Supporting Information

A combinatorial approach towards the synthesis of non-hydrolysable triazole-iduronic acid-hybrid inhibitors of human α-L-iduronidase: Discovery of enzyme stabilizers for the potential treatment of MPSI

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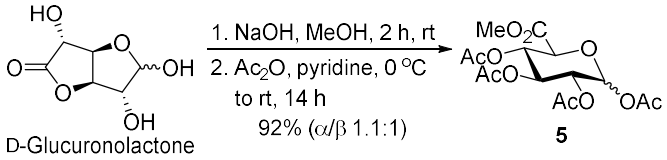
A. General Information

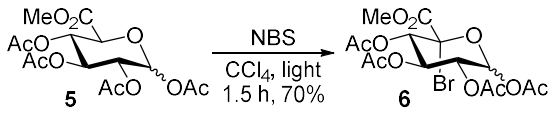
All solvents and reagents were obtained commercially and used without further purification. NMR spectra were recorded on a Bruker AVANCE 600 spectrometer in deuterium solvents at ambient temperature. Chemical shifts are reported in units of parts per million (ppm, δ) for solutions in chloroform-*d* (δ = 7.24 for ^{1}H, δ = 77.0 for ^{13}C) and coupling constants (*J*) are given in Hz. The splitting patterns are reported as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and dd (doublet of doublets). High resolution mass spectra were obtained on a Bruker Daltonics BioTOF III spectrometer (ESI-MS). Optical rotations were measured with a Perkin-Elmer Model 341 polarimeter. Flash column chromatography was carried out using Merck Kieselgel Si60 (40–63 μm). Reactions were monitored by analytical thin-layer chromatography (TLC) in silica gel 60 F254 plates and visualized by exposure to ultraviolet light at 254 nm and/or immersion in a staining solution (*p*-anisaldehyde or phosphomolybdic acid) followed by heating on a hot plate. Concentration refers to rotary evaporation. Parallel synthesis was performed on Buchi SynCore 96-well synthesizer and the reaction vessels (16 × 150 mm). Multiple-functional liquid handler (Freedom EVO, TECAN) was utilized for extraction and separation. Solvent evaporation was performed on Thermo Scientific Savant Explorer SpeedVac Concentrator Explorer-220. α-L-iduronidase (glycosaminoglycan a-L-iduronohydrolase, EC 3.2.1.76) is a lysosomal hydrolase.[S1] The substrate 4-methylumbelliferyl α-L-iduronide (4-MUI) used for activity assays was prepared from the reported papers with slight modification.[S2]

B. Chemistry section

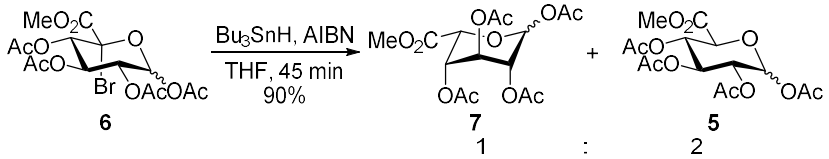
1. Preparation of iduronyl azides 3 and 4



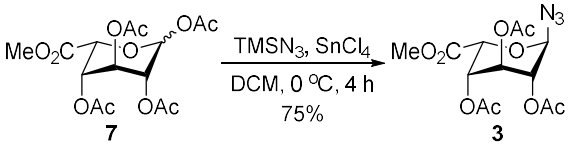
Compound 5. D-glucuronolactone (50.0 g, 283.9 mmol) and NaOH (120 mg, 0.01 equiv) in MeOH (350 mL) was stirred at room temperature for 2 h. The reaction was neutralized with HOAc (300 μL), and then MeOH was removed *in vacuo*. The residue was added pyridine (370 mL, 16 equiv) and Ac_2O (214 mL, 8 equiv) at 0 ºC and stirred overnight. After evaporation *in vacuo*, the residue was purified by flash column chromatography [silica gel, hexanes/ethyl acetate 1/1 (v/v)] to give **5** (98.2 g, 92%). The beta form can be obtained from recrystallization in hot ethanol to get (45.1 g). Beta form: ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.69 (d, 1H, *J* = 7.8 Hz), 5.23 (dd, 1H, *J* = 9.0, 9.3 Hz), 5.14 (dd, 1H, *J* = 9.3, 9.5 Hz), 5.05 (dd, 1H, *J*= 7.8, 9.0 Hz), 4.10 (d, 1H, *J* = 9.5 Hz), 3.65 (s, 3H), 2.02 (s, 3H), 1.94 (s, 6H), 1.93 (s, 3H); ^{13}C NMR (150 MHz,$CDCl_3$) δ 169.8, 169.3, 169.1, 168.7, 166.7, 91.3, 72.9, 71.7, 70.0, 68.8, 52.9, 20.7, 20.5, 20.4 × 2. HRMS calcd for $[C_{15}H_{20}O_{11}+Na]^+$ 399.0910, found 399.0898.



Compound 6. A mixture of **5** (10.0 g, 26.6 mmol) and NBS (18.9 g, 4 equiv) in dry CCl_4 (90 mL) was stirred for 1.5 under irradiation with two 250W tungsten light blubs. The reaction was quenched with 10% aqueous $Na_2S_2O_3$. The organic layer was washed with 10% aqueous $Na_2S_2O_3$, brine, dried over anhydrous $MgSO_4$, and concentrated. The residue was purified by flash column chromatography [silica gel, hexanes/ethyl acetate 3/1 (v/v)] to afford the title product **6** as a yellow solid (8.5 g, 70%). Beta form: ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.23 (d, 1H, J = 8.7 Hz), 5.48 (t, 1H, J = 9.5 Hz), 5.27 (d, 1H, J = 9.5 Hz), 5.19 (dd, 1H, J = 8.7, 9.5 Hz), 3.78 (s, 3H), 2.09 (s, 3H), 2.04 (s, 3H), 2.00 (s, 3H), 1.97 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.5, 169.0, 168.9, 168.2, 164.2, 90.8, 88.9, 70.7, 69.8, 69.1, 54.1, 20.6, 20.5, 20.4 × 2. HRMS calcd for $[C_{15}H_{19}BrO_{11}+Na]^+$ 477.0001, found 477.0003.

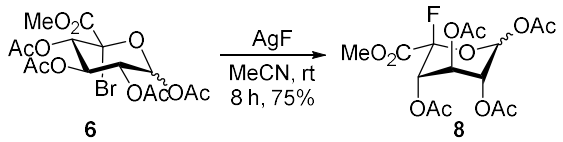


Compound 7. A mixture of **6** (8.7 g, 19.2 mmol), tributyltin hydride (44 mL, 2.5 equiv) and AIBN (723 mg, 0.23 equiv) in dry THF (64 mL) was refluxed for 45 min. After cooling and evaporation *in vacuo*, and the residue was treated with EtOAc and aqueous KF for 20 min. The mixture was filtered through Celite, the filtrate was concentrated, and purified by flash column chromatography [silica gel, toluene/ethyl acetate 2/1 (v/v)] to get **7** (2.2 g, 30%) and **5** (4.3 g, 60%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.26 (s, 1H), 5.14 (t, 1H, J = 3 Hz), 5.13 (d, 1H, J = 3.6 Hz), 4.84 (d, 1H, J = 2.4 Hz), 4.83 (s, 1H, J = 2.4 Hz), 3.76 (s, 3H), 2.10 (s, 3H), 2.08 (s, 3H), 2.07 (s, 3H), 2.05 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.3, 169.0, 168.5, 167.9, 167.6, 90.4, 68.2, 66.7, 66.2, 65.8, 52.7, 20.7, 20.6 × 2, 20.5.HRMS calcd for $[C_{15}H_{20}O_{11}+Na]^+$ 399.0801, found 399.0898.

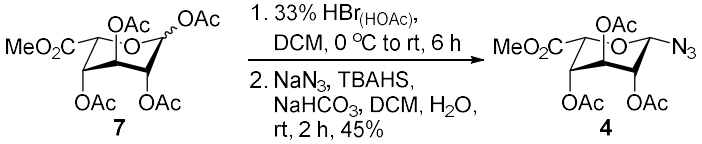


Compound 3. A mixture of **7** (300 mg, 0.9 mmol) in CH_2Cl_2 (9 mL) was added tin(IV) chloride (50 µL, 0.4 equiv) and trimethylsilyl azide (28 µL, 2.3 equiv) at 0 °C for 4 h. The reaction was quenched with saturated aqueous $NaHCO_3$ and stirred for 30 min. The mixture was filtered through Celite, the filtrate was diluted with EtOAc (60 mL) and washed with water (3 × 20 mL). The separated organic layer was dried over anhydrous $MgSO_4$, concentrated, and purified by column chromatography [silica gel,

hexanes/ethyl acetate 2/1 (v/v)] to afford the title product **3** (200 mg, 75%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.53 (d, 1H, J = 3.5 Hz, H-1), 5.14 (t, 1H, J = 4.5 Hz, H-3), 5.11 (dd, 1H, J = 4.8, 3.5 Hz, H-4), 4.90 (d, 1H, J = 3.4 Hz, H-5), 4.73 (t, 1H, J = 4.3 Hz, H-2), 3.78 (s, 3H, $CO_2\underline{CH_3}$), 2.09 (s, 3H, $CO\underline{CH_3}$), 2.07 (s, 3H, $CO\underline{CH_3}$), 2.05 (s, 3H, $CO\underline{CH_3}$); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.3, 169.2, 168.9, 167.9, 86.5, 68.5, 67.0, 66.6, 52.7, 20.7, 20.6, 20.5. HRMS calcd for $[C_{13}H_{17}N_3O_9+Na]^+$ 382.0857, found 382.0872.



Compound 8. A mixture of **6** (1.5 g, 3.3 mmol) and silver(I) fluoride (800 mg, 2 equiv) in acetonitrile (16 mL) was stirred at room temperature in the dark (the flask was coated by a layer of foil) for 8 h. The reaction mixture was concentrated, and purified by column chromatography [silica gel, hexanes/ethyl acetate 4/1 (v/v)] to afford the title product **8** as a yellow gel (900 mg, 75%). Alpha form: ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.16 (dd, 1H, J = 1.5, 2.5 Hz), 5.63 (dd, 1H, J = 12.0, 9.2 Hz), 5.42 (dd, 1H, J = 6.2, 9.2Hz), 5.16(dd, 1H, J = 2.8, 6.2Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.5, 168.5, 167.9, 163.6, 163.4, 106.3, 92.0, 72.3, 69.6, 69.5, 53.5, 20.8, 20.6, 20.5, 20,4 . HRMS calcd for $[C_{15}H_{19}FO_{11}+Na]^+$ 417.0805, found 417.0804.



Compound 4. A mixture of **7** (300 mg, 0.9 mmol) in dry CH_2Cl_2 (2 mL) was added acetic anhydride (300 µL, 0.3 equiv) and 30% $HBr_{(HOAc)}$ (1.2 mL, 4.8 mmol) at 0 °C for 6 h. The reaction was warmed up to room temperature. The mixture was diluted with CH_2Cl_2 (40 mL) and washed with saturated aqueous $NaHCO_3$ (2 × 20 mL). The organic layer was dried over anhydrous $MgSO_4$ and concentrated to get the crude iduronyl bromide as a yellow gel. A mixture of the crude iduronyl bromide (0.9 mmol), NaN_3 (100 mg, 1.9 equiv), and TBAHS (40 mg, 0.1 equiv) in dry CH_2Cl_2 (4 mL) and $NaHCO_3$ (4 mL, 1M aqueous solution) was stirred vigorously at room temperature for 2 h. The mixture was diluted with CH_2Cl_2 (60 mL), and washed with water (3 × 20 mL). The organic layer was dried over anhydrous $MgSO_4$, concentrated, and purified by column chromatography [silica gel, hexanes/ethyl acetate 2/1 (v/v)] to afford **4** (140 mg, 45%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.18 (t, 1H, J = 3.1 Hz, H-3), 5.08 (brs, 1H, H-4), 5.00 (d, 1H, J = 1.5 Hz, H-1), 4.90 (brs, 1H, H-2), 4.60 (d, 1H, J = 2.0 Hz, H-5), 3.77 (s, 3H, $CO_2\underline{CH_3}$), 2.12 (s, 6H, $CO\underline{CH_3}$), 2.07 (s, 3H, $CO\underline{CH_3}$); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.2, 169.1, 167.8, 166.8, 85.0, 73.7, 66.5, 65.9, 65.8, 52.7, 20.7, 20.6, 20.5. HRMS calcd for $[C_{13}H_{17}N_3O_9+Na]^+$ 382.0857, found 382.0872.

2. Preparation of iduronyl triazoles

General procedure 1 for CuAAC click reaction

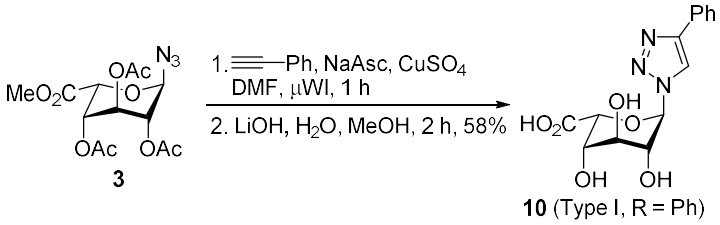
A mixture of an azide (1 mmol), alkyne (2 equiv), $CuSO_4$-$5H_2O$ (1M aqueous solution, 0.01 equiv, 10 μL), and sodium ascorbate (1M aqueous solution, 0.1 equiv, 100 μL) in DMF (400 μL) was irradiated in a microwave reactor reaction until the reaction was complete (TLC). The reaction was cooled to room temperature, then diluted with EtOAc (60 mL), and washed with water (3 × 20 mL). The organic layer was dried over anhydrous $MgSO_4$, concentrated, and purified by column chromatography [silica gel, hexanes/ethyl acetate 2/1 (v/v)] to afford iduronyl triazole.

General procedure 2 for CuAAC click reaction

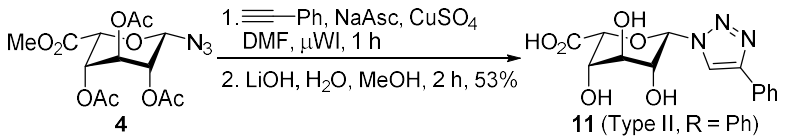
A mixture of an azide (1 mmol), alkyne (2 equiv), $CuSO_4$-$5H_2O$ (1M aqueous solution, 0.3 equiv, 300 μL), and sodium ascorbate (1M aqueous solution, 0.3 equiv, 300 μL) in *t*-BuOH/H_2O (400 μL) was stirred at room temperature for 48 h. Workup of the reaction mixture was carried out in the automated liquid-liquid extraction module. The mixture was diluted with H_2O (60 mL) and washed with EtOAc (3 × 20 mL). The aqueous layer was concentrated and purified by column chromatography [silica gel, ethyl acetate/methanol/water 7/2/1 (v/v)].

General procedure 3 for deprotection of esters

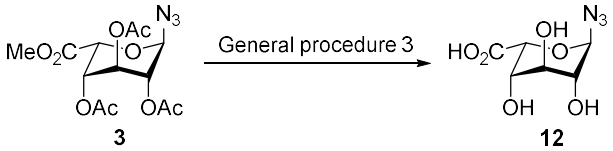
A mixture of an ester (1 mmol) in THF (5 mL) was added LiOH (2M aqeous solution, 500 μL, 1 equiv) at 0 °C and was stirred for 2 h. The reaction was adjusted pH value to approximately 7 by adding DOWEX 50WX8-200 ion-exchange resin. The mixture was filtered, the filtrate was concentrated and purified by column chromatography [silica gel, ethyl acetate/methanol/water 7/2/1 (v/v)].



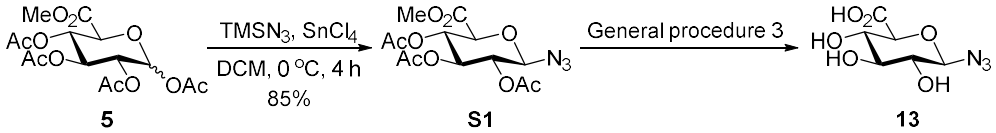
Compound 10. The preparation was accorded on General procedures 1 and 3. Compound **3** and phenylacetylene were used. Yield was 58%. ^{1}H NMR (600 MHz, D_2O) δ 8.57 (s, 1H), 7.82–7.83 (m, 2H), 7.47–7.54 (m, 3H), 6.12 (d, 1H, J = 9.0 Hz), 4.61 (d, 1H, J = 6.0 Hz), 4.12 (dd, 1H, J = 9.0, 9.2 Hz), 4.00 (dd, 1H, J = 6.0, 9.3 Hz), 3.78 (dd, 1H, J = 9.2, 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 147.6, 129.1 × 3, 128.9, 125.7 × 2, 121.5, 85.4, 74.3, 73.8, 72.1, 70.5. HRMS calcd for $[C_{14}H_{15}N_3O_6\text{-}H]^-$ 320.0891, found 320.0877.



Compound 11. The preparation was accorded on General procedures 1 and 3. Compound **4** and phenylacetylene were used. Yield was 53%. ^{1}H NMR (600 MHz, D_2O) δ 8.78 (s, 1H), 7.88–7.89 (m, 2H), 7.54–7.57 (m, 2H), 7.47–7.49 (m, 1H), 6.29 (s, 1H), 4.66 (s, 1H), 4.31 (dd, 1H, J = 2.7, 3.1 Hz), 4.15 (d, 1H, J = 1.3 Hz), 4.07 (d, 1H, J = 1.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.1, 147.0, 129.5, 129.2 × 2, 128.8, 125.7 × 2, 121.8, 85.3, 77.2, 69.1, 69.0, 68.9. HRMS calcd for $[C_{14}H_{15}N_3O_6+H]^+$ 322.1044, found 322.1034.



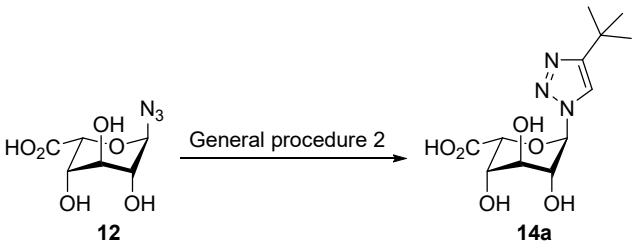
Compound 12. The preparation was accorded on General procedure 3. Yield was 83%. ^{1}H NMR (600 MHz, D_2O) δ 5.13 (d, 1H, J = 6.3 Hz), 4.48 (d, 1H, J = 4,7 Hz), 3.83 (dd, 1H, J = 7.3, 4.7 Hz), 3.67 (dd, 1H, J = 7.5, 14.0 Hz), 3.39 (dd, 1H, J= 6.3, 14.0 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.6, 88.6, 72.2, 72.2, 71.0, 70.3. HRMS calcd for $[C_6H_9N_3O_6-H]^-$ 218.0422, found 218.0408.



Compound S1. A mixture of **5** (3.1 g, 8.35 mmol) in CH_2Cl_2 (80 mL) was added tin(IV) chloride (500 µL, 0.5 equiv) and trimethylsilyl azide (500 µL, 2.4 equiv) at 0 °C for 4 h. The reaction was quenched with saturated aqueous $NaHCO_3$ and stirred for 30 min. The mixture was filtered through Celite, the filtrate was diluted with EtOAc (150 mL) and washed with water (3 × 20 mL). The separated organic layer was dried over anhydrous $MgSO_4$, concentrated, and purified by column chromatography [silica gel, hexanes/ethyl acetate 2/1 (v/v)] to afford the title product **S1** (2.5 g, 85%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.23 (t, 1H, J = 9.4 Hz, H-3), 5.19 (t, 1H, J = 9.5 Hz, H-4), 4.92 (t, 1H, J = 9.0 Hz, H-2), 4.68 (d, 1H, J = 8.7 Hz, H-1), 4.08 (d, 1H, J = 9.6 Hz, H-5), 3.73 (s, 1H, $CO_2C\underline{H_3}$), 2.03 (s, 3H, $CO\underline{CH_3}$), 1.99 (s, 3H, $\underline{CH_3}$), 1.98 (s, 3H, $\underline{CH_3}$); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.9, 169.2, 169.0, 166.4, 88.0, 74.1, 71.7, 70.3, 68.9, 53.0, 20.4 × 2, 20.3. HRMS calcd for $[C_{13}H_{17}N_3+Na]^+$ 382.0865, found 382.0857.

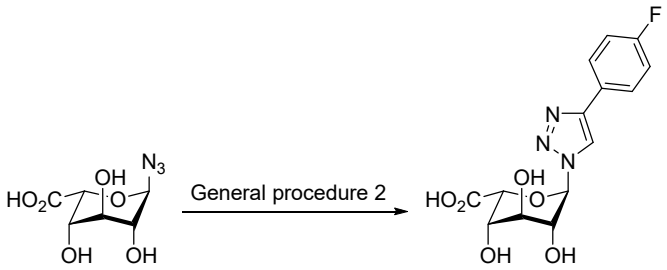
Compound 13. The preparation was accorded on General procedure 3. Yield was 80%. ^{1}H NMR (600 MHz, D_2O) δ 3.82 (d, 1H, J = 9.1 Hz), 3.52–3.57 (m, 2H), 3.32 (t, 1H, J = 8.7 Hz); ^{13}C NMR (150 MHz,

D_2O) δ 175.3, 89.9, 77.6, 75.5, 72.6, 71.4. HRMS calcd for $[C_6H_9N_3O_6\text{-}H]^-$ 218.0422, found 218.0408.



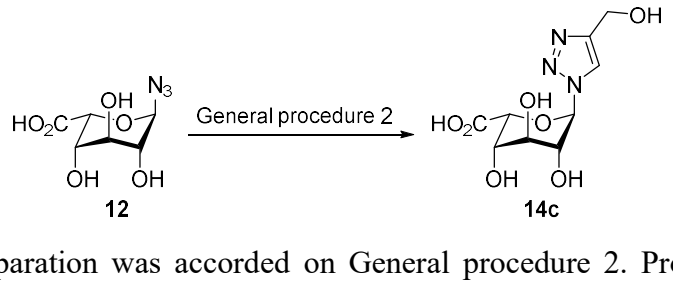
12 14a

Compound 14a. The preparation was accorded on General procedure 2. 2,2-Dimethyl-1-butyne was used. Yield was 63%. ^{1}H NMR (600 MHz, D_2O) δ 8.08 (s, 1H), 6.02 (d, 1H, J = 9.1 Hz), 4.56 (d, 1H, J = 6.0 Hz), 4.04 (dd, 1H, J = 9.1, 9.3 Hz), 3.95 (dd, 1H, J = 6.0, 9.4 Hz), 3.74 (dd, 1H, J = 9.3, 9.4 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 158.2, 120.5 , 85.1, 74.2, 73.8, 72.1, 70.4, 30.1, 29.3 × 3. HRMS calcd for $[C_{12}H_{19}N_3O_6\text{-}H]^-$ 300.1204, found 300.1190.



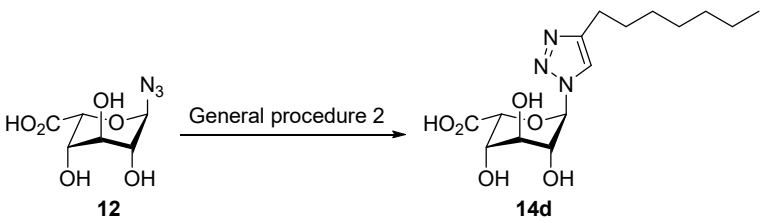
12 14b

Compound 14b. The preparation was accorded on General procedure 2. 1-Ethynyl-4-fluorobenzene was used. Yield was 63%. ^{1}H NMR (600 MHz, D_2O) δ 8.52 (s, 1H), 7.77–7.79 (m, 2H), 7.21–7.24 (m, 2H), 6.11 (d, 1H, J = 9.0 Hz), 4.61 (d, 1H, J= 6.0 Hz), 4.11 (dd, 1H, J = 9.0, 9.2 Hz), 3.99 (dd, 1H, J = 6.0, 9.3 Hz), 3.78 (dd, 1H, J = 9.2, 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 162.7, 146.9, 127.7 × 2, 125.4, 121.3, 115.9 × 2, 85.4, 74.3, 73.8, 72.1, 70.5. HRMS calcd for $[C_{14}\ H_{14}FN_3O_6\text{-}H]^-$ 338.0795, found 338.0783

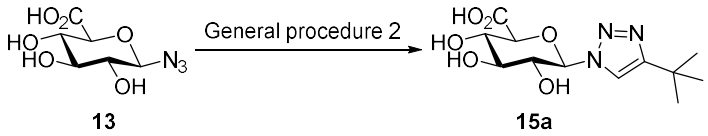


12 14c

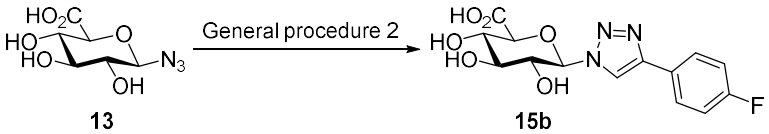
Compound 14c. The preparation was accorded on General procedure 2. Propargyl alcohol was used. Yield was 51%. ^{1}H NMR (600 MHz, D_2O) δ 8.26 (s, 1H), 6.06 (d, 1H, J = 9.2 Hz), 4.59 (d, 1H, J = 6.2 Hz), 4.08 (t, 1H, J = 9.2 Hz), 3.97 (dd, 1H, J = 6.2, 9.2 Hz), 3.75 (t, 1H, J = 9.2 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 147.0, 123.6 , 85.3, 74.2, 73.8, 72.1, 70.4. 54.5. HRMS calcd for $[C_9H_{13}N_3O_7\text{-}H]^-$ 274.0745, found 274.0670.



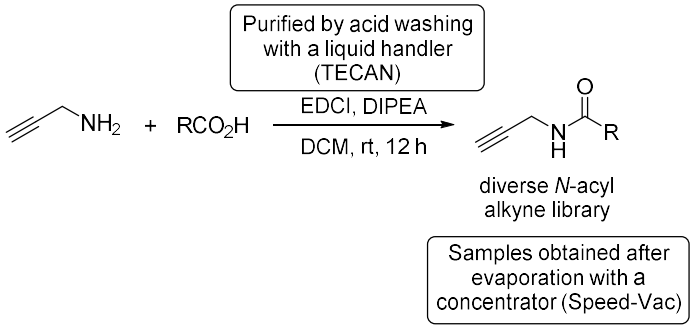
Compound 14d. The preparation was accorded on General procedure 2. 1-Nonyne was used. Yield was 60%. ^{1}H NMR (600 MHz, D_2O) δ 8.02 (s, 1H), 6.01 (d, 1H, J = 9.1 Hz), 4.54 (d, 1H, J = 6.0 Hz), 4.05 (dd, 1H, J = 9.1, 9.3 Hz), 3.95 (dd, 1H, J = 6.0, 9.4 Hz), 3.74 (dd, 1H, J = 9.3, 9.4 Hz), 2.74–2.76 (m, 2H), 1.67–1.69 (m, 2H), 1.28–1.33 (m, 8H), 0.86–0.88 (m, 3H); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 149.0, 122.5, 85.1, 74.2, 73.8, 72.1, 70.4, 30.9, 28.3, 28.0, 27.9, 24.3, 21.9, 13.3. HRMS calcd for $[C_{15}H_{25}N_3O_6\text{-}H]^-$ 342.1680, found 342.1660.



Compound 15a. The preparation was accorded on General procedure 2. 2,2-Dimethyl-1-butyne was used. Yield was 56%. ^{1}H NMR (600 MHz, D_2O) δ 8.09 (s, 1H), 5.74 (d, 1H, J = 9.2 Hz), 4.01–4.04 (m, 2H), 3.70–3.77 (m, 2H), 1.35 (s, 1H); ^{13}C NMR (150 MHz, D_2O) δ 174.9, 158.3, 120.2, , 87.1, 78.6, 75.7, 72.1, 71.4, 30.1, 29.2 × 3. HRMS calcd for $[C_{12}H_{19}N_3O_6\text{-}H]^-$ 300.1202, found 300.1190.



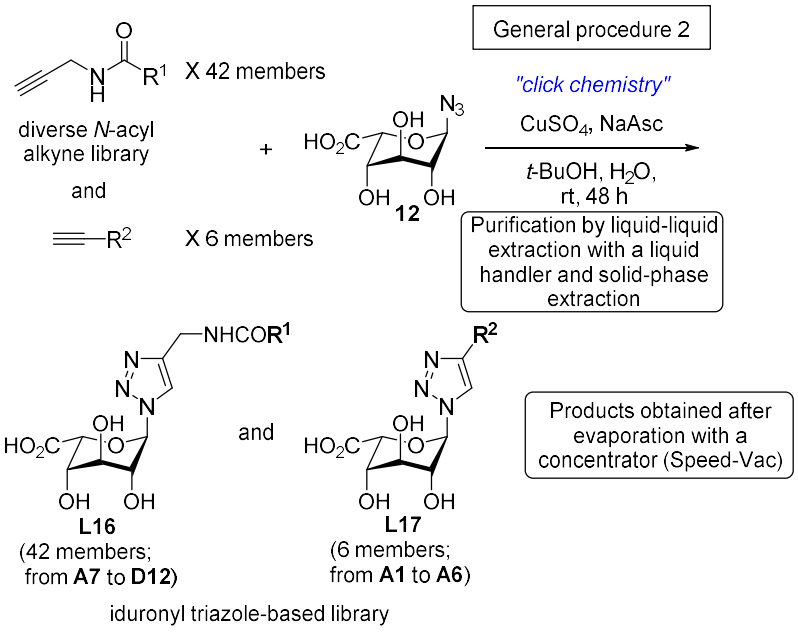
Compound 15b. The preparation was accorded on General procedure 2. 1-Ethynyl-4-fluorobenzene was used. Yield was 61%. ^{1}H NMR (600 MHz, D_2O) δ 8.46 (s, 1H), 7.69–7.71 (m, 2H), 7.17–7.20 (m, 2H), 5.78 (d, 1H, J = 9.2 Hz), 4.05–4.09 (m, 2H), 3.74–3.80 (m, 2H); ^{13}C NMR (150 MHz, D_2O) δ 174.9, 162.5, 146.9, 127.6, 125.3 × 2, 120.9, 115.9 × 2, 87.2, 78.8, 75.7, 72.2, 71.4. HRMS calcd for $[C_{14}H_{14}FN_3O_6\text{-}H]^-$ 338.0795, found 338.0783.



3. Parallel synthesis of an *N*-acyl propargylamine-based library

To a mixture of propargylamine (128 µL, 2 mmol), a carboxylic acid (2 mmol), and EDCI (460 mg, 1.2 equiv) in dry CH_2Cl_2 (5 mL) was added DIPEA (418 µL, 1.2 equiv). The mixture was stirred at room temperature for 12 h. After dilution with CH_2Cl_2 (30 mL), the mixture was washed with 1N $HCl_{(aq)}$ (3 × 10 mL) by assistance with a liquid handler (TECAN). The organic layer was dried over anhydrous $MgSO_4$, concentrated to get *N*-acyl propargylamine by assistance with a concentrator (Speed-Vac).

4. Parallel synthesis of a 48-membered library



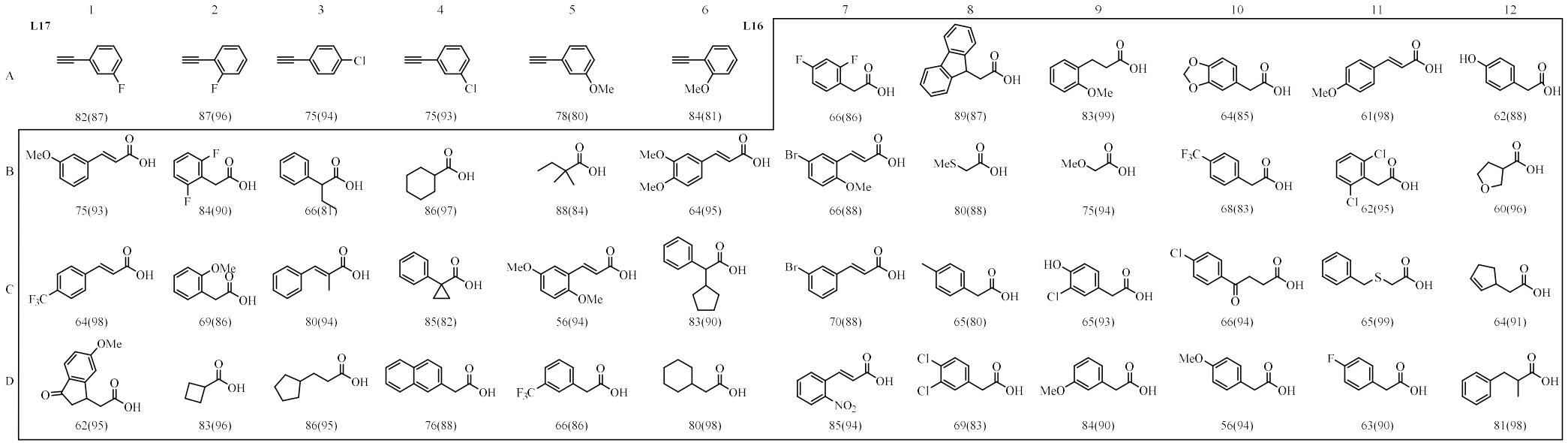


Figure S1. Alkyne library A1–A6 (for compound **L17**) and acid library A6–D12 (for compound **L16**) for preparation of *N*-acyl propargylamine-based library

Table S1. Yields and purities of iduronyl triazole-based library

	1	2	3	4	5	6	7	8	9	10	11	12
A	82[a](87)[b]	87(96)	75(94)	75(93)	78(80)	84(81)	66(86)	89(87)	83(99)	64(85)	61(98)	62(88)
B	75(93)	84(90)	66(81)	86(97)	88(84)	64(95)	66(88)	80(88)	75(94)	68(83)	62(95)	60(96)
C	64(98)	69(86)	80(94)	85(82)	56(94)	83(90)	70(88)	65(80)	65(93)	66(94)	65(99)	64(91)
D	62(95)	83(96)	86(95)	76(88)	66(86)	80(98)	85(94)	69(83)	84(90)	56(94)	63(90)	81(98)

[a] Yield was given after solid-liquid extraction. [b] Determined by HPLC.

Compound L17-A1. ^{1}H NMR (600 MHz, D_2O) δ 8.59 (s, 1H), 7.53–7.61 (m, 2H), 7.48–7.51 (m, 1H), 7.16–7.19 (m, 1H), 6.12 (d, 1H, J = 9.0 Hz), 4.61 (d, 1H, J = 6.0 Hz), 4.12 (dd, 1H, J = 9.2, 9.3 Hz), 4.00 (dd, 1H, J = 6.0, 9.2 Hz), 3.78 (dd, 1H, J = 9.0, 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 162.8, 146.6, 131.2, 130.9, 122.0, 121.6, 115.5, 112.5, 85.5, 74.3, 73.8, 72.1, 70.5. HRMS calcd for $[C_{14}H_{14}FN_3O_6\text{-}H]^-$ 338.0759, found 338.0783.

Compound L17-A2. NMR (600 MHz, D_2O) δ 8.58 (s, 1H), 7.42–7.99 (m, 2H), 7.30–7.33 (m, 1H), 7.24–7.28 (m, 1H), 6.14 (d, 1H, J = 9.0 Hz), 4.62 (d, 1H, J = 6.0 Hz), 4.15 (dd, 1H, J = 9.0, 9.3 Hz), 4.00 (dd, 1H, J = 6.0, 9.2 Hz), 3.79 (dd, 1H, J = 9.0, 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 159.1, 141.4, 130.5, 127.5 , 124.7, 123.9, 116.9, 115.9, 85.5, 74.3, 73.8, 72.1, 70.5. HRMS calcd for $[C_{14}H_{14}FN_3O_6\text{-}H]^-$ 338.0759, found 338.0783.

Compound L17-A3. ^{1}H NMR (600 MHz, D_2O) δ 8.52 (s, 1H), 7.67–7.69 (m, 2H), 7.43–7.44 (m, 2H), 6.12 (d, 1H, J = 9.0 Hz), 4.62 (d, 1H, J = 5.9 Hz), 4.12 (t, 1H, J = 9.0 Hz), 4.00 (dd, 1H, J = 6.0, 9.0 Hz), 3.78 (dd, 1H, J = 5.0, 9.0 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 146.6, 133.9, 129.0 × 2, 127.7 × 2, 127.0, 121.6, 85.5, 74.4, 73.7, 72.1, 70.5. HRMS calcd for $[C_{14}H_{14}ClN_3O_6\text{-}H]^-$ 354.0466, found 354.0487.

Compound L17-A4. ^{1}H NMR (600 MHz, D_2O) δ 8.49 (s, 1H), 7.67 (s, 1H), 7.59–7.60 (m, 1H), 7.34–7.37 (m, 1H), 6.10 (d, 1H, J = 9.0 Hz), 4.60 (d, 1H, J = 6.0 Hz), 4.11 (dd, 1H, J = 9.1, 9.3 Hz), 3.98 (dd, 1H, J = 6.0, 9.1 Hz), 3.78 (dd, 1H, J = 9.0, 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 146.3, 134.2, 130.8, 130.4, 128.5, 125.4, 123.9, 121.9, 85.5, 74.4, 73.8, 72.1, 70.5. HRMS calcd for $[C_{14}H_{14}ClN_3O_6\text{-}H]^-$ 354.0466, found 354.0487.

Compound L17-A5. ^{1}H NMR (600 MHz, D_2O) δ 8.55 (s, 1H), 7.39–7.44 (m, 2H), 7.34 (s, 1H), 7.00–7.01 (m, 1H), 6.12 (d, 1H, J = 9.0 Hz), 4.60 (d, 1H, J = 6.0 Hz), 4.11 (dd, 1H, J = 9.0, 9.3 Hz), 3.99 (dd, 1H, J = 6.0, 9.3 Hz), 3.87 (s, 1H), 3.78 (t, 1H, J = 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 159.2,

147.3, 130.4 × 2, 121.7,118.5, 114.5, 111.0, 85.5, 74.3, 73.8, 72.1, 70.5, 55.3. HRMS calcd for $[C_{15}H_{17}N_3O_7\text{-}H]^-$ 350.0961, found 350.0983.

Compound L17-A6. ^{1}H NMR (600 MHz, D_2O) δ 8.60 (s, 1H), 7.97–7.98 (m, 1H), 7.44–7.46 (m, 1H), 7.13–7.18 (m, 2H), 6.12 (d, 1H, J = 9.0 Hz), 4.60 (d, 1H, J = 6.0 Hz), 4.15 (dd, 1H, J = 9.0, 9.3 Hz), 3.99 (dd, 1H, J = 6.0, 9.3 Hz), 3.94 (s, 1H), 3.78 (t, 1H, J = 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 155.7, 143.1, 130.2, 127.3, 124.2, 121.1, 117.7, 111.9 , 85.4, 74.3, 73.8, 72.1, 70.5, 55.4. HRMS calcd for $[C_{15}H_{17}N_3O_7\text{-}H]^-$ 350.0959, found 350.0983.

Compound L16-A7. $[\alpha]_D^{25}$ –26.4 (c 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.00 (s, 1H), 7.24–7.20 (m, 1H), 6.91–6.86 (m, 2H), 5.91 (d, 1H, J = 9.1 Hz), 4.46 (d, 1H, J = 6.1 Hz), 4.42 (s, 2H), 3.91 (t, 1H, J = 9.1 Hz), 3.84 (dd, 1H, J = 9.1, 6.1 Hz), 3.62 (t, 1H, J = 9.1 Hz), 3.57 (s, 2H); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 173.6, 163.0, 161.7, 161.3, 160.0, 132.4, 132.3, 117.7, 111.4, 103.7, 85.3, 73.7, 72.1, 70.4, 35.1, 34.6. HRMS calcd for $[C_{17}H_{18}F_2N_4O_7\text{-}H]^-$ 427.1060, found 427.1056.

Compound L16-A10. $[\alpha]_D^{25}$ –31.7 (c 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7.91 (s, 1H), 6.77 (d, 1H, J = 7.9 Hz), 6.73 (s, 1H), 6.69 (d, 1H, J = 7.9 Hz), 5.90 (d, 1H, J = 9.1 Hz), 5.87 (s, 2H), 4.44 (d, 1H, J = 5.9 Hz), 4.39 (s, 2H), 3.87 (t, 1H, J = 9.1 Hz), 3.83–3.81 (m, 1H), 3.61 (t, 1H, J = 9.1 Hz), 3.45 (s, 2H); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 174.8, 147.3 × 2, 146.2, 128.4, 123.0, 122.5, 109.5, 108.6, 101.1, 85.3, 74.2, 73.7, 72.2, 70.4, 41.8, 34.6. HRMS calcd for $[C_{18}H_{20}N_4O_9\text{-}H]^-$ 435.1147, found 435.1138.

Compound L16-A11. $[\alpha]_D^{25}$ –29.7 (c 1.0 in H_2O); ^{1}H NMR(600 MHz, D_2O) δ 8.18 (s, 1H), 7.54–7.55 (m, 2H), 7.45 (d, 1H, 15.7Hz), 6.99–7.00 (m, 2H), 6.46 (d, 1H, 15.7 Hz), 6.03 (d, 1H, J = 9.0 Hz), 4.60 (s, 2H), 4.55 (s, 1H), 4.04 (t, 1H, J =9.0 Hz), 3.94 (s, 1H), 3.84 (s, 2H), 3.72 (dd, 1H, J = 9.2, 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ175.2, 168.9, 160.5, 144.9, 141.2, 129.7 × 2, 127.3, 123.3, 117.3, 114.3 × 2, 85.3, 74.2, 73.7, 72.1, 70.4, 55.3, 34.6. HRMS calcd for $[C_{19}H_{22}N_4O_8\text{-}H]^-$ 433.1354, found 433.1353.

Compound L16-A12. $[\alpha]_D^{25}$ –40.4 (c 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7.95 (s, 1H), 7.21 (br s, 2H), 6.90 (br s, 2H), 6.01–6.00 (m, 1H), 4.56 (br s, 1H), 4.51 (s, 2H), 3.98–3.95 (m, 2H), 3.74–3.73 (m, 1H), 3.57 (s, 2H); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 175.2, 154.6, 145.0, 130.5 × 2, 126.7, 122.9, 115.7 × 2, 85.3, 74.2, 73.7, 72.2, 70.4, 41.4, 34.6. HRMS calcd for $[C_{17}H_{20}N_4O_8\text{-}H]^-$ 407.1197, found 407.1193.

Compound L16-B1. $[\alpha]_D^{25}$ –35.8 (c 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.09 (s, 1H), 7.28 (d, 1H, J = 15.8 Hz), 7.21 (dd, 1H, J = 7.8, 8.0 Hz), 7.04 (d, 1H, J = 7.8 Hz), 6.95 (s, 1H), 6.85 (d, 1H, J = 8.0 Hz), 6.39 (d, 1H, J = 15.8 Hz), 5.94 (d, 1H, J = 9.1 Hz), 4.47 (s, 2H), 4.44 (d, 1H, J = 6.1 Hz), 3.94 (dd, 1H, J

= 9.1, 9.3 Hz), 3.83 (dd, 1H, *J* = 6.1, 9.3 Hz), 3.69 (s, 3H), 3.62 (t, 1H, *J* = 9.3 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 168.4, 159.0, 141.1, 135.7, 130.1 × 2, 120.9 × 2, 119.9, 115.8 × 2, 112.9, 85.3, 73.7, 72.1, 70.4, 55.2, 34.5. HRMS calcd for $[C_{19}H_{22}N_4O_8\text{-}H]^-$ 433.1354, found 433.1347.

Compound L16-B5. $[\alpha]_D^{25}$ –35.1 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.04 (s, 1H), 5.93 (d, 1H, *J* = 9.1 Hz), 4.48 (d, 1H, *J* = 6.1 Hz), 4.43 (s, 2H), 3.96 (t, 1H, *J* = 9.1 Hz), 3.87 (dd, 1H, *J* = 9.1, 6.1 Hz), 3.64 (t, 1H, *J* = 9.1 Hz), 1.45 (q, 2H, *J* = 7.5 Hz), 1.07 (s, 6H), 0.66 (t, 3H, *J* = 7.5 Hz); ^{13}C NMR (150 MHz, D_2O) δ 181.8, 175.3, 145.4, 123.3, 85.3, 74.3, 73.7, 72.1, 70.5, 42.3, 34.5, 33.3, 24.0, 8.4. HRMS calcd for $[C_{15}H_{24}N_4O_7\text{-}H]^-$ 371.1561, found 371.1572.

Compound L16-B6. $[\alpha]_D^{25}$ –31.5 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.18 (s, 1H), 7.32–7.31 (m, 1H), 7.06 (s, 1H), 7.02 (s, 1H), 6.89 (s, 1H), 6.37–6.35 (m, 1H), 6.02 (s, 1H), 4.56 (s, 2H), 4.53 (s, 1H), 4.021–4.018 (m, 1H), 3.91 (s, 1H), 3.78 (s, 6H), 3.70 (s, 1H); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 168.8, 149.8, 148.0, 144.9, 141.4, 127.4, 123.3, 122.6, 117.4, 111.4, 110.0, 85.3, 74.2, 73.7, 72.1, 70.4, 55.5, 55.4, 34.6. HRMS calcd for $[C_{20}H_{24}N_4O_9\text{-}H]^-$ 463.1460, found 463.1476.

Compound L16-B8. $[\alpha]_D^{25}$ –39.0 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.12 (s, 1H), 5.96 (d, 1H, *J* = 9.1 Hz), 4.49 (s, 3H), 3.98 (t, 1H, *J* = 9.1 Hz), 3.90–3.87 (m, 1H), 3.66 (t, 1H, *J* = 9.1 Hz), 3.22 (s, 2H), 3.70 (br s, 1H); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 172.7, 144.7, 123.4, 85.4, 74.3, 73.8, 72.1, 70.5, 36.8, 34.7, 14.9. HRMS calcd for $[C_{12}H_{18}N_4O_7S\text{-}H]^-$ 361.0812, found 361.0821.

Compound L16-C3 (18). $[\alpha]_D^{25}$ –27.1 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.17 (s, 1H), 7.36–744 (m, 4H), 7.34 (s, 1H), 7.24 (s, 1H), 6.03 (d, 1H, *J*= 9.2 Hz), 4.59 (s, 2H), 4.53 (d, 1H, *J* = 6.1 Hz), 4.03 (t, 1H, *J* = 9.2 Hz), 3.92 (dd, 1H, *J* = 6.1, 9.4 Hz), 3.71 (dd, 1H, *J* = 9.2, 9.4 Hz), 2.02 (s, 3H); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 172.9, 135.6, 134.6, 131.3, 129.3 × 2, 128.5 × 2, 128.2, 123.2, 85.3, 74.2, 73.7, 72.1, 70.4, 34.8, 13.4.HRMS calcd for $[C_{19}H_{22}N_4O_7\text{-}H]^-$ 417.1405, found 417.1397.

Compound L16-C5. $[\alpha]_D^{25}$ –21.8 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.10 (s, 1H), 7.54 (s, 1H), 6.93 (s, 1H), 6.85 (s, 2H), 6.47 (s, 1H), 5.94 (s, 1H), 4.50 (s, 2H), 4.45 (s, 1H), 3.93 (m, 1H), 3.83 (s, 1H), 3.70 (s, 3H), 3.67 (s, 3H), 3.61 (m, 1H); ^{13}C NMR (150 MHz, D_2O) δ 175.3, 168.8, 152.8, 152.4, 144.9, 136.1, 123.7, 123.3, 120.6, 117.0, 113.5, 113.2, 85.3, 74.2, 73.7, 72.1, 70.4, 56.3, 55.7, 34.6. HRMS calcd for $[C_{20}H_{24}N_4O_9\text{-}H]^-$ 463.1460, found 463.1450.

Compound L16-C7. $[\alpha]_D^{25}$ –38.5 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.09 (s, 1H), 7.69 (m, 1H), 7.44–7.47 (m, 1H), 7.34 (d, 1H, *J* = 15.7 Hz), 7.21–7.23 (m, 1H), 6.50 (d, 1H, *J* = 15.7 Hz), 5.91 (d, 1H,

J = 9.2 Hz), 4.52 (s, 2H), 4.44 (d, 1H, *J* = 6.1 Hz), 3.93 (t, 1H, *J* = 9.2 Hz), 3.82 (dd, 1H, *J* = 6.1, 9.4 Hz), 3.60 (dd, 1H, *J* = 9.2, 9.4 Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 168.2, 144.7, 140.0, 136.4, 132.6, 130.5, 130.4, 126.7, 123.3, 122.2, 120.9, 85.2, 74.2, 73.7, 72.1, 70.4, 34.6. HRMS calcd for $[C_{18}H_{19}BrN_4O_7\text{-}H]^-$ 481.0353, found 481.0370.

Compound L16-C8. $[\alpha]_D^{25}$ –24.8 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7.89 (s, 1H), 7.14 (d, 2H, *J* = 8.1 Hz), 7.10 (d, 2H, *J* = 8.1 Hz), 5.88 (d, 1H, *J* = 9.2 Hz), 4.45 (d, 1H, *J* = 6.1 Hz), 4.34 (s, 2H), 3.87 (t, 1H, *J* = 9.2 Hz), 3.82 (dd, 1H, *J* = 9.2, 6.1 Hz), 3.61 (t, 1H, *J* = 9.2 Hz), 3.49 (s, 2H), 2.22 (s, 3H); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 174.9, 144.9, 137.4, 131.7, 129.5 × 2, 129.0 × 2, 123.0, 85.3, 74.2, 73.7, 72.1, 70.4, 41.8, 34.5, 20.1 .HRMS calcd for $[C_{18}H_{22}N_4O_7\text{-}H]^-$ 405.1405, found 405.1420.

Compound L16-C9. $[\alpha]_D^{25}$ –20.0 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7.83 (s, 1H), 7.36 (s, 1H), 6.97 (d, 1H, *J* = 8.0 Hz), 6.86 (d, 1H, *J* = 8.0 Hz), 6.09 (d, 1H, *J* = 8.7 Hz), 4.63 (d, 1H, *J* = 6.0 Hz), 4.37 (s, 2H), 3.97 (dd, 1H, *J* = 6.0, 7.2 Hz), 3.91 (dd, 1H, *J* = 8.7, 8.8 Hz), 3.77 (t, 1H, *J* = 8.8 Hz), 3.42 (s, 2H); ^{13}C NMR (150 MHz, D_2O) δ 174.5, 173.0, 150.4, 130.3 × 2, 128.8 × 2, 127.9, 122.7, 120.2, 116.8, 85.4, 72.7, 71.7, 69.7, 41.0, 34.5.HRMS calcd for $[C_{17}H_{19}ClN_4O_8\text{-}H]^-$ 441.0808, found 441.0824.

Compound L16-D1. $[\alpha]_D^{25}$ –25.4 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7 .85 (s, 1H), 7.51–7.53 (m, 1H), 6.89–6.94 (m, 2H), 5.91 (dd, 1H, *J* = 9.0, 9.1 Hz), 4.46 (d, 1H, *J* = 6.1 Hz), 4.38 (d, 1H, *J* = 15.4 Hz), 4.29 (dd, 1H, *J* = 15.4, 15.5 Hz), 3.82–3.92 (m, 1H), 3.83–3.85 (m, 1H), 3.76–3.78 (m, 3H), 3.67–3.72 (m, 1H), 3.61–3.66 (m, 1H), 2.82–2.87 (m, 1H), 2.66–2.69 (m, 1H), 2.52–2.56 (m, 1H), 2.44–2.49 (m, 1H); ^{13}C NMR (150 MHz, D_2O) δ 208.87, 175.2, 173.8, 165.8, 161.3, 144.5, 128.8, 125.4, 123.1, 116.2, 109.1, 85.2, 74.2, 73.7, 72.1, 70.4, 55.8, 42.5, 40.1, 35.0, 34.1. HRMS calcd for $[C_{21}H_{24}N_4O_9\text{-}H]^-$ 475.1460, found 475.1479.

Compound L16-D3. $[\alpha]_D^{25}$ –34.6 (*c* 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 8.04 (s, 1H), 5.92 (d, 1H, *J* = 9.1 Hz), 4.44 (d, 1H, *J* = 6.2Hz), 4.39 (s, 2H), 3.92 (dd, 1H, *J* = 9.1, 9.2 Hz), 3.83 (dd, 1H, *J* = 6.2, 9.4 Hz), 3.61 (dd, 1H, *J* = 9.3, 9.4 Hz), 2.18–2.20 (m, 2H), 1.56–1.61 (m, 3H), 1.45–1.51 (m, 4H), 1.35–1.37 (m, 2H), 0.93–0.96 (m, 2H); ^{13}C NMR (150 MHz, D_2O) δ 177.4, 175.2, 123.2, 85.3, 74.2, 74.1, 73.7, 72.0, 70.4, 38.9, 34.9, 34.2, 31.8 × 2, 31.5, 24.6×2. HRMS calcd for $[C_{17}H_{26}N_4O_7\text{-}H]^-$ 397.1718, found 397.1718.

Compound L16-D7. $[\alpha]_D^{25}$ –37.8 (*c* 1.0 in H_2O); ^{1}H NMR(600 MHz, D_2O) δ 8.11 (s, 1H), 7.95 (d, 1H, *J* = 8.4 Hz), 7.77 (d, 1H, *J* = 15.7 Hz), 7.6–7.61 (m, 2H), 7.46–7.49 (m, 1H), 6.43 (d, 1H, *J* = 15.7 Hz), 5.93 (d, 1H, *J* = 9.2 Hz), 4.53 (s, 2H), 4.44 (d, 1H, *J* = 6.2 Hz), 3.94 (t, 1H, *J* = 9.2 Hz), 3.83 (dd, 1H, *J* = 6.2,

9.4Hz), 3.61 (t, 1H, J = 9.4Hz); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 167.6, 147.6, 144.6, 137.2, 134.1, 130.3, 130.2, 129.1, 124.8, 124.2, 123.4, 85.3, 74.2, 73.7, 72.1, 70.4, 34.5. HRMS calcd for $[C_{18}H_{19}N_5O_9\text{-}H]^-$ 448.1099, found 448.1115.

Compound L16-D8. $[\alpha]_D^{25}$ –24.1 (c 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7.93 (s, 1H), 7.39 (d, 1H, J = 8.3 Hz), 7.35 (d, 1H, J = 1.3 Hz), 7.08 (dd, 1H, J = 1.3, 8.3 Hz), 5.91 (d, 1H, J = 9.1 Hz), 4.44 (d, 1H, J = 6.0 Hz), 4.40 (s, 2H), 3.82–3.88 (m, 2H), 3.61 (t, 1H, J = 9.3 Hz), 3.51 (s, 2H); ^{13}C NMR (150 MHz, D_2O) δ 175.1, 173.6, 135.1, 131.7, 130.8 × 2, 130.5 × 2, 128.9 × 2, 123.0, 85.3, 73.6, 72.1, 70.3, 41.1, 34.5. HRMS calcd for $[C_{17}H_{18}Cl_2N_4O_7\text{-}H]^-$ 459.0469, found 459.0490.

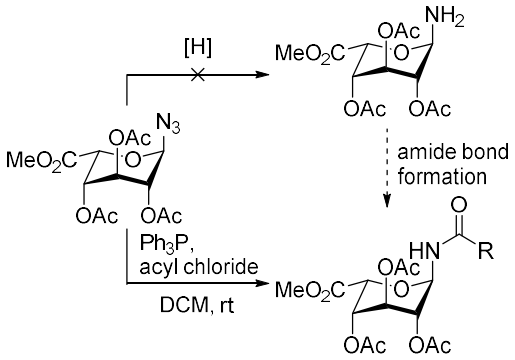
Compound L16-D9. $[\alpha]_D^{25}$ –30.0 (c 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7.87 (s, 1H), 7.23–7.25 (m, 1H), 6.83–6.85 (m, 2H), 6.80–6.81 (m, 1H), 5.88 (d, 1H, J = 9.1 Hz), 4.44 (d, 1H, J = 6.1 Hz), 4.39 (s, 2H), 3.82 (dd, 1H, J = 6.1, 9.2 Hz), 3.80–3.81 (m, 1H), 3.71 (s, 3H), 3.60 (t, 1H, J = 9.2 Hz), 3.52 (s, 2H); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 174.4, 159.0,136.4, 130.1, 122.9, 121.8, 114.4, 113.0, 112.0, 85.2, 74.2, 73.6, 72.1, 70.4, 55.2, 42.2, 34.5. HRMS calcd for $[C_{18}H_{22}N_4O_8\text{-}H]^-$ 421.1354, found 421.1344.

Compound L16-D10. $[\alpha]_D^{25}$ –31.5 (c 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7.87 (s, 1H), 7.13 (d, 2H, J = 8.8 Hz), 6.88 (d, 2H, J = 8.8 Hz), 5.88 (d, 1H, J = 9.2 Hz), 4.43 (d, 1H, J = 6.1 Hz), 4.38 (s, 2H), 3.85 (dd, 1H, J = 9.2, 9.3 Hz), 3.80–3.83 (m, 2H), 3.72 (s, 3H), 3.60 (t, 1H, J = 9.3 Hz), 3.47 (s, 2H); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 175.0, 157.9, 144.9, 130.3, 127.3, 122.9, 114.3,85.2, 74.1, 73.6, 72.1, 70.4, 55.3, 41.3, 34.5. HRMS calcd for $[C_{18}H_{22}N_4O_8\text{-}H]^-$ 421.1354, found 421.1367.

Compound L16-D11. $[\alpha]_D^{25}$ –34.0 (c 1.0 in H_2O); ^{1}H NMR (600 MHz, D_2O) δ 7.91 (s, 1H), 7.18–7.20 (m, 2H), 7.00–7.03 (m, 2H), 5.89 (d, 1H, J = 9.2 Hz), 4.44 (d, 1H, J = 6.1 Hz), 4.39 (s, 2H), 3.87 (t, 1H, J = 9.2 Hz), 3.83 (dd, 1H, J = 6.1, 9.4 Hz), 3.60 (dd, 1H, J = 9.2, 9.4 Hz), 3.52 (s, 2H); ^{13}C NMR (150 MHz, D_2O) δ 175.2, 174.6, 162.6, 160.9, 144.8, 130.8, 130.7, 123.0, 115.5, 115.4, 85.2, 74.2, 73.6, 72.1, 70.4, 41.3, 34.5. HRMS calcd for $[C_{17}H_{19}FN_4O_7\text{-}H]^-$ 409.1154, found 409.1167.

Compound L16-D12 (19). ^{1}H NMR (600 MHz, D_2O) δ 7.34 (s, 1H), 7.26–7.21 (m, 3H), 7.12–7.10 (m, 2H), 8.90 (dd, 1H, J = 9.1, 13.2 Hz), 4.50 (t, 1H, J = 5.4 Hz), 4.38 (dd, 1H, J = 11.5, 15.8 Hz), 4.13 (t, 1H, J = 15.4 Hz), 3.93 (t, 1H, J = 9.2 Hz), 3.89 (td, 1H, J = 4.1, 9.1 Hz), 3.68 (t, 1H, J = 9.4 Hz), 1.15–1.13 (m, 3H); ^{13}C NMR (150 MHz, D_2O) δ 179.0, 175.2, 144.9, 139.6, 128.9, 128.6, 126.6, 123.0, 85.3, 74.4, 73.8, 72.2, 70.5, 43.0, 39.7, 34.1, 17.1. HRMS calcd for $[C_{19}H_{24}N_4O_7\text{-}H]^-$ 419.1561, found 419.1556.

5. Attempts to reduce the protected azido iduronic acid intermediate and amidation



1. After hydrogenation, the reaction resulted in decomposition of starting material.
2. The amide bond formation at C1 using the glycosyl azide and acyl chloride by Staudinger ligation.

C. Biology section

Inhibition assay

Compounds were mixed with 4-methylberiilyl α-L-iduronic acid as substrate and rh-α-IDUA in pH 3.5 (citric phosphate) buffer, then assay was carried out at 37 °C for 15 min. Stop solution (0.4 mol/L K_2CO_3, pH 10.6) was then added and fluorescence was determined at 355 nm excitation and 460 nm emission. Inhibition was performed as relative enzyme activity to control. The active compounds were selected and further tested at lower concentration to determine their IC_{50} values. The assays performed in 96-wells of the microtiter plate contained citric phosphate buffer.

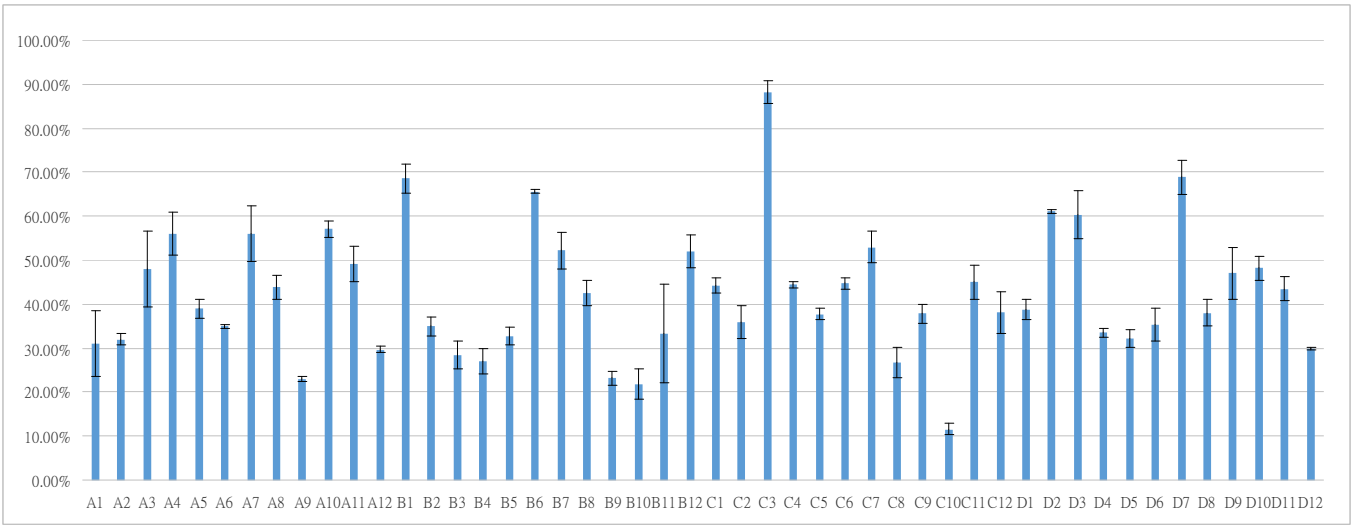


Figure S2. The inhibition activity of 48-membered iduronyl triazoles at 100 μM

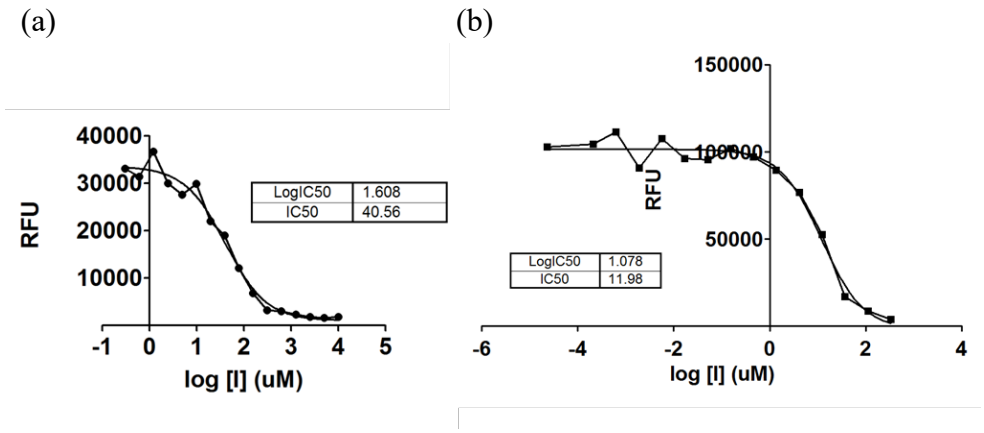


Figure S3. The IC_{50} plots of (a) compound **18** and (b) **2** versus rh-α-IDUA.

In vitro stabilization of rh-α-IDUA[S3]

An assessment of the ability of small molecules to stabilize rh-α-IDUA against denaturation was performed by using Aldurazyme. Enzyme aliquots (20 λ, pH 3.5) were incubated with 0, 100, 250 or 500 μM of small molecule on ice for 10 min. The samples were heated at 48 °C as a function of time in an

attempt to heat-inactivate (denature) enzyme, and then the samples were diluted into twenty-fold volume of 0.1 M citric phosphate buffer (pH 3.5). The enzyme was immediately incubated with substrate (0.5 mM 4-methyllumbelliferyl α-L-iduronic acid) for 15 min at 37 °C before quenching with glycine buffer. Liberated 4-methylumbelliferone was measured (excitation 355 nm, emission 460 nm). Enzyme activity was reported relative to unheated enzyme.

Thermal stability shift assay[S4]

The stability of rh-α-IDUA was assessed using a modified fluorescence thermal stability assay on a Rotor-Gene system in acidic buffer (citric phosphate, pH 3.5). Briefly, rh-α-IDUA (4 μg) was combined with SYPRO Orange and various concentrations of small molecules in a final reaction volume of 20 λ. A thermal gradient was applied to the plate at a rate of 1 °C per minute, during which time the fluorescence of SYPRO Orange was continuously monitored. The fluorescence intensity at each temperature was normalized to the maximum fluorescence after complete thermal denaturation.

TableS2. Thermal shift study of glycerol toward rh-α-IDUA.

Concentration/conditions	Tm (^{o}C)
0 mM (pH 3.5)	56.15
40 mM (pH 3.5)	56.32

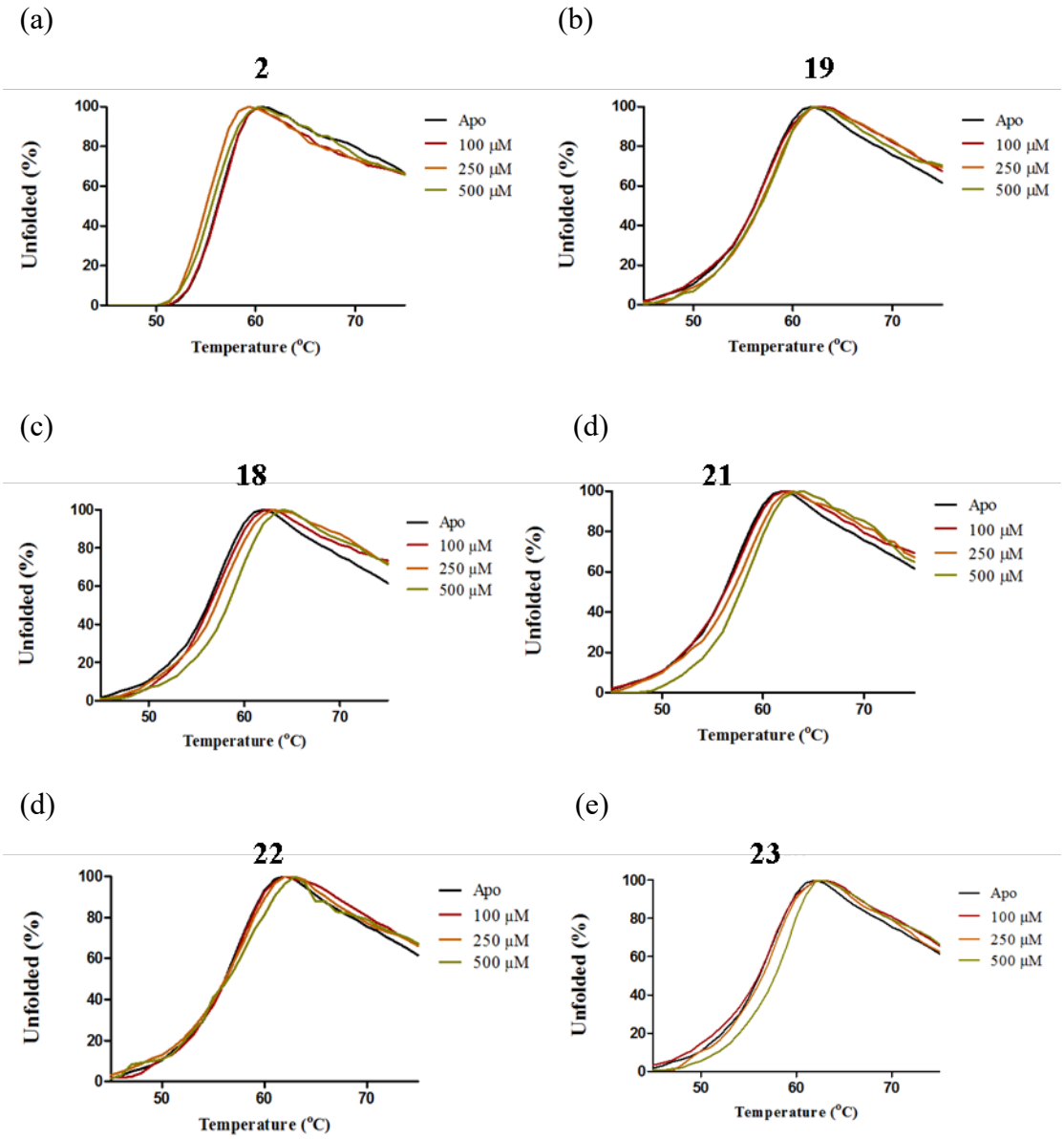
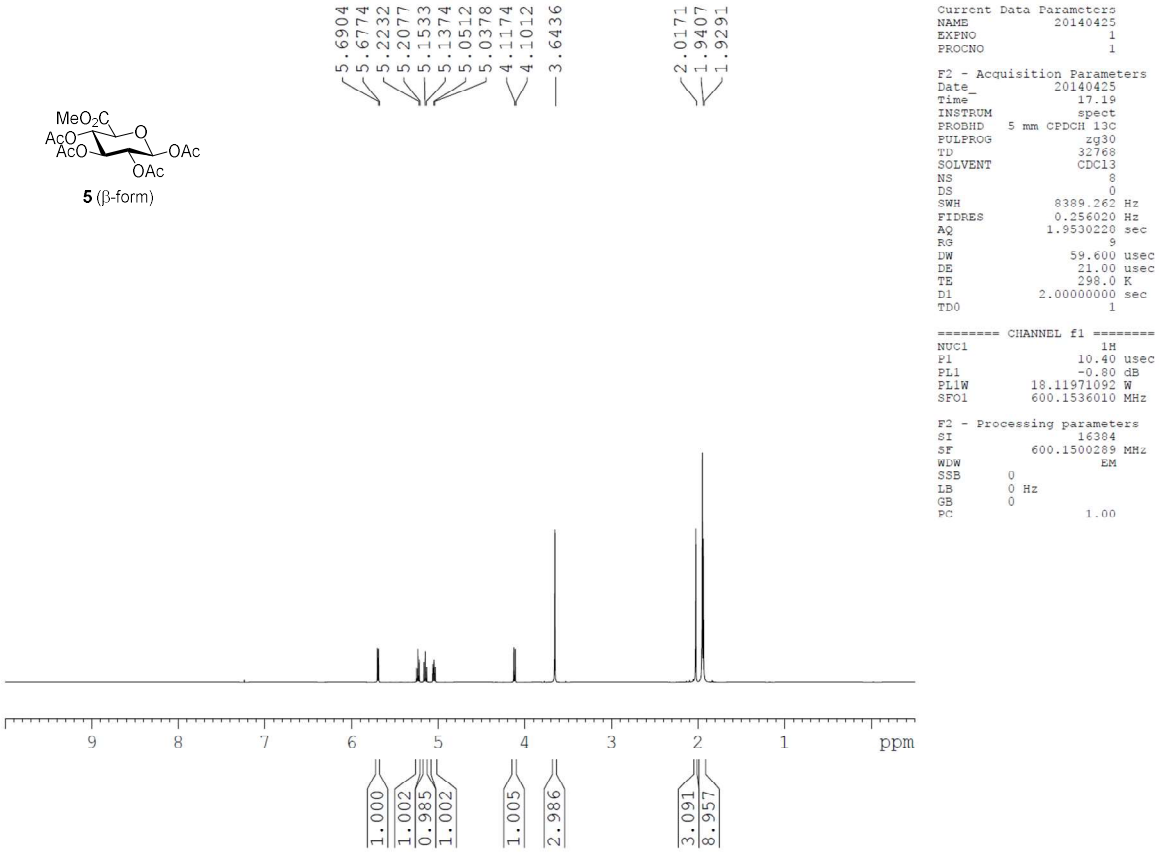


Figure S4. Thermal stability scans of rh-α-IDUA in the absence and presence of various concentrations of small molecules. All experiments were performed at pH 3.5, with the exception of Apo (pH 3.5, black). Unfolding of IDUA was monitored by changes in the fluorescence SYPRO Orange as a function of temperature.

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

^{1}H NMR and ^{13}C NMR of compound **5** in $CDCl_3$

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TD                      32768
SOLVENT                  CDCl3
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SWH                 8389.262 Hz
FIDRES              0.256020 Hz
AQ                  1.9530220 sec
RG                           9
DW                     59.600 usec
DE                     21.00 usec
TE                     298.0 K
D1                  2.00000000 sec
TD0                          1

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PL1W               18.11971092 W
SFO1               600.1536010 MHz

F2 - Processing parameters
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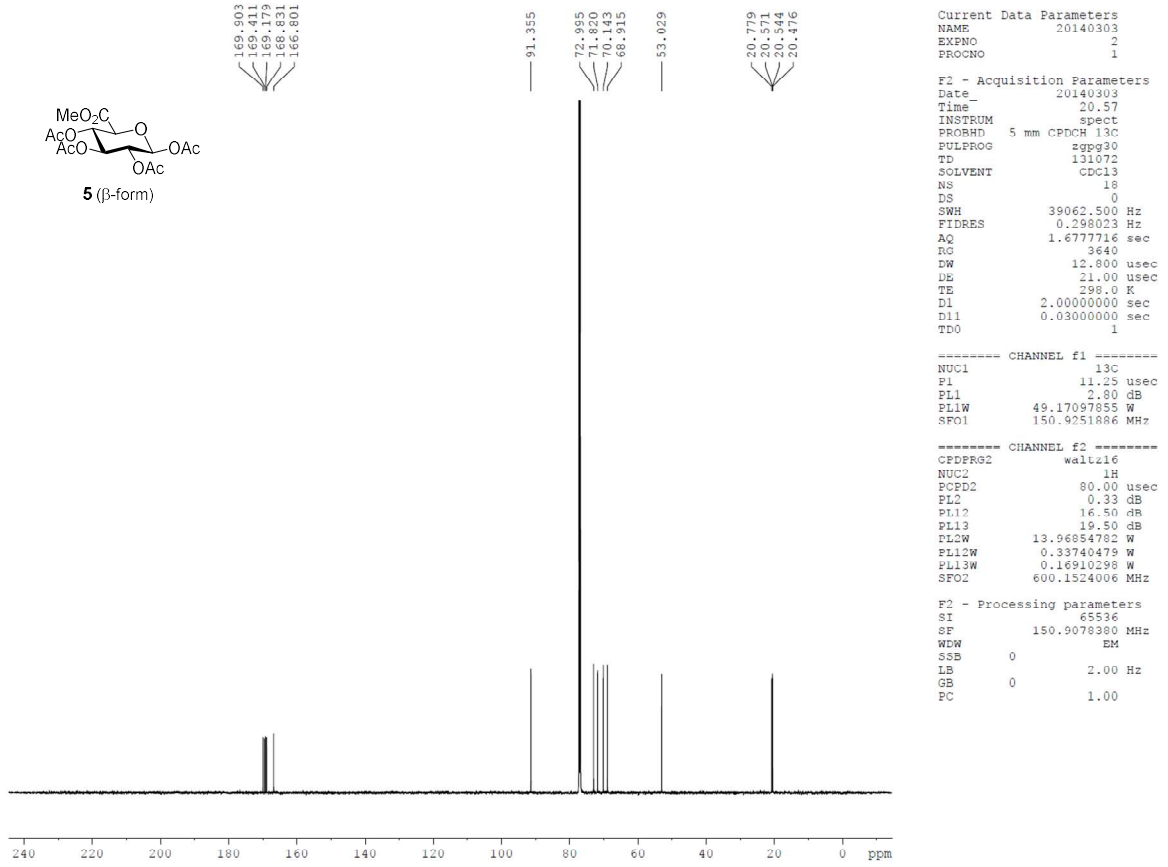


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PULPROG                zgpg30
TD                      131072
SOLVENT                  CDCl3
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DS                           0
SWH                39062.500 Hz
FIDRES              0.298023 Hz
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RG                        3640
DW                     12.800 usec
DE                     21.00 usec
TE                     298.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                      13C
P1                      11.25 usec
PL1                      2.80 dB
PL1W               49.17097855 W
SFO1               150.9251886 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      0.33 dB
PL12                    16.50 dB
PL13                    19.50 dB
PL2W               13.96854782 W
PL12W               0.33740479 W
PL13W               0.16910298 W
SFO2               600.1524006 MHz

F2 - Processing parameters
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SF                 150.9078380 MHz
WDW                         EM
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LB                       2.00 Hz
GB           0
PC                        1.00
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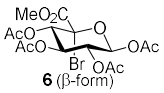
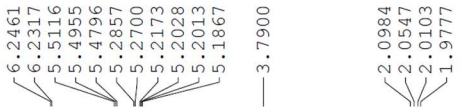
^{1}H NMR and ^{13}C NMR of compound **6** in $CDCl_3$



6 (β-form)

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PROCNO                       1

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PULPROG                  zg30
TD                      32768
SOLVENT                  CDCl3
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FIDRES                0.256020 Hz
AQ                    1.9530228 sec
RG                        28.5
DW                      59.600 usec
DE                      21.00 usec
TE                      298.0 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
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P1                      10.20 usec
PL1                     -0.80 dB
PL1W                18.11971092 W
SFO1                600.1536010 MHz

F2 - Processing parameters
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WDW                         EM
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PC                        1.00
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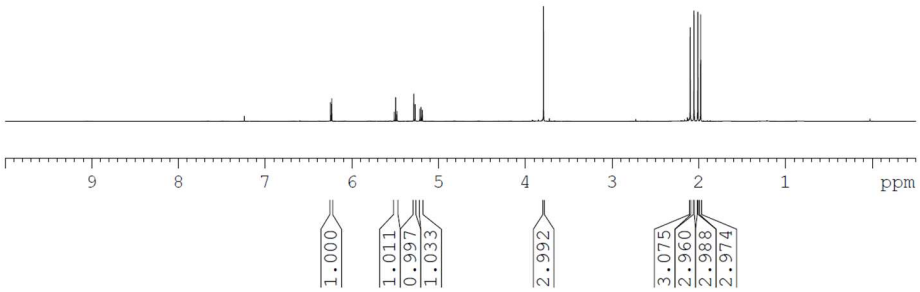
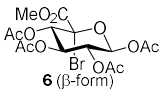
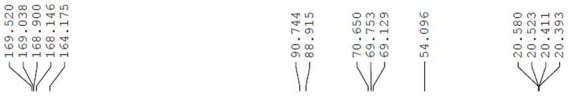




6 (β-form)

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PROCNO                       1

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TD                      131072
SOLVENT                  CDCl3
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FIDRES                0.298023 Hz
AQ                    1.6777716 sec
RG                        3640
DW                      12.800 usec
DE                      21.00 usec
TE                      297.9 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                      11.25 usec
PL1                      2.80 dB
PL1W                49.17097855 W
SFO1                150.9251886 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.33 dB
PL12                    16.50 dB
PL13                    19.50 dB
PL2W                13.96854782 W
PL12W                0.33740479 W
PL13W                0.16910298 W
SFO2                600.1524006 MHz

F2 - Processing parameters
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WDW                         EM
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LB                       2.00 Hz
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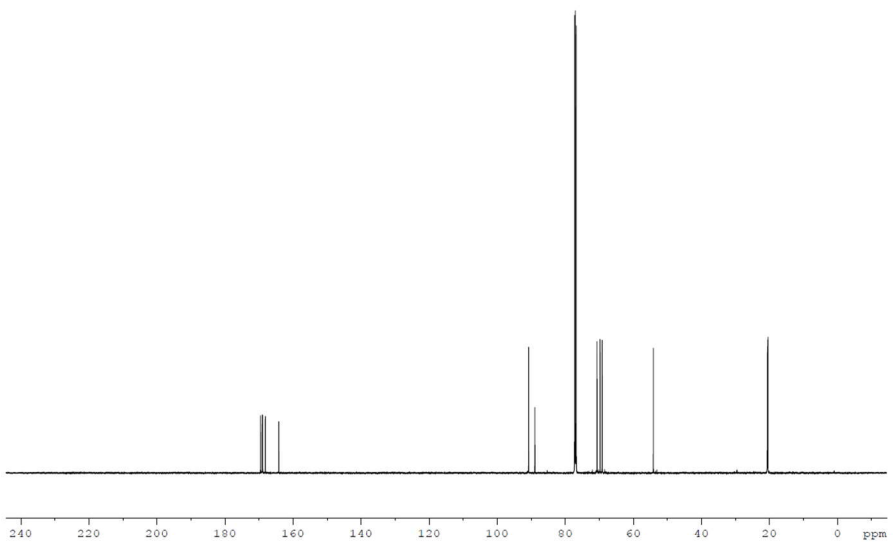
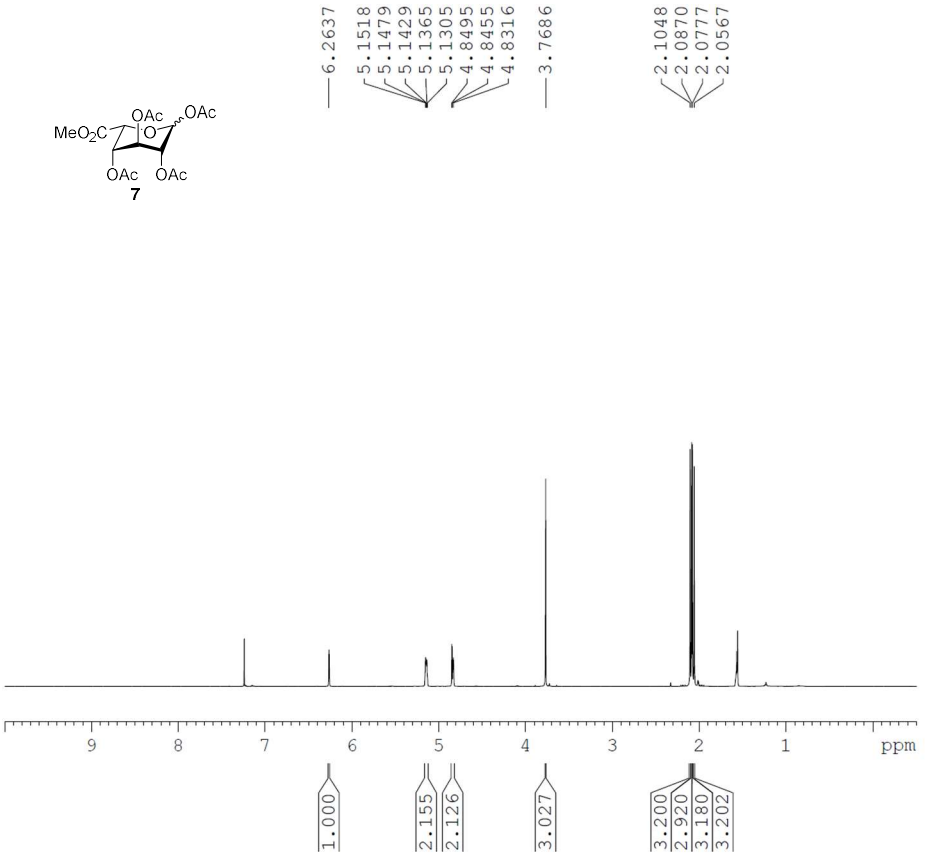


^{1}H NMR and ^{13}C NMR of compound **7** in $CDCl_3$

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PROCNO                       1

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PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
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TD0                          1

======== CHANNEL f1 ========
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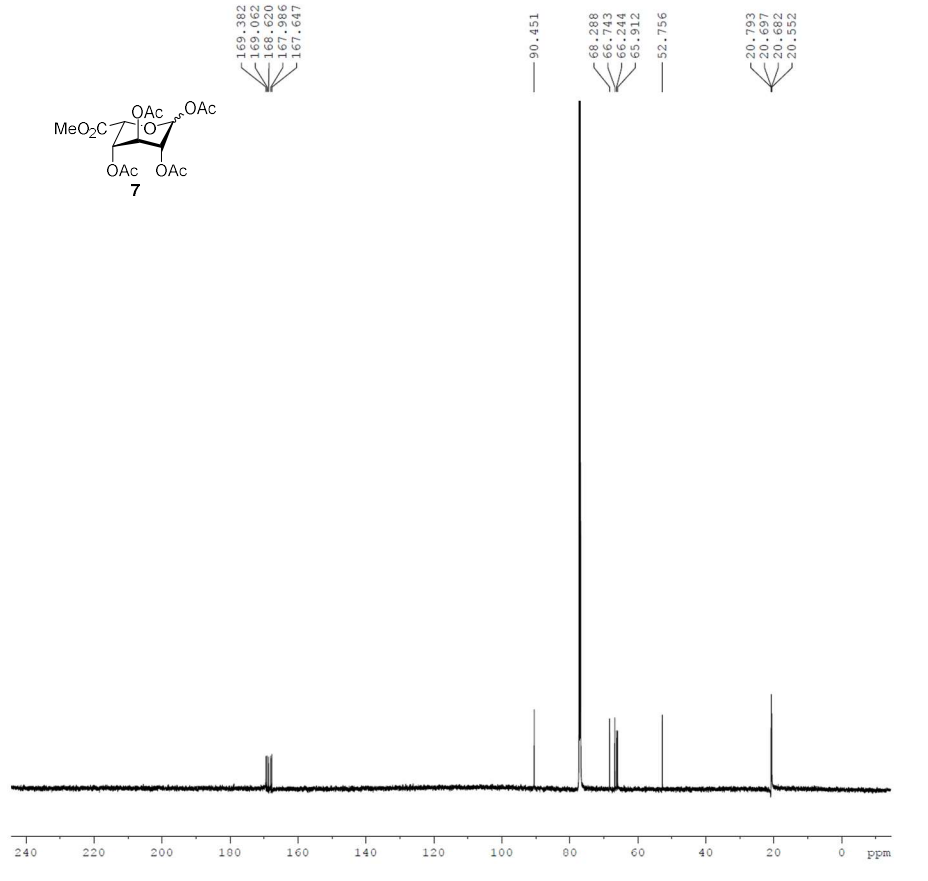


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PROCNO                       1

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TD                     131072
SOLVENT                 CDCl3
NS                        128
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FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                      2050
DW                    12.800 usec
DE                    21.00 usec
TE                    298.0 K
D1                2.00000000 sec
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TD0                          1

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PL1                      -1.82 dB
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SFO1             150.9201552 MHz

======== CHANNEL f2 ========
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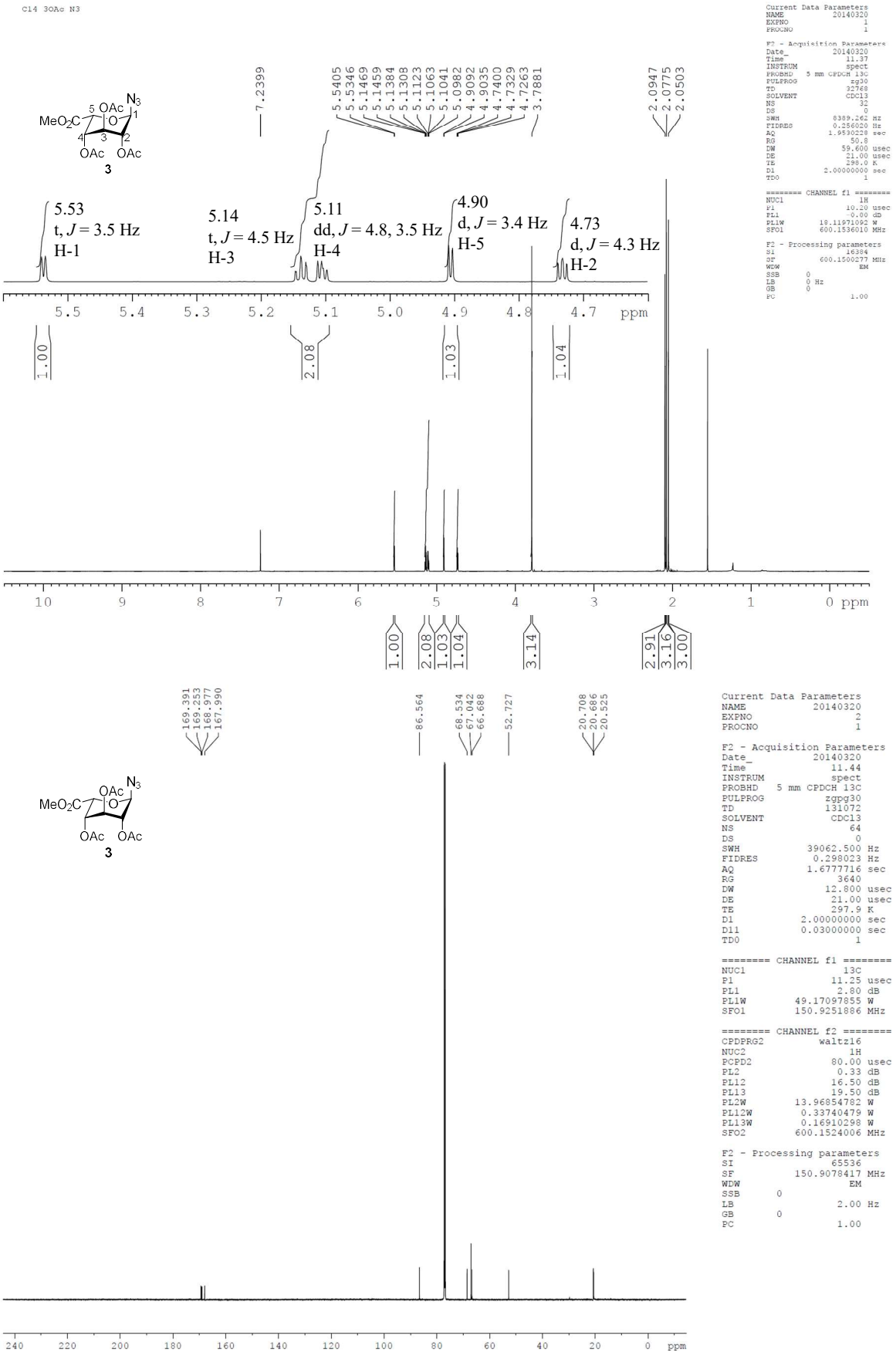
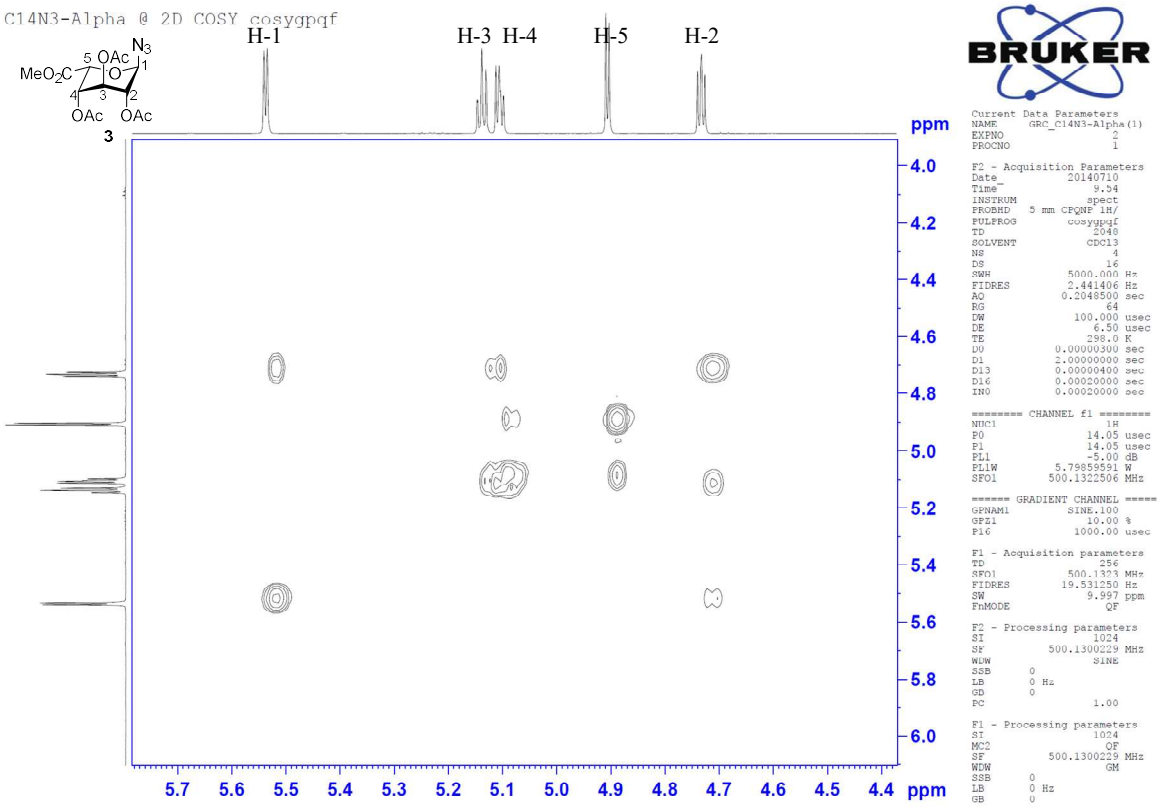
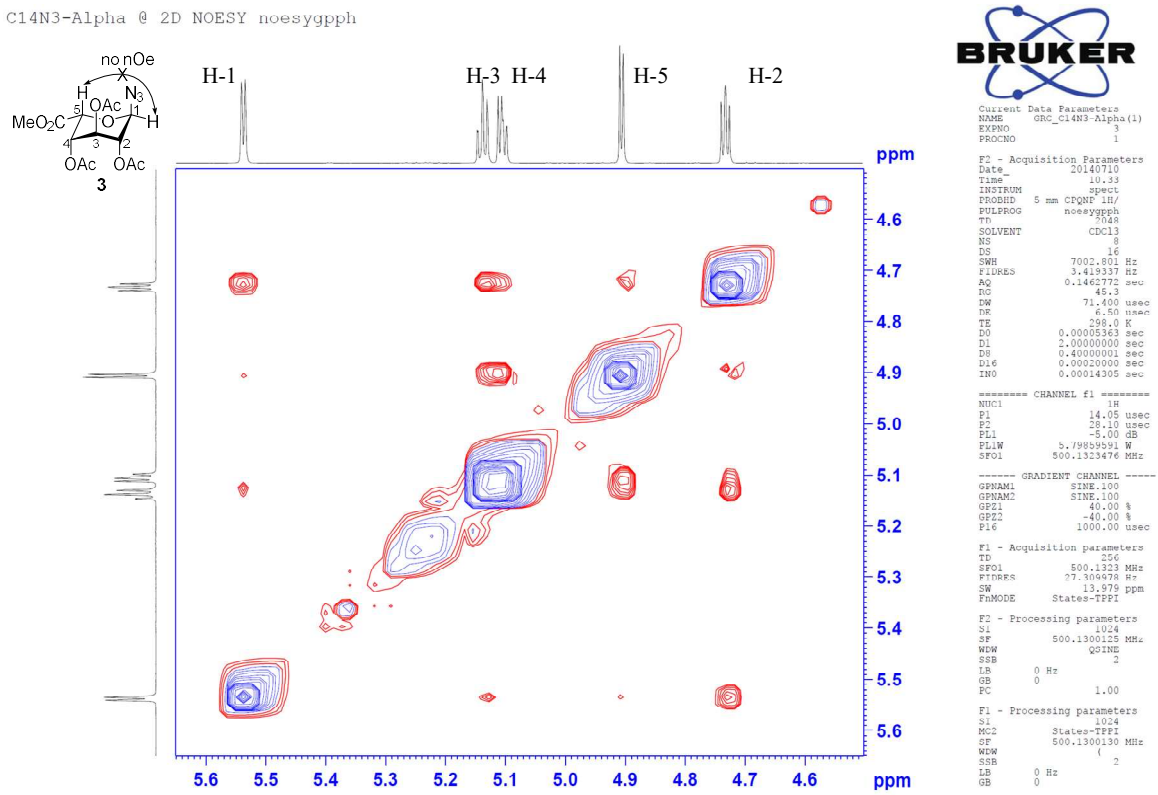
^{1}H NMR and ^{13}C NMR of compound **3** in $CDCl_3$

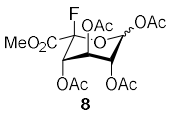


^{1}H 2D NMR of compound **3**

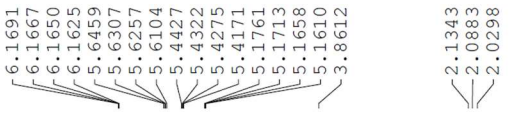




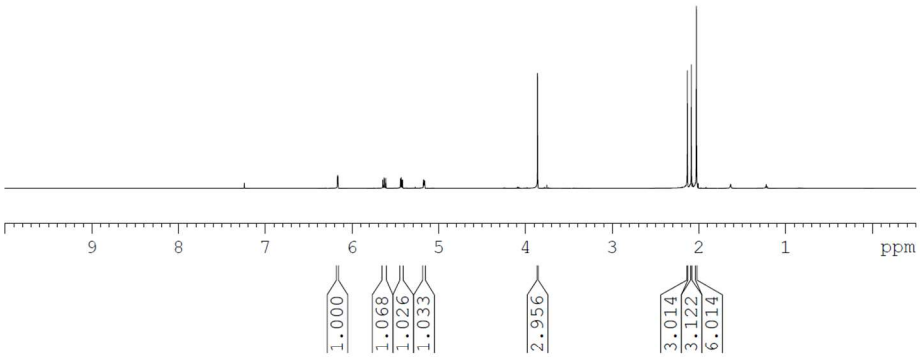
^{1}H NMR and ^{13}C NMR of compound **8** in $CDCl_3$

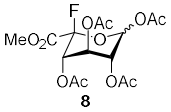


8




```
Current Data Parameters
NAME                  20140305
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140305
Time                     14.35
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                           18
DS                            0
SWH                  8389.262 Hz
FIDRES               0.256020 Hz
AQ                   1.9530228 sec
RG                           36
DW                     59.600 usec
DE                     21.00 usec
TE                     297.9 K
D1                   2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       10.20 usec
PL1                      -0.80 dB
PL1W                18.11971092 W
SFO1                600.1536010 MHz

F2 - Processing parameters
SI                       16384
SF                  600.1500278 MHz
WDW                         EM
SSB                  0
LB                   0 Hz
GB                   0
PC                           1.00
```

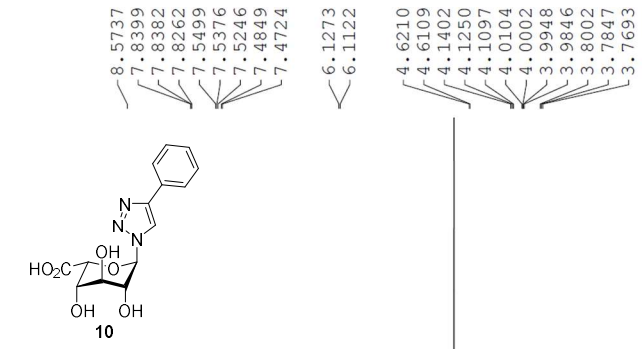


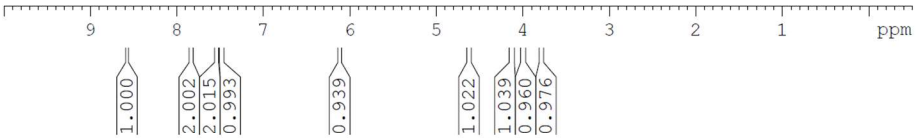


8

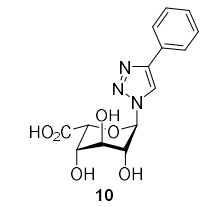
```
Current Data Parameters
NAME                  20140305
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140305
Time                     18.37
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                zgpg30
TD                     131072
SOLVENT                 CDCl3
NS                           32
DS                            0
SWH                39062.500 Hz
FIDRES               0.298023 Hz
AQ                   1.6777716 sec
RG                         3640
DW                     12.800 usec
DE                     21.00 usec
TE                     298.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       11.25 usec
PL1                       2.80 dB
PL1W                49.17097855 W
SFO1                150.9251886 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       0.33 dB
PL12                     16.50 dB
PL13                     19.50 dB
PL2W                13.96854782 W
PL12W                0.33740479 W
PL13W                0.16910298 W
SFO2                600.1524006 MHz

F2 - Processing parameters
SI                       65536
SF                  150.9078380 MHz
WDW                         EM
SSB                  0
LB                           2.00 Hz
GB                   0
PC                           1.00
```

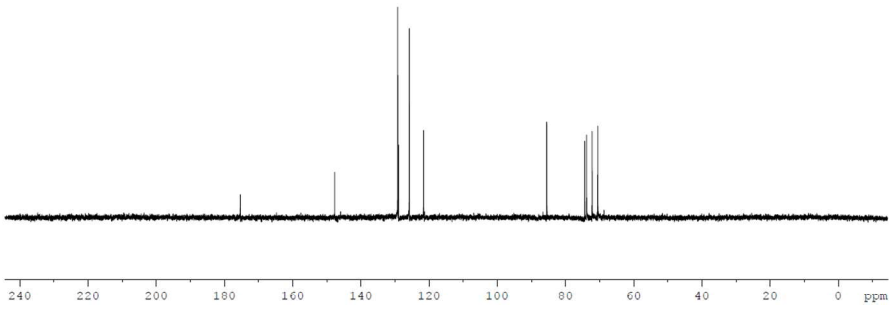
^{1}H NMR and ^{13}C NMR of compound **10** in D_2O





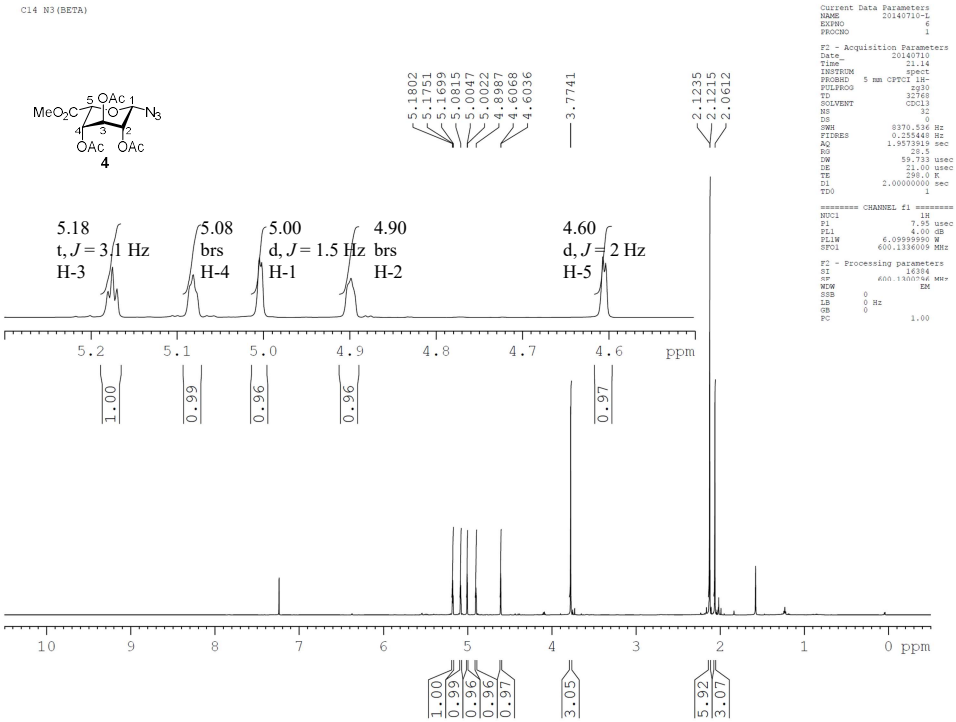

```
Current Data Parameters
NAME                  c14-ph
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140506
Time                  18.15
INSTRUM               spect
PROBHD    5 mm CPTCI 1H-
PULPROG                zg30
TD                    32768
SOLVENT                 D2O
NS                         18
DS                          0
SWH                8370.536 Hz
FIDRES            0.255448 Hz
AQ                1.9573919 sec
RG                      22.6
DW                    59.733 usec
DE                    21.00 usec
TE                    298.0 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                      7.95 usec
PL1                     4.00 dB
PL1W             6.09999990 W
SFO1            600.1336009 MHz

F2 - Processing parameters
SI                        16384
SF               600.1299450 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

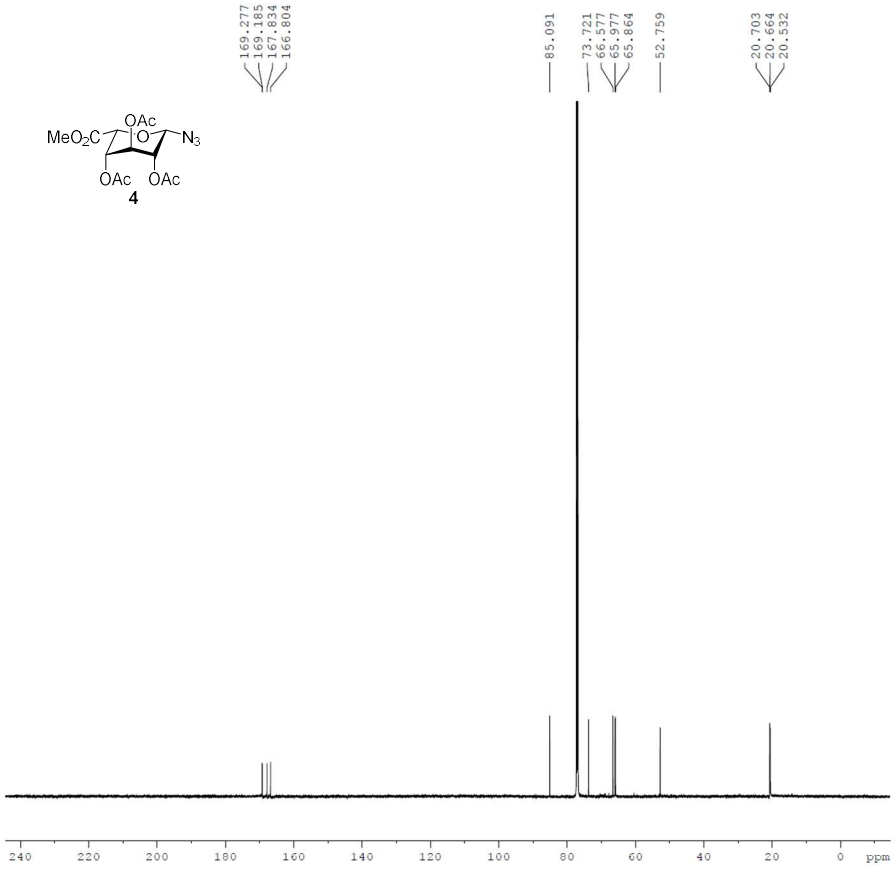





```
Current Data Parameters
NAME                  c14-ph
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140506
Time                  18.20
INSTRUM               spect
PROBHD    5 mm CPTCI 1H-
PULPROG              zgpg30
TD                   131072
SOLVENT                 D2O
NS                         64
DS                          0
SWH               39062.500 Hz
FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                      2050
DW                    12.800 usec
DE                    21.00 usec
TE                    298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                    10.05 usec
PL1                   -1.82 dB
PL1W            122.22216797 W
SFO1             150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 90.00 usec
PL2                     4.00 dB
PL12                   24.90 dB
PL13                   27.90 dB
PL2W             6.09999990 W
PL12W            0.04958267 W
PL13W            0.02485020 W
SFO2            600.1324005 MHz

F2 - Processing parameters
SI                        65536
SF               150.9028090 MHz
WDW                        EM
SSB          0
LB                    2.00 Hz
GB           0
PC                      1.00
```

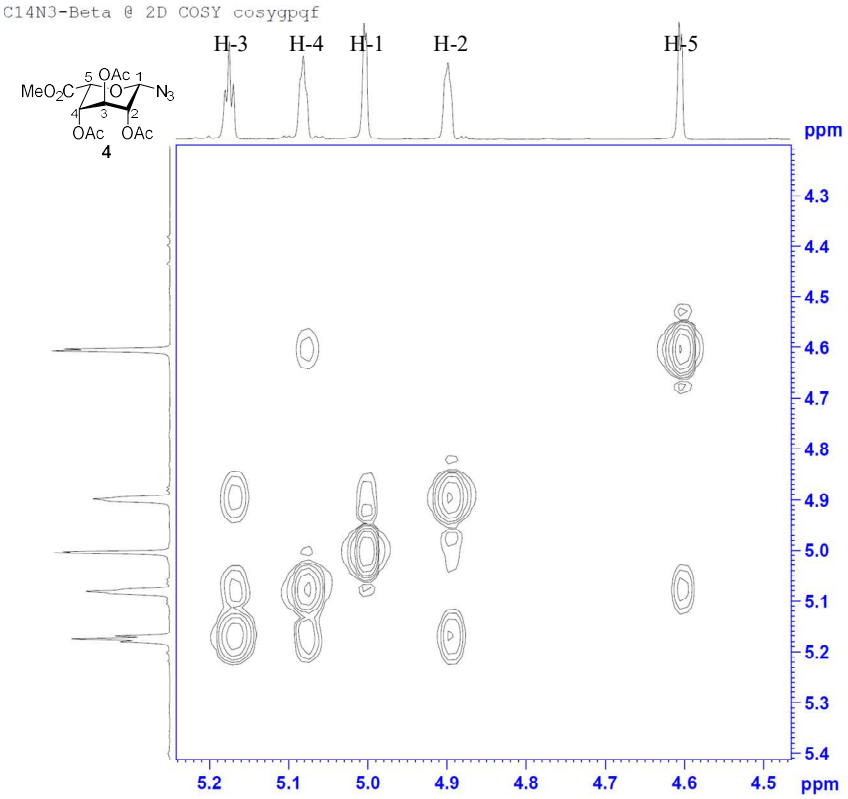
^{1}H NMR and ^{13}C NMR of compound **4** in $CDCl_3$

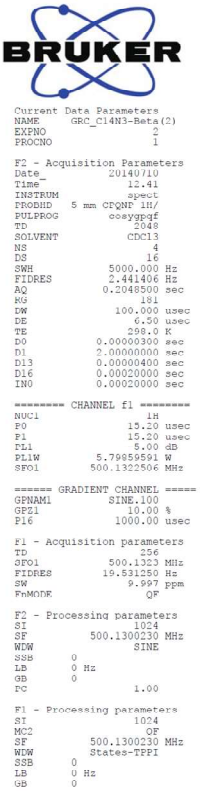


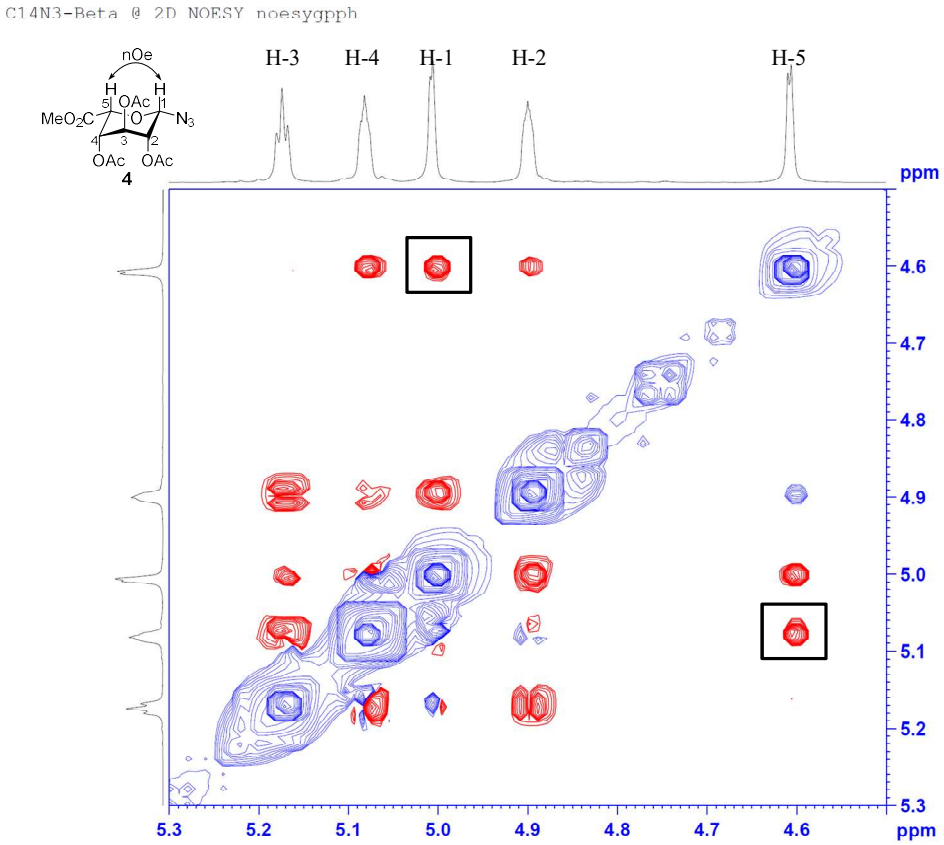


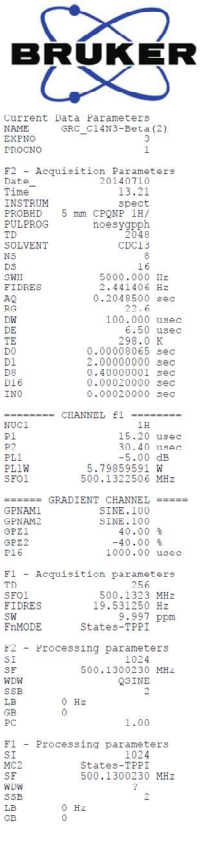

```
Current Data Parameters
NAME                  20140710-L
EXPNO                         7
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20140710
Time                     21.26
INSTRUM                  spect
PROBHD    5 mm CPTCI 1H-
PULPROG                 zgpg30
TD                      131072
SOLVENT                  CDCl3
NS                         128
DS                           0
SWH                  39062.500 Hz
FIDRES                0.298023 Hz
AQ                    1.6777716 sec
RG                         2050
DW                       12.800 usec
DE                       21.00 usec
TE                       298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                       10.05 usec
PL1                      -1.82 dB
PL1W               122.22216797 W
SFO1                150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                       4.00 dB
PL12                     24.90 dB
PL13                     27.90 dB
PL2W                6.09999990 W
PL12W               0.04958267 W
PL13W               0.02485020 W
SFO2                600.1324005 MHz

F2 - Processing parameters
SI                        65536
SF                  150.9028090 MHz
WDW                          EM
SSB                  0
LB                        2.00 Hz
GB                   0
PC                        1.00
```

^{1}H 2D NMR of compound **4**



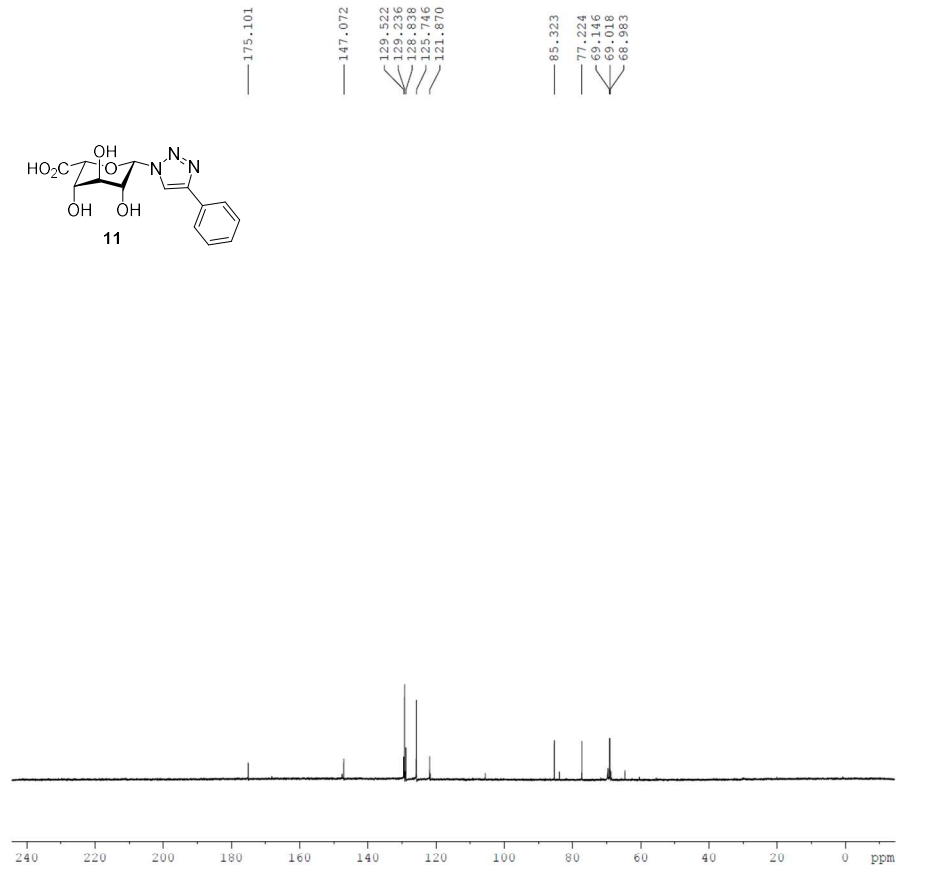






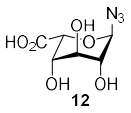
^{1}H NMR and ^{13}C NMR of compound **11** in D_2O


```
Current Data Parameters
NAME                  20140630
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140630
Time                     11.39
INSTRUM                  spect
PROBHD     5 mm CPTCI 1H-
PULPROG                  zg30
TD                      32768
SOLVENT                   D2O
NS                           64
DS                            0
SWH                  8370.536 Hz
FIDRES               0.255448 Hz
AQ                   1.9573919 sec
RG                          36
DW                      59.733 usec
DE                      21.00 usec
TE                      298.0 K
D1                   2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                         1H
P1                       7.95 usec
PL1                      4.00 dB
PL1W                6.09999990 W
SFO1               600.1336009 MHz

F2 - Processing parameters
SI                       16384
SF                 600.1299519 MHz
WDW                         EM
SSB                  0
LB                   0 Hz
GB                   0
PC                        1.00
```

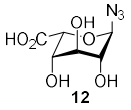



```
Current Data Parameters
NAME                  20140630
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140630
Time                     23.28
INSTRUM                  spect
PROBHD     5 mm CPTCI 1H-
PULPROG                zgpg30
TD                     131072
SOLVENT                   D2O
NS                         2048
DS                            0
SWH                39062.500 Hz
FIDRES               0.298023 Hz
AQ                   1.6777716 sec
RG                         2050
DW                      12.800 usec
DE                      21.00 usec
TE                      297.9 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                       10.05 usec
PL1                      -1.82 dB
PL1W              122.22216797 W
SFO1               150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                         1H
PCPD2                    90.00 usec
PL2                       4.00 dB
PL12                     24.90 dB
PL13                     27.90 dB
PL2W                6.09999990 W
PL12W               0.04958267 W
PL13W               0.02485020 W
SFO2               600.1324005 MHz

F2 - Processing parameters
SI                       65536
SF                 150.9028090 MHz
WDW                         EM
SSB                  0
LB                        2.00 Hz
GB                   0
PC                        1.00
```

^{1}H NMR and ^{13}C NMR of compound **12** in D_2O

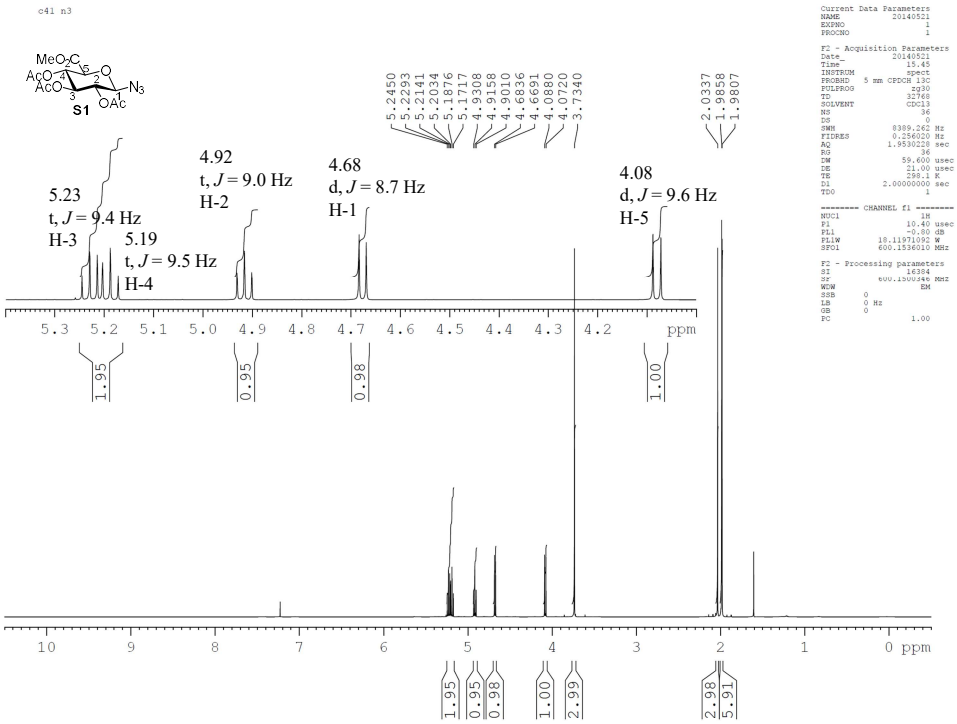


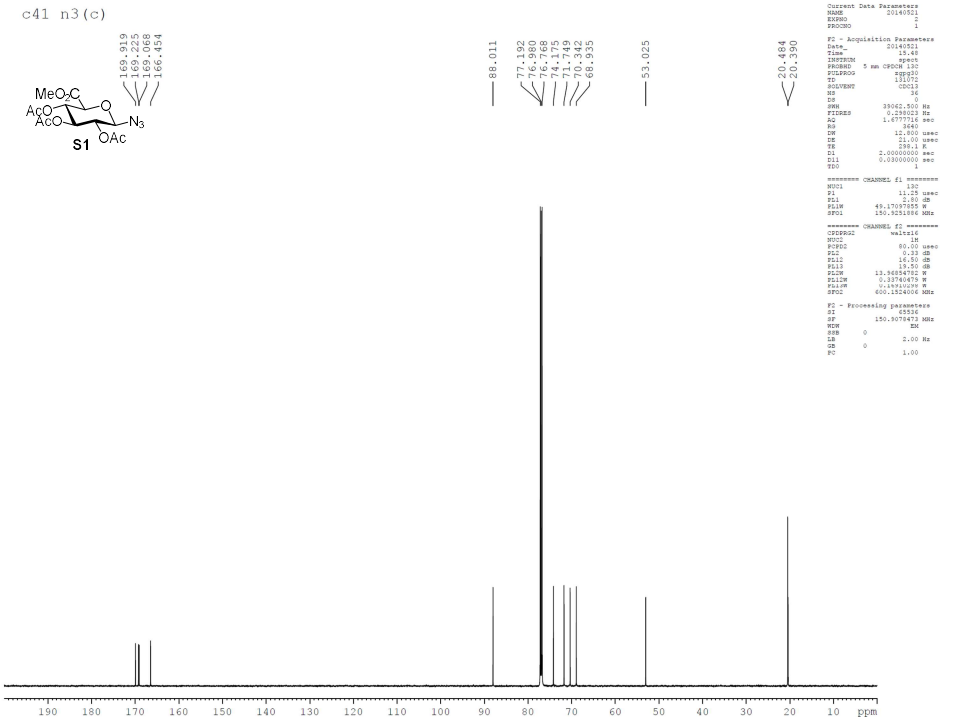

```
Current Data Parameters
NAME                  20140321
EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140321
Time                     20.06
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                  zg30
TD                      32768
SOLVENT                   D2O
NS                           32
DS                            0
SWH                   8389.262 Hz
FIDRES                0.256020 Hz
AQ                    1.953228 sec
RG                           28.5
DW                       59.600 usec
DE                       21.00 usec
TE                       298.0 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                         1H
P1                       10.20 usec
PL1                      -0.80 dB
PL1W                18.11971092 W
SFO1                600.1536010 MHz

F2 - Processing parameters
SI                       16384
SF                  600.1499441 MHz
WDW                         EM
SSB                  0
LB                   0 Hz
GB                   0
PC                        1.00
```



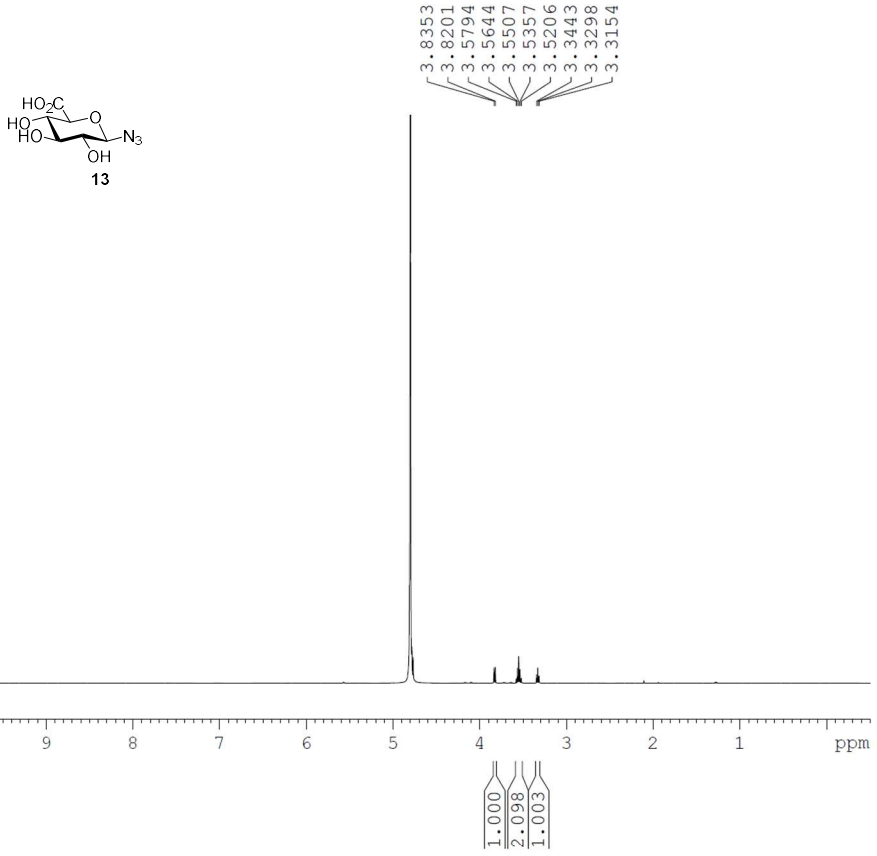

```
Current Data Parameters
NAME                  20140321
EXPNO                        8
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140321
Time                     20.51
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                zgpg30
TD                      131072
SOLVENT                   D2O
NS                          256
DS                            0
SWH                39062.500 Hz
FIDRES                0.298023 Hz
AQ                    1.6777716 sec
RG                         3640
DW                       12.800 usec
DE                       21.00 usec
TE                       297.9 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                       11.25 usec
PL1                       2.80 dB
PL1W                49.17097855 W
SFO1                150.9251886 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                         1H
PCPD2                    80.00 usec
PL2                       0.33 dB
PL12                     16.50 dB
PL13                     19.50 dB
PL2W                13.96854782 W
PL12W                0.33740479 W
PL13W                0.16910298 W
SFO2                600.1524006 MHz

F2 - Processing parameters
SI                       65536
SF                  150.9078380 MHz
WDW                         EM
SSB                  0
LB                        2.00 Hz
GB                   0
PC                        1.00
```

^{1}H NMR and ^{13}C NMR of compound **S1** in $CDCl_3$

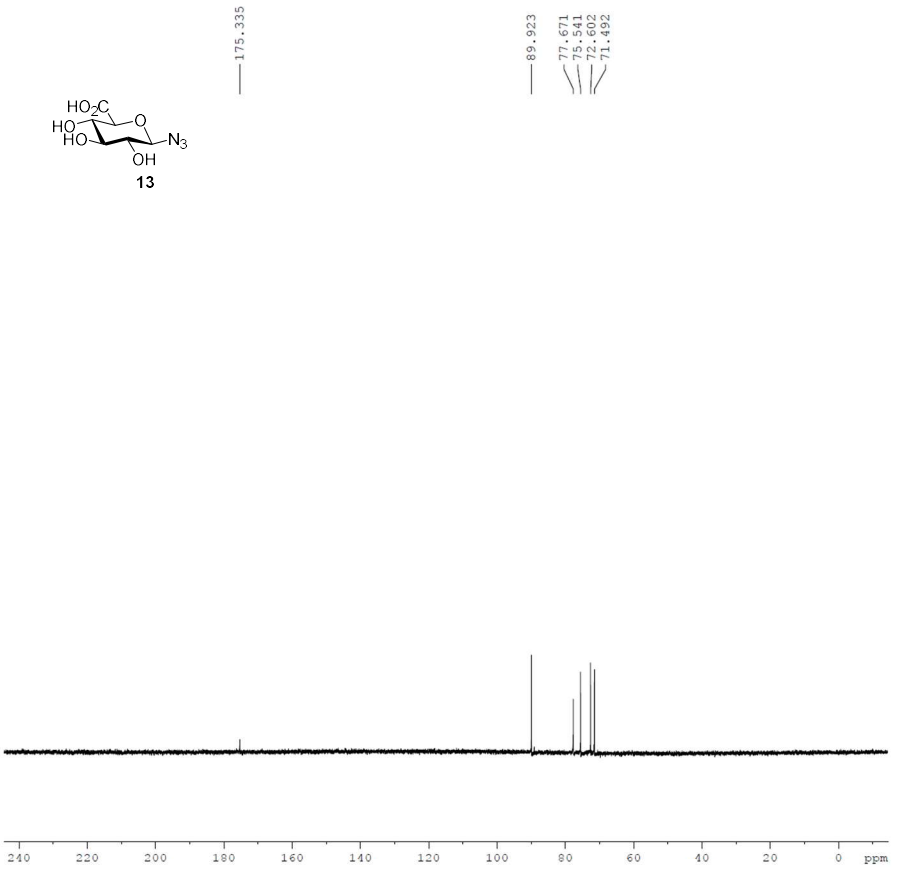




^{1}H NMR and ^{13}C NMR of compound **13** in D_2O

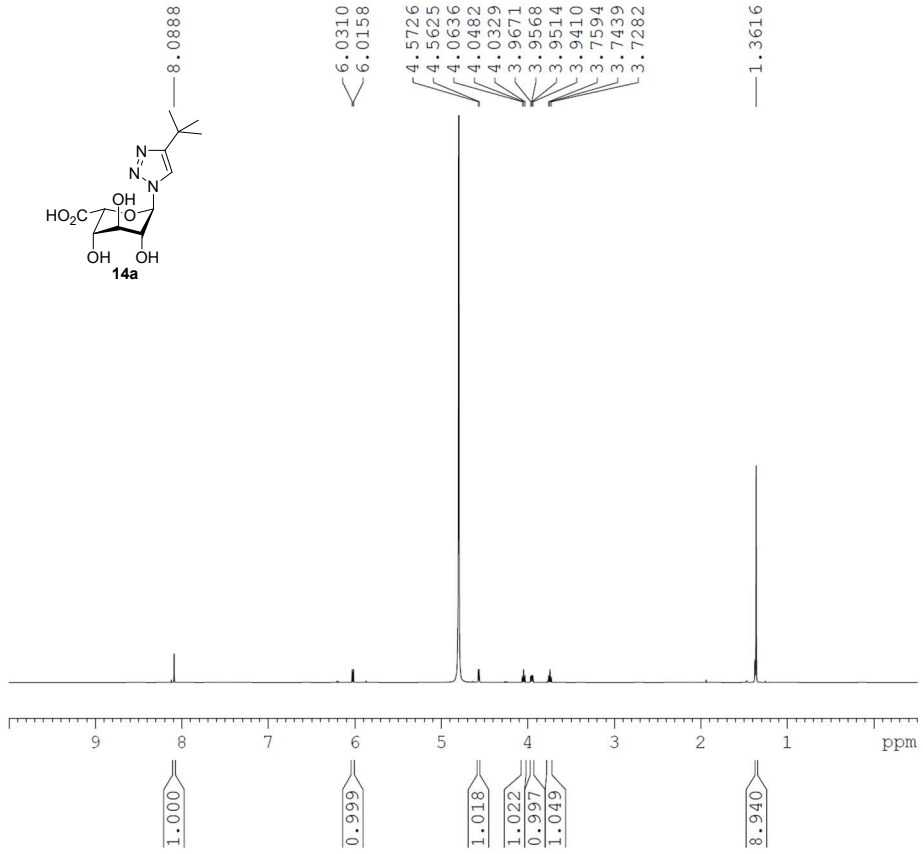



```
Current Data Parameters
NAME                  c41 n3
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140506
Time                  17.49
INSTRUM               spect
PROBHD    5 mm CPTCI 1H-
PULPROG                zg30
TD                    32768
SOLVENT                 D2O
NS                         18
DS                          0
SWH               8370.536 Hz
FIDRES            0.255448 Hz
AQ                1.9573919 sec
RG                      25.4
DW                    59.733 usec
DE                    21.00 usec
TE                    298.0 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                      7.95 usec
PL1                     4.00 dB
PL1W            6.09999990 W
SFO1           600.1336009 MHz

F2 - Processing parameters
SI                        16384
SF              600.1299421 MHz
WDW                       EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

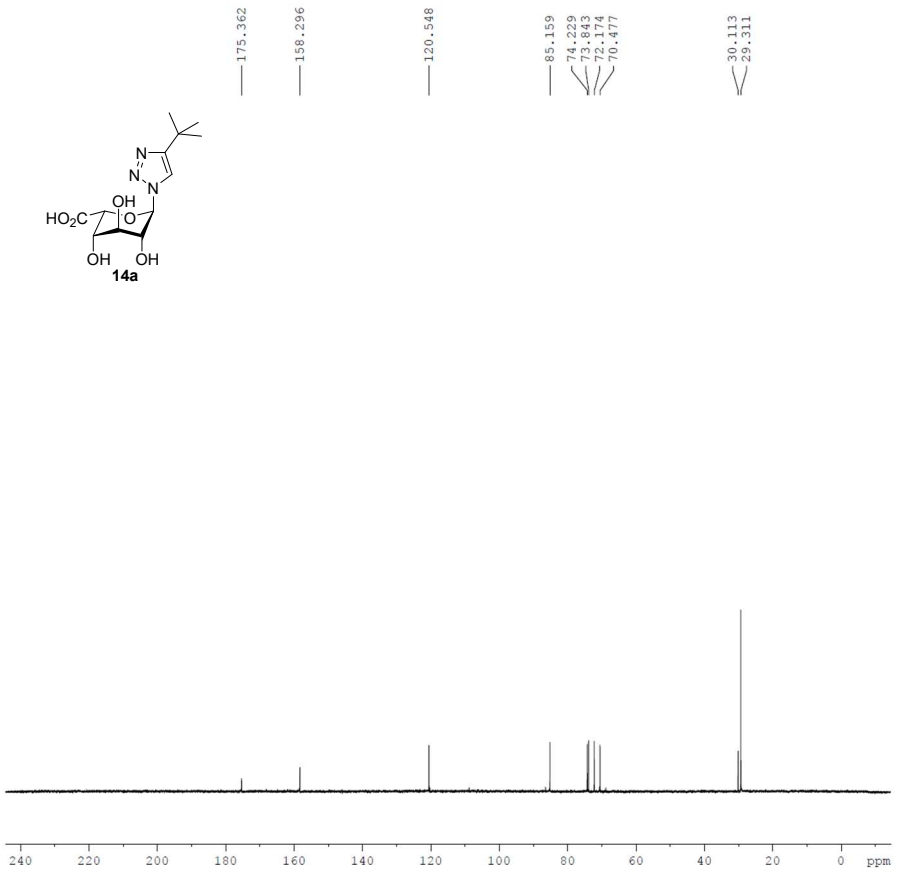



```
Current Data Parameters
NAME                  c41 n3
EXPNO                      6
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140506
Time                  17.54
INSTRUM               spect
PROBHD    5 mm CPTCI 1H-
PULPROG             zgpg30
TD                   131072
SOLVENT                 D2O
NS                         64
DS                          0
SWH              39062.500 Hz
FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                      2050
DW                   12.800 usec
DE                    21.00 usec
TE                    298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                    10.05 usec
PL1                   -1.82 dB
PL1W          122.22216797 W
SFO1           150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                 90.00 usec
PL2                     4.00 dB
PL12                   24.90 dB
PL13                   27.90 dB
PL2W            6.09999990 W
PL12W           0.04958267 W
PL13W           0.02485020 W
SFO2           600.1324005 MHz

F2 - Processing parameters
SI                        65536
SF              150.9028090 MHz
WDW                       EM
SSB          0
LB                    2.00 Hz
GB           0
PC                      1.00
```

^{1}H NMR and ^{13}C NMR of compound **14a** in D_2O

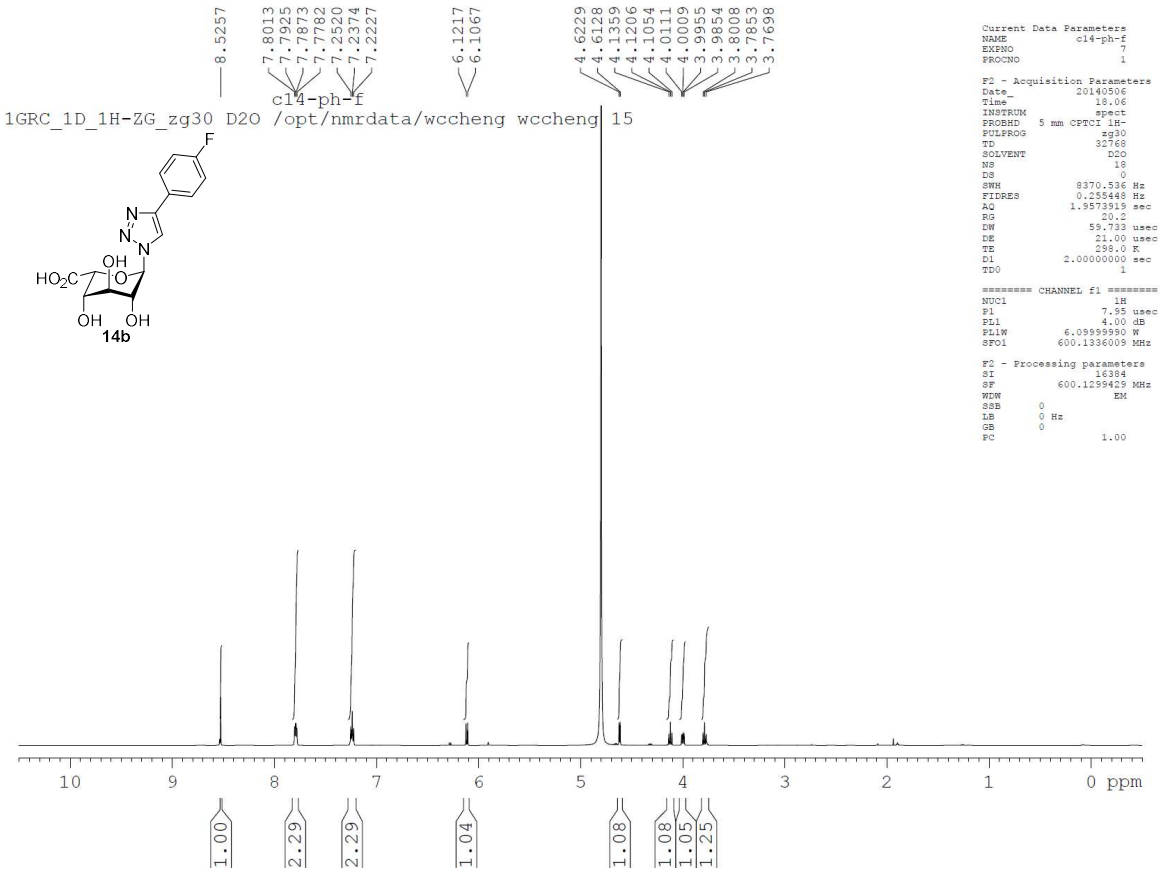


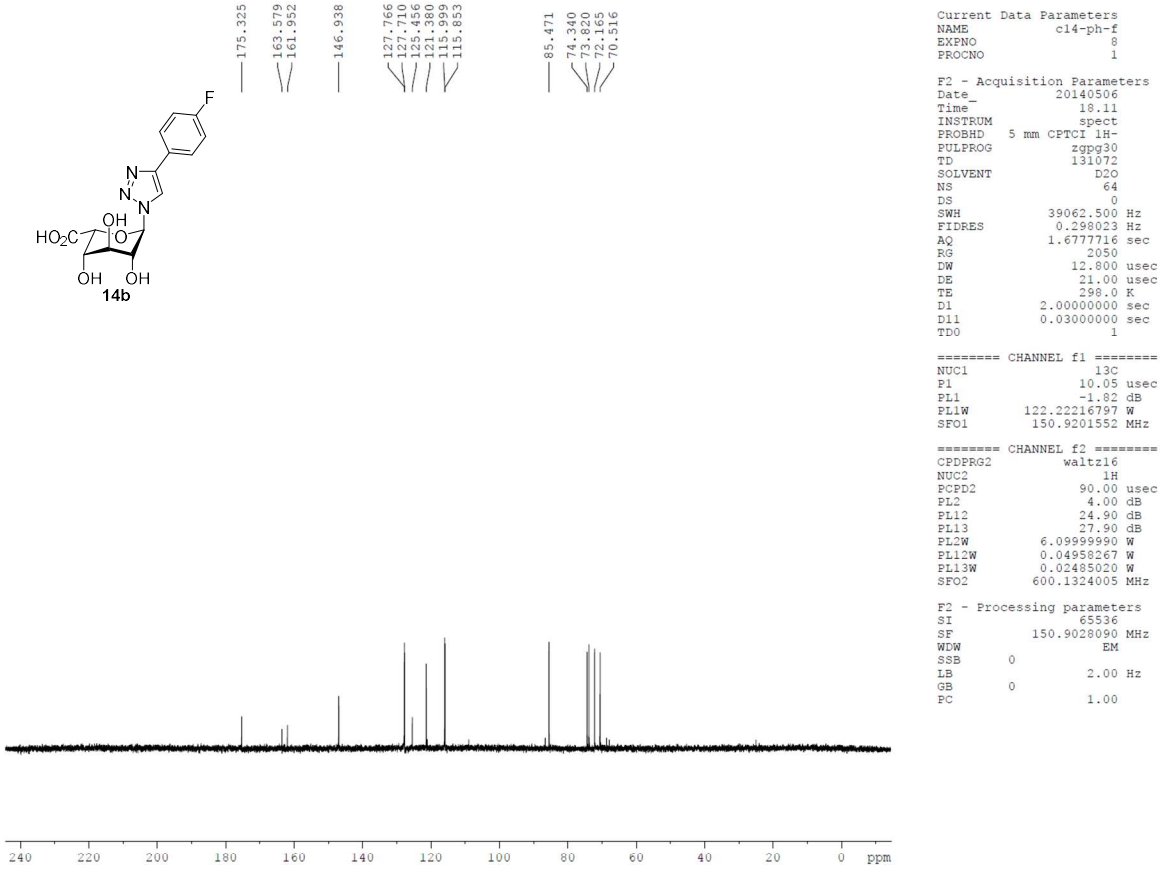

```
Current Data Parameters
NAME                  c14+
EXPNO                   12
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140506
Time                 18.23
INSTRUM              spect
PROBHD   5 mm CPTCI 1H-
PULPROG              zg30
TD                  32768
SOLVENT               D2O
NS                       18
DS                        0
SWH               8370.536 Hz
FIDRES               0.255448 Hz
AQ                1.9573919 sec
RG                       22.6
DW                   59.733 usec
DE                   21.00 usec
TE                   298.0 K
D1                2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                    7.95 usec
PL1                   4.00 dB
PL1W            6.09999990 W
SFO1           600.1336009 MHz

F2 - Processing parameters
SI                      16384
SF              600.1299432 MHz
WDW                     EM
SSB          0
LB           0 Hz
GB           0
PC                    1.00
```



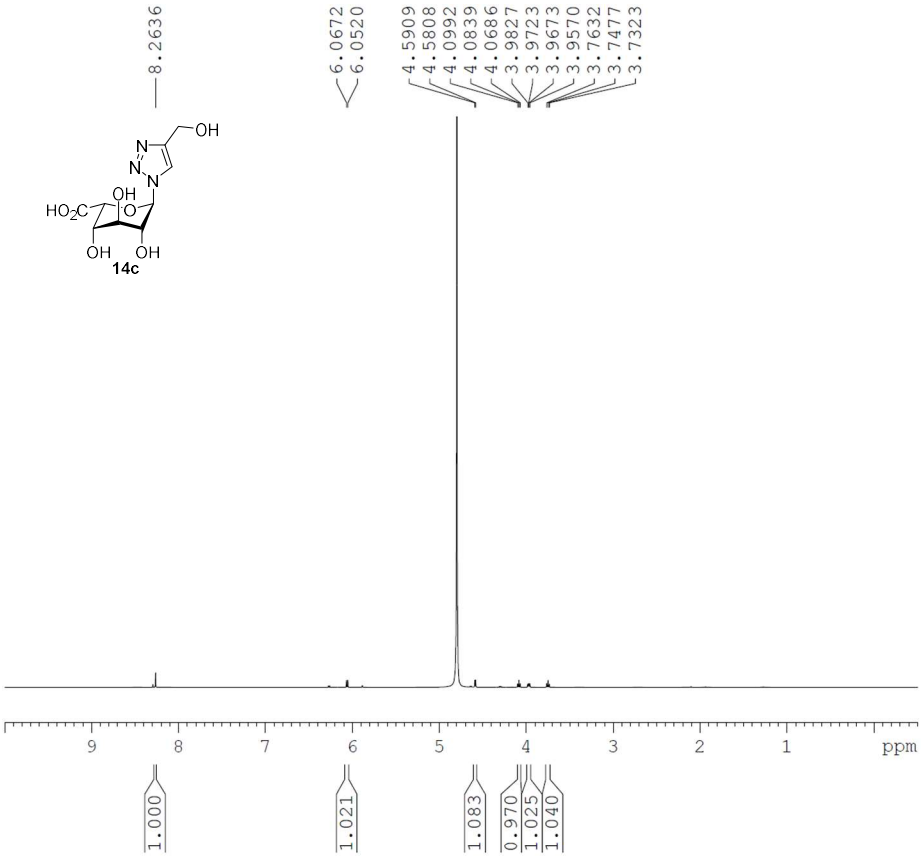

```
Current Data Parameters
NAME                  c14+
EXPNO                   14
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140506
Time                 18.28
INSTRUM              spect
PROBHD   5 mm CPTCI 1H-
PULPROG            zgpg30
TD                  131072
SOLVENT               D2O
NS                       64
DS                        0
SWH              39062.500 Hz
FIDRES               0.298023 Hz
AQ                1.6777716 sec
RG                     2050
DW                   12.800 usec
DE                   21.00 usec
TE                   298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.05 usec
PL1                  -1.82 dB
PL1W          122.22216797 W
SFO1           150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   4.00 dB
PL12                 24.90 dB
PL13                 27.90 dB
PL2W            6.09999990 W
PL12W           0.04958267 W
PL13W           0.02485020 W
SFO2           600.1324005 MHz

F2 - Processing parameters
SI                      65536
SF              150.9028090 MHz
WDW                     EM
SSB          0
LB                    2.00 Hz
GB           0
PC                    1.00
```

^{1}H NMR and ^{13}C NMR of compound **14b** in D_2O

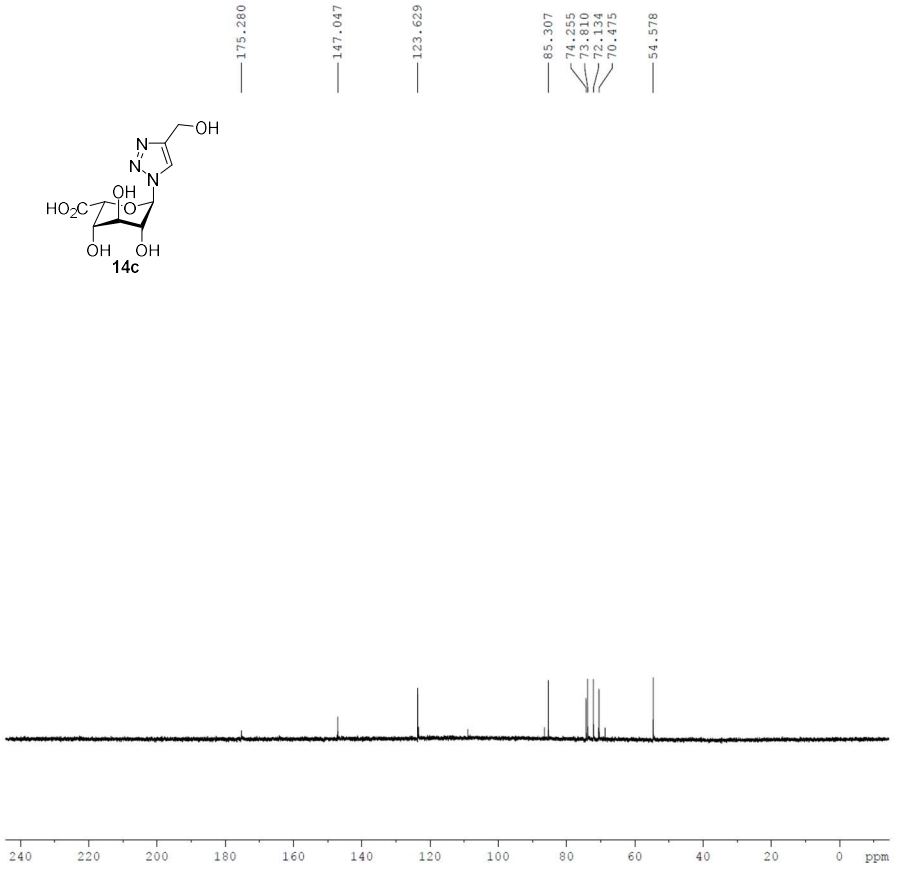




^{1}H NMR and ^{13}C NMR of compound **14c** in D_2O

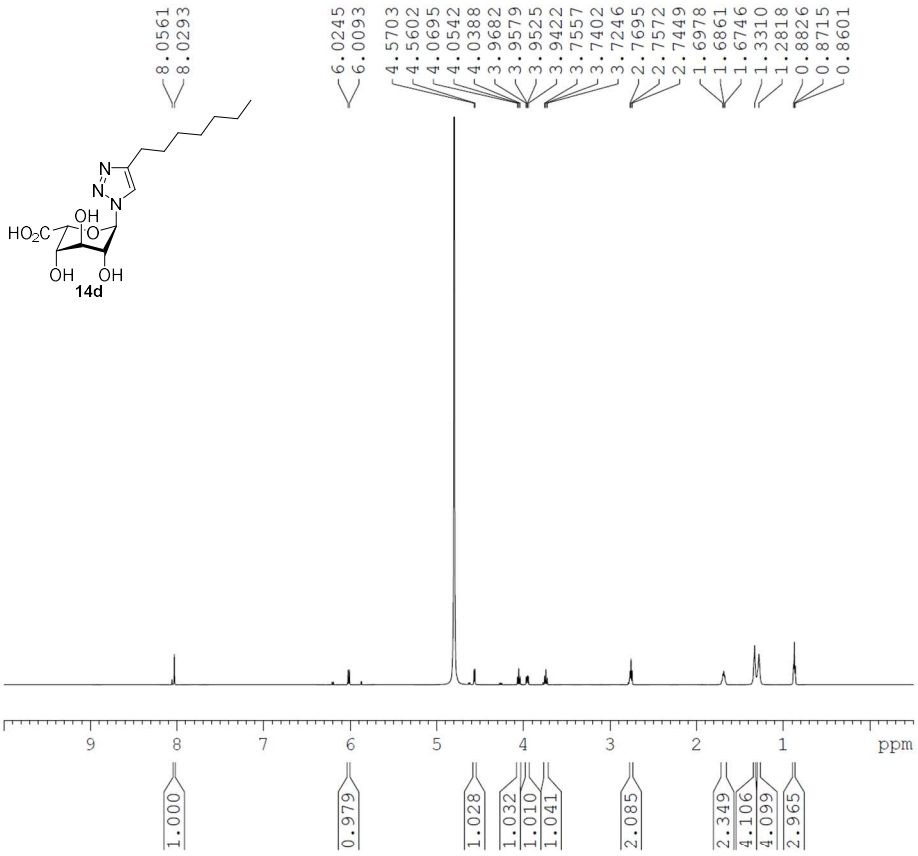



```
Current Data Parameters
NAME                  c14-oh
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140506
Time                  17.57
INSTRUM               spect
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                    32768
SOLVENT                 D2O
NS                         8
DS                         0
SWH                8370.536 Hz
FIDRES            0.255448 Hz
AQ                1.9573919 sec
RG                      25.4
DW                  59.733 usec
DE                  21.00 usec
TE                  298.0 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     7.95 usec
PL1                    4.00 dB
PL1W            6.09999990 W
SFO1           600.1336009 MHz

F2 - Processing parameters
SI                        16384
SF               600.1299442 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

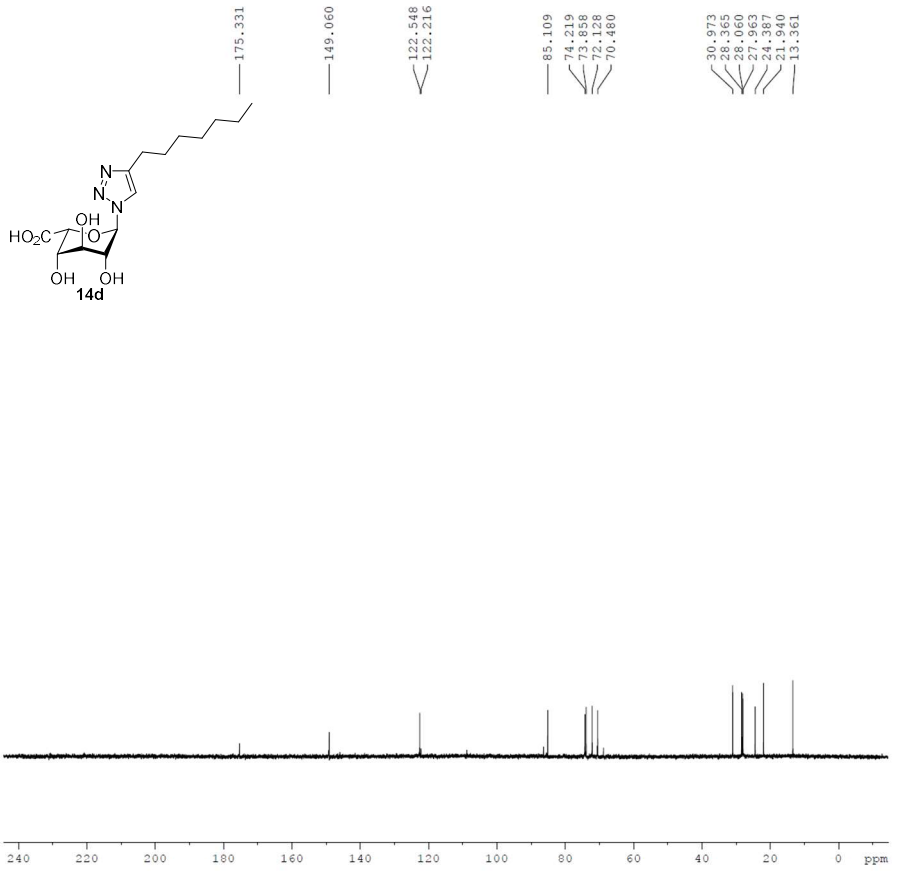



```
Current Data Parameters
NAME                  c14-oh
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140506
Time                  18.02
INSTRUM               spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zgpg30
TD                   131072
SOLVENT                 D2O
NS                        64
DS                         0
SWH               39062.500 Hz
FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                      2050
DW                  12.800 usec
DE                  21.00 usec
TE                  298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                    10.05 usec
PL1                   -1.82 dB
PL1W           122.22216797 W
SFO1            150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 90.00 usec
PL2                    4.00 dB
PL12                  24.90 dB
PL13                  27.90 dB
PL2W            6.09999990 W
PL12W           0.04958267 W
PL13W           0.02485020 W
SFO2           600.1324005 MHz

F2 - Processing parameters
SI                        65536
SF               150.9028090 MHz
WDW                        EM
SSB          0
LB                     2.00 Hz
GB           0
PC                      1.00
```

^{1}H NMR and ^{13}C NMR of compound **14d** in D_2O

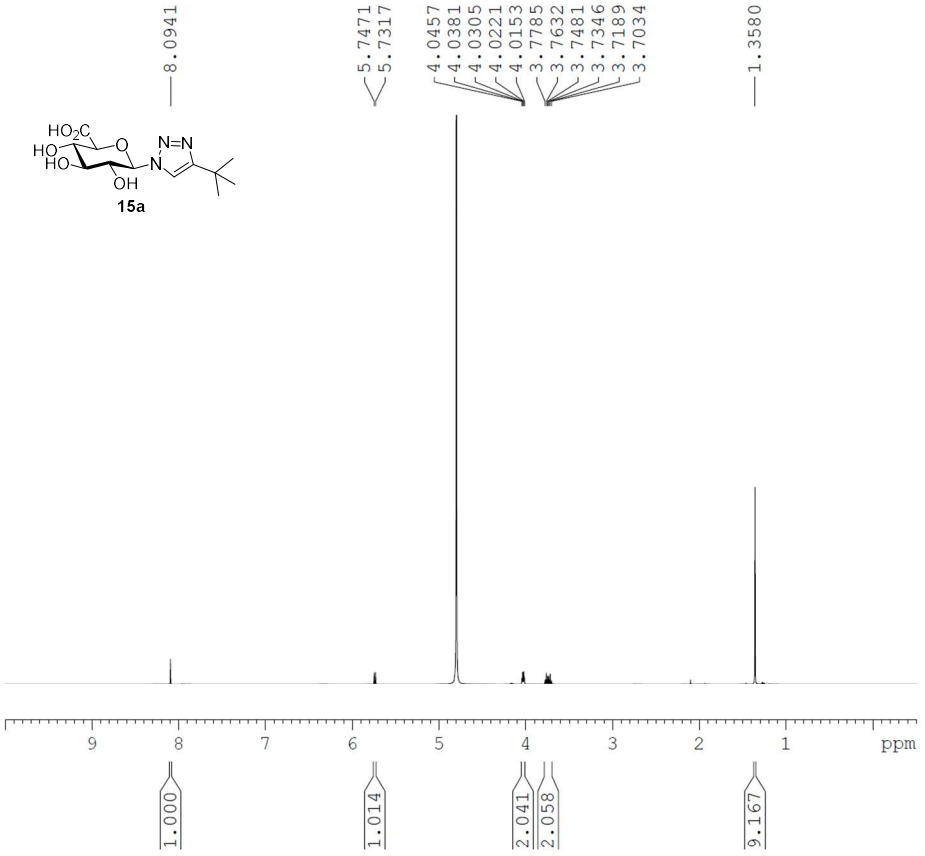



```
Current Data Parameters
NAME                  cl4more c
EXPNO                        15
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20140506
Time                     18.32
INSTRUM                  spect
PROBHD    5 mm CPTCI 1H-
PULPROG                  zg30
TD                      32768
SOLVENT                   D2O
NS                           18
DS                            0
SWH                   8370.536 Hz
FIDRES                0.255448 Hz
AQ                    1.9573919 sec
RG                           20.2
DW                       59.733 usec
DE                       21.00 usec
TE                       298.0 K
D1                    2.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        7.95 usec
PL1                       4.00 dB
PL1W                 6.09999990 W
SFO1                600.1336009 MHz

F2 - Processing parameters
SI                           16384
SF                  600.1299434 MHz
WDW                             EM
SSB                  0
LB                   0 Hz
GB                   0
PC                            1.00
```

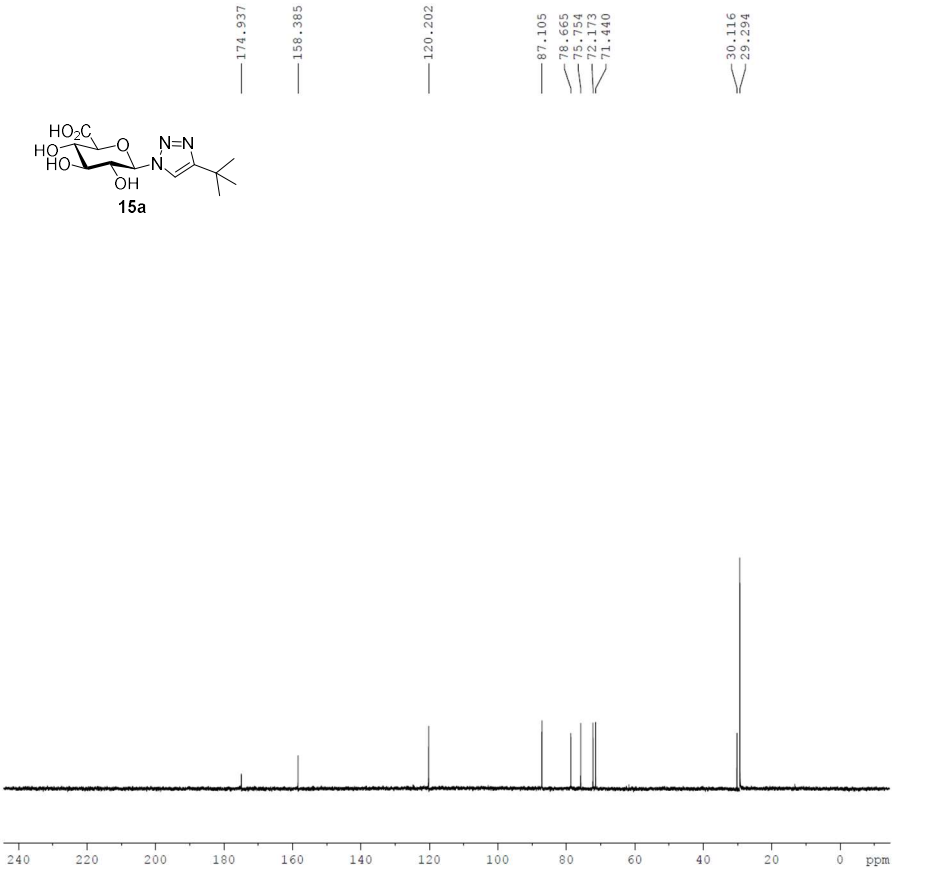



```
Current Data Parameters
NAME                  cl4more c
EXPNO                        17
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20140506
Time                     18.37
INSTRUM                  spect
PROBHD    5 mm CPTCI 1H-
PULPROG                zgpg30
TD                      131072
SOLVENT                   D2O
NS                           64
DS                            0
SWH                39062.500 Hz
FIDRES                0.298023 Hz
AQ                    1.6777716 sec
RG                         2050
DW                       12.800 usec
DE                       21.00 usec
TE                       298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                       10.05 usec
PL1                      -1.82 dB
PL1W             122.22216797 W
SFO1              150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                         1H
PCPD2                    90.00 usec
PL2                       4.00 dB
PL12                     24.90 dB
PL13                     27.90 dB
PL2W                 6.09999990 W
PL12W                0.04958267 W
PL13W                0.02485020 W
SFO2                600.1324005 MHz

F2 - Processing parameters
SI                           65536
SF                  150.9028090 MHz
WDW                             EM
SSB                  0
LB                        2.00 Hz
GB                   0
PC                            1.00
```

^{1}H NMR and ^{13}C NMR of compound **15a** in D_2O

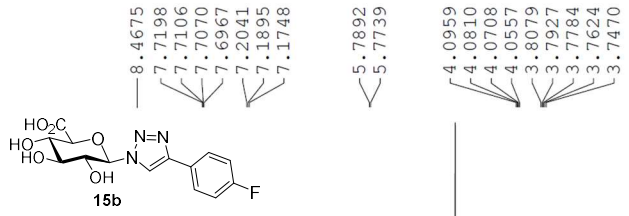


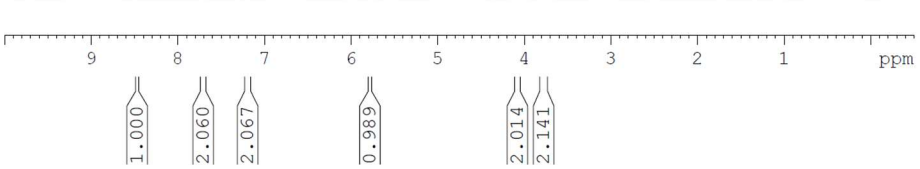

```
Current Data Parameters
NAME                  c41+
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140506
Time                 17.40
INSTRUM              spect
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  32768
SOLVENT               D2O
NS                       18
DS                        0
SWH               8370.536 Hz
FIDRES            0.255448 Hz
AQ                1.9573919 sec
RG                     22.6
DW                  59.733 usec
DE                  21.00 usec
TE                  298.0 K
D1                2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   7.95 usec
PL1                  4.00 dB
PL1W            6.09999990 W
SFO1           600.1336009 MHz

F2 - Processing parameters
SI                      16384
SF              600.1299429 MHz
WDW                     EM
SSB          0
LB           0 Hz
GB           0
PC                    1.00
```



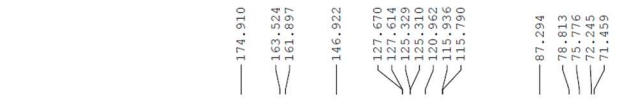

```
Current Data Parameters
NAME                  c41+
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140506
Time                 17.45
INSTRUM              spect
PROBHD    5 mm CPTCI 1H-
PULPROG            zgpg30
TD                 131072
SOLVENT               D2O
NS                       64
DS                        0
SWH              39062.500 Hz
FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                     2050
DW                  12.800 usec
DE                  21.00 usec
TE                  298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  10.05 usec
PL1                 -1.82 dB
PL1W       122.22216797 W
SFO1        150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   4.00 dB
PL12                 24.90 dB
PL13                 27.90 dB
PL2W            6.09999990 W
PL12W           0.04958267 W
PL13W           0.02485020 W
SFO2           600.1324005 MHz

F2 - Processing parameters
SI                      65536
SF              150.9028090 MHz
WDW                     EM
SSB          0
LB                    2.00 Hz
GB           0
PC                    1.00
```

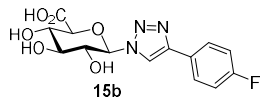
^{1}H NMR and ^{13}C NMR of compound **15b** in D_2O



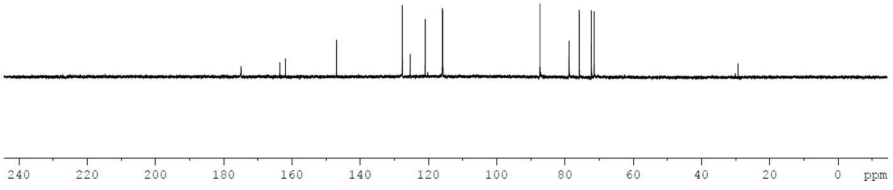



```
Current Data Parameters
NAME                  c41ph-f
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140506
Time                  17.31
INSTRUM               spect
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                    32768
SOLVENT                 D2O
NS                       18
DS                        0
SWH                8370.536 Hz
FIDRES            0.255448 Hz
AQ                1.9573919 sec
RG                     40.3
DW                   59.733 usec
DE                    21.00 usec
TE                    298.0 K
D1                2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                     1H
P1                     7.95 usec
PL1                    4.00 dB
PL1W            6.09999990 W
SFO1           600.1336009 MHz

F2 - Processing parameters
SI                      16384
SF              600.1299446 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```



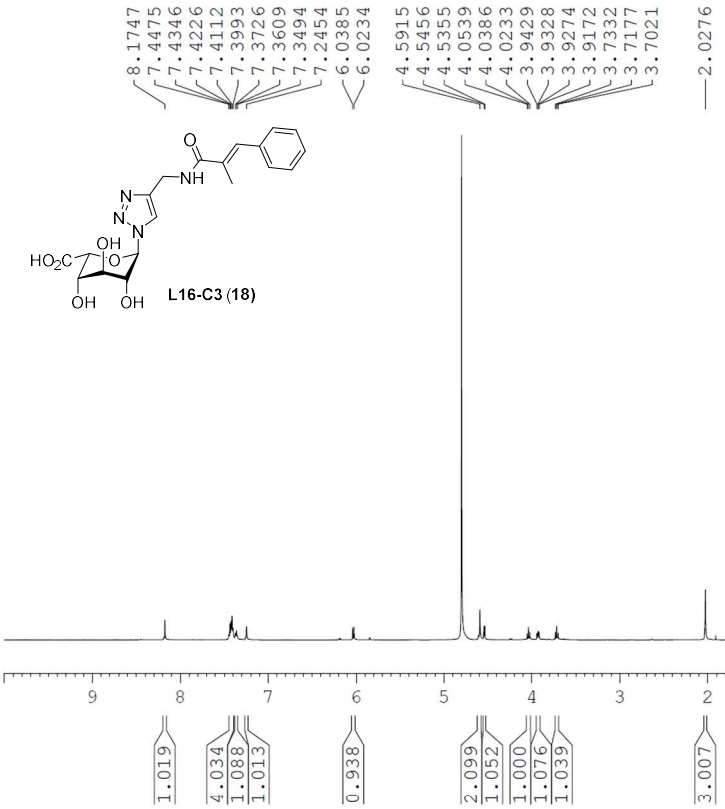



```
Current Data Parameters
NAME                  c41ph-f
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140506
Time                  17.37
INSTRUM               spect
PROBHD   5 mm CPTCI 1H-
PULPROG              zgpg30
TD                   131072
SOLVENT                 D2O
NS                       64
DS                        0
SWH               39062.500 Hz
FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                     2050
DW                   12.800 usec
DE                    21.00 usec
TE                    297.9 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                    13C
P1                    10.05 usec
PL1                   -1.82 dB
PL1W           122.22216797 W
SFO1           150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 90.00 usec
PL2                    4.00 dB
PL12                  24.90 dB
PL13                  27.90 dB
PL2W            6.09999990 W
PL12W           0.04958267 W
PL13W           0.02485020 W
SFO2           600.1324005 MHz

F2 - Processing parameters
SI                      65536
SF              150.9028090 MHz
WDW                        EM
SSB          0
LB                     2.00 Hz
GB           0
PC                     1.00
```



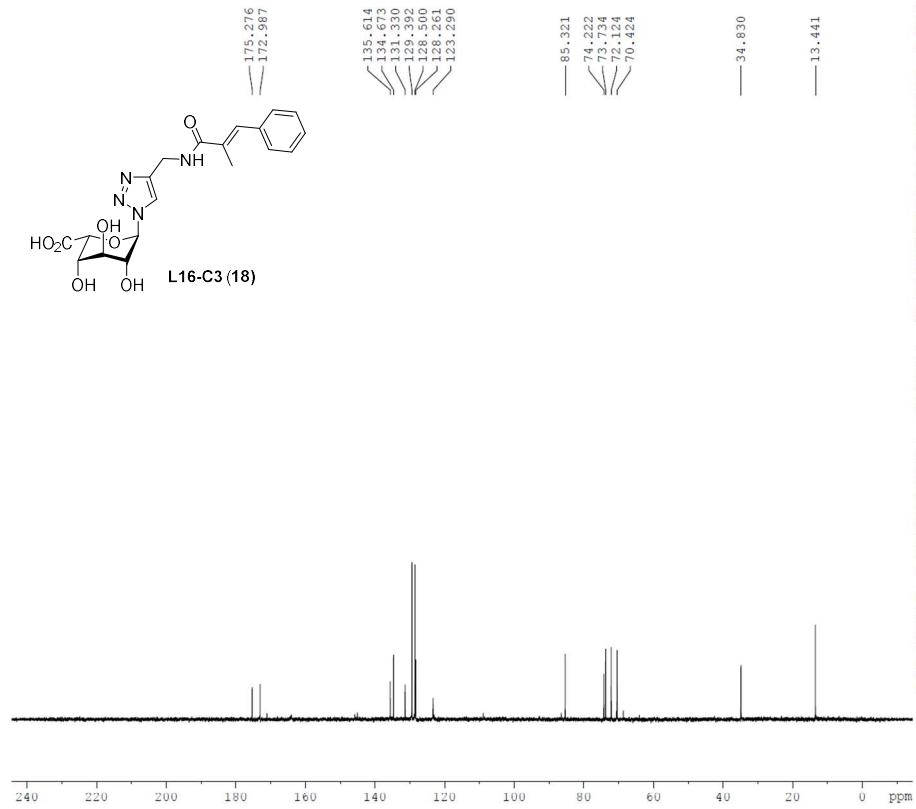
^{1}H NMR and ^{13}C NMR of compound **18** in D_2O

final-95



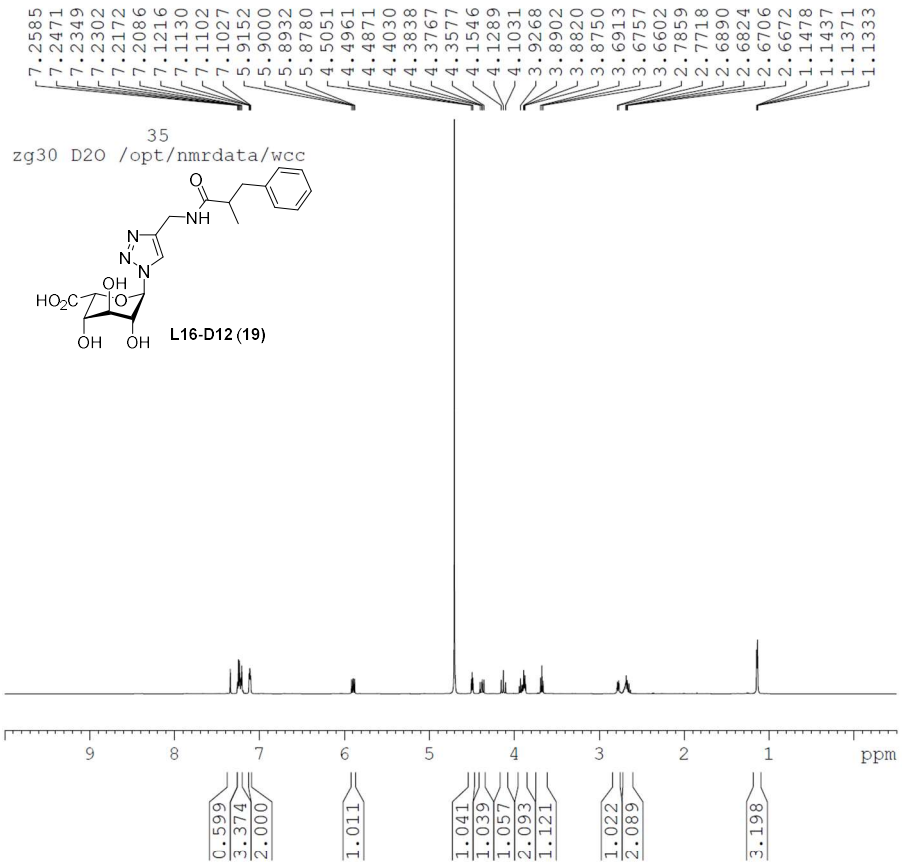

```
Current Data Parameters
NAME                  20140930
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140930
Time                     10.14
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                  zg30
TD                      32768
SOLVENT                   D2O
NS                         18
DS                          0
SWH                  8389.262 Hz
FIDRES               0.256020 Hz
AQ                   1.9530228 sec
RG                        45.2
DW                      59.600 usec
DE                      21.00 usec
TE                      298.0 K
D1                   2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       10.40 usec
PL1                      -0.80 dB
PL1W                18.11971092 W
SFO1               600.1536010 MHz

F2 - Processing parameters
SI                       16384
SF                 600.1499421 MHz
WDW                         EM
SSB             0
LB              0 Hz
GB              0
PC                       1.00
```

95
D2O /opt/nmr

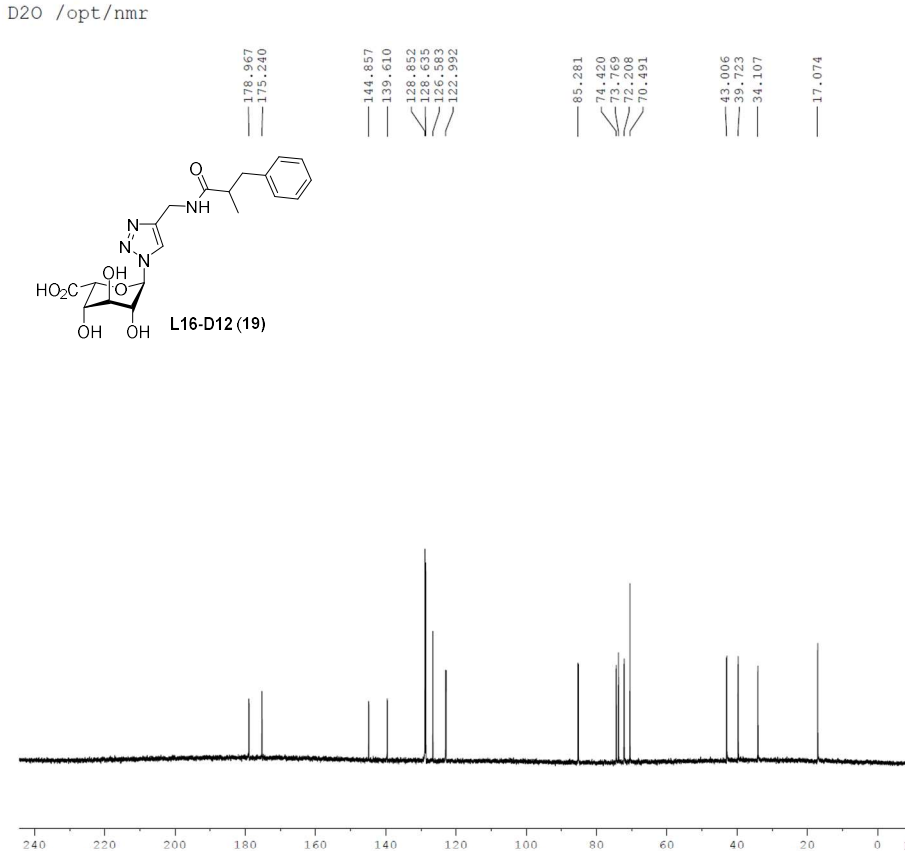



```
Current Data Parameters
NAME      20141104-yu chang
EXPNO                        9
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141104
Time                     21.32
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                zgpg30
TD                      131072
SOLVENT                   D2O
NS                        256
DS                          0
SWH                39062.500 Hz
FIDRES               0.298023 Hz
AQ                   1.6777716 sec
RG                       3640
DW                      12.800 usec
DE                      21.00 usec
TE                      298.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       11.15 usec
PL1                       2.80 dB
PL1W                49.17097855 W
SFO1               150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       0.33 dB
PL12                     16.50 dB
PL13                     19.50 dB
PL2W                13.96854782 W
PL12W                0.33740479 W
PL13W                0.16910298 W
SFO2               600.1524006 MHz

F2 - Processing parameters
SI                       65536
SF                 150.9078380 MHz
WDW                         EM
SSB             0
LB                       2.00 Hz
GB              0
PC                       1.00
```

^{1}H NMR and ^{13}C NMR of compound **19** in D_2O

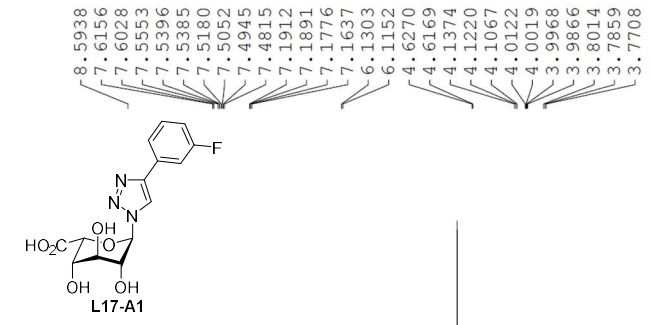


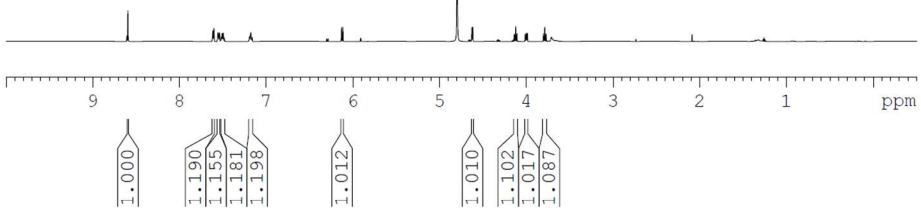

```
Current Data Parameters
NAME      20150116-yu chang
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20150106
Time              20.25
INSTRUM           spect
PROBHD    5 mm CPTCI 1H-
PULPROG             zg30
TD                 32768
SOLVENT              D2O
NS                  1024
DS                     0
SWH             8370.536 Hz
FIDRES             0.255448 Hz
AQ              1.9573919 sec
RG                   45.2
DW                59.733 usec
DE                21.00 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  8.10 usec
PL1                 4.00 dB
PL1W          6.09999990 W
SFO1         600.1336009 MHz

F2 - Processing parameters
SI                 16384
SF           600.1300000 MHz
WDW                   EM
SSB         0
LB          0 Hz
GB          0
PC                  1.00
```



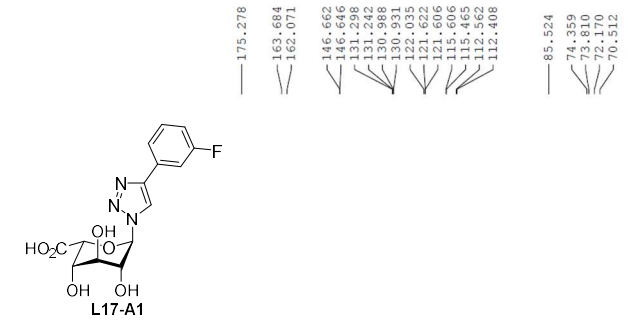

```
Current Data Parameters
NAME      20150107-yu chang
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20150107
Time              12.05
INSTRUM           spect
PROBHD    5 mm CPTCI 1H-
PULPROG           zgpg30
TD                131072
SOLVENT              D2O
NS                  1024
DS                     0
SWH            39062.500 Hz
FIDRES             0.298023 Hz
AQ              1.6777716 sec
RG                  2050
DW                12.800 usec
DE                21.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.15 usec
PL1               -1.82 dB
PL1W       122.22216797 W
SFO1        150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 4.00 dB
PL12               24.90 dB
PL13               27.90 dB
PL2W          6.09999990 W
PL12W         0.04958267 W
PL13W         0.02485020 W
SFO2         600.1324005 MHz

F2 - Processing parameters
SI                 65536
SF           150.9028090 MHz
WDW                   EM
SSB         0
LB                 2.00 Hz
GB          0
PC                  1.00
```

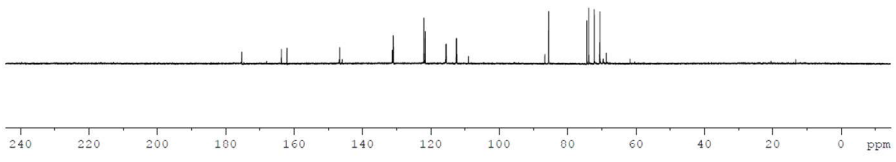
^{1}H NMR and ^{13}C NMR of compound **L17-A1** in D_2O





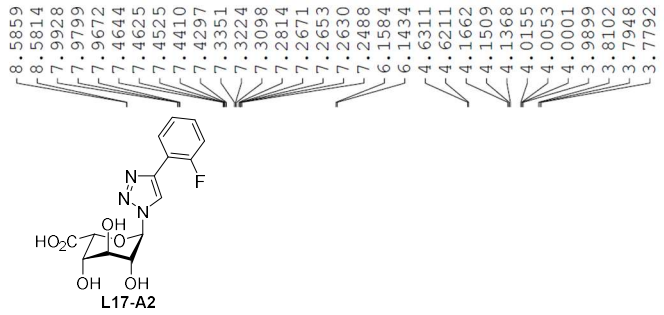

```
Current Data Parameters
NAME                  c14ph-f3
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140615
Time                     13.36
INSTRUM                  spect
PROBHD    5 mm CPTCI 1H-
PULPROG                  zg30
TD                      32768
SOLVENT                   D2O
NS                           64
DS                            0
SWH                   8370.536 Hz
FIDRES                0.255448 Hz
AQ                    1.9573919 sec
RG                         71.8
DW                       59.733 usec
DE                       21.00 usec
TE                       298.0 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                        7.95 usec
PL1                       4.00 dB
PL1W                6.09999990 W
SFO1               600.1336009 MHz

F2 - Processing parameters
SI                       16384
SF                  600.1299489 MHz
WDW                         EM
SSB              0
LB               0 Hz
GB               0
PC                        1.00
```

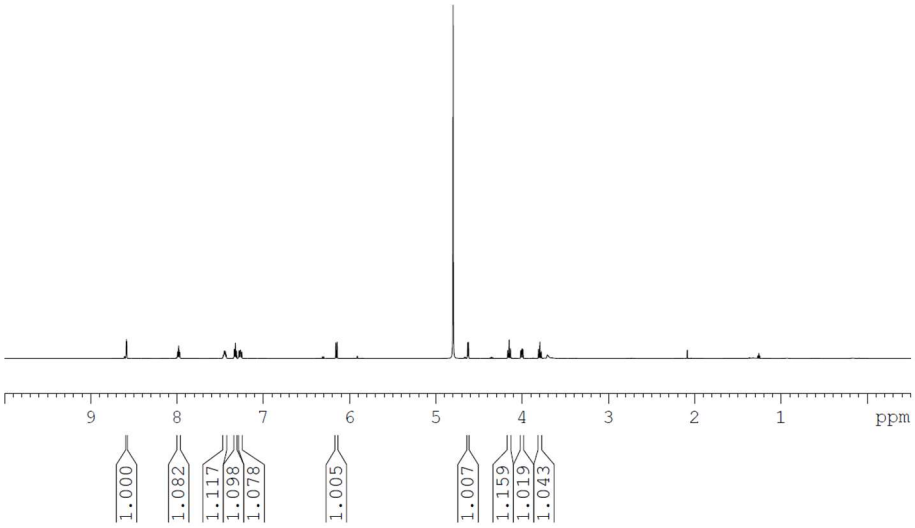




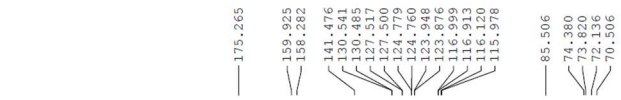

```
Current Data Parameters
NAME                  c14ph-f3
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140615
Time                     14.09
INSTRUM                  spect
PROBHD    5 mm CPTCI 1H-
PULPROG                zgpg30
TD                      131072
SOLVENT                   D2O
NS                          512
DS                            0
SWH                39062.500 Hz
FIDRES                0.298023 Hz
AQ                    1.6777716 sec
RG                         2050
DW                      12.800 usec
DE                       21.00 usec
TE                       298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       10.05 usec
PL1                      -1.82 dB
PL1W              122.22216797 W
SFO1               150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                       4.00 dB
PL12                     24.90 dB
PL13                     27.90 dB
PL2W                6.09999990 W
PL12W               0.04958267 W
PL13W               0.02485020 W
SFO2               600.1324005 MHz

F2 - Processing parameters
SI                       65536
SF                  150.9028090 MHz
WDW                         EM
SSB              0
LB                       2.00 Hz
GB               0
PC                        1.00
```

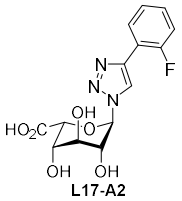
^{1}H NMR and ^{13}C NMR of compound **L17-A2** in D_2O



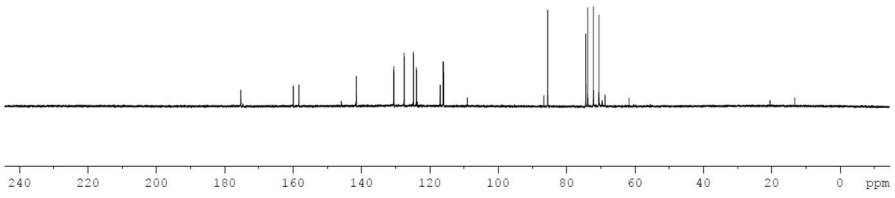



```
Current Data Parameters
NAME            c14ph-f2
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140615
Time              14.16
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG            zg30
TD                32768
SOLVENT             D2O
NS                    64
DS                     0
SWH            8370.536 Hz
FIDRES         0.255448 Hz
AQ             1.9573919 sec
RG                  45.2
DW                59.733 usec
DE                21.00 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 7.95 usec
PL1                4.00 dB
PL1W          6.09999990 W
SFO1         600.1336009 MHz

F2 - Processing parameters
SI                 16384
SF           600.1299469 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

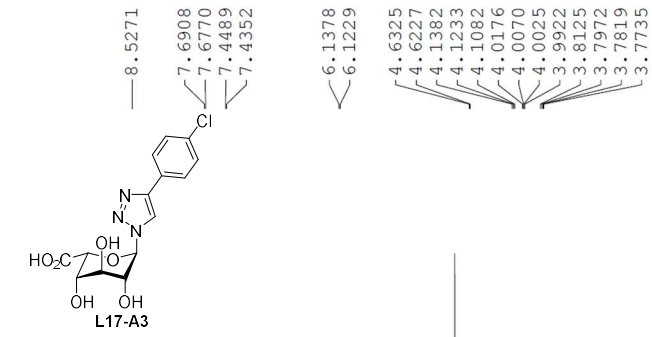


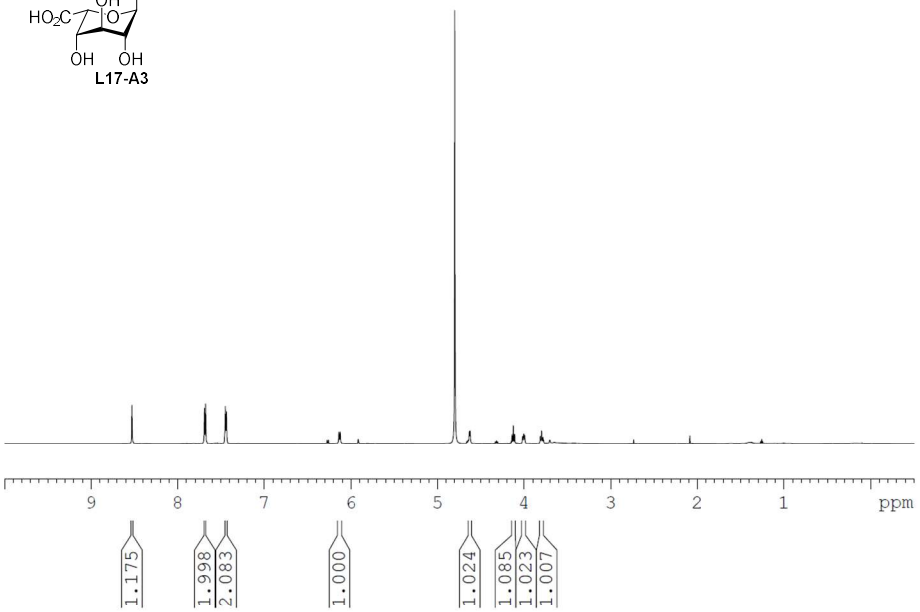



```
Current Data Parameters
NAME            c14ph-f2
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140615
Time              14.49
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD               131072
SOLVENT             D2O
NS                   512
DS                     0
SWH           39062.500 Hz
FIDRES         0.298023 Hz
AQ             1.6777716 sec
RG                  2050
DW                12.800 usec
DE                21.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.05 usec
PL1               -1.82 dB
PL1W       122.22216797 W
SFO1        150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                4.00 dB
PL12              24.90 dB
PL13              27.90 dB
PL2W          6.09999990 W
PL12W         0.04958267 W
PL13W         0.02485020 W
SFO2         600.1324005 MHz

F2 - Processing parameters
SI                 65536
SF           150.9028090 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.00
```

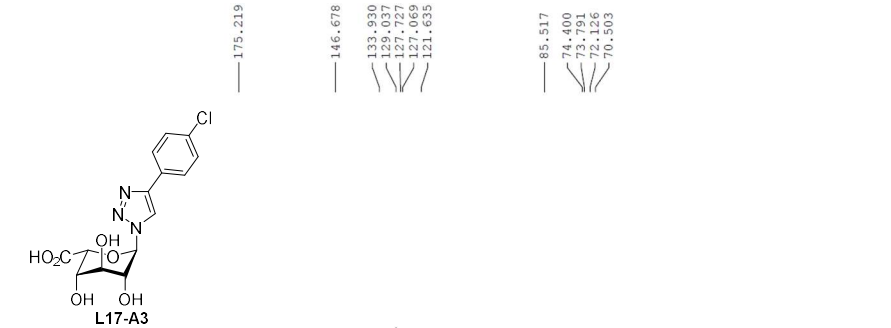


^{1}H NMR and ^{13}C NMR of compound **L17-A3** in D_2O



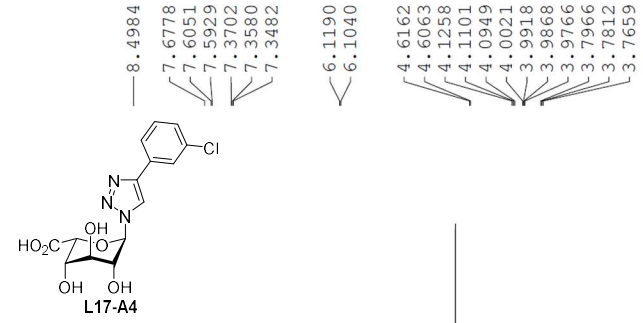


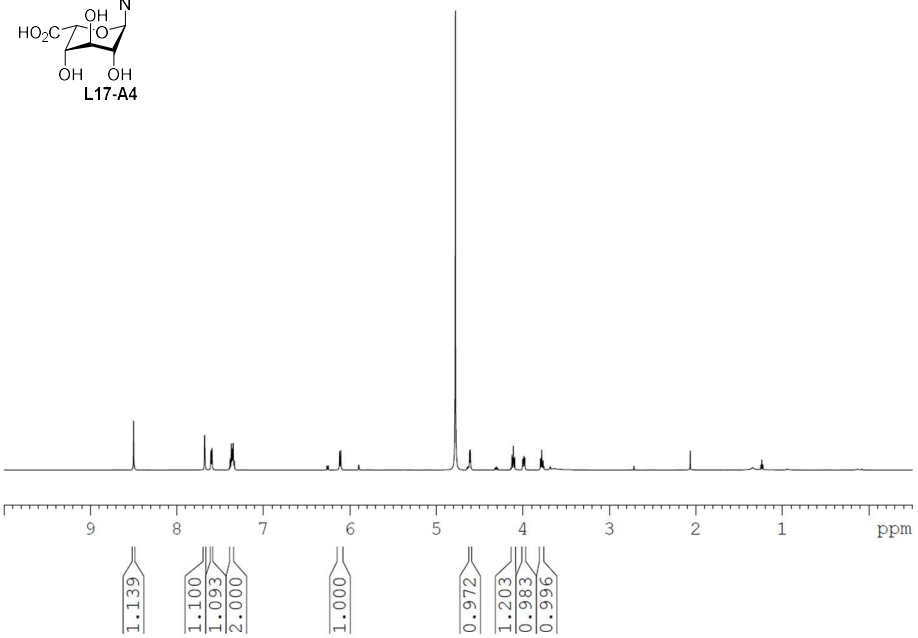

```
Current Data Parameters
NAME                  c14ph-cl 4
EXPNO                         5
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20140615
Time                      14.55
INSTRUM                   spect
PROBHD    5 mm CPTCI 1H-
PULPROG                   zg30
TD                       32768
SOLVENT                    D2O
NS                          64
DS                           0
SWH                   8370.536 Hz
FIDRES                0.255448 Hz
AQ                    1.9573919 sec
RG                         40.3
DW                       59.733 usec
DE                       21.00 usec
TE                       298.0 K
D1                    2.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        1H
P1                        7.95 usec
PL1                       4.00 dB
PL1W                6.09999990 W
SFO1               600.1336009 MHz

F2 - Processing parameters
SI                        16384
SF                  600.1299473 MHz
WDW                          EM
SSB             0
LB              0 Hz
GB              0
PC                        1.00
```



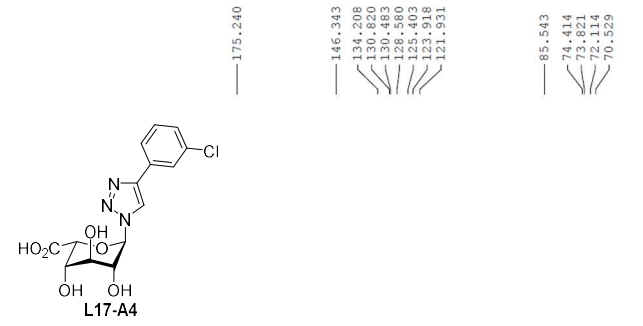

```
Current Data Parameters
NAME                  c14ph-cl 4
EXPNO                         6
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20140615
Time                      15.28
INSTRUM                   spect
PROBHD    5 mm CPTCI 1H-
PULPROG                 zgpg30
TD                      131072
SOLVENT                    D2O
NS                          512
DS                           0
SWH                  39062.500 Hz
FIDRES                0.298023 Hz
AQ                    1.6777716 sec
RG                         2050
DW                       12.800 usec
DE                       21.00 usec
TE                       298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                       13C
P1                       10.05 usec
PL1                      -1.82 dB
PL1W              122.22216797 W
SFO1               150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                       4.00 dB
PL12                     24.90 dB
PL13                     27.90 dB
PL2W                6.09999990 W
PL12W               0.04958267 W
PL13W               0.02485020 W
SFO2               600.1324005 MHz

F2 - Processing parameters
SI                        65536
SF                  150.9028090 MHz
WDW                          EM
SSB             0
LB                        2.00 Hz
GB              0
PC                        1.00
```

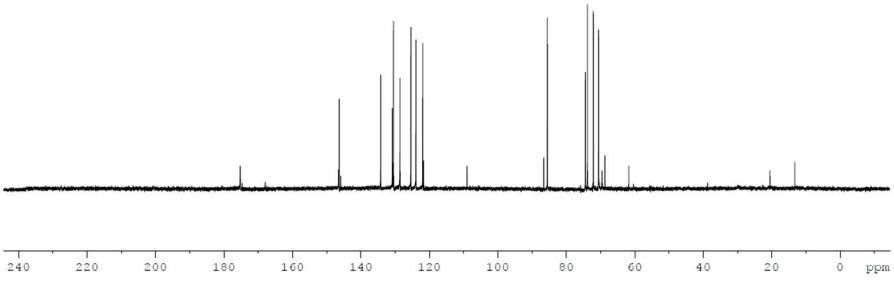
^{1}H NMR and ^{13}C NMR of compound **L17-A4** in D_2O





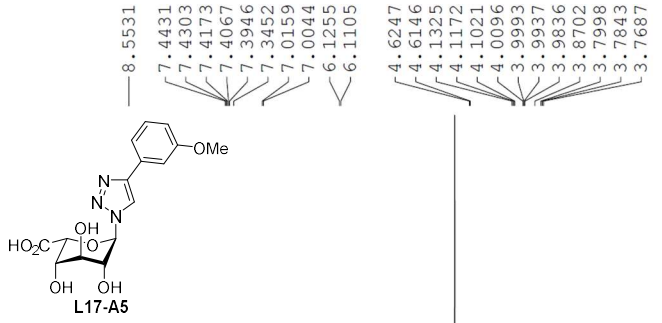

```
Current Data Parameters
NAME          c14ph-cl 3
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20140615
Time              15.35
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               32768
SOLVENT            D2O
NS                  64
DS                   0
SWH           8370.536 Hz
FIDRES        0.255448 Hz
AQ            1.9573919 sec
RG                40.3
DW              59.733 usec
DE              21.00 usec
TE              298.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                7.95 usec
PL1               4.00 dB
PL1W         6.09999990 W
SFO1        600.1336009 MHz

F2 - Processing parameters
SI                16384
SF          600.1299594 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                1.00
```

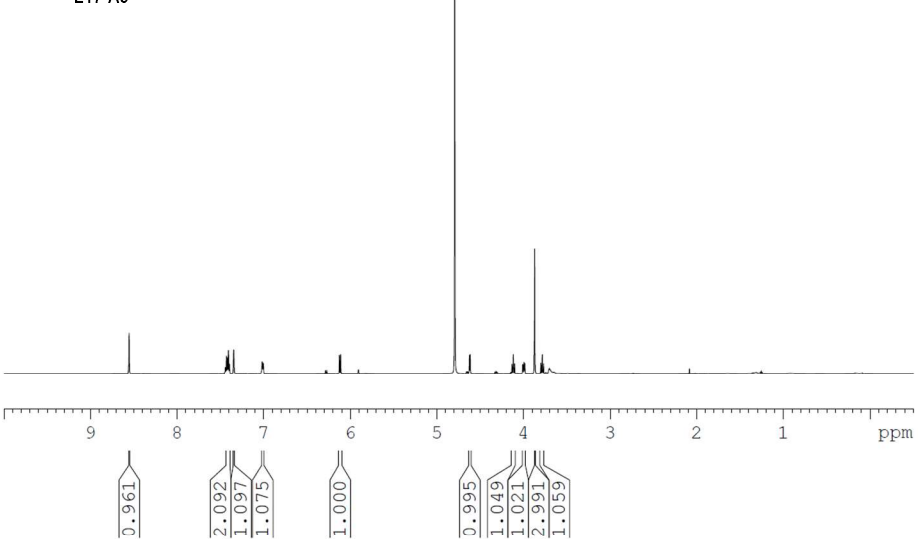




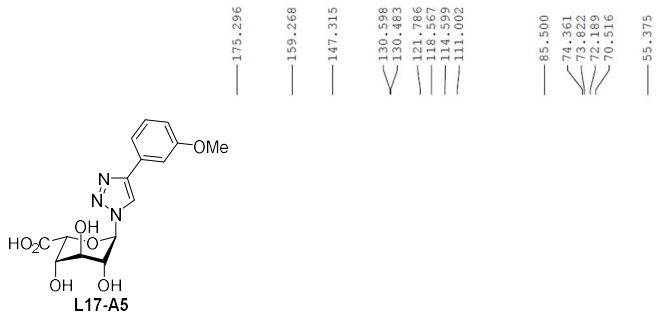

```
Current Data Parameters
NAME          c14ph-cl 3
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20140615
Time              16.08
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG         zgpg30
TD              131072
SOLVENT            D2O
NS                 512
DS                   0
SWH          39062.500 Hz
FIDRES        0.298023 Hz
AQ            1.6777716 sec
RG                2050
DW              12.800 usec
DE              21.00 usec
TE              298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1               10.05 usec
PL1              -1.82 dB
PL1W       122.22216797 W
SFO1        150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            90.00 usec
PL2               4.00 dB
PL12             24.90 dB
PL13             27.90 dB
PL2W         6.09999990 W
PL12W        0.04958267 W
PL13W        0.02485020 W
SFO2        600.1324005 MHz

F2 - Processing parameters
SI                65536
SF          150.9028090 MHz
WDW                  EM
SSB       0
LB               2.00 Hz
GB        0
PC                1.00
```

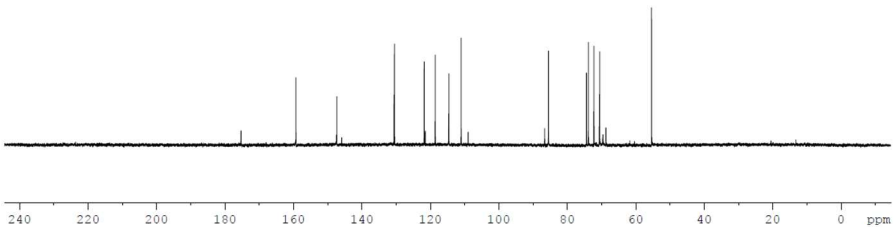
^{1}H NMR and ^{13}C NMR of compound **L17-A5** in D_2O





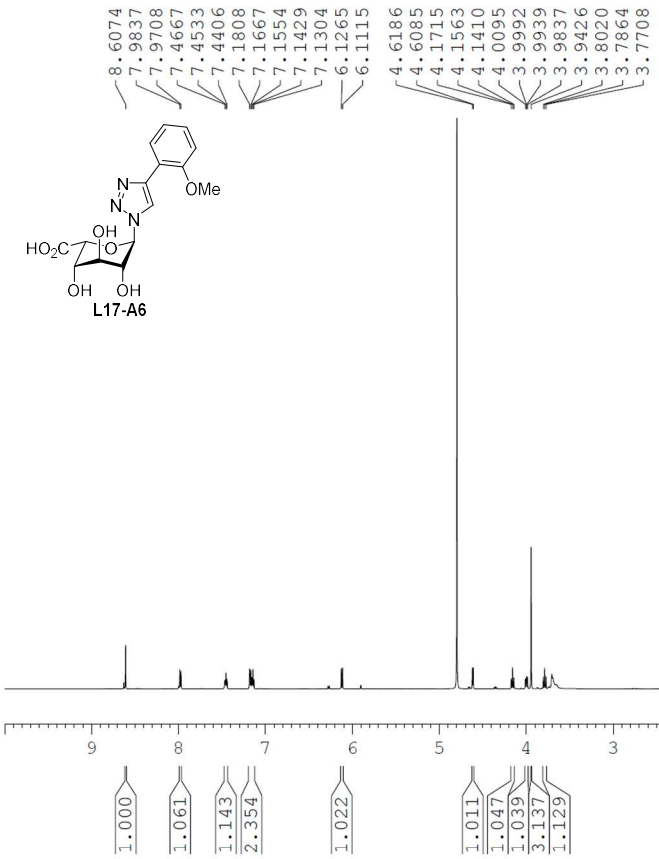

```
Current Data Parameters
NAME          c14ph-ome 3
EXPNO                   9
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140615
Time              16.14
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               32768
SOLVENT            D2O
NS                  64
DS                   0
SWH           8370.536 Hz
FIDRES        0.255448 Hz
AQ           1.9573919 sec
RG                45.2
DW              59.733 usec
DE              21.00 usec
TE              297.9 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               7.95 usec
PL1              4.00 dB
PL1W        6.09999990 W
SFO1       600.1336009 MHz

F2 - Processing parameters
SI                 16384
SF          600.1299509 MHz
WDW                EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



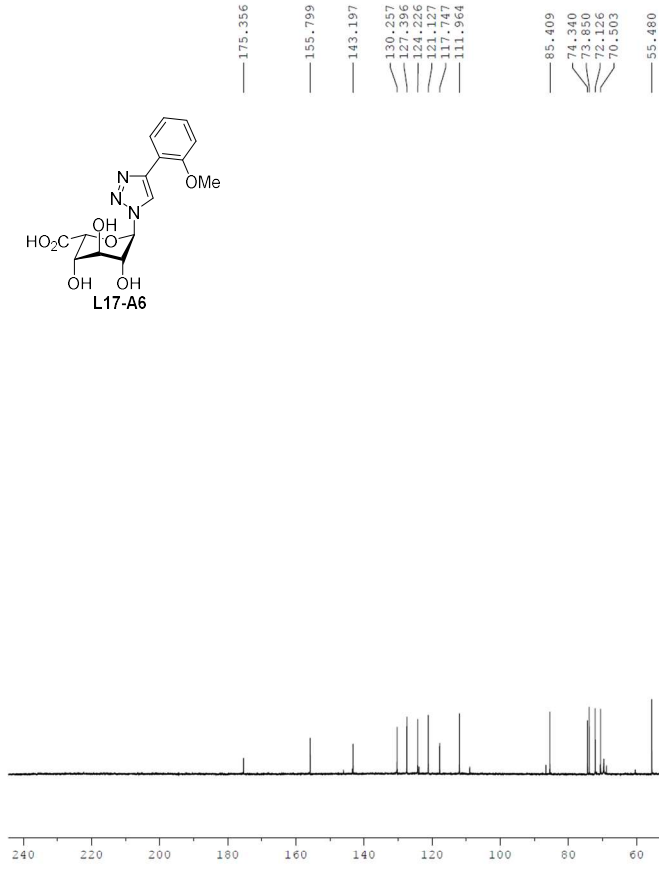



```
Current Data Parameters
NAME          c14ph-ome 3
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140615
Time              16.47
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD              131072
SOLVENT            D2O
NS                 512
DS                   0
SWH          39062.500 Hz
FIDRES        0.298023 Hz
AQ           1.6777716 sec
RG                2050
DW              12.800 usec
DE              21.00 usec
TE              298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               13C
P1              10.05 usec
PL1             -1.82 dB
PL1W       122.22216797 W
SFO1        150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           90.00 usec
PL2              4.00 dB
PL12            24.90 dB
PL13            27.90 dB
PL2W        6.09999990 W
PL12W       0.04958267 W
PL13W       0.02485020 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                 65536
SF          150.9028090 MHz
WDW                EM
SSB       0
LB              2.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR and ^{13}C NMR of compound **L17-A6** in D_2O

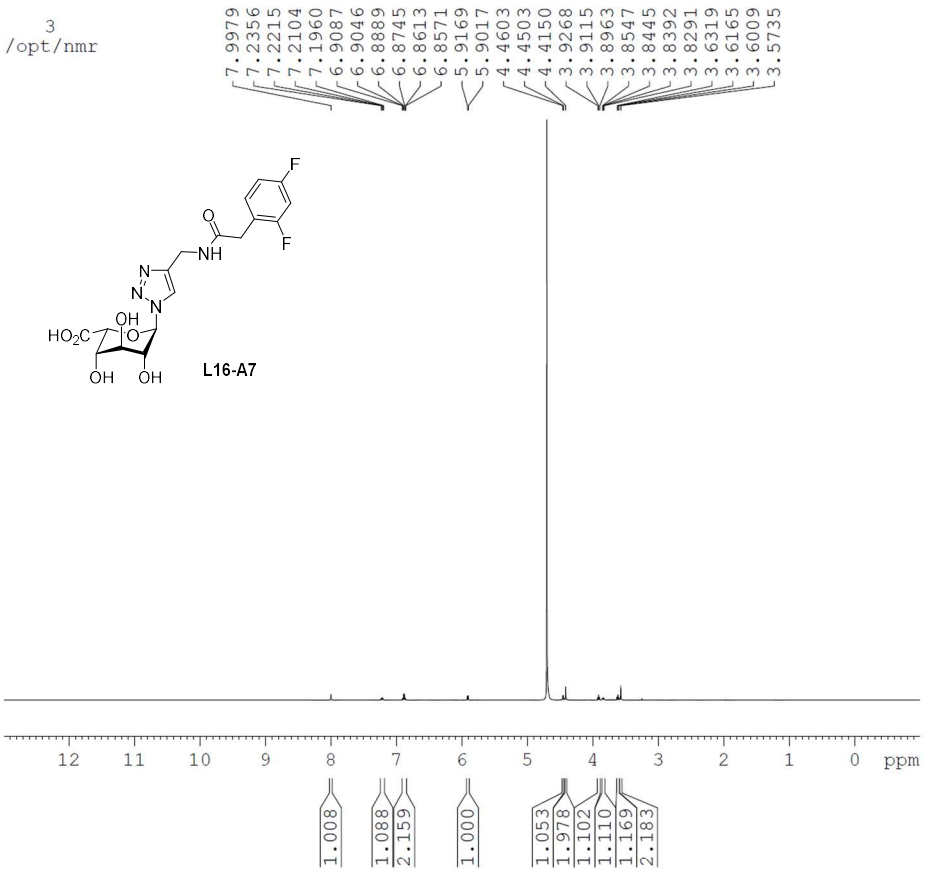



```
Current Data Parameters
NAME          c14ph-ome 2
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140615
Time              16.54
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               32768
SOLVENT             D2O
NS                   64
DS                    0
SWH           8370.536 Hz
FIDRES        0.255448 Hz
AQ           1.9573919 sec
RG                40.3
DW              59.733 usec
DE              21.00 usec
TE              298.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                 7.95 usec
PL1                4.00 dB
PL1W         6.09999990 W
SFO1        600.1336009 MHz

F2 - Processing parameters
SI                16384
SF          600.1299492 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                1.00
```

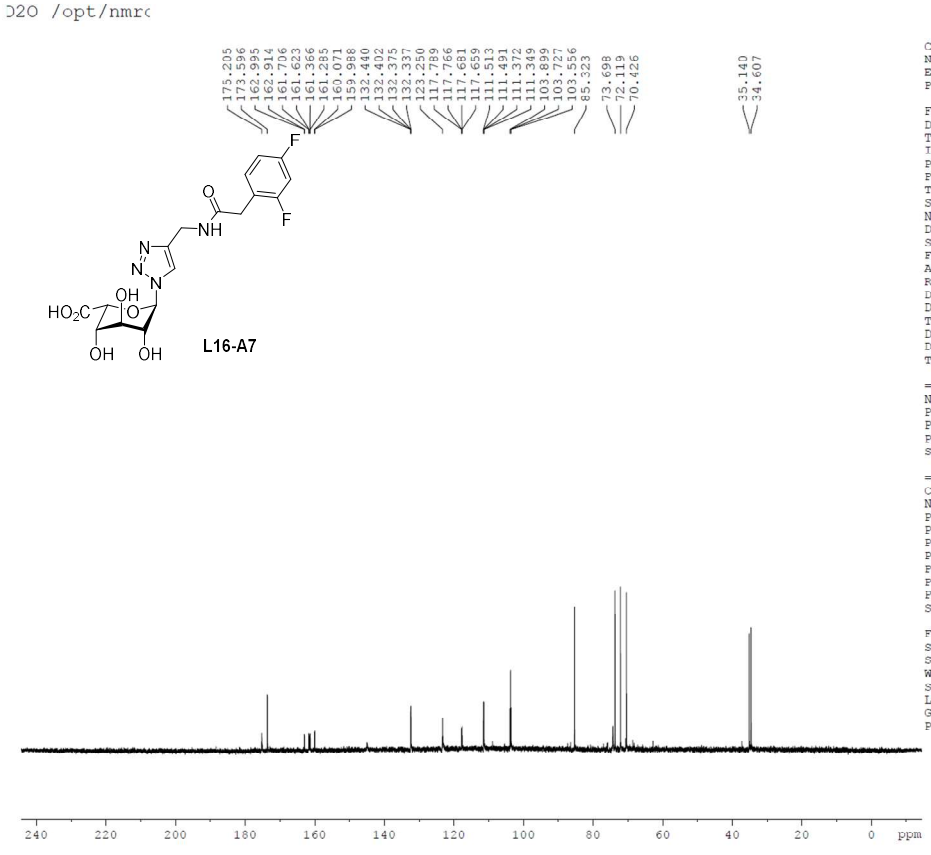



```
Current Data Parameters
NAME          c14ph-ome 2
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140615
Time              17.27
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG         zgpg30
TD              131072
SOLVENT             D2O
NS                  512
DS                    0
SWH          39062.500 Hz
FIDRES        0.298023 Hz
AQ           1.6777716 sec
RG                2050
DW              12.800 usec
DE              21.00 usec
TE              298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.05 usec
PL1               -1.82 dB
PL1W       122.22216797 W
SFO1        150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.00 dB
PL12              24.90 dB
PL13              27.90 dB
PL2W         6.09999990 W
PL12W        0.04958267 W
PL13W        0.02485020 W
SFO2        600.1324005 MHz

F2 - Processing parameters
SI                65536
SF          150.9028090 MHz
WDW                  EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-A7** in D_2O

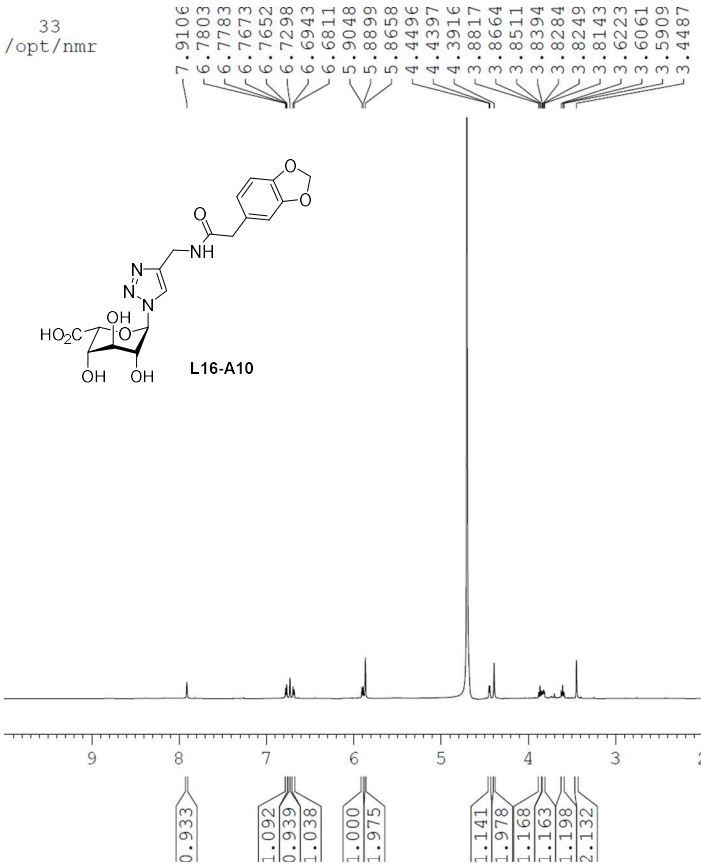



```
Current Data Parameters
NAME      20141117-yu chang
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141117
Time                 19.19
INSTRUM              spect
PROBHD   5 mm CPDCH 13C
PULPROG              zg30
TD                  32768
SOLVENT               D2O
NS                    512
DS                      0
SWH              8389.262 Hz
FIDRES           0.256020 Hz
AQ               1.9530228 sec
RG                   45.2
DW                 59.600 usec
DE                 21.00 usec
TE                 298.0 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.15 usec
PL1                 -0.80 dB
PL1W         18.11971092 W
SFO1         600.1536010 MHz

F2 - Processing parameters
SI                  16384
SF           600.1500000 MHz
WDW                    EM
SSB       0
LB        0 Hz
GB        0
PC                   1.00
```

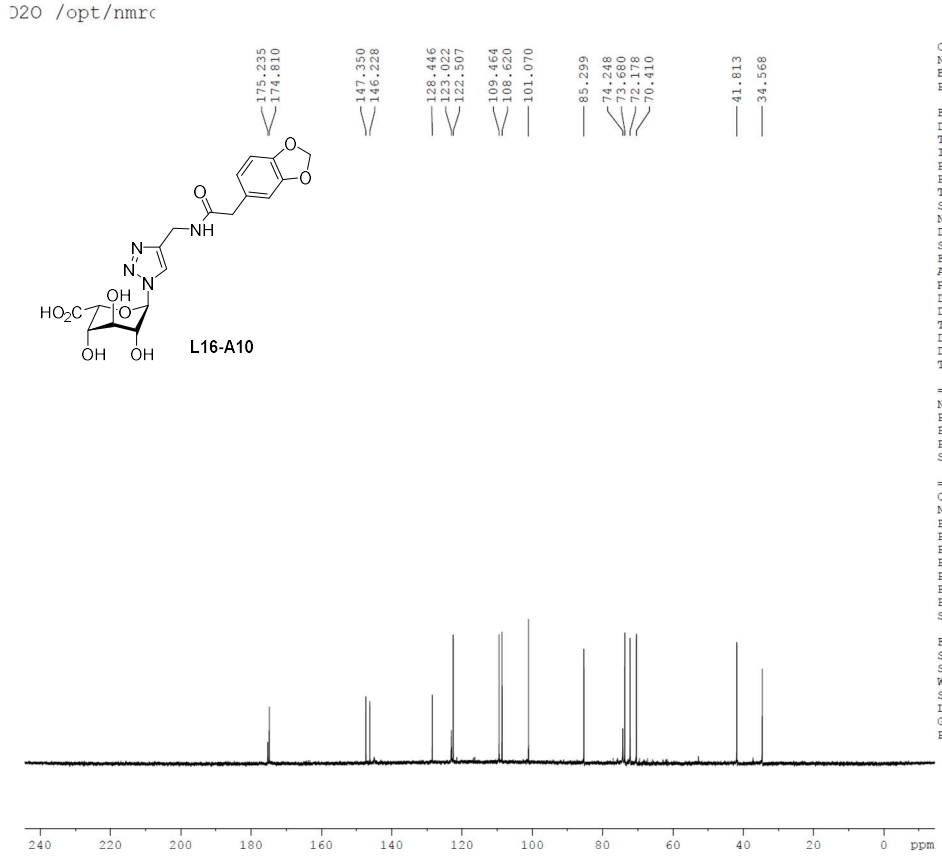



```
Current Data Parameters
NAME      20141117-yu chang
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141117
Time                 20.24
INSTRUM              spect
PROBHD   5 mm CPDCH 13C
PULPROG            zgpg30
TD                 131072
SOLVENT               D2O
NS                   1024
DS                      0
SWH              39062.500 Hz
FIDRES           0.298023 Hz
AQ               1.6777716 sec
RG                   3640
DW                 12.800 usec
DE                 21.00 usec
TE                 298.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  11.15 usec
PL1                  2.80 dB
PL1W         49.17097855 W
SFO1        150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  0.33 dB
PL12                16.50 dB
PL13                19.50 dB
PL2W         13.96854782 W
PL12W         0.33740479 W
PL13W         0.16910298 W
SFO2        600.1524006 MHz

F2 - Processing parameters
SI                  65536
SF          150.9070300 MHz
WDW                    EM
SSB       0
LB                   2.00 Hz
GB        0
PC                   1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-A10** in D_2O




```
Current Data Parameters
NAME      20141119-yu chang
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141119
Time                 19.17
INSTRUM              spect
PROBHD    5 mm CPDCH 13C
PULPROG               zg30
TD                   32768
SOLVENT                D2O
NS                       512
DS                         0
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                        36
DW                   59.600 usec
DE                   21.00 usec
TE                   298.0 K
D1                 2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.15 usec
PL1                    -0.80 dB
PL1W            18.11971092 W
SFO1            600.1536010 MHz

F2 - Processing parameters
SI                      16384
SF                600.1500000 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```




```
Current Data Parameters
NAME      20141119-yu chang
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141119
Time                 20.23
INSTRUM              spect
PROBHD    5 mm CPDCH 13C
PULPROG             zgpg30
TD                  131072
SOLVENT                D2O
NS                      1024
DS                         0
SWH               39062.500 Hz
FIDRES             0.298023 Hz
AQ                 1.6777716 sec
RG                      3640
DW                   12.800 usec
DE                   21.00 usec
TE                   298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.15 usec
PL1                     2.80 dB
PL1W            49.17097855 W
SFO1            150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.33 dB
PL12                   16.50 dB
PL13                   19.50 dB
PL2W            13.96854782 W
PL12W            0.33740479 W
PL13W            0.16910298 W
SFO2            600.1524006 MHz

F2 - Processing parameters
SI                      65536
SF                150.9078380 MHz
WDW                        EM
SSB          0
LB                      2.00 Hz
GB           0
PC                      1.00
```

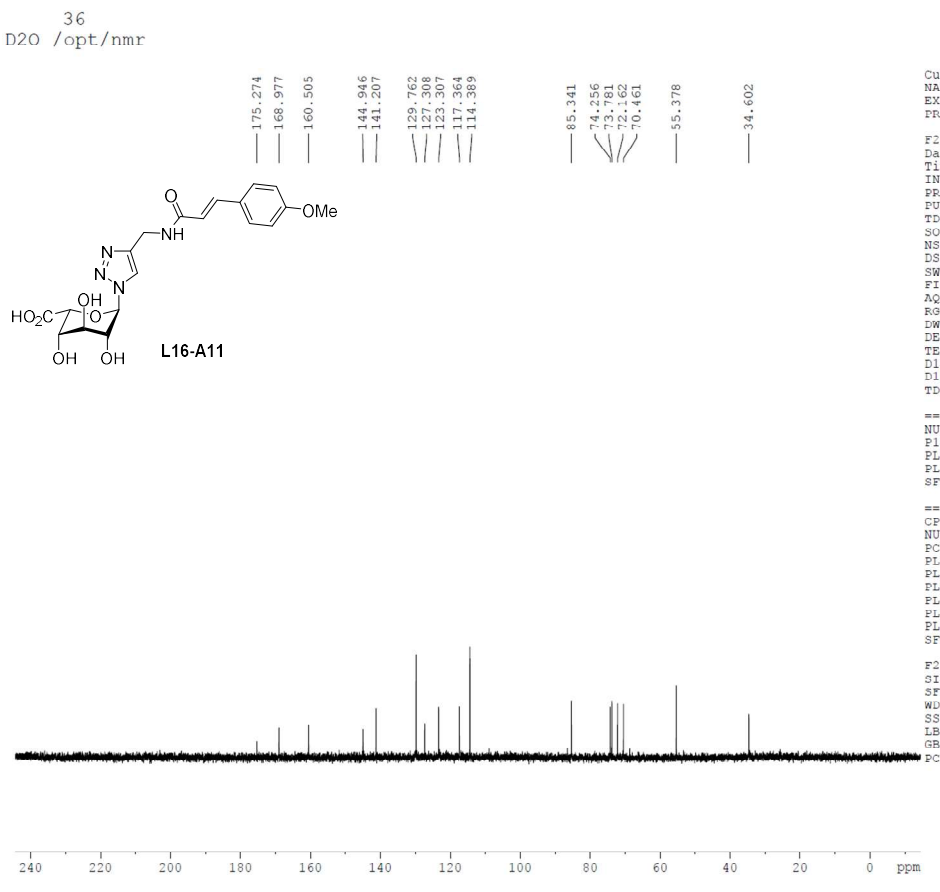
^{1}H NMR and ^{13}C NMR of compound **L16-A11** in D_2O

Current Data Parameters
NAME 36
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141002
Time 21.57
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32768
SOLVENT D2O
NS 18
DS 0
SWH 8370.536 Hz
FIDRES 0.255448 Hz
AQ 1.9573919 sec
RG 40.3
DW 59.733 usec
DE 21.00 usec
TE 297.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 4.00 dB
PL1W 6.09999990 W
SFO1 600.1336009 MHz

F2 - Processing parameters
SI 16384
SF 600.1299496 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 36
EXPNO 4
PROCNO 1

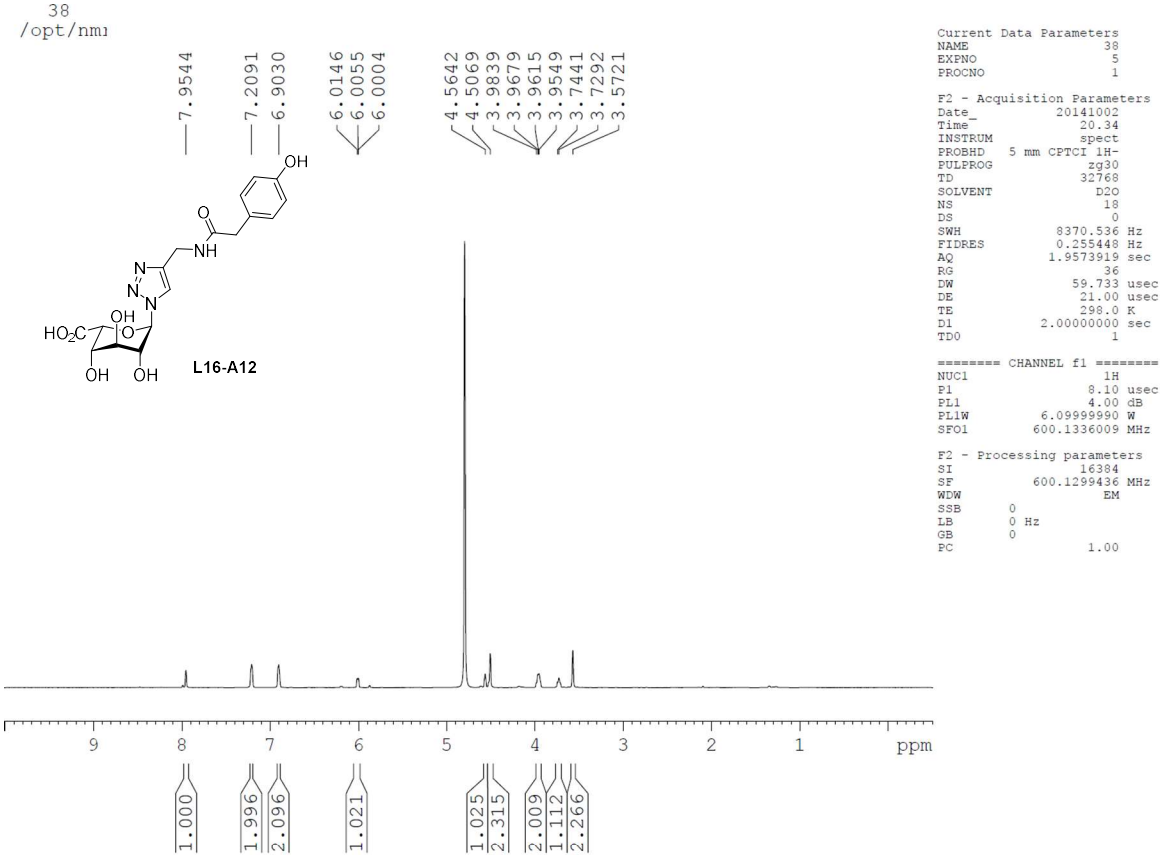
F2 - Acquisition Parameters
Date_ 20141002
Time 20.16
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 131072
SOLVENT D2O
NS 64
DS 0
SWH 39062.500 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 2050
DW 12.800 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.15 usec
PL1 -1.82 dB
PL1W 122.22216797 W
SFO1 150.9201552 MHz

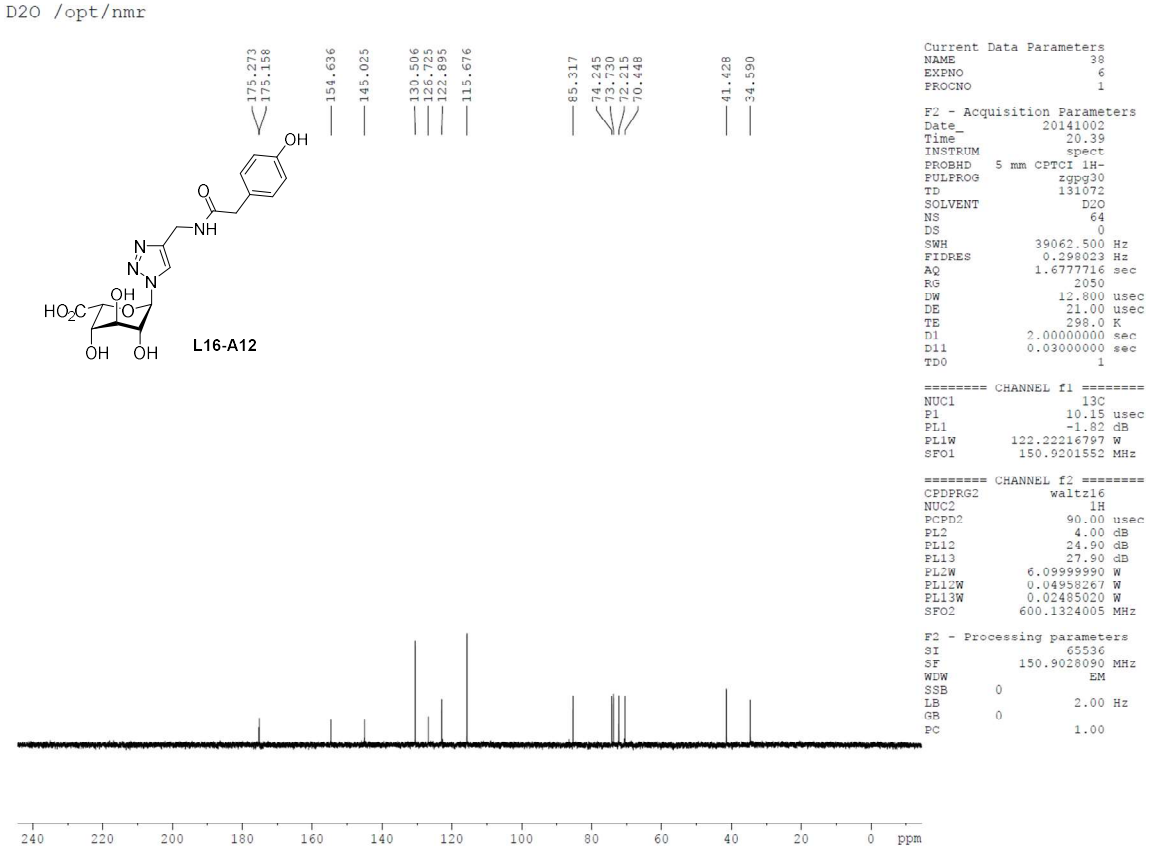
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.00 dB
PL12 24.90 dB
PL13 27.90 dB
PL2W 6.09999990 W
PL12W 0.04958267 W
PL13W 0.02485020 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 65536
SF 150.9028090 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

^{1}H NMR and ^{13}C NMR of compound **L16-A12** in D_2O

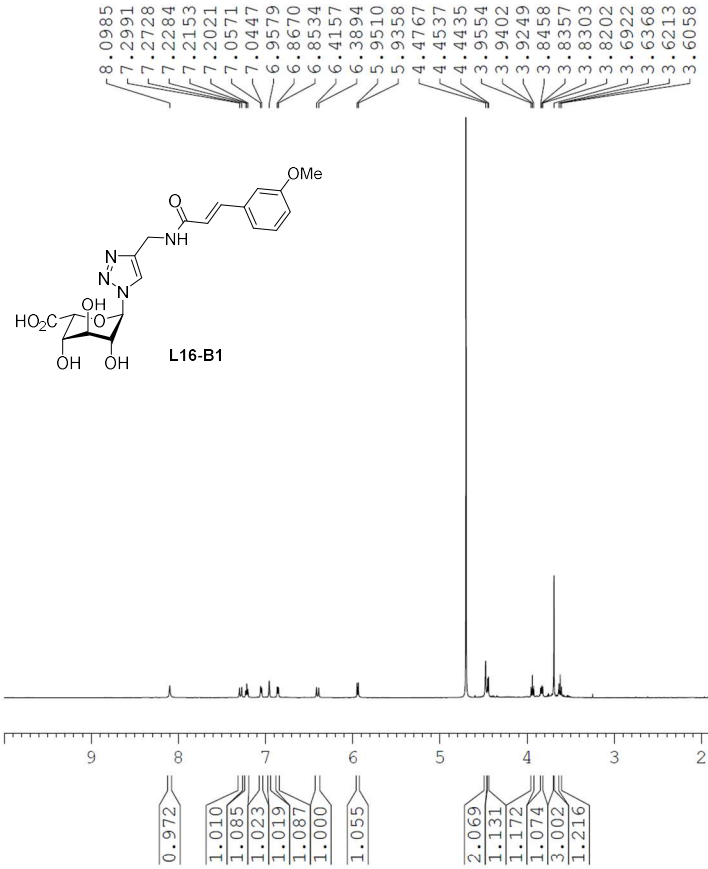



```
Current Data Parameters
NAME                  38
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141002
Time              20.34
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               32768
SOLVENT            D2O
NS                  18
DS                   0
SWH           8370.536 Hz
FIDRES        0.255448 Hz
AQ            1.9573919 sec
RG                  36
DW              59.733 usec
DE              21.00 usec
TE              298.0 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               8.10 usec
PL1              4.00 dB
PL1W        6.09999990 W
SFO1       600.1336009 MHz

F2 - Processing parameters
SI                 16384
SF         600.1299436 MHz
WDW                EM
SSB       0
LB        0 Hz
GB        0
PC               1.00
```



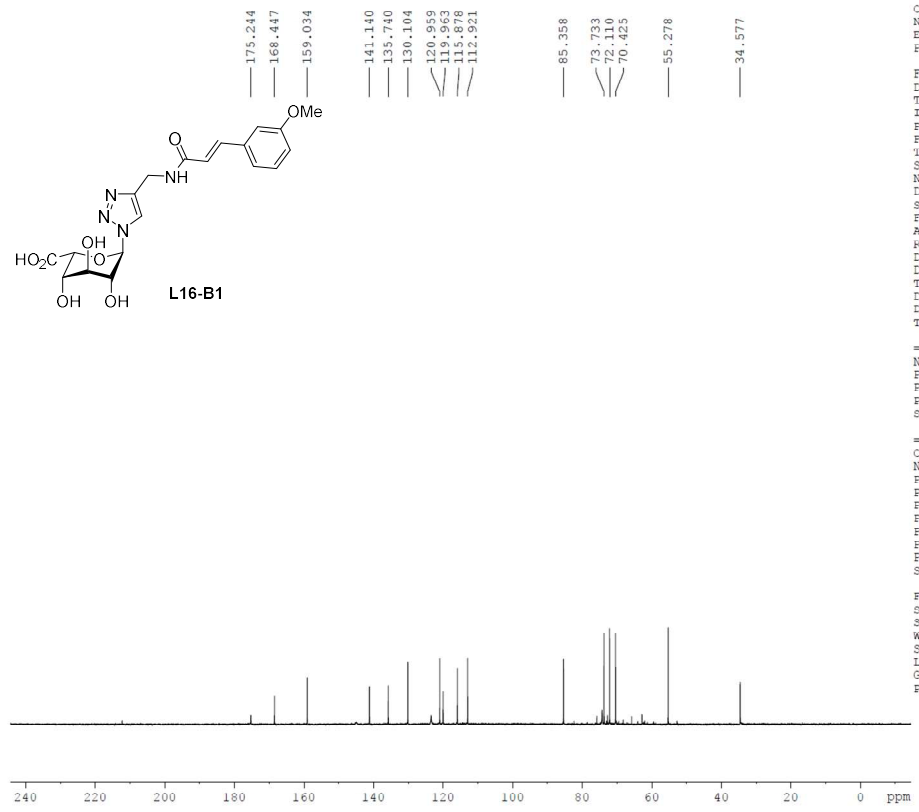

```
Current Data Parameters
NAME                  38
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141002
Time              20.39
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG         zgpg30
TD              131072
SOLVENT            D2O
NS                  64
DS                   0
SWH          39062.500 Hz
FIDRES        0.298023 Hz
AQ            1.6777716 sec
RG                2050
DW              12.800 usec
DE              21.00 usec
TE              298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               13C
P1              10.15 usec
PL1             -1.82 dB
PL1W       122.22216797 W
SFO1        150.9201552 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2               1H
PCPD2           90.00 usec
PL2              4.00 dB
PL12            24.90 dB
PL13            27.90 dB
PL2W        6.09999990 W
PL12W       0.04958267 W
PL13W       0.02485020 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                 65536
SF         150.9028090 MHz
WDW                EM
SSB       0
LB              2.00 Hz
GB        0
PC               1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-B1** in D_2O



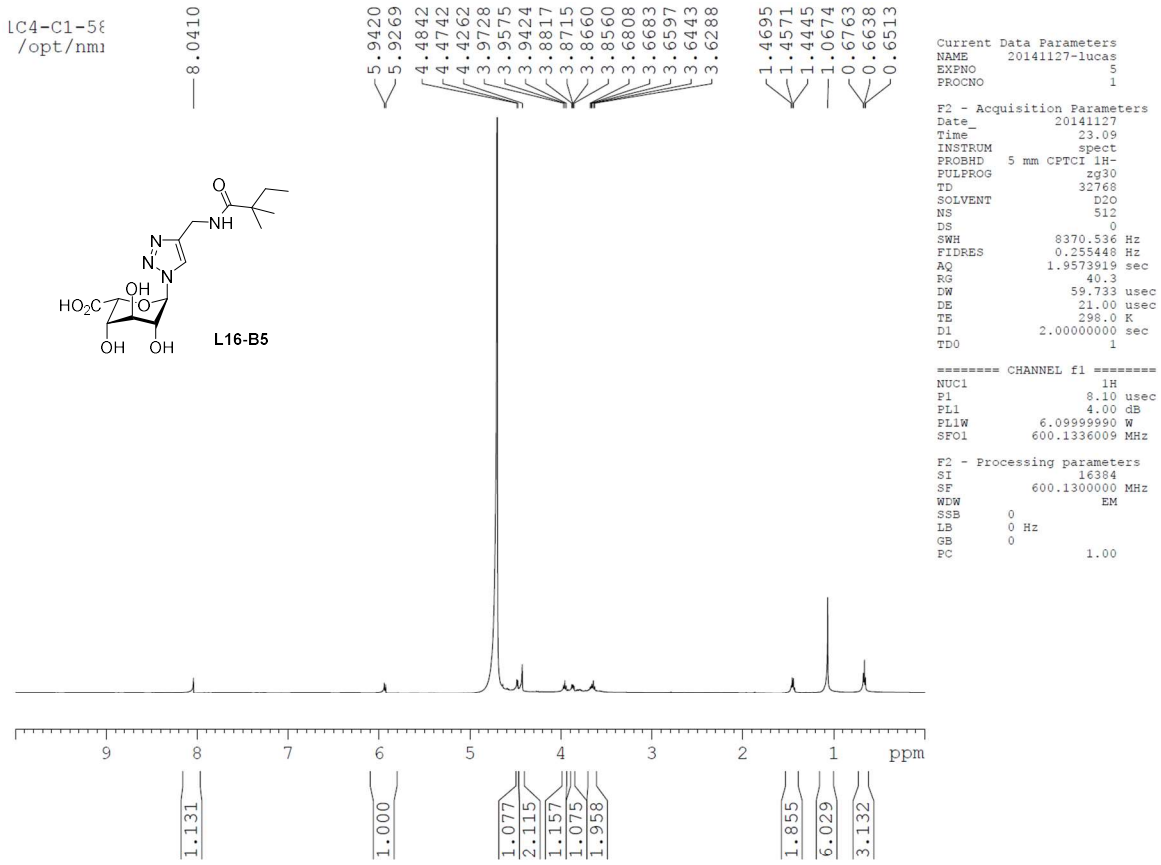

```
Current Data Parameters
NAME                  43
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141204
Time                4.59
INSTRUM            spect
PROBHD   5 mm CPDCH 13C
PULPROG             zg30
TD                 32768
SOLVENT              D2O
NS                   512
DS                     0
SWH             8389.262 Hz
FIDRES          0.256020 Hz
AQ              1.9530228 sec
RG                  71.8
DW                59.600 usec
DE                21.00 usec
TE                298.1 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.15 usec
PL1               -0.80 dB
PL1W         18.11971092 W
SFO1         600.1536010 MHz

F2 - Processing parameters
SI                 16384
SF            600.1500000 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

1C4-C1-43
D2O /opt/nmr




```
Current Data Parameters
NAME                  43
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141204
Time                6.04
INSTRUM            spect
PROBHD   5 mm CPDCH 13C
PULPROG           zgpg30
TD                131072
SOLVENT              D2O
NS                  1024
DS                     0
SWH            39062.500 Hz
FIDRES          0.298023 Hz
AQ              1.6777716 sec
RG                  5790
DW                12.800 usec
DE                21.00 usec
TE                298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.15 usec
PL1                2.80 dB
PL1W         49.17097855 W
SFO1        150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                0.33 dB
PL12              16.50 dB
PL13              19.50 dB
PL2W         13.96854782 W
PL12W         0.33740479 W
PL13W         0.16910298 W
SFO2        600.1524006 MHz

F2 - Processing parameters
SI                 65536
SF            150.9078380 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                  1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-B5** in D_2O

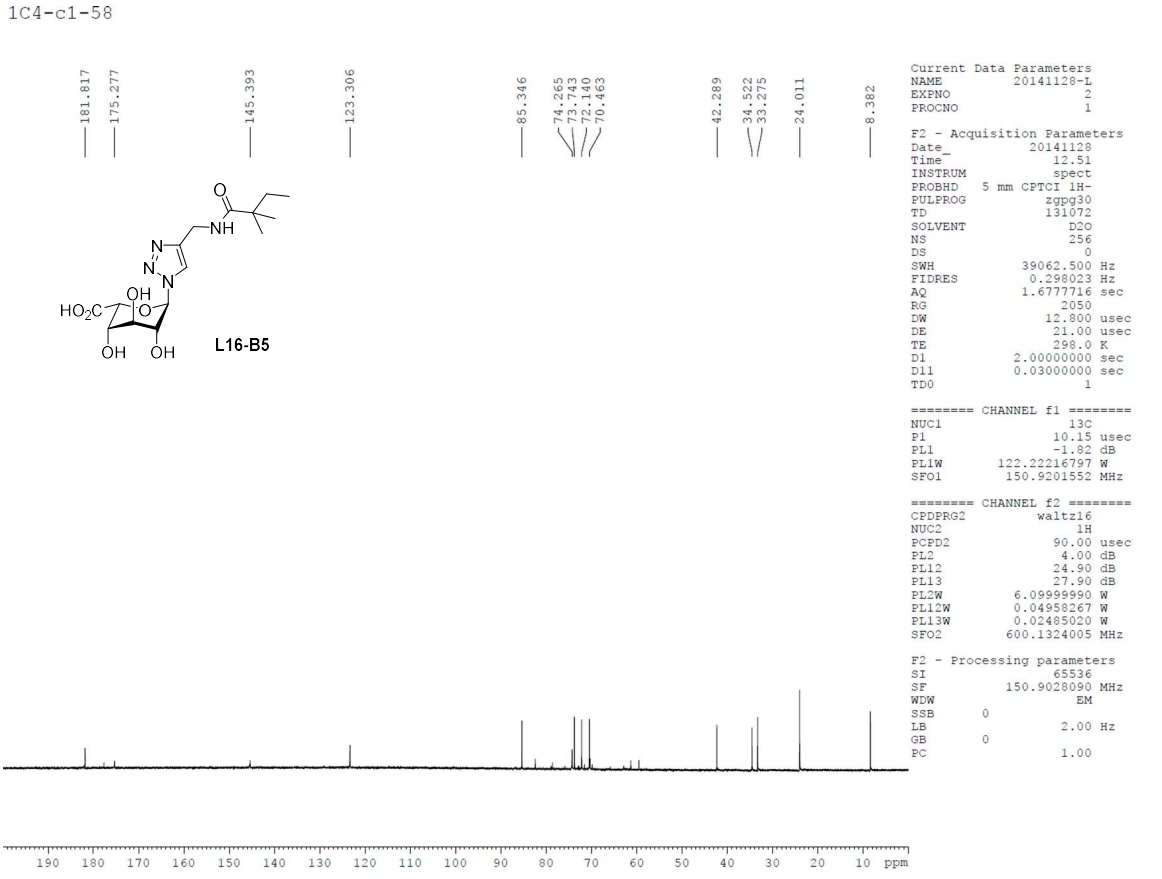


Current Data Parameters
NAME 20141127-lucas
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141127
Time 23.09
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32768
SOLVENT D2O
NS 512
DS 0
SWH 8370.536 Hz
FIDRES 0.255448 Hz
AQ 1.9573919 sec
RG 40.3
DW 59.733 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 4.00 dB
PL1W 6.09999990 W
SFO1 600.1336009 MHz

F2 - Processing parameters
SI 16384
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20141128-L
EXPNO 2
PROCNO 1

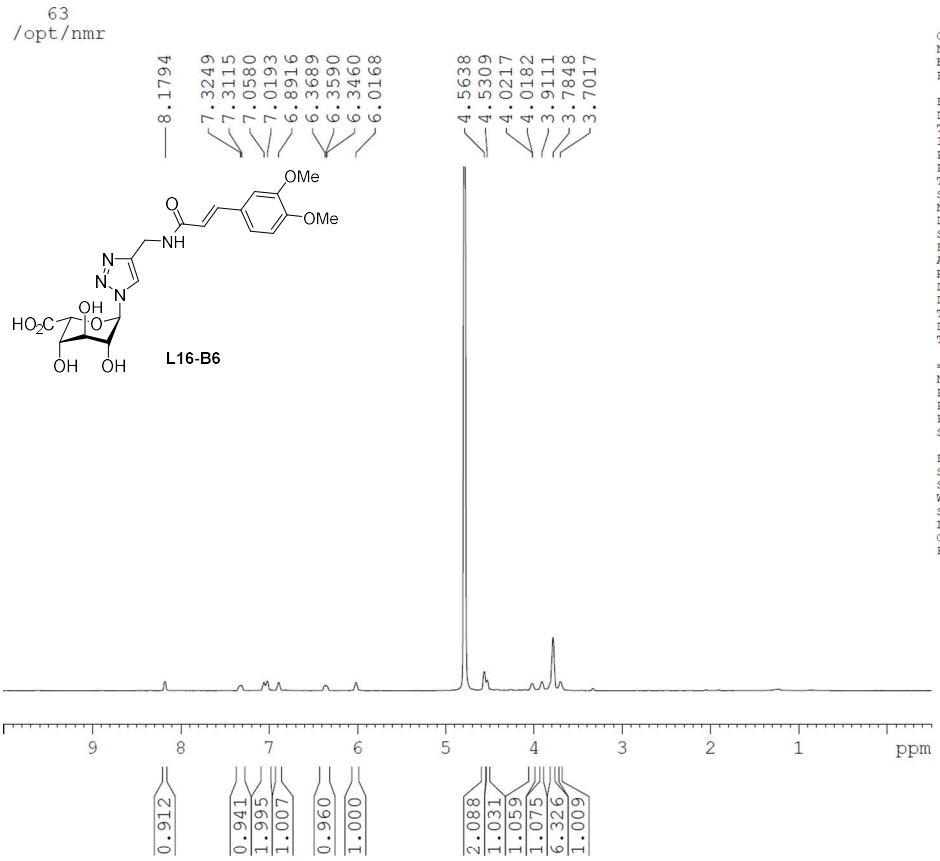
F2 - Acquisition Parameters
Date_ 20141128
Time 12.51
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 131072
SOLVENT D2O
NS 256
DS 0
SWH 39062.500 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 2050
DW 12.800 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.15 usec
PL1 -1.82 dB
PL1W 122.22216797 W
SFO1 150.9201552 MHz

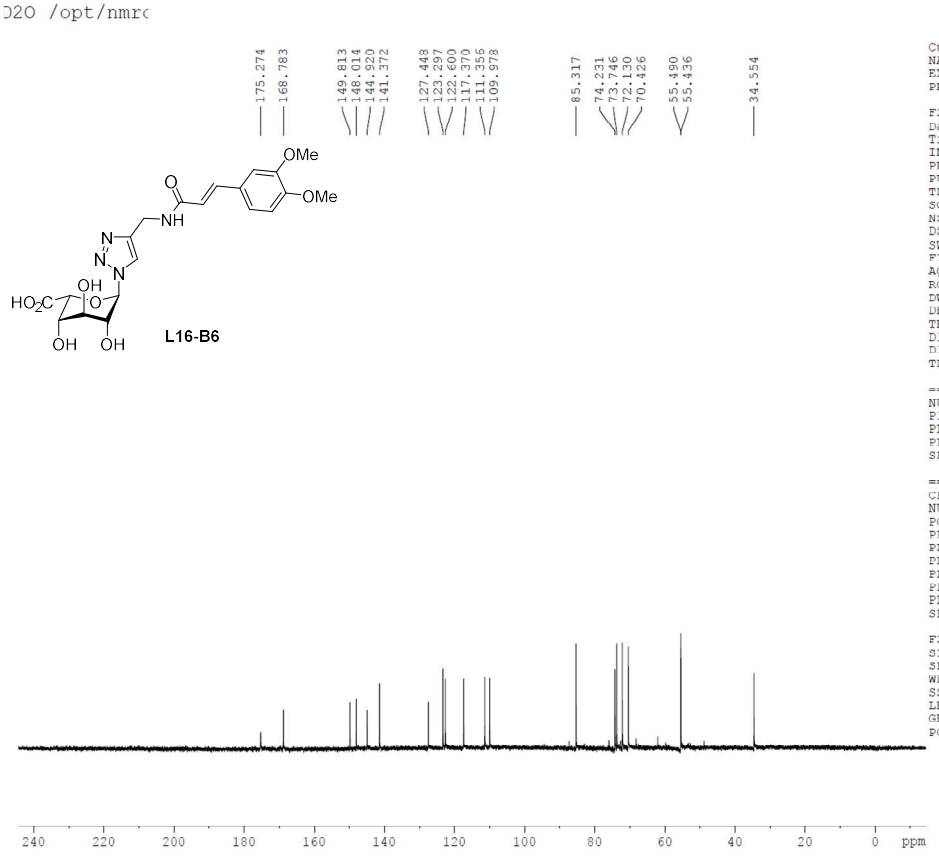
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.00 dB
PL12 24.90 dB
PL13 27.90 dB
PL2W 6.09999990 W
PL12W 0.04958267 W
PL13W 0.02485020 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 65536
SF 150.9028090 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

^{1}H NMR and ^{13}C NMR of compound **L16-B6** in D_2O

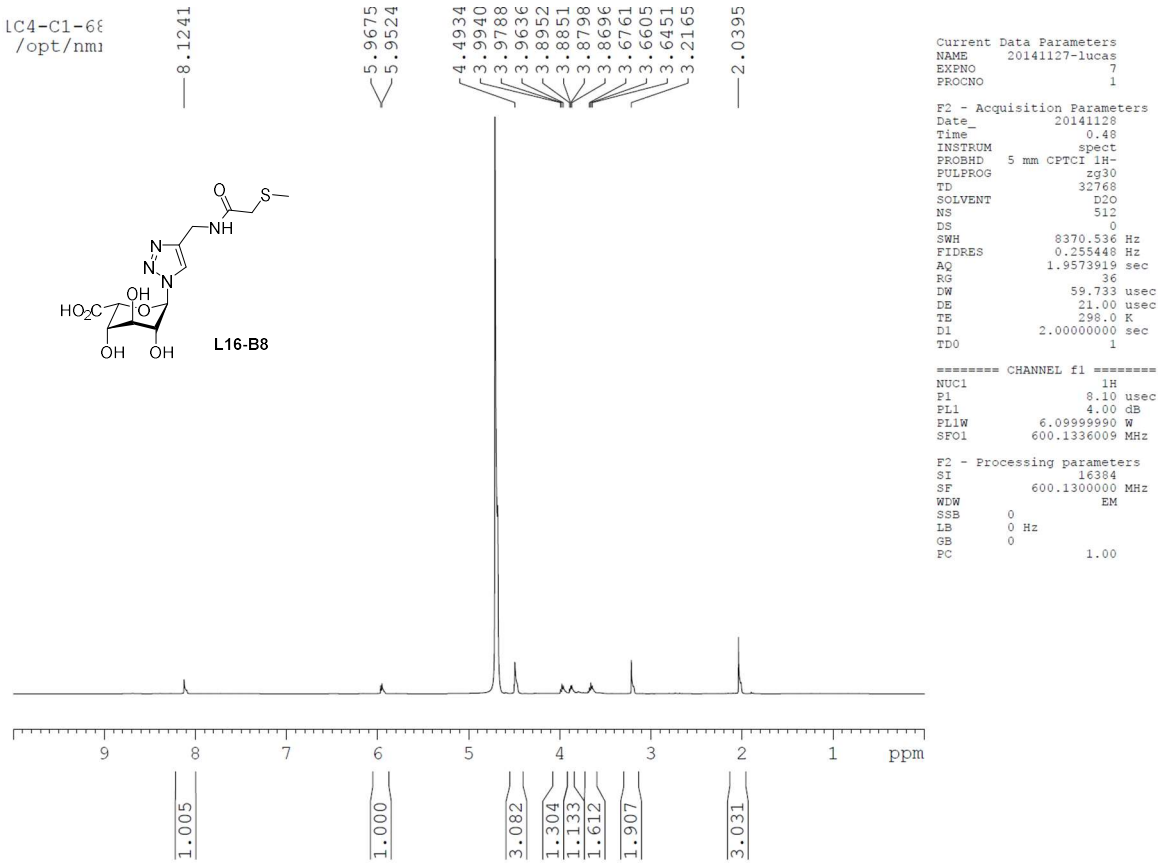



```
Current Data Parameters
NAME                  20141107
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141107
Time                     19.50
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                  zg30
TD                      32768
SOLVENT                   D2O
NS                        512
DS                          0
SWH                  8389.262 Hz
FIDRES               0.256020 Hz
AQ                   1.9530228 sec
RG                        40.3
DW                      59.600 usec
DE                      21.00 usec
TE                      298.0 K
D1                   2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      10.15 usec
PL1                     -0.80 dB
PL1W                18.11971092 W
SFO1                600.1536010 MHz

F2 - Processing parameters
SI                       16384
SF                  600.1499505 MHz
WDW                         EM
SSB          0
LB           0 Hz
GB           0
PC                        1.00
```




```
Current Data Parameters
NAME                  20141107
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141107
Time                     20.55
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG               zgpg30
TD                     131072
SOLVENT                   D2O
NS                       1024
DS                          0
SWH                 39062.500 Hz
FIDRES               0.298023 Hz
AQ                   1.6777716 sec
RG                        3640
DW                      12.800 usec
DE                      21.00 usec
TE                      298.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                      11.15 usec
PL1                      2.80 dB
PL1W                49.17097855 W
SFO1               150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.33 dB
PL12                    16.50 dB
PL13                    19.50 dB
PL2W                13.96854782 W
PL12W                0.33740479 W
PL13W                0.16910298 W
SFO2               600.1524006 MHz

F2 - Processing parameters
SI                       65536
SF                  150.9078380 MHz
WDW                         EM
SSB          0
LB                       2.00 Hz
GB           0
PC                        1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-B8** in D_2O

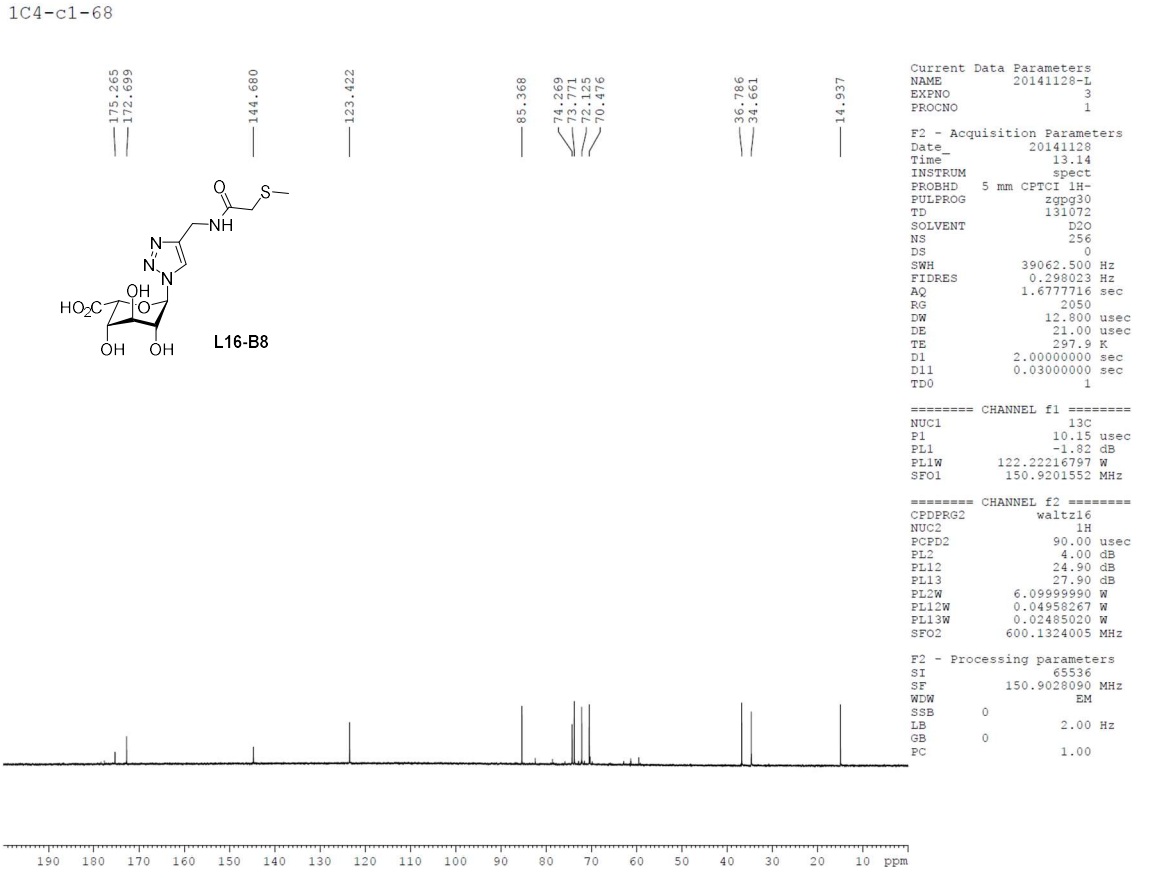


Current Data Parameters
NAME 20141127-lucas
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141128
Time 0.48
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32768
SOLVENT D2O
NS 512
DS 0
SWH 8370.536 Hz
FIDRES 0.255448 Hz
AQ 1.9573919 sec
RG 36
DW 59.733 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 4.00 dB
PL1W 6.09999990 W
SFO1 600.1336009 MHz

F2 - Processing parameters
SI 16384
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20141128-L
EXPNO 3
PROCNO 1

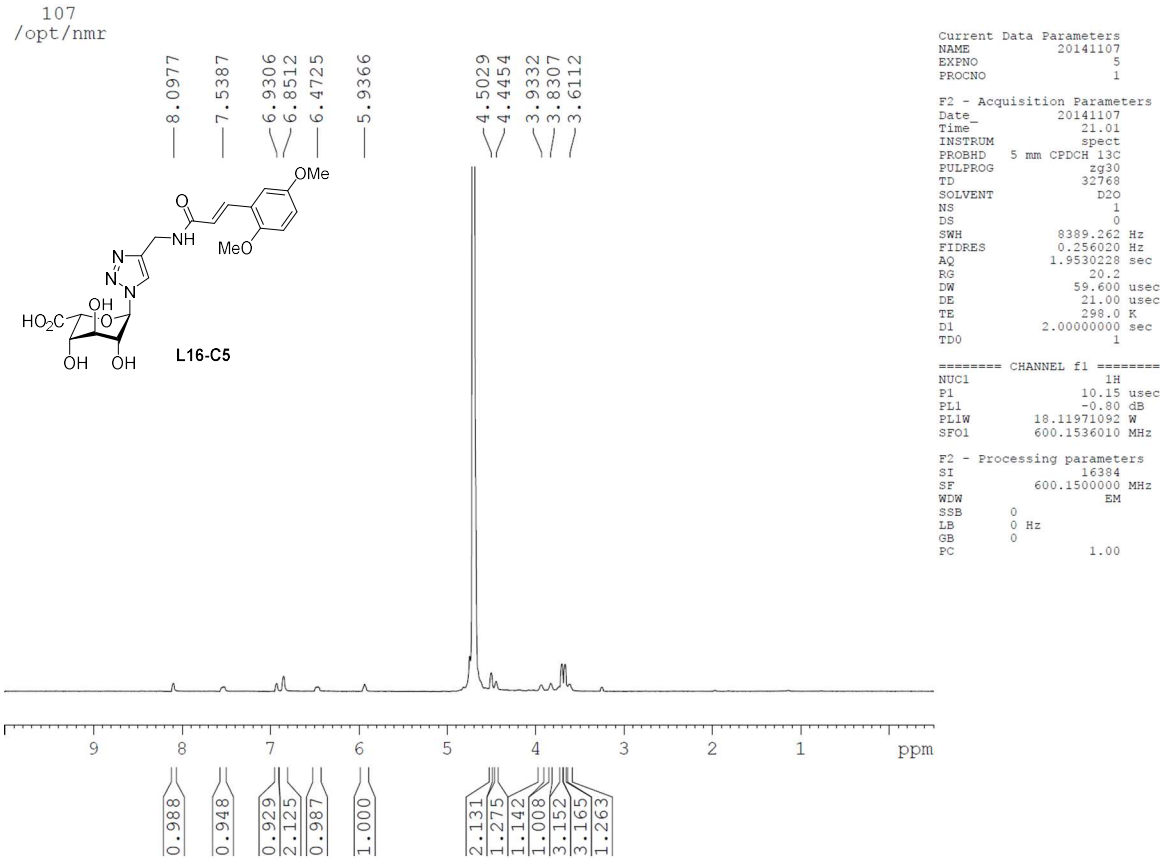
F2 - Acquisition Parameters
Date_ 20141128
Time 13.14
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 131072
SOLVENT D2O
NS 256
DS 0
SWH 39062.500 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 2050
DW 12.800 usec
DE 21.00 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.15 usec
PL1 -1.82 dB
PL1W 122.22216797 W
SFO1 150.9201552 MHz

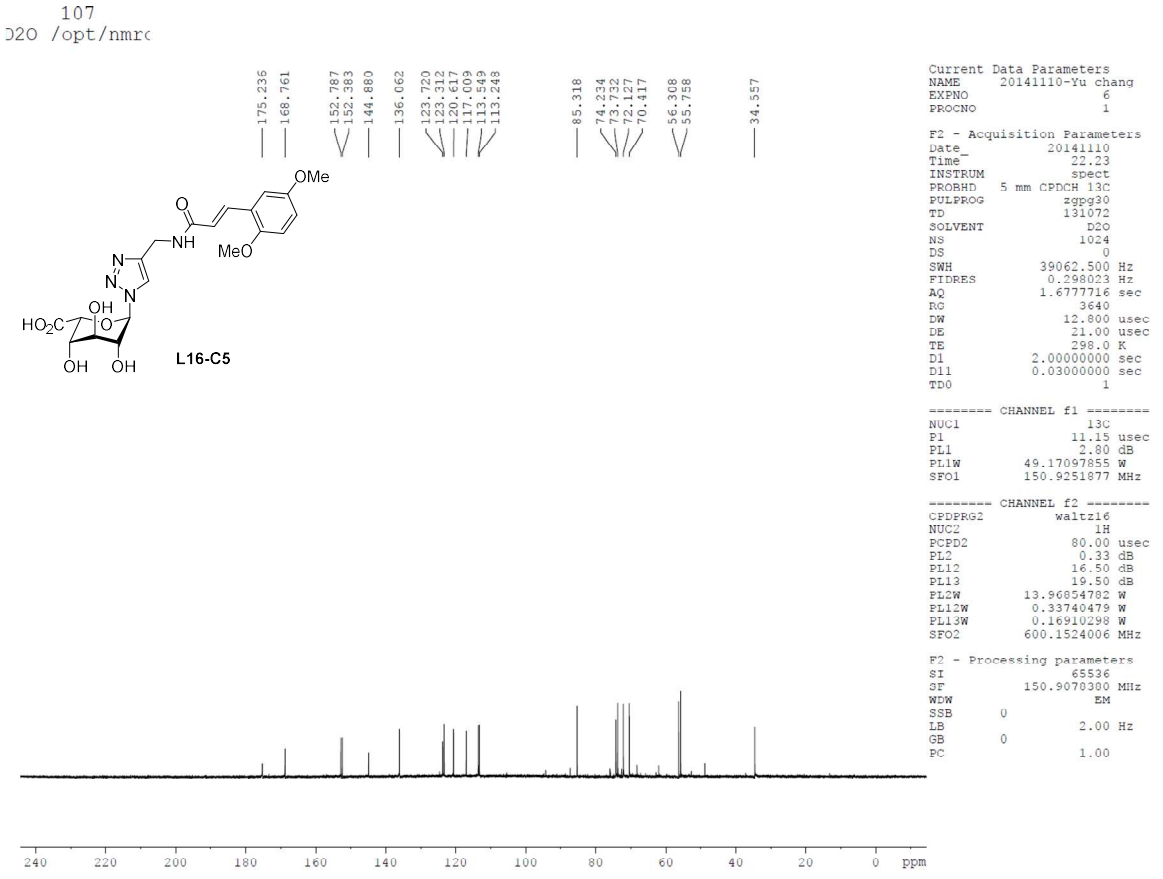
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.00 dB
PL12 24.90 dB
PL13 27.90 dB
PL2W 6.09999990 W
PL12W 0.04958267 W
PL13W 0.02485020 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 65536
SF 150.9028090 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

^{1}H NMR and ^{13}C NMR of compound **L16-C5** in D_2O

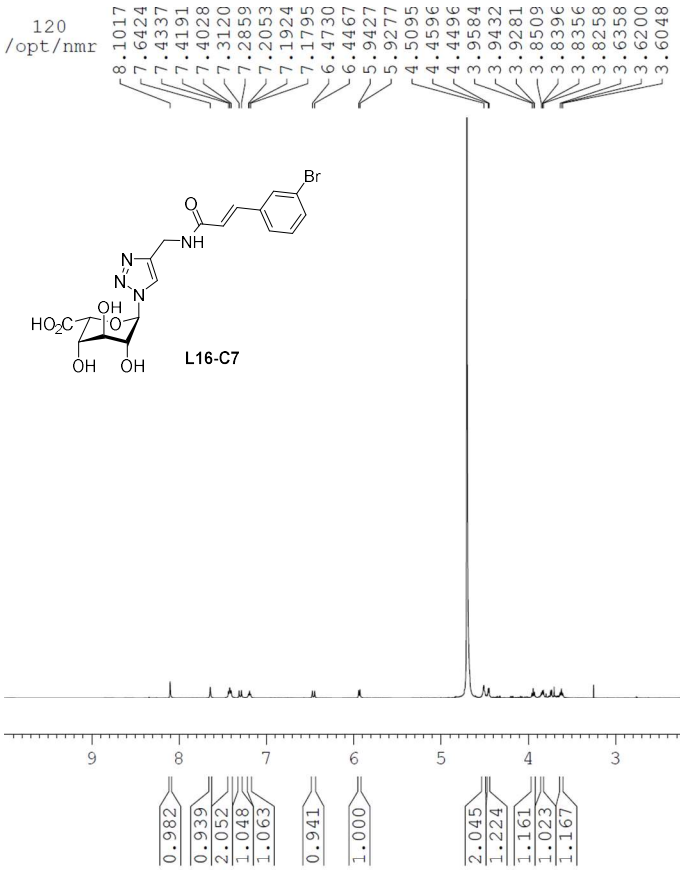



```
Current Data Parameters
NAME                  20141107
EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141107
Time                     21.01
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                  zg30
TD                      32768
SOLVENT                    D2O
NS                           1
DS                           0
SWH                 8389.262 Hz
FIDRES                 0.256020 Hz
AQ                  1.9530228 sec
RG                        20.2
DW                      59.600 usec
DE                      21.00 usec
TE                      298.0 K
D1                  2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      10.15 usec
PL1                     -0.80 dB
PL1W                18.11971092 W
SFO1                600.1536010 MHz

F2 - Processing parameters
SI                       16384
SF                  600.1500000 MHz
WDW                         EM
SSB                  0
LB                   0 Hz
GB                   0
PC                        1.00
```

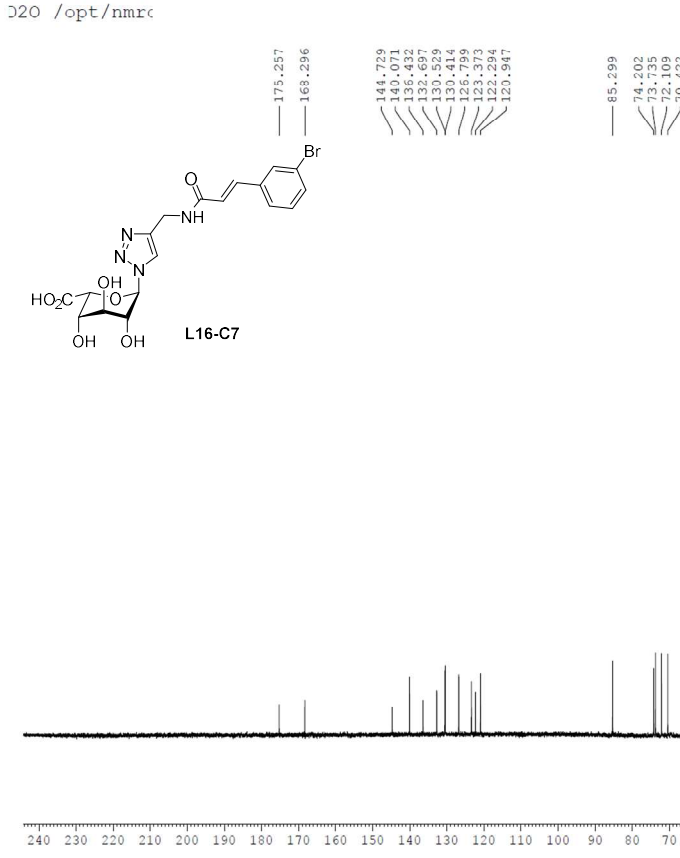



```
Current Data Parameters
NAME      20141110-Yu chang
EXPNO                        6
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141110
Time                     22.23
INSTRUM                  spect
PROBHD    5 mm CPDCH 13C
PULPROG                zgpg30
TD                     131072
SOLVENT                    D2O
NS                        1024
DS                           0
SWH                39062.500 Hz
FIDRES                 0.298023 Hz
AQ                  1.6777716 sec
RG                        3640
DW                      12.800 usec
DE                      21.00 usec
TE                      298.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                      11.15 usec
PL1                      2.80 dB
PL1W                49.17097855 W
SFO1                150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.33 dB
PL12                    16.50 dB
PL13                    19.50 dB
PL2W                13.96854782 W
PL12W                0.33740479 W
PL13W                0.16910298 W
SFO2                600.1524006 MHz

F2 - Processing parameters
SI                       65536
SF                  150.9070300 MHz
WDW                         EM
SSB                  0
LB                       2.00 Hz
GB                   0
PC                        1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-C7** in D_2O



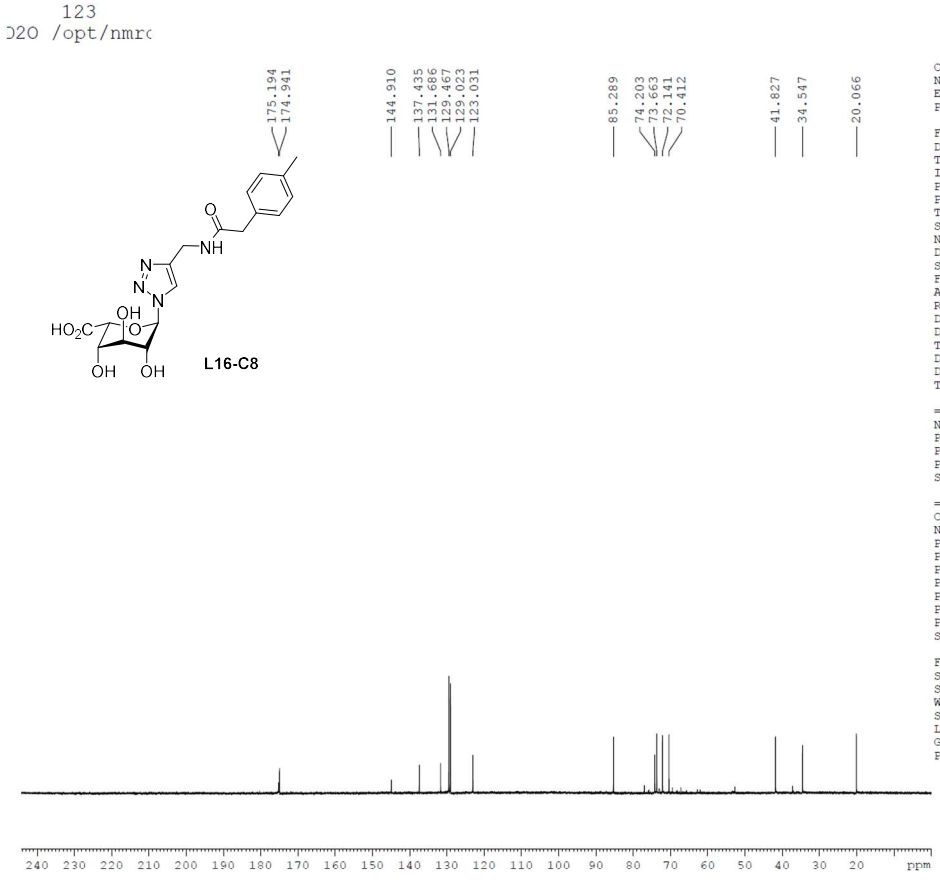

```
Current Data Parameters
NAME      20141117-yu chang
EXPNO                    13
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141117
Time                 22.55
INSTRUM              spect
PROBHD   5 mm CPDCH 13C
PULPROG               zg30
TD                   32768
SOLVENT                D2O
NS                       512
DS                         0
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                      50.8
DW                   59.600 usec
DE                   21.00 usec
TE                   298.1 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.15 usec
PL1                    -0.80 dB
PL1W            18.11971092 W
SFO1            600.1536010 MHz

F2 - Processing parameters
SI                       16384
SF                600.1500000 MHz
WDW                         EM
SSB          0
LB           0 Hz
GB           0
PC                       1.00
```




```
Current Data Parameters
NAME      20141205-lucas
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_              20141205
Time                 22.33
INSTRUM              spect
PROBHD   5 mm CPDCH 13C
PULPROG             zgpg30
TD                  131072
SOLVENT                D2O
NS                      1024
DS                         0
SWH               39062.500 Hz
FIDRES             0.298023 Hz
AQ                 1.6777716 sec
RG                      3640
DW                   12.800 usec
DE                   21.00 usec
TE                   298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.15 usec
PL1                     2.80 dB
PL1W            49.17097855 W
SFO1            150.9251077 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.33 dB
PL12                   16.50 dB
PL13                   19.50 dB
PL2W            13.96854782 W
PL12W            0.33740479 W
PL13W            0.16910298 W
SFO2            600.1524006 MHz

F2 - Processing parameters
SI                       65536
SF                150.9078380 MHz
WDW                         EM
SSB          0
LB                       2.00 Hz
GB           0
PC                       1.00
```

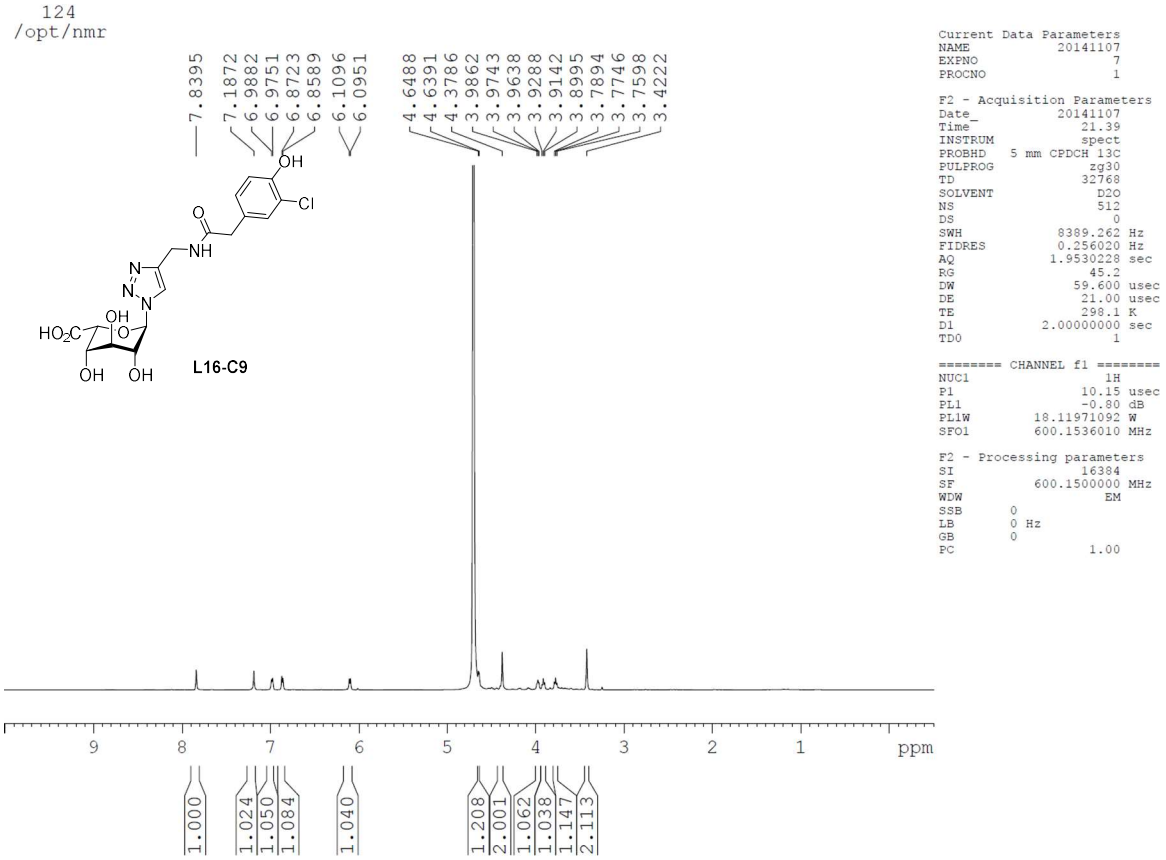
^{1}H NMR and ^{13}C NMR of compound **L16-C8** in D_2O


```
Current Data Parameters
NAME      20141119-yu chang
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141120
Time                   3.46
INSTRUM               spect
PROBHD   5 mm CPDCH 13C
PULPROG                zg30
TD                    32768
SOLVENT                 D2O
NS                      512
DS                        0
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                      45.2
DW                    59.600 usec
DE                    21.00 usec
TE                    298.0 K
D1                 2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.15 usec
PL1                    -0.80 dB
PL1W              18.11971092 W
SFO1              600.1536010 MHz

F2 - Processing parameters
SI                        16384
SF                600.1500000 MHz
WDW                          EM
SSB          0
LB           0 Hz
GB           0
PC                        1.00
```

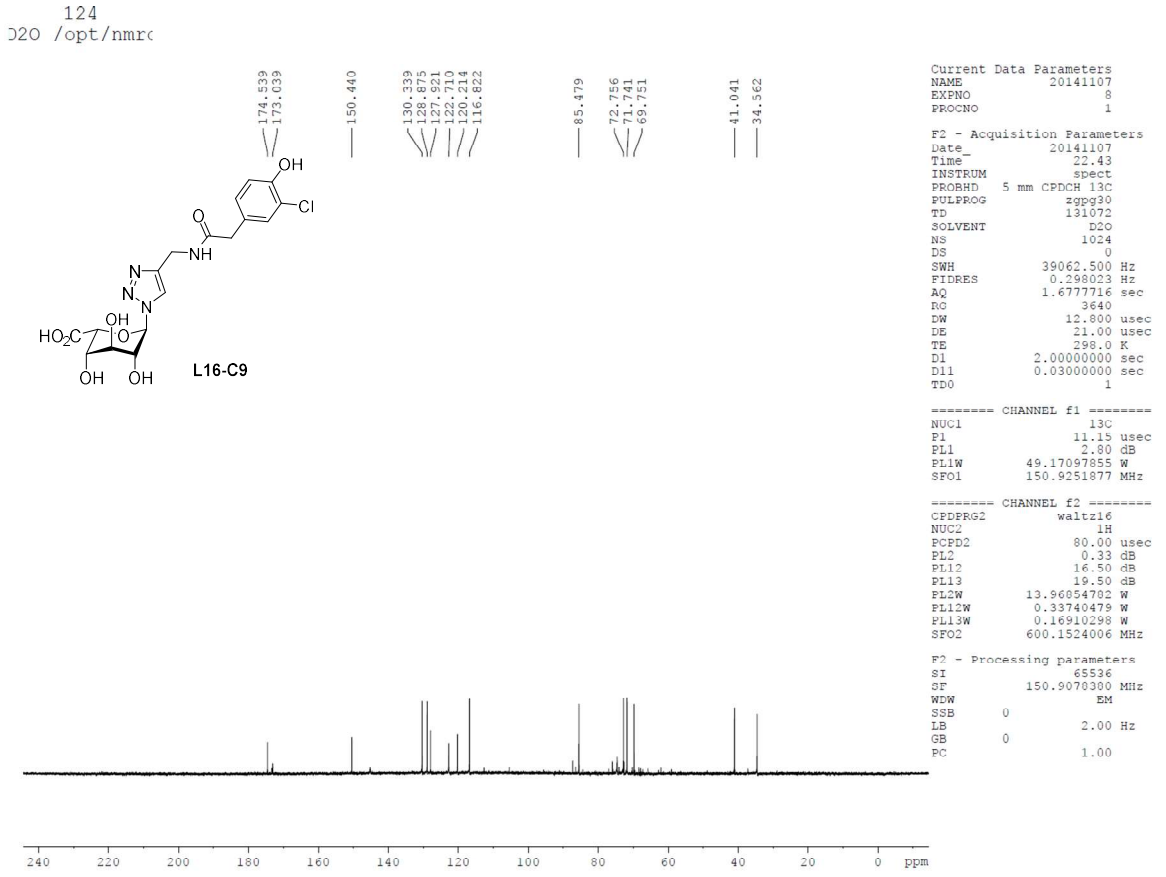



```
Current Data Parameters
NAME      201412008-lucas
EXPNO                    12
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141120
Time                   4.50
INSTRUM               spect
PROBHD   5 mm CPDCH 13C
PULPROG             zgpg30
TD                   131072
SOLVENT                 D2O
NS                     1024
DS                        0
SWH               39062.500 Hz
FIDRES             0.298023 Hz
AQ                 1.6777716 sec
RG                     3640
DW                   12.800 usec
DE                    21.00 usec
TE                    298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.15 usec
PL1                     2.80 dB
PL1W              49.17097855 W
SFO1              150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.33 dB
PL12                   16.50 dB
PL13                   19.50 dB
PL2W              13.96854782 W
PL12W              0.33740479 W
PL13W              0.16910298 W
SFO2              600.1524006 MHz

F2 - Processing parameters
SI                        65536
SF                150.9078380 MHz
WDW                          EM
SSB          0
LB                     2.00 Hz
GB           0
PC                        1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-C9** in D_2O

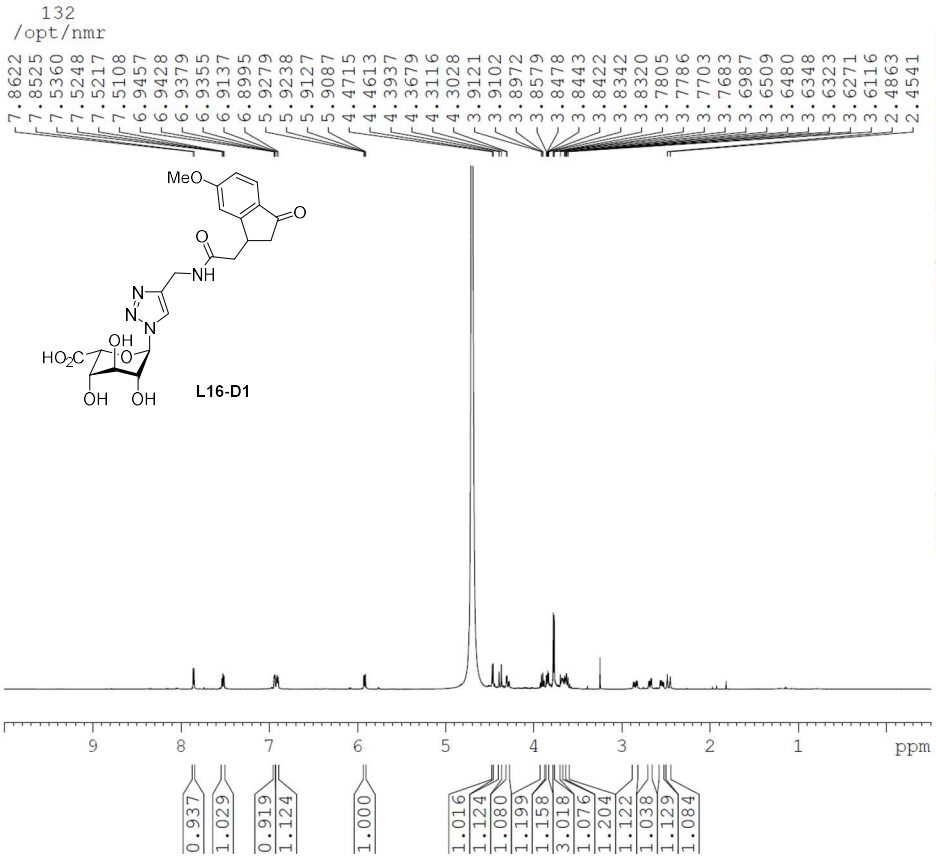



```
Current Data Parameters
NAME                  20141107
EXPNO                        7
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141107
Time                     21.39
INSTRUM                  spect
PROBHD     5 mm CPDCH 13C
PULPROG                  zg30
TD                      32768
SOLVENT                   D2O
NS                        512
DS                          0
SWH                  8389.262 Hz
FIDRES               0.256020 Hz
AQ                   1.9530228 sec
RG                        45.2
DW                      59.600 usec
DE                      21.00 usec
TE                      298.1 K
D1                   2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      10.15 usec
PL1                     -0.80 dB
PL1W                18.11971092 W
SFO1                600.1536010 MHz

F2 - Processing parameters
SI                       16384
SF                  600.1500000 MHz
WDW                         EM
SSB                 0
LB                  0 Hz
GB                  0
PC                       1.00
```




```
Current Data Parameters
NAME                  20141107
EXPNO                        8
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141107
Time                     22.43
INSTRUM                  spect
PROBHD     5 mm CPDCH 13C
PULPROG                zgpg30
TD                     131072
SOLVENT                   D2O
NS                       1024
DS                          0
SWH                 39062.500 Hz
FIDRES               0.298023 Hz
AQ                   1.6777716 sec
RG                        3640
DW                      12.800 usec
DE                      21.00 usec
TE                      298.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                      11.15 usec
PL1                      2.80 dB
PL1W                49.17097855 W
SFO1                150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.33 dB
PL12                    16.50 dB
PL13                    19.50 dB
PL2W                13.96054702 W
PL12W                0.33740479 W
PL13W                0.16910298 W
SFO2                600.1524006 MHz

F2 - Processing parameters
SI                       65536
SF                  150.9070300 MHz
WDW                         EM
SSB                 0
LB                      2.00 Hz
GB                  0
PC                       1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-D1** in D_2O

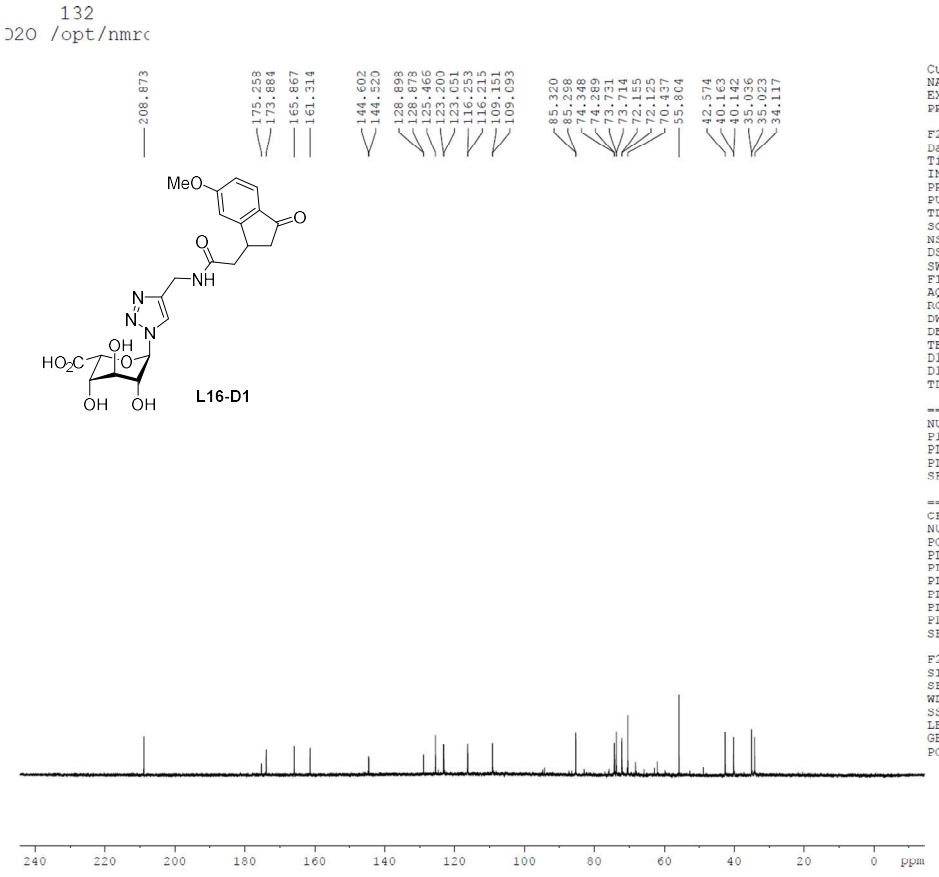


Current Data Parameters
NAME 20141107
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141108
Time 1.01
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 32768
SOLVENT D2O
NS 512
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 20.2
DW 59.600 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -0.80 dB
PL1W 18.11971092 W
SFO1 600.1536010 MHz

F2 - Processing parameters
SI 16384
SF 600.1500000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20141107
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141108
Time 2.05
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 131072
SOLVENT D2O
NS 1024
DS 0
SWH 39062.500 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 3640
DW 12.800 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.15 usec
PL1 2.80 dB
PL1W 49.17097855 W
SFO1 150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.33 dB
PL12 16.50 dB
PL13 19.50 dB
PL2W 13.96854702 W
PL12W 0.33740479 W
PL13W 0.16910298 W
SFO2 600.1524006 MHz

F2 - Processing parameters
SI 65536
SF 150.9078380 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

^{1}H NMR and ^{13}C NMR of compound **L16-D3** in D_2O

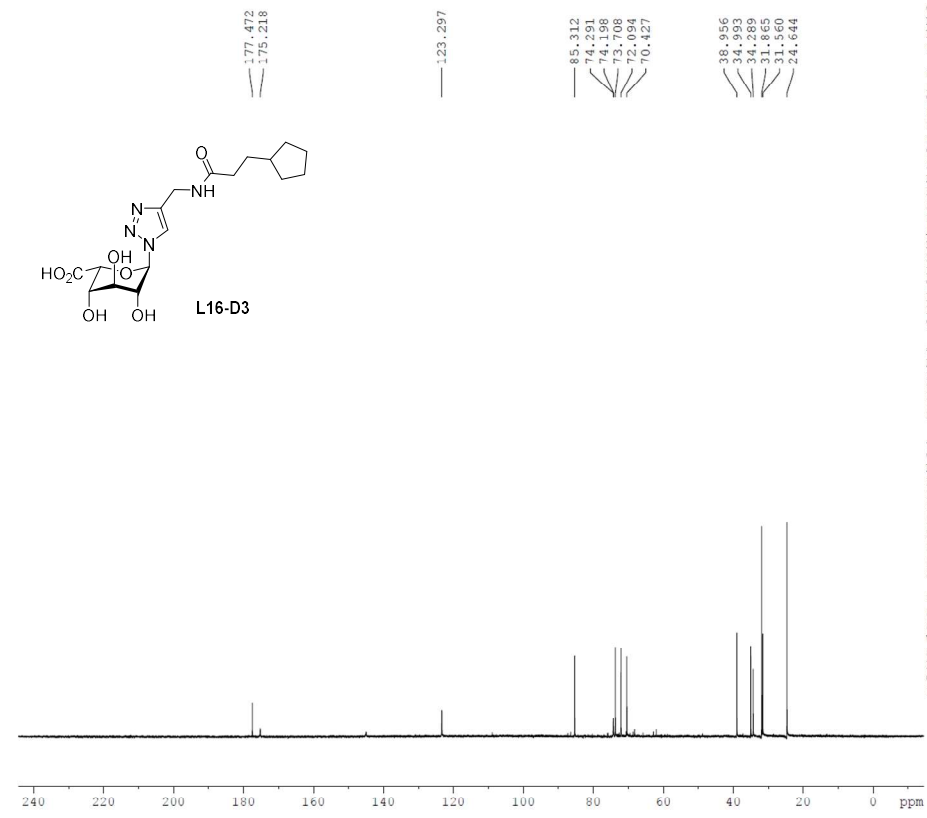
Current Data Parameters
NAME 20141117-yu chang
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141118
Time 0.37
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 32768
SOLVENT D2O
NS 512
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 45.2
DW 59.600 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -0.80 dB
PL1W 18.11971092 W
SFO1 600.1536010 MHz

F2 - Processing parameters
SI 16384
SF 600.1500000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

135
D2O /opt/nmrc



Current Data Parameters
NAME 20141117-yu chang
EXPNO 16
PROCNO 1

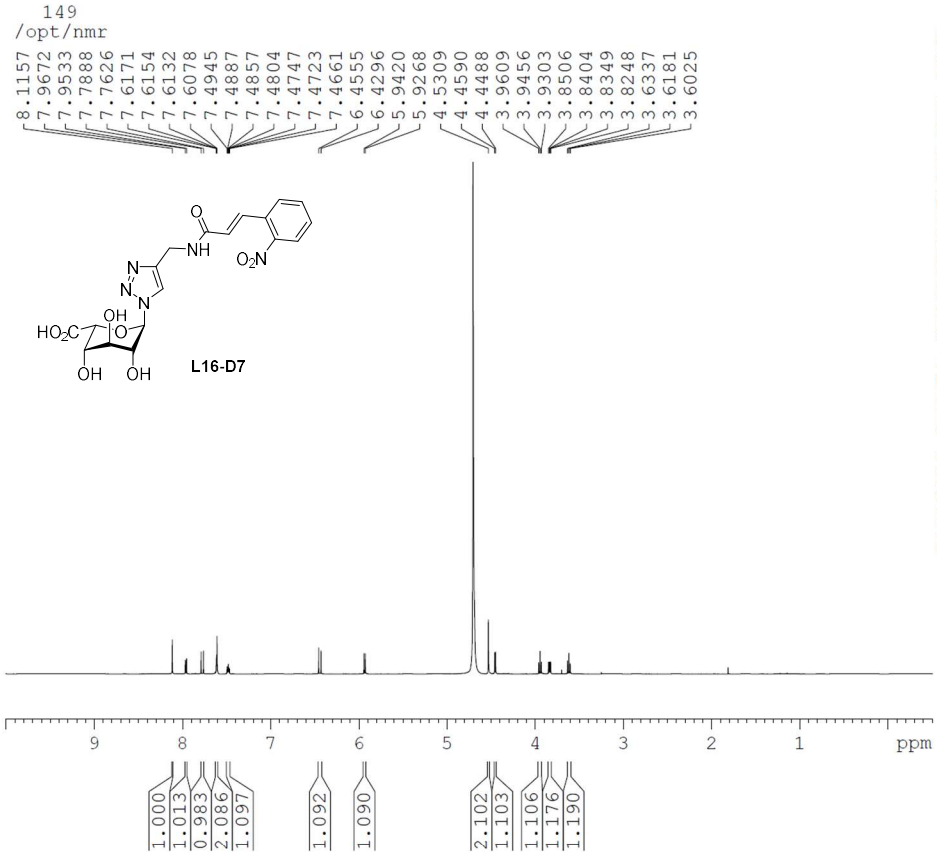
F2 - Acquisition Parameters
Date_ 20141118
Time 1.42
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 131072
SOLVENT D2O
NS 1024
DS 0
SWH 39062.500 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 3640
DW 12.800 usec
DE 21.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.15 usec
PL1 2.80 dB
PL1W 49.17097855 W
SFO1 150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.33 dB
PL12 16.50 dB
PL13 19.50 dB
PL2W 13.96054702 W
PL12W 0.33740479 W
PL13W 0.16910298 W
SFO2 600.1524006 MHz

F2 - Processing parameters
SI 65536
SF 150.9070300 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

^{1}H NMR and ^{13}C NMR of compound **L16-D7** in D_2O

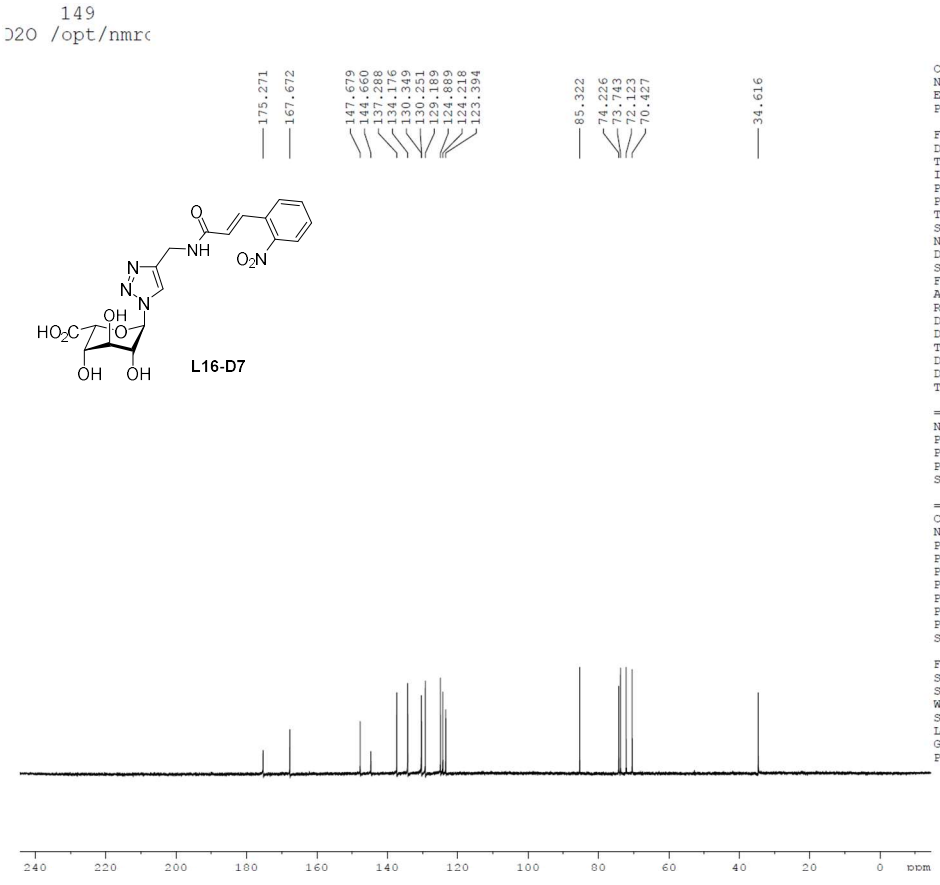


Current Data Parameters
NAME 20141107
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141108
Time 2.42
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 32768
SOLVENT D2O
NS 512
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 40.3
DW 59.600 usec
DE 21.00 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -0.80 dB
PL1W 18.11971092 W
SFO1 600.1536010 MHz

F2 - Processing parameters
SI 16384
SF 600.1500000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20141107
EXPNO 14
PROCNO 1

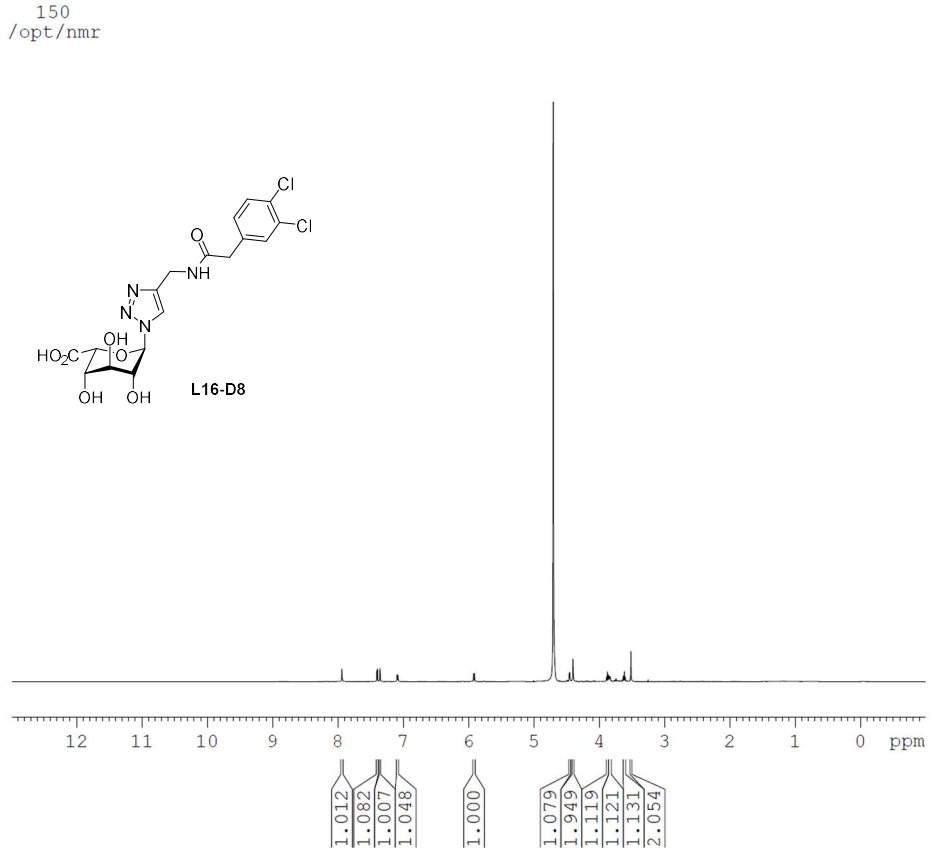
F2 - Acquisition Parameters
Date_ 20141108
Time 3.46
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 131072
SOLVENT D2O
NS 1024
DS 0
SWH 39062.500 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 3640
DW 12.800 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.15 usec
PL1 2.80 dB
PL1W 49.17097855 W
SFO1 150.9251877 MHz

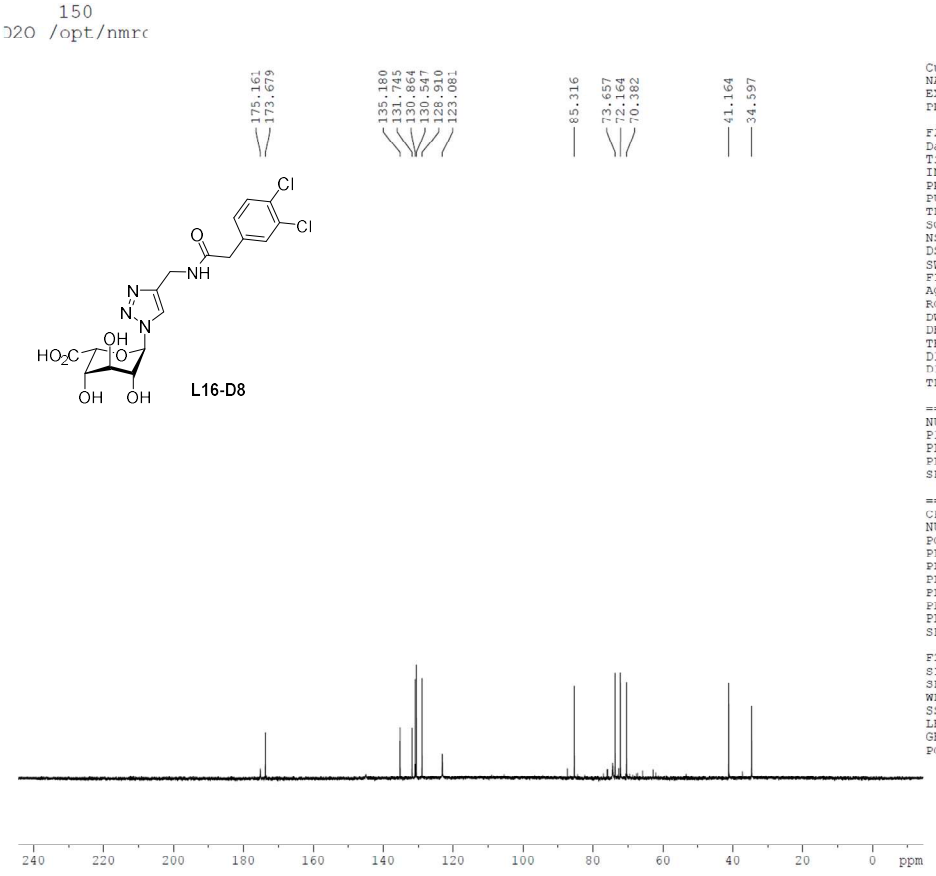
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.33 dB
PL12 16.50 dB
PL13 19.50 dB
PL2W 13.96854782 W
PL12W 0.33740479 W
PL13W 0.16910298 W
SFO2 600.1524006 MHz

F2 - Processing parameters
SI 65536
SF 150.9078380 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

^{1}H NMR and ^{13}C NMR of compound **L16-D8** in D_2O

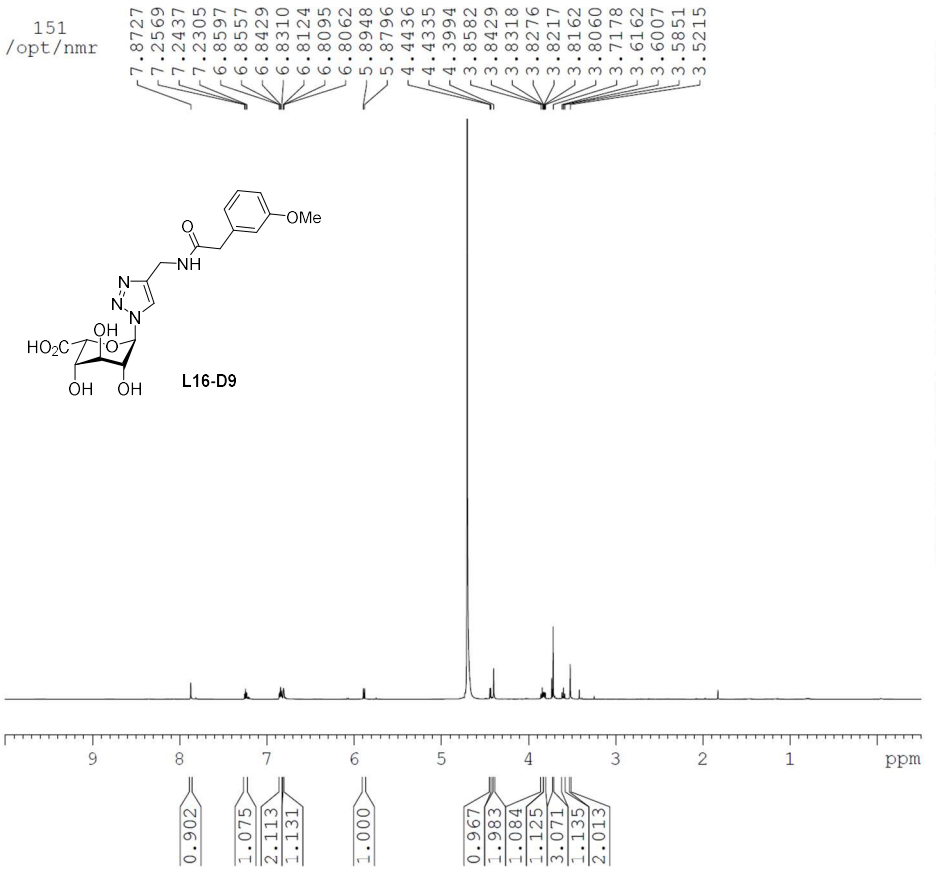



```
Current Data Parameters
NAME      20141119-yu chang
EXPNO                    13
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141120
Time                   5.27
INSTRUM               spect
PROBHD   5 mm CPDCH 13C
PULPROG                zg30
TD                    32768
SOLVENT                 D2O
NS                      512
DS                        0
SWH                8389.262 Hz
FIDRES            0.256020 Hz
AQ                1.9530228 sec
RG                     45.2
DW                   59.600 usec
DE                   21.00 usec
TE                   298.1 K
D1                2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.15 usec
PL1                   -0.80 dB
PL1W           18.11971092 W
SFO1           600.1536010 MHz

F2 - Processing parameters
SI                    16384
SF             600.1500000 MHz
WDW                      EM
SSB          0
LB           0 Hz
GB           0
PC                    1.00
```

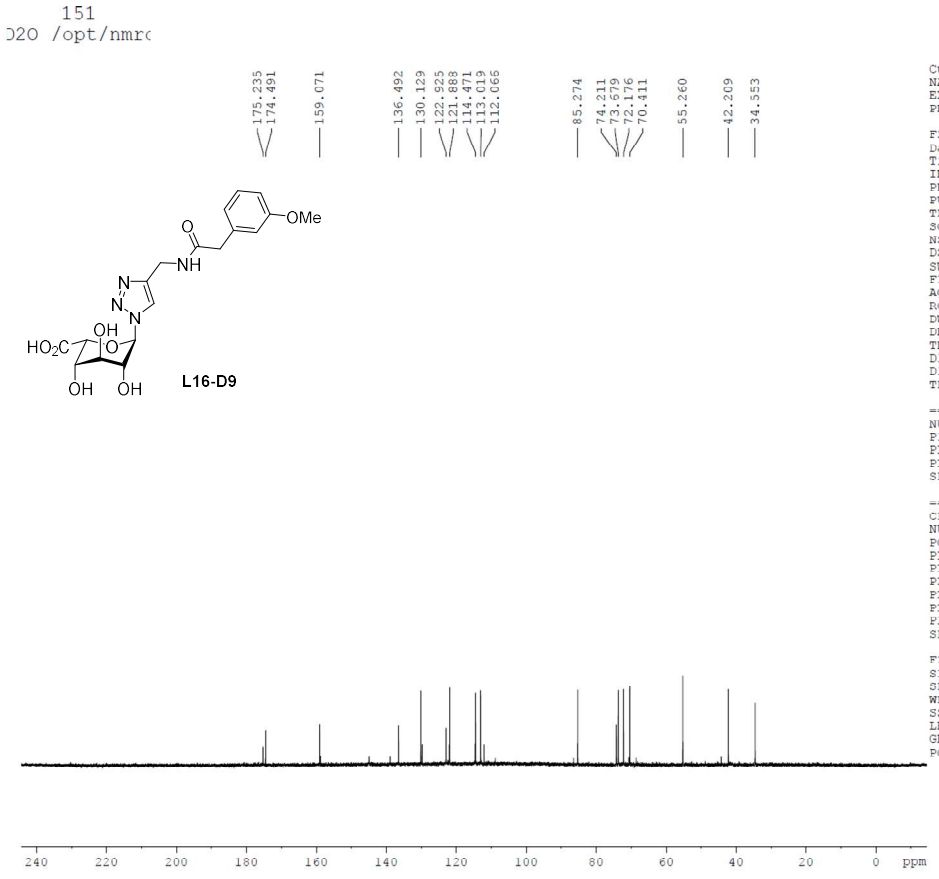



```
Current Data Parameters
NAME      20141119-yu chang
EXPNO                    14
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141120
Time                   6.31
INSTRUM               spect
PROBHD   5 mm CPDCH 13C
PULPROG             zgpg30
TD                   131072
SOLVENT                 D2O
NS                     1024
DS                        0
SWH               39062.500 Hz
FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                     3640
DW                   12.800 usec
DE                   21.00 usec
TE                   298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    11.15 usec
PL1                    2.80 dB
PL1W           49.17097855 W
SFO1          150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                    0.33 dB
PL12                  16.50 dB
PL13                  19.50 dB
PL2W           13.96854782 W
PL12W           0.33740479 W
PL13W           0.16910298 W
SFO2          600.1524006 MHz

F2 - Processing parameters
SI                    65536
SF             150.9078380 MHz
WDW                      EM
SSB          0
LB                    2.00 Hz
GB           0
PC                    1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-D9** in D_2O

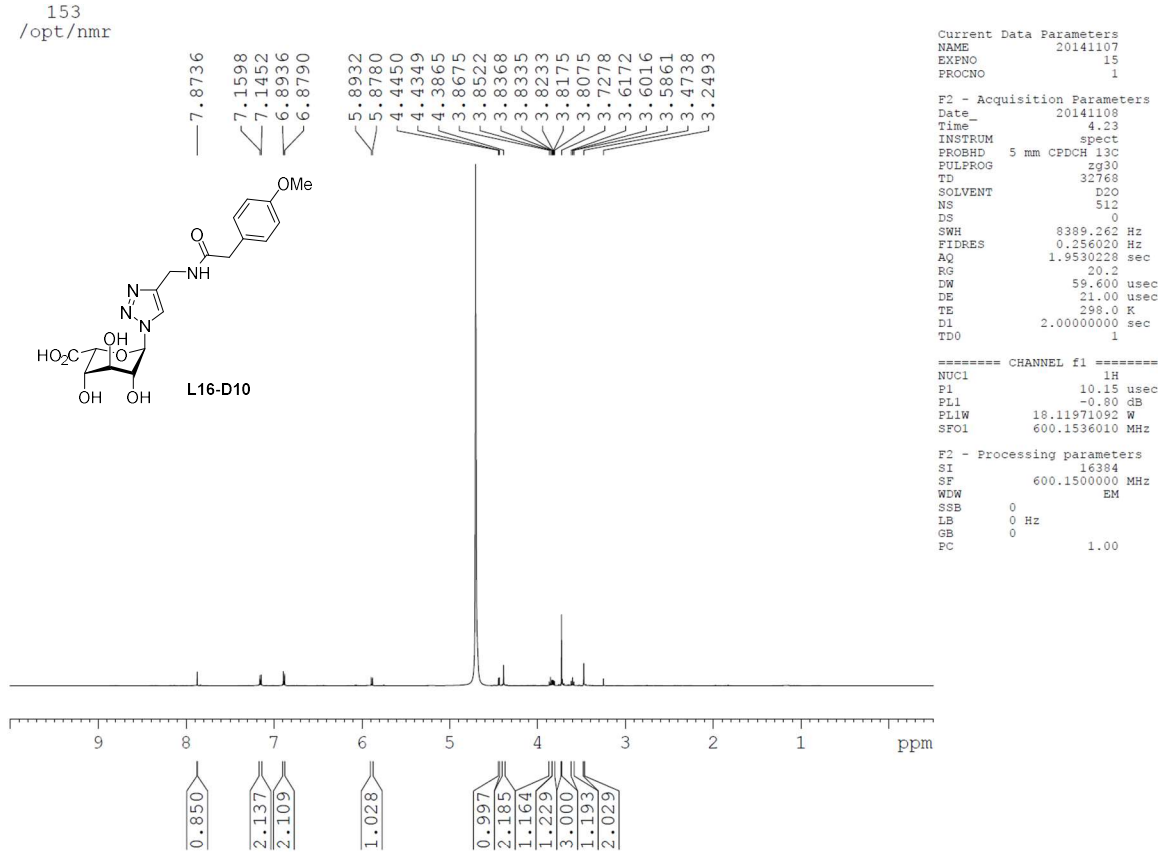



```
Current Data Parameters
NAME      20141117-yu chang
EXPNO                    19
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141118
Time                   4.00
INSTRUM               spect
PROBHD   5 mm CPDCH 13C
PULPROG                zg30
TD                    32768
SOLVENT                 D2O
NS                      512
DS                        0
SWH                8389.262 Hz
FIDRES            0.256020 Hz
AQ                1.9530228 sec
RG                     50.8
DW                   59.600 usec
DE                   21.00 usec
TE                   298.0 K
D1                2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.15 usec
PL1                   -0.80 dB
PL1W           18.11971092 W
SFO1           600.1536010 MHz

F2 - Processing parameters
SI                     16384
SF                600.1500000 MHz
WDW                       EM
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```




```
Current Data Parameters
NAME      20141117-yu chang
EXPNO                    20
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141118
Time                   5.04
INSTRUM               spect
PROBHD   5 mm CPDCH 13C
PULPROG            zgpg30
TD                   131072
SOLVENT                 D2O
NS                     1024
DS                        0
SWH               39062.500 Hz
FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                     3640
DW                   12.800 usec
DE                   21.00 usec
TE                   298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    11.15 usec
PL1                    2.80 dB
PL1W           49.17097855 W
SFO1           150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    0.33 dB
PL12                  16.50 dB
PL13                  19.50 dB
PL2W           13.96054702 W
PL12W           0.33740479 W
PL13W           0.16910298 W
SFO2           600.1524006 MHz

F2 - Processing parameters
SI                     65536
SF                150.9070300 MHz
WDW                       EM
SSB          0
LB                     2.00 Hz
GB           0
PC                     1.00
```

^{1}H NMR and ^{13}C NMR of compound **L16-D10** in D_2O

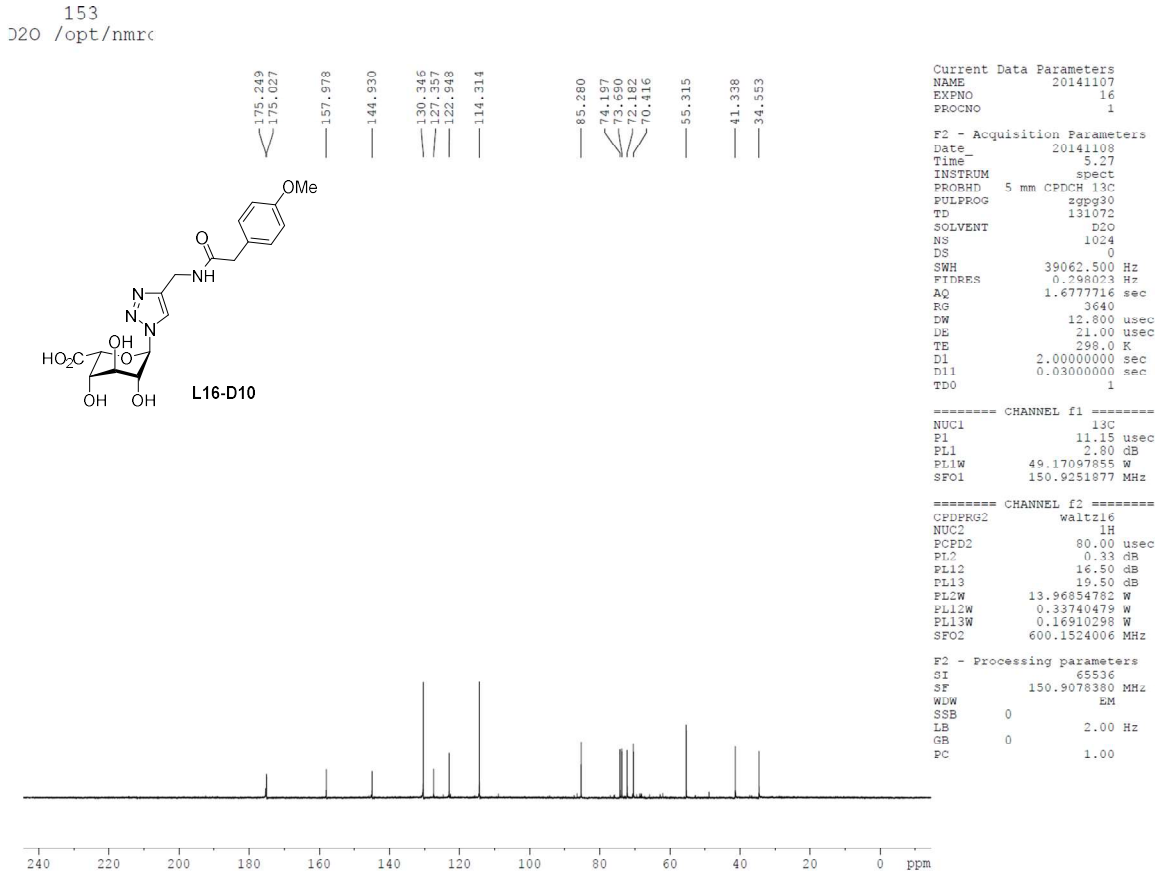


Current Data Parameters
NAME 20141107
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141108
Time 4.23
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 32768
SOLVENT D2O
NS 512
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 20.2
DW 59.600 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -0.80 dB
PL1W 18.11971092 W
SFO1 600.1536010 MHz

F2 - Processing parameters
SI 16384
SF 600.1500000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20141107
EXPNO 16
PROCNO 1

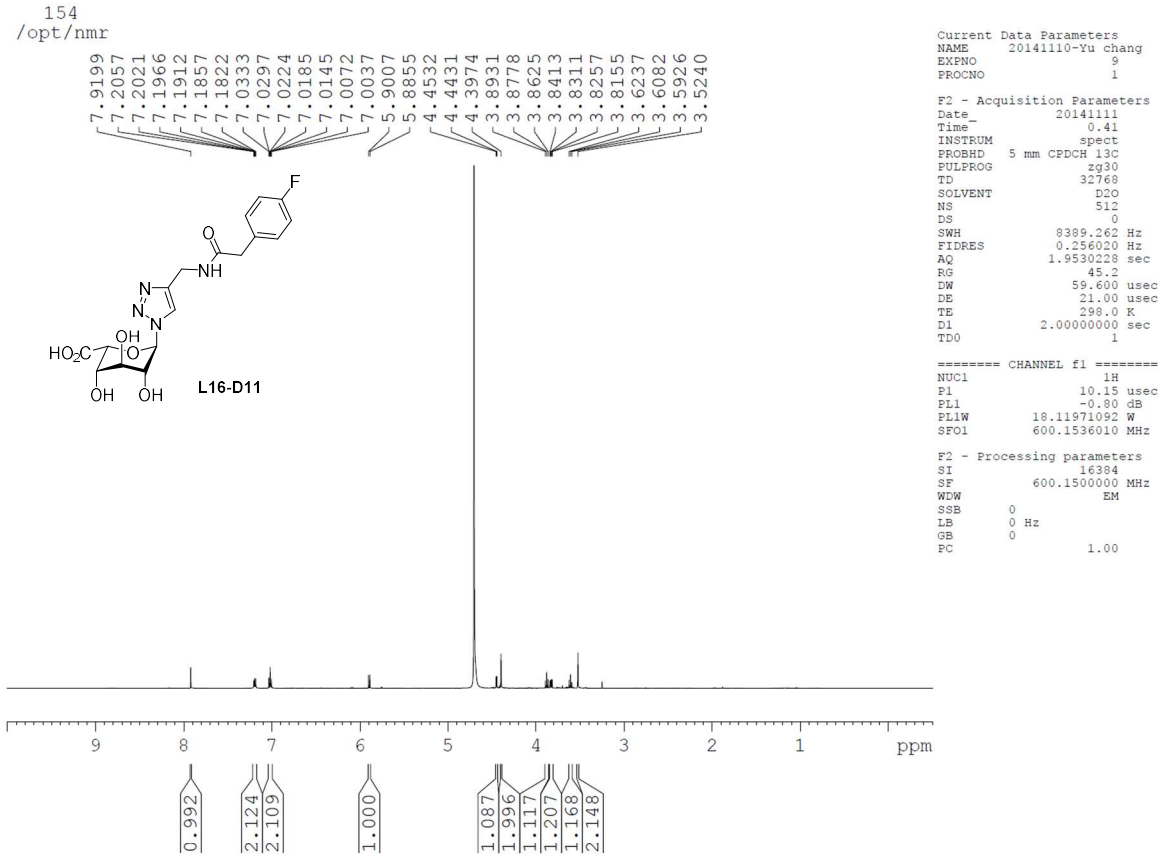
F2 - Acquisition Parameters
Date_ 20141108
Time 5.27
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 131072
SOLVENT D2O
NS 1024
DS 0
SWH 39062.500 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 3640
DW 12.800 usec
DE 21.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.15 usec
PL1 2.80 dB
PL1W 49.17097855 W
SFO1 150.9251877 MHz

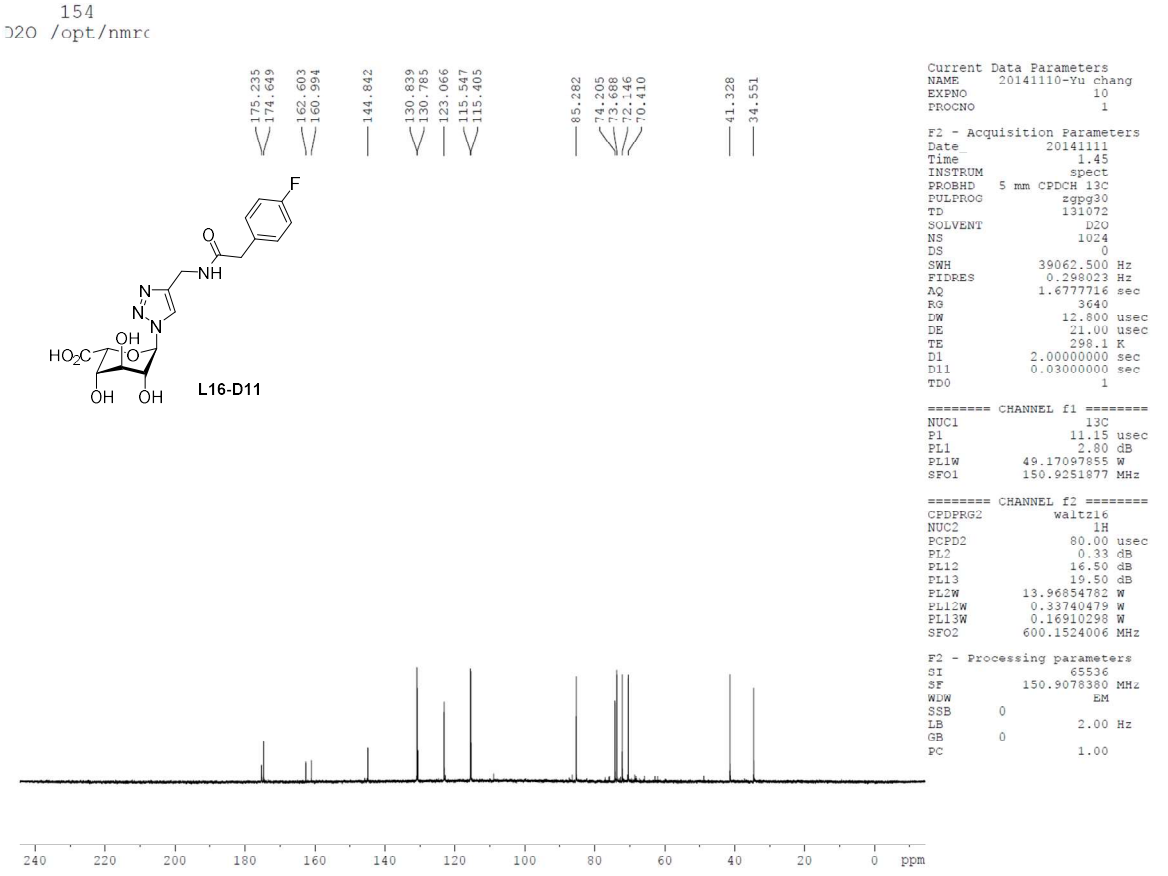
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.33 dB
PL12 16.50 dB
PL13 19.50 dB
PL2W 13.96854782 W
PL12W 0.33740479 W
PL13W 0.16910298 W
SFO2 600.1524006 MHz

F2 - Processing parameters
SI 65536
SF 150.9078380 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

^{1}H NMR and ^{13}C NMR of compound **L16-D11** in D_2O




```
Current Data Parameters
NAME      20141110-Yu chang
EXPNO                    9
PROCNO                   1

F2 - Acquisition Parameters
Date_              20141111
Time                   0.41
INSTRUM               spect
PROBHD   5 mm CPDCH 13C
PULPROG                zg30
TD                    32768
SOLVENT                 D2O
NS                      512
DS                        0
SWH                8389.262 Hz
FIDRES            0.256020 Hz
AQ                1.9530228 sec
RG                     45.2
DW                   59.600 usec
DE                   21.00 usec
TE                   298.0 K
D1                2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.15 usec
PL1                   -0.80 dB
PL1W           18.11971092 W
SFO1           600.1536010 MHz

F2 - Processing parameters
SI                    16384
SF             600.1500000 MHz
WDW                      EM
SSB          0
LB           0 Hz
GB           0
PC                    1.00
```




```
Current Data Parameters
NAME      20141110-Yu chang
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20141111
Time                   1.45
INSTRUM               spect
PROBHD   5 mm CPDCH 13C
PULPROG             zgpg30
TD                   131072
SOLVENT                 D2O
NS                     1024
DS                        0
SWH               39062.500 Hz
FIDRES            0.298023 Hz
AQ                1.6777716 sec
RG                     3640
DW                   12.800 usec
DE                   21.00 usec
TE                   298.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    11.15 usec
PL1                    2.80 dB
PL1W           49.17097855 W
SFO1           150.9251877 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    0.33 dB
PL12                  16.50 dB
PL13                  19.50 dB
PL2W           13.96854782 W
PL12W           0.33740479 W
PL13W           0.16910298 W
SFO2           600.1524006 MHz

F2 - Processing parameters
SI                    65536
SF             150.9078380 MHz
WDW                      EM
SSB          0
LB                    2.00 Hz
GB           0
PC                    1.00
```

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