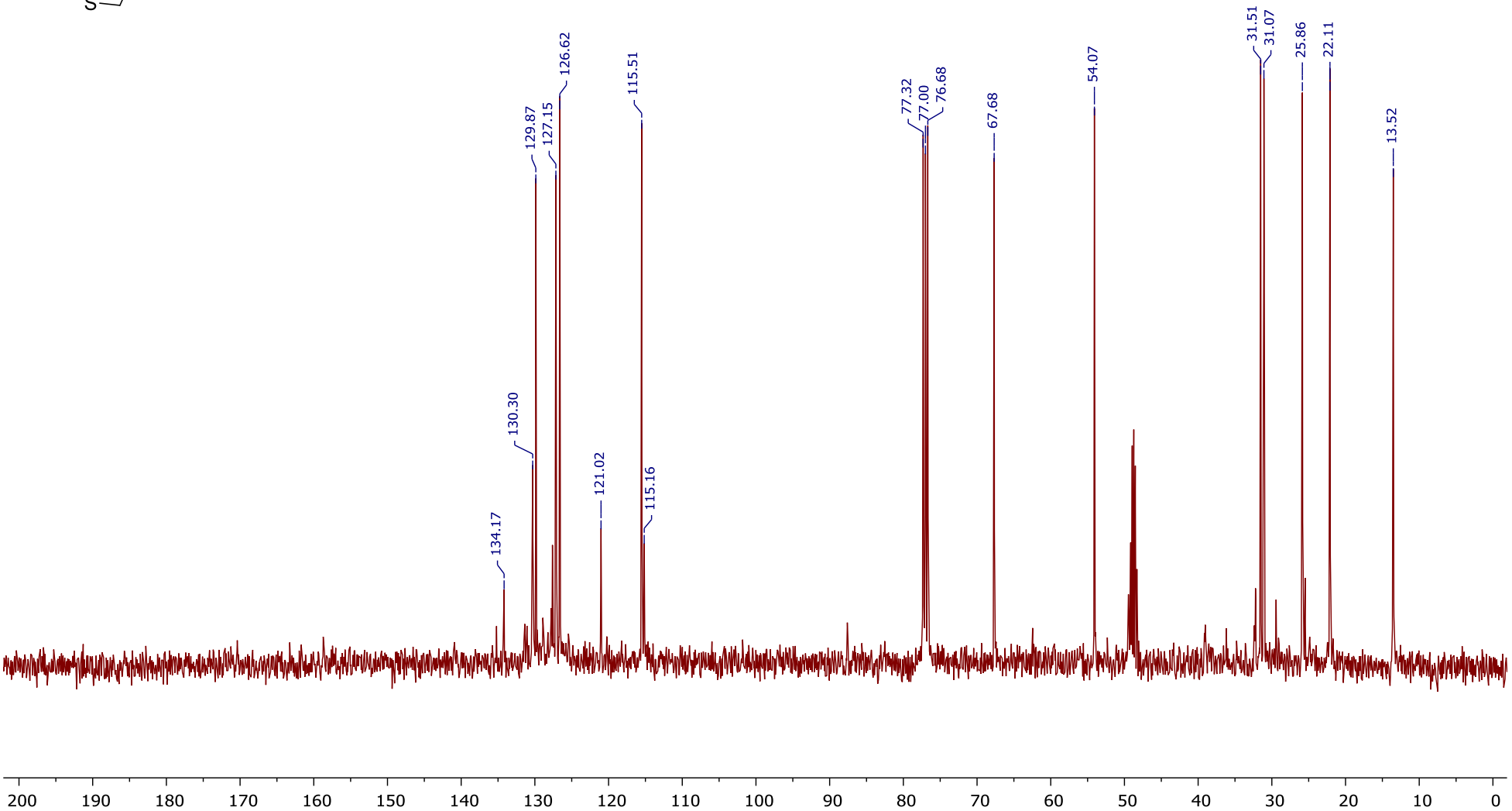
^{1}H NMR (400 MHz, $CDCl_3/CD_3OD$)



3-Butyl-5,6-dihydro-7a*H*-[1,3]thiazolo[3,2-*c*][1,2,3]triazolo[1,5-*a*]quinazoline (3m)

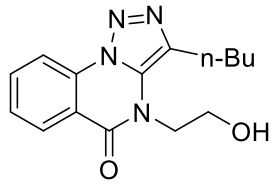
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3/CD_3OD$)





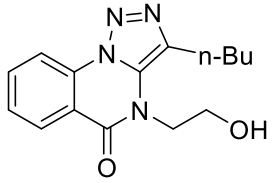
3-Butyl-4-(2-hydroxyethyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6a)

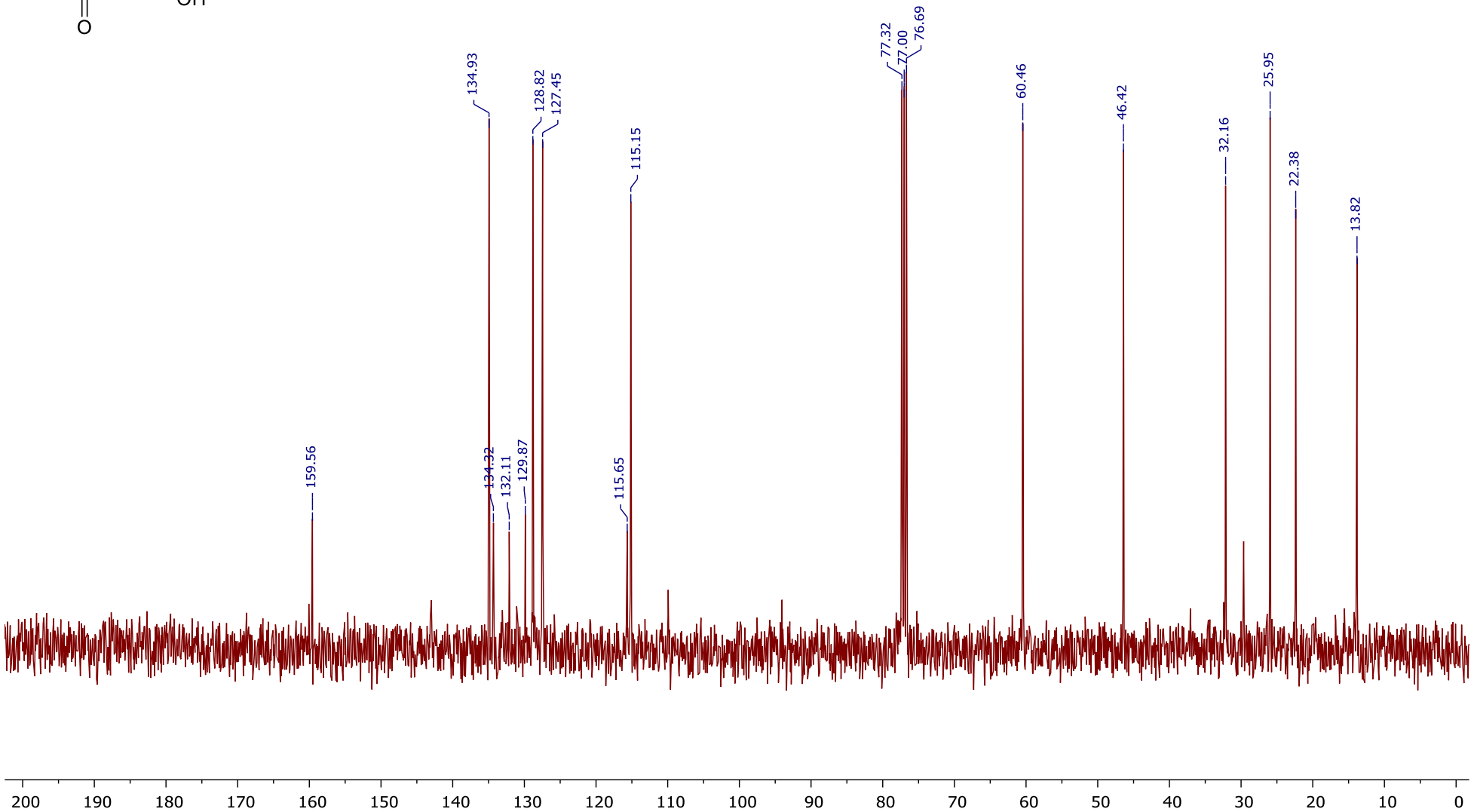
^{1}H NMR (400 MHz, $CDCl_3$)



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

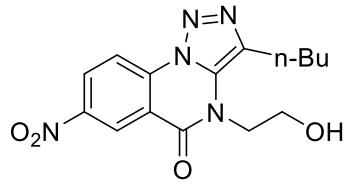
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)





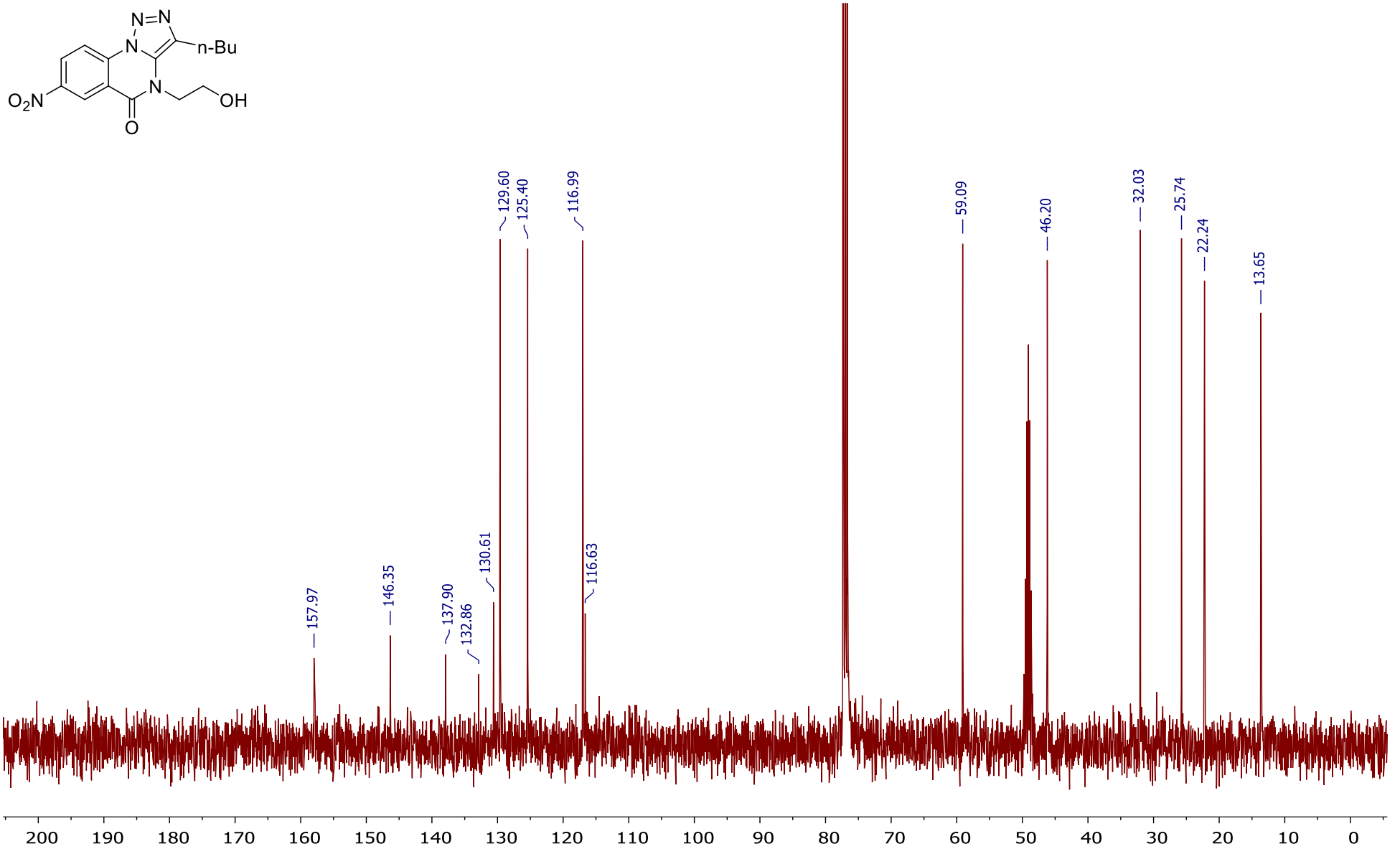
3-Butyl-4-(2-hydroxyethyl)-7-nitro[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6c)

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



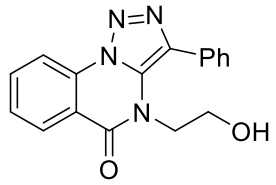
3-Butyl-4-(2-hydroxyethyl)-7-nitro[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6c)

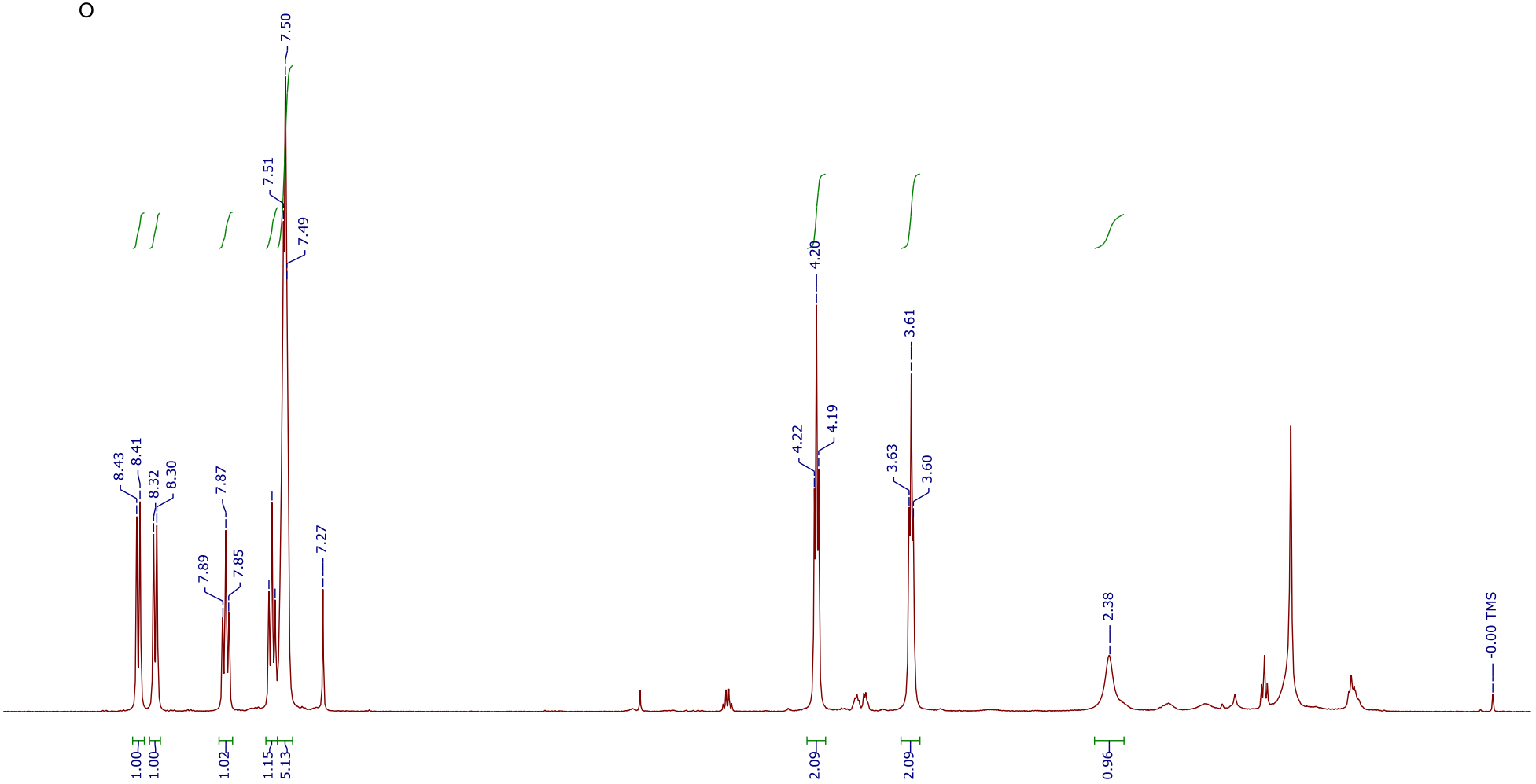
$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3/CD_3OD$)



4-(2-Hydroxyethyl)-3-phenyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6h)

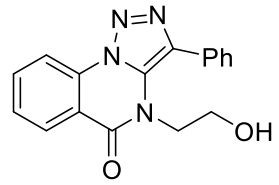
^{1}H NMR (400 MHz, $CDCl_3$)





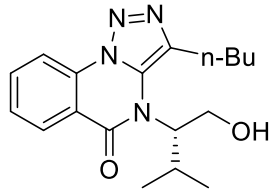
4-(2-Hydroxyethyl)-3-phenyl[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6h)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



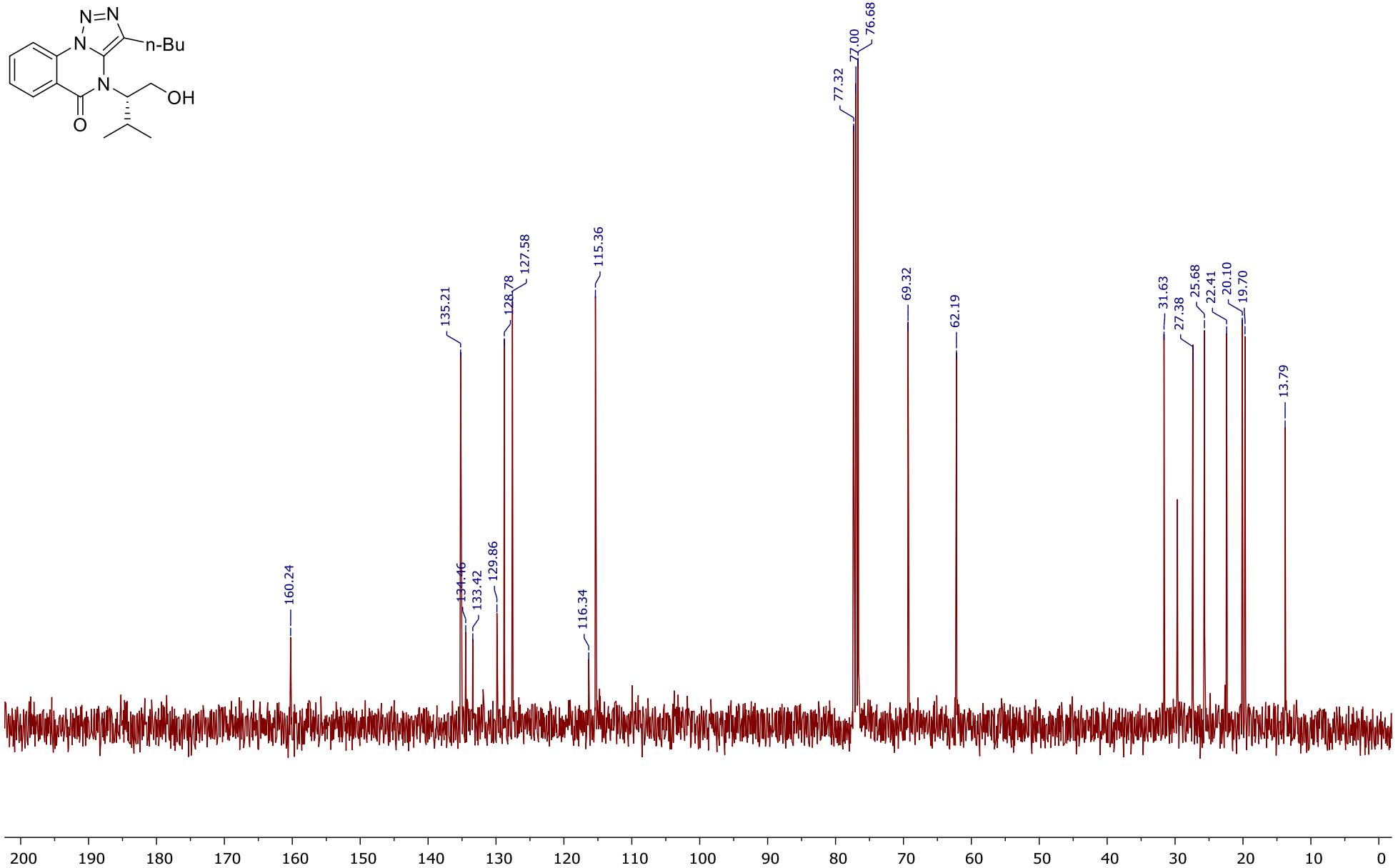
3-Butyl-4-[(1*S*)-1-(hydroxymethyl)-2-methylpropyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6j)

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



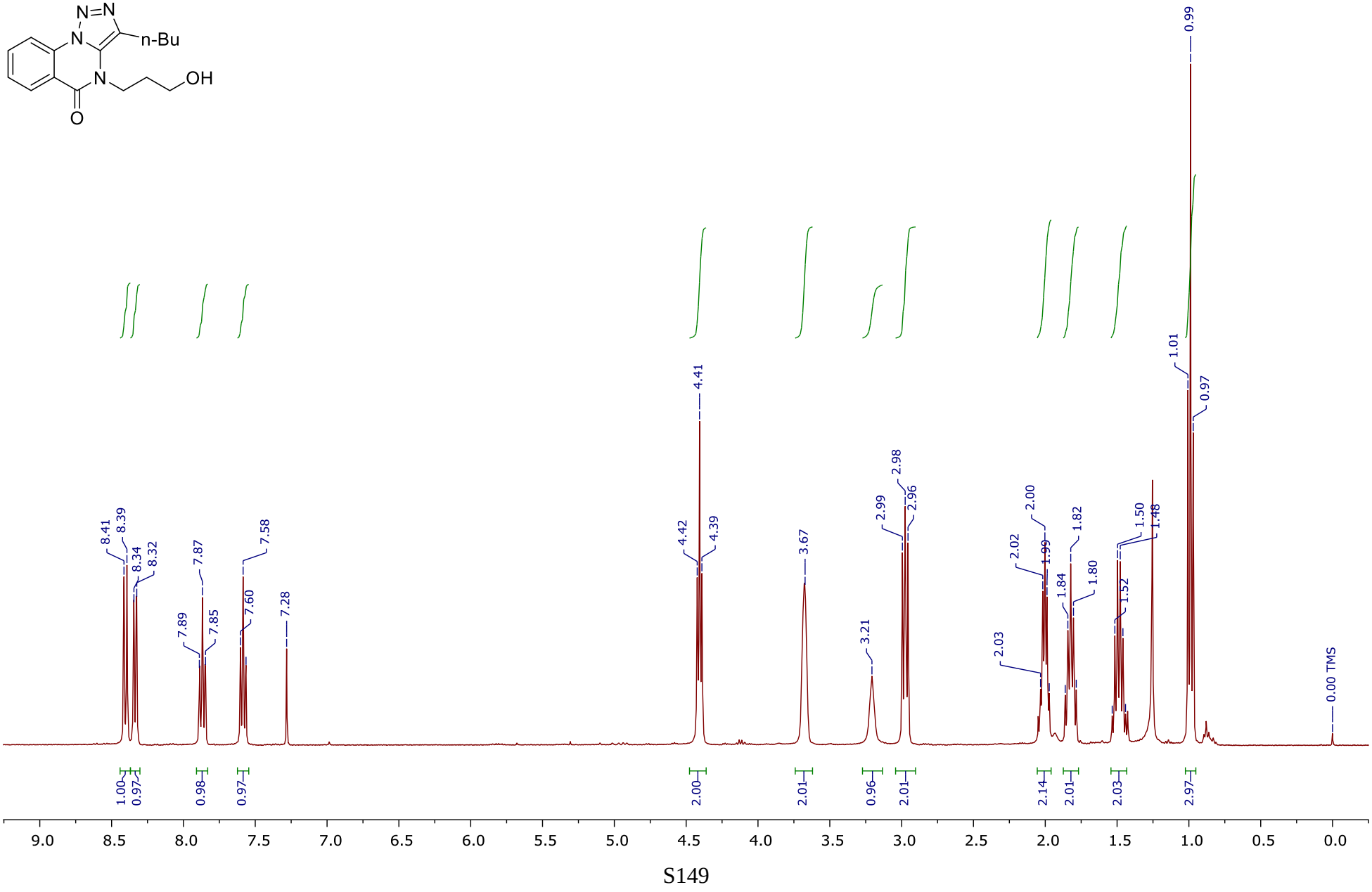
3-Butyl-4-[(1*S*)-1-(hydroxymethyl)-2-methylpropyl][1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6j)

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



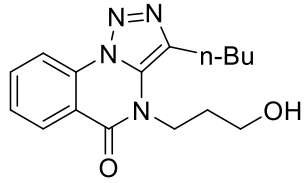
3-Butyl-4-(3-hydroxypropyl)[1,2,3]triazolo[1,5-*a*]quinazolin-5(4*H*)-one (6k)

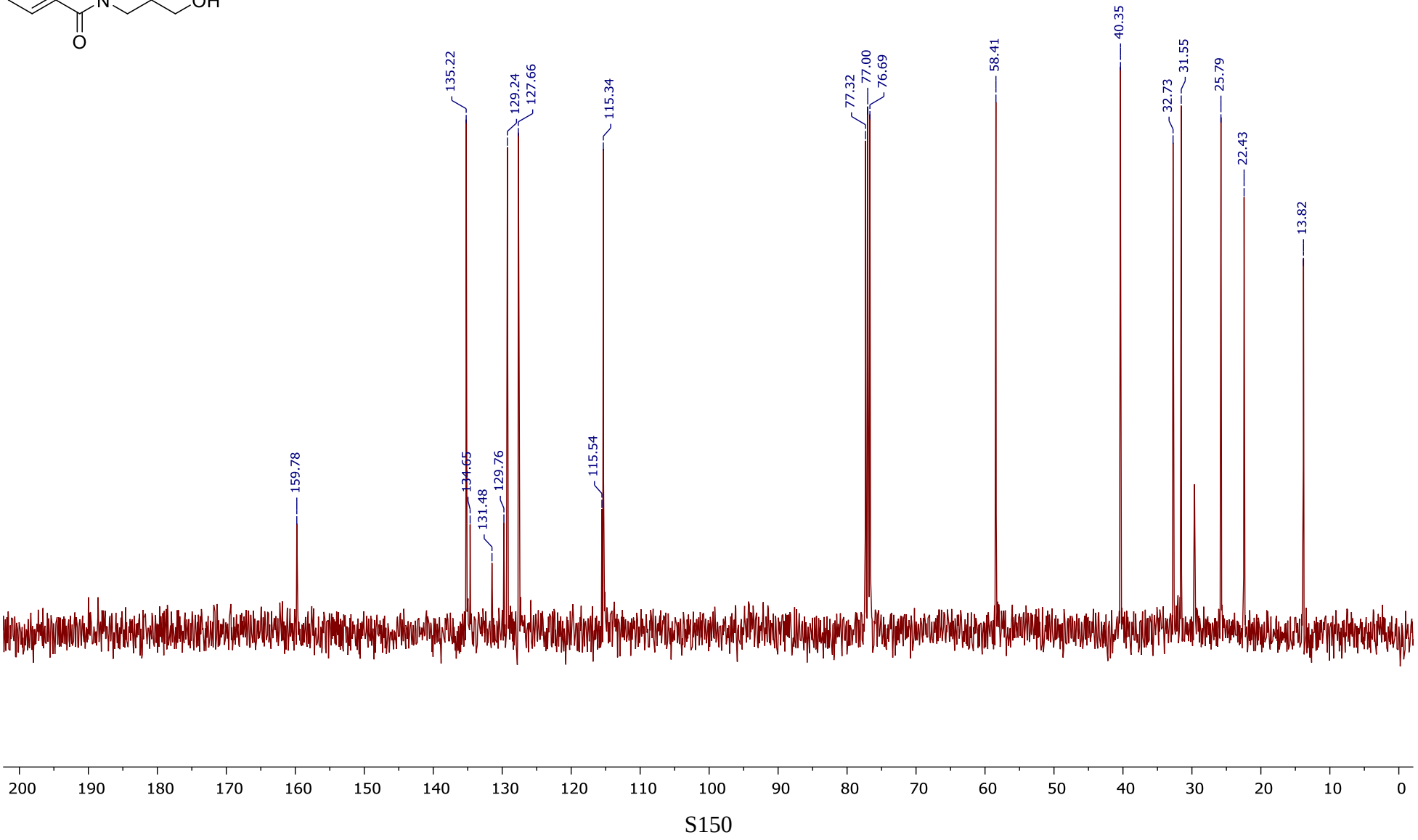
^{1}H NMR (400 MHz, $CDCl_3$)



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

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)





References

[1] Levesque, P.; Fournier, P. A. *J. Org. Chem.* **2010**, *75*, 7033.

[2] Gevondian, A. G.; Kotovshchikov, Y. N.; Latyshev, G. V.; Lukashev, N. V.; Beletskaya, I. P. *J. Org. Chem.* **2021**, *86*, 5639.

[3] Xu, W.; Chen, Q.-Y. *J. Org. Chem.* **2002**, *67*, 9421.

[4] Kotovshchikov, Y. N., Tatevosyan, S. S., Latyshev, G. V., Kugusheva, Z. R., Lukashev, N. V., Beletskaya, I. P. *New J. Chem*, **2023**, *47*, 12239.

[5] Kotovshchikov, Y. N.; Latyshev, G. V.; Navasardyan, M. A.; Erzunov, D. A.; Beletskaya, I. P.; Lukashev, N. V. *Org. Lett.* **2018**, *20*, 4467.

[6] Schulman, J. M.; Friedman, A. A.; Panteleev, J.; Lautens, M. *Chem. Comm.* **2012**, *48*, 55.

[7] Tatevosyan, S. S., Kotovshchikov, Y. N., Latyshev, G. V., Lukashev, N. V., Beletskaya, I.P. *Synthesis* **2022**, *54*, 369.

[8] Neese, F. *WIREs Comput. Mol. Sci.* **2025**, *15*, e70019.

[9] *(a)* Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 5656. *(b)* Lehtola, S.; Steigemann, C.; Oliveira, M. J. T.; Marques, M. A. L. *SoftwareX* **2018**, *7*, 1–5.

[10] (*a*) Caldeweyher, E.; Bannwarth, C.; Grimme, S. *J. Chem. Phys.* **2017**, *147*, 034112. (*b*) Caldeweyher, E.; Ehlert, S.; Hansen, A.; Neugebauer, H.; Spicher, S.; Bannwarth, C.; Grimme, S. *J. Chem. Phys.* **2019**, *150*, 154122.

[11] Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

[12] (*a*) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995. (*b*) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, *24*, 669.

[13] (*a*) Helmich-Paris, B.; De Souza, B.; Neese, F.; Izsák, R. *J. Chem. Phys.* **2021**, *155*, 104109. (*b*) Bykov, D.; Petrenko, T.; Izsák, R.; Kossmann, S.; Becker, U.; Valeev, E.; Neese, F. *Mol. Phys.* **2015**, *113*, 1961. (*c*) Neese, F.; Wennmohs, F.; Hansen, A.; Becker, U. *Chem. Phys.* **2009**, *356*, 98.

[14] Allouche, A. *J. Comput. Chem.* **2011**, *32*, 174.

[15] Pracht, P.; Grimme, S.; Bannwarth, C.; Bohle, F.; Ehlert, S.; Feldmann, G.; Gorges, J.; Müller, M.; Neudecker, T.; Plett, C.; Spicher, S.; Steinbach, P.; Wesołowski, P. A.; Zeller, F. *J. Chem. Phys.* **2024**, *160*, 114110.

[16] Grimme, S. *Chem. Eur. J.* **2012**, *18*, 9955.

[17] CYLview, 1.0b; C. Y. Legault, Université de Sherbrooke, 2009, **http://www.cylview.org**.

[18] (*a*) Laplaza, R.; Peccati, F.; A. Boto, R.; Quan, C.; Carbone, A.; Piquemal, J.-P.; Maday, Y.; Contreras-García, J. *WIREs Comp. Mol. Sci.* **2021**, *11*, e1497. (*b*) Contreras-García, J.; Johnson, E. R.; Keinan, S.; Chaudret, R.; Piquemal, J.-P.; Beratan, D. N.; Yang, W. *J. Chem. Theory Comput.* **2011**, *7*, 625.

[19] (*a*) Stone, J. An Efficient Library for Parallel Ray Tracing and Animation. Master's Thesis, Computer Science Department, University of Missouri-Rolla, 1998. (*b*) Humphrey, W.; Dalke, A.; Schulten, K. *J. Mol. Graph.* **1996**, *14*, 33.