Supplementary Information

Surfaces Presenting α-Phenyl Mannoside Derivatives Enable Formation of Stable, High Coverage, Non-pathogenic *Escherichia coli* Biofilms against Pathogen Colonization

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Content:

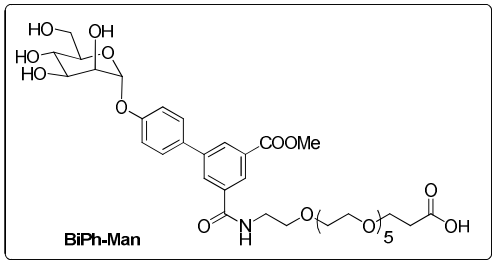
1. General Information

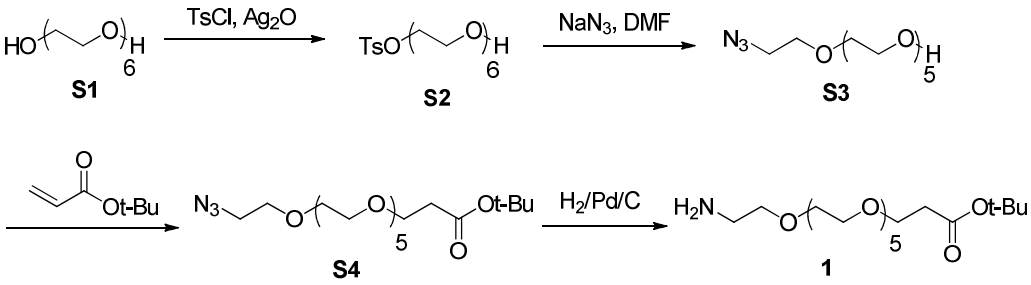
NMR spectra were recorded at 25 ^{o}C on JEOL ECX-400 and JEOL ECA-500 spectrometers. The chemical shifts were recorded in ppm relative to tetramethylsilane (TMS) and with the solvent resonance as the internal standard. ^{1}H NMR data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, br = broad), coupling constants (*J*) were reported in hertz (Hz), integration. ^{13}C NMR data were collected with complete proton decoupling. ESI-MS spectra were recorded on Thermo Finnigan LCQ Deca XP Plus LC/MSMS instrument using methanol solutions of the products through C18 column (Kinetex™ 5 μm XB-C18 100 Å, LC Column 50 × 4.6 mm, Phenomenex INC.) with gradient elution (10–95% Acetonitrile in H_2O, 12 min). Silicycle SiliaFlash F60 (40–63 μm) silica gel was used for the column chromatography.

2. Synthesis of mannosides

Synthesis of compound **Man** was described in our previous reports.[1]

2.1 Procedures for the synthesis of compound BiPh-Man





Compound **S3** was prepared in two steps according to the reported procedures.[2]

Synthesis of compound **S4**:

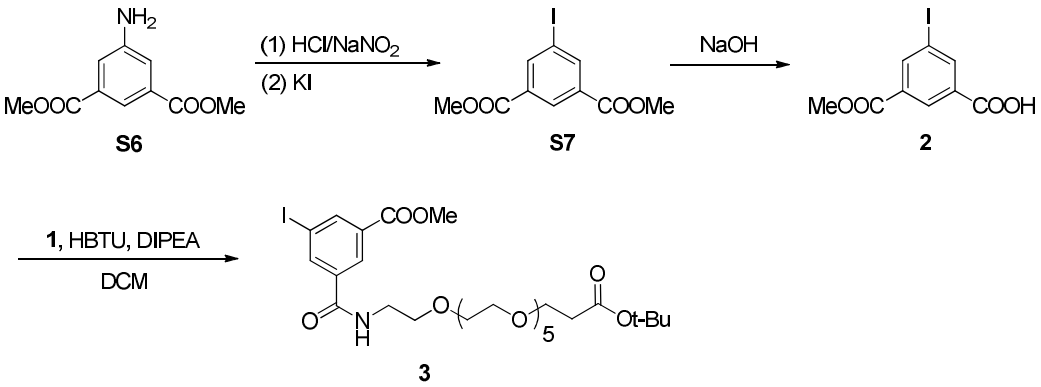
Under nitrogen atmosphere, to a solution of compound **S3** (2.8 g, 9.11 mmol) in anhydrous THF (15 mL) was added 60% sodium hydride suspended in mineral (10.6 mg, 0.05 equiv) at room temperature. After stirring for 10 minutes, *tert*-butyl acrylate (6.6 mL, 5 equiv) was added, and the mixture was allowed to stir for 12 h at room temperature. Followed the evaporation of the volatile components under reduced pressure, water (10 mL) and dichloromethane (15 mL) was added. The organic layer was separated, and the aqueous layer was extracted by dichloromethane (15 mL × 3). The combined organic layers were washed by brine (10 mL) and dried over anhydrous $MgSO_4$. After filtration and concentration, the residue was purified by silica gel column chromatography to afford the desired product **S4** (2.57 g, 65% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.70-3.6 (m, 24 H), 3.38 (t, J = 5.5 Hz, 2 H), 2.49 (t, J = 6.4 Hz, 2 H), 1.44 (s, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.95, 80.52, 70.72, 70.70, 70.6, 70.61, 70.52, 70.40, 70.08, 66.92, 50.69, 36.28, 28.13. MS (ESI): [M+Na^+] calcd for $C_{19}H_{37}N_3NaO_8$ = 458.2, Found 458.2.

Synthesis of compound **1**:

To a 50 mL round bottom flask was charged with compound **S4** (1.06 g, 2.43 mmol), Pd/C (259 mg, 10 mol%), and ethyl acetate (20 mL). The mixture was stirred and mildly bubbled by hydrogen for 4 hours at room temperature. Filtration and evaporation afforded the desired product **5** that was directly used for the next step without purification.

^{1}H NMR (500 MHz, $CDCl_3$): δ 3.55 (t, J = 6.3 Hz, 2 H), 3.50-3.40 (m, 20 H), 3.36 (t, J = 5.2 Hz, 2 H), 2.71 (t, J = 5.2 Hz, 2 H), 2.35 (t, J = 6.3 Hz, 2 H), 1.29 (s, 9 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 170.83, 80.39, 73.43, 70.53, 70.44, 70.32, 70.23, 66.83, 41.77, 36.19, 28.06. MS (ESI): [M+H^+] calcd for $C_{19}H_{40}NO_8$ = 410.3, Found 410.3.



Compound **3** was prepared according to the literature.[3]

Synthesis of compound **2**:

To a solution of compound **S7** (6.4 g, 20 mmol), methanol (40 mL), and dichloromethane (20 mL) was added sodium hydroxide (840 mg, 21 mmol). The mixture was allowed to stir at room temperature for 20 h. The solvents were removed under reduced pressure. Lots of white precipitate formed when water (9 mL), dichloromethane (10 mL), and ethyl acetate (10 mL) were added while stirring, which was collected by filtration, well washed with a mixture of dichloromethane (10 mL) and ethyl acetate (10 mL), and then with water (10 mL). After transferring the solid (mono sodium salt) to a separatory funnel, ethyl acetate (80 mL) and conc. HCl (3 mL) diluted with water (20 mL) were successively added. The mixture was vigorously shaken until the solid was disappeared. Then the organic layer was separated and the aqueous layer was extracted by ethyl acetate (25 mL). The organic layers were combined and washed by brine (20 mL), dried over $MgSO_4$, filtered, and concentrated. The solid obtained was washed with *n*-hexane/ethyl acetate (4/1, 10 mL), providing the desired product **2** as a white powder (4.28 g, 70% yield).

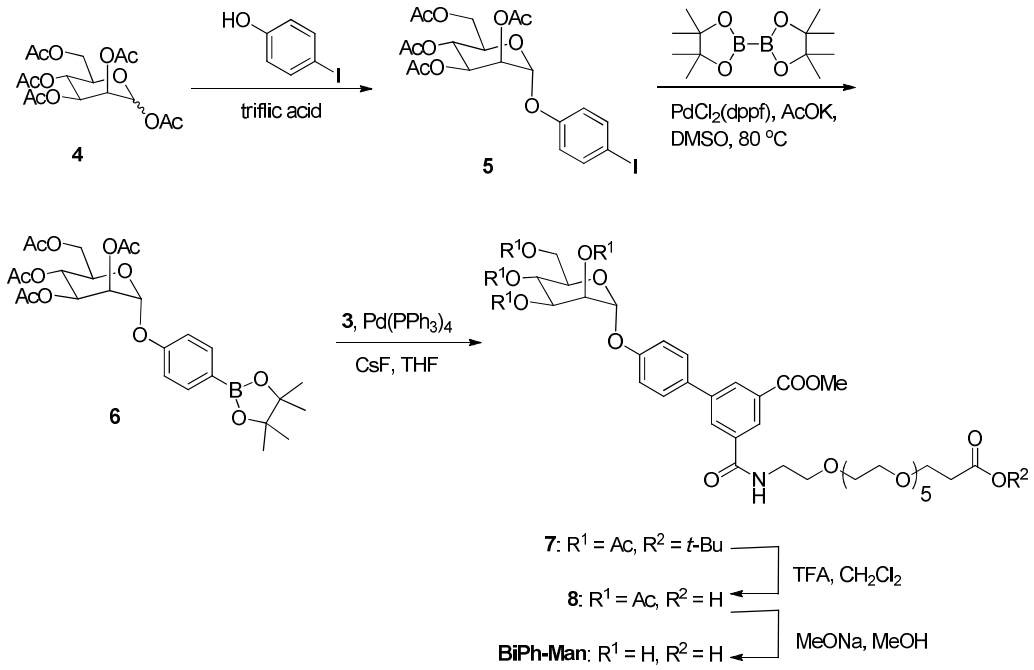
^{1}H NMR (400 MHz, CD_3COCD_3): δ 8.54 (m, 1 H), 8.51 (m, 1 H), 8.47 (m, 1 H), 3.91 (s, 3 H). ^{13}C NMR (100 MHz, CD_3COCD_3): δ 164.58, 164.33, 142.32, 141.91, 133.07, 132.52, 129.55, 93.32, 52.21.

Synthesis of compound **3**:

To a solution of compound **2** (306 mg, 1 mmol), HBTU (455 mg, 1.2 equiv), and dichloromethane (15 mL) was added diisopropylethylamine (524 uL, 3.0 equiv). After stirring for 30 min, amine **1** (451 mg, 1.1 equiv) was added and the resulting mixture was allowed to stir for 15 h. The reaction course could be followed by TLC (4% MeOH in ethyl acetate). When the reaction completed, the reaction mixture was washed by sat. NH_4Cl (10 mL), dried over $MgSO_4$, filtered,

concentrated, purified by silica gel column chromatography (eluent: ethyl acetate) to afford the desired product **3** as a yellow viscous oil (540 mg, 78% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.38 (m, 1 H), 8.35 (m, 1 H), 8.33 (m, 1 H), 7.34 (t, J = 5.5 Hz, 1 H), 3.86 (s, 3 H), 3.7-3.5 (m, 26 H), 2.43 (t, J = 6.4 Hz, 2 H), 1.37 (s, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.17, 165.39, 165.01, 140.93, 140.68, 136.58, 132.06, 127.46, 93.83, 80.77, 70.28, 70.19, 70.14, 70.10, 70.00, 69.83, 66.73, 52.68, 40.01, 36.05, 28.13. MS (ESI): [M+Na$^+$] calcd for $C_{28}H_{44}INNaO_{11}$ = 720.2, Found 720.1.



Compound **5** was prepared from pentaacetylmannoside (**4**) in 78% yield according to the literature.[4]

Synthesis of compound **6**:

Under N_2 atmosphere, a mixture of compound **5** (2.75 g, 5 mmol), bis(pinacolato)diboron (1.524 g, 1.2 equiv), AcOK (1.472 g, 3 equiv), $PdCl_2$(dppf) (122.5 mg, 0.03 equiv), and DMSO (12 mL) was stirred at 80 ^oC for 10 h. After cooling, water (50 mL) was added, and the resulting mixture was extracted with dichloromethane (30 mL × 3). The combined organic layers were washed with brine (20 mL×2), dried over $MgSO_4$, filtered, and concentrated. The residue obtained was subjected to the silica gel column chromatography for purification to afford the desired product **6** as a white foam powder (2.34 g, 85% yield).

^1H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.7 Hz, 2 H), 7.06 (d, J = 8.7 Hz, 2 H), 5.56-5.53 (m, 2 H), 5.43 (m, 1 H), 5.35 (t, J = 10.1 Hz, 1 H), 4.27 (dd, J = 5.0, 12.4 Hz, 1 H), 4.11-3.99 (m, 2 H), 2.18 (s, 3 H), 2.03 (s, 3 H), 2.02 (s, 3 H), 2.02 (s, 3 H), 1.31 (s, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.66, 170.06, 170.02, 169.84, 158.03, 136.66, 115.72, 95.46, 83.85, 69.41, 69.25, 68.92, 65.93, 62.10, 24.92, 20.97, 20.79. MS (ESI): [M+Na^+] calcd for $C_{26}H_{35}BNaO_{12}$ = 573.2, Found 573.3.

Synthesis of compound **7**:

Under N_2 atmosphere, a mixture of **7** (261 mg, 0.374 mmol), **6** (281 mg, 1.365 equiv), CsF (171 mg, 3 equiv), $Pd(PPh_3)_4$ (30.3 mg, 0.07 equiv), and THF (4 mL) was stirred at 80 ^oC for 12 h. The mixture was allowed to cool down to room temperature and the solvent was removed under reduced pressure. Dichloromethane (10 mL) was added, which was followed by filtration. The filter cake was thoroughly washed with dichloromethane. Concentrating the filtrate gave the crude product which was purified by silica gel column chromatography (gradient elution: from ethyl acetate to 2% MeOH in ethyl acetate). The desired product **7** was obtained as light yellow syrup (300 mg, 81% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.30 (m, 1 H), 8.26 (m, 1 H), 8.22 (m, 1 H), 7.55 (d, J = 8.7 Hz, 2 H), 7.13 (d, J = 8.7 Hz, 2 H), 5.53 (d, J = 2.3 Hz, 1 H), 5.51 (d, J = 3.7 Hz, 1 H), 5.42 (m, 1 H), 5.33 (t, J = 10.1 Hz, 1 H), 4.24 (dd, J = 5.0, 11.9 Hz, 1 H), 4.08-4.00 (m, 2 H), 3.89 (s, 3 H), 3.64-3.50 (m, 26 H), 2.41 (t, J = 6.4 Hz, 2 H), 2.15 (s, 3 H), 2.00 (s, 3 H), 1.99 (s, 3 H), 1.98 (s, 3 H), 1.36 (s, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.93, 170.56, 170.02, 170.00, 169.77, 166.56, 166.38, 155.71, 141.08, 135.68, 134.09, 130.96, 130.35, 128.50, 126.28, 116.98, 95.81, 80.52, 70.54, 70.48, 70.34, 70.31, 69.80, 69.35, 69.31, 68.88, 66.89, 65.89, 62.11, 52.47, 40.11, 36.26, 28.12, 20.95, 20.76. MS (ESI): [M+Na^+] calcd for $C_{48}H_{67}NNaO_{21}$ = 1016.4, Found 1016.3.

Synthesis of compound **8**:

To a solution of compound **7** (410 mg, 0.42 mmol) in dichloromethane (1 mL) was added trifluoroacetic acid (1 mL). The mixture was stirred for 15 h. The reaction was completed as detected by TLC (4% MeOH in ethyl acetate). After removing the volatile components under reduced pressure, the residue was purified by silica gel column chromatography (eluent: 0 to 50% MeOH in ethyl acetate), giving the product **8** as white foam powder (387 mg, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34 (m, 1 H), 8.27 (m, 1 H), 8.25 (m, 1 H), 7.57 (d, J = 8.7 Hz, 2 H), 7.13 (d, J = 8.7 Hz, 2 H), 5.54-5.50 (m, 2 H), 5.42 (m, 1 H), 5.33 (t, J = 10.1 Hz, 1 H), 4.24 (dd, J = 5.0, 11.9 Hz, 1 H), 4.06-4.00 (m, 2 H), 3.89 (s, 3 H), 3.70- 3.50 (m, 26 H), 2.51 (t, J = 6.4 Hz, 2 H), 2.16 (s, 3 H), 2.01 (s, 3 H), 1.99 (s, 3 H), 1.98 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.69, 170.64, 170.09, 170.05, 169.81, 166.90, 166.47, 155.70, 141.04, 135.52, 134.05, 130.96, 130.34, 128.51, 126.51, 116.99, 95.79, 70.22, 70.18, 70.11, 70.04, 69.91, 69.36, 69.30, 68.90, 66.56, 65.90, 62.13, 52.50, 40.04, 34.90, 20.95, 20.76. MS (ESI): [M+Na^+] calcd for $C_{44}H_{59}NNaO_{21}$ =

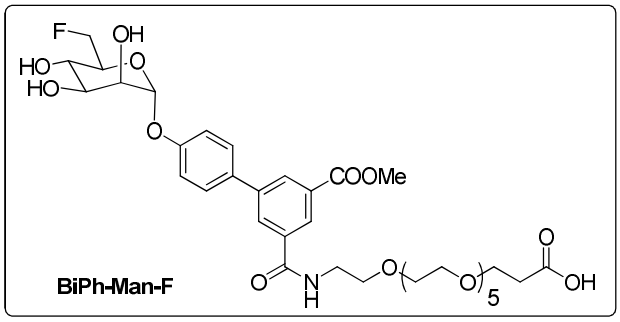
960.3, Found 960.6.

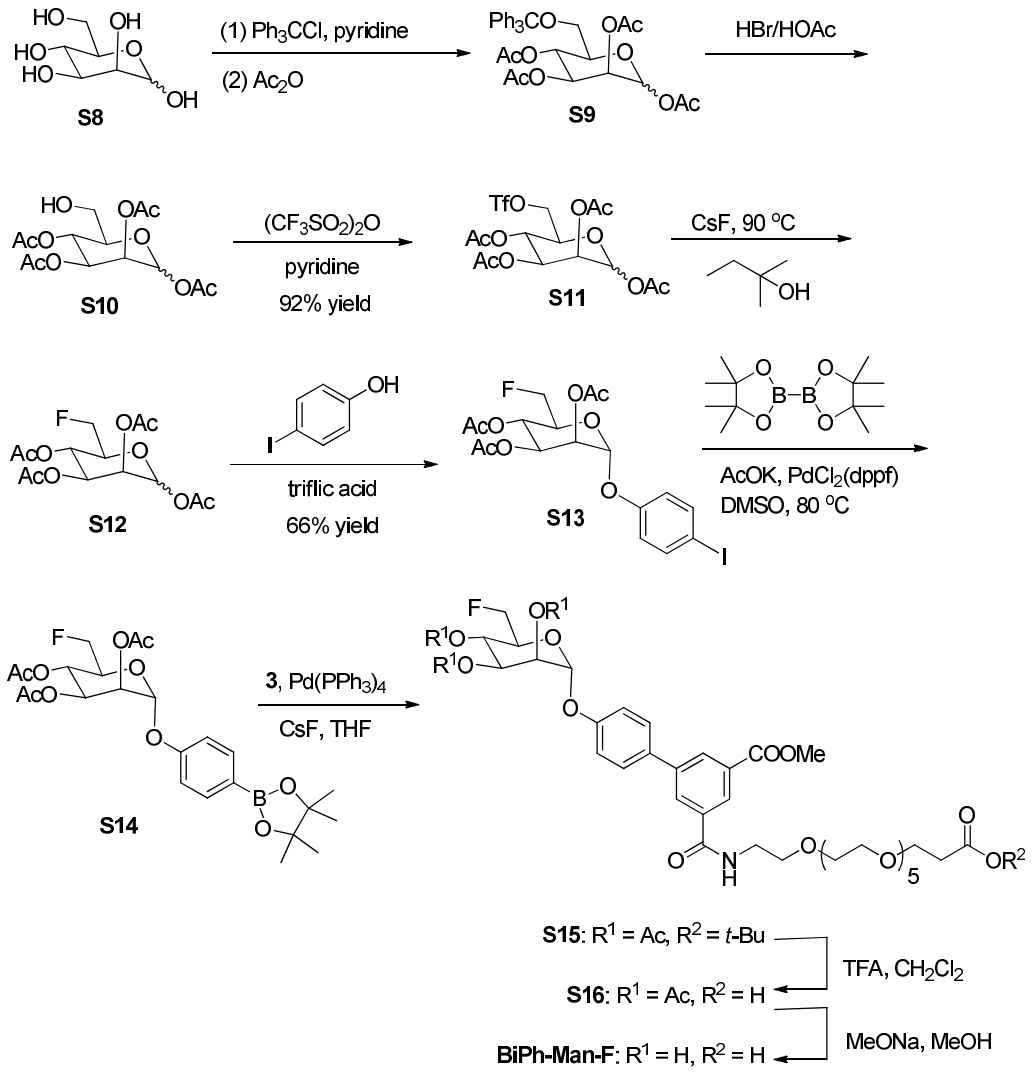
Synthesis of compound **BiPh-Man**:

Under N_2, sodium methoxide (68 mg, 3 equiv) was added to the solution of compound **8** (396 mg, 0.42 mmol) in anhydrous methanol (4 mL). After stirring for 12 h, the reaction was quenched and neutralized by acidic ion-exchange resin DOWEX-50W, filtered, washed with methanol, and concentrated to give the crude product. Further purification was performed by silica gel column chromatography (gradient elution from 5% to 50% MeOH in ethyl acetate) to give the pure product **BiPh-Man** as white foam powder (160 mg, 50% yield).

^{1}H NMR (400 MHz, CD_3OD): δ 8.35 (m, 1 H), 8.25 (m, 1 H), 8.22 (m, 1 H), 7.58 (d, J = 8.7 Hz, 2 H), 7.20 (d, J = 9.2 Hz, 2 H), 5.54 (d, J = 1.4 Hz, 1 H), 4.92 (s, 5 H), 4.04 (m, 1 H), 3.95-3.92 (m, 4 H), 3.80- 3.50 (m, 30 H), 2.49 (t, J = 6.4 Hz, 2 H). ^{13}C NMR (100 MHz, CD_3OD): δ 175.08, 167.65, 166.34, 156.84, 141.27, 135.33, 132.93, 130.97, 129.77, 129.55, 128.03, 126.39, 117.01, 98.75, 74.20, 71.09, 70.60, 70.09 70.04, 69.96, 69.90, 69.82, 69.32, 66.98, 66.80, 61.34, 51.75, 39.77, 35.12. MS (ESI): [M+Na^+] calcd for $C_{36}H_{51}NNaO_{17}$ = 792.3, Found 792.4.

2.2 Procedures for the synthesis of compound BiPh-Man-F





Compound **S10** was synthesized according to the literatures, which was obtained as a mixture of anomers (α/β = 1.2 :1).[5]

Compound **S12** was synthesized via two steps with compound **S11** as the intermediate according to the method used for the analogous transformations of methyl 1,3,4-tri-O-acetyl-α/β-D-fructofuranoside to methyl 1,3,4-tri-O-acetyl-6-deoxy-6-fluoro-α/β-D-fructofuranoside.[6]

Synthesis of compound **S11**:

At –10 ^{o}C, to a mixture of compound **S10** (α/β = 1.2 :1) (7.6 g, 21.8 mmol), pyridine (2.5 mL, 1.5 equiv), and dichloromethane (200 mL) was added triflic anhydride (4.0 mL, 1.1 equiv). After stirring for 45 min, water (100 mL) was added. The organic layer was separated and the aqueous layer was extracted with dichloromethane (30 mL × 3). The organic layers were combined, washed successively with 10% H_2SO_4 (80 mL), sat. $NaHCO_3$ (100 mL), and brine (100 mL), dried over $MgSO_4$, filtered, concentrated to give the crude product. Further purification by silica gel column chromatography (eluent: *n*-hexane/ethyl acetate: 2:1) provided the product **S11** as light yellow viscous oil (9.5 g, 92% yield), which was a mixture of anomers (α/β = 1.4 : 1).

^{1}H NMR (500 MHz, $CDCl_3$): for the α-anomer: δ 6.07 (d, J = 1.7 Hz, 1 H), 5.33 (m, 1 H), 5.28 (m, 1 H), 5.21 (m, 1 H), 4.51 (m, 2 H), 4.10 (m, 1 H), 2.14 (s, 6 H), 2.05 (s, 3 H), 1.98 (s, 3 H). For the β-anomer: δ 5.87 (d, 1.2 Hz, 1 H), 5.45 (dd, J = 1.2, 2.9 Hz, 1 H), 5.21 (m, 1 H), 5.14 (dd, J = 3.4, 9.8 Hz, 1 H), 4.53 (m, 2 H), 3.91 (m, 1 H), 2.17 (s, 3 H), 2.07 (s, 3 H), 2.05 (s, 3 H), 1.97 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 170.21, 169.99, 169.78, 169.70, 169.65, 168.33, 167.91, 118.54 (q, $^{1}J_{C, F}$ = 319.4 Hz), 90.25, 90.09, 73.43, 73.28, 72.48, 70.33, 70.24, 68.38, 68.10, 67.92, 65.33, 65.26, 20.81, 20.72, 20.64, 20.59, 20.55. ^{19}F NMR (470 MHz, $CDCl_3$): β-anomer: -74.30 (s); α-anomer: -74.41 (s).

Synthesis of compound **S12**:

To a solution of compound **S11** (9.5 g, 20 mmol) in *tert*-amyl alcohol (60 mL) was added CsF (9.12 g, 3.0 equiv) in one portion. The mixture was refluxed while stirring for 40 min, and then allowed to cool down to room temperature. After evaporating the *tert*-amyl alcohol under reduced pressure, ethyl acetate (30 mL) was added. The dark brown undissolved solid was removed by filtration. The filtrate was concentrated and the residue was purified by silica gel column chromatography (eluent: *n*-hexane/ethyl acetate: 3:1 to 2:1), providing the pure product **S12** as light yellow solid (4.0 g, 57% yield), which was a mixture of anomers (α/β = 4.7 : 1).

^{1}H NMR (500 MHz, $CDCl_3$): for the α-anomer: δ 6.08 (d, J = 1.7 Hz, 1 H), 5.35 (m, 2 H), 5.25 (s, 1 H), 4.48 (m, 2 H), 4.00 (m, 1 H), 2.14 (s, 6 H), 2.05 (s, 3 H), 2.00 (s, 3 H); For the β-anomer: δ 5.87 (s, 1 H), 5.47 (d, J = 2.3 Hz, 1 H), 5.34 (m, 1 H), 5.14 (dd, J = 3.5, 10.3 Hz, 1 H), 4.60 (m, 2 H), 3.90 (m, 1 H), 2.20 (s, 3 H), 2.09 (s, 3 H), 2.06 (s, 3 H), 2.00 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$): for the α-anomer: δ 170.13, 169.89, 169.58, 169.17, 90.57, 81.00 (d, $^{1}J_{C,F}$ = 176.1 Hz), 71.4 (d, $^{2}J_{C,F}$ = 19.2 Hz), 68.73, 68.30, 65.16 (d, $^{3}J_{C,F}$ = 6.4 Hz), 20.93, 20.84, 20.74; For the β-anomer: 170.32, 169.93, 169.61, 168.49, 90.31, 80.99 (d, $^{1}J_{C,F}$ = 175.2 Hz), 73.80 (d, $^{2}J_{C,F}$ = 19.2 Hz), 70.71, 68.18, 65.03 (d, $^{3}J_{C,F}$ = 6.4 Hz), 20.76, 20.63. ^{19}F NMR (470 MHz, $CDCl_3$): β-anomer: -231.94 (dt, $^{2}J_{H,F}$ = 47.7 Hz, $^{3}J_{H,F}$ = 21.6 Hz); α-anomer: -232.39 (dt, $^{2}J_{H,F}$ = 46.8 Hz, $^{3}J_{H,F}$ = 22.5 Hz).

Synthesis of compound **S13**:

The method used to synthesize compound **5** was applied.

At 0 ^{o}C, triflic acid (60 uL, 0.15 equiv) was added to a solution of compound **S12** (1.3 g, 3.7 mmol), 4-iodophenol (1.633 g, 2 equiv) in dry dichloromethane (60 mL). The mixture was stirred for

12 h at 0 ^{o}C. Trifilic acid was neutralized by addition of Et_3N (65 uL). After removing the solvent under reduced pressure, the residue was purified by silica gel column chromatography (eluent: *n*-hexane/ethyl acetate: 10:1 to 5:1) to provide the pure product **S13** as light yellow solid (1.25 g, 66% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.55 (d, 9.2 Hz, 2 H), 6.83 (d, J = 9.2 Hz, 2 H), 5.54 (dd, J = 3.4, 10.3 Hz, 1 H), 5.47 (d, J = 1.2 Hz, 1 H), 5.38-5.34 (m, 2 H), 4.49 (m, 1 H), 4.39 (m, 1 H), 4.02, (m, 1 H), 2.15 (s, 3 H), 2.03 (s, 3 H), 2.00 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 170.05, 169.66, 155.53, 138.65, 118.73, 95.78, 85.96, 81.16 (d, $^{1}J_{C, F}$ = 175.2 Hz), 70.03 (d, $^{2}J_{C, F}$ = 19.2 Hz), 69.18, 68.76, 65.30 (d, $^{3}J_{C, F}$ = 7.3 Hz), 20.93, 20.79, 20.76. ^{19}F NMR (470 MHz, $CDCl_3$): -232.56 (dt, $^{2}J_{H, F}$ = 47.7 Hz, $^{3}J_{H, F}$ = 23.4 Hz).

Synthesis of compound **S14**:

Under N_2 atmosphere, a mixture of compound **S13** (1.2 g, 2 mmol), bis(pinacolato)diboron (610 mg, 1.2 equiv), AcOK (589 mg, 3 equiv), $PdCl_2$(dppf) (49 mg, 0.03 equiv), and DMSO (12 mL) was stirred at 80 ^{o}C for 12 h. After cooling, water (20 mL) was added, and the resulting mixture was extracted with dichloromethane (10 mL × 3). The combined organic layers were washed with brine (10 mL×2), dried over $MgSO_4$, filtered, and concentrated. The residue obtained was subjected to the silica gel column chromatography for purification to afford the desired product **S14** as a white foam powder (820 mg, 80% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.73 (d, 8.1 Hz, 2 H), 7.05 (d, J = 8.6 Hz, 2 H), 5.57 (d, J = 1.2 Hz, 1 H), 5.54 (dd, J = 3.4, 10.3 Hz, 1 H), 5.40-5.34 (m, 2 H), 4.43 (d, J = 2.9 Hz, 1 H), 4.34 (d, J = 2.9 Hz, 1 H), 3.95, (m, 1 H), 2.15 (s, 3 H), 2.02 (s, 3 H), 2.00 (s, 3 H), 1.28 (s, 12 H). ^{13}C NMR (125

MHz, $CDCl_3$): δ 170.05, 170.02, 169.64, 157.98, 136.70, 115.56, 95.33, 83.80, 81.09 (d, $^1J_{C,F}$ = 176.1 Hz), 69.90 (d, $^2J_{C,F}$ = 18.3 Hz), 69.27, 68.88, 65.34 (d, $^3J_{C,F}$ = 6.4 Hz), 24.94, 24.90, 20.88, 20.76, 20.74. ^{19}F NMR (470 MHz, $CDCl_3$): -233.10 (dt, $^2J_{H,F}$ = 47.7 Hz, $^3J_{H,F}$ = 25.2 Hz).

Synthesis of compound **S15**:

Under N_2 atmosphere, a mixture of **3** (540 mg, 0.774 mmol), **S14** (592 mg, 1.5 equiv), CsF (365 mg, 3 equiv), $Pd(PPh_3)_4$ (65 mg, 0.07 equiv), and THF (15 mL) was stirred at 80 ^{o}C for 12 h. The mixture was allowed to cool down to room temperature and the solvent was removed under reduced pressure. Dichloromethane (10 mL) was added, which was followed by filtration. The filter cake was thoroughly washed with dichloromethane. Concentrating the filtrate gave the crude product which was purified by silica gel column chromatography (gradient elution: from ethyl acetate to 2% MeOH in ethyl acetate). The desired product **S15** was obtained as light yellow syrup (620 mg, 84% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.34 (m, 1 H), 8.29 (m, 1 H), 8.24 (m, 1 H), 7.58 (m, 2 H), 7.27 (t, J = 5.2 Hz, 1 H), 7.15 (m, 2 H), 5.57 (m, 2 H), 5.40 (m, 2 H), 4.49 (d, J = 2.9 Hz, 1 H), 4.40 (d, J = 3.5 Hz, 1 H), 4.06 (m, 1 H), 3.92 (s, 3 H), 3.70-3.50 (m, 26 H), 2.44 (t, J = 6.3 Hz, 2 H), 2.17 (s, 3 H), 2.04 (s, 3 H), 2.02 (s, 3 H), 1.39 (s, 9 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 171.00, 170.13, 170.09, 169.71, 166.65, 166.42, 155.75, 141.14, 135.66, 134.11, 130.99, 130.42, 130.30, 128.61, 126.39, 116.88, 95.78, 81.21 (d, $^1J_{C,F}$ = 175.2 Hz), 80.60, 70.55, 70.47, 70.41, 70.27, 70.07, 69.91, 69.30, 68.87, 66.88, 65.38 (d, $^3J_{C,F}$ = 6.4 Hz), 52.49, 40.10, 36.23, 28.14, 20.96, 20.81, 20.78. ^{19}F NMR (470 MHz, $CDCl_3$): -232.70 (dt, $^2J_{H,F}$ = 47.7 Hz, $^3J_{H,F}$ = 24.3 Hz). MS (ESI): [M+Na^+] calcd for $C_{46}H_{64}FNNaO_{19}$ = 976.4, Found 976.3.

Synthesis of compound **S16**:

To a solution of compound **S15** (620 mg, 0.65 mmol) in dichloromethane (2 mL) was added trifluoroacetic acid (2 mL). The mixture was stirred for 20 h. The reaction was completed as detected by TLC (4% MeOH in ethyl acetate). After removing the volatile components under reduced pressure, the residue was purified by silica gel column chromatography (eluent: 0 to 50% MeOH in ethyl acetate), giving the product **S16** as white foam powder (540 mg, 92% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.27 (s, 1 H), 8.16 (m, 2 H), 8.24 (m, 1 H), 7.86 (br s, 1 H), 7.48 (d, J = 8.6 Hz, 2 H), 7.04 (d, J = 8.6 Hz, 2 H), 5.48 (d, J = 1.8 Hz, 1 H), 5.45 (dd, J = 3.4, 10.3 Hz, 1 H), 5.34 (m, 1 H), 5.30 (t, J = 10.3 Hz, 1 H), 4.39 (d, J = 2.9 Hz, 1 H), 4.29 (d, J = 2.9 Hz, 1 H), 3.94 (m, 1 H), 3.79 (s, 3 H), 3.60-3.40 (m, 26 H), 2.44 (t, J = 6.3 Hz, 2 H), 2.07 (s, 3 H), 1.95 (s, 3 H), 1.91 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 174.39, 170.06, 170.02, 169.67, 166.98, 166.34, 155.63, 140.82, 135.39, 133.90, 130.85, 130.17, 130.11, 128.46, 126.69, 116.84, 95.67, 81.12 (d, $^{1}J_{C, F}$ = 175.2 Hz), 70.05, 69.94, 69.90, 69.81, 69.17, 68.84, 66.42, 65.19 (d, $^{3}J_{C, F}$ = 6.4 Hz), 52.38, 39.92, 34.69, 20.80, 20.66, 20.64. ^{19}F NMR (470 MHz, $CDCl_3$): -232.70 (dt, $^{2}J_{H, F}$ = 47.7, $^{3}J_{H, F}$ = 24.3 Hz). MS (ESI): [M+Na^+] calcd for $C_{42}H_{56}FNNaO_{19}$ = 920.3, Found 920.5.

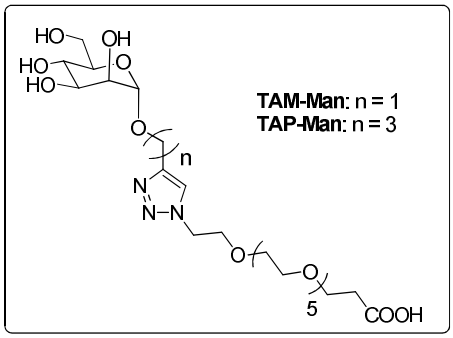
Synthesis of compound **BiPh-Man-F**:

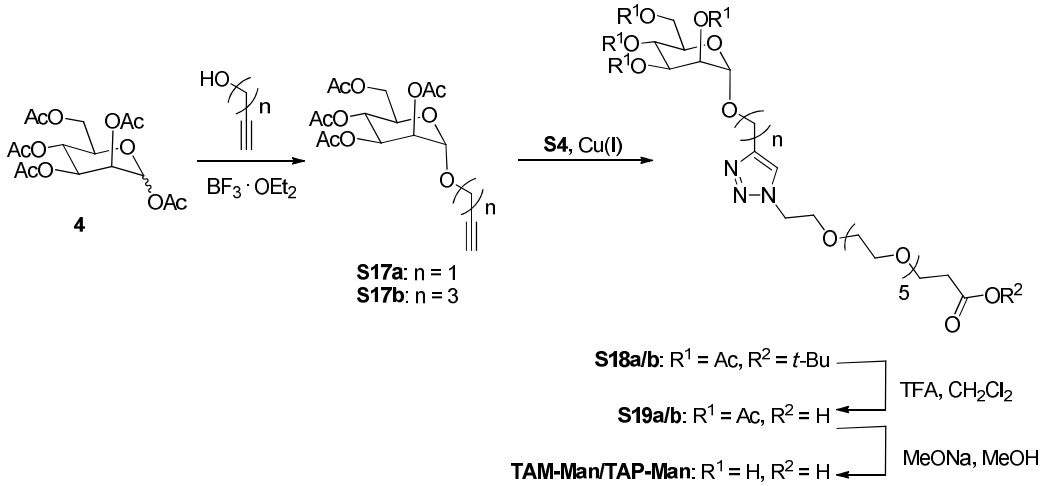
Under N_2, sodium methoxide (97 mg, 3 equiv) was added to the solution of compound **S16** (540 mg, 0.6 mmol) in anhydrous methanol (5 mL). After stirring for 19 h, the reaction was quenched and neutralized by acidic ion-exchange resin DOWEX-50W, filtered, washed with methanol, and concentrated to give the crude product. Further purification was performed by silica gel column chromatography (gradient elution from 0% to 20% MeOH in ethyl acetate) to give the pure product

BiPh-Man-F as white foam powder (264 mg, 57% yield).

^{1}H NMR (500 MHz, CD_3OD): δ 8.39 (s, 1 H), 8.31 (s, 1 H), 8.26 (s, 1 H), 7.64 (d, J = 8.6 Hz, 2 H), 7.20 (d, J = 8.6 Hz, 2 H), 5.55 (s, 1 H), 4.90 (br, 5 H), 4.70-4.48 (m, 2 H), 4.04 (t, J = 1.8 Hz, 1 H), 3.92 (m, 4 H), 3.78 (m, 2 H), 3.74-3.54 (m, 26 H), 2.51 (t, J = 6.3 Hz, 2 H). ^{13}C NMR (125 MHz, CD_3OD): δ 174.39, 167.75, 166.35, 156.72, 141.33, 135.38, 133.14, 131.05, 129.82, 129.58, 128.07, 126.43, 116.92, 98.73, 82.09 (d, $^{1}J_{C,F}$ = 172.5 Hz), 72.90 (d, $^{2}J_{C,F}$ = 18.3 Hz), 71.04, 70.43, 70.02, 69.94, 69.86, 69.79, 69.42, 66.42, 65.88 (d, $^{3}J_{C,F}$ = 6.4 Hz), 51.69, 39.70, 34.39. ^{19}F NMR (470 MHz, CD_3OD): -234.45 (dt, $^{2}J_{H,F}$ = 47.7, $^{3}J_{H,F}$ = 23.4 Hz). MS (ESI): [M+Na^+] calcd for $C_{36}H_{50}FNNaO_{16}$ = 794.3, Found 794.5.

2.3 Procedures for the synthesis of compound TAM-Man/TAP-Man





Compound **S17a** was prepared form **4** according to the reported procedure.[3]

Compound **S17b** was prepared form **4** according to the similar procedure for the preparation of **S17a**. Colorless thick oil; 32% yield;

^{1}H NMR (400 MHz, $CDCl_3$): δ 5.3-5.2 (m, 3 H), 4.78 (d, J = 1.4 Hz, 1 H), 4.25 (dd, J = 5.0, 12.4 Hz, 1 H), 4.06 (dd, J = 2.3, 12.4 Hz, 1 H), 3.98 (m, 1 H), 3.81 (m, 1 H), 3.51 (m, 1 H), 2.29 (m, 2 H), 2.12 (s, 3 H), 2.07 (s, 3 H), 2.01 (s, 3 H), 1.95-1.94 (m, 4 H), 1.79 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.77, 170.18, 170.00, 169.84, 97.66, 83.27, 69.62, 69.22, 69.16, 68.49, 66.50, 66.12, 62.46, 27.93, 21.01, 20.86, 20.81, 15.27. MS (ESI): [M+Na^+] calcd for $C_{19}H_{26}NaO_{10}$ = 437.1, Found 437.5.

Synthesis of compound **S18a** and **S18b**:

To a solution of alkyne **S17a** (206 mg, 0.533 mmol) and azide **S4** (279 mg, 1.2 equiv) in THF/H_2O (1:1, 3 mL) was added $CuSO_4$ (8.5 mg, 0.1 equiv) and sodium ascorbate (23 mg, 0.2 equiv). The mixture was stirred at room temperature for 20 h. Then, water (5 mL) and dichloromethane (5 mL) was added, transferred to a separatory funnel. The organic layer was separated and the aqueous layer was extracted with dichloromethane (5 mL × 3). The organic layers were combined, washed by brine (5 mL), dried over $MgSO_4$, filtered, and concentrated. The residue was purified by silica gel column chromatography (5% methanol in ethyl acetate) to give the desired product **S17a** as colorless viscous oil (450 mg, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (s, 1 H), 5.29-5.27 (m, 2 H), 5.21 (m, 1 H), 4.95 (d, J = 1.4 Hz, 1 H), 4.82 (d, J = 12.4 Hz, 1 H), 4.66 (d, J = 12.4 Hz, 1 H), 4.54 (t, J = 5.0 Hz, 2 H), 4.28 (dd, J = 5.0, 12.4 Hz, 1 H), 4.08 (m, 2 H), 3.87 (t, J = 5.5 Hz, 2 H), 3.68 (t, J = 6.4 Hz, 2 H), 3.62-3.55 (m, 20 H), 2.47 (t, J = 6.4 Hz, 2 H), 2.13 (s, 3 H), 2.10 (s, 3 H), 2.01 (s, 3 H), 1.95 (s, 3 H), 1.42 (s, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.87, 170.67, 169.96, 169.81, 169.70, 143.15, 124.43, 96.74, 80.44, 70.52, 70.44, 70.32, 69.37, 69.03, 68.60, 66.84, 65.98, 62.32, 60.84, 50.29, 36.21, 28.07, 20.89, 20.79, 20.71, 20.68. MS (ESI): [M+Na^+] calcd for $C_{36}H_{59}N_3NaO_{18}$ = 844.4, Found 844.3.

Compound **S18b** was prepared from **S17b** following the similar procedure for the preparation of **S18a**; colorless viscous oil; 71% yield;

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.46 (s, 1 H), 5.28-5.19 (m, 2 H), 5.17 (m, 1 H), 4.75 (d, J = 1.8 Hz, 1 H), 4.46 (t, J = 5.2 Hz, 2 H), 4.23 (dd, J = 5.7, 12.6 Hz, 1 H), 4.03 (dd, J = 2.3, 12.1 Hz, 1 H), 3.94 (m, 1 H), 3.80 (t, J = 5.2 Hz, 2 H), 3.72 (m, 1 H), 3.64 (t, J = 6.3 Hz, 2 H), 3.6-3.5 (m, 22 H), 3.46 (m, 1 H), 2.75 (t, J = 7.5 Hz, 2 H), 2.43 (t, J = 6.9 Hz, 2 H), 2.10 (s, 3 H), 2.03 (s, 3 H), 1.99 (s,

3 H), 1.94 (s, 3 H), 1.38 (s, 9 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 170.95, 170.73, 170.16, 169.97, 169.82, 146.96, 122.11, 97.62, 80.55, 70.60, 70.52, 70.39, 69.64, 69.19, 68.47, 67.59, 66.92, 66.15, 62.48, 50.15, 36.27, 29.00, 28.14, 22.37, 21.00, 20.83, 20.81. MS (ESI): [M+Na$^+$] calcd for C38H63N3NaO18 = 872.4, Found 872.4.

Synthesis of compound **S19a** and **S19b**:

To a solution of compound **S18a** (450 mg, 0.548 mmol) in dichloromethane (2 mL) was added trifluoroacetic acid (2 mL). The mixture was stirred for 15 h. After removing the volatile components under reduced pressure, the residue was purified by silica gel column chromatography (eluent: 3% to 5% methanol in dichloromethane), giving the product **S19a** as colorless viscous oil (326 mg, 79% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (br s, 1 H), 7.76 (s, 1 H), 5.23-5.20 (m, 2 H), 5.14 (m, 1 H), 4.88 (s, 1 H), 4.76 (d, J = 12.4, 1 H), 4.59 (d, J = 12.4 Hz, 1 H), 4.49 (t, J = 5.0 Hz, 2 H), 4.22 (dd, J = 5.0, 12.4 Hz, 1 H), 4.03-3.98 (m, 2 H), 3.81 (t, J = 5.0 Hz, 2 H), 3.66 (t, J = 6.0 Hz, 2 H), 3.60-3.50 (m, 20 H), 2.52 (t, J = 6.4 Hz, 2 H), 2.06 (s, 3 H), 2.03 (s, 3 H), 1.95 (s, 3 H), 1.88 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.71, 170.85, 170.12, 169.96, 169.82, 143.13, 124.61, 96.83, 70.53, 70.45, 70.39, 70.31, 69.41, 69.35, 69.08, 68.62, 66.54, 65.99, 62.35, 60.77, 50.42, 34.90, 20.95, 20.84, 20.76, 20.73. MS (ESI): [M+Na$^+$] calcd for $C_{32}H_{51}N_3NaO_{18}$ = 788.3, Found 788.4.

Compound **S19b** was prepared from **S18b** following the similar procedure for the preparation of **S19a**; colorless viscous oil; 91% yield;

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.85 (br s, 1 H), 7.50 (s, 1 H), 5.28-5.12 (m, 3 H), 4.74 (s, 1 H), 4.47 (t, J = 5.2 Hz, 2 H), 4.22 (dd, J = 5.2, 12.6 Hz, 1 H), 4.03 (dd, J = 1.8, 12.6 Hz, 1 H), 3.93 (m,

1 H), 3.81 (t, J = 5.2 Hz, 2 H), 3.71 (m, 3 H), 3.60-3.50 (m, 20 H), 3.44 (m, 1 H), 2.76 (t, J = 7.5 Hz, 2 H), 2.55 (t, J = 6.3 Hz, 2 H), 2.09 (s, 3 H), 2.03 (s, 3 H), 1.98 (s, 3 H), 1.93 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 174.58, 170.79, 170.20, 170.02, 169.85, 146.79, 122.44, 97.60, 70.57, 70.55, 70.51, 70.47, 70.43, 70.33, 69.61, 69.51, 69.20, 68.48, 67.56, 66.61, 66.15, 62.50, 50.33, 34.97, 28.93, 22.17, 20.97, 20.80, 20.77. MS (ESI): [M+H$^+$] calcd for $C_{34}H_{56}N_3O_{18}$ = 794.4, Found 794.5.

Synthesis of compound **TAM-Man** and **TAP-Man**:

To a solution of compound **S19a** (229 mg, 0.3 mmol) in anhydrous methanol (2 mL) was added sodium methoxide (25-30% w/w soln. in MeOH, 200 uL, 3.3 equiv). After the resulting solution was allowed to stir at room temperature for 5 hours, conc. HCl (83 uL, 3.3 equiv) dissolved in methanol (2 mL) was added while vigorously stirring. The solution was passed through a thin pad of silica gel, and washed thoroughly with methanol. After concentration, the product was obtained as colorless viscous oil (179 mg, 99% yield).

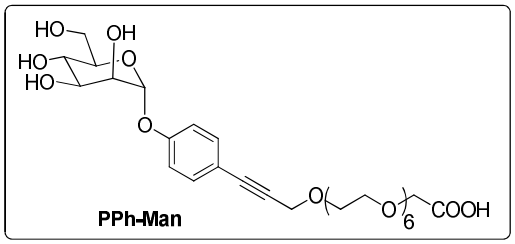
^{1}H NMR (400 MHz, CD_3OD): δ 8.13 (s, 1 H), 4.99 (br s, 5 H), 4.88 (d, J = 1.8 Hz, 1 H), 4.78 (d, J = 12.4 Hz, 1 H), 4.62 (m, 3 H), 3.91 (t, J = 5.0 Hz, 2 H), 3.85-3.80 (m, 2 H), 3.75-3.54 (m, 26 H), 2.57 (t, J = 6.0 Hz, 2 H). ^{13}C NMR (100 MHz, CD_3OD): δ 174.51, 143.73, 125.05, 99.49, 73.56, 71.11, 70.62, 69.85, 69.75, 69.71, 69.66, 69.62, 69.52, 69.02, 67.17, 66.25, 61.40, 59.42, 50.10, 34.10. MS (ESI): [M+Na$^+$] calcd for $C_{24}H_{43}N_3NaO_{14}$ = 620.3, Found 620.5.

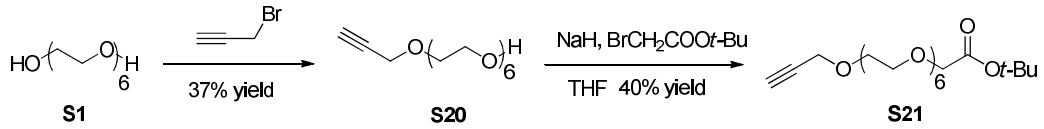
Compound **TAP-Man** was prepared from **S19b** following the similar procedure for the preparation of **TAM-Man**; colorless viscous oil; 95% yield;

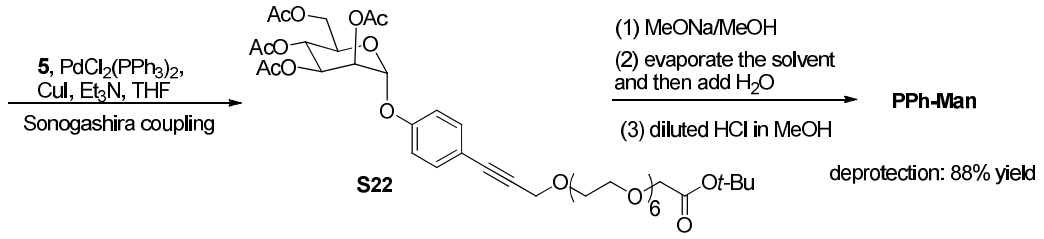
^{1}H NMR (500 MHz, CD_3OD): δ 7.85 (s, 1 H), 4.91 (br s, 5 H), 4.75 (s, 1 H), 4.56 (t, J = 5.2 Hz, 2 H), 3.89 (t, J = 5.2 Hz, 2 H), 3.80-3.74 (m, 3 H), 3.73-3.67 (m, 4 H), 3.63-3.61 (m, 21 H),

3.51-3.43 (m, 2 H), 2.78 (t, J = 7.5 Hz, 2 H), 2.57 (t, J = 5.8 Hz, 2 H), 1.95 (m, 2 H). ^{13}C NMR (125 MHz, CD_3OD): δ 174.60, 147.13, 122.84, 100.25, 73.29, 71.30, 70.81, 69.86, 69.73, 69.67, 69.64, 69.58, 69.52, 69.12, 67.22, 66.31, 61.37, 49.84, 34.20, 29.10, 21.84. MS (ESI): [M+Na^+] calcd for $C_{26}H_{47}N_3NaO_{14}$ = 648.3, Found 648.4.

2.4 Procedures for the synthesis of compound PPh-Man







Compound **S20** was prepared according to the literature.[7]

Synthesis of compound **S21**:

Under N_2, compound **S20** (747 mg, 2.33 mmol) in anhydrous THF (5 mL) was slowly added to a dry round bottom flask charged with 60% NaH (131 mg, 1.4 equiv) at 0 ^oC. When no gas (H_2) was released, the mixture was allowed to stir at room temperature for 30 min. After re-cooling the mixture to 0 ^oC, *tert*-butyl bromoacetate (688 uL, 2 equiv) was added. The reaction mixture was stirred at 0 ^oC for 1 h and at 25 ^oC for 24 h. The mixture was poured into water (10 mL), extracted with dichloromethane (15 mL × 3) and dried over $MgSO_4$. Filtration and concentration gave the crude product which was further purified by silica gel chromatography (*n*-hexane/ethyl acetate = 1 : 2), giving the pure product **S21** as a light yellow oil (400 mg, 40% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 4.14 (d, J = 2.3 Hz, 2 H), 3.97 (s, 2 H), 3.70-3.60 (m, 24 H), 2.41 (t, J = 2.3 Hz, 1 H), 1.42 (s, 9 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 169.73, 81.58, 79.70, 74.69, 70.75, 70.62, 70.45, 69.14, 69.06, 58.46, 28.17. MS (ESI): [M+Na^+] calcd for $C_{21}H_{38}NaO_9$ = 457.2, Found 457.2.

Synthesis of compound **S22**:

To a mixture of **S21** (400 mg, 0.92 mmol), **5** (550 mg, 1.1 equiv), Et_3N (3 mL), and THF (12 mL) was added $PdCl_2(PPh_3)_2$ (70 mg, 0.1 equiv) and CuI (38 mg, 0.2 equiv). The oxygen was excluded from the reaction system by bubbling the solution with nitrogen stream for 5 min. After stirred at room temperature for 4 h, the resulting dark red solution was concentrated, and the residue was purified by silica gel column chromatography (*n*-hexane/ethyl acetate: 1/2 to pure EA) to give the desired product **S22** as orange thick oil (410 mg, 52% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33 (d, J = 8.0 Hz, 2 H), 6.97 (d, J = 8.6 Hz, 2 H), 5.49 (m, 2 H), 5.38 (d, J = 1.2 Hz, 1 H), 5.30 (t, J = 9.8 Hz, 1 H), 4.35 (s, 2 H), 4.21 (m, 1 H), 4.00 (m, 2 H), 3.96 (s, 2 H), 3.70-3.60 (m, 24 H), 2.15 (s, 3 H), 2.00 (s, 3 H), 1.98 (s, 3 H), 1.97 (s, 3 H), 1.42 (s, 9 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 170.56, 169.99, 169.78, 169.73, 155.53, 133.34, 117.35, 116.43, 95.65, 85.67, 84.58, 81.57, 70.75, 70.68, 70.62, 70.52, 69.33, 69.27, 69.20, 69.06, 68.81, 65.86, 62.08, 59.24, 28.17, 20.94, 20.76. MS (ESI): [M+Na^+] calcd for $C_{41}H_{60}NaO_{19}$ = 879.4, Found 879.2.

Synthesis of compound **PPh-Man**:

To a solution of compound **S22** (223 mg, 0.26 mmol) in anhydrous methanol (5 mL) was added sodium methoxide (25-30% w/w soln. in MeOH, 250 uL, 5 equiv). After the resulting solution was

allowed to stir at room temperature for 5 hours, the volatile components including methanol, methyl acetate and *tert*-butanol was removed under reduced pressure. Then, water (50 uL) and methanol (3 mL) was added. After stirring for another 5 hours, conc. HCl (100 uL) dissolved in methanol (5 mL) was added while vigorously stirring. The residue obtained after evaporation of the solvent under reduced pressure was purified by silica gel column chromatography (ethyl acetate/methanol: 1:1 to 1:2) to give the pure product **PPh-Man** as colorless thick oil (145 mg, 88% yield).

^{1}H NMR (500 MHz, CD_3OD): δ 7.35 (d, J = 8.6 Hz, 2 H), 7.08 (d, J = 8.6 Hz, 2 H), 5.49 (d, J = 1.2 Hz, 1 H), 4.89 (s, 5 H), 4.39 (s, 2 H), 3.99 (m, 1.07), 3.95 (s, 2 H), 3.87 (dd, J = 3.4, 9.7 Hz), 3.76-3.62 (m, 27 H), 3.54 (m, 1 H). ^{13}C NMR (125 MHz, CD_3OD): δ 175.25, 156.76, 132.89, 116.51, 116.30, 98.68, 85.62, 83.80, 74.25, 71.00, 70.49, 69.80, 69.69, 69.55, 69.48, 69.44, 69.36, 69.30, 69.22, 69.17, 68.63, 66.91, 61.27, 58.46. MS (ESI): [M+Na^+] calcd for $C_{29}H_{44}NaO_{15}$ = 655.3, Found 655.4.

3. Images of bacterial biofilm and interference samples

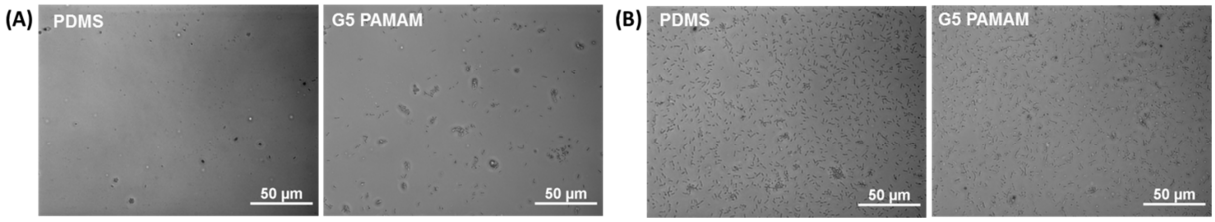


Fig. S1 The images of *fim*+ *E. coli* 83972 on the control surfaces (PDMS and G5 PAMAM). Representative reflected bright-field images of the adhered *fim*+ *E. coli* 83972 after 30 min incubation (A) and the corresponding biofilm formed after 48 h (B) on control surfaces (PDMS and G5 PAMAM). Each image is representative of up to 10 images obtained on random location at each surface and 3 experiments were repeated.

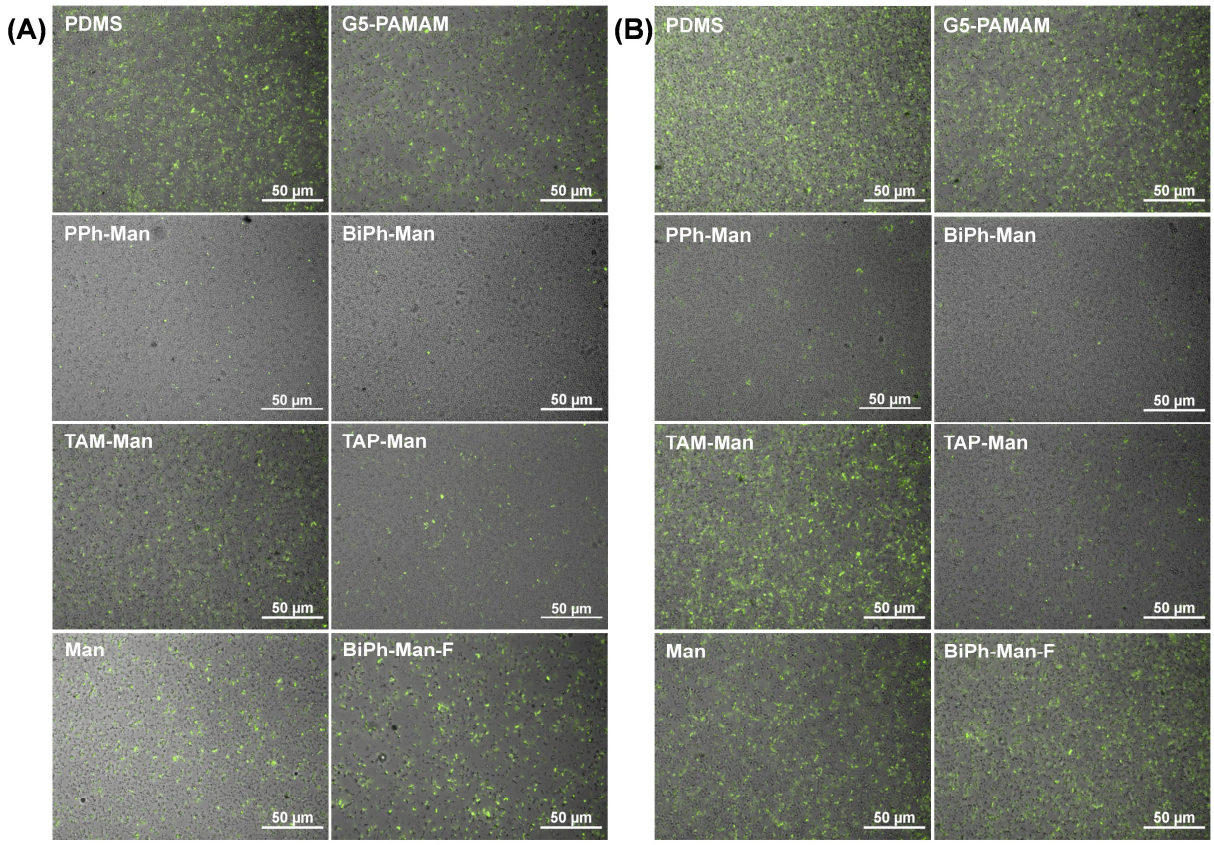


Fig. S2 Representative overlay of green fluorescence with reflected bright-field on mannoside-presenting and control surfaces with pre-formed *fim*+ *E. coli* 83972 biofilms after bacterial interference for (A) 5 days and (B) 11 days. See the Experimental section for detail conditions. Green fluorescence was generated from the adhered *E. faecalis* expressing GFP. Each image is representative of up to 10 images obtained on random locations at each surface and triplicate experiments were performed.

4. Viability of *fim*+ *E. coli* 83972 and *E. faecalis* undergo sonication and vortex

E. faecalis or *fim*+ *E. coli* 83972 was prepared as mentioned in text, and centrifuged (5000 rpm, 10 min) and then washed with PBS. The *E. faecalis* pellet was adjusted to OD_{600} 0.1 and *fim*+ *E. coli* 83972 was adjusted to OD_{600} 0.25 by addition of PBS or 0.01% SDS. Then the suspension was sonicated for 5 min, 10 min and 20 min, followed by vortexing for 1.5 min. Suspension without sonication or vortexing were control group. All the samples were diluted by factors of 10^2, 10^4, 10^6 and 10^8. Each diluted suspension (10 µL) was plated in duplicates on LB agar with chloramphenicol (20 µg/mL, for *fim*+ *E. coli* 83972), tetracycline (4 µg/mL, for *E. faecalis*). The plates were incubated at 37 ºC and the bacterial colonies formed were counted after 24 h and expressed as colony forming unit per mL (CFU/mL).

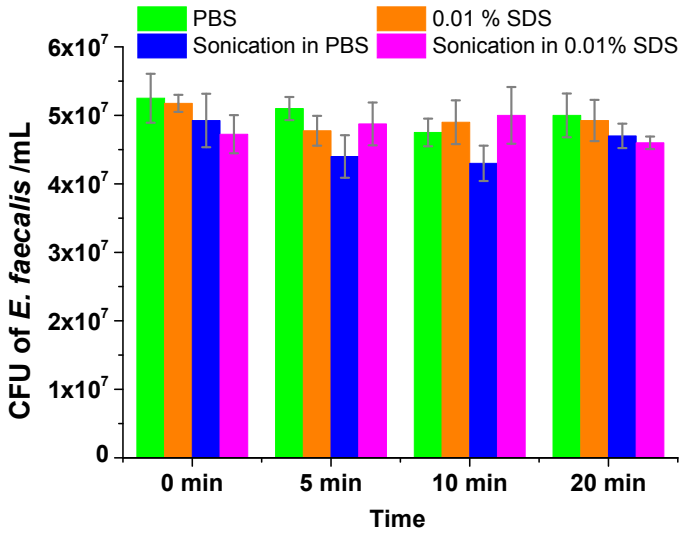


Fig. S3 Viability of *E. faecalis* underwent sonication and vortex in PBS and SDS.

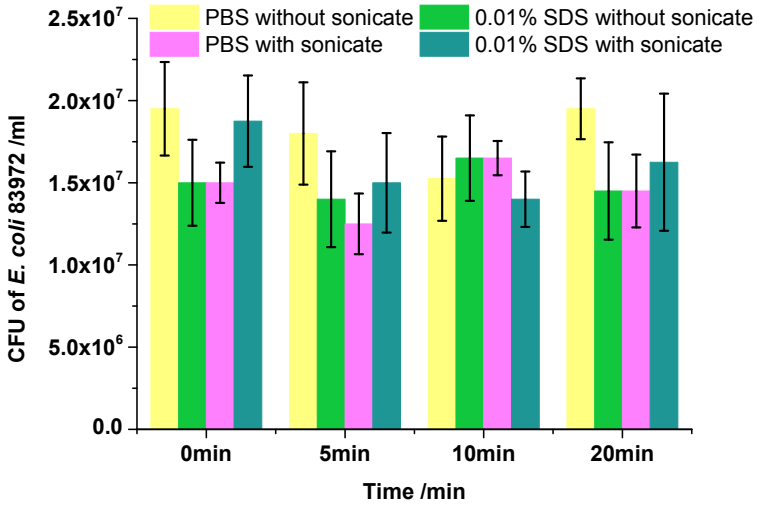
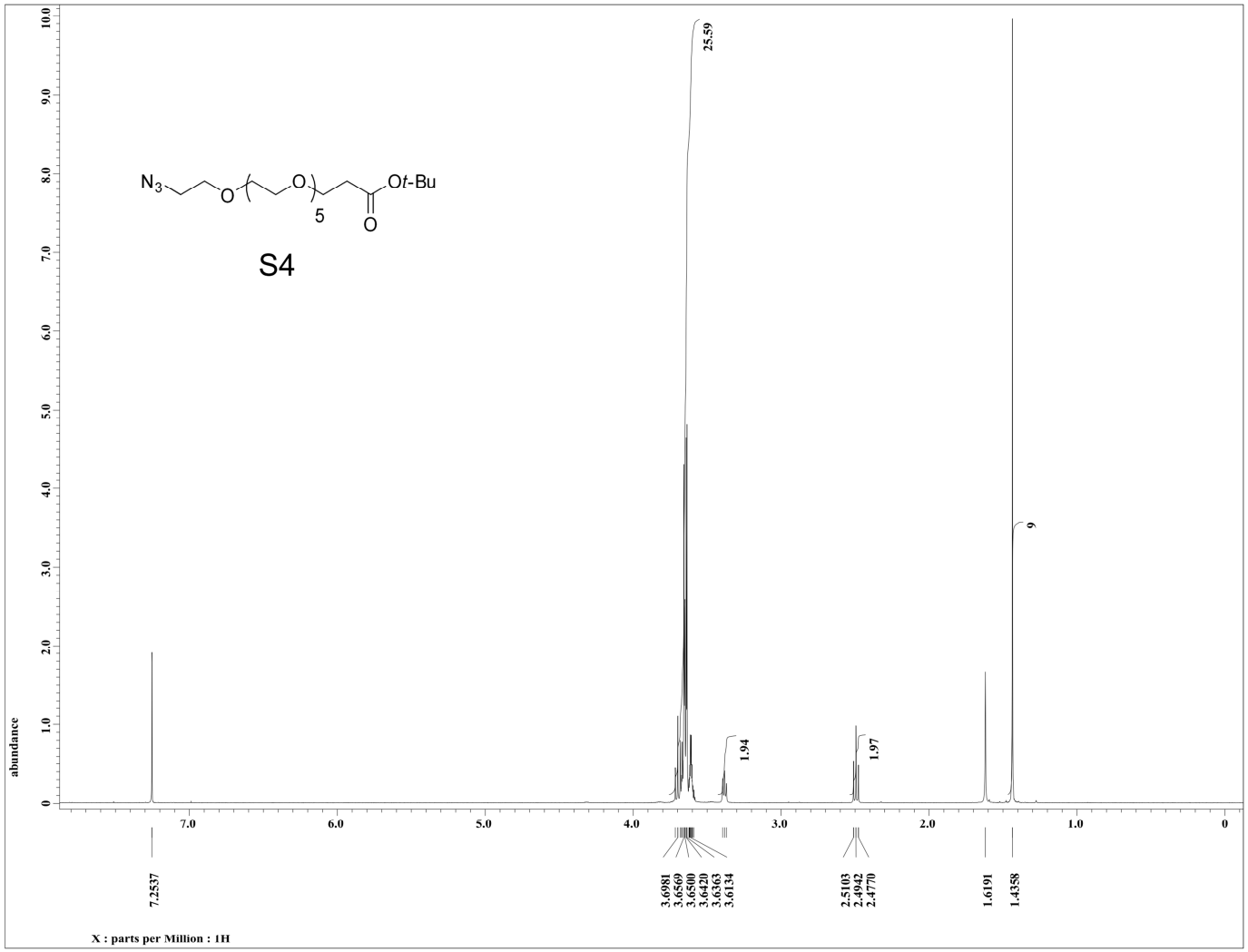
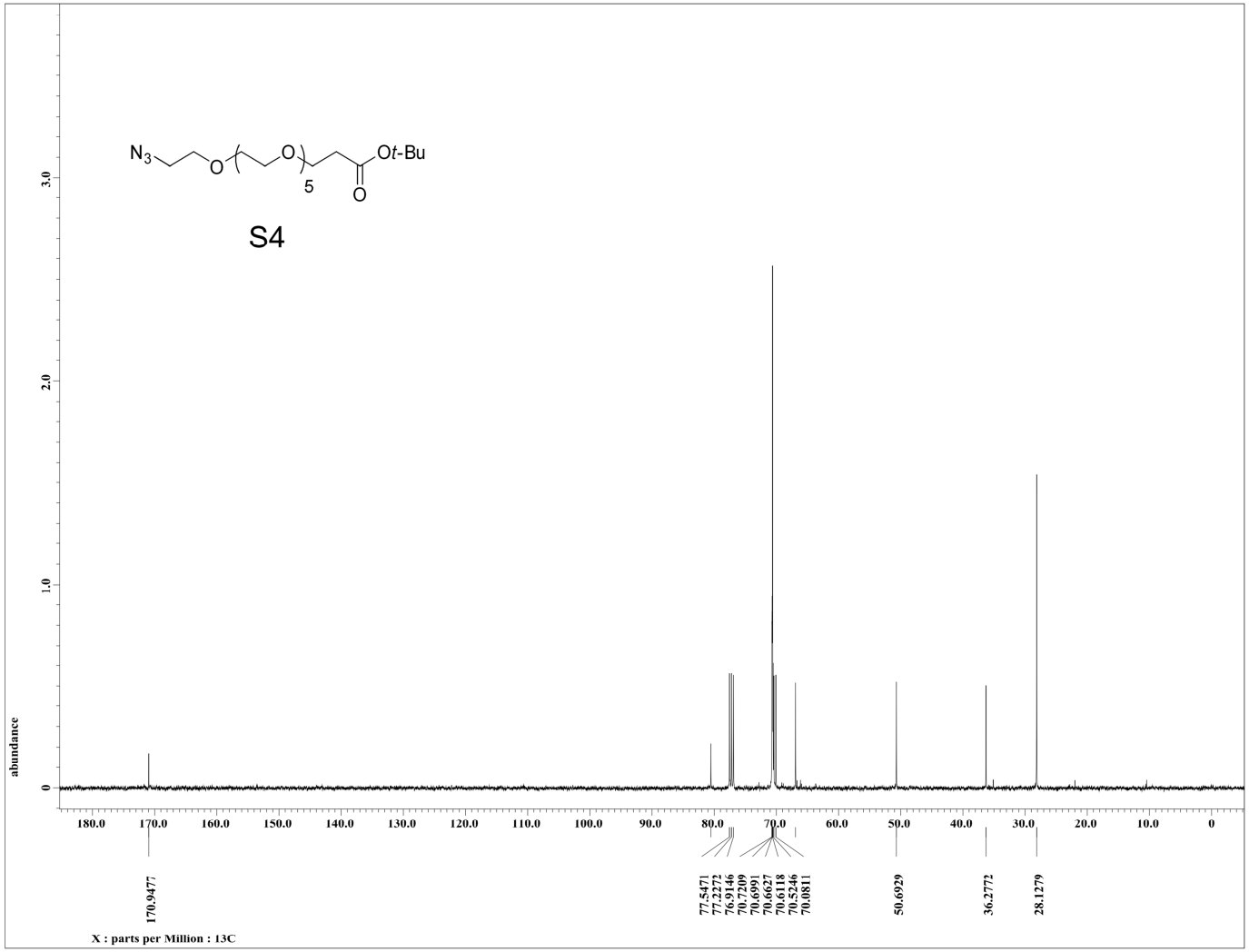
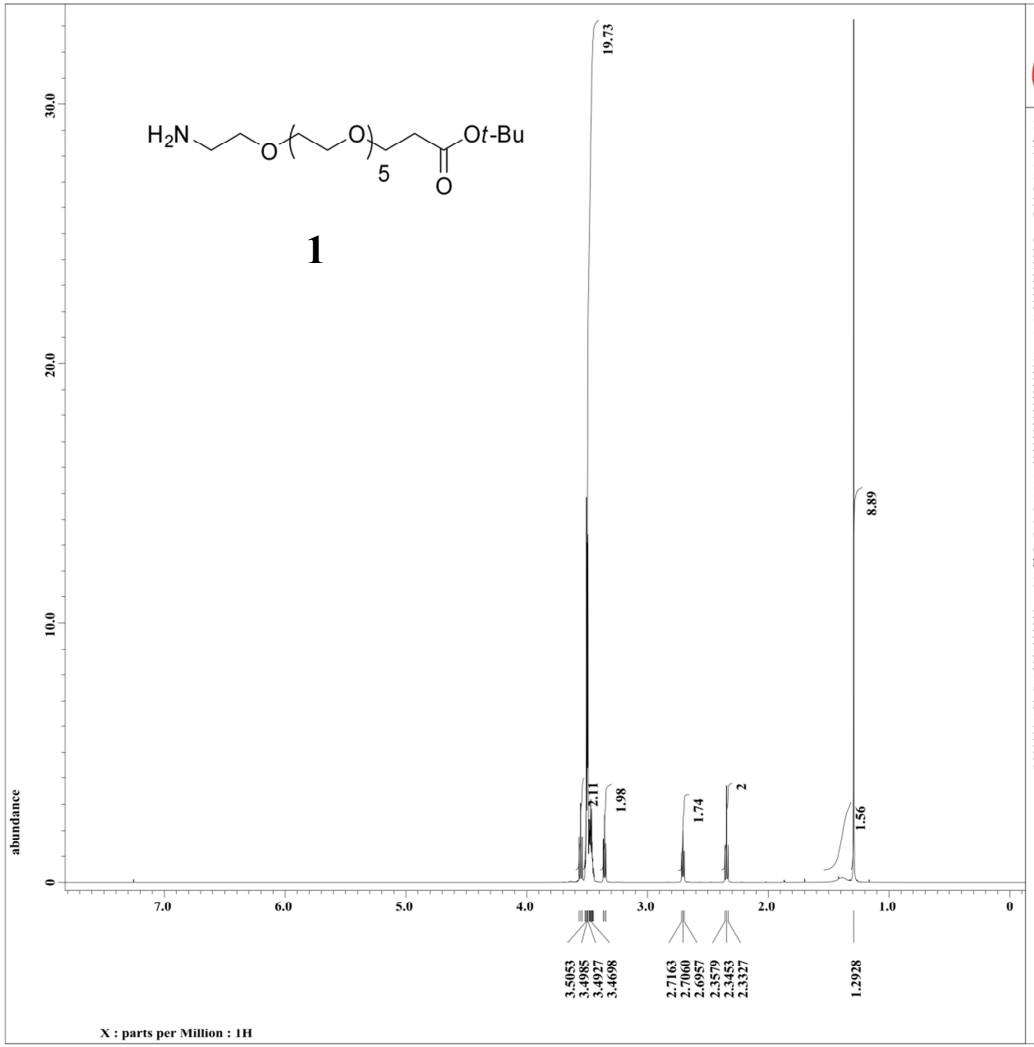


Fig. S4 Viability of *E. coli* 83972 underwent sonication and vortex in PBS and SDS.

5. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra




N3
O
O
5
O
Ot-Bu
O
S4
abundance
3.0
2.0
1.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.9477
77.5471
77.2272
76.9146
70.7209
70.6991
70.6627
70.6118
70.5246
70.0811
50.6929
36.2772
28.1279
X : parts per Million : 13C



JEOL

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Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = S#670602
Solvent           = CHLOROFORM-D
Creation_time     = 12-JUL-2010 18:12:10
Revision_time     = 12-JUL-2010 18:40:00
Current_time      = 26-JAN-2011 20:08:45

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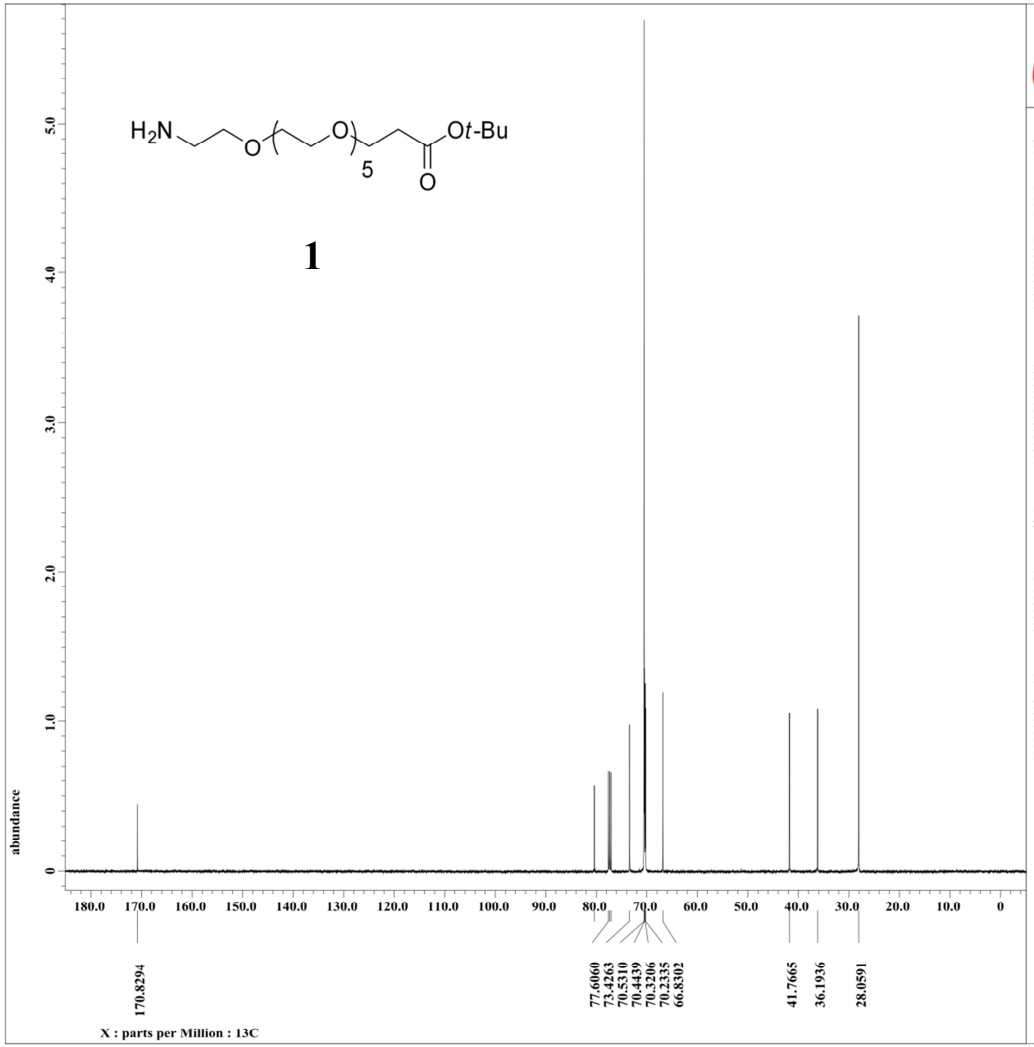
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 24
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 17.4[dC]
```

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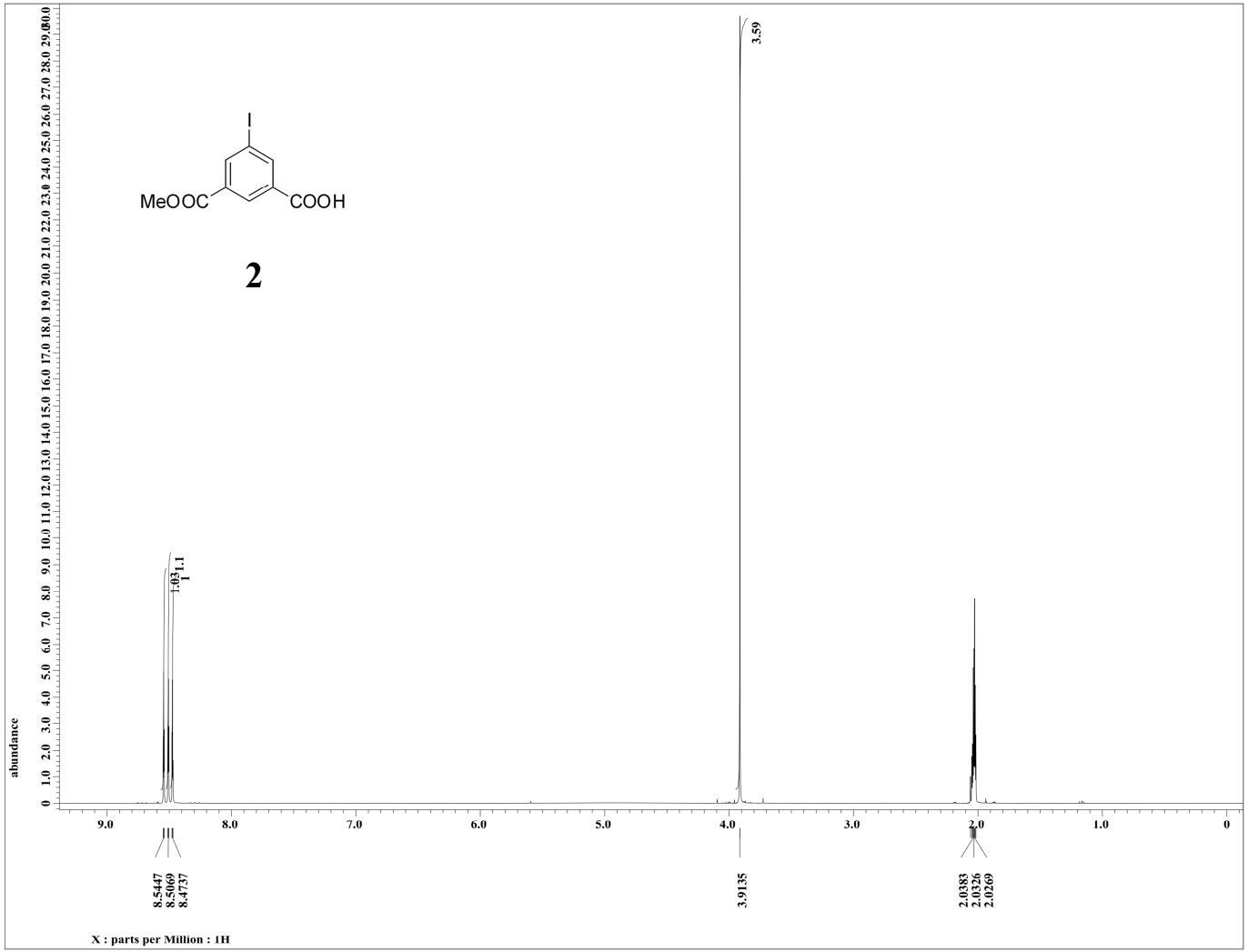
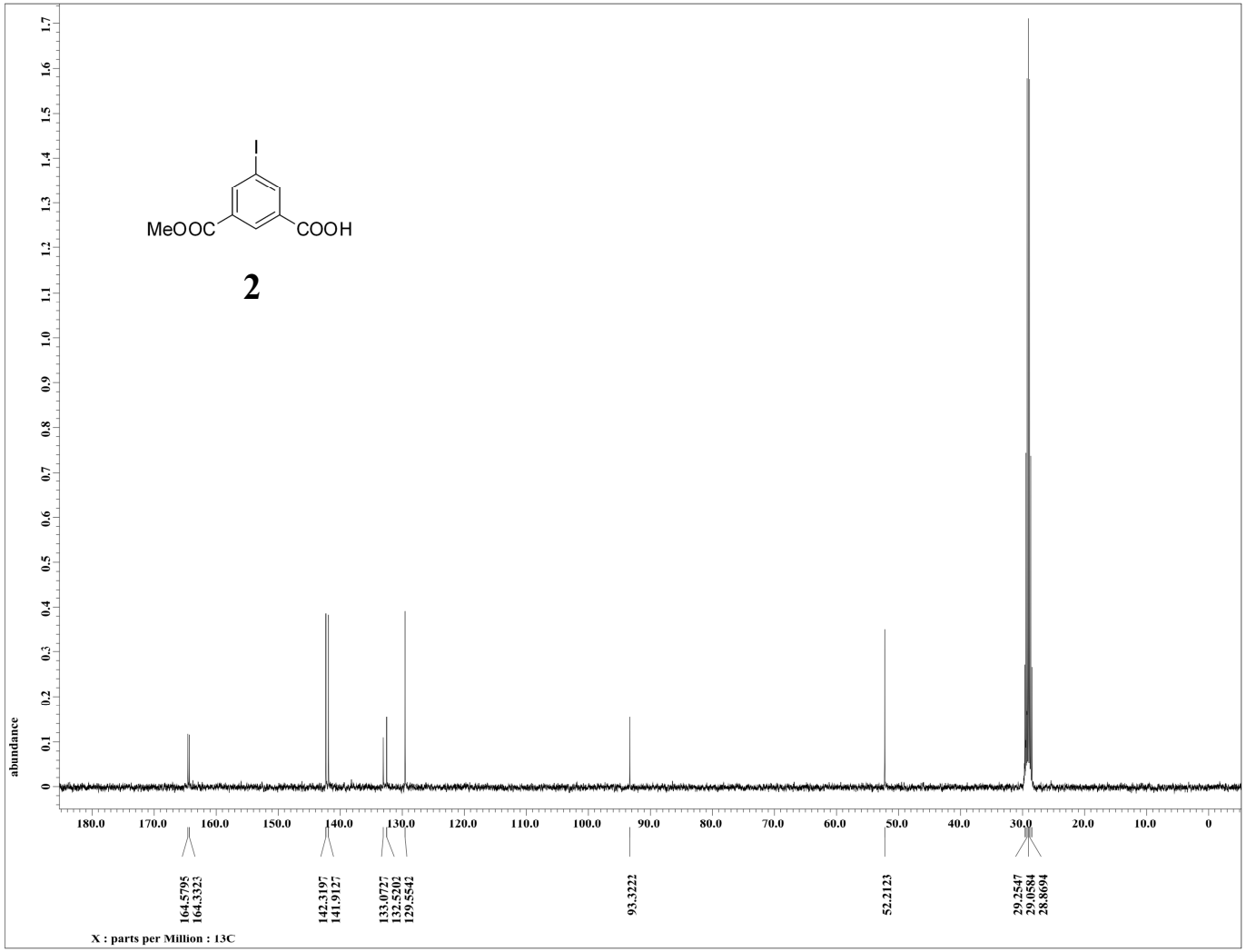
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = Junly_12_NO.1
Solvent           = CHLOROFORM-D
Creation_time     = 12-JUL-2010 18:27:05
Revision_time     = 26-JAN-2011 20:09:31
Current_time      = 26-JAN-2011 20:09:59

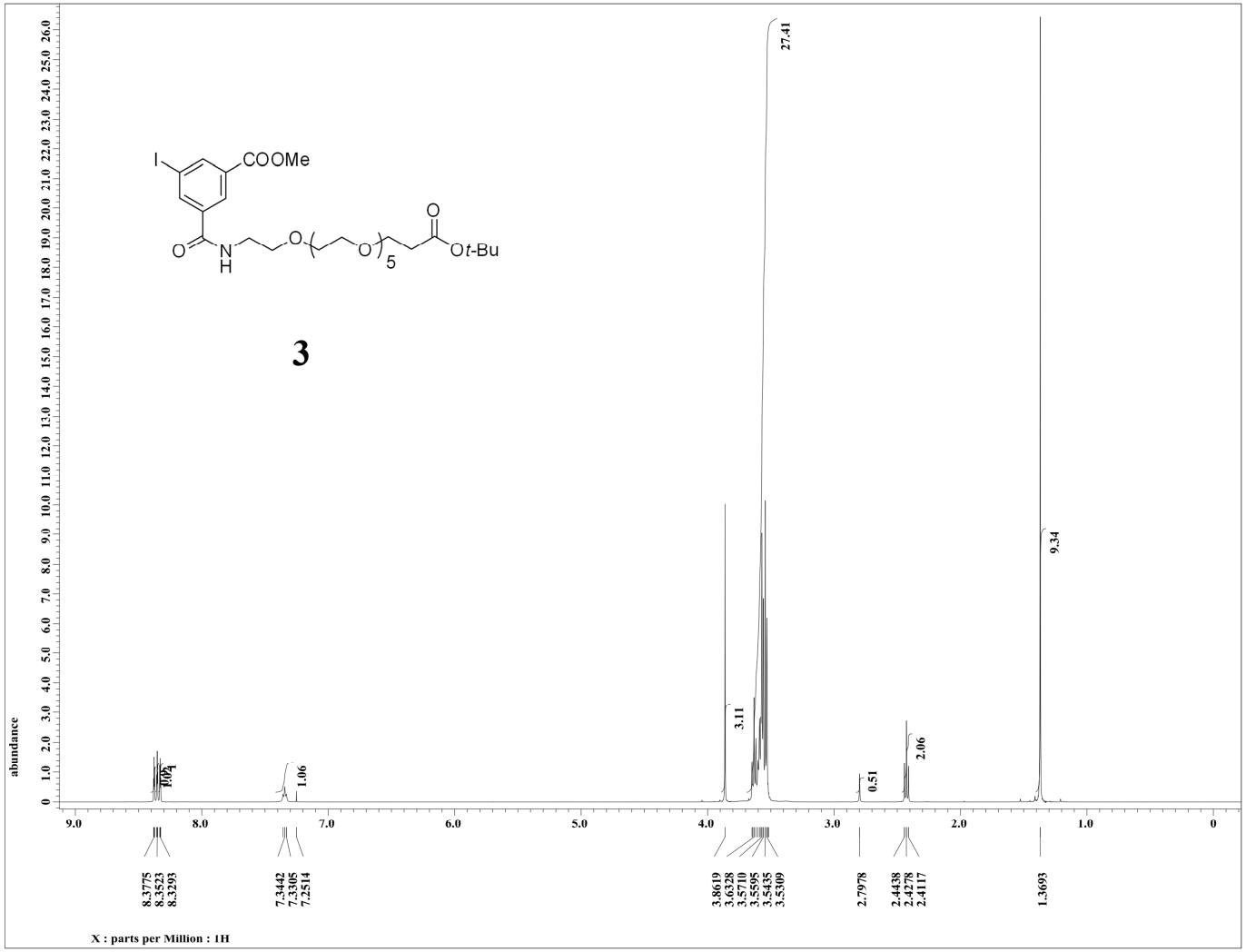
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

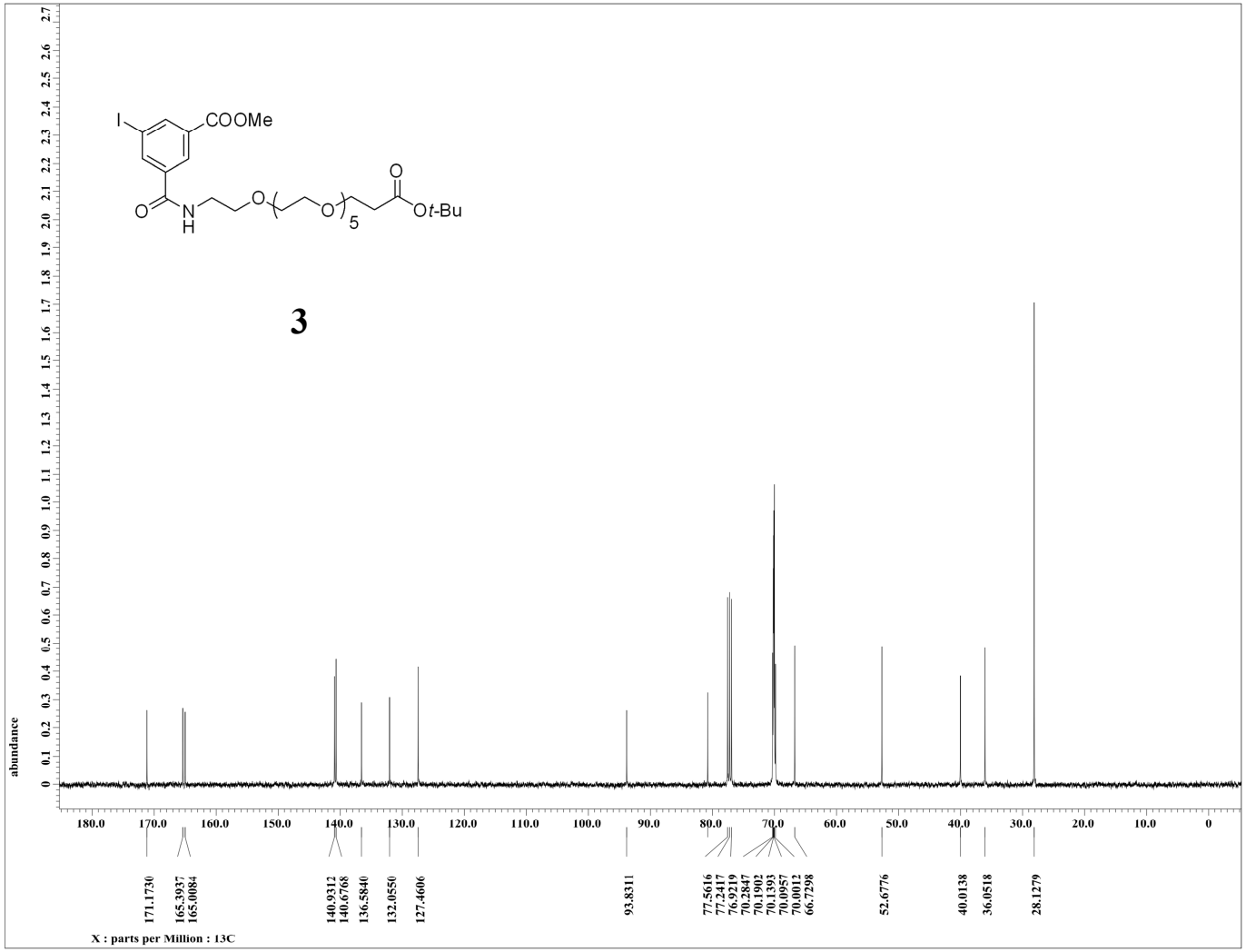
Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 300
Total_scans       = 300

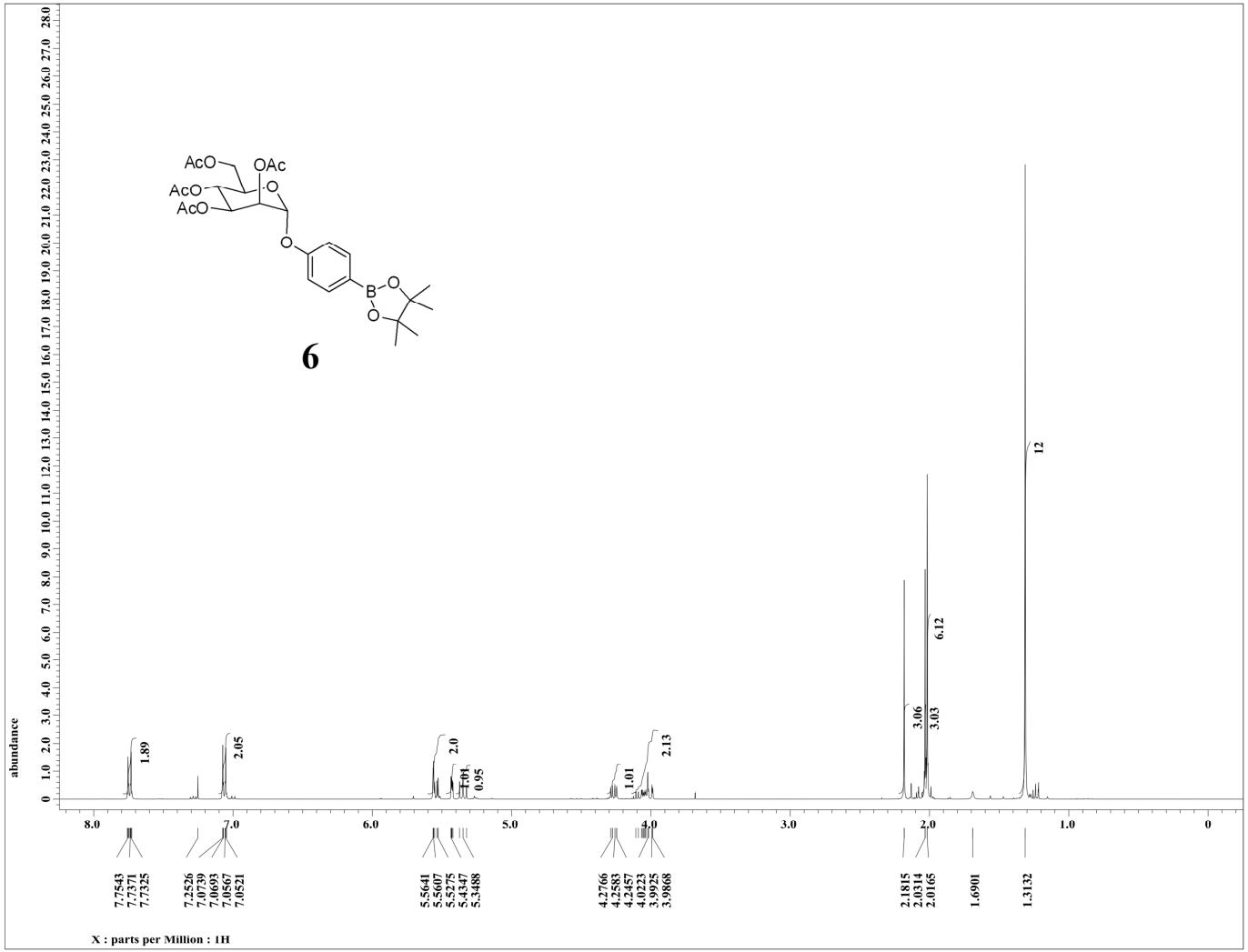
X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 58
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 18.1[dC]
```

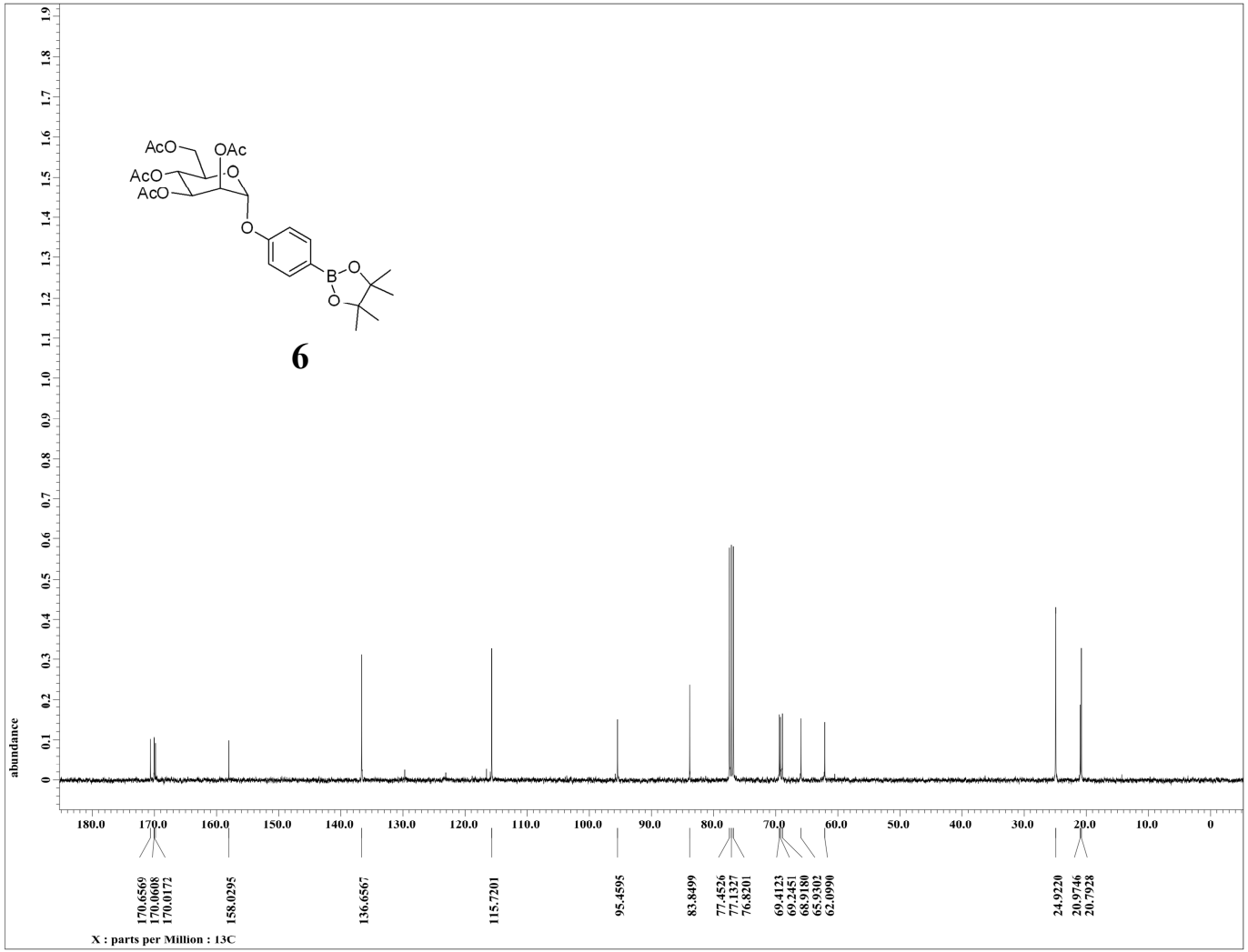

MeOOC
COOH
2
abundance
3.59
1.03
1.1
8.5447
8.5069
8.4737
3.9135
2.0383
2.0326
2.0269
X : parts per Million : 1H

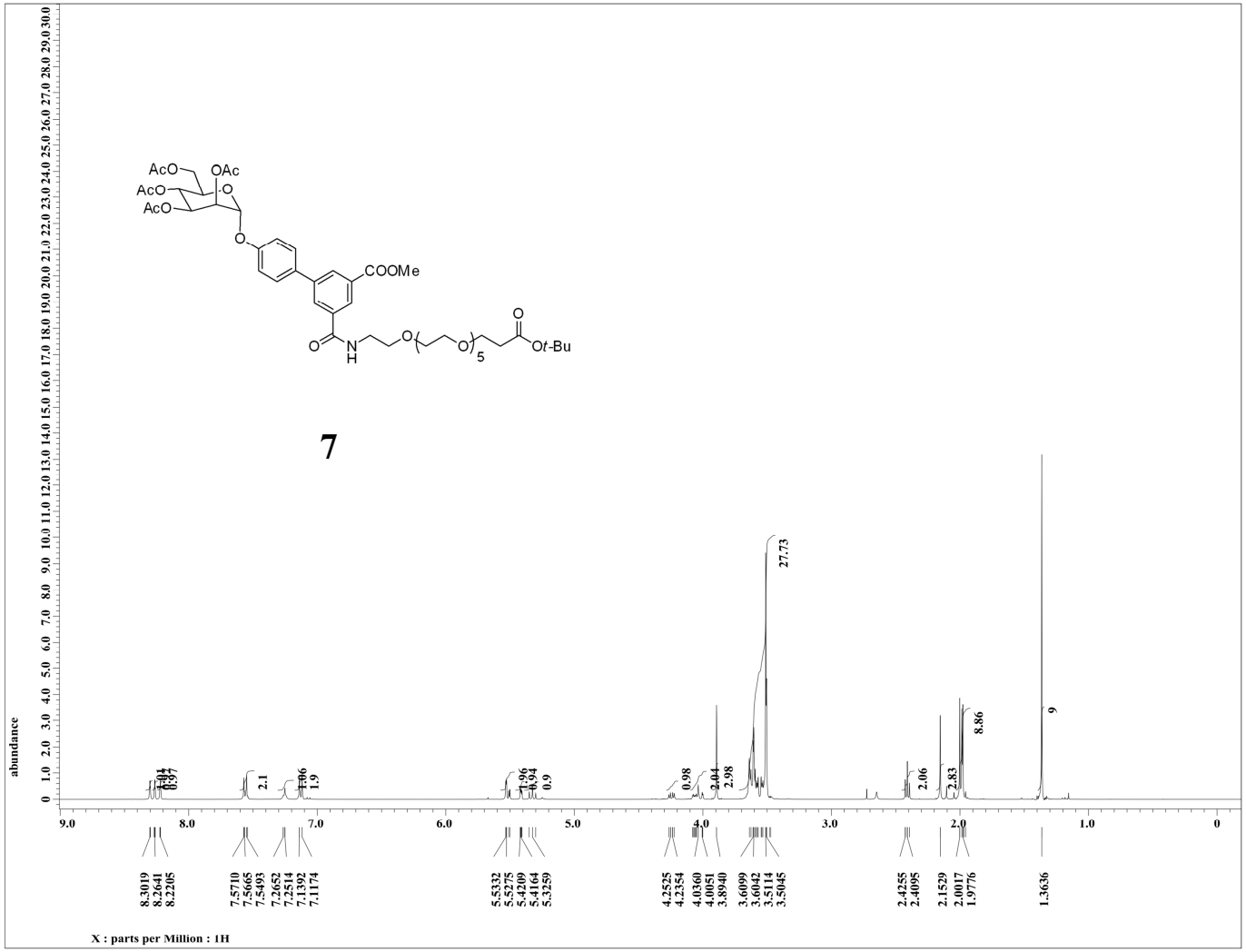

I
MeOOC
COOH
2
abundance
X : parts per Million : 13C
164.5795
164.3323
142.3197
141.9127
133.0727
132.5202
129.5542
93.3222
52.2123
29.2547
29.0584
28.8694

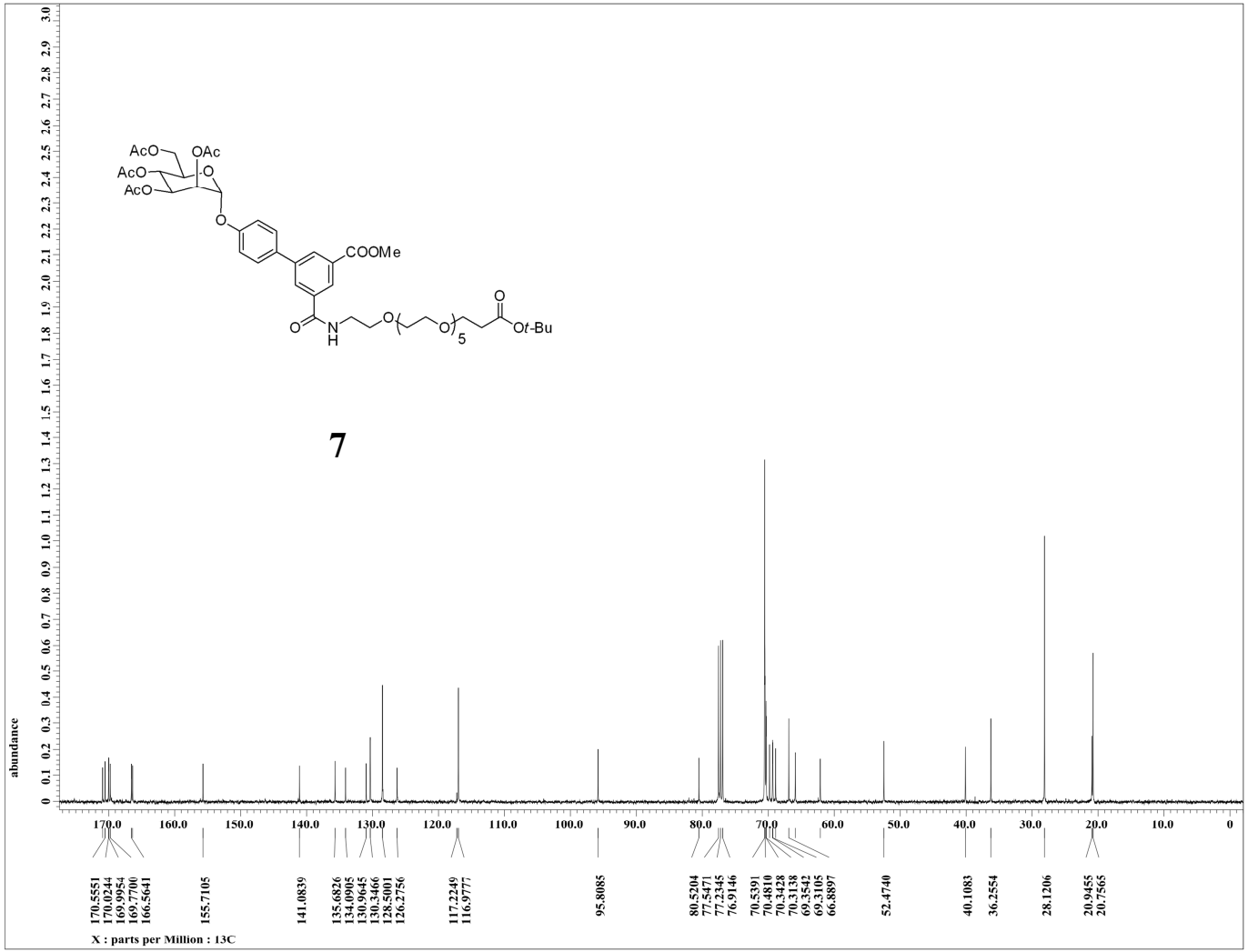

I
COOMe
O
N
H
O
O
5
O
Ot-Bu
3
abundance
X : parts per Million : 1H
27.41
9.34
3.11
2.06
1.06
0.51
8.3775
8.3523
8.3293
7.3442
7.3305
7.2514
3.8619
3.6328
3.5710
3.5595
3.5435
3.5309
2.7978
2.4438
2.4278
2.4117
1.3693

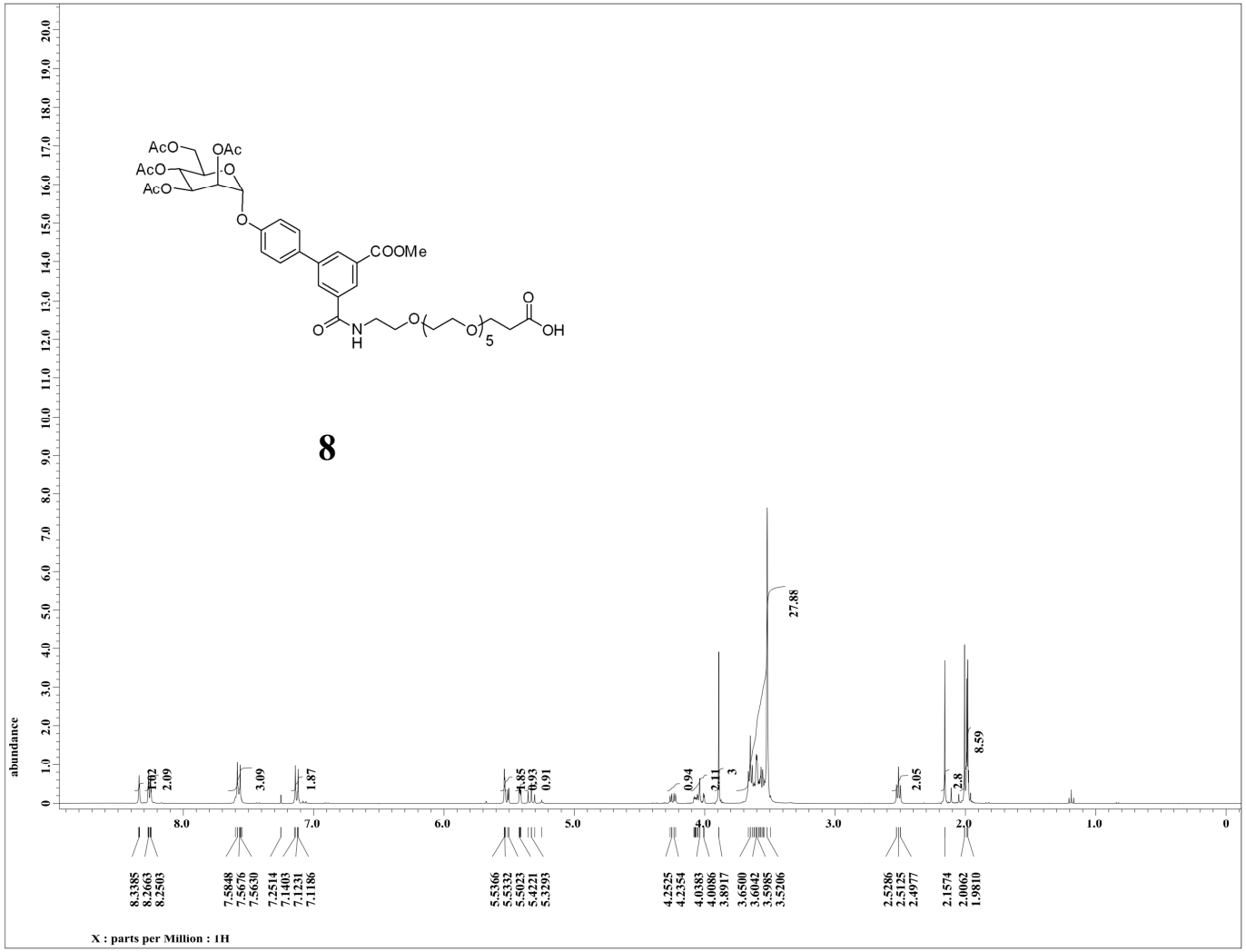

I
COOMe
O
N
H
O
O
O
5
O
Ot-Bu
3
abundance
X : parts per Million : 13C
171.1730
165.3937
165.0084
140.9312
140.6768
136.5840
132.0550
127.4606
93.8311
77.5616
77.2417
76.9219
70.2847
70.1902
70.1393
70.0957
70.0012
66.7298
52.6776
40.0138
36.0518
28.1279

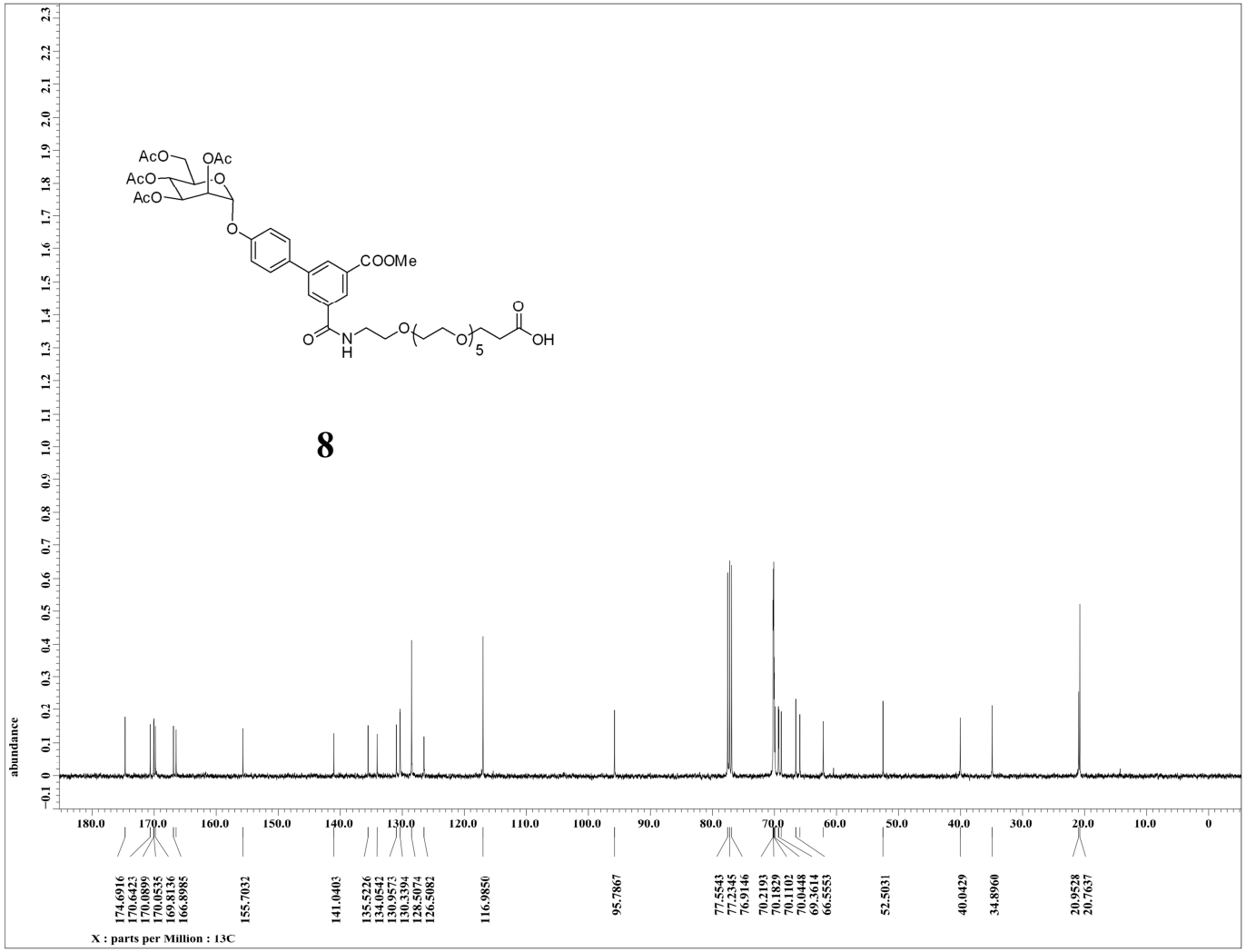

AcO
OAc
AcO
AcO
O
O
B
O
O
6
abundance
X : parts per Million : 1H
1.89
2.05
2.0
1.01
0.95
1.01
2.13
3.06
3.03
6.12
12
7.7543
7.7371
7.7325
7.2526
7.0739
7.0693
7.0567
7.0521
5.5641
5.5607
5.5275
5.4347
5.3488
4.2766
4.2583
4.2457
4.0223
3.9925
3.9868
2.1815
2.0314
2.0165
1.6901
1.3132

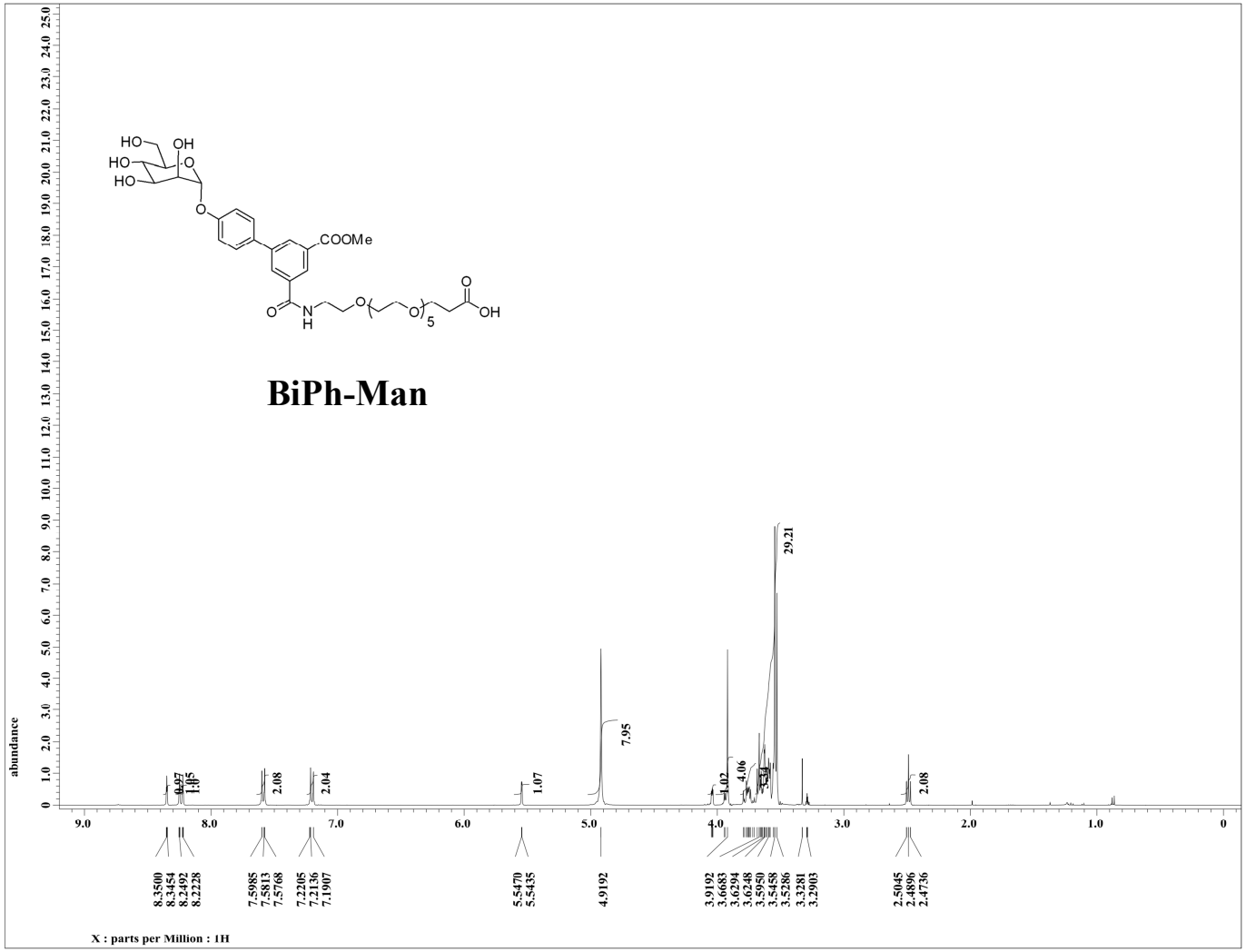

AcO
OAc
AcO
AcO
O
O
B
O
O
6
abundance
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.6569
170.0608
170.0172
158.0295
136.6567
115.7201
95.4595
83.8499
77.4526
77.1327
76.8201
69.4123
69.2451
68.9180
65.9302
62.0990
24.9220
20.9746
20.7928
X : parts per Million : 13C

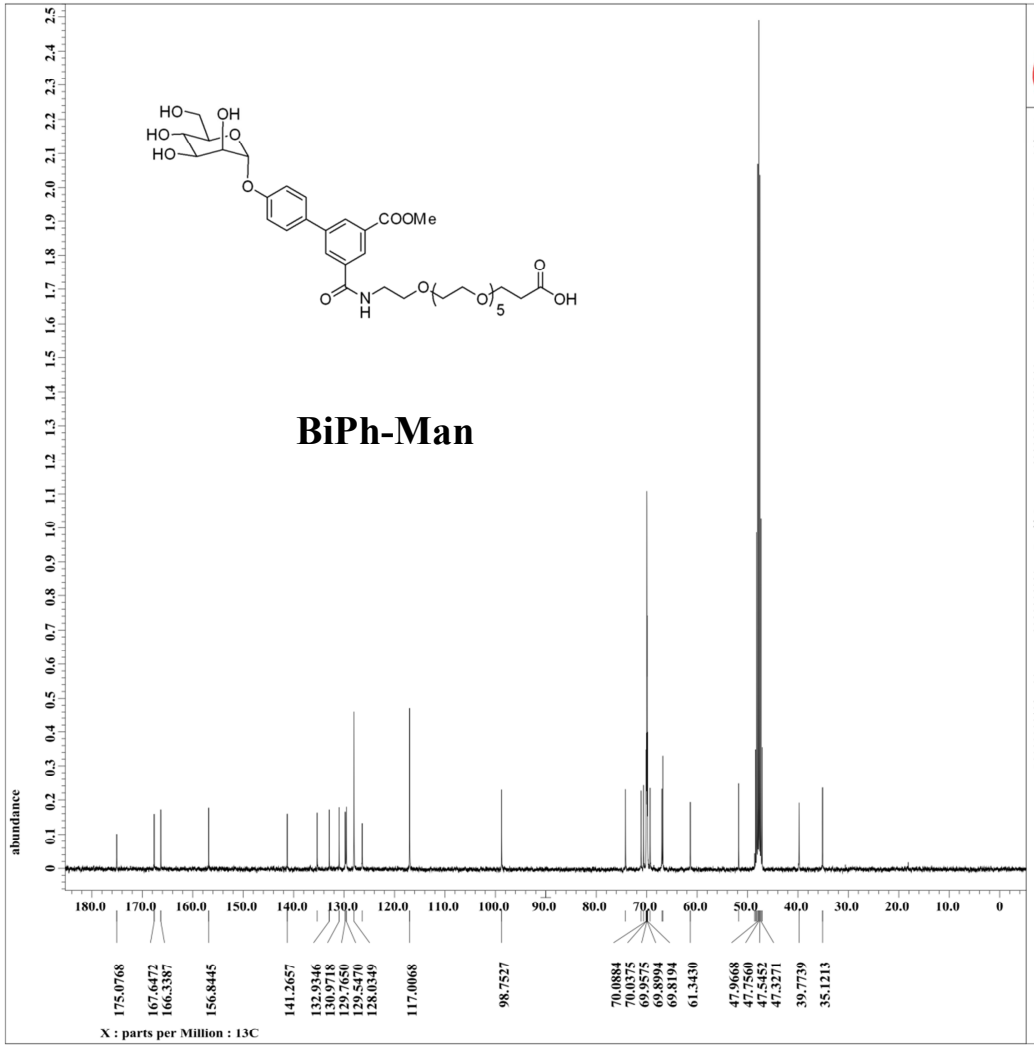

AcO
OAc
AcO
O
AcO
O
COOMe
O
N
H
O
O
O
5
O
Ot-Bu
7
abundance
X : parts per Million : 1H
27.73
8.86
9
2.1
1.9
0.9
0.98
2.98
2.06
2.83
8.3019
8.2641
8.2205
7.5710
7.5665
7.5493
7.2652
7.2514
7.1392
7.1174
5.5332
5.5275
5.4209
5.4164
5.3259
4.2525
4.2354
4.0360
4.0051
3.8940
3.6099
3.6042
3.5114
3.5045
2.4255
2.4095
2.1529
2.0017
1.9776
1.3636


AcO
OAc
AcO
AcO
O
COOMe
O
N
H
O
O
5
O
Ot-Bu
7
abundance
X : parts per Million : 13C
170.5551
170.0244
169.9954
169.7700
166.5641
155.7105
141.0839
135.6826
134.0905
130.9645
130.3466
128.5001
126.2756
117.2249
116.9777
95.8085
80.5204
77.5471
77.2345
76.9146
70.5391
70.4810
70.3428
70.3138
69.3542
69.3105
66.8897
52.4740
40.1083
36.2554
28.1206
20.9455
20.7565


AcO
OAc
AcO
AcO
O
COOMe
O
N
H
O
O
5
O
OH
8
abundance
27.88
8.59
3.09
1.87
2.09
2.02
0.94
2.11
3
4.85
4.93
0.91
2.05
2.8
8.3385
8.2663
8.2503
7.5848
7.5676
7.5630
7.2514
7.1403
7.1231
7.1186
5.5366
5.5332
5.5023
5.4721
5.3293
4.2525
4.2354
4.0383
4.0086
3.8917
3.6500
3.6042
3.5985
3.5206
2.5286
2.5125
2.4977
2.1574
2.0062
1.9810
X : parts per Million : 1H


AcO
OAc
AcO
AcO
O
COOMe
O
N
H
O
O
5
O
OH
8
abundance
X : parts per Million : 13C
174.6916
170.6423
170.0899
170.0535
169.8136
166.8985
155.7032
141.0403
135.5226
134.0542
130.9573
130.3394
128.5074
126.5082
116.9850
95.7867
77.5543
77.2345
76.9146
70.2193
70.1829
70.1102
70.0448
69.3614
66.5553
52.5031
40.0429
34.8960
20.9528
20.7637


HO
OH
HO
HO
O
O
COOMe
O
N
H
O
O
5
O
OH
BiPh-Man
abundance
X : parts per Million : 1H
29.21
7.95
4.06
2.08
2.04
1.07
1.02
2.08
8.3500
8.3454
8.2492
8.2228
7.5985
7.5813
7.5768
7.2205
7.2136
7.1907
5.5470
5.5435
4.9192
3.9192
3.6683
3.6294
3.6248
3.5950
3.5458
3.5286
3.3281
3.2903
2.5045
2.4896
2.4736

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Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = METHANOL-D3
Creation_time     = 10-SEP-2010 18:11:19
Revision_time     = 27-JAN-2011 20:33:25
Current_time      = 27-JAN-2011 20:33:44

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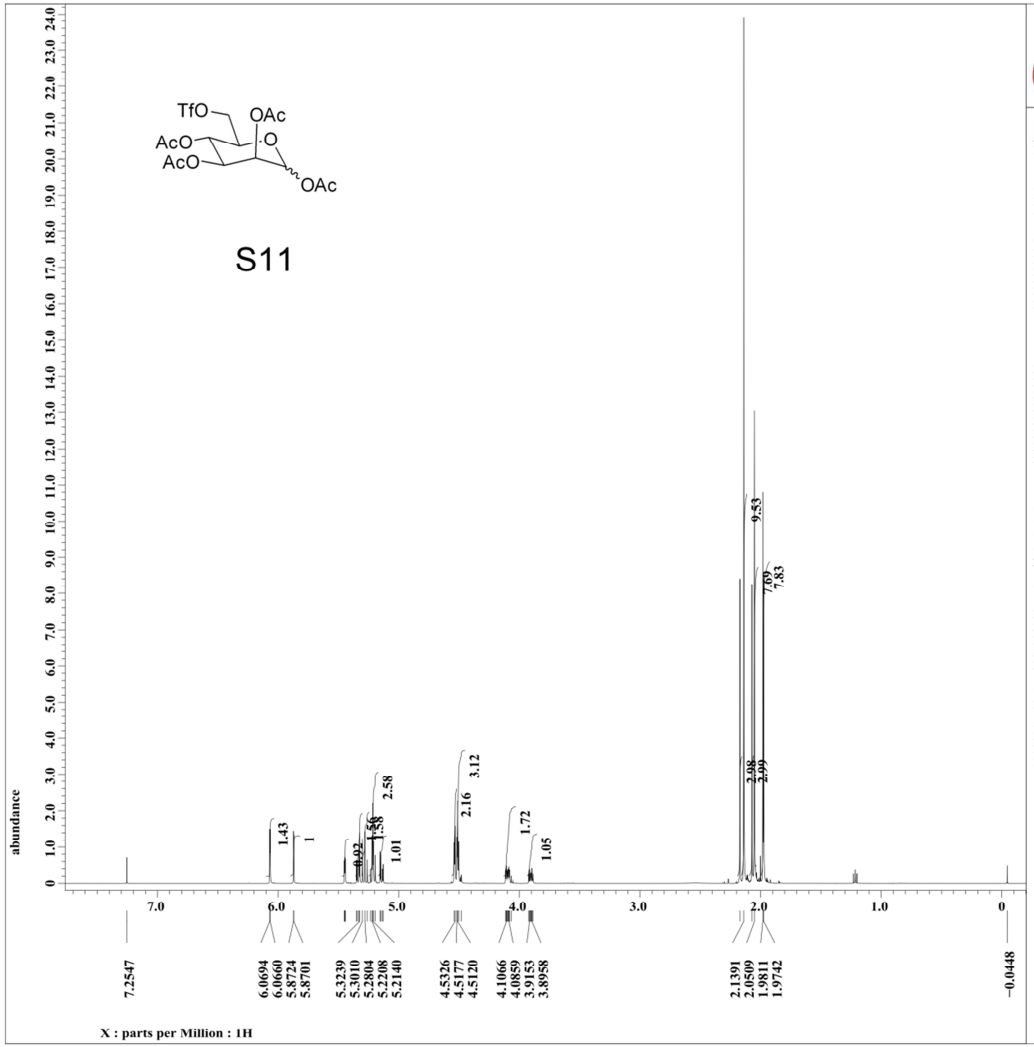
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.36839168[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 90.0[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.73078492[Hz]
X_sweep           = 23.94636015[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 490
Total_scans       = 490

X_90_width        = 12.4525[us]
X_acq_time        = 1.36839168[s]
X_angle           = 30[deg]
X_atn             = 6[dB]
X_pulse           = 4.15083333[us]
Irr_atn_dec       = 22[dB]
Irr_atn_noe       = 22[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 2.36839168[s]
Temp_get          = 20.4[dC]
```

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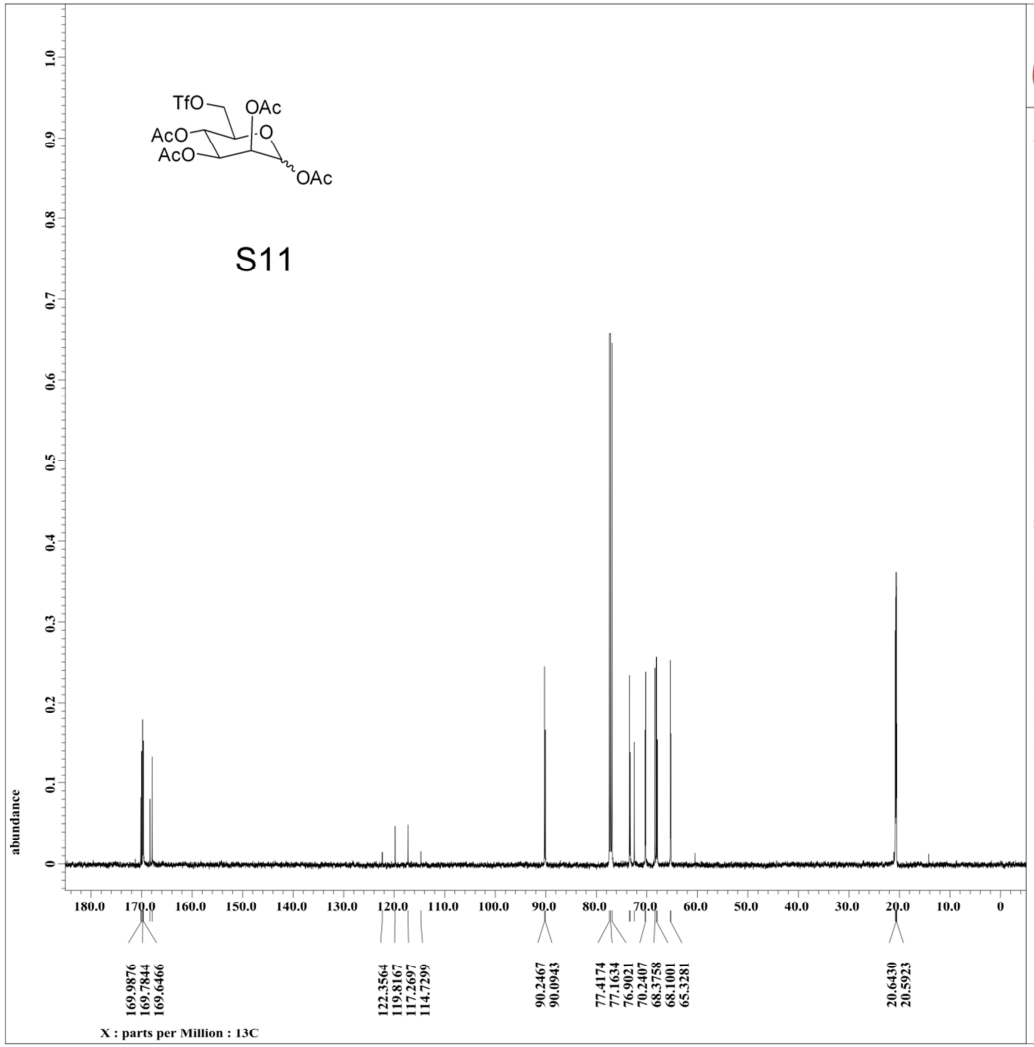
Filename          = 6-TfO-Ac4-mannose-h1-
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 10-JAN-2011 19:31:16
Revision_time     = 26-JAN-2011 20:56:04
Current_time      = 26-JAN-2011 20:57:36

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19.2[dC]
```

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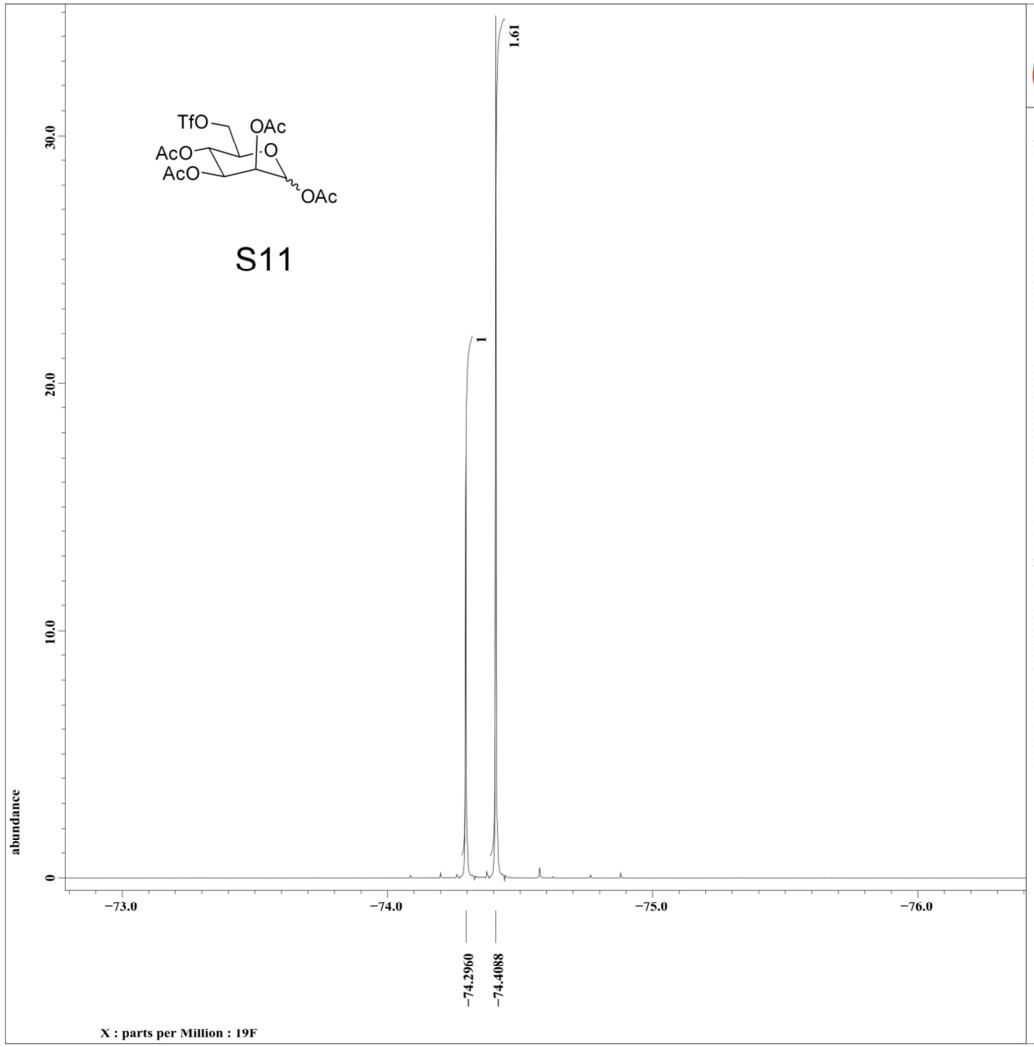
Filename          = c13default185to-5ppm-
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 10-JAN-2011 20:07:34
Revision_time     = 26-JAN-2011 20:58:37
Current_time      = 26-JAN-2011 20:59:53

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1024
Total_scans       = 1024

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 58
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 20.1[dC]
```

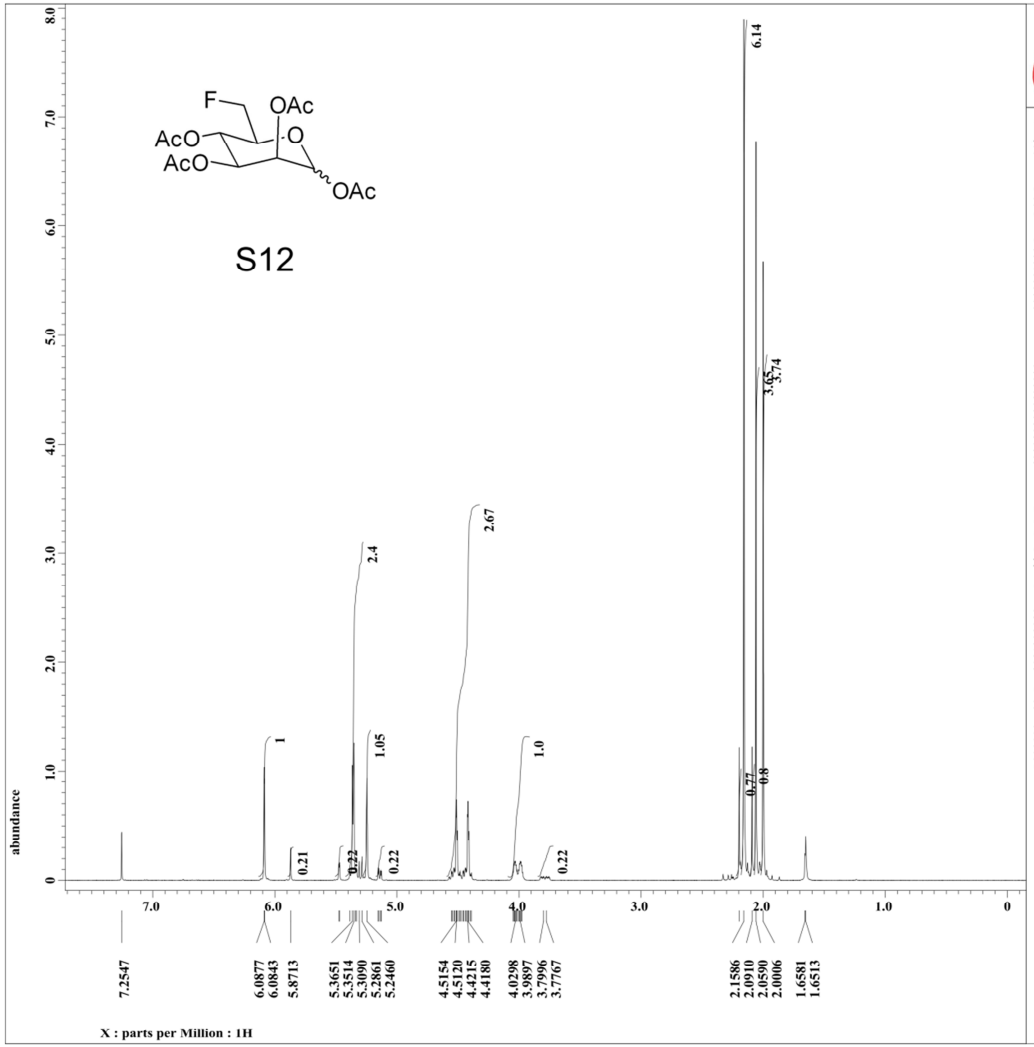



```
Filename          = test-9.jdf
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 10-JAN-2011 20:24:04
Revision_time     = 10-JAN-2011 20:59:53
Current_time      = 26-JAN-2011 21:10:39

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 52428
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.11149056[s]
X_domain          = 19F
X_freq            = 470.62046084[MHz]
X_offset          = -50[ppm]
X_points          = 65536
X_prescans        = 0
X_resolution      = 0.89969275[Hz]
X_sweep           = 58.96226415[kHz]
Irr_domain        = 19F
Irr_freq          = 470.62046084[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 470.62046084[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1
Total_scans       = 1

X_90_width        = 16[us]
X_acq_time        = 1.11149056[s]
X_angle           = 45[deg]
X_atn             = 2[dB]
X_pulse           = 8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 6.11149056[s]
Temp_get          = 19.2[dC]
```

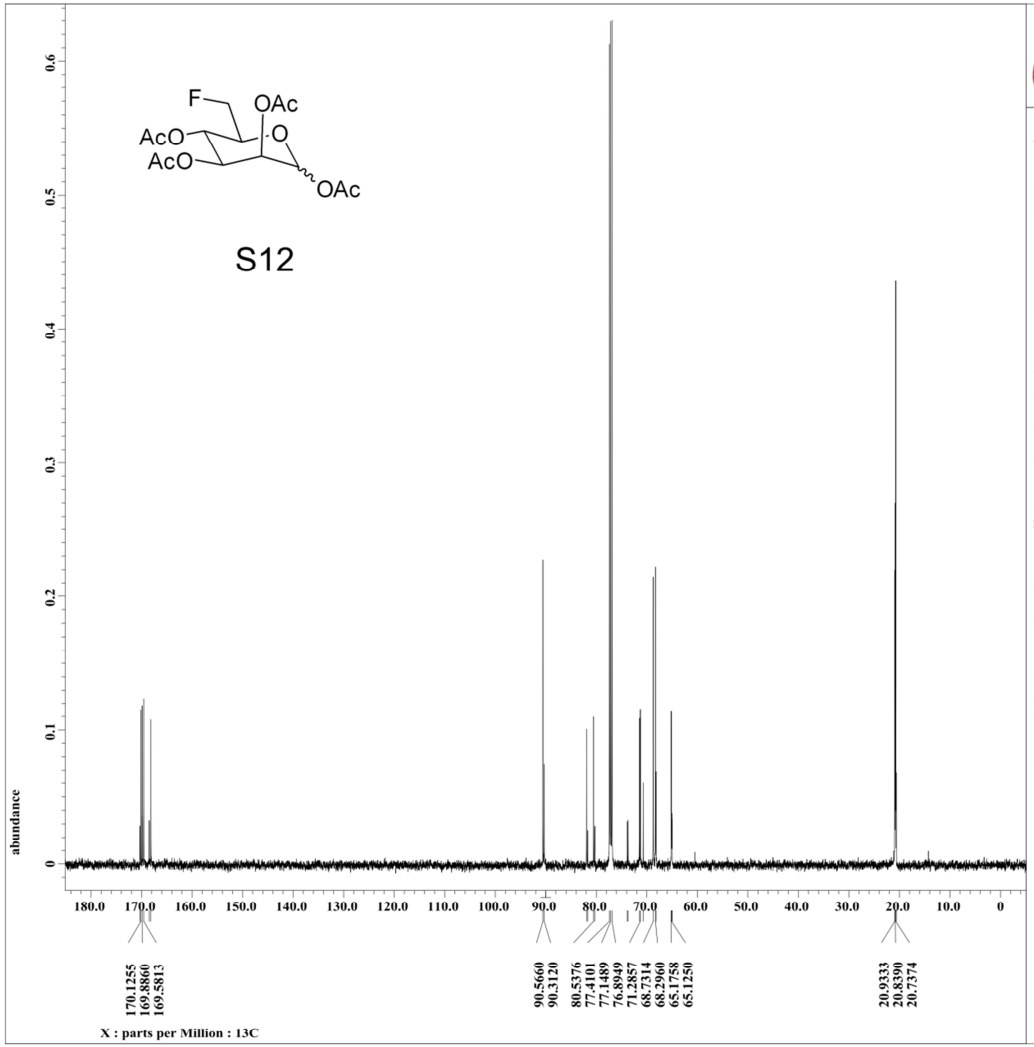



```
Filename          = 6-F-tetra-Ac-mannose-
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 12-NOV-2010 21:08:13
Revision_time     = 26-JAN-2011 21:01:18
Current_time      = 26-JAN-2011 21:02:18

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19.5[dC]
```

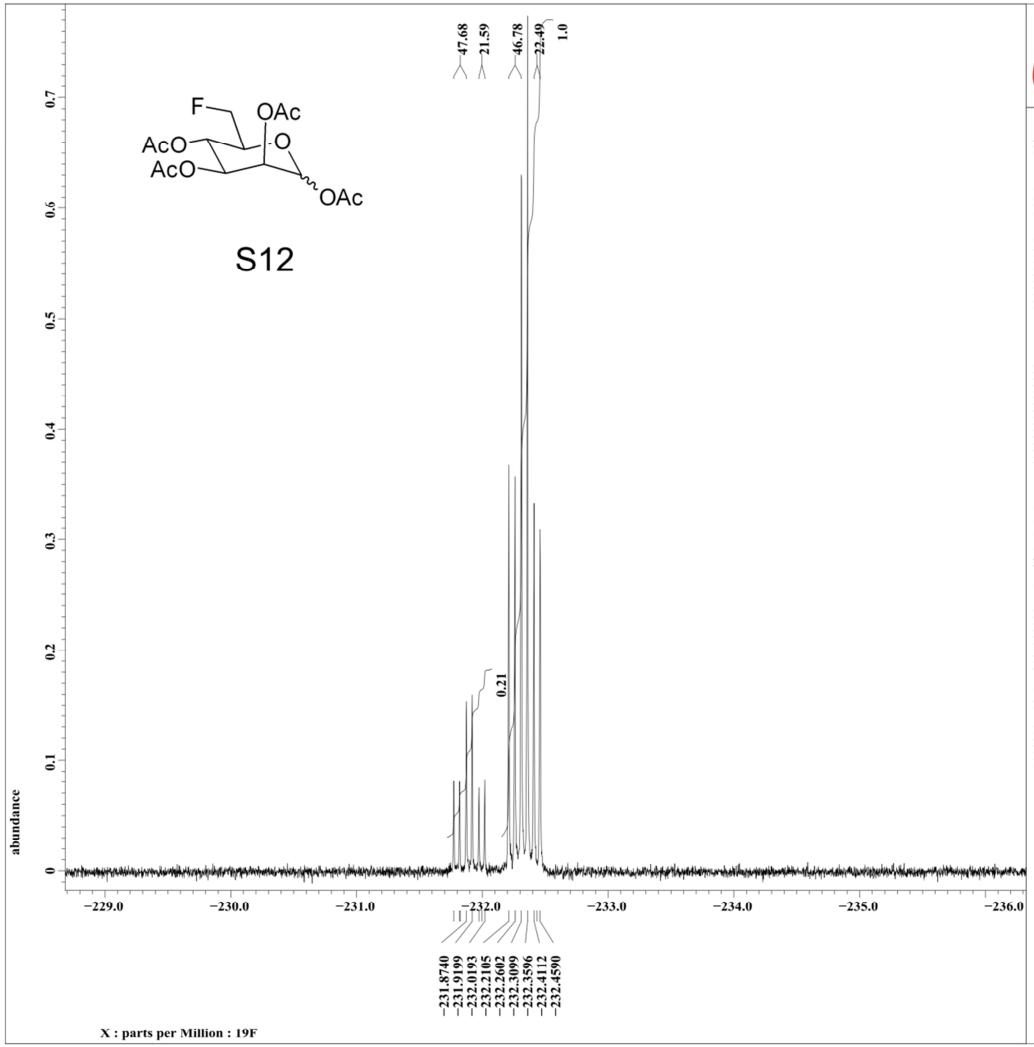


```
Filename          = c13default185to-5ppm-
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = up spot
Solvent           = CHLOROFORM-D
Creation_time     =  9-NOV-2010 14:45:16
Revision_time     = 26-JAN-2011 21:04:41
Current_time      = 26-JAN-2011 21:05:50

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1024
Total_scans       = 1024

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 58
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 20.2[dC]
```



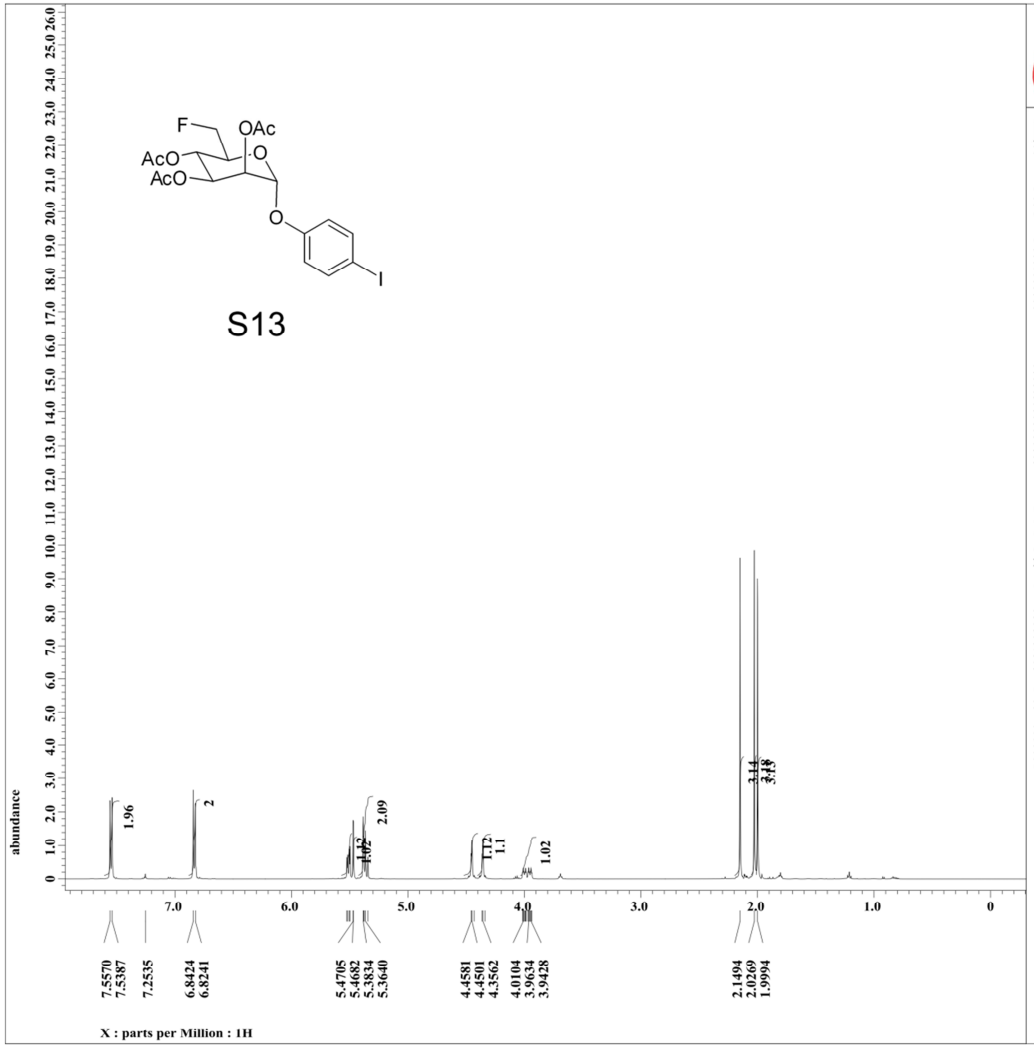
JEOL

```
Filename          = 6-F-tetra-Ac-mannose-
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 12-NOV-2010 21:22:29
Revision_time     = 12-NOV-2010 22:04:31
Current_time      = 26-JAN-2011 21:09:15

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 52428
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.11149056[s]
X_domain          = 19F
X_freq            = 470.62046084[MHz]
X_offset          = -200[ppm]
X_points          = 65536
X_prescans        = 0
X_resolution      = 0.89969275[Hz]
X_sweep           = 58.96226415[kHz]
Irr_domain        = 19F
Irr_freq          = 470.62046084[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 470.62046084[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1
Total_scans       = 1

X_90_width        = 16[us]
X_acq_time        = 1.11149056[s]
X_angle           = 45[deg]
X_atn             = 2[dB]
X_pulse           = 8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 6.11149056[s]
Temp_get          = 19.7[dC]
```



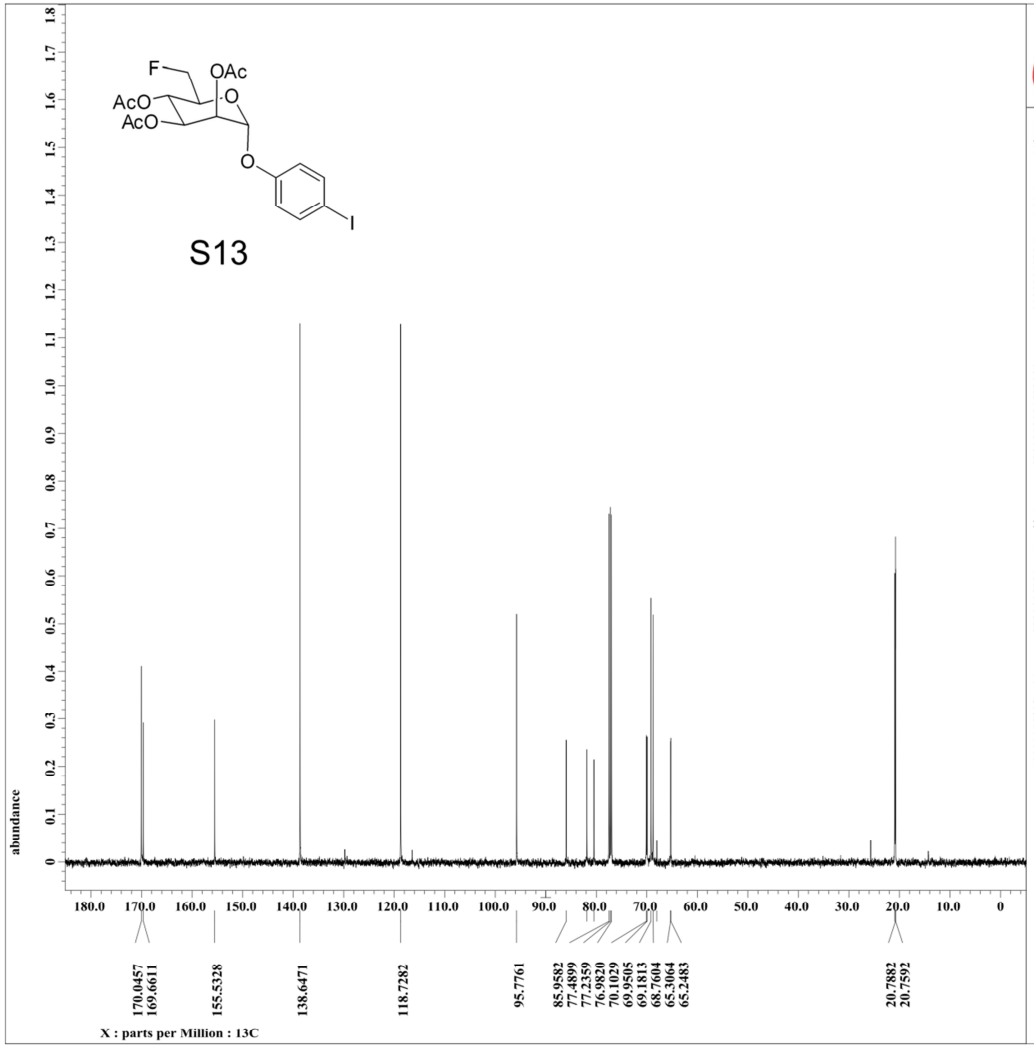
JEOL

```
Filename          = F-mannose-iodophenyl-
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 2
Solvent           = CHLOROFORM-D
Creation_time     = 15-NOV-2010 17:10:19
Revision_time     = 26-JAN-2011 21:16:23
Current_time      = 26-JAN-2011 21:17:56

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19.2[dC]
```

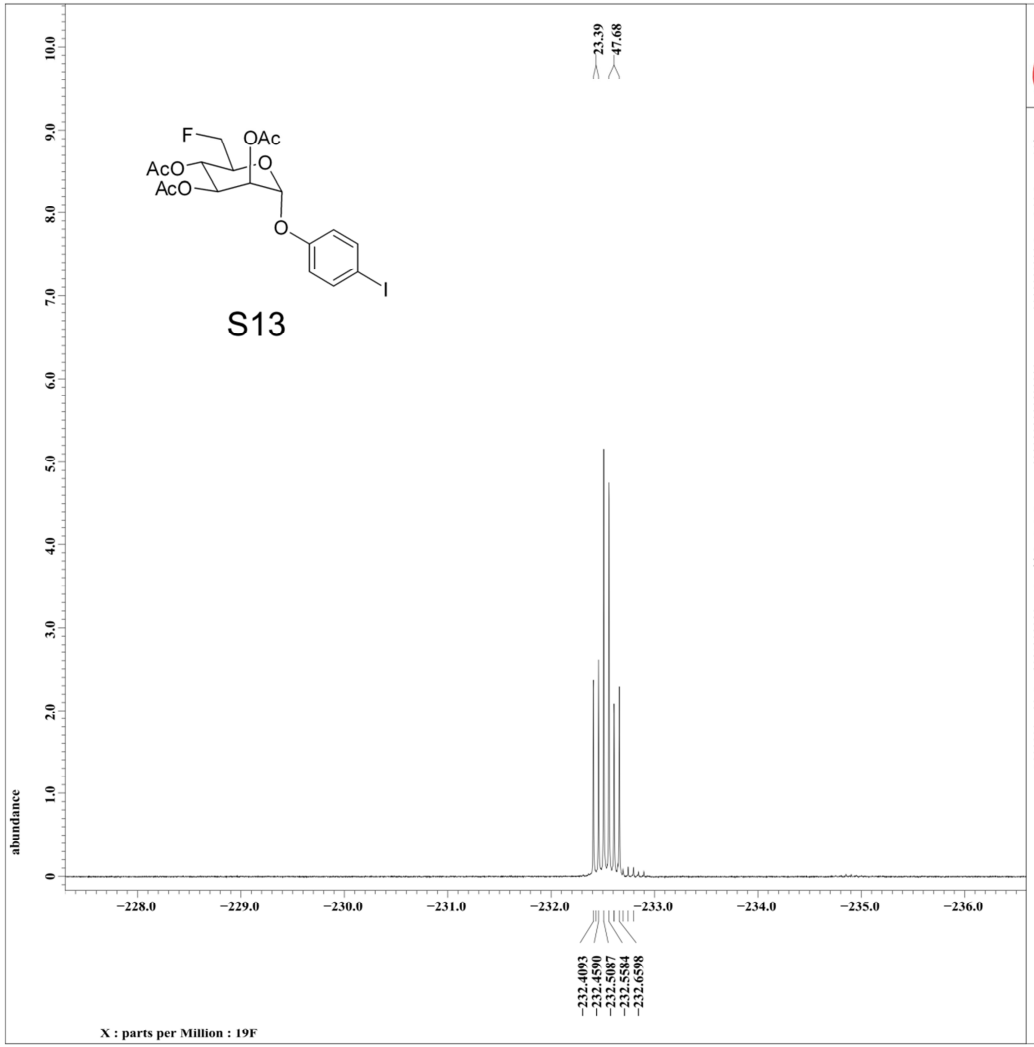



```
Filename          = F-mannose-iodophenyl-
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 2
Solvent           = CHLOROFORM-D
Creation_time     = 15-NOV-2010 17:19:22
Revision_time     = 26-JAN-2011 21:18:55
Current_time      = 26-JAN-2011 21:20:02

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 246
Total_scans       = 246

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 19.9[dC]
```

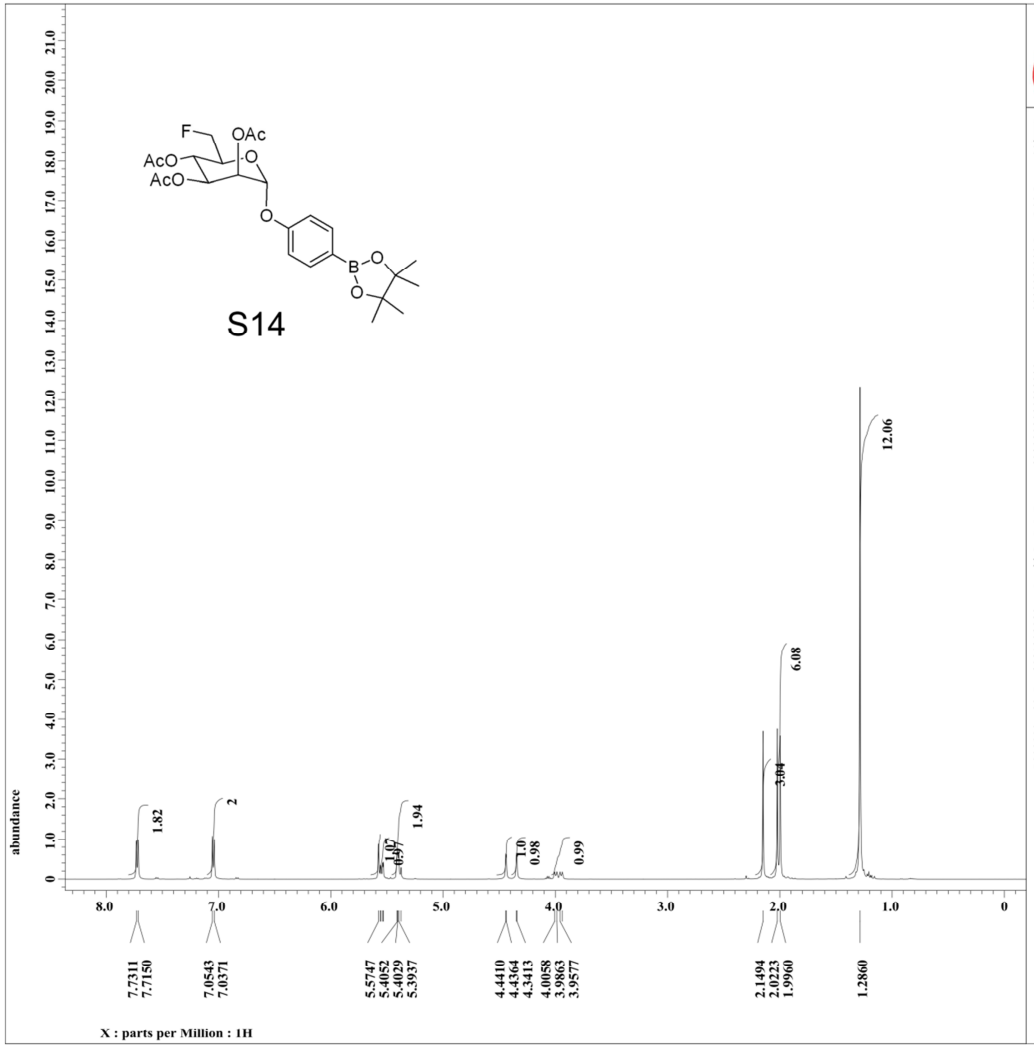



```
Filename          = F-mannose-iodophenyl-
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 15-NOV-2010 17:21:29
Revision_time     = 15-NOV-2010 17:55:33
Current_time      = 26-JAN-2011 21:12:34

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 52428
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.11149056[s]
X_domain          = 19F
X_freq            = 470.62046084[MHz]
X_offset          = -200[ppm]
X_points          = 65536
X_prescans        = 0
X_resolution      = 0.89969275[Hz]
X_sweep           = 58.96226415[kHz]
Irr_domain        = 19F
Irr_freq          = 470.62046084[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 470.62046084[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1
Total_scans       = 1

X_90_width        = 16[us]
X_acq_time        = 1.11149056[s]
X_angle           = 45[deg]
X_atn             = 2[dB]
X_pulse           = 8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 6.11149056[s]
Temp_get          = 19.6[dC]
```

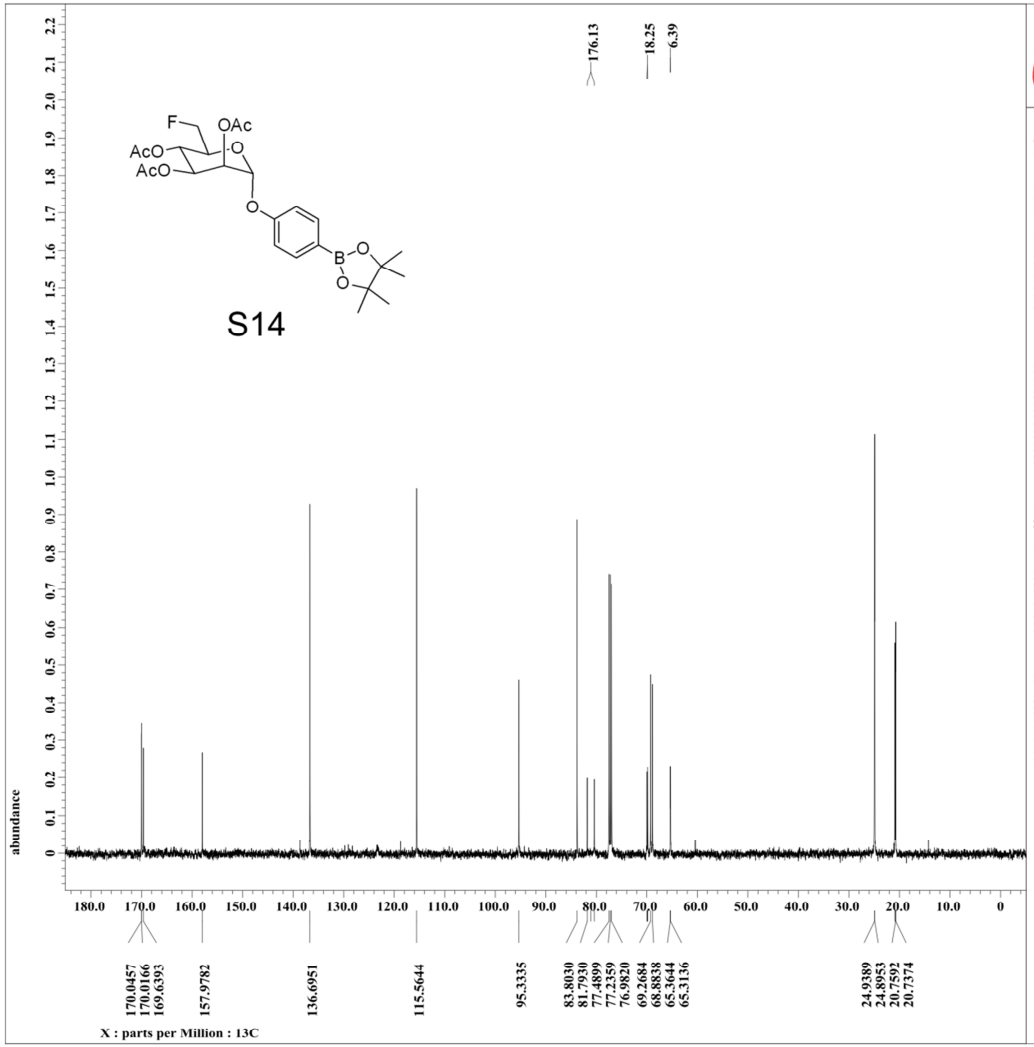



```
Filename          = h1default14to-1-117.j
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 2
Solvent           = CHLOROFORM-D
Creation_time     = 16-NOV-2010 22:19:27
Revision_time     = 26-JAN-2011 21:25:59
Current_time      = 26-JAN-2011 21:27:29

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 26
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19.3[dC]
```

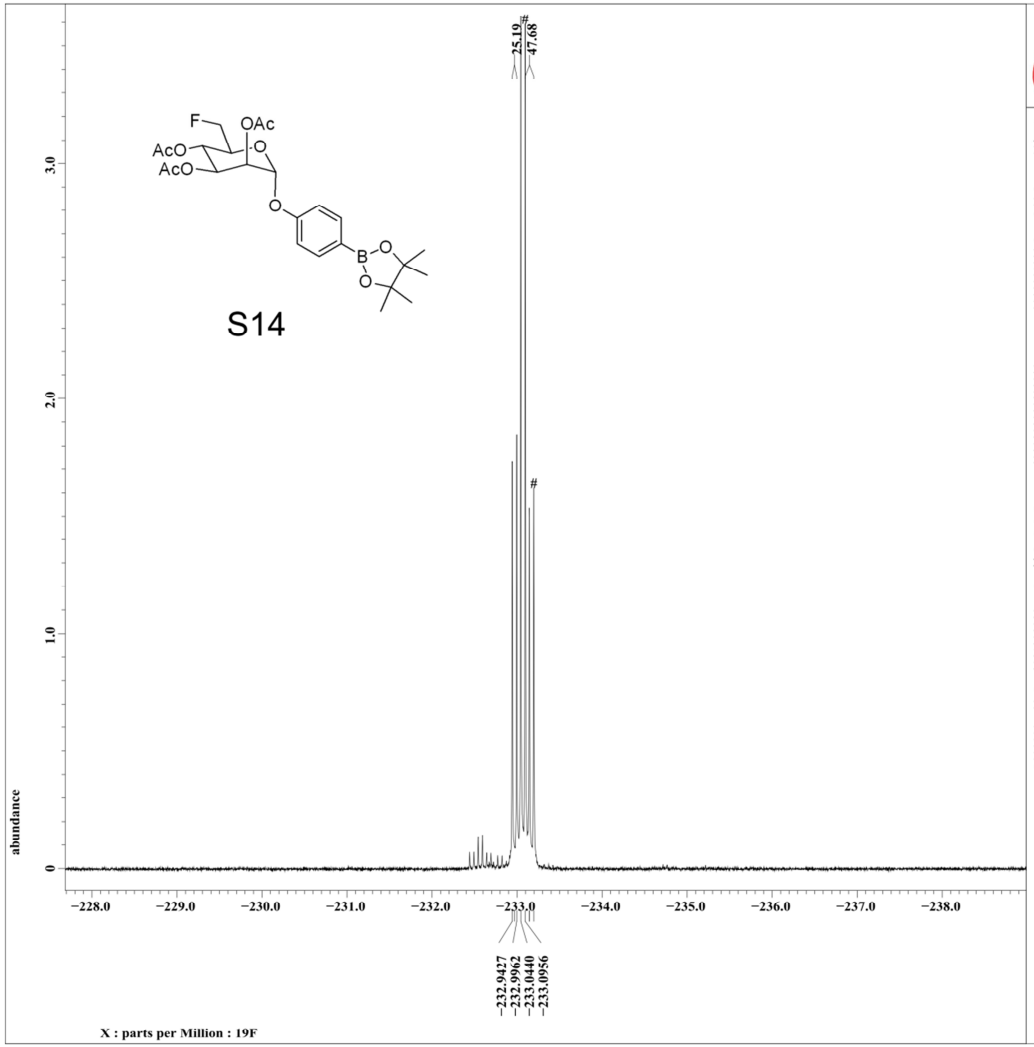


Filename = c13default185to-5ppm-
Author = Cai
Experiment = single_pulse_dec
Sample_id = 2
Solvent = CHLOROFORM-D
Creation_time = 16-NOV-2010 22:24:07
Revision_time = 16-NOV-2010 22:58:54
Current_time = 26-JAN-2011 21:32:59

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.09576192[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 90[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.912607[Hz]
X_sweep = 29.90430622[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 6.5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 103
Total_scans = 103

X_90_width = 11.77[us]
X_acq_time = 1.09576192[s]
X_angle = 30[deg]
X_atn = 9[dB]
X_pulse = 3.92333333[us]
Irr_atn_dec = 19.5[dB]
Irr_atn_noe = 19.5[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 1[s]
Recvr_gain = 60
Relaxation_delay = 1[s]
Repetition_time = 2.09576192[s]
Temp_get = 19.7[dC]



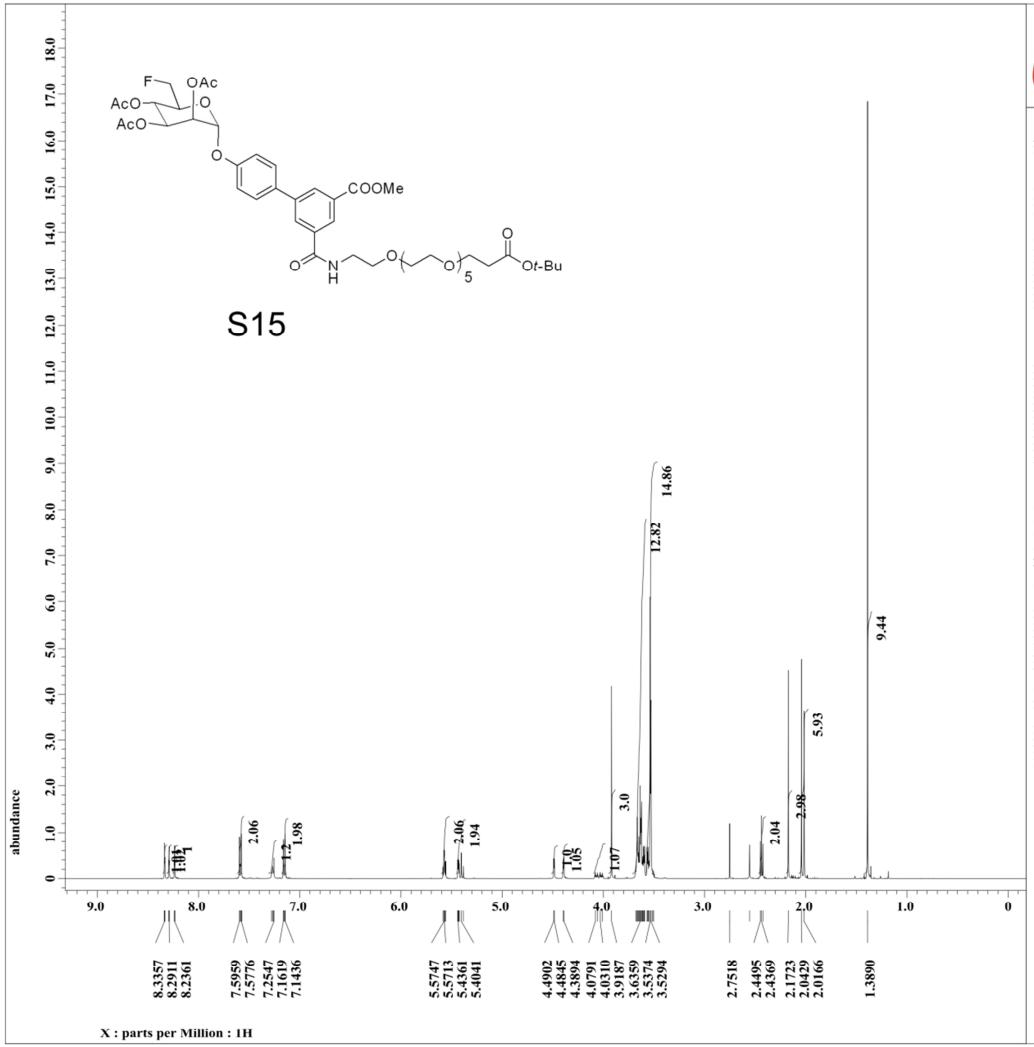
JEOL

```
Filename          = F19-5.jdf
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 2
Solvent           = CHLOROFORM-D
Creation_time     = 16-NOV-2010 22:26:47
Revision_time     = 26-JAN-2011 21:34:20
Current_time      = 26-JAN-2011 21:34:36

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 52428
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.11149056[s]
X_domain          = 19F
X_freq            = 470.62046084[MHz]
X_offset          = -200[ppm]
X_points          = 65536
X_prescans        = 0
X_resolution      = 0.89969275[Hz]
X_sweep           = 58.96226415[kHz]
Irr_domain        = 19F
Irr_freq          = 470.62046084[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 470.62046084[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1
Total_scans       = 1

X_90_width        = 16[us]
X_acq_time        = 1.11149056[s]
X_angle           = 45[deg]
X_atn             = 2[dB]
X_pulse           = 8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 6.11149056[s]
Temp_get          = 19.2[dC]
```

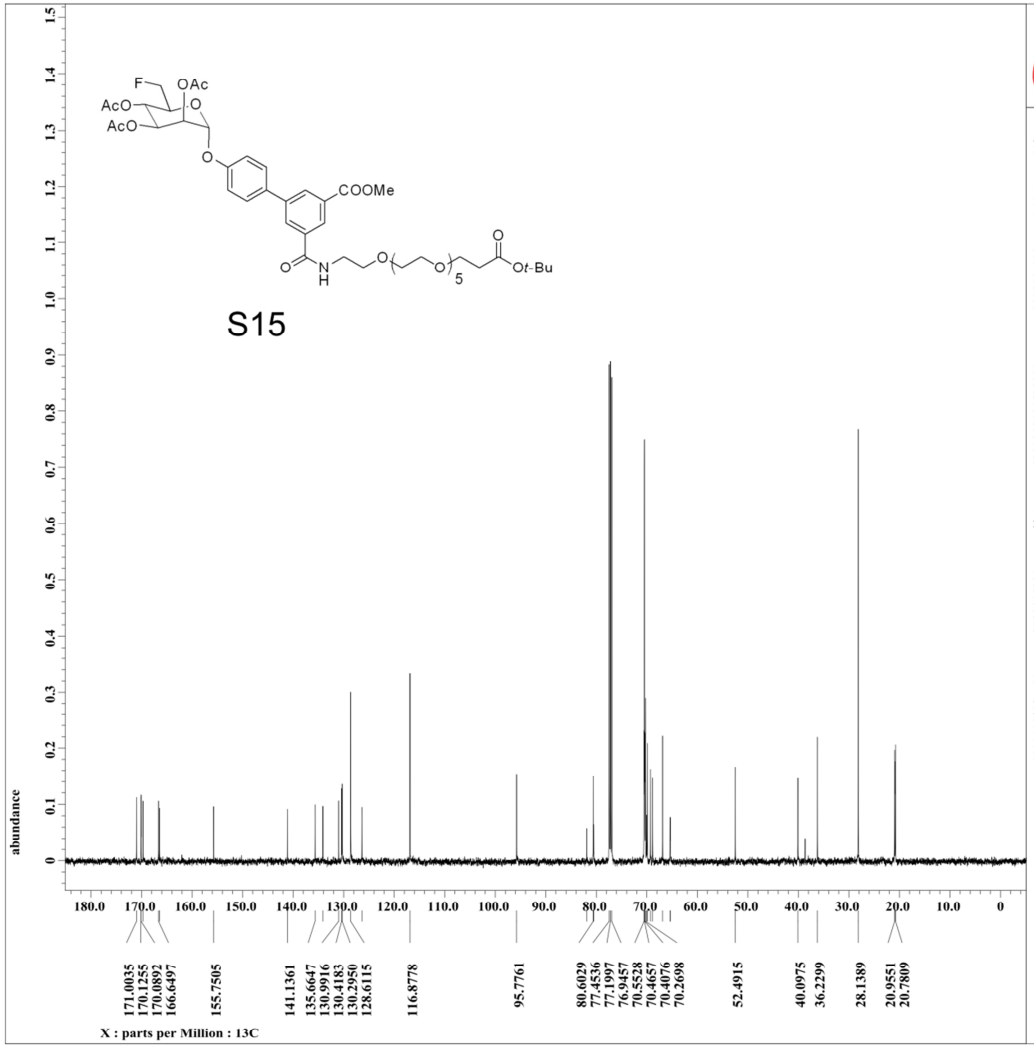



```
Filename          = Suzuki-Coupling-h1def
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 24-NOV-2010 15:10:26
Revision_time     = 26-JAN-2011 21:36:49
Current_time      = 26-JAN-2011 21:38:24

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19.2[dC]
```

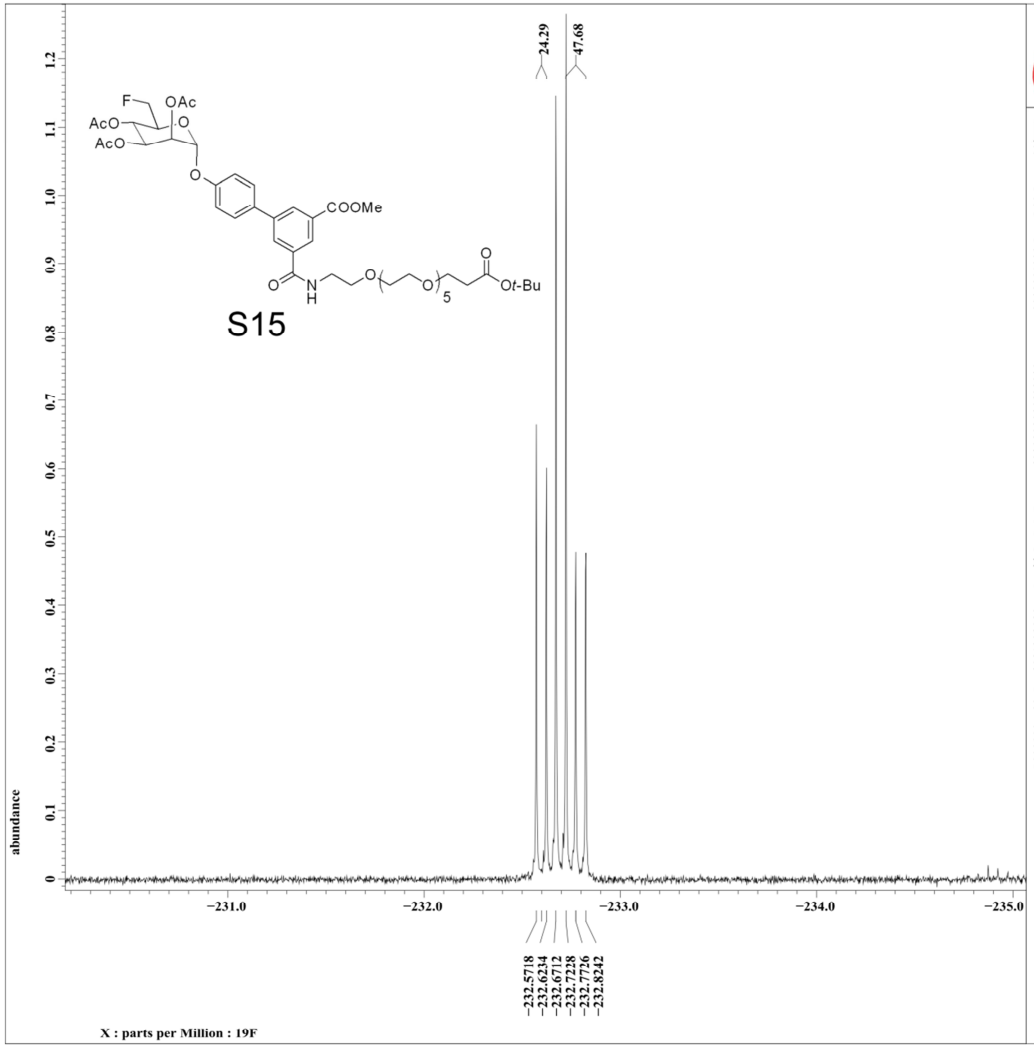



```
Filename          = Suzuki-Coupling-c13de
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 24-NOV-2010 15:29:58
Revision_time     = 26-JAN-2011 21:39:17
Current_time      = 26-JAN-2011 21:39:46

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 546
Total_scans       = 546

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 19.9[dC]
```

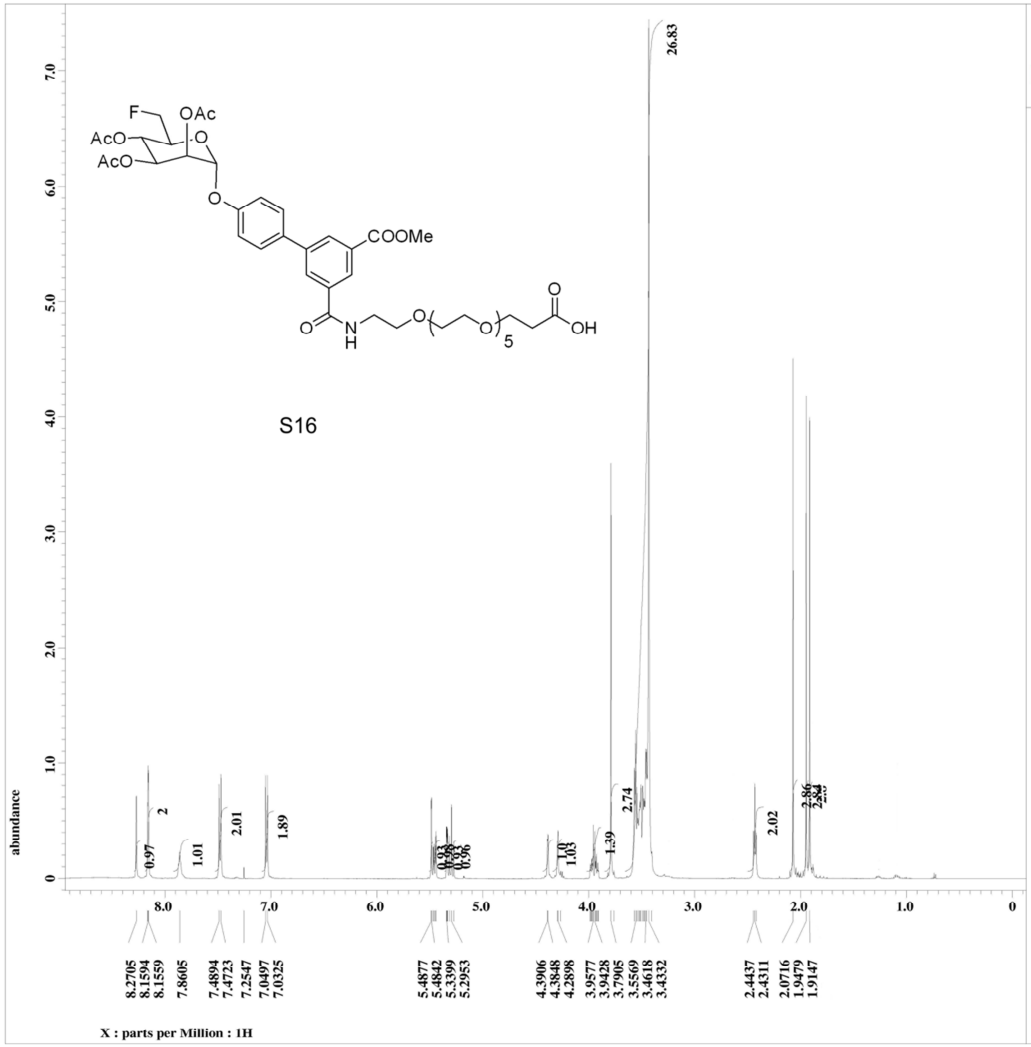



```
Filename          = Suzuki-Coupling-F19-3
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 24-NOV-2010 15:34:45
Revision_time     = 26-JAN-2011 21:40:31
Current_time      = 26-JAN-2011 21:41:10

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 52428
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.11149056[s]
X_domain          = 19F
X_freq            = 470.62046084[MHz]
X_offset          = -200[ppm]
X_points          = 65536
X_prescans        = 0
X_resolution      = 0.89969275[Hz]
X_sweep           = 58.96226415[kHz]
Irr_domain        = 19F
Irr_freq          = 470.62046084[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 470.62046084[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1
Total_scans       = 1

X_90_width        = 16[us]
X_acq_time        = 1.11149056[s]
X_angle           = 45[deg]
X_atn             = 2[dB]
X_pulse           = 8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 6.11149056[s]
Temp_get          = 19.3[dC]
```

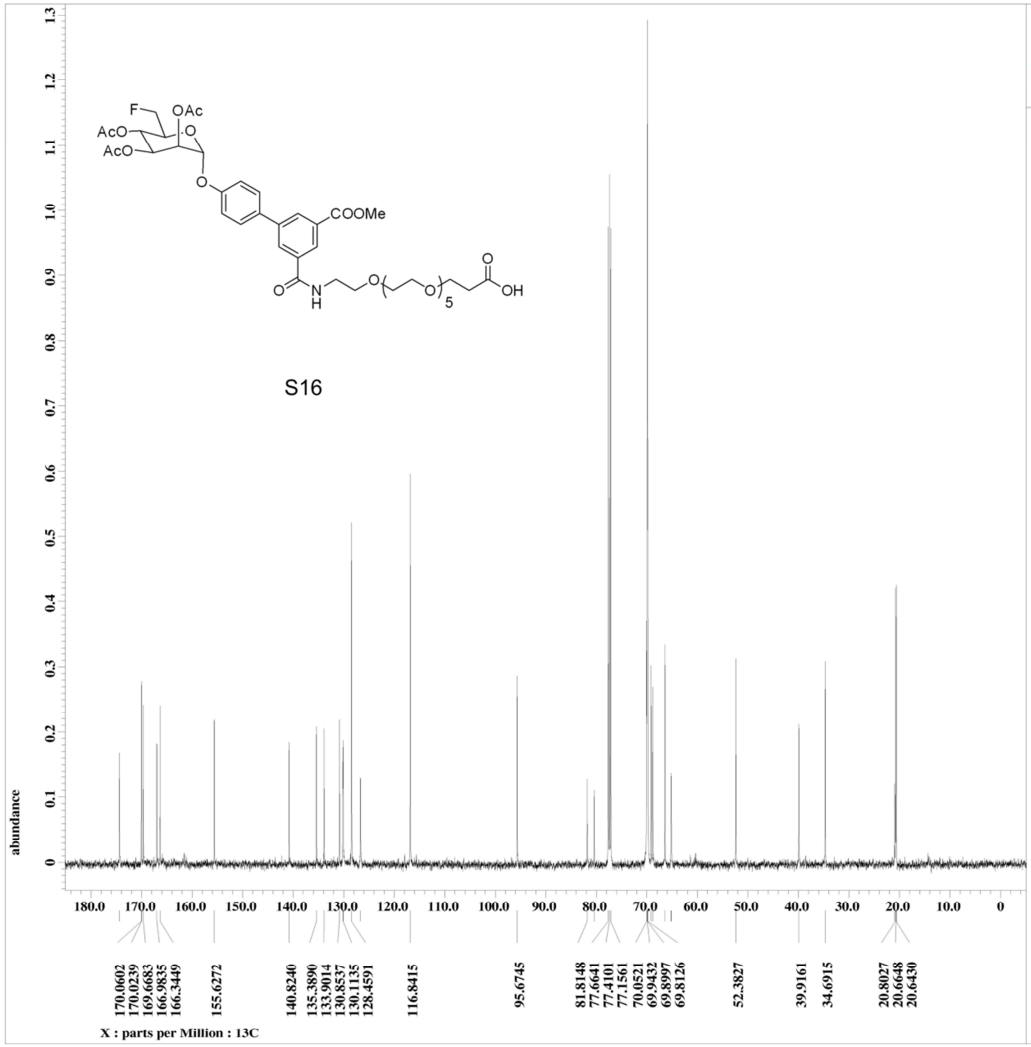


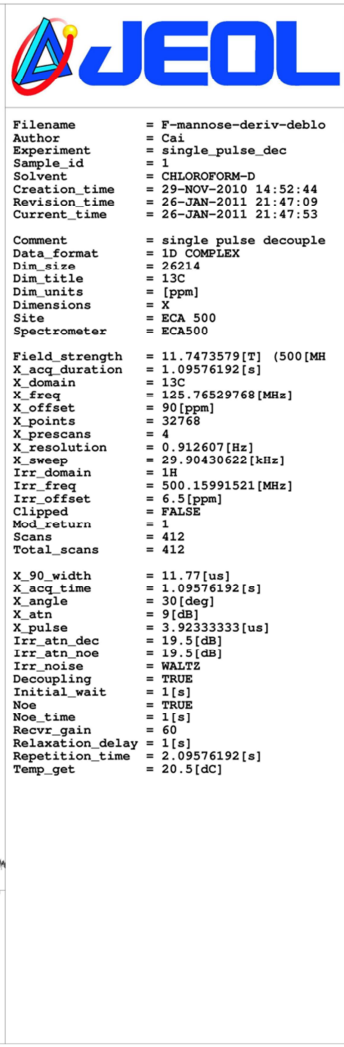

```
Filename          = H1-F-mannose-deriv-de
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 29-NOV-2010 14:37:53
Revision_time     = 26-JAN-2011 21:43:57
Current_time      = 26-JAN-2011 21:44:27

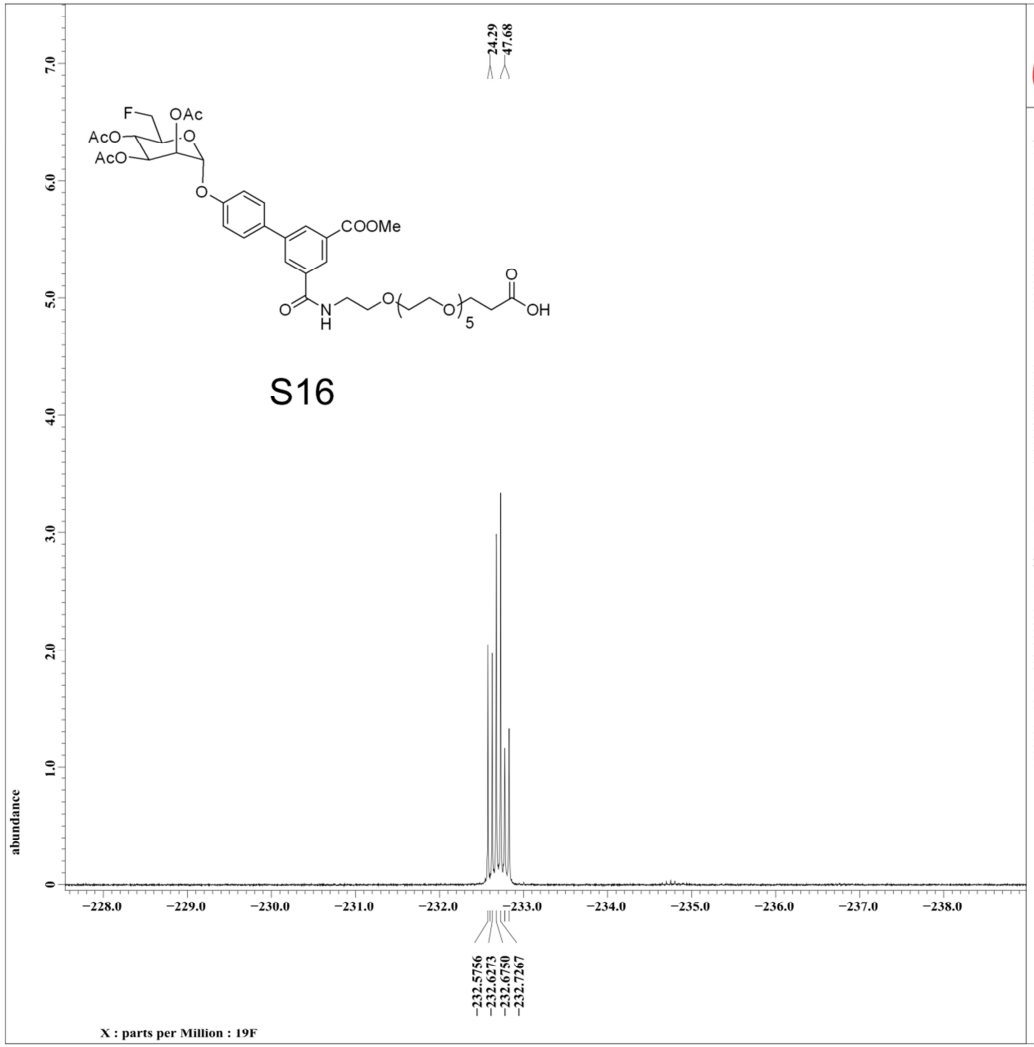
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.30438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 22
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19.8[dC]
```


F
OAc
AcO
AcO
O
COOMe
O
N
H
O
O
5
O
OH
S16
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.0602
170.0239
169.6683
166.9835
166.3449
155.6272
140.8240
135.3890
133.9014
130.8537
130.1135
128.4591
116.8415
95.6745
81.8148
77.6641
77.4101
77.1561
70.0521
69.9432
69.8997
69.8126
52.3827
39.9161
34.6915
20.8027
20.6648
20.6430
X : parts per Million : 13C


JEOL
Filename = F-mannose-deriv-deblo
Author = Cai
Experiment = single_pulse_dec
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 29-NOV-2010 14:52:44
Revision_time = 26-JAN-2011 21:47:09
Current_time = 26-JAN-2011 21:47:53
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = ECA500
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.09576192[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 90[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.912607[Hz]
X_sweep = 29.90430622[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 6.5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 412
Total_scans = 412
X_90_width = 11.77[us]
X_acq_time = 1.09576192[s]
X_angle = 30[deg]
X_atn = 9[dB]
X_pulse = 3.92333333[us]
Irr_atn_dec = 19.5[dB]
Irr_atn_noe = 19.5[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 1[s]
Recvr_gain = 60
Relaxation_delay = 1[s]
Repetition_time = 2.09576192[s]
Temp_get = 20.5[dC]

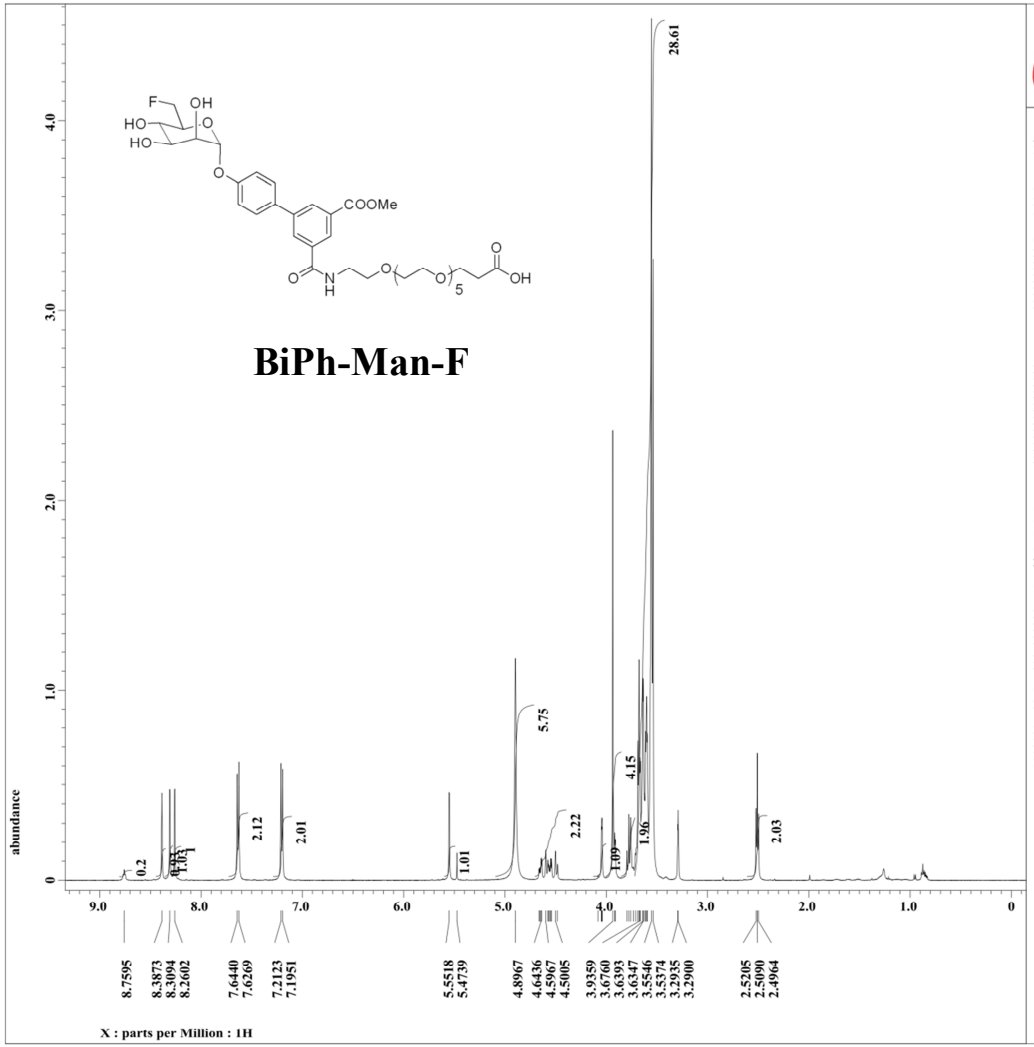



```
Filename          = f19-F-mannose-deriv-d
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 29-NOV-2010 14:55:13
Revision_time     = 29-NOV-2010 15:28:58
Current_time      = 26-JAN-2011 21:48:52

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 52428
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.11149056[s]
X_domain          = 19F
X_freq            = 470.62046084[MHz]
X_offset          = -200[ppm]
X_points          = 65536
X_prescans        = 0
X_resolution      = 0.89969275[Hz]
X_sweep           = 58.96226415[kHz]
Irr_domain        = 19F
Irr_freq          = 470.62046084[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 470.62046084[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1
Total_scans       = 1

X_90_width        = 16[us]
X_acq_time        = 1.11149056[s]
X_angle           = 45[deg]
X_atn             = 2[dB]
X_pulse           = 8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 6.11149056[s]
Temp_get          = 20.1[dC]
```

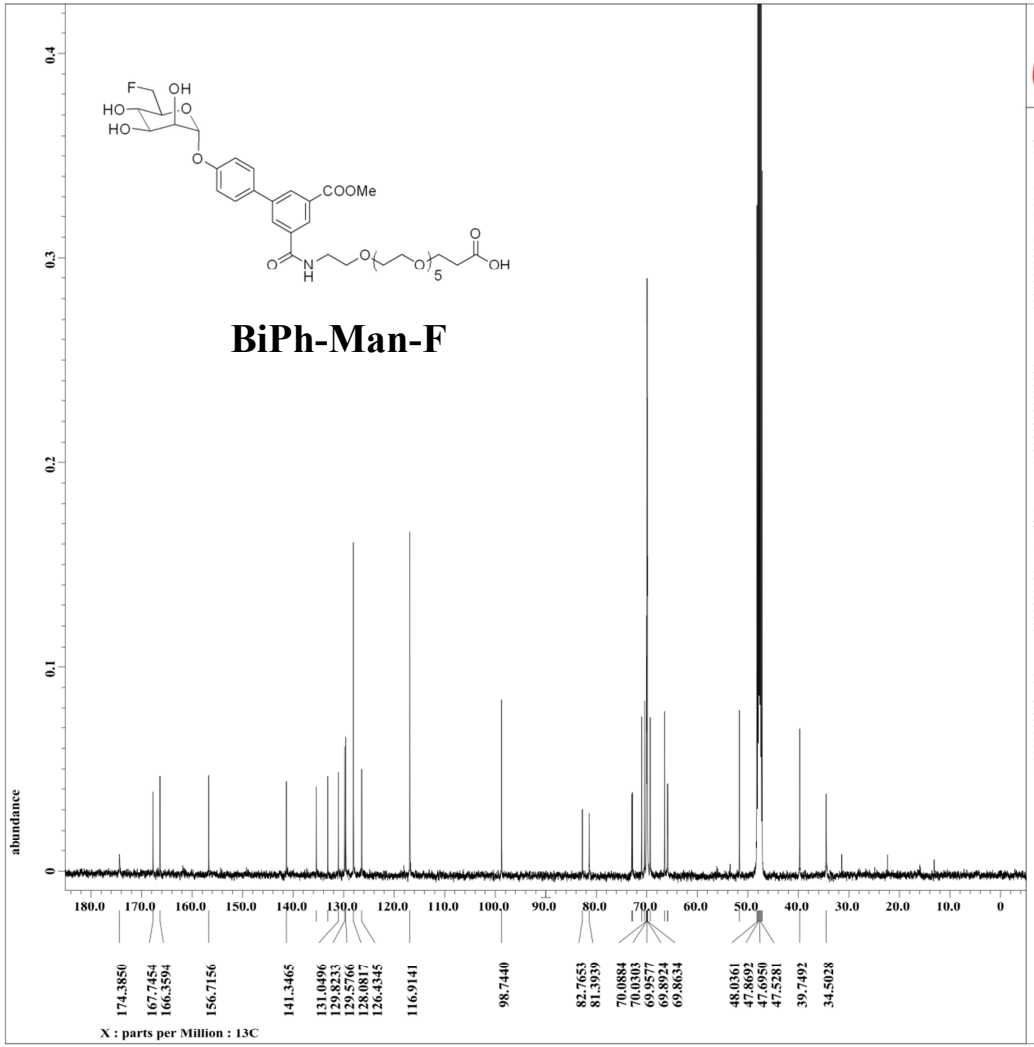



```
Filename          = F-mannose-biphenyl-OE
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = METHANOL-D3
Creation_time     =  7-DEC-2010 19:09:13
Revision_time     = 26-JAN-2011 21:50:03
Current_time      = 26-JAN-2011 21:50:54

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 4
Total_scans       = 4

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19[dC]
```

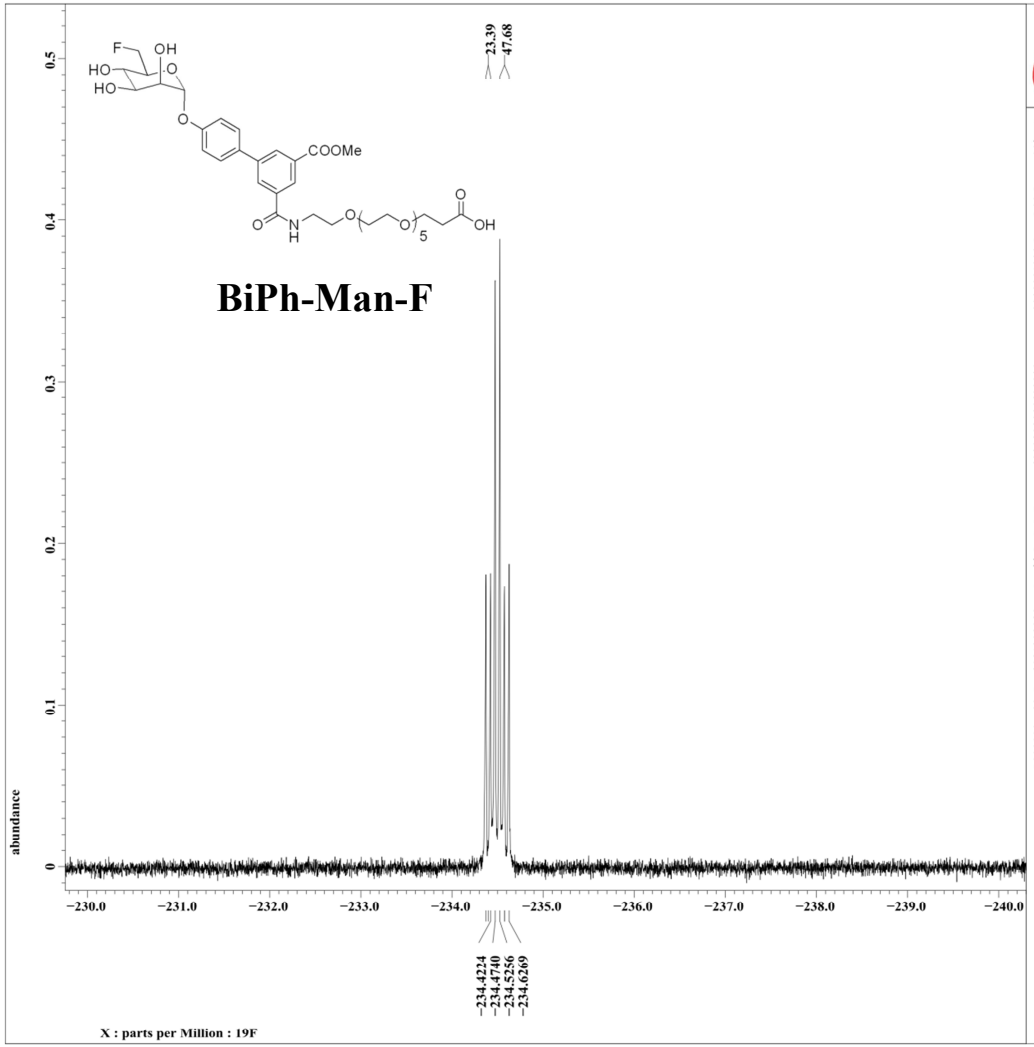



```
Filename          = F-mannose-biphenyl-OE
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = METHANOL-D3
Creation_time     =  7-DEC-2010 21:39:21
Revision_time     = 26-JAN-2011 21:54:00
Current_time      = 26-JAN-2011 21:54:31

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 4287
Total_scans       = 4287

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 19.8[dC]
```

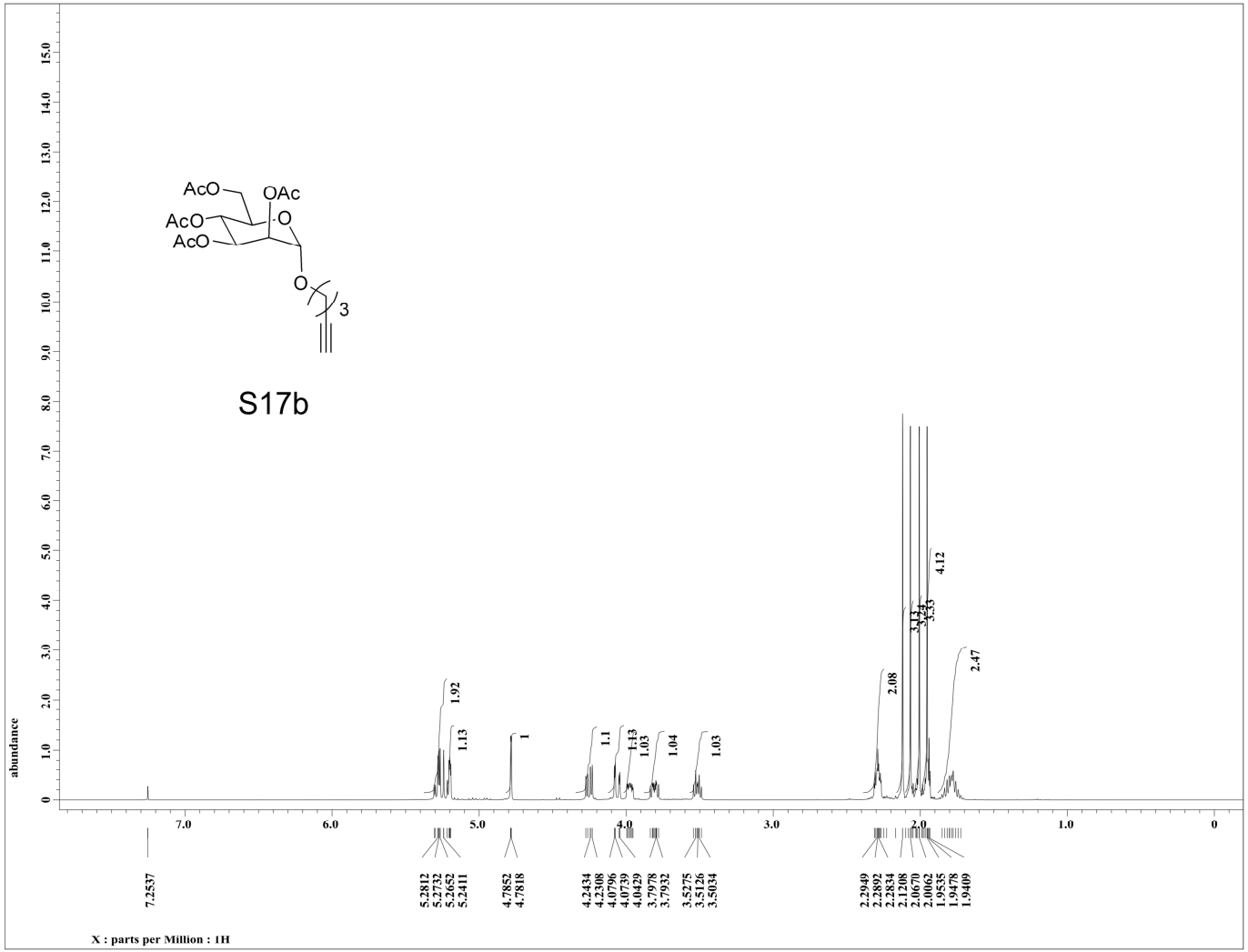


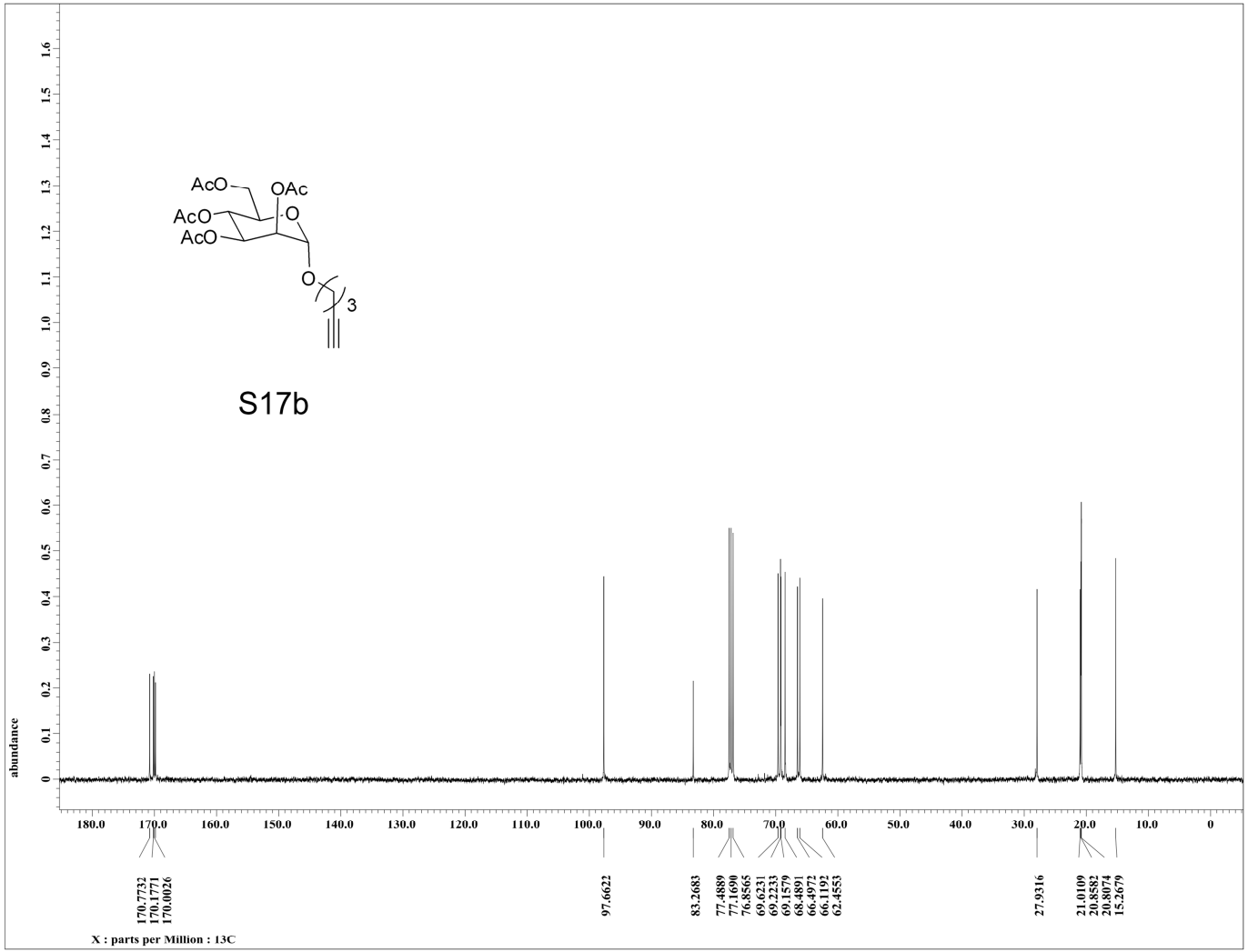

```
Filename          = F-mannose-biphenyl-OE
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = METHANOL-D3
Creation_time     =  3-DEC-2010 21:23:29
Revision_time     =  3-DEC-2010 21:58:31
Current_time      = 26-JAN-2011 21:55:52

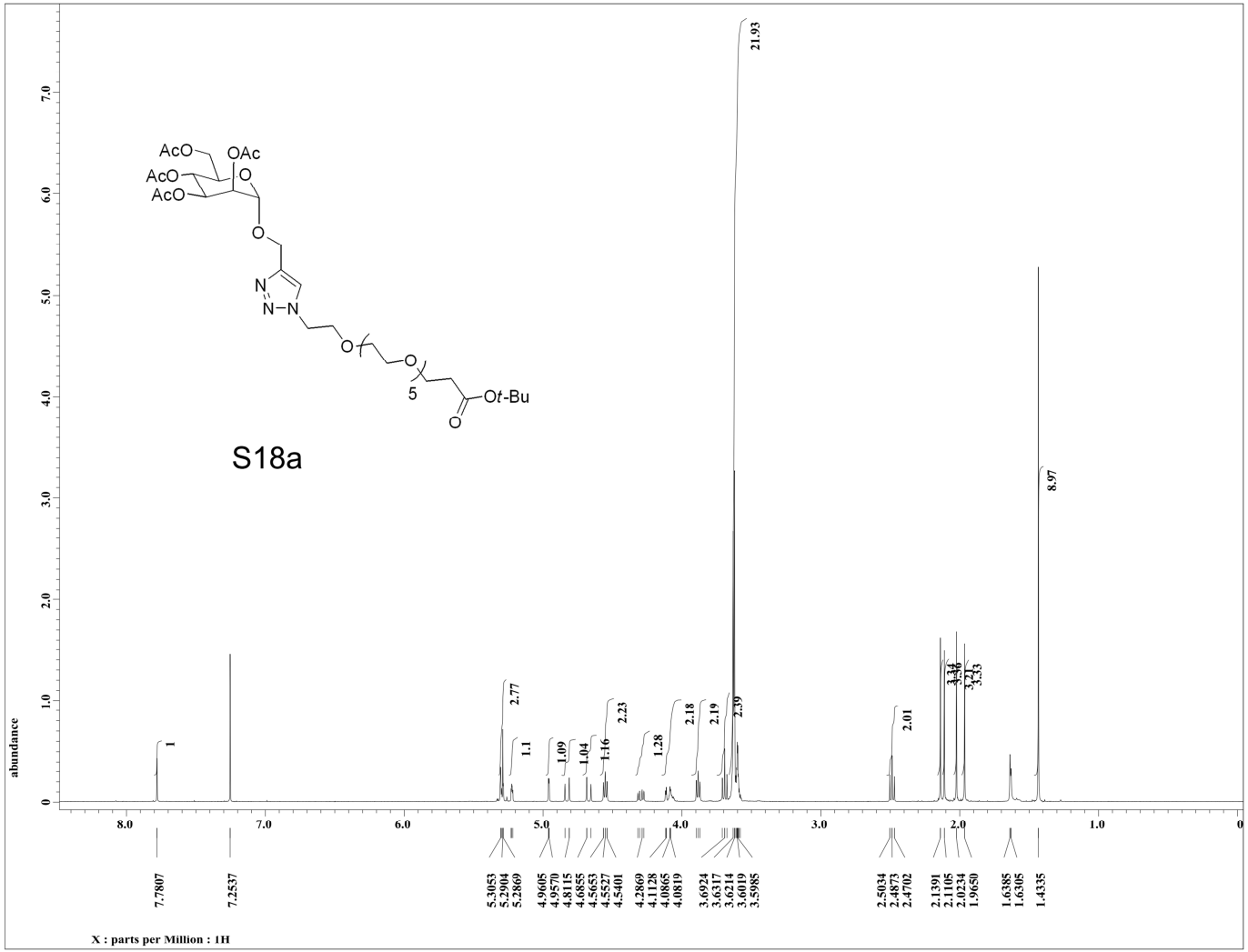
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 52428
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

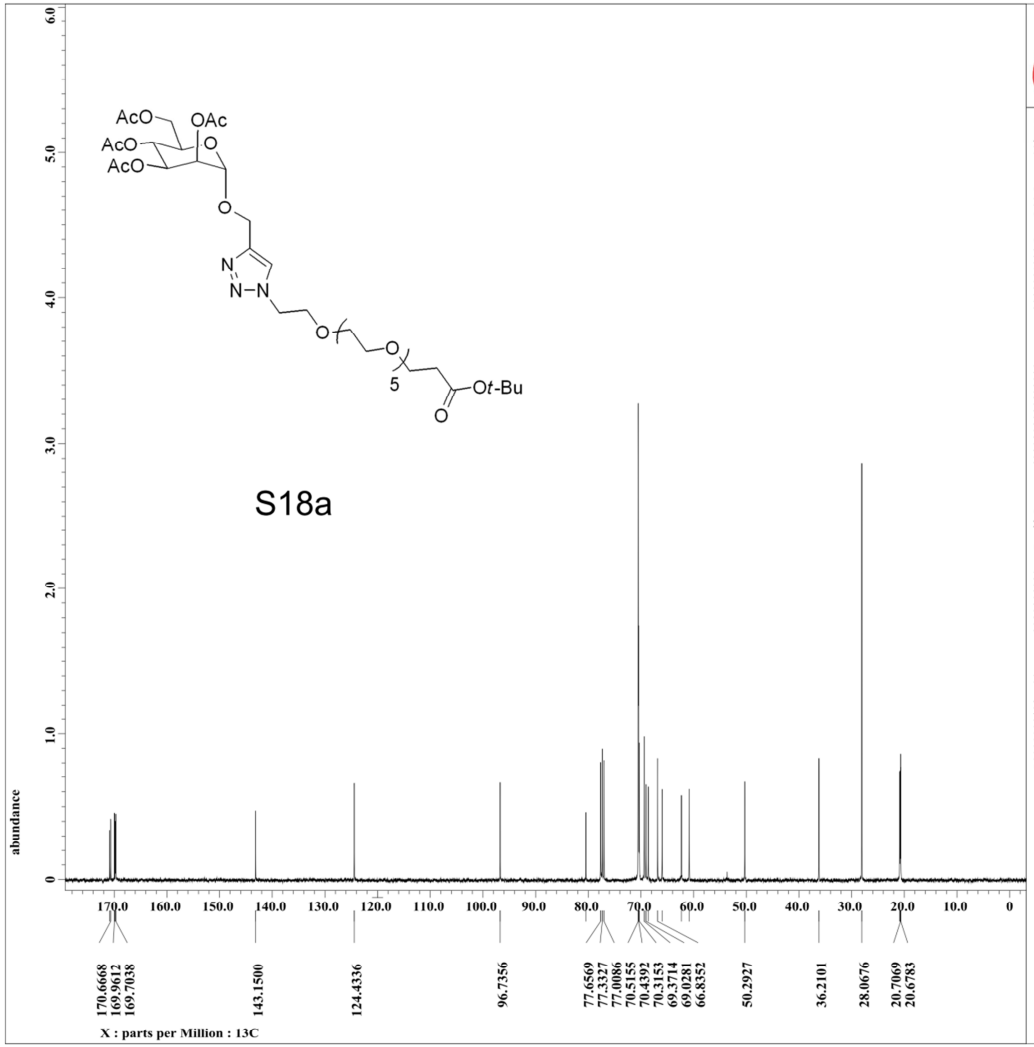
Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.11149056[s]
X_domain          = 19F
X_freq            = 470.62046084[MHz]
X_offset          = -200[ppm]
X_points          = 65536
X_prescans        = 0
X_resolution      = 0.89969275[Hz]
X_sweep           = 58.96226415[kHz]
Irr_domain        = 19F
Irr_freq          = 470.62046084[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 470.62046084[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1
Total_scans       = 1

X_90_width        = 16[us]
X_acq_time        = 1.11149056[s]
X_angle           = 45[deg]
X_atn             = 2[dB]
X_pulse           = 8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 6.11149056[s]
Temp_get          = 19.6[dC]
```


AcO
OAc
AcO
O
AcO
O
3
S17b
abundance
X : parts per Million : 1H
7.2537
5.2812
5.2732
5.2652
5.2411
4.7852
4.7818
4.2434
4.2308
4.0796
4.0739
4.0429
3.7978
3.7932
3.5275
3.5126
3.5034
2.2940
2.2892
2.2834
2.1208
2.0670
2.0062
1.9535
1.9478
1.9409
1.92
1.13
1
1.1
1.13
1.03
1.04
1.03
2.08
3.13
3.24
3.35
4.12
2.47


AcO
OAc
AcO
O
AcO
O
3
S17b
abundance
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.7732
170.1771
170.0026
97.6622
83.2683
77.4889
77.1690
76.8565
69.6231
69.2233
69.1579
68.4891
66.4972
66.1192
62.4553
27.9316
21.0109
20.8582
20.8074
15.2679
X : parts per Million : 13C


AcO
OAc
AcO
AcO
O
O
N
N–N
O
O
5
Ot-Bu
O
S18a
abundance
21.93
8.97
2.77
1.1
1.09
1.04
1.16
2.23
1.28
2.18
2.19
2.39
2.01
3.34
3.36
3.37
3.33
1
7.7807
7.2537
5.3053
5.2904
5.2869
4.9605
4.9570
4.8115
4.6855
4.5653
4.5527
4.5401
4.2869
4.1128
4.0865
4.0819
3.6924
3.6317
3.6214
3.6019
3.5985
2.5034
2.4873
2.4702
2.1391
2.1105
2.0234
1.9650
1.6385
1.6305
1.4335
X : parts per Million : 1H

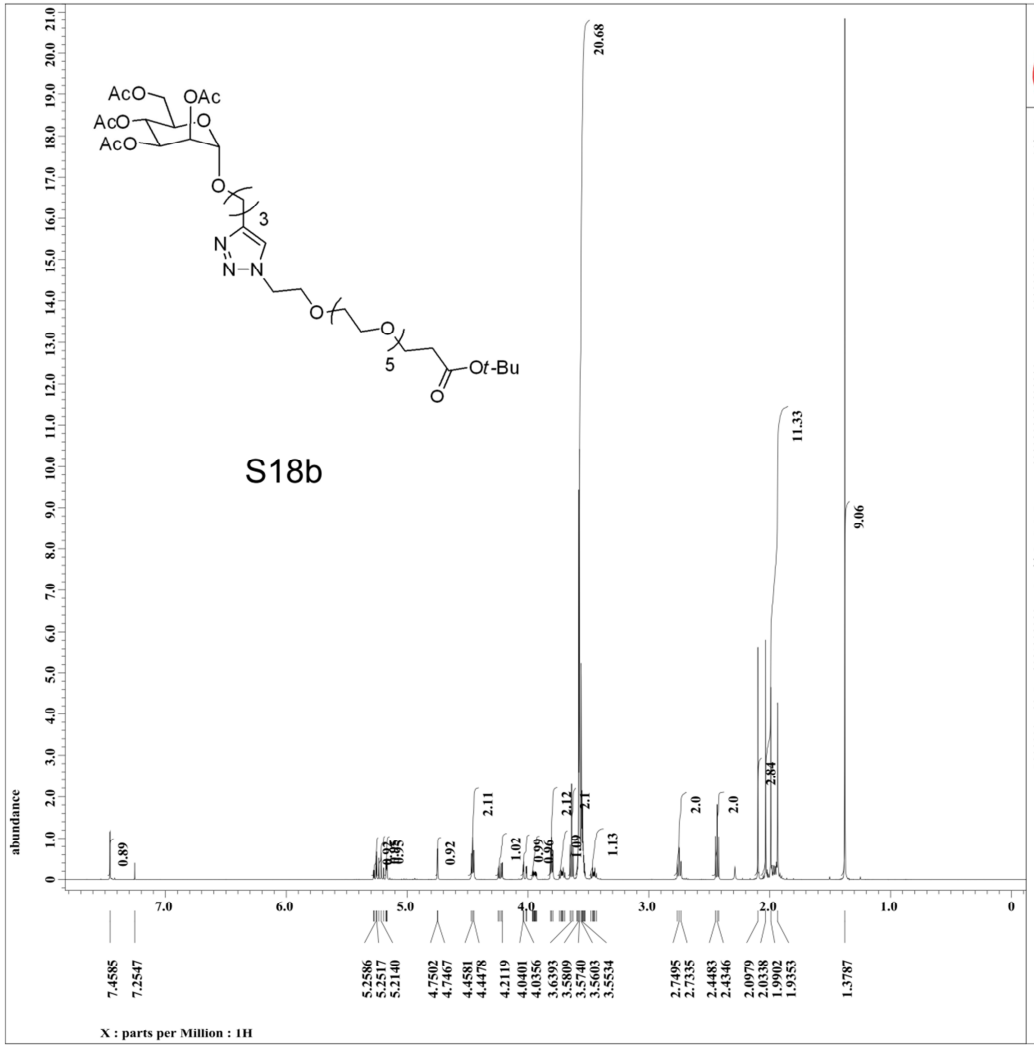



```
Filename          = 29-NO-13.jdf
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 29-JUN-2010 10:59:38
Revision_time     = 27-JAN-2011 20:52:28
Current_time      = 27-JAN-2011 20:53:43

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 120[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 204
Total_scans       = 204

X_90_width        = 12.4525[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 6[dB]
X_pulse           = 4.15083333[us]
Irr_atn_dec       = 22[dB]
Irr_atn_noe       = 22[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 2.04333312[s]
Temp_get          = 18.6[dC]
```

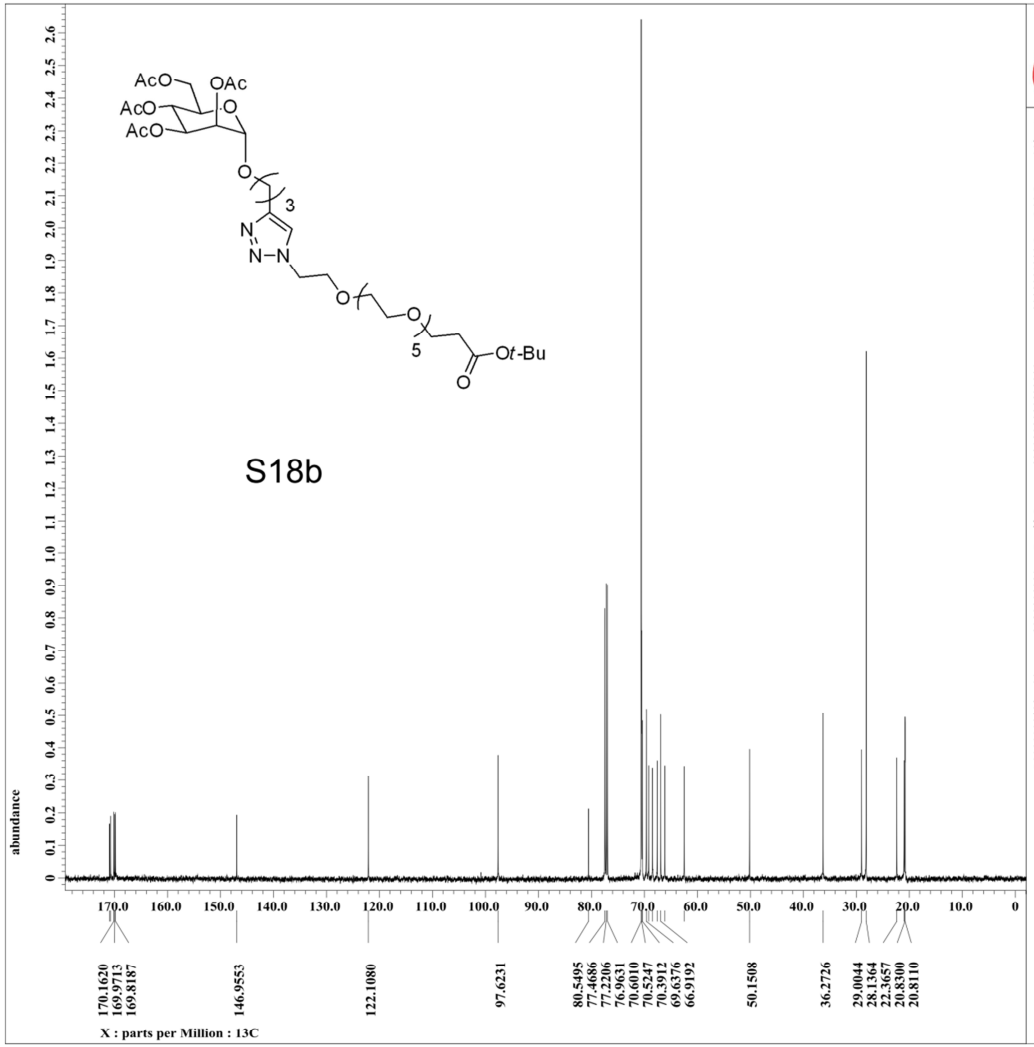


```
Filename          = h1default14to-1-117.j
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 3
Solvent           = CHLOROFORM-D
Creation_time     =  5-JUL-2010 21:34:32
Revision_time     = 26-JAN-2011 20:37:36
Current_time      = 26-JAN-2011 20:38:17

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 17.2[dC]
```



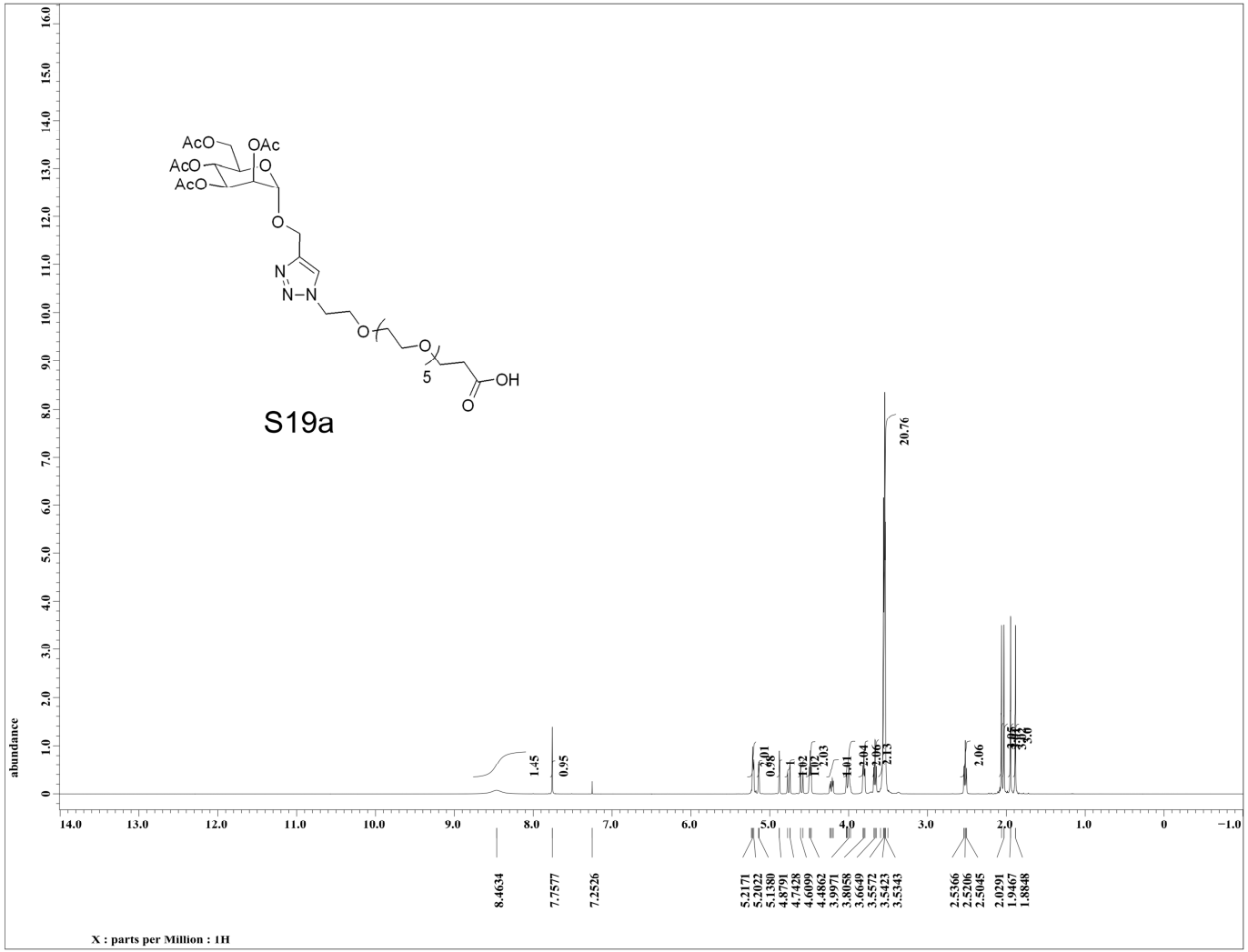
JEOL

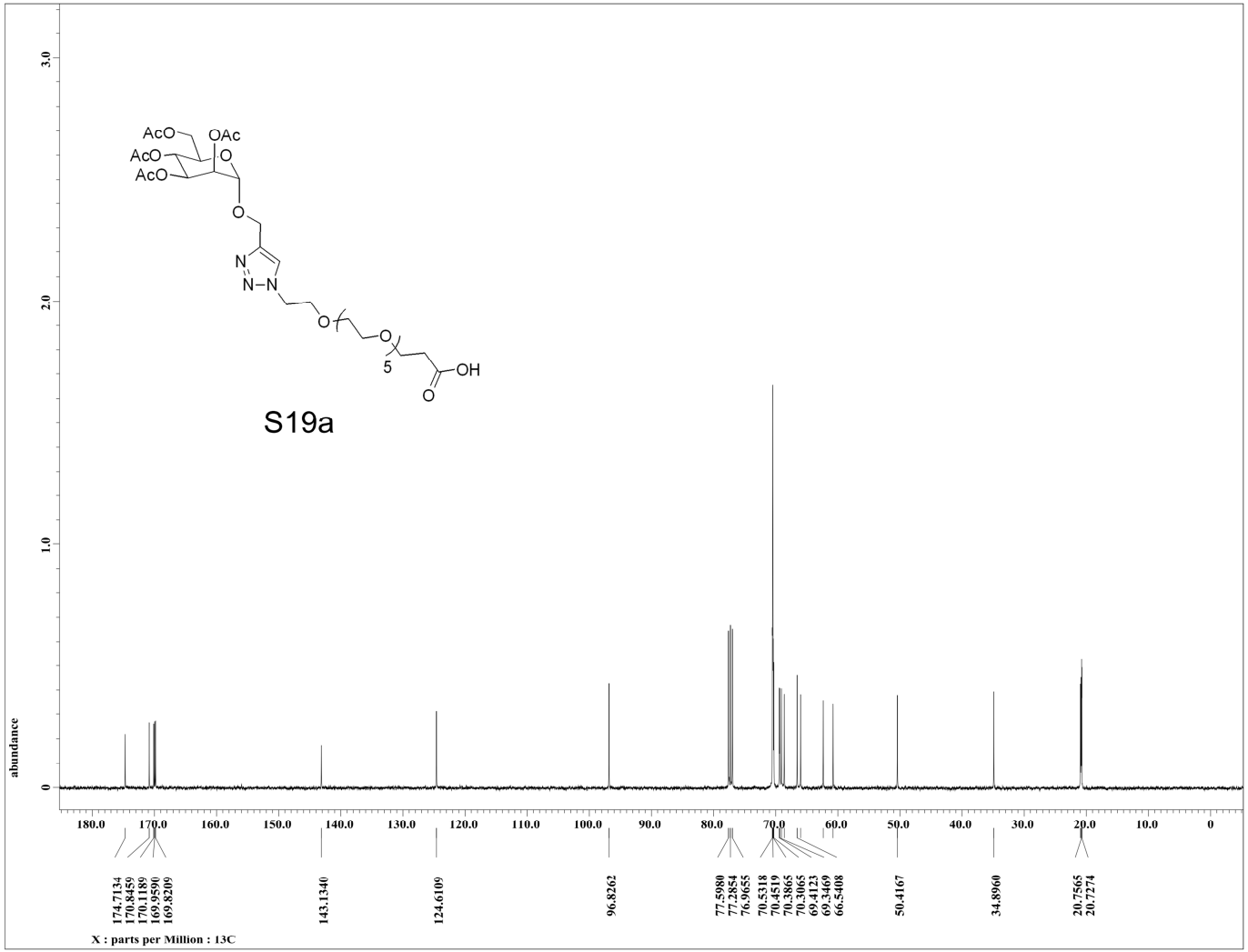
```
Filename          = c13default245to-5-2.j
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 3
Solvent           = CHLOROFORM-D
Creation_time     =  5-JUL-2010 21:48:19
Revision_time     =  5-JUL-2010 22:15:48
Current_time      = 26-JAN-2011 20:39:10

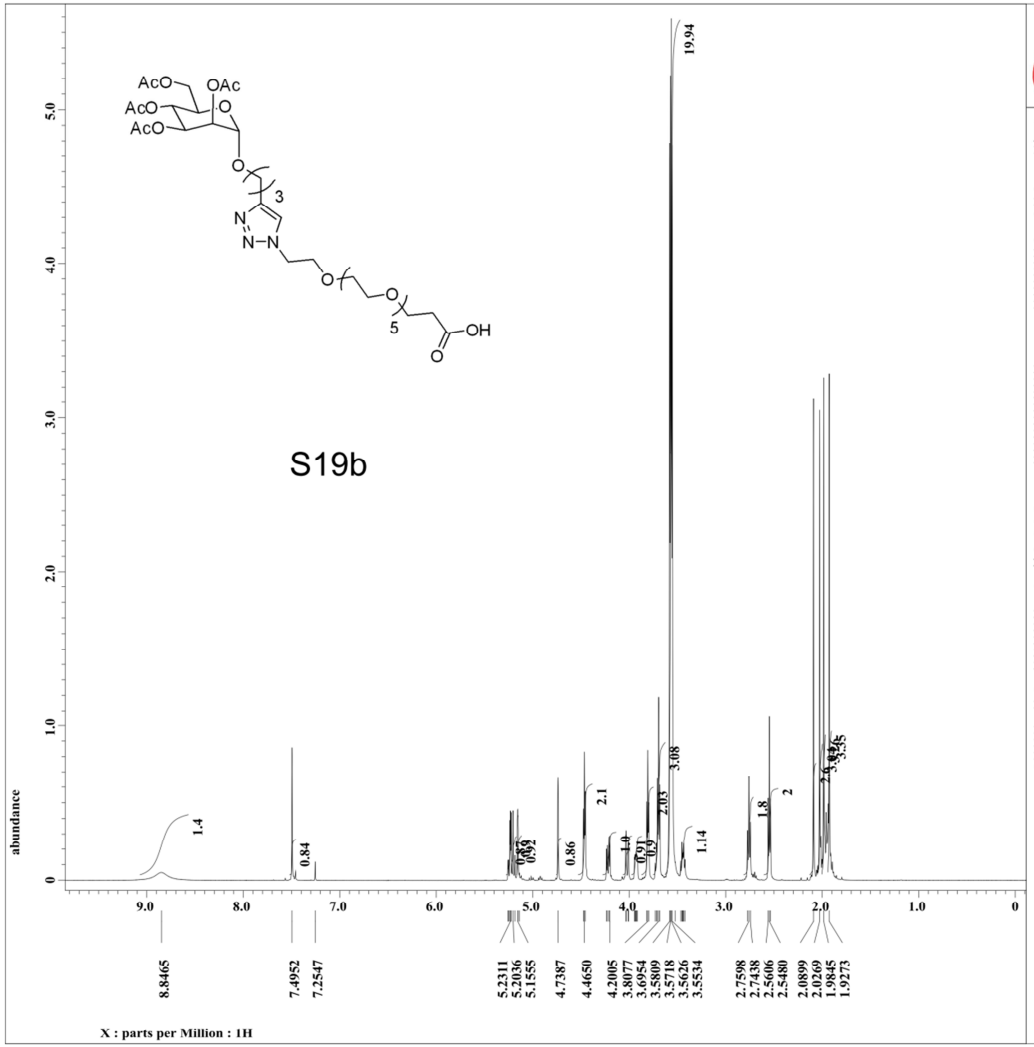
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 120[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 437
Total_scans       = 437

X_90_width        = 11.77[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 1.83361792[s]
Temp_get          = 17.9[dC]
```


S19a
abundance
X : parts per Million : 1H
20.76
1.45
0.95
2.06
8.4634
7.7577
7.2526


AcO
OAc
AcO
AcO
O
O
N
N–N
O
O
5
OH
O
S19a
abundance
3.0
2.0
1.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
174.7134
170.8459
170.1189
169.9590
169.8209
143.1340
124.6109
96.8262
77.5980
77.2854
76.9655
70.5318
70.4510
70.3865
70.3065
69.4123
69.3460
66.5408
50.4167
34.8960
20.7565
20.7274
X : parts per Million : 13C

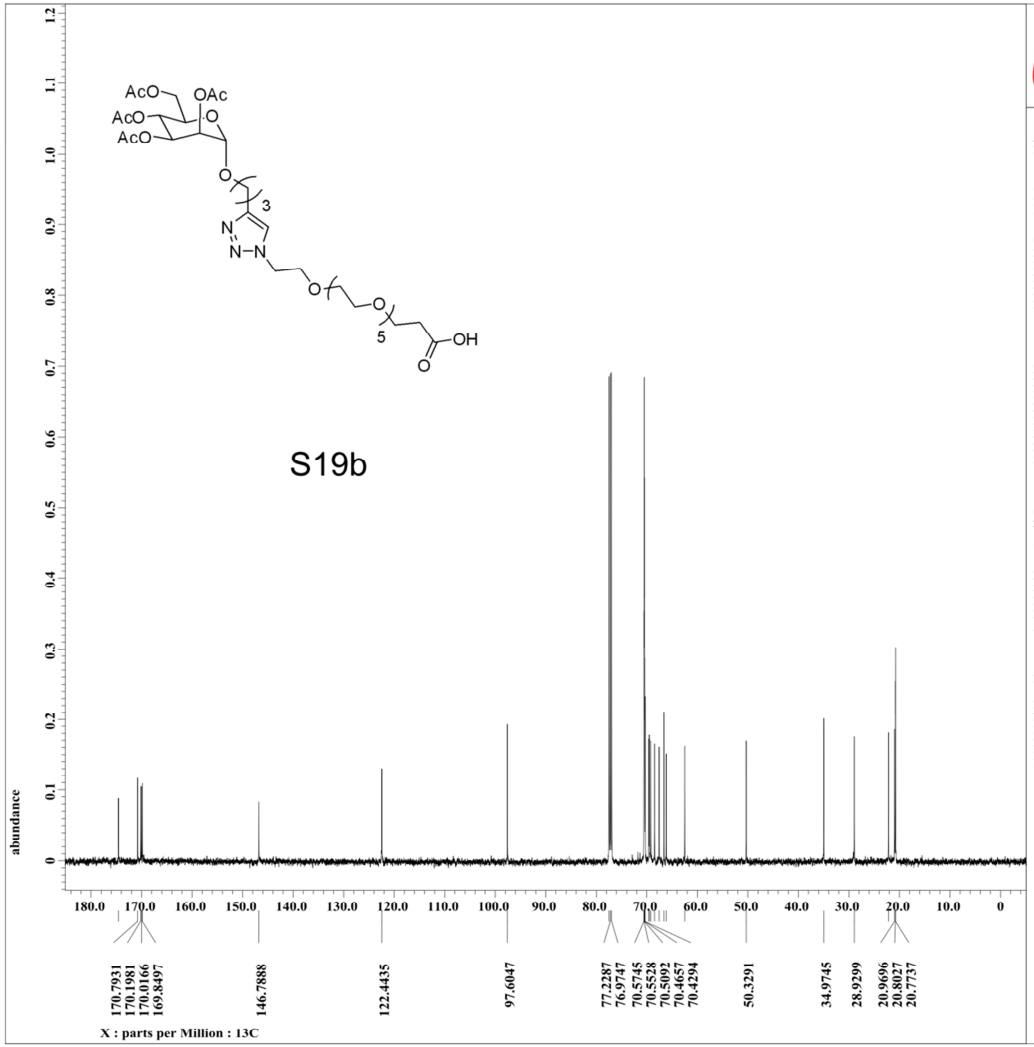



```
Filename          = h1default14to-1-117.j
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = long chain triazole m
Solvent           = CHLOROFORM-D
Creation_time     = 26-OCT-2010 21:29:09
Revision_time     = 26-JAN-2011 20:44:47
Current_time      = 26-JAN-2011 20:47:49

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19.6[dC]
```

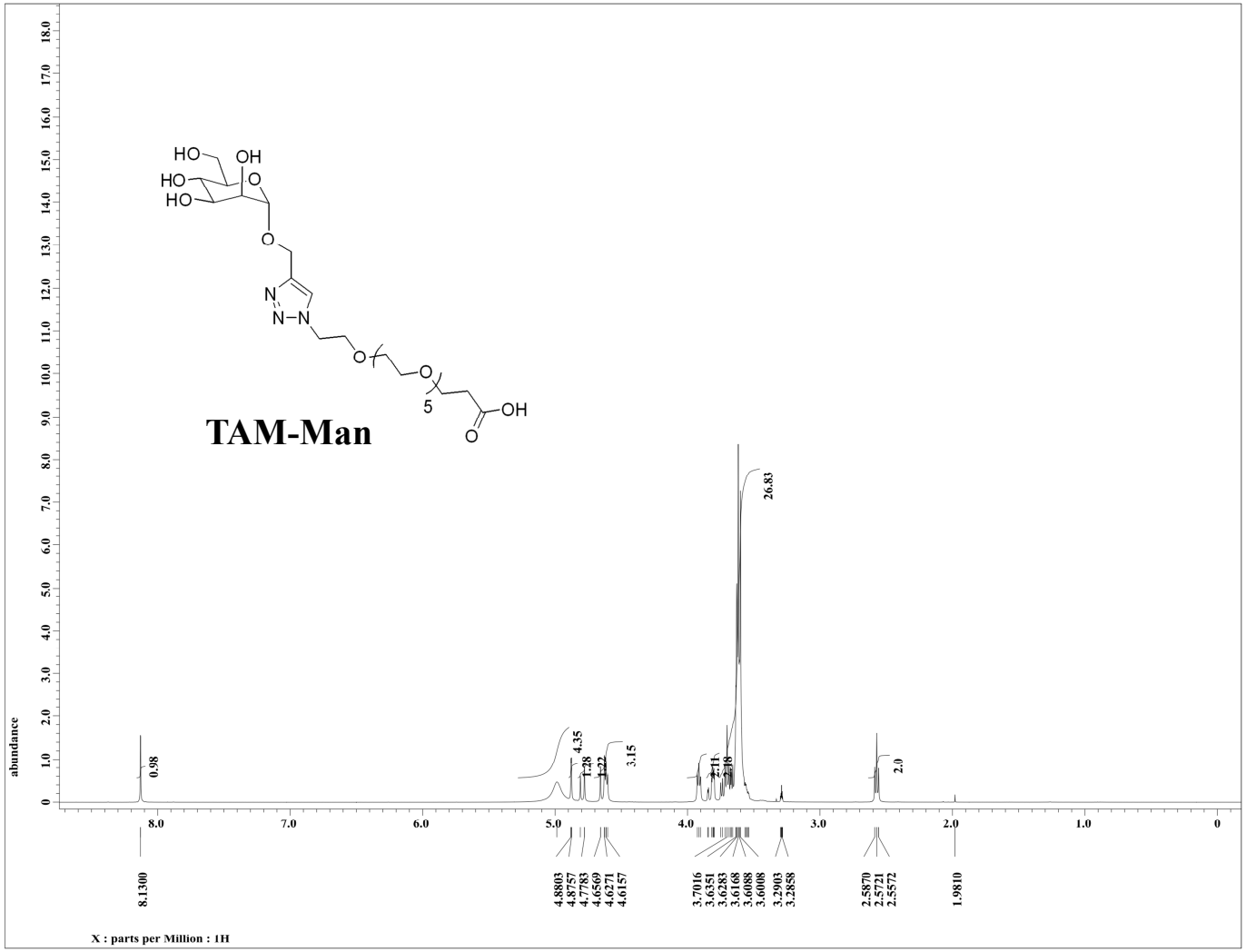


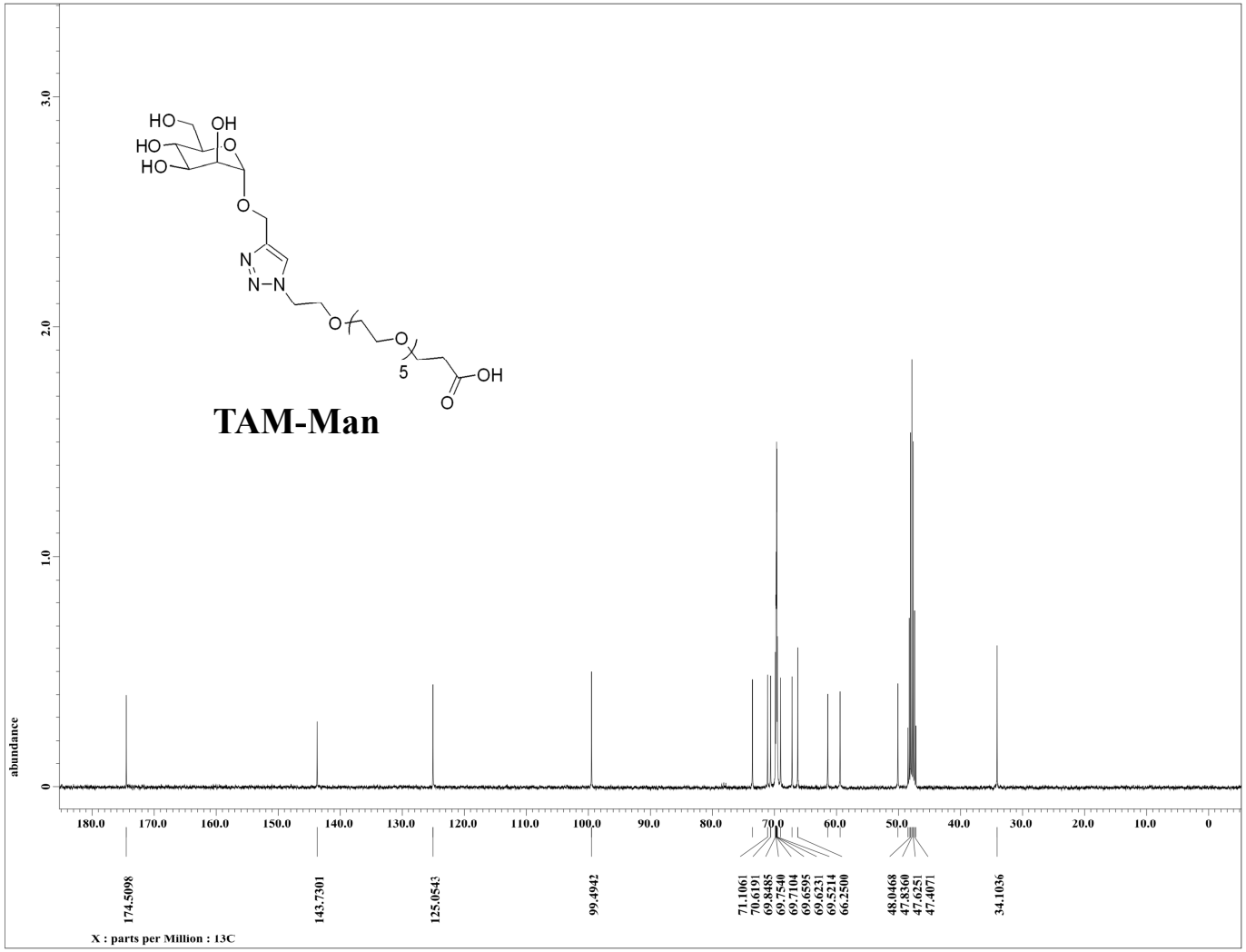

```
Filename          = c13default185to-5ppm-
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 26-OCT-2010 21:48:29
Revision_time     = 26-OCT-2010 22:20:28
Current_time      = 26-JAN-2011 20:48:47

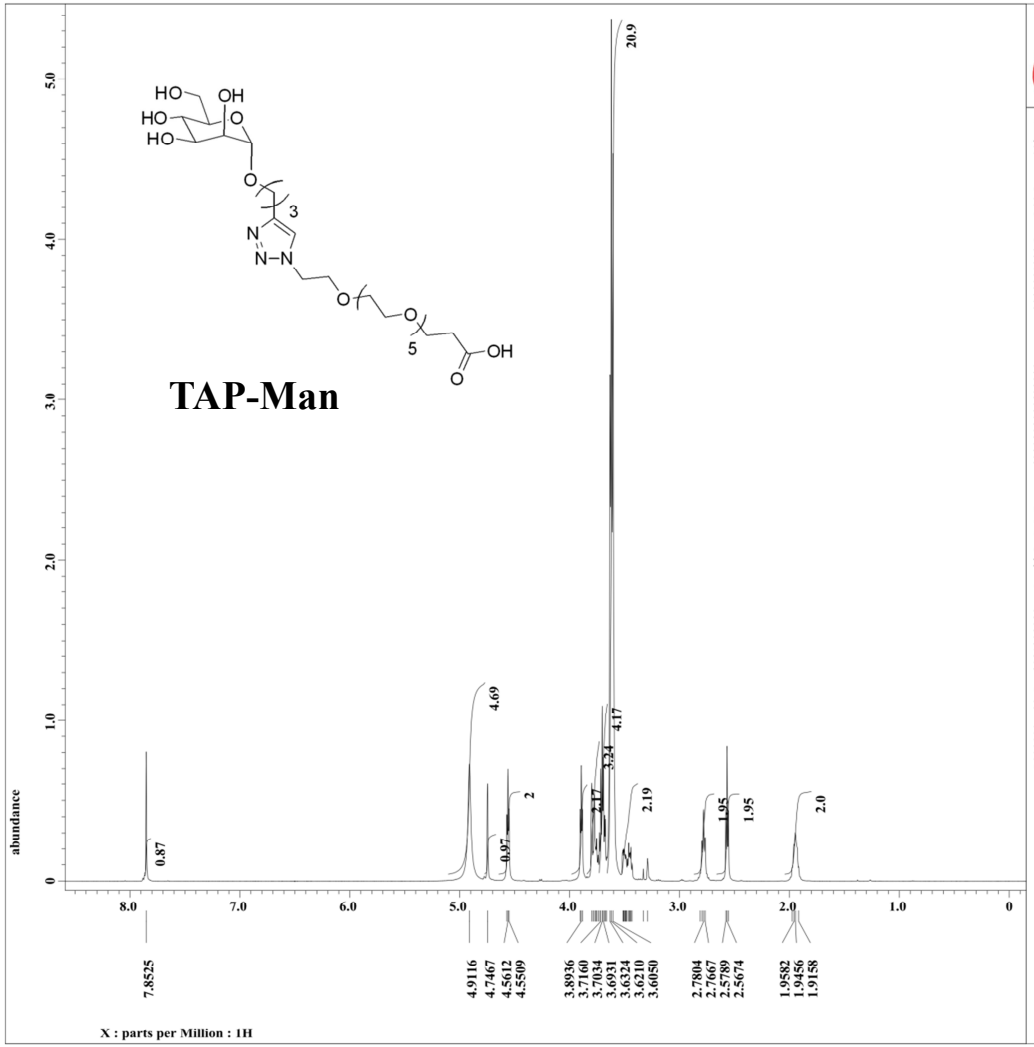
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 519
Total_scans       = 519

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 58
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 20.4[dC]
```


TAM-Man
abundance
X : parts per Million : 1H
0.98
4.35
1.28
1.22
3.15
26.83
2.0
8.1300
4.8803
4.8757
4.7783
4.6569
4.6271
4.6157
3.7016
3.6351
3.6283
3.6168
3.6088
3.6008
3.2903
3.2858
2.5870
2.5721
2.5572
1.9810


TAM-Man
abundance
X : parts per Million : 13C
174.5098
143.7301
125.0543
99.4942
71.1061
70.6191
69.8485
69.7540
69.7104
69.6595
69.6231
69.5214
66.2500
48.0468
47.8360
47.6251
47.4071
34.1036

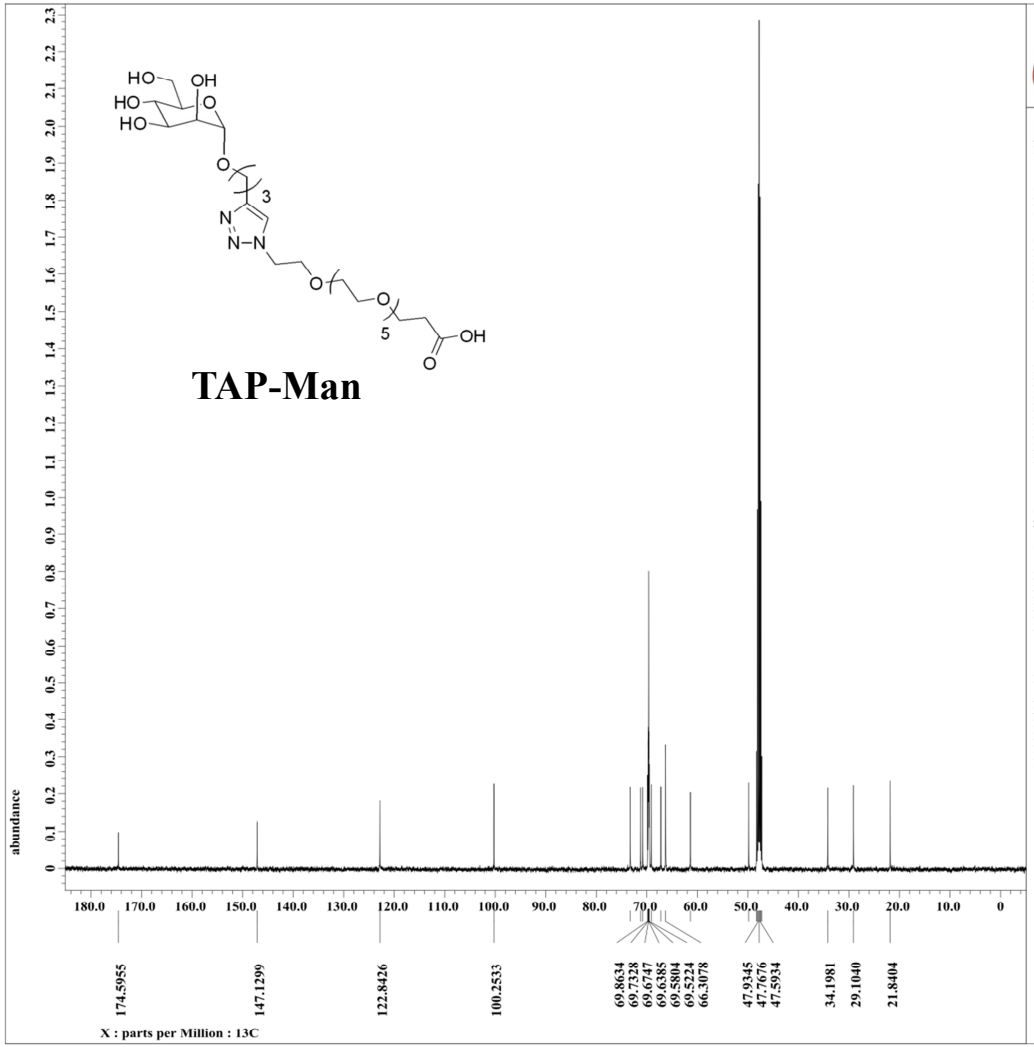



```
Filename          = h1default14to-1-87.jd
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = deprotect
Solvent           = METHANOL-D3
Creation_time     = 27-OCT-2010 15:34:49
Revision_time     = 27-OCT-2010 16:08:26
Current_time      = 26-JAN-2011 20:51:52

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 28
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 19.7[dC]
```

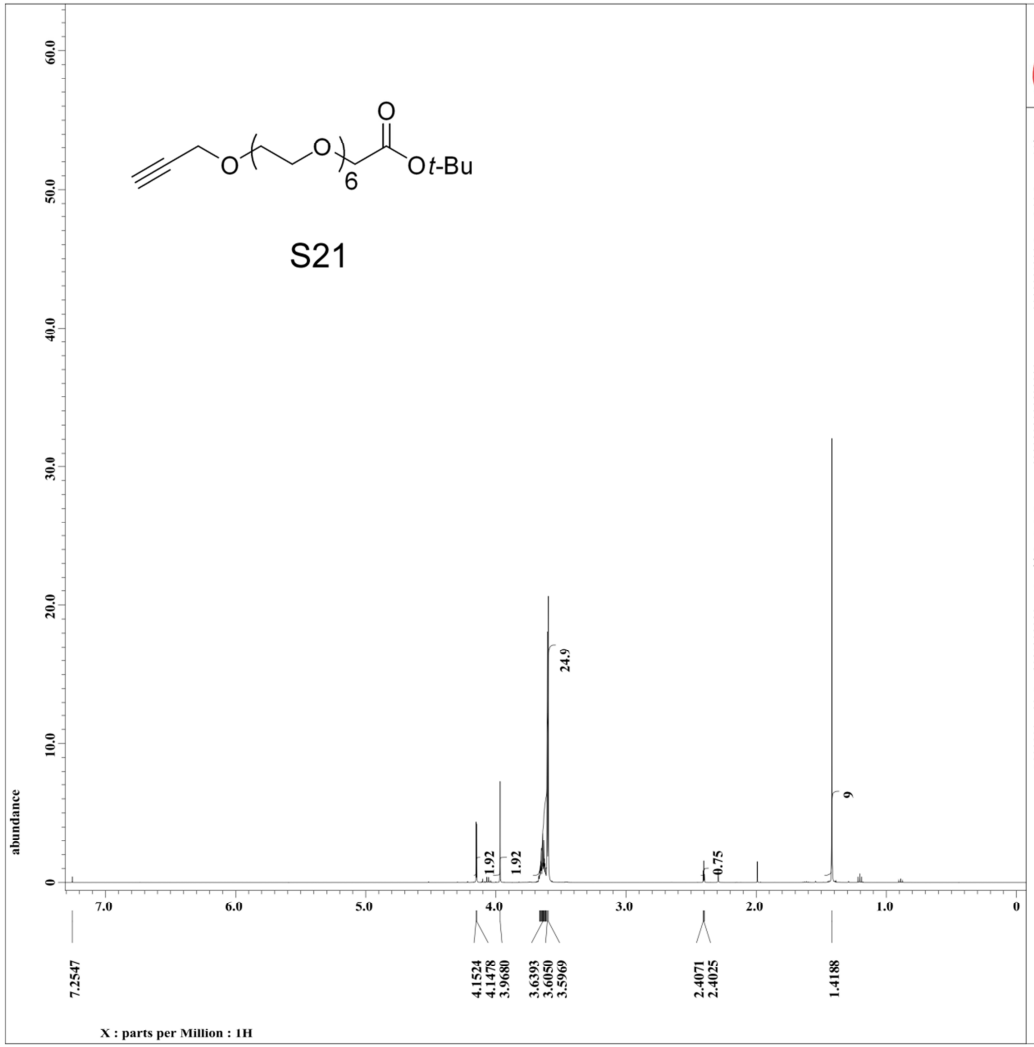



```
Filename          = c13default185to-5ppm-
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = deprotect
Solvent           = METHANOL-D3
Creation_time     = 27-OCT-2010 15:50:25
Revision_time     = 27-OCT-2010 16:21:53
Current_time      = 26-JAN-2011 20:52:33

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 436
Total_scans       = 436

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 20.4[dC]
```

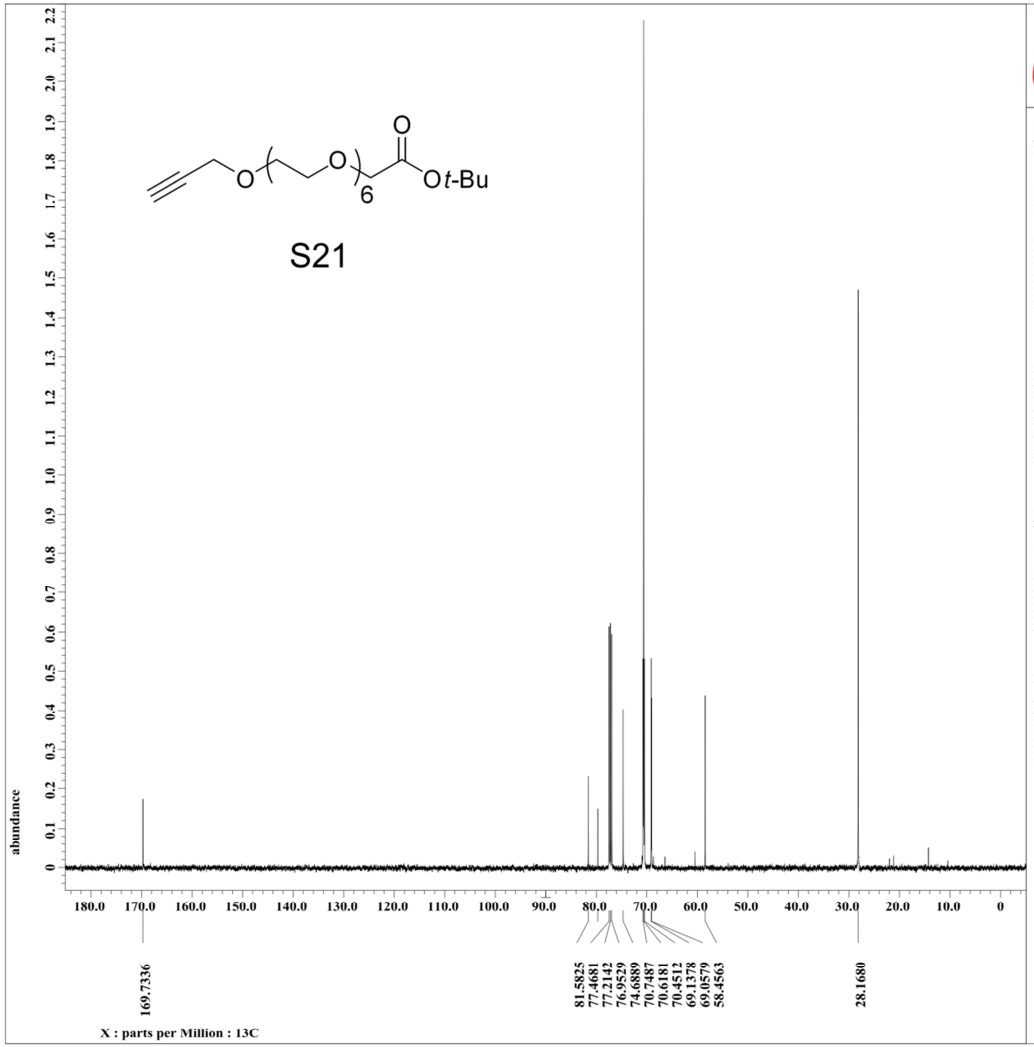



```
Filename          = July_13_NO.1_H1-7.jdf
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = July_13_NO.1
Solvent           = CHLOROFORM-D
Creation_time     = 13-JUL-2010 22:03:38
Revision_time     = 26-JAN-2011 20:14:39
Current_time      = 26-JAN-2011 20:15:54

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 16.9[dC]
```

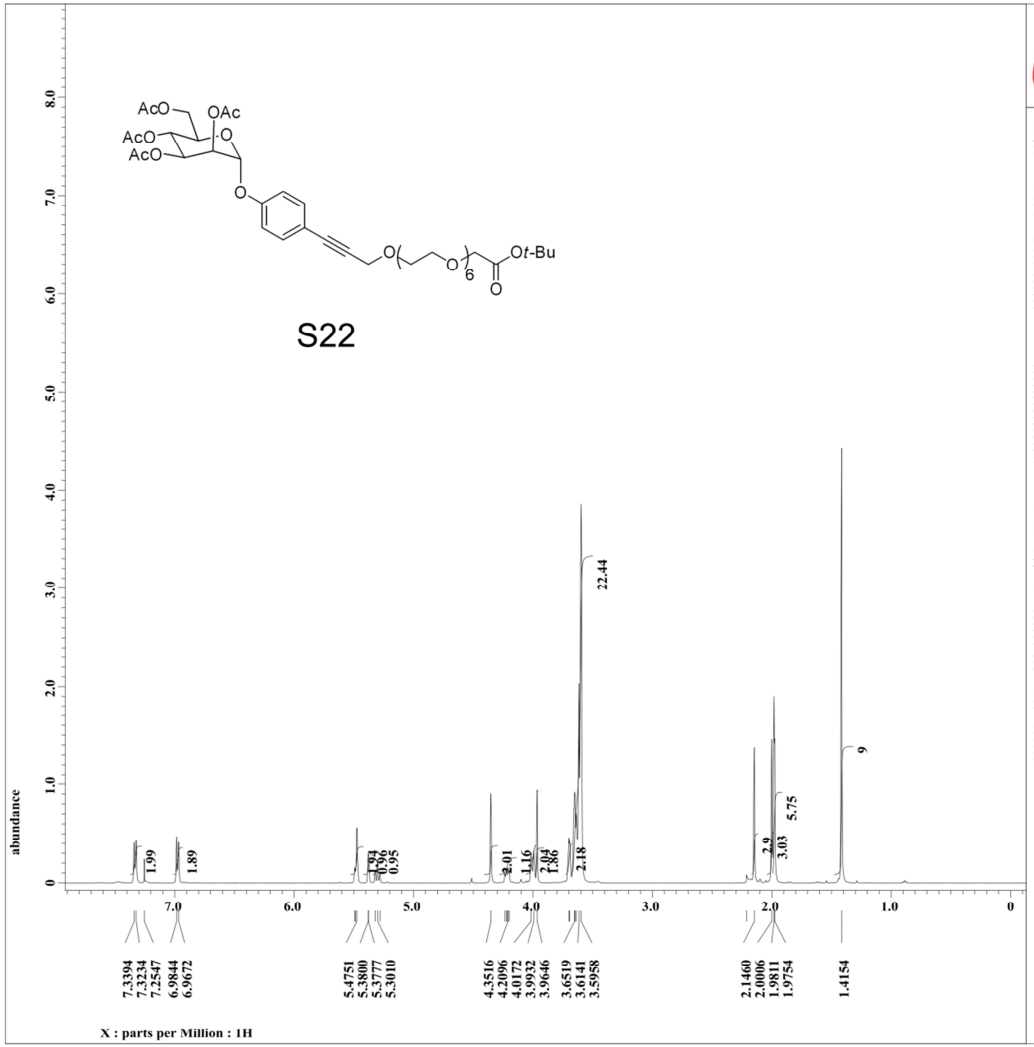



```
Filename          = July_13_NO.1_C13-5.jd
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = July_13_NO.1
Solvent           = CHLOROFORM-D
Creation_time     = 13-JUL-2010 22:12:49
Revision_time     = 26-JAN-2011 20:18:28
Current_time      = 26-JAN-2011 20:19:01

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 250
Total_scans       = 250

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 58
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 17.5[dC]
```



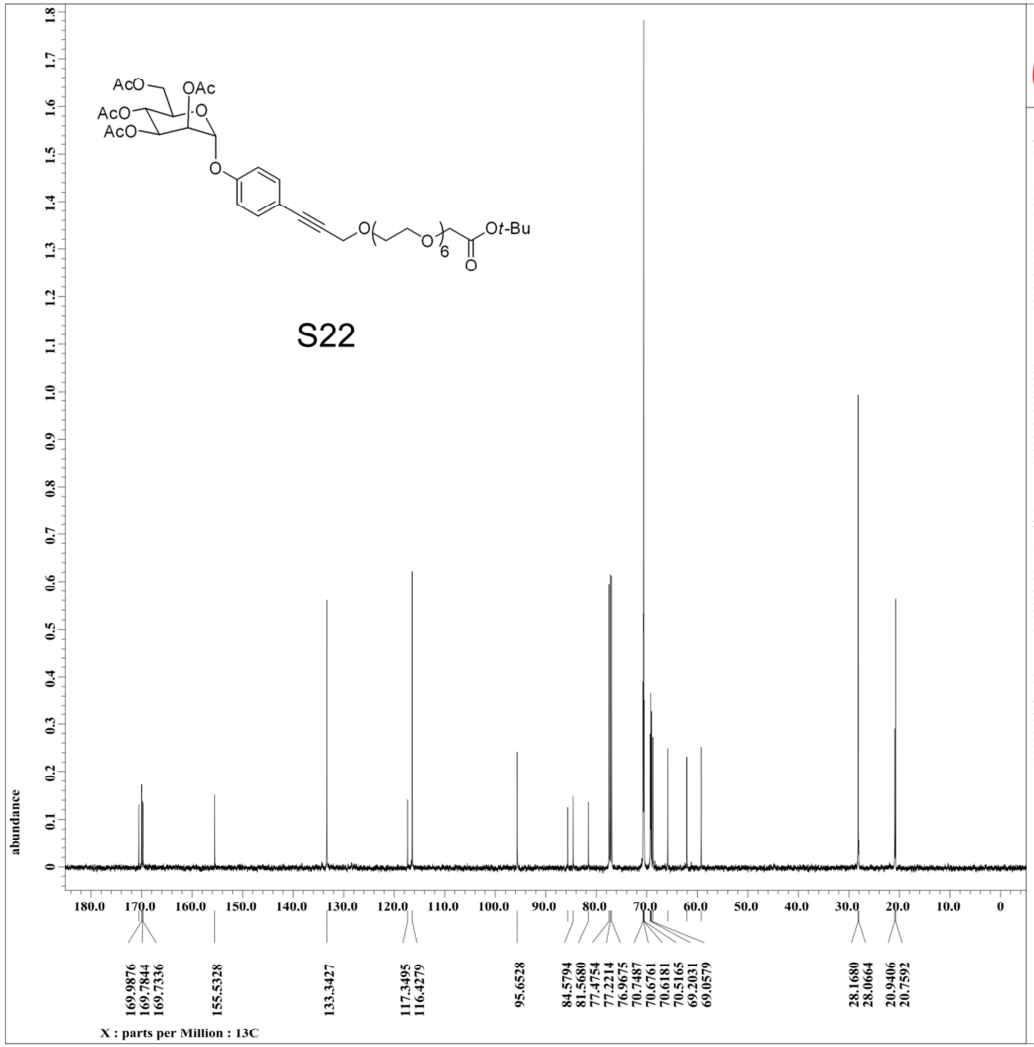
JEOL

```
Filename          = Junly_17_NO.1_h1defau
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = Junly_17_NO.1
Solvent           = CHLOROFORM-D
Creation_time     = 17-JUL-2010 18:34:41
Revision_time     = 26-JAN-2011 20:20:56
Current_time      = 26-JAN-2011 20:21:55

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 32
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 17.9[dC]
```

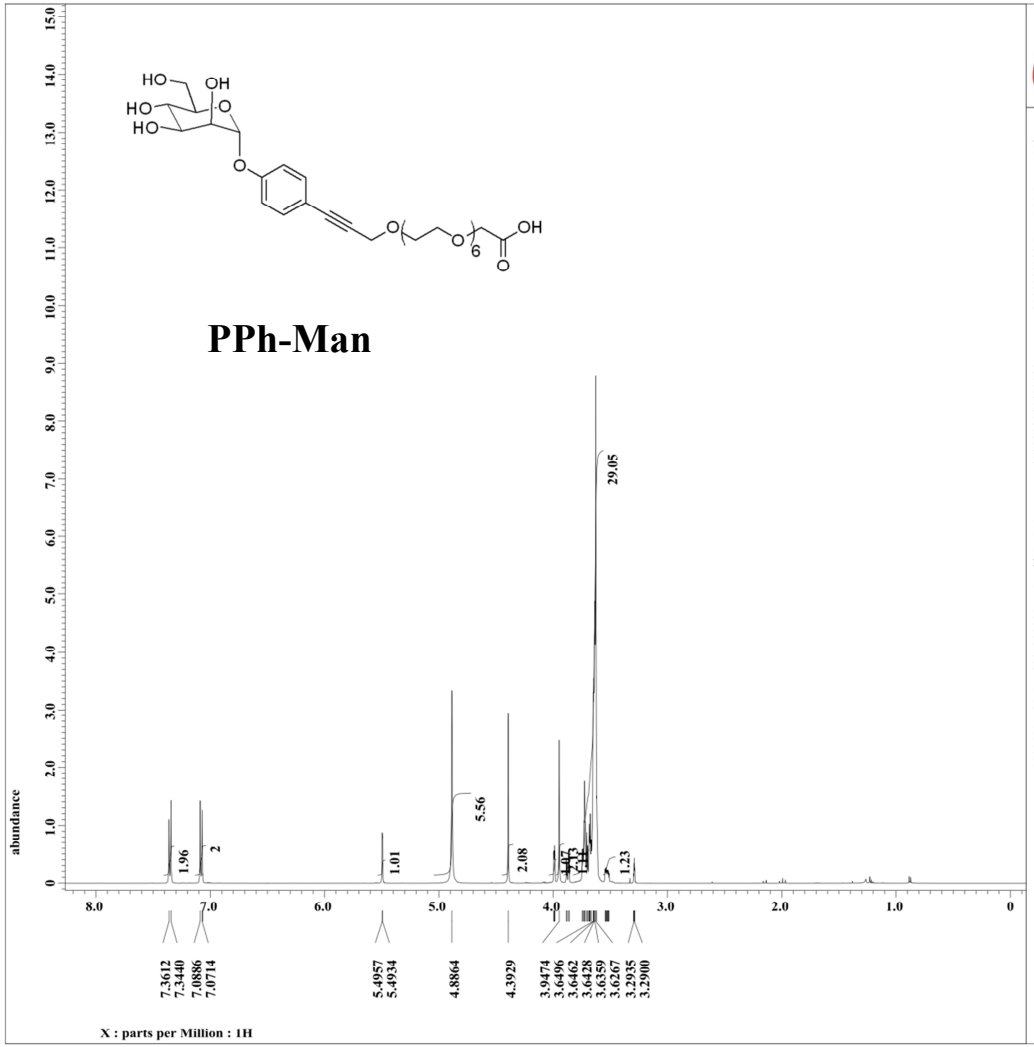


```
Filename          = Junly_17_NO.1_c13defa
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = Junly_17_NO.1
Solvent           = CHLOROFORM-D
Creation_time     = 17-JUL-2010 18:53:02
Revision_time     = 17-JUL-2010 19:25:33
Current_time      = 26-JAN-2011 20:22:54

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 512
Total_scans       = 512

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 18.5[dC]
```

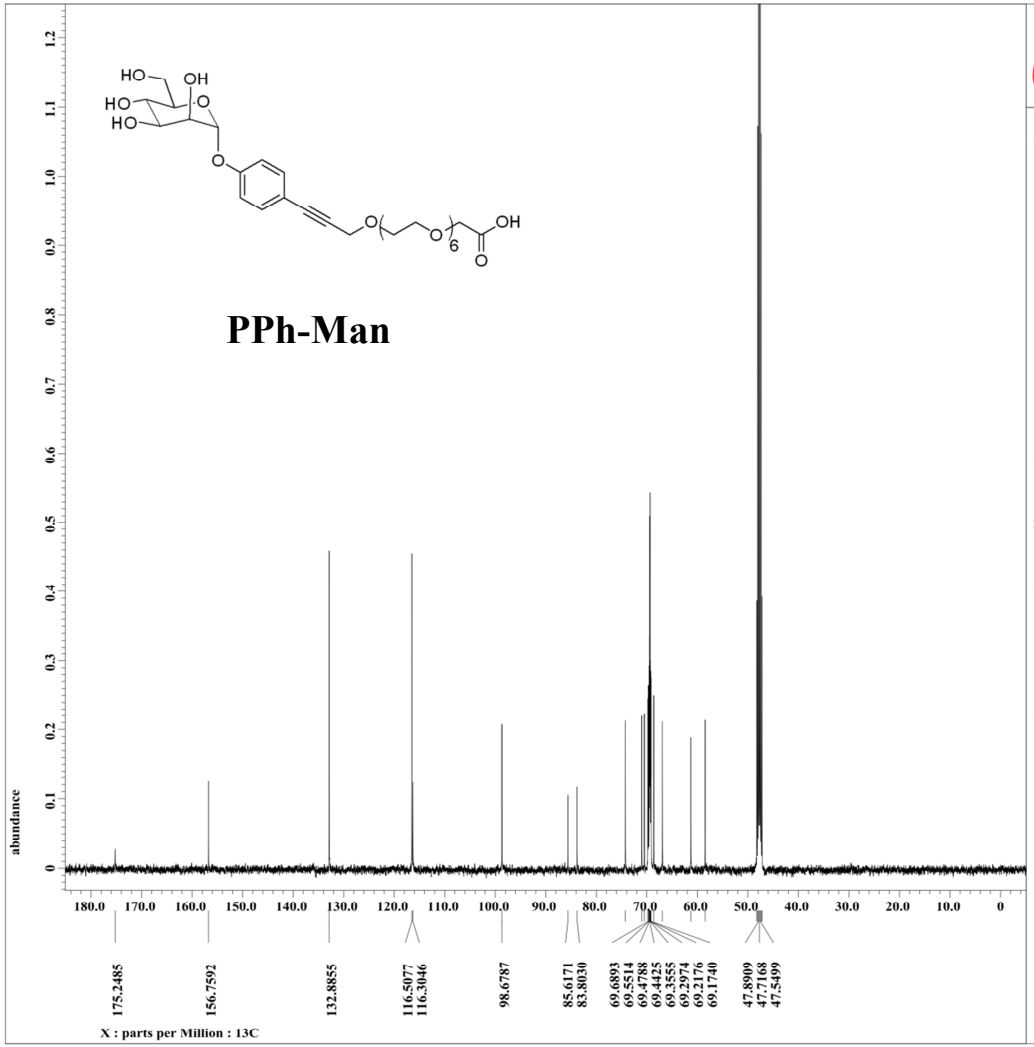



```
Filename          = h1_deprotect-4.jdf
Author            = Cai
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = METHANOL-D3
Creation_time     = 20-AUG-2010 14:08:34
Revision_time     = 20-AUG-2010 14:40:04
Current_time      = 26-JAN-2011 20:25:14

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 6.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.84[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 6.42[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 1[s]
Repetition_time   = 2.74587904[s]
Temp_get          = 21[dC]
```




```
Filename          = c13default185to-5ppm-
Author            = Cai
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = METHANOL-D3
Creation_time     = 20-AUG-2010 14:24:16
Revision_time     = 20-AUG-2010 14:54:19
Current_time      = 26-JAN-2011 20:26:24

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.09576192[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 90[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.912607[Hz]
X_sweep           = 29.90430622[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 6.5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 438
Total_scans       = 438

X_90_width        = 11.77[us]
X_acq_time        = 1.09576192[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.92333333[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 19.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 60
Relaxation_delay  = 1[s]
Repetition_time   = 2.09576192[s]
Temp_get          = 21.5[dC]
```

6. References:

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