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Supplementary material

SUPPLEMENTARY MATERIAL TO

Click mediated synthesis of functionalized glycolipids with peptide-peptoid linkages

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EXPERIMENTAL

A. General Information: The solvents used during the reaction were distilled before use, and dry solvents were prepared using standard methods. All reagents purchased from commercial sources were used without any purification. Column chromatography was performed over 100-200 mesh silica with ethyl acetate and hexane as the eluent. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer. All mass spectra were recorded in a Q-TOF electrospray ionization spectrometer. UV-Visible spectra were recorded on a Systronics PC-based double-beam UV-visible spectrophotometer (model-2202). Scanning Electron Microscopic studies were carried out using a Hitachi S3400 N microscope. All the Density Functional Theory (DFT) based computations were performed using the Gaussian 09W package. The geometries of Compounds **21** and **22**, which include iodine atoms in their structures, were optimized at B3LYP/def2svp level, and for all other compounds given in Figure 3, the geometry optimization was performed at B3LYP/6-31G(d) level. No symmetry was imposed in the molecules during optimization. The optimized structures obtained in the above processes were subjected to frequency calculations to find out whether these are maxima or minima in the potential energy surfaces.

B 1. General method for Cu(I) catalysed synthesis of 1,4-triazole linked glycolipids **4** & **6**: To a stirred mixture of azide (**3** or **5**, 1 mmol)[26] and alkyne (**1**, 1.1 mmol) in acetone (5 mL), solutions of copper sulphate (20 mol% in 1 mL water) and sodium ascorbate (40 mol% in 1.5 mL water) were added. The reaction continued until the starting material (**3** or **5**) was completely consumed at room temperature, as indicated by TLC. The crude product obtained after the aqueous workup was purified by column chromatography to obtain an analytically pure sample.

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Compound **4**: Yield 95% (520 mg), m.p. 175-179 °C, $[\alpha]_D$ -28.6° (c = 1.0, $CHCl_3$, 25 °C), ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H, triazole $-C\underline{H}$), 7.27 (t, 1H, J = 9.6 Hz, $N\underline{H}$), 5.98 (d, 1H, J = 8.4 Hz, H-1), 5.53-5.44 (m, 2H, H-2 & H-3), 5.31 (t, 1H, J = 9.6 Hz, H-4), 4.32-4.28 (dd, 1H, H-6a), 4.18-4.15 (dd, 1H, H-6b), 4.09-4.06 (m, 1H, H-5) 3.48-3.42 (m, 2H, NH-$C\underline{H}_2$-), 2.08, 2.06. 2.03, 1.87 (4s, 12H, 4 x $-COC\underline{H}_3$), 1.64-1.60 (m, 2H, $-NHCH_2\underline{CH_2}CH_2$), 1.38-1.27 (bs, 10H, 5 x $C\underline{H}_2$), 0.87 (t, 3H, $-C\underline{H}_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.6, 170.0, 169.4, 168.7, 159.4, 144.1, 124.4, 85.8, 75.1, 72.6, 70.5, 67.5, 61.4, 39.3, 31.8, 29.6, 29.3, 29.2, 27.0, 22.7, 20.7, 20.6 (x 2), 20.2, 14.1 ppm; ESI-MS HRMS: calculated 555.2666 for $[M+H]^+$, found 555.2667 for $C_{25}H_{39}N_4O_{10}$.

Compound **6**: Yield 90% (550 mg), m.p. 155-157 °C, $[\alpha]_D$ +11.2° (c = 1.3, $CHCl_3$, 25 °C), ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (s, 1H, triazole $-C\underline{H}$), 7.56 (d, 1H, J = 8.8 Hz, $N\underline{H}$), 7.29 (t, 1H, $N\underline{H}$), 5.33-5.27 (m, 2H, H-1 & H-2), 5.21-5.11 (ABq, 2H, $NHCOC\underline{H}_2$), 5.05 (t, 1H, J = 9.6 Hz, H-4), 4.94 (t, 1H, J = 9.6 Hz, H-3), 4.30-4.25 (dd, 1H, H-6a), 4.10-4.07 (dd, 1H, H-6b), 3.87-3.86 (m, 1H, H-5) 3.47-3.42 (m, 2H, NH-$C\underline{H}_2$-), 2.06. 2.03, 2.00 (3s, 12H, 4 x $-COC\underline{H}_3$), 1.64-1.59 (m, 2H, $-NHCH_2\underline{CH_2}CH_2$), 1.37-1.27 (bs, 10H, 5 x $C\underline{H}_2$), 0.87 (t, 3H, $-C\underline{H}_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.7, 170.6, 169.8, 169.5, 165.4, 159.7, 143.7, 127.1, 78.2, 73.8, 72.7, 70.4, 68.1, 61.7, 52.6, 39.3, 31.7, 29.5, 29.2, 29.1, 26.9, 22.6, 20.6, 20.5, 14.0 ppm; ESI-MS HRMS: calculated 612.2881 for $[M+H]^+$, found 612.2903 for $C_{27}H_{42}N_5O_{11}$.

2. General method for synthesis of 5-benzoyl 1,4-triazole linked glycolipids **7, 8, & 9:**

Per-*O*-acetylated glucopyranosyl azide/ azidoacetamide (**3** or **5**, 1 mmol) was taken along with *n*-alkyl propiolamide (**1** or **2**, 1.1 mmol) and Cu(I)Br (1.1 mmol) in a two necked RB flask under nitrogen. Dry acetonitrile (5 mL) was added to it, followed by DIEA (0.45 mL, 2.5 mmol). The reaction mixture was stirred at 0 °C for 10 minutes and benzoyl chloride (0.13 mL, 1.1 mmol) was added dropwise. The reaction was continued at room temperature until the per-*O*-acetylated glucopyranosyl azide/azidoacetamide was completely consumed, as indicated by TLC. The crude product, after aqueous workup, was purified by column chromatography and characterized based on NMR and ESI-MS spectroscopic data.

Compound **7**: Yield 75% (490 mg), m.p. 58-61 °C, $[\alpha]_D$ -39.8° (c = 0.7, $CHCl_3$, 25 °C), ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, 2H, J = 7.6 Hz), 7.61 (t, 1H, J = 7.6 Hz), 7.45 (t, 2H, J = 7.6 Hz), 7.07 (t, 2H, J = 6.0 Hz, $N\underline{H}$), 5.89-5.80 (m, 2H, H-1 & H-2), 5.34 (t, 1H, J = 9.2 Hz, H-3), 5.11 (t, 1H, J = 9.6 Hz, H-4), 3.92-3.88 (dd, 1H, H-6a), 3.80-3.76 (m, 2H, H-6b & H-5), 3.33-3.28 (q, 2H, NH-$C\underline{H}_2$-), 2.03, 2.00. 1.96, 1.81 (4s, 12H, 4 x $-COC\underline{H}_3$), 1.53-1.50 (m, 2H, $-NHCH_2C\underline{H}_2$), 1.29-1.25 (bs, 10H, 5 x $C\underline{H}_2$), 0.86 (t, 3H, $-C\underline{H}_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.2 (Triazole-$\underline{C}$=O), 170.3, 170.2, 169.2, 168.7 (4 x $-\underline{C}OCH_3$), 158.3 (NH-$\underline{C}$O), 142.2, 136.5, 135.8, 134.7, 129.6, 128.7, 85.3 (C-1), 75.0, 72.8, 70.1, 67.3, 61.3, 39.4, 31.8, 29.8, 29.6, 29.3, 29.2, 27.0, 22.7, 20.6 (x 2), 20.5, 20.4, 14.2 ppm; ESI-MS HRMS: calculated 659.2928 for $[M+H]^+$, found 659.2924 for $C_{32}H_{43}N_4O_{11}$.

Compound **8**: Yield 70% (500 mg), syrup, $[\alpha]_D$ -53.0° (c = 0.2, $CHCl_3$, 25 °C), ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 7.6 Hz, 2H), 7.61 (t, J = 7.6 Hz, 1H), 7.45 (t, J = 7.6 Hz, 2H), 7.07 (t, 1H, NH), 5.89-5.80 (m, 2H, H-1 & H-2), 5.34 (t, 1H, J = 9.2 Hz, H-3), 5.11 (t, 1H, J = 9.6 Hz, H-4), 3.91-3.88 (dd, 1H, H-6a), 3.79-3.76 (m, 2H, H-6b & H-5), 3.33-3.28 (q, 2H, NH-$C\underline{H}_2$-), 2.03, 2.00. 1.96, 1.81 (4s, 12H, 4 x $-COC\underline{H}_3$), 1.53 (m, 2H, $-NHCH_2C\underline{H}_2$), 1.25 (bs,18H, 9 x $C\underline{H}_2$), 0.87 (t, 3H, $-C\underline{H}_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.1 (Triazole-$\underline{C}$=O), 170.2, 170.1, 169.0, 168.6 (4 x $-\underline{C}OCH_3$), 158.2, 142.1, 136.4, 135.7, 134.5, 129.4, 128.6, 85.2, 74.9, 72.7, 70.0, 67.2, 61.2, 39.2, 31.8, 29.6, 29.5, 29.4, 29.3, 29.2, 26.8, 22.6, 20.5, 20.4, 20.3, 14.2 ppm; ESI-MS HRMS: calculated 715.3554 for $[M+H]^+$, found 715.3528 for $C_{36}H_{51}N_4O_{11}$.

Compound **9**: Yield 70% (540 mg), syrup, $[\alpha]_D$ -14.2° (c = 0.3, $CHCl_3$, 25 °C), ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 7.6 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.46 (t, 2H, *J* = 7.6 Hz,), 7.20 (t, 1H, *J* = 6.0 Hz, N$\underline{H}$), 7.06 (d, 1H, *J* = 9.2 Hz, C-1N$\underline{H}$-), 5.26-5.19 (m, 3H, H-2 & -NHCOC$\underline{H}_2$-), 5.13 (t, 1H, *J* = 9.2 Hz, H-1), 5.02 (t, 1H, *J* = 9.2 Hz, H-4), 4.86 (t, 1H, *J* = 9.6 Hz, H-3), 4.26-4.22 (dd, 1H, H-6a), 4.03-4.00 (dd, 1H, H-6b), 3.76-3.73 (m, 1H, H-5) 3.32-3.27 (q, 2H, NH-C$\underline{H}_2$-), 2.05, 2.01. 1.99 (x 2) (4s, 12H, 4 x -COC$\underline{H}_3$), 1.53-1.50 (m, 2H, -$NHCH_2C\underline{H}_2$), 1.24 (bs,18H, 9 x C$\underline{H}_2$), 0.87 (t, 3H, - C$\underline{H}_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ186.8 (Triazole-$\underline{C}$=O), 171.4, 170.7, 169.9, 169.6 (4 x –$\underline{C}OCH_3$), 165.1, 158.6 (2 x NH-CO), 142.5, 136.5, 135.3, 134.7, 129.8, 128.9, 128.6, 78.3 (C-1), 73.7, 72.5, 70.5, 68.1, 61.7, 51.7, 39.4, 32.0, 29.7, 29.6 (x 2), 29.4, 29.3, 26.9, 22.7, 20.8, 20.6, 14.2 ppm; ESI-MS HRMS: calculated 772.3769 for $[M+H]^+$, found 772.3758 for $C_{38}H_{54}N_5O_{12}$.

3. Synthesis of **11**: To a mixture of aniline (0.3 mL, 3.2 mmol) and potassium carbonate (900 mg, 6.5 mmol) in dry acetonitrile (10 mL), propargyl bromide (0.3 mL, 3.5 mmol) was added at 0 °C. After stirring the reaction mixture for 12 h at room temperature, chloroacetyl chloride (5 mmol) was added to the reaction mixture at 0 °C. The reaction mixture was allowed to cool to room temperature over a period of 30 minutes and stirred for 24 h at room temperature. After completion of the reaction, as indicated by TLC, the reaction mixture was filtered and the filtrate was concentrated to dryness. The crude reaction mixture was purified by column chromatography to give the title compound in 50% overall yield.

Compound **11:** Yield 50% (330 mg), ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 7.48-7.46 (m, 3H), 7.35-7.33 (m, 2H), 4.50 (d, 2H, *J* = 2.4 Hz, N-$\underline{CH_2}$-), 3.84 (s, 2H, CO-C$\underline{H}_2$-Cl), 2.24 (t, 1H, *J* = 2 Hz, alkyne C$\underline{H}$) ppm; ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 165.9, 140.2, 130.1, 129.3, 128.2, 120.2, 78.2, 72.9, 41.7, 39.2 ppm. ESI-MS HRMS: Calculated for $C_{11}H_{11}NOCl$ ($[M+H]^+$): 208.0529; found 208.0527.

4. Synthesis of triazole-linked chloroacetamide functionalized glycoconjugates **12** & **13**:

Synthesis was done following the same procedure as that of compounds **4** and **6**.

Compound **12**: Yield 90% (450 mg), m.p. 80-81 °C, $[\alpha]_D$ -10.0° (c = 0.4, $CHCl_3$, 25 °C), ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 7.80 (s, 1H, triazole C$\underline{H}$), 7.16 (s, 1H, N$\underline{H}$), 5.87-5.85 (m, 1H, H-1), 5.45-5.38 (m, 2H, H-2 & H-3), 5.26-5.21 (m, 1H, H-4), 4.62-4.55 (m, 2H, C$\underline{H}_2$NH), 4.33-4.28 (m, 1H, H-6a), 4.17-4.14 (m, 1H, H-6b), 4.07 (s, 2H, C$\underline{H}_2$Cl), 4.02-3.98 (m, 1H, H-5), 2.09, 2.06, 2.03, 1.87 (4s, 12H, 4 x –COC$\underline{H}_3$) ppm; ^{13}C-NMR ($CDCl_3$, 100 MHz): δ170.6, 170.0, 169.4, 168.9, 166.2, 144.7, 121.0, 85.9, 75.3, 72.7, 70.5, 67.8, 61.6, 42.6, 35.3, 20.8, 20.6 (x 2), 20.2 ppm; ESI-MS HRMS: Calculated for $C_{19}H_{26}N_4O_{10}Cl$ ($[M+H]^+$): 505.1337; found 505.1330.

Compound **13**: Yield: 92% (530 mg), m.p. 89-90 °C, $[\alpha]_D$ -8.3° (c = 0.4, $CHCl_3$, 25 °C), ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 7.96 (s, 1H, triazole C$\underline{H}$), 7.42-7.37 (m, 3H), 7.18-7.16 (m, 2H), 5.83 (d, 1H, *J* = 8.8 Hz, H-1), 5.43-5.39 (m, 2H, H-2 & H-3), 5.25 (t, 1H, *J* = 9.6 Hz, H-4), 5.09-4.79 (ABq, 2H, NC$\underline{H}_2$), 4.35-4.30 (m, 1H, H-6a), 4.18-4.15 (m, 1H, H-6b), 4.02-3.98 (m, 1H, H-5), 3.87 (s, 2H, C$\underline{H}_2$Cl), 2.11, 2.07, 2.03, 1.87 (4s, 12H, 4 x –COC$\underline{H}_3$) ppm; ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 170.7, 170.0, 169.4, 168.8, 166.4, 144.3, 141.0, 130.1, 129.1, 128.0, 122.3, 86.0, 75.3, 72.5, 70.7, 67.7, 61.5, 45.7, 42.0, 20.8, 20.6, 20.2 ppm; ESI-MS HRMS: Calculated for $C_{25}H_{30}N_4O_{10}Cl$ ($[M+H]^+$): 581.1650; found 581.1673.

5. Synthesis of triazole-linked azide functionalized glycoconjugates **14** & **15**:

Triazole-linked chloroacetamide functionalized glycoconjugate (**12** or **13**, 0.5 mmol) was dissolved in acetone (14 mL) and an aqueous solution (7 mL) of sodium azide (160 mg, 2.5

mmol) was added to it. The reaction mixture was stirred at 60 °C for 24 h. After completion of the reaction, acetone was removed by applying vacuum. Ethyl acetate (50 mL) was added to the reaction mixture and the organic layer after aqueous workup gave the desired compound (**14** or **15**).

Compound **14**: Yield 92% (240 mg), m.p. 89-90 °C, $[\alpha]_D$ -3.5° (c = 0.3, $CHCl_3$, 25 °C), ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 7.84 (s, 1H, triazole C-H), 7.09 (s, 1H, NH), 5.89-5.87 (m, 1H, H-1), 5.46-5.40 (m, 2H, H-2 & H-3), 5.28-5.23 (m, 1H, H-4), 4.62-4.53 (m, 2H, NHCH_2), 4.33-4.28 (m, 1H, H-6a), 4.17-4.14 (m, 1H, H-6b), 4.05-3.99 (m, 3H, H-5 & CH_2N_3), 2.09, 2.07, 2.03, 1.87 (4s, 12H, 4 x –COCH_3) ppm; ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 170.6, 170.0, 169.4, 169.0, 167.0, 144.8, 121.1, 85.8, 75.2, 72.6, 70.5, 67.7, 61.5, 52.6, 34.8, 20.8, 20.6 (x 2), 20.2 ppm; ESI-MS HRMS: Calculated for $C_{19}H_{25}N_7O_{10}Na$ ([M+Na]$^+$): 534.1561; found 534.1556.

Compound **15**: Yield 94% (275 mg), m.p. 81-84 °C, $[\alpha]_D$ -22.7° (c = 0.3, $CHCl_3$, 25 °C), ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 7.97 (s, 1H, triazole C-H), 7.41-7.37 (m, 3H), 7.14-7.12 (m, 2H), 5.84 (d, 1H, *J* = 8.8 Hz, H-1), 5.46-5.37 (m, 2H, H-2 & H-3), 5.26 (t, 1H, *J* = 9.6 Hz, H-4), 5.09-4.80 (ABq, 2H, NHCH_2-), 4.35-4.30 (m, 1H, H-6a), 4.18-4.15 (m, 1H, H-6b), 4.03-3.99 (m, 1H, H-5), 3.64-3.61 (m, 2H, CH_2N_3), 2.11, 2.07, 2.03, 1.87 (4s, 12H, 4 x –COCH_3) ppm; ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 170.7, 170.0, 169.4, 168.9, 167.6, 144.3, 140.5, 130.2, 129.1, 128.0, 122.3, 85.9, 75.2, 72.5, 70.7, 67.7, 61.5, 50.9, 45.3, 20.8, 20.6, 20.2 ppm; ESI-MS HRMS: Calculated for $C_{25}H_{30}N_7O_{10}$ ([M+H]$^+$): 588.2054; found 588.2048.

6. Synthesis of bis-triazole-linked glycolipids **17**, **18**, & **19**:

Synthesis was done following the same procedure as that of compounds **4** and **6**.

Compound **17**: Yield 94% (240 mg), $[\alpha]_D$ +23.5° (c = 0.2, $CHCl_3$, 25 °C), ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.32 (s, 1H, triazole C-H), 7.86 (s, 1H, triazole C-H), 7.33 (s, 1H, NH), 5.87-5.85 (m, 1H, H-1), 5.43-5.41 (m, 2H, H-2 & H-3), 5.27-5.23 (m, 1H, H-4), 5.16-5.08 (m, 2H, COCH_2-N), 4.56-4.54 (m, 2H, -O-CH_2-triazole), 4.35-4.28 (m, 3H, H-6a & O-CH_2-CH$_2$-), 4.18-4.14 (m, 1H, H-6b), 4.04-4.02 (m, 1H, H-5), 2.07, 2.02, 1.84 (3s, 12H, 4 x –COCH$_3$), 1.77-1.72 (m, 2H, O-CH$_2$-CH_2-), 1.40-1.26 (bs, 10H, 5 x CH_2), 0.88 (t, 3H, -CH_3) ppm; ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 170.6, 170.0, 169.4, 169.0, 164.7, 160.7, 144.6, 140.7, 129.3, 121.5, 85.9, 75.3, 72.6, 70.6, 67.8, 65.6, 61.6, 52.7, 35.2, 31.9, 29.3, 29.2, 28.7, 26.0, 22.7, 20.8, 20.7, 20.6, 20.2, 14.1 ppm; ESI-MS HRMS: Calculated for $C_{30}H_{45}N_7O_{11}K$ ([M+K]$^+$): 718.2814; found 718.2816.

Compound **18**: Yield 92% (275 mg), $[\alpha]_D$ +22.8° (c = 0.3, $CHCl_3$, 25 °C), ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.29 (s, 1H, triazole C-H), 7.85 (s, 1H, triazole C-H), 7.26-7.18 (m, 2H, 2x NH), 5.87-85 (d, 1H, H-1), 5.43-5.41 (m, 2H, H-2 & H-3), 5.29-5.25 (m, 1H, H-4), 5.14 (s, 2H, N-CH_2-CO), 4.53-4.52 (m, 2H, NH-CH_2-triazole), 4.32-4.28 (m, 1H, H-6a), 4.19-4.15 (m, 1H, H-6b), 4.04-4.02 (m, 1H, H-5), 3.45-3.40 (m, 2H, CO-NH-CH_2), 2.07, 2.06, 2.02, 1.85 (4s, 12H, 4 x –COCH_3), 1.62-1.59 (m, 2H, NH-CH$_2$-CH_2), 1.25 (bs, 18H, 9 x CH_2), 0.87 (t, 3H, -CH_3) ppm; ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 170.6, 170.0, 169.4, 169.1, 164.9, 159.8, 144.6, 144.0, 127.2, 121.5, 85.9, 75.3, 72.6, 70.6, 67.8, 61.6, 52.9, 39.4, 35.1, 32.0, 29.8, 29.7, 29.6, 29.4, 27.1, 22.8, 20.8, 20.6, 20.6, 20.2, 14.2 ppm; ESI-MS HRMS: Calculated for $C_{34}H_{52}N_8O_{11}Na$ ([M+Na]$^+$): 771.3653; found 771.3659.

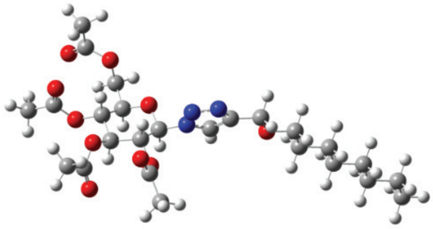
Compound **19**: Yield 92% (275 mg), $[\alpha]_D$ -26.5° (c = 0.3, $CHCl_3$, 25 °C), ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.20 (s, 1H, triazole C-H), 7.91 (s, 1H, triazole C-H), 7.48-7.43 (m, 3H), 7.26-7.23 (m, 2H), 7.11 (t, 1H, NH), 5.82 (d, 1H, *J* = 8.8 Hz, H-1), 5.43-5.36 (m, 2H, H-2 & H-3), 5.26 (t, 1H, *J* = 9.6 Hz, H-4), 5.14-4.75 (m, 4H, CO-CH_2-triazole & N-CH_2-triazole), 4.33-4.29 (m, 1H, H-6a), 4.19-4.16 (m, 1H, H-6b), 4.01-3.97 (m, 1H, H-5), 3.45-3.40 (m, 2H, NH-C$\underline{H}_2$), 2.10, 2.06, 2.04, 1.88 (4s, 12H, 4 x –COC$\underline{H}_3$), 1.62-1.58 (m, 2H, CO-NH-CH$_2$-C$\underline{H}_2$), 1.37-1.26 (bs, 18H, 9 x C$\underline{H}_2$), 0.87 (t, 3H, -C$\underline{H}_3$) ppm; ^{13}C-NMR (CDCl$_3$, 100 MHz): δ 170.6, 170.0, 169.3, 168.9, 164.6, 160.0, 144.0, 143.7, 140.2, 130.5, 129.5, 128.3, 127.3, 122.5, 86.0, 75.4, 72.5, 70.9, 67.9, 61.5, 51.7, 45.6, 39.3, 32.0, 29.7, 29.6, 29.4, 27.0, 22.8, 20.8, 20.6, 20.3, 14.2 ppm; ESI-MS HRMS: Calculated for $C_{40}H_{56}N_8O_{11}K$ ([M+K]$^+$): 863.3705; found 863.3708.

C. Optimized structures of the synthesized glycolipids[1]

To understand the stability of the glycolipids, the geometries of these molecules were optimized using B3LYP density functional theory method. The optimized structures thus obtained were used for frequency calculations. In each case, positive frequencies were obtained, which implies that the optimized structures have the minimum potential energy surfaces and hence are stable. The optimized energies, zero point energies, and the energies obtained after zero point energy correction are given in Table S-I. Table S-I also includes the corresponding computed dipole moments of the optimized structures.

TABLE S-I. The computed optimized energies and dipole moments of different glycolipids

Glycolipids	Energy (Hartree)	Zero Point Energy (ZPE) (Hartree)	ZPE corrected Energy (Hartree)	Dipole moment (Debye)
Compound **20**	-1892.6572228	0.6452809	-1892.011942	4.6002
Compound **21**	-2188.4529957	0.6300699	-2187.822926	4.2163
Compound **4**	-1946.8434404	0.640086	-1946.203354	1.7310
Compound **22**	-2242.6021772	0.6249956	-2241.977182	1.4714
Compound **23**	-4517.9400722	0.6300275	-4517.310045	1.2438
Compound **24**	-4725.9556611	0.685842	-4725.269819	4.7129
Compound **8**	-2448.4788797	0.8450222	-2447.633858	1.9814
Compound **9**	-2656.4962833	0.9017656	-2655.594518	4.2192
Compound **6**	-2154.8592204	0.6963938	-2154.162827	5.9574
Compound **17**	-2381.0080409	0.7691367	-2380.238904	7.9441
Compound **18**	-2592.4501362	0.8781671	-2591.571969	8.1417
Compound **19**	-2823.4965783	0.9592672	-2822.537311	2.1175



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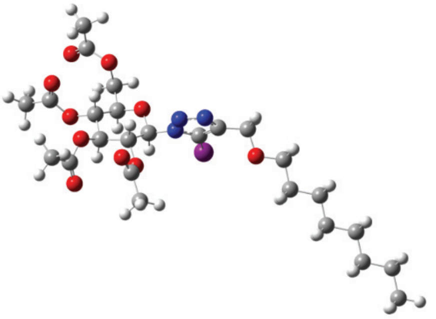

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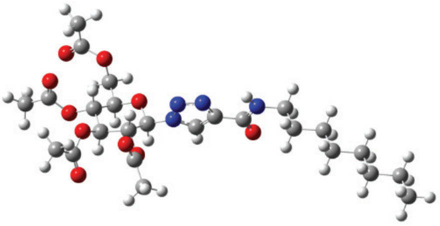

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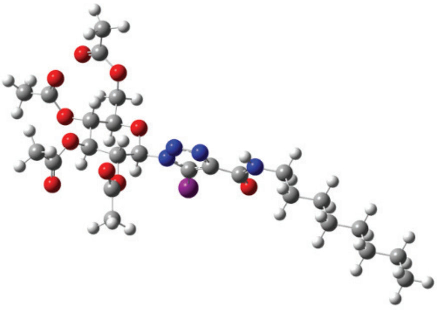

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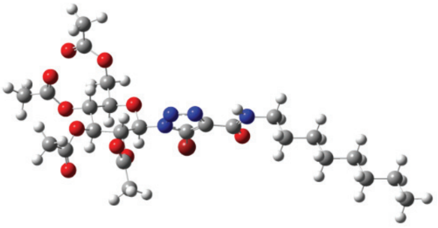

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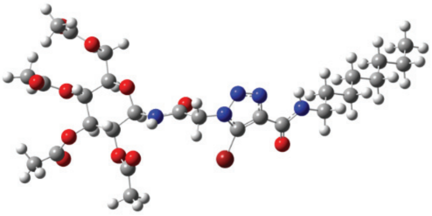

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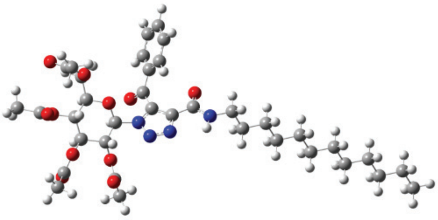

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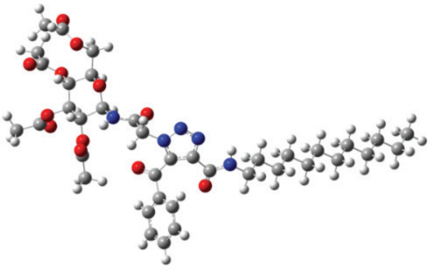

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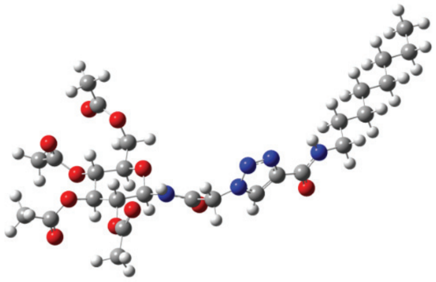

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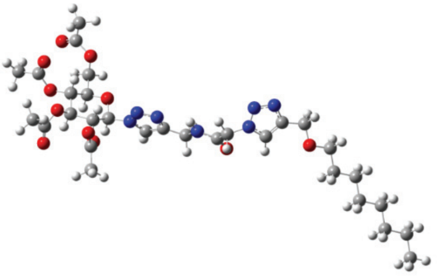

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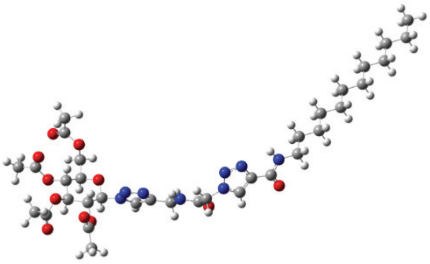

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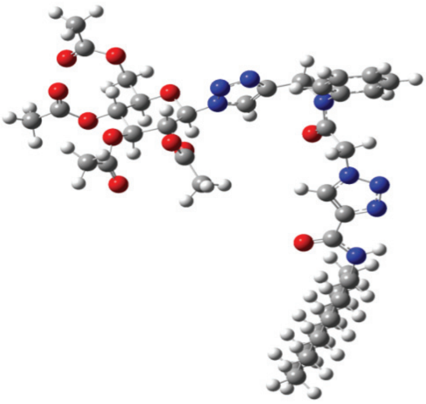

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REFERENCES

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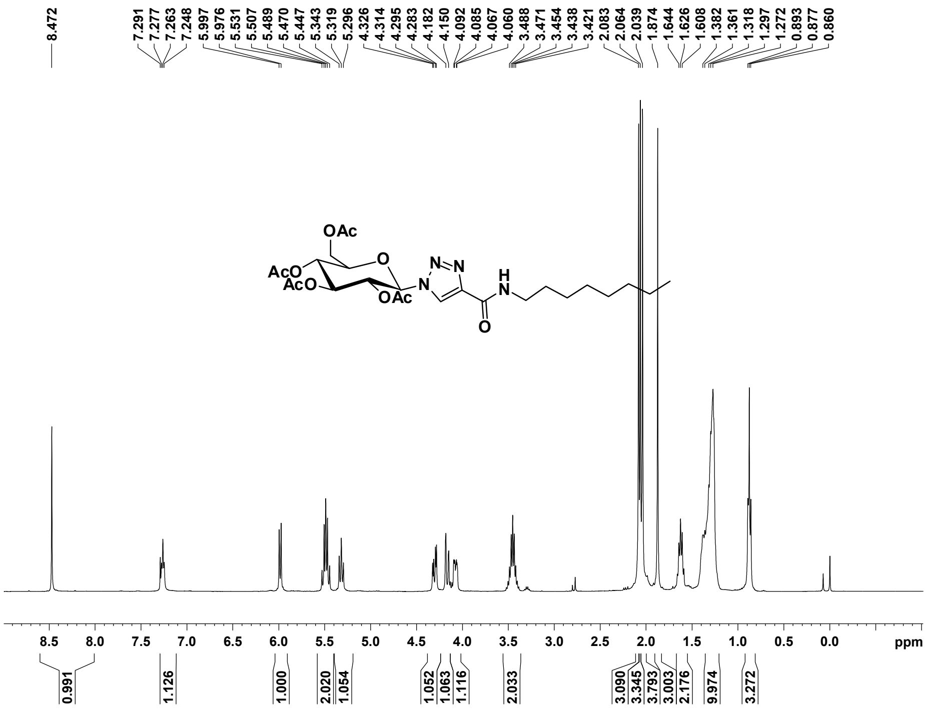

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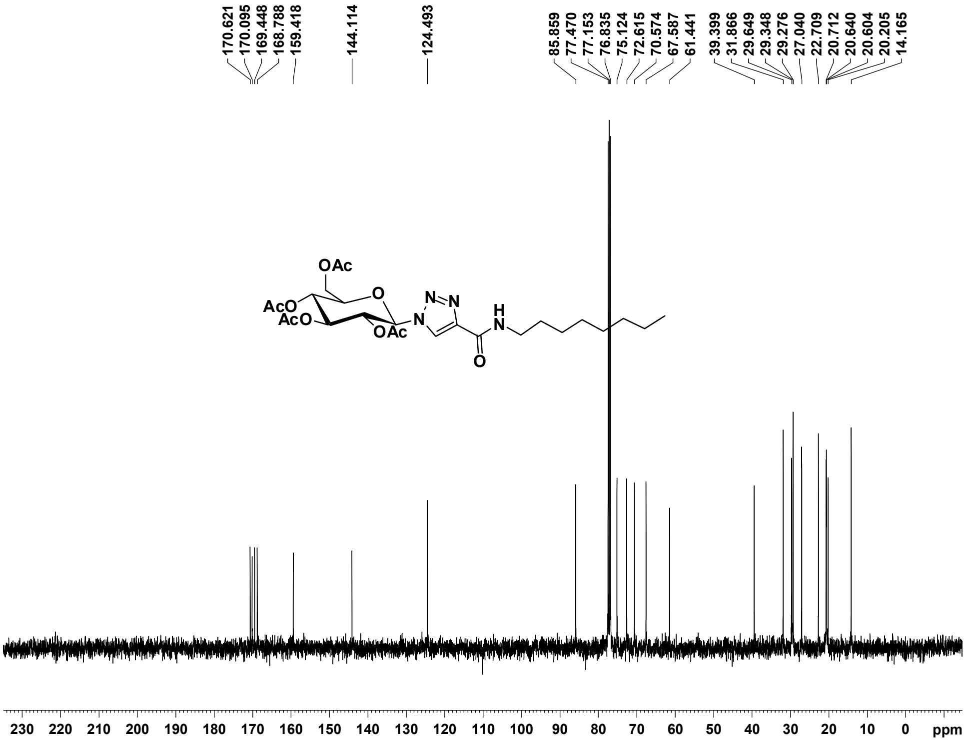


Figure S2 ^{13}C NMR (100 MHz, CDCl$_3$) spectrum of **4**

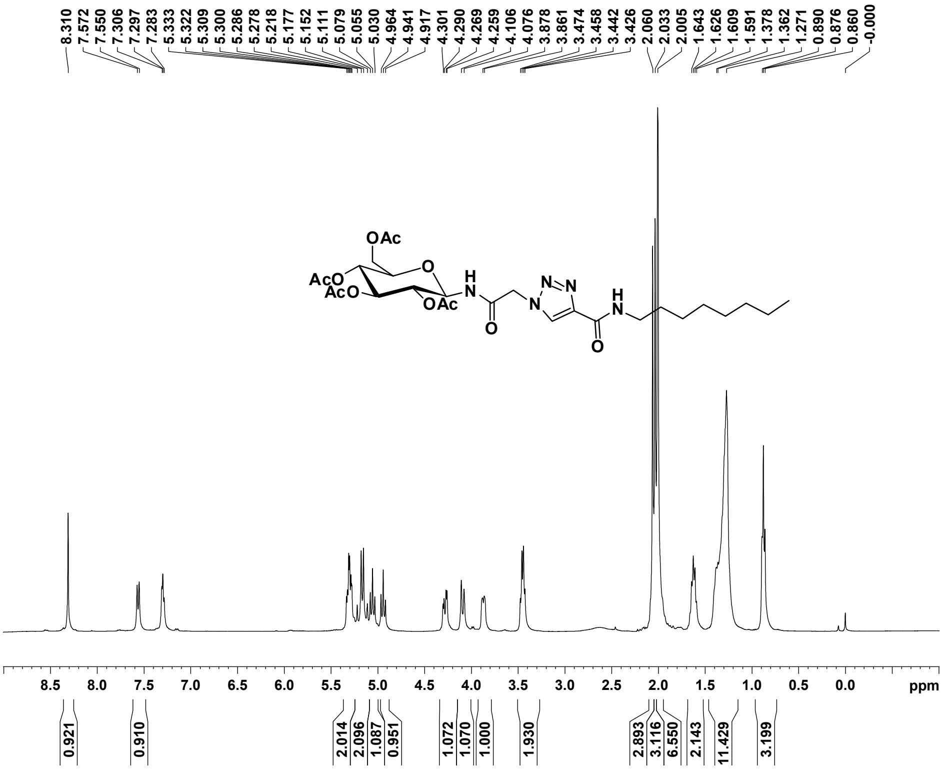
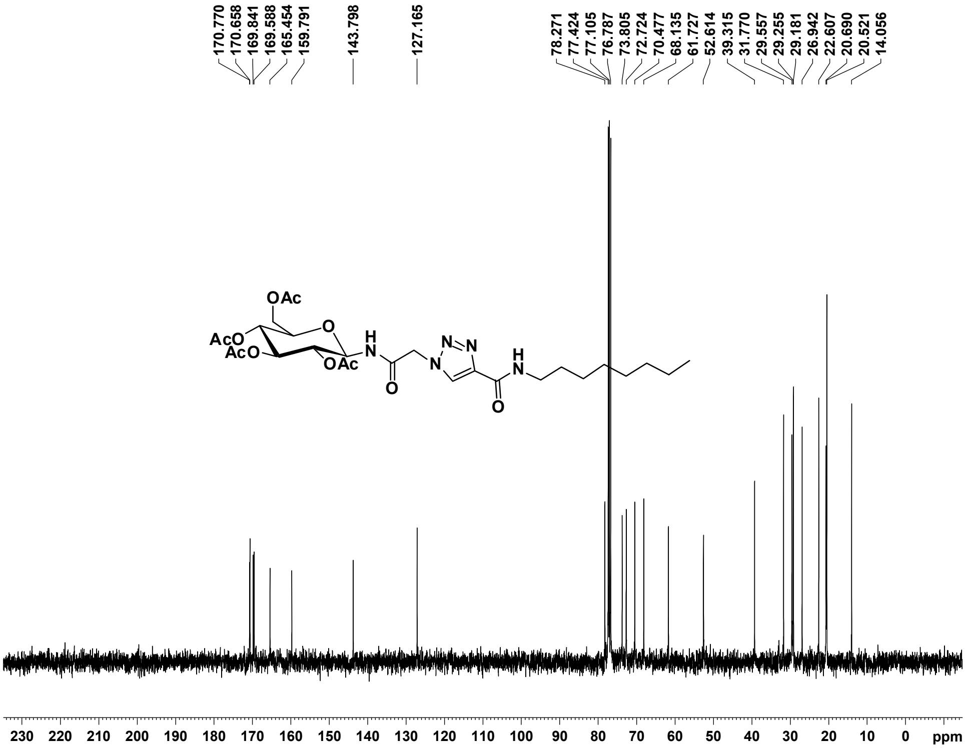


Figure S3 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6**



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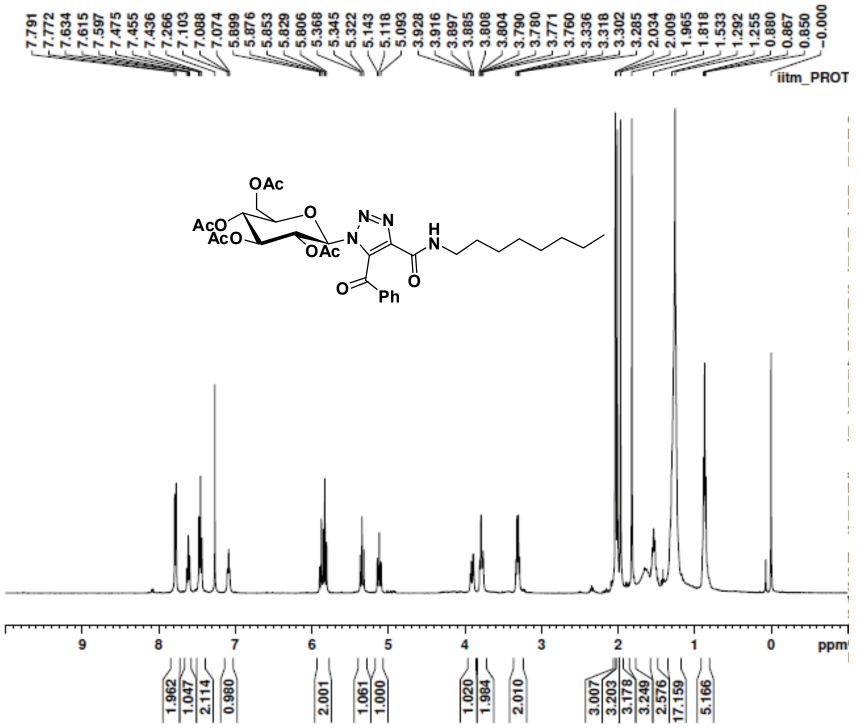

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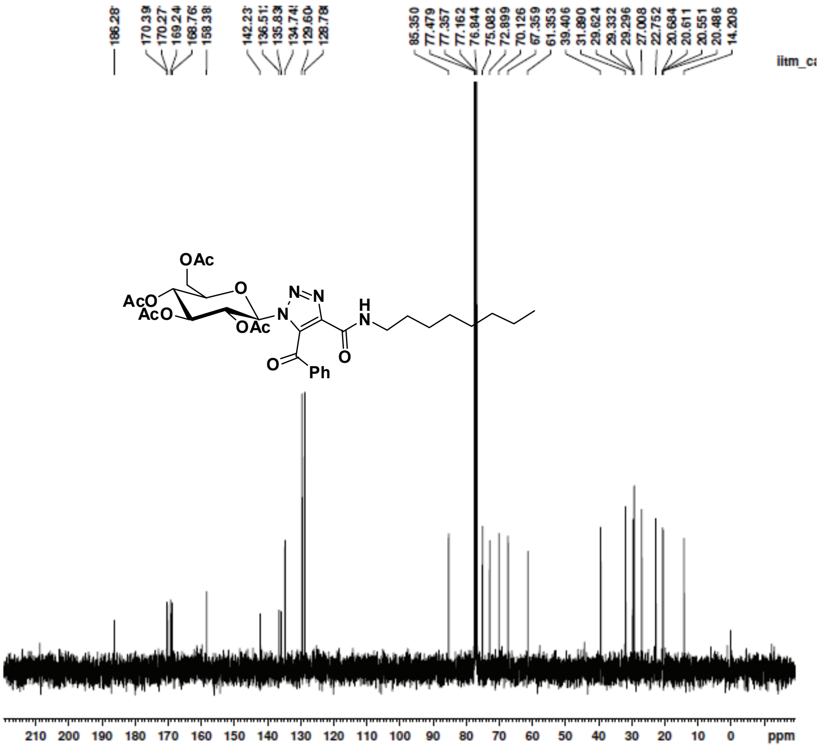


Figure S6 ^{13}C NMR (100 MHz, CDCl$_3$) spectrum of **7**

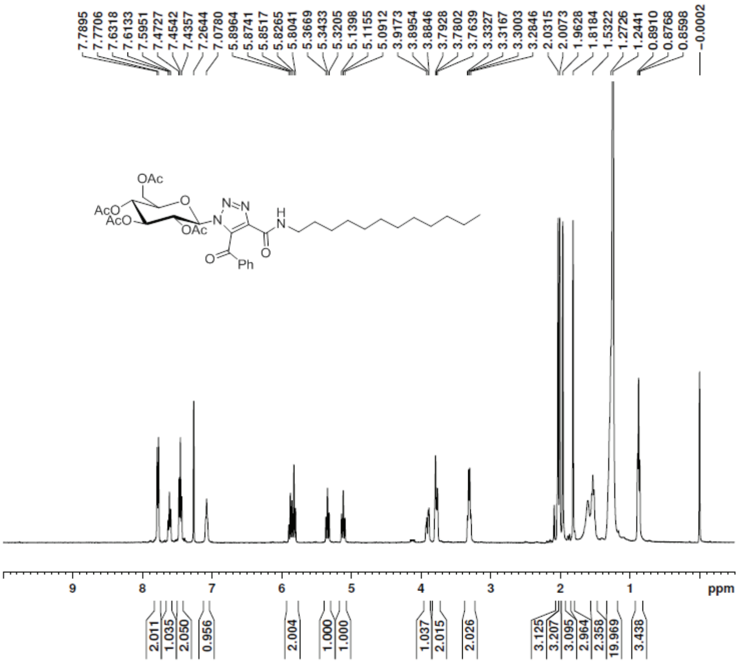
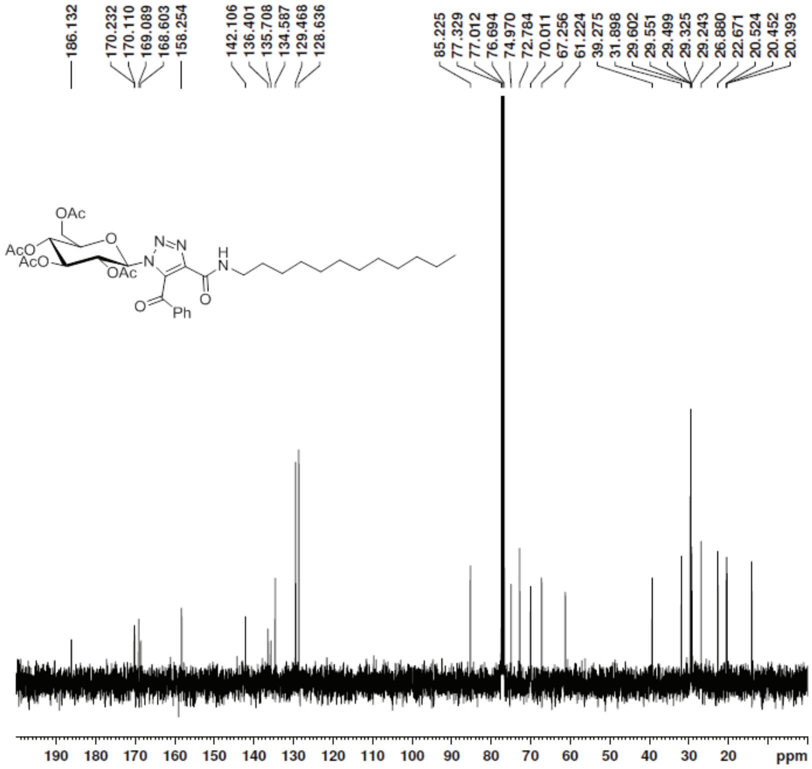


Figure S7 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8**



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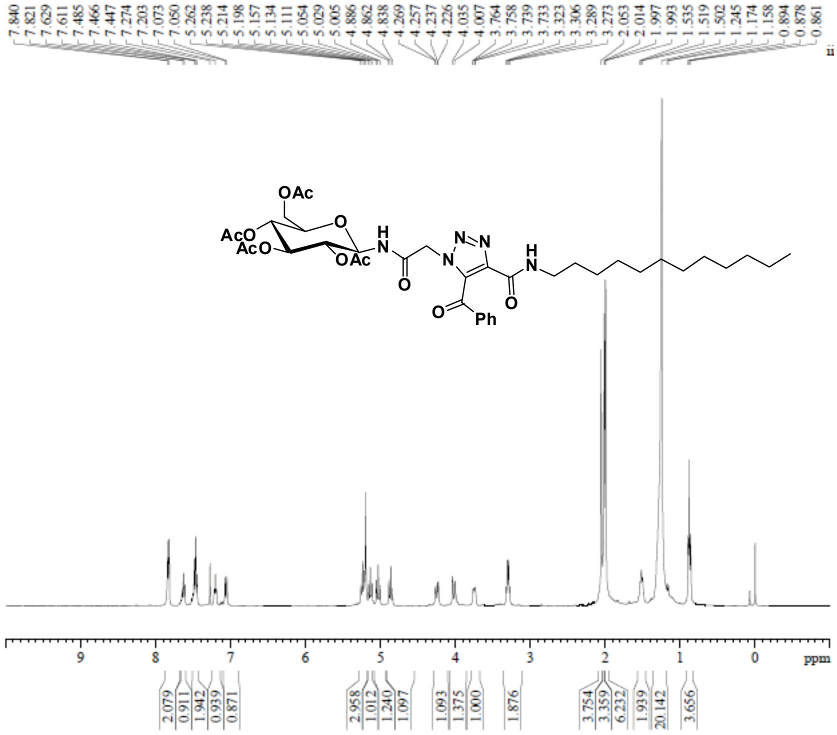


Figure S9 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **9**

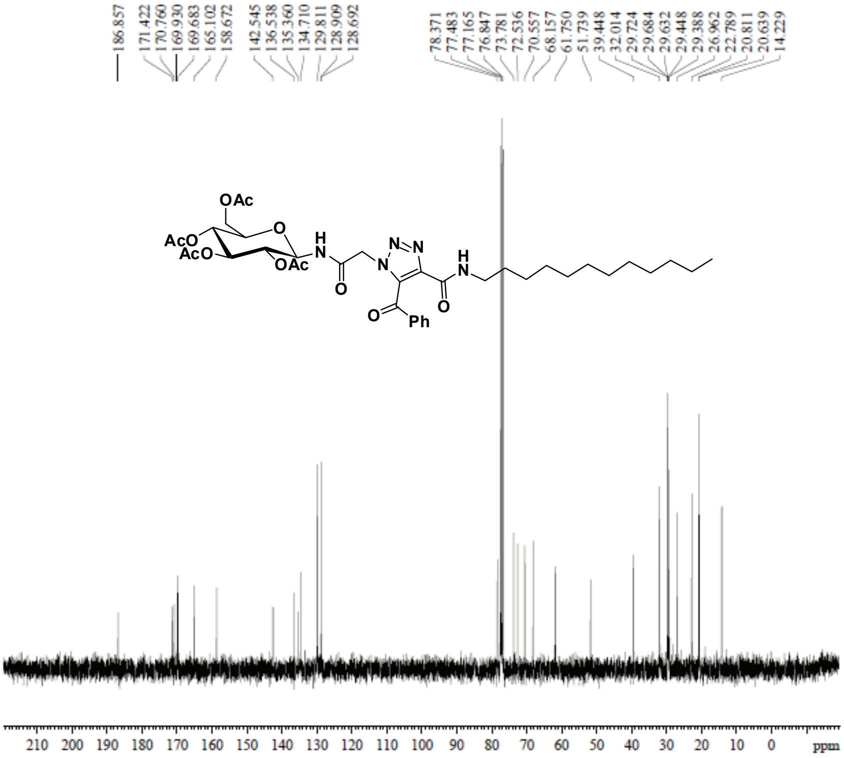


Figure S10 ^{13}C NMR (100 MHz, CDCl$_3$) spectrum of **9**

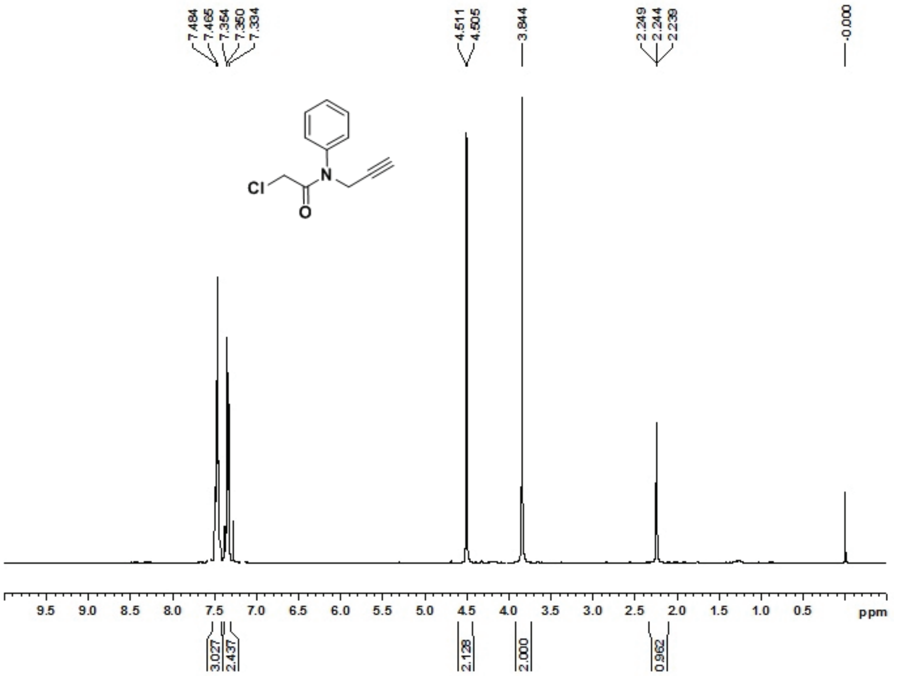


Figure S11 ^{1}H NMR (400 MHz, $CDCl_3$) of compound **11**

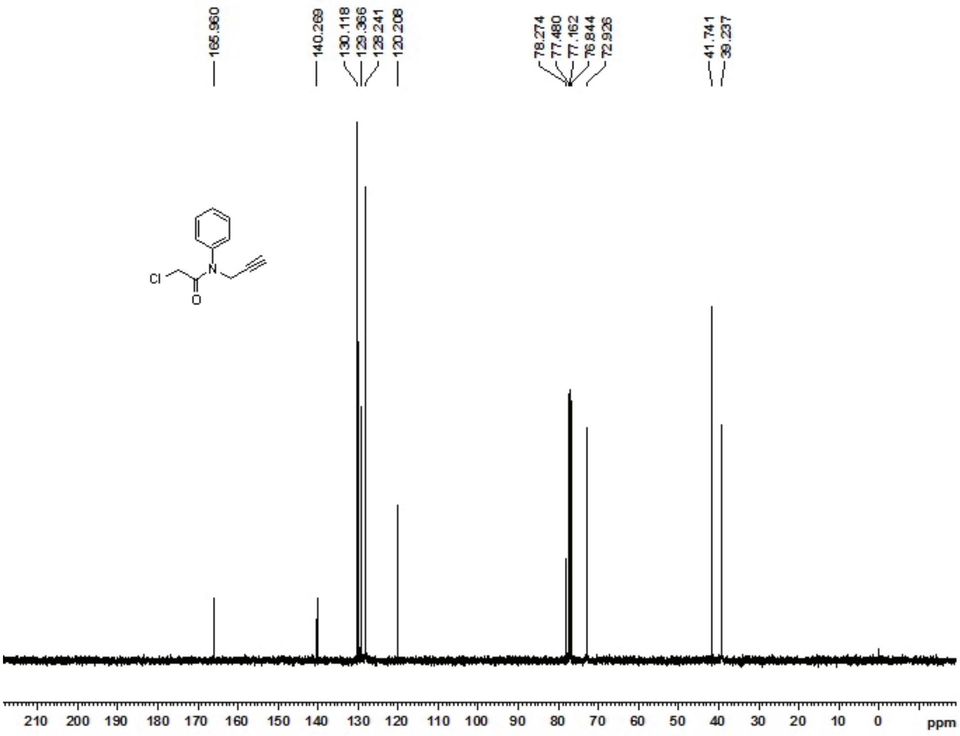


Figure S12 ^{13}C NMR (100 MHz, CDCl$_3$) of compound **11**

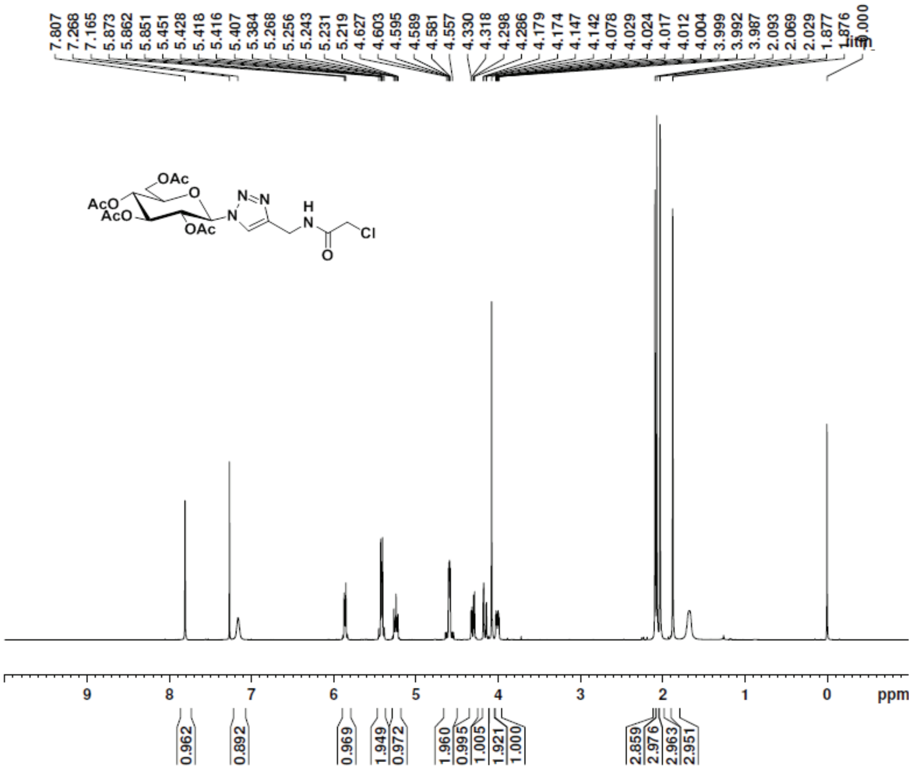
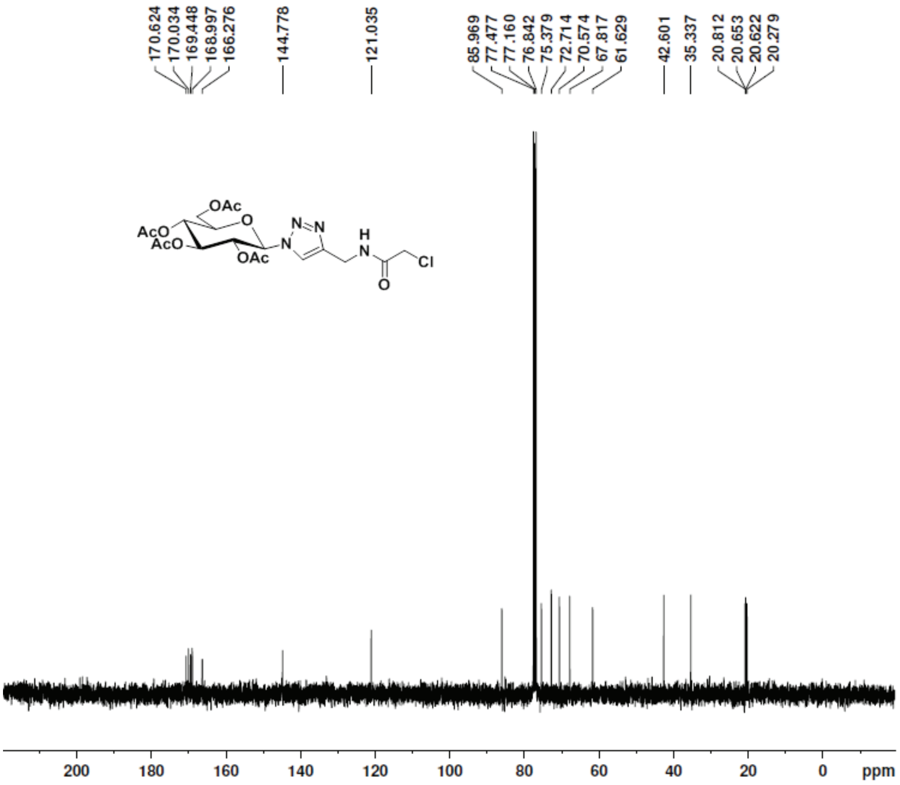


Figure S13 ^{1}H NMR (400 MHz, $CDCl_3$) of compound **12**



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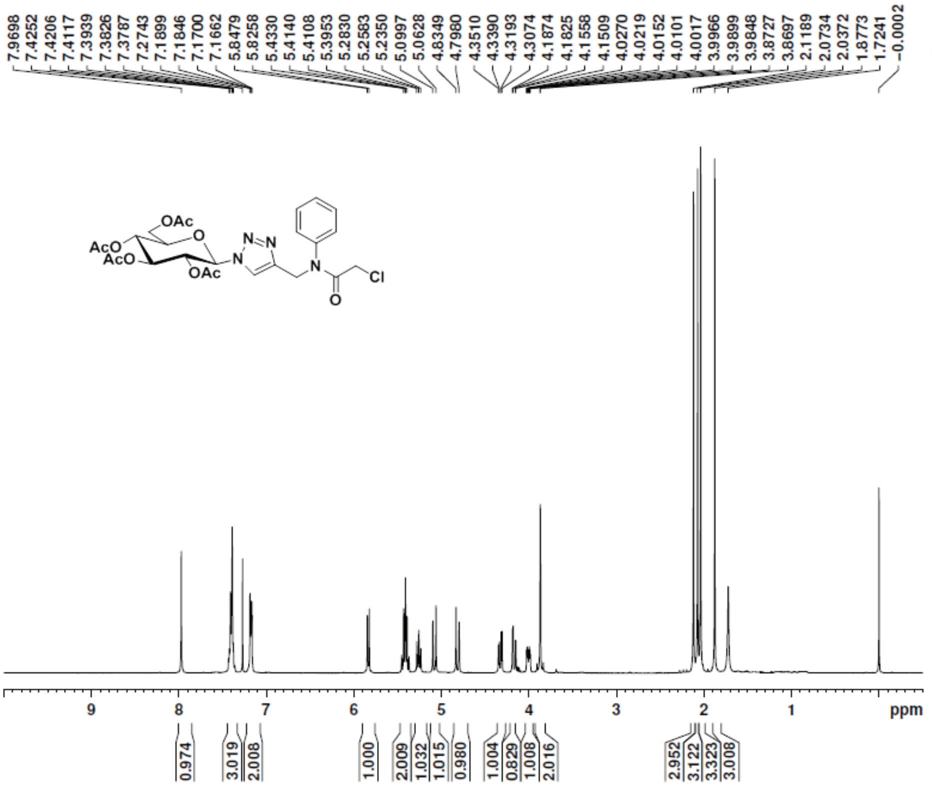

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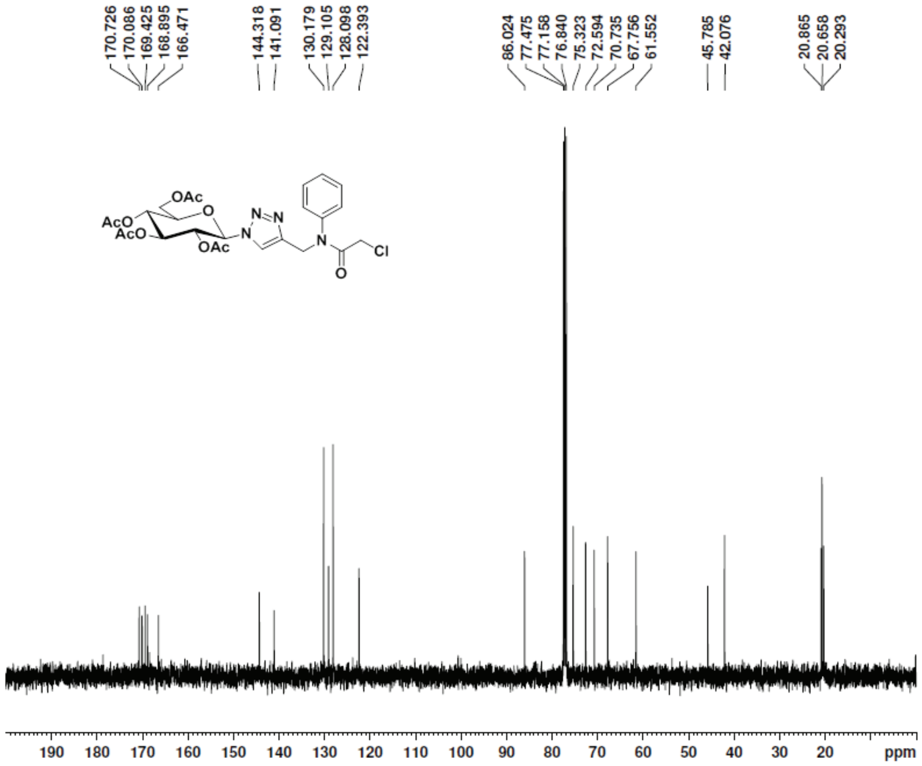

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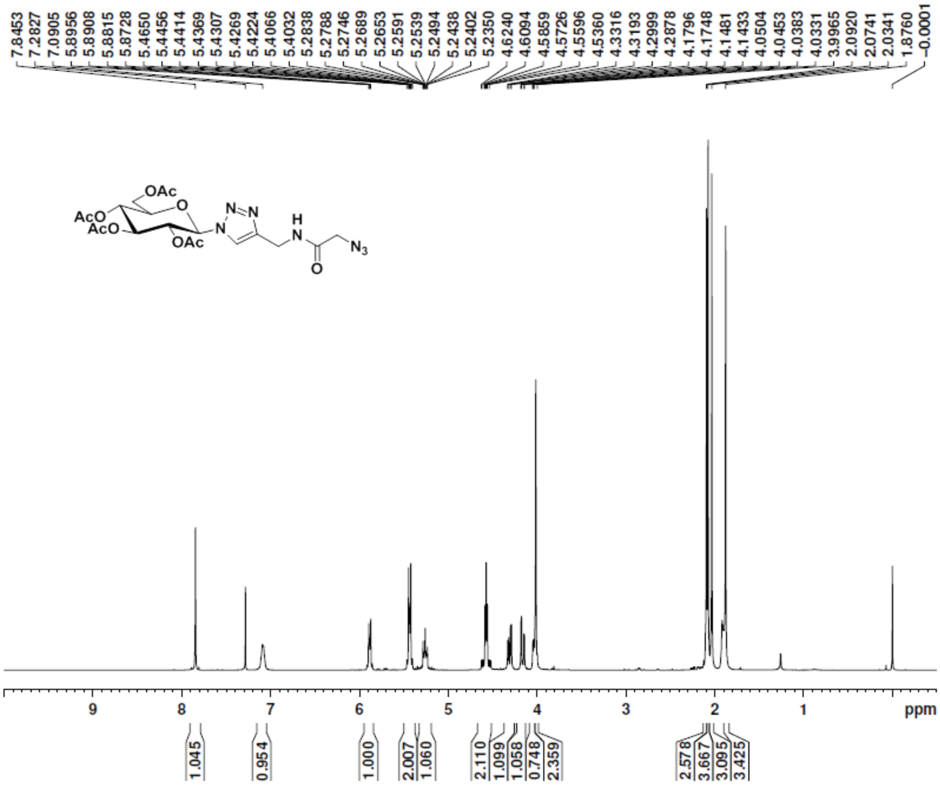


Figure S17 ^{1}H NMR (400 MHz, CDCl$_3$) of compound **14**

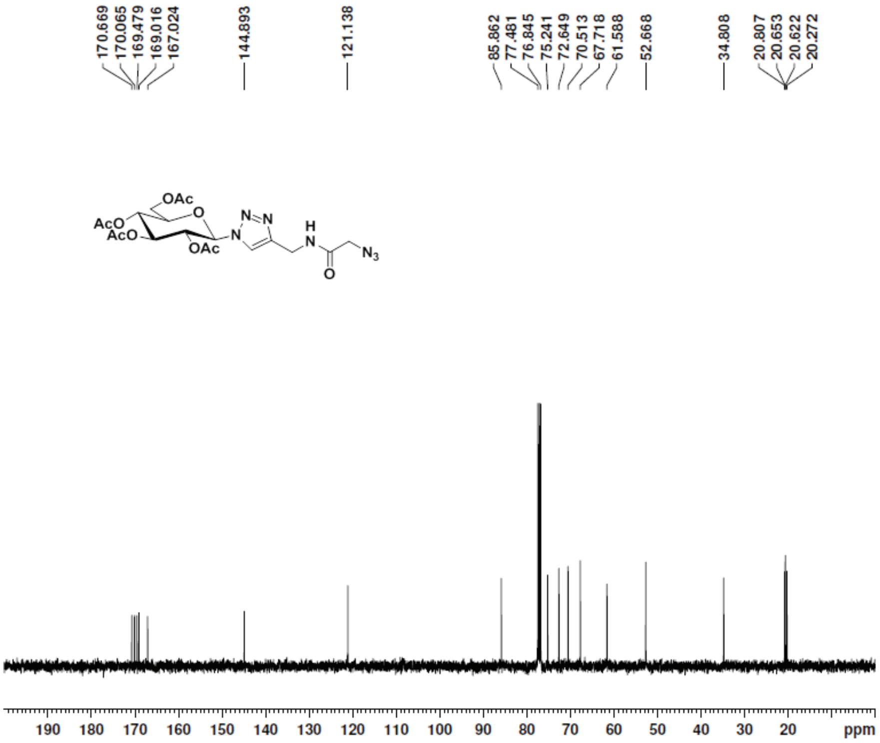


Figure S18 ^{13}C NMR (100 MHz, CDCl$_3$) of compound **14**

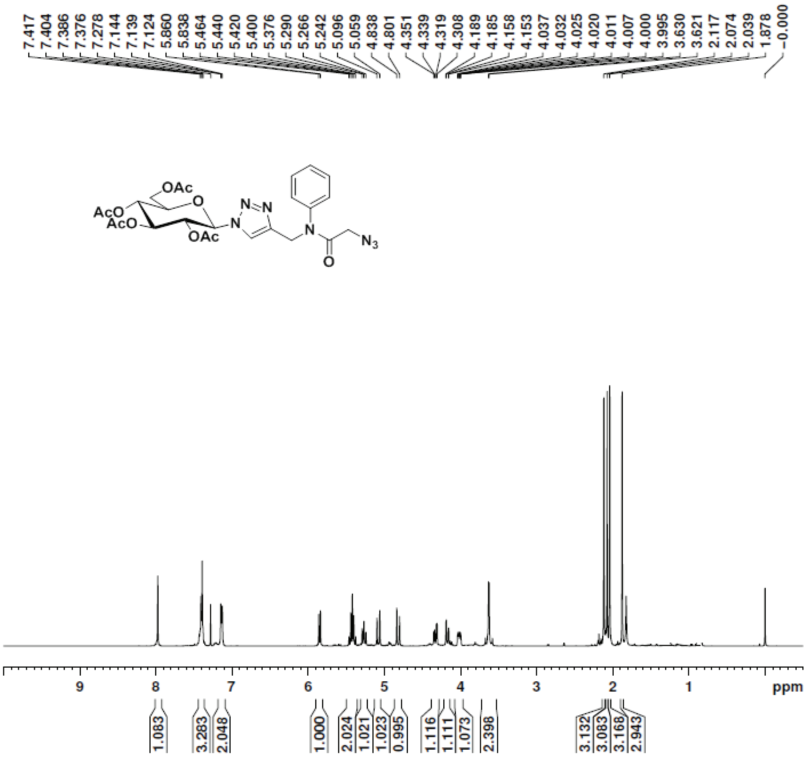
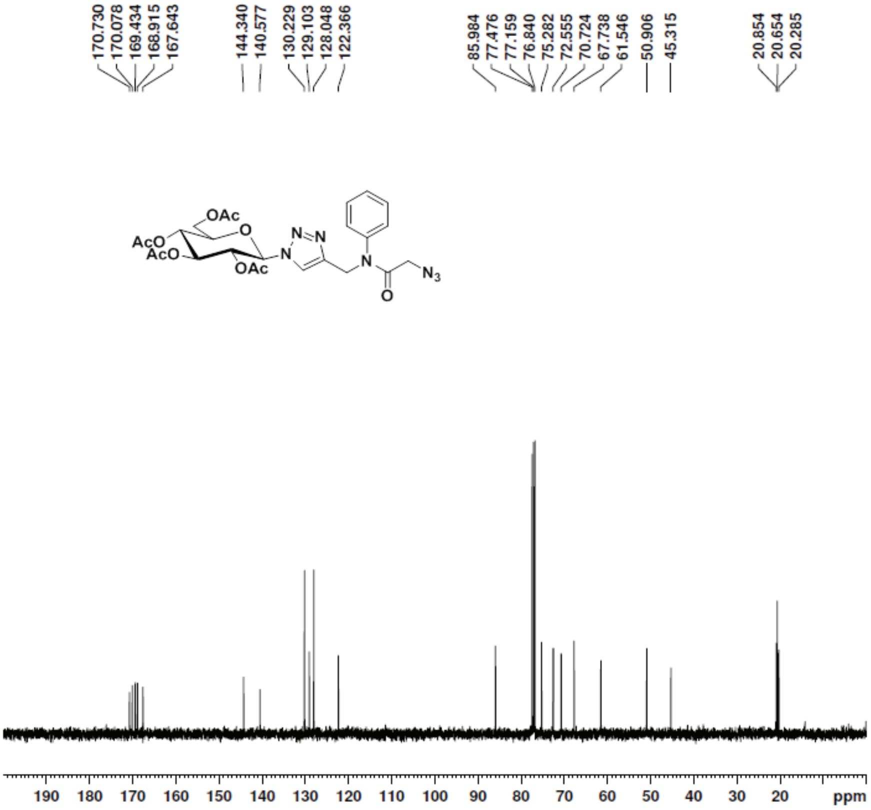


Figure S19 ^{1}H NMR (400 MHz, CDCl$_3$) of compound **15**



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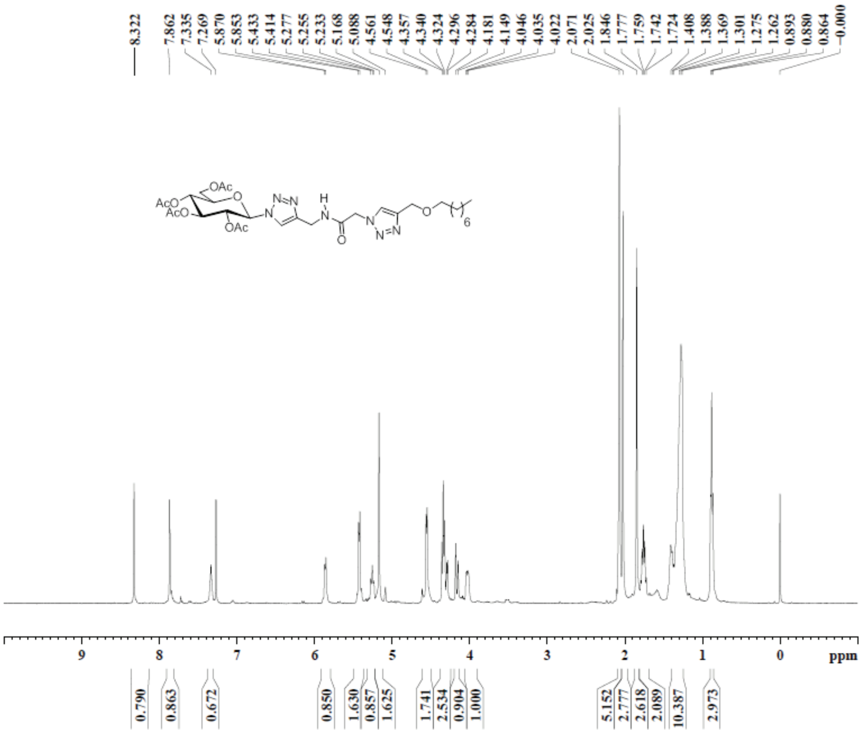
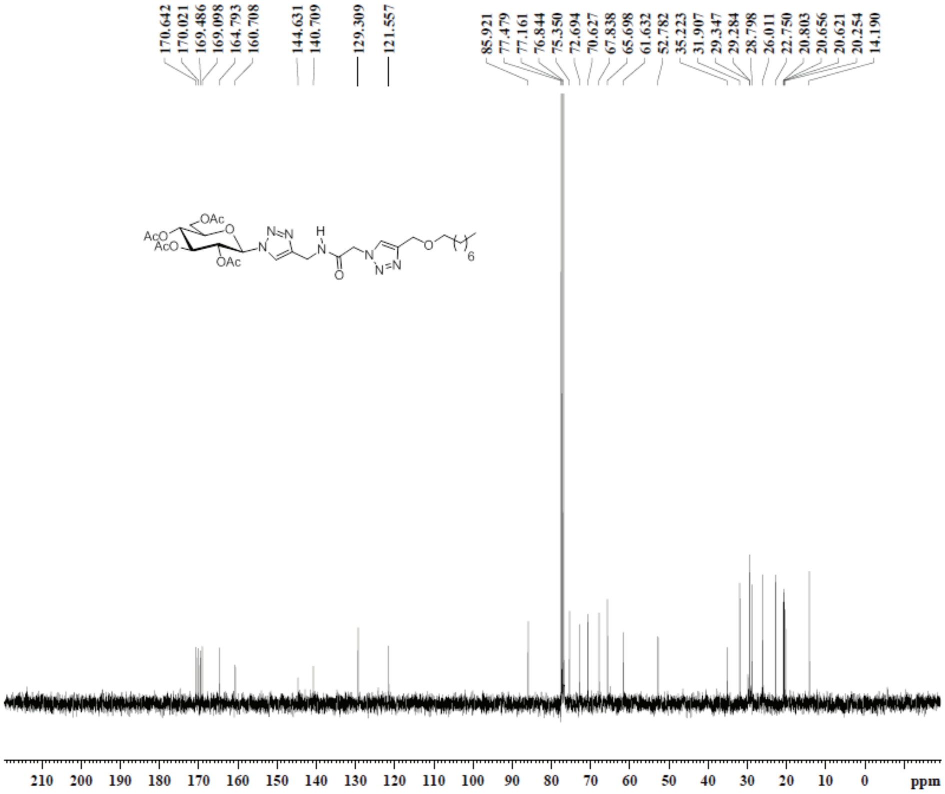


Figure S21 ^{1}H NMR (400 MHz, CDCl$_3$) of compound **17**



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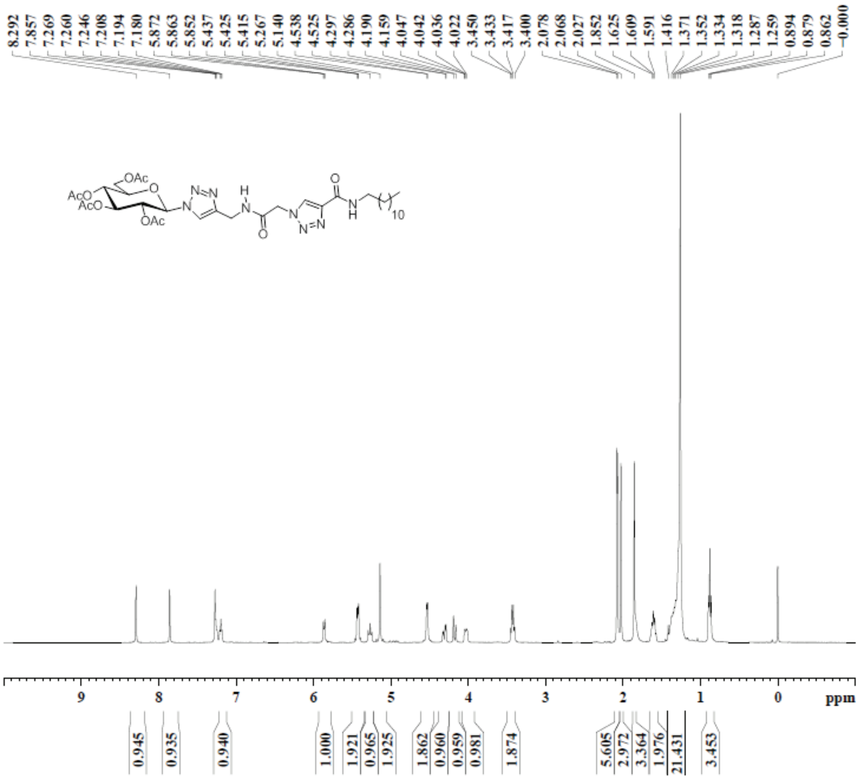
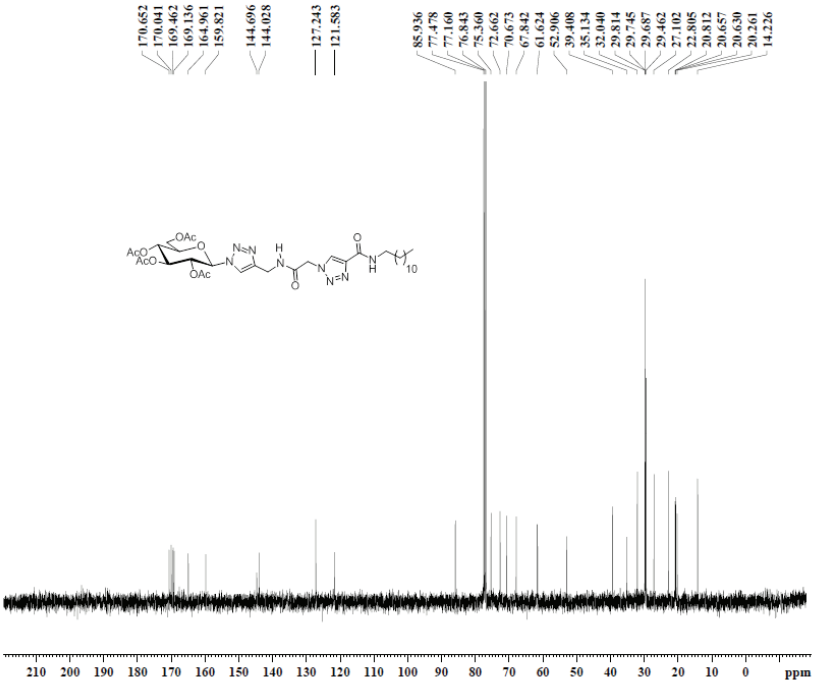


Figure S23 ^{1}H NMR (400 MHz, CDCl$_3$) of compound **18**



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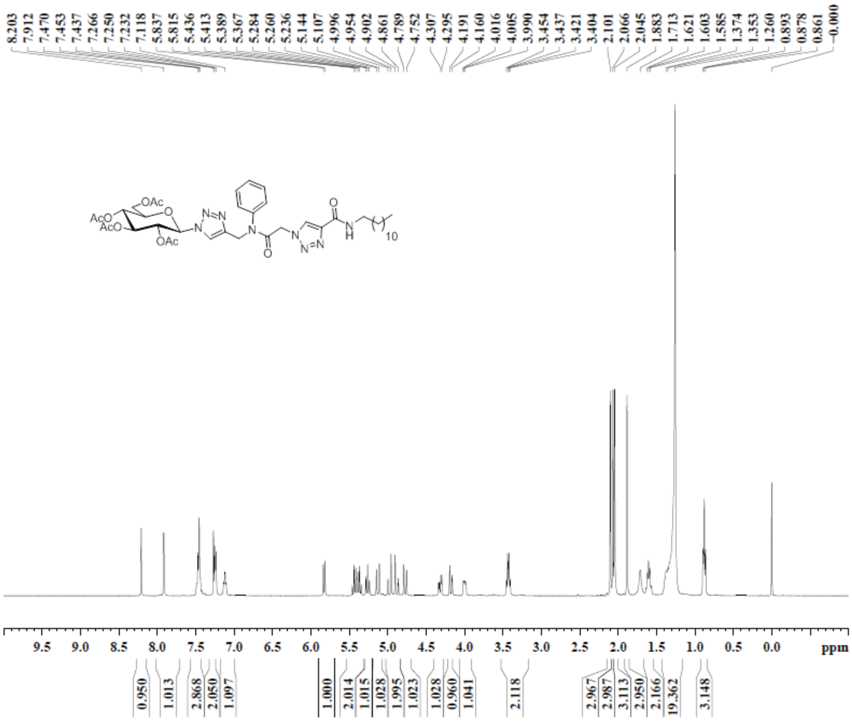

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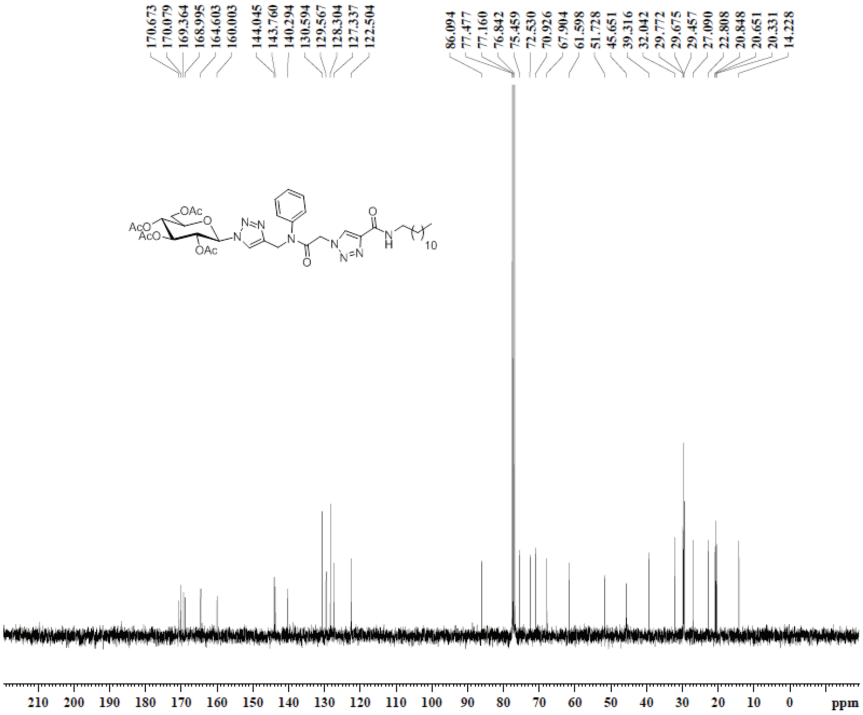

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