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Supporting Information

for

Anomeric 1,2,3-triazole-linked sialic acid derivatives show selective inhibition towards a bacterial neuraminidase over a trypanosome *trans*-sialidase

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Analytical data, ^{1}H and ^{13}C NMR spectra of compounds 1, 2a–h and 3a–h, and calculated LogP of compounds 3a–h

CONTENT

Analytical data of compounds 1, 2a–h and 3a–h

Compound **1**:

Methyl 4,7,8,9-tetra-*O*-acetyl-2-azido-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-galactonon-2-ulopyranosonate (**1**) [25,26]

Yield: 72% (370 mg; 0.72 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.36-5.31 (2H, m, H-8, H-7), 5.29 (1H, d, $J_{AcNH,5}$ = 10.0 Hz, CH_3CONH), 5.05 (1H, ddd, $J_{4,3ax}$ = 11.7 Hz, $J_{4,5}$ = 10.3 Hz, $J_{4,3eq}$ = 4.8 Hz, H-4), 4.38-4.32 (1H, m, H-9a), 4.16-4.10 (1H, m, H-9b), 4.05 (1H, q, $J_{5,4}$ = $J_{5,AcNH}$ = $J_{5,6}$ = 10.3 Hz, H-5), 3.91-3.86 (4H, m, H-6, CO_2CH_3), 2.56 (1H, dd, $J_{3eq,3ax}$ = 13.1 Hz, $J_{3eq,4}$ = 4.8 Hz, H-3_{eq}), 2.14 (3H, s, CH_3CO), 2.12 (3H, s, CH_3CO), 2.03 (6H, s, 2x CH_3CO), 1.88 (3H, s, CH_3CONH), 1.87-1.79 (1H, m, H-3_{ax}). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.7, 170.4, 170.2, 170.1 (4x $CH_3\underline{C}O$, C-1), 167.2 ($CH_3\underline{C}ONH$), 89.1 (C-2), 74.1 (C-6), 69.6 (C-8), 68.9 (C-4), 67.6 (C-7), 62.2 (C-9), 53.6 ($CO_2\underline{C}H_3$), 49.4 (C-5), 36.7 (C-3), 23.3 ($\underline{C}H_3CONH$), 21.1, 20.9, 20.8, 20.8 (4x $\underline{C}H_3CO$). HRMS (ESI): *m/z* calculated for $C_{20}H_{28}N_4NaO_{12}$ $[M+Na]^+$: 539.1601; found: 539.1608.

Compounds **2a–h**:

Methyl 4,7,8,9-tetra-*O*-acetyl-2-{4-[2-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-*galacto*non-2-ulopyranosonate (**2a**)

Yield: 70% (28 mg; 0.041 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (1H, s, C*H*-triazole), 7.88 (1H, d, *J* = 7.7 Hz, H-Ph), 7.76 (1H, dd, *J* = 8.0 Hz, *J* =1.3 Hz, H-Ph), 7.63 (1H, td, *J* = 7.7, 1.3 Hz, H-Ph), 7.50 (1H, t, *J* = 7.7 Hz, H-Ph), 5.47-5.37 (3H, m, H-8, H-7, CH_3CONH), 5.23 (1H, ddd, *J* = 11.8 Hz, *J* = 10.2 Hz, *J* = 4.5 Hz, H-4), 4.41 (1H, dd, *J* = 10.8 Hz, *J* = 2.2 Hz, H-6), 4.25 (1H, dd, *J* = 12.4 Hz, *J* = 2.6 Hz, H-9a), 4.15 (1H, q, *J* = 10.3 Hz, H-5), 4.08 (1H, dd, *J* = 12.5 Hz, *J* = 5.6 Hz, H-9b), 3.79 (3H, s, CO_2CH_3), 3.48 (1H, dd, *J* = 13.3 Hz, *J* = 4.5 Hz, H-3_{eq}), 2.80 (1H, dd, *J* = 13.4 Hz, *J* = 11.8 Hz, H-3_{ax}), 2.15 (3H, s, CH_3CO), 2.13 (3H, s, CH_3CO), 2.08 (3H, s, CH_3CO), 2.03 (3H, s, CH_3CO), 1.92 (3H, s, CH_3CONH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0, 170.7, 170.4, 170.2, 170.2 (4x $CH_3\underline{C}O$, C-1), 166.7 ($CH_3\underline{C}ONH$), 145.2 ($\underline{C}CH$-triazole), 132.1 (Ph-$\underline{C}H$), 132.0 (Ph-$\underline{C}H$), 129.2 ($C_{quat.}$), 128.7 (Ph-$\underline{C}H$), 128.3 ($C_{quat.}$), 127.9 ($C_{quat.}$), 126.4 (Ph-$\underline{C}H$), 122.3 ($\underline{C}H$-triazole), 88.6 (C-2), 74.0 (C-6), 68.7 (C-4), 68.3 (C-8), 67.1 (C-7), 62.4 (C-9), 54.1 ($CO_2\underline{C}H_3$), 49.5 (C-5), 36.0 (C-3), 23.3 ($\underline{C}H_3CONH$), 21.2, 21.0, 20.9, 20.8 (4x $\underline{C}H_3CO$). HRMS (ESI): *m/z* calculated for $C_{29}H_{33}F_3N_4NaO_{12}$ $[M+Na]^+$: 709.1945; found: 709.1925.

Methyl 4,7,8,9-tetra-*O*-acetyl-2-{4-[3-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-*galacto*non-2-ulopyranosonate (**2b**)

Yield: 62% (28 mg; 0.041 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (1H, s, C*H*-triazole), 8.21 (1H, d, *J* = 1.8 Hz, H-Ph), 8.09 (1H, dt, *J* = 7.2 Hz, *J* =1.7 Hz, H-Ph), 7.62-7.53 (2H, m, H-Ph), 5.50 (1H, ddd, *J* = 8.0 Hz, *J* = 6.4 Hz, *J* = 2.7 Hz, H-8), 5.44-5.38 (2H, m, CH_3CON*H*, H-7), 5.20 (1H, ddd, *J* = 12.0 Hz, *J* = 10.3 Hz, *J* = 4.4 Hz, H-4), 4.44-4.34 (2H, m, H-6, H-9a), 4.16 (1H, q, *J* = 10.4 Hz, H-5), 4.03 (1H, dd, *J* = 12.4 Hz, *J* = 6.4 Hz, H-9b), 3.80 (3H, s, CO_2C*H*$_3$), 3.54 (1H, dd, *J* = 13.2 Hz, *J* = 4.4 Hz, H-3$_{eq}$), 2.73 (1H, dd, *J* = 13.3 Hz, *J* = 12.0 Hz, H-3$_{ax}$), 2.19 (3H, s, C*H*$_3$CO), 2.12 (3H, s, C*H*$_3$CO), 2.09 (3H, s, C*H*$_3$CO), 2.08 (3H, s, C*H*$_3$CO), 1.91 (3H, s, C*H*$_3$CONH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0, 170.9, 170.7, 170.4, 170.2 (4x $CH_3\underline{C}O$, C-1), 166.6 ($CH_3\underline{C}ONH$), 147.2 (<u>C</u>CH-triazole), 131.2 ($C_{quat.}$), 131.1 ($C_{quat.}$), 129.5 (Ph-<u>C</u>H), 129.1 (Ph-<u>C</u>H), 125.4 ($C_{quat.}$), 125.1 (Ph-<u>C</u>H), 122.9 (Ph-<u>C</u>H), 119.8 (triazole-<u>C</u>H), 88.7 (C-2), 74.3 (C-6), 68.7 (C-4), 68.6 (C-8), 67.4 (C-7), 62.5 (C-9), 54.3 ($CO_2\underline{C}H_3$), 49.4 (C-5), 36.0 (C-3), 23.3 ($\underline{C}H_3CONH$), 21.4, 21.0, 20.9, 20.8 (4x $\underline{C}H_3CO$). HRMS (ESI): *m/z* calculated for $C_{29}H_{33}F_3N_4NaO_{12}$ $[M+Na]^+$: 709.1945; found: 709.1923.

Methyl 4,7,8,9-tetra-*O*-acetyl-2-{4-[4-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-*galacto*non-2-ulopyranosonate (**2c**)

Yield: 78% (24 mg; 0.035 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (1H, s, C*H*-triazole), 8.03 (2H, d, *J* = 8.1 Hz, H-Ph), 7.69 (2H, d, *J* = 8.2 Hz, H-Ph), 5.51 (1H, ddd, *J* = 8.6 Hz, *J* = 5.9 Hz, *J* = 2.7 Hz, H-8), 5.43-5.35 (2H, m, CH_3CON*H*, H-7), 5.20 (1H, ddd, *J* = 12.0 Hz, *J* = 10.3 Hz, *J* = 4.4 Hz, H-4), 4.40-4.31 (2H, m, H-6, H-9a), 4.15 (1H, q, *J* = 10.3 Hz, H-5), 4.06 (1H, dd, *J* = 12.4 Hz, *J* = 5.9 Hz, H-9b), 3.79 (3H, s, CO_2C*H*$_3$), 3.54 (1H, dd, *J* = 13.2 Hz, *J* = 4.5 Hz, H-3$_{eq}$), 2.72 (1H, dd, *J* = 13.2 Hz, *J* = 12.0 Hz, H-3$_{ax}$), 2.20 (3H, s, C*H*$_3$CO), 2.11 (3H, s, C*H*$_3$CO), 2.09 (3H, s, C*H*$_3$CO), 2.08 (3H, s, C*H*$_3$CO), 1.92 (3H, s, C*H*$_3$CONH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0, 170.8, 170.7, 170.4, 170.2 (4x $CH_3\underline{C}O$, C-1), 166.6 ($CH_3\underline{C}ONH$), 147.2 (<u>C</u>CH-triazole), 133.6 ($C_{quat.}$), 130.5 ($C_{quat.}$), 130.2 ($C_{quat.}$), 126.2 (2x Ph-<u>C</u>H), 126.0 (2x Ph-<u>C</u>H), 120.0 (triazole-<u>C</u>H), 88.6 (C-2), 74.1 (C-6), 68.5 (C-4), 68.2 (C-8), 67.1 (C-7), 62.5 (C-9), 54.3 ($CO_2\underline{C}H_3$), 49.4 (C-5), 36.0 (C-3), 23.3 ($\underline{C}H_3CONH$), 21.4, 21.0, 20.9, 20.9 (4x $\underline{C}H_3CO$). HRMS (ESI): *m/z* calculated for $C_{29}H_{33}F_3N_4NaO_{12}$ $[M+Na]^+$: 709.1945; found: 709.1921.

Methyl 4,7,8,9-tetra-*O*-acetyl-2-[4-(pyridine-2-yl)-1*H*-1,2,3-triazol-1-yl]-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-*galacto*non-2-ulopyranosonate (**2d**)

Yield: 71% (30 mg; 0.048 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (1H, dt, *J* = 4.9 Hz, *J* = 1.3 Hz, H-Py), 8.50 (1H, s, C*H*-triazole), 8.13 (1H, dd, *J* = 7.9 Hz, *J* = 1.2 Hz, H-Py), 7.77 (1H, td, *J* = 7.7 Hz, *J* = 1.8 Hz, H-Py), 7.25-7.20 (1H, m, H-Py), 5.50 (1H,

ddd, *J* = 8.4 Hz, *J* = 5.3 Hz, *J* = 2.9 Hz, H-8), 5.45 (1H, d, *J* = 9.8 Hz, $CH_3CON\mathit{H}$), 5.39 (1H, dd, *J* = 8.6 Hz, *J* = 2.2 Hz, H-7), 5.23 (1H, ddd, *J* = 11.8 Hz, *J* = 10.2 Hz, *J* = 4.5 Hz, H-4), 4.38 (1H, ddd, *J* = 10.8 Hz, *J* = 2.2 Hz, H-6), 4.25 (1H, dd, *J* = 12.5 Hz, *J* = 2.9 Hz, H-9a), 4.18-4.08 (2H, m, H-5, H9-b), 3.79 (3H, s, $CO_2C\mathit{H}_3$), 3.48 (1H, dd, *J* = 13.3 Hz, *J* = 4.5 Hz, H-3_{eq}), 2.71 (1H, dd, *J* = 13.3 Hz, *J* = 11.9 Hz, H-3_{ax}), 2.17 (3H, s, $C\mathit{H}_3CO$), 2.10 (3H, s, $C\mathit{H}_3CO$), 2.07 (3H, s, $C\mathit{H}_3CO$), 2.06 (3H, s, $C\mathit{H}_3CO$), 1.91 (3H, s, $C\mathit{H}_3CONH$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.7, 170.4, 170.3, 170.1 (4x $CH_3\underline{C}O$, C-1), 166.5 ($CH_3\underline{C}ONH$), 149.9 (<u>C</u>CH-triazole), 149.8 (Py-<u>C</u>H), 148.9 ($C_{quat.}$), 137.0 (Py-<u>C</u>H), 123.2 (Py-<u>C</u>H), 121.1 (Py-<u>C</u>H), 120.7 (triazole-<u>C</u>H), 88.7 (C-2), 73.9 (C-6), 68.6 (C-4), 68.3 (C-8), 67.0 (C-7), 62.3 (C-9), 54.2 ($CO_2\underline{C}H_3$), 49.5 (C-5), 36.5 (C-3), 23.3 ($\underline{C}H_3CONH$), 21.3, 21.0, 20.9, 20.9 (4x $\underline{C}H_3CO$). HRMS (ESI): *m/z* calculated for $C_{27}H_{33}N_5NaO_{12}$ $[M+Na]^+$: 642.2023; found: 642.2014.

Methyl 4,7,8,9-tetra-*O*-acetyl-2-{4-[(*N*-methylbenzylamino)methyl]-1*H*-1,2,3-triazol-1-yl}-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-*galacto*non-2-ulopyranosonate (**2e**)

Yield: 71% (26 mg; 0.038 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (1H, s, C*H*-triazole), 7.39-7.21 (5H, m, H-Ph), 5.45 (1H, ddd, *J* = 8.4 Hz, *J* = 5.6 Hz, *J* = 2.7 Hz, H-8), 5.42-5.35 (2H, m, $CH_3CON\mathit{H}$, H-7), 5.18 (1H, ddd, *J* = 12.0 Hz, *J* = 10.3 Hz, *J* = 4.5 Hz, H-4), 4.35-4.25 (2H, m, H-6, H-9a), 4.16-4.04 (2H, m, H-5, H-9b), 3.76 (3H, s, $CO_2C\mathit{H}_3$), 3.74 (2H, s, $C\mathit{H}_2$), 3.57 (2H, s, $C\mathit{H}_2$), 3.44 (1H, dd, *J* = 13.3 Hz, *J* = 4.5 Hz, H-3_{eq}), 2.68 (1H, dd, *J* = 13.3 Hz, *J* = 12.0 Hz, H-3_{ax}), 2.25 (3H, s, $NC\mathit{H}_3$), 2.17 (3H, s, $C\mathit{H}_3CO$), 2.11 (3H, s, $C\mathit{H}_3CO$), 2.07 (3H, s, $C\mathit{H}_3CO$), 2.04 (3H, s, $C\mathit{H}_3CO$), 1.91 (3H, s, $C\mathit{H}_3CONH$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0, 170.7, 170.4, 170.3, 170.2 (4x $CH_3\underline{C}O$, C-1), 166.7 ($CH_3\underline{C}ONH$), 145.9 (<u>C</u>CH-triazole), 138.7 ($C_{quat.}$), 129.3 (2x Ph-<u>C</u>H), 128.4 (2x Ph-<u>C</u>H), 127.2 (Ph-<u>C</u>H), 121.8 (triazole-<u>C</u>H), 88.5 (C-2), 73.9 (C-6), 68.7 (C-4), 68.2 (C-8), 67.1 (C-7), 62.4 (C-9), 61.4 ($\underline{C}H_2$), 54.1 ($CO_2\underline{C}H_3$), 51.9 ($\underline{C}H_2$), 49.4 (C-5), 42.2 ($N\underline{C}H_3$), 36.2 (C-3), 23.3 ($\underline{C}H_3CONH$), 21.3, 21.0, 20.9, 20.8 (4x $\underline{C}H_3CO$). HRMS (ESI): *m/z* calculated for $C_{31}H_{42}N_5O_{12}$ $[M+H]^+$: 676.2830; found: 676.2813.

Methyl 4,7,8,9-tetra-*O*-acetyl-2-[4-(1-hydroxypropyl)-1*H*-1,2,3-triazol-1-yl]-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-*galacto*non-2-ulopyranosonate (**2f**)

Yield: 54% (24 mg; 0.040 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (1H, d, *J* = 4.3 Hz, C*H*-triazole), 5.57 (1H, d, *J* = 9.8 Hz, $CH_3CON\mathit{H}$), 5.44-5.34 (2H, H-8, H-7), 5.16 (1H, ddd, *J* = 11.9 Hz, *J* = 10.3 Hz, *J* = 4.4 Hz, H-4), 4.84-4.78 (1H, m, C*H*OH), 4.37-4.28 (2H, m, H-6, H-9a), 4.12 (1H, q, *J* = 10.3 Hz, H-5), 4.02 (1H, ddd, *J* = 12.5 Hz, *J* = 5.7 Hz, *J* = 1.8 Hz, H9-b), 3.77 (3H, s, $CO_2C\mathit{H}_3$), 3.43 (1H, dd, *J* = 13.3 Hz, *J* = 4.5 Hz, H-3_{eq}), 2.78 (1H, d, *J* = 19.5 Hz, O*H*), 2.66 (1H, dd, *J* = 13.3 Hz, *J* = 12.0 Hz, H-3_{ax}), 2.15 (3H, s, $C\mathit{H}_3CO$), 2.10 (3H, s, $C\mathit{H}_3CO$), 2.06 (3H, s, $C\mathit{H}_3CO$), 2.04 (3H, s, $C\mathit{H}_3CO$), 1.98-1.91 (2H, m, $C\mathit{H}_2CH_3$), 1.89 (3H, s, $C\mathit{H}_3CONH$), 1.01 (3H, td, *J* = 7.4 Hz, *J* = 1.1 Hz, $CH_2C\mathit{H}_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0, 170.8, 170.5, 170.4,

170.2 (4x $CH_3\underline{C}O$, C-1), 166.5 ($CH_3\underline{C}ONH$), 152.0 (<u>C</u>CH-triazole), 119.8 (triazole-<u>C</u>H), 88.6 (C-2), 74.1 (C-6), 68.6 (C-4, C-8), 68.3 (CHOH), 67.2 (C-7), 62.5 (C-9), 54.2 ($CO_2\underline{C}H_3$), 49.3 (C-5), 36.1 (C-3), 30.1 ($\underline{C}H_2CH_3$), 23.2 ($\underline{C}H_3CONH$), 21.3, 21.0, 20.9, 20.9 (4x $\underline{C}H_3CO$), 9.9 ($CH_2\underline{C}H_3$). HRMS (ESI): *m/z* calculated for $C_{25}H_{36}N_4NaO_{13}$ $[M+Na]^+$: 236.2177; found: 236.2166.

Methyl 4,7,8,9-tetra-*O*-acetyl-2-[4-(2-hydroxypropyl)-1*H*-1,2,3-triazol-1-yl]-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-*galacto*non-2-ulopyranosonate (**2g**)

Yield: 45% (20 mg; 0.033 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (1H, d, *J* = 3.8 Hz, C*H*-triazole), 5.46-5.35 (3H, m, H-8, $CH_3CON\mathit{H}$, H-7), 5.16 (1H, ddd, *J* = 12.0 Hz, *J* = 10.3 Hz, *J* = 4.4 Hz, H-4), 4.34-4.28 (2H, m, H-6, H-9a), 4.21-4.14 (1H, m, C*H*OH), 4.11 (1H, q, *J* = 10.4 Hz, H-5), 4.04 (1H, ddd, *J* = 12.5 Hz, *J* = 5.8 Hz, *J* = 1.9 Hz, H9-b), 3.78 (3H, s, $CO_2C\mathit{H}_3$), 3.43 (1H, dd, *J* = 13.2 Hz, *J* = 4.5 Hz, H-3_{eq}), 3.05 (1H, s, O*H*), 2.91 (1H, dd, *J* = 15.1 Hz, *J* = 3.5 Hz, CH_2CHOH), 2.79 (1H, ddd, *J* = 15.4 Hz, *J* = 8.5 Hz, *J* = 2.5 Hz, CH_2CHOH), 2.67 (1H, dd, *J* = 13.3 Hz, *J* = 12.1 Hz, H-3_{ax}), 2.17 (3H, s, CH_3CO), 2.12 (3H, s, CH_3CO), 2.07 (3H, s, CH_3CO), 2.05 (3H, s, CH_3CO), 1.90 (3H, s, CH_3CONH), 1.29 (3H, dd, *J* = 6.2 Hz, *J* = 1.4 Hz, CH_3CHOH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0, 170.8, 170.5, 170.4, 170.2 (4x $CH_3\underline{C}O$, C-1), 166.6 ($CH_3\underline{C}ONH$), 146.2 (<u>C</u>CH-triazole), 120.9 (triazole-<u>C</u>H), 88.5 (C-2), 74.0 (C-6), 68.6 (C-4), 68.4 (C-8), 67.1 (C-7, CHOH), 62.5 (C-9), 54.2 ($CO_2\underline{C}H_3$), 49.4 (C-5), 36.1 (C-3), 35.0 ($\underline{C}H_2CHOH$), 23.3 ($\underline{C}H_3CONH$), 23.0 ($\underline{C}H_3CHOH$), 21.3, 21.0, 20.9, 20.9 (4x $\underline{C}H_3CO$). HRMS (ESI): *m/z* calculated for $C_{25}H_{36}N_4NaO_{13}$ $[M+Na]^+$: 236.2177; found: 236.2166.

Methyl 4,7,8,9-tetra-*O*-acetyl-2-(4-phenylmethyl-1*H*-1,2,3-triazol-1-yl)-5-acetamido-2,3,5-trideoxy-D-*glycero*-α-D-*galacto*non-2-ulopyranosonate (**2h**)

Yield: 49% (24 mg; 0.038 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (1H, s, C*H*-triazole), 7.34-7.28 (4H, m, H-Ph), 7.24-7.19 (1H, m, H-Ph), 5.44 (1H, d, *J* = 9.8 Hz, $CH_3CON\mathit{H}$), 5.40 (1H, ddd, *J* = 8.3 Hz, *J* = 5.6 Hz, *J* = 2.6 Hz, H-8), 5.35 (1H, dd, *J* = 8.5 Hz, *J* = 2.2 Hz, H-7), 5.15 (1H, ddd, *J* = 11.9 Hz, *J* = 10.2 Hz, *J* = 4.5 Hz, H-4), 4.31-4.24 (2H, m, H-6, H-9a), 4.14-4.02 (4H, m, H-5, H-9b, CH_2), 3.76 (3H, s, $CO_2C\mathit{H}_3$), 3.42 (1H, dd, *J* = 13.3 Hz, *J* = 4.5 Hz, H-3_{eq}), 2.65 (1H, dd, *J* = 13.3 Hz, *J* = 12.0 Hz, H-3_{ax}), 2.13 (3H, s, CH_3CO), 2.09 (3H, s, CH_3CO), 2.06 (3H, s, CH_3CO), 2.04 (3H, s, CH_3CO), 1.89 (3H, s, CH_3CONH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.7, 170.4, 170.3, 170.2 (4x $CH_3\underline{C}O$, C-1), 166.6 ($CH_3\underline{C}ONH$), 147.8 (<u>C</u>CH-triazole), 138.8 ($C_{quat.}$), 128.9 (2x Ph-<u>C</u>H), 128.7 (2x Ph-<u>C</u>H), 126.6 (Ph-<u>C</u>H), 120.5 (triazole-<u>C</u>H), 88.5 (C-2), 73.9 (C-6), 68.7 (C-4), 68.3 (C-8), 67.1 (C-7), 62.4 (C-9), 54.1 ($CO_2\underline{C}H_3$), 49.4 (C-5), 36.1 (C-3), 32.1 ($\underline{C}H_2$), 23.3 ($\underline{C}H_3CONH$), 21.3, 21.0, 20.9, 20.8 (4x $\underline{C}H_3CO$). HRMS (ESI): *m/z* calculated for $C_{29}H_{36}N_4NaO_{12}$ $[M+Na]^+$: 655.2227; found: 655.2215.

Compounds **3a–h**:

5-Acetamido-3,5-dideoxy-2-{4-[2-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-D-*glycero*-α-D-*galacto*-non-2-ulopyranosidic acid (**3a**)

Yield: 85% (20 mg; 0.040 mmol); $[\alpha]_D^{20}$ -26.6 (c 1, H_2O). ^{1}H NMR (400 MHz, D_2O) δ 8.33 (1H, s, C*H*-triazole), 7.89 (1H, d, *J* = 7.8 Hz, H-Ph), 7.73 (1H, t, *J* = 7.6 Hz, H-Ph), 7.69-7.60 (2H, m, H-Ph), 4.10-3.84 (5H, ms - overlapped signals, H-4, H-5, H-6, H-7, H-9a), 3.70-3.61 (2H, m, H-8, H-9b), 3.39-3.30 (1H, m, H-3_{eq}), 2.35 (1H, t, *J* = 11.4 Hz, H-3_{ax}), 2.08 (3H, s, CH_3CONH). ^{13}C NMR (101 MHz, D_2O) δ 175.0 (C-1), 170.5 (CH_3CONH), 144.5 (CCH-triazole), 132.3 (Ph-CH), 132.0 (Ph-CH), 129.4 (Ph-CH), 127.8 ($C_{quat.}$), 126.4 (Ph-CH), 122.5 (CH-triazole), 91.0 (C-2), 74.2, 71.4, 68.1, 68.0, (C-4, C-6, C-7, C-8), 62.6 (C-9), 51.5 (C-5), 39.5 (C-3), 22.1 (CH_3CONH). HRMS (ESI): *m/z* calculated for $C_{20}H_{23}F_3N_4NaO_8$ $[M+Na]^+$: 527.1360; found: 527.1352.

5-Acetamido-3,5-dideoxy-2-{4-[3-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-D-*glycero*-α-D-*galacto*-non-2-ulopyranosidic acid (**3b**)

Yield: 98% (23 mg; 0.046 mmol); $[\alpha]_D^{20}$ -20.0 (c 1, H_2O). ^{1}H NMR (400 MHz, D_2O) δ 8.51 (1H, s, C*H*-triazole), 7.96 (1H, s, H-Ph), 7.90 (1H, d, *J* = 7.8 Hz, H-Ph), 7.61 (1H, d, *J* = 7.9 Hz, H-Ph), 7.53 (1H, d, *J* = 7.8 Hz, H-Ph), 4.11-3.88 (5H, ms - overlapped signals, H-4, H-5, H-6, H-7, H-9a), 3.72-3.63 (2H, m, H-8, H-9b), 3.38-3.29 (1H, m, H-3_{eq}), 2.29 (1H, t, *J* = 11.5 Hz, H-3_{ax}), 2.09 (3H, s, CH_3CONH). ^{13}C NMR (101 MHz, D_2O) δ 175.0 (C-1), 170.4 (CH_3CONH), 145.9 (CCH-triazole), 129.9 ($C_{quat.}$), 129.6 (Ph-CH), 129.0 (Ph-CH), 125.1 (Ph-CH), 122.2 (Ph-CH), 120.2 (CH-triazole), 91.0 (C-2), 74.2, 71.3, 68.1, 68.0, (C-4, C-6, C-7, C-8), 62.7 (C-9), 51.6 (C-5), 39.8 (C-3), 22.0 (CH_3CONH). HRMS (ESI): *m/z* calculated for $C_{20}H_{23}F_3N_4NaO_8$ $[M+Na]^+$: 527.1360; found: 527.1346.

5-Acetamido-3,5-dideoxy-2-{4-[4-(trifluoromethyl)phenyl]-1*H*-1,2,3-triazol-1-yl}-D-*glycero*-α-D-*galacto*-non-2-ulopyranosidic acid (**3c**)

Yield: 69% (14 mg; 0.028 mmol); $[\alpha]_D^{20}$ -18.3 (c 1, H_2O). ^{1}H NMR (400 MHz, D_2O) δ 8.58 (1H, s, C*H*-triazole), 7.90 (2H, d, *J* = 8.1 Hz, H-Ph), 7.76 (2H, d, *J* = 8.2 Hz, H-Ph), 4.11-3.84 (5H, ms - overlapped signals, H-4, H-5, H-6, H-7, H-9a), 3.71-3.64 (2H, m, H-8, H-9b), 3.33 (1H, dd, *J* = 12.5 Hz, *J* = 3.9 Hz, H-3_{eq}), 2.30 (1H, t, *J* = 11.5 Hz, H-3_{ax}), 2.08 (3H, s, CH_3CONH). ^{13}C NMR (101 MHz, D_2O) δ 175.0 (C-1), 170.5 (CH_3CONH), 146.0 (CCH-triazole), 132.9 ($C_{quat.}$), 129.8 ($C_{quat.}$), 126.0 (4x Ph-CH), 120.6 (CH-triazole), 91.0 (C-2), 74.2, 71.3, 68.1, 68.0, (C-4, C-6, C-7, C-8), 62.7 (C-9), 51.5 (C-5), 39.8 (C-3), 22.0 (CH_3CONH). HRMS (ESI): *m/z* calculated for $C_{20}H_{23}F_3N_4NaO_8$ $[M+Na]^+$: 527.1360; found: 527.1351.

5-Acetamido-3,5-dideoxy-2-[4-(pyridine-2-yl)-1*H*-1,2,3-triazol-1-yl]-D-*glycero*-α-D-*galacto*-non-2-ulopyranosidic acid (**3d**)

Yield: 71% (17 mg; 0.040 mmol); $[\alpha]_D^{20}$ -32.0 (c 1, H_2O). ^{1}H NMR (400 MHz, D_2O) δ 8.57 (1H, s, C*H*-triazole), 8.50 (1H, s, H-Py), 7.90 (2H, d, *J* = 4.3 Hz, H-Py), 7.39 (1H, q, *J* = 4.6 Hz, H-Py), 4.09-3.88 (5H, ms - overlapped signals, H-4, H-5, H-6, H-7, H-9a), 3.71-3.64 (2H, m, H-8, H-9b), 3.36 (1H, dd, *J* = 12.5 Hz, *J* = 4.0 Hz, H-3_{eq}), 2.30 (1H, t, *J* = 11.5 Hz, H-3_{ax}), 2.08 (3H, s, CH_3CONH). ^{13}C NMR (101 MHz, D_2O) δ 175.0 (C-1), 170.5 (CH_3CONH), 149.0 (Py-CH), 146.6 (CCH-triazole), 138.4 (Py-CH), 124.0 (Py-CH), 121.3 (Py-CH), 121.1 (CH-triazole), 91.0 (C-2), 74.2, 71.3, 68.1, 68.0, (C-4, C-6, C-7, C-8), 62.7 (C-9), 51.5 (C-5), 39.7 (C-3), 22.1 (CH_3CONH). HRMS (ESI): *m/z* calculated for $C_{18}H_{24}N_5O_8$ $[M+H]^+$: 438.1619; found: 438.1623.

5-Acetamido-3,5-dideoxy-2-{4-[(*N*-methylbenzylamino)methyl]-1*H*-1,2,3-triazol-1-yl}-D-*glycero*-α-D-*galacto*-non-2-ulopyranosidic acid (**3e**)

Yield: 82% (18 mg; 0.037 mmol); $[\alpha]_D^{20}$ -18.1 (c 1, H_2O). ^{1}H NMR (400 MHz, D_2O) δ 8.18 (1H, s, C*H*-triazole), 7.48-7.42 (3H, m, H-Ph), 7.41-7.37 (2H, m, H-Ph), 4.06-3.83 (9H, ms - overlapped signals, H-4, H-5, H-6, H-7, H-9a, 2x CH_2), 3.69-3.60 (2H, m, H-8, H-9b), 3.28 (1H, dd, *J* = 12.6 Hz, *J* = 3.8 Hz, H-3_{eq}), 2.42 (3H, s, NCH_3), 2.24 (1H, t, *J* = 11.5 Hz, H-3_{ax}), 2.07 (3H, s, CH_3CONH). ^{13}C NMR (101 MHz, D_2O) δ 175.0 (C-1), 170.5 (CH_3CONH), 140.6 (CCH-triazole), 130.3 (2x Ph-CH), 128.8 (2x Ph-CH), 128.6 (Ph-CH), 123.6 (CH-triazole), 90.9 (C-2), 74.1, 71.3, 68.0, 67.9, (C-4, C-6, C-7, C-8), 62.7 (C-9), 60.0 (CH_2), 51.5 (C-5), 49.7 (CH_2), 40.3 (NCH_3), 39.6 (C-3), 22.0 (CH_3CONH). HRMS (ESI): *m/z* calculated for $C_{22}H_{32}N_5O_8$ $[M+H]^+$: 494.2245; found: 494.2249.

5-Acetamido-3,5-dideoxy-2-[4-(1-hydroxypropyl)-1*H*-1,2,3-triazol-1-yl]-D-*glycero*-α-D-*galacto*-non-2-ulopyranosidic acid (**3f**)

Yield: 100% (20 mg; 0.048 mmol); $[\alpha]_D^{20}$ -24.7 (c 1, H_2O). ^{1}H NMR (400 MHz, D_2O) δ 8.14 (1H, s, C*H*-triazole), 4.84 (1H, t, *J* = 6.9 Hz, C*H*OH), 4.06-3.83 (5H, ms - overlapped signals, H-4, H-5, H-6, H-7, H-9a), 3.69-3.60 (2H, m, H-8, H-9b), 3.27 (1H, dd, *J* = 12.7 Hz, *J* = 3.9 Hz, H-3_{eq}), 2.26 (1H, t, *J* = 11.0 Hz, H-3_{ax}), 2.07 (3H, s, CH_3CONH), 1.95-1.85 (2H, m, CH_2CH$_3$), 0.90 (3H, t, *J* = 7.4 Hz, CH$_2$CH_3). ^{13}C NMR (101 MHz, D_2O) δ 175.0 (C-1), 170.6 (CH_3CONH), 150.1 (CCH-triazole), 120.6 (CH-triazole), 90.8 (C-2), 74.1, 71.3, 68.1, 68.0, (C-4, C-6, C-7, C-8), 67.4 (CHOH), 62.7 (C-9), 51.5 (C-5), 39.6 (C-3), 29.0 (CH_2CH$_3$), 22.0 (CH_3CONH) 9.0 (CH$_2$CH$_3$). HRMS (ESI): *m/z* calculated for $C_{16}H_{26}N_4NaO_9$ $[M+Na]^+$: 441.1592; found: 441.1590.

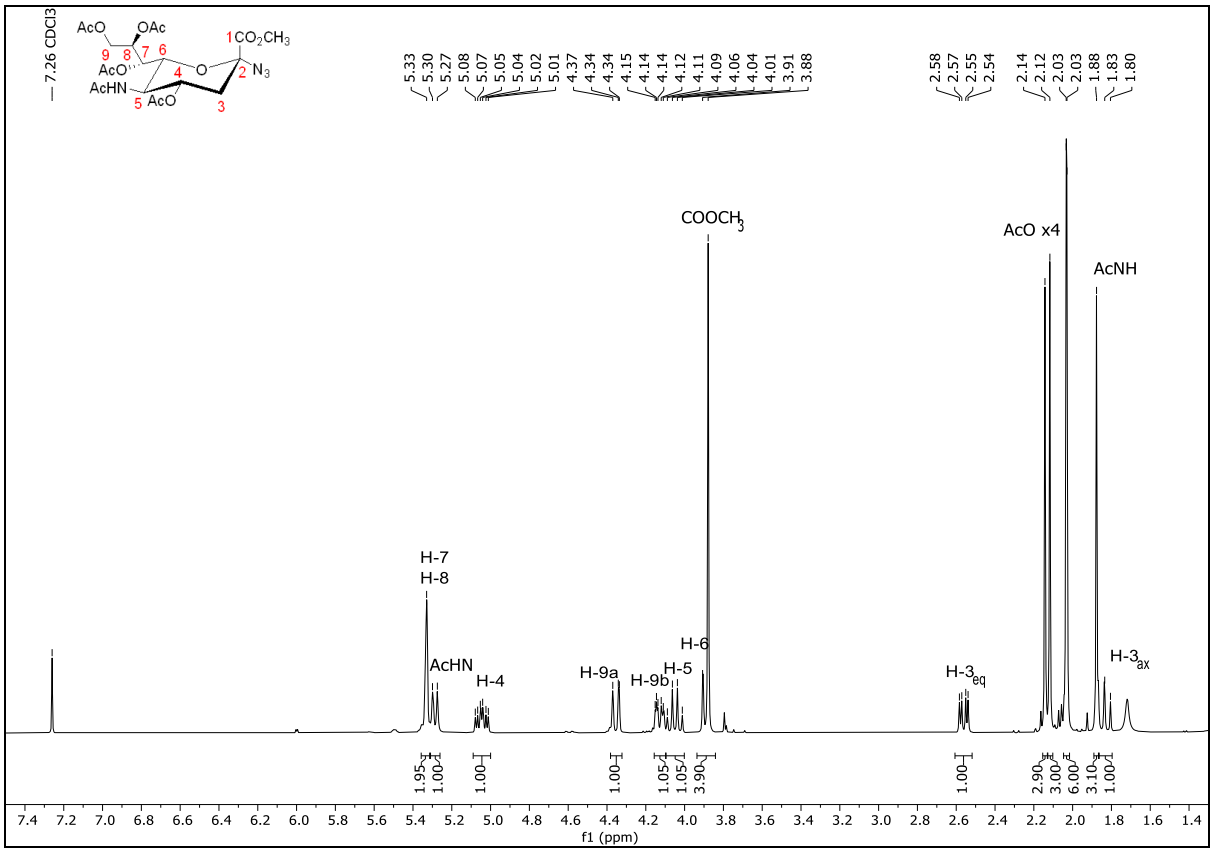
5-Acetamido-3,5-dideoxy-2-[4-(2-hydroxypropyl)-1*H*-1,2,3-triazol-1-yl]-D-*glycero*-α-D-*galacto*-non-2-ulopyranosidic acid (**3g**)

Yield: 94% (16 mg; 0.038 mmol); $[\alpha]_D^{20}$ -34.5 (c 1, H_2O). ^{1}H NMR (400 MHz, D_2O) δ 8.03 (1H, s, C*H*-triazole), 4.13 (1H, h, *J* = 6.4 Hz, C*H*OH), 4.05-3.83 (5H, ms - overlapped signals, H-4, H-5, H-6, H-7, H-9a), 3.69-3.60 (2H, m, H-8, H-9b), 3.25 (1H, dd, *J* = 12.6 Hz, *J* = 4.0 Hz, H-3_{eq}), 2.96-2.83 (2H, m, CH_2CHOH), 2.27 (1H, t, *J* = 11.5 Hz, H-3_{ax}), 2.07 (3H, s, CH_3CONH), 1.21 (3H, d, *J* = 6.2 Hz, CH_3CHOH). ^{13}C NMR (101 MHz, D_2O) δ 175.0 (C-1), 170.8 (CH_3<u>C</u>ONH), 144.5 (<u>C</u>CH-triazole), 121.7 (<u>C</u>H-triazole), 90.7 (C-2), 74.0, 71.3, 68.1, 68.0, (C-4, C-6, C-7, C-8), 66.9 (<u>C</u>HOH), 62.7 (C-9), 51.5 (C-5), 39.6 (C-3), 33.9 (CH_2CHOH), 22.0 (<u>C</u>H_3CONH) 21.4 (CH_3<u>C</u>HOH). HRMS (ESI): *m/z* calculated for $C_{16}H_{26}N_4NaO_9$ $[M+Na]^+$: 441.1592; found: 441.1592.

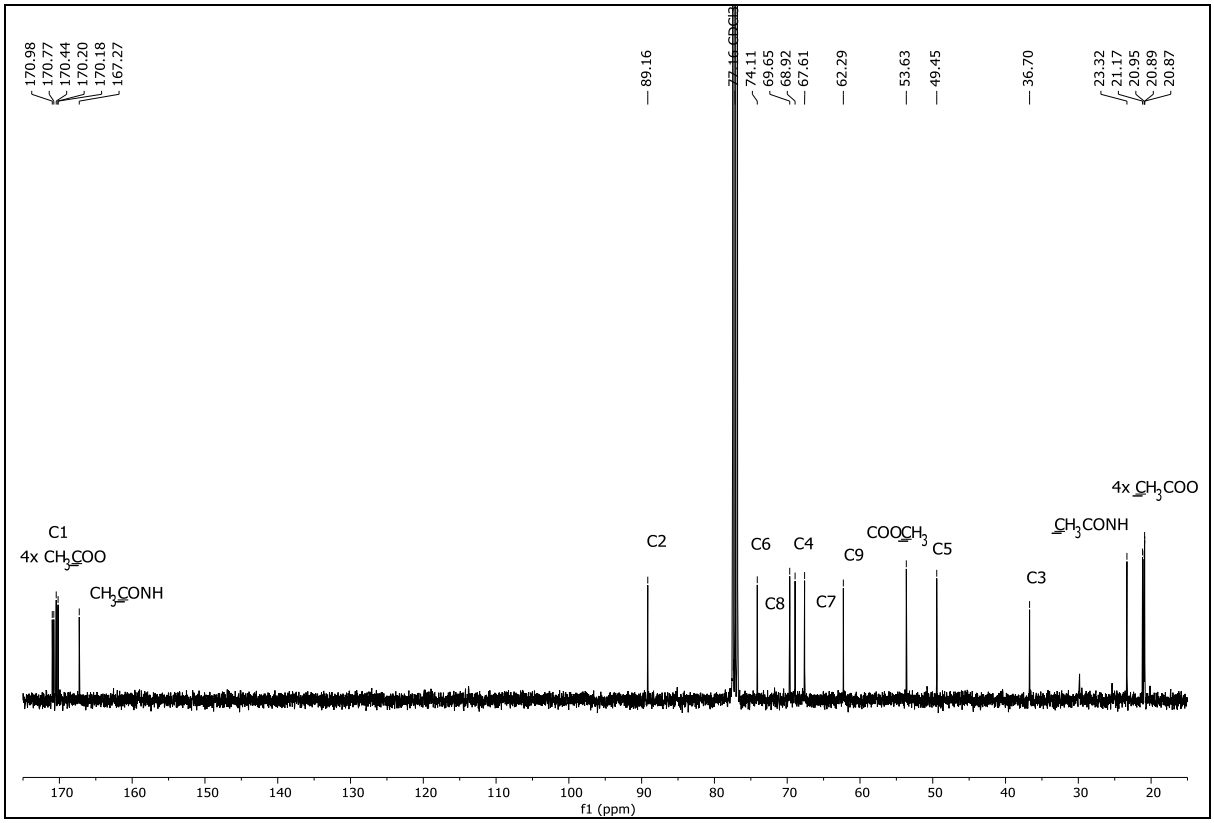
5-Acetamido-3,5-dideoxy-2-(4-phenylmethyl-1*H*-1,2,3-triazol-1-yl)-D-*glycero*-α-D-*galacto*-non-2-ulopyranosidic acid (**3h**)

Yield: 74% (15 mg; 0.033 mmol); $[\alpha]_D^{20}$ -38.4 (c 1, H_2O). ^{1}H NMR (400 MHz, D_2O) δ 7.99 (1H, s, C*H*-triazole), 7.41-7.34 (2H, m, H-Ph), 7.34-7.27 (3H, m, H-Ph), 4.09 (2H, s, CH_2), 4.03-3.81 (5H, ms - overlapped signals, H-4, H-5, H-6, H-7, H-9a), 3.67-3.58 (2H, m, H-8, H-9b), 3.23 (1H, dd, *J* = 12.5 Hz, *J* = 3.9 Hz, H-3_{eq}), 2.21 (1H, t, *J* = 11.8 Hz, H-3_{ax}), 2.06 (3H, s, CH_3CONH). ^{13}C NMR (101 MHz, D_2O) δ 175.0 (C-1), 170.7 (CH_3<u>C</u>ONH), 147.3 (<u>C</u>CH-triazole), 139.0 ($C_{quat.}$), 128.9 (2x Ph-<u>C</u>H), 128.6 (2x Ph-<u>C</u>H), 126.7 (Ph-<u>C</u>H), 121.1 (<u>C</u>H-triazole), 90.7 (C-2), 74.0, 71.2, 68.1, 68.0, (C-4, C-6, C-7, C-8), 62.7 (C-9), 51.5 (C-5), 39.7 (C-3), 30.80 (<u>C</u>H_2), 22.0 (<u>C</u>H_3CONH). HRMS (ESI): *m/z* calculated for $C_{20}H_{26}N_4NaO_8$ $[M+Na]^+$: 473.1643; found: 473.1638.

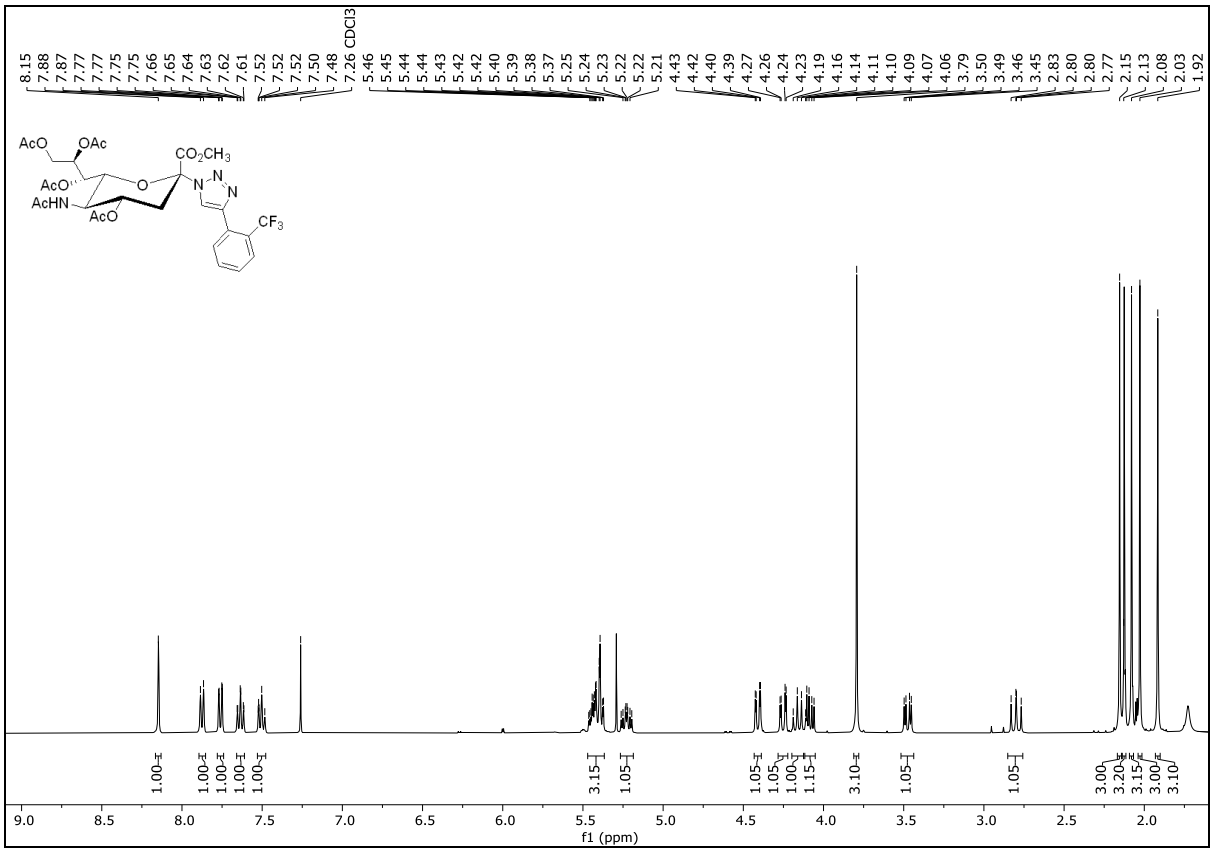
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1**



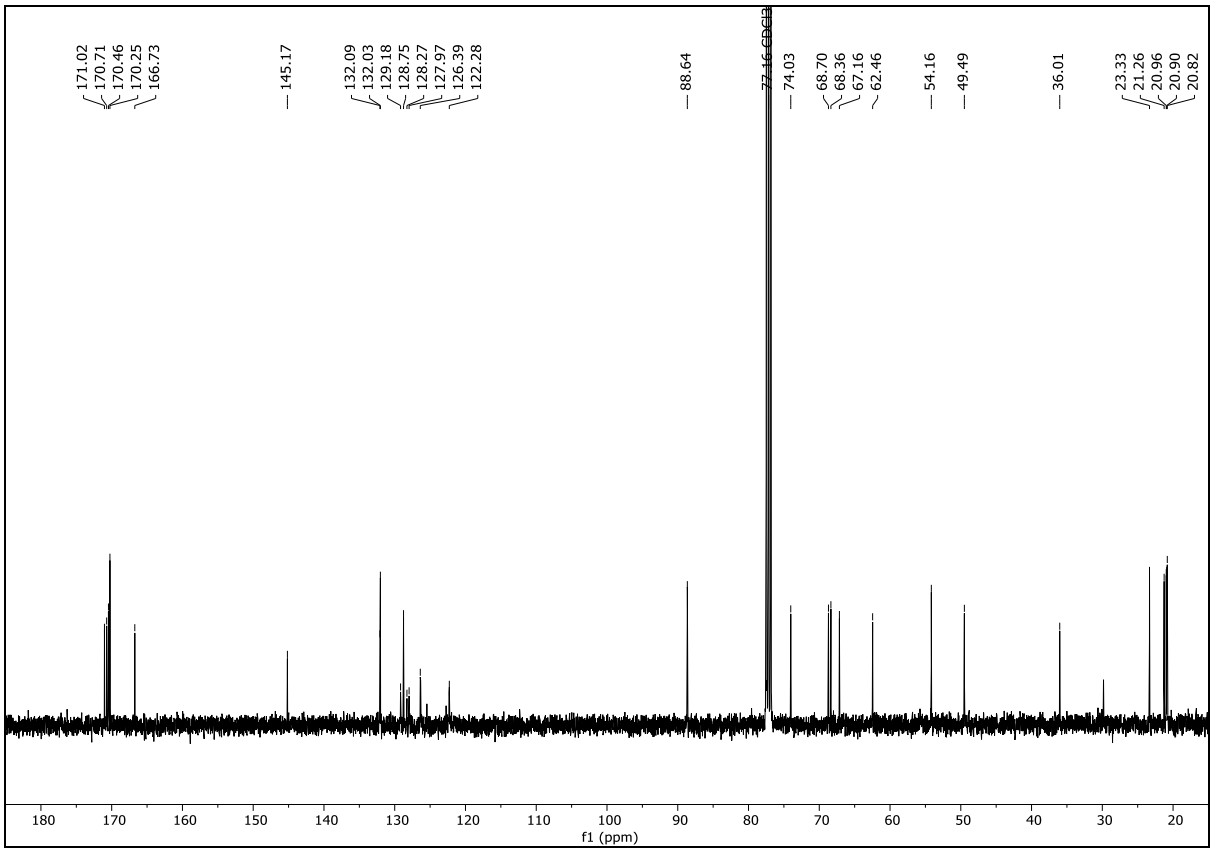
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **1**



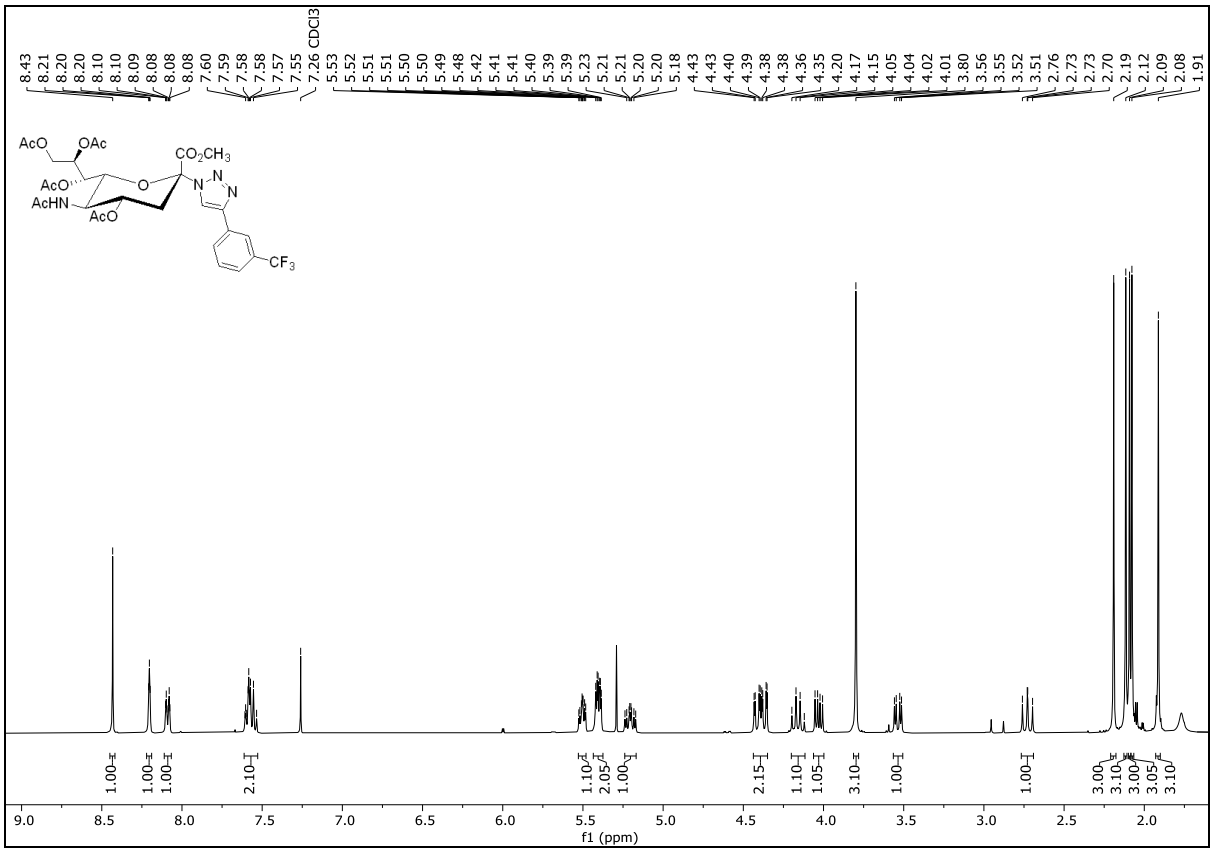
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2a**



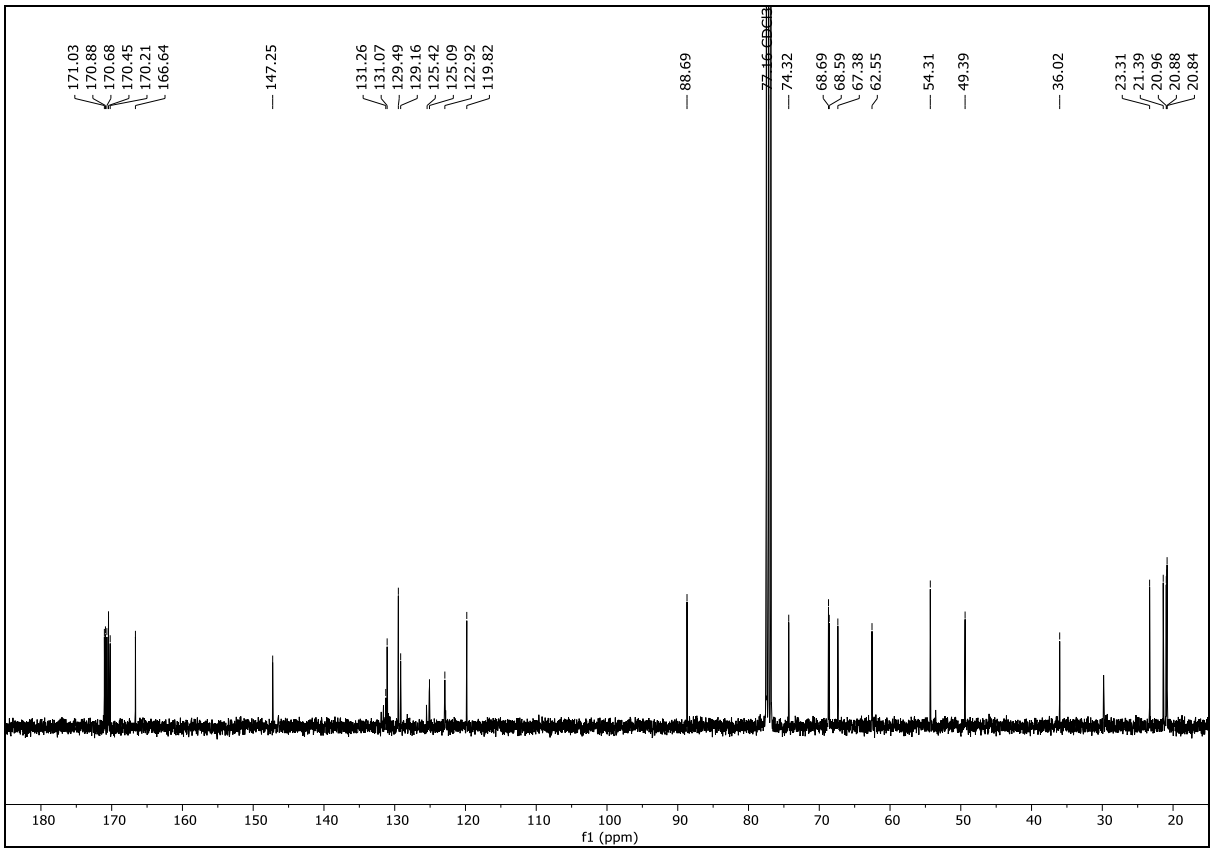
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **2a**



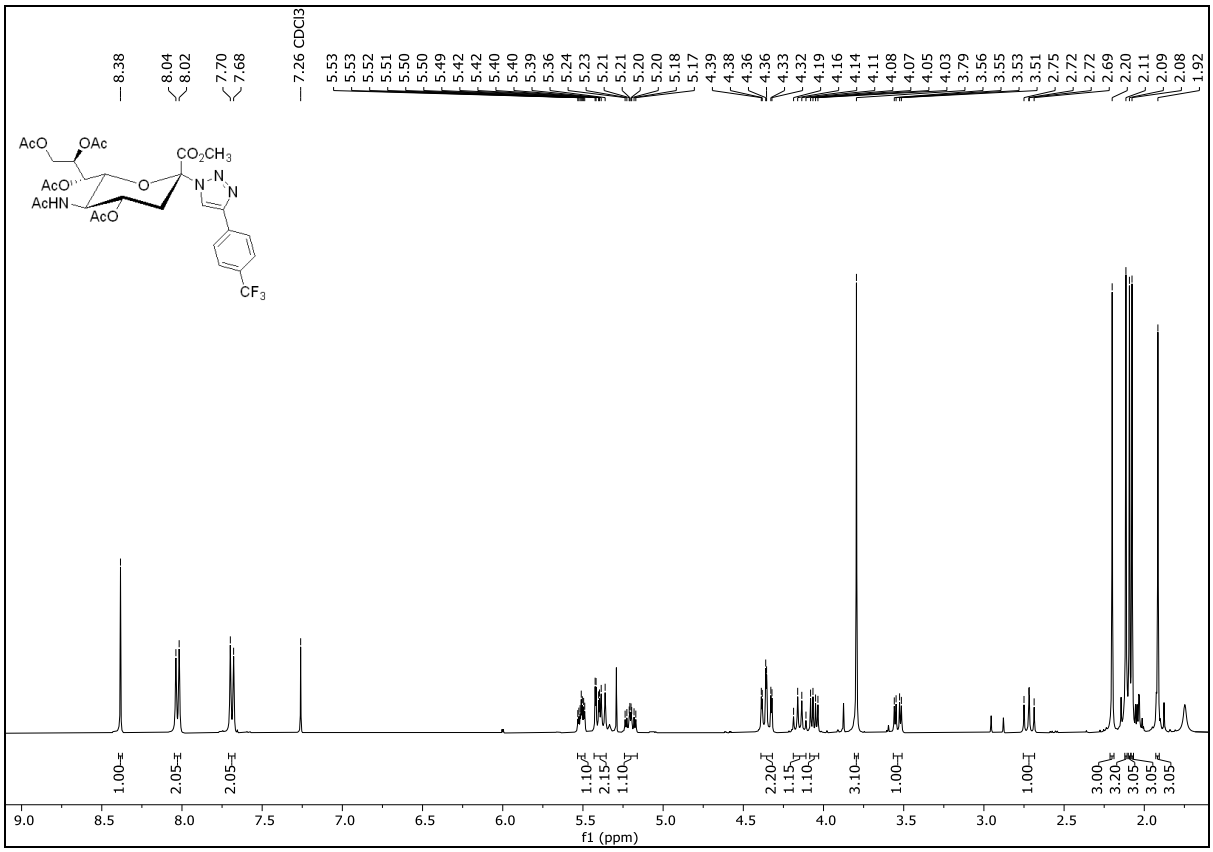
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2b**



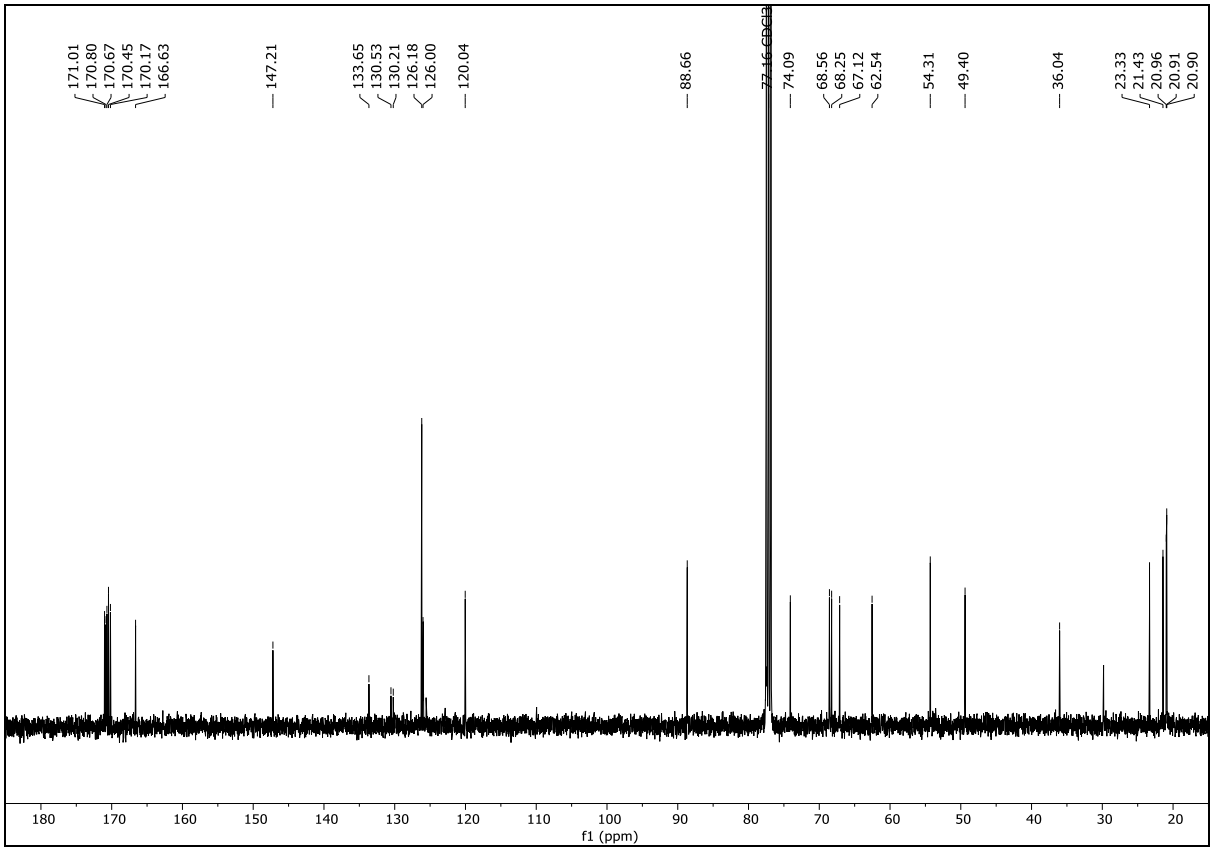
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **2b**



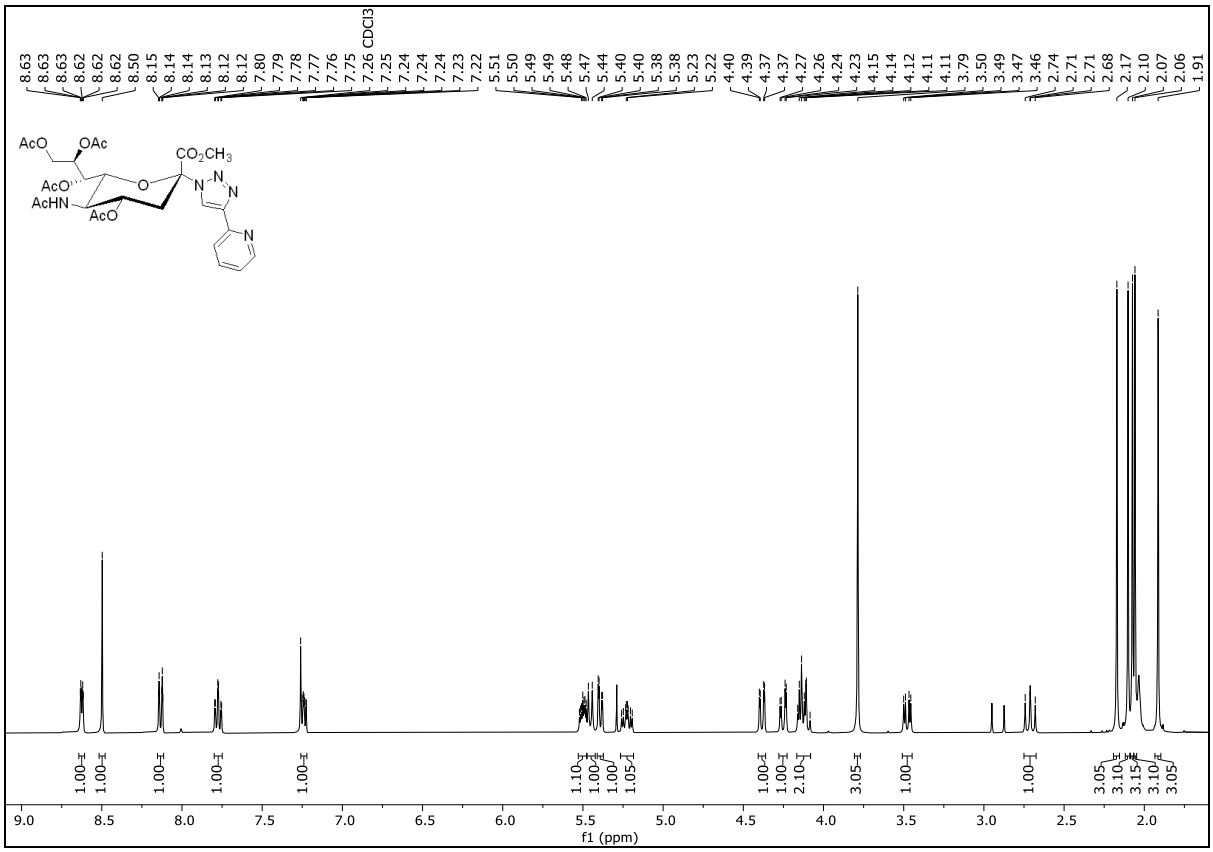
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2c**



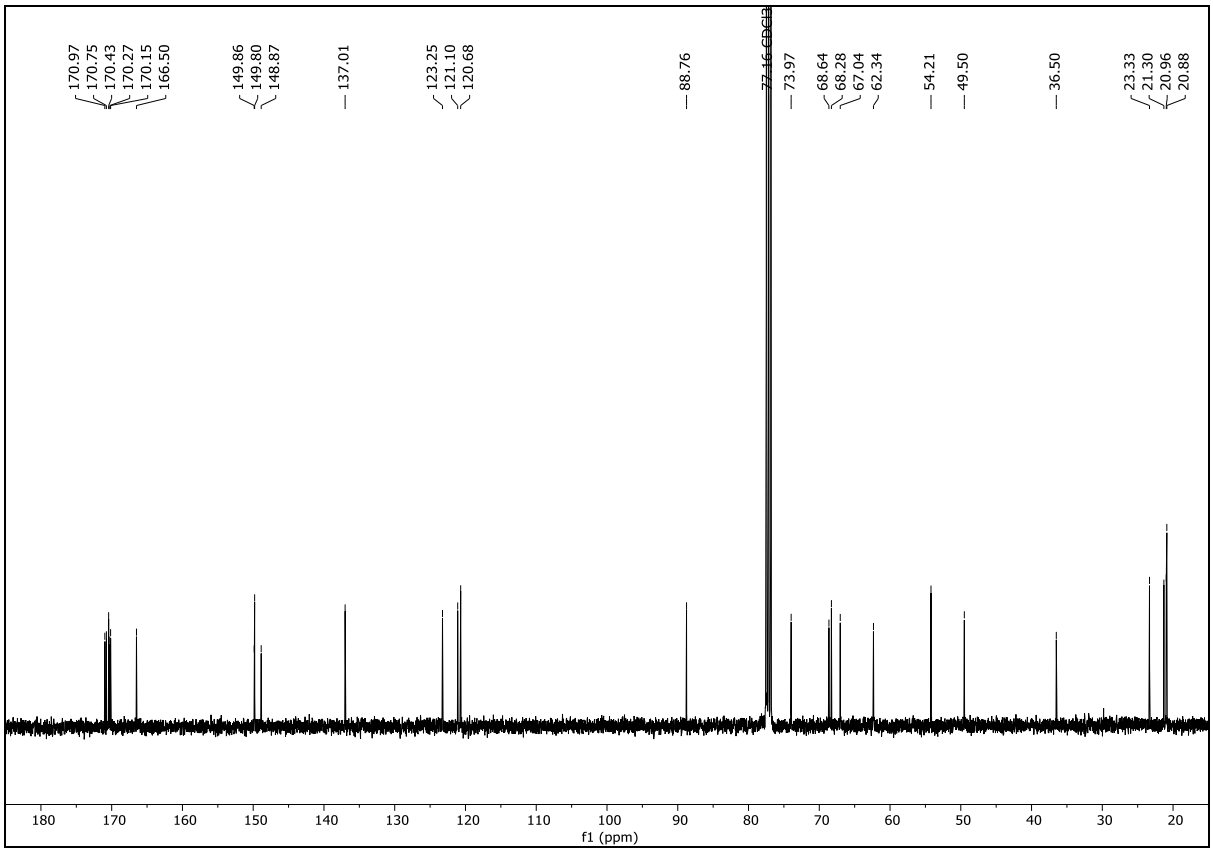
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **2c**



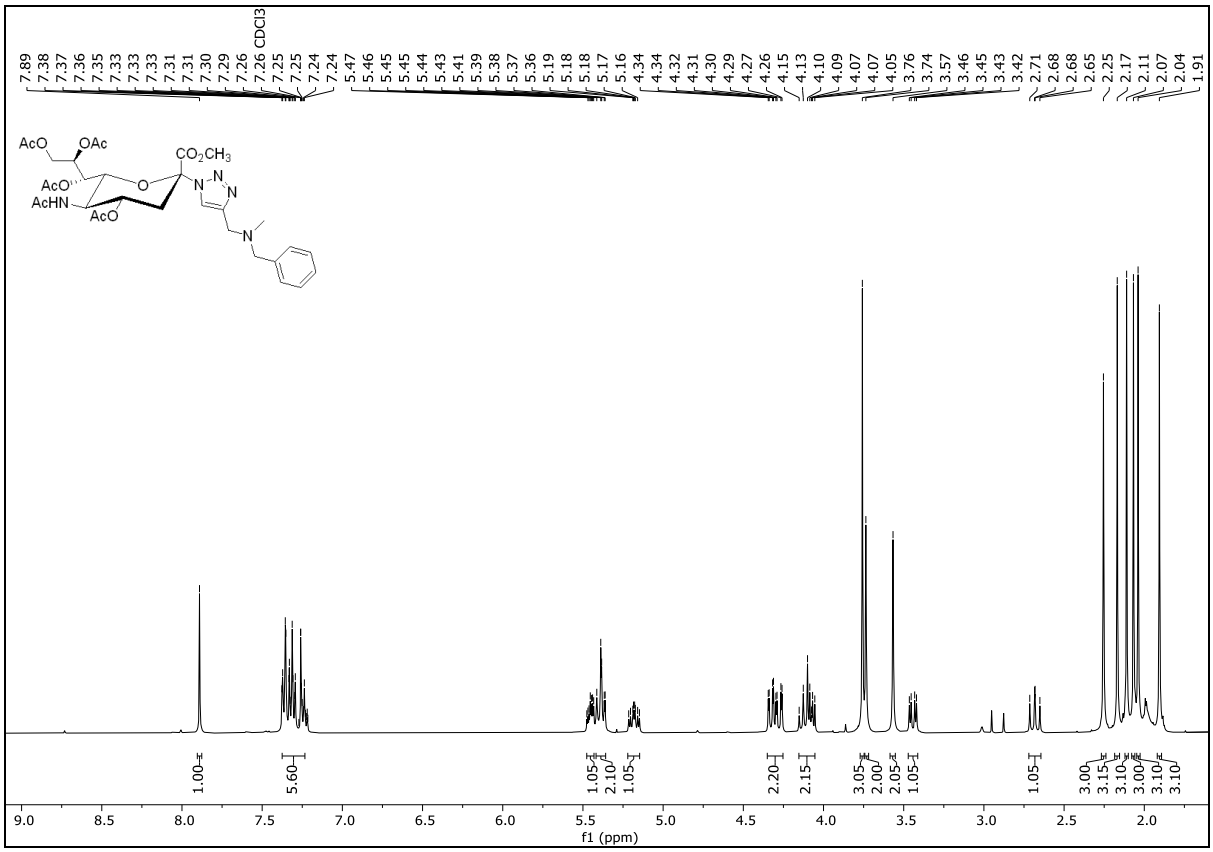
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2d**



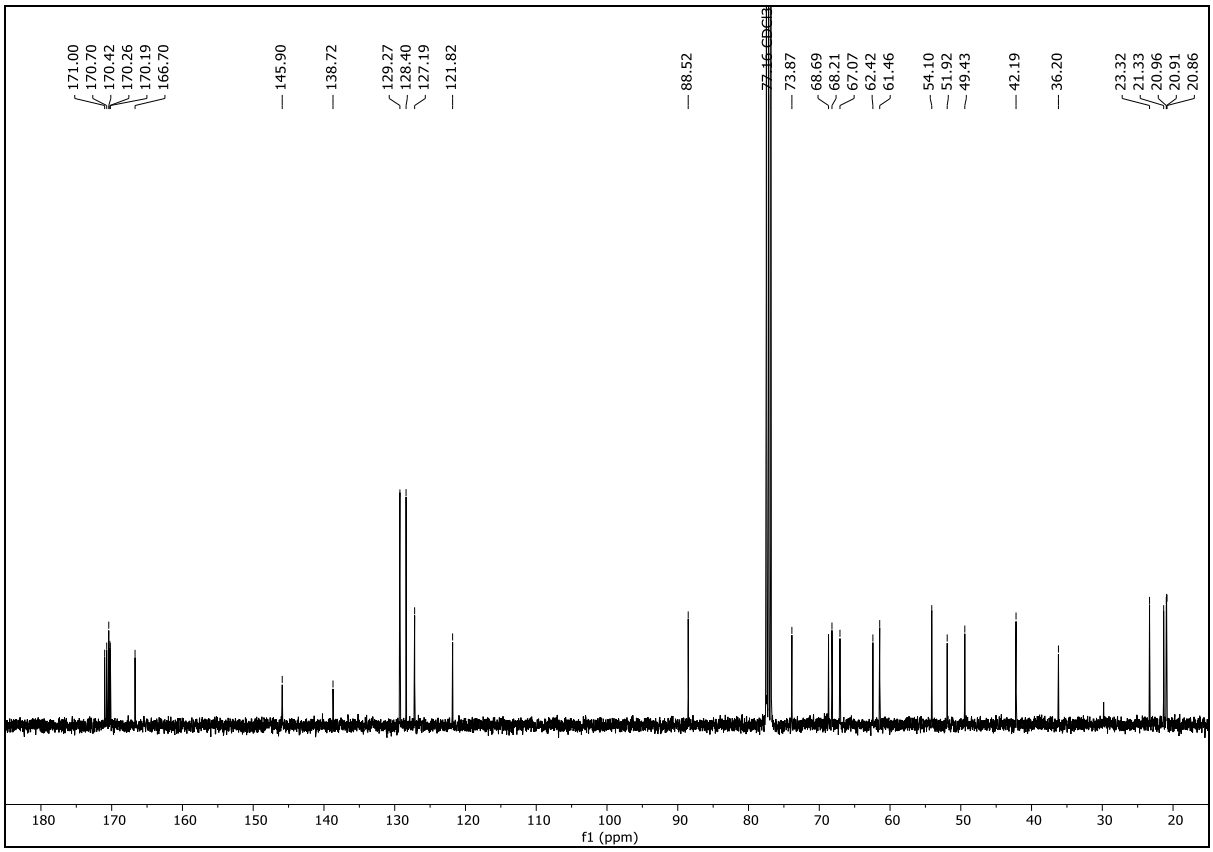
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **2d**



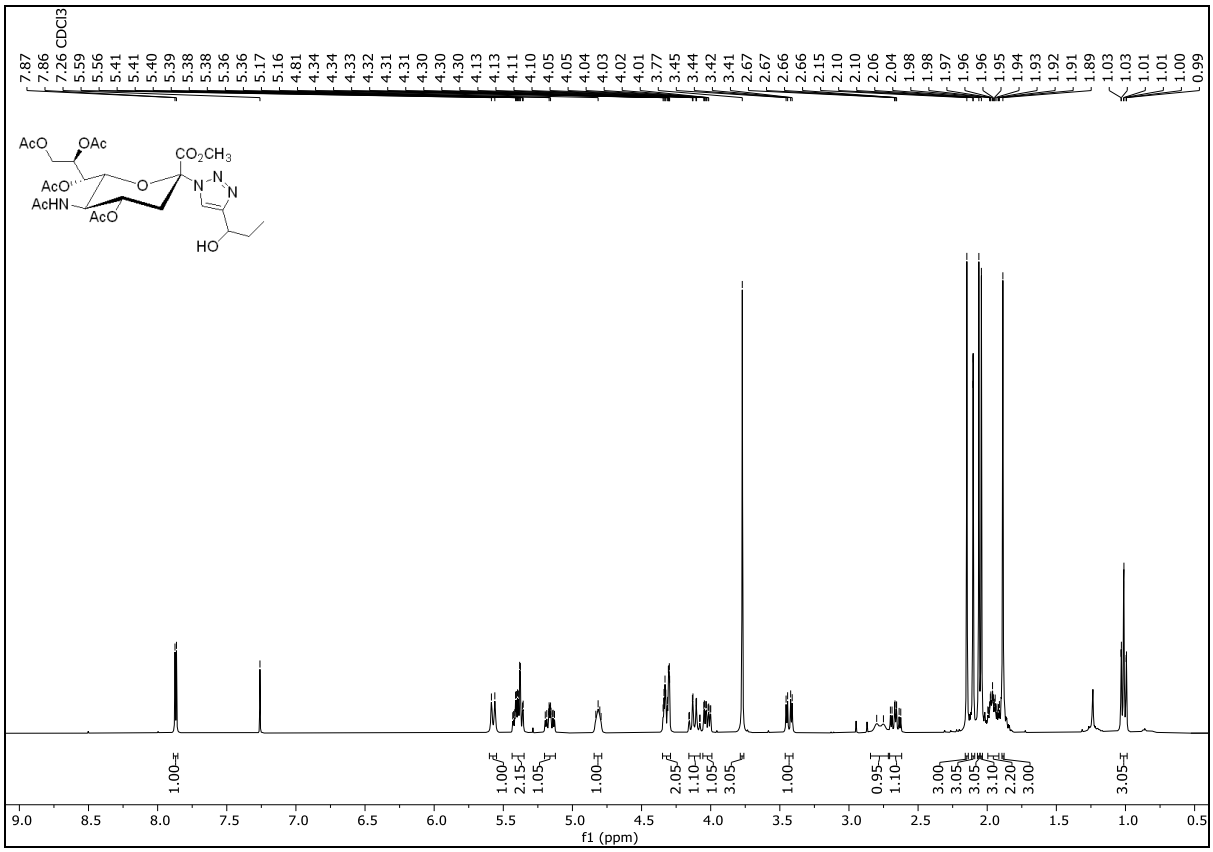
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2e**



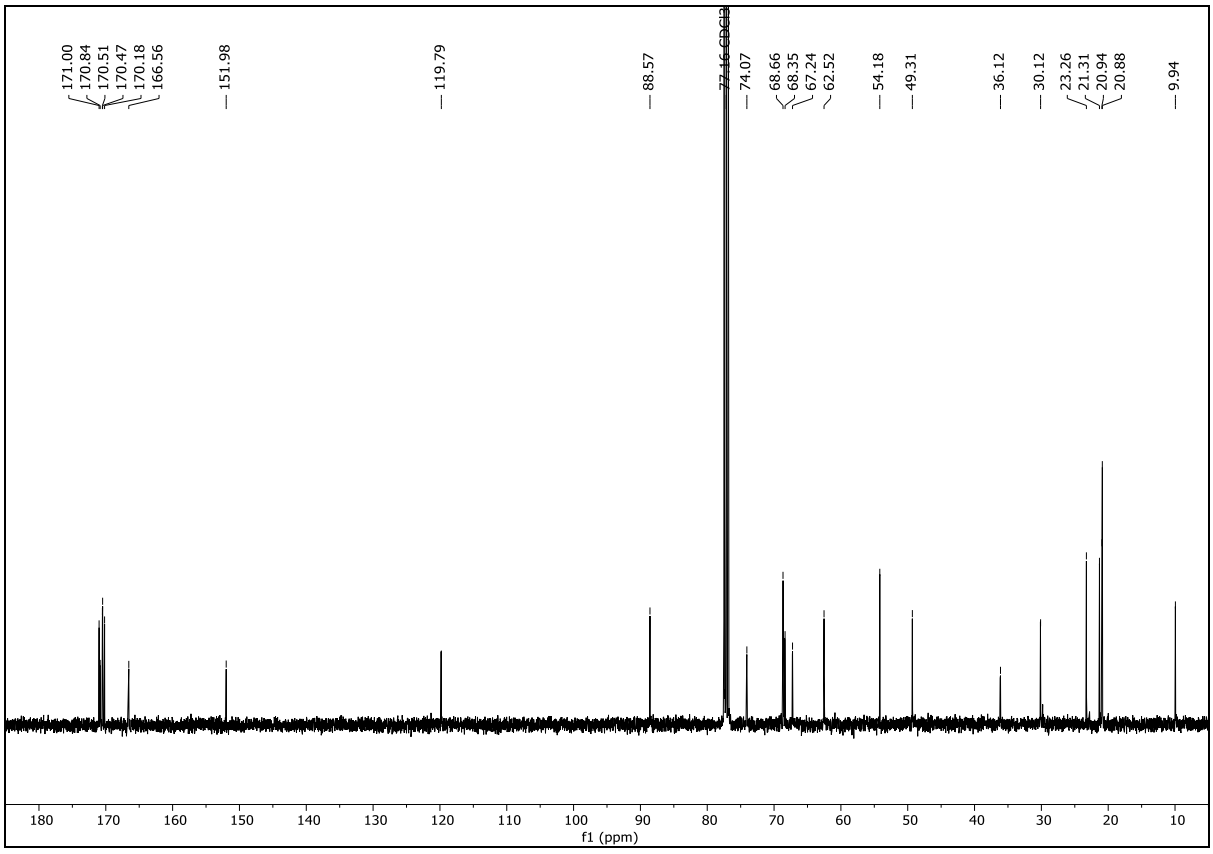
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **2e**



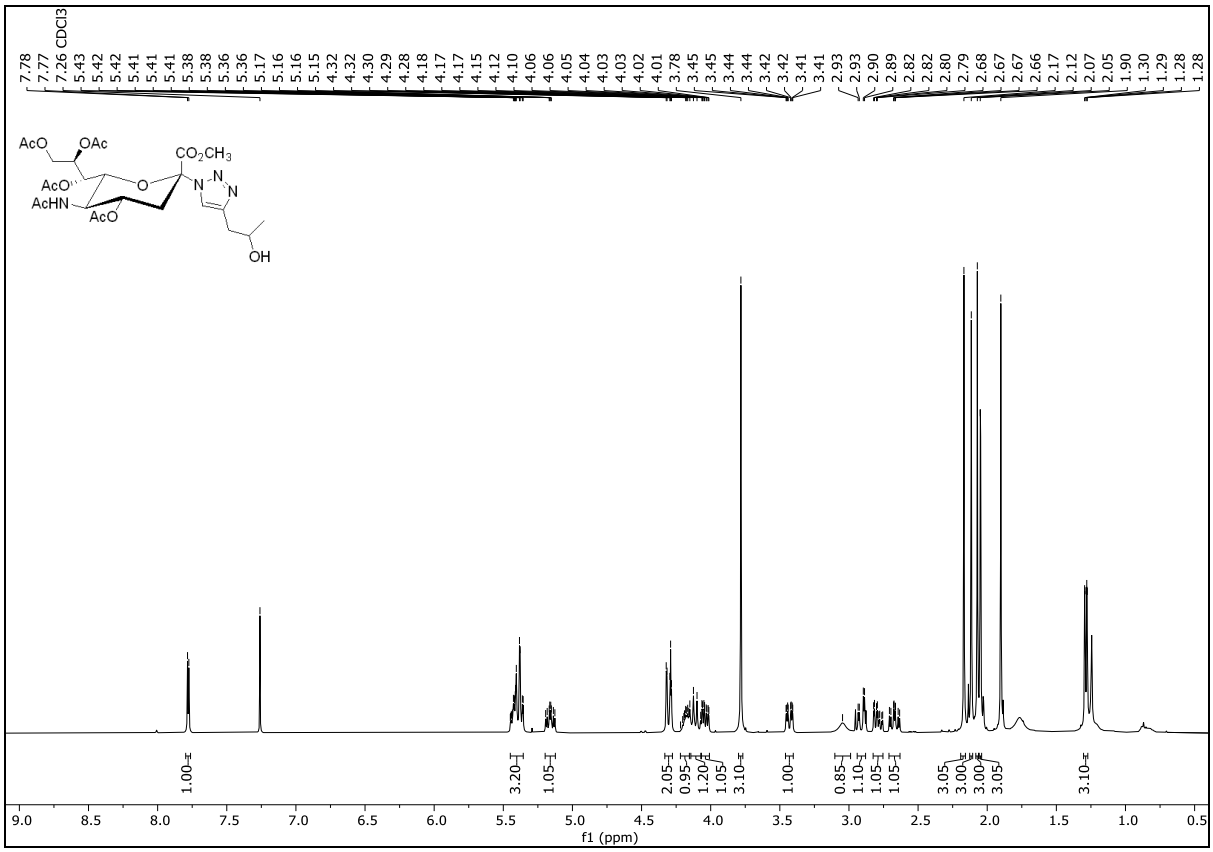
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2f**



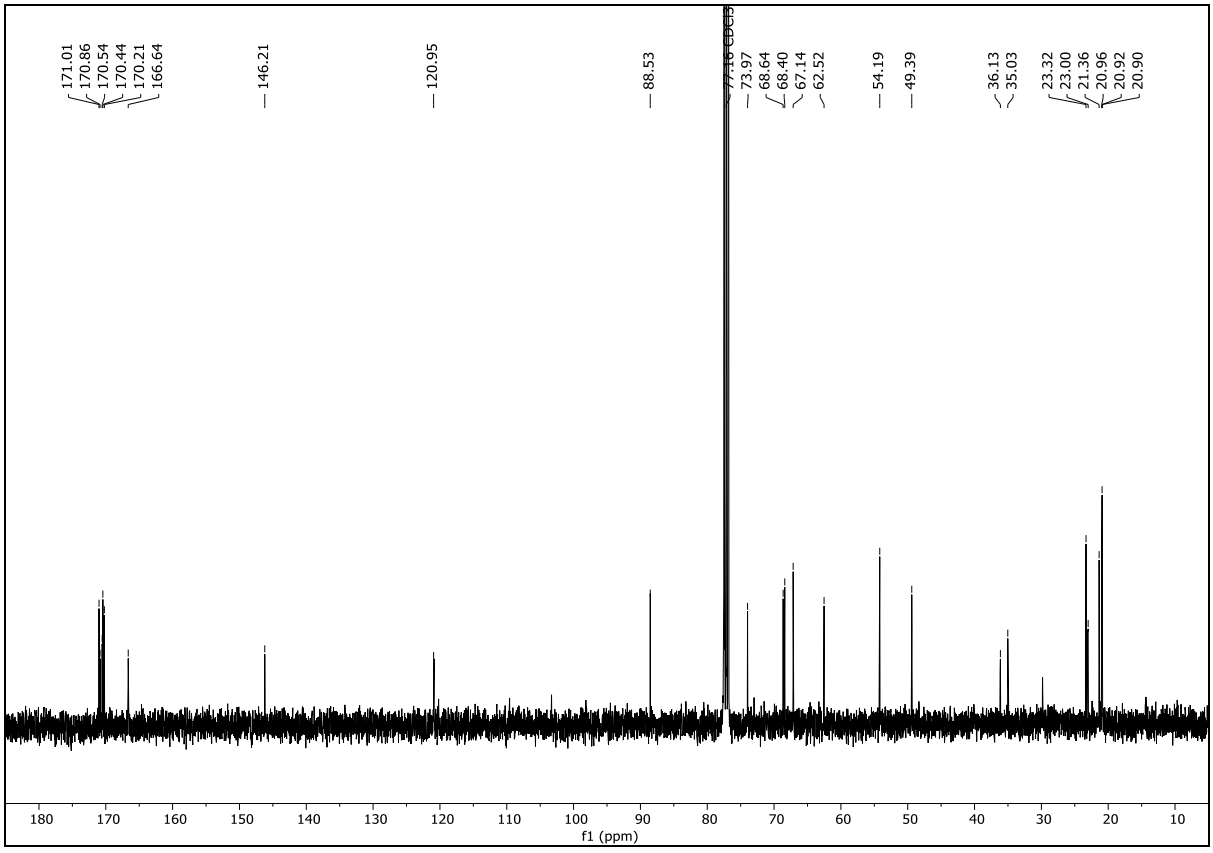
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **2f**



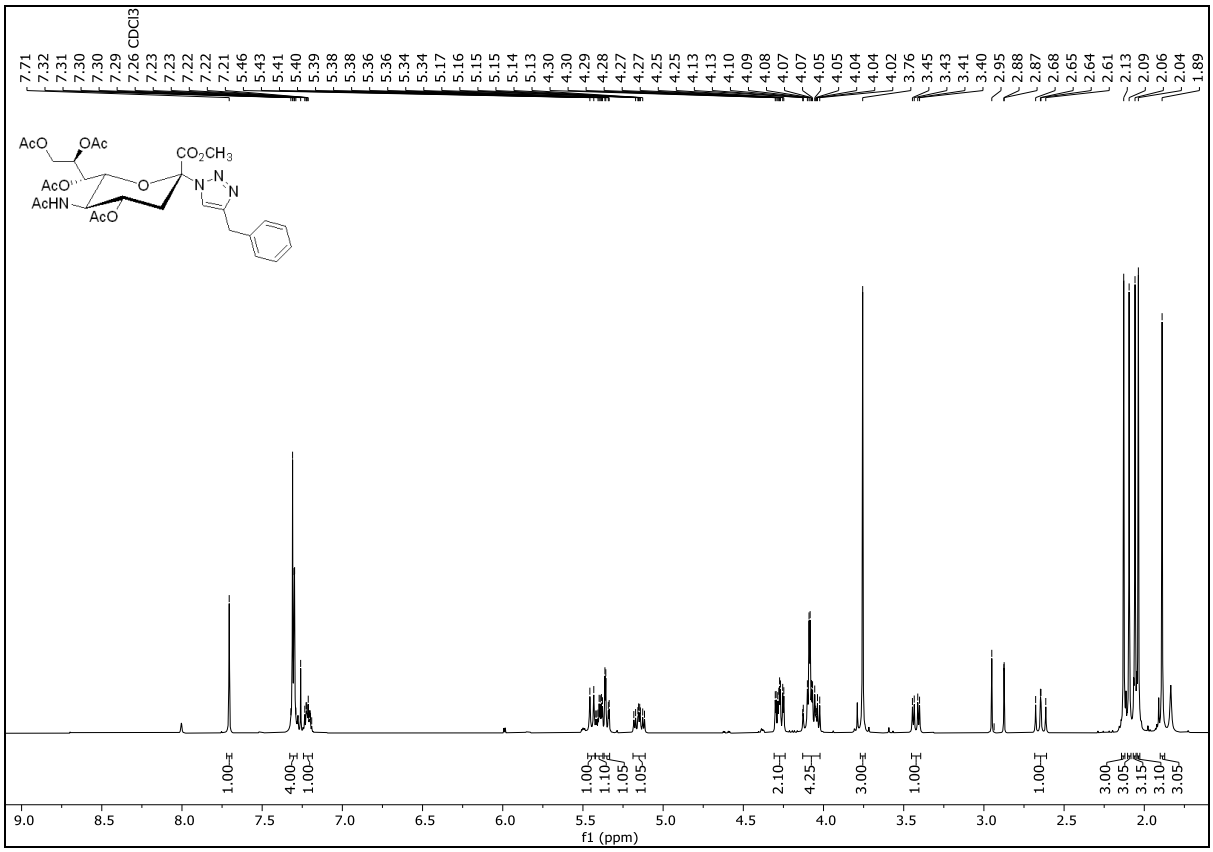
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2g**



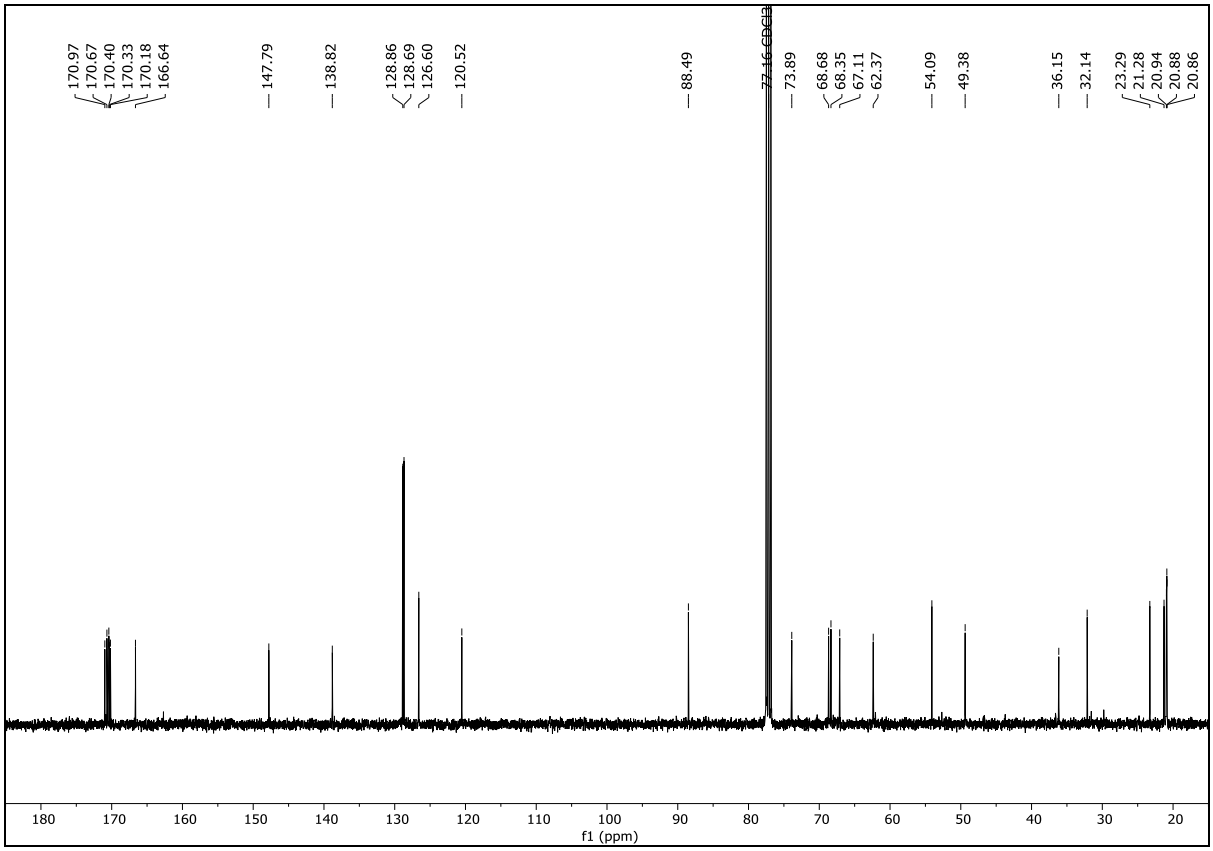
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **2g**



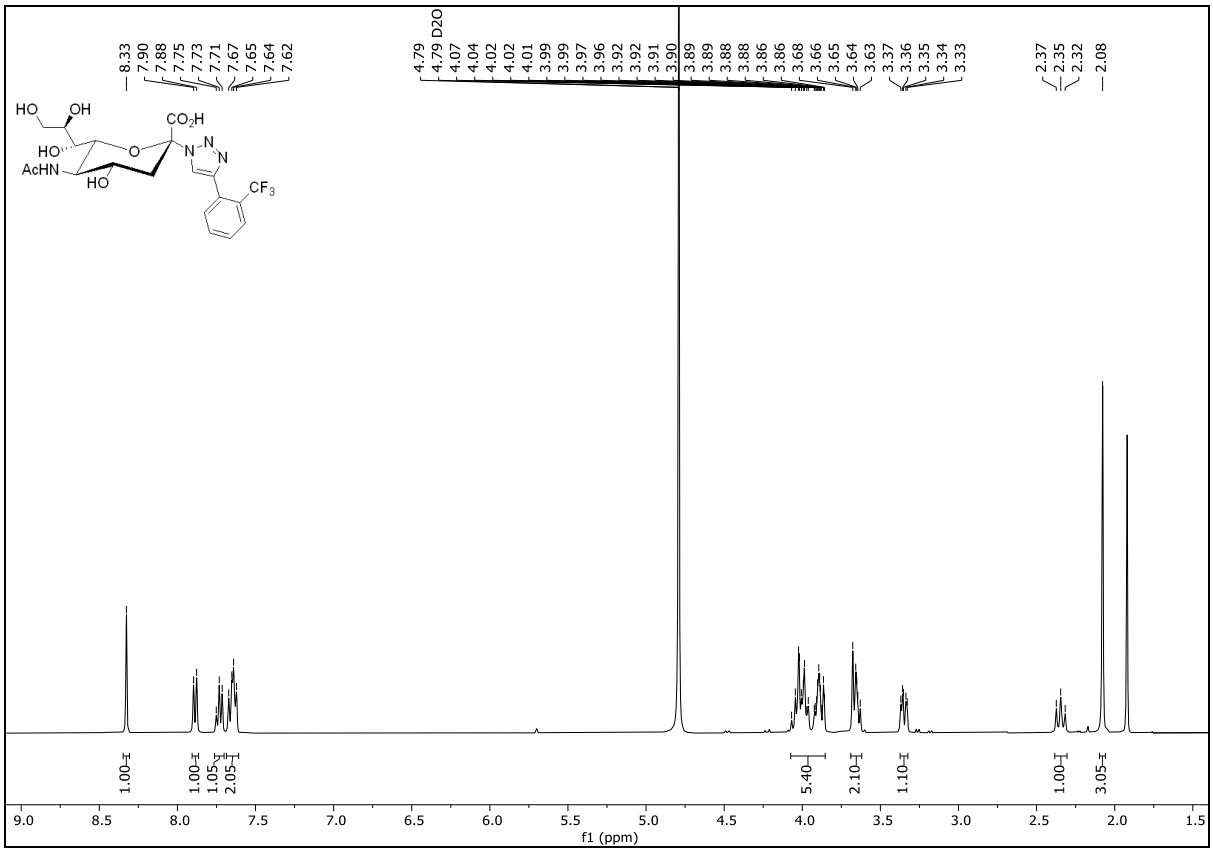
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2h**



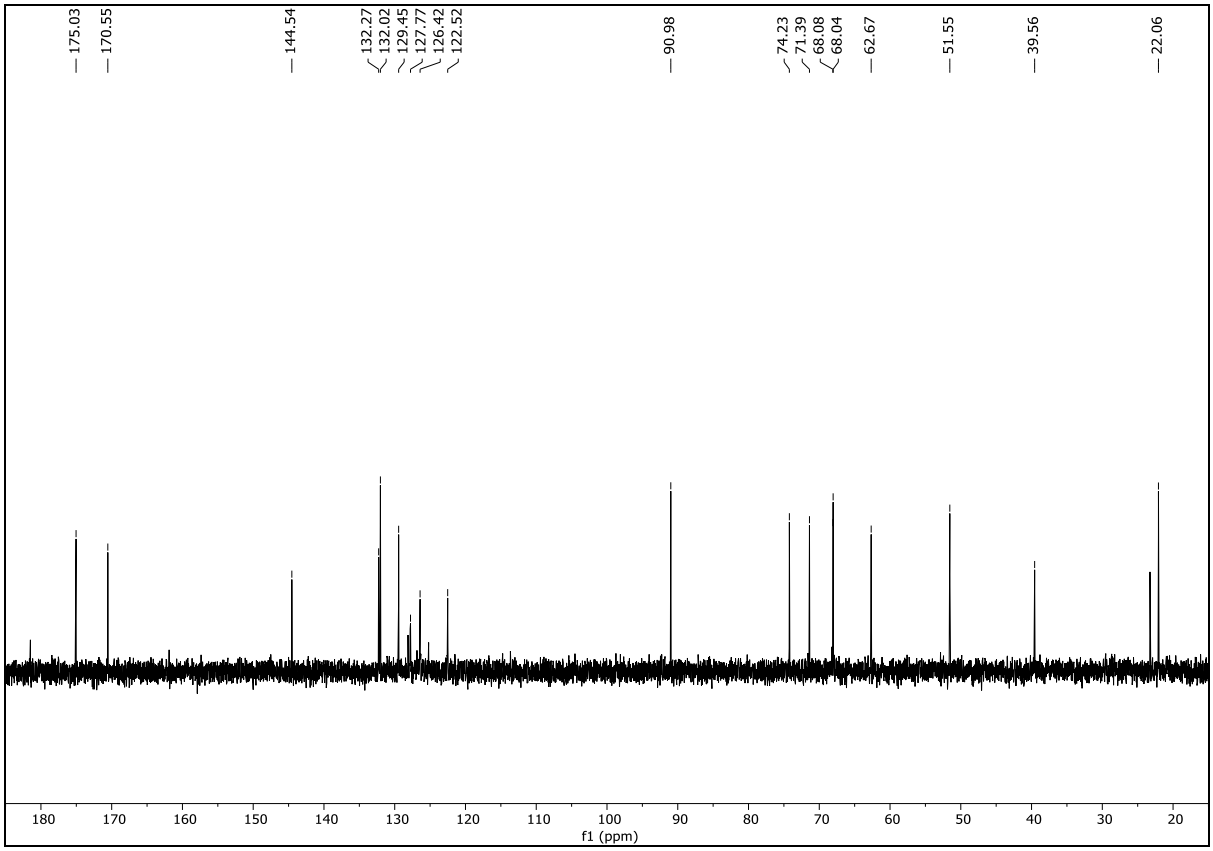
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **2h**



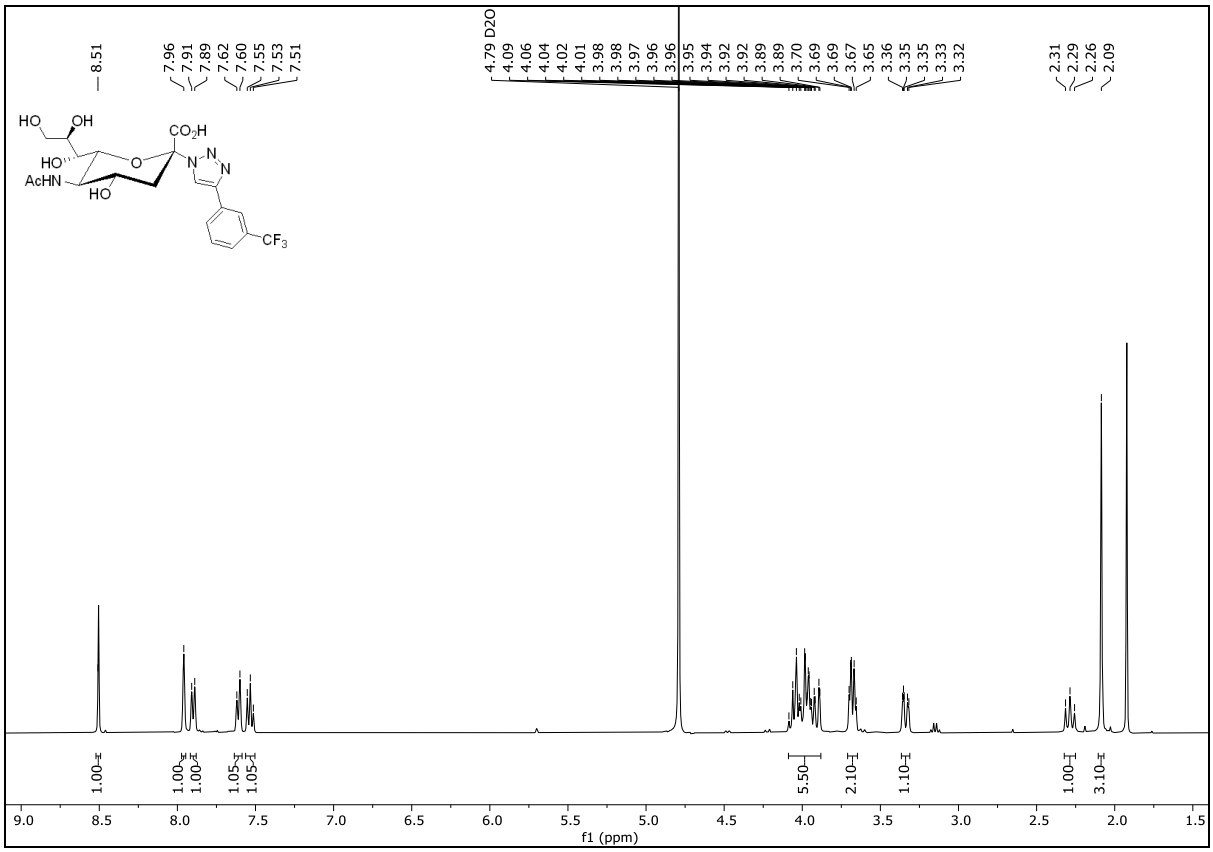
^{1}H NMR (400 MHz, D_2O) spectrum of compound **3a**



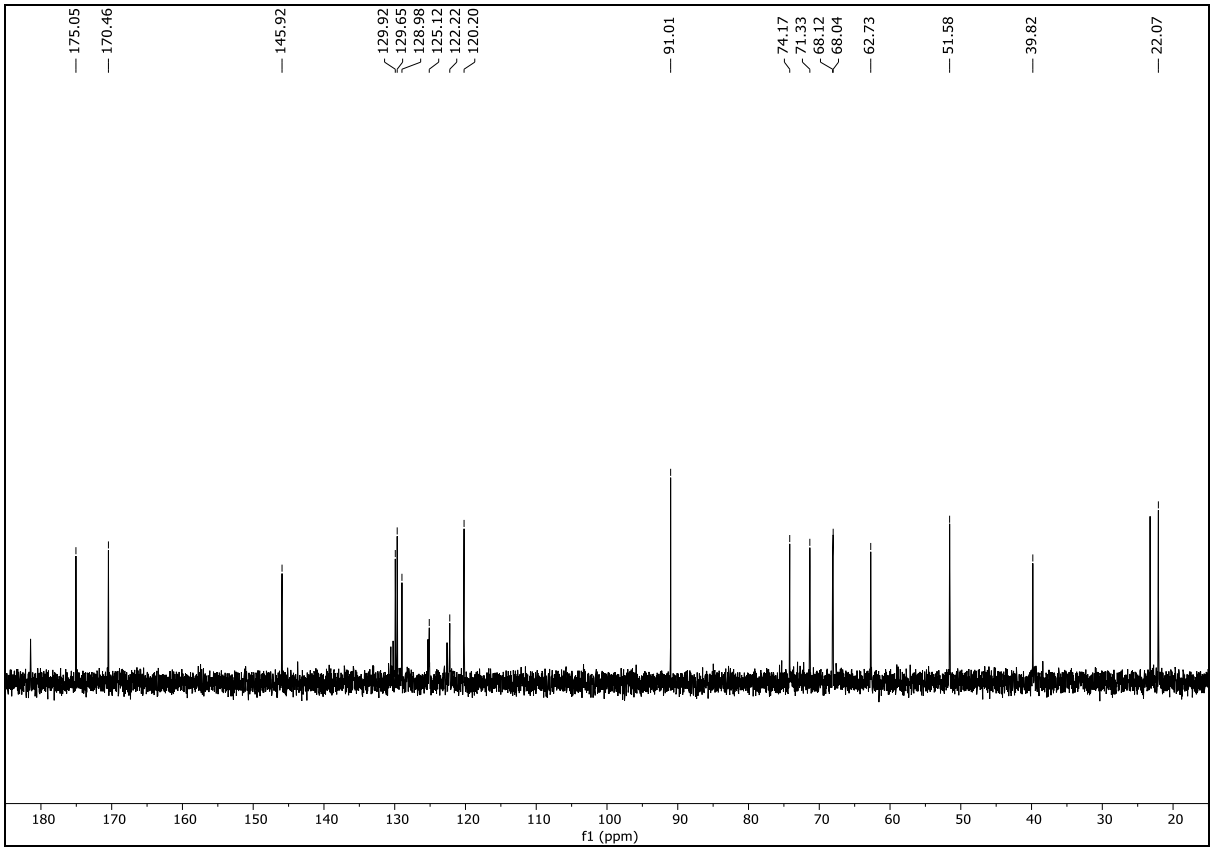
^{13}C NMR (101 MHz, D_2O) spectrum of compound **3a**



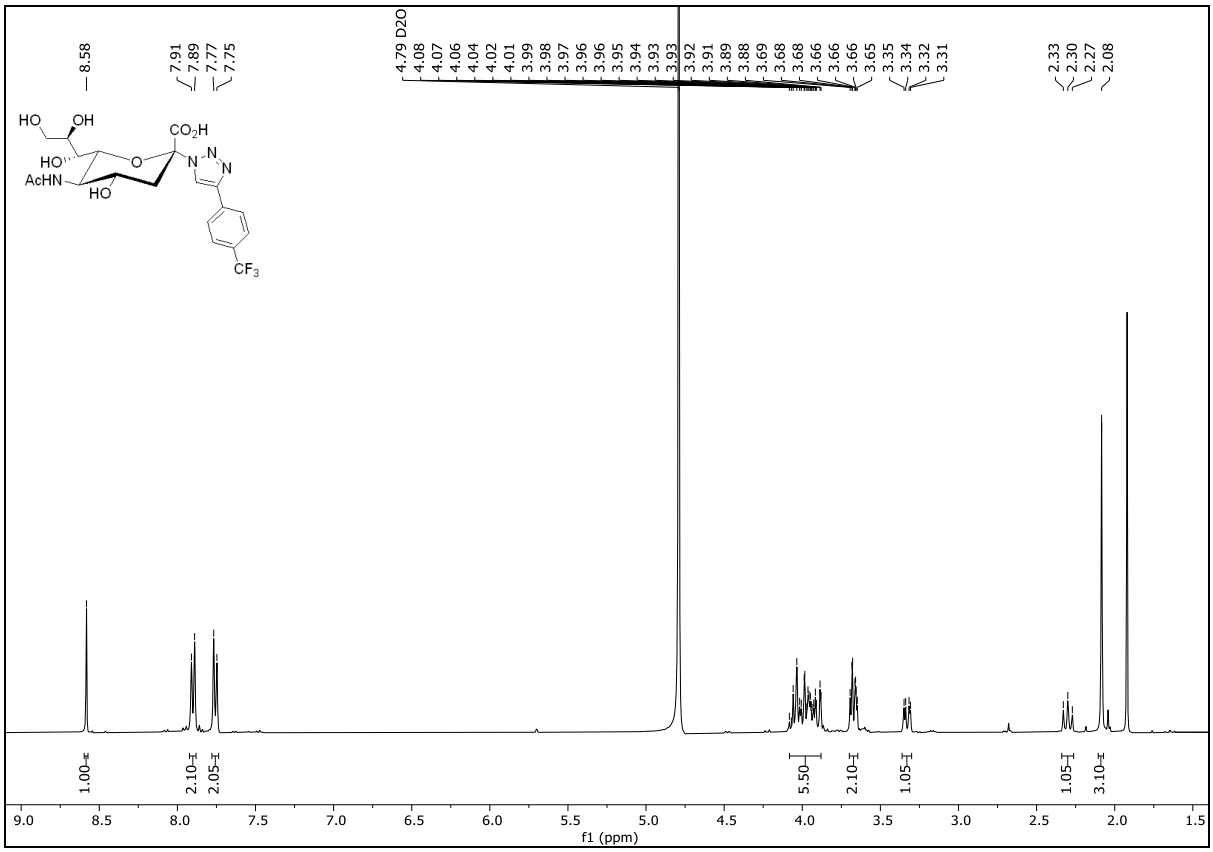
^{1}H NMR (400 MHz, D_2O) spectrum of compound **3b**



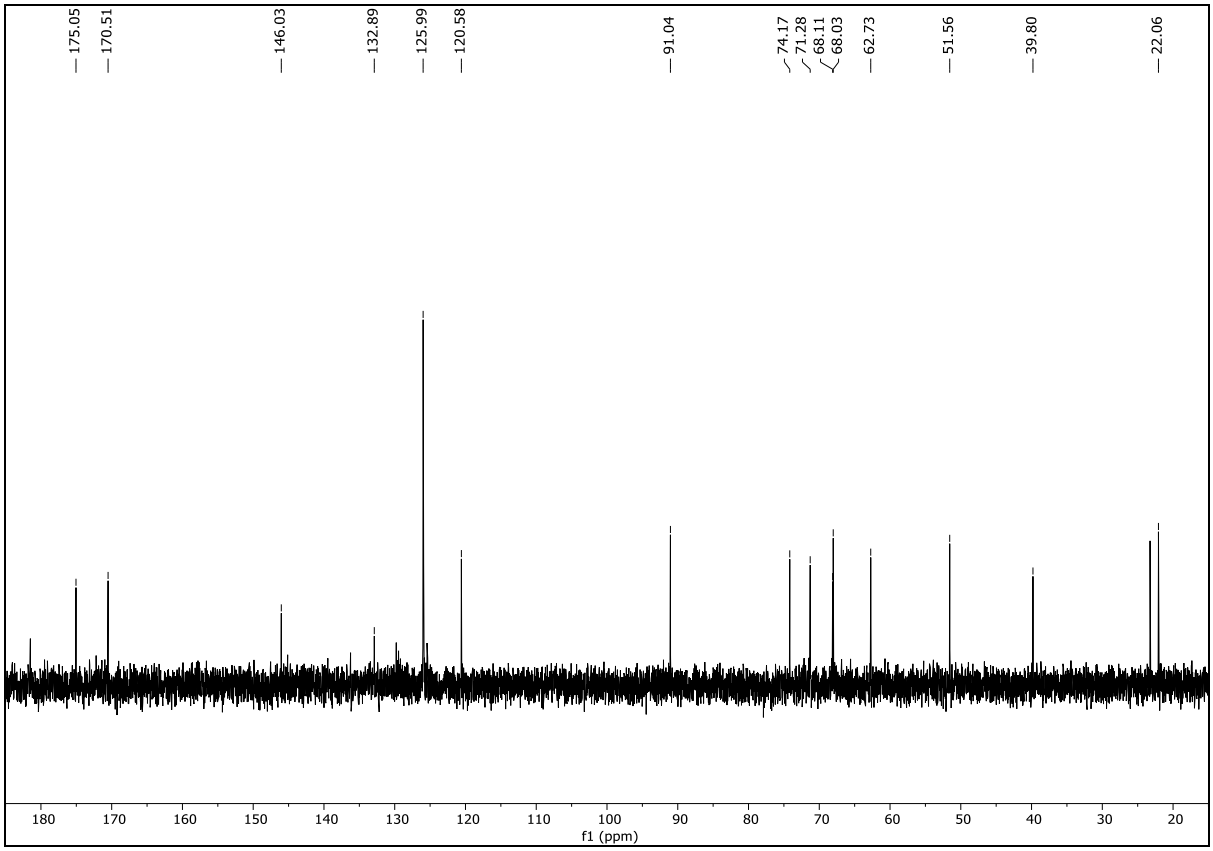
^{13}C NMR (101 MHz, D_2O) spectrum of compound **3b**



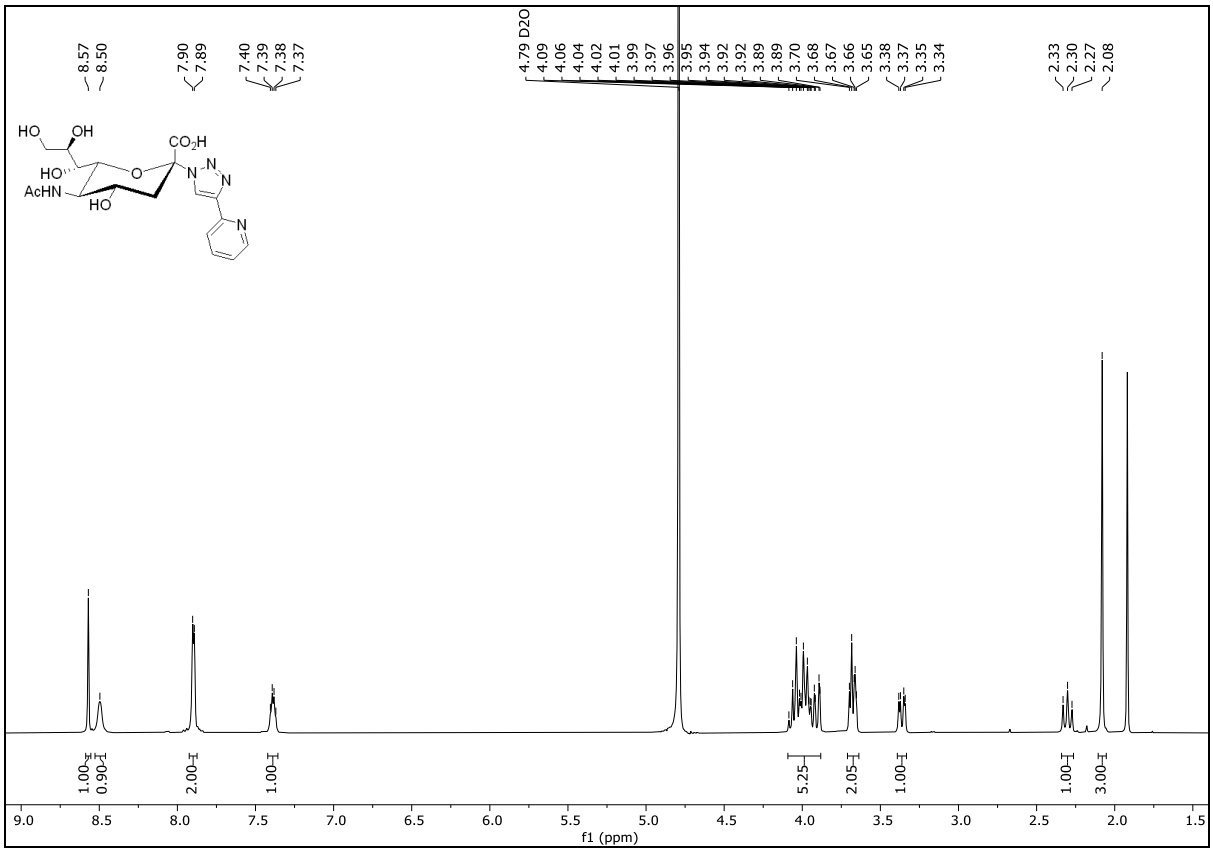
^{1}H NMR (400 MHz, D_2O) spectrum of compound **3c**



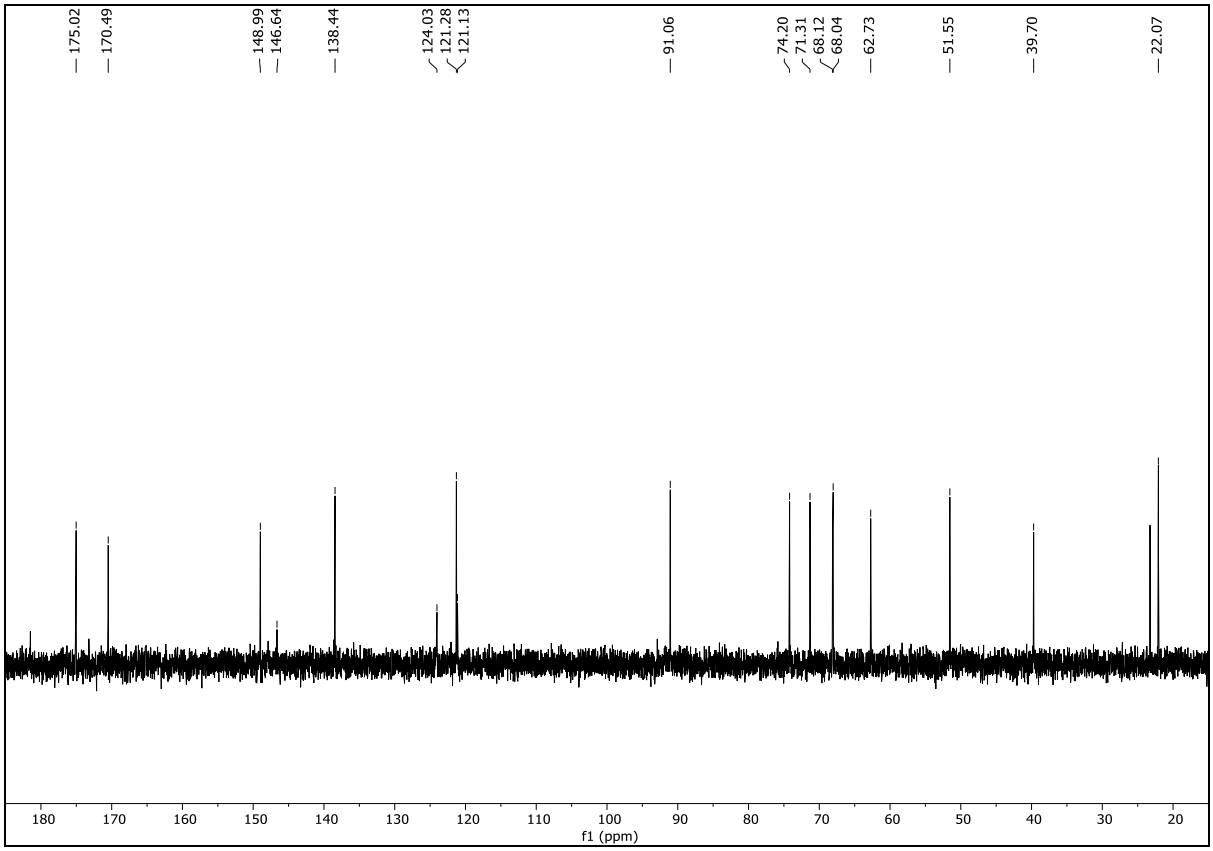
^{13}C NMR (101 MHz, D_2O) spectrum of compound **3c**



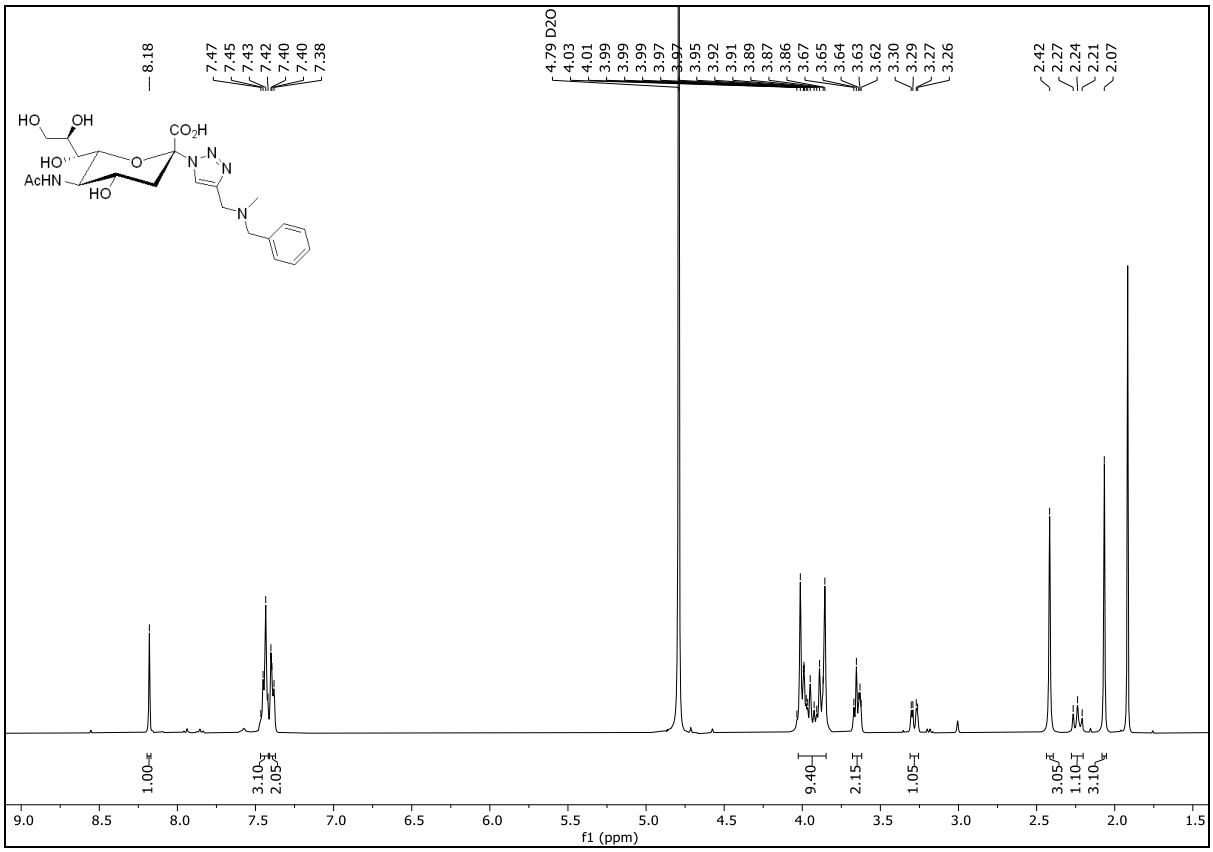
^{1}H NMR (400 MHz, D_2O) spectrum of compound **3d**



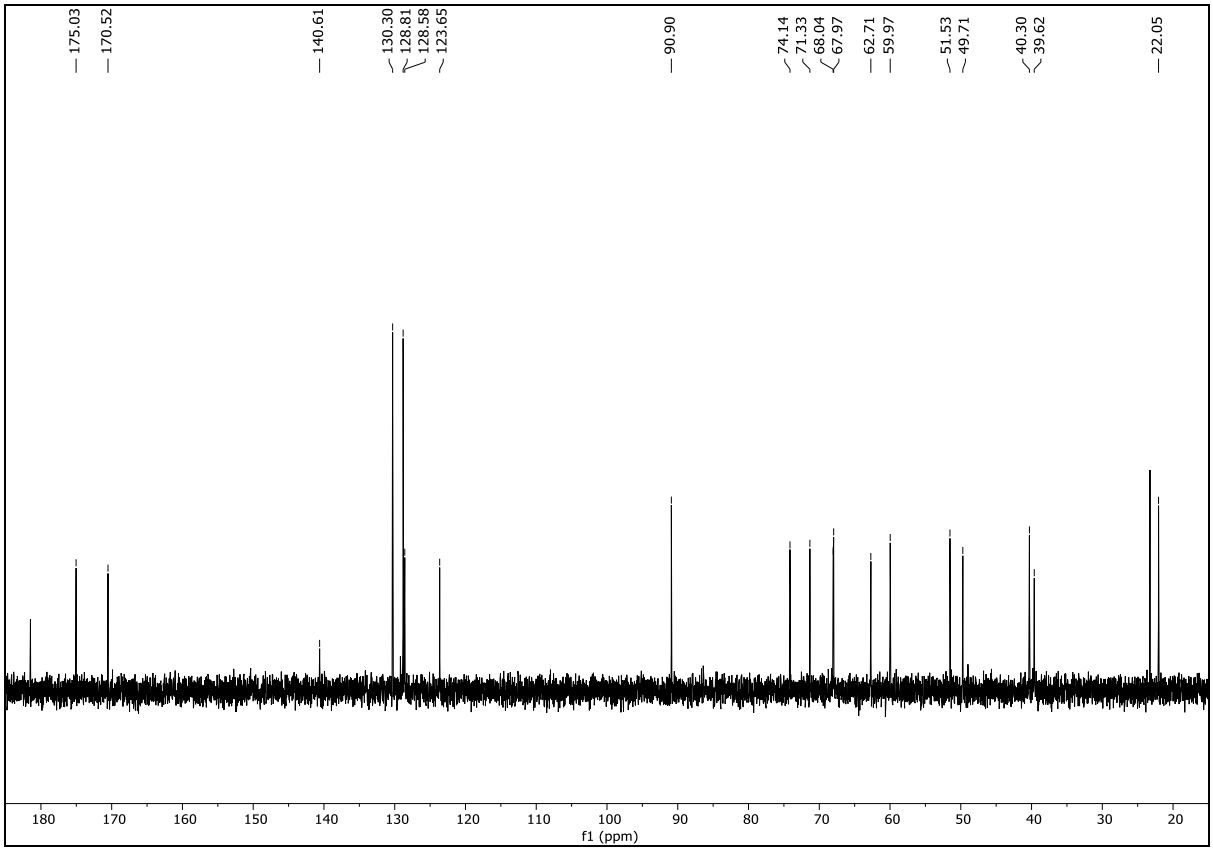
^{13}C NMR (101 MHz, D_2O) spectrum of compound **3d**



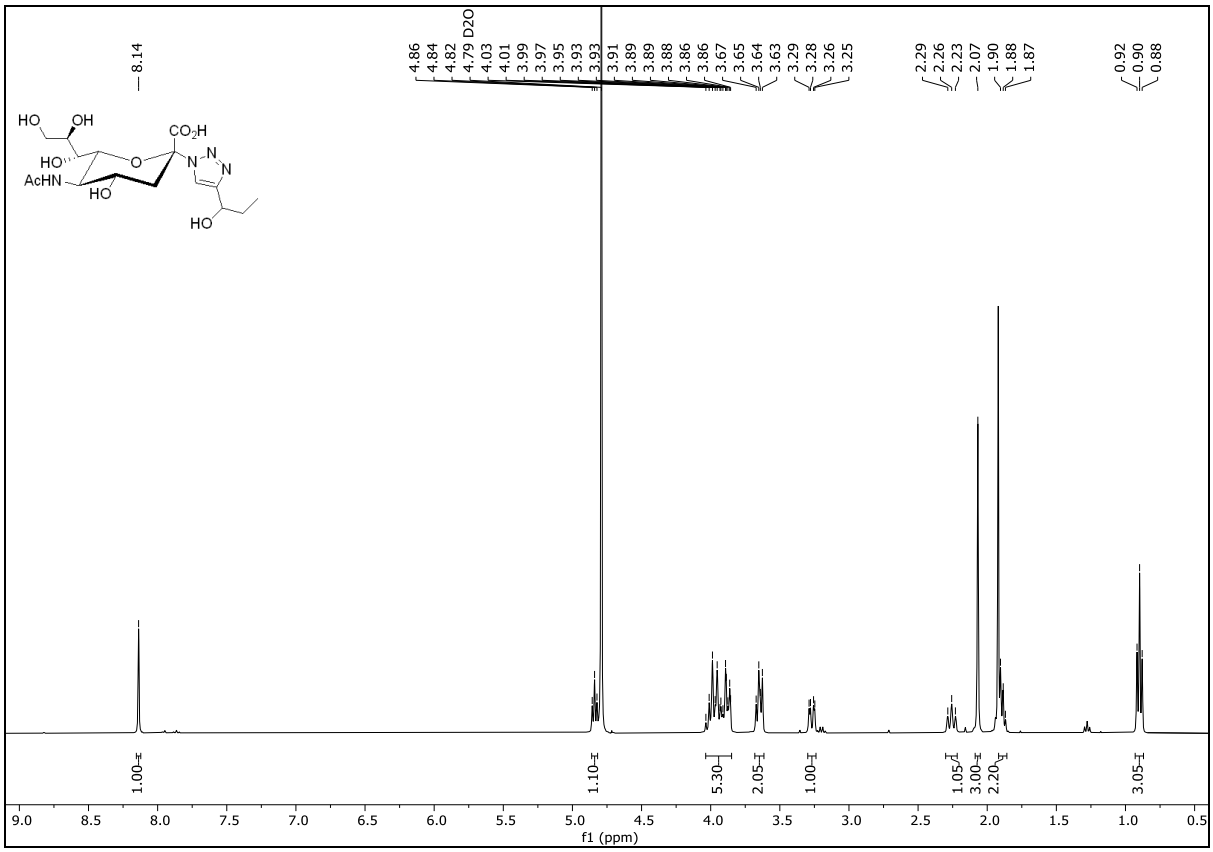
^{1}H NMR (400 MHz, D_2O) spectrum of compound **3e**



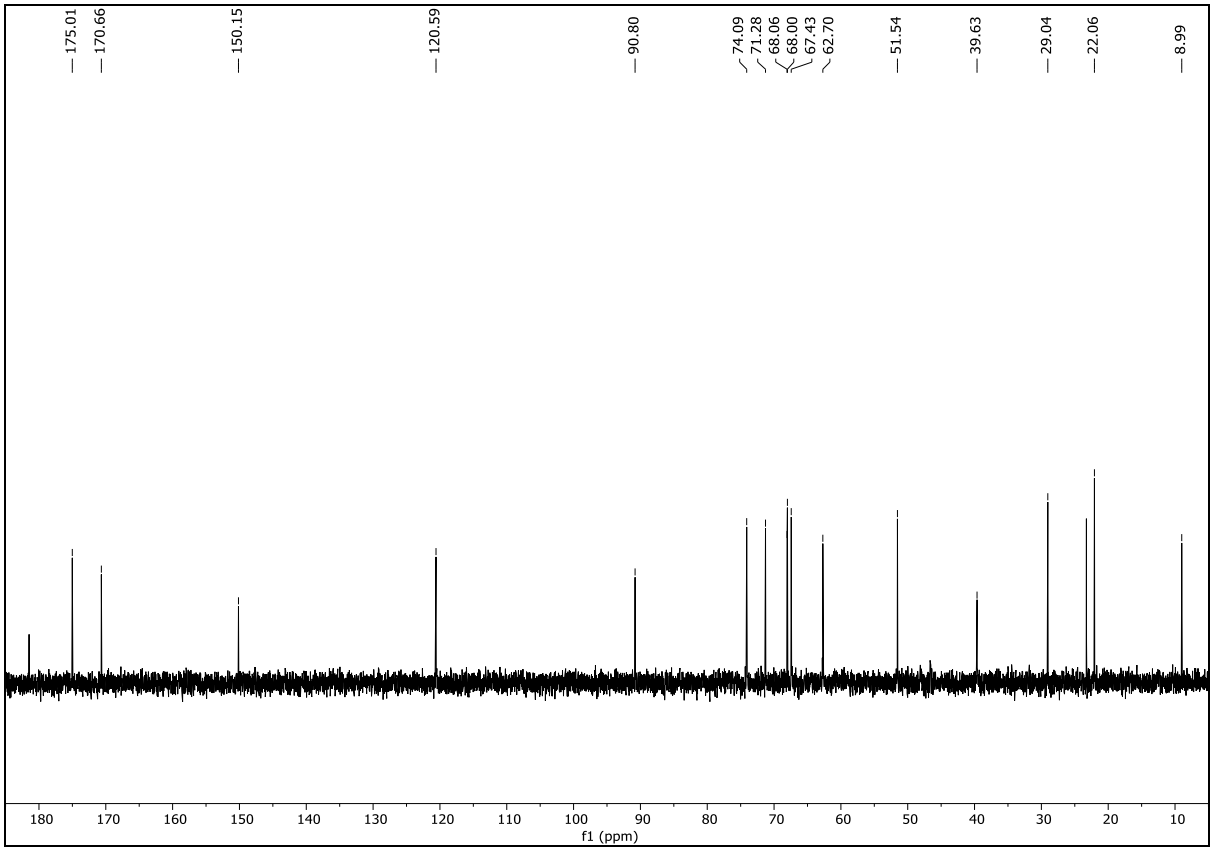
^{13}C NMR (101 MHz, D_2O) spectrum of compound **3e**



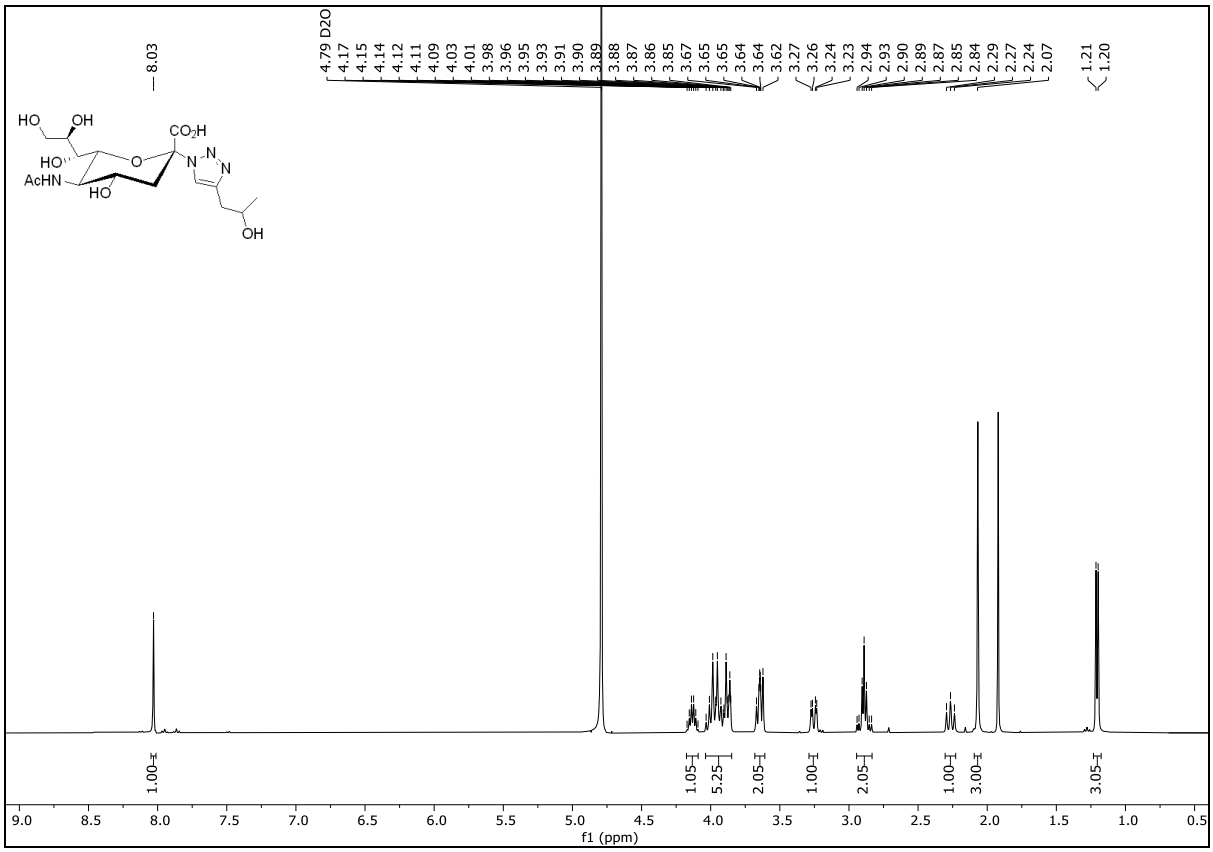
^{1}H NMR (400 MHz, D_2O) spectrum of compound **3f**



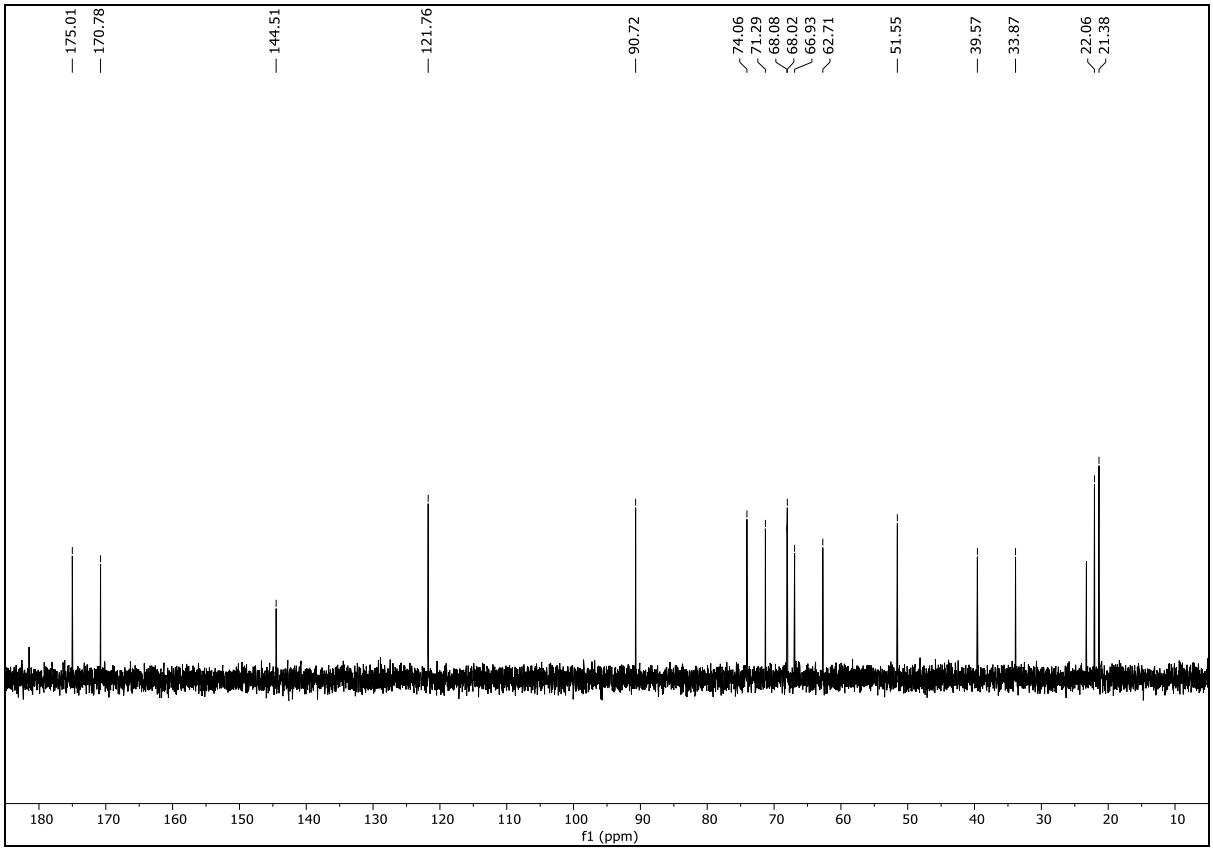
^{13}C NMR (101 MHz, D_2O) spectrum of compound **3f**



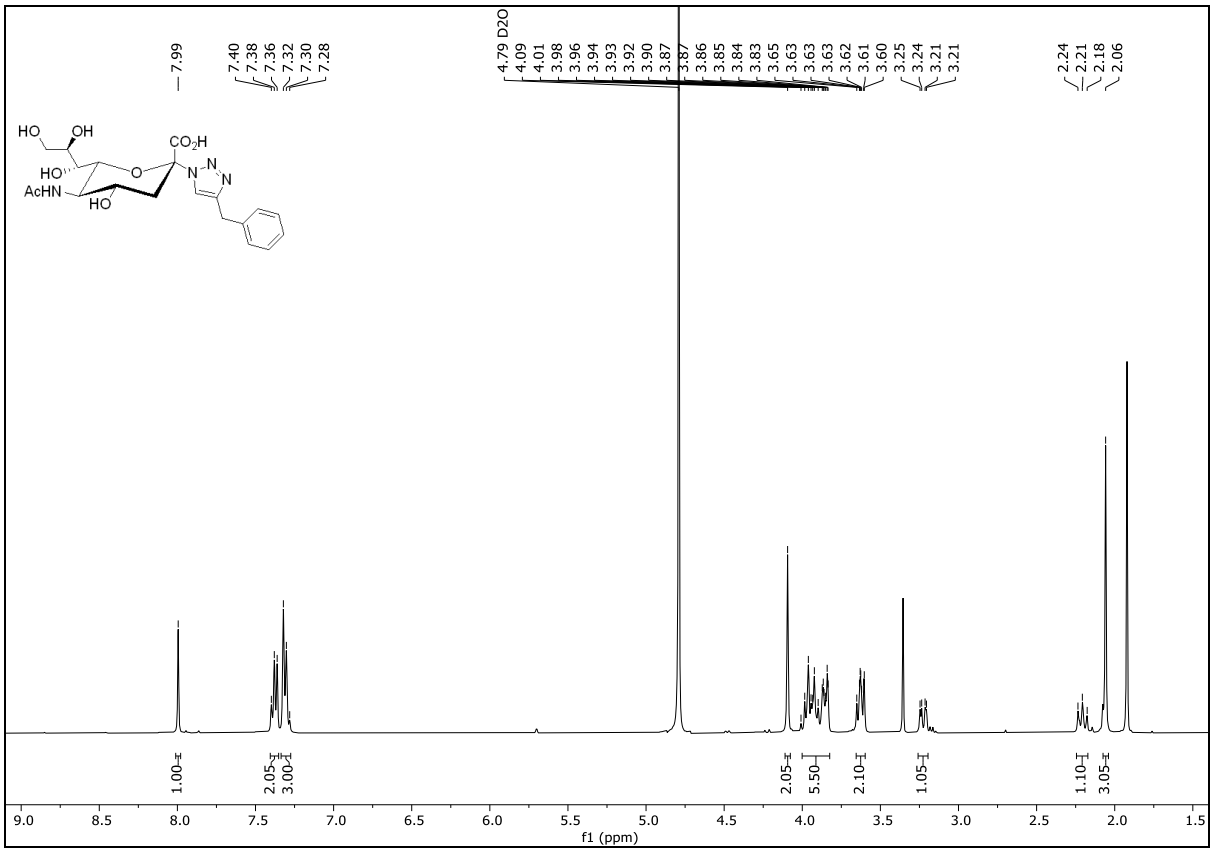
^{1}H NMR (400 MHz, D_2O) spectrum of compound **3g**



^{13}C NMR (101 MHz, D_2O) spectrum of compound **3g**



^{1}H NMR (400 MHz, D_2O) spectrum of compound **3h**



^{13}C NMR (101 MHz, D_2O) spectrum of compound **3h**

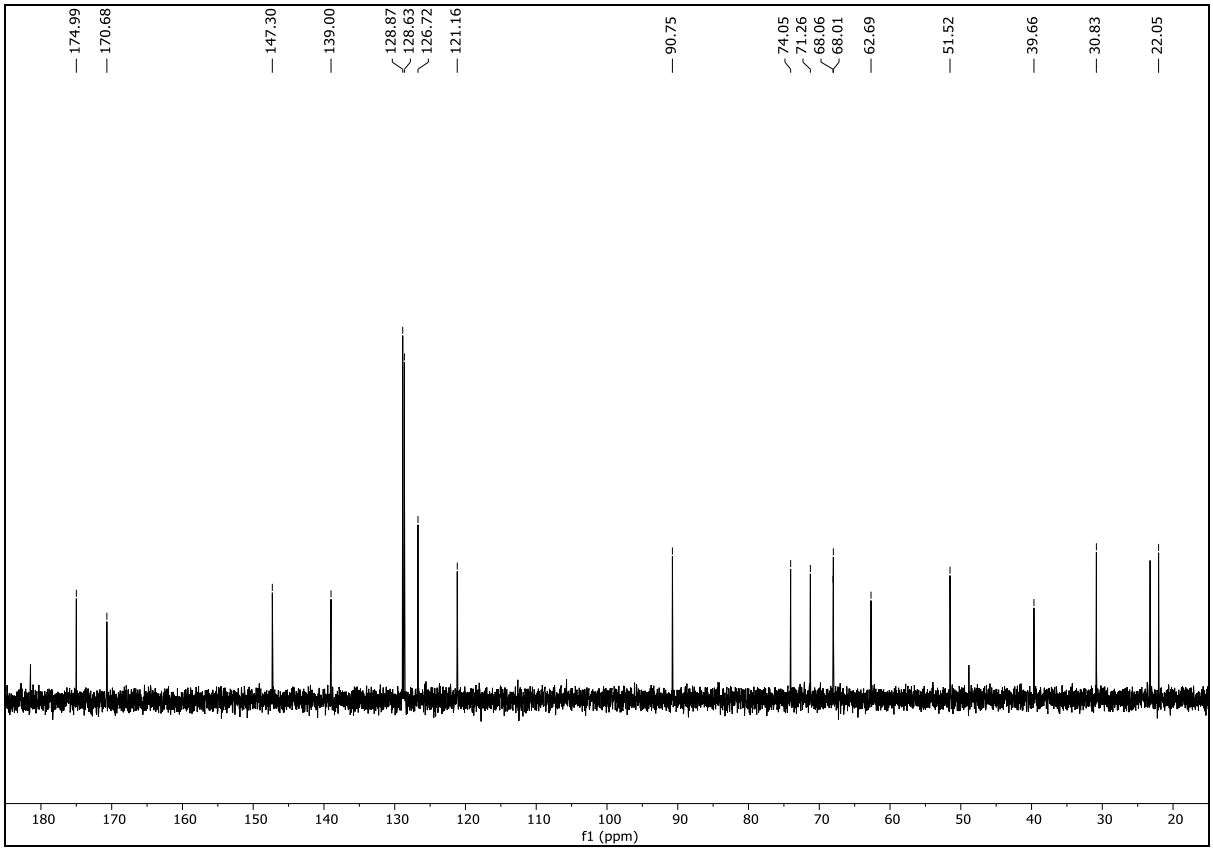
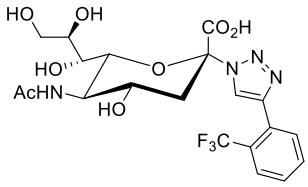
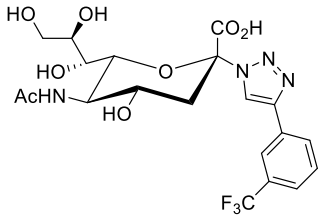
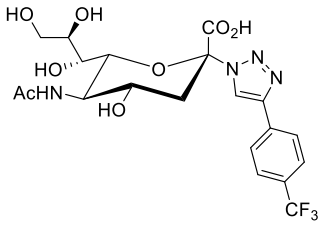
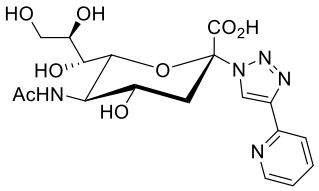
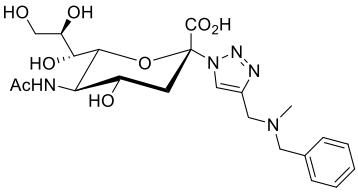
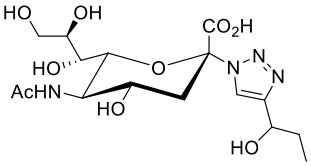
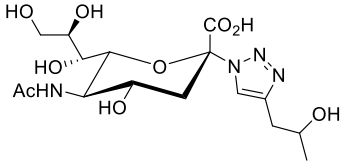
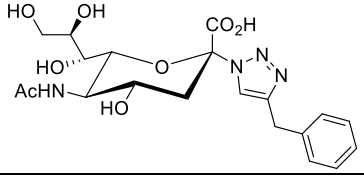


Table S1. Calculated LogP* of compounds **3a–h**.

Compound	Structure	LogP
3a		**0.08**
3b		**0.08**
3c		**0.08**
3d		**-1.76**
3e		**-0.84**
3f		**-2.29**
3g		**-2.67**
3h		**-0.56**

* Calculated with CambridgeSoft software (ChemDraw's Chemical Properties).