

Supporting Information

Phenanthroline-Catalyzed Stereoselective Formation of α -1,2-*Cis* 2-Deoxy-2-Fluoro Glycosides

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1. General Information

Methods and Reagents. All reactions were performed in oven-dried flasks fitted with septa under a positive pressure of nitrogen atmosphere. Organic solutions were concentrated using a Buchi rotary evaporator below 40 °C at 25 torr. Analytical thin-layer chromatography was routinely used to monitor the progress of the reactions. Analytical thin-layer chromatography was performed using pre-coated glass plates with 230-400 mesh silica gel impregnated with a fluorescent indicator (250 nm). Visualization was then achieved using UV light, iodine, or ceric ammonium molybdate. Flash column chromatography was performed using 40-63 µm silica gel (SiliaFlash F60 from Silicycle) or a Teledyne Isco CombiFlash R_f system utilizing normal phase pre-column cartridges and gold high performance columns. Dry solvents were obtained from a SG Waters solvent system utilizing activated alumina columns under an argon pressure or purchased from Sigma-Aldrich in Sure/Seal™ bottles. All chemicals and reagents were obtained from commercial vendors and used without further purification, unless otherwise noted.

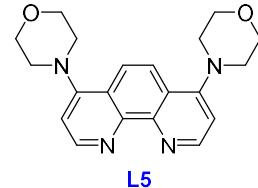
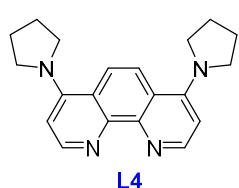
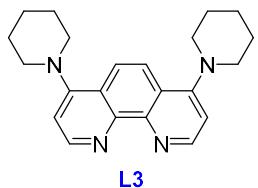
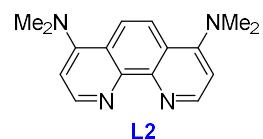
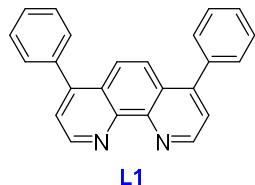
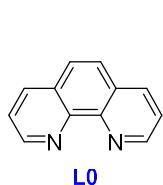
Instrumentation. All proton (¹H) nuclear magnetic resonance spectra were recorded on a 400 or 500 MHz spectrometer. All carbon (¹³C) nuclear magnetic resonance spectra were recorded on a 101 or 125 MHz NMR spectrometer. All fluorine (¹⁹F) nuclear magnetic resonance spectra were recorded on a 376 MHz NMR spectrometer. Chemical shifts are expressed in parts per million (δ scale) and are referenced to residual CHCl₃ (¹H: δ 7.26 ppm, ¹³C: δ 77.16 ppm) and C₆D₆ (¹H: δ 7.16 ppm, ¹³C: δ 128.06 ppm). Data are presented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and bs = broad singlet), integration, and coupling constant in hertz (Hz). Infrared (IR) spectra were reported in cm⁻¹. High resolution TOF mass spectrometry utilizing electrospray ionization in positive mode or electron ionization was performed to confirm the identity of the compounds.

Abbreviations were used as follows: MTBE (*tert*-butyl methyl ether), IBO (isobutylene oxide), DTBMP (di-*tert*-butylmethylpyridine) and DFT (density functional theory).

2. Preparation of Phenanthroline and Pyridine-Based Catalysts

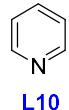
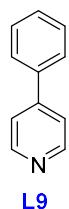
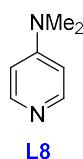
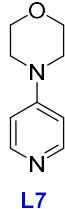
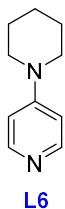
Phenanthroline-Based Catalysts

While **L0** and **L1** catalysts are commercially available, **L2 – L5** catalysts were prepared according to literature procedure.^{1,2}

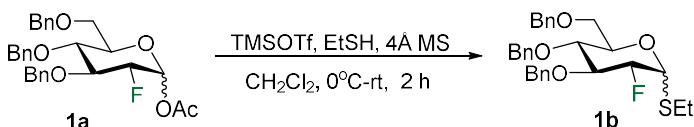


Pyridine-Based Catalysts

All **L6 – L10** catalysts are commercially available.



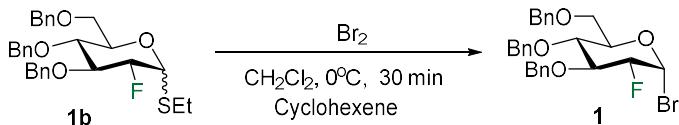
3. Synthesis of Glycosyl Halides



A 50 mL oven-dried Schlenk flask was charged with **1a** (2.1 g, 4.25 mmol) and dry CH_2Cl_2 (21 mL). Ethylthiol (1.2 mL, 17 mmol) and 4 \AA of crushed molecular sieves (2.1 g) were then added to the solution. The resulting solution was stirred at room temperature for 30 min and cooled to 0°C. After the mixture had been stirring for 5 min at 0°C, trimethylsilyl trifluoromethanesulfonate was added (1.15 mL, 6.38 mmol). The reaction mixture was stirred at 0°C for 2 h and then allowed to warm to room temperature. After the reaction mixture had been stirring for 1.5 h, almost all of starting material **1a** disappeared by TLC (20% ethyl acetate in hexanes). The mixture was quenched with CH_3OH and concentrated *in vacuo*. The crude residue was purified by silica gel column chromatography (5% ethyl acetate in hexane \rightarrow 10% ethyl acetate in hexane \rightarrow 15% ethyl acetate in hexane \rightarrow 20% ethyl acetate in hexane \rightarrow 30% ethyl acetate in hexane) to give **1b** (1.284 g, 61%) as a clear oil.

$^1\text{H NMR}$ (400 MHz, CDCl_3) α/β mixture, inseparable, δ 7.42 – 7.12 (m, 36.7H), 5.56 (d, J = 5.7 Hz, 1H), 4.94 (d, J = 11.2 Hz, 2.3H), 4.90 – 4.82 (m, 3.8H), 4.82 – 4.70 (m, 3.5H), 4.68 – 4.40 (m, 11.5H), 4.37 – 4.28 (m, 1.1H), 4.23 (d, J = 9.9 Hz, 1.3H), 3.95 (dt, J = 12.4, 9.1 Hz, 1.5H), 3.85 – 3.73 (m, 4.6H), 3.73 – 3.61 (m, 5.6H), 3.55 – 3.46 (m, 1.9H), 2.85 – 2.72 (m, 3.8H), 2.72 – 2.55 (m, 2.8H), 1.39 – 1.29 (m, 8.1H).

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -186.36 (dd, J = 49.4, 15.1 Hz, β -anomer), -188.38 (dd, J = 50.6, 12.5 Hz, α -anomer).



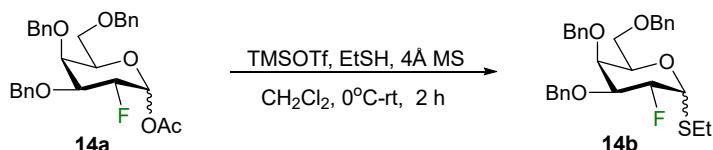
A 25 mL oven-dried Schlenk flask was charged with **1b** (1.267 g, 2.56 mmol) and CH_2Cl_2 (12.5 mL). The solution was cooled to 0°C, and bromine (0.263 mL) was then added. The resulting solution turned dark purple. After the reaction mixture had been stirring for 15 min, almost all of starting material **1b** disappeared by TLC (5% ethyl acetate in toluene). Cyclohexene was added dropwise until the solution turned pale yellow. The resulting mixture was concentrated *in vacuo*. The crude residue was purified by silica gel column chromatography (1% ethyl acetate in toluene \rightarrow 2% ethyl acetate in toluene \rightarrow 3% ethyl acetate in toluene \rightarrow 4% ethyl acetate in toluene \rightarrow 5% ethyl acetate in toluene \rightarrow 10% ethyl acetate in toluene) to give **1** (1.120 g, 85%) as a pale yellow oil.

¹H NMR (CDCl₃, 400 MHz): δ 7.38-7.15 (15H, m, Ph) 6.56 (1H, d, J = 4.0 Hz, H-C1), 4.91 (1H, d, J = 11.2 Hz, Bn), 4.85 (1H, d, J = 10.8 Hz, Bn), 4.77 (1H, d, J = 10.8 Hz, Bn), 4.58 (1H, d, J = 12.0 Hz, Bn), 4.52 (1H, d, J = 11.2 Hz, Bn), 4.48 (1H, d, J = 12.0 Hz, Bn), 4.49 (1H, ddd, J = 49.6, 8.8, 6.8 Hz, H-C2), 4.17 (1H, dt, J = 11.2, 9.2 Hz, H-C3), 4.08 (1H, brd, J = 10.0 Hz, H-C5), 3.81 (1H, t, J = 9.6 Hz, H-C4), 3.79 (1H, dd, J = 11.2, 1.2 Hz, H-C6), 3.68 (1H, dd, J = 11.2, 1.2 Hz, H-C6)

¹³C NMR (CDCl₃, 150 MHz): δ 137.9 (Ph), 137.7 (Ph), 137.5 (Ph), 128.4-127.9 (Ph) 90.0 (d, ¹J_{CF} 196.0 Hz, C2), 88.0 (d, ²J_{CF} 25.7 Hz, C1), 80.9 (d, ²J_{CF} 15.5 Hz, C3), 75.4 (Bn), 75.3 (d, ³J_{CF} 10.5 Hz, C4), 75.2 (Bn), 75.1 (d, ⁴J_{CF} 1.0 Hz, C5), 73.5 (Bn), 67.3 (C6)

¹⁹F NMR (376 MHz, CDCl₃) δ = -186.19 (dd, ²J_{FH} 49.7 Hz, ³J_{FH} 11.3 Hz)

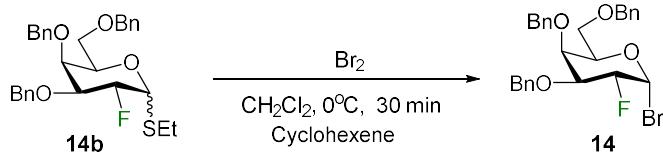
HRMS (ESI): calc. for C₂₇H₃₂BrFO₄N [M + NH₄]⁺, 532.1498; found, 532.1501.



A 50 mL oven-dried Schlenk flask was charged with **14a** (6.0 g, 12.1 mmol) and dry CH₂Cl₂ (21 mL). Ethylthiol (3.5 mL, 49 mmol) and 4Å of crushed molecular sieves (6.0 g) were then added to the solution. The resulting solution was stirred at room temperature for 30 min and cooled to 0°C. After the mixture had been stirring for 5 min at 0°C, trimethylsilyl trifluoromethanesulfonate was added (3.3 mL, 18.2 mmol). The reaction mixture was stirred at 0°C for 2 h and then allowed to warm to room temperature. After the reaction mixture had been stirring for 1.5 h, almost all of starting material **14a** disappeared by TLC (20% ethyl acetate in hexanes). The mixture was quenched with CH₃OH and concentrated *in vacuo*. The crude residue was purified by silica gel column chromatography (5% ethyl acetate in hexane → 10% ethyl acetate in hexane → 15% ethyl acetate in hexane → 20% ethyl acetate in hexane → 30% ethyl acetate in hexane) to give **14b** (3.15 g, 53%) as a pale yellow solid.

¹H NMR (400 MHz, CDCl₃) α/β mixture, inseparable, δ 7.44 – 7.26 (m, 167.7H), 5.62 (d, J = 5.8 Hz, 1H), 4.97 (dd, J = 11.5, 1.6 Hz, 12.4H), 4.89 – 4.79 (m, 18.2H), 4.76 – 4.68 (m, 18.5H), 4.63 (dd, J = 11.5, 1.7 Hz, 12.4H), 4.53 – 4.40 (m, 35.9H), 4.40 – 4.33 (m, 1.4H), 4.15 (ddd, J = 14.2, 7.1, 1.3 Hz, 2.3H), 4.02 (d, J = 1.6 Hz, 12.2H), 3.93 – 3.78 (m, 3.2H), 3.71 – 3.56 (m, 47.7H), 2.84 – 2.69 (m, 24.6H), 2.68 – 2.55 (m, 3.5H), 2.07 (d, J = 1.2 Hz, 2.6H), 1.31 (dtd, J = 8.6, 7.3, 1.5 Hz, 41.1H).

¹⁹F NMR (376 MHz, CDCl₃) δ -195.90 (ddd, J = 50.6, 12.7, 2.7 Hz, β-anomer), -197.42 (dd, J = 51.3, 10.5 Hz, α-anomer).



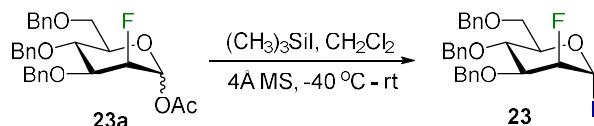
A 50 mL oven-dried Schlenk flask was charged with **14b** (3.15 g, 6.3 mmol) and CH_2Cl_2 (30 mL). The solution was cooled to 0°C , and bromine (0.651 mL) stirring for 15 min, almost all of starting material **14b** disappeared by TLC (5% ethyl acetate in toluene). Cyclohexene was added dropwise until the solution turned pale yellow. The resulting mixture was concentrated in *vacuo*. The crude residue was purified by silica gel column chromatography (1% ethyl acetate in toluene \rightarrow 2% ethyl acetate in toluene \rightarrow 3% ethyl acetate in toluene \rightarrow 4% ethyl acetate in toluene \rightarrow 5% ethyl acetate in toluene \rightarrow 10% ethyl acetate in toluene) to give **14** (2.1 g, 65%) as a light tan solid.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.48 – 7.14 (m, 15H), 6.62 (d, $J = 4.0$ Hz, 1H), 4.94 (d, $J = 11.2$ Hz, 1H), 4.92 (ddd, $J = 50.6, 9.2, 4.1$ Hz, 1H) 4.84 (d, $J = 11.9$ Hz, 1H), 4.70 (d, $J = 11.8$ Hz, 1H), 4.56 (d, $J = 11.1$ Hz, 1H), 4.50 (d, $J = 11.8$ Hz, 1H), 4.43 (d, $J = 11.8$ Hz, 1H), 4.22 (t, $J = 6.5$ Hz, 1H), 4.09 (dd, $J = 9.4, 2.9$ Hz, 1H), 4.06 – 4.00 (m, 1H), 3.66 – 3.52 (m, 2H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 137.94, 137.85, 137.52, 128.50, 128.47, 128.34, 128.22, 127.91, 127.86, 127.61, 89.80 (d, $J = 26.0$ Hz), 88.09 (d, $J = 192.3$ Hz), 77.62 (d, $J = 15.2$ Hz), 75.26, 74.61 (d, $J = 8.3$ Hz), 74.23 (d, $J = 1.0$ Hz), 73.54, 73.21 (d, $J = 2.3$ Hz), 67.43.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -194.11 (ddd, $J = 50.6, 9.2, 4.1$ Hz).

HRMS (ESI): calc. for $\text{C}_{27}\text{H}_{32}\text{BrFO}_4\text{N} [\text{M} + \text{NH}_4]^+$, 532.1498; found, 532.1494.

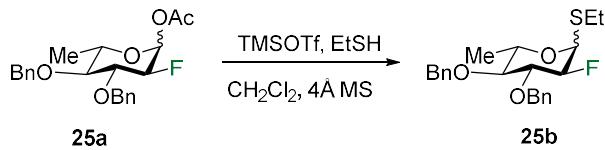


A 25 mL oven-dried Schlenk flask was charged with **23a** (1.06 g, 2.15 mmol), CH_2Cl_2 (11 mL), and 4 Å MS (1.1 g) was added and stirred. The mixture was stirred at room temperature for 30 min and then cooled to -40°C . Trimethylsilyl iodide was added dropwise (0.46 mL, 3.22 mmol) to the mixture. The mixture was stirred for 2 h at -40°C , warmed to 0°C and stirred for 2 h, and finally warmed to room temperature. The reaction mixture was quenched with Et_3N (0.60 mL, 4.3 mmol) and concentrated in *vacuo*. The crude residue was purified by silica gel column chromatography (2.5% ethyl acetate in toluene \rightarrow 5% ethyl acetate in toluene \rightarrow 10% ethyl acetate in toluene \rightarrow 15% ethyl acetate in toluene) to give **23** (0.44 g, 37%).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.47 – 7.17 (m, 15H), 6.93 (d, $J = 11.6$ Hz, 1H), 4.91 (d, $J = 49.7$ Hz, 1H), 4.90 (d, $J = 10.7$ Hz, 1H), 4.78 (d, $J = 9.8$ Hz, 2H), 4.63 (d, $J = 12.1$ Hz, 1H), 4.58 (d, $J = 10.7$ Hz, 1H), 4.51 (d, $J = 12.1$ Hz, 1H), 4.46 (ddd, $J = 27.0, 9.6, 2.2$ Hz, 1H), 4.11 (t, $J = 9.8$ Hz, 1H), 3.85 (dd, $J = 11.1, 3.8$ Hz, 1H), 3.73 – 3.63 (m, 2H).

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -172.89 (ddd, $J = 49.7, 26.9, 11.7$ Hz).

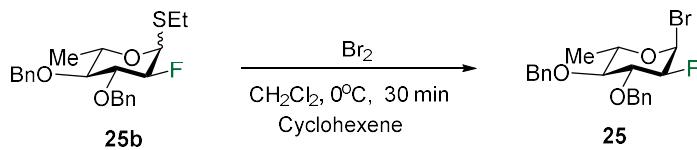
HRMS (ESI): calc. for $C_{27}H_{32}O_4NFI$ [M + NH₄]⁺, 580.1355; found, 580.1341.



A 25 mL oven-dried Schlenk flask was charged with **25a** (1.29 g, 3.32 mmol) and dry CH₂Cl₂ (16 mL). Ethylthiol (0.96 mL, 13.3 mmol) and 4Å of crushed molecular sieves (1.6 g) were then added to the solution. The resulting solution was stirred at room temperature for 30 min and cooled to 0°C. After the mixture had been stirring for 5 min at 0°C, trimethylsilyl trifluoromethanesulfonate was added (0.6 mL, 3.3 mmol). The reaction mixture was stirred at 0°C for 2 h and then allowed to warm to room temperature. After the reaction mixture had been stirring for 1.5 h, almost all of starting material **25a** disappeared by TLC (20% ethyl acetate in hexanes). The mixture was quenched with CH₃OH and concentrated *in vacuo*. The crude residue was purified by silica gel column chromatography (2.5% ethyl acetate in hexanes → 5% ethyl acetate in hexanes → 10% ethyl acetate in hexanes → 15% ethyl acetate in hexanes → 20% ethyl acetate in hexanes) to give **25b** (1.04 g, 80%) as a clear oil.

¹H NMR (400 MHz, CDCl₃) α/β mixture, inseparable, δ 7.40 – 7.27 (m, 11.9H), 5.43 (d, J = 5.8 Hz, 1H), 4.95 – 4.86 (m, 2.5H), 4.74 (ddd, J = 50.8, 9.2, 5.8 Hz, 1.5H), 4.73 (d, J = 11.1 Hz, 1.1H), 4.63 (d, J = 11.0 Hz, 1.2H), 4.48 (dd, J = 9.7, 1.5 Hz, 0.3H), 4.44 – 4.38 (m, 0.3H), 4.44 – 4.25 (m, 0.3H), 4.16 (dq, J = 12.4, 6.2 Hz, 1.2H), 3.91 (dt, J = 12.4, 9.1 Hz, 1.2H), 3.75 (dt, J = 15.6, 8.5 Hz, 0.5H), 3.42 (dt, J = 15.7, 6.1 Hz, 0.4H), 3.21 (t, J = 9.1 Hz, 0.4H), 3.15 (t, J = 9.2 Hz, 1.2H), 2.75 (ddd, J = 15.1, 7.5, 2.7 Hz, 0.6H), 2.69 – 2.57 (m, 2.3H), 1.36 – 1.23 (m, 8H).

¹⁹F NMR (376 MHz, CDCl₃) δ -186.23 (dd, J = 49.5, 15.1 Hz, β -anomer), -188.29 (dd, J = 50.7, 12.5 Hz, α -anomer).



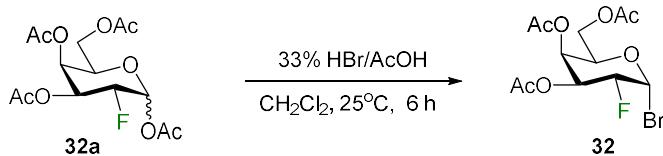
A 10 mL oven-dried Schlenk flask was charged with **25b** (0.30 g, 0.77 mmol) and CH₂Cl₂ (3.8 mL). The solution was cooled to 0°C, and bromine (0.651 mL) was added, stirring for 15 min, almost all of starting material **25b** disappeared by TLC (5% ethyl acetate in toluene). Cyclohexene was added dropwise until the solution turned pale yellow. The resulting mixture was concentrated *in vacuo*. The crude residue was purified by silica gel column chromatography (1% ethyl acetate in hexanes → 2% ethyl acetate in hexanes → 3% ethyl acetate in hexanes → 4% ethyl acetate in hexanes → 5% ethyl acetate in hexanes → 10% ethyl acetate in hexanes) to give **25** (0.174 g, 55%) as a clear oil.

¹H NMR (400 MHz, CDCl₃) δ 7.33 (dq, *J* = 16.7, 7.8 Hz, 1H), 6.48 (d, *J* = 4.0 Hz, 1H), 4.91 (d, *J* = 10.9 Hz, 2H), 4.77 (d, *J* = 10.9 Hz, 1H), 4.64 (d, *J* = 10.9 Hz, 1H), 4.46 (ddd, *J* = 49.9, 9.0, 4.1 Hz, 1H), 4.14 (dt, *J* = 10.9, 9.0 Hz, 1H), 4.06 (m, 1H), 3.24 (t, *J* = 9.3 Hz, 1H), 1.32 (d, *J* = 6.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 137.90, 137.67, 128.46, 128.44, 128.06, 127.99, 127.96, 127.90, 90.37 (d, *J* = 196.6 Hz), 87.65 (d, *J* = 26.2 Hz), 81.24 (d, *J* = 8.4 Hz), 80.76 (d, *J* = 15.6 Hz), 75.57, 75.19 (d, *J* = 2.6 Hz), 72.03, 17.36.

¹⁹F NMR (376 MHz, CDCl₃) δ -185.84 (dd, *J* = 49.8, 11.2 Hz).

HRMS (ESI): calc. for C₂₀H₂₆O₄BrFN [M + NH₄]⁺, 426.1080; found, 426.1085.



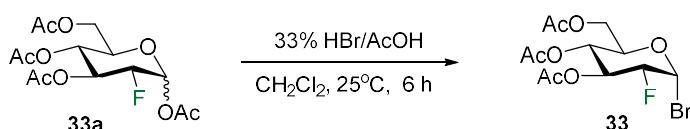
To a solution of **32a** (1.0 g, 2.85 mmol) in CH₂Cl₂ (15 mL) at 0 °C was added 33% HBr/AcOH (18 mL, 250 mmol). The reaction mixture was stirred at 0 °C for 20 min and then warmed to room temperature. After the mixture had been stirring for 6 h, TLC (30% ethyl acetate in hexanes) indicated that it was complete. The reaction mixture was diluted with CH₂Cl₂ and quenched with saturated aqueous NaHCO₃ solution. The two layers were separated, and the aqueous layer was back extracted twice with CH₂Cl₂. The combined organic extracts were dried over MgSO₄, filtered, and concentrated *in vacuo*. The crude residue was purified by silica gel column chromatography to give **32** (0.88 g, 84%) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 6.59 (d, *J* = 4.1 Hz, 1H), 5.50 (s, 1H), 5.43 (td, *J* = 10.0, 3.4 Hz, 1H), 4.73 (ddd, *J* = 50.1, 10.0, 4.2 Hz, 1H), 4.48 (t, *J* = 6.5 Hz, 1H), 4.11 (qd, *J* = 11.5, 6.6 Hz, 2H), 2.11 (s, 3H), 2.02 (s, 3H), 2.02 (s, 3H).

¹³C NMR (101 MHz, D₂O) δ 167.67 (s), 167.10 (s), 167.06 (s), 84.17 (d, *J* = 25.5 Hz), 81.55 (d, *J* = 195.0 Hz), 68.60 (s), 66.32 (d, *J* = 18.0 Hz), 64.86 (d, *J* = 7.6 Hz), 58.02 (s), 18.02 (s), 17.95 (s), 17.88 (s).

¹⁹F NMR (376 MHz, CDCl₃) δ -195.02 (ddd, *J* = 50.0, 9.9, 2.4 Hz).

HRMS (ESI): calc. for C₁₂H₂₀O₇BrFN [M + NH₄]⁺, 388.0407; found, 388.0404.



To a solution of **33a** (2.5 g, 7.12 mmol) in CH₂Cl₂ (45 mL) at 0 °C was added 33% HBr/AcOH (38 mL, 250 mmol). The reaction mixture was stirred at 0 °C for 20 min and then warmed to room

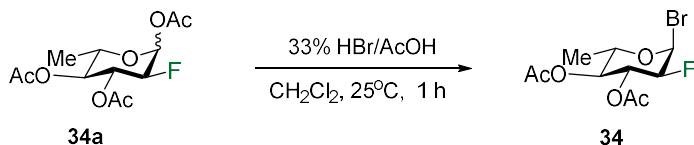
temperature. After the mixture had been stirring for 6 h, TLC (30% ethyl acetate in hexanes) indicated that it was complete. The reaction mixture was diluted with CH₂Cl₂ and quenched with saturated aqueous NaHCO₃ solution. The two layers were separated, and the aqueous layer was back extracted twice with CH₂Cl₂. The combined organic extracts were dried over MgSO₄, filtered, and concentrated *in vacuo*. The crude residue was purified by silica gel column chromatography to give **33** (1.85 g, 70%) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 6.52 (d, *J* = 4.1 Hz, 1H), 5.70 – 5.55 (m, 1H), 5.11 (t, *J* = 9.8 Hz, 1H), 4.54 (ddd, *J* = 49.4, 9.3, 4.3 Hz, 1H), 4.37 – 4.27 (m, 2H), 4.12 (d, *J* = 10.8 Hz, 1H), 2.09 (s, 3H), 2.08 (s, 3H), 2.06 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 170.39, 169.75, 169.45, 86.29 (d, *J* = 198.7 Hz), 85.26 (d, *J* = 25.1 Hz), 72.13, 71.06 (d, *J* = 18.6 Hz), 66.59 (d, *J* = 7.2 Hz), 60.84, 20.63, 20.62, 20.51.

¹⁹F NMR (376 MHz, CDCl₃) δ -188.58 (dd, *J* = 49.3, 11.2 Hz).

HRMS (ESI): calc. for C₁₂H₂₀O₇BrFN [M + NH₄]⁺, 388.0407; found, 388.0402.



To a solution of **34a** (0.385 g, 1.30 mmol) in CH₂Cl₂ (6.5 mL) at 0 °C was added 33% HBr/AcOH (3.6 mL, 250 mmol). The reaction mixture was stirred at 0 °C for 20 min and then warmed to room temperature. After the mixture had been stirring for 1 h, TLC (20% ethyl acetate in hexanes) indicated that it was complete. The reaction mixture was diluted with CH₂Cl₂ and quenched with saturated aqueous NaHCO₃ solution. The two layers were separated, and the aqueous layer was back extracted twice with CH₂Cl₂. The combined organic extracts were dried over MgSO₄, filtered, and concentrated *in vacuo*. The crude residue was purified by silica gel column chromatography to give **34** (0.337 g, 83%) as a white solid.

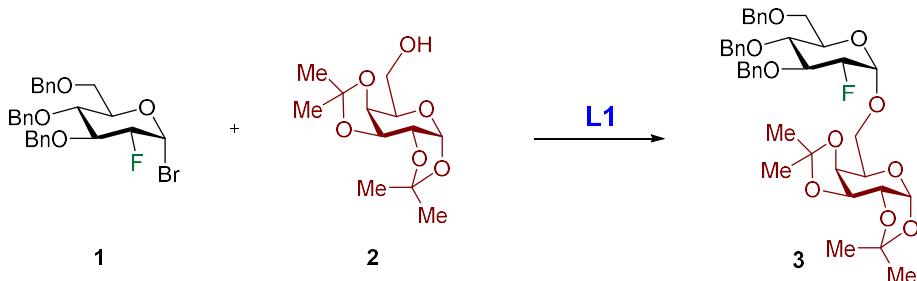
¹H NMR (400 MHz, CDCl₃) δ 6.48 (d, *J* = 4.1 Hz, 1H), 5.58 (dt, *J* = 20.6, 9.5 Hz, 1H), 4.83 (t, *J* = 9.8 Hz, 1H), 4.49 (ddd, *J* = 49.6, 9.4, 4.2 Hz, 1H), 4.19 (dq, *J* = 12.4, 6.2 Hz, 1H), 2.07 (s, 3H), 2.06 (s, 3H), 1.25 (d, *J* = 6.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 169.81, 169.74, 86.72 (d, *J* = 198.4 Hz), 85.72 (d, *J* = 24.8 Hz), 71.93 (d, *J* = 7.2 Hz), 71.00 (d, *J* = 18.4 Hz), 70.42 (d, *J* = 1.1 Hz), 20.66, 20.62, 16.81.

¹⁹F NMR (376 MHz, CDCl₃) δ -188.21 (dd, *J* = 49.6, 11.3 Hz).

HRMS (APCI): calc. for C₁₀H₁₅O₅BrF [M + H]⁺, 313.0087; found, 313.0081.

4. Procedure for Phenanthroline (**L1** or **L3**)-Catalyzed Glycosylation



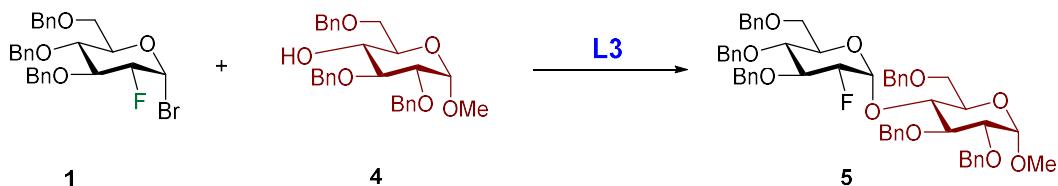
A 10 mL oven-dried Schlenk flask was charged with **L1** (5 mg, 0.015 mmol), **1** (52 mg, 0.1 mmol), **2** (78 mg, 0.3 mmol), IBO (18 μ L, 0.2 mmol), and MTBE (200 μ L). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) \rightarrow 20% ethyl acetate in hexanes (100 mL) \rightarrow 30% ethyl acetate in hexanes (100 mL)] to give **3** (59 mg, 85%) with $\alpha:\beta = 10:1$.

¹H NMR (400 MHz, CDCl₃) δ 7.44 – 7.09 (m, 15H), 5.52 (d, *J* = 5.0 Hz, 1H), 5.11 (d, *J* = 3.8 Hz, 1H), 4.90 (d, *J* = 11.0 Hz, 1H), 4.83 (t, *J* = 10.0 Hz, 1H), 4.76 (d, *J* = 11.0 Hz, 1H), 4.67 – 4.56 (m, 2.5H), 4.53 – 4.43 (m, 2.5H), 4.35 – 4.27 (m, 2H), 4.10 (dt, *J* = 12.1, 9.1 Hz, 1H), 4.02 (t, *J* = 6.1 Hz, 1H), 3.93 – 3.64 (m, 6H), 1.55 (s, 3H), 1.45 (s, 3H), 1.35 (s, 3H), 1.34 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 138.47, 138.18, 137.89, 128.37, 128.33, 127.93, 127.91, 127.84, 127.69, 127.68, 127.66, 109.25, 108.60, 96.79 (d, *J* = 21.0 Hz), 96.25, 91.19 (d, *J* = 192.0 Hz), 80.65 (d, *J* = 16.2 Hz), 76.82 (d, *J* = 8.4 Hz), 75.06 (d, *J* = 2.7 Hz), 75.03, 73.46, 70.73, 70.68, 70.57, 70.16, 68.12, 66.94, 66.24, 53.43, 29.71, 26.15, 25.98, 24.95, 24.45.

¹⁹F NMR (376 MHz, CDCl₃) δ -199.09 (dd, *J* = 49.5, 12.2 Hz).

HRMS (ESI): calc. for C₃₉H₅₁O₁₀NF [M + NH₄]⁺, 712.3492; found, 712.3511.



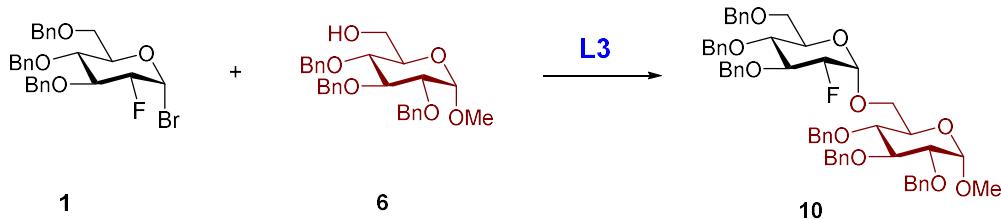
A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **1** (103 mg, 0.2 mmol), **4** (46 mg, 0.1 mmol), IBO (18 μ L, 0.2 mmol), and MTBE (200 μ L). The resulting mixture was stirred at 50°C for 48 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [0.5% ethyl acetate in toluene (50 mL) \rightarrow 1% ethyl acetate in toluene (100 mL) \rightarrow 2% ethyl acetate in toluene (100 mL) \rightarrow 3% ethyl acetate in toluene (100 mL) \rightarrow 4% ethyl acetate in toluene (100 mL) \rightarrow 5% ethyl acetate in toluene (100 mL) \rightarrow 10% ethyl acetate in toluene (100 mL)] to give **5** (61 mg, 68%) with $\alpha:\beta = 10:1$.

¹H NMR (CDCl₃, 400 MHz): δ 7.39–7.13 (30H, m) 5.75 (1H, d, J = 4.0 Hz), 5.03 (1H, d, J = 10.4 Hz), 4.91 (1H, d, J = 11.0 Hz), 4.84–4.76 (4H, m), 4.66–4.62 (2H, m), 4.56–4.39 (5H, m), 4.30 (1H, d, J = 12.1), 4.07–3.97 (2H, m), 3.89 (1H, t, J = 9.1 Hz), 3.81 (1H, dd, J = 15.0, 5.1 Hz), 3.77–3.62 (4H, m), 3.61–3.52 (2H, m), 3.42 (3H, s), 3.38 (1H, d, J = 10.5 Hz)

¹³C NMR (CDCl₃, 101 MHz): δ 136.12, 135.87, 135.61, 135.59, 135.47, 135.24, 125.89, 125.80, 125.76, 125.74, 125.71, 125.56, 125.36, 125.31, 125.14, 125.11, 125.09, 124.88, 124.72, 95.24, 94.43 (d, J = 20.9 Hz, C1), 88.21 (d, J = 192.9 Hz, C2), 79.07, 77.91 (d, J = 16.3, C3), 77.72, 74.02, 72.81, 72.57, 72.51 (d, J = 2.6 Hz, C4), 70.91, 70.75, 70.71, 68.31, 66.94, 66.80, 65.30, 52.73.

¹⁹F NMR (376 MHz, CDCl₃) δ -197.22 (dd, J = 49.6, 11.6 Hz).

HRMS (ESI): calc. for C₅₅H₆₃O₁₀NF [M + NH₄]⁺, 916.4431; found, 916.4440.



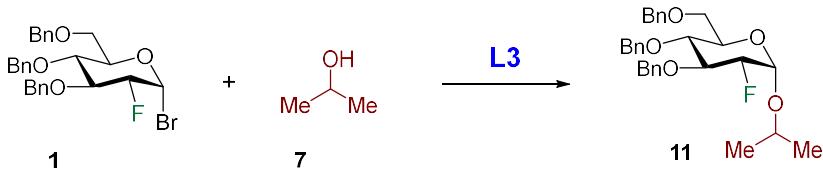
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **1** (103 mg, 0.2 mmol), **6** (46 mg, 0.1 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL) → 30% ethyl acetate in hexanes (100 mL)] to give **10** (80 mg, 89%) with α:β = 8:1.

¹H NMR (400 MHz, CDCl₃) δ 7.49 – 7.00 (m, 30H), 5.15 (d, J = 3.7 Hz, 1H), 5.00 (d, J = 10.8 Hz, 1H), 4.94 (d, J = 11.2 Hz, 1H), 4.89 (d, J = 11.1 Hz, 1H), 4.87 – 4.78 (m, 3H), 4.75 (d, J = 11.1 Hz, 1H), 4.69 (d, J = 12.1 Hz, 1H), 4.65 – 4.48 (m, 4H), 4.45 (dd, J = 11.4, 3.1 Hz, 2H), 4.05 (dt, J = 25.8, 9.1 Hz, 2H), 3.88 – 3.73 (m, 4H), 3.66 (dd, J = 16.5, 6.3 Hz, 2H), 3.61 – 3.52 (m, 3H), 3.38 (s 3H).

¹³C NMR (101 MHz, CDCl₃) δ 138.69, 138.31, 138.22, 138.18, 137.87, 128.46, 128.41, 128.39, 128.36, 128.30, 128.07, 128.05, 128.04, 127.88, 127.87, 127.78, 127.71, 127.69, 127.64, 97.85, 96.49 (d, J = 21.1 Hz), 91.17 (d, J = 193.3 Hz), 82.16, 80.32 (d, J = 16.4 Hz), 80.19, 77.72, 76.82 (d, J = 8.5 Hz), 75.82, 75.05, 74.94 (d, J = 2.6 Hz), 74.92, 73.44, 73.38, 70.17 (d, J = 0.9 Hz), 68.14, 66.21, 55.09.

¹⁹F NMR (376 MHz, CDCl₃) δ -198.55 (dd, J = 49.6, 12.4).

HRMS (ESI): calc. for C₅₅H₆₃O₁₀NF [M + NH₄]⁺, 916.4431; found, 916.4464.



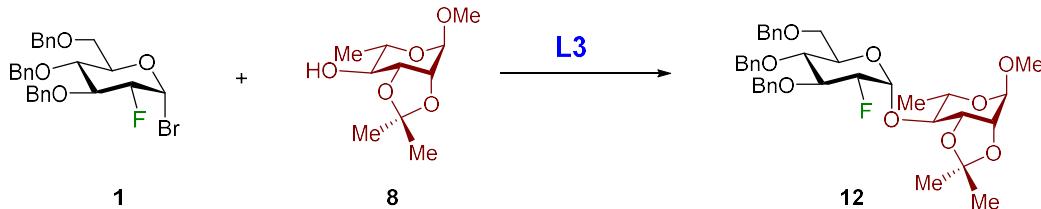
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **1** (52 mg, 0.1 mmol), **7** (23 μ L, 0.3 mmol), IBO (18 μ L, 0.2 mmol), and MTBE (200 μ L). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [2.5% ethyl acetate in hexanes (100 mL) \rightarrow 5% ethyl acetate in hexanes (100 mL) \rightarrow 10% ethyl acetate in hexanes (100 mL) \rightarrow 15% ethyl acetate in hexanes (100 mL) \rightarrow 20% ethyl acetate in hexanes (100 mL)] to give **11** (42 mg, 85%) with $\alpha:\beta = 7:1$.

¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.10 (m, 15H), 5.12 (d, *J* = 3.9 Hz, 1H), 4.91 (d, *J* = 11.0 Hz, 1H), 4.83 (d, *J* = 10.7 Hz, 1H), 4.76 (d, *J* = 11.0 Hz, 1H), 4.63 (d, *J* = 12.1 Hz, 1H), 4.51 (m, 1H), 4.49 (d, *J* = 5.4 Hz, 1H), 4.46 (d, *J* = 4.0 Hz, 1H), 4.09 (dt, *J* = 12.1, 9.1 Hz, 1H), 3.98 – 3.90 (m, 1H), 3.92 – 3.86 (m, 1H), 3.75 (dd, *J* = 10.6, 3.6 Hz, 1H), 3.70 – 3.62 (m, 2H), 1.24 (d, *J* = 6.3 Hz, 3H), 1.20 (d, *J* = 6.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 138.52, 138.05, 137.89, 128.36, 127.96, 127.89, 127.87, 127.75, 127.69, 127.64, 94.64 (d, *J* = 20.7 Hz), 91.07 (d, *J* = 191.6 Hz), 80.86 (d, *J* = 16.1 Hz), 75.22, 75.09 (d, *J* = 2.3 Hz), 73.47, 70.41, 70.05, 68.28, 23.21, 21.46.

¹⁹F NMR (376 MHz, CDCl₃) δ -198.51 (dd, *J* = 49.9, 12.1 Hz).

HRMS (ESI): calc. for C₃₀H₃₉O₅NF [M + NH₄]⁺, 512.2807; found, 512.2804.



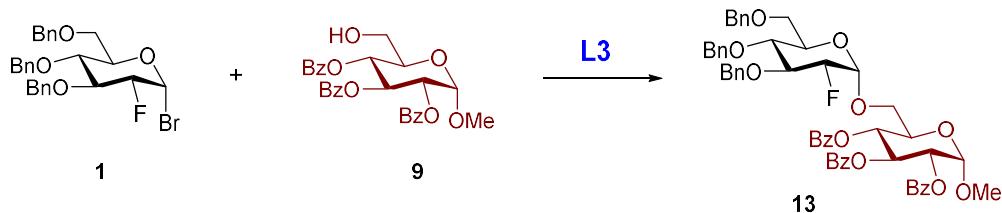
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **1** (103 mg, 0.2 mmol), **8** (22 mg, 0.1 mmol), IBO (18 μ L, 0.2 mmol), and MTBE (200 μ L). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [5% ethyl acetate in hexanes (100 mL) \rightarrow 10% ethyl acetate in hexanes (100 mL) \rightarrow 15% ethyl acetate in hexanes (100 mL) \rightarrow 20% ethyl acetate in hexanes (100 mL) \rightarrow 30% ethyl acetate in hexanes (100 mL)] to give **12** (40 mg, 61%) with $\alpha:\beta > 20:1$.

¹H NMR (CDCl₃, 400 MHz): δ 7.38–7.17 (15H, m), 5.14 (1H, d, *J* = 4.0 Hz), 4.89 (1H, d, *J* = 11.2 Hz), 4.85 (1H, d, *J* = 10.8 Hz), 4.84 (1H, s), 4.76 (1H, d, *J* = 10.8 Hz), 4.62 (1H, d, *J* = 12.0 Hz), 4.54 (1H, ddd, *J* = 49.6, 9.2, 4.0 Hz) 4.52 (1H, d, *J* = 10.4 Hz), 4.50 (1H, d, *J* = 12.0 Hz), 4.10–4.00 (4H, m), 3.83–3.64 (4H, m), 3.36 (4H, m) 1.46 (3H, s), 1.32 (3H, d, *J* = 6.4 Hz), 1.27 (3H, s)

¹³C NMR (CDCl₃, 101 MHz) δ 138.44, 138.24, 137.95, 128.38, 128.35, 128.34, 127.94, 127.90, 127.71, 127.67, 109.05, 97.87, 97.39 (d, *J* = 20.5 Hz), 91.43 (d, *J* = 191.8 Hz), 80.71 (d, *J* = 15.8 Hz), 76.74, 75.99, 75.23, 75.09 (d, *J* = 2.6 Hz), 73.53, 70.17, 67.78, 64.75, 54.74, 28.12, 26.35, 17.13.

¹⁹F NMR (376 MHz, CDCl₃) δ -197.77 (dd, *J* = 49.8, 12.1 Hz).

HRMS (ESI): calc. for C₃₇H₄₉O₉NF [M + NH₄]⁺, 670.3386; found, 670.3389.



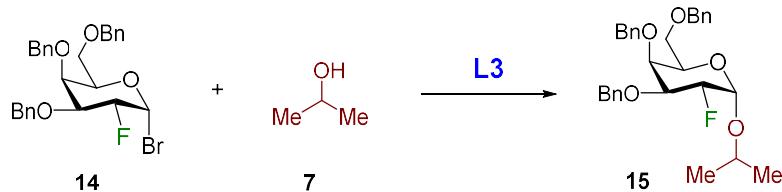
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3mg, 0.015mmol), **1** (140mg, 0.25 mmol), **9** (46mg, 0.1 mmol), IBO (18μL, 0.2 mmol), and MTBE (200μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL) → 30% ethyl acetate in hexanes (100 mL)] to give **13** (80 mg, 85%) with α:β = 7:1.

¹H NMR (400 MHz, CDCl₃) δ 7.98 (d, *J* = 7.2 Hz, 2H), 7.94 (d, *J* = 7.3 Hz, 2H), 7.86 (d, *J* = 7.3 Hz, 2H), 7.51 (t, *J* = 7.0 Hz, 2H), 7.44 – 7.24 (m, 20H), 7.18 – 7.12 (m, 2H), 6.16 (t, *J* = 9.6 Hz, 1H), 5.50 (t, *J* = 9.9 Hz, 1H), 5.30 – 5.22 (m, 2H), 4.90 (d, *J* = 11.0 Hz, 1H), 4.81 (d, *J* = 10.9 Hz, 1H), 4.72 (d, *J* = 11.1 Hz, 1H), 4.56 (dd, *J* = 7.5, 4.9 Hz, 2H), 4.51 (d, *J* = 10.9 Hz, 1H), 4.46 (d, *J* = 12.2 Hz, 1H), 4.35 – 4.29 (m, 1H), 4.33 (dt, *J* = 50.8, 8.0 Hz, 1H), 4.06 (dd, *J* = 11.6, 1.7 Hz, 1H), 3.85 – 3.73 (m, 2H), 3.68 (dd, *J* = 17.9, 7.1 Hz, 2H), 3.63 – 3.57 (m, 1H), 3.48 (s, 3H), 3.44 (d, *J* = 7.7 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 163.24, 163.21, 162.66, 135.83, 135.72, 135.27, 130.74, 130.45, 127.35, 127.33, 127.08, 126.68, 126.51, 126.38, 125.81, 125.79, 125.77, 125.74, 125.70, 125.66, 125.42, 125.27, 125.18, 125.09, 125.05, 125.02, 94.23, 91.70 (d, *J* = 453.5 Hz), 77.74 (d, *J* = 16.4 Hz), 72.41, 72.37 (d, *J* = 2.7 Hz), 70.85, 69.55, 67.98, 67.68, 67.05, 65.79, 65.47, 64.09, 52.90.

¹⁹F NMR (376 MHz, CDCl₃) δ -195.61 (dd, *J* = 51.5, 15.8 Hz).

HRMS (ESI): calc. for C₅₅H₅₇O₁₃NF [M + NH₄]⁺, 958.3814; found, 958.3808.



A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **14** (52 mg, 0.1 mmol), **7** (23 μL, 0.3 mmol), IBO (18μL, 0.2 mmol), 4Å M.S. (30 mg, crushed) and MTBE (200

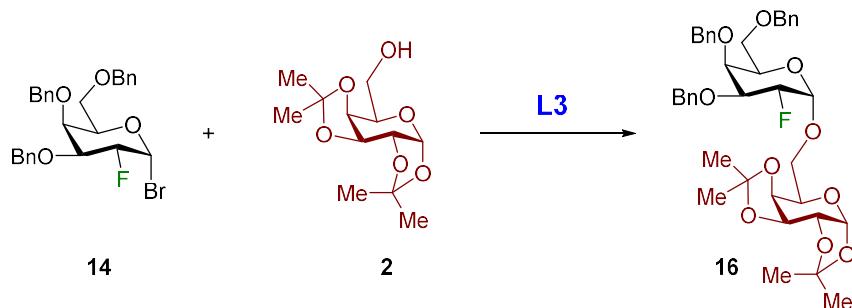
μL). The resulting mixture was stirred at 25°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [5% ethyl acetate in hexanes (100 mL) \rightarrow 10% ethyl acetate in hexanes (100 mL) \rightarrow 15% ethyl acetate in hexanes (100 mL) \rightarrow 20% ethyl acetate in hexanes (100 mL)] to give **15** (30 mg, 60%) with $\alpha:\beta = 9:1$.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.45 – 7.15 (m, 15H), 5.13 (d, $J = 3.9$ Hz, 1H), 4.94 (ddd, $J = 50.8, 9.7, 4.0$ Hz, 1H), 4.94 (d, $J = 11.3$ Hz, 1H), 4.82 (d, $J = 11.8$ Hz, 1H), 4.69 (d, $J = 11.8$ Hz, 1H), 4.56 (d, $J = 11.3$ Hz, 1H), 4.50 (d, $J = 11.8$ Hz, 1H), 4.43 (d, $J = 11.8$ Hz, 1H), 4.03 (td, $J = 12.2, 4.8$ Hz, 3H), 3.92 (dp, $J = 12.4, 6.2$ Hz, 1H), 3.64 – 3.49 (m, 2H), 1.24 (d, $J = 6.2$ Hz, 3H), 1.19 (d, $J = 6.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 138.47, 137.95, 128.38, 128.37, 128.21, 128.18, 127.71, 127.70, 127.59, 127.55, 127.44, 95.07 (d, $J = 20.8$ Hz), 89.09 (d, $J = 187.8$ Hz), 77.45, 75.75 (d, $J = 8.2$ Hz), 74.95, 73.46, 73.06 (d, $J = 2.2$ Hz), 70.31, 69.29, 68.65.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -207.38 (ddd, $J = 50.5, 9.5, 4.7$ Hz).

HRMS (ESI): calc. for $\text{C}_{30}\text{H}_{36}\text{O}_5\text{NF}$ [$\text{M} + \text{H}]^+$, 495.2541; found, 495.2526.



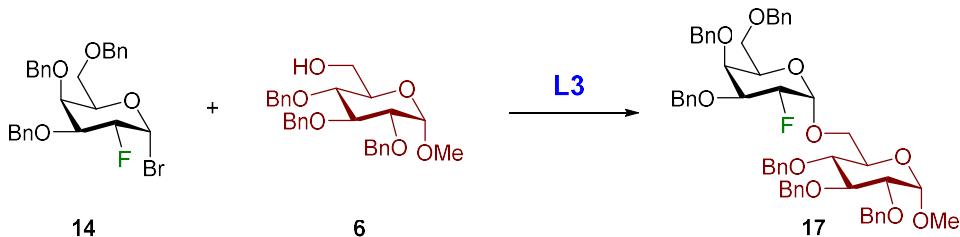
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **14** (52 mg, 0.1 mmol), **2** (78 mg, 0.3 mmol), IBO (18 μL , 0.2 mmol), 4 \AA M.S. (30 mg, crushed) and MTBE (200 μL). The resulting mixture was stirred at 25°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) \rightarrow 20% ethyl acetate in hexanes (200 mL) \rightarrow 30% ethyl acetate in hexanes (50 mL)] to give **16** (45 mg, 65%) with $\alpha:\beta = 12:1$.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.49 – 7.09 (m, 15H), 5.51 (d, $J = 5.0$ Hz, 1H), 5.10 (d, $J = 3.8$ Hz, 1H), 4.96 (ddd, $J = 50.4, 9.6, 3.6$ Hz, 1H), 4.92 (d, $J = 11.3$ Hz, 1H), 4.80 (d, $J = 11.9$ Hz, 1H), 4.68 (d, $J = 11.9$ Hz, 1H), 4.59 (dd, $J = 8.1, 2.3$ Hz, 1H), 4.57 (d, $J = 11.4$ Hz, 1H), 4.49 (d, $J = 11.8$ Hz, 1H), 4.43 (d, $J = 11.8$ Hz, 1H), 4.30 (dd, $J = 5.0, 2.3$ Hz, 1H), 4.27 (dd, $J = 8.0, 1.6$ Hz, 1H), 4.10 (t, $J = 6.6$ Hz, 1H), 4.07 – 3.97 (m, 3H), 3.83 (dd, $J = 10.6, 6.6$ Hz, 1H), 3.75 (dd, $J = 10.6, 6.2$ Hz, 1H), 3.63 – 3.49 (m, 2H), 1.52 (s, 3H), 1.42 (s, 3H), 1.33 (s, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 138.44, 138.39, 137.96, 128.38, 128.37, 128.22, 127.79, 127.69, 127.60, 127.57, 127.46, 109.27, 108.56, 96.92 (d, $J = 20.9$ Hz), 89.20 (d, $J = 188.1$ Hz), 77.15, 75.52 (d, $J = 8.4$ Hz), 74.96, 73.33, 72.91 (d, $J = 2.0$ Hz), 70.87, 70.63, 70.61, 69.23, 68.30, 66.97, 66.44, 26.11, 25.95, 24.97, 24.43.

¹⁹F NMR (376 MHz, CDCl₃) δ -208.04 (ddd, *J* = 50.1, 9.7, 4.6 Hz).

HRMS (ESI): calc. for C₃₉H₅₁O₁₀NF [M + NH₄]⁺, 712.3492; found, 712.3511.



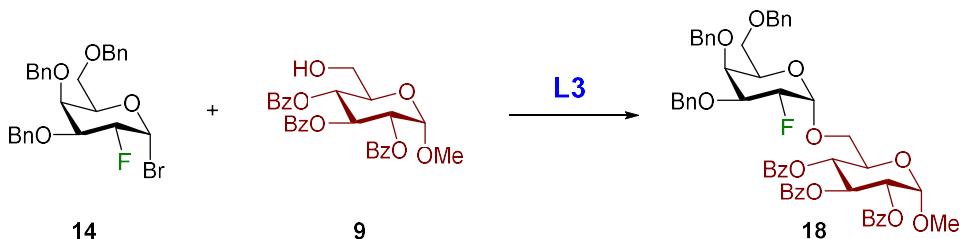
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **14** (52 mg, 0.1 mmol), **6** (139 mg, 0.3 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 25°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (200 mL) → 30% ethyl acetate in hexanes (50 mL)] to give **17** (76 mg, 85%) with α:β = 11:1.

¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.18 (m, 30H), 5.12 (d, *J* = 3.7 Hz, 1H), 5.02 – 4.82 (m, 4H), 4.81 (d, *J* = 4.8 Hz, 1H), 4.78 (d, *J* = 5.1 Hz, 1H), 4.76 (d, *J* = 10.2 Hz, 1H), 4.66 (d, *J* = 11.7 Hz, 2H), 4.58 (d, *J* = 3.5 Hz, 1H), 4.56 (d, *J* = 6.7 Hz, 1H), 4.53 (d, *J* = 6.4 Hz, 1H), 4.43 (d, *J* = 11.8 Hz, 1H), 4.37 (d, *J* = 11.8 Hz, 1H), 4.02 – 3.90 (m, 4H), 3.82 – 3.71 (m, 3H), 3.56 – 3.46 (m, 4H), 3.31 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 138.74, 138.40, 138.28, 138.19, 138.17, 137.88, 128.42, 128.37, 128.36, 128.22, 128.18, 128.02, 127.85, 127.72, 127.71, 127.65, 127.62, 127.61, 127.60, 127.53, 97.79, 96.88 (d, *J* = 21.0 Hz), 89.12 (d, *J* = 188.1 Hz), 82.08, 80.14, 77.90, 77.19, 76.40 (d, *J* = 16.0 Hz), 75.78, 75.49 (d, *J* = 8.6 Hz), 74.93, 73.38, 73.35, 72.65 (d, *J* = 2.1 Hz), 70.06, 69.43, 68.49, 66.47, 54.97, 29.69.

¹⁹F NMR (376 MHz, CDCl₃) δ -207.36 – -207.57 (m).

HRMS (ESI): calc. for C₅₅H₆₃O₁₀NF [M + NH₄]⁺, 916.4431; found, 916.4474.



A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **14** (52 mg, 0.1 mmol), **9** (140 mg, 0.25 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (200 mL)].

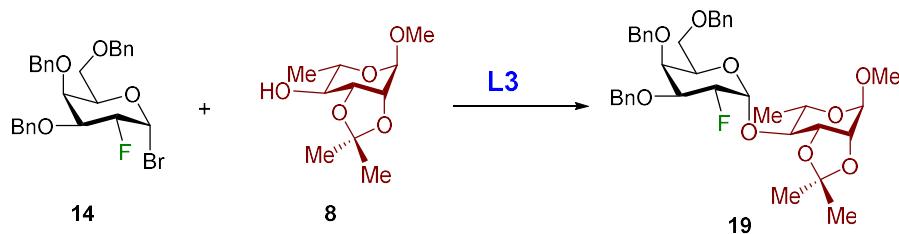
in hexanes (200 mL) → 30% ethyl acetate in hexanes (50 mL)] to give **18** (76 mg, 85%) with $\alpha:\beta = 11:1$.

¹H NMR (400 MHz, CDCl₃) ¹H NMR (400 MHz, cdcl₃) δ 7.99 (d, *J* = 7.2 Hz, 2H), 7.92 (d, *J* = 7.2 Hz, 2H), 7.86 (d, *J* = 7.2 Hz, 2H), 7.55 – 7.20 (m, 20H), 6.13 (t, *J* = 9.9 Hz, 1H), 5.56 (t, *J* = 9.9 Hz, 1H), 5.27 (dd, *J* = 10.2, 3.6 Hz, 1H), 5.19 (d, *J* = 3.6 Hz, 1H), 5.07 (d, *J* = 3.7 Hz, 1H), 4.92 (d, *J* = 11.4 Hz, 1H), 4.80 (d, *J* = 12.0 Hz, 1H), 4.69 (d, *J* = 12.0 Hz, 1H), 4.55 (d, *J* = 11.3 Hz, 1H), 4.39 (d, *J* = 11.9 Hz, 1H), 4.32 (d, *J* = 11.9 Hz, 1H), 4.29 – 4.24 (m, 1H), 4.05 (dd, *J* = 9.9, 2.7 Hz, 1H), 4.00 (dd, *J* = 12.5, 4.3 Hz, 2H), 3.92 (dd, *J* = 11.1, 6.2 Hz, 1H), 3.66 (dd, *J* = 11.1, 1.9 Hz, 1H), 3.50 – 3.40 (m, 2H), 3.37 (s, 2H).

¹³C NMR (101 MHz, CDCl₃) ¹³C NMR (101 MHz, cdcl₃) δ 165.78, 165.77, 165.32, 138.39, 138.35, 137.95, 133.33, 133.30, 133.02, 129.92, 129.80, 129.64, 129.27, 129.11, 128.97, 128.38, 128.37, 128.35, 128.23, 128.21, 127.64, 127.63, 127.60, 127.58, 96.80, 96.80 (d, *J* = 20.7 Hz), 89.07 (d, *J* = 189.1 Hz), 75.54 (d, *J* = 8.5 Hz), 74.94, 73.28, 72.83 (d, *J* = 2.1 Hz), 72.06, 70.64, 69.46, 68.40, 68.30, 66.50, 55.34.

¹⁹F NMR (376 MHz, CDCl₃) δ -207.97 (ddd, *J* = 50.1, 10.2, 4.1 Hz).

HRMS (ESI): calc. for C₅₅H₅₇O₁₃NF [M + NH₄]⁺, 958.3814; found, 958.3808.



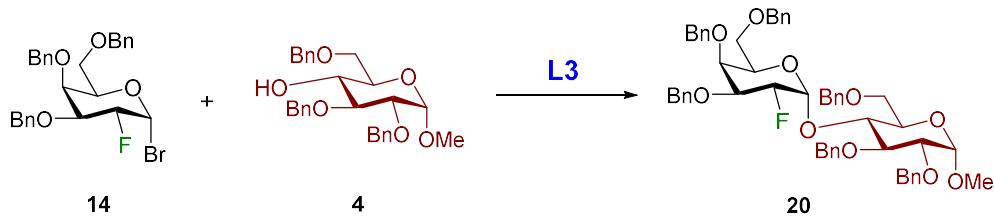
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **14** (52 mg, 0.1 mmol), **8** (66 mg, 0.3 mmol), IBO (18 μ L, 0.2 mmol), and MTBE (200 μ L). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL) → 30% ethyl acetate in hexanes (100 mL)] to give **19** (53 mg, 81%) with $\alpha:\beta = 8:1$.

¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.23 (m, 15H), 5.13 (d, *J* = 3.9 Hz, 1H), 4.97 (ddd, *J* = 50.4, 10.0, 4.0 Hz, 1H) 4.95 (d, *J* = 11.3 Hz, 1H), 4.84 (s, 1H), 4.77 (d, *J* = 11.9 Hz, 1H), 4.68 (d, *J* = 11.9 Hz, 1H), 4.59 (d, *J* = 11.3 Hz, 1H), 4.49 (d, *J* = 11.9 Hz, 1H), 4.41 (d, *J* = 11.9 Hz, 1H), 4.24 (dd, *J* = 9.0, 4.9 Hz, 1H), 4.10 (m, 3H), 3.98 (td, *J* = 10.0, 2.9 Hz, 1H), 3.70 (dt, *J* = 6.2, 4.6 Hz, 1H), 3.65 (d, *J* = 9.0 Hz, 1H), 3.56 – 3.49 (m, 1H), 3.36 (s, 3H), 3.35 – 3.29 (m, 1H), 1.40 (s, 3H), 1.30 (d, *J* = 6.3 Hz, 3H), 1.26 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 138.66, 138.35, 137.98, 128.41, 128.38, 128.19, 128.05, 127.89, 127.77, 127.59, 127.49, 127.42, 109.10, 97.89, 97.54 (d, *J* = 20.6 Hz), 89.41 (d, *J* = 188.1 Hz), 80.80, 76.96, 76.90 (d, *J* = 16.0 Hz), 75.98, 75.34 (d, *J* = 8.2 Hz), 75.06, 73.49, 72.74 (d, *J* = 1.7 Hz), 68.93, 67.50, 64.81, 54.74, 27.97, 26.39, 17.18.

¹⁹F NMR (376 MHz, CDCl₃) δ -206.98 (ddd, *J* = 50.5, 10.2, 4.1 Hz).

HRMS (ESI): calc. for C₃₇H₄₉O₉NF [M + NH₄]⁺, 670.3386; found, 670.3366.



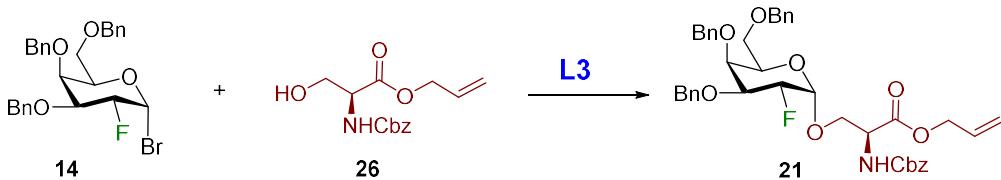
A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **14** (103 mg, 0.2 mmol), **4** (46 mg, 0.1 mmol), IBO (18 μL, 0.2 mmol), 4Å M.S. (30 mg, crushed), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 48 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [5% ethyl acetate in hexanes (100 mL) → 10% ethyl acetate in hexanes (100 mL) → 15% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL) → 30% ethyl acetate in hexanes (100 mL)] to give **20** (67 mg, 75%) with α:β = 10:1.

¹H NMR (400 MHz, CDCl₃) δ 7.53 – 6.99 (m, 30H), 5.74 (d, *J* = 4.1 Hz, 1H), 4.98 (d, *J* = 10.2 Hz, 1H), 4.92 (ddd, *J* = 50.4, 10.0, 4.0 Hz, 1H), 4.89 (d, *J* = 11.4 Hz, 1H), 4.82 – 4.75 (m, 3H), 4.69 – 4.61 (m, 2H), 4.59 (d, *J* = 3.4 Hz, 1H), 4.55 (d, *J* = 5.7 Hz, 1H), 4.52 (d, *J* = 6.5 Hz, 1H), 4.41 (d, *J* = 12.1 Hz, 1H), 4.33 (d, *J* = 11.6 Hz, 1H), 4.27 (d, *J* = 11.7 Hz, 1H), 4.03 – 3.97 (m, 1H), 3.90 (m, 3H), 3.80 (m, 2H), 3.69 (m, 2H), 3.54 (dd, *J* = 9.6, 3.5 Hz, 1H), 3.48 – 3.36 (m, 2H), 3.41 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 138.57, 138.35, 138.30, 138.25, 138.05, 137.83, 128.46, 128.42, 128.36, 128.33, 128.26, 128.19, 128.13, 128.02, 128.01, 127.92, 127.83, 127.74, 127.71, 127.65, 127.48, 127.45, 127.38, 127.33, 97.83, 97.35 (d, *J* = 20.9 Hz), 88.66 (d, *J* = 188.5 Hz), 81.61, 80.19, 76.86 (d, *J* = 16.2 Hz), 75.41, 75.31, 75.23, 75.20, 74.95, 73.47, 73.35, 73.01, 72.94 (d, *J* = 1.9 Hz), 69.94, 69.58, 68.53, 55.28.

¹⁹F NMR (376 MHz, CDCl₃) δ -206.11 (ddd, *J* = 50.3, 9.6, 4.0 Hz).

HRMS (ESI): calc. for C₅₅H₆₃O₁₀NF [M + NH₄]⁺, 916.4431; found, 916.4460.



A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **14** (52 mg, 0.1 mmol), **26** (83 mg, 0.3 mmol), IBO (18 μL, 0.2 mmol), 4Å M.S. (30 mg, crushed), and MTBE (200 μL). The resulting mixture was stirred at 25°C for 48 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [5% ethyl acetate in hexanes (100 mL)]

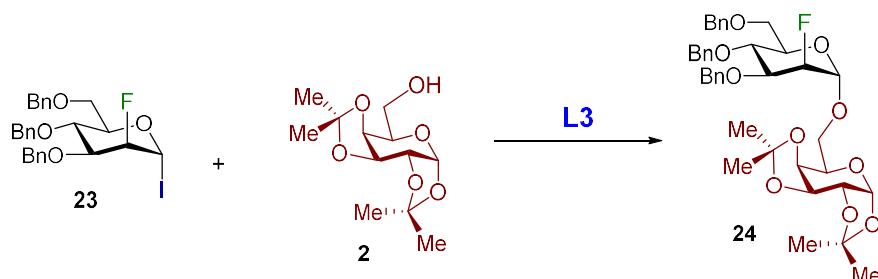
→ 10% ethyl acetate in hexanes (100 mL) → 15% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL)] to give **21** (38 mg, 73%) with $\alpha:\beta = 7:1$.

¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.21 (m, 20H), 5.97 (d, *J* = 8.4 Hz, 1H), 5.88 (ddd, *J* = 16.0, 10.4, 5.2 Hz, 1H), 5.32 (d, *J* = 17.2 Hz, 1H), 5.22 (d, *J* = 10.4 Hz, 1H), 5.11 (d, *J* = 12.1 Hz, 1H), 5.07 (d, *J* = 12.5 Hz, 1H), 4.98 (d, *J* = 3.3 Hz, 1H), 4.92 (ddd, *J* = 48–52, 10.0, 4.0 Hz, 1H) 4.89 (d, *J* = 11.4 Hz, 1H), 4.77 (d, *J* = 11.9 Hz, 1H), 4.68 – 4.62 (m, 2H), 4.58 (d, *J* = 8.6 Hz, 1H), 4.52 (d, *J* = 11.3 Hz, 1H), 4.47 (d, *J* = 12.0 Hz, 1H), 4.36 (d, *J* = 11.9 Hz, 1H), 4.16 (dd, *J* = 10.5, 2.7 Hz, 1H), 3.98 – 3.92 (m, 3H), 3.89 (t, *J* = 10.0 Hz, 1H), 3.50 (dt, *J* = 15.9, 9.2 Hz, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 169.51, 156.03, 138.20, 138.14, 137.79, 136.16, 131.51, 128.49, 128.40, 128.37, 128.24, 128.21, 128.16, 127.75, 127.69, 127.52, 118.79, 98.36 (d, *J* = 21.6 Hz), 88.88 (d, *J* = 188.7 Hz), 75.34 (d, *J* = 8.4 Hz), 74.91, 73.40, 72.98 (d, *J* = 2.0 Hz), 70.44, 70.06, 68.48, 67.09, 66.25, 54.72, 29.69.

¹⁹F NMR (376 MHz, CDCl₃) δ -207.79 (ddd, *J* = 11.9, 9.5, 3.1 Hz).

HRMS (ESI): calc. for C₄₁H₄₅O₉NF [M + H]⁺, 714.3073; found, 714.3061.



A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **23** (56 mg, 0.1 mmol), **2** (78 mg, 0.3 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [0.5% ethyl acetate in toluene (50 mL) → 1% ethyl acetate in toluene (100 mL) → 2% ethyl acetate in toluene (100 mL) → 3% ethyl acetate in toluene (100 mL) → 4% ethyl acetate in toluene (100 mL) → 5% ethyl acetate in toluene (100 mL) → 10% ethyl acetate in toluene (100 mL)] to give **24** (42 mg, 60%) with $\alpha:\beta = 2:1$.

α-isomer 24:

¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.11 (m, 15H), 5.51 (d, *J* = 5.0 Hz, 1H), 5.06 (d, *J* = 6.3 Hz, 1H), 4.85 (d, *J* = 10.8 Hz, 1H), 4.79 (d, *J* = 22.5 Hz, 1H), 4.75 – 4.64 (m, 3H), 4.59 (dd, *J* = 14.4, 7.2 Hz, 2H), 4.51 (d, *J* = 11.5 Hz, 2H), 4.32 (dd, *J* = 4.9, 2.3 Hz, 1H), 4.15 (d, *J* = 8.0 Hz, 1H), 4.01 – 3.93 (m, 2H), 3.88 (dd, *J* = 15.2, 13.2 Hz, 1H), 3.84 – 3.76 (m, 3H), 3.74 – 3.66 (m, 2H), 1.52 (s, 3H), 1.43 (s, 3H), 1.33 (s, 6H).

¹³C NMR (101 MHz, CDCl₃) δ 138.22, 138.18, 138.00, 128.39, 128.31, 128.30, 128.01, 127.81, 127.78, 127.73, 127.66, 127.52, 109.41, 108.60, 97.09 (d, *J* = 29.3 Hz), 96.28, 86.72 (d, *J* = 176.6 Hz), 78.58 (d, *J* = 17.2 Hz), 75.27, 74.28, 73.41, 72.17, 71.78, 70.86, 70.62, 70.53, 68.54, 65.93, 65.45, 26.11, 25.94, 24.89, 24.53.

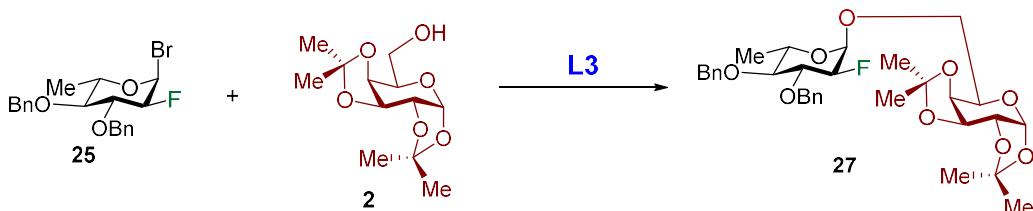
¹⁹F NMR (376 MHz, CDCl₃) δ -204.35 (ddd, *J* = 49.7, 29.3, 7.3 Hz).

HRMS (ESI): calc. for C₃₉H₅₁O₁₀NF [M + NH₄]⁺, 712.3492; found, 712.3509.

β-isomer 24:

¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.14 (m, 15H), 5.53 (d, *J* = 4.9 Hz, 1H), 4.94 (dd, *J* = 51.6, 1.6 Hz, 1H), 4.88 (d, *J* = 10.8 Hz, 1H), 4.78 (d, *J* = 11.8 Hz, 1H), 4.65 (d, *J* = 11.8 Hz, 1H), 4.64 (d, *J* = 12.1 Hz, 1H), 4.61 – 4.49 (m, 4H), 4.31 (dd, *J* = 4.9, 2.2 Hz, 1H), 4.21 (d, *J* = 8.0 Hz, 1H), 4.14 (d, *J* = 11.5 Hz, 1H), 4.05 (d, *J* = 7.8 Hz, 1H), 3.87 (t, *J* = 9.5 Hz, 1H), 3.80 – 3.66 (m, 3H), 3.57 (dd, *J* = 27.0, 9.2 Hz, 1H), 3.45 (dd, *J* = 9.5, 3.2 Hz, 1H), 1.54 (s, 3H), 1.43 (s, 3H), 1.33 (s, 3H), 1.31 (s, 3H).

¹⁹F NMR (376 MHz, CDCl₃) δ -220.10 (ddd, *J* = 51.2, 28.6, 18.4 Hz).



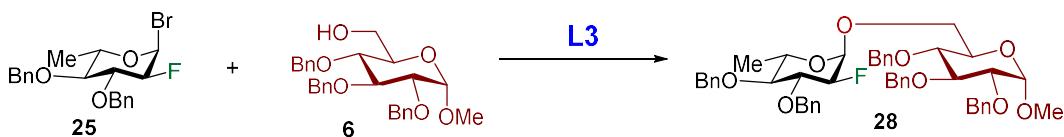
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **25** (41 mg, 0.1 mmol), **2** (78 mg, 0.3 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL) → 30% ethyl acetate in hexanes (100 mL)] to give **27** (52 mg, 88%) with α:β > 20:1.

¹H NMR (400 MHz, CDCl₃) δ 7.42 – 7.15 (m, 10H), 5.53 (d, *J* = 4.9 Hz, 1H), 5.06 (d, *J* = 3.6 Hz, 1H), 4.89 (d, *J* = 11.0 Hz, 2H), 4.74 (d, *J* = 11.0 Hz, 1H), 4.66 – 4.59 (m, 2H), 4.48 (ddd, *J* = 49.4, 9.2, 3.7 Hz, 1H), 4.32 – 4.26 (m, 2H), 4.09 – 3.97 (m, 2H), 3.97 – 3.84 (m, 2H), 3.67 (dd, *J* = 10.1, 6.1 Hz, 1H), 3.14 (t, *J* = 9.3 Hz, 1H), 1.56 (s, 3H), 1.44 (s, 3H), 1.34 (s, 6H), 1.25 (d, *J* = 6.3 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 138.45, 138.25, 128.35, 127.96, 127.82, 127.71, 127.65, 109.18, 108.63, 96.20, 95.86 (d, *J* = 20.7 Hz), 91.48 (d, *J* = 192.1 Hz), 82.84 (d, *J* = 8.1 Hz), 80.44 (d, *J* = 16.0 Hz), 75.19, 75.01 (d, *J* = 2.8 Hz), 70.89, 70.60, 70.55, 66.75, 66.65 (d, *J* = 1.0 Hz), 65.62, 26.09, 25.97, 24.93, 24.40, 17.61.

¹⁹F NMR (376 MHz, CDCl₃) δ -198.87 (dd, *J* = 49.6, 12.2 Hz).

HRMS (ESI): calc. for C₃₂H₄₅O₉FN [M + NH₄]⁺, 606.3078; found, 606.3070.



A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **25** (41 mg, 0.1 mmol), **6** (139 mg, 0.3 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture

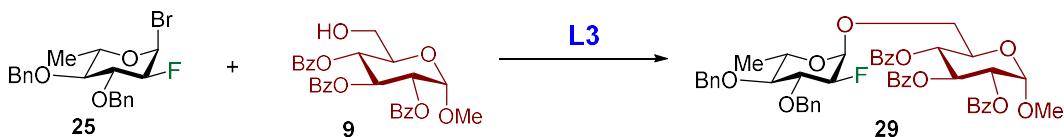
was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL) → 30% ethyl acetate in hexanes (100 mL) → 40% ethyl acetate in hexanes (100 mL) → 50% ethyl acetate in hexanes (100 mL)] to give **28** (67 mg, 85%) with $\alpha:\beta = 7:1$.

¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.24 (m, 25H), 4.98 (d, *J* = 10.7 Hz, 1H), 4.92 (d, *J* = 7.6 Hz, 1H), 4.90 – 4.86 (m, 2H), 4.83 (d, *J* = 7.0 Hz, 1H), 4.81 (d, *J* = 8.4 Hz, 1H), 4.75 (d, *J* = 11.0 Hz, 1H), 4.69 (d, *J* = 12.1 Hz, 1H), 4.64 (d, *J* = 3.4 Hz, 1H), 4.61 (d, *J* = 3.2 Hz, 1H), 4.59 (d, *J* = 3.5 Hz, 1H), 4.45 (ddd, *J* = 49.5, 9.3, 3.8 Hz, 1H), 4.10 – 4.00 (m, 1H), 3.98 (d, *J* = 9.3 Hz, 1H), 3.89 – 3.80 (m, 2H), 3.77 (dd, *J* = 10.1, 3.4 Hz, 1H), 3.67 – 3.56 (m, 2H), 3.54 (dd, *J* = 9.6, 3.6 Hz, 1H), 3.37 (s, 3H), 3.13 (t, *J* = 9.3 Hz, 1H), 1.23 (d, *J* = 6.2 Hz, 3H).

¹³C NMR (101 MHz, cdcl₃) δ 138.67, 138.47, 138.40, 138.18, 138.07, 128.48, 128.44, 128.43, 128.42, 128.38, 128.12, 128.09, 128.06, 128.01, 127.90, 127.87, 127.77, 127.70, 127.67, 97.94, 96.51 (d, *J* = 20.6 Hz), 91.51 (d, *J* = 192.3 Hz), 82.94 (d, *J* = 8.2 Hz), 82.12, 80.30 (d, *J* = 16.1 Hz), 80.11, 77.65, 75.90, 75.51, 75.08 (d, *J* = 2.7 Hz), 75.02 (d, *J* = 0.8 Hz), 73.41, 69.91, 66.60 (d, *J* = 2.8 Hz), 55.12, 17.71.

¹⁹F NMR (376 MHz, CDCl₃) δ -198.33 (dd, *J* = 49.6, 12.2 Hz).

HRMS (ESI): calc. for C₄₈H₅₇O₉FN [M + NH₄]⁺, 810.4017; found, 810.4012.



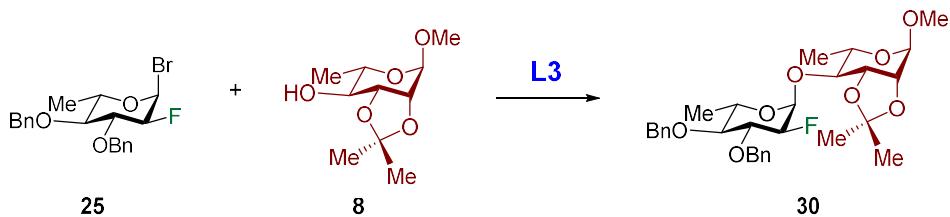
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **25** (41 mg, 0.1 mmol), **9** (102 mg, 0.2 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [10% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL) → 30% ethyl acetate in hexanes (100 mL) → 40% ethyl acetate in hexanes (100 mL) → 50% ethyl acetate in hexanes (100 mL)] to give **29** (49 mg, 59%) with $\alpha:\beta = 11:1$.

¹H NMR (400 MHz, CDCl₃) δ 7.97 (dd, *J* = 10.0, 8.0 Hz, 3H), 7.86 (d, *J* = 7.3 Hz, 2H), 7.56 – 7.23 (m, 20H), 6.14 (t, *J* = 9.8 Hz, 1H), 5.50 (t, *J* = 9.9 Hz, 1H), 5.26 (dd, *J* = 10.1, 3.6 Hz, 1H), 5.21 (d, *J* = 3.6 Hz, 1H), 5.04 (d, *J* = 3.8 Hz, 1H), 4.87 (d, *J* = 11.0 Hz, 1H), 4.81 (d, *J* = 11.0 Hz, 1H), 4.64 (d, *J* = 11.1 Hz, 1H), 4.61 (d, *J* = 11.0 Hz, 1H), 4.45 (ddd, *J* = 49.4, 9.3, 3.9 Hz, 1H), 4.31 – 4.25 (m, 1H), 3.96 (dt, *J* = 12.1, 9.1 Hz, 1H), 3.84 (dd, *J* = 11.7, 2.3 Hz, 1H), 3.76 (dt, *J* = 11.7, 7.3 Hz, 2H), 3.48 (s, 3H), 3.10 (t, *J* = 9.2 Hz, 1H), 1.19 (d, *J* = 6.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 165.81, 165.75, 165.32, 138.41, 138.17, 133.36, 133.30, 133.01, 129.92, 129.88, 129.65, 129.25, 129.08, 128.92, 128.39, 128.37, 128.34, 128.32, 128.22, 127.97, 127.88, 127.72, 127.63, 96.79, 96.77 (d, *J* = 20.7 Hz), 91.41 (d, *J* = 192.5 Hz), 82.76 (d, *J* = 8.4 Hz), 80.21 (d, *J* = 16.3 Hz), 75.26, 74.93 (d, *J* = 2.8 Hz), 72.06, 70.45, 69.78, 69.38, 66.83 (d, *J* = 1.5 Hz), 66.53, 55.51, 17.64.

¹⁹F NMR (376 MHz, CDCl₃) δ -199.05 (dd, *J* = 49.4, 12.1 Hz).

HRMS (ESI): calc. for C₄₈H₅₁O₁₂FN [M + NH₄]⁺, 852.3395; found, 852.3390.



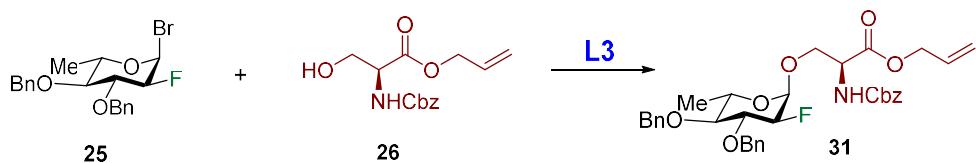
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **25** (82 mg, 0.2 mmol), **8** (22 mg, 0.1 mmol), IBO (18 μL, 0.2 mmol), 4Å MS (30 mg, crushed) and MTBE (200 μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography [2.5% ethyl acetate in hexanes (100 mL) → 5% ethyl acetate in hexanes (100 mL) → 10% ethyl acetate in hexanes (100 mL) → 15% ethyl acetate in hexanes (100 mL) → 20% ethyl acetate in hexanes (100 mL)] to give **30** (53 mg, 96%) with α:β > 20:1.

¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.27 (m, 10H), 5.58 (d, *J* = 4.0 Hz, 1H), 4.90 (d, *J* = 11.0 Hz, 2H), 4.86 (s, 1H), 4.74 (d, *J* = 10.9 Hz, 1H), 4.63 (d, *J* = 10.9 Hz, 1H), 4.50 (ddd, *J* = 49.5, 9.4, 4.1 Hz, 1H), 4.27 (t, *J* = 6.4 Hz, 1H), 4.11 (d, *J* = 5.7 Hz, 1H), 3.96 (dt, *J* = 11.7, 9.2 Hz, 1H), 3.81 (dq, *J* = 12.6, 6.2 Hz, 1H), 3.73 (dq, *J* = 12.6, 6.2 Hz, 1H), 3.53 (dd, *J* = 9.7, 7.3 Hz, 1H), 3.37 (s, 3H), 3.14 (t, *J* = 9.3 Hz, 1H), 1.54 (s, 3H), 1.35 (s, 3H), 1.31 (d, *J* = 6.2 Hz, 3H), 1.25 (d, *J* = 6.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 138.38, 138.04, 128.41, 128.39, 128.08, 127.98, 127.85, 127.72, 109.37, 97.98, 94.42 (d, *J* = 20.6 Hz), 91.27 (d, *J* = 192.2 Hz), 82.64 (d, *J* = 8.1 Hz), 80.45 (d, *J* = 16.1 Hz), 78.33, 78.00, 75.95, 75.49, 75.11 (d, *J* = 2.9 Hz), 67.09 (d, *J* = 1.1 Hz), 63.64, 54.80, 27.91, 26.32, 18.19, 17.63 (d, *J* = 0.6 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -198.68 (dd, *J* = 49.5, 11.8 Hz).

HRMS (ESI): calc. for C₃₀H₄₃O₈FN [M + NH₄]⁺, 564.2973; found, 564.2967.



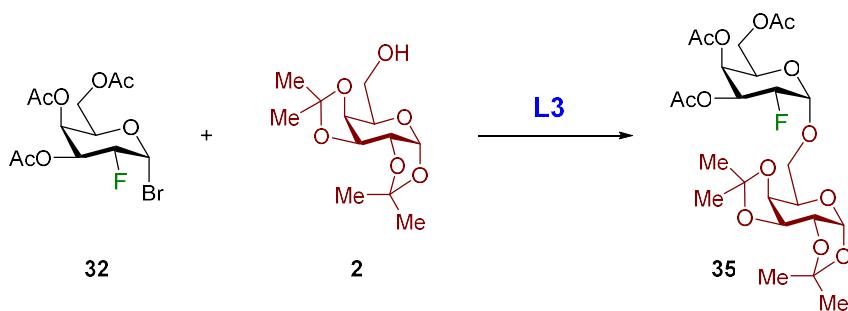
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **25** (41 mg, 0.1 mmol), **26** (84 mg, 0.3 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography to give **31** (47 mg, 78%) with α:β = 13:1.

¹H NMR (400 MHz, CDCl₃) ¹H NMR (400 MHz, cdcl₃) δ 7.46 – 7.09 (m, 15H), 5.89 (ddd, *J* = 16.4, 11.0, 5.9 Hz, 1H), 5.68 (d, *J* = 8.8 Hz, 1H), 5.30 (d, *J* = 17.1 Hz, 1H), 5.20 (d, *J* = 10.3 Hz, 1H), 5.15 (s, 2H), 4.88 (d, *J* = 4.6 Hz, 1H), 4.85 (d, *J* = 11.2 Hz, 2H), 4.71 (d, *J* = 11.0 Hz, 1H), 4.67 – 4.57 (m, 3H), 4.44 (ddd, *J* = 49.3, 9.3, 3.8 Hz, 1H), 4.23 (d, *J* = 7.9 Hz, 1H), 3.89 (dt, *J* = 12.1, 9.1 Hz, 1H), 3.69 (dd, *J* = 9.7, 2.7 Hz, 1H), 3.62 (td, *J* = 12.6, 6.3 Hz, 1H), 3.09 (t, *J* = 9.2 Hz, 1H), 1.55 (s, 1H), 1.21 (d, *J* = 6.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) ¹³C NMR (101 MHz, cdcl₃) δ 169.44, 156.00, 138.26, 138.15, 136.13, 131.31, 128.53, 128.36, 128.31, 128.21, 128.14, 127.98, 127.77, 127.71, 127.70, 119.36, 96.61 (d, *J* = 20.9 Hz), 91.28 (d, *J* = 193.0 Hz), 82.53 (d, *J* = 8.5 Hz), 80.20 (d, *J* = 16.2 Hz), 75.24, 75.08 (d, *J* = 2.7 Hz), 68.31, 67.17, 67.07, 66.46, 54.20, 17.65.

¹⁹F NMR (376 MHz, cdcl₃) ¹⁹F NMR (376 MHz, cdcl₃) δ -198.88 (dd, *J* = 49.3, 12.1 Hz).

HRMS (ESI): calc. for C₃₄H₄₂O₈NF [M + NH₄]⁺, 625.2925; found, 625.2920.



A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **32** (74 mg, 0.2 mmol), **2** (26 mg, 0.1 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 48 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography to give **35** (35 mg, 64%) with α:β = 7:1.

35 α-isomer:

¹H NMR (400 MHz, CDCl₃) δ 5.52 – 5.46 (m, 2H), 5.41 (td, *J* = 10.6, 3.5 Hz, 1H), 5.16 (d, *J* = 3.7 Hz, 1H), 4.75 (ddd, *J* = 50.0, 10.1, 3.7 Hz, 1H), 4.60 (dd, *J* = 7.9, 2.2 Hz, 1H), 4.37 (t, *J* = 6.5 Hz, 1H), 4.30 (dd, *J* = 4.9, 2.3 Hz, 1H), 4.26 (dd, *J* = 7.9, 1.5 Hz, 1H), 4.15 – 4.04 (m, 2H), 4.00 (t, *J* = 5.7 Hz, 1H), 3.87 – 3.74 (m, 2H), 2.12 (s, 3H), 2.04 (s, 3H), 2.02 (s, 3H), 1.55 (s, 3H), 1.43 (s, 3H), 1.32 (s, 6H).

¹⁹F NMR (376 MHz, CDCl₃) δ -208.51 (ddd, *J* = 50.0, 10.7, 3.0 Hz).

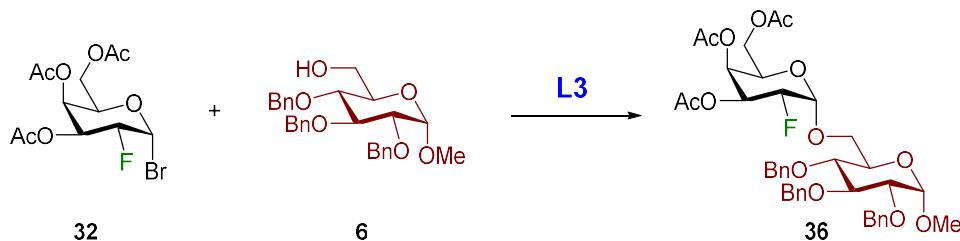
¹³C NMR (101 MHz, CDCl₃) δ 170.38, 170.01, 169.90, 109.27, 108.71, 96.73 (d, *J* = 20.7 Hz), 96.23, 85.36 (d, *J* = 191.0 Hz), 70.77, 70.61, 70.60, 68.79 (d, *J* = 7.6 Hz), 68.17 (d, *J* = 18.8 Hz), 67.67, 66.56, 66.51 (d, *J* = 0.9 Hz), 61.47, 26.10, 25.95, 24.94, 24.35, 20.70, 20.65, 20.55.

HRMS (ESI): calc. for C₂₄H₃₉O₁₃FN [M + NH₄]⁺, 568.2405; found, 568.2400.

35 β-isomer:

¹H NMR (400 MHz, CDCl₃) δ 5.53 (d, *J* = 5.0 Hz, 1H), 5.41 (s, 1H), 5.15 – 5.05 (m, 1H), 4.78 (dd, *J* = 7.7, 3.6 Hz, 1H), 4.61 (dd, *J* = 7.9, 2.4 Hz, 1H), 4.51 (ddd, *J* = 51.3, 9.7, 7.8 Hz, 1H), 4.31 (dd, *J* = 4.9, 2.4 Hz, 1H), 4.26 (d, *J* = 7.9 Hz, 1H), 4.14 (ddd, *J* = 23.5, 11.2, 6.8 Hz, 2H), 4.07 – 3.99 (m, 2H), 3.92 (t, *J* = 7.3 Hz, 1H), 3.89 – 3.84 (m, 1H), 2.13 (s, 3H), 2.05 (s, 6H), 1.53 (s, 3H), 1.45 (s, 3H), 1.34 (s, 3H), 1.33 (s, 3H).

¹⁹F NMR (376 MHz, CDCl₃) δ -206.64 (ddt, *J* = 51.5, 13.4, 2.9 Hz).



A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **32** (74 mg, 0.2 mmol), **6** (46 mg, 0.1 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 48 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography to give **36** (53 mg, 70%) with α:β = 9:1.

36 α-isomer:

¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.27 (m, 15H), 5.43 (brs, 1H), 5.35 (td, *J* = 10.5, 3.5 Hz, 1H), 5.20 (d, *J* = 3.7 Hz, 1H), 4.98 (d, *J* = 10.8 Hz, 1H), 4.93 (d, *J* = 11.3 Hz, 1H), 4.84 – 4.74 (m, 2.5H), 4.69 – 4.63 (m, 1.5H), 4.61 (d, *J* = 8.3 Hz, 1H), 4.59 (s, 1H), 4.17 (t, *J* = 6.6 Hz, 1H), 4.10 – 3.94 (m, 3H), 3.85 – 3.72 (m, 3H), 3.54 – 3.43 (m, 2H), 3.38 (s, 3H), 2.12 (s, 3H), 2.03 (s, 3H), 1.98 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 170.27, 169.97, 169.92, 138.61, 138.24, 138.13, 128.44, 128.41, 128.38, 128.02, 128.00, 127.88, 127.72, 127.70, 127.61, 97.85, 96.39 (d, *J* = 20.7 Hz), 85.19 (d, *J* = 191.5 Hz), 82.07, 80.12, 77.72, 75.78, 74.97, 73.38, 70.04, 68.65 (d, *J* = 7.5 Hz), 68.17 (d, *J* = 18.8 Hz), 66.65, 66.41, 61.51, 55.13, 20.64, 20.64, 20.53.

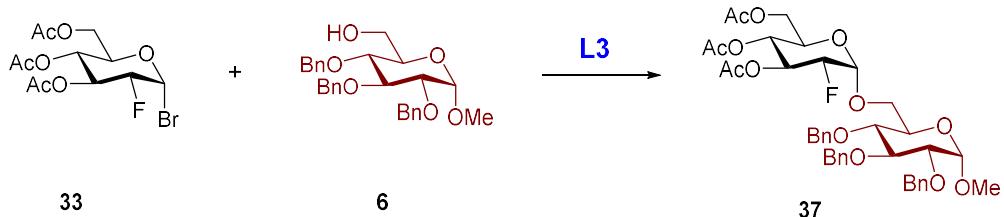
¹⁹F NMR (376 MHz, CDCl₃) δ -208.07 (ddd, *J* = 50.0, 10.8, 3.3 Hz).

HRMS (ESI): calc. for C₃₀H₄₃O₈FN [M + NH₄]⁺, 564.2973; found, 564.2978.

36 β-isomer:

¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.22 (m, 15H), 5.38 (brs, 1H), 5.10 – 5.01 (m, 1H), 4.98 (d, *J* = 10.8 Hz, 1H), 4.91 (d, *J* = 11.1 Hz, 1H), 4.82 (d, *J* = 10.8 Hz, 1H), 4.79 (d, *J* = 12.2 Hz, 1H), 4.65 (d, *J* = 12.2 Hz, 1H), 4.62 – 4.55 (m, 2.5H), 4.52 – 4.44 (m, 1.5H), 4.16 – 4.05 (m, 3H), 3.99 (t, *J* = 9.2 Hz, 1H), 3.84 (t, *J* = 6.9 Hz, 1H), 3.80 – 3.73 (m, 2H), 3.61 (t, *J* = 9.3 Hz, 1H), 3.54 (dd, *J* = 9.6, 3.4 Hz, 1H), 3.37 (s, 3H), 2.09 (s, 3H), 2.04 (d, *J* = 5.1 Hz, 3H), 2.03 (s, 3H).

¹⁹F NMR (376 MHz, CDCl₃) δ -206.10 – -206.37 (m).



A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **33** (74 mg, 0.2 mmol), **6** (46 mg, 0.1 mmol), IBO (18 μ L, 0.2 mmol), and MTBE (200 μ L). The resulting mixture was stirred at 50°C for 48 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography to give **37** (54 mg, 72%) with $\alpha:\beta = 7:1$.

37 α -isomer:

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.46 – 7.13 (m, 15H), 5.51 (dt, $J = 11.8, 9.5$ Hz, 1H), 5.17 (d, $J = 3.7$ Hz, 1H), 4.99 (d, $J = 9.8$ Hz, 1H), 4.98 (d, $J = 11.0$ Hz, 1H), 4.94 (d, $J = 11.4$ Hz, 1H), 4.80 (d, $J = 10.8$ Hz, 1H), 4.79 (d, $J = 12.1$ Hz, 1H), 4.67 (d, $J = 12.1$ Hz, 1H), 4.62 (d, $J = 11.4$ Hz, 1H), 4.59 (d, $J = 3.5$ Hz, 1H), 4.46 (ddd, $J = 49.2, 9.6, 3.8$ Hz, 1H), 4.16 (dd, $J = 12.6, 4.5$ Hz, 1H), 4.06 – 3.94 (m, 3H), 3.86 – 3.70 (m, 3H), 3.58 – 3.46 (m, 2H), 3.38 (s, 3H), 2.06 (s, 3H), 2.03 (s, 3H), 2.02 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 170.52, 169.97, 169.60, 138.61, 138.25, 138.13, 128.43, 128.41, 128.37, 128.02, 128.00, 127.86, 127.71, 127.67, 127.61, 97.89, 95.93 (d, $J = 20.4$ Hz), 87.16 (d, $J = 195.4$ Hz), 82.10, 80.12, 77.56, 75.79, 74.91, 73.40, 70.66 (d, $J = 19.6$ Hz), 70.10, 68.02 (d, $J = 7.1$ Hz), 67.23 (d, $J = 0.8$ Hz), 66.59, 61.64, 55.15, 20.72, 20.67, 20.57.

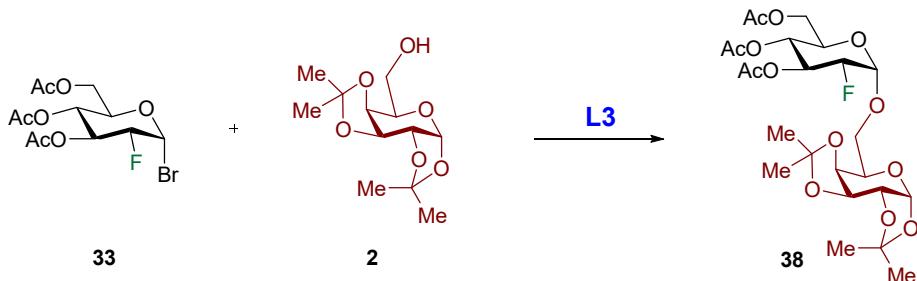
$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -201.15 (dd, $J = 49.2, 12.0$ Hz).

HRMS (ESI): calc. for $\text{C}_{30}\text{H}_{43}\text{O}_8\text{FN} [\text{M} + \text{NH}_4]^+$, 564.2973; found, 564.2978.

37 β -isomer:

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.40 – 7.21 (m, 15H), 5.27 (dt, $J = 14.6, 9.3$ Hz, 1H), 5.02 – 4.95 (m, 2H), 4.91 (d, $J = 11.2$ Hz, 1H), 4.81 (d, $J = 10.8$ Hz, 1H), 4.79 (d, $J = 12.1$ Hz, 1H), 4.65 (d, $J = 12.1$ Hz, 1H), 4.61 – 4.55 (m, 2H), 4.50 – 4.44 (m, 1H), 4.33 (dt, $J = 50.4, 8.6$ Hz, 1H), 4.21 (dd, $J = 12.3, 4.6$ Hz, 1H), 4.13 – 4.06 (m, 2H), 3.99 (t, $J = 9.3$ Hz, 1H), 3.83 – 3.70 (m, 2H), 3.68 – 3.55 (m, 2H), 3.53 (dd, $J = 9.6, 3.5$ Hz, 1H), 3.36 (s, 3H), 2.07 (s, 3H), 2.04 (s, 3H), 2.02 (s, 3H).

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -199.16 (ddd, $J = 50.5, 14.5, 2.6$ Hz).



A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **33** (74 mg, 0.2 mmol), **2** (26 mg, 0.1 mmol), IBO (18 μ L, 0.2 mmol), and MTBE (200 μ L). The resulting mixture was stirred at 50°C for 48 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography to give **38** (37 mg, 67%) with $\alpha:\beta = 10:1$.

38 α -isomer:

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 5.58 – 5.51 (m, 1H), 5.50 (d, $J = 4.9$ Hz, 1H), 5.13 (d, $J = 3.7$ Hz, 1H), 5.03 (t, $J = 9.9$ Hz, 1H), 4.61 (dd, $J = 7.9, 2.3$ Hz, 1H), 4.49 (ddd, $J = 49.2, 9.5, 3.8$ Hz, 1H), 4.34 – 4.24 (m, 3H), 4.20 – 4.14 (m, 1H), 4.08 (dd, $J = 12.4, 1.9$ Hz, 1H), 4.02 (t, $J = 5.7$ Hz, 1H), 3.87 – 3.79 (m, 2H), 2.08 (s, 3H), 2.06 (s, 3H), 2.03 (s, 3H), 1.57 (s, 3H), 1.43 (s, 3H), 1.34 (s, 3H), 1.32 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 170.63, 170.04, 169.65, 109.28, 108.73, 96.51 (d, $J = 20.5$ Hz), 96.21, 87.33 (d, $J = 195.2$ Hz), 70.82 (d, $J = 19.6$ Hz), 70.71, 70.60, 70.55, 68.12, 67.93 (d, $J = 7.2$ Hz), 67.24 (d, $J = 0.9$ Hz), 66.62, 61.70, 26.10, 25.93, 24.94, 24.34, 20.73, 20.70, 20.59.

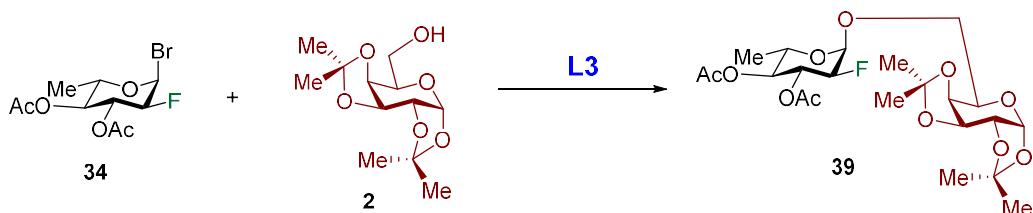
$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -201.41 (dd, $J = 49.3, 12.0$ Hz).

HRMS (ESI): calc. for $\text{C}_{24}\text{H}_{39}\text{O}_{13}\text{FN}$ [$\text{M} + \text{NH}_4$]⁺, 568.2405; found, 568.2400.

38 β -isomer:

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 5.52 (d, $J = 5.0$ Hz, 1H), 5.31 (dt, $J = 14.7, 9.2$ Hz, 1H), 5.02 (t, $J = 9.7$ Hz, 1H), 4.76 (dd, $J = 7.7, 2.5$ Hz, 1H), 4.60 (dd, $J = 7.9, 2.2$ Hz, 1H), 4.33 – 4.28 (m, 1H), 4.31 (dt, $J = 50.4, 8.4$ Hz, 1H), 4.25 (m, 1H), 4.11 (dd, $J = 12.3, 2.0$ Hz, 1H), 4.06 – 3.98 (m, 2H), 3.85 (dd, $J = 12.6, 7.9$ Hz, 1H), 3.71 (ddd, $J = 10.0, 4.6, 2.2$ Hz, 1H), 3.65 (d, $J = 6.7$ Hz, 1H), 2.08 (s, 3H), 2.07 (s, 3H), 2.02 (s, 3H), 1.53 (s, 3H), 1.44 (s, 3H), 1.33 (s, 6H).

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -199.39 (ddd, $J = 50.6, 14.7, 2.4$ Hz).



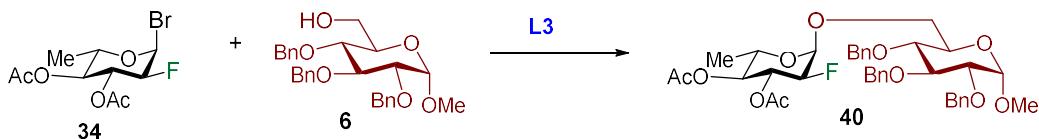
A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **34** (37 mg, 0.1 mmol), **2** (78 mg, 0.3 mmol), IBO (18 μ L, 0.2 mmol), and MTBE (200 μ L). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography to give **39** (37 mg, 76%) with $\alpha:\beta = 11:1$.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 5.51 (d, $J = 4.8$ Hz, 1H), 5.47 (dt, $J = 11.6, 9.6$ Hz, 1H), 5.12 (d, $J = 3.7$ Hz, 1H), 4.72 (t, $J = 9.7$ Hz, 1H), 4.63 (dd, $J = 7.9, 2.1$ Hz, 1H), 4.46 (ddd, $J = 49.4, 9.6, 3.8$ Hz, 1H), 4.35 – 4.28 (m, 2H), 4.13 – 4.01 (m, 2H), 3.90 (dd, $J = 9.8, 7.3$ Hz, 1H), 3.67 (dd, $J = 9.9, 6.0$ Hz, 1H), 2.05 (s, 3H), 2.03 (s, 3H), 1.54 (s, 3H), 1.44 (s, 3H), 1.34 (d, $J = 3.9$ Hz, 3H), 1.33 (s, 3H), 1.15 (d, $J = 6.3$ Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 170.15, 169.88, 109.11, 108.71, 96.14, 95.38 (d, *J* = 20.0 Hz), 87.63 (d, *J* = 195.1 Hz), 73.41 (d, *J* = 6.9 Hz), 70.77, 70.75 (d, *J* = 19.2 Hz), 70.57, 70.52, 66.51, 65.63, 65.09 (d, *J* = 1.1 Hz), 26.04, 25.96, 24.91, 24.37, 20.79, 20.68, 16.94.

¹⁹F NMR (376 MHz, cdcl₃) δ -201.45 (dd, *J* = 49.4, 12.0 Hz).

HRMS (ESI): calc. for C₂₂H₃₇O₁₁FN [M + NH₄]⁺, 510.2351; found, 510.2345.



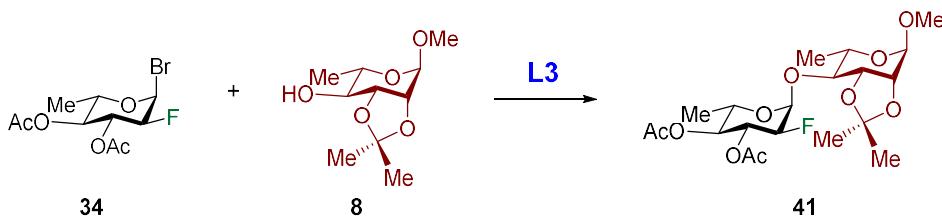
A 10 mL oven-dried Schlenk flask was charged with **L3** (5.3 mg, 0.015 mmol), **34** (41 mg, 0.1 mmol), **6** (139 mg, 0.3 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 24 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography to give **40** (67 mg, 85%) with α:β = 8:1.

¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.23 (m, 15H), 5.50 (dt, *J* = 12.0, 9.5 Hz, 1H), 4.98 (d, *J* = 10.9 Hz, 1H), 4.95 (d, *J* = 3.8 Hz, 1H), 4.91 (d, *J* = 11.2 Hz, 1H), 4.81 (d, *J* = 11.7 Hz, 2H), 4.73 (d, *J* = 9.7 Hz, 1H), 4.68 (d, *J* = 11.9 Hz, 1H), 4.58 (dd, *J* = 9.4, 3.5 Hz, 2H), 4.44 (ddd, *J* = 49.4, 9.6, 3.9 Hz, 1H), 3.99 (t, *J* = 9.3 Hz, 1H), 3.92 (dd, *J* = 9.9, 6.3 Hz, 1H), 3.87 (d, *J* = 10.9 Hz, 1H), 3.79 (dd, *J* = 10.1, 3.9 Hz, 1H), 3.64 (dd, *J* = 10.9, 4.9 Hz, 1H), 3.57 (dd, *J* = 5.7, 3.8 Hz, 1H), 3.54 (d, *J* = 10.0 Hz, 1H), 3.37 (s, 3H), 2.05 (s, 3H), 2.04 (s, 3H), 1.13 (d, *J* = 6.3 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 170.07, 169.92, 138.71, 138.41, 138.23, 128.43, 128.38, 128.35, 128.08, 127.94, 127.85, 127.72, 127.64, 127.55, 98.03, 96.24 (d, *J* = 20.1 Hz), 87.65 (d, *J* = 195.1 Hz), 82.13, 80.19, 77.61, 75.75, 74.95, 73.50, 73.43 (d, *J* = 7.2 Hz), 70.75 (d, *J* = 19.4 Hz), 69.91, 67.20, 65.05, 55.13, 20.76, 20.70, 17.06.

¹⁹F NMR (376 MHz, CDCl₃) δ -200.82 (dd, *J* = 49.4, 12.1 Hz).

HRMS (ESI): calc. for C₃₈H₄₉O₁₁FN [M + NH₄]⁺, 714.3290; found, 714.3284.



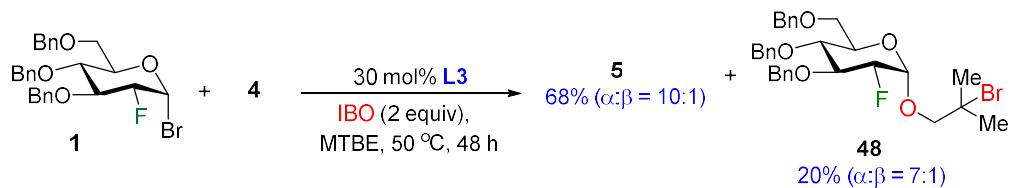
A 10 mL oven-dried Schlenk flask was charged with **L3** (10.5 mg, 0.03 mmol), **34** (31 mg, 0.1 mmol), **8** (66 mg, 0.3 mmol), IBO (18 μL, 0.2 mmol), and MTBE (200 μL). The resulting mixture was stirred at 50°C for 48 h. The reaction mixture concentrated *in vacuo* and purified by silica gel column chromatography to give **41** (23 mg, 52%) with α:β > 20:1.

¹H NMR (400 MHz, CDCl₃) δ 5.66 (d, *J* = 3.7 Hz, 1H), 5.42 (dd, *J* = 20.4, 10.4 Hz, 1H), 4.86 (s, 1H), 4.73 (t, *J* = 9.7 Hz, 1H), 4.46 (ddd, *J* = 49.4, 9.7, 4.0 Hz, 1H), 4.25 (t, *J* = 6.3 Hz, 1H), 4.09 (d, *J* = 5.6 Hz, 1H), 3.93 (td, *J* = 12.4, 6.1 Hz, 1H), 3.75 (td, *J* = 12.3, 6.1 Hz, 1H), 3.53 (dd, *J* = 9.3, 7.8 Hz, 1H), 3.38 (s, 3H), 2.06 (s, 3H), 2.04 (s, 3H), 1.53 (s, 3H), 1.33 (s, 3H), 1.33 (s, 3H), 1.17 (d, *J* = 6.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 170.07, 169.86, 109.40, 97.96, 93.90 (d, *J* = 20.2 Hz), 87.39 (d, *J* = 195.0 Hz), 78.31, 78.13, 75.96, 73.28 (d, *J* = 7.0 Hz), 70.48 (d, *J* = 19.2 Hz), 65.51, 63.46, 54.80, 27.90, 26.25, 20.72 (d, *J* = 8.1 Hz), 18.19, 17.07.

¹⁹F NMR (376 MHz, CDCl₃) δ -201.34 (dd, *J* = 49.4, 11.6 Hz).

HRMS (ESI): calc. for C₂₀H₃₅O₁₀FN [M + NH₄]⁺, 468.2245; found, 468.2240.



¹H NMR (400 MHz, CDCl₃) δ 7.42 – 7.10 (m, 19H), 5.29 (d, *J* = 3.9 Hz, 1H), 5.08 (d, *J* = 3.8 Hz, 0.2H), 4.90 (dd, *J* = 11.1, 5.9 Hz, 1.3H), 4.83 (d, *J* = 10.7 Hz, 1.5H), 4.76 (d, *J* = 11.0 Hz, 1.5H), 4.64 (d, *J* = 12.1 Hz, 1.6H), 4.54 (dd, *J* = 9.3, 4.0 Hz, 0.8H), 4.46 (dd, *J* = 11.4, 7.0 Hz, 2.8H), 4.42 (dd, *J* = 9.4, 4.0 Hz, 0.6H), 4.16 – 4.01 (m, 2.3H), 3.88 (d, *J* = 10.2 Hz, 0.5H), 3.76 (dt, *J* = 8.5, 4.3 Hz, 1.7H), 3.66 (ddd, *J* = 19.8, 14.1, 10.9 Hz, 2.7H), 3.57 (d, *J* = 10.1 Hz, 0.3H), 3.50 – 3.38 (m, 2H), 1.78 (d, *J* = 4.1 Hz, 0.9H), 1.41 (d, *J* = 7.6 Hz, 5.4H).

¹³C NMR (101 MHz, CDCl₃) δ 138.49, 138.10, 137.88, 128.36, 128.35, 127.93, 127.91, 127.85, 127.72, 127.68, 127.65, 91.41 (d, *J* = 40.1 Hz), 90.35 (d, *J* = 131.2 Hz), 80.64 (d, *J* = 16.0 Hz), 76.87 (d, *J* = 8.3 Hz), 76.54, 75.16, 75.04 (d, *J* = 2.8 Hz), 73.48, 70.33, 68.27, 41.85, 25.17, 24.83.

¹⁹F NMR (376 MHz, CDCl₃) α -isomer: δ -197.14 (dd, *J* = 50.2, 11.7 Hz), **β -isomer:** -199.12 (dd, *J* = 49.3, 12.2 Hz).

HRMS (ESI): calc. for C₃₁H₄₀O₅BrFN [M + NH₄]⁺, 604.2074; found, 604.2068.

5. DFT Calculations

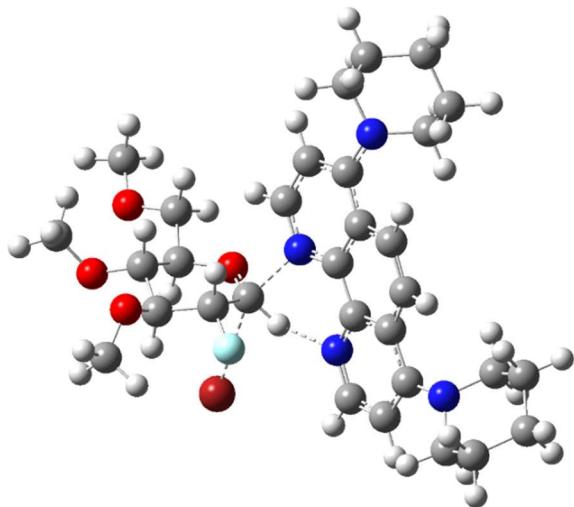
Cartesian coordinates for the reactants, intermediates, products and transition structures are collected in Section 8. Total energies, relative energies and selected geometrical parameters are also available in the accompanying spreadsheet. Three dimensional structures for the coupling of methanol with glycosyl bromide (reactant) to form α -1,2-*cis* glycoside (product) using catalyst **L3** are given below. Structures for the other reactions can be generated from the Cartesian coordinates in Section 8.

Color Assignment to Each Atom in the Structures of TS1, TS2, and Int1 for Catalyst L3

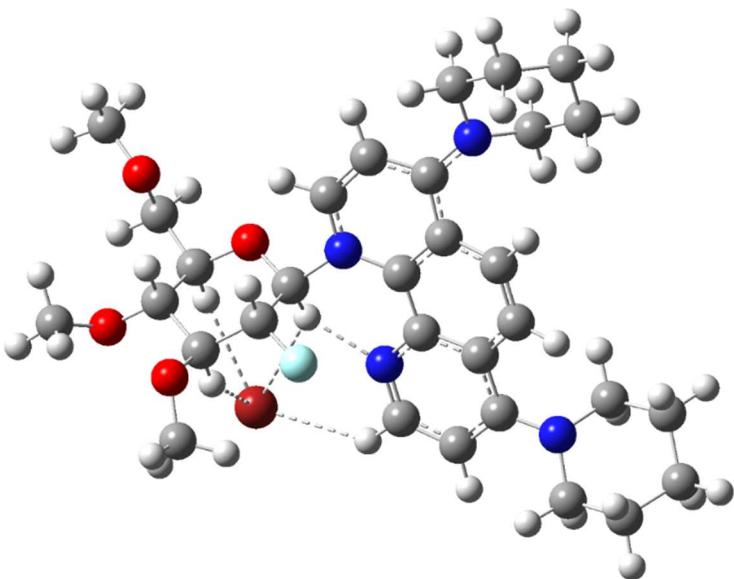
White = hydrogen; Gray = Carbon, **Blue** = Nitrogen, **Red** = Oxygen

Light Blue = Fluoride, **Marron** = Bromide

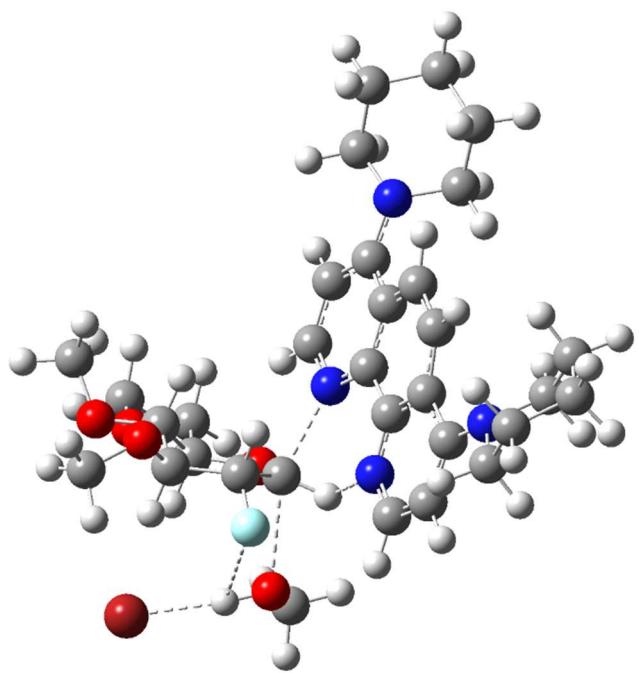
TS1 for L3



Int1 for L3



TS2 for L3



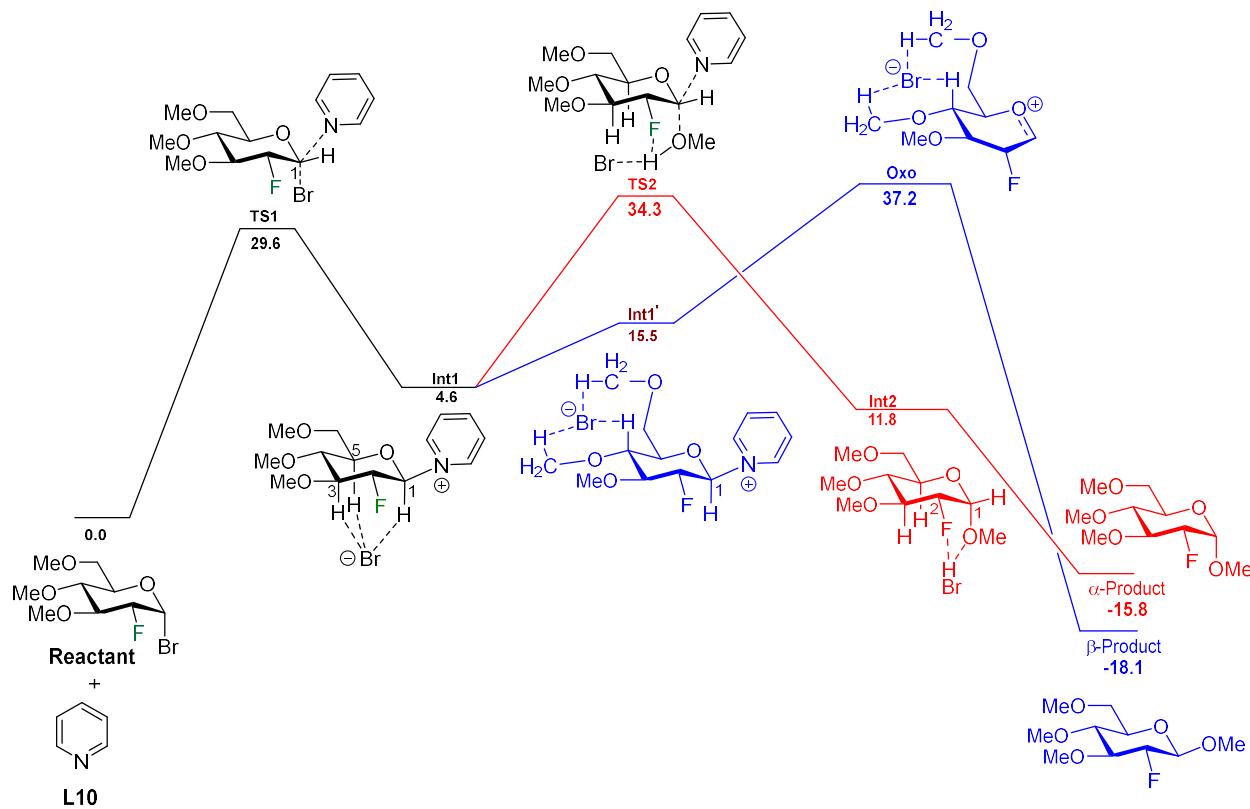
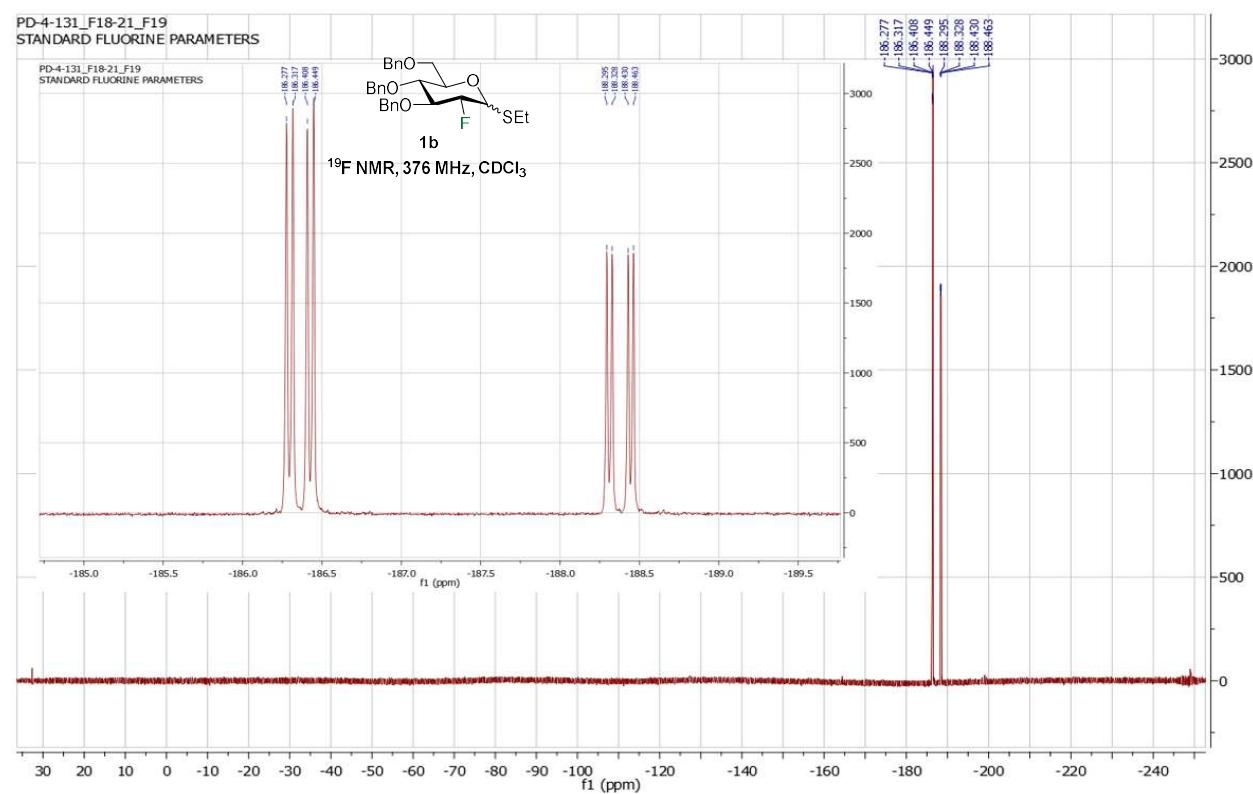
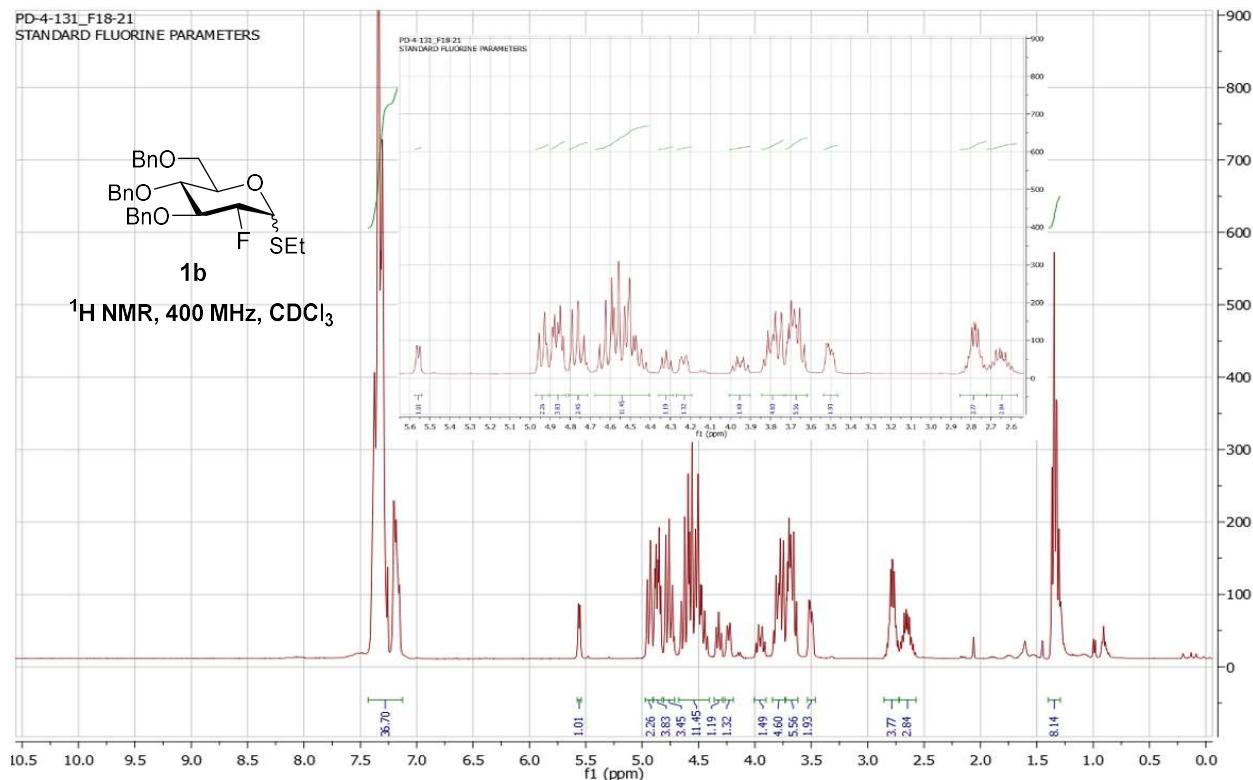


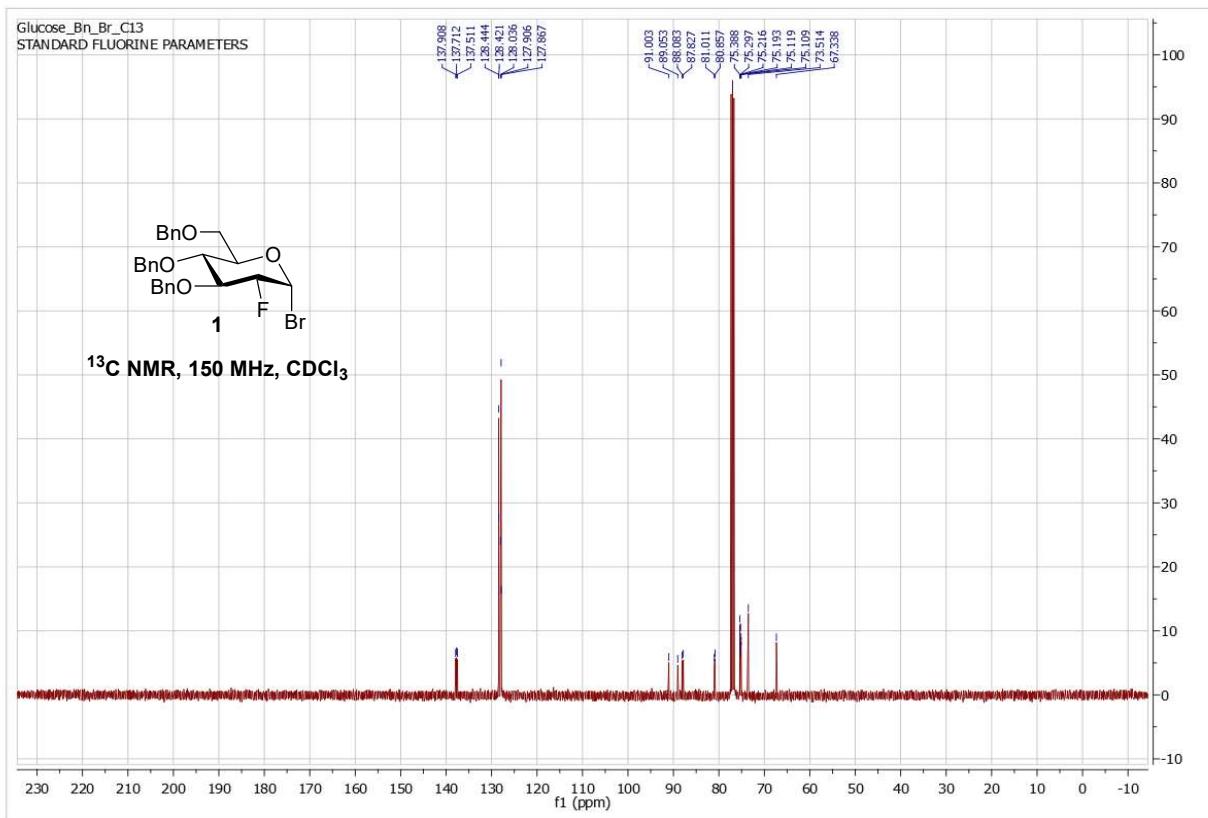
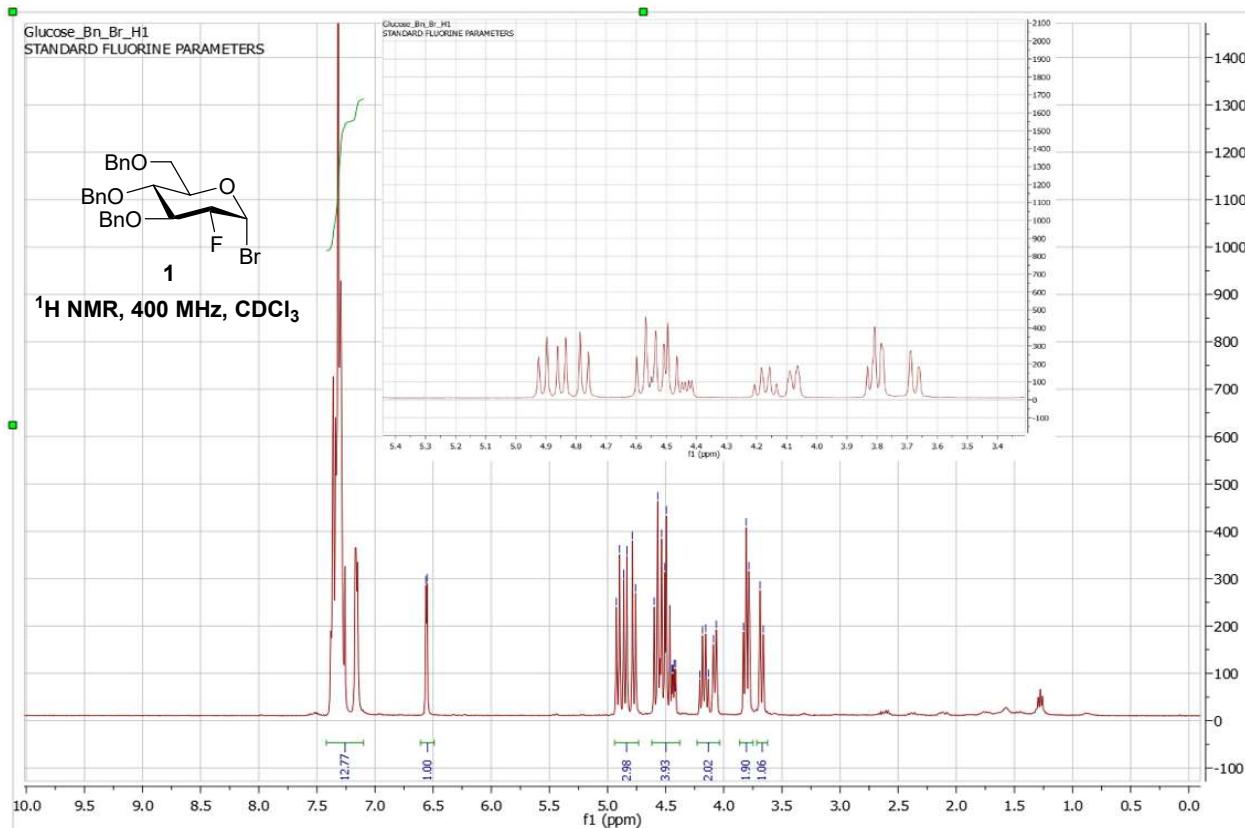
Figure S1. Reaction coordinate diagrams showing the diverging pathways for formation of α - (red) and β - (blue) glycosylation product using pyridine **L10**.

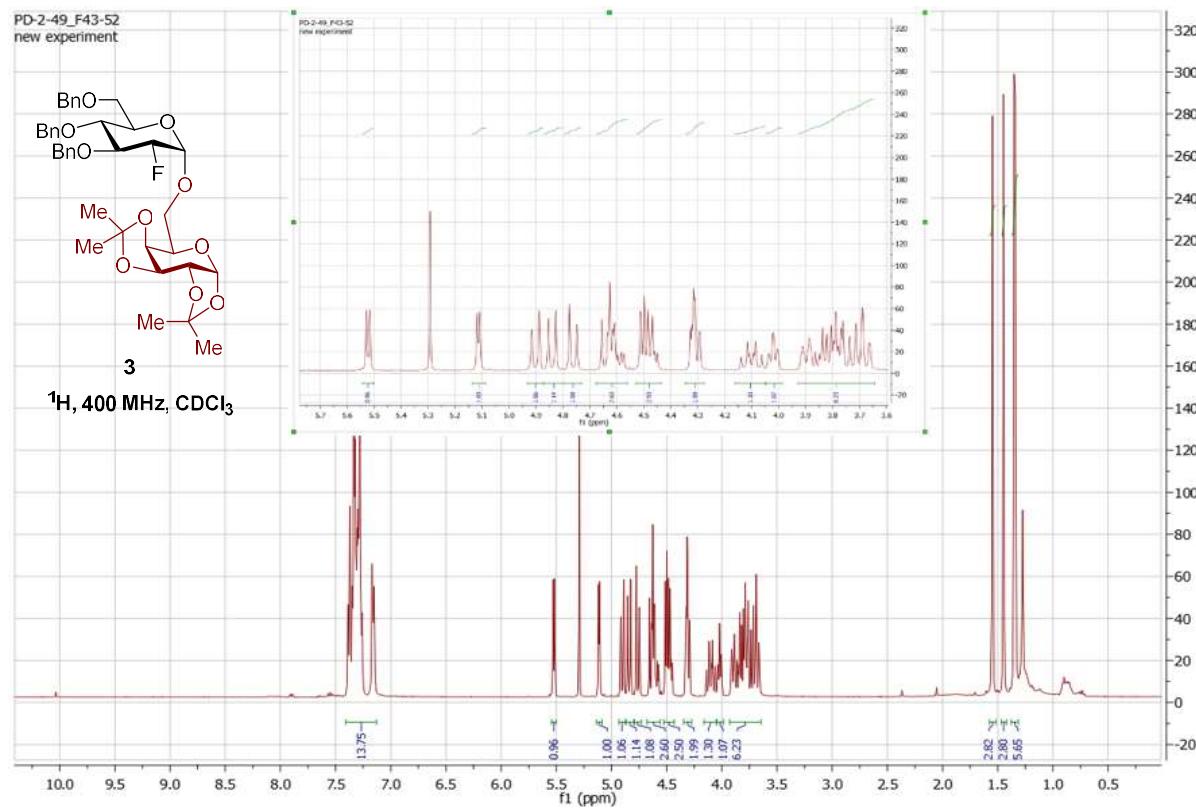
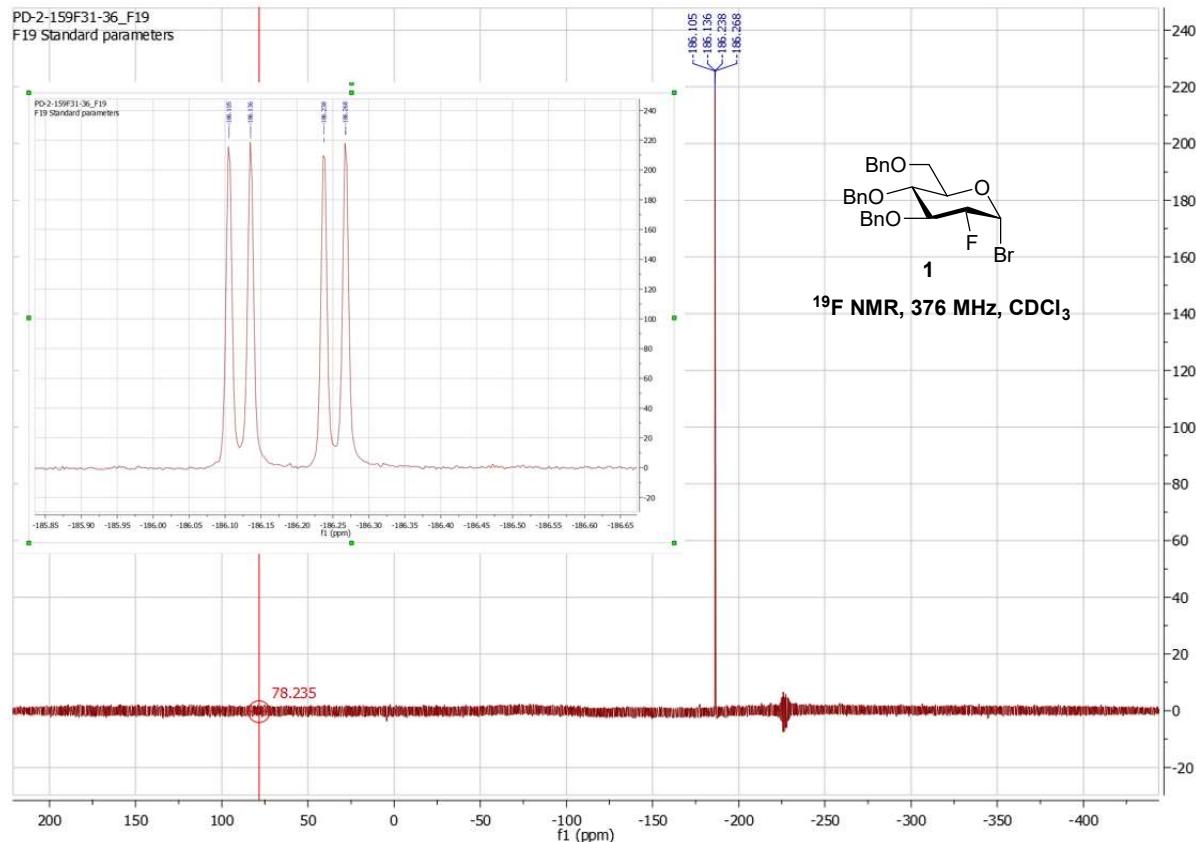
6. References

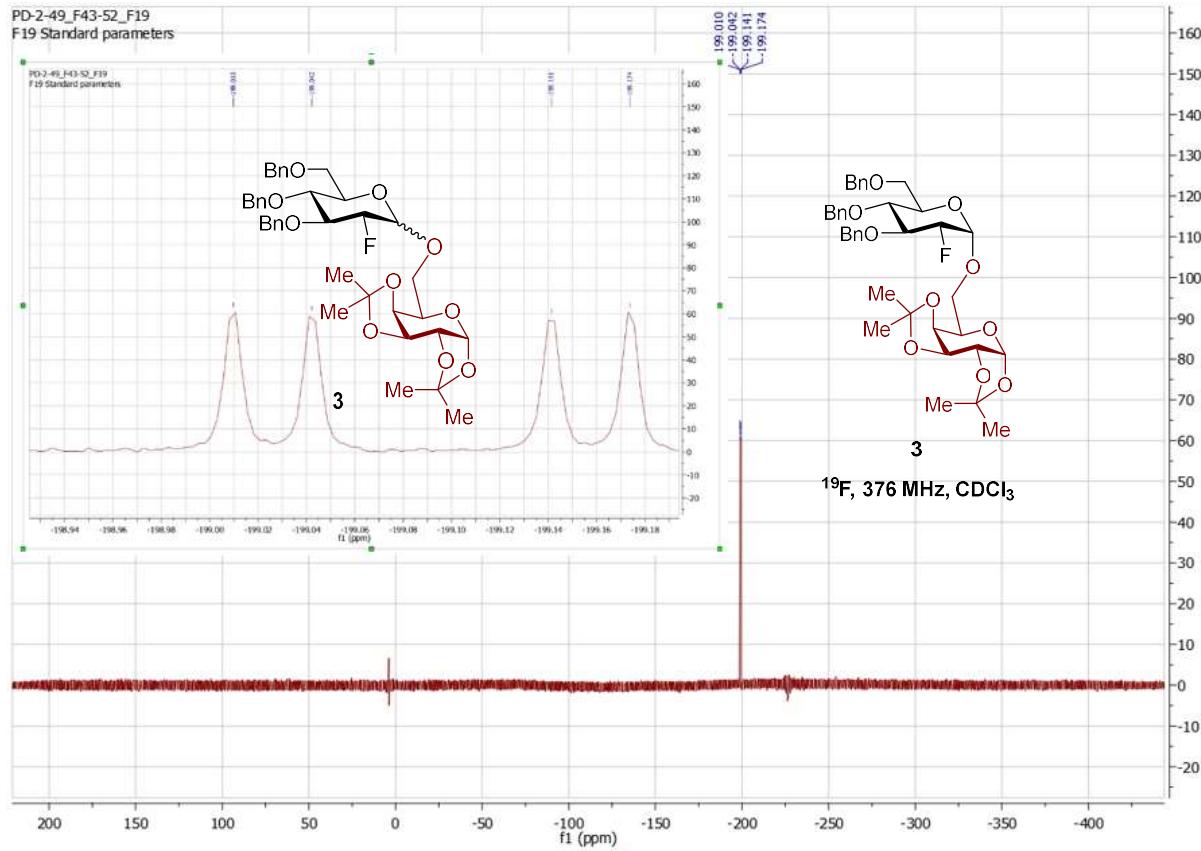
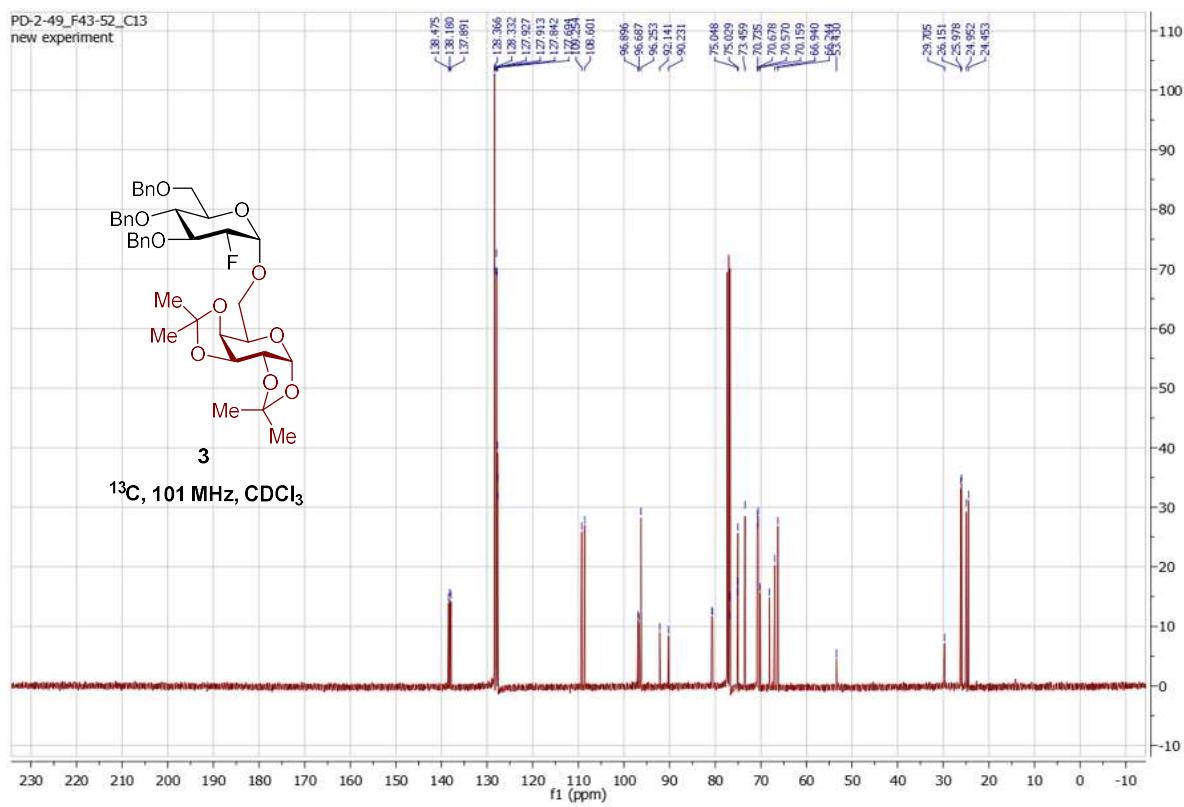
- El-Atawy, M. A.; Ferretti, F.; Ragagni, F. Palladium-catalyzed intramolecular cyclization of nitroalkenes: Synthesis of thienopyrroles. *Eur. J. Org. Chem.* **2017**, 1902-1910.
- Larsen, M. A.; Oeschger, R. J.; Hartwig, J. F. Effect of ligand structure on the electron density and activity of iridium catalysts for the borylation of alkanes. *ACS Catal.* **2020**, 10, 3415-3424.

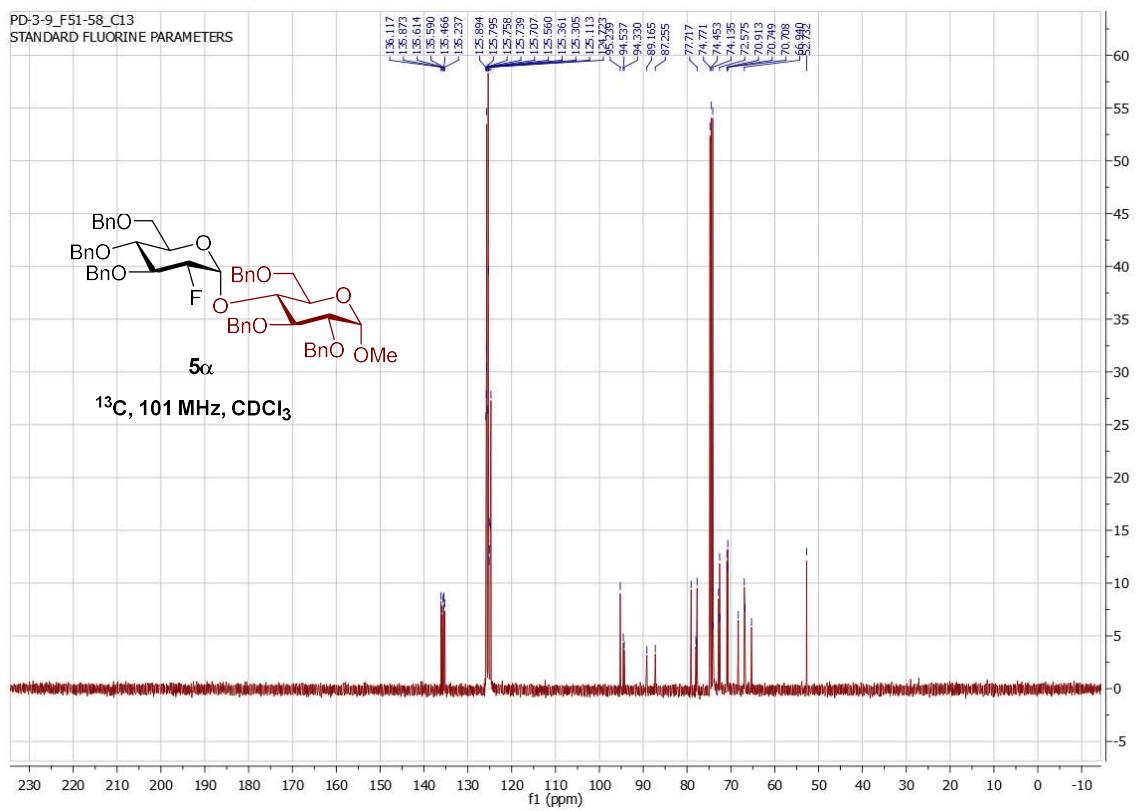
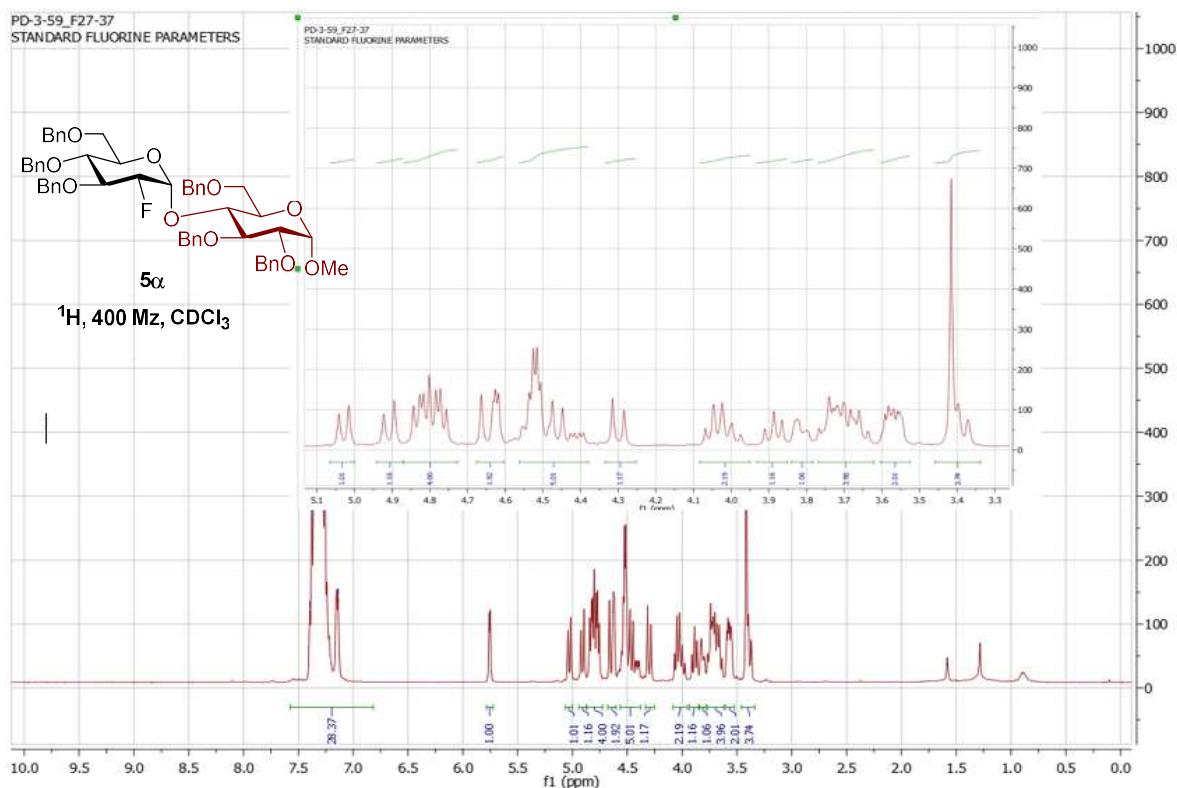
7. Spectral Data

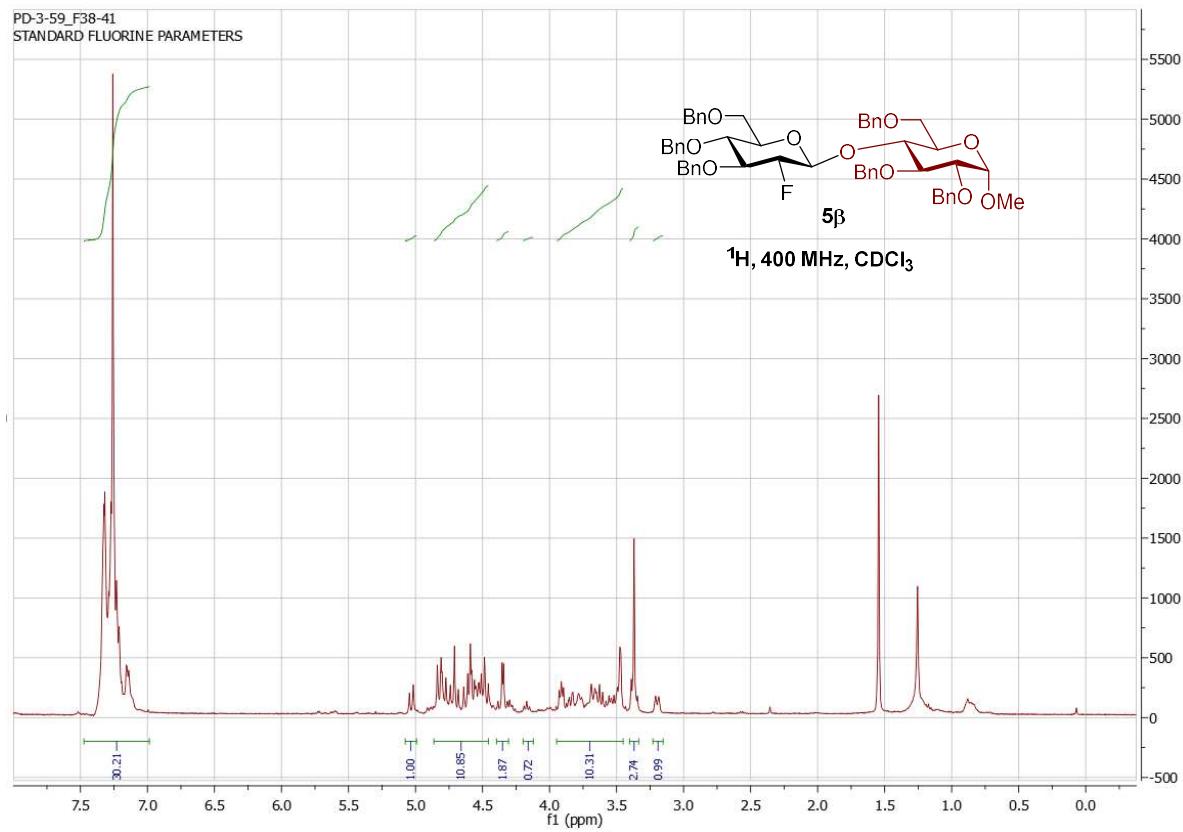
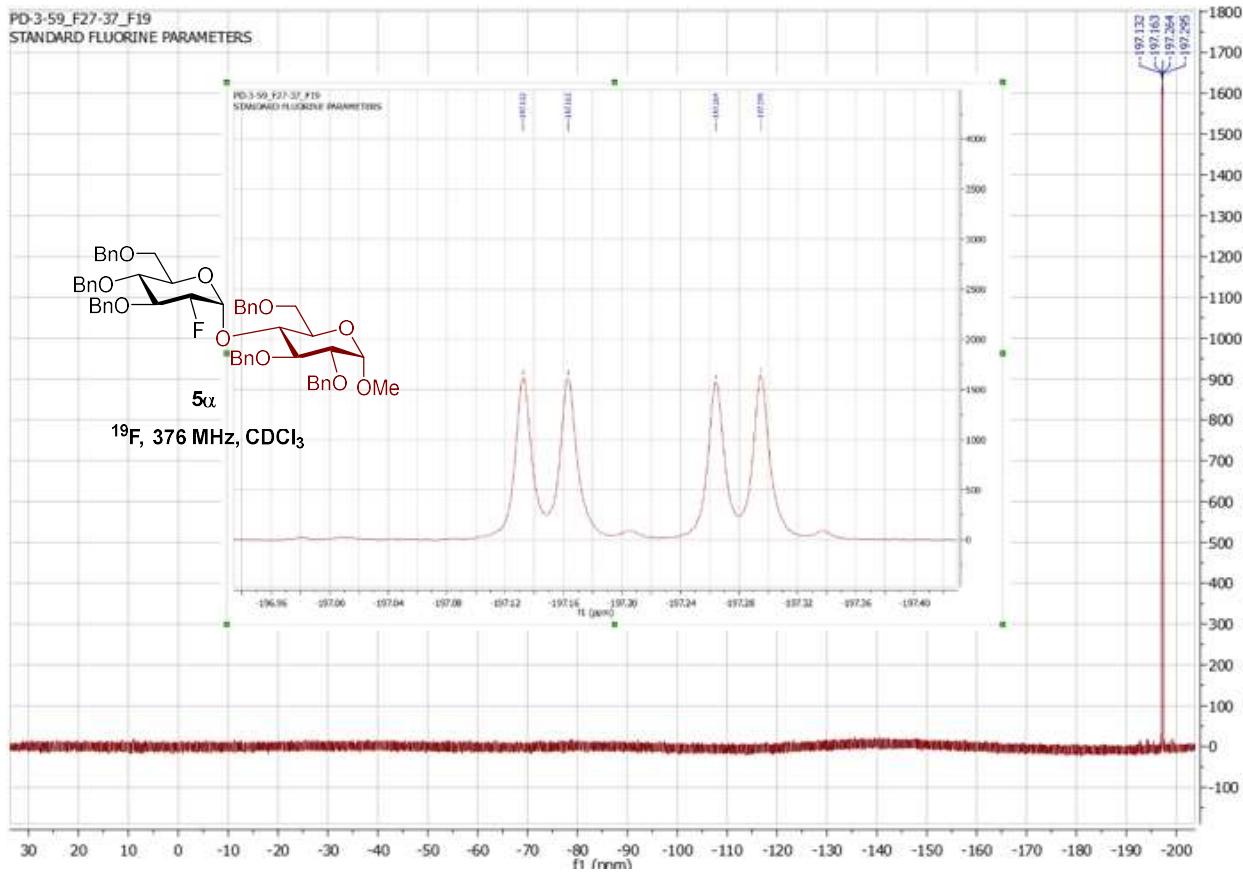


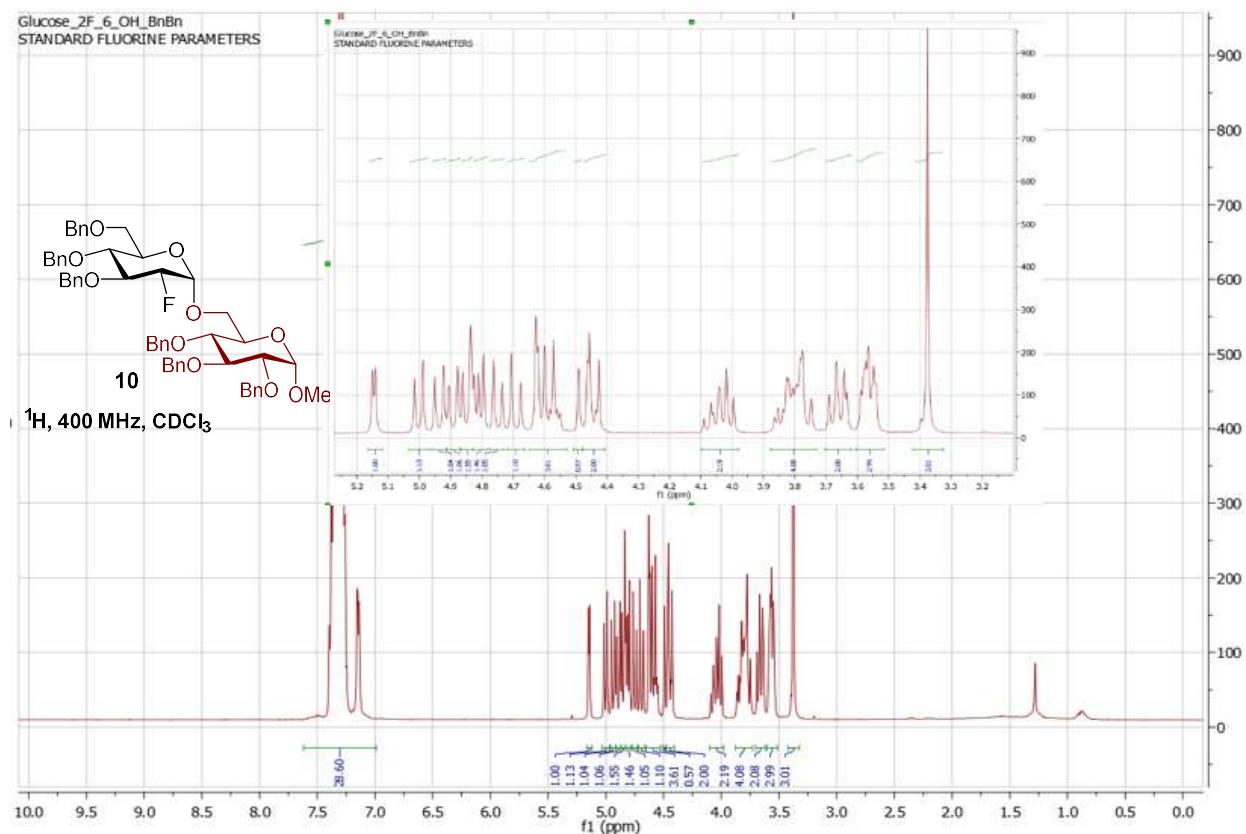
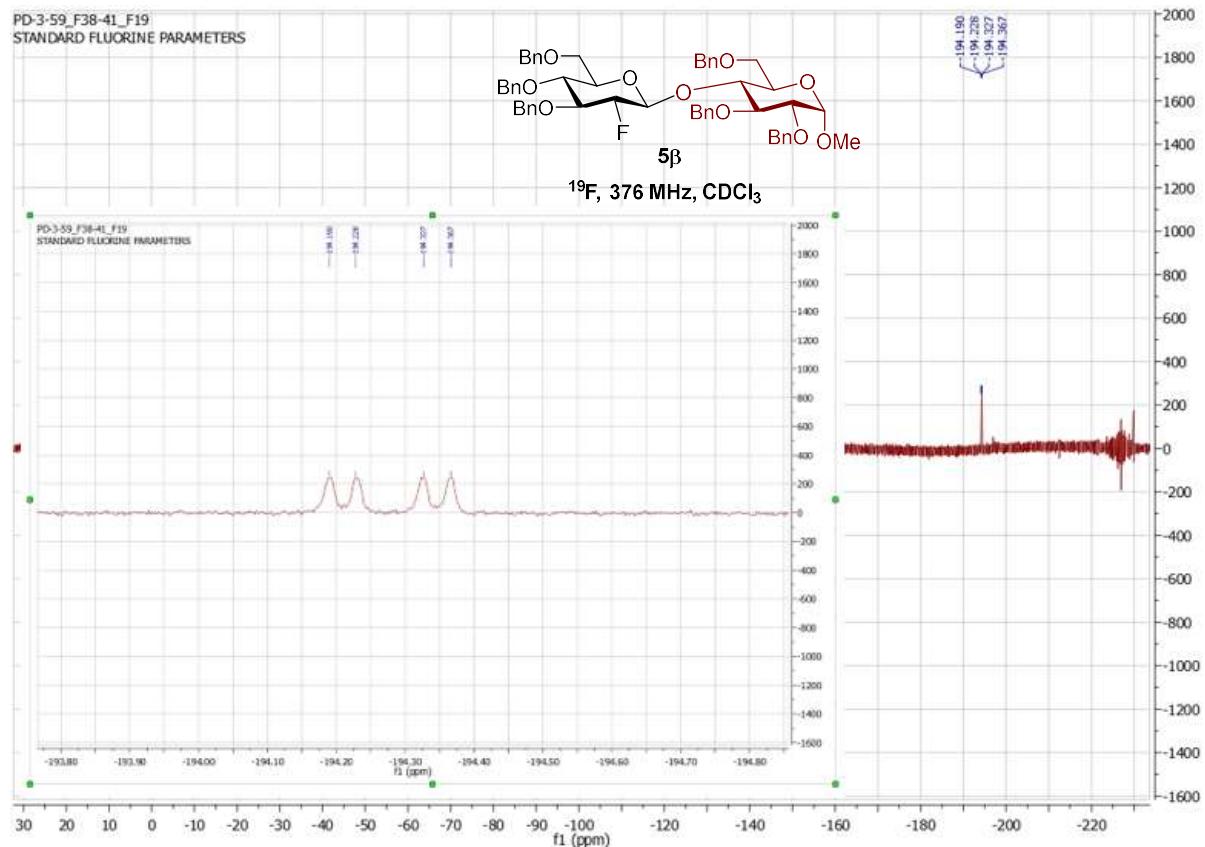


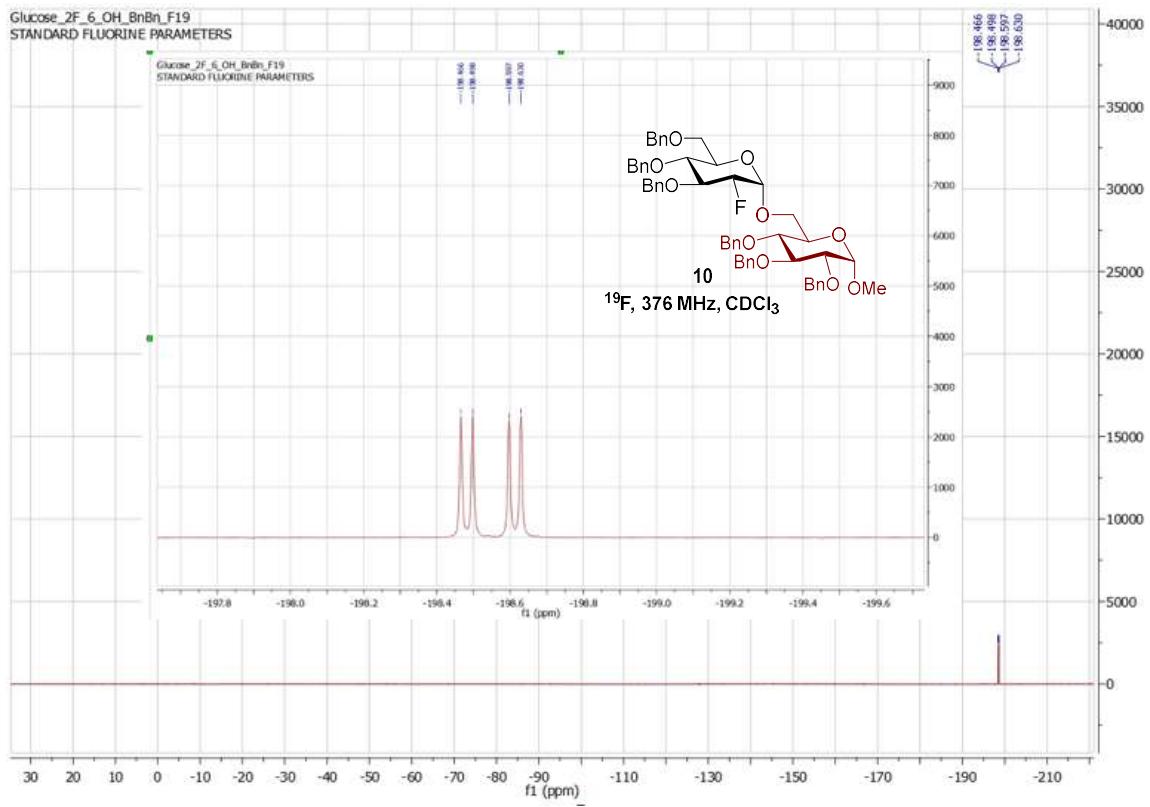
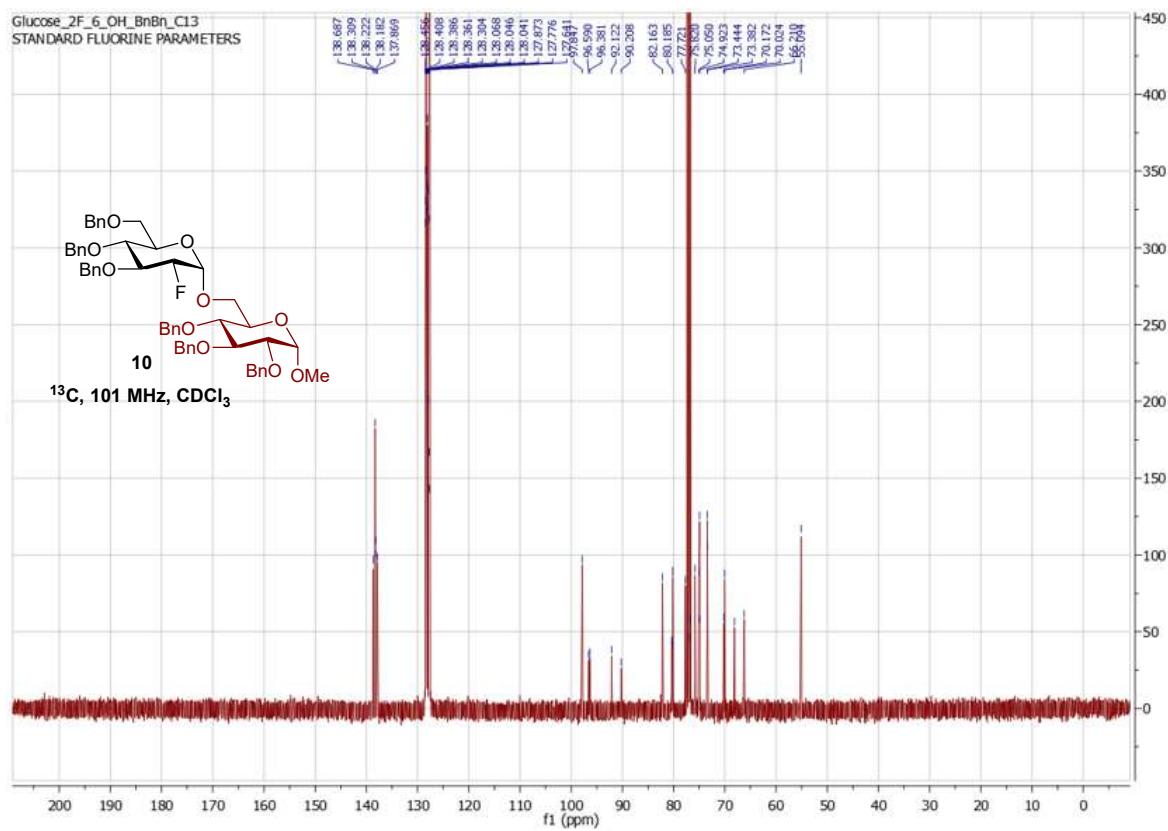


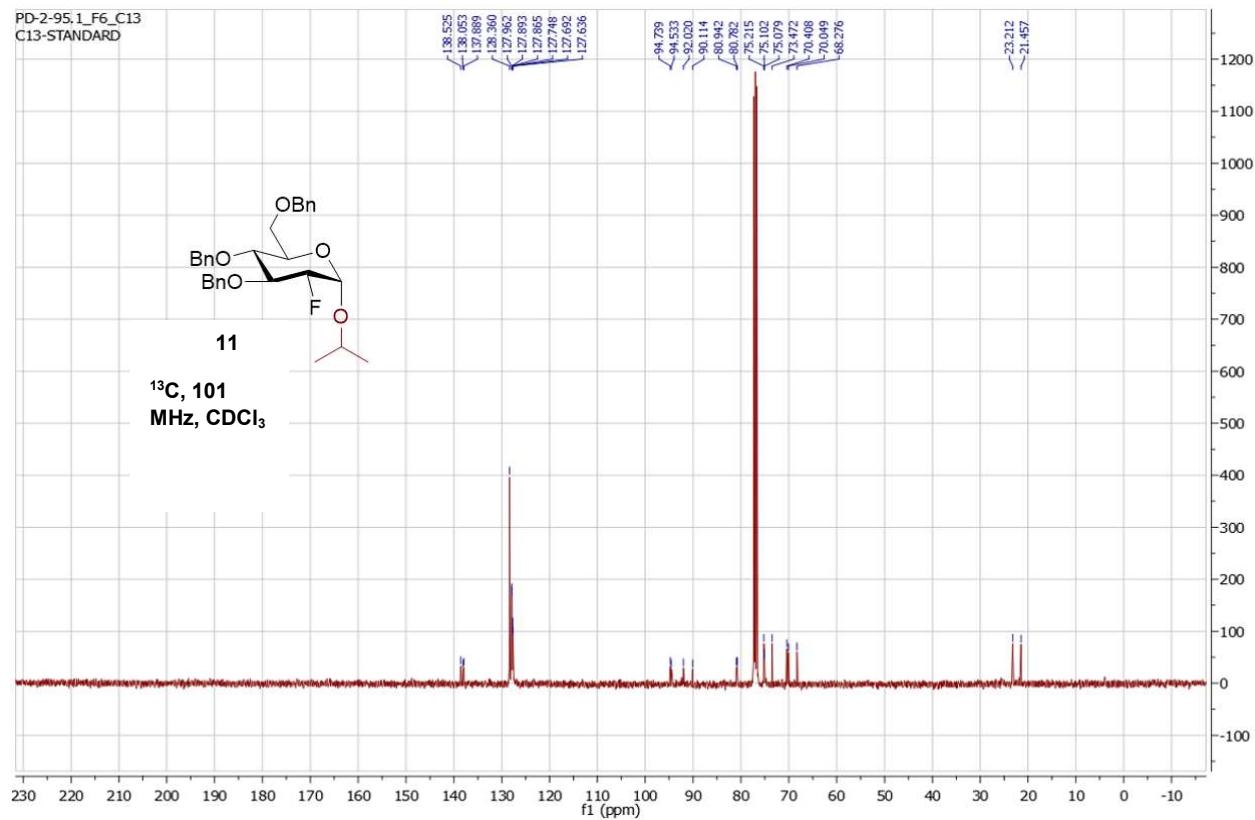
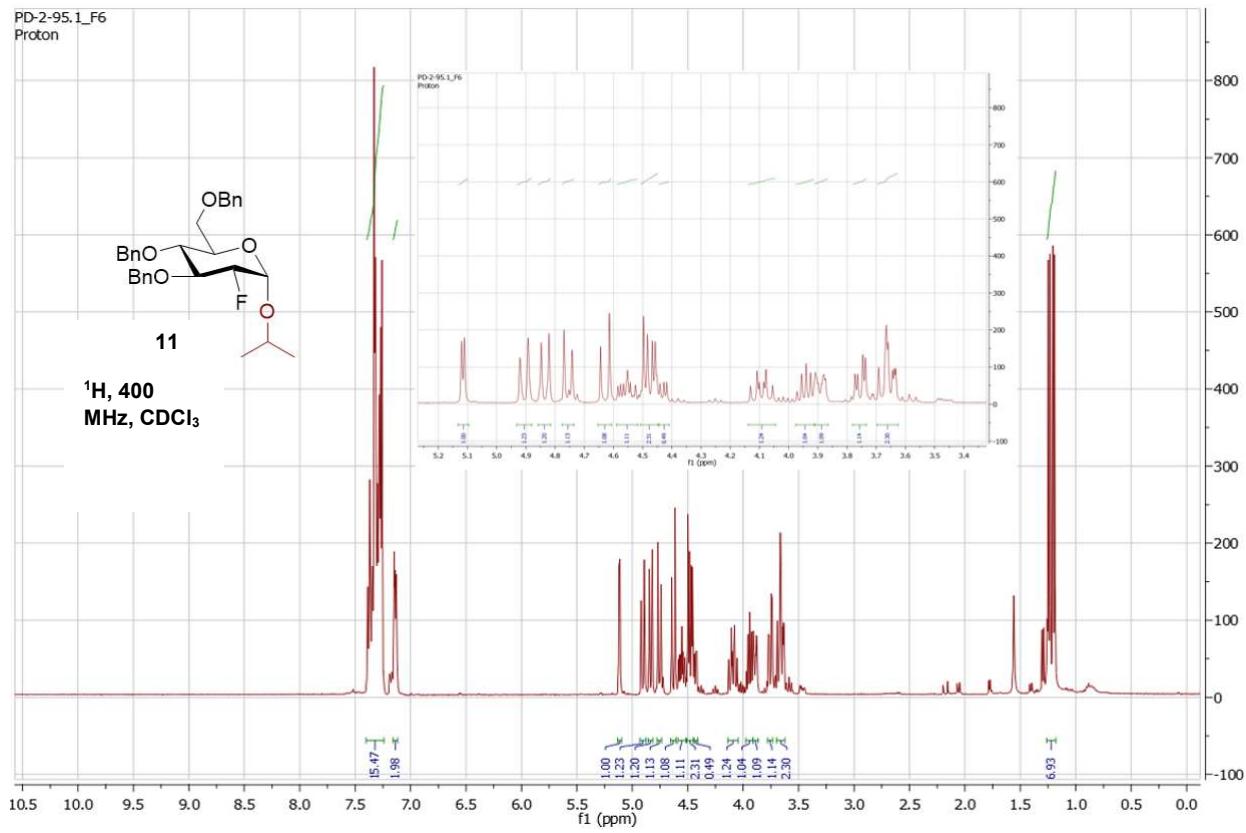


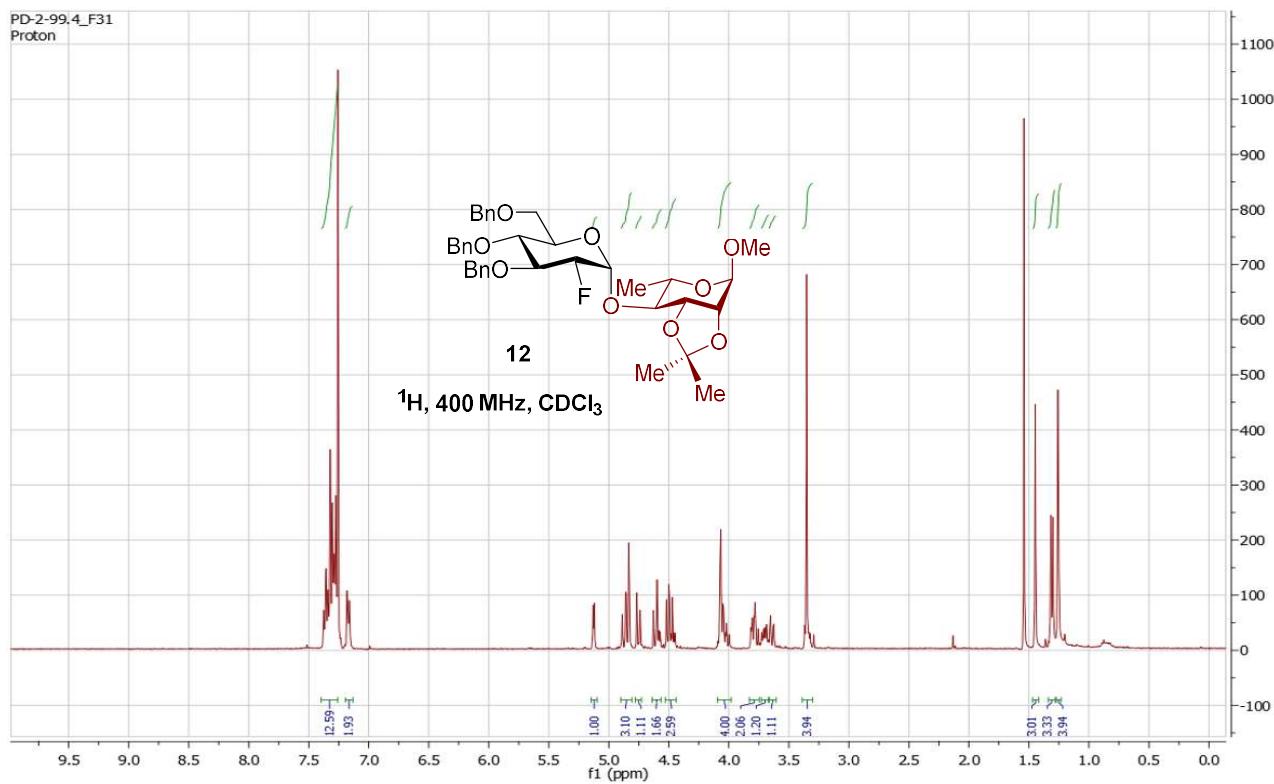
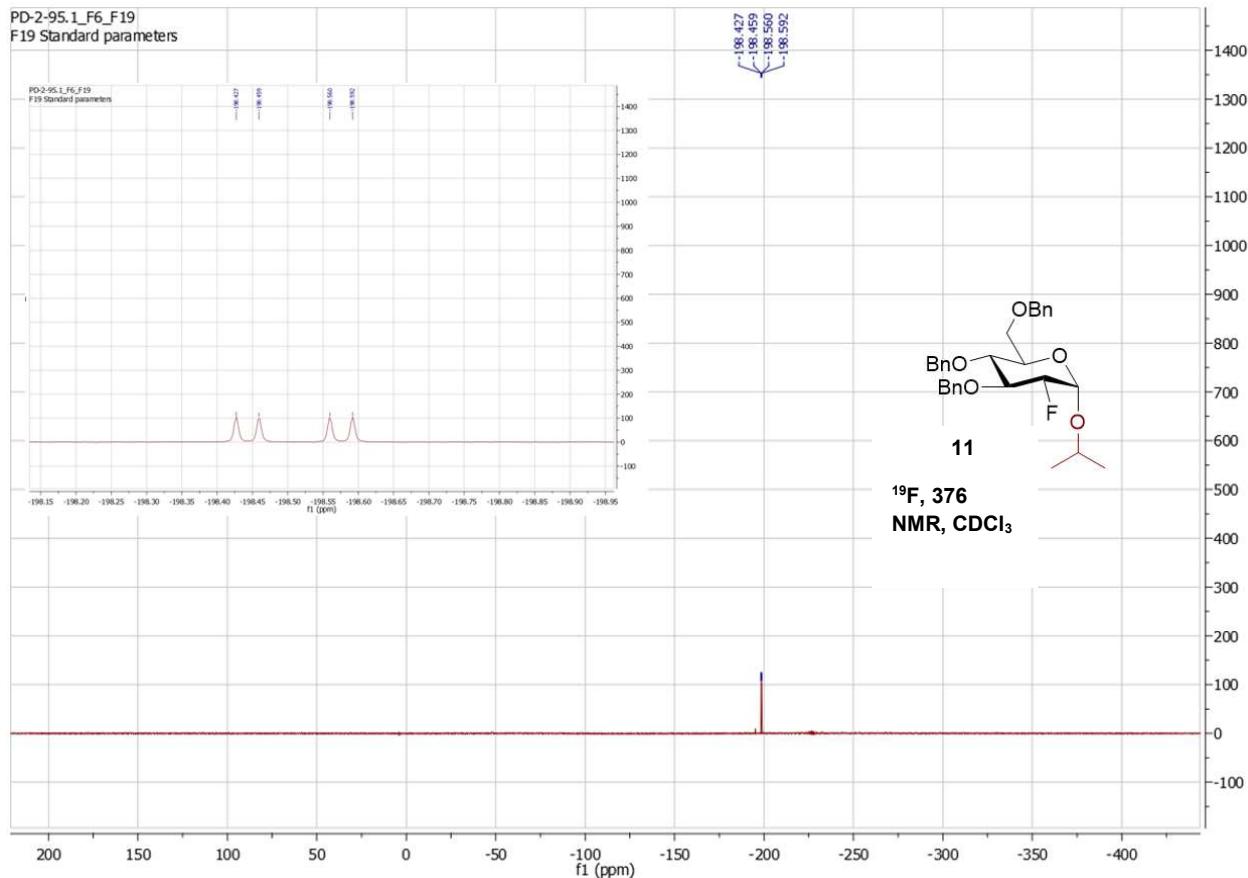




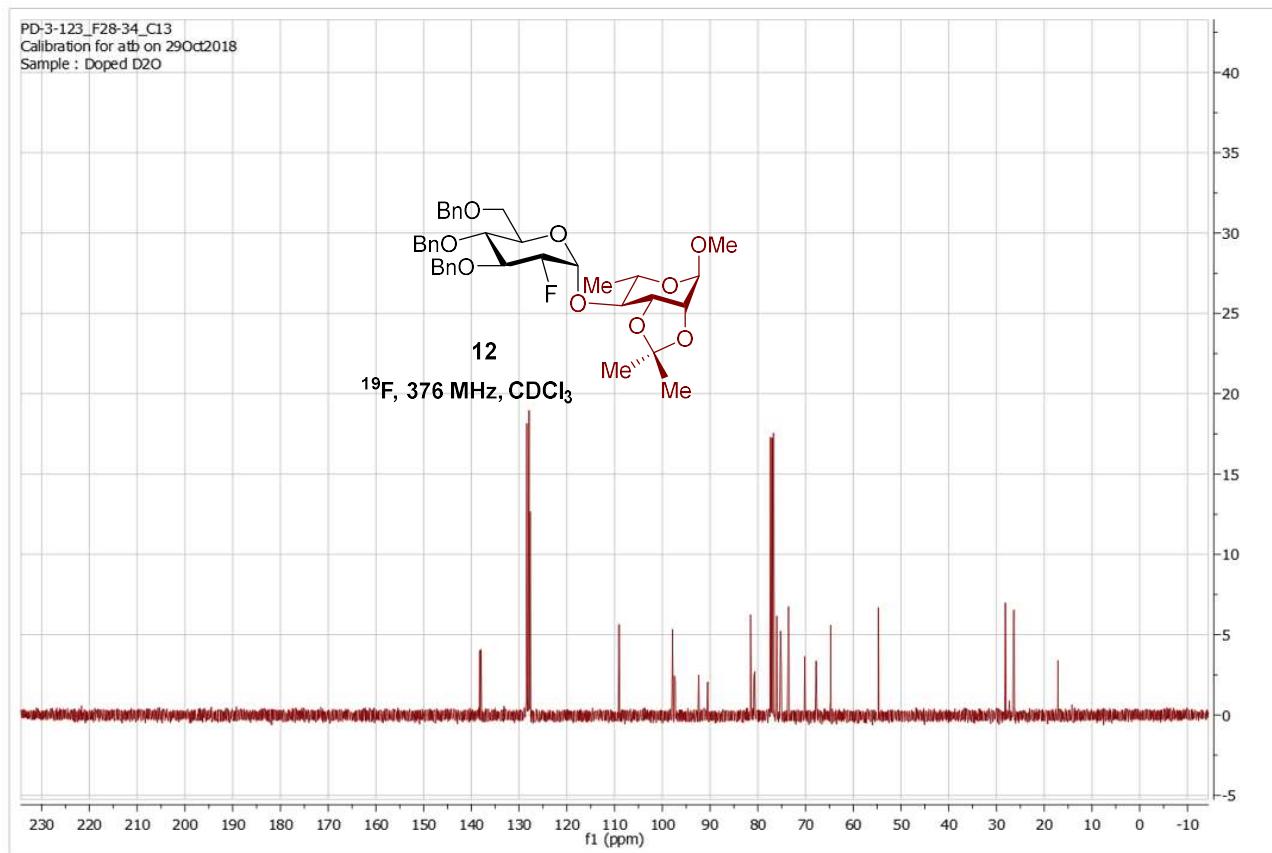






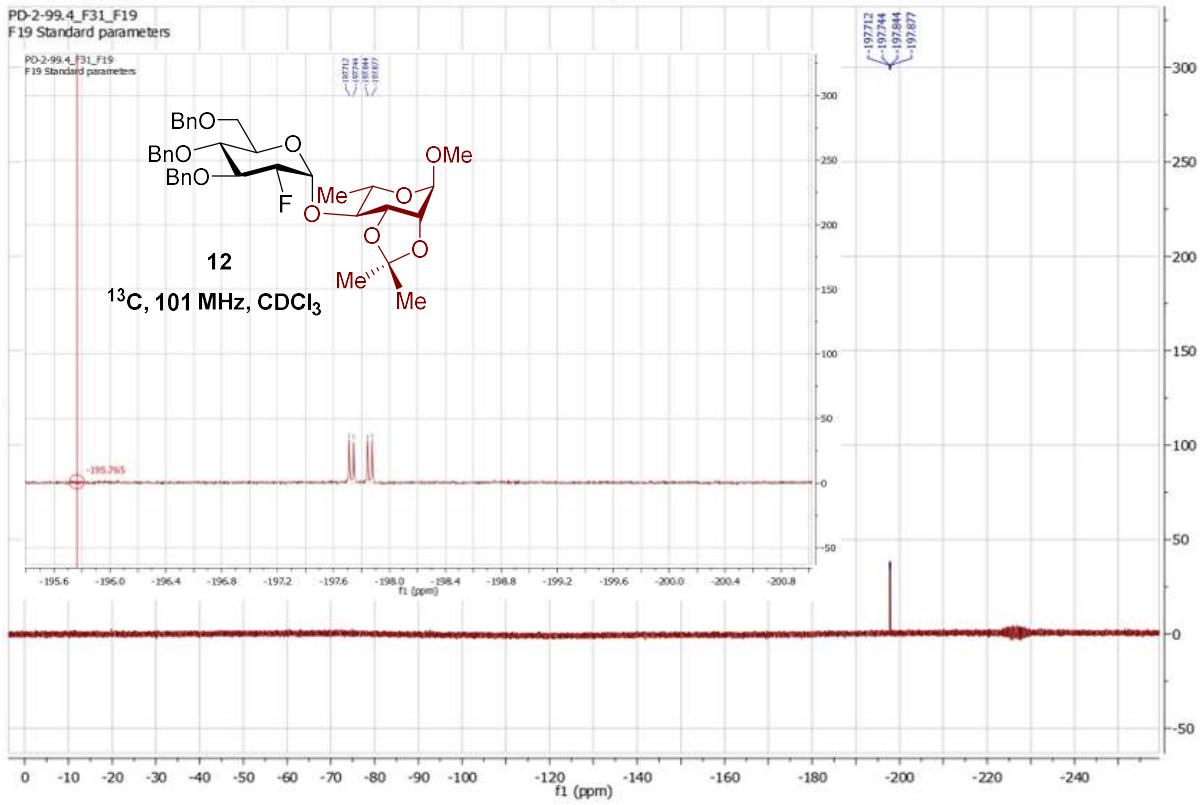
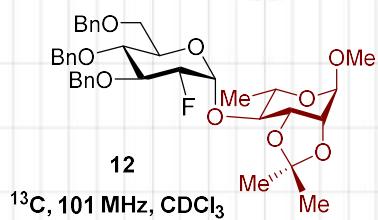


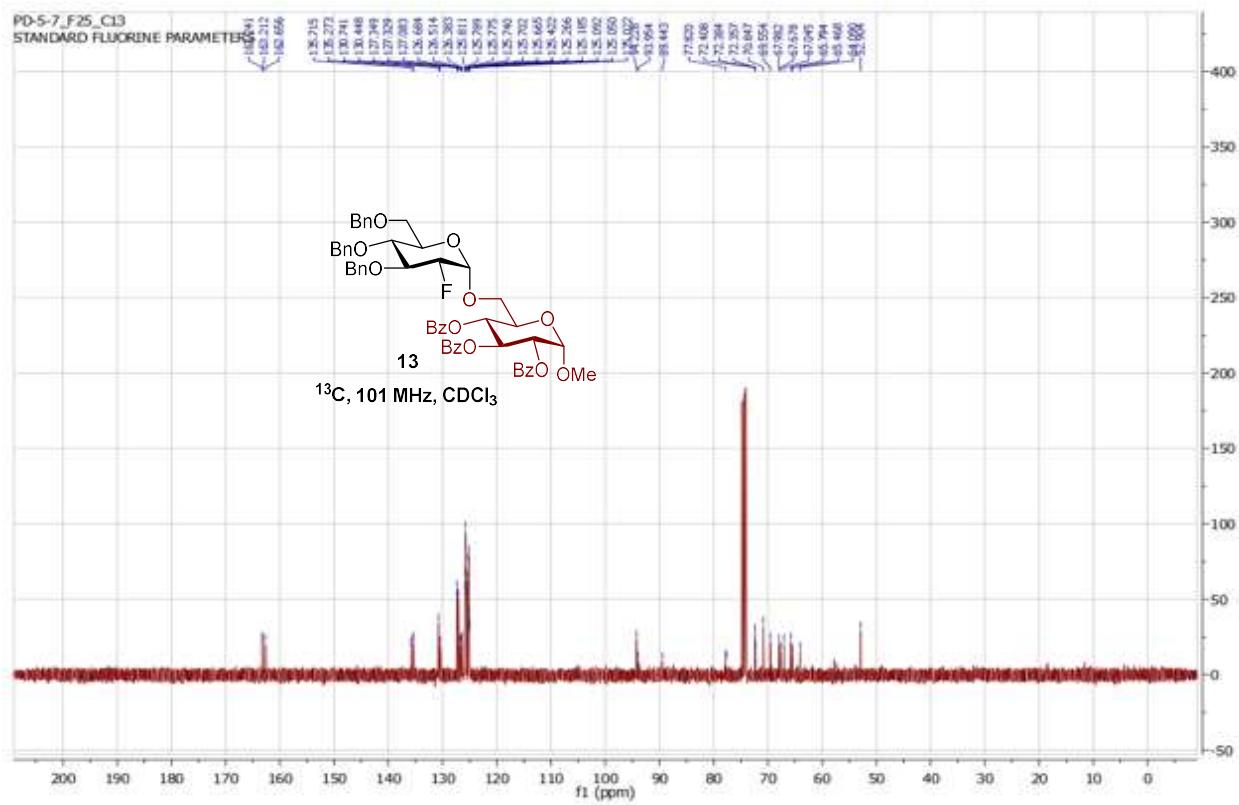
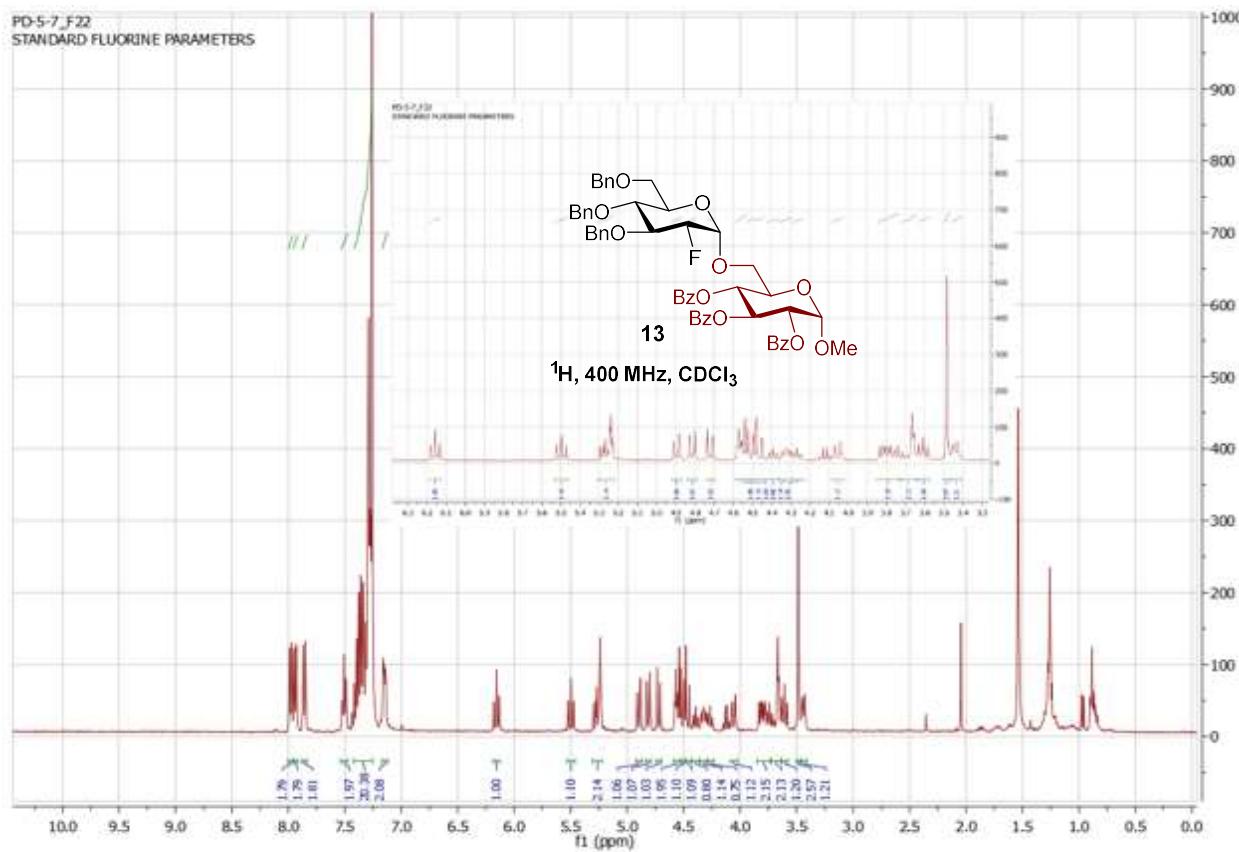
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Calibration for atb on 29Oct2018
Sample : Doped D2O

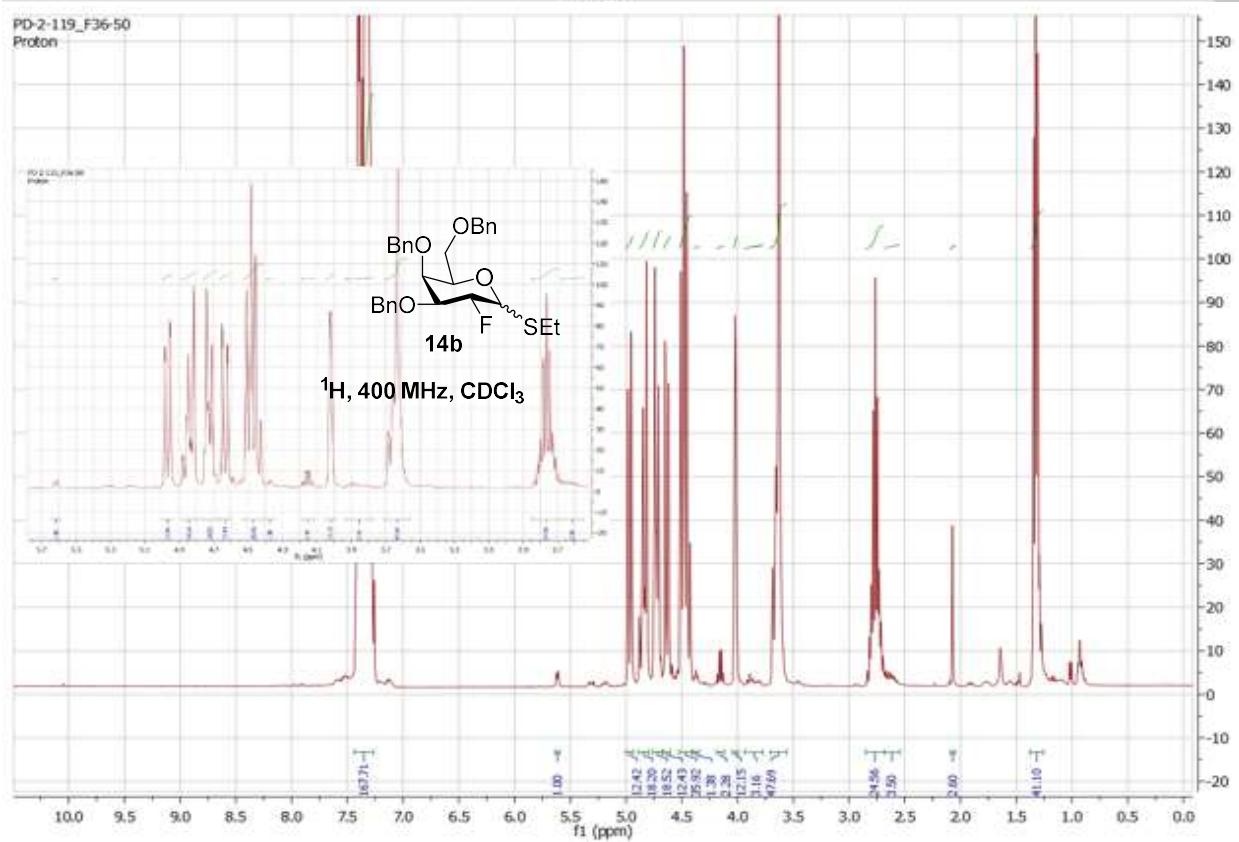
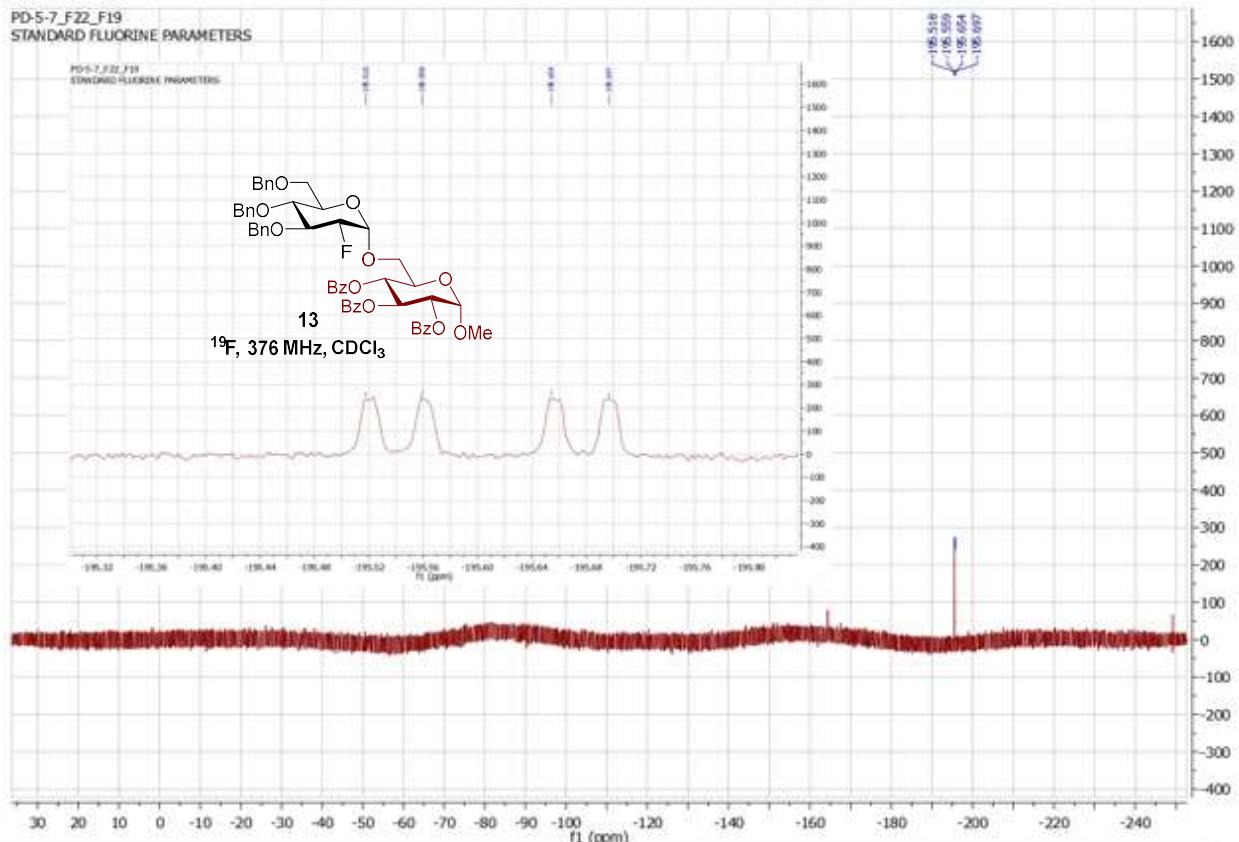


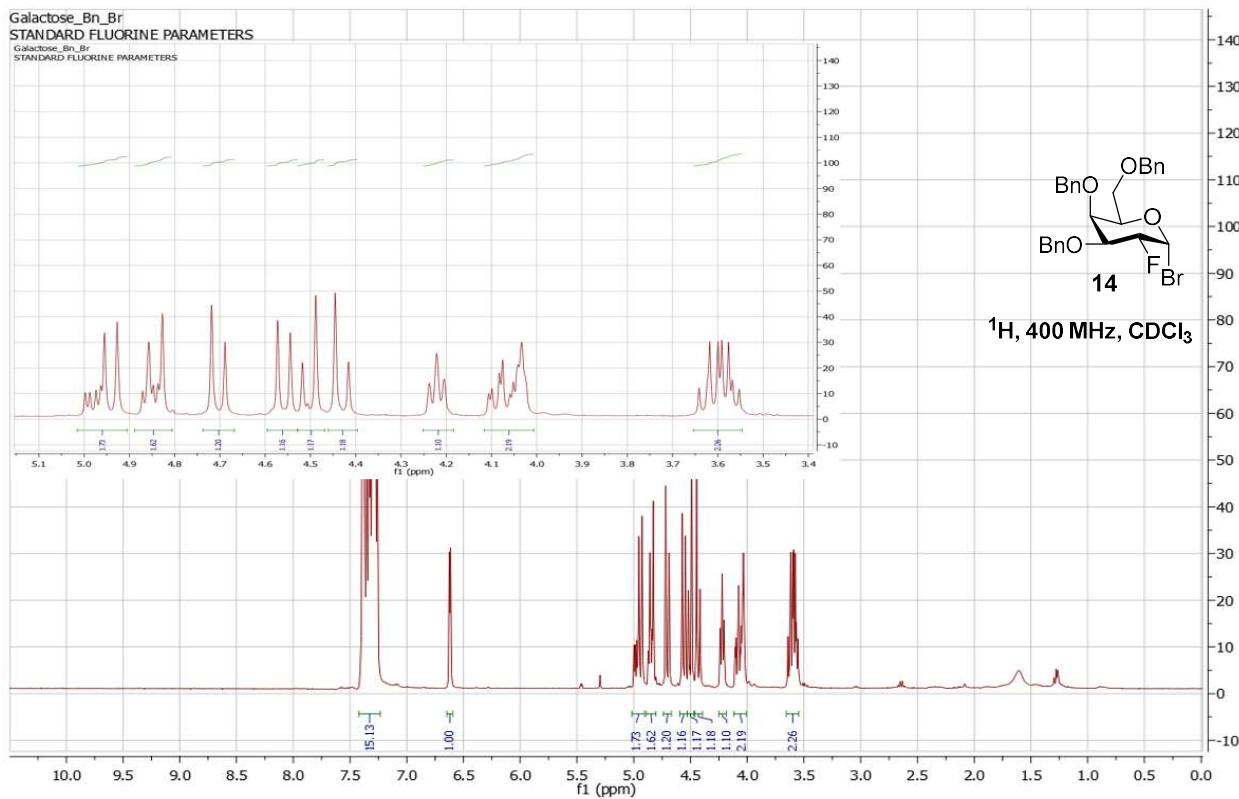
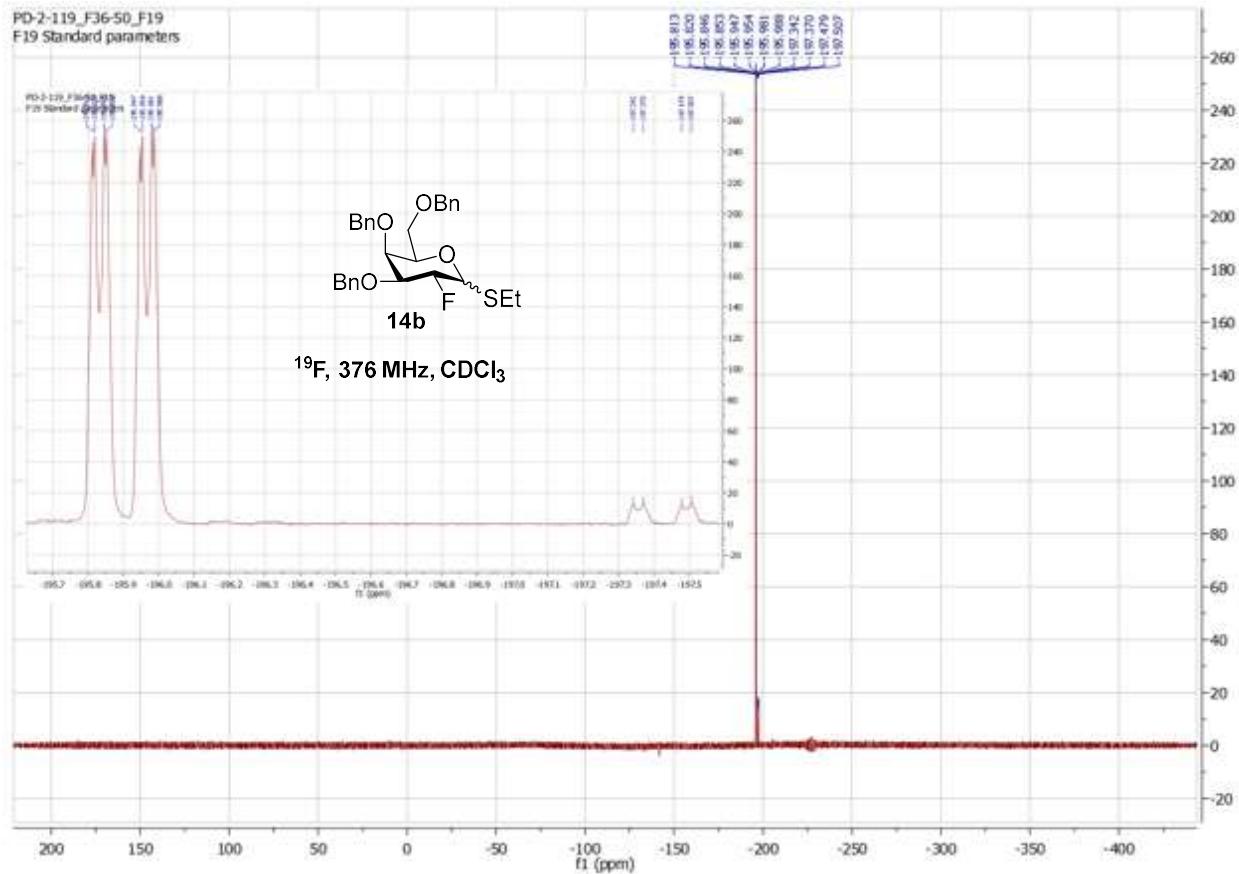
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F19 Standard parameters

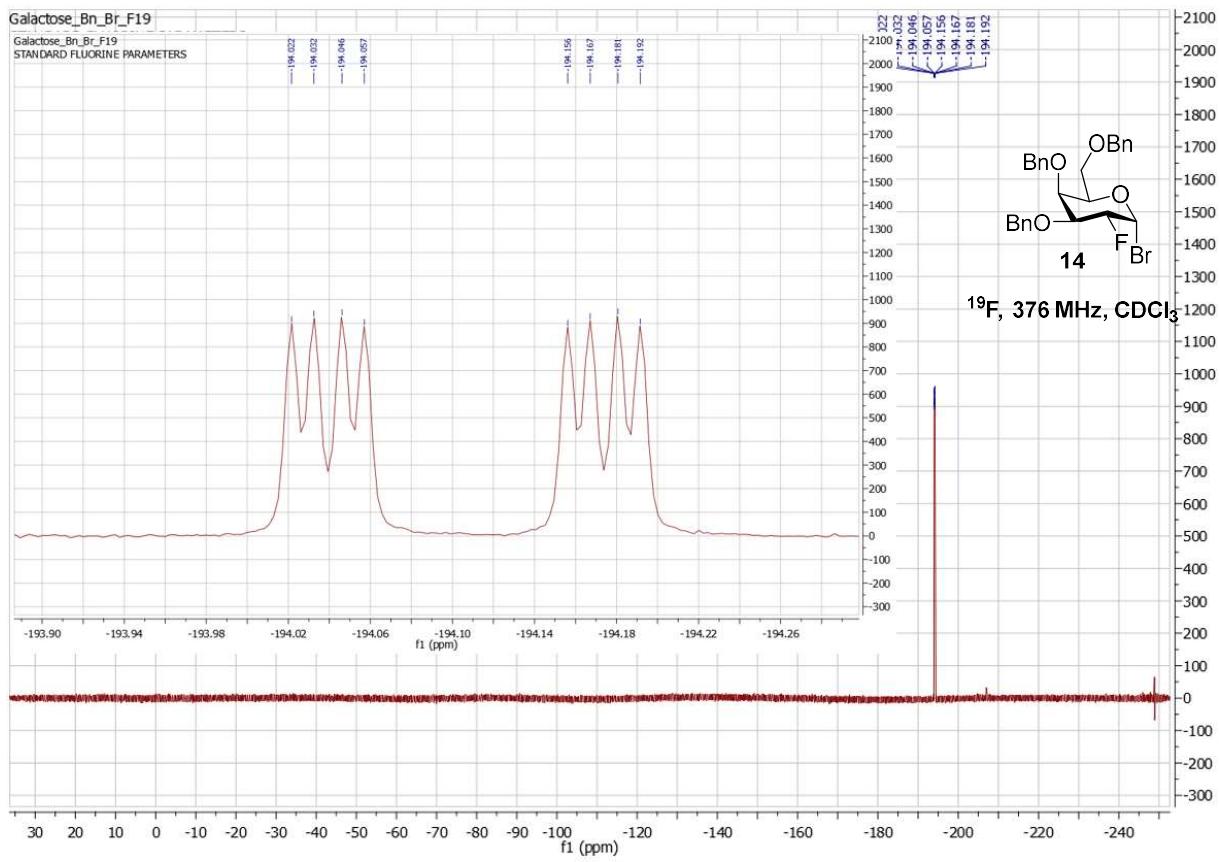
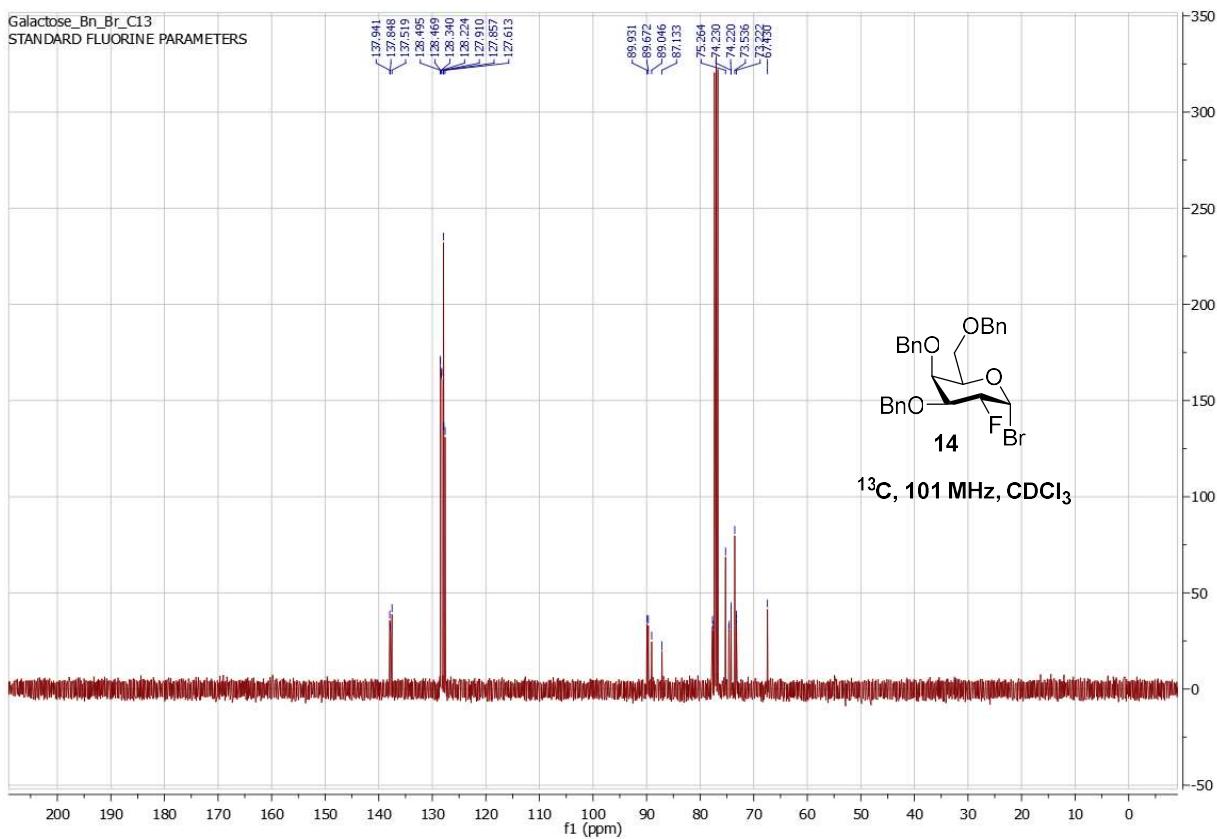
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F19 Standard parameters

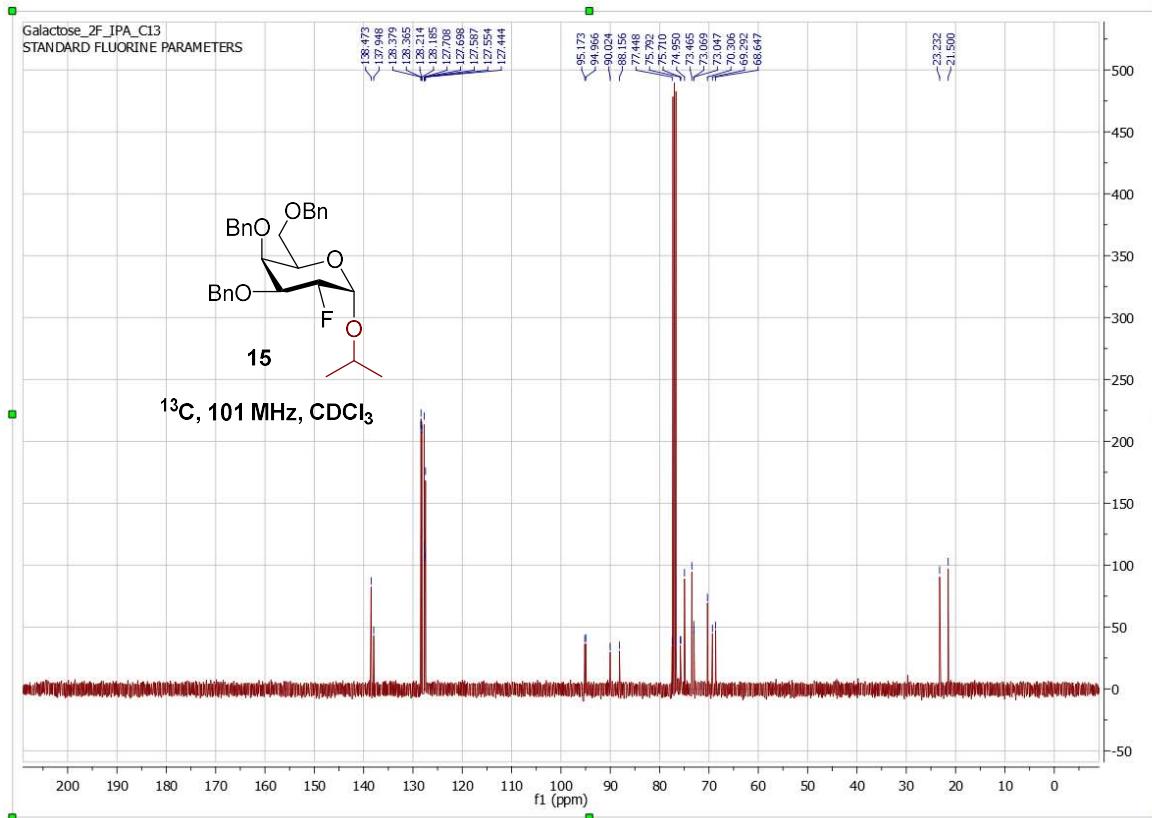
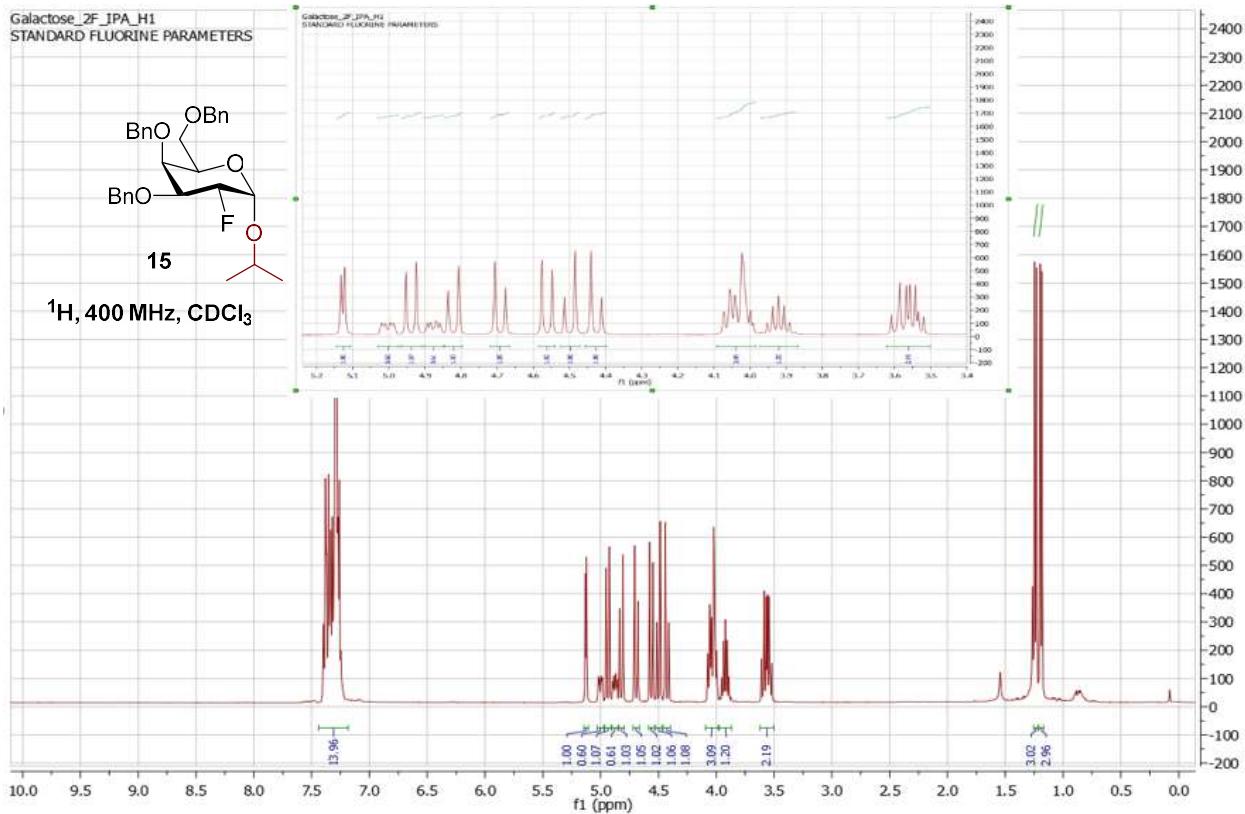


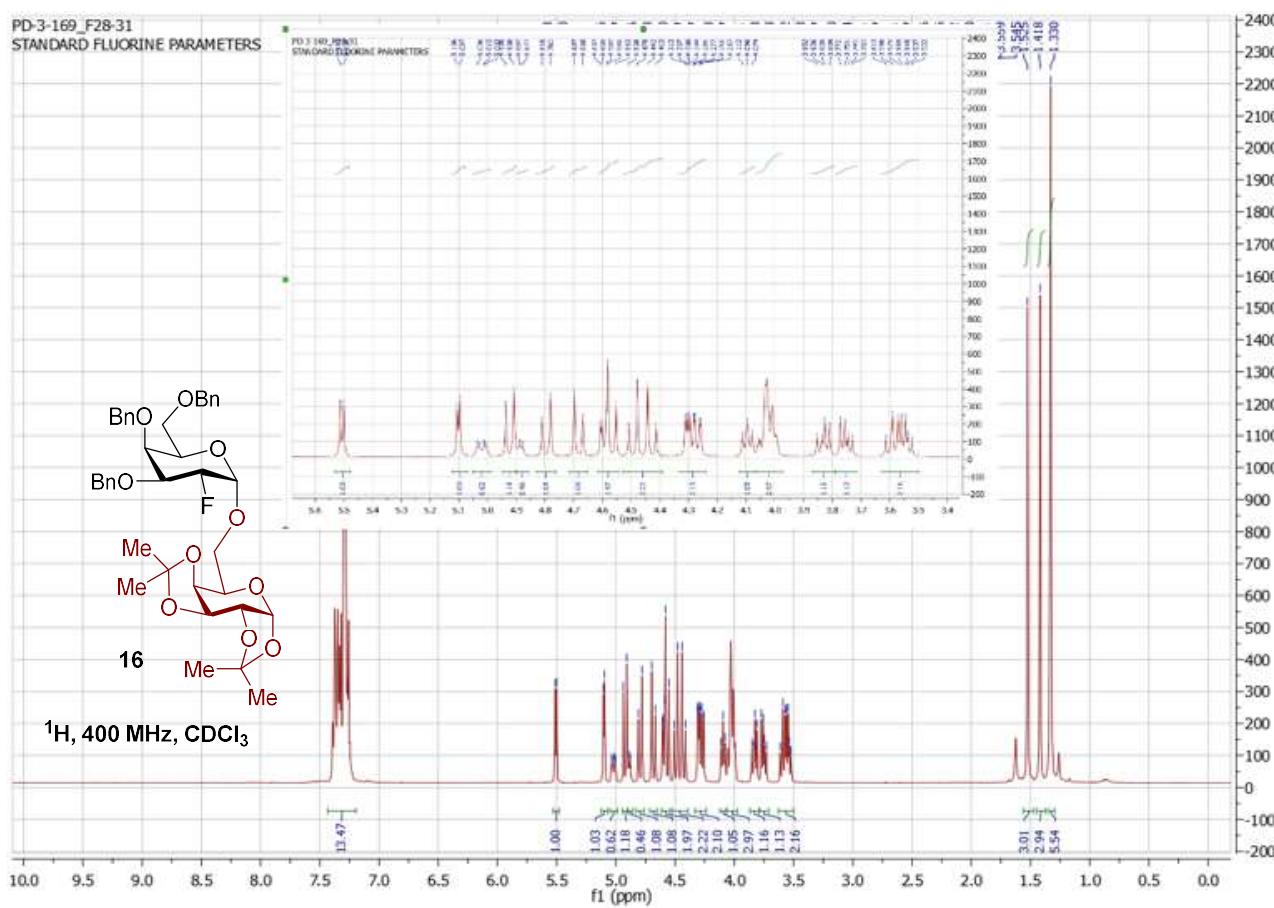
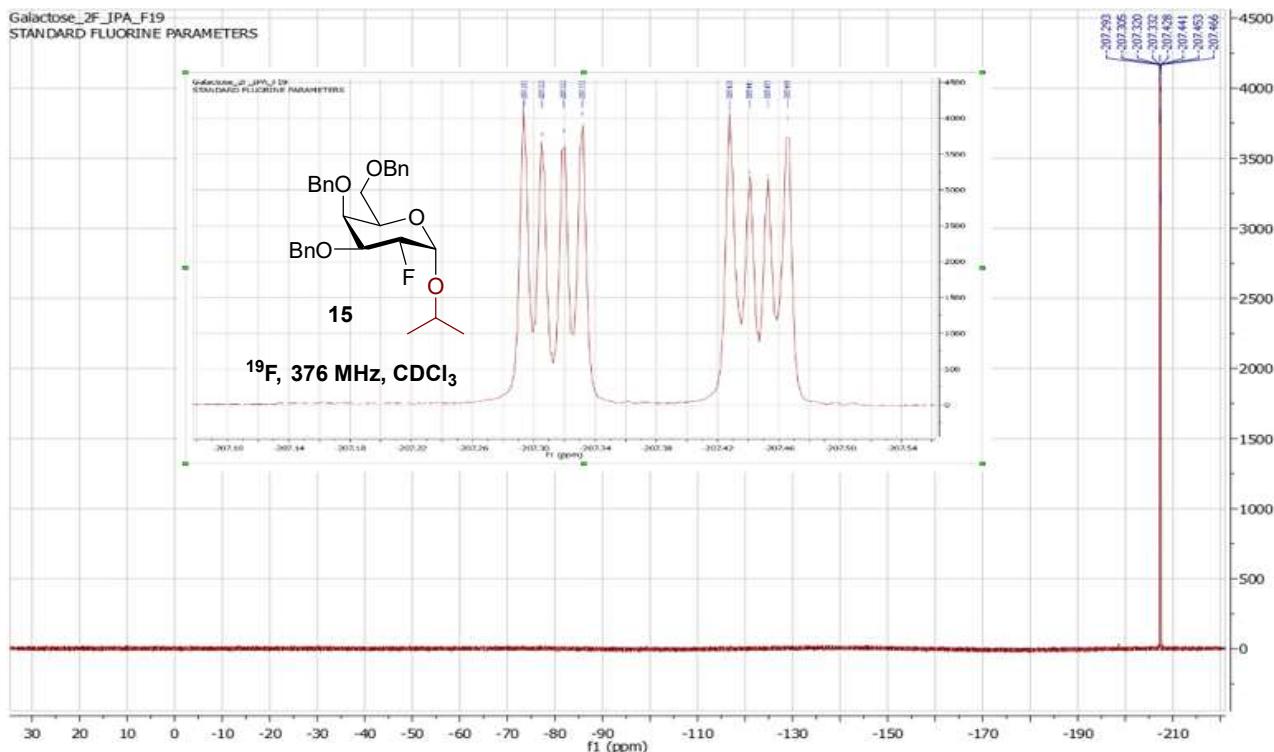


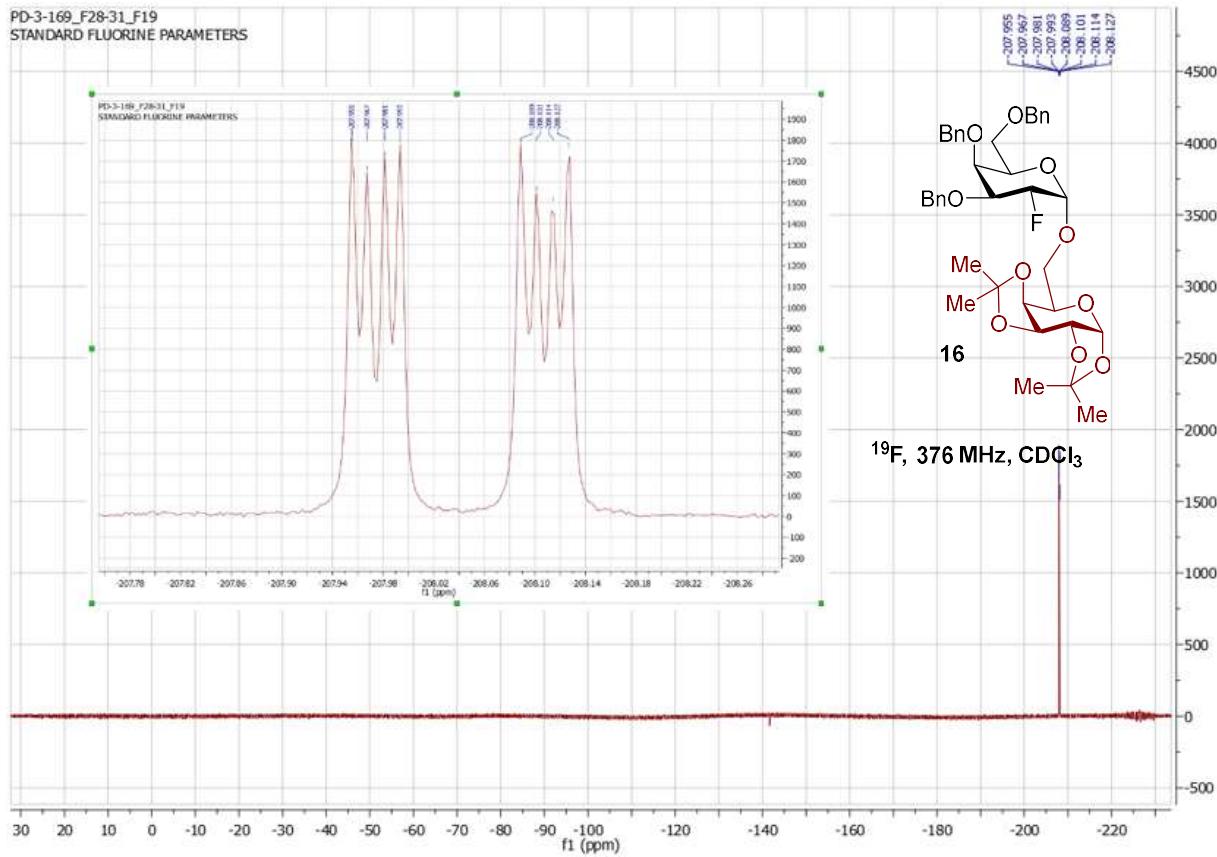
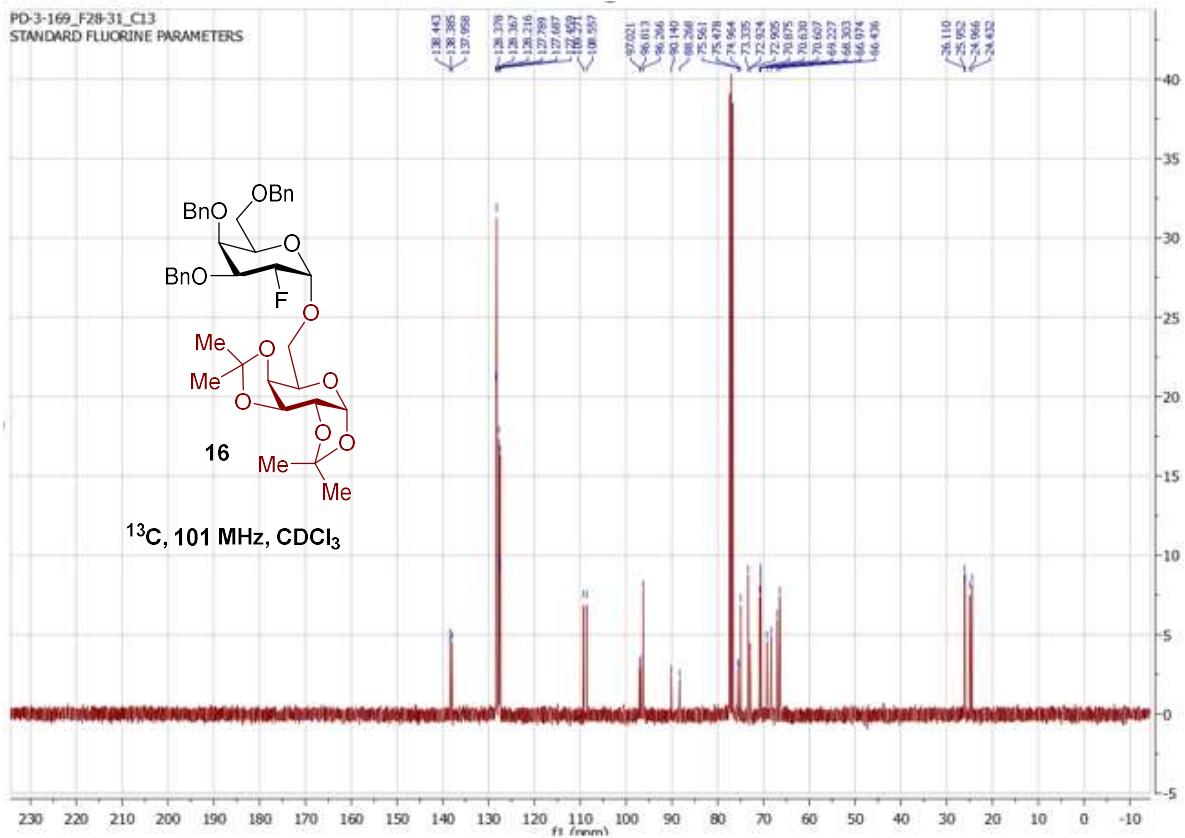


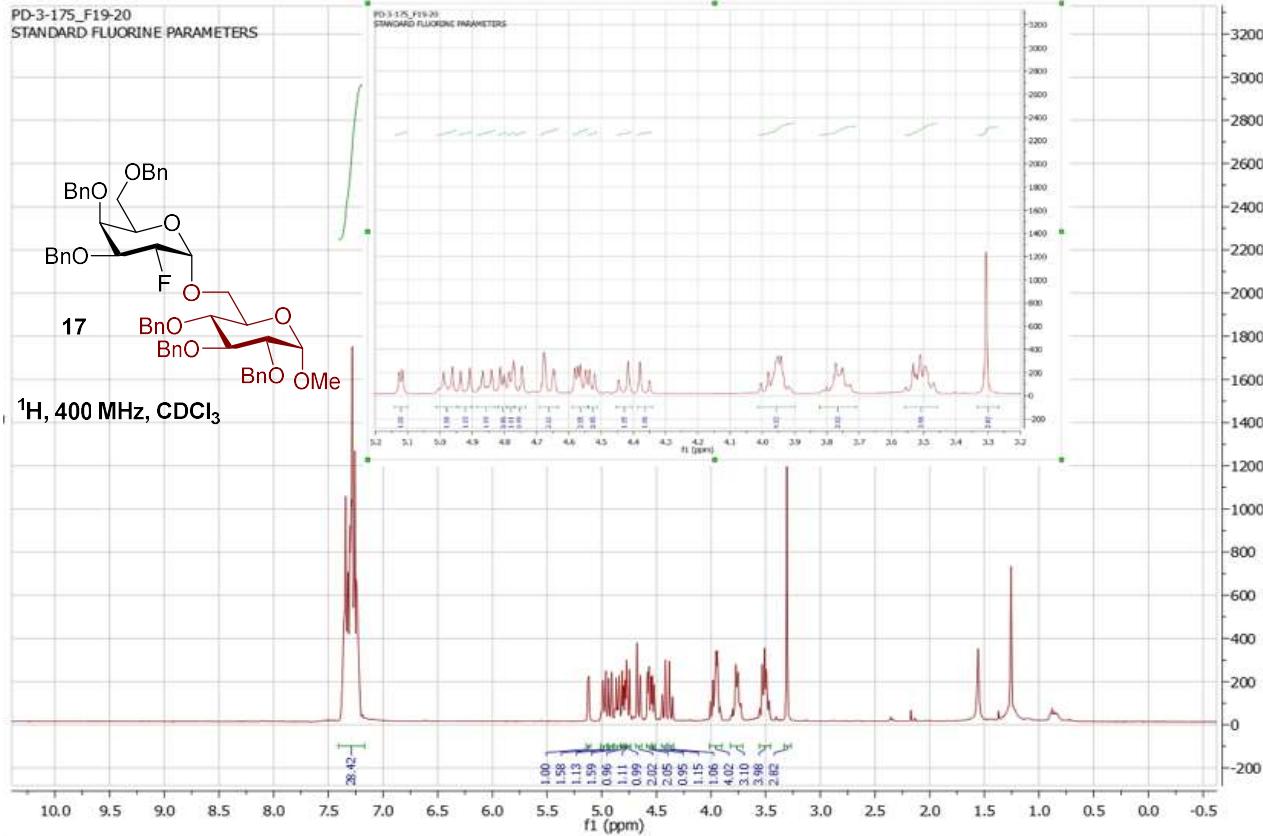


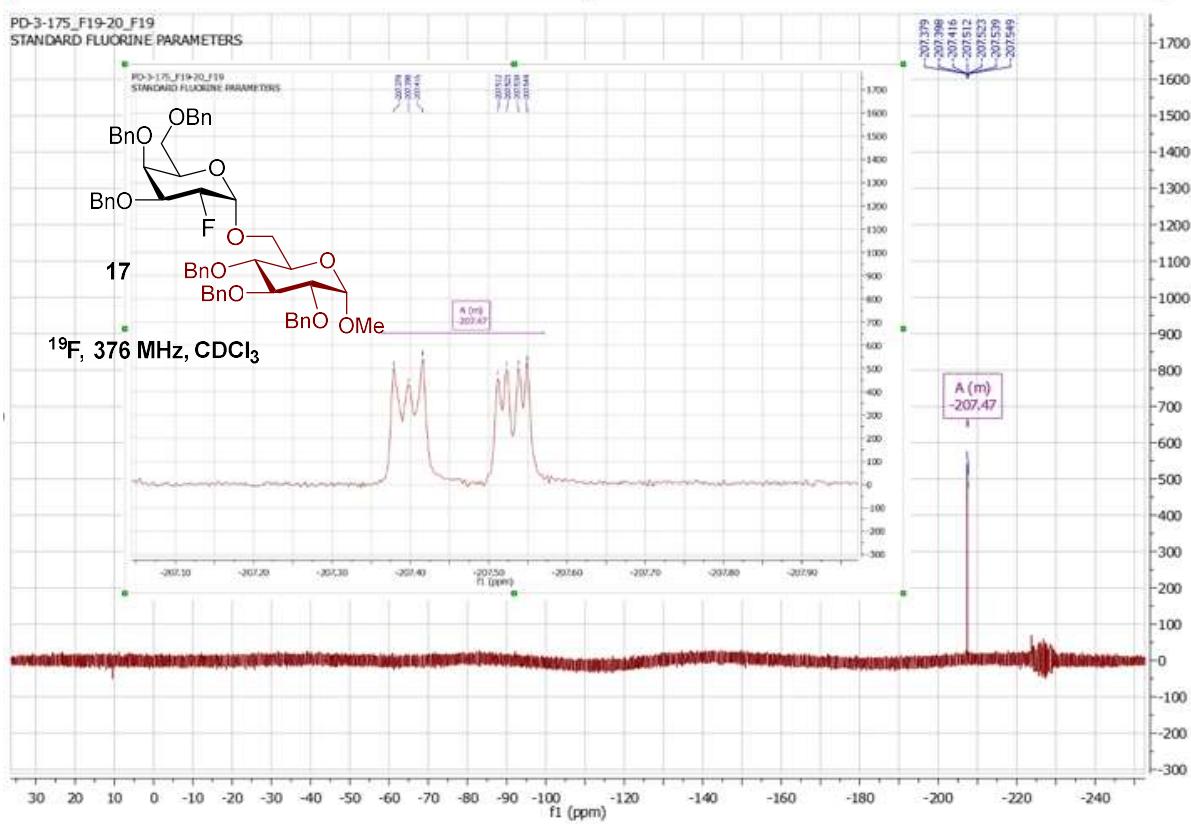
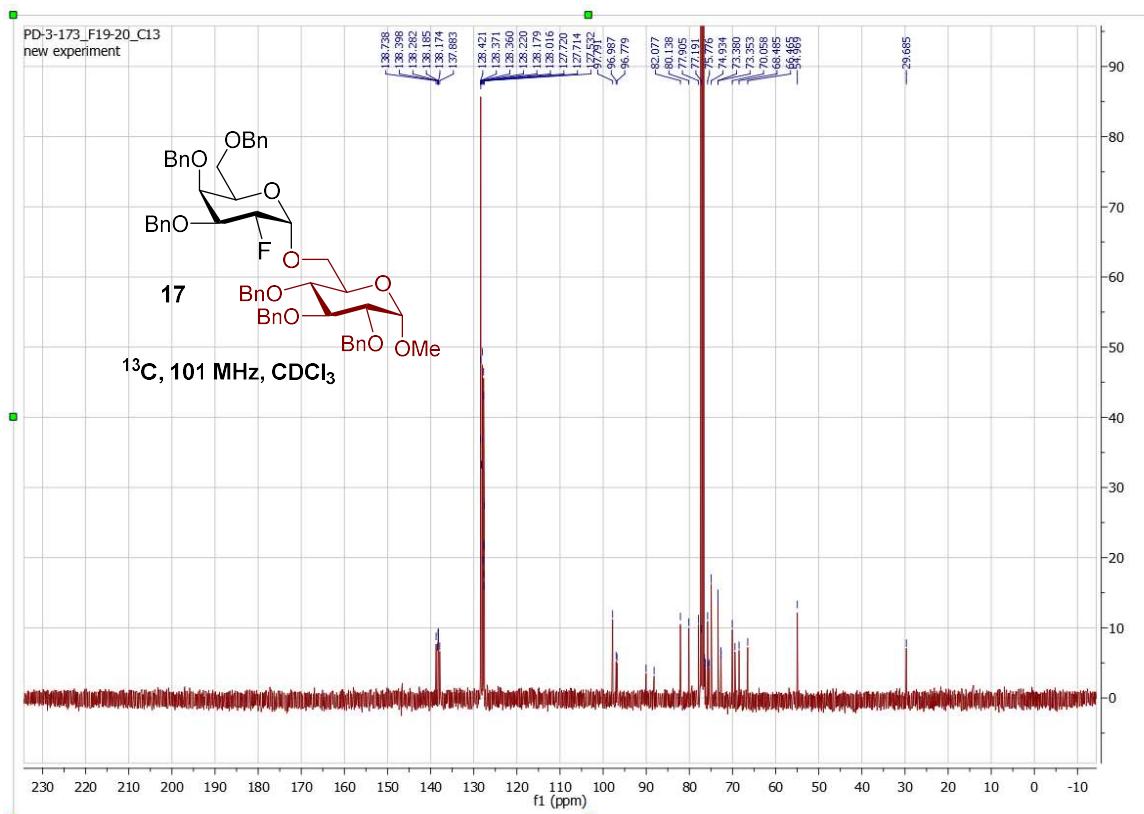






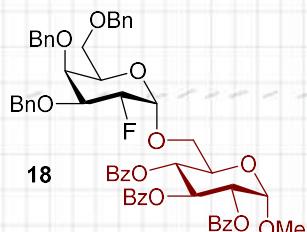




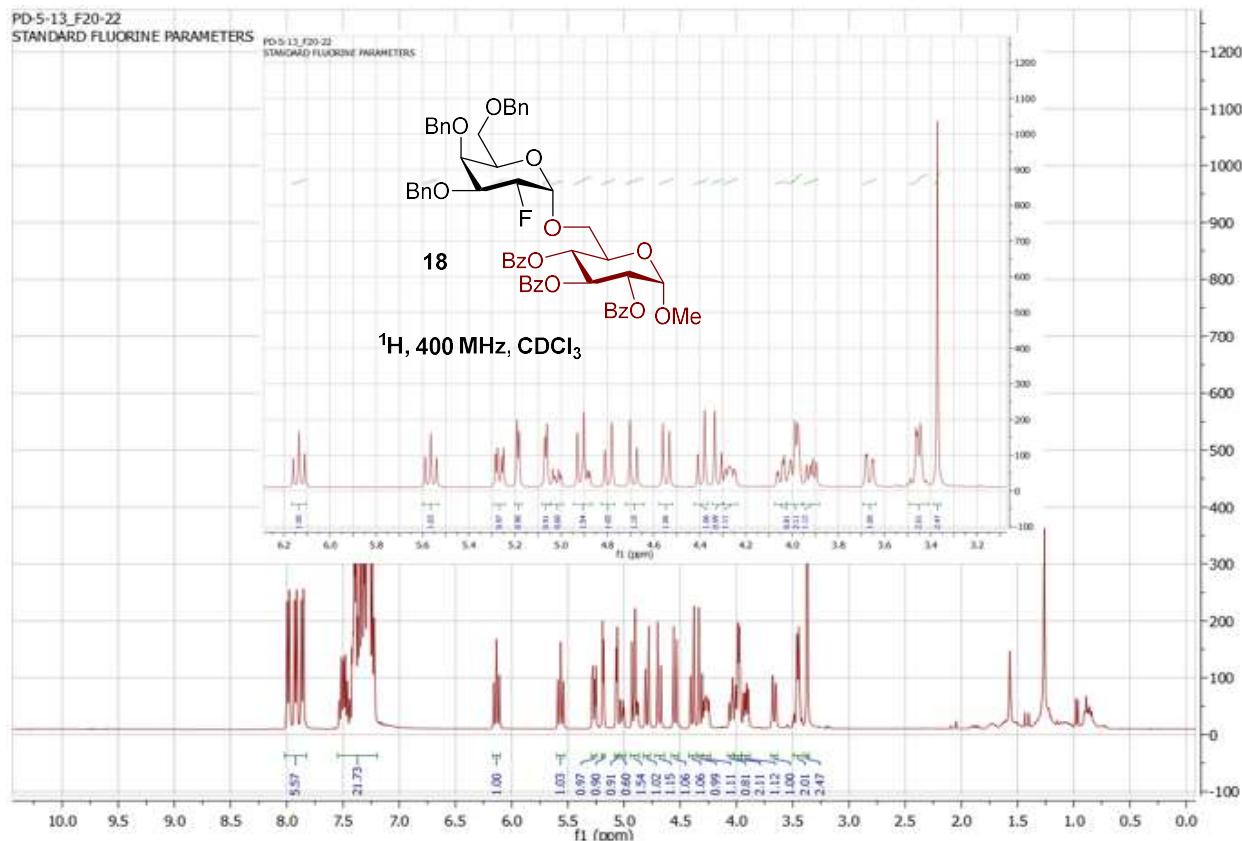


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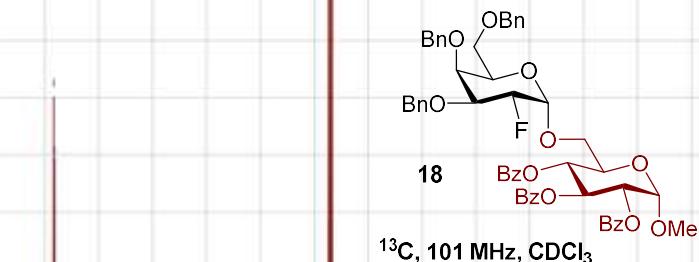
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STANDARD FLUORINE PARAMETERS



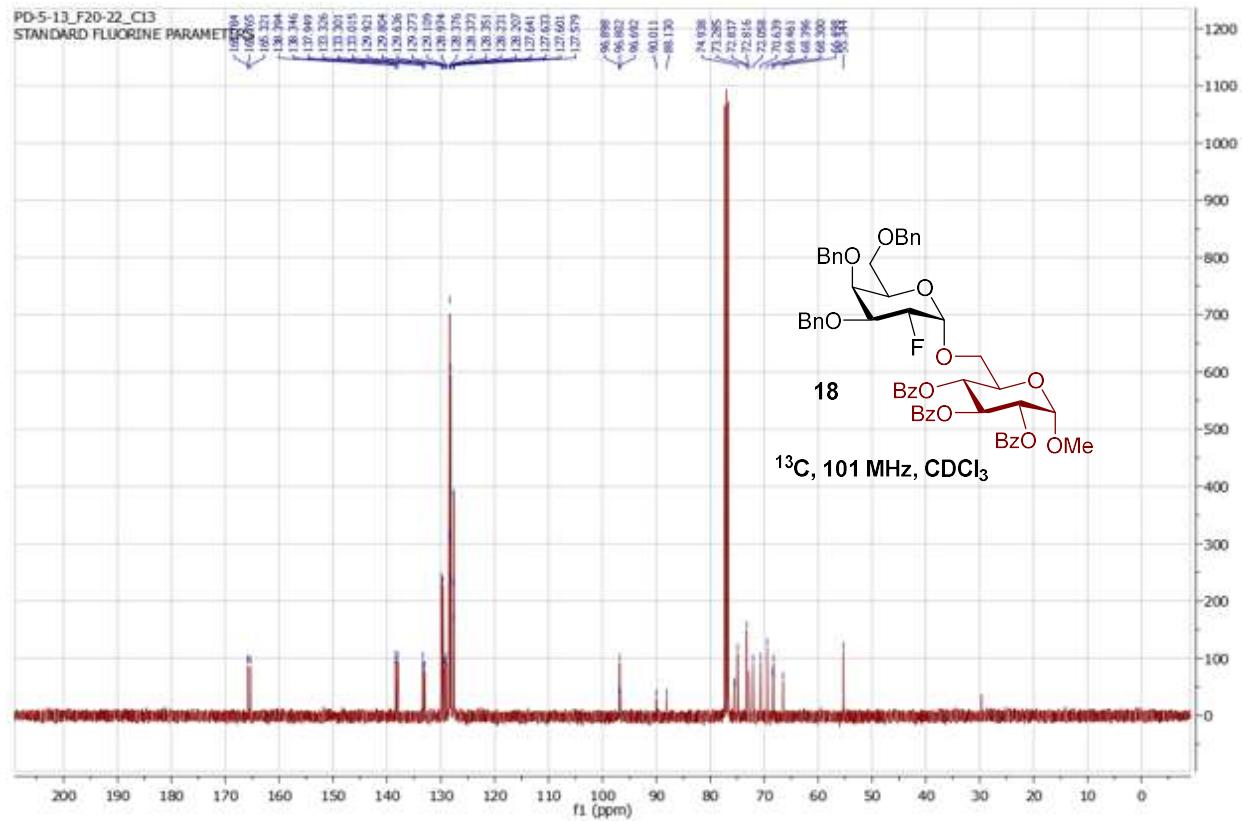
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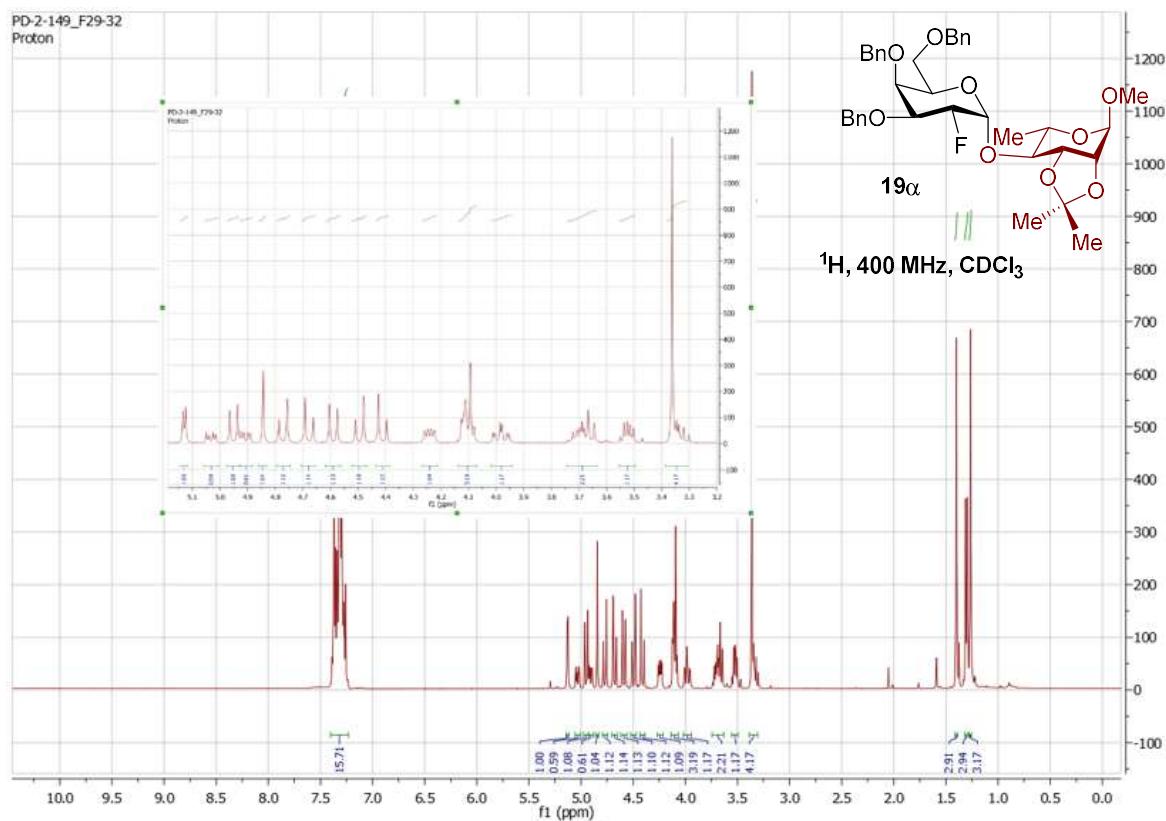
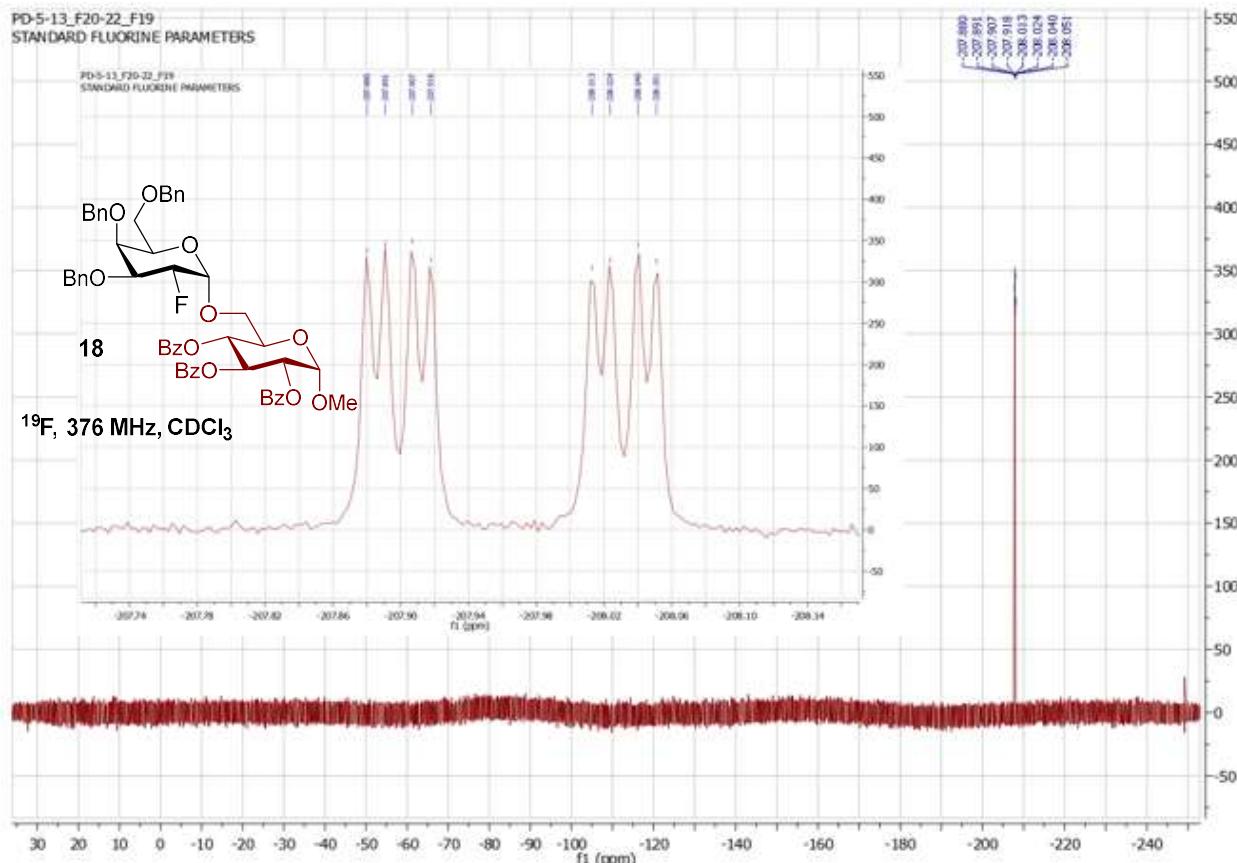


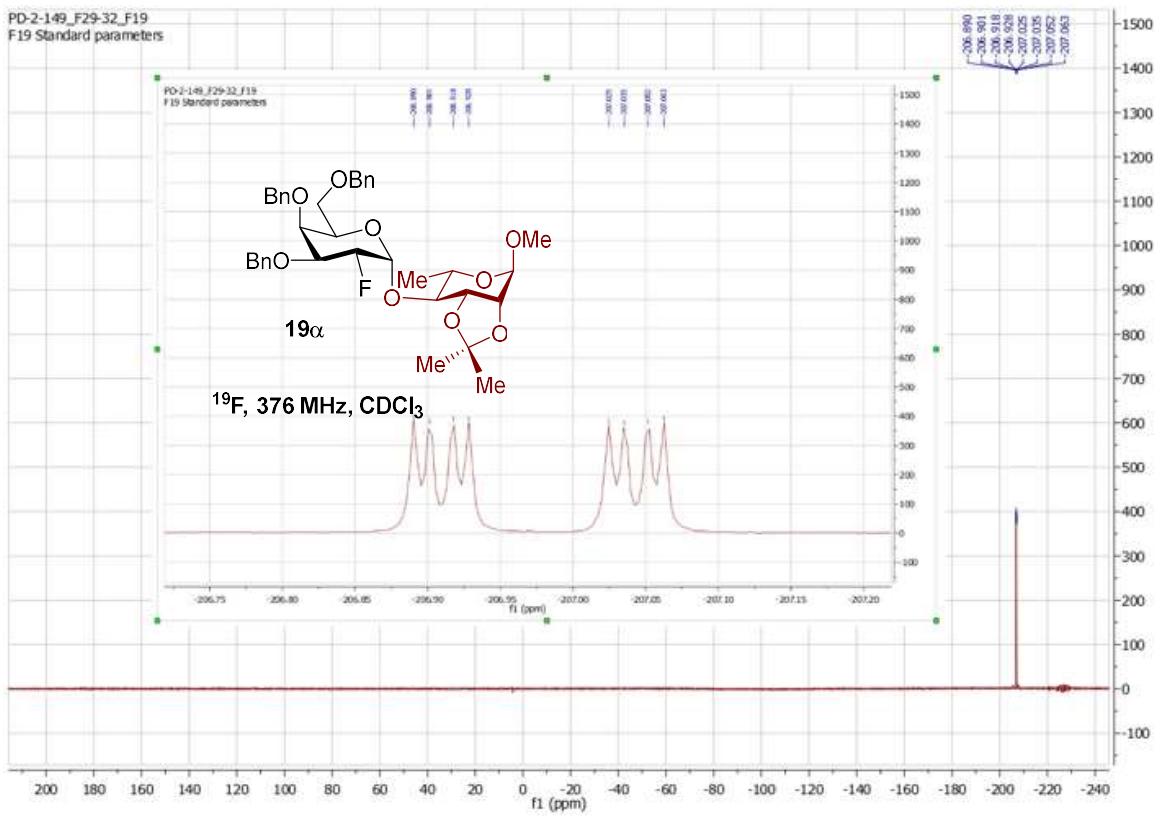
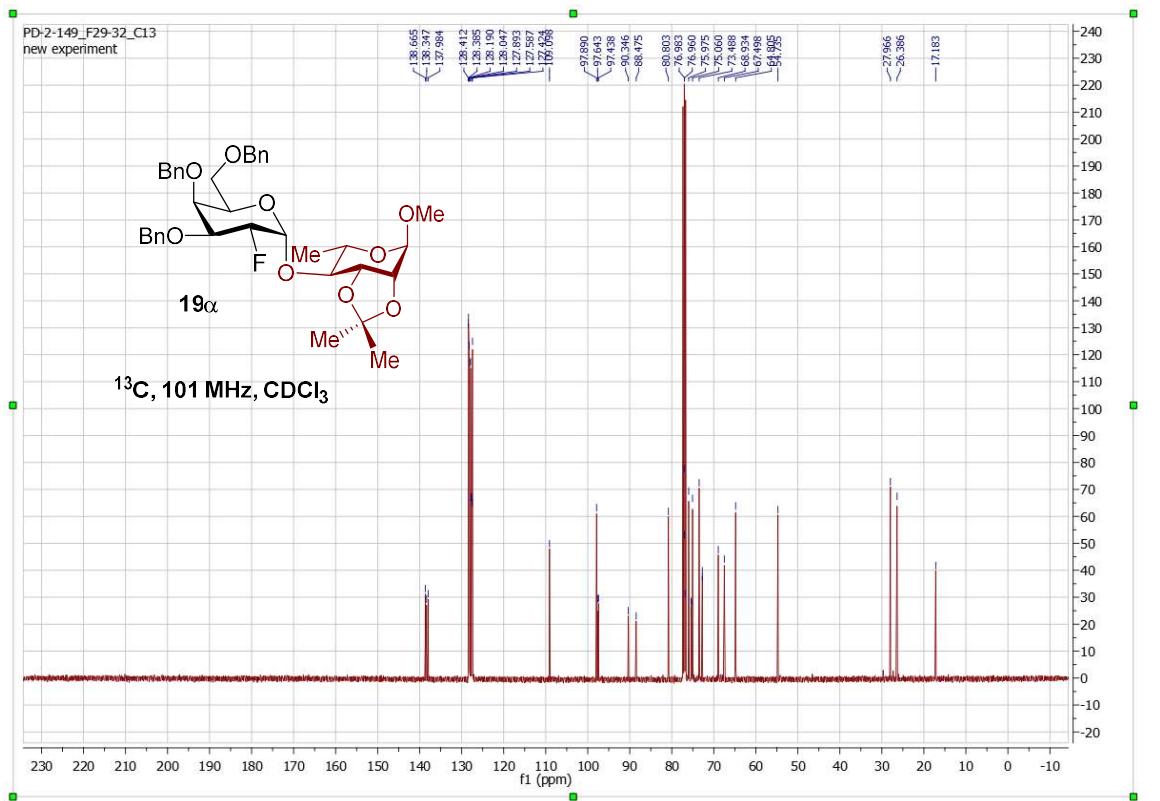
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STANDARD FLUORINE PARAMETERS

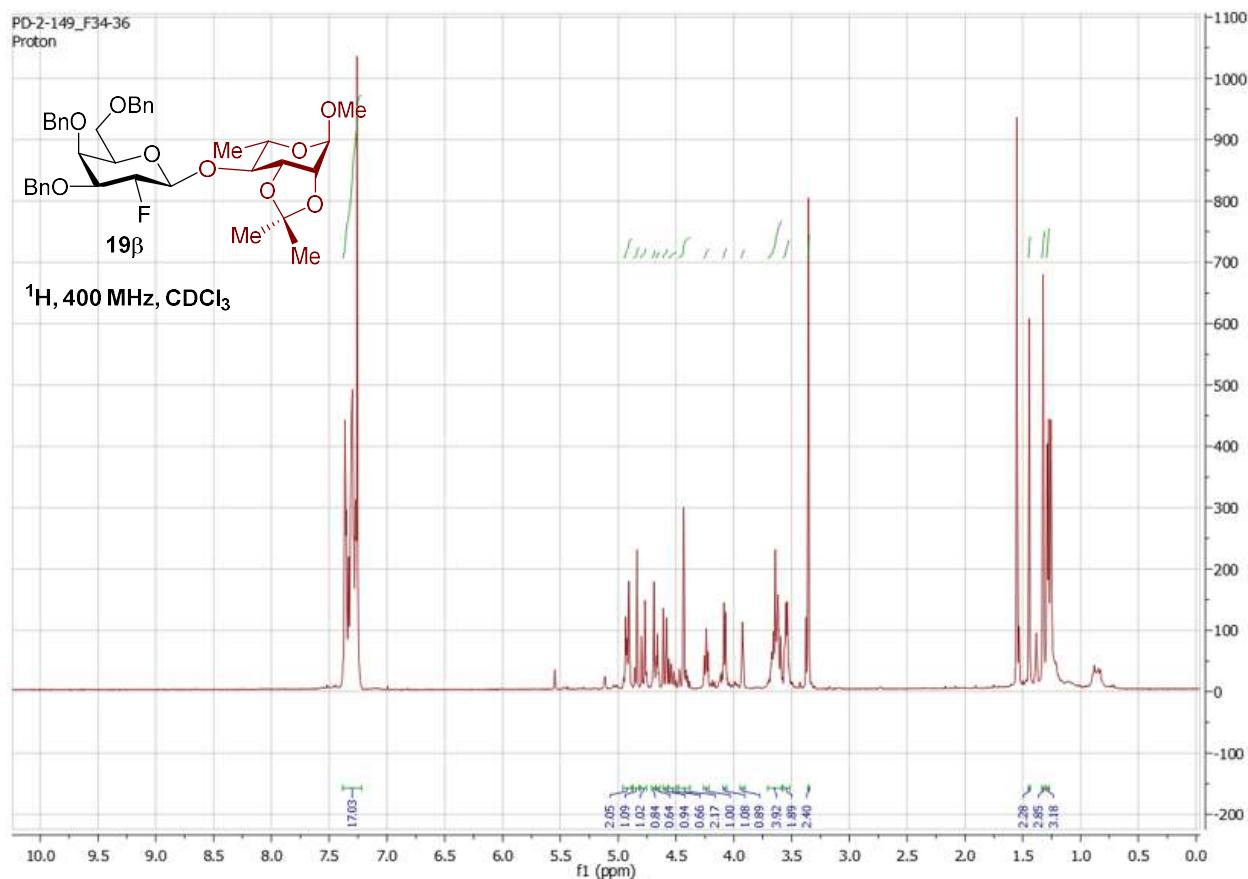


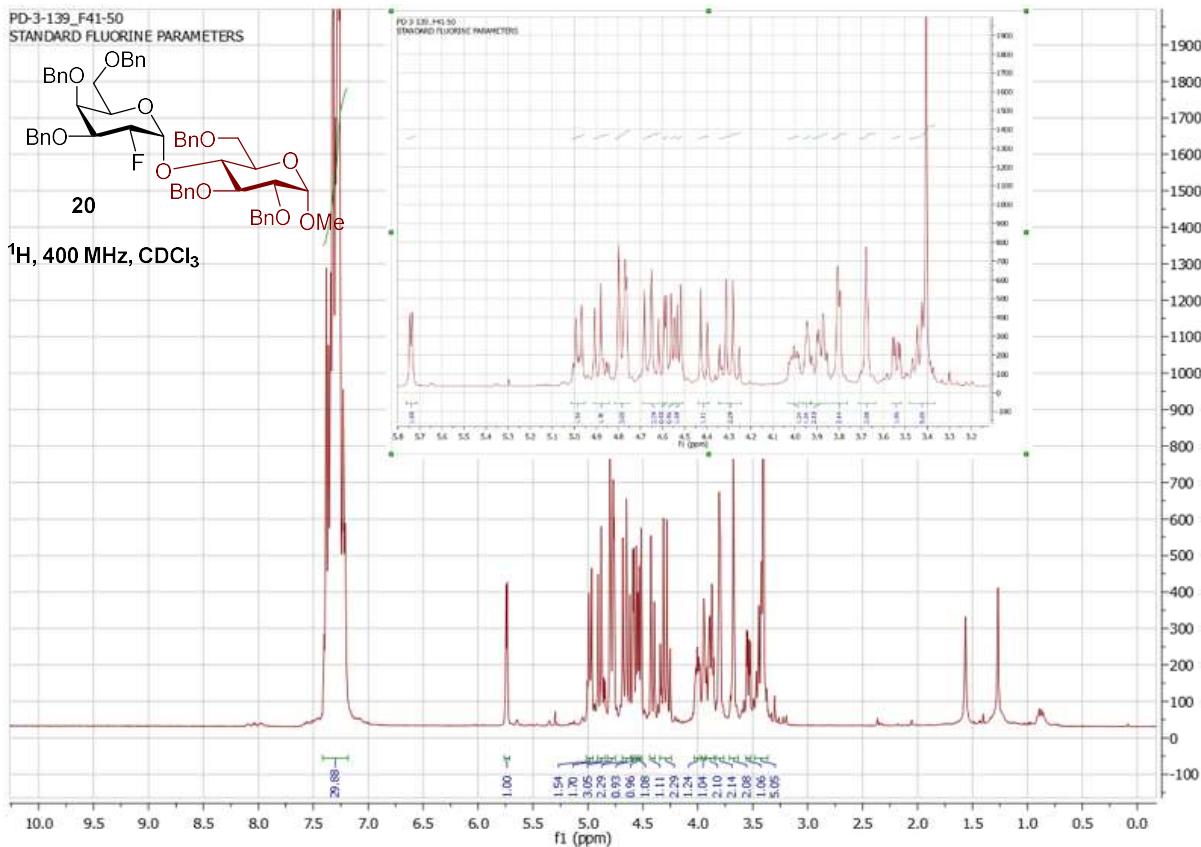
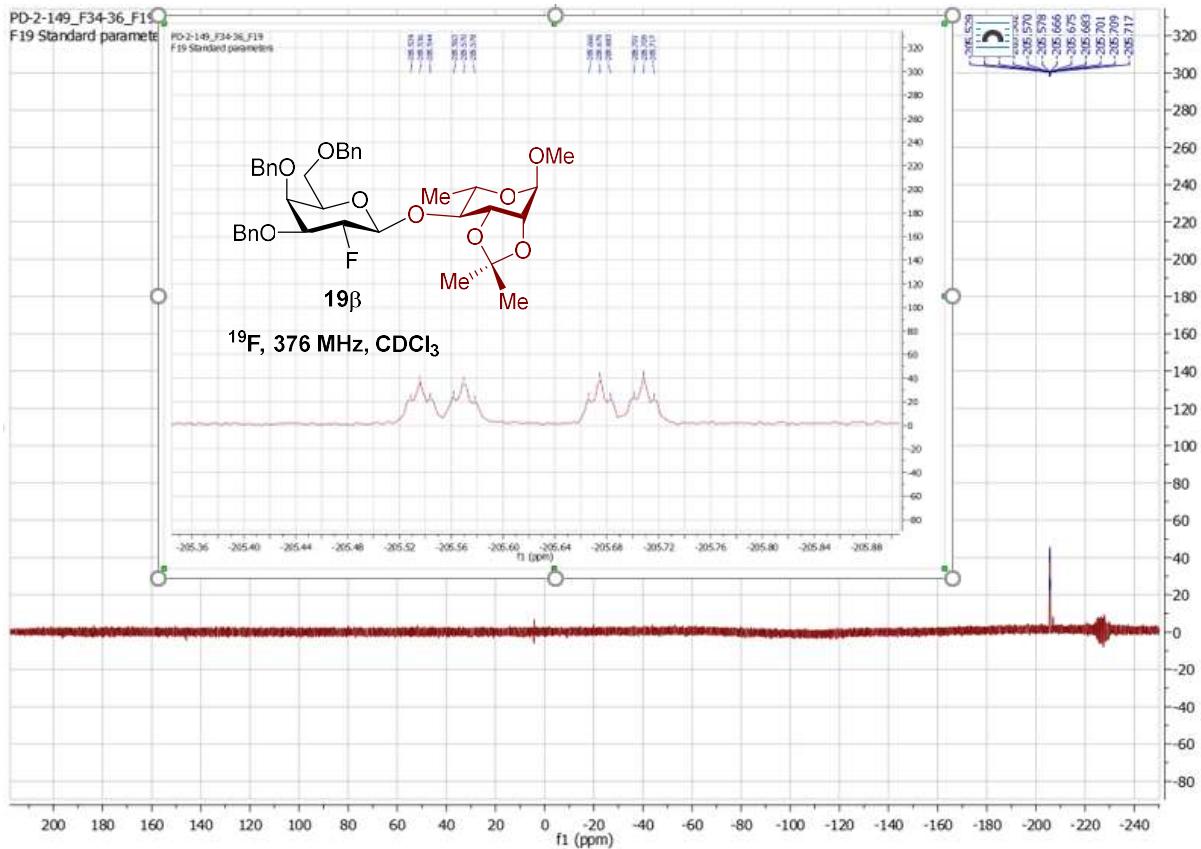
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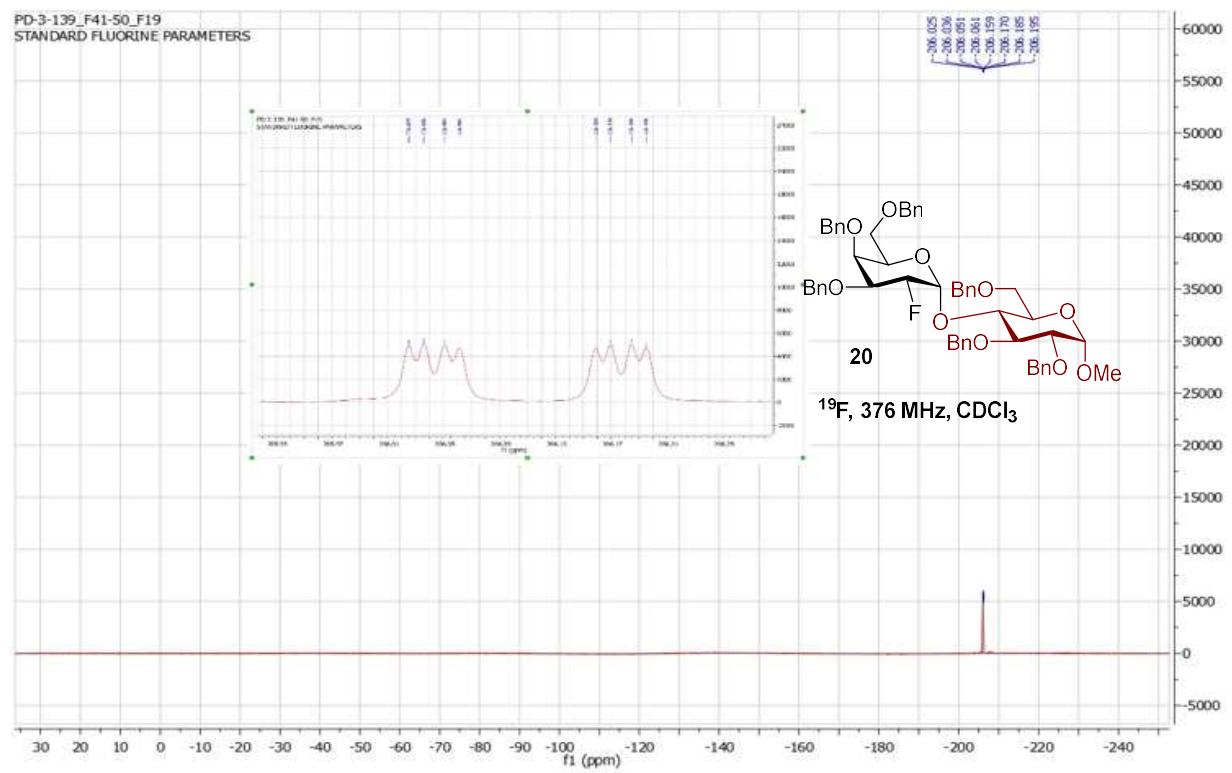
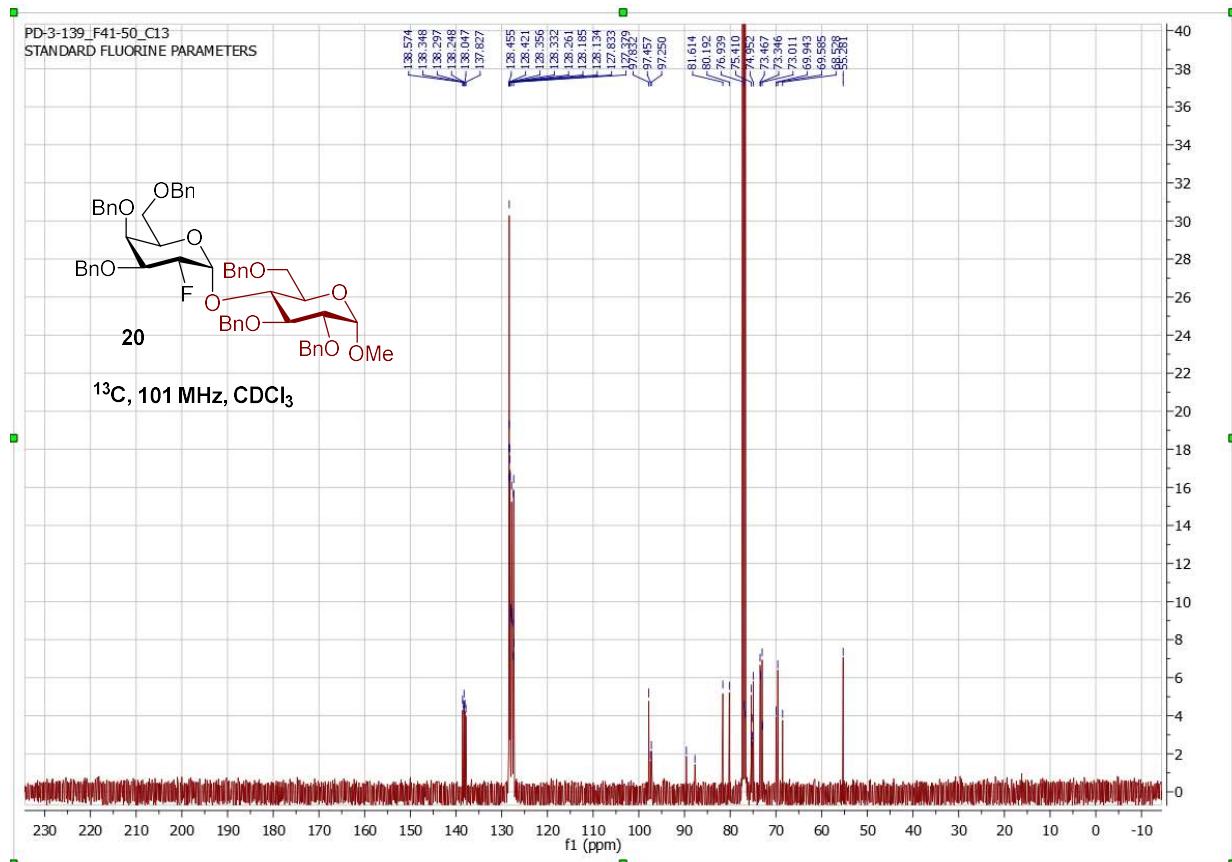


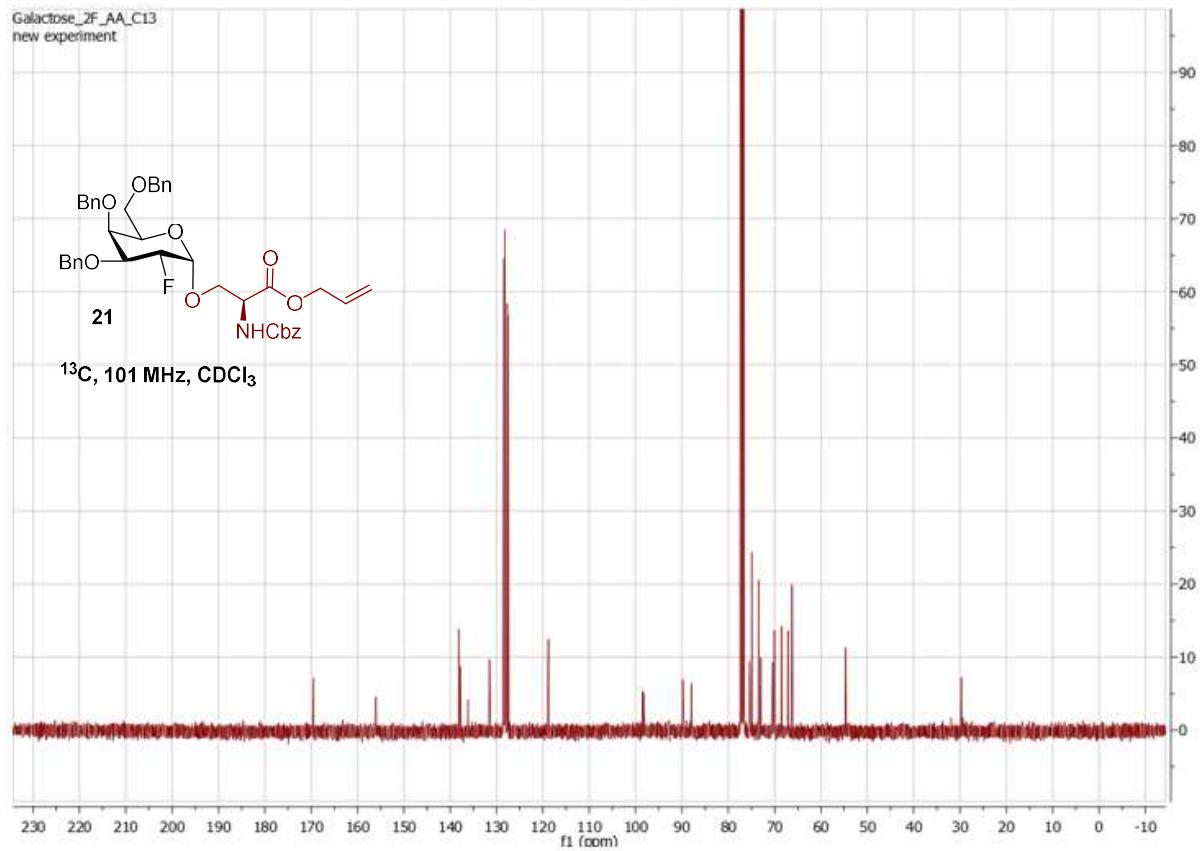
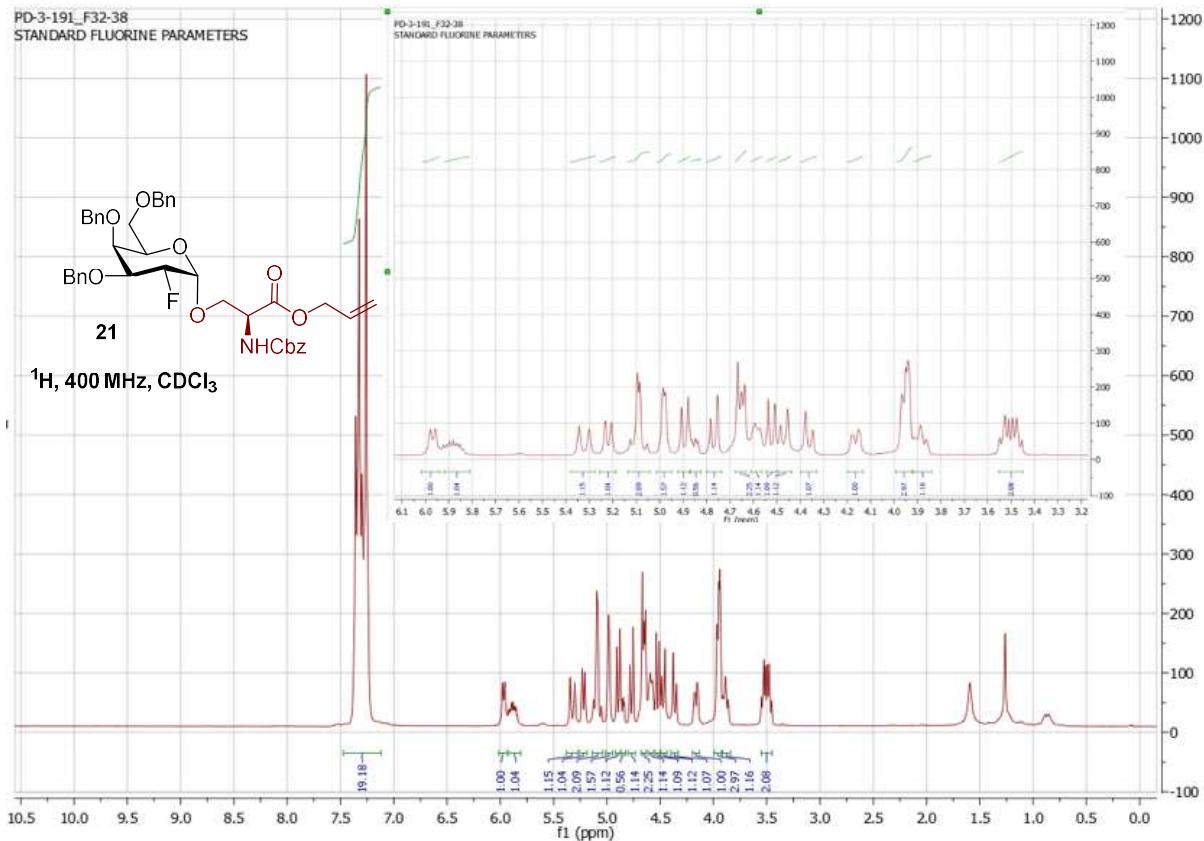




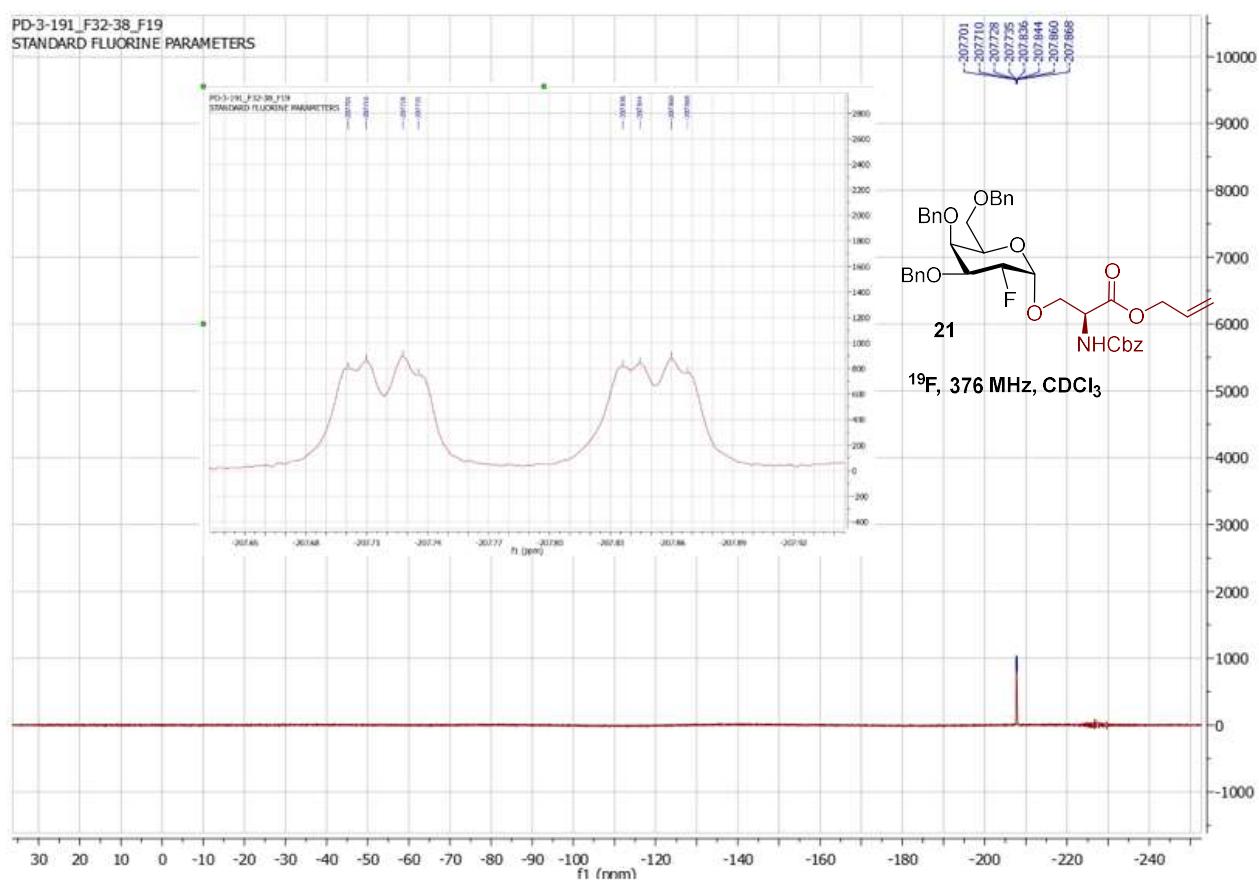


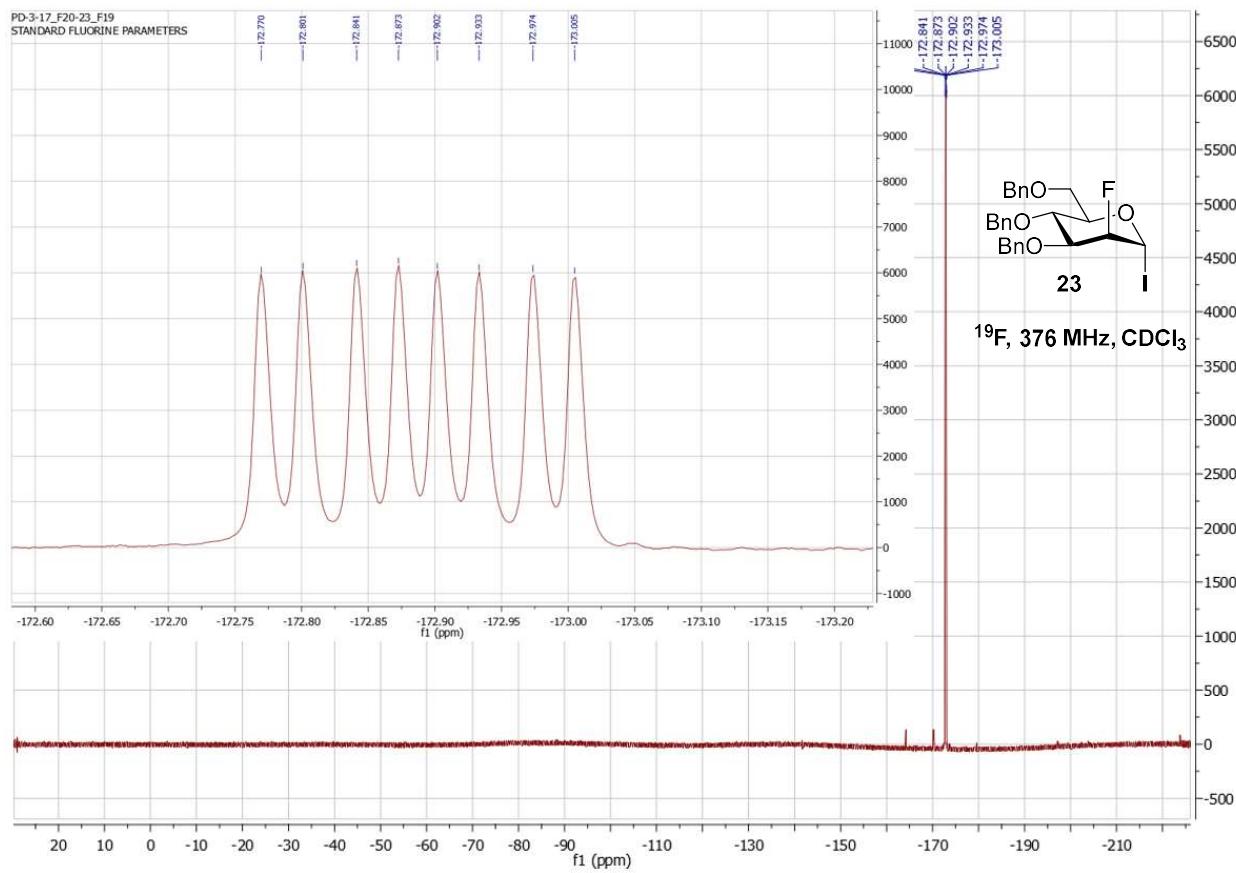
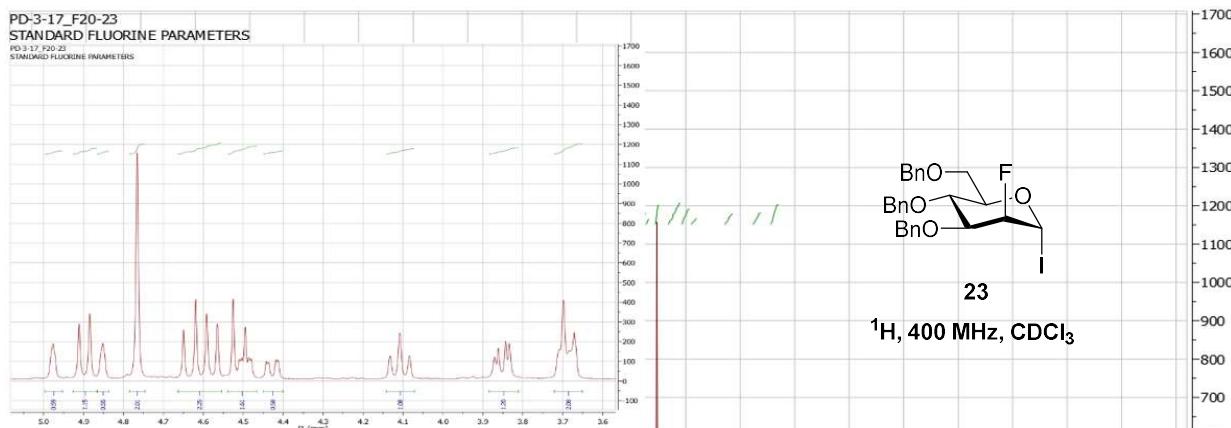


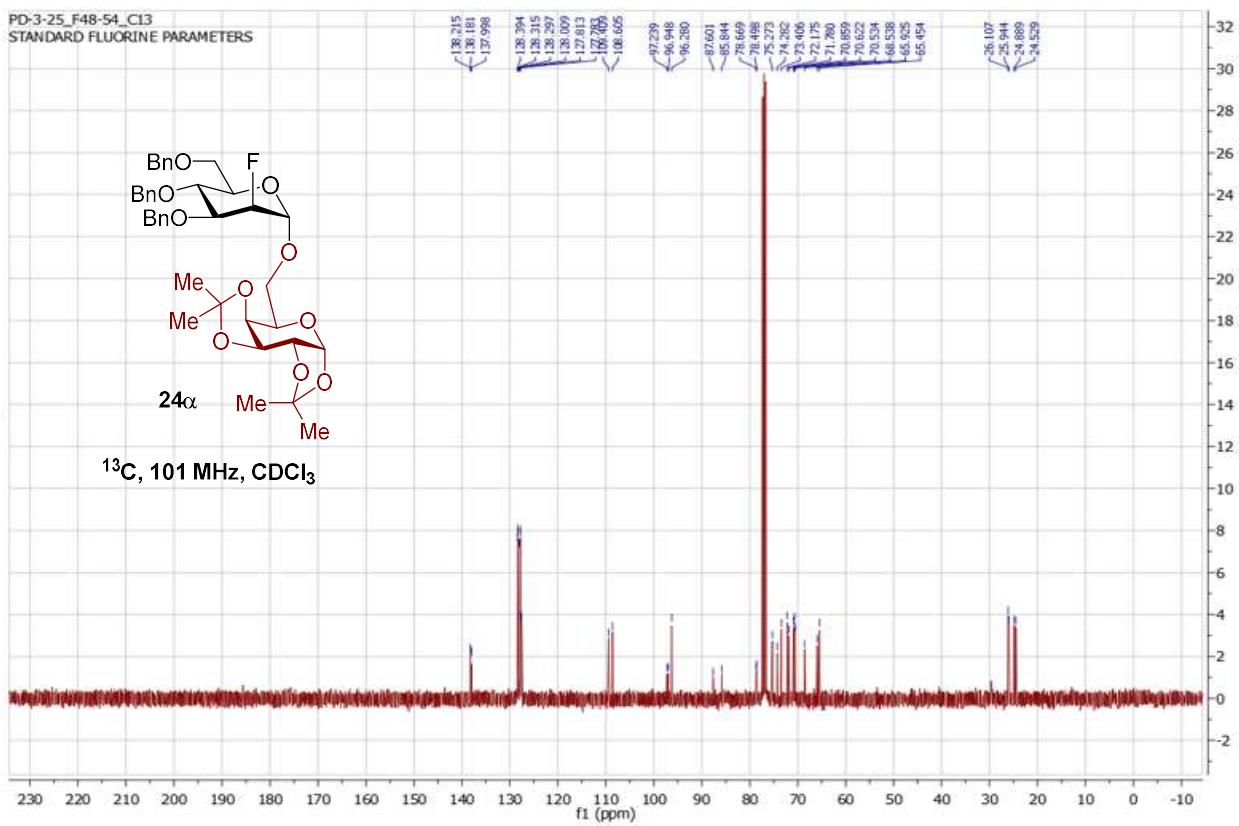
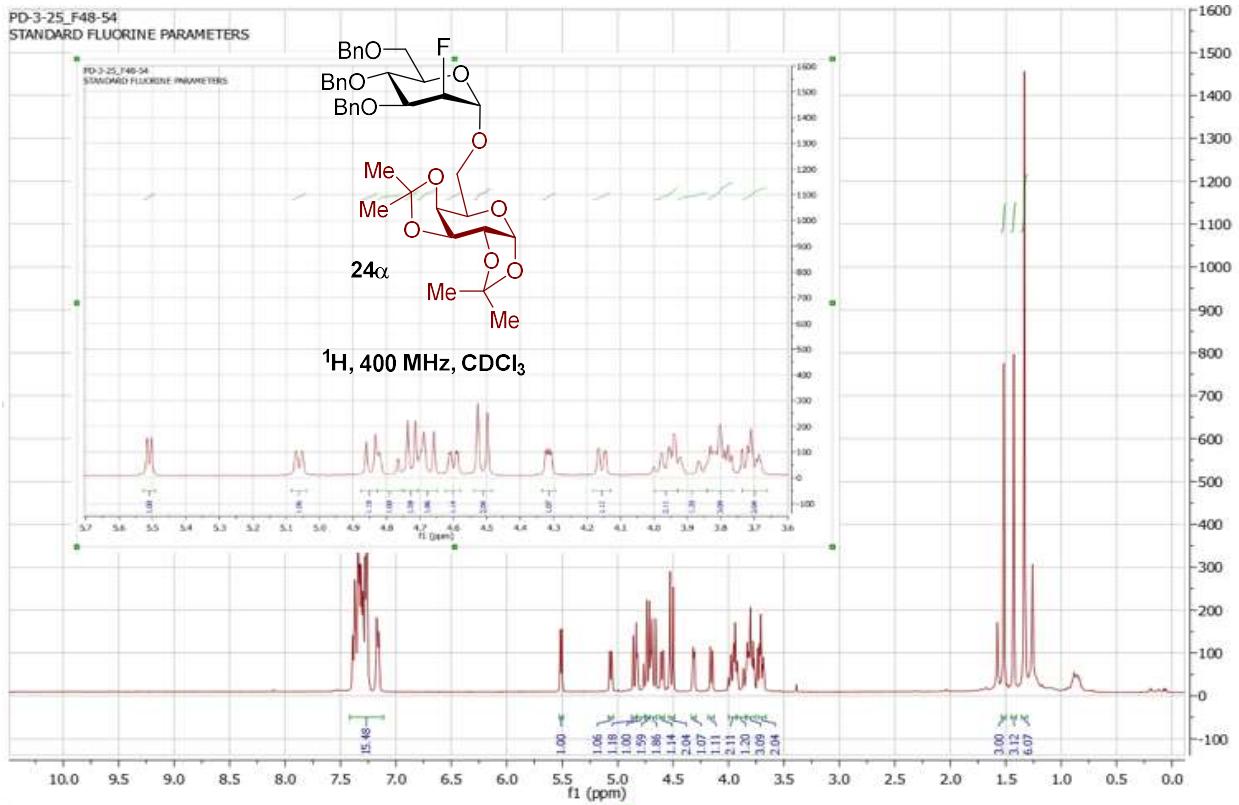


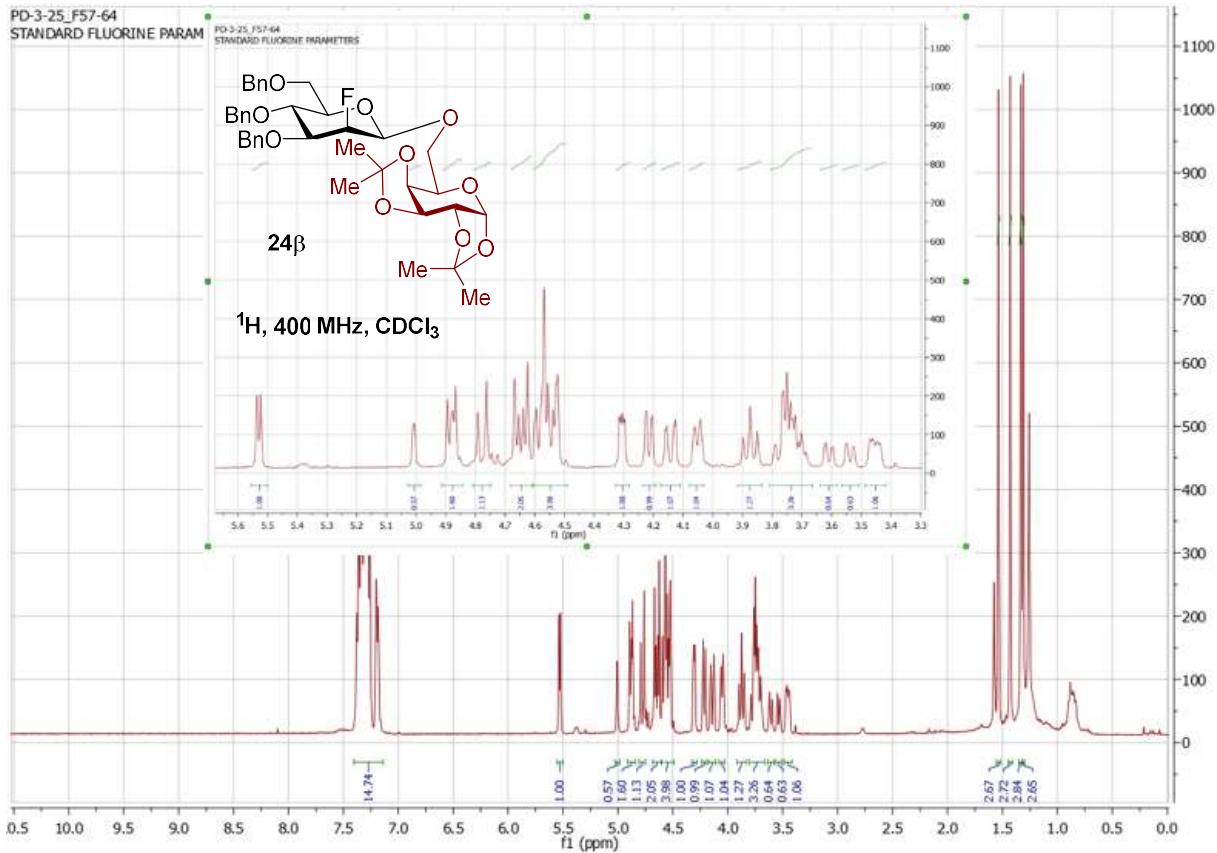
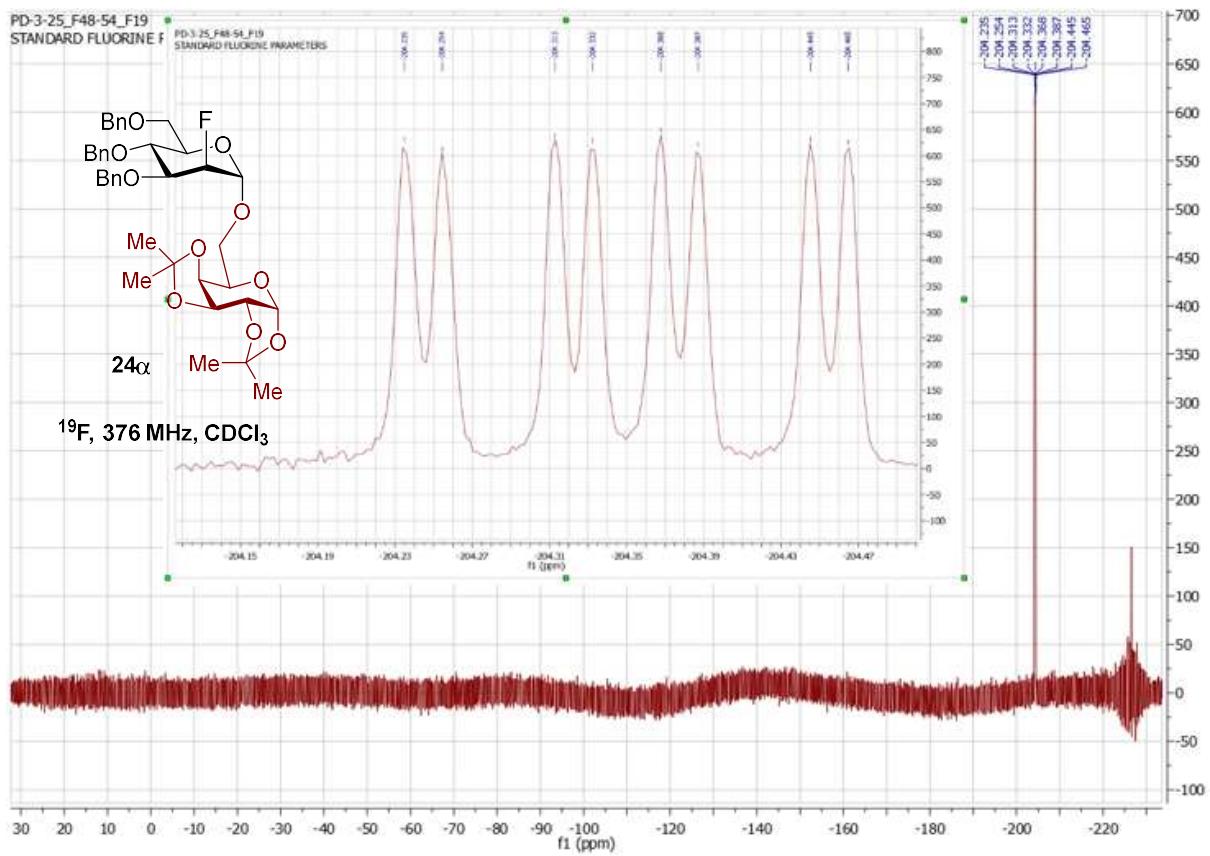


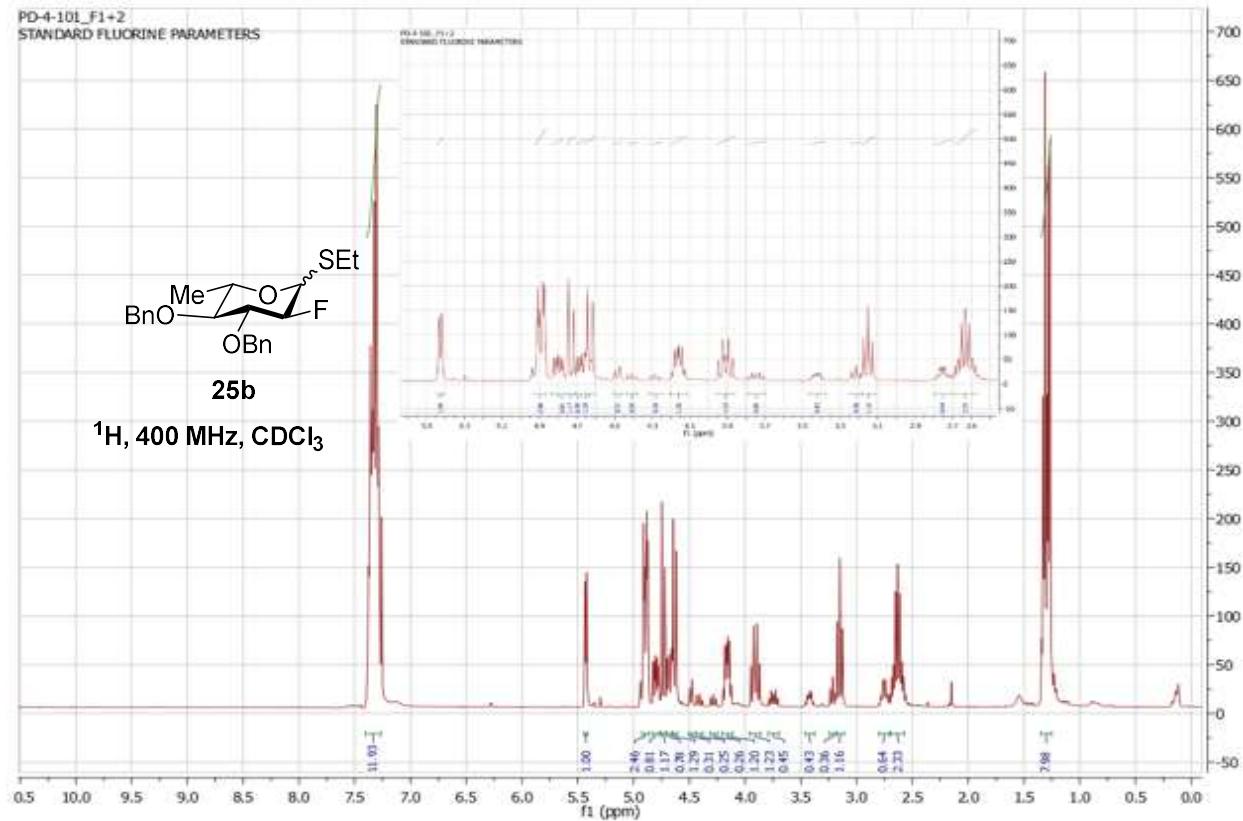
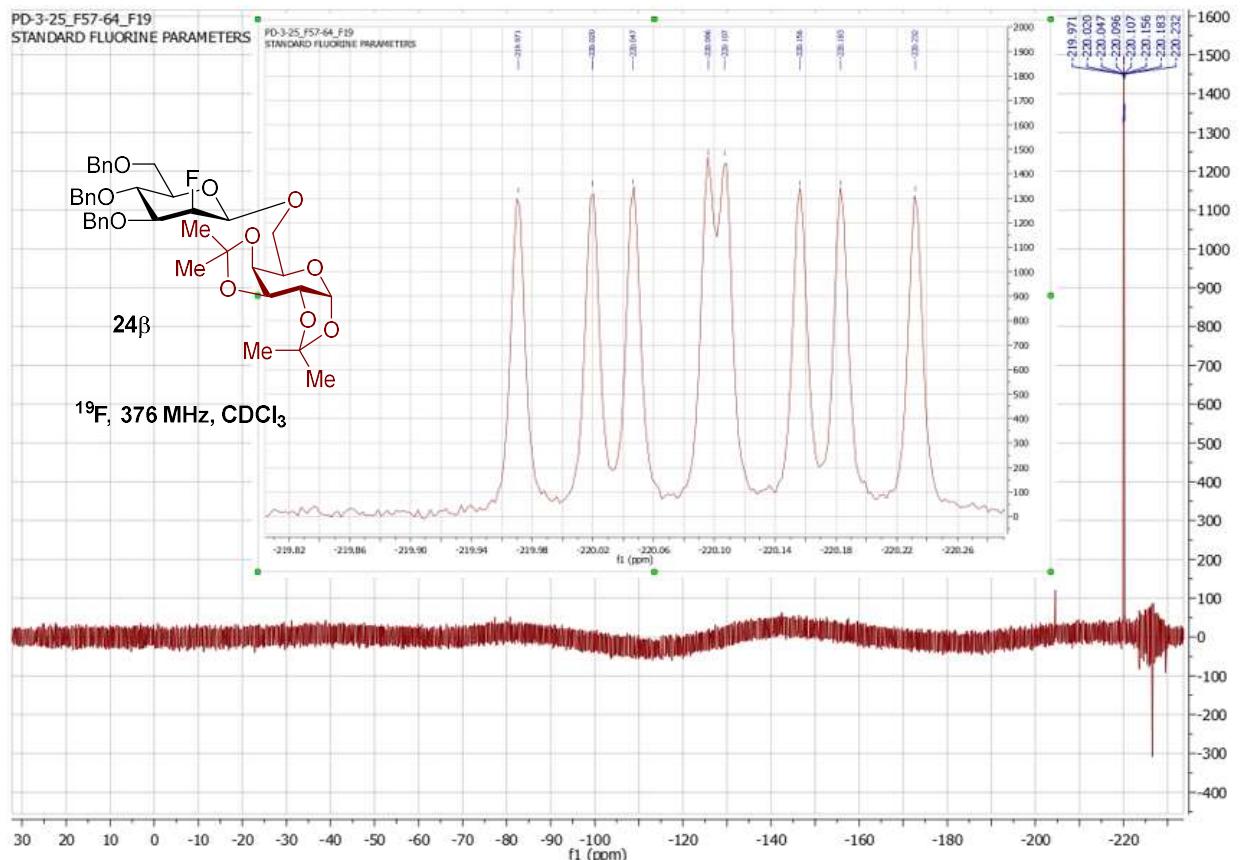
PD-3-191_F32-38_F19
STANDARD FLUORINE PARAMETERS





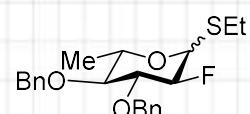






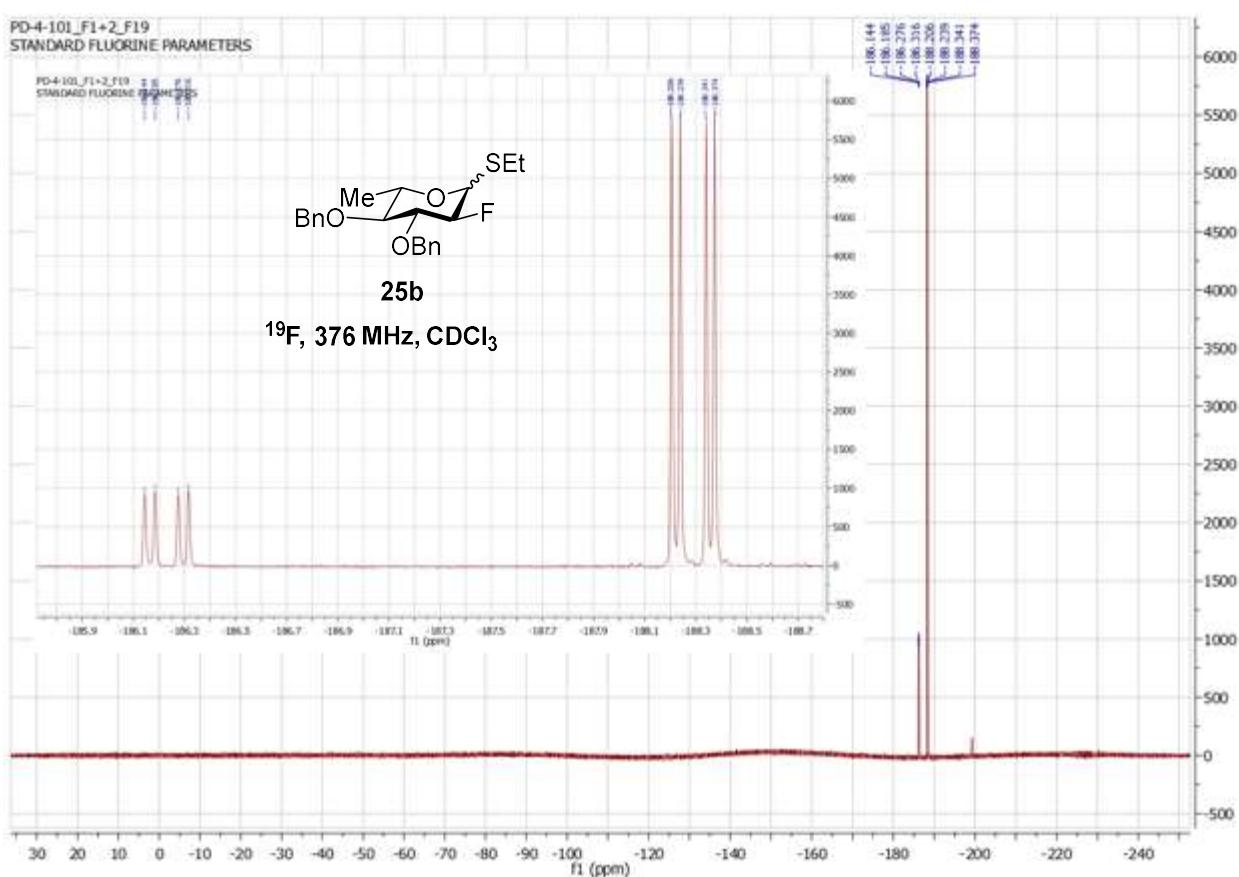
PD-4-101_F1+2_F19
STANDARD FLUORINE PARAMETERS

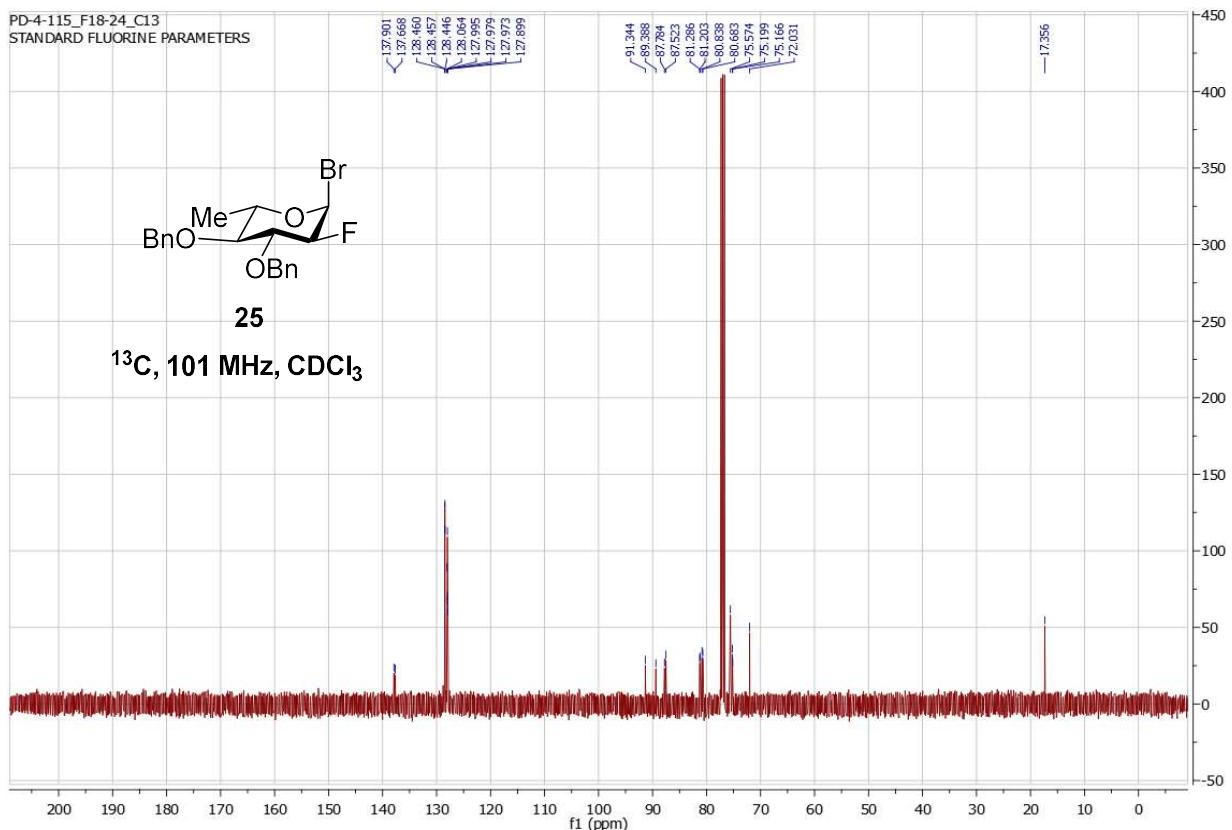
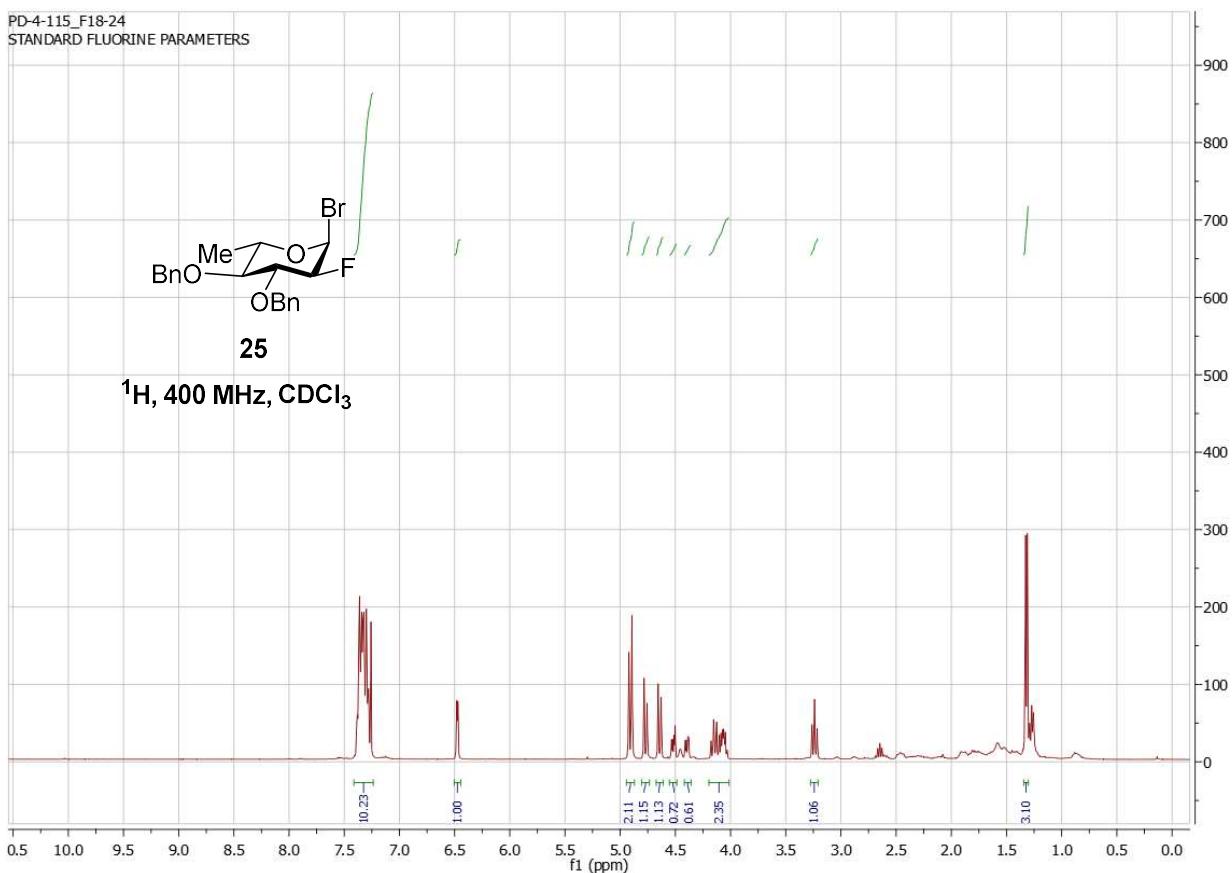
PD-4_101_F1+2_F19
STANDARD FLUORINE PARAMETERS

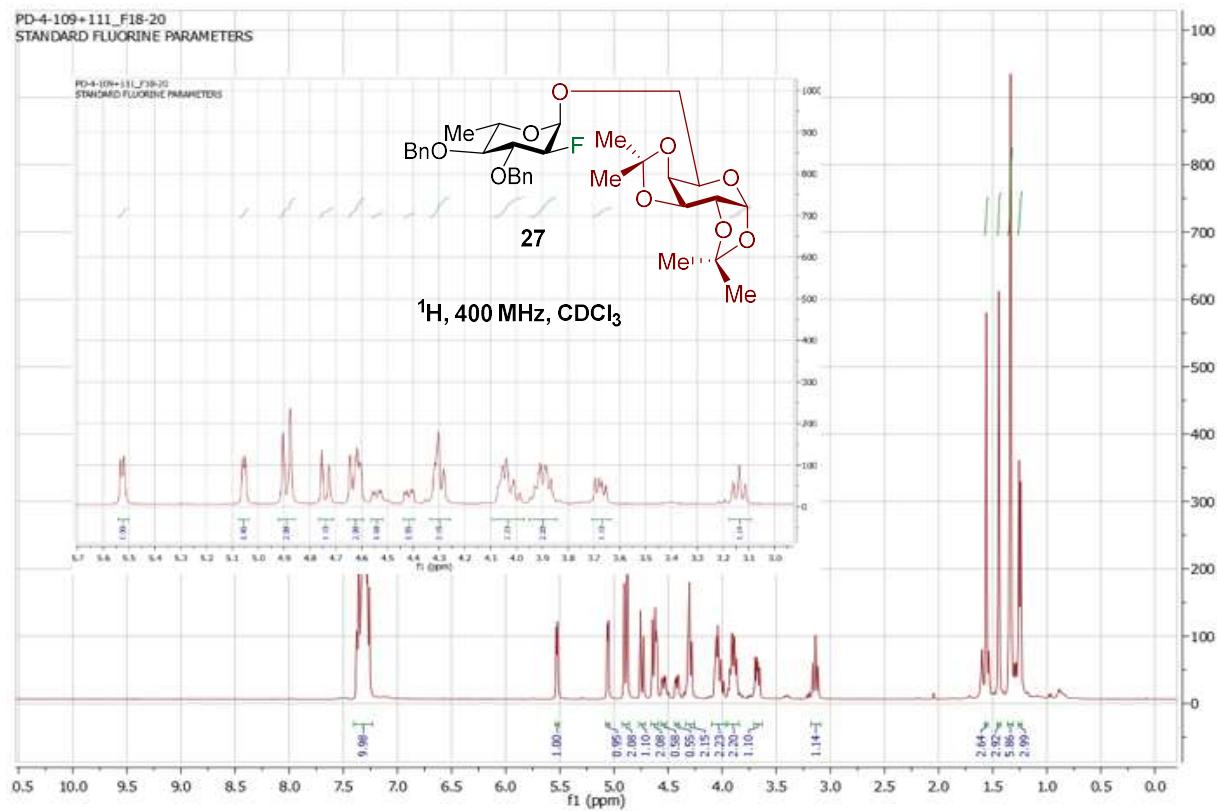
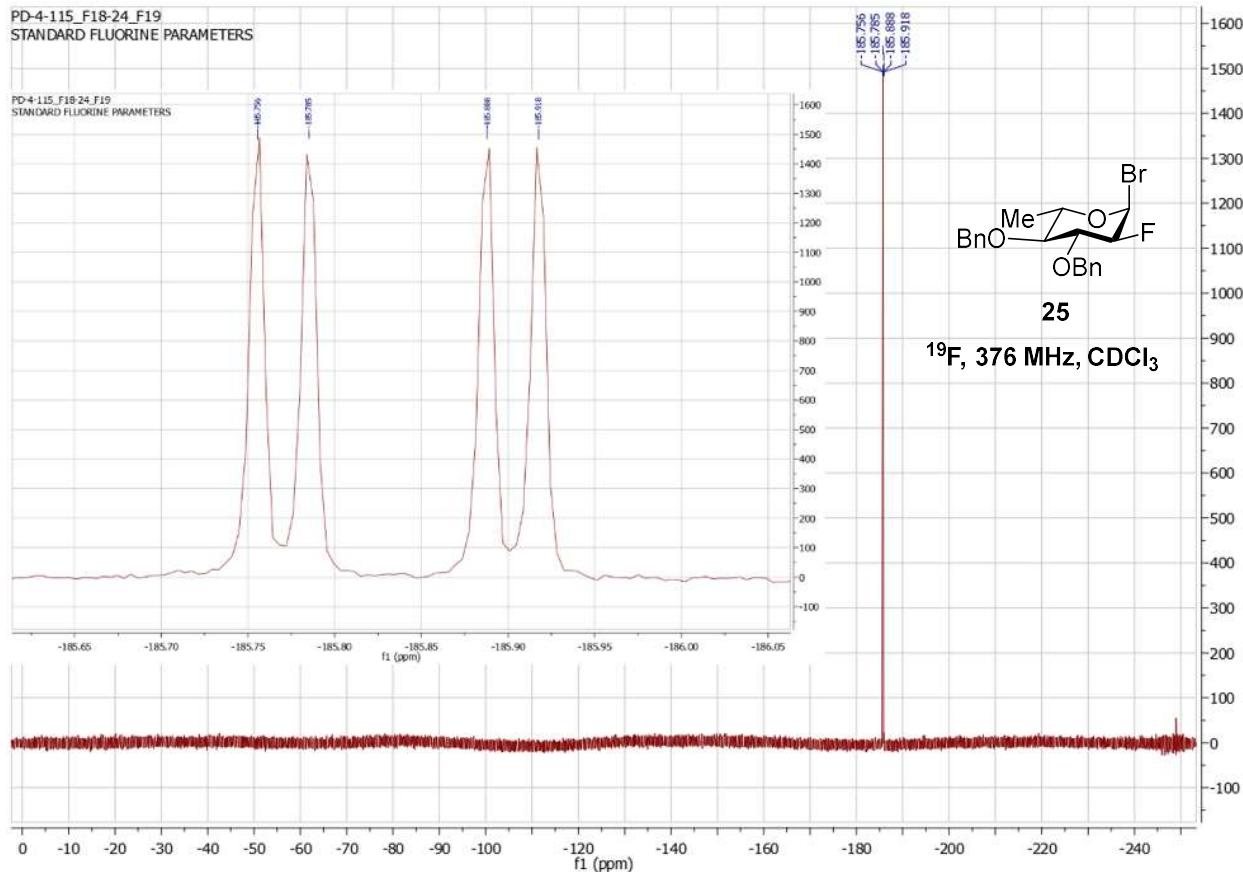


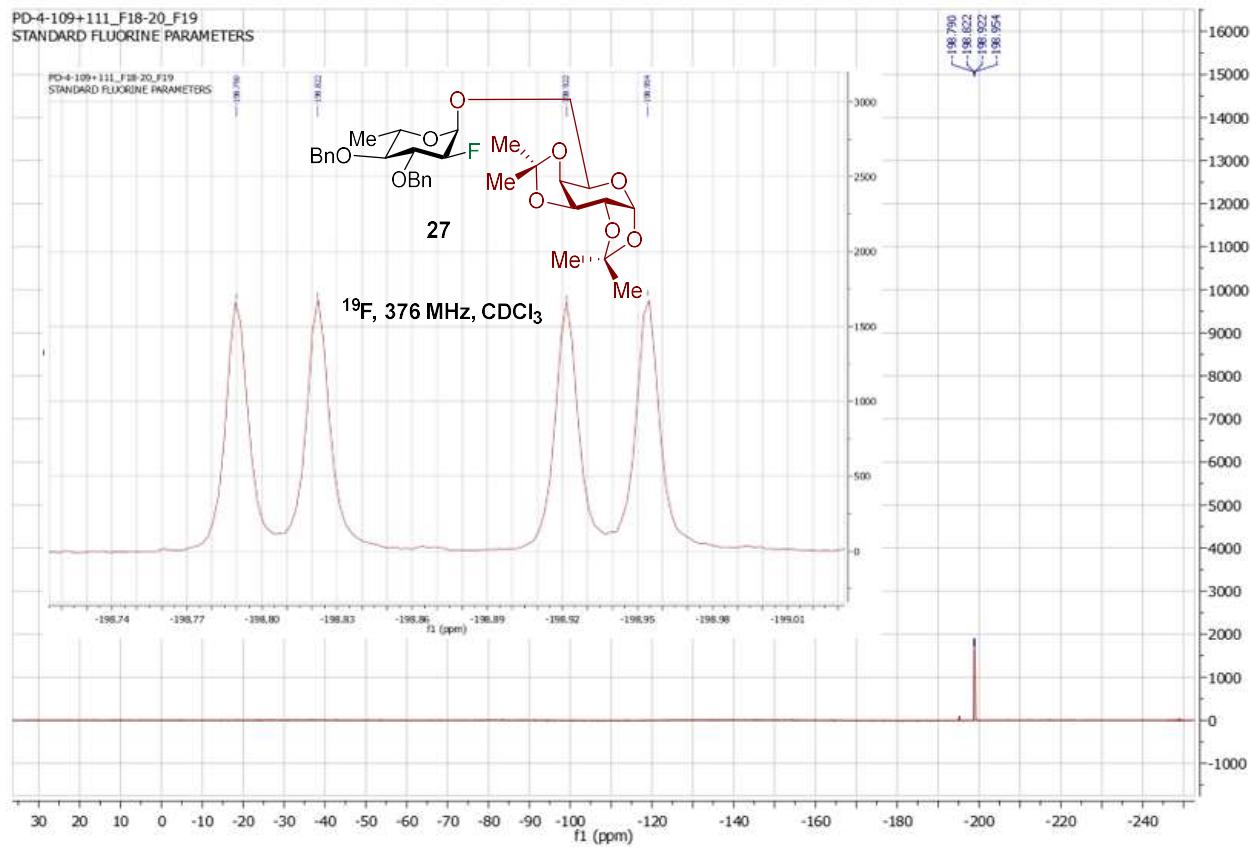
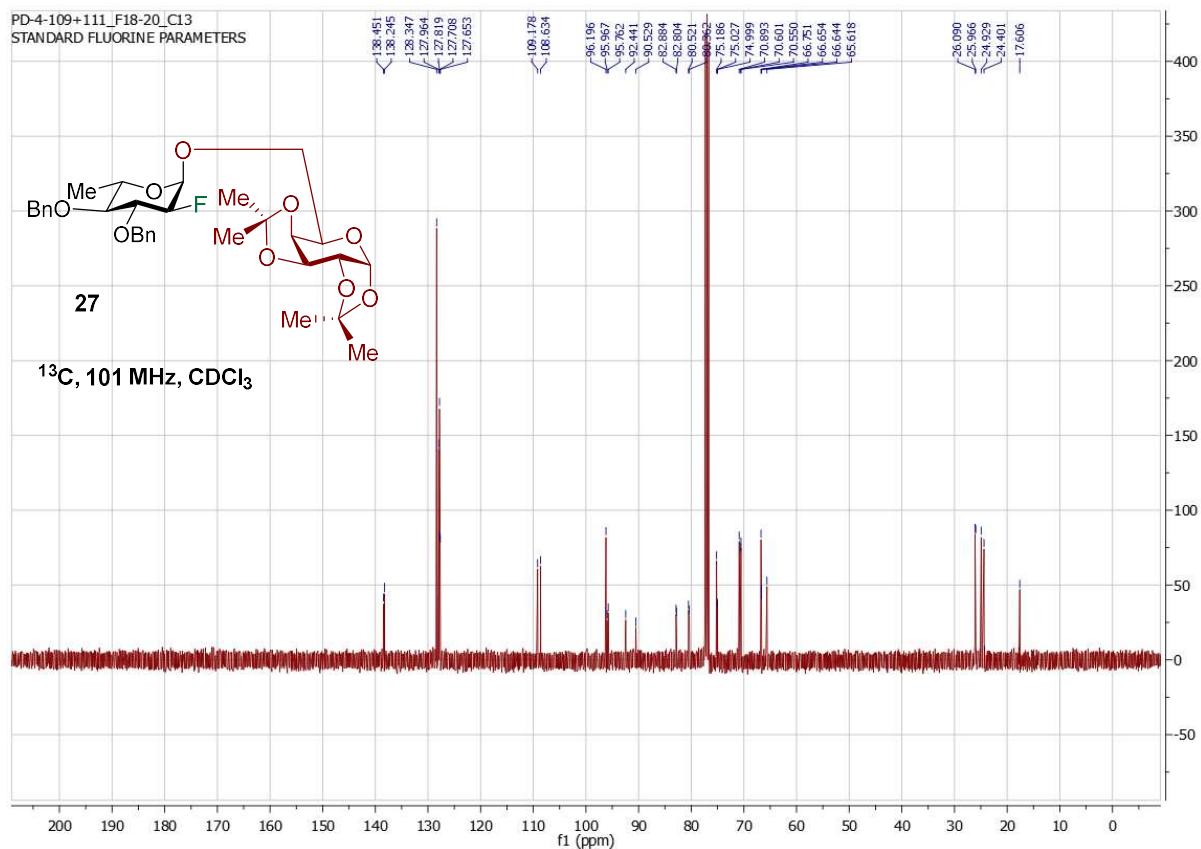
25b

^{19}F , 376 MHz, CDCl_3



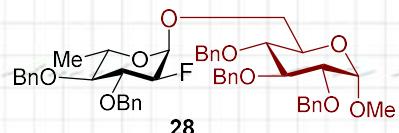






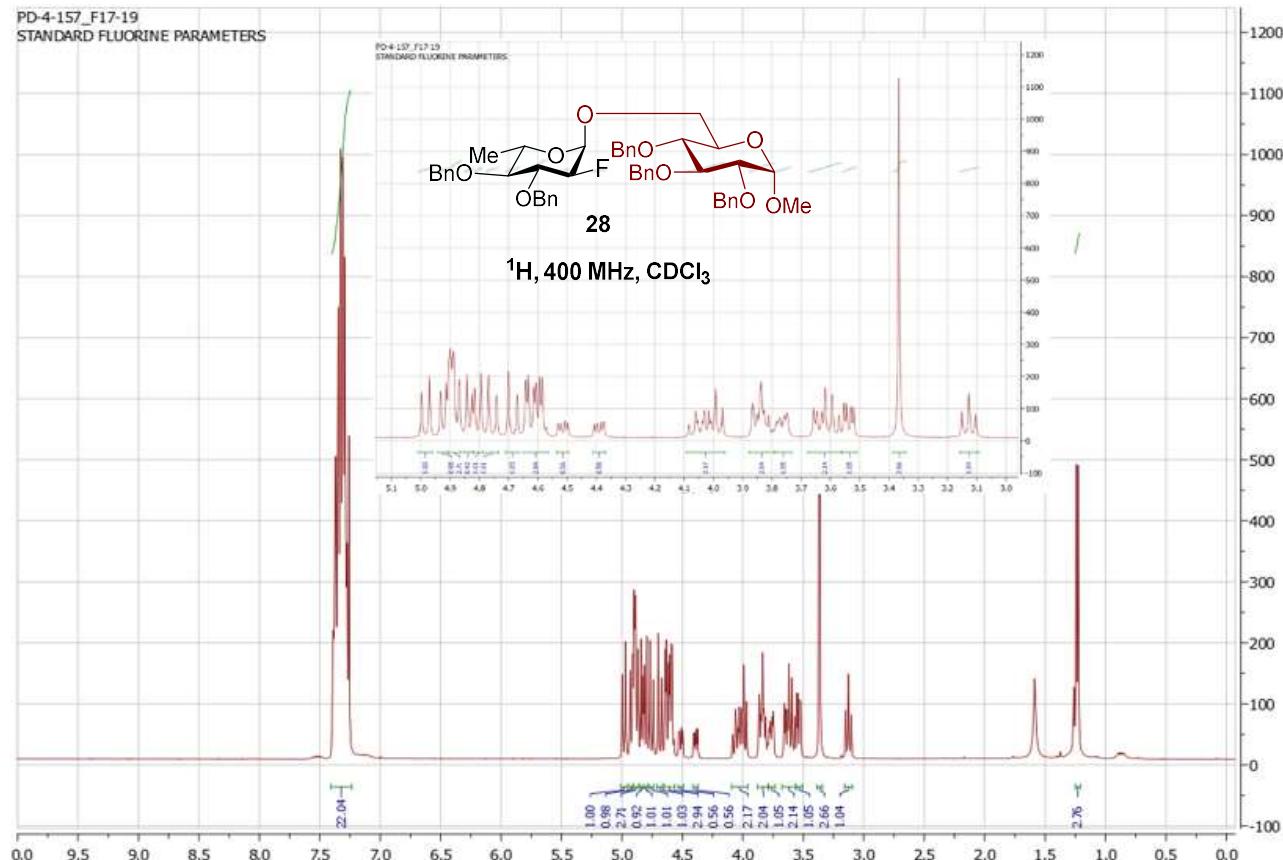
PD-4-157_F17-19
STANDARD FLUORINE PARAMETERS

PD-4-157_F17-19
STANDARD FLUORINE PARAMETERS



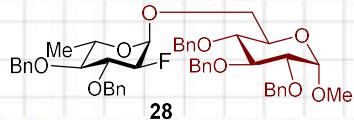
28

^1H , 400 MHz, CDCl_3



Peak Position (ppm)	Assignment
7.6	Ar
4.5 - 5.5	Olefins
3.0 - 4.0	Aliphatic
1.4	OMe

PD-4-157_F17-19_F19
STANDARD FLUORINE PARAMETERS

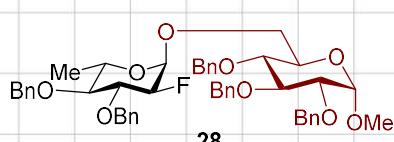


28

PD-4-157_F17-19_F19
STANDARD FLUORINE PARAMETERS

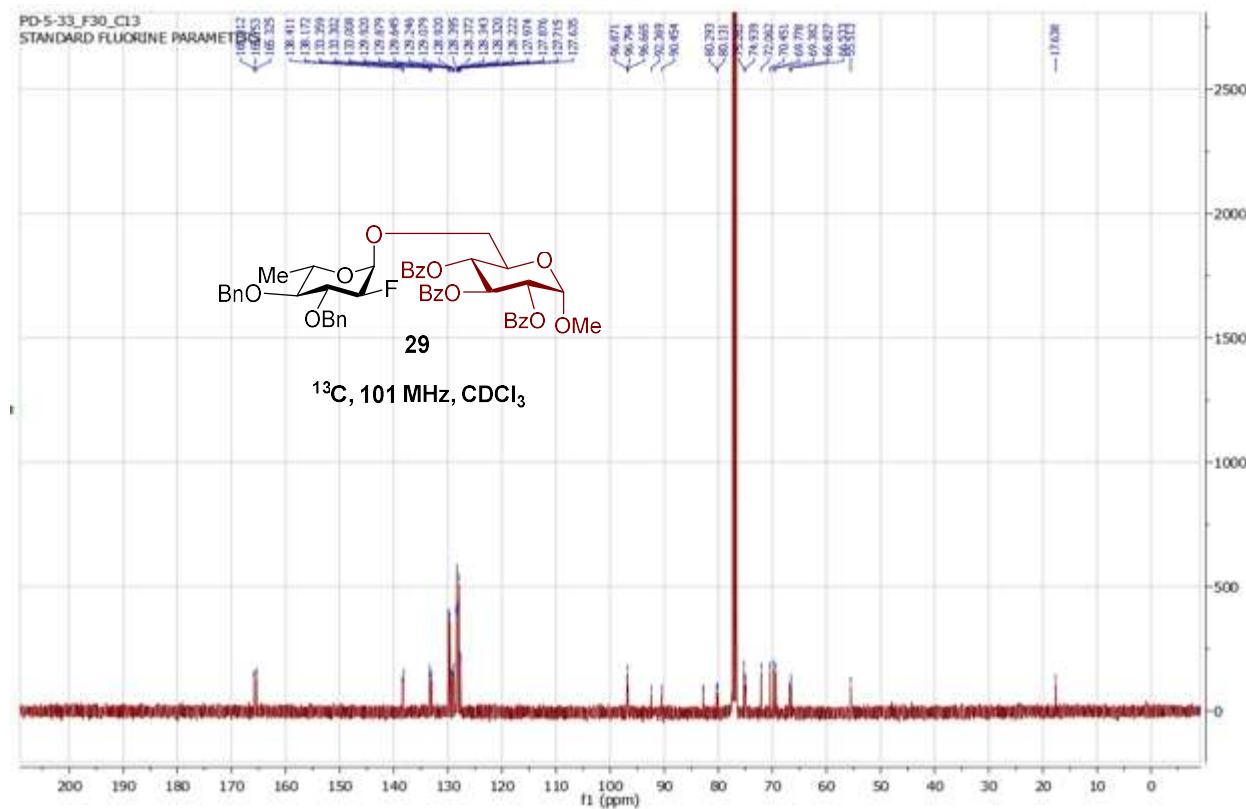
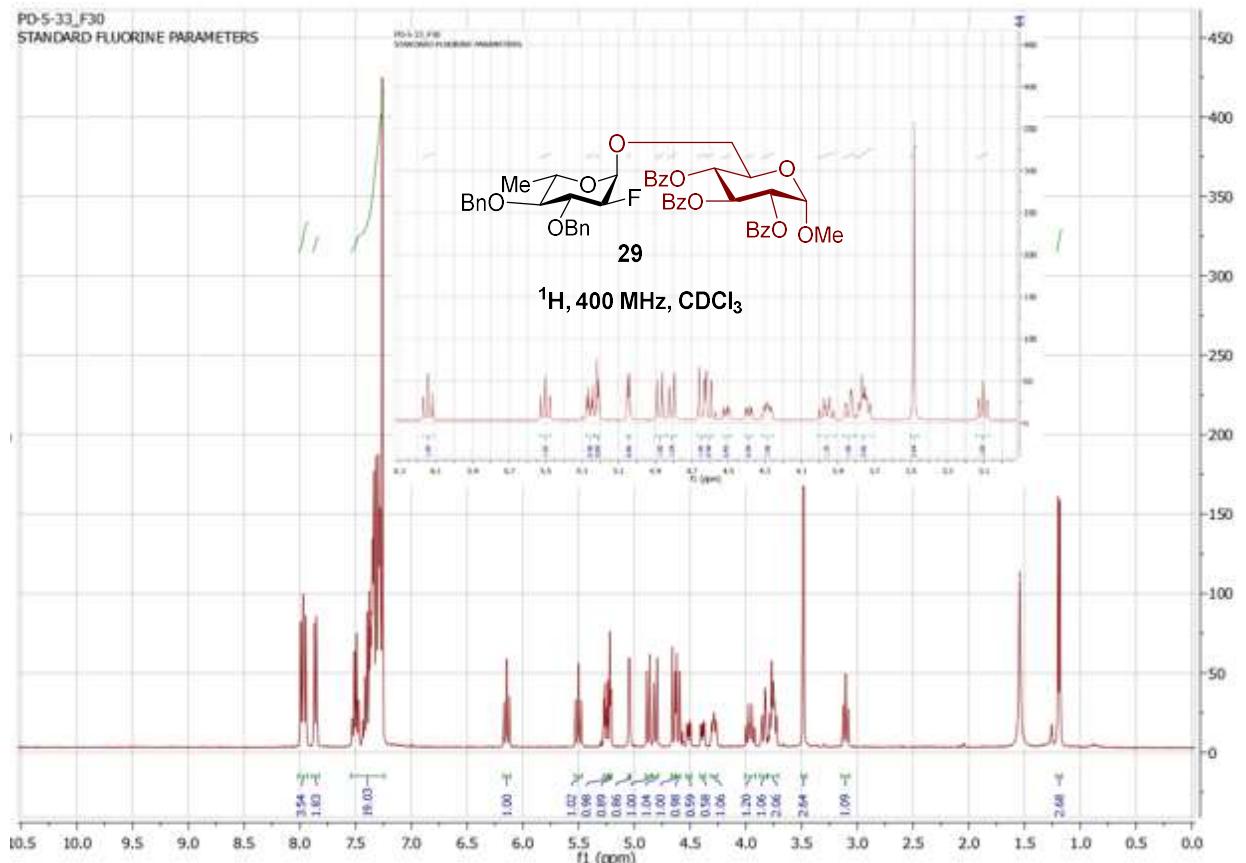
^{19}F , 376 MHz, CDCl_3

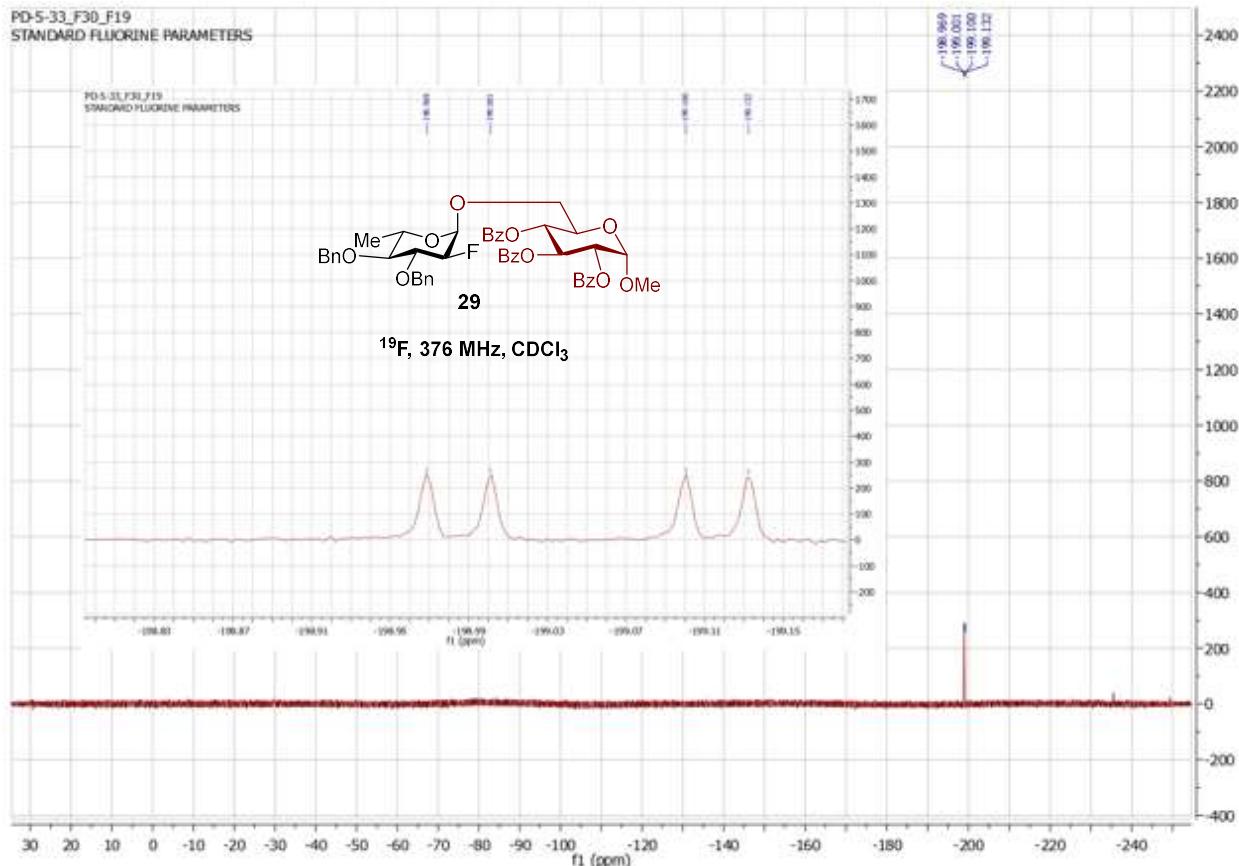
PD-4-157_F17-19_C13
STANDARD FLUORINE PARAMETERS



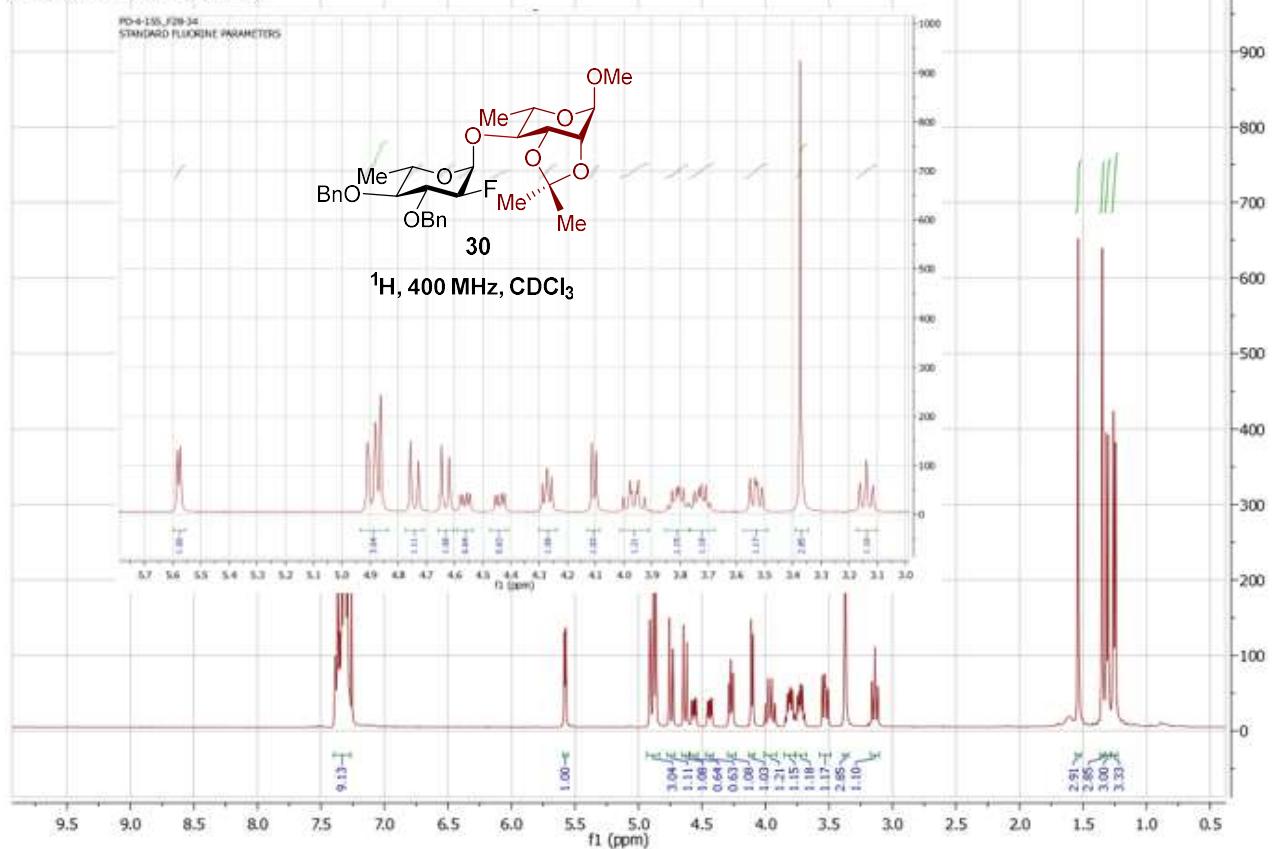
28

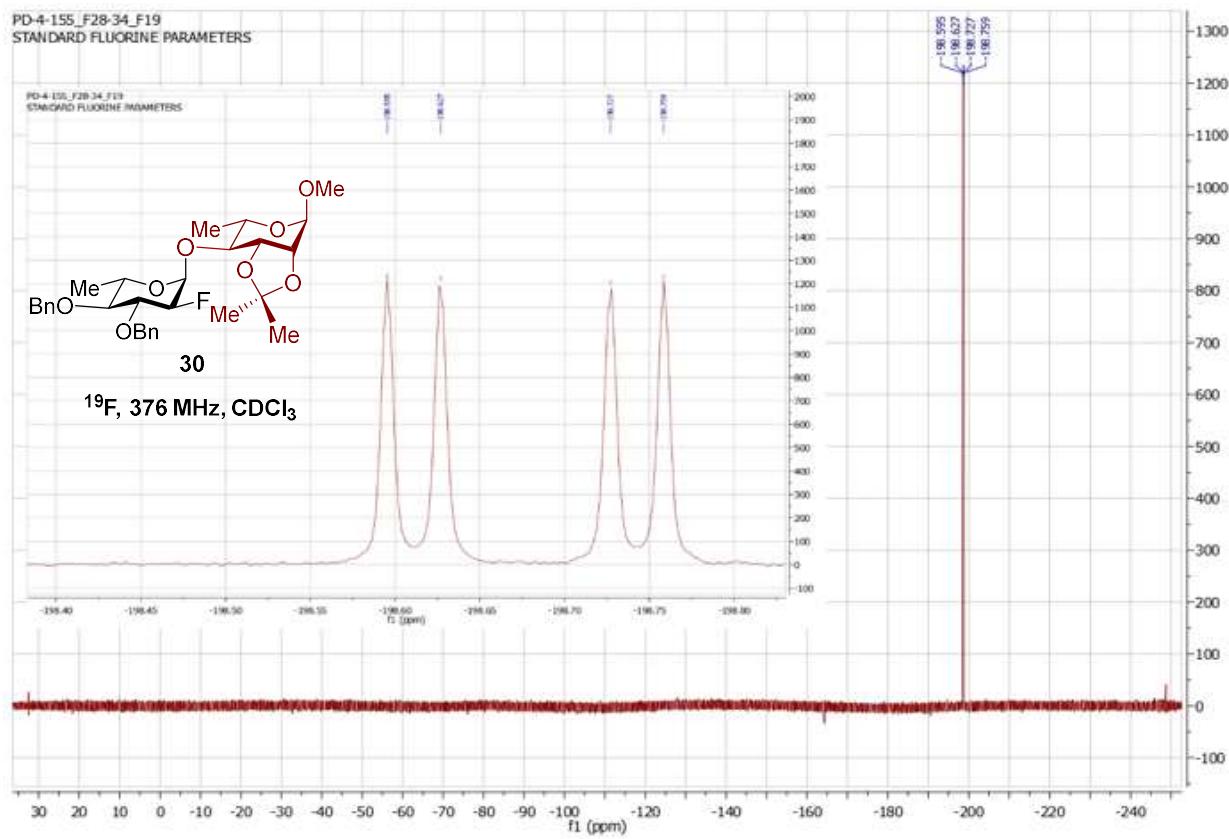
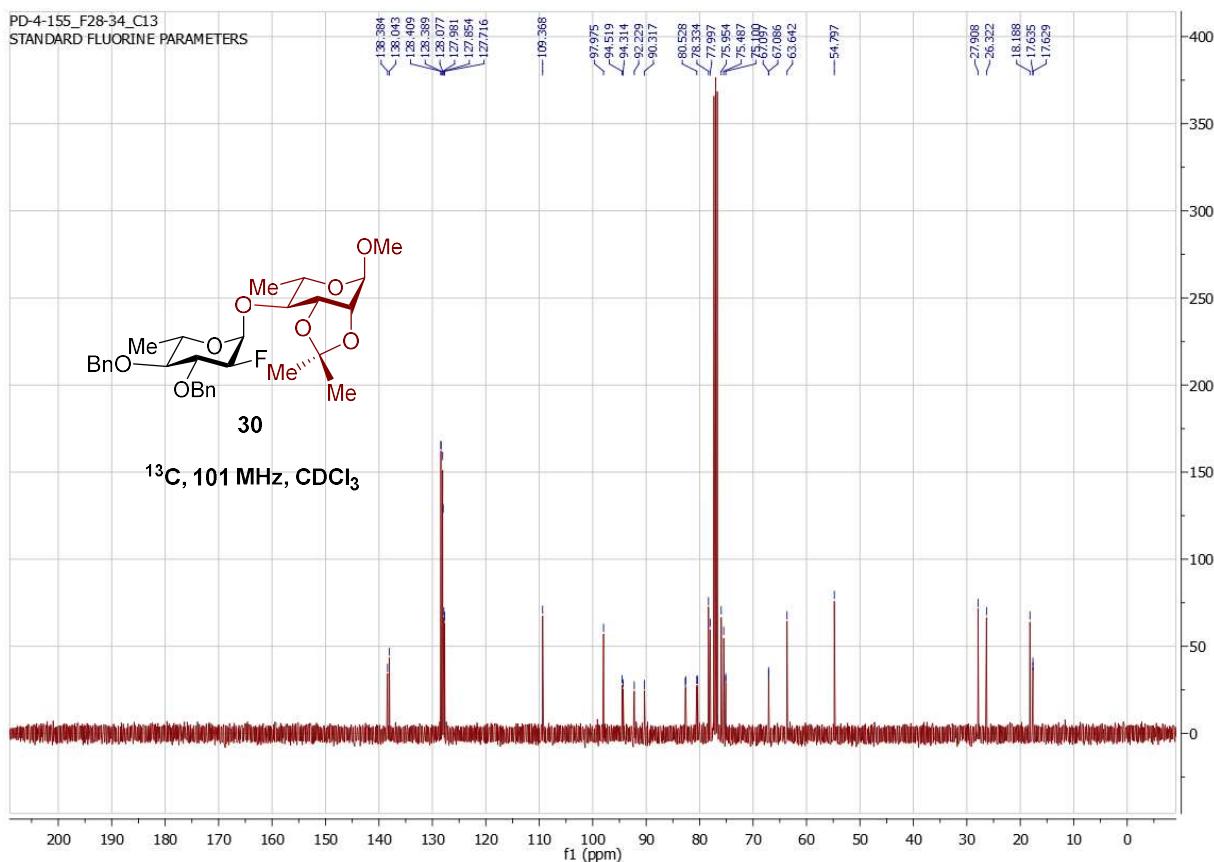
^{13}C , 101 MHz, CDCl_3



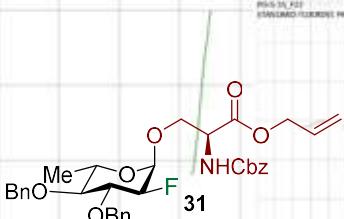


PD-4-155_F28-34
STANDARD FLUORINE PARAMETERS

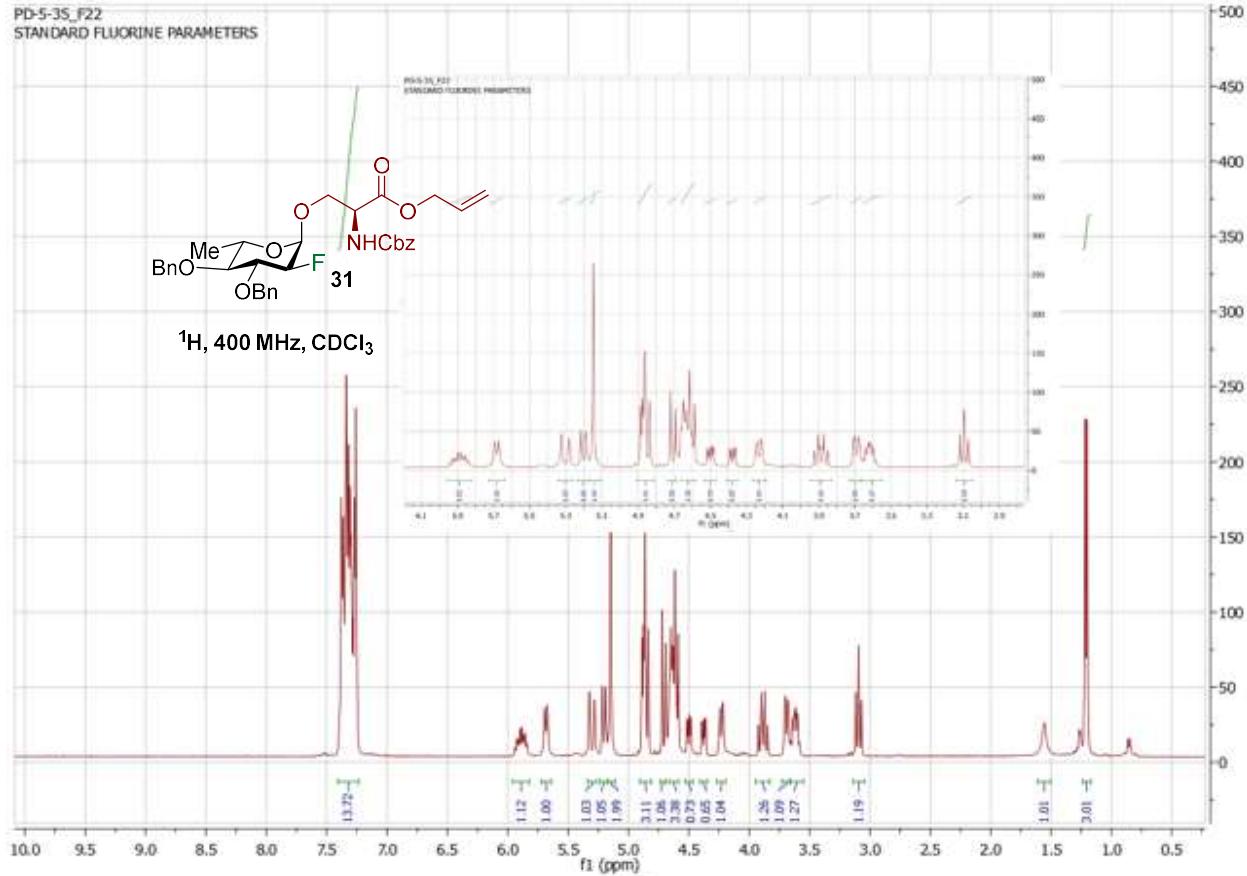




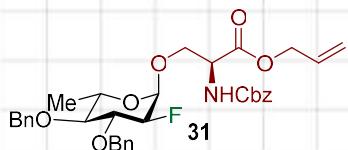
PD-5-35_F22
STANDARD FLUORINE PARAMETERS



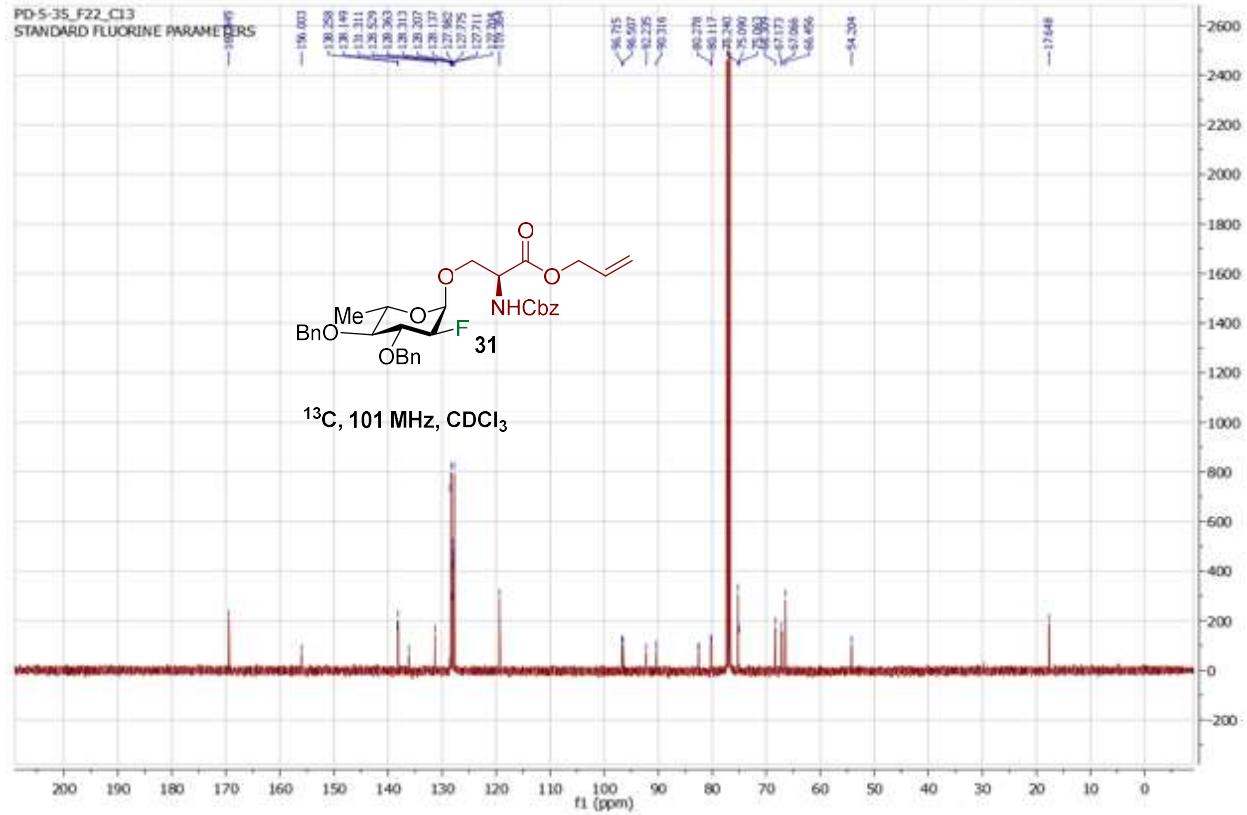
¹H, 400 MHz, CDCl₃



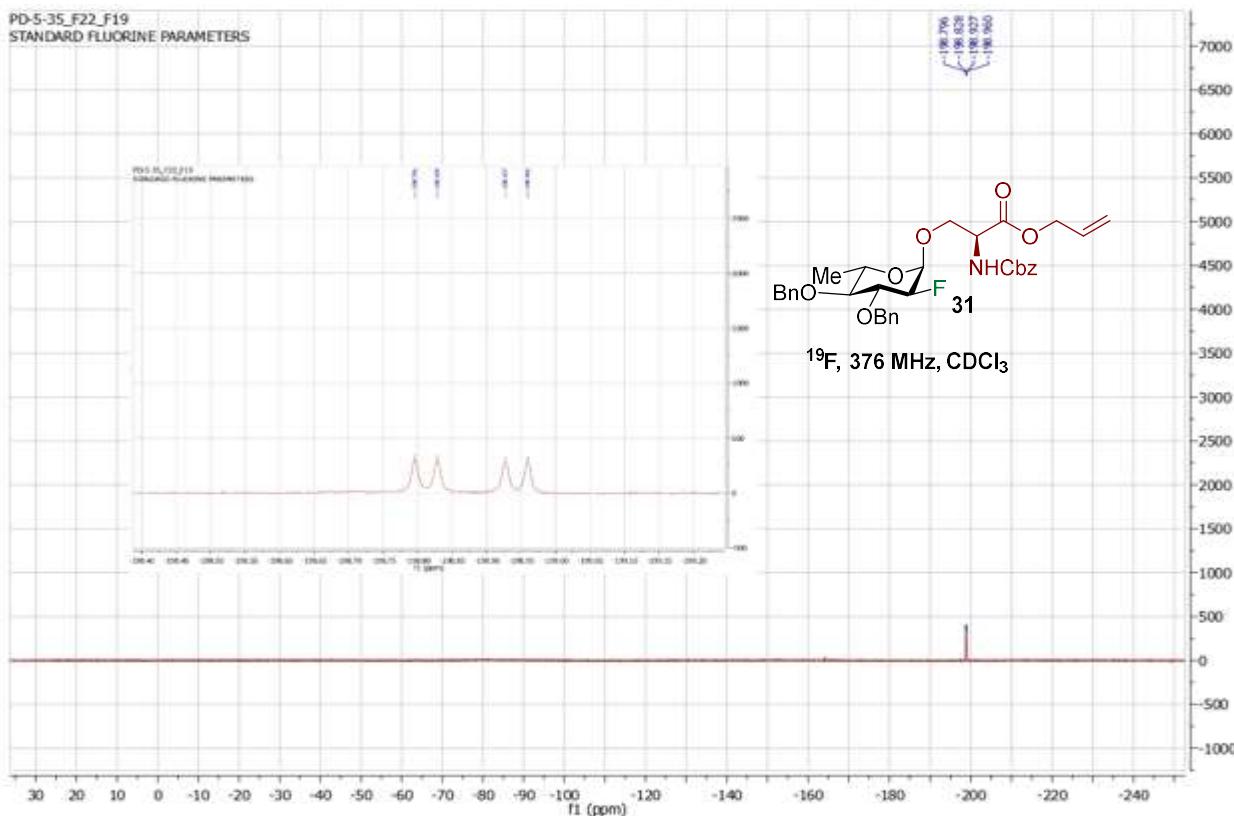
PD-5-35_F22_C13
STANDARD FLUORINE PARAMETERS



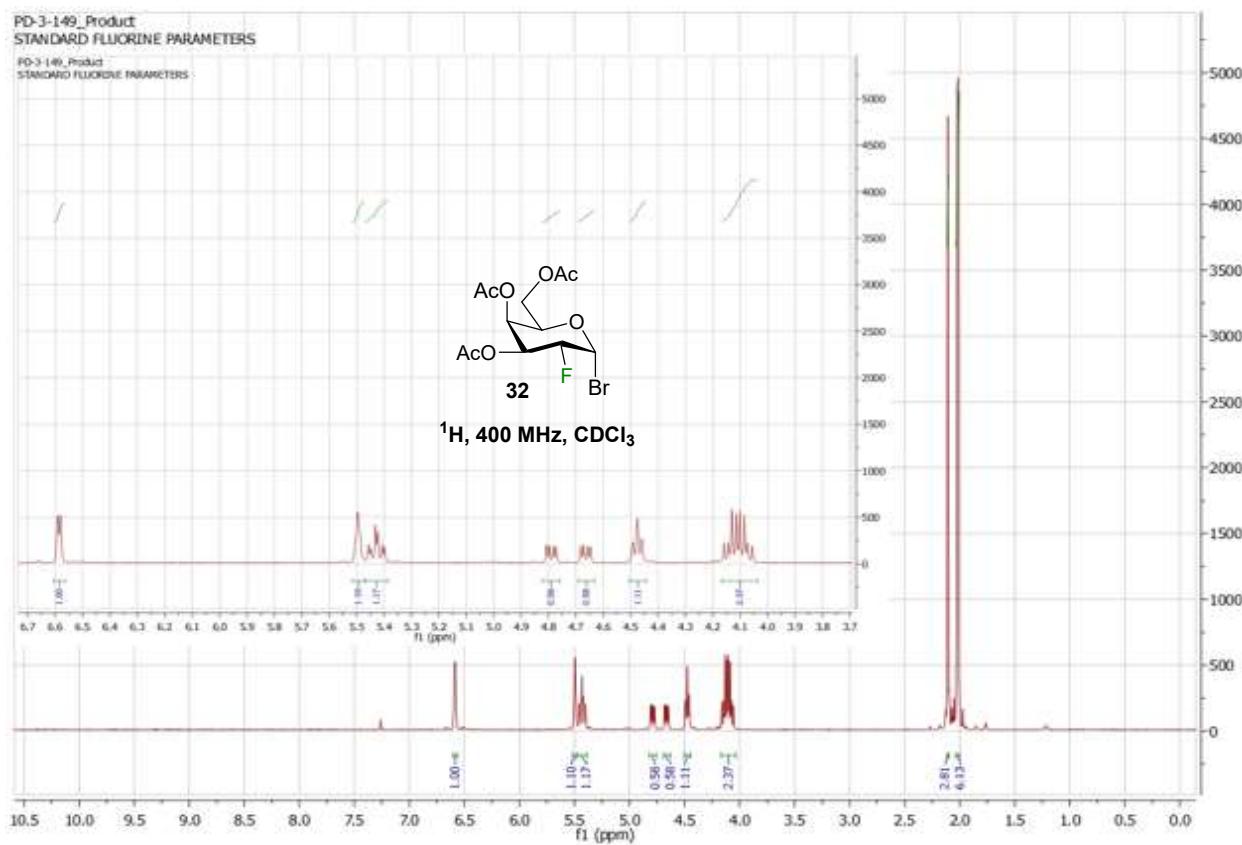
¹³C, 101 MHz, CDCl₃



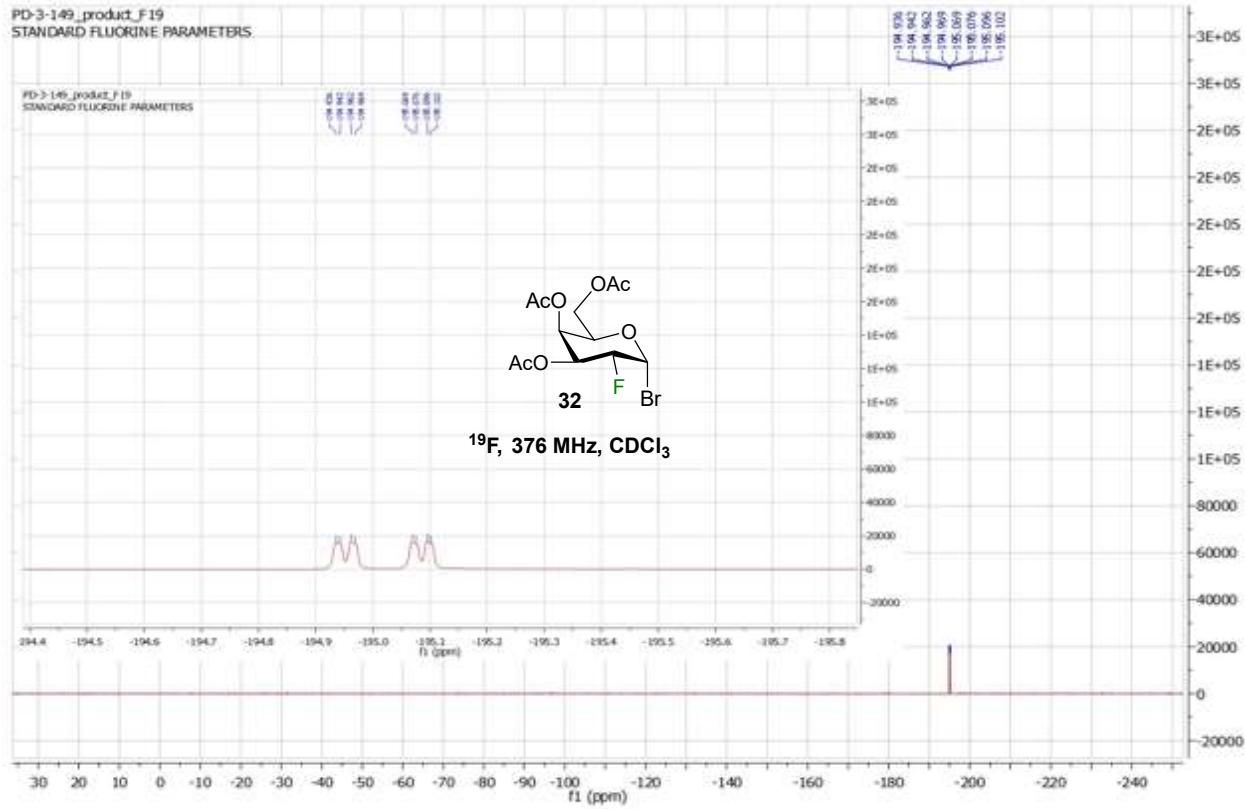
PD-5-35_F22_F19
STANDARD FLUORINE PARAMETERS



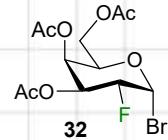
PD-3-149_Product
STANDARD FLUORINE PARAMETERS
PD-3-149_Product
STANDARD FLUORINE PARAMETERS



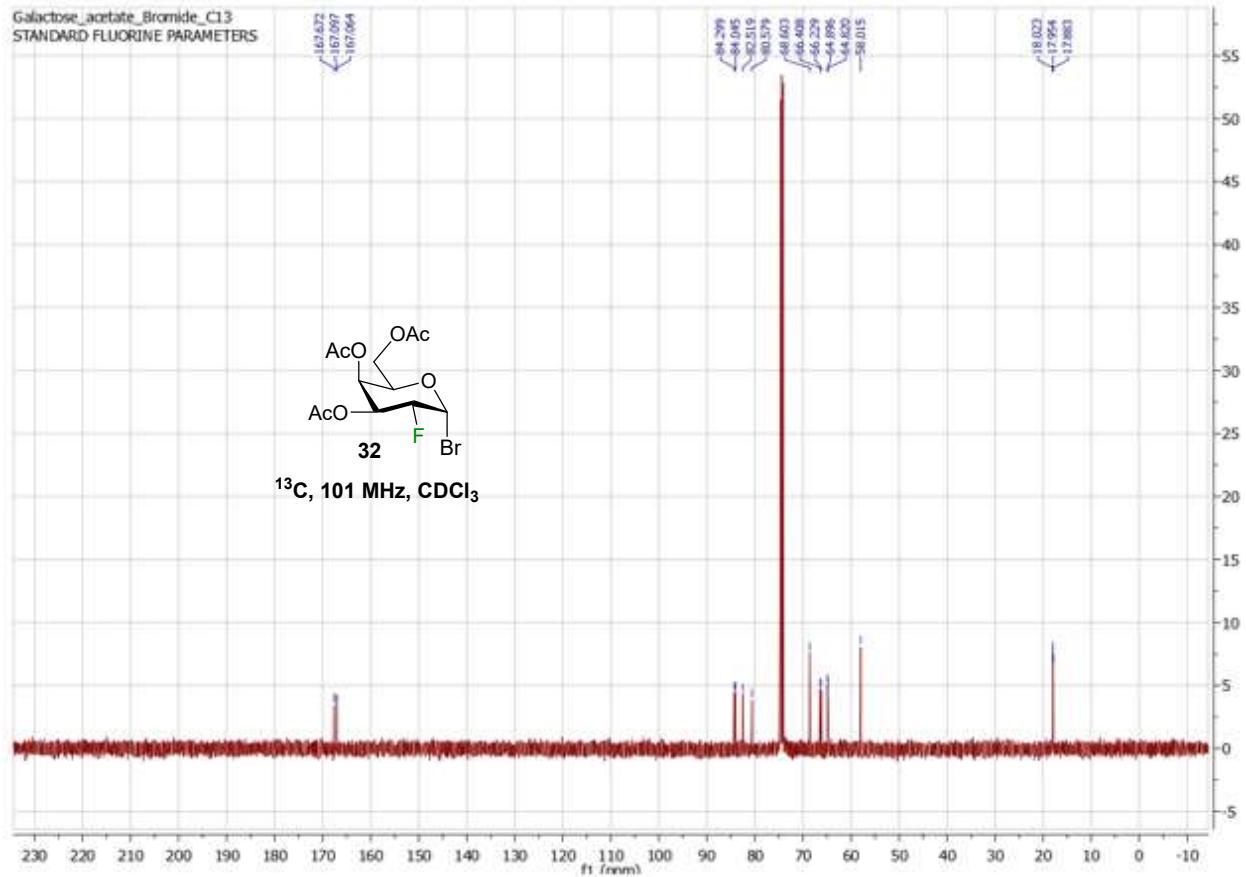
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STANDARD FLUORINE PARAMETERS

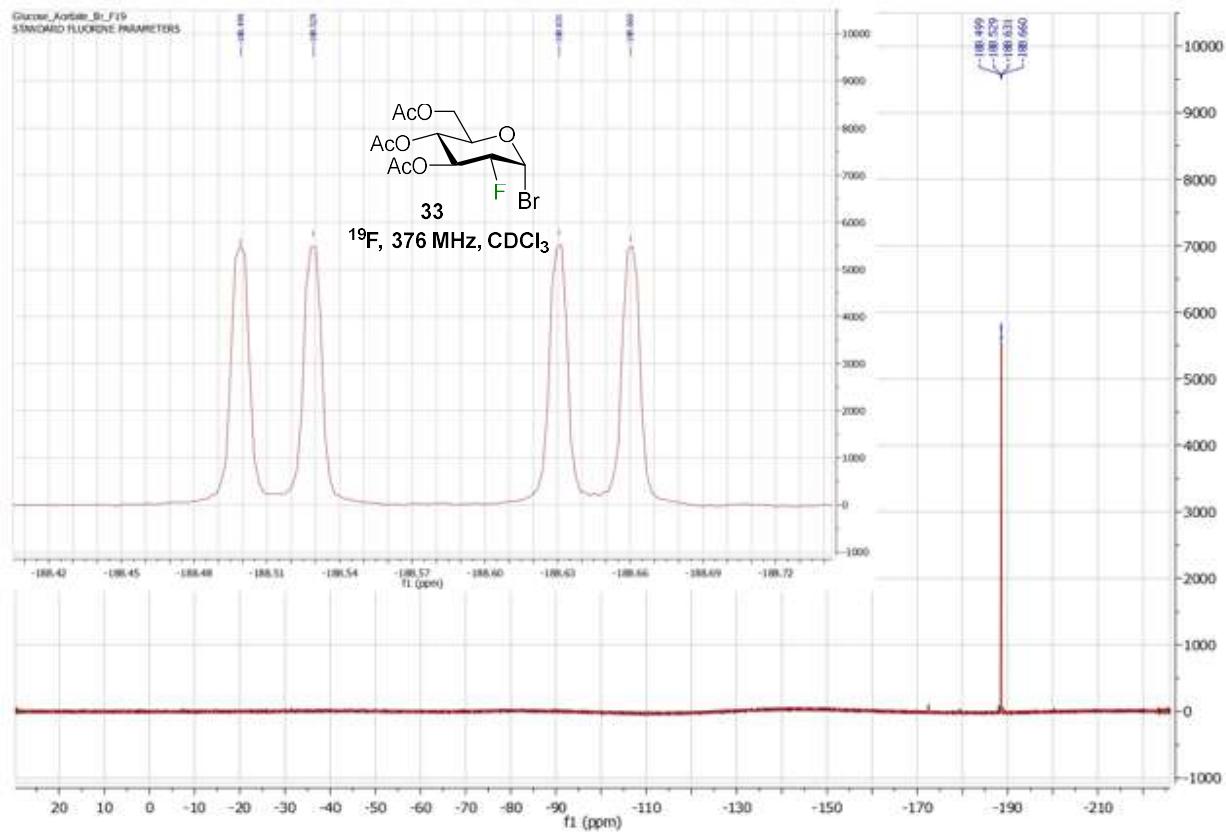
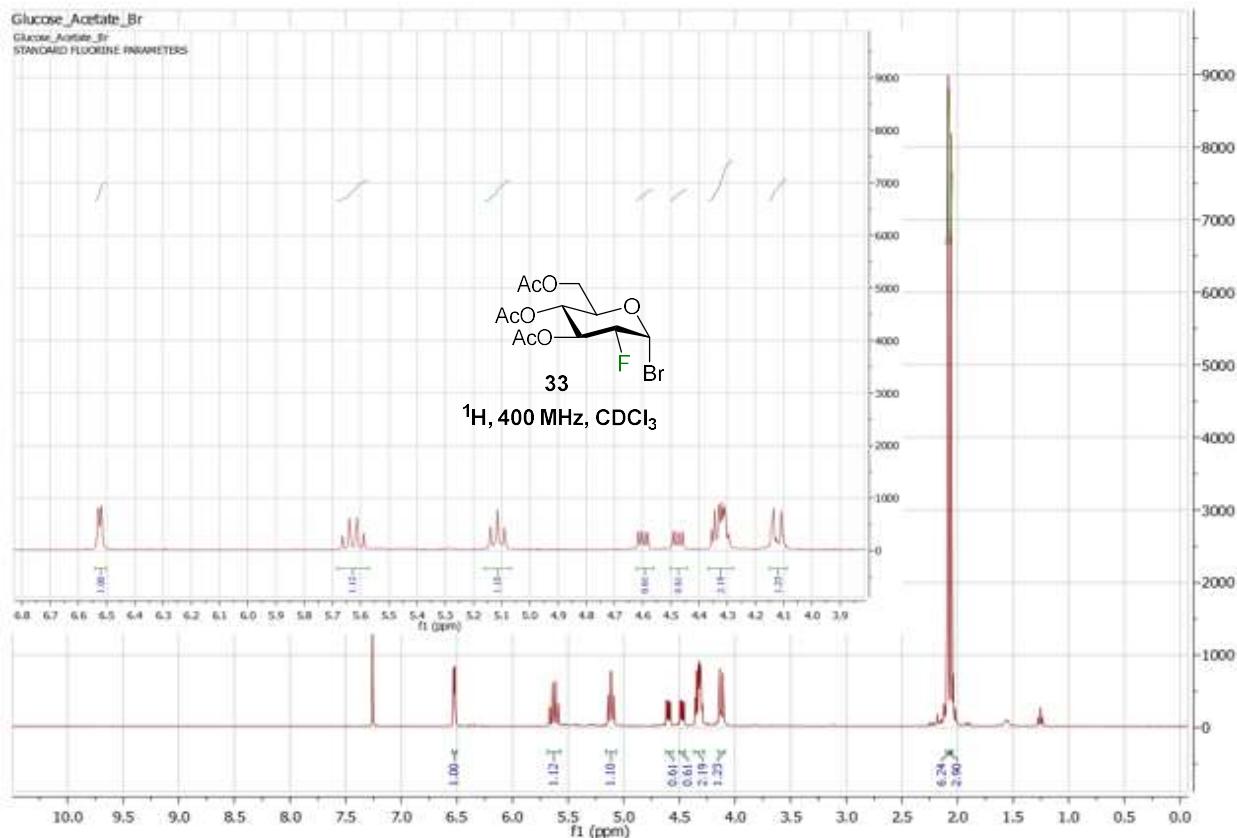


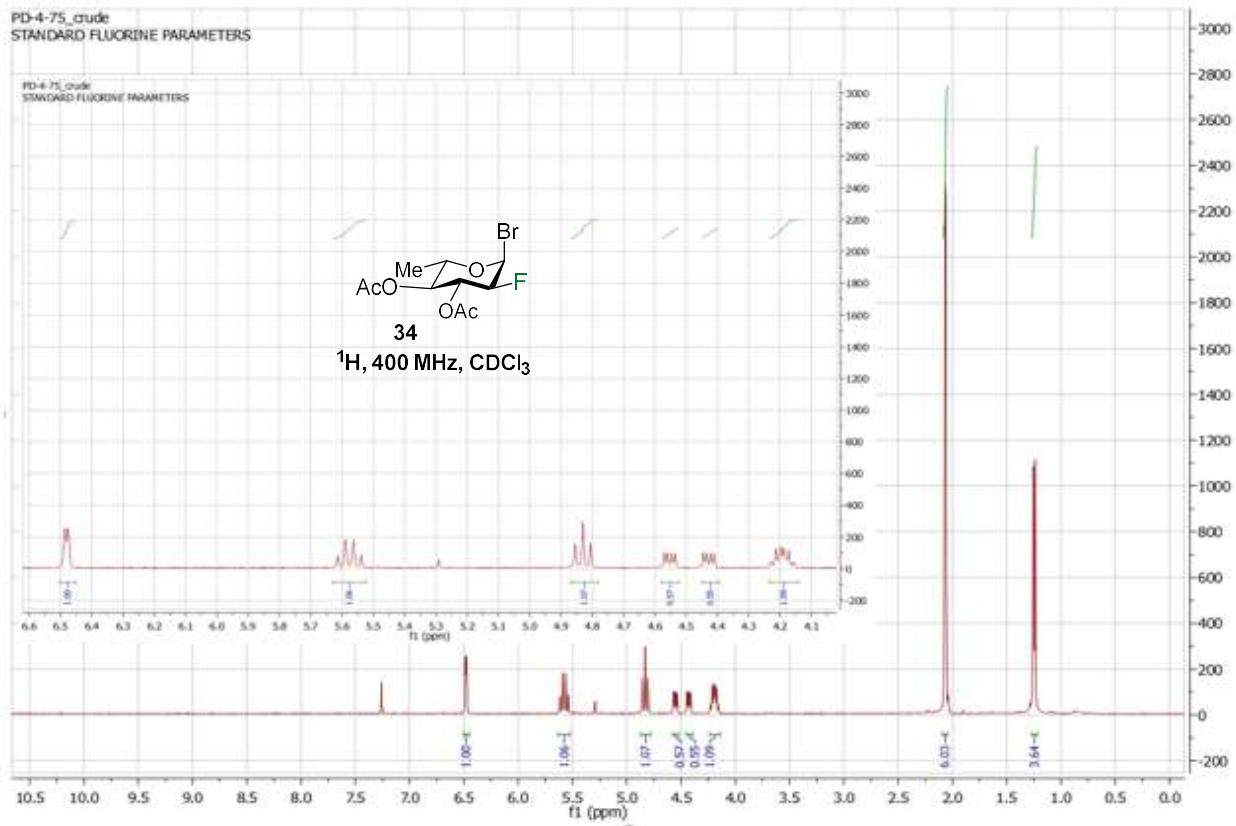
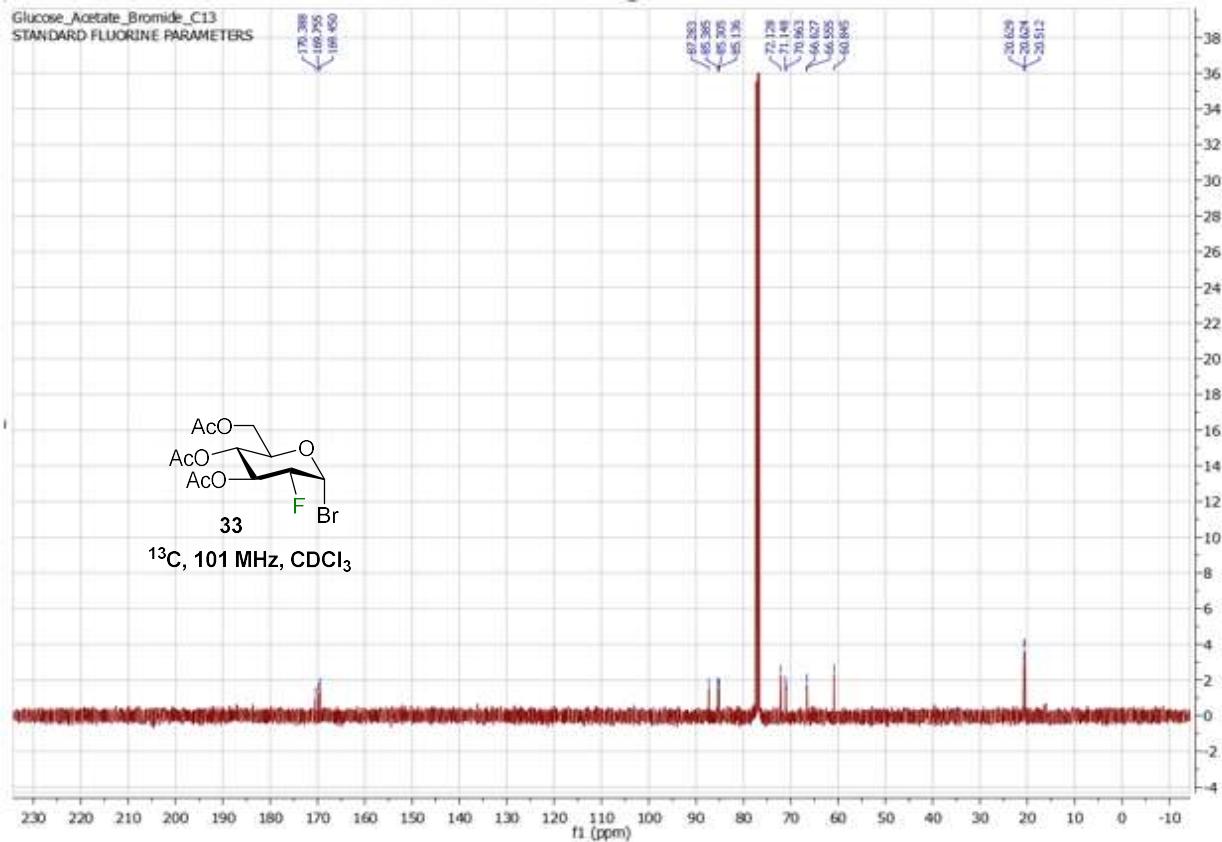
Galactose_acetate_Bromide_C13
STANDARD FLUORINE PARAMETERS

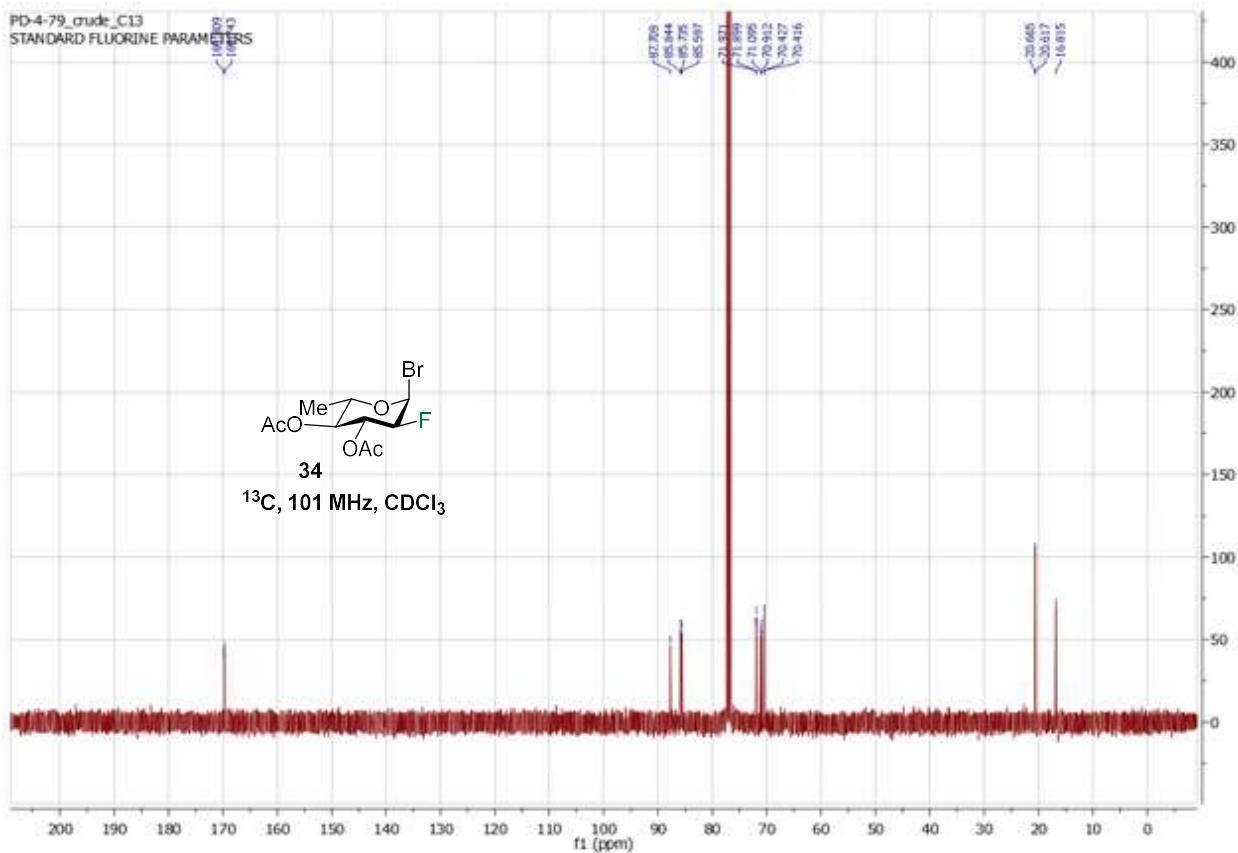
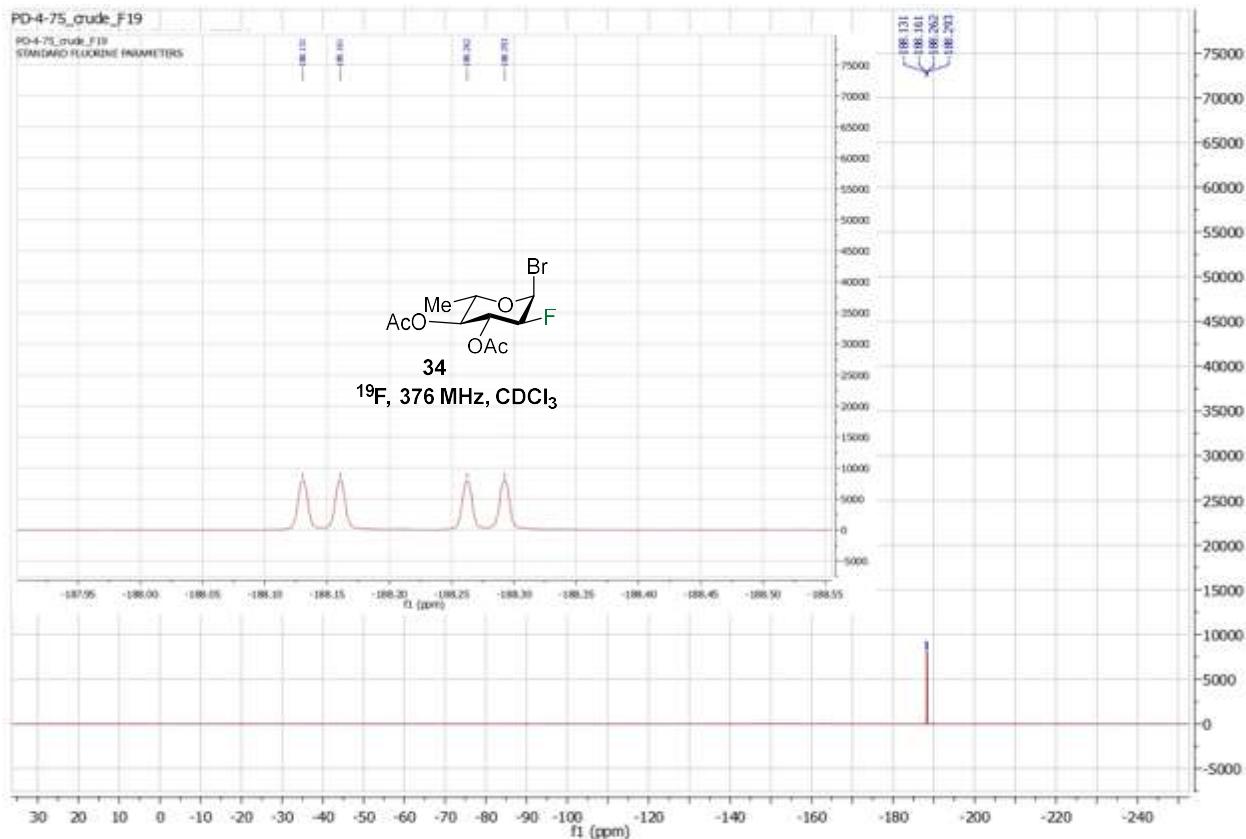


¹³C, 101 MHz, CDCl₃

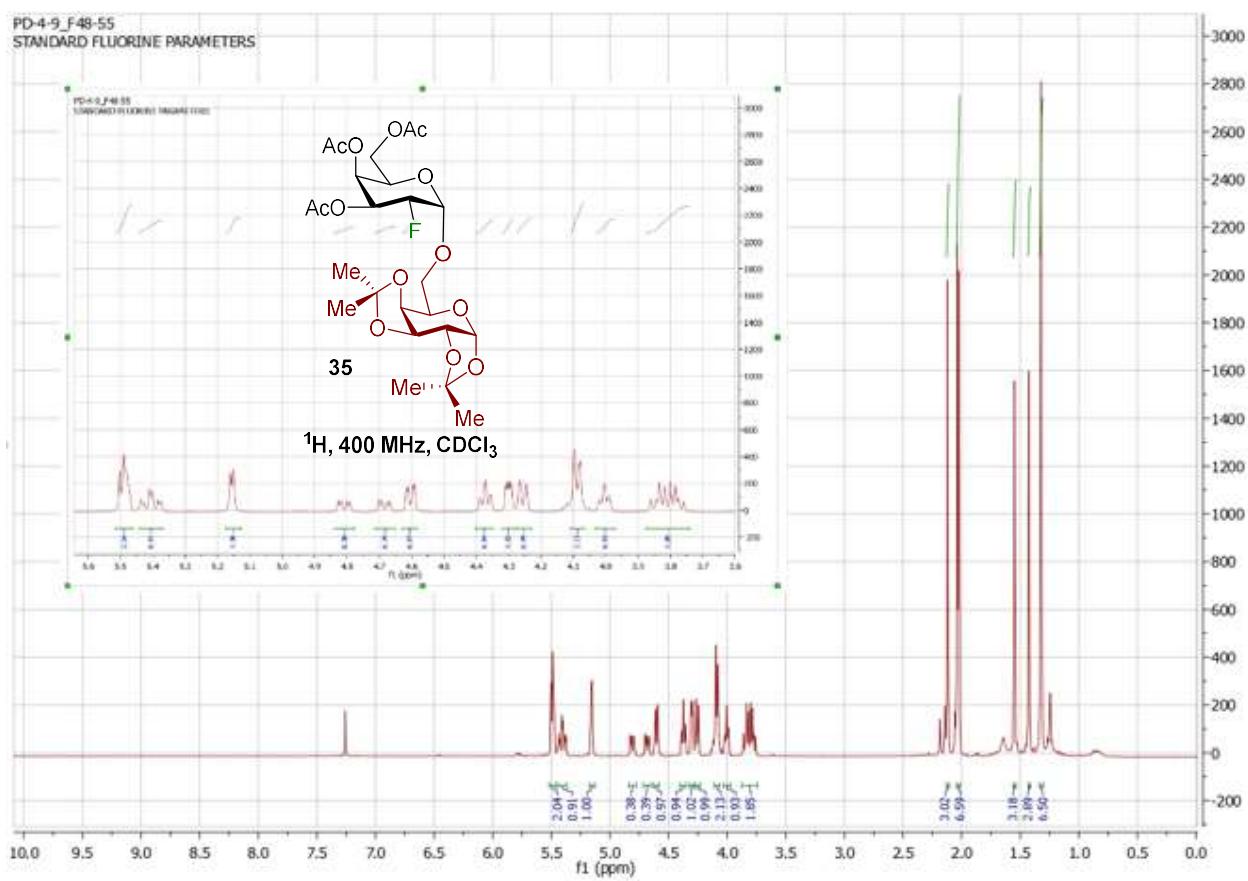




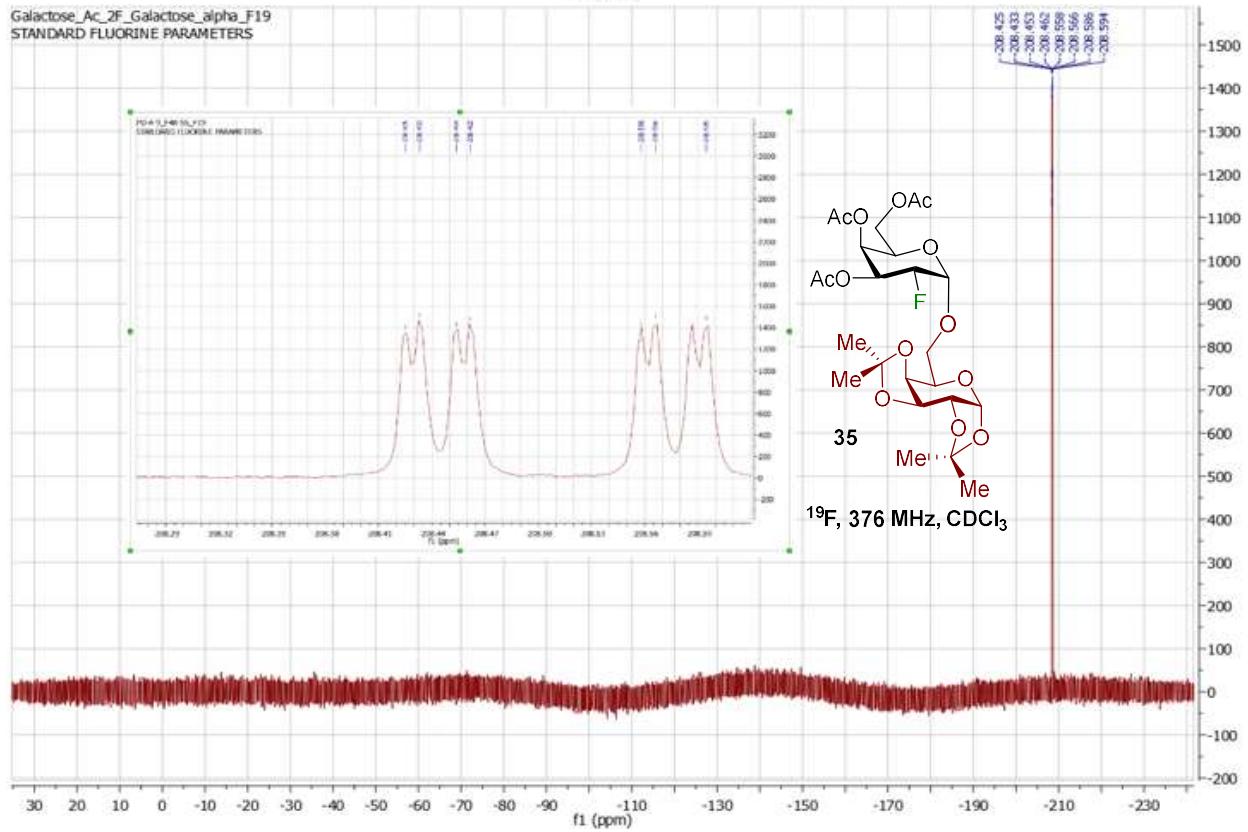


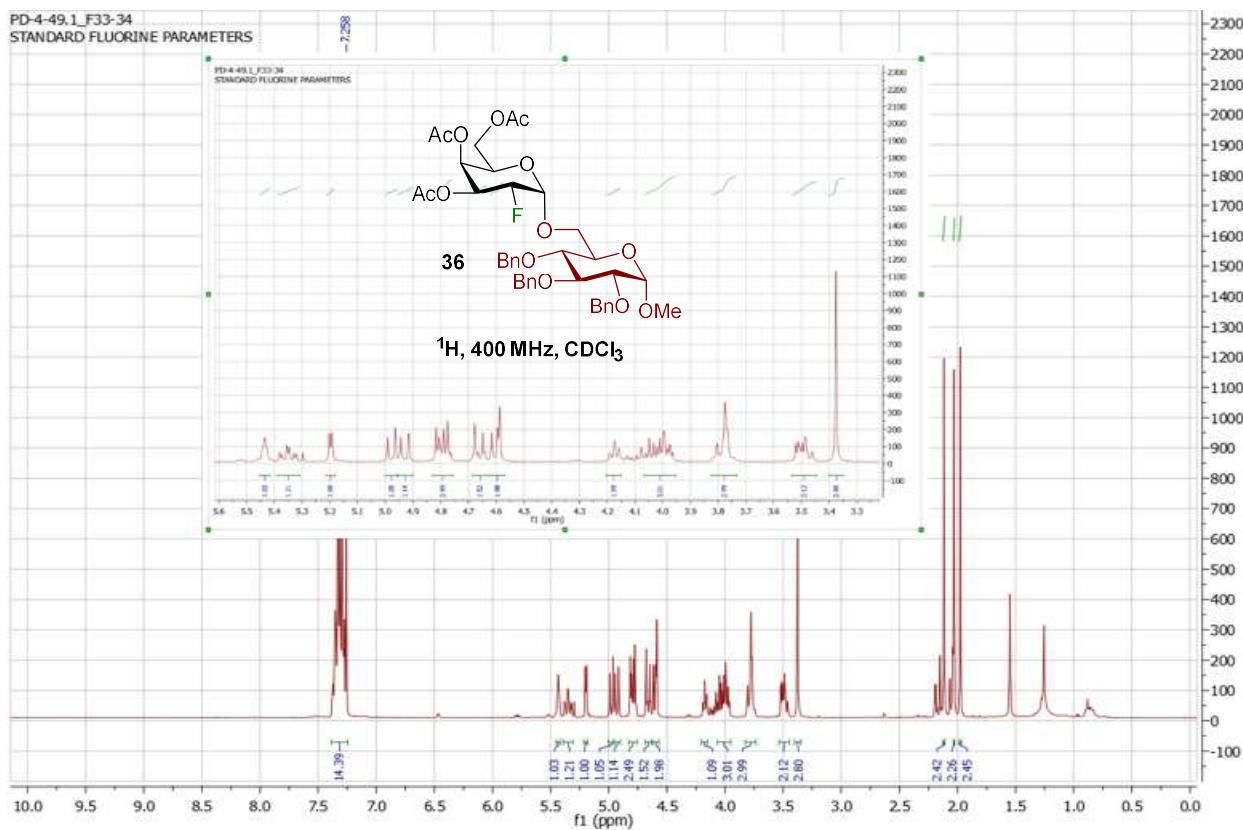
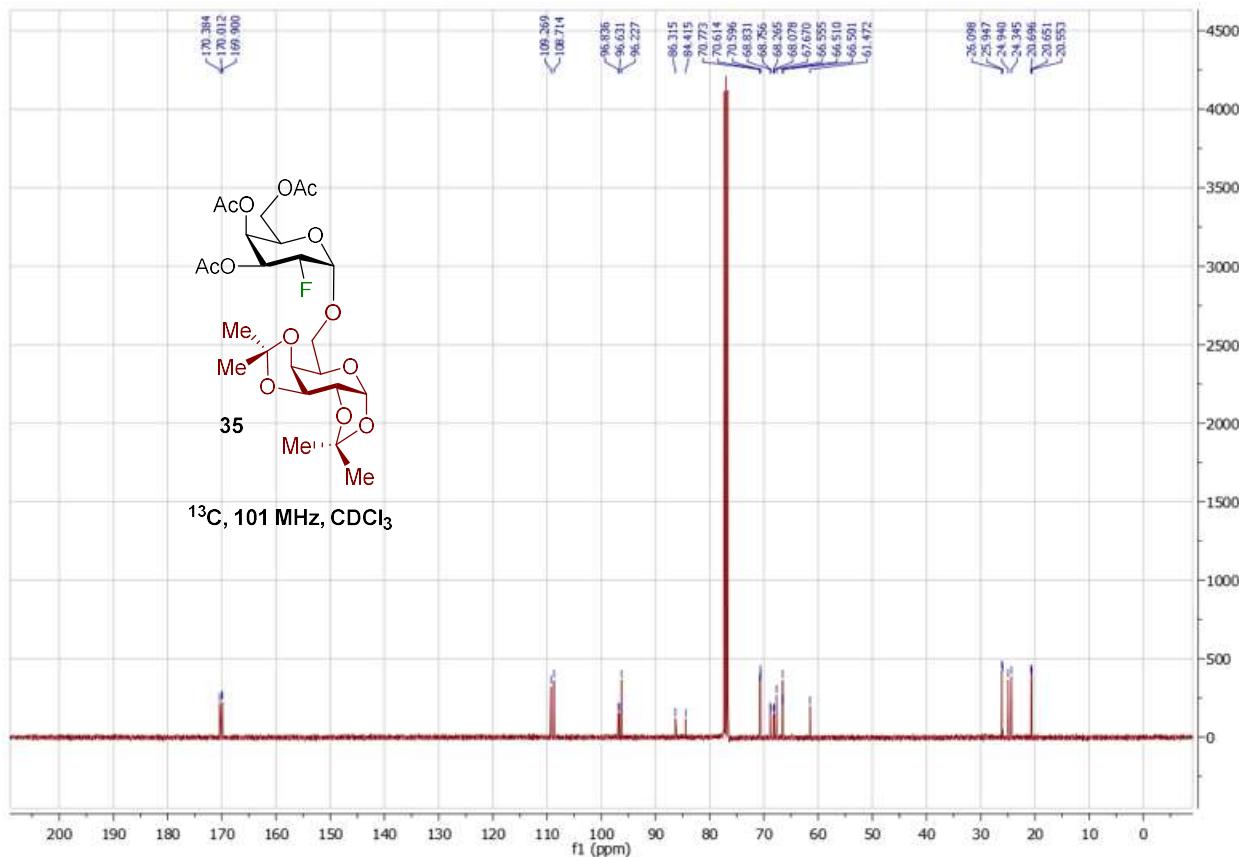


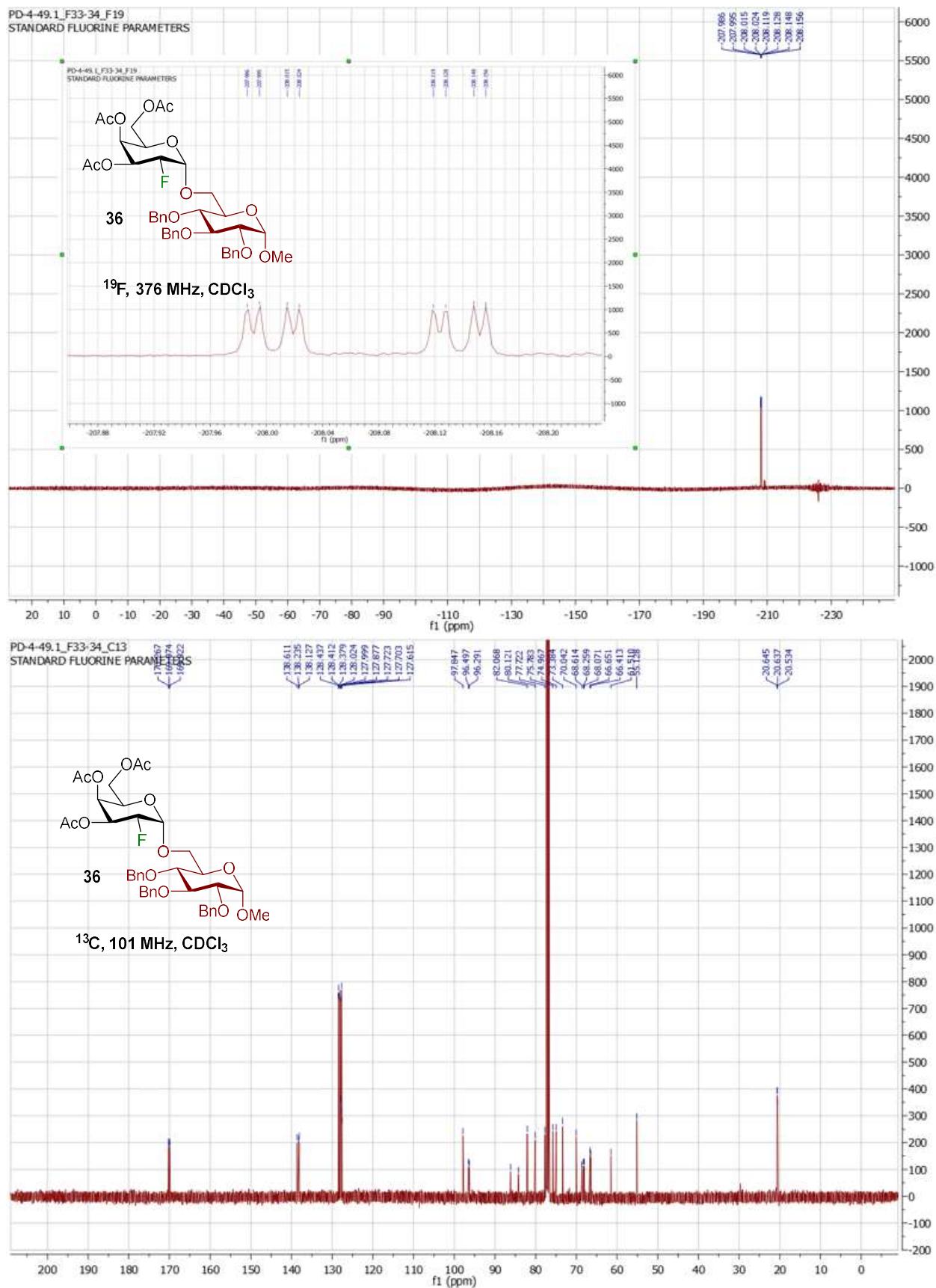
PD-4-9_F48-55
STANDARD FLUORINE PARAMETERS

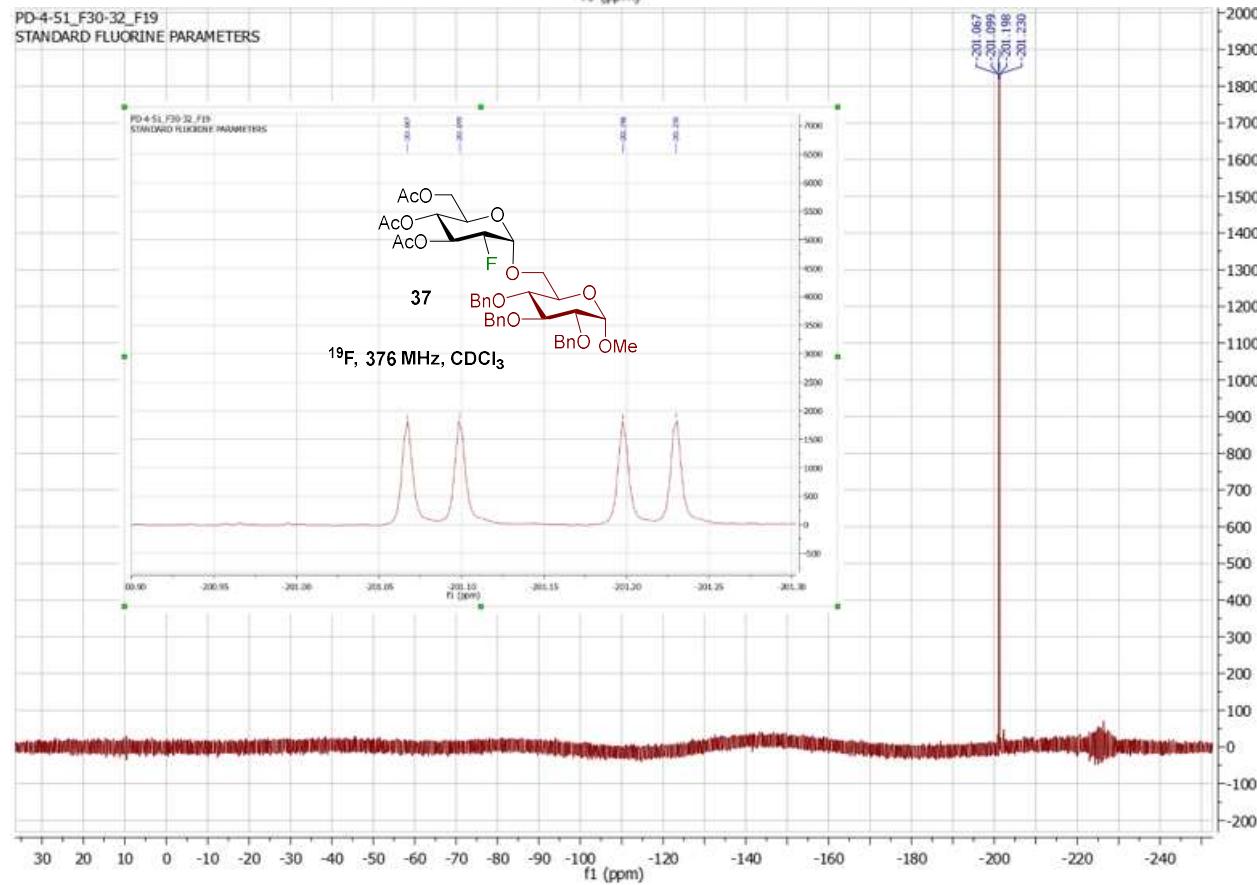
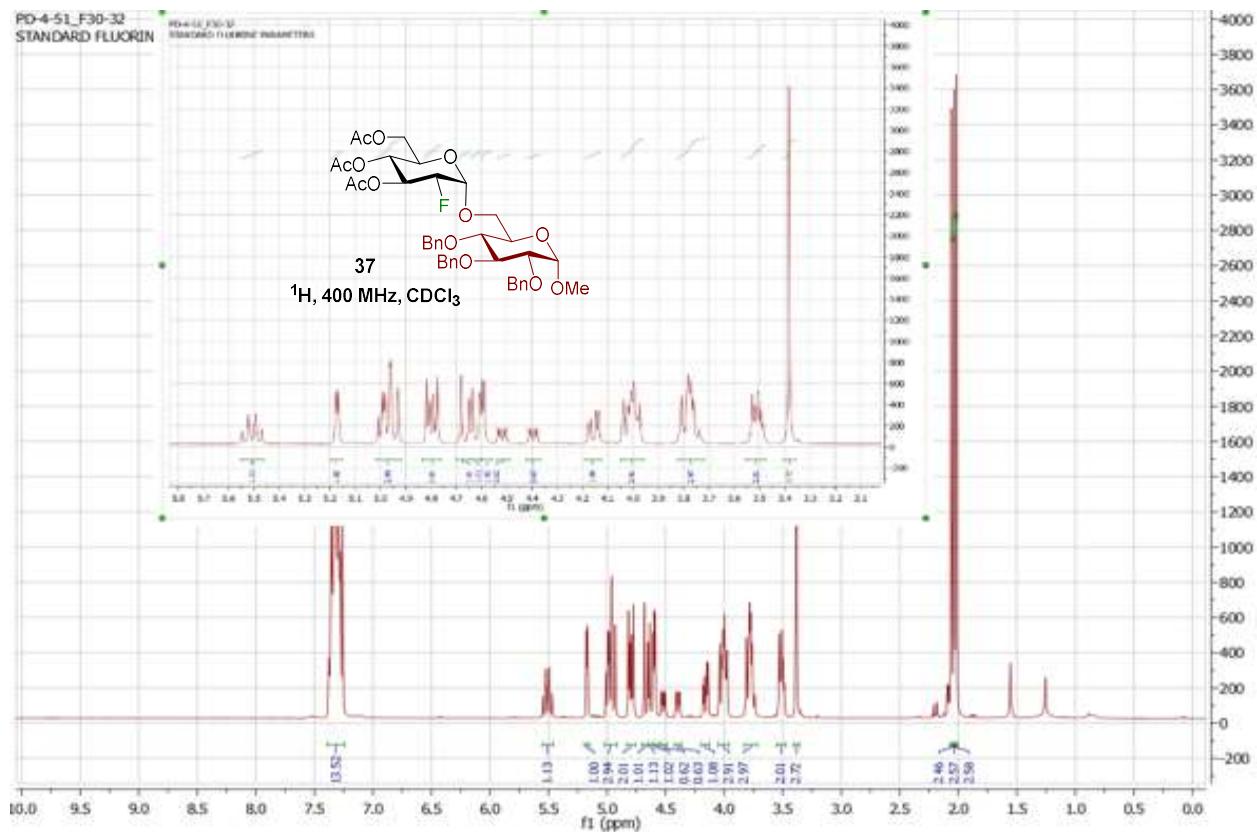


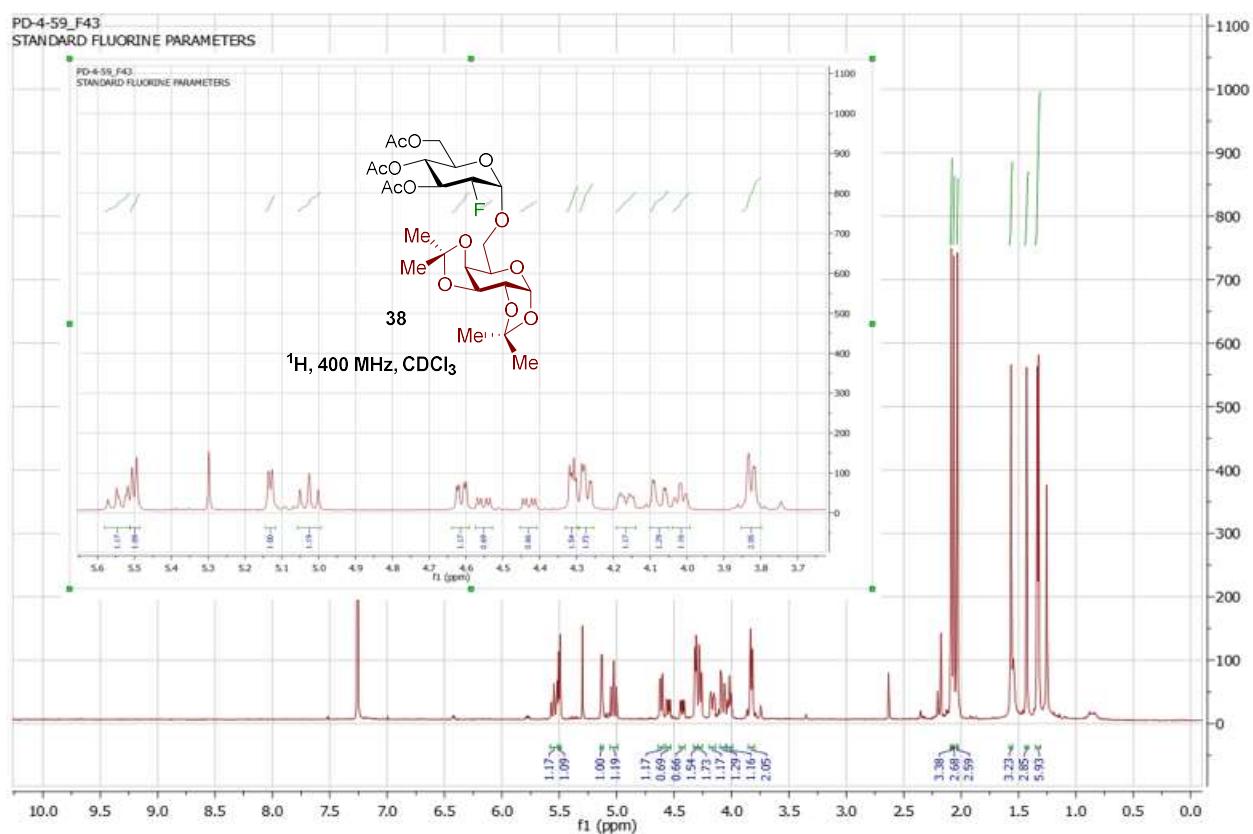
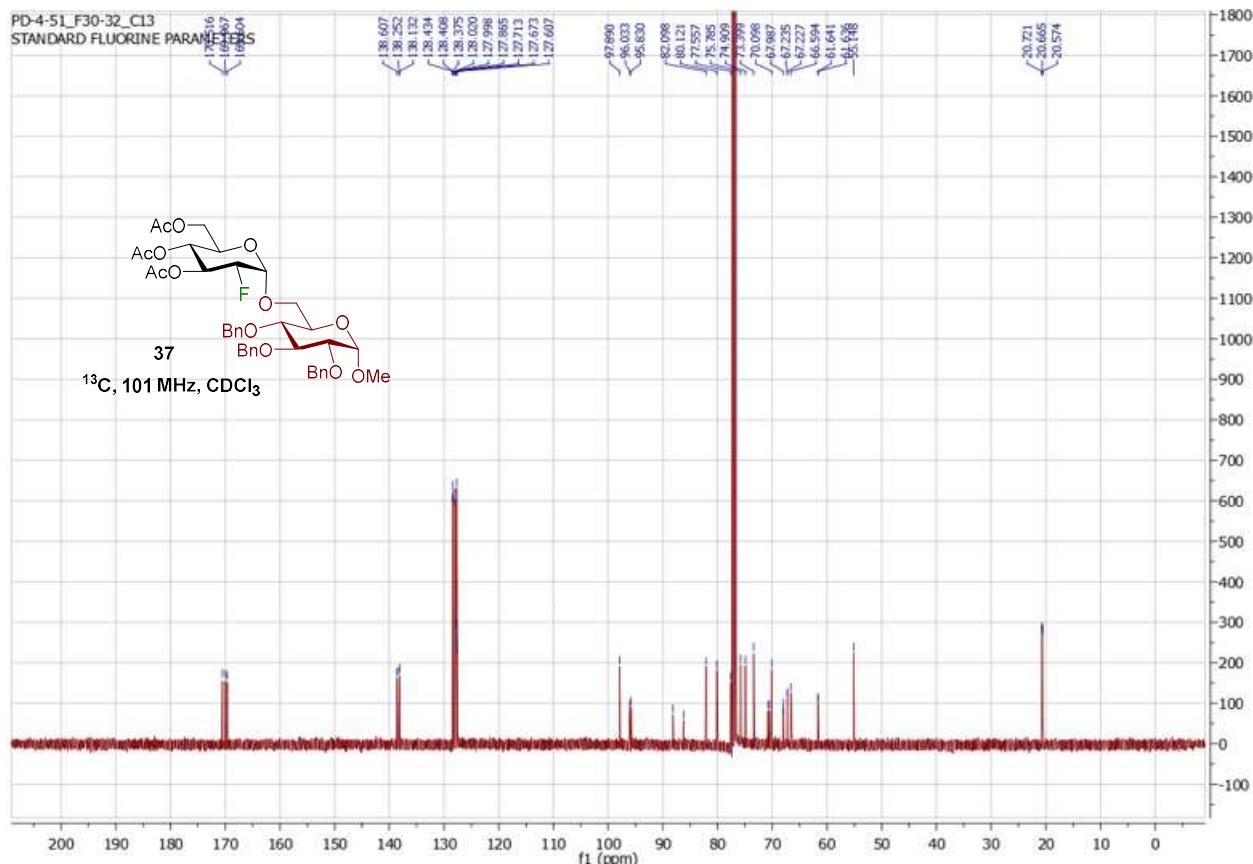
Galactose_Ac_2F_Galactose_alpha_F19
STANDARD FLUORINE PARAMETERS

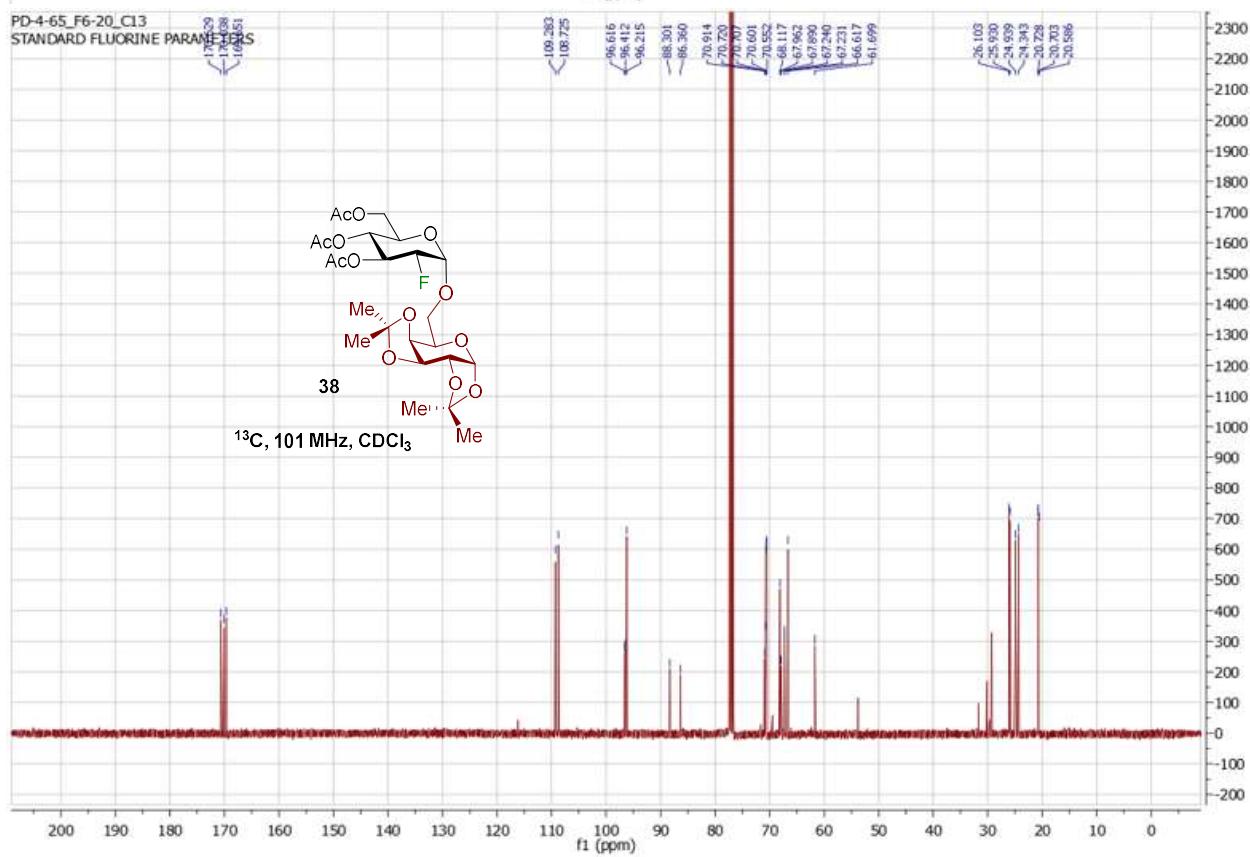
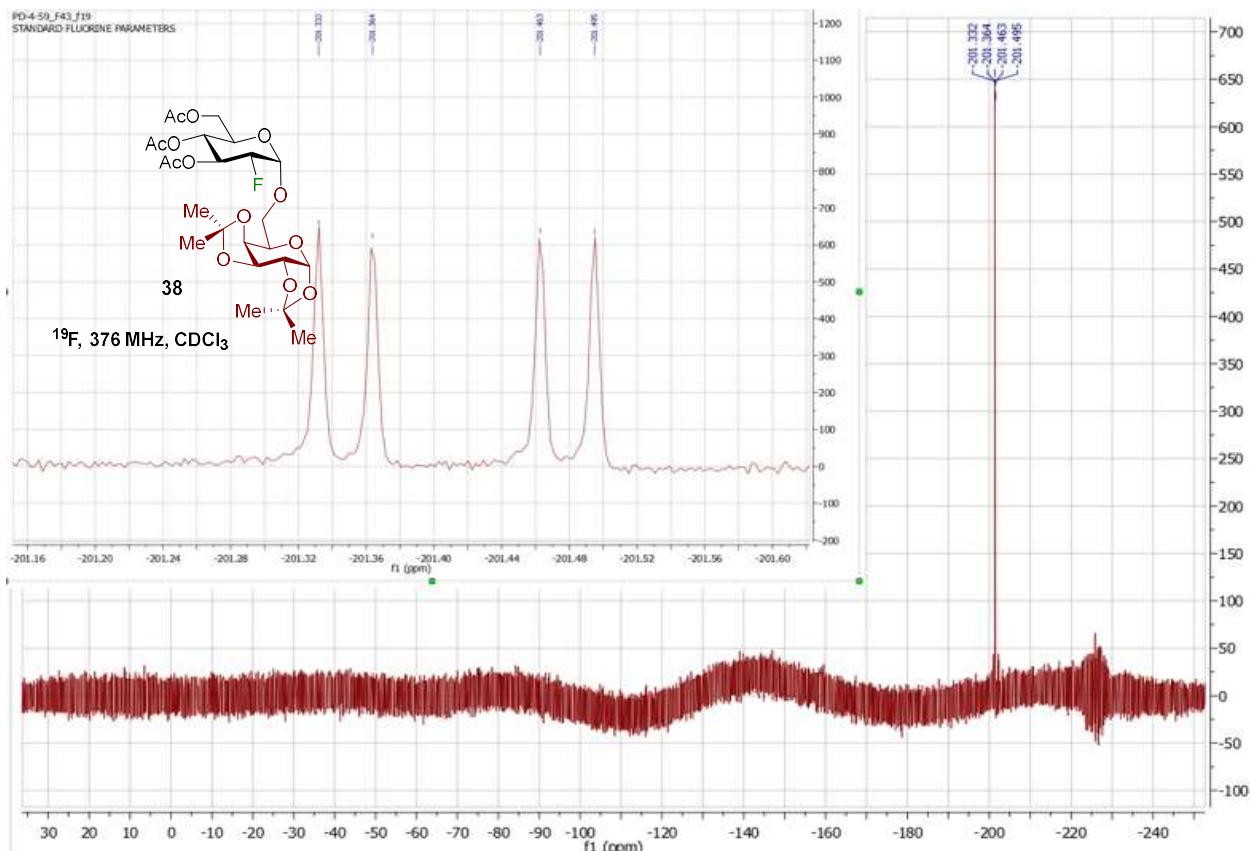


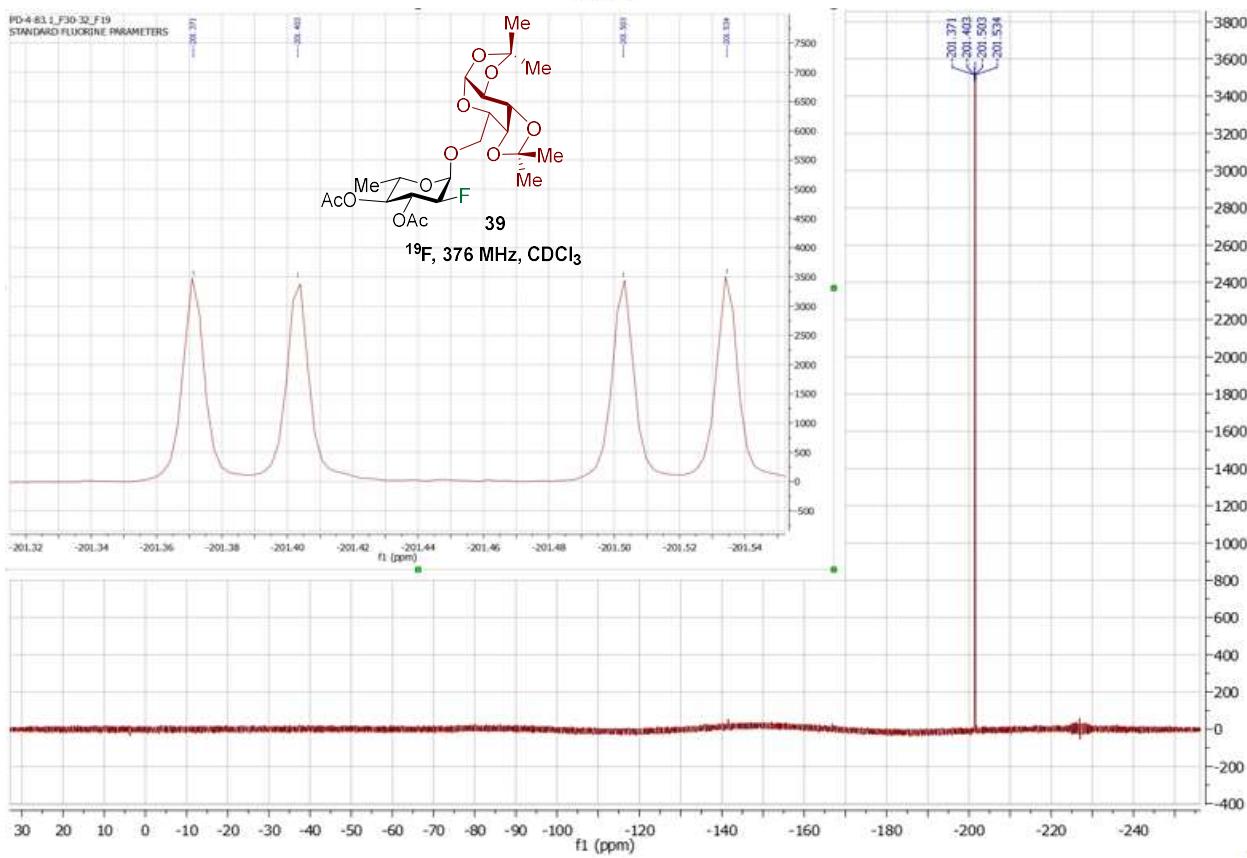
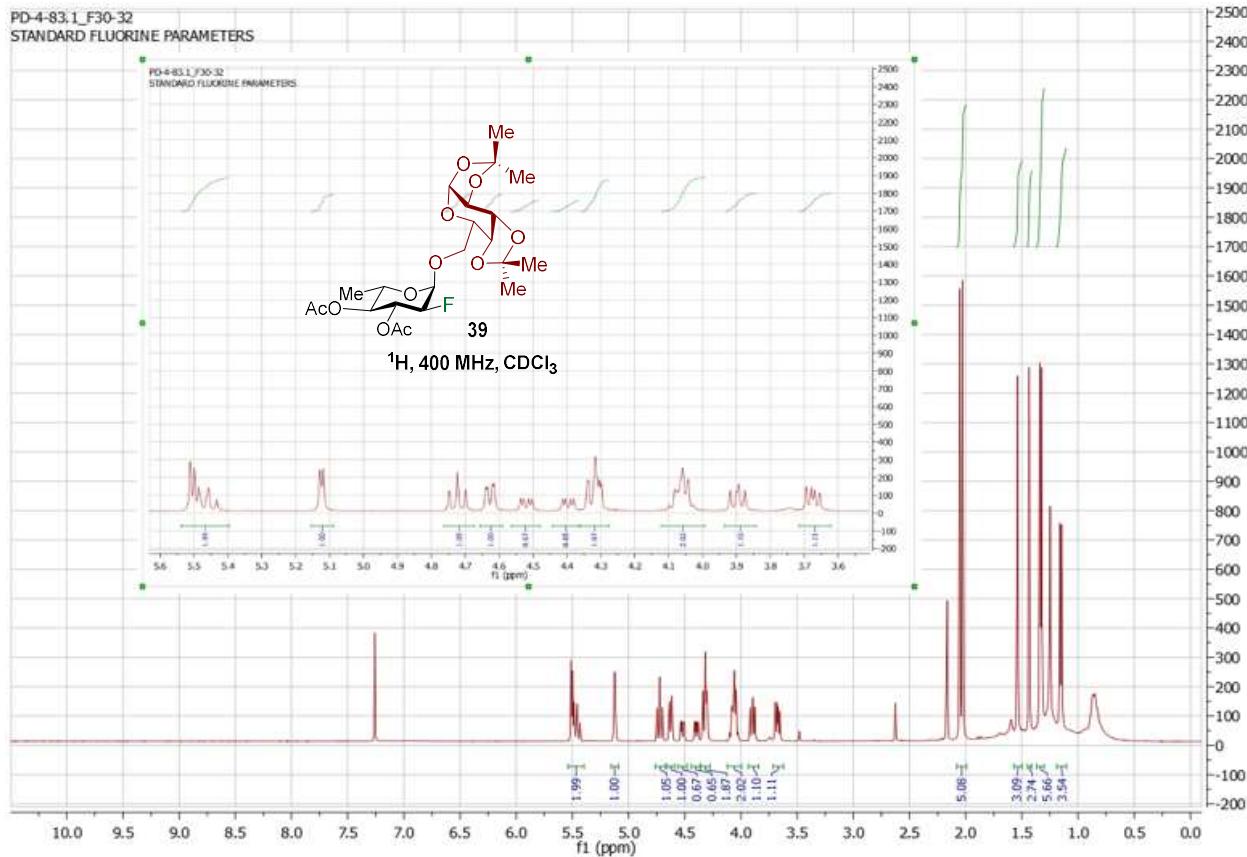


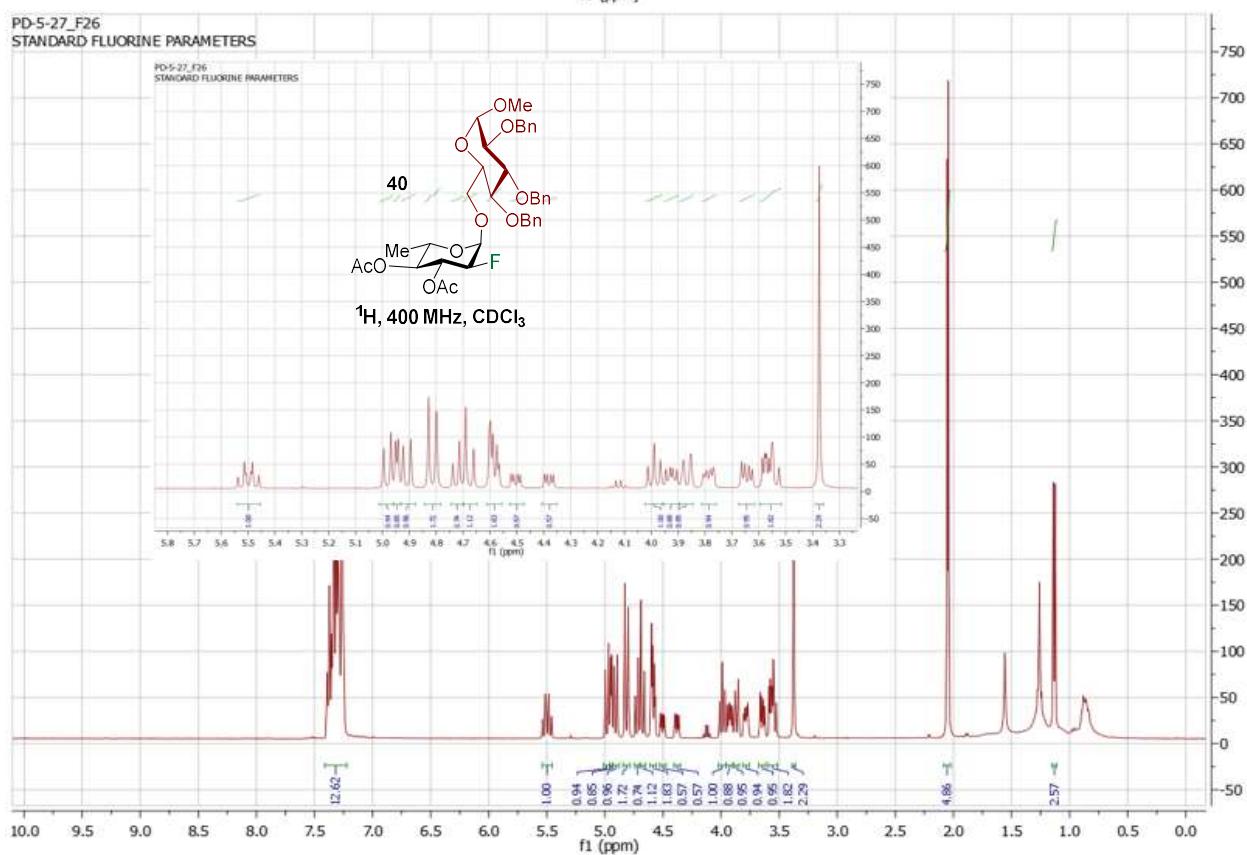
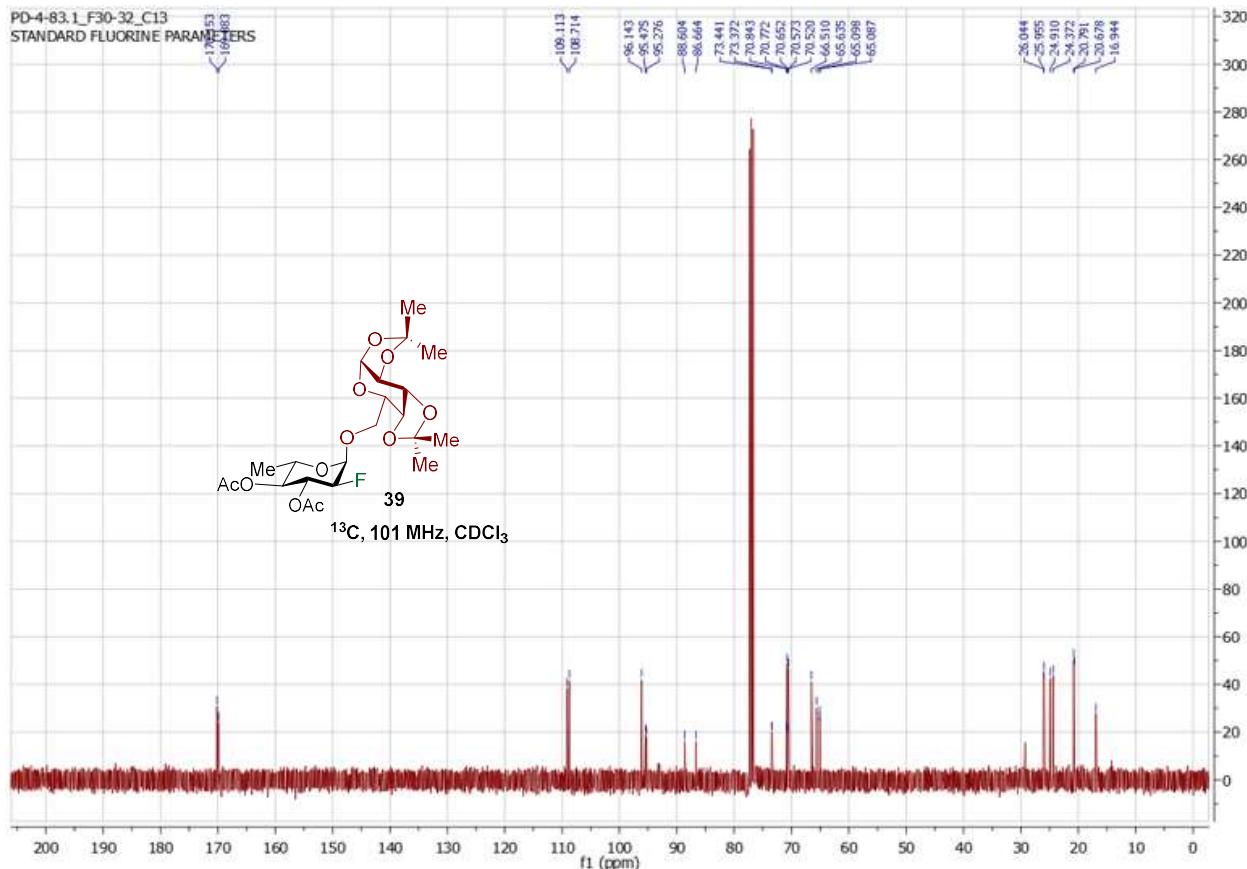




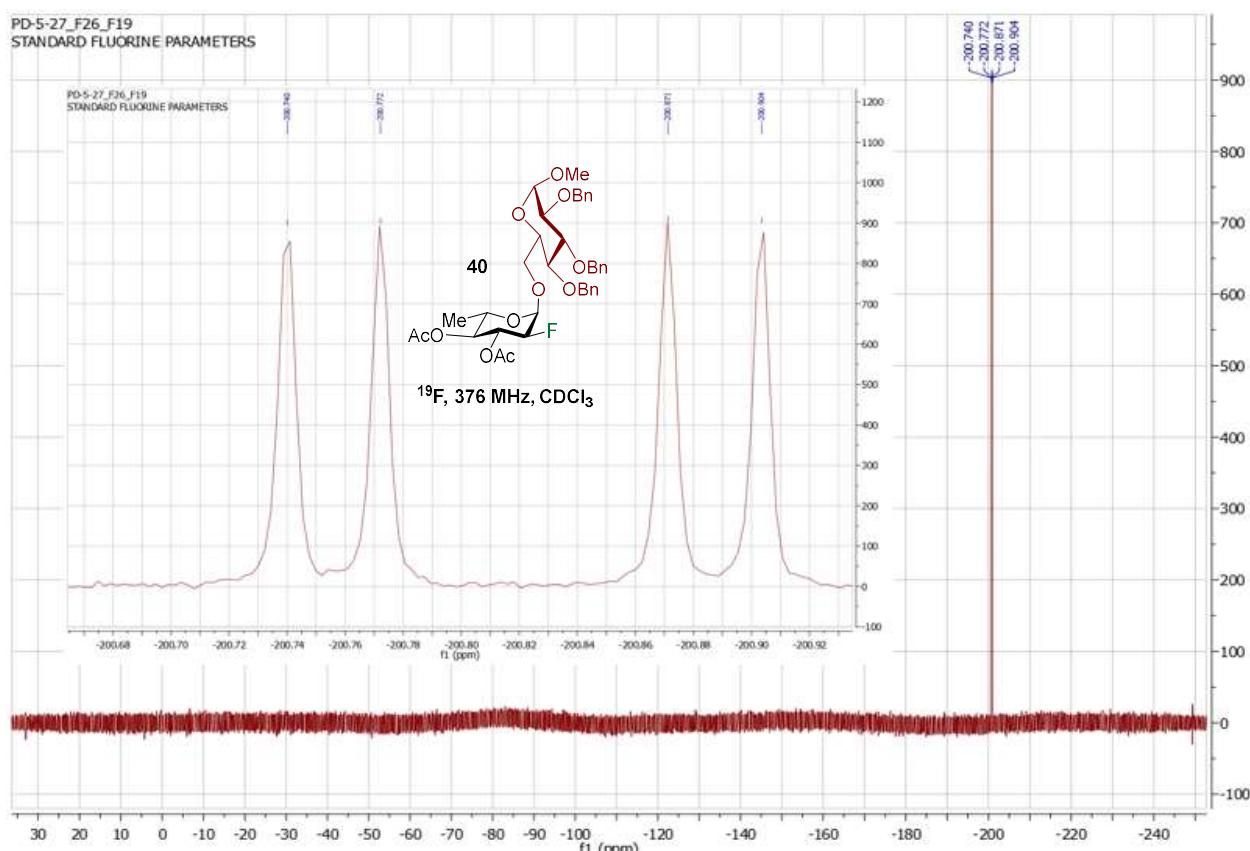




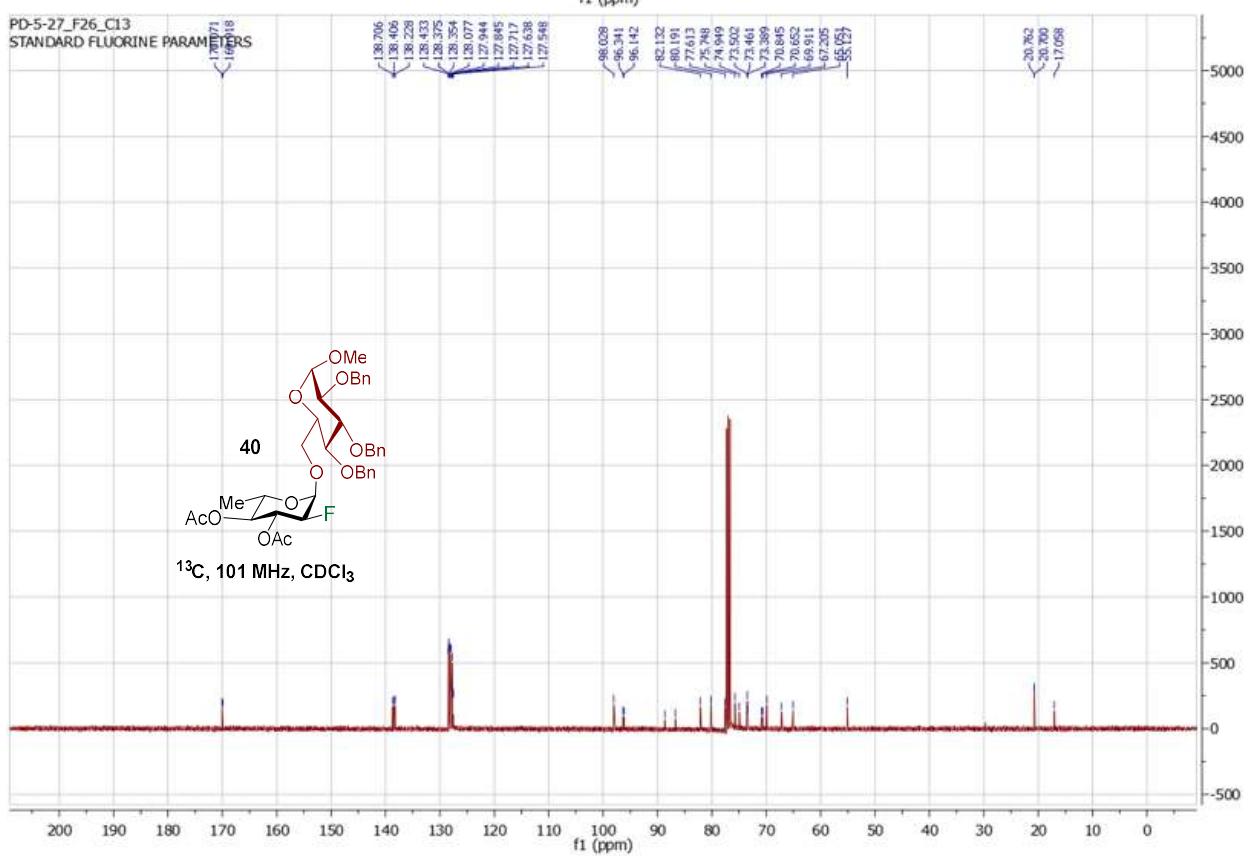




PD-5-27_F26_F19
STANDARD FLUORINE PARAMETERS

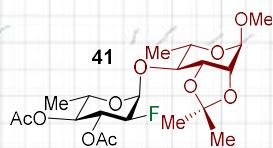


PD-5-27_F26_C13
STANDARD FLUORINE PARAMETERS

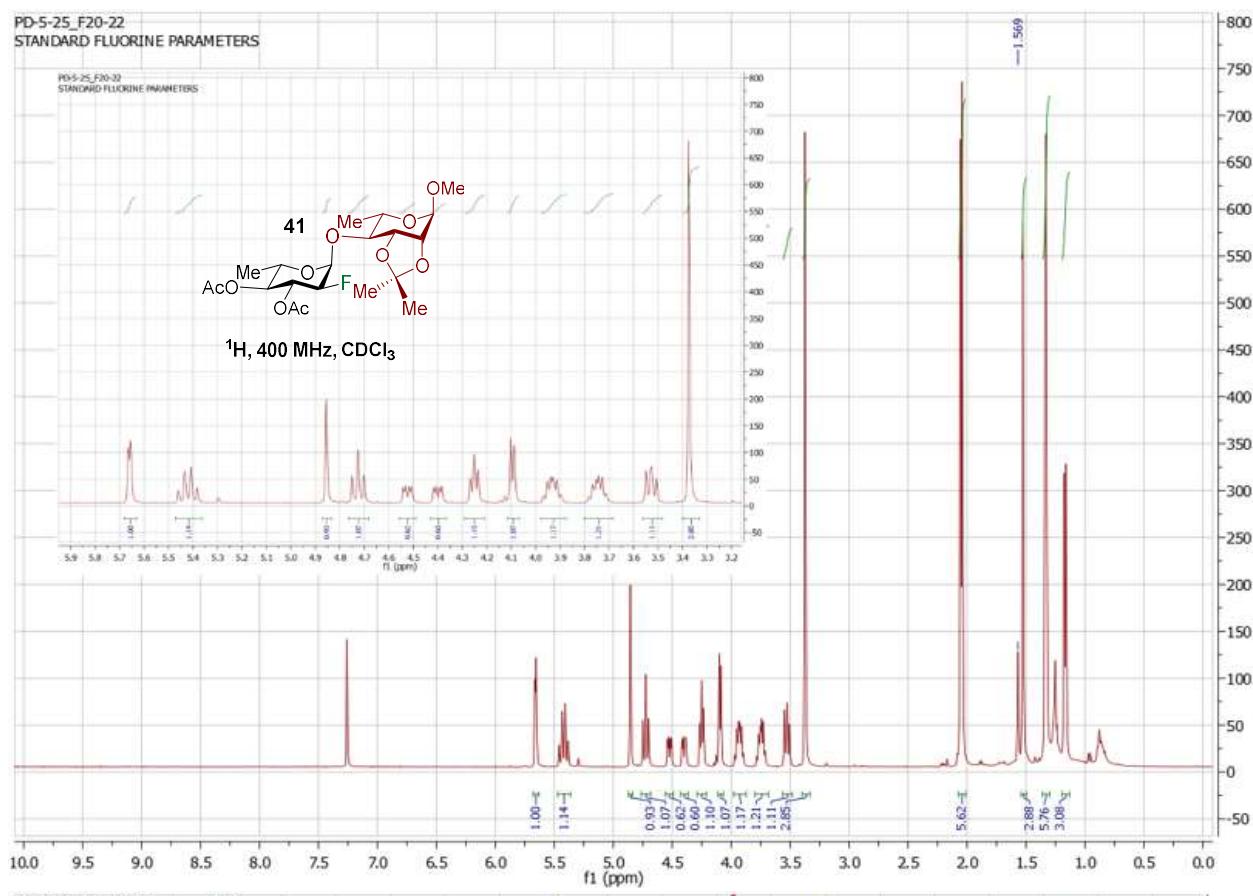


PD-5-25_F20-22
STANDARD FLUORINE PARAMETERS

PD-5-25_F20-22
STANDARD FLUORINE PARAMETERS

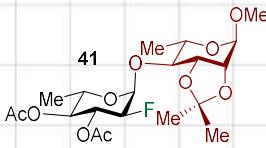


^1H , 400 MHz, CDCl_3

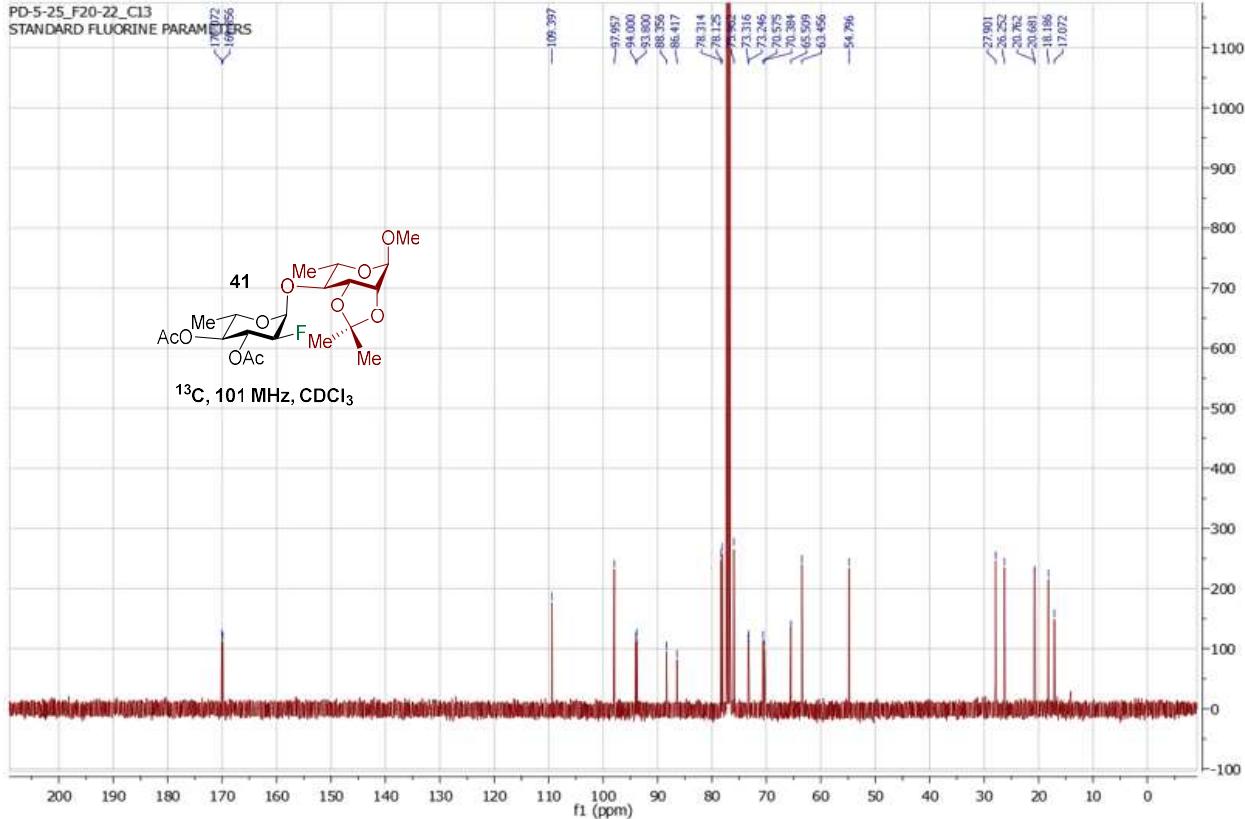


PD-5-25_F20-22_C13
STANDARD FLUORINE PARAMETERS

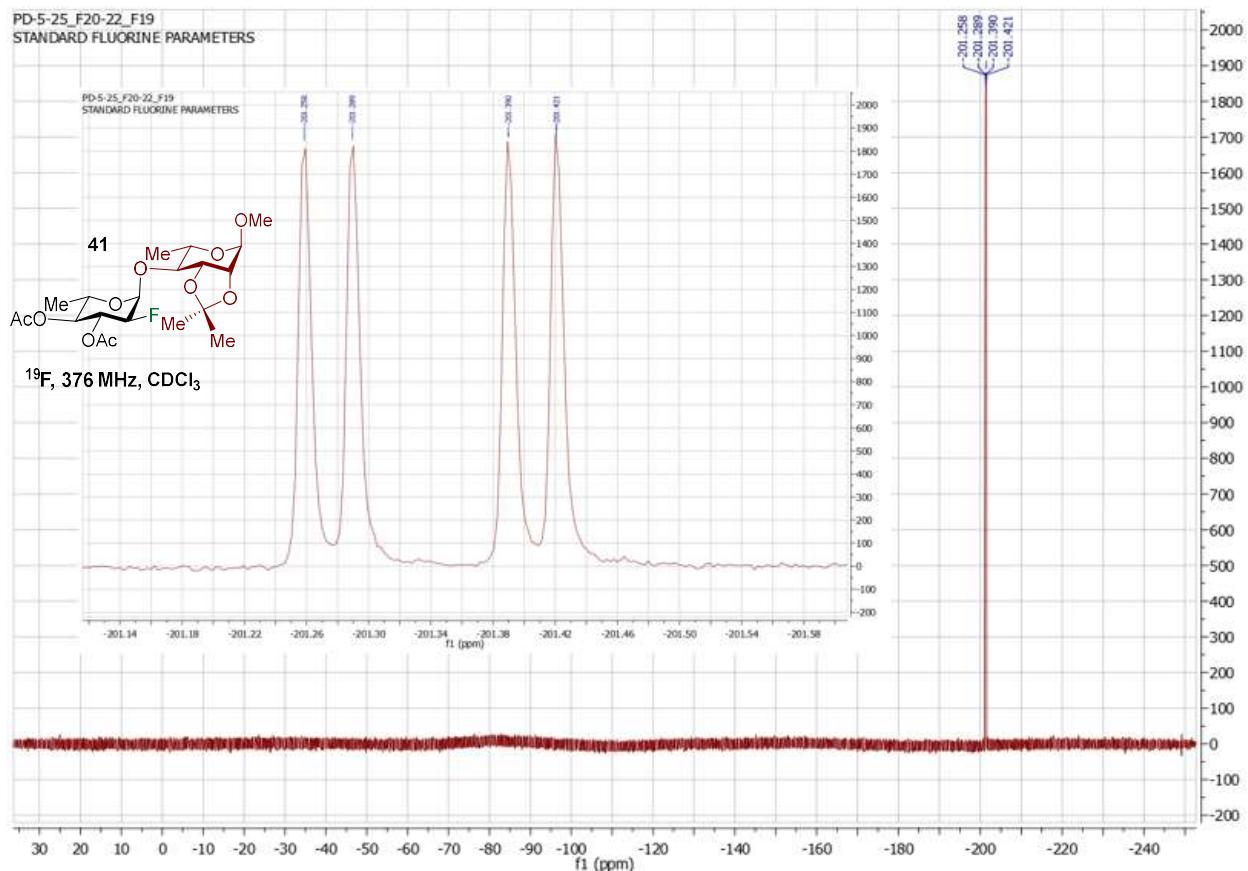
170.72, 165.66



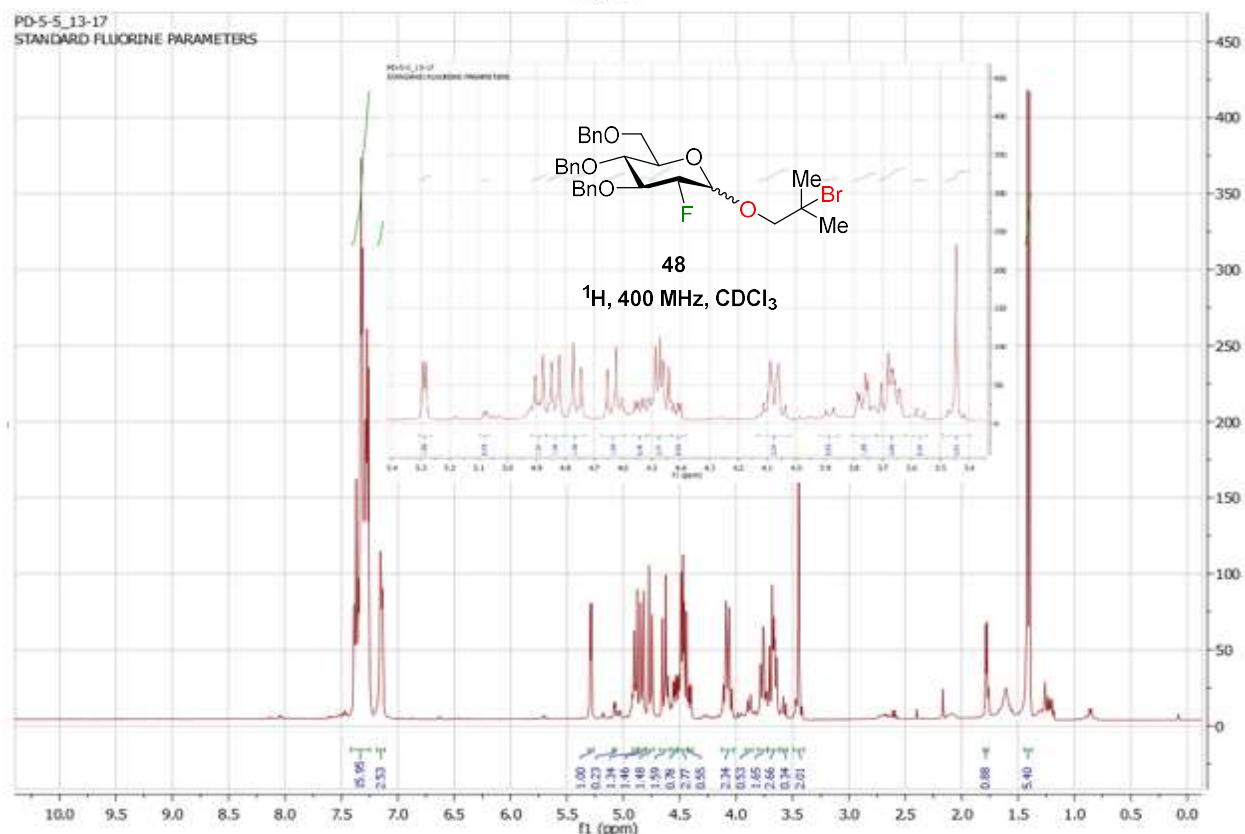
^{13}C , 101 MHz, CDCl_3

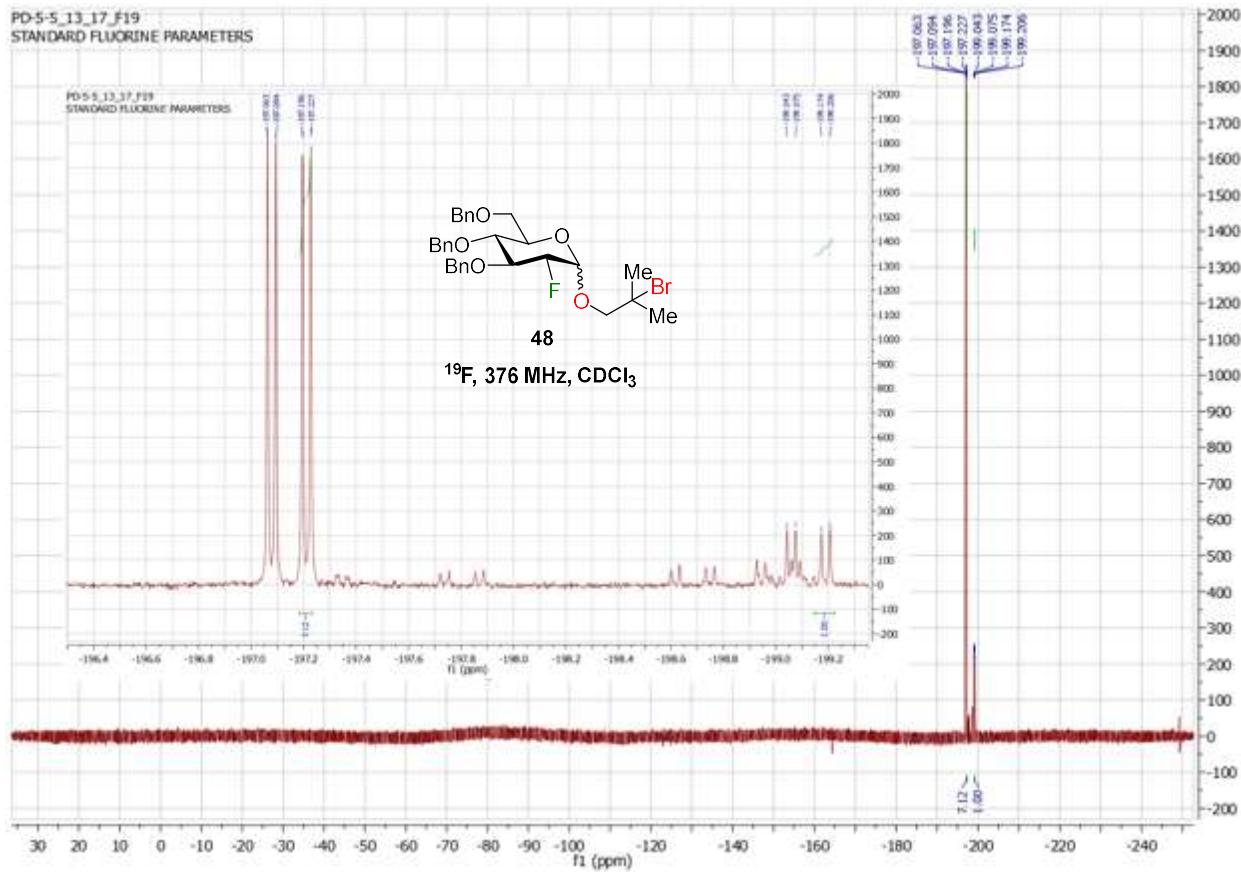
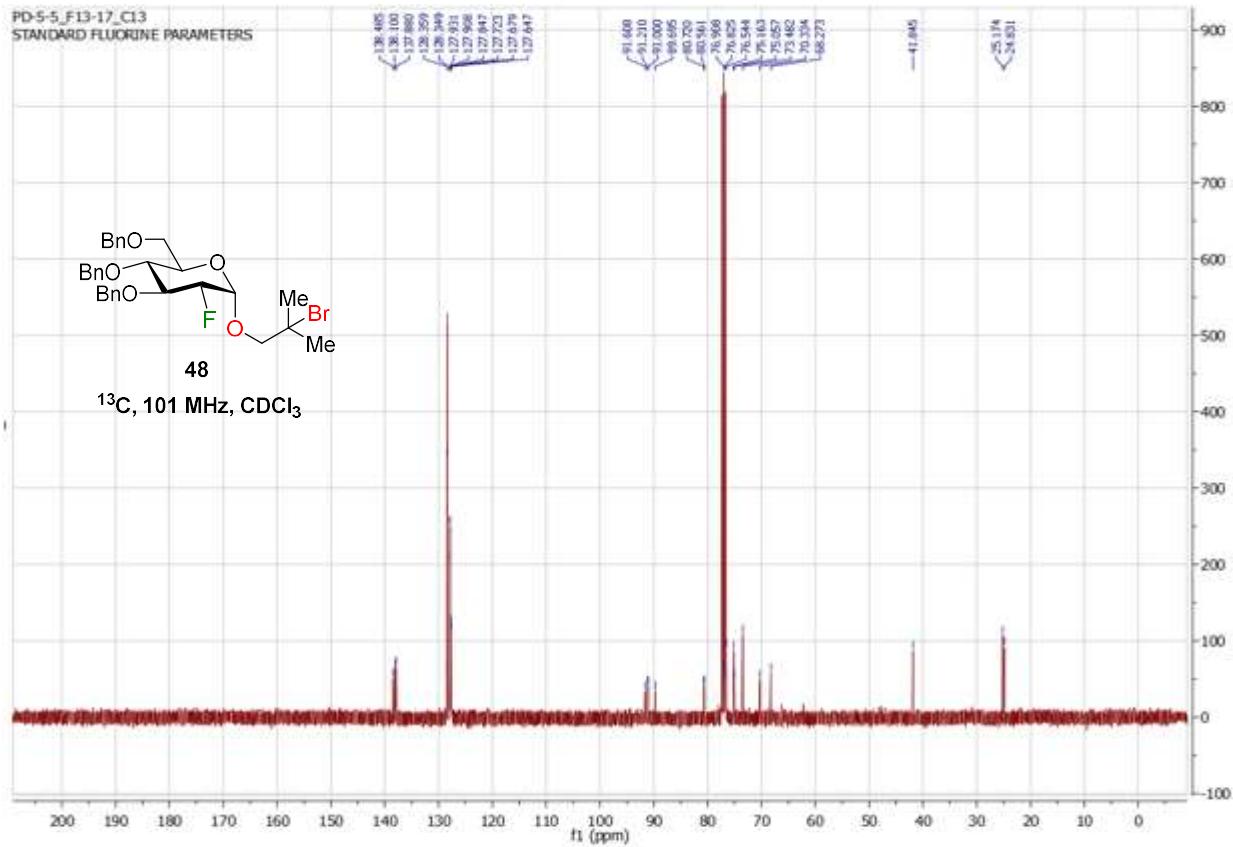


PD-5-25_F20-22_F19
STANDARD FLUORINE PARAMETERS



PD-5-5_13-17
STANDARD FLUORINE PARAMETERS





8. Cartesian Coordinates for Calculated Structures

L0 Catalyst

Charge= 0 Multiplicity= 1

E (UB3LYP): -571.883945 A.U.

ΔG (Thermal Corrections): 0.136194 A.U.

G (UB3LYP): -571.747751 A.U.

C	1.418532	0.871965	0.000048
C	2.833067	0.841156	0.000103
C	3.485573	-0.376793	0.000037
C	2.704920	-1.554137	-0.000137
N	1.384319	-1.558682	-0.000135
H	4.577127	-0.440203	0.000074
C	0.729385	-0.377494	-0.000019
C	-1.418532	0.871965	-0.000048
C	0.682123	2.104847	0.000048
C	-0.682123	2.104847	-0.000047
H	1.241578	3.045142	0.000071
H	-1.241578	3.045142	-0.000071
H	3.200261	-2.534224	-0.000235
C	-0.729385	-0.377494	0.000019
C	-2.704920	-1.554137	0.000137
C	-2.833067	0.841156	-0.000104
C	-3.485573	-0.376793	-0.000037
H	-3.200261	-2.534224	0.000234
H	-4.577127	-0.440203	-0.000076
N	-1.384319	-1.558682	0.000135
H	-3.390906	1.782795	-0.000239
H	3.390906	1.782795	0.000238

C	5.227044	-1.379392	-0.052415
C	4.480496	-2.445524	-0.516760
C	3.131905	-2.218569	-0.872363
N	2.554732	-1.039482	-0.758776
H	4.916333	-3.442365	-0.622649
C	3.246545	0.005646	-0.271275
C	3.361821	2.424691	0.264996
C	5.356200	1.048519	0.513789
C	4.752823	2.269224	0.584001
H	6.413231	0.931362	0.769022
H	5.313580	3.156577	0.889876
H	2.500276	-3.027381	-1.259477
C	2.583826	1.291641	-0.120986
C	0.678080	2.633872	-0.297529
C	2.730241	3.688250	0.322092
C	1.387483	3.803453	0.016538
H	-0.397264	2.657280	-0.502113
H	0.871008	4.765403	0.036619
O	-1.904614	-0.720890	2.772115
C	-1.867010	-1.997015	3.375007
H	-2.685799	-2.645065	3.003105
H	-0.901736	-2.509370	3.199971
H	-1.999052	-1.845944	4.460059
O	-4.014940	-0.248586	0.939754
C	-4.863020	0.532859	1.743294
H	-4.467154	0.638980	2.772866
H	-5.031925	1.537327	1.307643
H	-5.832911	0.008889	1.791017
C	-3.135443	1.673713	-1.352610
H	-2.806553	1.759028	-2.409783
H	-2.774029	2.582890	-0.820151
O	-4.526110	1.566448	-1.263724
C	-5.201280	2.666179	-1.816543
H	-4.941089	3.614063	-1.297192
H	-4.972090	2.789553	-2.896758
H	-6.282815	2.484853	-1.701774
H	3.318110	4.565363	0.607413
H	6.281176	-1.500837	0.214365

L0 TS1

Charge= 0 Multiplicity= 1

E (UB3LYP): -3899.690467 A.U.

ΔG (Thermal Corrections): 0.365308 A.U.

G (UB3LYP): -3899.325159 A.U.

C	-0.110721	-0.030669	-0.446245
O	-1.075599	0.579910	-1.104586
C	-0.304498	-0.269542	1.039495
H	-0.143621	0.676836	1.582127
C	-1.719000	-0.727724	1.374513
H	-1.880199	-1.725756	0.934354
C	-2.714692	0.254662	0.757344
H	-2.597183	1.229544	1.269604
C	-2.479243	0.439028	-0.748227
H	-2.813772	-0.479835	-1.255104
F	0.640162	-1.161470	1.503595
H	0.570575	-0.668630	-1.003151
Br	-0.996239	-2.819696	-1.344259
N	1.248852	1.442593	-0.347170
C	4.624243	-0.104469	0.077210

L0 Int 1

Charge= 0 Multiplicity= 1

E (UB3LYP): -3899.721067 A.U.

ΔG (Thermal Corrections): 0.368077 A.U.

G (UB3LYP): -3899.352990 A.U.

C	-0.020881	0.592785	-0.173264
O	-1.098166	1.246343	-0.763816
C	-0.359676	0.275208	1.291623
H	-0.526241	1.220506	1.837917

C	-1.618430	-0.580347	1.360488	
H	-1.431661	-1.537597	0.836396	ΔG (Thermal Corrections): 0.412961 A.U.
C	-2.751463	0.144970	0.628836	G (UB3LYP): -4015.076431 A.U.
H	-2.970274	1.091581	1.155103	
C	-2.314867	0.476523	-0.804645	C 0.147033 -0.296849 -0.794173
H	-2.126591	-0.473077	-1.340799	O -0.788465 0.442458 -1.287247
F	0.708899	-0.362983	1.907628	C 0.149096 -0.751695 0.665413
H	0.272706	-0.316876	-0.712954	H 1.043014 -0.342249 1.154464
Br	-0.931137	-2.853077	-1.519048	C -1.066752 -0.299967 1.463378
N	1.132803	1.571577	-0.186444	H -1.882502 -1.028032 1.287990
C	4.330640	-0.440381	0.017378	C -1.554090 1.063629 0.970641
C	4.758017	-1.786948	-0.085240	H -0.741311 1.808398 1.086039
C	3.847171	-2.775678	-0.399537	C -1.937352 0.931217 -0.506525
C	2.500830	-2.404803	-0.622010	H -2.713790 0.148088 -0.598472
N	2.088912	-1.159746	-0.509147	F 0.252035 -2.125841 0.715441
H	4.151355	-3.822256	-0.484708	H 0.731918 -0.869302 -1.503729
C	2.941778	-0.175982	-0.187911	N 1.749312 1.109719 -0.703634
C	3.426873	2.228090	0.141988	C 4.900517 -0.672810 0.189744
C	5.250015	0.620869	0.287392	C 5.352188 -2.008927 0.310825
C	4.813206	1.909219	0.328989	C 4.495031 -3.049064 0.005082
H	6.305630	0.379133	0.438535	C 3.189155 -2.739306 -0.435212
H	5.504478	2.736124	0.508442	N 2.747364 -1.502394 -0.558659
H	1.718913	-3.126031	-0.900441	H 4.811466 -4.091650 0.091724
C	2.464730	1.195061	-0.075234	C 3.556685 -0.474410 -0.240907
C	0.769373	2.867190	-0.169868	C 3.930624 1.972253 -0.120258
C	3.016939	3.577734	0.166380	C 5.743992 0.453758 0.464974
C	1.687049	3.900084	-0.014102	C 5.280614 1.726153 0.301484
H	-0.299372	3.045881	-0.274363	H 6.771155 0.270761 0.792756
H	1.331996	4.932007	-0.014647	H 5.927254 2.587307 0.490107
O	-1.983597	-0.782619	2.710778	H 2.482599 -3.537258 -0.691677
C	-1.669153	-2.063129	3.214018	C 3.046069 0.879141 -0.359389
H	-2.194927	-2.860746	2.651940	C 1.325487 2.343491 -0.906411
H	-0.581427	-2.266720	3.179629	C 3.443001 3.284764 -0.317445
H	-2.002770	-2.089284	4.265668	C 2.140955 3.475854 -0.736133
O	-3.905543	-0.658555	0.565367	H 0.283217 2.452872 -1.214568
C	-4.916562	-0.322235	1.485261	H 1.732640 4.472472 -0.917518
H	-4.565348	-0.400787	2.531183	O -0.693406 -0.244005 2.820623
H	-5.299738	0.705903	1.312967	C -1.618479 -0.839447 3.708399
H	-5.745031	-1.035103	1.332002	H -2.612097 -0.359514 3.648504
C	-3.333866	1.295059	-1.561968	H -1.734144 -1.922979 3.505465
H	-2.930169	1.535572	-2.567889	H -1.214411 -0.709708 4.727143
H	-4.241130	0.673924	-1.699398	O -2.670432 1.436004 1.732183
O	-3.633972	2.474974	-0.852840	C -2.702507 2.774770 2.161648
C	-4.605408	3.265520	-1.482692	H -1.838575 3.010698 2.817151
H	-4.276245	3.603659	-2.489425	H -2.724540 3.488868 1.316856
H	-5.567574	2.722131	-1.602374	H -3.630915 2.902531 2.742658
H	-4.778523	4.153913	-0.851456	C -2.391094 2.196303 -1.223784
H	3.767849	4.356142	0.325126	H -2.334093 2.006927 -2.316791
H	5.814123	-2.020260	0.079493	H -1.708995 3.045868 -0.998223
			O -3.697801 2.496315 -0.831736	
			C -4.221882 3.628540 -1.475714	
			H -3.630169 4.542655 -1.252026	
			H -4.252184 3.496581 -2.578451	
			H -5.250579 3.773228 -1.106775	

L0 TS 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -4015.489392 A.U.

O	-1.052196	-2.411878	-1.742111	O	-3.253004	1.727200	1.625142
C	-1.582714	-2.091337	-3.000513	C	-3.200540	2.716266	2.620470
H	-2.176562	-1.153041	-2.996164	H	-2.571012	2.400802	3.477083
H	-0.744158	-1.962940	-3.710826	H	-2.826348	3.682650	2.228899
H	-2.242538	-2.894060	-3.393553	H	-4.232790	2.868175	2.980547
H	-1.827852	-2.498895	-1.113839	C	-1.979120	3.262102	-0.738011
Br	-3.751152	-2.270808	-0.104489	H	-1.794187	3.401726	-1.824701
H	6.376767	-2.199543	0.643642	H	-1.113440	3.704562	-0.198168
H	4.109598	4.133963	-0.142170	O	-3.177311	3.876516	-0.352769
				C	-3.176558	5.262930	-0.563547
				H	-2.380405	5.770657	0.023225
L0 Int 2				H	-3.028858	5.518104	-1.635613
Charge= 0 Multiplicity= 1				H	-4.156470	5.651571	-0.239106
E (UB3LYP): -4015.521273 A.U.				O	-1.772308	-0.848615	-1.640075
ΔG (Thermal Corrections): 0.406797 A.U.				C	-1.836815	-0.748453	-3.054645
G (UB3LYP): -4015.114476 A.U.				H	-1.978591	0.300088	-3.370677
				H	-0.915295	-1.148582	-3.519851
C	-0.702733	-0.148153	-1.042180	H	-2.701787	-1.347115	-3.380728
O	-0.884005	1.237499	-1.127958	H	-2.476632	-2.350403	-1.055607
C	-0.602387	-0.583598	0.415476	Br	-3.365602	-3.503872	-0.842022
H	0.337380	-0.184717	0.819572	H	5.382580	3.523482	-0.582984
C	-1.792252	-0.106851	1.232632	H	5.975742	-3.077770	0.901181
H	-2.702239	-0.631110	0.889052				
C	-2.020872	1.393045	1.030080				
H	-1.186022	1.930266	1.517602				
C	-2.035618	1.763716	-0.462521				
H	-2.957265	1.352609	-0.911256				
F	-0.523722	-1.975253	0.471111				
H	0.241278	-0.359274	-1.567757				
N	2.267223	1.188924	-0.500142				
C	4.912428	-1.259095	0.368811				
C	4.999003	-2.637462	0.677688				
C	3.848958	-3.404404	0.693918				
C	2.618724	-2.777215	0.396588				
N	2.510405	-1.495215	0.100675				
H	3.878363	-4.471483	0.930405				
C	3.620000	-0.728617	0.083738				
C	4.663489	1.500522	-0.251205				
C	6.065527	-0.403424	0.337980				
C	5.945980	0.923022	0.039862				
H	7.043796	-0.840048	0.560435				
H	6.826362	1.572385	0.018198				
H	1.685971	-3.353744	0.405964				
C	3.491692	0.688029	-0.233580				
C	2.147498	2.471526	-0.790376				
C	4.503529	2.871651	-0.562019				
C	3.240892	3.364462	-0.834270				
H	1.131140	2.821511	-1.006340				
H	3.081114	4.417942	-1.079727				
O	-1.583122	-0.338232	2.609313				
C	-2.211358	-1.492020	3.119739				
H	-3.315450	-1.427091	3.028462				
H	-1.869205	-2.413924	2.612014				
H	-1.950364	-1.557255	4.189949				

C	5.532914	-1.915668	0.835373	C	-0.737773	2.122437	-0.626461
C	5.390850	-2.816243	-0.226085	C	1.421604	3.096121	-0.182170
H	2.831375	-1.287227	-1.890689	C	0.062396	3.252297	-0.431923
H	4.815149	-0.093904	1.754341	H	-1.816716	2.212634	-0.785058
H	4.304338	-3.279811	-2.042639	H	-0.386215	4.246216	-0.483081
H	6.292882	-2.087580	1.604229	O	-3.245670	-0.962890	2.815870
H	6.040984	-3.694241	-0.293758	C	-3.274840	-2.228392	3.440865
C	-3.712659	-0.556985	0.049966	H	-4.187706	-2.794615	3.167349
C	-4.704304	-0.792920	-0.919688	H	-2.388108	-2.838181	3.182281
C	-3.581398	-1.467837	1.115296	H	-3.280379	-2.051070	4.529981
C	-5.533133	-1.915646	-0.835029	O	-5.476881	-0.342182	1.185648
C	-4.414753	-2.586457	1.202955	C	-6.177440	0.528708	2.037919
C	-5.390804	-2.816297	0.226327	H	-5.677889	0.626860	3.022280
H	-4.815602	-0.093825	-1.754057	H	-6.303901	1.532261	1.586404
H	-2.830919	-1.287399	1.890399	H	-7.178104	0.090325	2.192996
H	-6.293284	-2.087510	-1.603715	C	-4.669555	1.450264	-1.238710
H	-4.303814	-3.280006	2.042562	H	-4.443423	1.479301	-2.325476
H	-6.040914	-3.694306	0.294091	H	-4.179822	2.337135	-0.775430
				O	-6.048116	1.467426	-1.009526
				C	-6.683728	2.597005	-1.549094
				H	-6.295182	3.540184	-1.107224
				H	-6.556210	2.653416	-2.651404
				H	-7.759167	2.515179	-1.319924
				C	2.266737	4.297242	0.027352
				C	1.873188	5.279620	0.953114
C	-1.715791	-0.474759	-0.571476	C	3.435818	4.504049	-0.727546
O	-2.692052	0.195689	-1.150791	C	2.639045	6.433747	1.132100
C	-1.788199	-0.677552	0.931663	C	4.193481	5.664152	-0.555164
H	-1.493907	0.258097	1.435470	C	3.800511	6.629492	0.378003
C	-3.197967	-1.006268	1.407324	H	0.969549	5.126417	1.549716
H	-3.482464	-1.993931	1.007797	H	3.739830	3.762151	-1.470449
C	-4.163888	0.045989	0.864212	H	2.326589	7.183350	1.865060
H	-3.916001	1.016660	1.335709	H	5.094269	5.816698	-1.156982
C	-4.061215	0.178633	-0.661178	H	4.398036	7.535643	0.515194
H	-4.515497	-0.720041	-1.107666	C	4.913493	-2.577215	-0.001886
F	-0.889442	-1.645357	1.330963	C	5.201343	-3.595190	0.923902
H	-1.141337	-1.169673	-1.176476	C	5.980467	-1.939743	-0.660281
Br	-2.891869	-3.187618	-1.335710	C	6.523130	-3.956167	1.196551
N	-0.252087	0.893681	-0.634244	C	7.301288	-2.306904	-0.392380
C	3.003284	-0.890956	-0.214864	C	7.577048	-3.312699	0.539962
C	3.500867	-2.229300	-0.305289	H	4.379696	-4.095973	1.443744
C	2.614201	-3.227131	-0.693664	H	5.772371	-1.165560	-1.403795
C	1.291997	-2.890743	-1.041361	H	6.729869	-4.743964	1.927175
N	0.835560	-1.656228	-0.992129	H	8.119734	-1.807683	-0.919809
H	2.950447	-4.263913	-0.770634	H	8.612253	-3.596919	0.751511
C	1.636318	-0.668555	-0.556173				
C	1.947942	1.767060	-0.148103				
C	3.801394	0.216818	0.221300				
C	3.305167	1.487773	0.226284				
H	4.824232	0.037586	0.554676				
H	3.937618	2.313062	0.554461				
H	0.582018	-3.655659	-1.378568				
C	1.080237	0.673889	-0.450100				

L1 Int 1

Charge= 0 Multiplicity= 1

E (UB3LYP): -4362.058883 A.U.

ΔG (Thermal Corrections): 0.517299 A.U.

G (UB3LYP): -4361.541584 A.U.

C -1.572675 0.288541 -0.233458

O	-2.614823	1.024910	-0.791307	C	3.544812	6.213845	1.016585
C	-1.884756	-0.002172	1.242950	C	4.798939	5.151137	-0.760777
H	-1.943547	0.951028	1.797591	C	4.650045	6.194273	0.159624
C	-3.211681	-0.741653	1.362739	H	1.730316	5.211660	1.627246
H	-3.130786	-1.712016	0.835885	H	3.969494	3.320045	-1.548423
C	-4.302214	0.082536	0.673025	H	3.423844	7.025524	1.739842
H	-4.409854	1.047676	1.200116	H	5.653723	5.138511	-1.443245
C	-3.893982	0.365766	-0.778899	H	5.394403	6.994671	0.206336
H	-3.811627	-0.598956	-1.314839	C	4.395498	-2.975744	-0.025660
F	-0.856070	-0.737659	1.817739	C	4.637063	-4.013492	0.891170
H	-1.370937	-0.639330	-0.782292	C	5.469829	-2.479832	-0.785840
Br	-2.781529	-3.058493	-1.563327	C	5.923901	-4.531892	1.055803
N	-0.348283	1.178440	-0.288141	C	6.754497	-3.004438	-0.625747
C	2.690189	-1.073290	-0.093227	C	6.986420	-4.028652	0.298405
C	3.013290	-2.462239	-0.214214	H	3.809085	-4.405553	1.488552
C	1.988192	-3.346180	-0.524908	H	5.292962	-1.692919	-1.524203
C	0.688147	-2.855514	-0.755819	H	6.096488	-5.333284	1.780461
N	0.393825	-1.576798	-0.657223	H	7.577976	-2.614858	-1.231865
H	2.194474	-4.414514	-0.626777	H	7.993681	-4.436822	0.424812
C	1.332963	-0.683273	-0.317689				
C	1.997474	1.688767	-0.003579				
C	3.658550	-0.084533	0.261417				
C	3.329464	1.236615	0.277620				
H	4.672054	-0.393402	0.519239				
H	4.081676	1.978742	0.542139				
H	-0.153209	-3.504425	-1.039166				
C	0.962084	0.723666	-0.202141	C	-1.518481	-0.599105	-0.901048
C	-0.619448	2.496254	-0.264512	O	-2.464989	0.197542	-1.259998
C	1.699768	3.085540	-0.040327	C	-1.381391	-1.121678	0.527662
C	0.367782	3.461720	-0.169207	H	-0.429820	-0.757175	0.935932
H	-1.674846	2.752020	-0.336747	C	-2.491118	-0.672686	1.468873
H	0.079343	4.513098	-0.207224	H	-3.347757	-1.363555	1.347340
O	-3.540538	-0.910218	2.727060	C	-2.973053	0.729483	1.090618
C	-3.329688	-2.214861	3.221646	H	-2.124247	1.440268	1.151237
H	-3.955820	-2.957919	2.688177	C	-3.513055	0.676180	-0.342371
H	-2.269684	-2.523578	3.139153	H	-4.316485	-0.084150	-0.387726
H	-3.615935	-2.207980	4.287479	F	-1.313595	-2.498571	0.507111
O	-5.528423	-0.609420	0.663644	H	-1.006016	-1.131707	-1.692100
C	-6.464906	-0.174018	1.620066	N	0.148798	0.776913	-0.897112
H	-6.079511	-0.277491	2.651689	C	3.312781	-1.114990	-0.349820
H	-6.757904	0.884023	1.452129	C	3.729791	-2.483127	-0.310424
H	-7.361616	-0.807666	1.508428	C	2.790059	-3.454664	-0.636737
C	-4.864969	1.269285	-1.502464	C	1.475939	-3.074716	-0.966880
H	-4.481471	1.468441	-2.525116	N	1.070786	-1.819812	-0.972581
H	-5.829416	0.732422	-1.599275	H	3.059759	-4.513177	-0.615006
O	-5.028912	2.474518	-0.790924	C	1.946737	-0.847219	-0.657626
C	-5.946715	3.348939	-1.389402	C	2.387015	1.593553	-0.445765
H	-5.627513	3.650012	-2.410965	C	4.209278	-0.012174	-0.163083
H	-6.959294	2.897152	-1.466985	C	3.769214	1.278497	-0.223468
H	-6.011230	4.252766	-0.759596	H	5.270569	-0.210986	-0.008885
C	2.741635	4.134239	0.043251	H	4.484075	2.095591	-0.123939
C	2.590506	5.196914	0.952245	H	0.724924	-3.832850	-1.217673
C	3.855924	4.123631	-0.816342	C	1.465609	0.525675	-0.662995

C	-0.266032	2.022756	-1.022940		L1 Int 2
C	1.906081	2.939091	-0.514615		Charge= 0 Multiplicity= 1
C	0.572137	3.132437	-0.853843		E (UB3LYP): -4477.858896 A.U.
H	-1.326312	2.162283	-1.248077		ΔG (Thermal Corrections): 0.556451 A.U.
H	0.156988	4.138646	-0.939539		G (UB3LYP): -4477.302445 A.U.
O	-1.976935	-0.696870	2.779984		
C	-2.832454	-1.290515	3.735817	C	-2.425505
H	-3.800484	-0.762041	3.804536	O	-2.621642
H	-3.024401	-2.356519	3.500113	C	-2.265362
H	-2.316655	-1.229421	4.709548	H	-1.311926
O	-3.986566	1.103583	1.983624	C	-3.424432
C	-3.933556	2.427107	2.456304	H	-4.343517
H	-2.991876	2.621820	3.010382	C	-3.672818
H	-4.038114	3.170899	1.644174	H	-2.822395
H	-4.782386	2.553822	3.148601	C	-3.752129
C	-4.007943	1.980708	-0.951382	H	-4.685945
H	-4.063000	1.843497	-2.052301	F	-2.178968
H	-3.292514	2.809761	-0.755742		-2.058573
O	-5.264975	2.275529	-0.417395	N	0.538226
C	-5.829168	3.447400	-0.946125	C	3.197488
H	-5.200222	4.340059	-0.737946	C	3.276950
H	-5.973857	3.374277	-2.045313	C	2.089311
H	-6.812201	3.587290	-0.467178	C	0.866247
O	-2.845151	-2.614963	-1.821719	N	0.773147
C	-3.459907	-2.219058	-3.019342	H	2.097885
H	-4.023519	-1.267294	-2.924169	C	1.903257
H	-2.674240	-2.078306	-3.785432	C	2.951433
H	-4.170904	-2.984630	-3.396568	C	4.352387
H	-3.572317	-2.704938	-1.137637	C	4.235417
Br	-5.392570	-2.449212	0.037894	H	5.344999
C	2.769524	4.115762	-0.246845	H	5.135930
C	3.507515	4.220461	0.946180	H	-0.076897
C	2.816093	5.175966	-1.169236	C	1.777590
C	4.276578	5.356708	1.205761	C	0.406287
C	3.594952	6.306538	-0.912587	C	2.786042
C	4.326651	6.400382	0.275597	C	1.493636
H	3.459746	3.416712	1.685624	H	-0.618474
H	2.250542	5.103335	-2.102487	H	1.316676
H	4.836510	5.428415	2.142897	O	-3.157673
H	3.630883	7.117920	-1.645600	C	-3.766554
H	4.933482	7.287757	0.478749	H	-4.873442
C	5.109013	-2.885626	0.064586	H	-3.452436
C	5.696353	-2.439931	1.262723	H	-3.456281
C	5.834102	-3.766263	-0.757323	O	-4.881328
C	6.978419	-2.859761	1.624096	C	-4.795749
C	7.119518	-4.178799	-0.398682	H	-4.125241
C	7.695704	-3.726529	0.792720	H	-4.450022
H	5.134206	-1.778195	1.927261	H	-5.812551
H	5.389831	-4.116703	-1.693160	C	-3.725947
H	7.417067	-2.512205	2.564289	H	-3.582231
H	7.674049	-4.856491	-1.054703	H	-2.847881
H	8.701420	-4.051875	1.075286	O	-4.918115
				C	-4.945561

H	-4.135337	5.679596	0.365603	C	-0.734726	1.187434	0.032536
H	-4.842315	5.492691	-1.277849	C	-2.688233	2.376237	0.091438
H	-5.918100	5.543422	0.164214	C	-2.870068	-0.031763	-0.079167
O	-3.511782	-0.843105	-1.625804	C	-3.485214	1.220957	-0.010300
C	-3.634047	-0.670614	-3.029443	H	-3.183201	3.354971	0.164155
H	-3.803323	0.390413	-3.284186	H	-4.571279	1.322936	0.011373
H	-2.726012	-1.030375	-3.550841	N	-1.368920	2.377821	0.143329
H	-4.502537	-1.265676	-3.352779	N	-3.593365	-1.222836	-0.136653
H	-4.161135	-2.390483	-1.101138	N	3.595625	-1.214297	-0.171711
Br	-5.010522	-3.579947	-0.926771	C	-3.345539	-2.251093	0.872279
C	4.564576	-3.533865	0.217097	H	-3.479003	-3.259402	0.439301
C	5.440438	-3.202141	1.266700	H	-2.326846	-2.178251	1.277489
C	4.905575	-4.599490	-0.634313	H	-4.053074	-2.144073	1.723060
C	6.627740	-3.913681	1.454093	C	4.981605	-1.133933	-0.594795
C	6.096836	-5.306012	-0.450657	H	5.317339	-2.139485	-0.904564
C	6.962018	-4.965064	0.593873	H	5.081736	-0.458758	-1.460476
H	5.178049	-2.393052	1.953561	H	5.665498	-0.784337	0.210197
H	4.235285	-4.864460	-1.456907	C	3.373734	-2.269784	0.814396
H	7.293211	-3.648181	2.281160	H	3.512581	-3.265282	0.354179
H	6.350719	-6.126395	-1.128781	H	4.091436	-2.176315	1.658412
H	7.894135	-5.519320	0.739589	H	2.359766	-2.218621	1.234780
C	3.931361	3.821876	-0.273261	C	-4.986954	-1.165310	-0.537994
C	4.843711	3.789514	0.796894	H	-5.322525	-2.183411	-0.803216
C	4.093094	4.802242	-1.267974	H	-5.657532	-0.788588	0.265861
C	5.892167	4.709921	0.865645	H	-5.106561	-0.523930	-1.426563
C	5.146540	5.717656	-1.202518				
C	6.049583	5.674294	-0.135539				
H	4.718064	3.049017	1.591408				
H	3.393707	4.834112	-2.108352				
H	6.587779	4.676151	1.709686				
H	5.263277	6.467430	-1.990959				
H	6.873750	6.392113	-0.082666				

L2 Catalyst

Charge= 0 Multiplicity= 1

E (UB3LYP): -839.954262 A.U.

ΔG (Thermal Corrections): 0.272353 A.U.

G (UB3LYP): -839.681909 A.U.

C	1.428005	-0.044150	-0.126832	C	-1.048208	-0.375709	-0.551030
C	2.866743	-0.028359	-0.065885	O	-2.010549	0.273894	-1.169387
C	3.478961	1.221468	0.053434	C	-1.161596	-0.580236	0.949266
C	2.679999	2.370709	0.199112	H	-0.861247	0.349896	1.458773
N	1.360251	2.369752	0.229670	C	-2.585555	-0.882140	1.399219
H	4.564881	1.323240	0.083365	H	-2.871438	-1.876041	1.017407
C	0.728718	1.185055	0.057456	C	-3.529686	0.164297	0.809110
C	-1.431050	-0.045197	-0.137091	H	-3.285265	1.144556	1.262052
C	0.683737	-1.224135	-0.458749	C	-3.390758	0.256237	-0.716067
C	-0.683579	-1.226552	-0.456289	H	-3.823304	-0.659778	-1.149269
H	1.224346	-2.121426	-0.766915	F	-0.287774	-1.562360	1.368240
H	-1.222758	-2.126782	-0.759171	H	-0.395629	-1.018313	-1.134196
H	3.173229	3.344923	0.325005	Br	-2.186726	-3.075313	-1.296358
			N	0.399325	1.075238	-0.553011	
			C	3.684971	-0.590680	0.021377	
			C	4.260304	-1.906299	-0.095134	
			C	3.412026	-2.934597	-0.515872	
			C	2.100961	-2.629904	-0.916984	
			N	1.593519	-1.412618	-0.904493	
			H	3.766700	-3.962234	-0.598179	
			C	2.340580	-0.406055	-0.409158	

C	2.536393	2.022080	0.083257		G (UB3LYP): -4167.297059 A.U.
C	4.375899	0.506154	0.623524		
C	3.837007	1.762185	0.626466	C	-0.891960
H	5.333222	0.328963	1.115411	O	-1.894565
H	4.378051	2.572439	1.114608	C	-1.333590
H	1.440803	-3.422894	-1.289678	H	-1.458286
C	1.731302	0.913663	-0.305475	C	-2.652667
C	-0.132943	2.286373	-0.491656	H	-2.511617
C	1.973576	3.351700	0.025675	C	-3.686899
C	0.593271	3.442759	-0.226909	H	-3.855756
H	-1.208233	2.344431	-0.690069	C	-3.149266
H	0.081154	4.403234	-0.263336	H	-2.995037
N	5.588215	-2.129772	0.245466	F	-0.343751
C	6.639539	-1.355113	-0.407486	H	-0.635423
H	6.246070	-0.414776	-0.815498	Br	-2.017591
C	6.002048	-3.485202	0.554624	N	0.314345
H	6.129830	-4.117652	-0.350555	C	3.406502
H	5.270707	-3.967130	1.222905	C	3.782034
H	7.074868	-1.930078	-1.252020	C	2.757845
N	2.735865	4.469199	0.239341	C	1.444289
C	2.089898	5.731339	0.556075	N	1.112668
H	1.273681	5.578279	1.279250	H	2.966126
C	4.077295	4.620346	-0.317725	C	2.041188
H	4.080258	5.474292	-1.022092	C	2.652863
H	4.374781	3.725455	-0.879923	C	4.328402
H	1.684510	6.239439	-0.343297	C	3.969375
O	-2.667578	-0.805056	2.805672	H	5.316450
C	-2.717084	-2.054913	3.458819	H	4.677703
H	-3.625940	-2.624177	3.177523	H	0.616147
H	-1.827475	-2.674528	3.235583	C	1.641392
H	-2.747338	-1.852702	4.543300	C	0.020358
O	-4.852703	-0.206371	1.112144	C	2.333578
C	-5.574390	0.704733	1.901427	C	0.963261
H	-5.103392	0.847943	2.894548	H	-1.041799
H	-5.684977	1.686795	1.400988	H	0.617485
H	-6.580834	0.276580	2.047886	N	5.114163
C	-3.999992	1.501663	-1.347136	C	6.111534
H	-3.724304	1.512251	-2.422699	H	5.788010
H	-3.554297	2.410468	-0.882942	C	5.403361
O	-5.388471	1.491157	-1.183061	H	5.289360
C	-6.022116	2.594833	-1.774902	H	4.746652
H	-5.675862	3.555455	-1.335151	H	6.275481
H	-5.843855	2.632786	-2.871072	N	3.283869
H	-7.105273	2.493269	-1.594902	C	2.941435
H	7.452713	-1.120279	0.303238	H	2.276268
H	6.973110	-3.447250	1.077993	C	4.545417
H	4.828854	4.820486	0.467939	H	4.620029
H	2.834201	6.399590	1.019943	H	4.574732
				H	2.456656
				O	-3.104782
				C	-2.907369
				H	-3.458070
				H	-1.836398
					2.654955
					3.167674
					2.576691
					3.187320

L2 Int 1

Charge= 0 Multiplicity= 1

E (UB3LYP): -4167.802489 A.U.

ΔG (Thermal Corrections): 0.505430 A.U.

H	-3.294848	-2.132112	4.201288	C	2.677115	3.107666	-0.168435
O	-4.899674	-0.549501	0.417346	C	1.322216	3.317903	-0.470174
C	-5.921577	-0.128743	1.287712	H	-0.557771	2.390926	-0.957985
H	-5.628463	-0.232344	2.349358	H	0.911067	4.321068	-0.578320
H	-6.210525	0.926966	1.098224	N	5.714956	-2.702146	0.342137
H	-6.798157	-0.771369	1.095082	C	6.836770	-2.050174	-0.326893
C	-4.076664	1.320713	-1.684735	H	6.519101	-1.124391	-0.824440
H	-3.595711	1.546178	-2.659779	C	6.001092	-4.073104	0.720251
H	-5.003050	0.747291	-1.886344	H	6.046879	-4.761805	-0.150642
O	-4.366125	2.511548	-0.988517	H	5.241528	-4.444545	1.426413
C	-5.250644	3.351997	-1.677066	H	7.256404	-2.720379	-1.105633
H	-4.836550	3.678404	-2.656171	N	3.542176	4.156186	0.020946
H	-6.228337	2.858419	-1.867757	C	3.012405	5.482825	0.281816
H	-5.423244	4.245261	-1.052322	H	2.173848	5.431093	0.994100
H	7.077371	-1.918482	-0.297125	C	4.887426	4.165608	-0.547045
H	6.448665	-4.094009	0.710019	H	4.957137	4.972050	-1.303108
H	3.868756	6.164372	0.674790	H	5.110593	3.217456	-1.053570
H	5.417487	4.157182	0.052264	H	2.670171	5.996273	-0.640917
O				O	-1.676003	-0.607999	2.763221
C				C	-2.625657	-1.251168	3.588626

L2 TS 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -4283.564780 A.U.

ΔG (Thermal Corrections): 0.545904 A.U.

G (UB3LYP): -4283.018876 A.U.

C	-0.818532	-0.424947	-0.846917	H	-2.738319	2.666116	2.997353
O	-1.701856	0.409227	-1.277474	H	-3.611853	3.279622	1.539948
C	-0.813325	-0.953236	0.585134	H	-4.532343	2.600965	2.914829
H	0.078711	-0.553572	1.085424	C	-3.268798	2.179806	-1.096596
C	-2.032021	-0.546985	1.401573	H	-3.201740	2.073539	-2.200216
H	-2.861375	-1.240875	1.163492	H	-2.569923	2.992668	-0.799890
C	-2.484405	0.861912	1.013262	O	-4.573862	2.479991	-0.698331
H	-1.657533	1.577531	1.194347	C	-5.061553	3.671497	-1.257555
C	-2.850879	0.853367	-0.474824	H	-4.448899	4.549917	-0.959333
H	-3.643562	0.098658	-0.634781	H	-5.083305	3.626045	-2.367592
F	-0.695253	-2.326378	0.583151	H	-6.090237	3.814852	-0.887855
H	-0.202291	-0.921262	-1.585299	O	-2.101643	-2.336108	-1.758164
N	0.888208	0.961610	-0.664455	C	-2.576506	-1.966711	-3.026831
C	3.980237	-0.982845	0.057212	H	-3.214994	-1.059281	-3.004241
C	4.412877	-2.357334	0.021467	H	-1.707725	-1.762081	-3.680005
C	3.445146	-3.315454	-0.302261	H	-3.172955	-2.777750	-3.495013
C	2.160270	-2.901008	-0.683584	H	-2.907351	-2.475904	-1.172673
N	1.779795	-1.638209	-0.752506	Br	-4.835533	-2.344008	-0.222558
H	3.685095	-4.378654	-0.320220	H	5.656649	4.351994	0.224784
C	2.653723	-0.686195	-0.365632	H	3.808427	6.095545	0.737174
C	3.104081	1.734783	-0.033460	H	7.643297	-1.810530	0.390082
C	4.786409	0.073398	0.585530	H	6.981835	-4.102147	1.225278
C	4.373301	1.375156	0.525977				
H	5.728285	-0.168538	1.079382				
H	4.995725	2.151779	0.969990				
H	1.412450	-3.649718	-0.971822				
C	2.191332	0.694486	-0.367246				
C	0.491076	2.222480	-0.700016				

L2 Int 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -4283.592609 A.U.

ΔG (Thermal Corrections): 0.542621 A.U.

G (UB3LYP): -4283.049988 A.U.

C	-1.710028	-0.109721	-1.078755	C	-4.118634	2.426865	2.873545
O	-1.901760	1.276371	-1.038698	H	-3.460329	2.051677	3.683304
C	-1.581121	-0.674916	0.331480	H	-3.761679	3.423241	2.546236
H	-0.629622	-0.316994	0.746428	H	-5.139460	2.543513	3.276841
C	-2.751407	-0.273702	1.214707	C	-3.004775	3.249954	-0.453591
H	-3.669601	-0.766871	0.847263	H	-2.840108	3.482359	-1.527600
C	-2.983889	1.237501	1.150534	H	-2.135604	3.657424	0.107371
H	-2.134766	1.732251	1.658021	O	-4.203864	3.813892	0.000853
C	-3.040267	1.733263	-0.304135	C	-4.222714	5.212922	-0.089491
H	-3.969707	1.352154	-0.763503	H	-3.422721	5.678903	0.526041
F	-1.508188	-2.066525	0.258509	H	-4.096199	5.561737	-1.137674
H	-0.774146	-0.265820	-1.636728	H	-5.201439	5.559477	0.282851
N	1.263941	1.163135	-0.403568	O	-2.786089	-0.761486	-1.720331
C	3.934923	-1.310264	0.287552	C	-2.876513	-0.533311	-3.118161
C	4.056906	-2.738620	0.415238	H	-3.036067	0.537697	-3.334729
C	2.871767	-3.478731	0.396810	H	-1.958592	-0.876702	-3.633196
C	1.651056	-2.822823	0.161828	H	-3.739977	-1.111218	-3.483594
N	1.532871	-1.526267	-0.056165	H	-3.498106	-2.292583	-1.256950
H	2.877945	-4.562742	0.515356	Br	-4.403765	-3.447563	-1.134505
C	2.648244	-0.766403	0.011722	H	6.669992	3.775997	-0.744754
C	3.653713	1.510236	-0.072842	H	5.334956	5.663996	0.154288
C	5.028160	-0.415937	0.528759	H	7.345515	-3.054447	0.102949
C	4.893408	0.933819	0.356804	H	6.389180	-4.869768	1.488107
H	5.967017	-0.819712	0.911614				
H	5.726071	1.594215	0.604592				
H	0.722504	-3.406221	0.127104				
C	2.504050	0.675711	-0.172966				
C	1.126118	2.470094	-0.530532				
C	3.494334	2.920765	-0.310023				
C	2.189870	3.387658	-0.493039				
H	0.104689	2.828484	-0.707906				
H	1.984801	4.446176	-0.656974				
N	5.303585	-3.329315	0.596362				
C	6.355179	-3.087425	-0.386455				
H	6.194016	-2.138907	-0.915399				
C	5.357603	-4.667695	1.151098				
H	5.082019	-5.455623	0.416399				
H	4.689608	-4.749731	2.023459				
H	6.372566	-3.897910	-1.146380				
N	4.596473	3.769648	-0.307337				
C	4.373545	5.187694	-0.105221				
H	3.673467	5.351777	0.729621				
C	5.708143	3.500551	-1.214169				
H	5.599167	4.090350	-2.149499				
H	5.745425	2.439300	-1.493087				
H	3.976499	5.699830	-1.009026				
O	-2.511269	-0.626146	2.560507				
C	-3.133456	-1.817828	2.982142				
H	-4.239264	-1.740257	2.927345				
H	-2.811613	-2.692151	2.384792				
H	-2.844420	-1.980480	4.034686				
O	-4.198257	1.516451	1.807837				

L3 Catalyst

Charge= 0 Multiplicity= 1

E (UB3LYP): -1073.558177 A.U.

ΔG (Thermal Corrections): 0.400767 A.U.

G (UB3LYP): -1073.157410 A.U.

C	1.426588	0.759428	-0.074791
C	2.863087	0.772991	-0.004554
C	3.479850	2.019555	0.108547
C	2.683798	3.175394	0.222179
N	1.363706	3.179000	0.231564
H	4.566048	2.114580	0.154092
C	0.729115	1.993711	0.076402
C	-1.428298	0.760641	-0.105996
C	0.685161	-0.431428	-0.373084
C	-0.681668	-0.432523	-0.380322
H	1.231860	-1.336729	-0.645422
H	-1.224999	-1.339473	-0.654656
H	3.178260	4.150135	0.338092
C	-0.733830	1.996812	0.040717
C	-2.690363	3.183688	0.073978
C	-2.865814	0.774044	-0.059487
C	-3.484755	2.023949	-0.007077
H	-3.186416	4.162943	0.128873
H	-4.571438	2.121013	0.014121
N	-1.371036	3.187614	0.125228
N	3.580971	-0.425195	-0.083531
C	3.397018	-1.399531	1.005693

H	2.354518	-1.373562	1.353023	C	2.476536	-3.312026	-0.616832
C	3.784606	-2.808082	0.555546	C	1.152397	-2.981296	-0.953543
H	3.084642	-3.136806	-0.236042	N	0.679869	-1.750224	-0.941761
C	5.220827	-2.829904	0.018803	H	2.802208	-4.349634	-0.695839
H	5.922388	-2.631232	0.852885	C	1.479174	-0.752178	-0.516704
C	5.402511	-1.756183	-1.059917	C	1.781699	1.678801	-0.111755
H	4.794843	-2.015396	-1.947135	C	3.600585	0.124393	0.372818
C	4.963925	-0.376307	-0.556600	C	3.101766	1.396183	0.369373
H	5.652901	-0.040442	0.251388	H	4.578746	-0.077283	0.812272
H	5.473106	-3.828582	-0.381158	H	3.685974	2.209657	0.801624
H	3.672541	-3.505012	1.405785	H	0.451647	-3.762729	-1.272544
H	6.456770	-1.702075	-1.386454	C	0.921249	0.590987	-0.430109
H	5.030292	0.358243	-1.375105	C	-0.892235	2.034901	-0.607627
H	4.030869	-1.100126	1.870913	C	1.268690	3.024010	-0.184822
N	-3.578767	-0.428254	-0.096660	C	-0.107094	3.169283	-0.409773
C	-4.964758	-0.400473	-0.562963	H	-1.969531	2.130121	-0.778698
H	-5.036992	0.299618	-1.410600	H	-0.574967	4.151103	-0.473266
C	-5.407102	-1.799455	-1.006653	N	4.713159	-2.535874	0.013205
H	-4.806804	-2.094471	-1.887675	C	5.708049	-1.881297	-0.851755
C	-5.217119	-2.829664	0.112201	H	5.343497	-0.887743	-1.145543
H	-5.910960	-2.597488	0.944085	C	7.062153	-1.782582	-0.154630
C	-3.776268	-2.786960	0.634319	H	6.969021	-1.111079	0.719584
H	-3.083142	-3.145828	-0.150123	C	7.537497	-3.165423	0.301815
C	-3.386013	-1.362252	1.026746	H	7.762228	-3.783262	-0.589201
H	-4.013257	-1.030252	1.884774	C	6.453003	-3.855264	1.134041
H	-5.473438	-3.843223	-0.245479	H	6.313707	-3.311458	2.086716
H	-6.463895	-1.757527	-1.326601	C	5.113395	-3.888907	0.394214
H	-3.655686	-3.450074	1.510059	H	5.196865	-4.546076	-0.499801
H	-2.341019	-1.323768	1.364872	H	8.475505	-3.083866	0.879273
H	-5.648115	-0.031335	0.235178	H	7.792631	-1.325471	-0.845758
				H	6.759000	-4.888873	1.385332
				H	4.335121	-4.313091	1.047231

L3 TS1

Charge= 0 Multiplicity= 1

E (UB3LYP): -4401.369964 A.U.

ΔG (Thermal Corrections): 0.627400 A.U.

G (UB3LYP): -4400.742564 A.U.

C	-1.904750	-0.582506	-0.548962	H	2.816563	5.725268	2.081834
O	-2.856051	0.081616	-1.170388	C	3.869428	6.396677	0.309605
C	-1.993557	-0.732042	0.960050	C	4.398328	5.030170	-0.136669
H	-1.643780	0.199905	1.433315	H	4.743560	4.454997	0.742770
C	-3.418868	-0.957849	1.448868	C	3.305566	4.241658	-0.851498
H	-3.754212	-1.950991	1.107538	H	3.013601	4.776559	-1.780555
C	-4.330808	0.107255	0.841644	H	5.261612	5.145726	-0.815616
H	-4.030336	1.092825	1.247851	H	3.661763	3.249252	-1.154488
C	-4.225777	0.132205	-0.688533	H	3.657686	7.013136	-0.585376
H	-4.700657	-0.783752	-1.075085	H	4.632540	6.936684	0.897336
F	-1.153041	-1.736956	1.392827	H	2.146308	7.213707	1.371943
H	-1.298383	-1.278393	-1.121358	H	1.181005	5.951279	-0.514955
Br	-3.171245	-3.263117	-1.178514	O	-3.465553	-0.830314	2.852992
N	-0.411324	0.802211	-0.634399	C	-3.560342	-2.054052	3.549161
C	2.838229	-0.965574	-0.152289	H	-4.501881	-2.586971	3.306954
C	3.367885	-2.298454	-0.260853	H	-2.707080	-2.723528	3.327897

H	-3.555589	-1.815149	4.626563	H	-0.056237	4.493103	-0.006332
O	-5.660069	-0.189937	1.192861	N	4.152967	-2.931918	0.005319
C	-6.323137	0.788848	1.951685	C	5.125838	-2.434809	-0.981185
H	-5.822346	0.959829	2.925730	H	4.868682	-1.405411	-1.265613
H	-6.404948	1.749475	1.406106	C	6.548980	-2.511702	-0.434887
H	-7.342785	0.412296	2.141896	H	6.642904	-1.819528	0.423096
C	-4.805315	1.372557	-1.356216	C	6.880241	-3.939231	0.011363
H	-4.545706	1.335389	-2.435223	H	6.920538	-4.596239	-0.879052
H	-4.325121	2.283401	-0.931963	C	5.809995	-4.460348	0.974650
O	-6.190909	1.410777	-1.172641	H	5.849915	-3.887503	1.919669
C	-6.799150	2.513248	-1.792682	C	4.405731	-4.321539	0.381616
H	-6.418080	3.476762	-1.389549	H	4.302978	-4.997243	-0.496241
H	-6.634936	2.509744	-2.891691	H	7.878165	-3.978127	0.483169
H	-7.882272	2.450774	-1.595464	H	7.254700	-2.170606	-1.213257
				H	5.990880	-5.520841	1.224288
				H	3.652330	-4.625407	1.124661
L3 Int 1				H	5.049407	-3.051664	-1.903850
Charge= 0 Multiplicity= 1				N	2.606729	3.964866	-0.031852
E (UB3LYP): -4401.405423 A.U.				C	2.372550	5.359238	0.356785
ΔG (Thermal Corrections): 0.632265 A.U.				H	1.540854	5.395383	1.073882
G (UB3LYP): -4400.773158 A.U.				C	3.630213	5.943546	1.008300
C	-1.741261	0.309560	-0.164523	H	3.806388	5.414918	1.963285
O	-2.745862	1.060559	-0.781385	C	4.860657	5.804995	0.108782
C	-2.135105	0.037531	1.294271	C	5.043550	4.347334	-0.324956
H	-2.210491	0.996423	1.837540	H	5.319770	3.725643	0.547112
C	-3.474237	-0.684798	1.354916	C	3.756489	3.811534	-0.943782
H	-3.379580	-1.662699	0.844045	H	3.521735	4.392097	-1.859399
C	-4.516670	0.142988	0.599278	H	5.858341	4.256514	-1.064468
H	-4.643138	1.114157	1.110959	H	3.854611	2.762953	-1.247939
C	-4.026487	0.410302	-0.830700	H	4.731341	6.437586	-0.790404
H	-3.924888	-0.561592	-1.350970	H	5.761462	6.170867	0.631659
F	-1.144720	-0.703960	1.927865	H	3.437858	7.003213	1.251069
H	-1.536256	-0.629586	-0.690548	H	2.086398	5.957521	-0.532381
Br	-3.004960	-3.096620	-1.467287	O	-3.878949	-0.833985	2.702696
N	-0.504217	1.166786	-0.180272	C	-3.701868	-2.133204	3.222364
C	2.502898	-1.123266	0.007647	H	-4.300171	-2.880470	2.663131
C	2.828713	-2.517839	-0.131817	H	-2.640391	-2.447486	3.202134
C	1.778016	-3.401495	-0.374764	H	-4.046835	-2.114005	4.270725
C	0.479726	-2.895495	-0.566532	O	-5.749226	-0.536073	0.529417
N	0.191746	-1.611336	-0.507784	C	-6.728936	-0.082151	1.431279
H	1.953448	-4.473466	-0.473513	H	-6.400109	-0.181618	2.482826
C	1.151260	-0.721272	-0.210640	H	-6.999956	0.978120	1.240716
C	1.853612	1.635596	0.067806	H	-7.626674	-0.705710	1.277495
C	3.466918	-0.161879	0.426460	C	-4.955278	1.308769	-1.614172
C	3.157104	1.165983	0.430655	H	-4.510230	1.506842	-2.611900
H	4.443213	-0.502707	0.774023	H	-5.910676	0.769184	-1.768448
H	3.887544	1.893313	0.783700	O	-5.167905	2.516161	-0.918599
H	-0.371415	-3.547256	-0.812014	C	-6.050443	3.383602	-1.575695
C	0.804326	0.693823	-0.114964	H	-5.669923	3.683729	-2.576556
C	-0.744748	2.493267	-0.083985	H	-7.054226	2.926695	-1.715286
C	1.593408	3.055850	0.002094	H	-6.159082	4.289136	-0.954248
C	0.242167	3.446304	0.002350				
H	-1.796305	2.769836	-0.135518				

L3 TS 2

Charge= 0 Multiplicity= 1
E (UB3LYP): -4517.168533 A.U.
ΔG (Thermal Corrections): 0.676461 A.U.
G (UB3LYP): -4516.492072 A.U.

C	-1.693033	-0.556543	-0.888208	N	2.792263	3.915352	-0.128457
O	-2.575420	0.300520	-1.274167	C	2.316220	5.251088	0.229151
C	-1.653822	-1.117875	0.531150	H	1.437383	5.148534	0.883403
H	-0.732290	-0.758480	1.007555	C	3.415423	6.024466	0.963275
C	-2.829089	-0.693879	1.401097	H	3.609315	5.522791	1.929337
H	-3.683238	-1.365270	1.187722	C	4.709441	6.085035	0.147414
C	-3.264863	0.729730	1.048653	C	5.142838	4.677330	-0.273528
H	-2.415469	1.424360	1.205292	H	5.448882	4.095711	0.616111
C	-3.688725	0.746904	-0.424192	C	3.997942	3.952297	-0.974084
H	-4.496731	0.004160	-0.563825	H	3.744272	4.486697	-1.914936
F	-1.579386	-2.493765	0.492693	H	6.011551	4.721270	-0.954025
H	-1.118811	-1.056006	-1.658101	C	4.285455	2.931569	-1.255673
N	0.032379	0.791396	-0.733830	H	4.542237	6.698470	-0.759055
C	3.118449	-1.205426	-0.137146	C	5.507634	6.581323	0.727024
C	3.530397	-2.582758	-0.188264	H	3.045951	7.040348	1.188832
C	2.547887	-3.528932	-0.489216	H	2.000211	5.811122	-0.677591
C	1.250898	-3.099910	-0.816883	O	-2.420874	-0.781107	2.746639
N	0.881513	-1.833098	-0.858188	C	-3.351466	-1.415374	3.600319
H	2.780239	-4.593582	-0.525528	H	-4.321250	-0.885617	3.616843
C	1.780046	-0.891605	-0.503635	C	-3.527381	-2.467000	3.297191
C	2.283033	1.518148	-0.188755	H	-2.915573	-1.405446	4.614244
C	3.970168	-0.163153	0.346567	C	-4.340026	1.080861	1.876372
C	3.574664	1.144147	0.306225	H	-4.304043	2.380162	2.412524
H	4.930619	-0.428733	0.791053	H	-3.401847	2.534869	3.040188
H	4.222664	1.920223	0.715978	C	-4.341638	3.161683	1.630313
H	0.484722	-3.838274	-1.082273	H	-5.198349	2.488979	3.048474
C	1.339761	0.495399	-0.485659	C	-4.114400	2.084908	-1.014252
C	-0.341016	2.058968	-0.759247	H	-4.092057	1.989918	-2.120687
C	1.877178	2.896079	-0.300950	H	-3.395108	2.886984	-0.737511
C	0.523351	3.137946	-0.561298	O	-5.399509	2.394003	-0.561842
H	-1.394287	2.247929	-0.981879	C	-5.897537	3.594716	-1.091639
H	0.133144	4.150744	-0.658758	H	-5.265557	4.465016	-0.810477
N	4.849443	-2.926853	0.089571	H	-5.963252	3.558877	-2.200278
C	5.899981	-2.387478	-0.789269	C	-6.909534	3.744128	-0.680629
H	5.620936	-1.378443	-1.121045	O	-3.072256	-2.416716	-1.793630
C	7.254604	-2.376749	-0.086272	C	-3.590108	-2.009056	-3.033205
H	7.214912	-1.668417	0.762500	H	-4.197895	-1.082798	-2.967016
C	7.610823	-3.776714	0.423179	H	-2.744634	-1.818926	-3.720528
H	7.786027	-4.443799	-0.443109	C	-4.231994	-2.791946	-3.489052
C	6.469468	-4.341805	1.272962	H	-3.855780	-2.547181	-1.177291
H	6.372443	-3.752525	2.203585	Br	-5.742860	-2.382358	-0.144944
C	5.134457	-4.292557	0.525757				
H	5.165511	-4.988482	-0.341675				
H	8.550214	-3.752566	1.003521				
H	8.023165	-2.007443	-0.788468				
H	6.678079	-5.386249	1.564943				
H	4.321667	-4.624546	1.189842				
H	5.961948	-3.020681	-1.701809				

L3 Int 2

Charge= 0 Multiplicity= 1
E (UB3LYP): -4517.196643 A.U.
ΔG (Thermal Corrections): 0.671100 A.U.
G (UB3LYP): -4516.525543 A.U.

H	-4.694166	-0.860878	0.676944	H	6.872859	3.839101	-1.746200
C	-4.109589	1.134041	1.184825	H	4.846342	2.386294	-1.498243
H	-3.356657	1.611829	1.839026	H	5.845860	6.066152	-1.430089
C	-3.968189	1.716040	-0.231926	H	7.085929	5.845930	-0.177566
H	-4.819373	1.357599	-0.837904	H	4.905598	6.782859	0.749704
F	-2.440352	-2.088561	0.336857	H	3.287488	5.678600	-0.747473
H	-1.502783	-0.178415	-1.347418	O	-3.791929	-0.800587	2.542170
N	0.405263	1.212640	-0.213526	C	-4.437453	-2.025402	2.805222
C	3.025950	-1.362796	0.256066	H	-5.525703	-1.963912	2.596511
C	3.113936	-2.795664	0.322163	H	-4.011756	-2.858324	2.213811
C	1.913342	-3.506967	0.316660	H	-4.297059	-2.242526	3.878027
C	0.699476	-2.811713	0.168797	O	-5.413555	1.352426	1.671682
N	0.606335	-1.503253	0.020719	C	-5.510889	2.180689	2.801230
H	1.899284	-4.595688	0.381069	H	-4.974133	1.750542	3.670992
C	1.743770	-0.774446	0.066926	H	-5.127553	3.201171	2.604048
C	2.815677	1.471524	0.013170	H	-6.582549	2.259060	3.053880
C	4.161542	-0.513090	0.461895	C	-3.930530	3.239186	-0.284329
C	4.061132	0.845056	0.345441	H	-3.641562	3.537563	-1.314958
H	5.105508	-0.965492	0.771020	H	-3.136672	3.611340	0.399577
H	4.924999	1.476126	0.561880	O	-5.179279	3.773623	0.058189
H	-0.244990	-3.369209	0.146653	C	-5.197412	5.175607	0.052554
C	1.636364	0.677171	-0.057208	H	-4.480156	5.602126	0.787150
C	0.303345	2.525841	-0.297873	H	-4.948871	5.588538	-0.949473
C	2.691142	2.891866	-0.166955	H	-6.216161	5.498598	0.325478
C	1.399270	3.407323	-0.282905	O	-3.479560	-0.694579	-1.729103
H	-0.712895	2.921369	-0.418640	C	-3.379491	-0.400238	-3.113891
H	1.225386	4.476745	-0.409184	H	-3.521431	0.679114	-3.299324
N	4.361060	-3.413843	0.418034	H	-2.395098	-0.712536	-3.512671
C	5.296986	-3.224737	-0.701015	H	-4.177112	-0.964980	-3.621793
H	5.182259	-2.211261	-1.108149	H	-4.181624	-2.271030	-1.452582
C	6.737195	-3.476591	-0.262661	Br	-5.041160	-3.466381	-1.509518
H	7.027684	-2.706581	0.476601				
C	6.877800	-4.870157	0.357418				
H	6.719916	-5.633832	-0.428894				
C	5.841612	-5.066887	1.467498				
H	6.070525	-4.391255	2.312413				
C	4.424846	-4.763045	0.973416				
H	4.123962	-5.521652	0.216491				
H	7.899268	-5.021210	0.749754				
H	7.406354	-3.366088	-1.134644				
H	5.873366	-6.100940	1.854452				
H	3.714005	-4.830935	1.811459				
H	5.030351	-3.932295	-1.517727				
N	3.831728	3.695198	-0.191298				
C	3.686182	5.113432	0.124859				
H	2.960183	5.216212	0.946252				
C	5.034179	5.705116	0.544720				
H	5.348572	5.224561	1.489661				
C	6.104247	5.479509	-0.527032				
C	6.181833	3.995524	-0.898666				
H	6.572874	3.415143	-0.042030				
C	4.802048	3.459986	-1.271838				
H	4.444884	3.969839	-2.194457				

L4 Catalyst

Charge= 0 Multiplicity= 1

E (UB3LYP): -994.874196 A.U.

ΔG (Thermal Corrections): 0.341975 A.U.

G (UB3LYP): -994.532221 A.U.

C	1.426011	0.496054	-0.126440
C	2.863108	0.509684	-0.049027
C	3.477727	1.757866	0.075874
C	2.678671	2.908358	0.214038
N	1.358636	2.908889	0.234326
H	4.563609	1.857726	0.109086
C	0.726708	1.725326	0.054985
C	-1.429900	0.494550	-0.154869
C	0.685558	-0.680719	-0.475968
C	-0.681596	-0.683612	-0.481762
H	1.230161	-1.570207	-0.798592
H	-1.220527	-1.576405	-0.805664
H	3.171766	3.882445	0.341250
C	-0.736358	1.727652	0.019577

C	-2.692312	2.913704	0.064828	C	3.119856	-0.833005	-0.067459
C	-2.868048	0.505653	-0.098324	C	3.665533	-2.158850	-0.192771
C	-3.487400	1.756684	-0.037355	C	2.793746	-3.168783	-0.609140
H	-3.188742	3.892305	0.128343	C	1.485278	-2.835473	-0.998054
H	-4.573707	1.856262	-0.029001	N	1.004159	-1.607613	-0.978265
N	-1.373371	2.917059	0.126467	H	3.124323	-4.204463	-0.689023
N	3.586947	-0.674716	-0.138533	C	1.776528	-0.618819	-0.486403
C	3.404796	-1.753109	0.846713	C	2.036990	1.803074	-0.004649
H	2.352288	-2.048148	0.954236	C	3.837321	0.244683	0.537900
C	4.306914	-2.875756	0.310470	C	3.329629	1.513536	0.540982
H	3.724275	-3.556608	-0.332244	H	4.783737	0.037459	1.038761
C	5.394643	-2.138329	-0.520261	H	3.878629	2.310999	1.042332
H	5.367069	-2.466451	-1.572166	H	0.804126	-3.613454	-1.364484
C	5.020866	-0.647141	-0.415181	C	1.199472	0.714406	-0.375957
H	5.582213	-0.168806	0.417030	C	-0.633286	2.132907	-0.532301
H	4.730086	-3.475592	1.132606	C	1.511756	3.146052	-0.076481
H	6.414173	-2.319899	-0.143211	C	0.129902	3.273320	-0.294885
H	5.225100	-0.073626	-1.334115	H	-1.711694	2.215981	-0.701936
H	3.758007	-1.406539	1.842264	H	-0.357379	4.246735	-0.318416
N	-3.584604	-0.684482	-0.140539	O	-3.153935	-0.944528	2.818543
C	-5.022536	-0.673943	-0.398721	C	-3.208957	-2.202398	3.455865
H	-5.241193	-0.143210	-1.339722	H	-4.133942	-2.752351	3.189156
C	-5.396976	-2.168850	-0.430181	H	-2.335769	-2.833631	3.202587
H	-5.402670	-2.541960	-1.467265	H	-3.209515	-2.014657	4.543351
C	-4.284883	-2.871602	0.397866	O	-5.367228	-0.279398	1.185687
H	-3.709067	-3.564973	-0.237627	C	-6.045645	0.626936	2.017775
C	-3.382484	-1.726252	0.880522	H	-5.543688	0.734783	3.000045
H	-3.723735	-1.345480	1.867659	H	-6.147992	1.623459	1.544777
H	-6.404105	-2.333242	-0.013979	H	-7.056916	0.217183	2.182509
H	-4.683924	-3.451395	1.246040	C	-4.529967	1.452909	-1.264661
H	-2.327215	-2.012484	0.983575	H	-4.289027	1.471421	-2.348455
H	-5.572163	-0.158255	0.418736	H	-4.040504	2.339893	-0.802082
O	-5.911877	1.483565	-1.054848	O	-5.911877	1.483565	-1.054848
C	-6.528915	2.616403	-1.607977	C	-6.528915	2.616403	-1.607977

L4 TS1

Charge= 0 Multiplicity= 1

E (UB3LYP): -4322.685917 A.U.

ΔG (Thermal Corrections): 0.570984 A.U.

G (UB3LYP): -4322.114933 A.U.

C	-1.608622	-0.507783	-0.571755	H	5.980362	-0.623770	-0.537707
O	-2.573296	0.164823	-1.161073	C	7.339601	-2.220669	0.173584
C	-1.689254	-0.720644	0.929654	H	7.600941	-1.532724	0.994389
H	-1.362549	0.201100	1.438071	C	6.927246	-3.607893	0.736772
C	-3.107148	-1.003552	1.409689	H	7.018917	-3.622703	1.834573
H	-3.420350	-1.986758	1.021481	C	5.455390	-3.779204	0.318744
C	-4.044379	0.068724	0.856540	H	5.388827	-4.357134	-0.627595
H	-3.769269	1.037931	1.316118	H	8.206179	-2.274992	-0.504448
C	-3.940812	0.179906	-0.670364	H	7.547923	-4.427382	0.341252
H	-4.411038	-0.716373	-1.105441	H	4.838429	-4.292456	1.073369
F	-0.822451	-1.719508	1.322458	H	6.108042	-2.028368	-1.626850
H	-0.987848	-1.162645	-1.175862	N	2.313892	4.240770	0.098306
Br	-2.820596	-3.179300	-1.319467	C	1.736938	5.574086	0.293103
N	-0.132269	0.909678	-0.601143	H	1.057405	5.560484	1.160446

C	2.955225	6.510036	0.478828	H	-2.383434	-2.530484	3.137844
H	2.991647	6.927842	1.496983	H	-3.821035	-2.245655	4.178806
C	4.192226	5.630046	0.183390	O	-5.449660	-0.564715	0.448410
H	4.655830	5.286250	1.123692	C	-6.450995	-0.146260	1.343480
C	3.615585	4.430174	-0.563208	H	-6.143500	-0.277589	2.397965
H	3.444834	4.672971	-1.633011	H	-6.725145	0.917935	1.181336
H	2.891549	7.357733	-0.221781	H	-7.341063	-0.770074	1.150863
H	4.962785	6.153680	-0.404361	C	-4.624668	1.335225	-1.626354
H	4.247744	3.536382	-0.521452	H	-4.154987	1.571618	-2.604296
H	1.145959	5.879278	-0.593197	H	-5.564630	0.783031	-1.824408
				O	-4.880932	2.516810	-0.901858
				C	-5.762303	3.385953	-1.558009
				H	-5.359923	3.724084	-2.538017
				H	-6.751957	2.913491	-1.740386
				H	-5.907650	4.269775	-0.913219
				N	4.482943	-2.846733	0.066099
				C	5.555025	-2.302096	-0.783406
C	-1.434099	0.338263	-0.123449	H	5.588949	-1.205018	-0.764461
O	-2.431975	1.096776	-0.744596	C	6.820011	-2.964189	-0.220549
C	-1.859538	0.011861	1.314775	H	7.280758	-2.315591	0.542588
H	-1.955555	0.947749	1.893841	C	6.316819	-4.286246	0.420238
C	-3.192520	-0.723156	1.322178	H	6.557037	-4.311229	1.495179
H	-3.077416	-1.684652	0.784700	C	4.791727	-4.267456	0.211415
C	-4.223376	0.119063	0.566647	H	4.522299	-4.830032	-0.707603
H	-4.368609	1.074840	1.101878	H	7.568090	-3.130588	-1.011950
C	-3.701208	0.430792	-0.843203	H	6.767501	-5.179106	-0.041177
H	-3.573425	-0.525813	-1.385685	H	4.224554	-4.699130	1.051320
F	-0.873523	-0.744047	1.939193	H	5.382963	-2.614333	-1.835362
H	-1.203477	-0.581351	-0.672235	N	2.824055	4.064766	0.066606
Br	-2.649592	-3.087278	-1.504265	C	2.524990	5.492367	0.292679
N	-0.209585	1.208695	-0.083372	H	2.143289	5.617458	1.319598
C	2.820729	-1.048777	0.092568	C	3.859179	6.229406	0.050238
C	3.167456	-2.434421	-0.086316	H	4.076970	6.954248	0.849834
C	2.130225	-3.321810	-0.377653	C	4.912642	5.114592	-0.046597
C	0.834833	-2.821411	-0.596681	H	5.283104	4.834785	0.955531
N	0.532889	-1.541097	-0.517978	C	4.117965	3.956524	-0.636127
H	2.315019	-4.390530	-0.489155	H	3.939303	4.110685	-1.719011
C	1.473219	-0.652595	-0.159727	H	3.812245	6.785934	-0.900242
C	2.139813	1.702942	0.206022	H	5.777283	5.390385	-0.670678
C	3.748091	-0.094233	0.597502	H	4.593012	2.979829	-0.512750
C	3.425496	1.231116	0.624641	H	1.743786	5.845064	-0.403355
H	4.702005	-0.436479	1.000283				
H	4.126296	1.943896	1.057615				
H	-0.003510	-3.475202	-0.878828				
C	1.106274	0.754590	-0.024494				
C	-0.470584	2.523516	0.098127				
C	1.860598	3.124444	0.149848				
C	0.497826	3.488132	0.220193				
H	-1.527431	2.784338	0.083351				
H	0.177889	4.524950	0.300375				
O	-3.627471	-0.916227	2.655336				
C	-3.448766	-2.228729	3.139730				
H	-4.023171	-2.965079	2.542347				

H	-3.421755	-1.339603	1.163343	C	2.576218	5.383454	0.114598
C	-3.025124	0.761345	1.044430	H	1.857092	5.445578	0.946813
H	-2.190426	1.466016	1.232236	C	3.861455	6.209778	0.347271
C	-3.401835	0.780978	-0.441002	H	3.938921	6.537181	1.395831
H	-4.201275	0.035024	-0.608153	C	5.027350	5.260274	-0.027768
F	-1.279224	-2.439021	0.540432	H	5.537762	4.899276	0.880802
H	-0.781773	-1.000889	-1.601711	C	4.343640	4.086673	-0.728765
N	0.333164	0.854510	-0.655905	H	4.163838	4.315577	-1.800269
C	3.421403	-1.125073	-0.015113	H	3.852934	7.115253	-0.279733
C	3.844543	-2.499560	-0.078127	H	5.782011	5.738840	-0.671769
C	2.865885	-3.450646	-0.384683	H	4.911232	3.150550	-0.679309
C	1.572084	-3.025517	-0.726498	H	2.059165	5.722580	-0.806157
N	1.198889	-1.759916	-0.775501	N	5.155272	-2.847378	0.194880
H	3.099271	-4.515081	-0.411416	C	6.280200	-2.274535	-0.562106
C	2.087942	-0.816023	-0.403652	H	6.259257	-1.177605	-0.581128
C	2.570507	1.596255	-0.069152	C	7.510102	-2.850613	0.150107
C	4.245636	-0.083083	0.512497	H	7.841984	-2.162895	0.945256
C	3.843092	1.222469	0.471739	C	7.015679	-4.189425	0.761178
H	5.185746	-0.345111	0.999516	H	7.169833	-4.198542	1.851903
H	4.468190	1.991855	0.925522	C	5.512883	-4.245070	0.427032
H	0.810809	-3.766852	-0.997786	H	5.343206	-4.854539	-0.485694
C	1.639149	0.568601	-0.387439	H	8.351167	-2.983613	-0.548804
C	-0.050055	2.119322	-0.672705	H	7.542426	-5.062892	0.345549
C	2.159621	2.973126	-0.196867	H	4.896367	-4.668410	1.235814
C	0.801829	3.203958	-0.459261	H	6.231380	-2.630166	-1.613218
H	-1.103016	2.302082	-0.901600				
H	0.400238	4.212950	-0.542255				
O	-2.216340	-0.745030	2.763068				
C	-3.165960	-1.390542	3.586713				
H	-4.140844	-0.870109	3.575518				
H	-3.322290	-2.443058	3.276352				
H	-2.760847	-1.378854	4.613318				
O	-4.133125	1.096307	1.835749				
C	-4.123370	2.388731	2.389393				
H	-3.249474	2.537218	3.057255				
H	-4.128891	3.180022	1.616078				
H	-5.044544	2.487943	2.987431				
C	-3.814075	2.120749	-1.037395				
H	-3.756347	2.032458	-2.143117				
H	-3.106644	2.923245	-0.732795				
O	-5.113462	2.424561	-0.623972				
C	-5.596274	3.628577	-1.160284				
H	-4.974623	4.497433	-0.852871				
H	-5.626861	3.601099	-2.270699				
H	-6.620932	3.773749	-0.780287				
O	-2.698533	-2.388015	-1.797284				
C	-3.186688	-1.983816	-3.049986				
H	-3.817910	-1.072551	-2.996919				
H	-2.324786	-1.769165	-3.709108				
H	-3.795232	-2.778328	-3.530954				
H	-3.497321	-2.534280	-1.204317				
Br	-5.413069	-2.406528	-0.225491				
N	3.048313	4.005644	-0.033801				

L5 Catalyst

Charge= 0 Multiplicity= 1

E (UB3LYP): -1145.366953 A.U.

ΔG (Thermal Corrections): 0.353141 A.U.

G (UB3LYP): -1145.013812 A.U.

C 1.425715 0.741896 -0.087198

C 2.860997 0.757689 -0.018488

C 3.479366 2.001850 0.099104

C 2.683227 3.157172 0.221320

N 1.363315 3.159061 0.235032

H 4.565772 2.096146 0.140055

C 0.728434 1.975154 0.074149

C -1.428603 0.742653 -0.114379

C 0.684504 -0.446663 -0.395451

C -0.682307 -0.447919 -0.401383

H 1.231298 -1.348240 -0.679807

H -1.225593 -1.351332 -0.687247

H 3.177252 4.131542 0.340636

C -0.734416 1.978035 0.041559

C -2.691032 3.164974 0.086321

C -2.864867 0.757961 -0.065793

C -3.485382 2.005478 -0.003320

H -3.186719 4.143774 0.148944

H -4.572148 2.101465 0.017278

N -1.371838 3.167487 0.136576

N 3.579899 -0.441262 -0.103237

C	3.415418	-1.417613	0.984381	N	0.687996	-1.734369	-0.911582
H	2.362207	-1.480962	1.293582	H	2.811026	-4.332411	-0.665163
C	3.910219	-2.785859	0.528155	C	1.485052	-0.735829	-0.485907
H	3.251390	-3.166093	-0.282925	C	1.784984	1.693993	-0.075026
O	5.252376	-2.727420	0.083620	C	3.604164	0.140582	0.410829
C	5.411040	-1.793789	-0.967227	C	3.103843	1.411701	0.409907
H	4.823916	-2.109936	-1.856519	H	4.579339	-0.062343	0.856349
C	4.969566	-0.391343	-0.549757	H	3.682896	2.224405	0.850439
H	5.644880	-0.023515	0.253435	H	0.456499	-3.746155	-1.240658
H	3.879375	-3.500378	1.367763	C	0.925512	0.606647	-0.398154
H	6.480476	-1.789372	-1.236375	C	-0.889126	2.051122	-0.573876
H	5.053977	0.289985	-1.412105	C	1.269935	3.036757	-0.145523
H	4.007016	-1.093941	1.868318	C	-0.103842	3.185202	-0.371159
N	-3.579181	-0.444747	-0.111850	H	-1.966443	2.145696	-0.745209
C	-4.972679	-0.413844	-0.548362	H	-0.570665	4.168020	-0.427053
H	-5.066420	0.237852	-1.432338	N	4.720545	-2.517249	0.038986
C	-5.415326	-1.829917	-0.915658	C	5.717014	-1.878295	-0.832744
H	-4.836664	-2.173712	-1.800213	H	5.425185	-0.843709	-1.059876
O	-5.244684	-2.729259	0.162599	C	7.082394	-1.901869	-0.158911
C	-3.897808	-2.771147	0.594093	H	7.059768	-1.260327	0.748206
H	-3.246769	-3.175067	-0.211782	O	7.465913	-3.217857	0.183802
C	-3.401807	-1.388654	1.002755	C	6.513405	-3.829071	1.030271
H	-3.985424	-1.039339	1.882117	H	6.448483	-3.280194	1.993681
H	-6.487395	-1.835428	-1.174017	C	5.129769	-3.874676	0.387383
H	-3.855875	-3.458933	1.455259	H	5.164033	-4.531613	-0.508038
H	-2.345695	-1.441261	1.303483	H	7.850210	-1.510339	-0.846166
H	-5.641314	-0.020268	0.248123	H	6.869867	-4.852289	1.231480

L5 TS1

Charge= 0 Multiplicity= 1

E (UB3LYP): -4473.177473 A.U.

ΔG (Thermal Corrections): 0.580268 A.U.

G (UB3LYP): -4472.597205 A.U.

C	-1.890402	-0.564638	-0.534811	C	4.315391	5.171717	-0.127074
O	-2.841697	0.090776	-1.166853	H	4.701872	4.664766	0.782776
C	-1.997970	-0.713042	0.972687	C	3.295240	4.277568	-0.817448
H	-1.678436	0.228039	1.449659	H	2.986592	4.751058	-1.772424
C	-3.425501	-0.971888	1.438164	H	5.161578	5.371014	-0.804322
H	-3.735278	-1.969286	1.084991	H	3.737784	3.302188	-1.056199
C	-4.348573	0.079319	0.822950	H	2.234594	7.281241	1.252854
H	-4.075732	1.067837	1.241563	H	1.137942	5.940361	-0.493576
C	-4.219250	0.118356	-0.705241	O	-3.497130	-0.854611	2.841952
H	-4.675822	-0.800728	-1.105977	C	-3.576249	-2.084797	3.529046
F	-1.139667	-1.696620	1.419514	H	-4.501893	-2.636367	3.268297
H	-1.278894	-1.262654	-1.099089	H	-2.705127	-2.734005	3.317365
Br	-3.093918	-3.270960	-1.189650	H	-3.594003	-1.852738	4.607781
N	-0.406540	0.819355	-0.604011	O	-5.677387	-0.248194	1.147943
C	2.844035	-0.948367	-0.119984	C	-6.370602	0.705686	1.911813
C	3.372502	-2.280186	-0.232017	H	-5.887805	0.870826	2.895822
C	2.484155	-3.295096	-0.587455	H	-6.462575	1.672798	1.379545
C	1.158963	-2.965640	-0.923248	H	-7.385431	0.306604	2.080538

C	-4.804864	1.356576	-1.371602	O	6.806397	-3.953617	-0.062600				
H	-4.535456	1.328037	-2.448467	C	5.870167	-4.419653	0.888265				
H	-4.336369	2.269127	-0.937895	H	5.968999	-3.848015	1.835418				
O	-6.192071	1.381174	-1.199698	C	4.436272	-4.298375	0.379151				
C	-6.805650	2.480389	-1.820529	H	4.299978	-4.971547	-0.494025				
H	-6.436733	3.445821	-1.410770	H	7.303361	-2.332897	-1.180134				
H	-6.632724	2.482444	-2.918169	H	6.112042	-5.476118	1.087859				
H	-7.889634	2.407088	-1.632083	H	3.739204	-4.613360	1.171815				
				H	5.045071	-2.997218	-1.899475				
				N	2.588074	3.981274	-0.040488				
L5 Int 1											
Charge= 0 Multiplicity= 1				C	2.348818	5.376113	0.332667				
E (UB3LYP): -4473.211992 A.U.				H	1.542752	5.427717	1.078703				
ΔG (Thermal Corrections): 0.584709 A.U.				C	3.626662	5.948872	0.948500				
G (UB3LYP): -4472.627283 A.U.				H	3.825976	5.430569	1.910078				
				O	4.736534	5.824192	0.086563				
C	-1.736804	0.301522	-0.175619	C	4.982334	4.474697	-0.253136				
O	-2.748028	1.042336	-0.792215	H	5.255689	3.891983	0.652429				
C	-2.121417	0.037450	1.287175	C	3.762739	3.851672	-0.917803				
H	-2.199043	0.999805	1.823946	H	3.543949	4.400893	-1.854880				
C	-3.456356	-0.691575	1.360045	H	5.836597	4.465401	-0.948813				
H	-3.358423	-1.673217	0.857109	H	3.945640	2.803225	-1.180564				
C	-4.507170	0.124047	0.602561	H	3.490346	7.023387	1.150546				
H	-4.637503	1.098083	1.107752	H	2.054507	5.971344	-0.554309				
C	-4.025364	0.384064	-0.831547	O	-3.853730	-0.830967	2.710830				
H	-3.919703	-0.590554	-1.345717	C	-3.667694	-2.124372	3.241946				
F	-1.123404	-0.694222	1.920483	H	-4.264889	-2.879858	2.692733				
H	-1.528354	-0.639614	-0.696954	H	-2.604727	-2.433474	3.219892				
Br	-2.971414	-3.113764	-1.454970	H	-4.007953	-2.096801	4.291620				
N	-0.504326	1.166987	-0.201025	O	-5.735231	-0.563660	0.543252				
C	2.512796	-1.106626	0.016718	C	-6.715106	-0.108216	1.444414				
C	2.844988	-2.498951	-0.117571	H	-6.382083	-0.196170	2.495658				
C	1.802807	-3.390058	-0.363964	H	-6.993804	0.948421	1.245231				
C	0.502539	-2.891842	-0.565649	H	-7.609039	-0.739174	1.299150				
N	0.208533	-1.608914	-0.513881	C	-4.962671	1.271723	-1.617070				
H	1.985096	-4.461470	-0.456039	H	-4.524067	1.464149	-2.618734				
C	1.160570	-0.712738	-0.213120	H	-5.916033	0.725982	-1.761956				
C	1.849638	1.648457	0.059495	O	-5.177535	2.483267	-0.929606				
C	3.468161	-0.139235	0.441936	C	-6.070098	3.340216	-1.587263				
C	3.152169	1.187121	0.437690	H	-5.698566	3.634510	-2.593179				
H	4.440992	-0.474880	0.803949	H	-7.071992	2.876092	-1.715851				
H	3.875586	1.918757	0.797310	H	-6.179703	4.249987	-0.972238				
H	-0.344402	-3.548560	-0.812629								
C	0.805606	0.700899	-0.125635								
C	-0.753079	2.492796	-0.119667								
C	1.580361	3.064780	-0.017162	L5 TS 2							
C	0.229420	3.451186	-0.034759	Charge= 0 Multiplicity= 1							
H	-1.805980	2.762838	-0.179136	E (UB3LYP): -4588.976146 A.U.							
H	-0.070641	4.497760	-0.052383	ΔG (Thermal Corrections): 0.630034 A.U.							
N	4.172356	-2.906010	0.027713	G (UB3LYP): -4588.346112 A.U.							
C	5.151440	-2.420891	-0.955706								
H	4.972635	-1.362280	-1.189782								
C	6.561778	-2.606959	-0.411950								
H	6.707857	-1.948491	0.471553								

H	-3.670564	-1.379082	1.172376	C	2.301371	5.266352	0.224776
C	-3.264258	0.719095	1.048090	H	1.464243	5.198331	0.936999
H	-2.420306	1.418485	1.213645	C	3.433719	6.069993	0.861336
C	-3.679379	0.740778	-0.427098	H	3.689707	5.619136	1.843397
H	-4.483164	-0.004988	-0.574059	O	4.576521	6.118726	0.033601
F	-1.557423	-2.491562	0.484992	C	5.058840	4.822429	-0.256083
H	-1.100414	-1.050308	-1.655688	H	5.399847	4.322043	0.675383
N	0.037029	0.796932	-0.719960	C	3.989336	3.974660	-0.930308
C	3.124587	-1.193311	-0.105614	H	3.724511	4.434112	-1.905298
C	3.542259	-2.567104	-0.169216	H	5.924334	4.941686	-0.927819
C	2.569593	-3.516356	-0.487199	H	4.369513	2.964551	-1.129549
C	1.272788	-3.090965	-0.821786	H	3.108218	7.109759	1.026256
N	0.898937	-1.825457	-0.855432	H	1.945262	5.786961	-0.688841
H	2.808208	-4.579358	-0.530327	N	4.862836	-2.907383	0.113169
C	1.788463	-0.882926	-0.483713	C	5.920658	-2.363564	-0.750851
C	2.279610	1.526100	-0.148969	H	5.711348	-1.316325	-1.007969
C	3.965097	-0.152087	0.430	C	7.267398	-2.473437	-0.048692
C	3.565134	1.153925	0.363624	H	7.275423	-1.812592	0.844664
H	4.918275	-0.418261	0.859710	O	7.544282	-3.806715	0.328028
H	4.201734	1.929141	0.792467	C	6.534247	-4.325733	1.168955
H	0.512274	-3.830283	-1.099983	H	6.493924	-3.752134	2.119181
C	1.342476	0.501999	-0.460796	C	5.162164	-4.282768	0.501156
C	-0.339881	2.063209	-0.746509	H	5.161427	-4.961556	-0.378251
C	1.871175	2.901247	-0.266368	H	6.809110	-5.367931	1.398587
C	0.521496	3.143510	-0.540236	H	4.399526	-4.635949	1.213097
H	-1.391844	2.249653	-0.976446	H	8.075427	-2.155207	-0.727553
H	0.130972	4.156116	-0.638390	H	5.955858	-2.942728	-1.698113
O	-2.422810	-0.796190	2.743649				
C	-3.353861	-1.445023	3.586059				
H	-4.328778	-0.924785	3.598034				
H	-3.516991	-2.496287	3.274929				
H	-2.926063	-1.437018	4.603441				
O	-4.346972	1.059459	1.870333				
C	-4.321277	2.355409	2.415070				
H	-3.424865	2.510127	3.051018				
H	-4.356316	3.141706	1.637543				
H	-5.221095	2.456031	3.044523				
C	-4.107324	2.079462	-1.014209				
H	-4.079898	1.988501	-2.120861				
H	-3.391751	2.882888	-0.731493				
O	-5.395059	2.383186	-0.566161				
C	-5.894976	3.583817	-1.094625				
H	-5.266940	4.455325	-0.808415				
H	-5.956099	3.550839	-2.203584				
H	-6.909064	3.728679	-0.687216				
O	-3.046426	-2.422351	-1.815722				
C	-3.570530	-2.005854	-3.049446				
H	-4.186952	-1.086136	-2.971907				
H	-2.728243	-1.799611	-3.736156				
H	-4.205876	-2.789140	-3.514106				
H	-3.826568	-2.561434	-1.197763				
Br	-5.712064	-2.411361	-0.153298				
N	2.784650	3.923486	-0.086755				

L5 Int 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -4589.005313 A.U.

ΔG (Thermal Corrections): 0.622266 A.U.

G (UB3LYP): -4588.383047 A.U.

C	1.746396	-0.821346	-0.036944	H	-2.957614	3.600744	0.394376
C	2.784644	1.439973	-0.059363	O	-5.021528	3.815275	0.307377
C	4.143992	-0.522096	0.445478	C	-5.006991	5.217199	0.329402
C	4.026475	0.833946	0.321230	H	-4.196656	5.613110	0.979497
H	5.081632	-0.957885	0.795112	H	-4.871463	5.645584	-0.687651
H	4.870414	1.479178	0.571627	H	-5.977491	5.556033	0.729290
H	-0.207889	-3.443435	-0.002905	O	-3.687445	-0.653551	-1.759017
C	1.620665	0.627629	-0.171529	C	-3.769145	-0.327511	-3.138012
C	0.268779	2.455389	-0.462672	H	-3.901850	0.759490	-3.279941
C	2.642919	2.856757	-0.244702	H	-2.858766	-0.657091	-3.675002
C	1.350228	3.353589	-0.408406	H	-4.645727	-0.857290	-3.542858
H	-0.748339	2.834581	-0.619120	H	-4.398452	-2.221234	-1.416780
H	1.165110	4.420568	-0.539179	Br	-5.298350	-3.386379	-1.387068
N	4.385804	-3.421657	0.421173				
C	5.358987	-3.242458	-0.664649				
H	5.336947	-2.208720	-1.035796				
C	6.755940	-3.590281	-0.168538				
H	7.068163	-2.856043	0.604892				
O	6.805622	-4.901827	0.356125				
C	5.877059	-5.071368	1.407792				
H	6.134232	-4.403866	2.257519				
C	4.448589	-4.777140	0.956856				
H	4.142915	-5.530236	0.198848				
H	7.475840	-3.549030	-1.002339				
H	5.959052	-6.117549	1.744882				
H	3.769547	-4.860622	1.820289				
H	5.097014	-3.911236	-1.512731				
N	3.771862	3.679350	-0.226359				
C	3.593150	5.099036	0.057563				
H	2.892570	5.217655	0.899443				
C	4.941995	5.707832	0.432445				
H	5.292532	5.254893	1.384140				
O	5.905038	5.515379	-0.583451				
C	6.089830	4.142215	-0.864309				
H	6.507843	3.622475	0.024322				
C	4.782396	3.477728	-1.273652				
H	4.426732	3.929404	-2.224777				
H	6.822036	4.076856	-1.685729				
H	4.943466	2.405880	-1.452730				
H	4.838860	6.795600	0.577506				
H	3.179539	5.642073	-0.819676				
O	-3.431201	-0.838523	2.514165				
C	-4.069482	-2.051031	2.842644				
H	-5.173857	-1.957263	2.785640				
H	-3.752166	-2.882739	2.185069				
H	-3.790755	-2.293482	3.882505				
O	-5.091432	1.373483	1.908198				
C	-5.009998	2.183528	3.052143				
H	-4.370320	1.724497	3.832979				
H	-4.630073	3.197722	2.818874				
H	-6.034108	2.283949	3.451439				
C	-3.837225	3.261194	-0.194901				
H	-3.668351	3.575603	-1.247171				

L6 Catalyst

Charge= 0 Multiplicity= 1

E (UB3LYP): -499.247830 A.U.

ΔG (Thermal Corrections): 0.193202 A.U.

G (UB3LYP): -499.054628 A.U.

L6 TS1

Charge= 0 Multiplicity= 1

E (UB3LYP): -3827.060235 A.U.

ΔG (Thermal Corrections): 0.418808 A.U.

G (UB3LYP): -3826.641427 A.U.

C	-1.092912	-0.901296	-0.715709	H	-3.507802	5.411012	-0.766119
O	-1.374277	0.280248	-1.194953	C	3.208625	-1.509314	-0.116595
C	-1.325953	-1.213196	0.747684	H	3.776864	-2.348039	0.281699
H	-0.476128	-0.817998	1.325047	C	1.828197	-1.609729	-0.128852
C	-2.575708	-0.545705	1.304552	H	1.333375	-2.511191	0.250309
H	-3.464935	-1.024215	0.865052				
C	-2.561498	0.932911	0.908909				
H	-1.718950	1.419292	1.436999				
C	-2.390092	1.133555	-0.604738				
H	-3.331887	0.841362	-1.095339				
F	-1.329872	-2.581766	0.935507				
H	-0.856188	-1.686477	-1.425820	C	-0.779750	-0.157313	0.089629
Br	-3.494402	-2.078893	-1.630124	O	-1.274034	0.962788	-0.587378
N	1.027438	-0.635235	-0.578094	C	-1.474895	-0.289103	1.443871
C	1.592232	0.481049	-1.045157	H	-1.296590	0.601000	2.071679
C	3.846886	-0.330951	-0.605153	C	-2.971007	-0.477185	1.214702
C	2.961914	0.684798	-1.072045	H	-3.119815	-1.443831	0.697211
H	0.905753	1.251023	-1.415227	C	-3.503505	0.639404	0.307996
H	3.331408	1.628821	-1.468955	H	-3.450389	1.591718	0.862465
N	5.203212	-0.192568	-0.638331	C	-2.644684	0.786628	-0.958403
C	5.869828	1.093518	-0.851077	H	-2.734226	-0.133336	-1.565698
H	5.209322	1.795710	-1.371916	F	-0.937428	-1.384737	2.113205
C	6.349938	1.671822	0.486520	H	-0.933418	-1.089961	-0.495693
H	5.465372	1.903351	1.109002	Br	-0.824305	-3.032979	-1.845810
C	7.260519	0.675934	1.217245	N	0.668358	0.002683	0.235882
C	6.606876	-0.708850	1.319755	C	1.206407	1.198562	0.587451
H	5.742687	-0.671385	2.009135	C	2.553202	1.351178	0.779907
C	6.119811	-1.174943	-0.057218	H	0.504144	2.026982	0.686653
H	6.980855	-1.267848	-0.744035	H	2.907737	2.343780	1.048652
H	7.320296	-1.446675	1.728329	O	-3.687016	-0.446518	2.428710
H	5.649861	-2.163911	-0.008051	C	-3.947523	-1.709367	3.004671
H	8.212022	0.582820	0.658624	H	-4.546803	-2.347927	2.324025
H	7.518264	1.055992	2.221584	H	-3.017979	-2.248271	3.267765
H	6.881009	2.623485	0.305522	H	-4.529072	-1.530444	3.924832
H	6.735490	0.916213	-1.515052	O	-4.827878	0.361641	-0.083317
O	-2.577438	-0.618793	2.712433	C	-5.816410	1.131274	0.563110
C	-3.410884	-1.625686	3.246345	H	-5.807478	0.973416	1.657890
H	-4.474880	-1.448907	2.989632	H	-5.688747	2.213577	0.354516
H	-3.123053	-2.633687	2.891114	H	-6.792491	0.807597	0.162944
H	-3.300231	-1.589179	4.343471	C	-3.066914	1.960502	-1.816467
O	-3.787041	1.508286	1.287490	H	-2.342983	2.069929	-2.650919
C	-3.710895	2.514540	2.266886	H	-4.058559	1.730634	-2.255384
H	-3.291125	2.128394	3.216679	O	-3.121044	3.133886	-1.043320
H	-3.109989	3.378713	1.921958	C	-3.531786	4.258041	-1.774320
H	-4.742003	2.861234	2.451397	H	-2.833138	4.487581	-2.607842
C	-1.968366	2.538536	-1.017897	H	-4.547328	4.122774	-2.205353
H	-1.769566	2.532005	-2.110631	H	-3.552855	5.118530	-1.084164
H	-1.013136	2.798822	-0.509644	C	1.473682	-1.076458	0.055111
O	-2.974352	3.453543	-0.695002	H	0.970289	-1.990964	-0.293389
C	-2.656113	4.772855	-1.054415	C	2.829971	-0.988495	0.240497
H	-1.745082	5.134999	-0.530607	H	3.409756	-1.891240	0.060574
H	-2.488838	4.872650	-2.148405	C	3.448724	0.240700	0.631136

L6 Int 1

Charge= 0 Multiplicity= 1

E (UB3LYP): -3827.116260 A.U.

ΔG (Thermal Corrections): 0.422920 A.U.

G (UB3LYP): -3826.693340 A.U.

C	5.464614	1.624384	1.079848	H	-0.233864	2.314916	0.297603
C	5.733063	-0.731662	0.587634	O	-1.969623	3.368503	0.725938
C	6.262572	2.029623	-0.165396	C	-1.422382	4.655265	0.591618
H	6.148018	1.475733	1.934939	H	-0.365652	4.691651	0.934513
H	4.754767	2.406289	1.368712	H	-1.458678	5.008418	-0.460661
C	6.539583	-0.433540	-0.681158	H	-2.021974	5.337809	1.216235
H	6.408817	-0.783872	1.460029	O	-2.970188	-1.928352	-0.999362
H	5.221453	-1.697179	0.521	C	-2.870190	-2.976755	-1.935810
C	7.245425	0.923587	-0.569385	H	-2.314177	-2.675127	-2.847938
H	6.798831	2.972806	0.040375	H	-2.344555	-3.820818	-1.458105
H	5.553377	2.227815	-0.990413	H	-3.874879	-3.319786	-2.252261
H	7.272833	-1.243295	-0.842072	H	-3.461859	-1.148422	-1.445780
H	5.852055	-0.436384	-1.547128	Br	-4.373283	0.415372	-2.447336
H	7.740274	1.179326	-1.522566	C	6.460101	-1.196555	-0.194084
H	8.042699	0.852923	0.195336	C	6.108627	0.881231	-1.373773
N	4.775859	0.350492	0.845028	C	7.047569	-0.474151	1.024922
				H	7.264505	-1.420645	-0.918263
				H	6.011750	-2.156470	0.085994

L6 TS 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -3942.855550 A.U.

ΔG (Thermal Corrections): 0.464854 A.U.

G (UB3LYP): -3942.390696 A.U.

C	-0.966213	-1.047783	-0.477519
O	-1.257216	0.165457	-0.756373
C	-1.088105	-1.611610	0.916633
H	-0.159811	-1.397972	1.465776
C	-2.232416	-0.966673	1.685007
H	-3.190019	-1.260014	1.228443
C	-2.078024	0.556123	1.594687
H	-1.156021	0.833539	2.139988
C	-1.990832	1.059188	0.146479
H	-3.003171	1.092247	-0.292611
F	-1.201549	-2.986800	0.838380
H	-0.635222	-1.668099	-1.305384
N	1.320563	-0.766192	-0.384956
C	1.844175	0.296657	-1.005509
C	4.135847	-0.469622	-0.694106
C	3.205021	0.496442	-1.175005
H	1.130523	1.035476	-1.388604
H	3.529543	1.401598	-1.685993
O	-2.174705	-1.331872	3.041713
C	-3.067075	-2.361541	3.416750
H	-4.121419	-2.059933	3.255615
H	-2.874820	-3.299022	2.860788
H	-2.911100	-2.546571	4.492721
O	-3.203607	1.160930	2.177109
C	-2.969319	1.858500	3.377912
H	-2.589336	1.187709	4.172660
H	-2.260067	2.695086	3.227563
H	-3.939214	2.274859	3.698685
C	-1.295025	2.402572	-0.025703
H	-1.299652	2.656938	-1.106128

H	-0.233864	2.314916	0.297603
O	-1.969623	3.368503	0.725938
C	-1.422382	4.655265	0.591618
H	-0.365652	4.691651	0.934513
H	-1.458678	5.008418	-0.460661
H	-2.021974	5.337809	1.216235
O	-2.970188	-1.928352	-0.999362
C	-2.870190	-2.976755	-1.935810
H	-2.314177	-2.675127	-2.847938
H	-2.344555	-3.820818	-1.458105
H	-3.874879	-3.319786	-2.252261
H	-3.461859	-1.148422	-1.445780
Br	-4.373283	0.415372	-2.447336
C	6.460101	-1.196555	-0.194084
C	6.108627	0.881231	-1.373773
C	7.047569	-0.474151	1.024922
H	7.264505	-1.420645	-0.918263
H	6.011750	-2.156470	0.085994
C	6.676084	1.708030	-0.213340
H	6.928392	0.579962	-2.051441
H	5.400978	1.462501	-1.975821
C	7.661738	0.871124	0.613845
H	7.806788	-1.117601	1.504486
H	6.240529	-0.312658	1.763923
H	7.171791	2.611607	-0.611115
H	5.838064	2.047122	0.424076
H	7.989910	1.433030	1.506131
H	8.568039	0.680956	0.006715
C	2.173721	-1.686370	0.082722
H	1.728599	-2.555601	0.583161
C	3.550876	-1.588835	-0.032681
H	4.156874	-2.388969	0.389493
N	5.483107	-0.342851	-0.871275

L6 Int 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -3942.881405 A.U.

ΔG (Thermal Corrections): 0.463930 A.U.

G (UB3LYP): -3942.417475 A.U.

C	-2.401831	0.809541	-1.510815
O	-1.279704	1.624170	-1.350478
C	-2.050962	-0.637241	-1.178023
H	-1.302179	-0.996196	-1.901998
C	-1.501209	-0.750834	0.236638
H	-2.297003	-0.486621	0.956025
C	-0.344395	0.233841	0.448185
H	0.522823	-0.131966	-0.124432
C	-0.702281	1.648900	-0.037645
H	-1.419468	2.080430	0.682726
F	-3.191830	-1.424554	-1.323737
H	-2.694206	0.908125	-2.571275
N	0.950321	-1.459065	-2.699887

C	1.610475	-0.294777	-2.777546	Charge= 0 Multiplicity= 1
C	3.118159	-0.814934	-0.941894	E (UB3LYP): -535.153205 A.U.
C	2.670818	0.071946	-1.957913	ΔG (Thermal Corrections): 0.168567 A.U.
H	1.261535	0.413421	-3.539921	G (UB3LYP): -534.984638 A.U.
H	3.129725	1.048439	-2.109735	
O	-1.021650	-2.051214	0.501209	C 2.984510 1.131936 -0.035519
C	-1.938565	-2.907393	1.145642	C 1.594030 1.195756 -0.011960
H	-2.235297	-2.509294	2.137996	C 0.831091 0.000022 -0.016957
H	-2.852533	-3.071235	0.544866	C 1.594014 -1.195715 -0.011498
H	-1.428980	-3.875012	1.291695	C 2.984497 -1.131929 -0.035080
O	-0.055820	0.278734	1.828159	N 3.697670 -0.000006 -0.050236
C	1.206761	-0.217251	2.194659	H 3.555785 2.069808 -0.037326
H	1.308749	-1.291377	1.947280	H 1.124053 2.178407 0.008693
H	2.024183	0.349479	1.710514	H 1.124013 -2.178340 0.009709
H	1.296696	-0.095286	3.288320	H 3.555755 -2.069813 -0.036493
C	0.489914	2.586393	-0.200066	C -1.287706 -1.223515 0.270638
H	0.105059	3.573378	-0.534936	C -1.287754 1.223388 0.271174
H	1.138054	2.192821	-1.009267	C -2.714506 -1.154972 -0.262796
O	1.206674	2.711461	0.998071	H -1.306662 -1.396244 1.367666
C	2.244582	3.650728	0.916780	H -0.799619 -2.087637 -0.199819
H	2.963978	3.408108	0.106227	C -2.714523 1.155074 -0.262331
H	1.857930	4.676907	0.733756	H -1.306794 1.395528 1.368295
H	2.781180	3.642147	1.880417	H -0.799661 2.087779 -0.198759
O	-3.470427	1.205100	-0.681995	H -3.283536 -2.028275 0.095028
C	-4.062831	2.451724	-1.016735	H -2.693463 -1.179711 -1.373408
H	-3.328711	3.272682	-0.938681	H -3.283563 2.028227 0.095847
H	-4.476741	2.427818	-2.043352	H -2.693456 1.180277 -1.372934
H	-4.878827	2.622396	-0.297410	N -0.549734 0.000018 -0.036490
H	-4.614463	0.125062	0.144633	O -3.391289 -0.000045 0.180821
Br	-5.650399	-0.401373	1.043400	
N	4.112637	-0.509380	-0.054222	
C	1.390912	-2.315289	-1.769293	L7 TS1
H	0.854123	-3.268109	-1.689737	Charge= 0 Multiplicity= 1
C	2.442016	-2.063126	-0.894298	E (UB3LYP): -3862.964251 A.U.
H	2.696501	-2.822160	-0.156100	ΔG (Thermal Corrections): 0.394954 A.U.
C	4.526514	-1.495269	0.947787	G (UB3LYP): -3862.569297 A.U.
H	4.809508	-2.429753	0.428586	
H	3.681895	-1.742376	1.620221	C -1.080113 -0.825831 -0.677921
C	5.726555	-0.999146	1.757670	O -1.351557 0.379012 -1.102176
H	6.125765	-1.848443	2.337761	C -1.445720 -1.244808 0.730403
H	5.407327	-0.239970	2.493384	H -0.673651 -0.863576 1.416591
C	6.796715	-0.418847	0.829584	C -2.769332 -0.656473 1.198933
H	7.136709	-1.219677	0.148225	H -3.590908 -1.128418 0.637545
H	7.680243	-0.106051	1.411548	C -2.769029 0.846781 0.909128
C	6.231255	0.766319	0.007955	H -2.006109 1.317890 1.557834
H	6.541613	0.678713	-1.047392	C -2.447506 1.163474 -0.559934
H	6.624064	1.729377	0.379417	H -3.324675 0.887235 -1.165864
C	4.699255	0.819323	0.080963	F -1.415520 -2.622815 0.825851
H	4.377423	1.257995	1.044193	H -0.768604 -1.558542 -1.415546
H	4.309328	1.480741	-0.699686	Br -3.356025 -1.986293 -1.917889

L7 Catalyst

H	0.912579	1.356970	-1.169463	H	1.022367	0.051788	-2.214589
H	3.333188	1.764363	-1.046445	H	2.977473	-1.511615	-0.442882
N	5.150670	0.005021	0.016895	O	1.425271	1.338689	0.039582
C	5.825880	1.131101	-0.631009	F	0.612488	-1.791978	-1.512152
H	5.188089	2.024258	-0.600933	C	3.455236	-2.706526	-2.536332
C	7.132072	1.473388	0.077981	H	3.854534	-2.950690	-3.535199
H	6.906930	1.899462	1.079006	H	4.175203	-3.056007	-1.768915
C	7.330658	-0.646719	0.970789	H	2.497820	-3.240605	-2.391623
H	7.110179	-0.264019	1.990149	O	3.292561	-1.303029	-2.488820
C	6.037093	-1.121426	0.317352	C	5.773423	0.438430	-1.666990
H	6.269739	-1.674855	-0.615378	H	6.773992	0.247558	-1.243587
H	8.027534	-1.495473	1.059749	H	5.583346	-0.276756	-2.486962
H	5.548067	-1.815528	1.013061	H	5.757666	1.468571	-2.081675
H	7.678375	2.229647	-0.508319	O	4.846881	0.291942	-0.612982
H	6.028591	0.887379	-1.694024	C	3.385160	2.638955	0.426060
O	-2.910211	-0.829672	2.590835	H	3.063151	3.269457	-0.432201
C	-3.761579	-1.891416	2.967252	H	4.492306	2.578859	0.405794
H	-4.799120	-1.723027	2.614784	C	3.417477	4.463918	1.888029
H	-3.407871	-2.864962	2.577037	H	3.024554	4.788406	2.866510
H	-3.763642	-1.928838	4.069897	H	4.528637	4.489833	1.925463
O	-4.048546	1.355683	1.192129	H	3.084939	5.190280	1.113811
C	-4.114632	2.291140	2.240344	O	2.931593	3.173586	1.639260
H	-3.780729	1.851693	3.200953	C	-1.246622	1.297339	-0.550046
H	-3.516243	3.196617	2.020036	C	-2.612918	1.405765	-0.559820
H	-5.172411	2.589674	2.337302	C	-3.436240	0.380347	0.007377
C	-2.026950	2.604130	-0.824785	C	-2.726749	-0.702918	0.611118
H	-1.723137	2.684714	-1.890054	C	-1.355603	-0.753530	0.595350
H	-1.133441	2.844615	-0.206362	N	-0.624080	0.231786	0.012136
O	-3.084745	3.471080	-0.537153	H	-0.595964	2.064068	-0.970706
C	-2.775801	4.818862	-0.780871	H	-3.035239	2.302338	-1.008184
H	-1.924438	5.166779	-0.156722	H	-3.240399	-1.520245	1.112805
H	-2.518190	4.995448	-1.847235	H	-0.773266	-1.556987	1.074929
H	-3.667740	5.415649	-0.527927	C	-5.648690	-0.523280	0.673491
C	3.150290	-1.378555	0.286348	C	-5.534444	1.591796	-0.533207
H	3.702857	-2.223348	0.693306	C	-6.865263	-0.875502	-0.178717
C	1.775810	-1.499147	0.167848	H	-5.979125	-0.074714	1.629940
H	1.268657	-2.417799	0.483279	H	-5.102567	-1.446253	0.897034
O	7.973002	0.350206	0.208888	C	-6.757395	1.134968	-1.325999
				H	-5.855941	2.215320	0.323176
				H	-4.907780	2.204647	-1.190685
				H	-7.552238	-1.505972	0.407902
				H	-6.535635	-1.448039	-1.071414
				H	-7.362762	2.013417	-1.601343
				H	-6.422895	0.630489	-2.257359
				N	-4.787428	0.436745	-0.025834
C	3.497528	0.519304	-0.945215	O	-7.579805	0.274612	-0.572328
C	2.837277	1.239649	0.246802	Br	1.301120	-2.410178	2.330392
C	0.831879	0.076640	-0.046413				
C	1.278421	-0.584345	-1.349532				
C	2.785163	-0.803902	-1.271116				
H	3.027420	0.654527	1.164775				
H	3.421479	1.173438	-1.836503				
H	1.110039	-0.579827	0.806487				

L7 Int 1

Charge= 0 Multiplicity= 1

E (UB3LYP): -3863.015673 A.U.

ΔG (Thermal Corrections): 0.398376 A.U.

G (UB3LYP): -3862.617297 A.U.

C	3.497528	0.519304	-0.945215
C	2.837277	1.239649	0.246802
C	0.831879	0.076640	-0.046413
C	1.278421	-0.584345	-1.349532
C	2.785163	-0.803902	-1.271116
H	3.027420	0.654527	1.164775
H	3.421479	1.173438	-1.836503
H	1.110039	-0.579827	0.806487

L7 TS 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -3978.759631 A.U.

ΔG (Thermal Corrections): 0.440944 A.U.

G (UB3LYP): -3978.318687 A.U.

C	-0.960636	-0.944857	-0.562598	H	7.591228	-0.428269	1.525565
O	-1.279499	0.286785	-0.685838	H	7.863950	2.382710	-0.668730
C	-1.156673	-1.707071	0.725204	H	7.248809	1.825342	0.923267
H	-0.278549	-1.546031	1.367202	C	2.142385	-1.604630	0.064476
C	-2.377430	-1.215574	1.489656	H	1.692821	-2.567741	0.335818
H	-3.287383	-1.469350	0.925178	C	3.520149	-1.453422	0.084455
C	-2.280790	0.308161	1.629051	H	4.125453	-2.311164	0.372832
H	-1.413518	0.532161	2.278599	N	5.456474	0.014906	-0.216510
C	-2.109623	1.018946	0.278167	O	8.273652	0.440763	-0.228251
H	-3.087824	1.087188	-0.228701				
F	-1.208619	-3.059384	0.444830				
H	-0.567054	-1.434477	-1.448915				
N	1.295231	-0.626887	-0.279935				
C	1.820003	0.546620	-0.644549				
C	4.103544	-0.202735	-0.262328				
C	3.182538	0.807100	-0.656370	C	-2.146484	-0.159991	-1.566098
H	1.109789	1.322595	-0.953205	O	-1.222879	0.878247	-1.418735
H	3.513908	1.791420	-0.982772	C	-2.005221	-1.161085	-0.424356
O	-2.398032	-1.773175	2.780523	H	-0.999892	-1.606706	-0.473120
C	-3.282143	-2.864066	2.940104	C	-2.183519	-0.483878	0.925586
H	-4.332340	-2.562415	2.754172	H	-3.221783	-0.118554	1.022170
H	-3.027332	-3.705082	2.267211	C	-1.246820	0.722879	1.035970
H	-3.189658	-3.203143	3.985459	H	-0.219094	0.331939	1.120439
O	-3.469605	0.786937	2.203206	C	-1.323681	1.633119	-0.202994
C	-3.350176	1.311965	3.504746	H	-2.286962	2.172455	-0.174963
H	-3.000273	0.545977	4.223635	F	-2.946351	-2.176024	-0.593975
H	-2.666960	2.182639	3.528016	H	-1.910447	-0.634904	-2.534901
H	-4.356683	1.648197	3.806098	N	1.340080	-1.199952	-0.243492
C	-1.456075	2.392408	0.352404	C	1.941657	-0.416435	-1.146790
H	-1.395055	2.800609	-0.677934	C	4.175018	-0.826886	-0.273044
H	-0.417684	2.287962	0.738947	C	3.314523	-0.204088	-1.214643
O	-2.217946	3.219297	1.182070	H	1.280992	0.085298	-1.863412
C	-1.717707	4.529335	1.267127	H	3.696056	0.450585	-1.997464
H	-0.686978	4.550872	1.682780	O	-1.878097	-1.368799	1.982522
H	-1.702744	5.027419	0.274674	C	-2.993533	-1.999416	2.569770
H	-2.383339	5.095983	1.938919	H	-3.684319	-1.260136	3.025856
O	-2.911309	-1.791219	-1.344879	H	-3.562041	-2.608963	1.841996
C	-2.726760	-2.714422	-2.393040	H	-2.610554	-2.660646	3.365885
H	-3.700160	-3.033408	-2.815329	O	-1.612903	1.456296	2.183312
H	-2.121151	-2.294153	-3.222942	C	-0.610646	1.586696	3.158012
H	-2.212015	-3.602151	-1.988066	H	-0.297095	0.600901	3.556848
H	-3.382747	-0.966128	-1.725692	H	0.278975	2.121711	2.770877
Br	-4.236874	0.712211	-2.585545	H	-1.037244	2.181215	3.984653
C	6.397201	-1.105036	-0.147870	C	-0.191241	2.649434	-0.295904
C	6.037277	1.238485	-0.770967	H	-0.229242	3.113353	-1.305126
C	7.730332	-0.669188	0.449939	H	0.783989	2.124684	-0.211207
H	6.561518	-1.518663	-1.164116	O	-0.327467	3.621038	0.704659
H	5.992754	-1.906002	0.484170	C	0.715122	4.558195	0.704998
C	7.393536	1.538166	-0.140153	H	1.702471	4.079177	0.882869
H	6.147390	1.141695	-1.870670	H	0.771868	5.114943	-0.255963
H	5.380543	2.094662	-0.566788	H	0.519524	5.276947	1.518548
H	8.455710	-1.494521	0.367680	O	-3.474527	0.311762	-1.577226

C	-3.831144	1.085196	-2.713449	Charge= 0 Multiplicity= 1
H	-3.215675	1.999424	-2.779326	E (UB3LYP): -3710.261598 A.U.
H	-3.712475	0.496396	-3.643721	ΔG (Thermal Corrections): 0.354941 A.U.
H	-4.888795	1.365983	-2.590964	G (UB3LYP): -3709.906657 A.U.
H	-4.878318	-0.511814	-0.870311	
Br	-6.220981	-0.806650	-0.351145	C -0.216756 -0.785673 -0.644515
N	5.538964	-0.620257	-0.265937	O -0.534398 0.407894 -1.068993
C	2.142810	-1.806178	0.637740	C -0.621434 -1.240032 0.741942
H	1.651832	-2.452308	1.376551	H 0.097675 -0.824117 1.464508
C	3.526972	-1.667774	0.668550	C -1.996190 -0.732431 1.154306
H	4.082744	-2.220774	1.424582	H -2.762780 -1.246163 0.553335
C	6.404701	-1.458597	0.560948	C -2.072292 0.770545 0.873395
H	6.566673	-2.443370	0.073952	H -1.369765 1.281592 1.559189
H	5.935953	-1.636052	1.538467	C -1.703473 1.116600 -0.577911
C	7.747888	-0.781462	0.812441	H -2.531275 0.787339 -1.225462
H	8.424511	-1.485448	1.323213	F -0.519339 -2.615254 0.827526
H	7.596687	0.101107	1.470250	H 0.181938 -1.486905 -1.370173
C	7.560731	0.529757	-1.080845	Br -2.350047 -2.063077 -1.994052
H	8.095909	0.815741	-2.000765	N 1.833209 -0.372969 -0.191843
H	7.405259	1.442114	-0.465913	C 2.363651 0.799459 -0.549707
C	6.207673	-0.071086	-1.444779	C 4.599547 0.100460 0.091250
H	5.598437	0.725925	-1.890900	C 3.713844 1.087312 -0.428606
H	6.345728	-0.864870	-2.209001	H 1.665206 1.540341 -0.954796
O	8.376584	-0.386961	-0.386398	H 4.071595 2.067918 -0.740392
			N 5.931944 0.328445 0.228175	
			O -2.189434 -0.926804 2.537193	

L8 Catalyst

Charge= 0 Multiplicity= 1	C -2.999117 -2.035388 2.866966
E (UB3LYP): -382.449604 A.U.	H -4.027900 -1.917849 2.470805
ΔG (Thermal Corrections): 0.128741 A.U.	H -2.578033 -2.984994 2.484650
G (UB3LYP): -382.320863 A.U.	H -3.047016 -2.084630 3.968133
	O -3.392052 1.199052 1.100194
C 0.187786 -0.000097 0.000254	C -3.561179 2.127797 2.142692
C -0.569423 1.200971 -0.009559	H -3.241372 1.709532 3.117528
C -0.569546 -1.201081 0.009741	H -3.012444 3.069564 1.946581
C -1.959359 1.134460 -0.009577	H -4.638834 2.359000 2.194250
H -0.086818 2.178420 -0.020140	C -1.366214 2.582894 -0.819591
C -1.959476 -1.134415 0.009463	H -1.010852 2.686822 -1.866693
H -0.087078 -2.178598 0.020214	H -0.526109 2.881119 -0.153423
H -2.534251 2.070317 -0.018568	O -2.494058 3.376191 -0.590682
H -2.534464 -2.070215 0.018227	C -2.262809 4.742352 -0.817244
N -2.670943 0.000058 -0.000117	H -1.472344 5.144247 -0.147076
N 1.554609 -0.000029 0.000448	H -1.958857 4.939322 -1.867741
C 2.280098 1.256287 0.016702	H -3.205254 5.277549 -0.614367
H 3.359711 1.051145 0.053226	C 4.005627 -1.142363 0.455949
H 2.076732 1.863199 -0.887262	H 4.598844 -1.962980 0.857614
H 2.020448 1.867598 0.902352	C 2.642557 -1.323580 0.293973
C 2.280309 -1.256204 -0.017080	H 2.168602 -2.273354 0.566705
H 2.075839 -1.864462 0.885685	C 6.499656 1.602442 -0.182081
H 2.021926 -1.866272 -0.903966	H 6.331403 1.795686 -1.258386
H 3.359951 -1.050860 -0.051749	H 6.067999 2.444262 0.391403
	H 7.583883 1.589081 -0.003420
	C 6.798949 -0.709710 0.761989
	H 6.490229 -1.011601 1.780250

L8 TS1

H 6.800621 -1.611297 0.120463
H 7.827782 -0.327595 0.817761

L8 Int 1

Charge= 0 Multiplicity= 1

E (UB3LYP): -3710.313688 A.U.

ΔG (Thermal Corrections): 0.357950 A.U.

G (UB3LYP): -3709.955738 A.U.

C 2.822 0.456225 -0.828196
C 2.087235 1.224535 0.289042
C 0.087533 0.088 -0.112850
C 0.620815 -0.634022 -1.353534
C 2.113900 -0.869747 -1.155041
H 2.201814 0.668076 1.236968
H 2.813698 1.078677 -1.744905
H 0.285438 -0.549716 0.781490
H 0.437859 -0.026407 -2.257362
H 2.233393 -1.546497 -0.288122
O 0.695942 1.335110 -0.023226
Br 0.347854 -2.318141 2.382803
F -0.049130 -1.838509 -1.522309
C 2.847465 -2.829706 -2.289671
H 3.313035 -3.119974 -3.246653
H 3.506168 -3.154885 -1.459107
H 1.874621 -3.346248 -2.191928
O 2.701786 -1.423744 -2.311156
C 5.138629 0.327807 -1.387584
H 6.105168 0.138904 -0.890562
H 4.995058 -0.411342 -2.195687
H 5.165631 1.344169 -1.834563
O 4.140169 0.226290 -0.395828
C 2.641965 2.622072 0.461897
H 2.396912 3.225893 -0.439903
H 3.746282 2.546457 0.529254
C 2.593015 4.496127 1.859934
H 2.126656 4.862404 2.790227
H 3.697560 4.505714 1.989130
H 2.339580 5.198997 1.035709
O 2.104975 3.205545 1.617029
C -1.912164 1.304847 -0.853127
C -3.270284 1.442077 -0.977203
C -4.149972 0.471587 -0.400857
C -3.526646 -0.603528 0.301833
C -2.159509 -0.679751 0.397127
N -1.365240 0.262689 -0.177192
H -1.207691 2.024213 -1.271121
H -3.649810 2.304679 -1.521777
H -4.111624 -1.381436 0.789376
H -1.630709 -1.468481 0.956251
N -5.488238 0.571337 -0.513859
C -6.083756 1.696288 -1.224542
H -5.772847 1.711897 -2.284912

H -7.177462 1.606310 -1.187708
H -5.801238 2.658319 -0.760321
C -6.352319 -0.444789 0.076648
H -6.132813 -1.444844 -0.338412
H -6.231667 -0.485960 1.174256
H -7.399829 -0.201356 -0.147399

L8 TS 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -3826.056806 A.U.

ΔG (Thermal Corrections): 0.400599 A.U.

G (UB3LYP): -3825.656207 A.U.

C -0.158276 -0.898994 -0.597991
O -0.537566 0.319666 -0.676355
C -0.305982 -1.716708 0.662138
H 0.573308 -1.544662 1.298973
C -1.534242 -1.305756 1.461149
H -2.441768 -1.585016 0.904347
C -1.506933 0.216216 1.645269
H -0.634128 0.464055 2.278973
C -1.405418 0.969995 0.311612
H -2.392660 0.984236 -0.181939
F -0.306631 -3.058769 0.331520
H 0.266039 -1.332666 -1.499260
N 2.083848 -0.464569 -0.298232
C 2.543949 0.741016 -0.650900
C 4.858988 0.097810 -0.297024
C 3.896000 1.073678 -0.665030
H 1.789994 1.482676 -0.939904
H 4.179507 2.081066 -0.962284
O -1.506584 -1.901118 2.734809
C -2.329811 -3.041178 2.873866
H -3.396925 -2.790656 2.709190
H -2.040454 -3.848631 2.174312
H -2.205697 -3.403839 3.907981
O -2.702626 0.617546 2.262110
C -2.574696 1.124509 3.569660
H -2.162007 0.366177 4.263089
H -1.940986 2.031867 3.591584
H -3.589101 1.398156 3.905909
C -0.849598 2.384003 0.409369
H -0.821492 2.812181 -0.614198
H 0.194748 2.346914 0.791614
O -1.665941 3.141182 1.253977
C -1.259421 4.481645 1.359691
H -0.232478 4.569638 1.775959
H -1.280332 4.995246 0.375233
H -1.962956 4.989209 2.040113
O -2.058655 -1.806320 -1.397049
C -1.837297 -2.685369 -2.476082
H -1.246803 -2.213773 -3.289091
H -1.290053 -3.566358 -2.100527

H	-2.797873	-3.024654	-2.911295	H	4.094732	-2.644484	0.645889
H	-2.575607	-0.994930	-1.748608	O	4.597938	-2.220269	-1.326509
Br	-3.532573	0.653698	-2.550720	C	5.492286	-3.291183	-1.471812
C	2.979187	-1.400535	0.042895	H	6.058712	-3.487542	-0.535823
H	2.576525	-2.384687	0.312855	H	4.969914	-4.229104	-1.760463
C	4.347576	-1.181345	0.063210	H	6.206958	-3.024479	-2.268438
H	5.006578	-1.999303	0.352131	O	-0.021547	-0.351212	-0.250605
N	6.191301	0.368798	-0.294280	C	-0.745478	-1.375106	-0.923088
C	7.144199	-0.662753	0.080829	H	-0.057057	-2.104666	-1.384709
H	6.952737	-1.037914	1.103297	H	-1.424115	-1.898593	-0.228099
H	7.111791	-1.523938	-0.613871	H	-1.335091	-0.882278	-1.711125
H	8.159742	-0.243064	0.058183	H	-0.635106	1.237535	-0.617792
C	6.668787	1.677331	-0.709723	Br	-1.141700	2.450600	-1.284154
H	6.376973	1.905905	-1.752320	C	-3.291384	-2.255586	1.814952
H	6.275992	2.480249	-0.057923	H	-3.133231	-3.240763	2.273457
H	7.765927	1.697357	-0.650980	C	-4.285206	-2.113442	0.851421

L8 Int 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -3826.086681 A.U.

ΔG (Thermal Corrections): 0.399783 A.U.

G (UB3LYP): -3825.686898 A.U.

C	0.647918	-0.760556	0.921518
O	1.660632	-1.686114	0.655097
C	1.248795	0.479344	1.580982
H	1.663409	0.186028	2.558596
C	2.344283	1.091875	0.720700
H	1.894015	1.486404	-0.207221
C	3.374609	0.030627	0.319935
H	3.950513	-0.235978	1.225805
C	2.700244	-1.240835	-0.224499
H	2.283755	-1.007525	-1.220210
F	0.251599	1.421478	1.821883
H	-0.061150	-1.266532	1.598077
C	-4.492175	-0.846320	0.243580
C	-3.648931	0.199198	0.702714
C	-2.690737	-0.067495	1.672891
N	-2.486783	-1.269175	2.233335
H	-3.717961	1.208531	0.299309
H	-2.024965	0.738840	1.998099
O	3.016981	2.117176	1.416709
C	2.607780	3.427263	1.090450
H	2.800102	3.657331	0.022393
H	1.534274	3.594161	1.300582
H	3.203754	4.116653	1.712388
O	4.211035	0.594279	-0.662118
C	5.578996	0.642887	-0.343924
H	5.767063	1.264428	0.554615
H	6.003885	-0.367603	-0.186726
H	6.094316	1.103903	-1.204158
C	3.626860	-2.444818	-0.342725
H	3.004951	-3.330451	-0.594393

H	4.094732	-2.644484	0.645889
O	4.597938	-2.220269	-1.326509
C	5.492286	-3.291183	-1.471812
H	6.058712	-3.487542	-0.535823
H	4.969914	-4.229104	-1.760463
H	6.206958	-3.024479	-2.268438
O	-0.021547	-0.351212	-0.250605
C	-0.745478	-1.375106	-0.923088
H	-0.057057	-2.104666	-1.384709
H	-1.424115	-1.898593	-0.228099
H	-1.335091	-0.882278	-1.711125
H	-0.635106	1.237535	-0.617792
Br	-1.141700	2.450600	-1.284154
C	-3.291384	-2.255586	1.814952
H	-3.133231	-3.240763	2.273457
C	-4.285206	-2.113442	0.851421
H	-4.883763	-2.982294	0.577056
N	-5.435362	-0.646140	-0.723892
C	-5.590345	0.667211	-1.323107
H	-6.376282	0.625087	-2.090855
H	-5.883157	1.428946	-0.574897
H	-4.656152	1.009475	-1.807756
C	-6.275322	-1.746459	-1.157869
H	-6.873001	-2.161043	-0.323262
H	-6.972916	-1.388681	-1.928695
H	-5.679733	-2.572898	-1.592592

L9 Catalyst

Charge= 0 Multiplicity= 1

E (UB3LYP): -479.571245 A.U.

ΔG (Thermal Corrections): 0.135910 A.U.

G (UB3LYP): -479.435335 A.U.

C	2.889360	-1.150149	0.000116
C	1.483412	-1.201297	-0.000630
C	0.772568	0.000261	-0.000956
C	1.483432	1.201686	-0.000289
C	2.889443	1.149964	0.000594
N	3.591253	-0.000233	0.000733
H	3.489028	-2.077781	0.000273
H	0.963472	-2.167740	-0.001210
H	0.963908	2.168362	-0.000422
H	3.489469	2.077455	0.001032
C	-0.767432	-0.000003	-0.000441
C	-1.465161	1.208154	-0.000774
C	-1.464730	-1.208028	0.000249
C	-2.859873	1.208193	0.000263
H	-0.915132	2.160367	-0.000541
C	-2.859868	-1.208163	0.000291
H	-0.914969	-2.160337	0.000332
C	-3.557497	-0.000334	0.000436
H	-3.409899	2.160436	0.000634

H -3.409390 -2.160791 0.000419
H -4.657177 -0.000054 0.001195

L9 TS1

Charge= 0 Multiplicity= 1
E (UB3LYP): -3807.385850 A.U.
ΔG (Thermal Corrections): 0.362241 A.U.
G (UB3LYP): -3807.023609 A.U.

C 7.661460 -0.822525 0.039936
H 5.891129 -2.010631 -0.269281
C 7.311508 1.541566 0.411694
H 5.263958 2.210723 0.427477
C 8.181062 0.453945 0.279098
H 8.334805 -1.677299 -0.073135
H 7.708946 2.542043 0.606473
H 9.262004 0.601089 0.362010

C -0.857169 -0.832831 -0.594642
O -1.156813 0.336257 -1.096660
C -1.247961 -1.174529 0.828511
H -0.510613 -0.724872 1.512311
C -2.605371 -0.608221 1.222023
H -3.390408 -1.142658 0.664289
C -2.648463 0.874462 0.842452
H -1.921366 1.410893 1.481860
C -2.296287 1.113032 -0.634184
H -3.144086 0.765620 -1.245080
F -1.174221 -2.542461 1.008656
H -0.564706 -1.616154 -1.289191
Br -3.112955 -2.133425 -1.824419
N 1.175231 -0.501911 -0.259607
C 1.943502 -1.471408 0.246384
C 1.723224 0.640882 -0.670087
C 3.933216 -0.124382 -0.047050
C 3.093095 0.872047 -0.579261
H 1.037357 1.383826 -1.090637
H 3.501626 1.814773 -0.948330
O -2.781807 -0.707432 2.616640
C -3.627604 -1.761152 3.027658
H -4.658040 -1.627193 2.641681
H -3.250197 -2.747996 2.697622
H -3.656417 -1.741043 4.130342
O -3.952407 1.352138 1.059549
C -4.081052 2.348238 2.044442
H -3.761252 1.981523 3.039727
H -3.507226 3.258901 1.784052
H -5.150656 2.614421 2.093025
C -1.920309 2.549282 -0.977905
H -1.586028 2.575685 -2.036789
H -1.056680 2.862911 -0.349692
O -3.018029 3.389749 -0.775532
C -2.751543 4.732263 -1.089604
H -1.936123 5.149423 -0.459968
H -2.463933 4.856050 -2.155667
H -3.673573 5.306908 -0.901839
H 1.432278 -2.384991 0.567599
C 3.320483 -1.321883 0.371519
H 3.906521 -2.129723 0.814020
C 5.396748 0.075306 0.065511
C 6.282229 -1.011308 -0.062079
C 5.932553 1.355126 0.302108

L9 Int 1

Charge= 0 Multiplicity= 1
E (UB3LYP): -3807.430929 A.U.
ΔG (Thermal Corrections): 0.365132 A.U.
G (UB3LYP): -3807.065797 A.U.

C 3.404091 0.579883 -0.841005
C 2.660337 1.277551 0.313401
C 0.709991 0.056000 -0.084705
C 1.244667 -0.599049 -1.359029
C 2.752621 -0.767306 -1.196208
H 2.814680 0.697241 1.240854
H 3.350266 1.229759 -1.736890
H 0.949558 -0.591318 0.789279
H 1.013889 0.029261 -2.236883
H 2.922105 -1.464530 -0.354271
O 1.258477 1.331693 0.024805
Br 1.030251 -2.440293 2.266832
F 0.630708 -1.827305 -1.553813
C 3.555804 -2.652286 -2.409157
H 4.012149 -2.886976 -3.385448
H 4.249944 -2.968790 -1.604733
H 2.612816 -3.220540 -2.307045
O 3.338906 -1.254974 -2.381005
C 5.714822 0.581526 -1.445622
H 6.697865 0.416313 -0.973425
H 5.587956 -0.131295 -2.279673
H 5.688288 1.614801 -1.851436
O 4.740760 0.396491 -0.440893
C 3.149393 2.693519 0.526404
H 2.867936 3.314485 -0.352791
H 4.256607 2.667677 0.582244
C 3.029521 4.510540 1.994689
H 2.552968 4.820719 2.940010
H 4.133233 4.561641 2.119839
H 2.741790 5.232123 1.198590
O 2.595208 3.209847 1.704796
C -1.359299 1.272186 -0.621449
C -2.734988 1.345961 -0.689720
C -3.533776 0.274651 -0.231350
C -2.859331 -0.844120 0.293869
C -1.477650 -0.879730 0.344506
N -0.757036 0.171404 -0.114666

H	-0.697648	2.076254	-0.942015	C	-1.691777	4.615803	-1.230414				
H	-3.185377	2.259787	-1.079325	H	-0.732377	4.943572	-0.774998				
H	-3.406275	-1.714184	0.659376	H	-1.569447	4.614854	-2.334705				
H	-0.894896	-1.706163	0.781934	H	-2.478075	5.339872	-0.960882				
C	-5.008019	0.330778	-0.294298	O	-2.478095	-2.194133	-1.499751				
C	-5.793492	-0.354743	0.652992	C	-2.462531	-1.955942	-2.888602				
C	-5.657769	1.070495	-1.301645	H	-2.422491	-0.875922	-3.138003				
C	-7.186057	-0.295785	0.597211	H	-1.573491	-2.450295	-3.321538				
H	-5.313668	-0.915264	1.458791	H	-3.363780	-2.379142	-3.373915				
C	-7.050636	1.118142	-1.362258	H	-3.338555	-1.788047	-1.149502				
H	-5.072227	1.589367	-2.064506	Br	-5.052125	-0.630217	-0.754972				
C	-7.819248	0.438164	-0.411504	C	3.732237	-1.474010	0.449822				
H	-7.780176	-0.823033	1.349123	H	4.327415	-2.212056	0.991321				
H	-7.538895	1.686160	-2.159365	C	2.353240	-1.639880	0.362273				
H	-8.911500	0.479966	-0.456734	H	1.860016	-2.507853	0.815140				
L9 TS 2											
Charge= 0 Multiplicity= 1											
E (UB3LYP): -3923.180685 A.U.											
ΔG (Thermal Corrections): 0.410278 A.U.											
G (UB3LYP): -3922.770407 A.U.											
C	-0.601702	-1.132043	-0.612227	C	5.799472	-0.127938	-0.066913				
O	-0.877118	0.002385	-1.149780	C	6.688028	-1.219461	-0.062208				
C	-0.957757	-1.493052	0.819462	C	6.331731	1.173247	-0.002732				
H	-0.062099	-1.359732	1.443517	C	8.067409	-1.014994	0.000670				
C	-2.033870	-0.592580	1.400029	H	6.298577	-2.238270	-0.134436				
H	-3.020122	-0.834779	0.962219	C	7.710945	1.376363	0.068315				
C	-1.686540	0.855992	1.029414	H	5.660201	2.035506	0.019195				
H	-0.670434	1.084113	1.409252	C	8.583743	0.283285	0.068216				
C	-1.709940	1.022920	-0.493973	H	8.743297	-1.875240	-0.007899				
H	-2.741008	0.838263	-0.847337	H	8.105941	2.394720	0.129744				
F	-1.292022	-2.825828	0.884296	H	9.664763	0.443195	0.120936				
H	-0.203074	-1.895201	-1.273612	L9 Int 2							
N	1.567149	-0.757990	-0.262023	Charge= 0 Multiplicity= 1							
C	2.115298	0.313694	-0.836162	E (UB3LYP): -3923.215029 A.U.							
C	4.335828	-0.345250	-0.136483	ΔG (Thermal Corrections): 0.407147 A.U.							
C	3.484831	0.562606	-0.794255	G (UB3LYP): -3922.807882 A.U.							
H	1.431013	0.993851	-1.354740	C	1.205346	-0.810861	1.030214				
H	3.883980	1.446424	-1.296309	O	2.182563	-1.718819	0.617551				
O	-2.028227	-0.760135	2.796051	C	1.872524	0.423942	1.633690				
C	-3.314596	-0.858650	3.377237	H	2.407314	0.118831	2.547300				
H	-3.928653	0.034620	3.164551	C	2.848724	1.063330	0.657206				
H	-3.853943	-1.755643	3.012853	H	2.284874	1.472093	-0.199794				
H	-3.166879	-0.949107	4.466842	C	3.828743	0.020462	0.108561				
O	-2.632869	1.710437	1.608678	H	4.514056	-0.262077	0.929494				
C	-2.112807	2.774981	2.367497	C	3.098558	-1.243548	-0.377462				
H	-1.530025	2.407499	3.236649	H	2.555848	-0.990477	-1.305182				
H	-1.479242	3.449394	1.760101	F	0.903705	1.350340	2.011741				
H	-2.974721	3.353460	2.739434	H	0.596560	-1.340477	1.782224				
C	-1.178978	2.342845	-1.037324	C	-3.841987	-0.800554	0.866295				
H	-1.036614	2.230482	-2.133503	C	-2.987808	0.212949	1.332488				
H	-0.182941	2.564280	-0.594106	C	-2.004803	-0.093412	2.273389				
O	-2.093476	3.358390	-0.751023	N	-1.819283	-1.319223	2.777296				
			H	-3.081200	1.238376	0.970382					
			H	-1.317159	0.686327	2.615693					
			O	3.593156	2.080951	1.287506					
			C	3.145115	3.394103	1.031334					

H	3.215174	3.642491	-0.047463	H	-0.000499	2.480752	0.000192
H	2.101551	3.551648	1.364133	H	-2.070842	-1.313868	-0.000368
H	3.804914	4.076361	1.593753	H	-2.166922	1.185352	-0.000237
O	4.533062	0.613360	-0.955949	H	2.166543	1.186034	0.000365
C	5.929816	0.667488	-0.808535	H	2.071329	-1.313092	0.000202
H	6.223587	1.272910	0.072467				
H	6.376962	-0.342177	-0.725637				
H	6.331657	1.149594	-1.716291				
C	4.008842	-2.436242	-0.643097				
H	3.364752	-3.320250	-0.838663				
H	4.598105	-2.657646	0.273369				
O	4.847018	-2.177047	-1.734157				
C	5.721793	-3.235732	-2.020848	C	0.848136	-0.537467	-0.524602
H	6.401944	-3.452971	-1.169001	O	0.289108	0.548002	-0.992008
H	5.172275	-4.169669	-2.269015	C	0.441256	-1.081340	0.829724
H	6.329743	-2.940405	-2.892416	H	0.971769	-0.514006	1.610485
O	0.384931	-0.388144	-0.036177	C	-1.045903	-0.918130	1.111174
C	-0.405339	-1.409244	-0.634687	H	-1.610037	-1.590538	0.445849
H	0.230533	-2.135178	-1.170720	C	-1.447639	0.528287	0.811461
H	-1.005438	-1.938248	0.125503	H	-0.943983	1.182306	1.548931
H	-1.075771	-0.914018	-1.353264	C	-1.050745	0.964299	-0.607059
H	-0.238300	1.200560	-0.336862	H	-1.720895	0.456052	-1.317896
Br	-0.803519	2.421747	-0.940384	F	0.856737	-2.394609	0.940168
C	-4.870681	-0.533138	-0.168133	H	1.379785	-1.169910	-1.232030
C	-6.091636	-1.232814	-0.175956	Br	-0.896239	-2.278142	-2.053268
C	-4.640816	0.425045	-1.173611	N	2.680769	0.270453	0.018697
C	-7.053531	-0.980625	-1.156322	C	2.930716	1.545219	-0.276058
C	-5.600576	0.672225	-2.157230	C	4.182481	2.114890	-0.037838
C	-6.811299	-0.028299	-2.151980	H	2.102811	2.112001	-0.714713
H	-6.301809	-1.966155	0.607238	H	4.363284	3.163674	-0.285947
H	-3.692000	0.967750	-1.201438	O	-1.307564	-1.172078	2.472416
H	-8.000773	-1.528188	-1.139075	C	-1.885804	-2.434066	2.733067
H	-5.398106	1.414199	-2.935530	H	-2.878253	-2.532303	2.249324
H	-7.564220	0.167223	-2.921503	H	-1.239479	-3.264555	2.389789
C	-2.643789	-2.284753	2.355165	H	-2.014684	-2.510917	3.826042
H	-2.482979	-3.285248	2.776065	O	-2.844571	0.633747	0.922461
C	-3.654893	-2.082016	1.414587	C	-3.313388	1.480320	1.943380
H	-4.266953	-2.927069	1.090332	H	-2.989681	1.130899	2.943637
				H	-2.983167	2.526526	1.792206
				H	-4.415546	1.454649	1.899910
				C	-1.041407	2.470901	-0.835500
				H	-0.645481	2.663106	-1.855281
				H	-0.341204	2.946583	-0.112756
				O	-2.333631	2.982791	-
					0.692443		

L10 Catalyst

Charge= 0 Multiplicity= 1
E (UB3LYP): -248.406079 A.U.
ΔG (Thermal Corrections): 0.061489 A.U.
G (UB3LYP): -248.344590 A.U.

C	-1.144395	-0.725432	-0.000204	C	-2.407427	4.366954	-0.917760
C	-1.201093	0.672127	-0.000126	H	-1.778989	4.936233	-0.199197
C	-0.000249	1.386235	0.000087	H	-2.084928	4.633575	-1.947053
C	1.200849	0.672570	0.000206	H	-3.459325	4.669739	-0.785936
C	1.144648	-0.725024	0.000112	C	4.905226	-0.023680	0.813014
N	0.000262	-1.415433	-0.000086	H	5.662501	-0.682630	1.244726
				C	3.627384	-0.512706	0.544839

H	3.344955	-1.549502	0.755166
C	5.185087	1.313964	0.515704
H	6.178335	1.727937	0.712058

L10 Int 1

Charge= 0 Multiplicity= 1

E (UB3LYP): -3576.256986 A.U.
 ΔG (Thermal Corrections): 0.291128 A.U.
 G (UB3LYP): -3575.965858 A.U.

C	2.235535	-0.149015	-0.584150
C	1.589363	0.968344	0.256586
C	-0.566686	0.278395	-0.316802
C	-0.087773	-0.771985	-1.320172
C	1.253332	-1.307539	-0.826353
H	1.416776	0.592279	1.280933
H	2.515847	0.270976	-1.570330
H	-0.674000	-0.192176	0.687779
H	0.016387	-0.321649	-2.322381
H	1.074895	-1.815018	0.140202
O	0.331574	1.341502	-0.320618
Br	-1.414111	-1.587227	2.437866
F	-1.018557	-1.795149	-1.418422
C	1.599933	-3.565030	-1.498807
H	2.090846	-4.131203	-2.307999
H	2.048324	-3.864150	-0.530074
H	0.523638	-3.818118	-1.484552
O	1.818680	-2.193107	-1.764646
C	4.493451	-0.917438	-0.698367
H	5.296794	-1.242675	-0.016177
H	4.271243	-1.730764	-1.411857
H	4.849813	-0.031746	-1.265372
O	3.376244	-0.600778	0.104666
C	2.459720	2.204252	0.321139
H	2.519028	2.663548	-0.690361
H	3.482376	1.886278	0.608865
C	2.700190	4.266023	1.399947
H	2.214004	4.897831	2.162402
H	3.735058	4.036777	1.735773
H	2.768056	4.843063	0.451482
O	1.928514	3.105054	1.252938
C	-2.046122	1.895591	-1.428186
C	-3.308554	2.331722	-1.790683
C	-4.252868	0.469859	-0.577983
C	-2.969606	0.067449	-0.233813
N	-1.905996	0.783614	-0.670578
H	-1.123690	2.403690	-1.707037
H	-3.407551	3.232866	-2.399207
H	-5.103338	-0.110112	-0.213404
H	-2.736967	-0.780005	0.430371
C	-4.429891	1.608610	-1.365592
H	-5.434902	1.937505	-1.643825

L10 TS 2

Charge= 0 Multiplicity= 1
 E (UB3LYP): -3692.009613 A.U.
 ΔG (Thermal Corrections): 0.333701 A.U.
 G (UB3LYP): -3691.675912 A.U.

C	0.754586	-0.910687	-0.369940
O	0.139781	0.114581	-0.822408
C	0.846261	-1.218140	1.105979
H	1.725375	-0.708363	1.527464
C	-0.372358	-0.714491	1.866448
H	-1.252971	-1.304221	1.570795
C	-0.602409	0.755508	1.497673
H	0.259528	1.337683	1.876598
C	-0.743640	0.968122	-0.015839
H	-1.753434	0.663495	-0.342192
F	1.053912	-2.574566	1.267577
H	1.109766	-1.625499	-1.108218
N	2.852194	-0.155821	-0.605844
C	3.028534	0.917842	-1.376705
C	4.300287	1.406278	-1.683073
H	2.121538	1.398051	-1.760168
H	4.410747	2.291003	-2.315082
O	-0.138733	-0.788704	3.250701
C	-0.759786	-1.880785	3.898396
H	-1.863040	-1.828987	3.807464
H	-0.412703	-2.851679	3.495732
H	-0.487783	-1.819252	4.965367
O	-1.797670	1.187378	2.093656
C	-1.659812	2.158066	3.105062
H	-1.062070	1.778114	3.956241
H	-1.201954	3.087012	2.714304
H	-2.676871	2.392287	3.462099
C	-0.442556	2.378028	-0.505108
H	-0.572573	2.392402	-1.607278
H	0.617942	2.632607	-0.283022
O	-1.312838	3.274250	0.120339
C	-1.150818	4.599326	-0.318027
H	-0.127449	4.980071	-0.109850
H	-1.343442	4.696725	-1.407313
H	-1.878919	5.220964	0.228589
O	-1.096421	-2.329710	-0.490860
C	-0.830487	-3.516936	-1.198665
H	-0.417190	-3.322020	-2.210782
H	-0.097913	-4.108511	-0.623239
H	-1.749630	-4.123780	-1.324427
H	-1.756299	-1.775924	-1.036850
Br	-3.000214	-0.631366	-2.261735
C	3.908509	-0.809105	-0.113327
H	3.698037	-1.690568	0.503225
C	5.216191	-0.394798	-0.368945
H	6.059072	-0.950337	0.049749
C	5.412802	0.736181	-1.167214

H 6.424398 1.089534 -1.387471

L10 Int 2

Charge= 0 Multiplicity= 1

E (UB3LYP): -3692.039784 A.U.

ΔG (Thermal Corrections): 0.328051 A.U.

G (UB3LYP): -3691.711733 A.U.

C -0.292432 -0.269947 -0.910086
O 0.593659 -1.325191 -1.144494
C -0.395907 -0.007827 0.588197
H -0.847098 -0.893026 1.060171
C 0.965584 0.281447 1.199302
H 1.350092 1.233438 0.792207
C 1.964224 -0.819339 0.824094
H 1.677052 -1.733820 1.375921
C 1.935956 -1.127467 -0.683913
H 2.399666 -0.277812 -1.215241
F -1.260768 1.064382 0.810535
H -1.267393 -0.599620 -1.304003
C -5.385398 -0.840514 0.763712
C -4.037172 -0.643182 0.450009
N -3.279465 -1.577694 -0.135398
H -5.960589 -0.043309 1.242915
H -3.540100 0.305064 0.682753
O 0.886905 0.343638 2.606073
C 0.825931 1.647240 3.141392
H 1.740112 2.227524 2.899813
H -0.055256 2.208246 2.776220
H 0.753480 1.544044 4.237472
O 3.248393 -0.383683 1.202807
C 3.915879 -1.192970 2.137625
H 3.361938 -1.251536 3.096118
H 4.088799 -2.216175 1.750700
H 4.897516 -0.725289 2.326896
C 2.653861 -2.413496 -1.075446
H 2.446071 -2.607092 -2.149633
H 2.221173 -3.261561 -0.501183
O 4.030315 -2.296867 -0.846127
C 4.744507 -3.457367 -1.178666
H 4.416811 -4.332373 -0.576490
H 4.631596 -3.718204 -2.253471
H 5.810595 -3.264996 -0.971293
O 0.122480 0.921929 -1.539021
C 0.037687 0.910699 -2.957071
H 0.691339 0.130809 -3.385472
H -1.004347 0.736357 -3.287460
H 0.373364 1.899548 -3.306556
H -0.093905 2.552949 -0.896690
Br -0.018845 4.003154 -0.665924
C -3.843093 -2.753231 -0.430514
H -3.196163 -3.498819 -0.909509
C -5.181838 -3.050691 -0.157787

H -5.593802 -4.029389 -0.419670
C -5.969485 -2.070969 0.452438
H -7.022058 -2.263856 0.682179

α-Glycosyl-Br

Charge= 0 Multiplicity= 1

E (UB3LYP): -3327.835423 A.U.

ΔG (Thermal Corrections): 0.206786 A.U.

G (UB3LYP): -3327.628637 A.U.

C 0.285737 1.396747 0.151401
C 1.210887 0.173698 0.064496
C -0.444511 -1.274981 0.982549
C -1.451193 -0.133640 1.099891
C -1.187720 0.978632 0.093094
H 1.126998 -0.262712 -0.945252
H 0.460072 1.909880 1.116700
H -1.343777 0.277897 2.119124
H -1.390055 0.595632 -0.922757
O 0.839380 -0.826803 1.024811
F -2.743568 -0.611806 0.982498
C -3.208059 2.165784 -0.344846
H -3.712153 3.097750 -0.049112
H -3.038267 2.188834 -1.438127
H -3.867860 1.313939 -0.108887
O -1.986669 2.107390 0.366293
C 0.560862 3.629292 -0.652554
H 0.833469 4.152814 -1.581081
H -0.443083 3.954579 -0.335522
H 1.288909 3.910165 0.133229
O 0.603663 2.243427 -0.928337
C 2.656453 0.537069 0.319784
H 2.785155 0.780164 1.395282
H 2.886293 1.451086 -0.261291
C 4.845831 -0.272929 0.152675
H 5.413617 -1.150740 -0.190521
H 5.197743 0.615960 -0.410160
H 5.073129 -0.105216 1.225356
O 3.483342 -0.527767 -0.063585
Br -0.832090 -2.353485 -0.707320
H -0.582377 -2.019810 1.774329

α-Glycosyl-OMe

Charge= 0 Multiplicity= 1

E (UB3LYP): -868.826317 A.U.

ΔG (Thermal Corrections): 0.248643 A.U.

G (UB3LYP): -868.577674 A.U.

C 0.242405 1.071526 -0.183560
C -1.001002 0.189457 0.002232
C 1.467673 -1.037645 -0.792609
C 1.520667 0.247459 0.027407

H	-1.048551	-0.119194	1.060840	H	-1.134089	3.152852	-0.834256
H	0.249050	1.464548	-1.218905	H	-2.067044	2.797986	0.655866
H	1.531640	-0.786622	-1.864182	H	-1.036278	4.261281	0.569613
H	1.575189	-0.020938	1.097941	O	1.875445	1.374665	-0.997441
O	-0.918079	-0.961512	-0.838151	C	2.948524	2.282615	-0.946154
F	2.557345	-1.847171	-0.490944	H	2.725104	3.142439	-0.287547
C	3.788875	0.858800	0.446766	H	3.883728	1.799099	-0.610899
H	4.549061	1.563986	0.070158	H	3.106189	2.659178	-1.968551
H	3.593101	1.086862	1.515014	C	3.173236	-1.186558	0.194053
H	4.187780	-0.169931	0.371976	H	3.189086	-2.292369	0.278403
O	2.631061	1.040142	-0.339255	H	3.648351	-0.786602	1.114279
C	0.625072	3.382654	0.281422	O	3.849692	-0.758888	-0.955550
H	0.508651	4.097009	1.114277	C	5.202553	-1.134725	-0.970159
H	1.685852	3.353069	-0.025648	H	5.762972	-0.700738	-0.117511
H	0.015636	3.740302	-0.575333	H	5.326600	-2.235977	-0.932612
O	0.176668	2.129096	0.747735	H	5.646061	-0.763514	-1.906002
C	-2.288164	0.911068	-0.334501	O	-1.014229	-1.556679	0.360603
H	-2.352008	1.053738	-1.434905	C	-1.076595	-2.961941	0.150115
H	-2.267756	1.912437	0.141468	H	-0.072871	-3.380424	-0.024346
C	-4.617774	0.732415	-0.154749	H	-1.535620	-3.470012	1.016709
H	-5.399589	0.079605	0.269385	H	-1.698608	-3.127271	-0.739755
H	-4.721266	1.745958	0.291526	H	-2.486993	-0.719506	-0.251935
H	-4.787540	0.822541	-1.250088	Br	-3.602668	-0.296447	-1.085188
O	-3.374605	0.156034	0.137584				
C	0.168872	-1.806650	-0.551137				
C	-0.938854	-3.100189	1.071886				
H	-0.820339	-3.416306	2.120682				
H	-1.896801	-2.560184	0.957592				
H	-0.957964	-3.999368	0.422434				
O	0.166902	-2.272325	0.759588				
H	0.077555	-2.647831	-1.264679				

α-Glycosyl-OMe HBr

Charge= 0 Multiplicity= 1

E (UB3LYP): -3443.628961 A.U.

ΔG (Thermal Corrections): 0.250647 A.U.

G (UB3LYP): -3443.378314 A.U.

C	-0.242242	-1.155794	1.465555
O	1.120755	-1.398599	1.278402
C	-0.474377	0.335824	1.685853
H	0.038320	0.635497	2.613217
C	0.060290	1.152969	0.519948
H	-0.529220	0.917580	-0.382972
C	1.517837	0.782162	0.228519
H	2.134620	1.177003	1.056751
C	1.718074	-0.741238	0.151444
H	1.257073	-1.097076	-0.785766
F	-1.834256	0.569163	1.861267
H	-0.532322	-1.734218	2.360279
O	0.006990	2.532891	0.802257
C	-1.116066	3.205164	0.270999

HBr

Charge= 0 Multiplicity= 1

E (UB3LYP): -2574.794460 A.U.

ΔG (Thermal Corrections): -0.013269 A.U.

G (UB3LYP): -2574.807729 A.U.

Br 0.000000000 0.000000000 0.039703

H 0.000000000 0.000000000 -1.389601

IBO

Charge= 0 Multiplicity= 1

E (UB3LYP): -232.547655 A.U.

ΔG (Thermal Corrections): 0.084323 A.U.

G (UB3LYP): -232.463332 A.U.

C	-1.245287	-0.000041	-0.576293
H	-1.673558	-0.927941	-0.985760
H	-1.673610	0.927774	-0.985896
C	0.130162	0.000003	-0.053723
C	0.933560	1.281647	-0.050361
H	1.594417	1.318803	0.835625
H	1.570980	1.347410	-0.951120
H	0.270797	2.163000	-0.023586
C	0.933488	-1.281705	-0.050270
H	1.569511	-1.348302	-0.951955
H	1.595689	-1.318247	0.834736
H	0.270606	-2.162914	-0.021773
O	-1.004546	0.000124	0.829201

IBOHBr

Charge= 0 Multiplicity= 1

E (UB3LYP): -2807.389785 A.U.

ΔG (Thermal Corrections): 0.093021 A.U.

G (UB3LYP): -2807.296764 A.U.

Br	1.619645	-0.000002	0.027862
C	-0.094847	-0.000004	-0.935571
H	-0.089356	-0.896430	-1.570927
H	-0.089343	0.896423	-1.570925
C	-1.330083	-0.000004	-0.024127
C	-1.411238	1.264927	0.834489
H	-2.361095	1.275159	1.400505
H	-0.583876	1.319887	1.561687
H	-1.380887	2.165218	0.195868
C	-1.411336	-1.265000	0.834389
H	-0.584023	-1.320049	1.561635

H	-2.361230	-1.275235	1.400341
H	-1.380983	-2.165242	0.195701
O	-2.392261	0.000075	-0.988213
H	-3.233664	0.000223	-0.498443

MeOH

Charge= 0 Multiplicity= 1

E (UB3LYP): -115.785128 A.U.

ΔG (Thermal Corrections): 0.027819 A.U.

G (UB3LYP): -115.757309 A.U.

H	1.141829	0.764115	-0.000157
C	-0.656961	0.019648	0.000027
H	-1.037543	0.551508	0.898785
H	-1.037886	0.550798	-0.899121
H	-1.093206	-0.994560	0.000339
O	0.746072	-0.123718	-0.000001