

Supporting Information

Synthesis and biological evaluation of selective phosphonate-bearing 1,2,3-triazole-linked sialyltransferase inhibitors

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Additional Synthesis

Uridine Synthons:

5'-O-Propargyl-2',3'-O-isopropylidenuridine (7)

The acetonide protected 5'-O-propargyluridine compound (**7**) was synthesised by the method described by Sun *et al.*, and spectral data matched those reported.¹

5'-O-Propargyluridine (8)

Protected propargyl uridine (**7**, 540 mg, 1.68 mmol) was dissolved in 10 mL 9:1 ACN/H₂O, with indium triflate (5% mol equiv.), for 4 hours at reflux. After reaction, the mixture was evaporated under reduced pressure and the crude product purified by column chromatography (DCM:MeOH, 9:1), to give a white foam (436 mg, 92 %). R_f 0.46 (Silica, DCM:MeOH, 9:1). Spectral data matched those previously reported.¹

Synthesis of α -hydroxyphosphonates:

All α -hydroxyphosphonates (compounds **10a-g**) were synthesised as per the method of Montgomery *et al.*,² and **10a-d** and **10g** are characterised in that work. ¹H, ¹³C, ³¹P, and ¹⁹F NMR spectra for **10e** and **10f** is provided in the supplementary information.

Dibenzyl α -hydroxy(3-trifluoromethyl)benzylphosphonate (10e)

From 3-trifluoromethylbenzaldehyde (300 mg, 1.72 mmol), and purified by column chromatography with a 9:1 Toluene/Acetone eluent to yield a white solid (752 mg, 78 %). R_f 0.26 (Silica, Toluene/Acetone, 9:1). ¹H NMR (400 MHz, CDCl₃): 7.71 (s, 1H), 7.59 (d, 1H, *J* = 7.8 Hz), 7.54 (d, 1H, *J* = 7.6 Hz), 7.42-7.36 (m, 1H), 7.32-7.20 (m, 10H), 5.10 (d, 1H, ²*J*_(H,P) = 10.1 Hz), 5.04-4.91 (m, 4H), 4.59-4.38 (bs, 1H). ¹³C NMR (100 MHz, CDCl₃): 137.4, 135.7 (d, ²*J*_(C,P) = 5.8 Hz), 130.4 (d, ³*J*_(C,F) = 5.6 Hz), 128.7, 128.6, 128.0, 127.0, 124.9, 124.0 (q, ¹*J*_(C,F) = 270.6 Hz), 123.9, 70.5 (2 x d, ¹*J*_(C,P) = 157.6 Hz), 69.0-68.5 (m). ³¹P NMR (162 MHz, CDCl₃): 21.1 ¹⁹F NMR (376 MHz, CDCl₃): -62.6 ESI-HRMS: *m/z* calculated for C₂₂H₂₀F₃O₄PNa [M + Na]⁺ 459.0949, found 459.0967.

Dibenzyl α -hydroxy(3-[1,1,2,2-tetrafluoroethoxy])benzyl phosphonate (10f)

From 3-(1,1,2,2-tetrafluoroethoxy) benzaldehyde (861 mg, 4.34 mmol), and purified by column chromatography with a 9:1 Toluene/Acetone eluent to yield a white solid (1750 mg, 70 %). R_f 0.85 (Silica, Toluene/Acetone, 9:1). ¹H NMR (400 MHz, CDCl₃): 7.37-7.14 (m, 14H), 5.87 (tt, 1H, ²*J*_(H,F) = 53.0 Hz, ³*J*_(H,F) = 2.5 Hz), 5.05 (d, 1H, ²*J*_(H,P) = 10.5 Hz), 5.01-4.90 (m, 4H), 2.70-2.36 (bs, 1H). ¹³C NMR (125 MHz, CDCl₃): 148.2, 139.2, 135.9 (t, ³*J*_(C,P) = 5.6 Hz), 129.4, 128.5-127.9 (m), 125.3 (d, ³*J*_(C,P) = 5.6 Hz), 121.0 (d, ⁴*J*_(C,F) = 1.8 Hz), 120.5 (d, ³*J*_(C,P) = 5.6 Hz), 116.5 (tt, ¹*J*_(C,F) = 270.3 Hz, ²*J*_(C,F) = 27.8 Hz), 107.7 (tt, ¹*J*_(C,F) = 249.9 Hz, ²*J*_(C,F) = 41.6 Hz), 70.3 (d, ¹*J*_(C,P) = 160.1 Hz), 68.9 (d, ²*J*_(C,P) =

7.4 Hz), 68.5 (d, $^2J_{(C,P)} = 7.5$ Hz). ^{31}P NMR (162 MHz, CDCl_3): 21.2 ^{19}F NMR (376 MHz, CDCl_3): -88.0 (t, $J = 5.4$ Hz), -136.7 (t, $J = 5.4$ Hz). ESI-HRMS: m/z calculated for $\text{C}_{22}\text{H}_{20}\text{F}_3\text{O}_4\text{PNa}$ $[\text{M} + \text{H}]^+$ 485.1141, found 485.1143.

Synthesis of α -azidophosphonates:

Dibenzyl α -hydroxyphosphonate (**10a-g**, 1 equiv.) and triphenylphosphine (3 equiv.), were dissolved in dry THF under an inert atmosphere at 0 °C. Freshly prepared HN_3 (30 mL) was added, along with diisopropylazodicarboxylate (DIAD, 3 equiv.) dropwise, and the reaction was allowed to warm to room temperature. Upon completion (judged by TLC), the reaction mixture was taken up in CH_2Cl_2 (10 mL), washed with saturated NaHCO_3 solution (3 x 5 mL) and brine (3 x 5 mL). The organic phase was separated and dried with anhydrous MgSO_4 and evaporated, with the resultant product purified by column chromatography. The α -azidophosphonates proved difficult to purify, as the hydrazine by-product of DIAD seemed to ‘stick’ to the desired product during column chromatography, and would not readily precipitate when the crude product was taken up in a non-polar solvent such as hexane. This was not deemed an issue, as the hydrazine did not impact the proceeding click reaction and so it was not necessary for the α -azidophosphonate to be completely purified. ^1H , ^{13}C , ^{31}P , and ^{19}F NMR spectra for these compounds is provided.

Dibenzyl α -azido-3-phenoxybenzylphosphonate (11a)

From **10a** (1.25 g, 2.71 mmol): purified by column chromatography using a Toluene/Acetone (1:1) eluent, to yield a white solid (1.095 g, 83.7%). R_f 0.48 (Silica, Toluene/Acetone, 1:1). ^1H NMR (400 MHz, CDCl_3): 7.23-7.18 (m, 12H), 7.18-7.13 (m, 2H), 7.08 (s, 1H), 7.00 (t, $J = 7.3$ Hz, 1H), 6.92 (d, $J = 7.7$ Hz, 3H), 4.97-4.82 (m, 4H), 4.67 (d, $^2J_{(H,P)} = 16.0$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3): 157.6, 156.8, 135.9, 135.8, 134.3, 130.2, 129.9, 128.6, 128.2, 123.7, 123.2, 119.2, 118.7, 68.8, 61.3 (d, $^2J_{(C,P)} = 157.2$ Hz). ^{31}P NMR (162 MHz, CDCl_3): 19.2. ESI-HRMS: m/z calculated for $\text{C}_{27}\text{H}_{24}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M} + \text{Na}]^+$: 508.1406, found 508.1402.

Dibenzyl α -azido-3-cyclopentoxybenzylphosphonate (11b)

From **10b** (232 mg, 0.512 mmol): purified by column chromatography using a DCM/EtOAc (99:1) eluent, to give a white solid (195 mg, 80%). R_f 0.68 (Silica, DCM:EtOAc, 99:1). ^1H NMR (400 MHz, CDCl_3): 7.35-7.18 (m, 11H), 6.95-6.92 (m, 2H), 6.87-6.84 (m, 1H, H4), 5.04-4.82 (m, 4H), 4.68 (d, 1H, $J = 16.8$ Hz), 4.65 (m, 1H), 1.89-1.70 (m, 6H), 1.63-1.53 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3): 158.3 (d, $J = 2.4$ Hz), 135.8 (d, $J = 5.8$ Hz), 135.7 (d, $J = 5.9$ Hz), 133.1 (d, $J = 3.6$ Hz), 129.7 (d, $J = 1.5$ Hz), 128.6, 128.5, 128.09, 128.05, 120.3 (d, $J = 6.7$ Hz), 116.5 (d, $J = 2.6$ Hz), 115.0 (d, $J = 6.0$ Hz), 79.2, 68.83 (d, $J = 6.8$ Hz), 68.79 (d, $J = 7.2$ Hz), 61.8 (d, $J = 158.7$ Hz), 32.7, 24.0. ^{31}P NMR (162 MHz, CDCl_3): 19.3. ESI-HRMS: m/z calculated for $\text{C}_{26}\text{H}_{28}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M} + \text{Na}]^+$: 500.1716, found 500.1709.

Dibenzyl α -azido-3-phenoxy-4-fluorobenzylphosphonate (11c)

From **10c** (179 mg, 0.375 mmol): purified by column chromatography using a DCM/EtOAc (99:1) eluent, to give a white solid (141 mg, 75%). R_f 0.83 (Silica, DCM:EtOAc, 99:1). **$^1\text{H NMR}$ (500 MHz, CDCl_3):** 7.31-7.18 (m, 12H), 7.12-7.05 (m, 4H), 6.92-6.90 (m, 2H), 5.01-4.88 (m, 4H), 4.61 (d, 1H, $J_{(H,P)} = 16.3$ Hz). **$^{13}\text{C NMR}$ (125 MHz, CDCl_3):** 156.8, 154.3 (d, $J = 251.1$ Hz), 144.0 (dd, $J = 12.1$, 2.8 Hz), 135.5 (2 x d, $J = 5.8$ Hz), 129.8, 128.9 (d, $J = 3.9$ Hz), 128.7, 128.6 (d, $J = 3.2$ Hz), 128.13, 128.08, 126.4 (d, $J = 6.1$ Hz), 124.5 (2 x d, $J = 6.4$ Hz), 123.5, 121.4 (d, $J = 4.5$ Hz), 117.5, 117.3 (dd, $J = 19.2$, 2.2 Hz), 68.9 (2 x d, $J = 6.8$ Hz), 60.9 (d, $J = 159.2$ Hz). **$^{31}\text{P NMR}$ (202 MHz, CDCl_3):** 18.8. **$^{19}\text{F NMR}$ (376 MHz, CDCl_3):** -131.7. **ESI-HRMS:** m/z calculated for $\text{C}_{27}\text{H}_{23}\text{FN}_3\text{O}_4\text{PNa}$ [$\text{M} + \text{Na}$] $^+$: 526.1308, found 526.1321.

Dibenzyl α -azido-4-fluorobenzylphosphonate (11d)

From **10d** (400 mg, 1.04 mmol): purified by column chromatography using a DCM/EtOAc (99:1) eluent, to give a white solid (379 mg, 89%). R_f 0.68 (Silica, DCM:EtOAc, 99:1). **$^1\text{H NMR}$ (500 MHz, CDCl_3):** 7.36-7.27 (m, 10H), 7.21-7.19 (m, 2H), 7.00 (dd, $^3J_{(H,F)} = 8.5$ Hz, 2H), 5.04-4.86 (m, 4H), 4.69 (d, 1H, $J_{(H,P)} = 16.3$ Hz). **$^{13}\text{C NMR}$ (125 MHz, CDCl_3):** 162.9 (dd, $^1J_{(C,F)} = 248.0$ Hz, $^5J_{(C,P)} = 3.0$ Hz), 135.6 (2 x d, $^2J_{(C,P)} = 18.4$ Hz), 130.2 (dd, $^3J_{(C,P)} = 8.3$ Hz, $^3J_{(C,F)} = 6.4$ Hz), 128.6 (m), 128.2, 128.1, 127.8 (t, $^3J_{(C,P)} = 3.4$ Hz), 115.8 (dd, $^2J_{(C,F)} = 22.0$ Hz), 68.9 (m), 61.1 (d, $^1J_{(C,P)} = 160.9$ Hz). **$^{31}\text{P NMR}$ (202 MHz, CDCl_3):** 19.2. **$^{19}\text{F NMR}$ (376 MHz, CDCl_3):** -112.3 (2 x s). **ESI-HRMS:** m/z calculated for $\text{C}_{21}\text{H}_{19}\text{FN}_3\text{O}_3\text{PNa}$ [$\text{M} + \text{Na}$] $^+$: 434.1046, found 434.1066.

Dibenzyl α -azido-3-trifluoromethylbenzylphosphonate (11e)

From **10e** (600 mg, 1.38 mmol): purified by column chromatography using a DCM/EtOAc (99:1) eluent, to give a white solid (608 mg, 96%). R_f 0.77 (Silica, DCM:EtOAc, 99:1). **$^1\text{H NMR}$ (400 MHz, CDCl_3):** 7.61 (bs, 1H), 7.57 (bs, 1H), 7.55 (bs, 1H), 7.41 (t, 1H, $J = 7.8$ Hz), 7.20-7.33 (m, 10H), 4.94-5.03 (m, 4H), 4.79 (d, 1H, $J = 16.5$ Hz). **$^{13}\text{C NMR}$ (100 MHz, CDCl_3):** 135.4-135.6 (m), 133.5 (d, $J = 3.7$ Hz), 131.6 (d, $J = 4.4$ Hz), 131.0 (dq, $J = 33.3$, 2.4 Hz), 129.1 (d, $J = 2.2$ Hz), 128.8, 128.69, 128.67, 128.2, 125.0 (quint, $J = 3.5$ Hz), 125.0 (sext, $J = 3.5$ Hz), 123.8 (q, $J = 272.7$ Hz), 69.1, 69.0, 61.4 (d, $J = 157.7$ Hz). **$^{31}\text{P NMR}$ (162 MHz, CDCl_3):** 18.5. **$^{19}\text{F NMR}$ (376 MHz, CDCl_3):** -62.6. **ESI-HRMS:** m/z calculated for $\text{C}_{22}\text{H}_{19}\text{F}_3\text{N}_3\text{O}_3\text{PNa}$ [$\text{M} + \text{Na}$] $^+$: 484.1014, found 484.1037.

Dibenzyl α -azido-3-(1,1,2,2-tetrafluoroethoxy)benzyl phosphonate (11f)

From **10f** (331 mg, 0.840 mmol): purified by column chromatography using a DCM/EtOAc (4:1) eluent, to give a white solid (289 mg, 83%). R_f 0.95 (Silica, DCM:EtOAc, 4:1). **$^1\text{H NMR}$ (500 MHz, CDCl_3):** 7.36-7.20 (m, 14H), 5.89 (tt, 1H, $J = 53.1$, 2.8 Hz), 5.02-4.90 (m, 4H), 4.73 (d, 1H, $J = 16.5$ Hz). **$^{13}\text{C NMR}$ (125 MHz, CDCl_3):** 148.9, 135.6 (d, $J = 6.1$ Hz), 135.5 (d, $J = 6.2$ Hz), 134.3 (d, $J = 4.6$ Hz), 130.0 (d, $J = 1.8$ Hz), 128.7, 128.64, 128.62, 128.19, 128.17, 126.3 (d, $J = 6.3$ Hz), 121.9 (d, $J = 2.4$ Hz), 121.5 (d, $J = 6.2$ Hz), 116.5 (tt, $J = 272.5$, 28.7 Hz), 107.6 (tt, $J = 252.0$, 41.2 Hz), 69.1 (m), 61.3

(d, $J = 158.7$ Hz). ^{31}P NMR (162 MHz, CDCl_3): 18.6. ^{19}F NMR (376 MHz, CDCl_3): -88.1 (t, $J = 6.8$ Hz), -136.7 (dt, $J = 53.0, 5.7$ Hz). ESI-HRMS: m/z calculated for $\text{C}_{23}\text{H}_{20}\text{F}_4\text{N}_3\text{O}_4\text{PNa}$ $[\text{M} + \text{Na}]^+$: 532.1025, found 532.1035.

Dibenzyl α -azido-(3-benzothiophene)methylphosphonate (11g)

From **10g** (460 mg, 1.08 mmol): purified by column chromatography, with a Hexane/EtOAc (1:1) eluent. This afforded a clear oil (390 mg, 80 %). R_f 0.73 (Silica, Hexane/EtOAc, 1:1). ^1H NMR (500 MHz, CDCl_3): 7.86-7.75 (m, 3H), 7.38-7.35 (m, 2H), 7.34-7.29 (m, 5H), 7.27-7.21 (m, 3H), 7.14-7.11 (m, 2H), 5.01 (d, 1H, $J = 16.8$ Hz), 5.13-4.79 (m, 4H) ^{13}C NMR (125 MHz, CDCl_3): 140.0, 137.3 (2 x s), 135.6 (2 x s), 135.4 (2 x s), 128.56, 128.54, 128.48, 128.43, 128.1, 128.0, 127.5 (d, $J = 7.5$ Hz), 126.1, 124.9, 124.5, 122.7, 121.9, 68.9-68.8 (m), 55.4 (d, $J = 162.7$ Hz) ^{31}P NMR (202 MHz, CDCl_3): 19.1. ESI-HRMS: m/z calculated for $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_3\text{PSNa}$ $[\text{M} + \text{Na}]^+$: 472.08552, found 472.08550.

CuAAC ‘click’ coupling to form 1,2,3-triazoles:

An α -azidophosphonate (**11a-g**, 1 equiv.), **8** (1.2 equiv.), $\text{Cu}(\text{OAc})_2$ (0.25 equiv.), and sodium ascorbate (0.5 equiv.) were suspended in a mixture of THF and water (1:1) and stirred at room temperature until starting material disappeared (4-12 hours). Upon completion (judged by TLC), the reaction mixture was concentrated under reduced pressure and extracted with EtOAc. The organic layer washed with brine, dried with anhydrous MgSO_4 , filtered and evaporated, with the resultant product purified by column chromatography.

5'-O-[1-(Dibenzoxyphosphoryl-3-phenoxyphenylmethyl)-1,2,3-triazol-4-yl]methyluridine (12a)

From **11a** (150 mg, 0.309 mmol): purified by column chromatography to give white solid (100 mg, 51%). R_f 0.64 (DCM/MeOH, 9:1). ^1H NMR (400 MHz, CDCl_3): 9.18 (2 x bs, 1H), 8.04 (2 x s, 1H), 7.73 (2 x d, $J = 8.2$ Hz), 7.33-7.21 (m, 10H), 7.16-7.09 (m, 6H), 7.00-6.92 (m, 3H), 6.13 (2 x d, 1H, $J = 21.6$ Hz), 5.80 (2 x d, 1H, $J = 2.3$ Hz), 5.63 (2 x d, 1H, $J = 8.1$ Hz), 4.97-4.80 (m, 4H), 4.69-4.59 (m, 2H), 4.39 (bs, 1H), 4.20-4.15 (m, 3H), 3.86-3.51 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3): 163.3, 158.0 (2 x s), 156.3 (2 x s), 151.0, 144.6, 140.4 (2 x s), 135.1 (m), 133.6 (2 x s), 130.6 (2 x s), 129.9 (2 x s), 128.8, 128.7, 128.1 (m), 123.9 (2 x s), 123.0 (2 x s), 119.3 (2 x s), 118.8 (2 x s), 102.3 (2 x s), 90.7 (2 x s), 83.8 (2 x s), 75.4 (2 x s), 70.5 (2 x s), 69.7 (2 x s), 69.2 (2 x s), 69.0 (2 x s), 64.4 (2 x s), 61.7 (d, $J = 159.1$ Hz). ^{31}P NMR (162 MHz, CDCl_3): 16.4. ESI-HRMS: m/z calculated for $\text{C}_{39}\text{H}_{38}\text{N}_5\text{O}_{10}\text{PNa}$ $[\text{M} + \text{Na}]^+$: 790.2271, found 790.2254.

5'-O-[1-(Dibenzoxyphosphoryl-3-cyclopentoxyphenylmethyl)-1,2,3-triazol-4-yl]methyluridine (12b)

From **11b** (156 mg, 0.326 mmol): purified by column chromatography with a 9:1 DCM/MeOH eluent to afford a white foam (129 mg, 52 %). R_f 0.68 (DCM/MeOH, 9:1). ^1H NMR (500 MHz, CDCl_3): 8.80 (2 x s, 1H), 8.02 (2 x s, 1H), 7.72 (2 x d, 1H, $J = 8.2$ Hz), 7.31-7.23 (m, 7H), 7.19-7.17 (m, 2H), 7.11-

7.03 (m, 4H), 6.89-6.86 (m, 1H), 6.11 (2 x d, 1H, $J = 21.3$ Hz), 5.79 (2 x d, 1H, $J = 3.4$ Hz), 4.96-4.60 (m, 4H), 4.70-4.60 (m, 3H), 4.553 (2 x dd, 1H, $J = 8.1, 2.0$ Hz), 2.4-4.10 (m, 4H), 3.86-3.45 (m, 3H), 1.91-1.72 (m, 6H), 1.67-1.57 (m, 2H). **^{13}C NMR (125 MHz, CDCl_3):** 163.0, 158.6 (2 x s), 150.8, 144.5, 140.3 (2 x s), 135.2-135.0 (m), 132.9 (2 x s), 130.3 (2 x s), 128.8-128.6 (m), 128.1 (m), 123.0, 120.4 (m), 116.6 (2 x s), 116.0 (2 x d, $J = 7.1$ Hz), 102.2, 91.0, 84.0 (2 x s), 79.4, 75.6, 70.7 (2 x s), 69.7 (2 x s), 69.1 (2 x s), 68.9 (2 x s), 63.4 (2 x s), 62.0 (2 x d, $J = 155.4$ Hz), 32.8, 24.1. **^{31}P NMR (162 MHz, CDCl_3):** 16.8. **ESI-HRMS:** m/z calculated for $\text{C}_{39}\text{H}_{38}\text{N}_5\text{O}_{10}\text{PNa}$ $[\text{M} + \text{Na}]^+$: 782.2567, found 782.2598.

5'-O-[1-(Dibenzoxyphosphoryl-3-phenoxy-4-fluorophenylmethyl)-1,2,3-triazol-4-yl]methyluridine (12c)

From **11c** (59.9 mg, 0.119 mmol): purified by column chromatography using a DCM/MeOH (9:1) eluent, to give a white solid (51.1 mg, 66%). R_f 0.67 (Silica, DCM:MeOH, 9:1). **^1H NMR (400 MHz, MeOD):** 8.16 (s, 1H), 7.86 (2 x d, 1H, $J = 8.2$ Hz), 7.34-7.10 (m, 19H), 6.90-6.88 (m, 2H), 6.54 (2 x d, 1H, $J = 22.2$ Hz), 5.88 (d, 1H, $J = 4.5$ Hz), 5.53 (2 x d, 1H, $J = 8.3$ Hz), 5.03-4.94 (m, 4H), 4.68 (m, 2H), 4.12 (m, 3H), 3.79 (m, 2H). **^{13}C NMR (100 MHz, MeOD):** 164.6, 151.0, 149.0, 144.5, 140.8, 135.4, 129.6, 128.4, 127.8, 126.9, 124.3, 123.3, 121.9, 121.6 (d, $J = 17.2$ Hz), 117.2, 101.4, 89.0, 83.4, 74.5, 70.2, 69.4-69.2 (m), 63.4, 60.6 (d, $J = 155.1$ Hz). **^{31}P NMR (162 MHz, MeOD):** 16.3. **^{19}F NMR (376 MHz, MeOD):** -131.6 (2 x s). **ESI-HRMS:** m/z calculated for $\text{C}_{55}\text{H}_{49}\text{FN}_5\text{O}_{14}\text{PNa}$ $[\text{M} + \text{Na}]^+$: 808.2158, found 808.2160.

5'-O-[1-(Dibenzoxyphosphoryl-4-fluorophenylmethyl)-1,2,3-triazol-4-yl]methyluridine (12d)

From **11d** (109 mg, 0.265 mmol): purified by column chromatography with a 9:1 DCM/MeOH eluent to afford a white foam (106 mg, 57 %). R_f 0.62 (DCM/MeOH, 9:1). **^1H NMR (400 MHz, CDCl_3):** 9.52 (2 x s, 1H), 8.01 (2 x s, 1H), 7.74 (m, 1H, $J = 8.1$ Hz), 7.50-7.46 (m, 2H), 7.30-7.24 (m, 6H), 7.17-7.15 (m, 2H), 7.11-7.08 (m, 2H), 7.01 (2 x t, 2H, $J = 8.6$ Hz), 6.15 (2 x d, 1H, $J = 22.2$ Hz), 5.82 (2 x d, 1H, $J = 3.0$ Hz), 5.59 (2 x d, 1H, $J = 8.4$ Hz), 4.96-4.80 (m, 4H), 4.59-4.67 (m, 3H), 4.22-4.16 (m, 3H), 3.86-3.49 (m, 3H). **^{13}C NMR (100 MHz, CDCl_3):** 163.5 (2 x s), 163.4 (2 x d, $J = 274.4$ Hz), 151.0, 144.7 (2 x s), 140.5 (2 x s), 134.9-135.1 (m), 130.8 (m), 128.8, 128.68, 128.65, 128.15, 128.12, 128.09, 122.9 (2 x s), 116.3 (2 x d, $J = 21.3$ Hz), 103.0 (2 x s), 102.3 (2 x s), 90.7 (2 x s), 83.8, 75.4 (2 x s), 70.5 (2 x s), 69.8 (2 x s), 69.3 (2 x s), 69.1 (2 x s), 64.4, 61.2 (d, $J = 155.8$ Hz). **^{31}P NMR (162 MHz, CDCl_3):** 16.5. **^{19}F NMR (376 MHz, CDCl_3):** -111.0 (2 x m). **ESI-HRMS:** m/z calculated for $\text{C}_{39}\text{H}_{38}\text{N}_5\text{O}_{10}\text{PNa}$ $[\text{M} + \text{Na}]^+$: 716.1898, found 716.1899.

5'-O-[1-(Dibenzoxyphosphoryl-3-trifluoromethylphenylmethyl)-1,2,3-triazol-4-yl]methyluridine (12e)

From **11e** (159 mg, 0.344 mmol): purified by column chromatography with a 9:1 DCM/MeOH eluent to afford a white foam (156 mg, 60 %). R_f 0.56 (DCM/MeOH, 9:1). **^1H NMR (400 MHz, MeOD):** 8.85-8.34 (2 x s, 1H), 8.31-8.11 (2 x s, 1H), 7.71 (2 x d, 1H, $J = 8.2$ Hz), 7.41-7.34 (m, 7H), 7.25-7.21

(m, 2H), 7.18-7.10 (m, 4H), 6.93-6.90 (m, 1H), 6.18-6.12 (2 x d, 1H, $J = 22.0$ Hz), 5.80 (2 x d, 1H, $J = 2.3$ Hz), 5.71-5.66 (m, 1H), 5.13-4.79 (m, 4H), 4.68-4.59 (m, 2H), 4.49 (bs, 1H), 4.18-4.14 (m, 3H), 3.86-3.50 (m, 3H). **^{13}C NMR (100 MHz, MeOD):** 162.6 (2 x s), 150.0, 144.7 (2 x s), 140.6 (2 x s), 135.0, 134.8 (2 x s), 134.7 (2 x s), 132.7 (2 x s), 131.9 (m), 129.8 (2 x s), 128.9-128.2 (m), 126.3 (m), 125.6 (m), 123.5 (q, $J = 272.7$ Hz), 123.0 (2 x s), 103.2 (2 x s), 90.2 (2 x s), 83.6 (2 x s), 75.3 (2 x s), 70.9 (2 x s), 69.7 (m), 69.5 (m), 68.9 (2 x s), 65.0 (2 x s), 61.6 (d, $J = 155.3$ Hz). **^{31}P NMR (162 MHz, MeOD):** 15.6. **^{19}F NMR (376 MHz, MeOD):** -62.7 (2 x s). **ESI-HRMS:** m/z calculated for $\text{C}_{34}\text{H}_{33}\text{F}_3\text{N}_5\text{O}_9\text{PNa}$ $[\text{M} + \text{Na}]^+$: 765.2158, found 765.2182.

5'-O-[1-(Dibenzoxyphosphoryl-3-(1,1,2,2-tetrafluoroethoxy)phenylmethyl)-1,2,3-triazol-4-yl]methyluridine (12f)

From **11f** (18.5 mg, 0.0363 mmol): purified by column chromatography with a 9:1 DCM/MeOH eluent to afford a white foam (12.1 mg, 52 %). R_f 0.61 (Silica, DCM:MeOH, 9:1). **^1H NMR (500 MHz, MeOD):** 8.21 (s, 1H), 7.86 (2 x d, 1H, $J = 8.2$ Hz), 7.50-7.43 (m, 3H), 7.32-7.29 (m, 7H), 7.21-7.19 (m, 4H), 6.54 (2 x d, 1H, $J = 22.4$ Hz), 6.32 (tt, 1H, $J = 52.5, 3.0$ Hz), 5.88 (d, 1H, $J = 4.5$ Hz), 5.55 (2 x d, 1H, $J = 8.0$ Hz), 5.07-4.94 (m, 4H), 4.68 (m, 2H), 4.12 (m, 3H), 3.79 (m, 2H). **^{13}C NMR (125 MHz, MeOD):** 164.6, 151.0, 149.0, 144.6, 140.9, 135.3, 134.4, 130.2, 128.6-127.8 (m), 128.4, 128.3, 128.1, 128.0, 127.9, 127.8, 127.5, 127.4 (2 x s), 126.9, 124.4, 122.3, 121.9, 121.6 (d, $J = 17.2$ Hz), 116.6 (t, $J = 271.0$ Hz), 108.0 (t, $J = 250.6$ Hz), 101.5, 89.1, 83.4, 74.5, 70.2, 69.5-69.2 (m), 65.5, 63.5, 60.6 (d, $J = 155.1$ Hz). **^{31}P NMR (162 MHz, MeOD):** 16.1. **^{19}F NMR (376 MHz, MeOD):** -89.8, -139.2. **ESI-HRMS:** m/z calculated for $\text{C}_{35}\text{H}_{33}\text{F}_4\text{N}_5\text{O}_{10}\text{P}$ $[\text{M} - \text{H}]^-$: 790.1901, found 790.1902.

5'-O-[1-(Dibenzoxyphosphorylbenzothiophen-3-ylmethyl)-1,2,3-triazol-4-yl]methyluridine (12g)

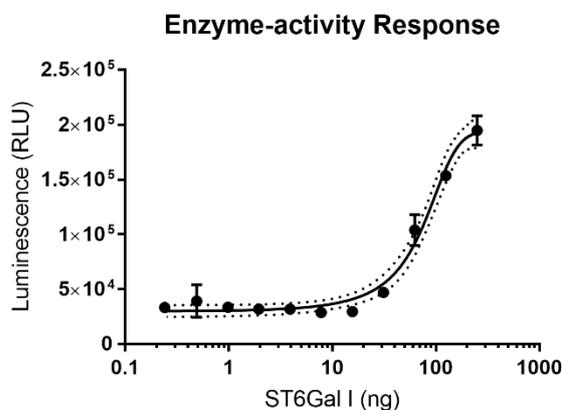
From **11g** (105 mg, 0.234 mmol): purified by column chromatography with a 9:1 DCM/MeOH eluent to afford a white foam (97.7 mg, 57 %). R_f 0.65 (DCM/MeOH, 9:1). **^1H NMR (500 MHz, CDCl_3):** 8.95 (2 x s, 1H), 8.22 (2 x s, 1H), 7.88-7.80 (m, 2H), 7.67-7.64 (m, 2H), 7.38-7.35 (m, 2H), 7.32-7.29 (m, 3H), 7.08-7.07 (m, 2H), 7.24-7.17 (m, 5H), 6.59 (2 x d, 1H, $J = 20.9$ Hz), 5.80 (2 x d, 1H, $J = 3.1$ Hz), 5.62 (2 x d, 1H, $J = 8.1$ Hz), 5.01-4.75 (m, 4H), 4.63-4.53 (m, 2H), 4.20-4.13 (m, 4H), 3.82-3.56 (m, 3H). **^{13}C NMR (125 MHz, CDCl_3):** 163.0, 150.9 (2 x s), 144.8 (2 x s), 140.3 (2 x s), 139.8 (2 x s), 137.2 (d, $J = 10.7$ Hz), 135.03, 134.99, 134.8 (2 x d, $J = 5.1$ Hz), 129.0-128.6 (m), 128.14, 128.08 (2 x s), 125.5 (2 x s), 125.3 (2 x s), 125.0 (2 x s), 123.0 (2 x s), 122.8 (2 x s), 121.2, 102.2 (2 x s), 90.9 (2 x s), 83.9, 75.5 (2 x s), 70.6 (2 x s), 69.8-69.7 (m), 69.4-69.3 (m), 69.0 (2 x s), 64.5 (2 x s), 54.9 (d, $J = 159.1$ Hz). **^{31}P NMR (162 MHz, CDCl_3):** 16.6 (2 x s). **ESI-HRMS:** m/z calculated for $\text{C}_{35}\text{H}_{34}\text{N}_5\text{O}_9\text{PSNa}$ $[\text{M} + \text{Na}]^+$: 754.1717, found 754.1713.

CMP-Glo based Sialyltransferase Inhibition Assay

Recombinant human ST3Gal I and ST6Gal I were obtained from R&D Systems, CMP-Neu5Ac (purified prior to use by size exclusion chromatography), Gal- β 1,3-GalNAc and LacNAc were from Carbosynth. Assays were performed in a sodium cacodylate buffer (5.0 mM sodium cacodylate, 15.0 μ M NaCl, 0.05 % Triton X-100). Assays were performed in a solid white 96-well plate, in a 25 μ L volume for one hour, incubated at room temperature. CMP detection reagent was prepared as per Promega's guidelines, and 25 μ L was added, with luminescence measured after a further hour of incubation. In each assay a CMP standard curve was established in duplicate, with concentrations ranging from 0-100 μ M.

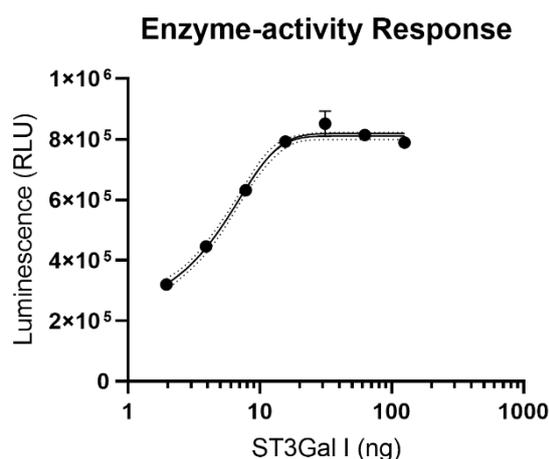
Enzyme activity curve

To determine the amount of enzyme to use in each assay, an assay was performed using amounts of enzyme ranging from 0-500 ng/well. The amount of enzyme was added in 15 μ L of assay buffer, to which was added 10 μ L of a mixture containing 25 μ M CMP-Neu5Ac and 2.5 mM acceptor (Gal- β 1,3-GalNAc and LacNAc for ST3Gal I and ST6Gal I respectively). The resultant sigmoidal activity curve of luminescence vs quantity of enzyme showed a linear region of response, which gave a guideline as to the amount of enzyme that should be used for subsequent reactions.



Interpolation	
	Luminescence (RLU)
	Y
Sigmoidal, 4PL, X is log(concentration)	
Best-fit values	
Top	193637
Bottom	3751
LogIC50	68.26
HillSlope	0.01169
IC50	1.824e+068
Span	189886
95% CI (asymptotic)	
Top	178245 to 209028
Bottom	-30104 to 37606
LogIC50	50.31 to 86.21
HillSlope	0.006578 to 0.01679
IC50	2.038e+050 to 1.632e+086
Span	147449 to 232323
Goodness of Fit	
Degrees of Freedom	20
R square	0.9756
Adjusted R square	0.972
Absolute Sum of Squares	1724622611

Figure S1. Enzyme-activity curve for ST6Gal I in the CMP-Glo™ assay. The assay gave a $R^2 = 0.9756$ for the sigmoidal response curve.

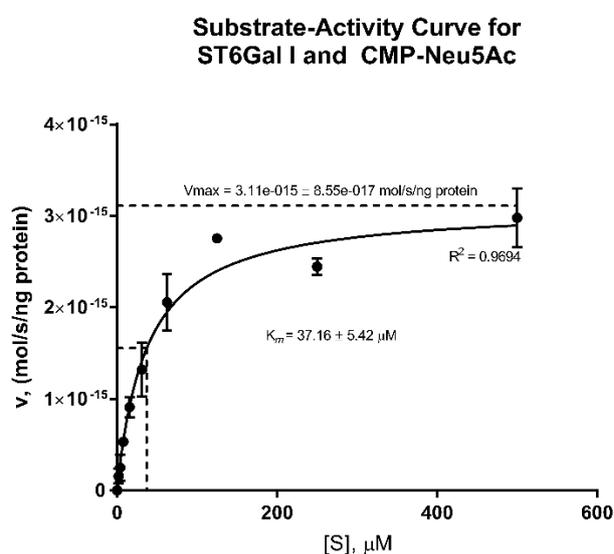


Interpolation		A
Table of results		Luminescence (RLU)
Sigmoidal, 4PL, X is log(concentration)		
Best-fit values		
Top	810208	
Bottom	-84327	
LogIC50	2.630	
HillSlope	0.1191	
IC50	426.1	
Span	894534	
95% CI (asymptotic)		
Top	798418 to 821997	
Bottom	-553712 to 385059	
LogIC50	-1.206 to 6.465	
HillSlope	0.08058 to 0.1576	
IC50	0.06229 to 2914808	
Span	421453 to 1367616	
Goodness of Fit		
Degrees of Freedom	16	
R squared	0.9942	
Adjusted R squared	0.9931	
Sum of Squares	4195321444	

Figure S2. Enzyme-activity curve for ST3Gal I in the CMP-Glo™ assay. The assay gave a $R^2 = 0.9942$ for the sigmoidal response curve.

Determination of CMP-Neu5Ac K_m against hST6Gal I

CMP-Neu5Ac was diluted to 1250, 625, 312.5, 156.3, 78.1, 39.1, 19.5, 9.8, 4.9, 2.4, 1.2, and 0 μM , while the enzyme was diluted to 60 ng/5 μL . In duplicate on a solid white 96-well plate, 10 μL of donor, 10 μL of 2.5 mM acceptor, and 5 μL of enzyme were added. The assay was then performed as per the general procedure detailed above. The K_m was calculated using non-linear regression analysis with GraphPad Prism 7.



Nonlin fit		v, (mol/s/ng protein)
		Y
1	Michaelis-Menten	
2	Best-fit values	
3	Vmax	3.11e-015
4	Km	37.16
5	Std. Error	
6	Vmax	8.547e-017
7	Km	5.422
8	95% CI (profile likelihood)	
9	Vmax	2.847e-015 to 3.396e-015
10	Km	27.44 to 50.23
11	Goodness of Fit	
12	Degrees of Freedom	17
13	R square	0.9694
14	Absolute Sum of Squares	6.589e-031
15	Sy.x	1.969e-016
16	Constraints	
17	Km	Km > 0
18		

Figure S3. Non-linear regression analysis in Michaelis-Menten equation of CMP-Neu5Ac with recombinant hST6Gal I. This is the same data as from our previous work.²

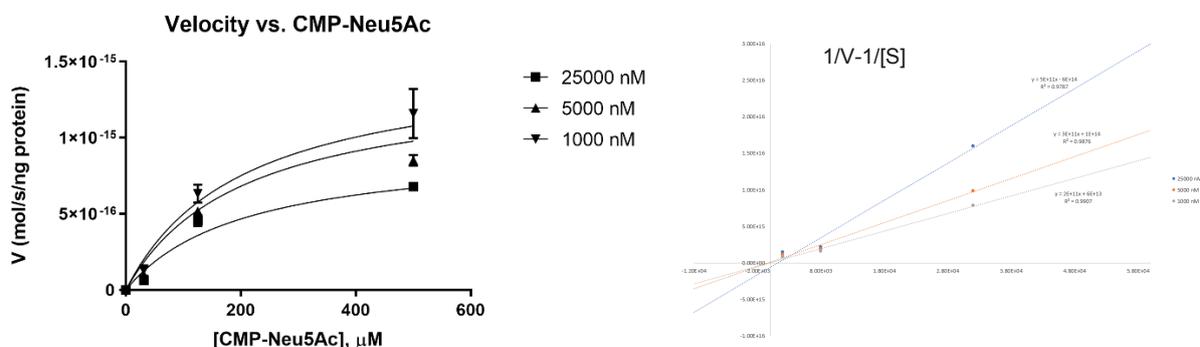
Single point inhibition at 100 and 10 μM

Enzyme was diluted to 20 ng/5 μL and 60 ng/5 μL for ST3Gal I and ST6Gal I respectively. To a solid white 96 well plate, 10 μL of a mixture of 2.5 mM acceptor and 250 μM donor in assay buffer, 10 μL

of a 250 or 25 μM solution of inhibitor in assay buffer (for inhibition at 100 or 10 μM respectively), and 5 μL of enzyme solution were added to each well in duplicate. A positive control with no inhibitor was also prepared, as well as a negative control where no enzyme was present. The assay was then performed as per the general procedure detailed above. Percentage inhibition was calculated relative to the positive control, with the negative control used as a blank.

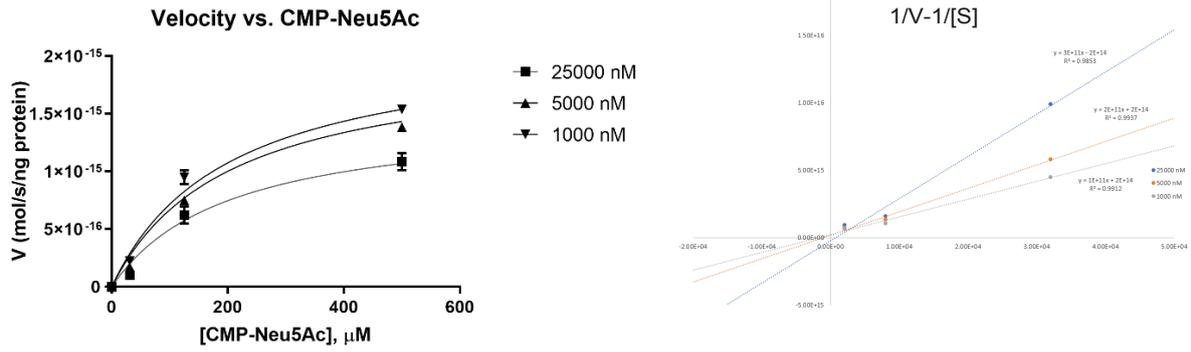
Determination of inhibitor K_i against hST6Gal I

CMP-Neu5Ac was diluted to 2500, 625, 156.3, 39.1, and 9.8, while the enzyme was diluted to 60 ng/5 μL . Inhibitors were diluted to three concentrations, usually between 0.5-62.5 μM . To a solid white 96 well plate, 5 μL of CMP-Neu5Ac solution, 5 μL of 5 mM acceptor in assay buffer, 10 μL of inhibitor solution, and 5 μL of enzyme solution were added to each well in duplicate. The assay was then performed as per the general procedure detailed above. The K_i 's were calculated using non-linear regression analysis with GraphPad Prism 8.



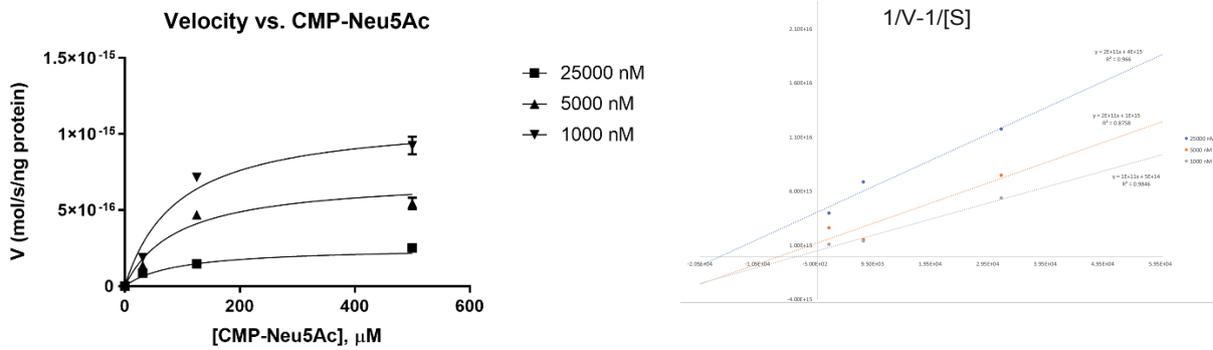
Nonlin fit Table of results		A 25000 nM	B 5000 nM	C 1000 nM	D Global (shared)
1	Noncompetitive inhibition				
2	Best-fit values				
3	Vmax	1.556e-015	1.556e-015	1.556e-015	1.556e-015
4	I	= 25000	= 5000	= 1000	
5	Ki	38374	38374	38374	38374
6	KM	204.0	204.0	204.0	204.0
7	Std. Error				
8	Vmax	5.820e-017	5.820e-017	5.820e-017	5.820e-017
9	Ki	10940	10940	10940	10940
10	KM	51.95	51.95	51.95	51.95
11	95% CI (asymptotic)				
12	Vmax	1.434e-015 to 1.679e-015	1.434e-015 to 1.679e-015	1.434e-015 to 1.679e-015	1.434e-015 to 1.679e-015
13	Ki	15390 to 61358	15390 to 61358	15390 to 61358	15390 to 61358
14	KM	94.87 to 313.2	94.87 to 313.2	94.87 to 313.2	94.87 to 313.2
15	Goodness of Fit				
16	Degrees of Freedom				18
17	R squared	0.9419	0.9382	0.9378	0.9418

Figure S4. Non-linear regression analysis in of velocity vs [CMP-NeuAc] with recombinant hST6Gal I at three 13a-s concentrations.



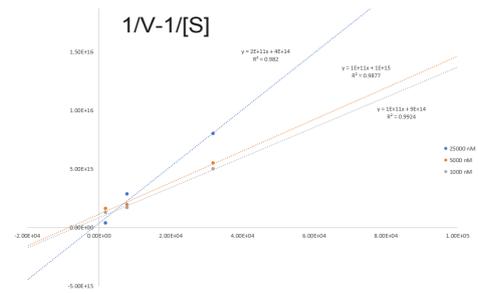
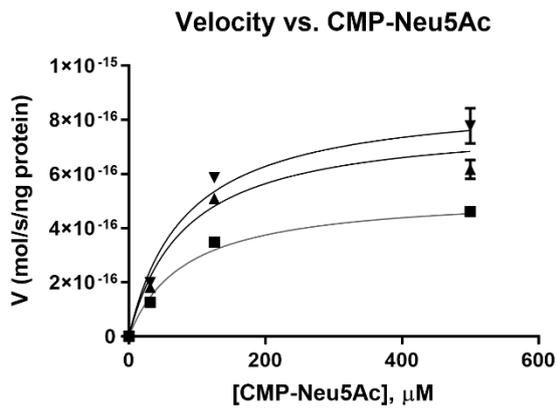
Nonlin fit Table of results		A 25000 nM	B 5000 nM	C 1000 nM	D Global (shared)
1	Noncompetitive inhibition				
2	Best-fit values				
3	Vmax	2.200e-015	2.200e-015	2.200e-015	2.200e-015
4	I	= 25000	= 5000	= 1000	
5	Ki	53686	53686	53686	53686
6	KM	201.9	201.9	201.9	201.9
7	Std. Error				
8	Vmax	4.707e-017	4.707e-017	4.707e-017	4.707e-017
9	Ki	10220	10220	10220	10220
10	KM	29.35	29.35	29.35	29.35
11	95% CI (asymptotic)				
12	Vmax	2.101e-015 to 2.299e-015	2.101e-015 to 2.299e-015	2.101e-015 to 2.299e-015	2.101e-015 to 2.299e-015
13	Ki	32214 to 75159	32214 to 75159	32214 to 75159	32214 to 75159
14	KM	140.3 to 263.6	140.3 to 263.6	140.3 to 263.6	140.3 to 263.6
15	Goodness of Fit				
16	Degrees of Freedom				18
17	R squared	0.9635	0.9868	0.9805	0.9797

Figure S5. Non-linear regression analysis of velocity vs [CMP-NeuAc] with recombinant hST6Gal I at three **13a-7** concentrations.



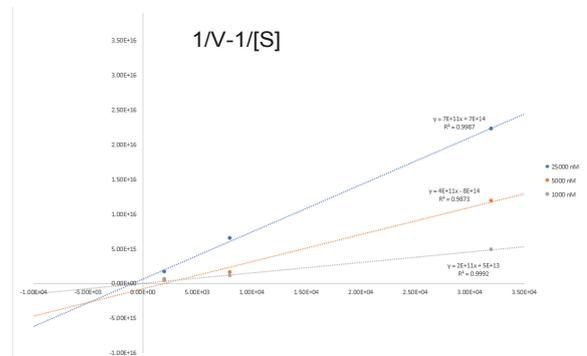
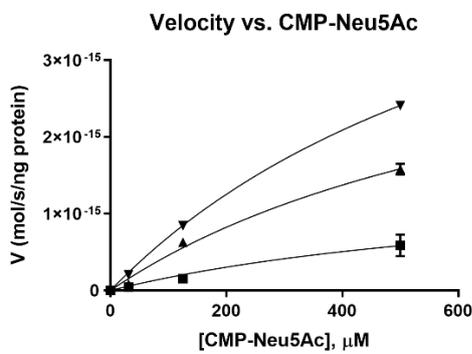
Nonlin fit Table of results		A 25000 nM	B 5000 nM	C 1000 nM	D Global (shared)
1	Noncompetitive inhibition				
2	Best-fit values				
3	Vmax	1.291e-015	1.291e-015	1.291e-015	1.291e-015
4	I	= 25000	= 5000	= 1000	
5	Ki	6163	6163	6163	6163
6	KM	92.70	92.70	92.70	92.70
7	Std. Error				
8	Vmax	3.813e-017	3.813e-017	3.813e-017	3.813e-017
9	Ki	1044	1044	1044	1044
10	KM	21.72	21.72	21.72	21.72
11	95% CI (asymptotic)				
12	Vmax	1.211e-015 to 1.372e-015	1.211e-015 to 1.372e-015	1.211e-015 to 1.372e-015	1.211e-015 to 1.372e-015
13	Ki	3968 to 8357	3968 to 8357	3968 to 8357	3968 to 8357
14	KM	47.06 to 138.3	47.06 to 138.3	47.06 to 138.3	47.06 to 138.3
15	Goodness of Fit				
16	Degrees of Freedom				18
17	R squared	0.9180	0.9314	0.9594	0.9649

Figure S6. Non-linear regression analysis of velocity vs [CMP-NeuAc] with recombinant hST6Gal I at three **13c-s** concentrations.



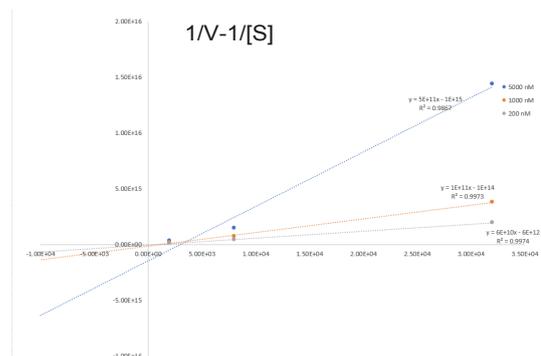
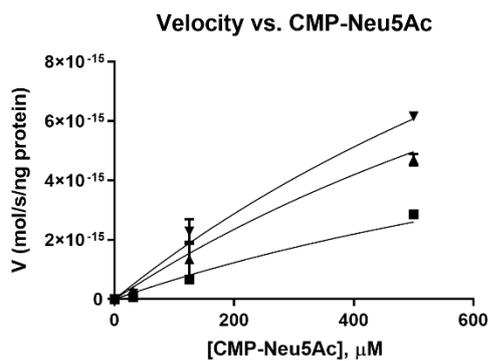
Nonlin fit Table of results		A 25000 nM	B 5000 nM	C 1000 nM	D Global (shared)
1	Noncompetitive inhibition				
2	Best-fit values				
3	Vmax	9.114e-016	9.114e-016	9.114e-016	9.114e-016
4	I =	= 25000	= 5000	= 1000	
5	Ki	34414	34414	34414	34414
6	KM	82.03	82.03	82.03	82.03
7	Std. Error				
8	Vmax	2.086e-017	2.086e-017	2.086e-017	2.086e-017
9	Ki	5762	5762	5762	5762
10	KM	13.09	13.09	13.09	13.09
11	95% CI (asymptotic)				
12	Vmax	8.675e-016 to 9.552e-016	8.675e-016 to 9.552e-016	8.675e-016 to 9.552e-016	8.675e-016 to 9.552e-016
13	Ki	22309 to 46519	22309 to 46519	22309 to 46519	22309 to 46519
14	KM	54.53 to 109.5	54.53 to 109.5	54.53 to 109.5	54.53 to 109.5
15	Goodness of Fit				
16	Degrees of Freedom				18
17	R squared	0.9856	0.9569	0.9681	0.9705

Figure S7. Non-linear regression analysis of velocity vs [CMP-NeuAc] with recombinant hST6Gal I at three 13c-I concentrations.



Nonlin fit Table of results		A 25000 nM	B 5000 nM	C 1000 nM	D Global (shared)
1	Noncompetitive inhibition				
2	Best-fit values				
3	Vmax	7.204e-015	7.204e-015	7.204e-015	7.204e-015
4	I =	= 25000	= 5000	= 1000	
5	Ki	6677	6677	6677	6677
6	KM	799.5	799.5	799.5	799.5
7	Std. Error				
8	Vmax	1.100e-016	1.100e-016	1.100e-016	1.100e-016
9	Ki	585.3	585.3	585.3	585.3
10	KM	149.3	149.3	149.3	149.3
11	95% CI (asymptotic)				
12	Vmax	6.973e-015 to 7.435e-015	6.973e-015 to 7.435e-015	6.973e-015 to 7.435e-015	6.973e-015 to 7.435e-015
13	Ki	5448 to 7907	5448 to 7907	5448 to 7907	5448 to 7907
14	KM	485.8 to 1113	485.8 to 1113	485.8 to 1113	485.8 to 1113
15	Goodness of Fit				
16	Degrees of Freedom				18
17	R squared	0.8898	0.9893	0.9992	0.9929

Figure S8. Non-linear regression analysis of velocity vs [CMP-NeuAc] with recombinant hST6Gal I at three 13f-s concentrations.

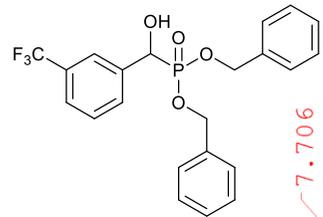


	Nonlin fit Table of results			
	A 5000 nM	B 1000 nM	C 200 nM	D Global (shared)
1	Noncompetitive inhibition			
2	Best-fit values			
3	Vmax	2.487e-014	2.487e-014	2.487e-014
4	I	= 5000	= 1000	= 200.0
5	Ki	3385	3385	3385
6	KM	1432	1432	1432
7	Std. Error			
8	Vmax	7.149e-016	7.149e-016	7.149e-016
9	Ki	604.7	604.7	604.7
10	KM	769.4	769.4	769.4
11	95% CI (asymptotic)			
12	Vmax	2.337e-014 to 2.637e-014	2.337e-014 to 2.637e-014	2.337e-014 to 2.637e-014
13	Ki	2115 to 4655	2115 to 4655	2115 to 4655
14	KM	-184.2 to 3049	-184.2 to 3049	-184.2 to 3049
15	Goodness of Fit			
16	Degrees of Freedom			18
17	R squared	0.9732	0.9593	0.9744

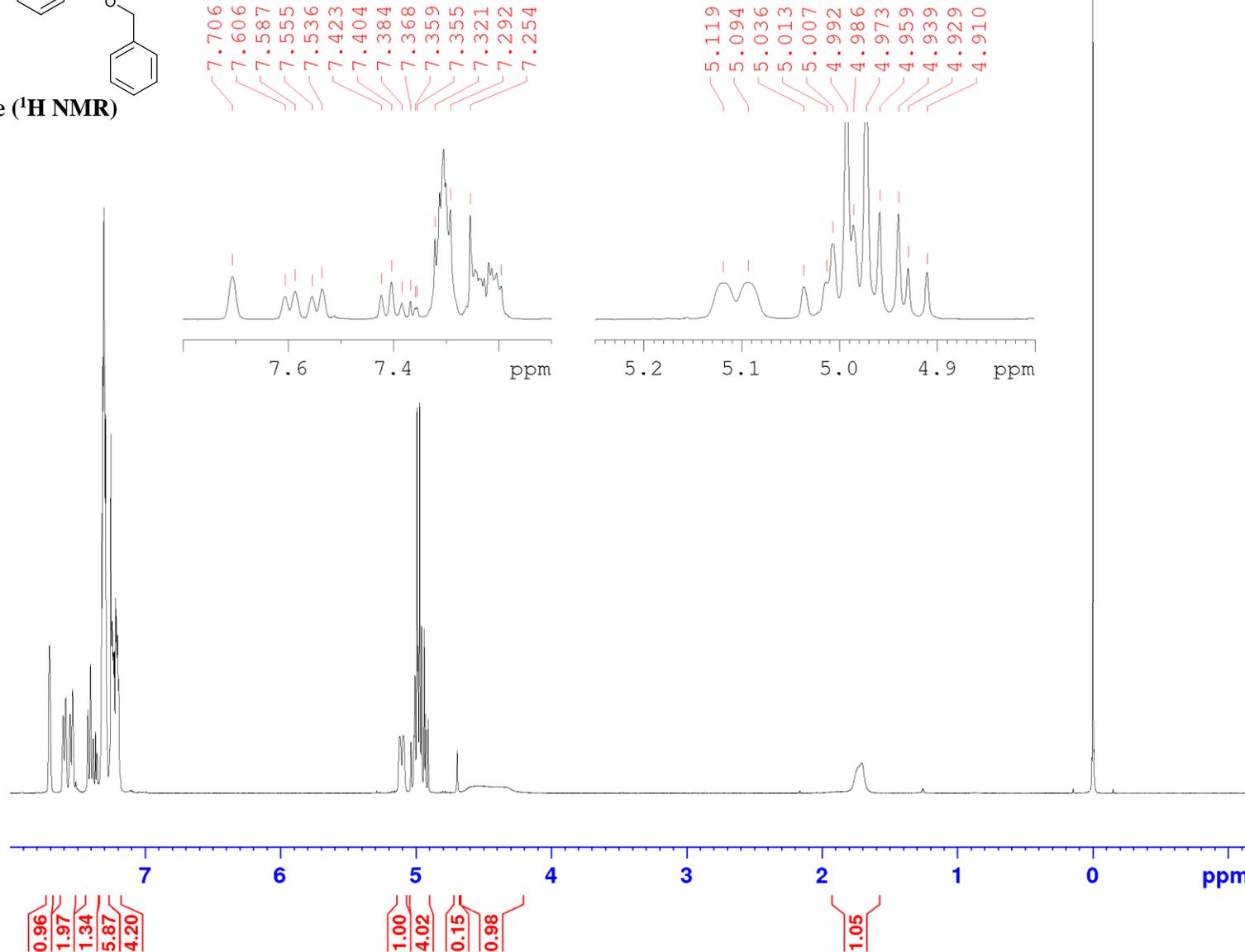
Figure S9. Non-linear regression analysis of velocity vs [CMP-NeuAc] with recombinant hST6Gal I at three **13f-I** concentrations.

References:

1. J. Sun, R. Liu, Q. Fu, J. Zang, Q. Tao, J. Wu and H. Zhu, *Helv. Chim. Acta*, 2014, **97**, 733-743.
2. A. P. Montgomery, C. Dobie, R. Szabo, L. Hallam, M. Ranson, H. Yu and D. Skropeta, *Bioorg. Med. Chem.*, 2020, **28**, 115561.



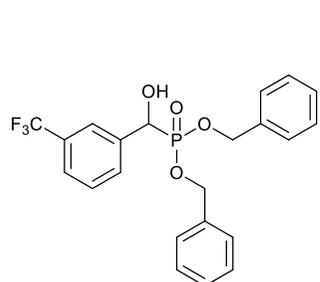
10e (¹H NMR)



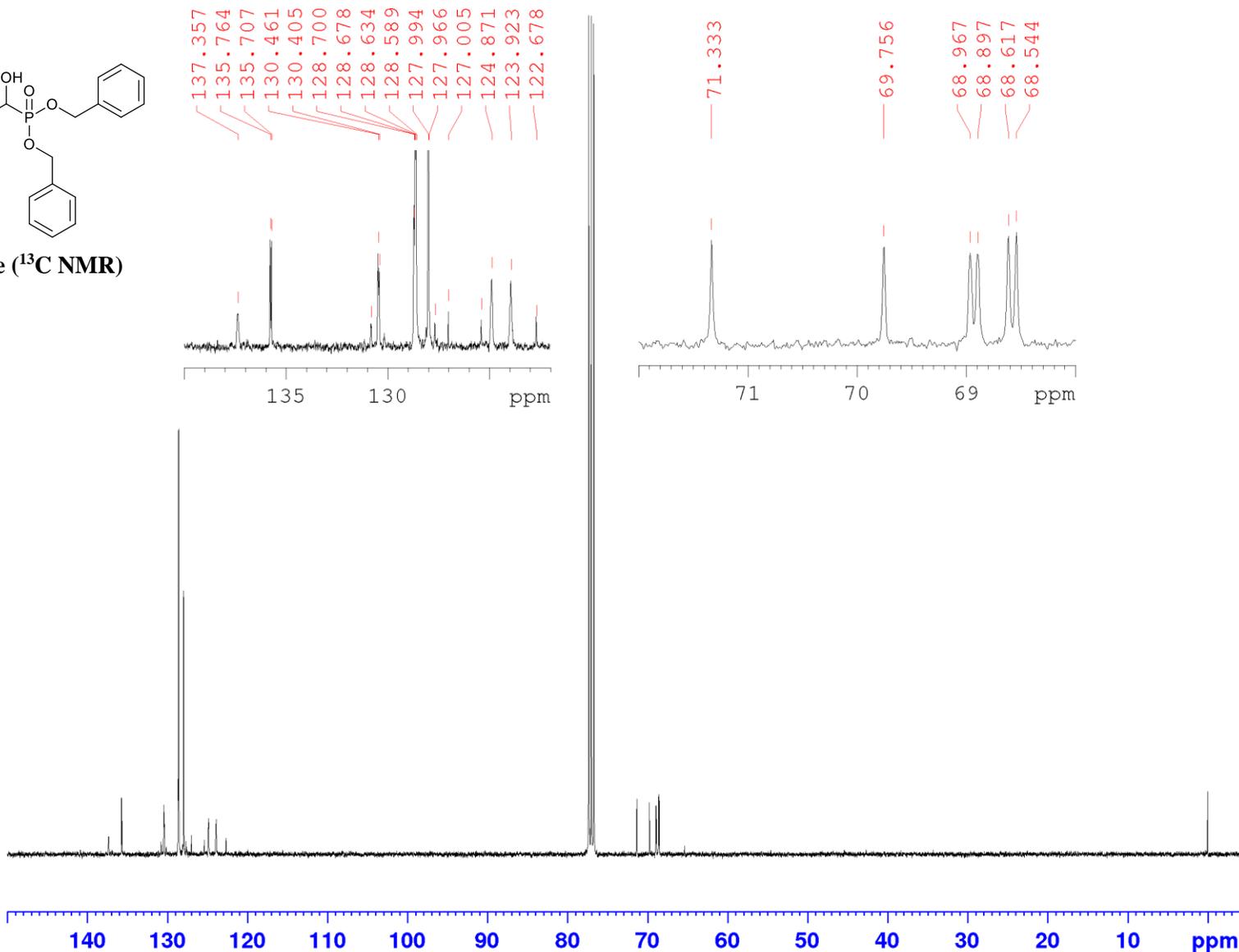
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NAME CD36
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171019
Time 16.49 h
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PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 144.7
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters
SI 65536
SF 400.1600119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



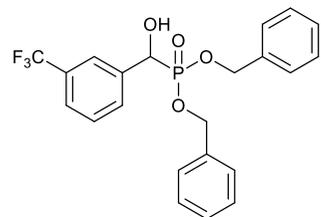
10e (¹³C NMR)



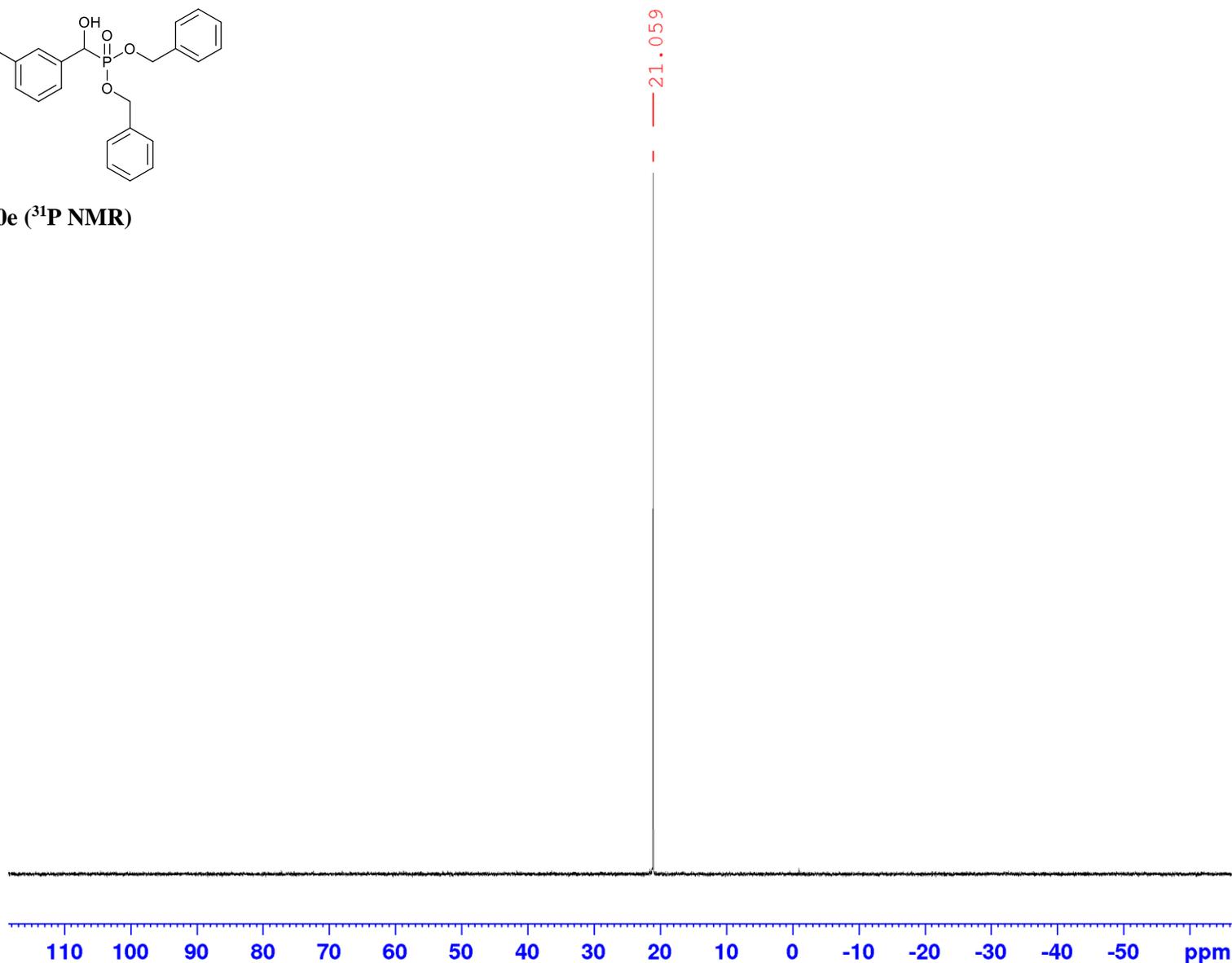
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NAME CD36
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171020
Time 0.07 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 196.38
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6303741 MHz
NUC1 13C
P1 10.00 usec
PLW1 55.50099945 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



10e (^{31}P NMR)

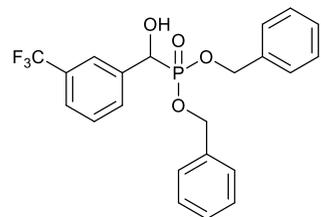


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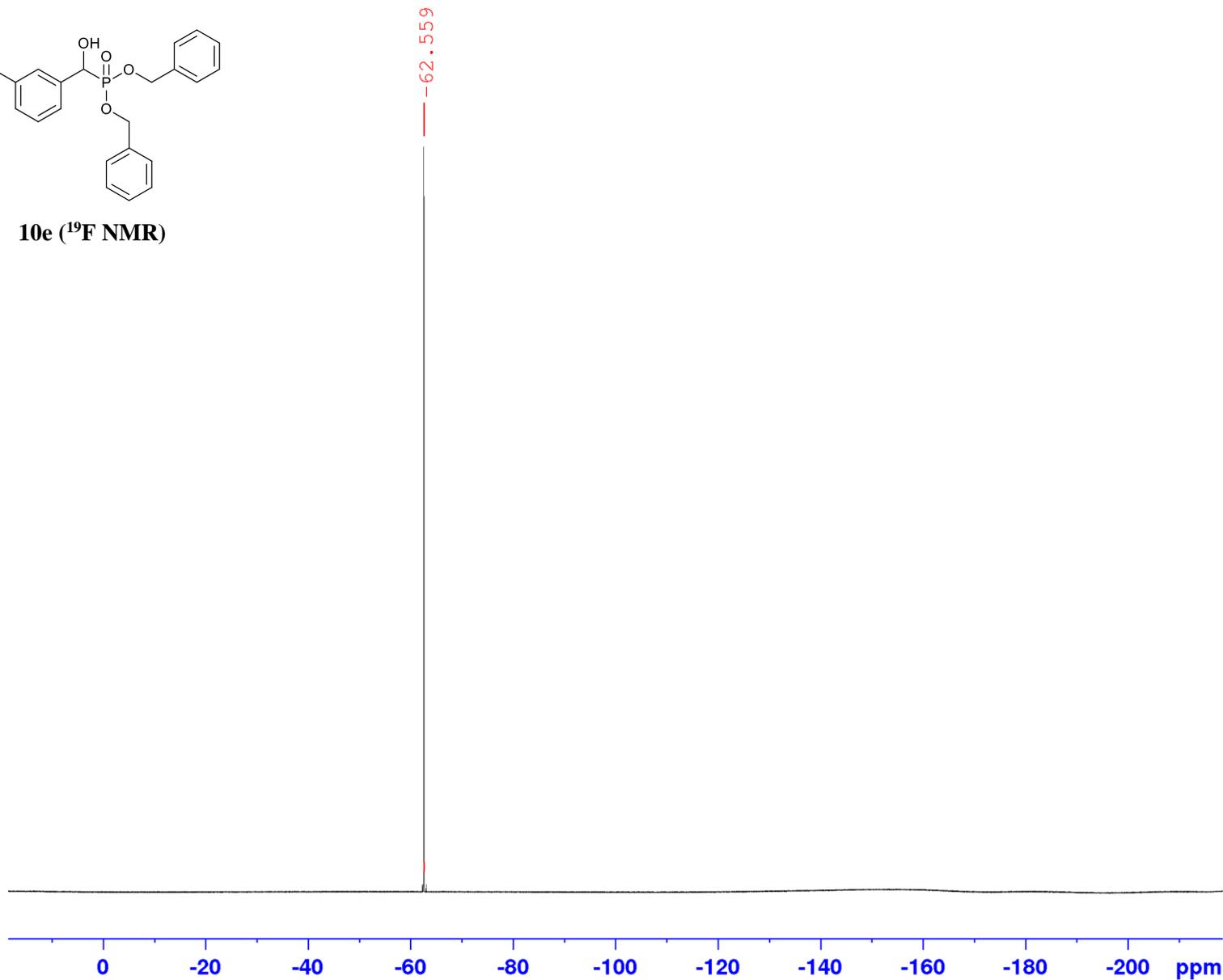
Current Data Parameters
NAME             CD36
EXPNO            9
PROCNO          1

F2 - Acquisition Parameters
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Time             1.25 h
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PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS               16
DS               4
SWH              64102.563 Hz
FIDRES           1.956255 Hz
AQ               0.5111808 sec
RG               196.38
DW               7.800 usec
DE               6.50 usec
TE               297.6 K
D1               2.0000000 sec
D11              0.0300000 sec
TD0              1
SFO1             161.9796378 MHz
NUC1             31P
P1               15.00 usec
PLW1             11.77099991 W
SFO2             400.1616006 MHz
NUC2             1H
CPDPRG[2]        waltz16
PCPD2            90.00 usec
PLW2             11.52400017 W
PLW12            0.27886000 W
PLW13            0.14026000 W

F2 - Processing parameters
SI               32768
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WDW              EM
SSB              0
LB               1.00 Hz
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PC               1.40
  
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10e (¹⁹F NMR)

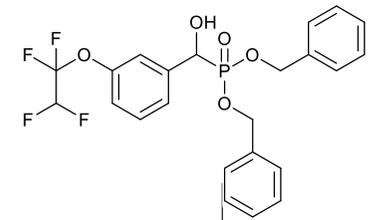


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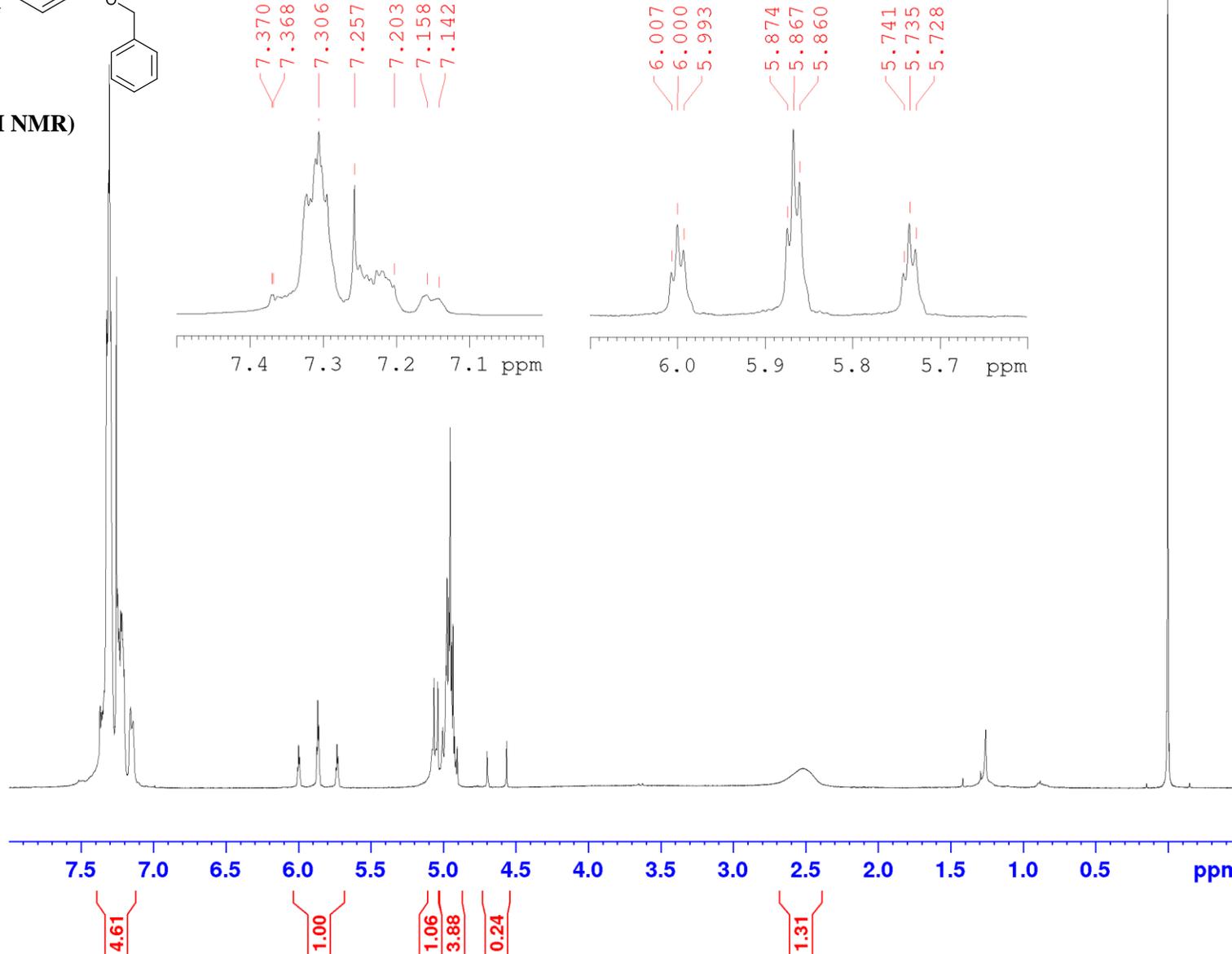
Current Data Parameters
NAME           CD36
EXPNO          8
PROCNO         1

F2 - Acquisition Parameters
Date_          20171020
Time           1.23 h
INSTRUM        spect
PROBHD         Z108618_0921 (
PULPROG        zgfhigqn.2
TD             131072
SOLVENT        CDCl3
NS             16
DS             4
SWH            89285.711 Hz
FIDRES         1.362392 Hz
AQ             0.7340032 sec
RG             196.38
DW             5.600 usec
DE             6.50 usec
TE             297.5 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0            1
SFO1           376.4889418 MHz
NUC1           19F
P1             15.00 usec
PLW1           17.75399971 W
SFO2           400.1616006 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         90.00 usec
PLW2           11.52400017 W
PLW12          0.27886000 W

F2 - Processing parameters
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SF             376.5265944 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB            0
PC             1.00
  
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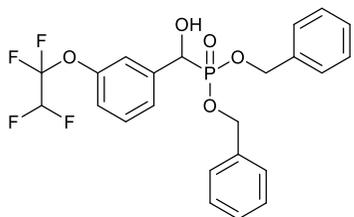
10f (¹H NMR)



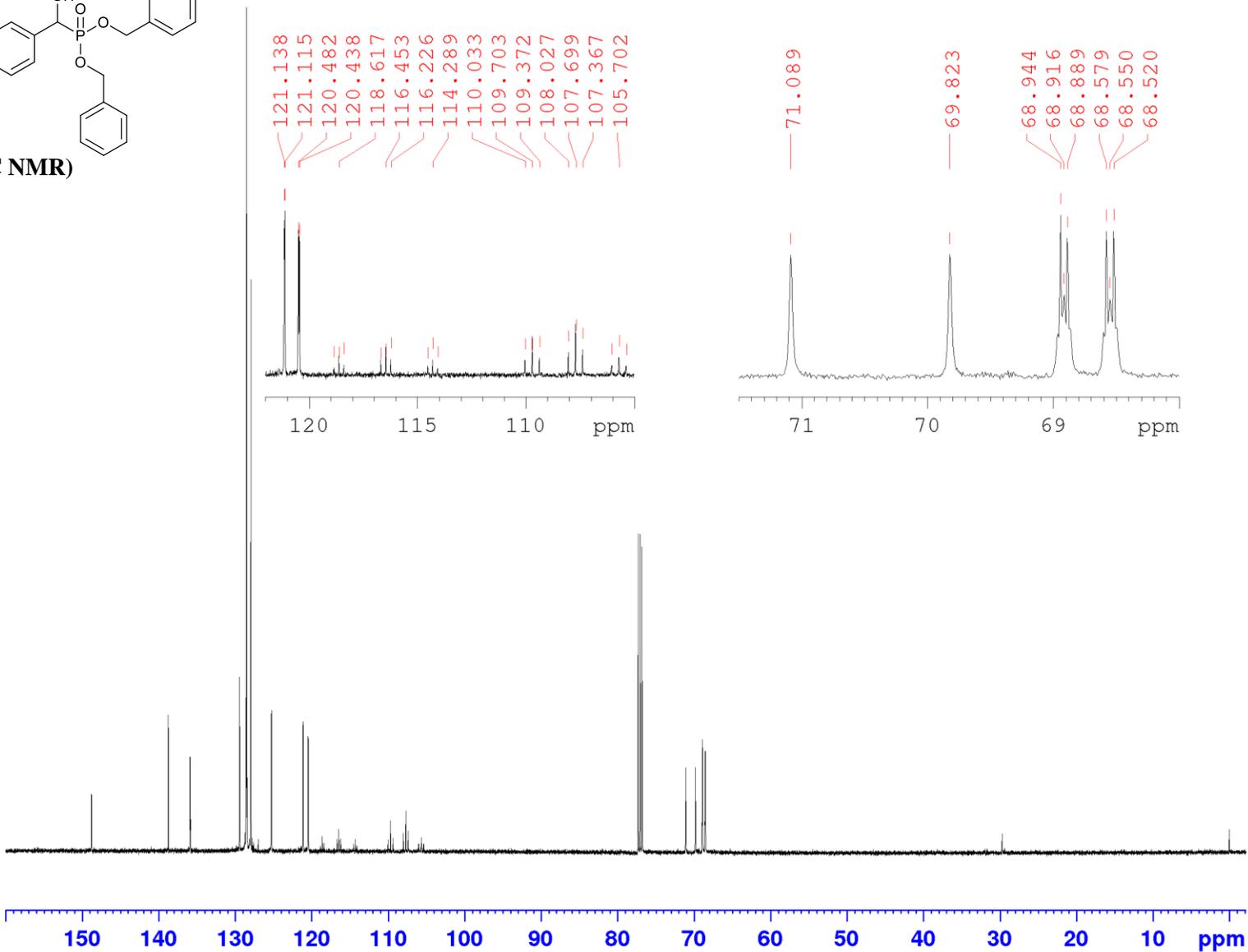
Current Data Parameters
NAME CD9
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190205
Time 10.54 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 158.68
DW 62.400 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters
SI 65536
SF 400.1600108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

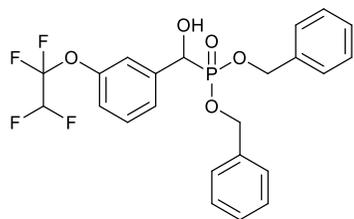


10f (¹³C NMR)

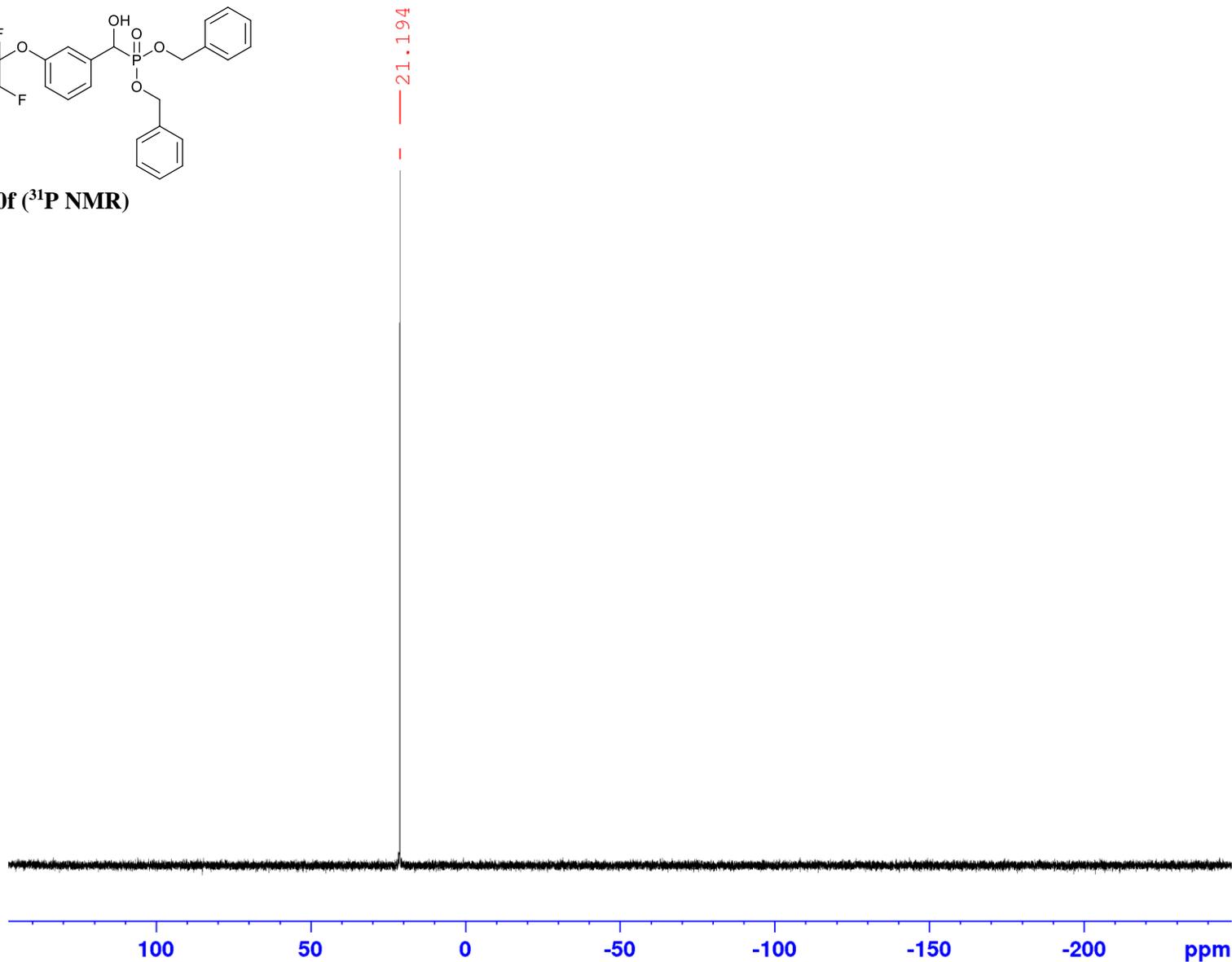


Current Data Parameters
 NAME CD2170330_CD9_Carbon01.fid
 EXPNO 1
 PROCNO 1

F2 - Processing parameters
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 SF 125.6600690 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



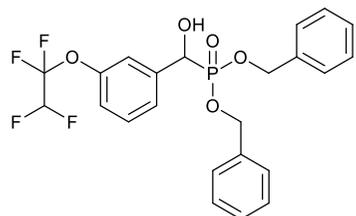
10f (³¹P NMR)



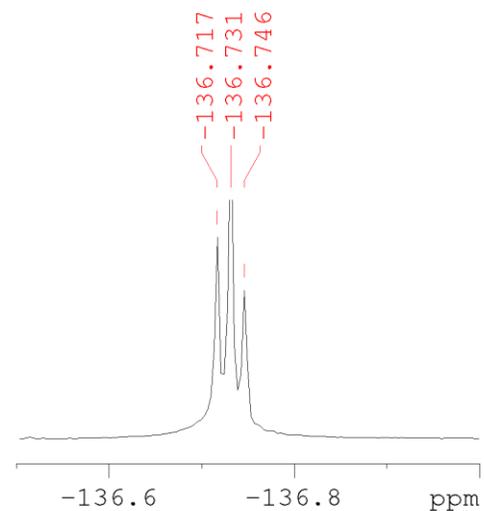
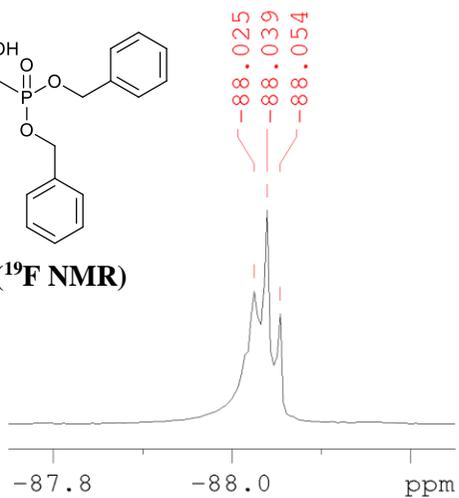
Current Data Parameters
 NAME CD9
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190205
 Time 10.57 h
 INSTRUM spect
 PROBHD Z108618_0921 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 64102.563 Hz
 FIDRES 1.956255 Hz
 AQ 0.5111808 sec
 RG 196.38
 DW 7.800 usec
 DE 50.00 usec
 TE 299.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 161.9796378 MHz
 NUC1 31P
 P1 15.00 usec
 PLW1 11.77099991 W
 SFO2 400.1616006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 11.52400017 W
 PLW12 0.27886000 W
 PLW13 0.14026000 W

F2 - Processing parameters
 SI 32768
 SF 161.9877372 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



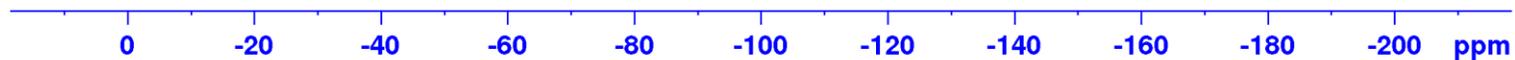
10f (¹⁹F NMR)

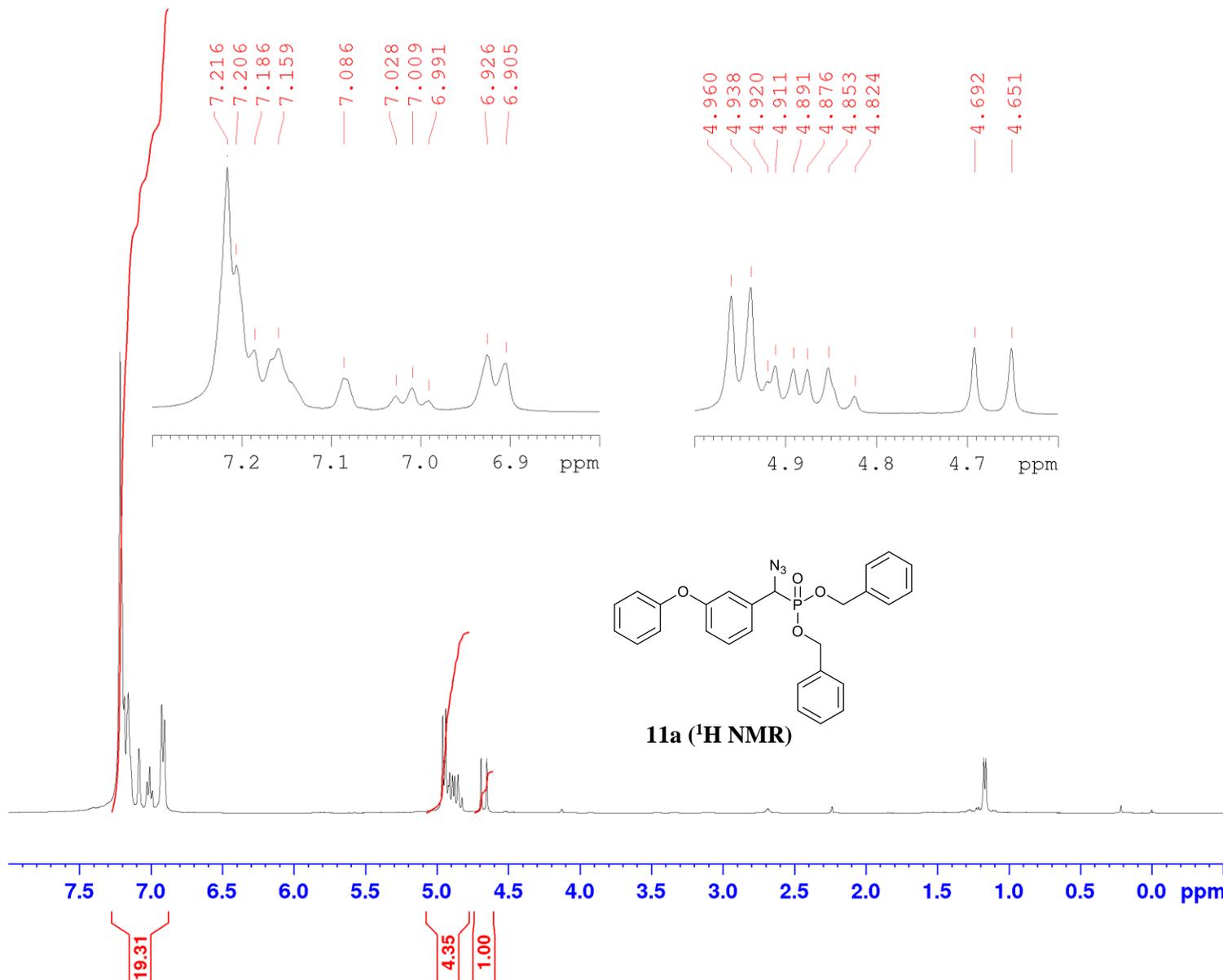


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Current Data Parameters
NAME          CD9
EXPNO        3
PROCNO       1

F2 - Acquisition Parameters
Date_        20190205
Time         10.59 h
INSTRUM      spect
PROBHD       Z108618_0921 (
PULPROG      zgfhigqn.2
TD           131072
SOLVENT      CDCl3
NS           16
DS           4
SWH          89285.711 Hz
FIDRES       1.362392 Hz
AQ           0.7340032 sec
RG           196.38
DW           5.600 usec
DE           120.00 usec
TE           299.8 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0          1
SFO1         376.4889418 MHz
NUC1         19F
P1           15.00 usec
PLW1         17.75399971 W
SFO2         400.1616006 MHz
NUC2         1H
CPDPRG[2]    waltz16
PCPD2        90.00 usec
PLW2         11.52400017 W
PLW12        0.27886000 W

F2 - Processing parameters
SI           65536
SF           376.5265944 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB          0
PC           1.00
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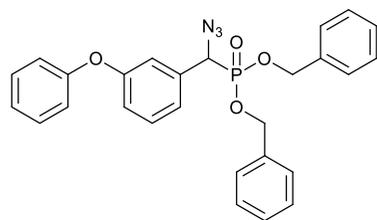




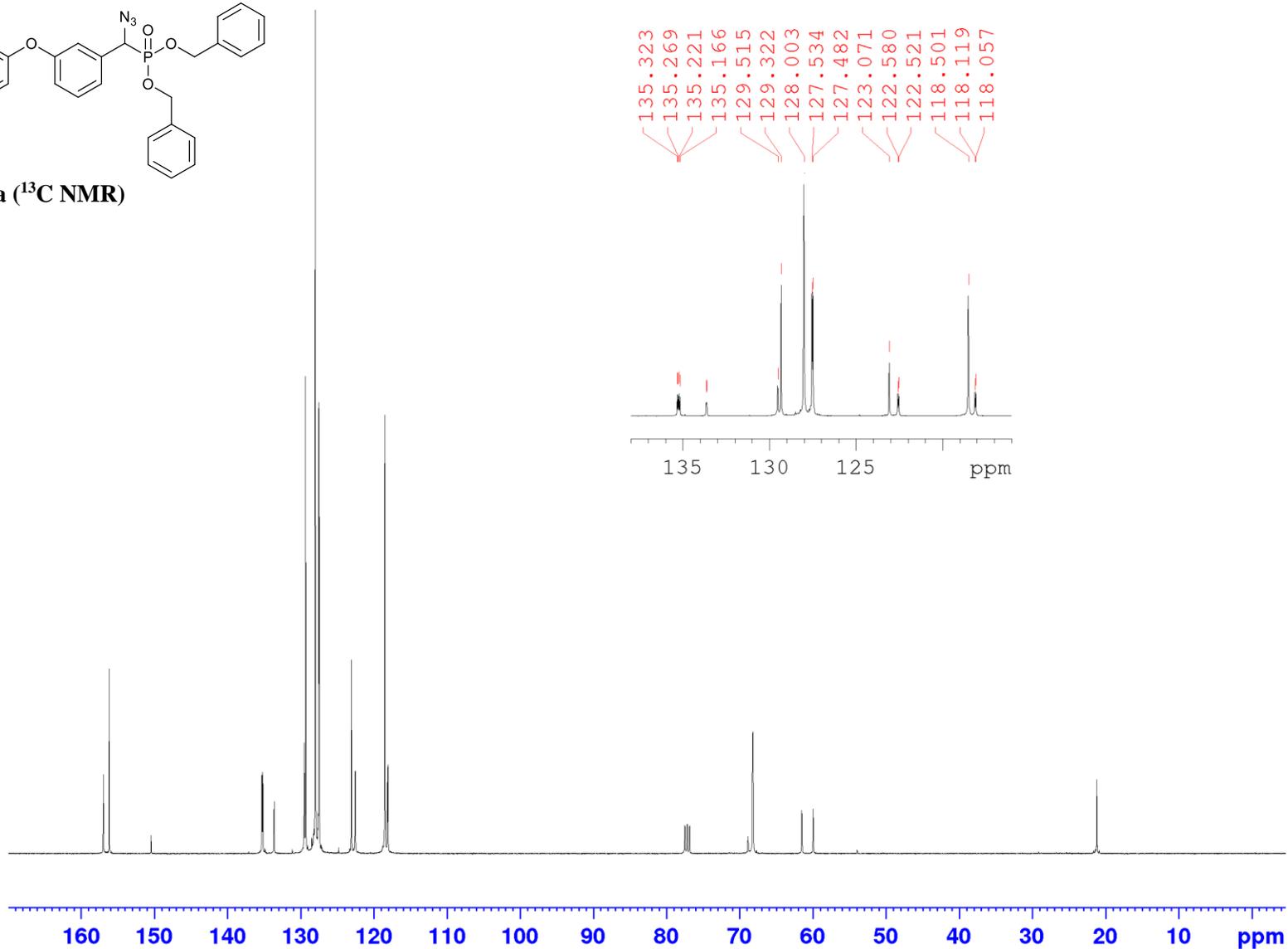
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NAME LH14 H
EXPNO 1
PROCNO 1

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Date_ 20180419
Time 15.10 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 6.39
DW 62.400 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters
SI 65536
SF 400.1600261 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



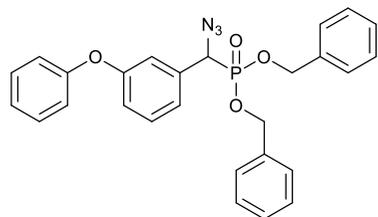
11a (¹³C NMR)



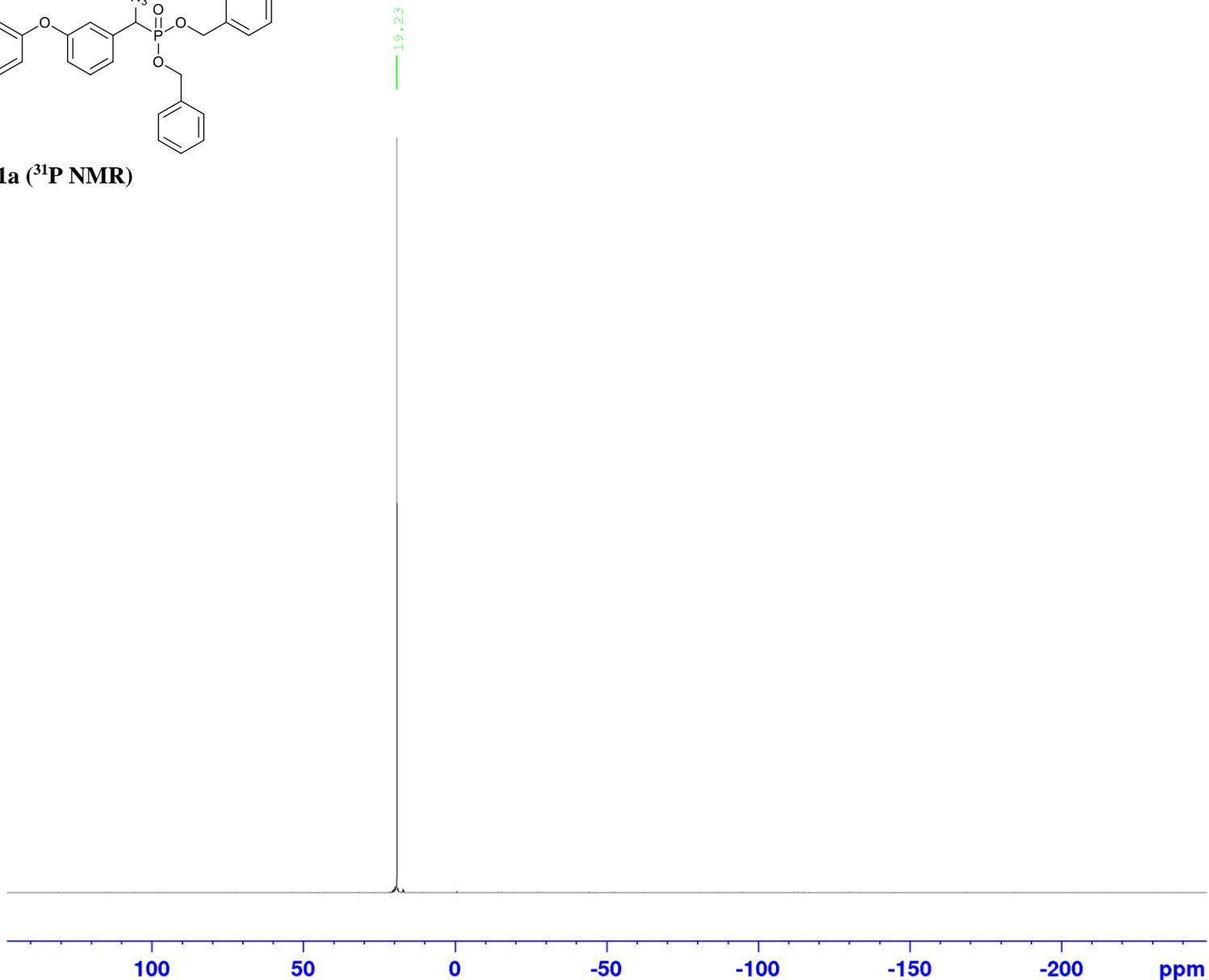
Current Data Parameters
NAME LH14 (C and P)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180423
Time 17.30 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 196.38
DW 20.800 usec
DE 6.50 usec
TE 301.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6303741 MHz
NUC1 13C
P1 10.00 usec
PLW1 55.50099945 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

F2 - Processing parameters
SI 32768
SF 100.6203756 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



11a (³¹P NMR)



Current Data Parameters
NAME LHL4 (C and P)
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180423
Time 17.33 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 use
DE 6.50 use
TE 301.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 use
PLW1 11.77099991 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 use
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

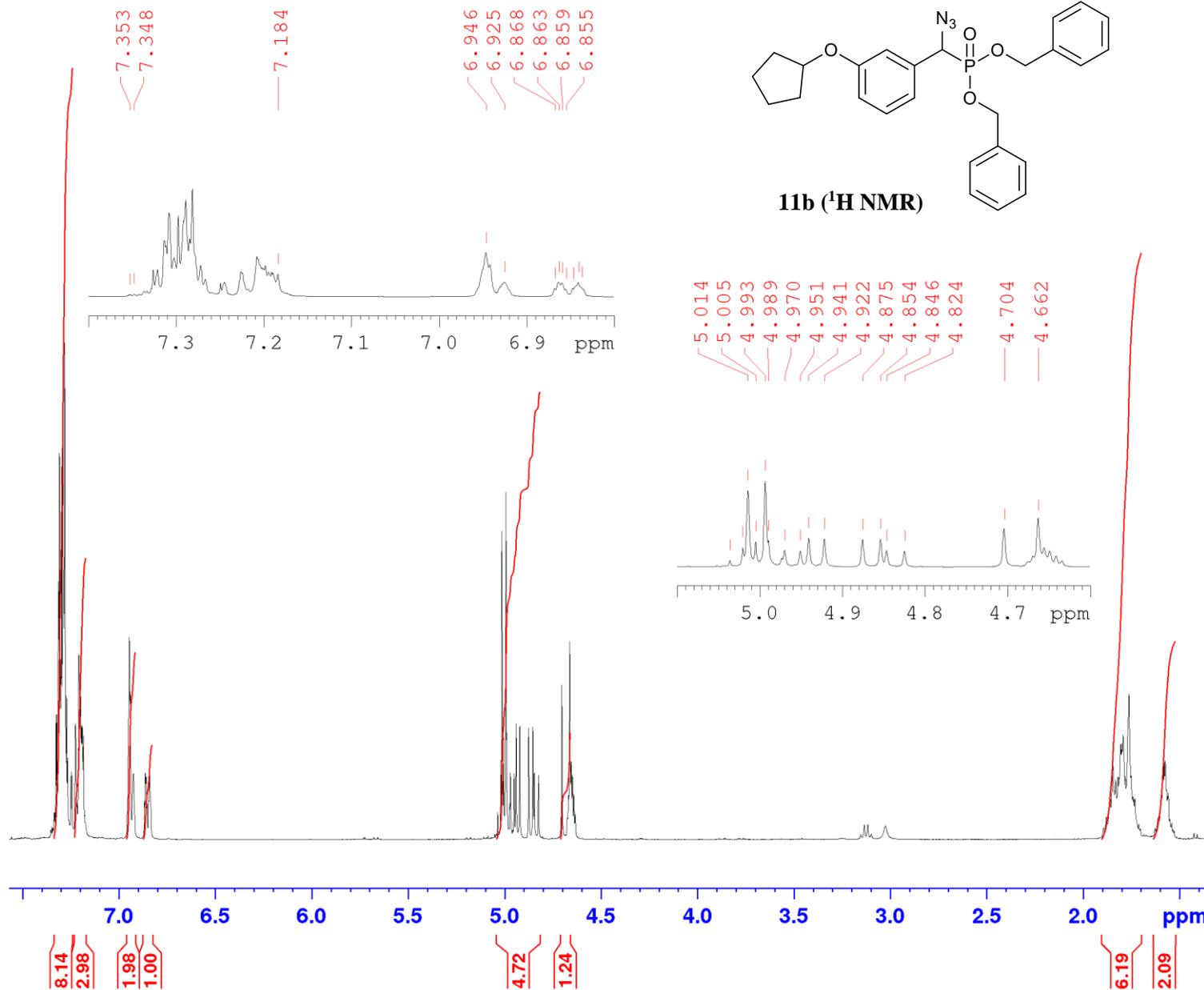
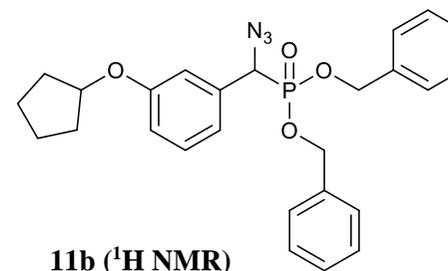
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PC 1.40



Current Data Parameters
NAME CD95 P3P36
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190801
Time 16.39 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 30.94
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters
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SF 400.1600137 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

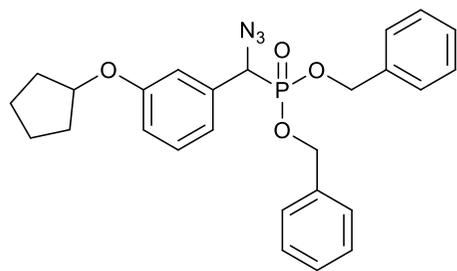
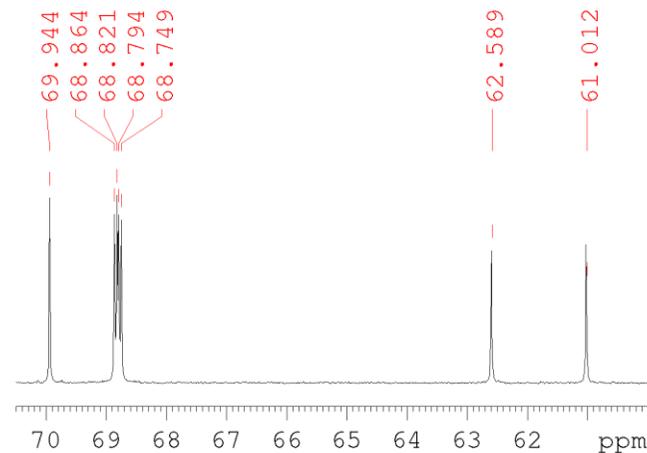
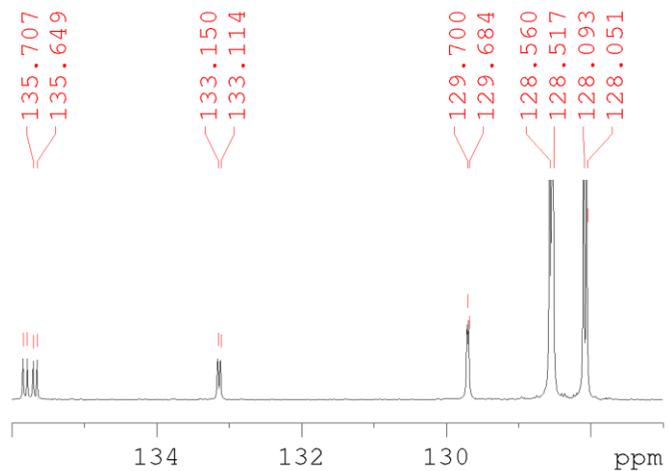




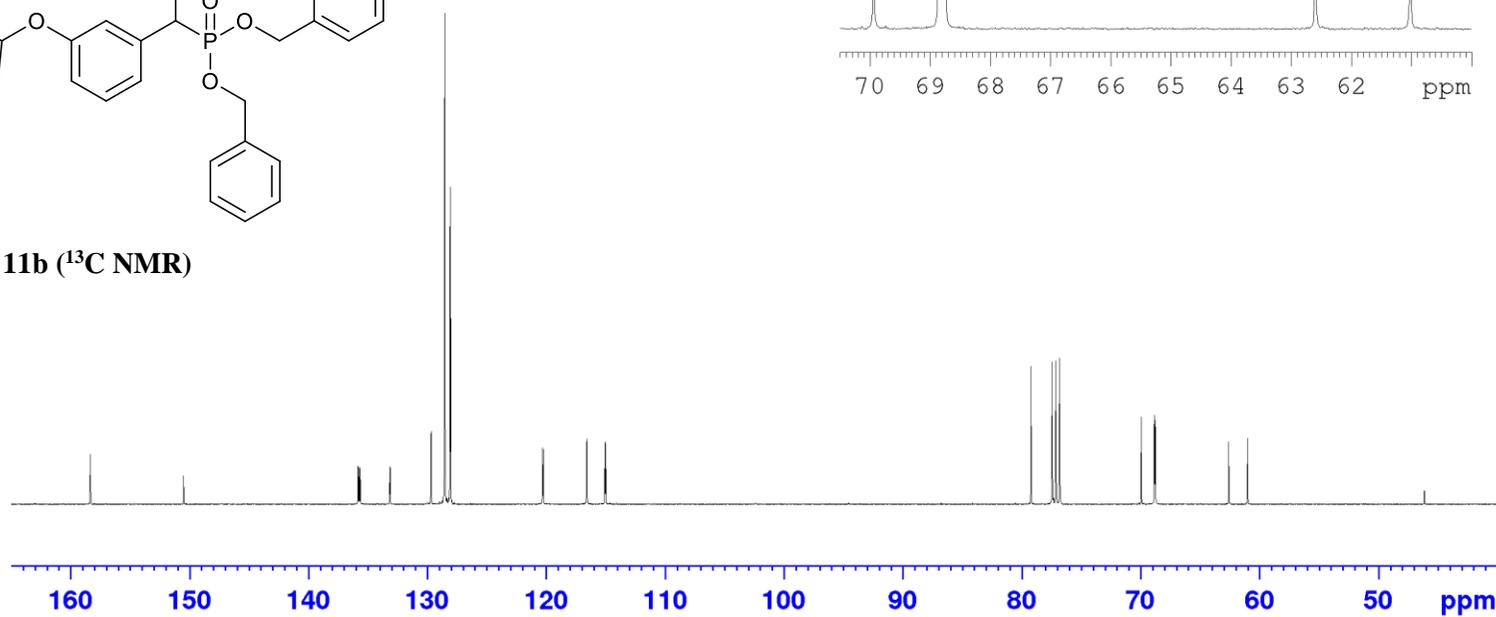
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NAME CD95 P3P36
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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PROBHD Z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2300
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 196.38
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6303741 MHz
NUC1 13C
P1 10.00 usec
PLW1 55.50099945 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



11b (¹³C NMR)

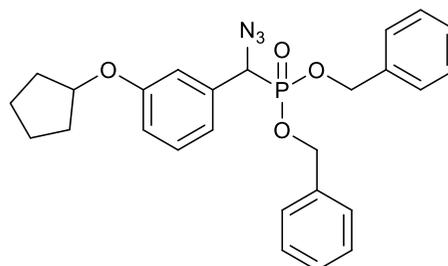




Current Data Parameters
NAME CD95 P3P36
EXPNO 6
PROCNO 1

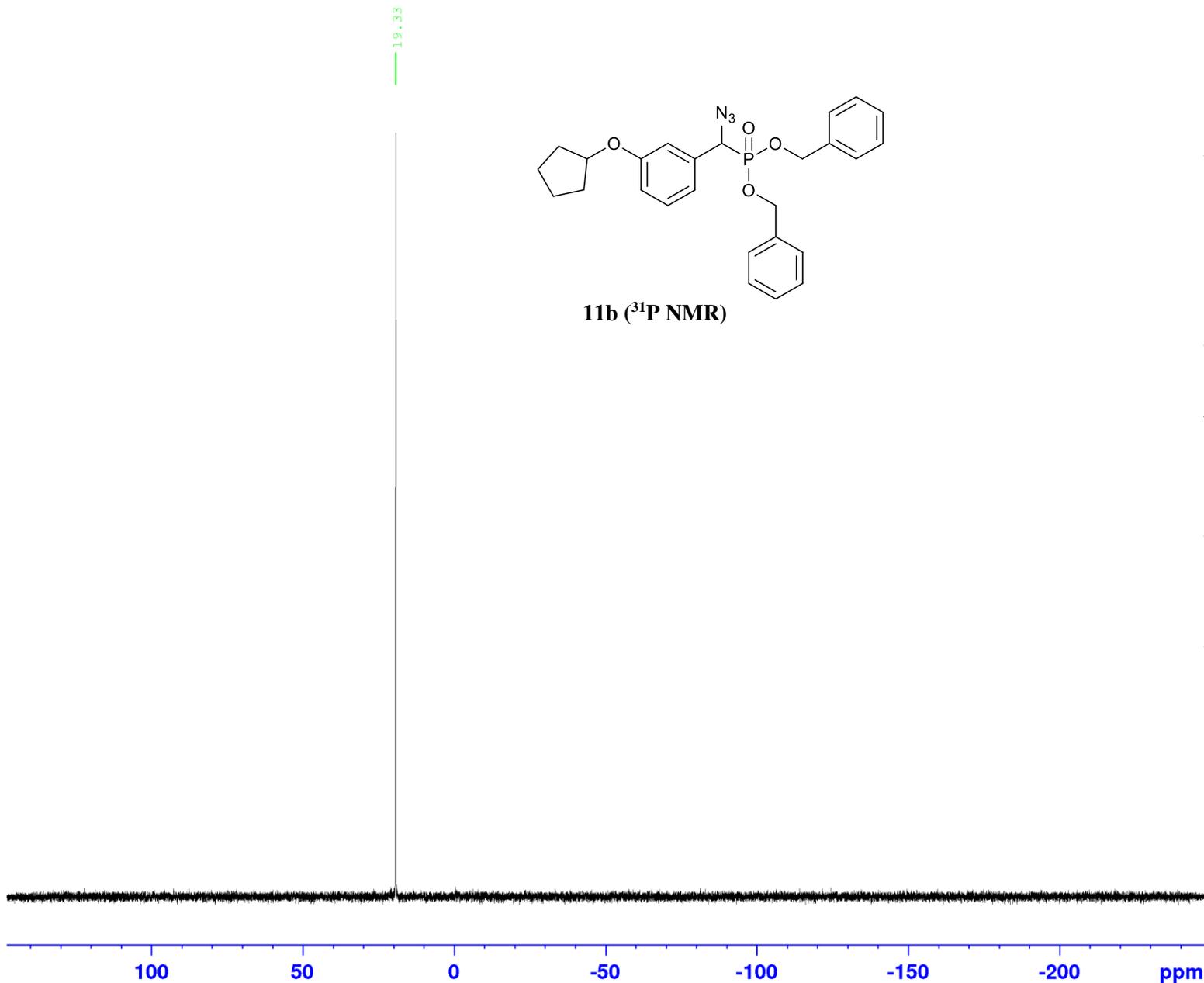
F2 - Acquisition Parameters
Date_ 20190802
Time 6.07 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 usec
DE 50.00 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 usec
PLW1 11.77099991 W

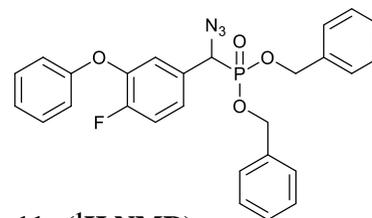
F2 - Processing parameters
SI 32768
SF 161.9877372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



11b (^{31}P NMR)

19.33





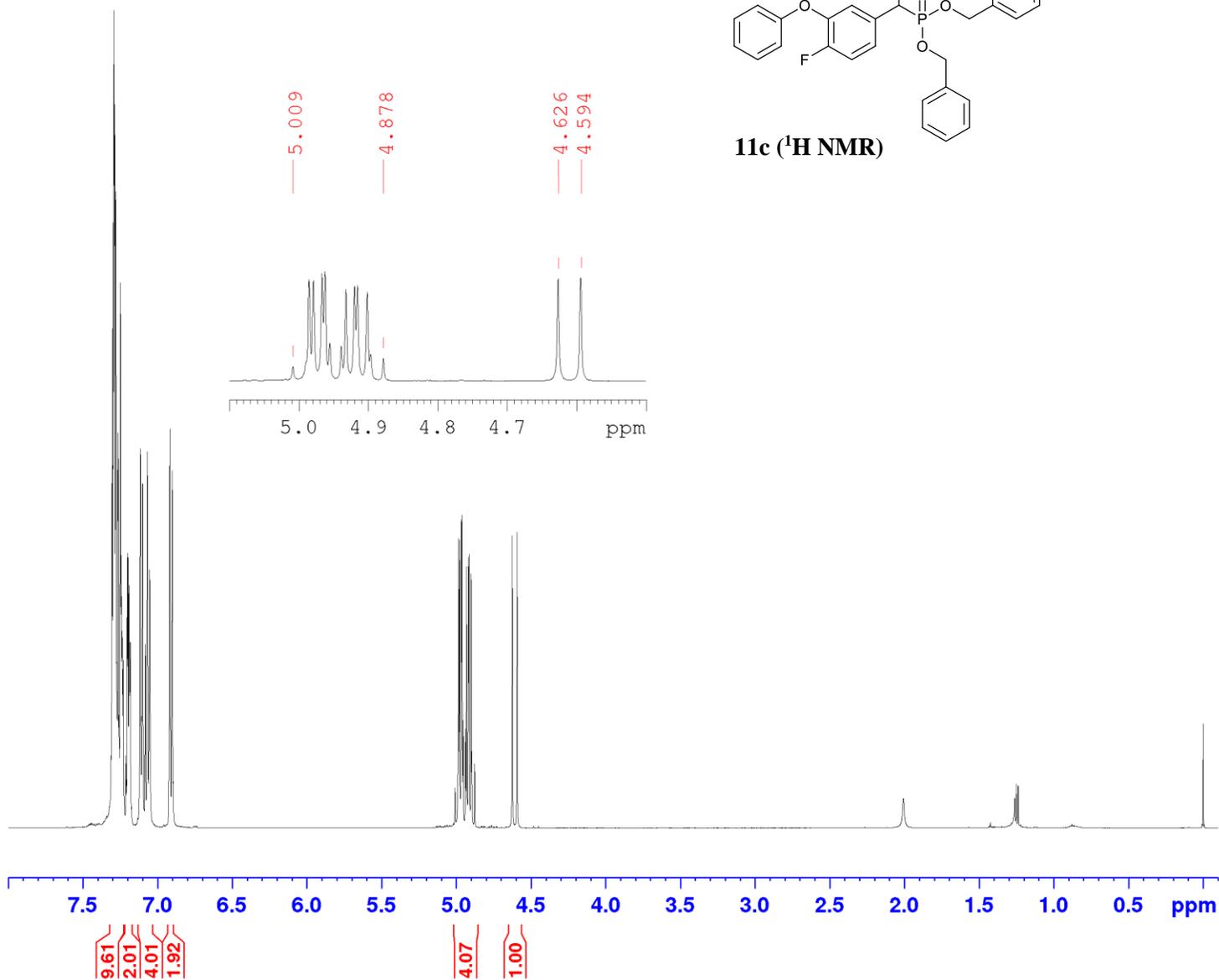
11c (¹H NMR)



Current Data Parameters
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 EXPNO 1
 PROCNO 1

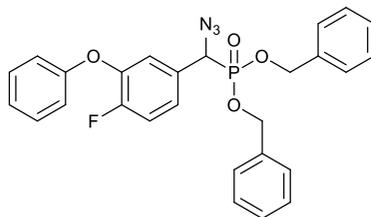
F2 - Acquisition Parameters
 Date_ 20180427
 Time 10.57 h
 INSTRUM CAB AV4 500 MHZ BASIC
 PROBHD Z150364_0005 (zq30
 PULPROG
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 10.9863
 DW 50.000 usec
 DE 16.23 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 499.7470859 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 15.53100014 W

F2 - Processing parameters
 SI 65536
 SF 499.7440342 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

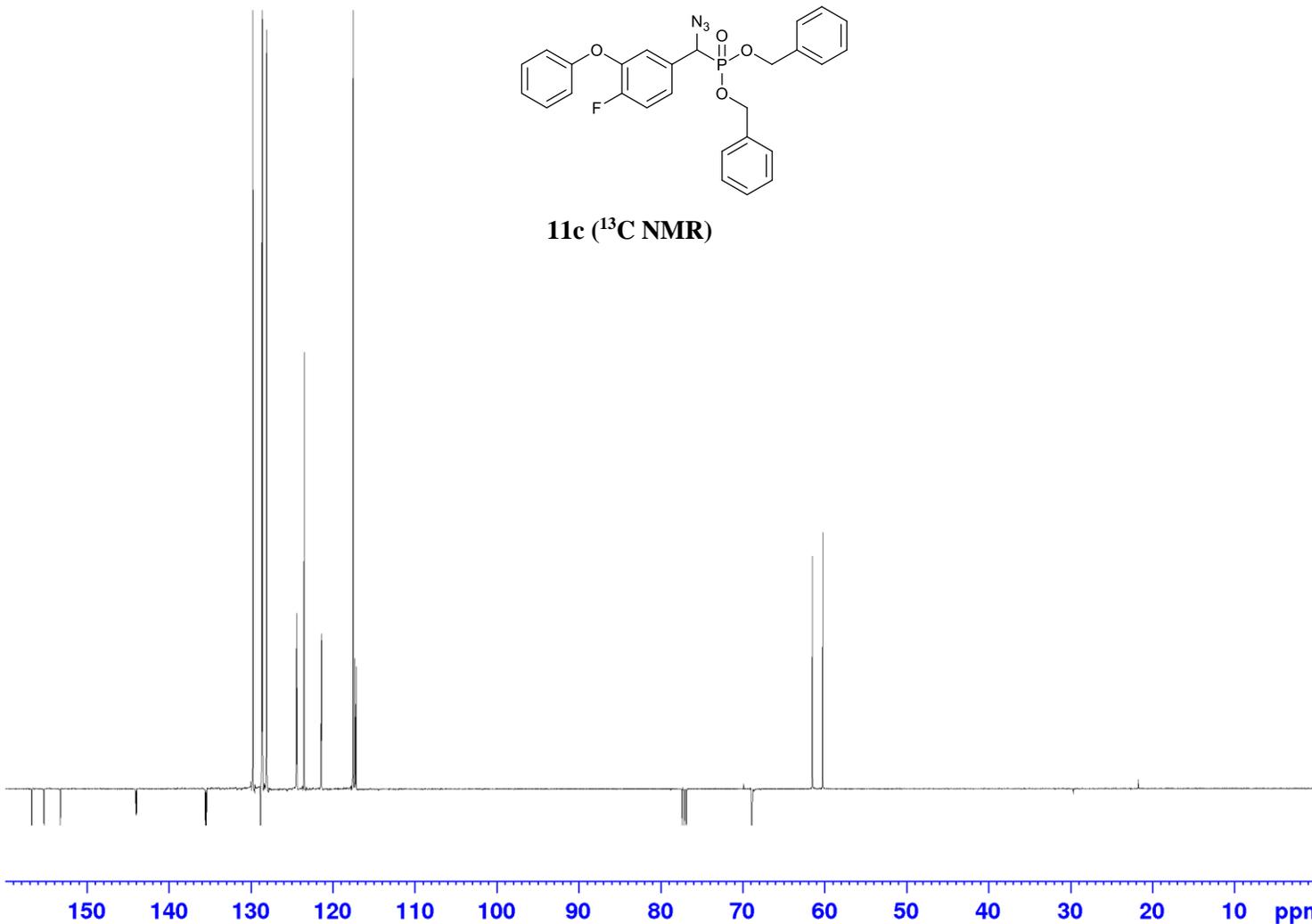


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153.26
144.07
143.97
135.60
135.55
135.49
135.45
129.79
128.89
128.86
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128.67
128.61
128.59
128.13
128.08
124.50
124.45
124.40
123.52
121.45
121.41
117.54
117.34
117.33
117.19
117.18

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77.12
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68.83
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60.24



11c (¹³C NMR)

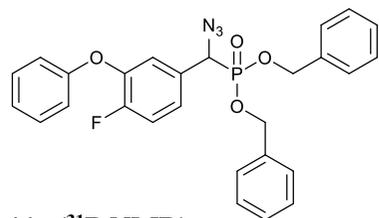


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Current Data Parameters
NAME          CD58
EXPNO         2
PROCNO        1

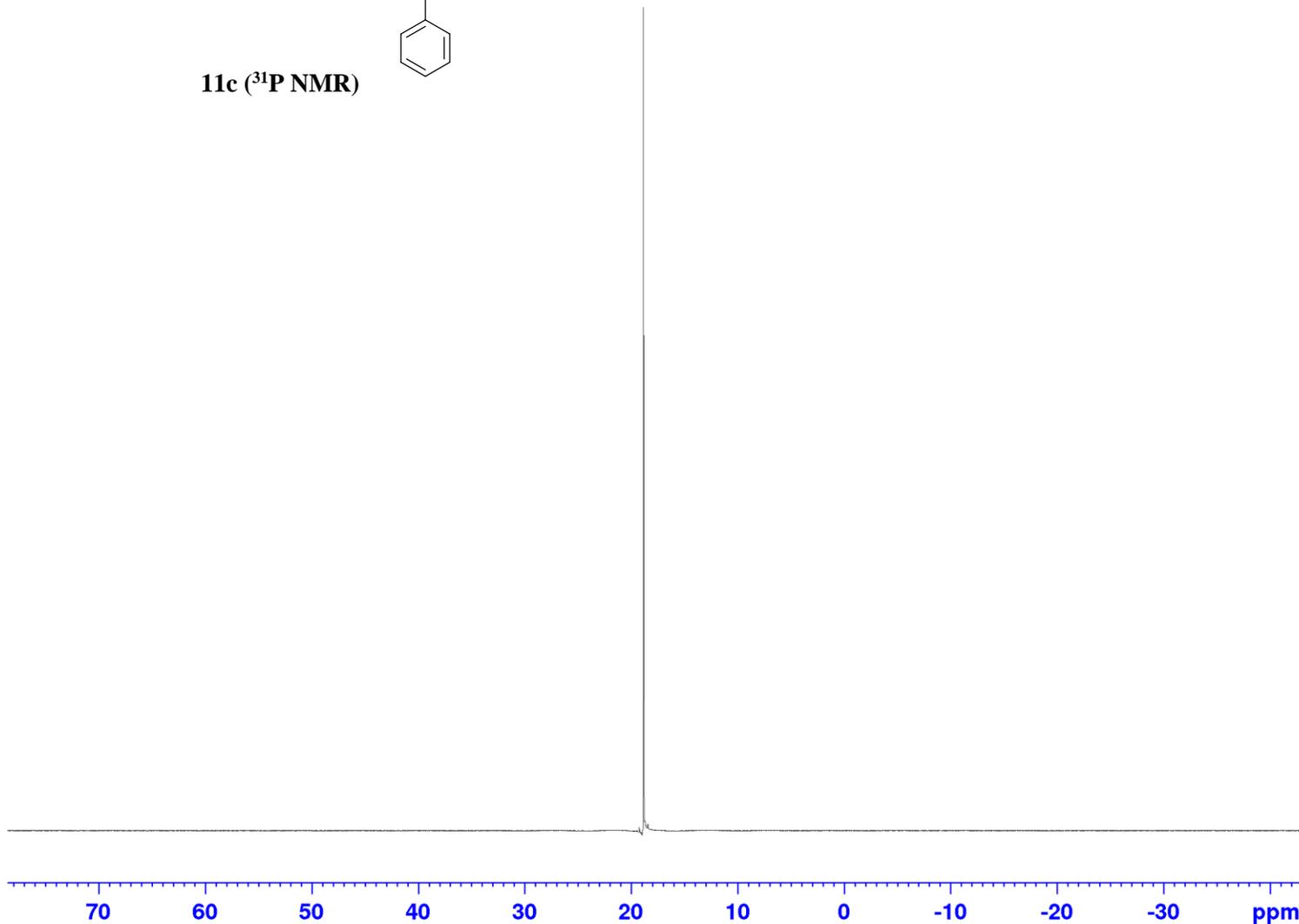
F2 - Acquisition Parameters
Date_         20180427
Time_         11.25 h
INSTRUM       CAB AV4 500 MHZ BASIC
PROBHD        Z150364_0005 (
PULPROG       deptgpgpp
TD            65536
SOLVENT       CDCl3
NS            512
DS            8
SWH           30120.482 Hz
FIDRES        0.919204 Hz
AQ            1.0878977 sec
RG            101
DW            16.600 usec
DE            18.00 usec
TE            298.0 K
CNST2         145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
D16           0.00020000 sec
TDO           1
SFO1          125.6732948 MHz
NUC1          13C
P1            10.00 usec
P13           2000.00 usec
PLWO          0 W
PLW1          51.23600006 W
SPNAM[5]      Crp60comp.4
SPOAL5        0.500
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SPW5          7.82830000 W
SFO2          499.7459990 MHz
NUC2          1H
CNST12        1.5000000
CPDPRG[2]     waltz16
P0            18.00 usec
P3            12.00 usec
P4            24.00 usec
PCPD2         80.00 usec
PLW2          15.53100014 W
PLW12         0.34306911 W
GPNAM[1]      SMSQ10.100
GPZ1          31.00 %
GPNAM[2]      SMSQ10.100
GPZ2          31.00 %
GPNAM[3]      SMSQ10.100
GPZ3          31.00 %
P16           1000.00 usec

F2 - Processing parameters
SI            32768
SF            125.6607401 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
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11c (³¹P NMR)

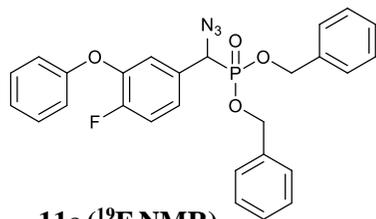
18.85
18.83



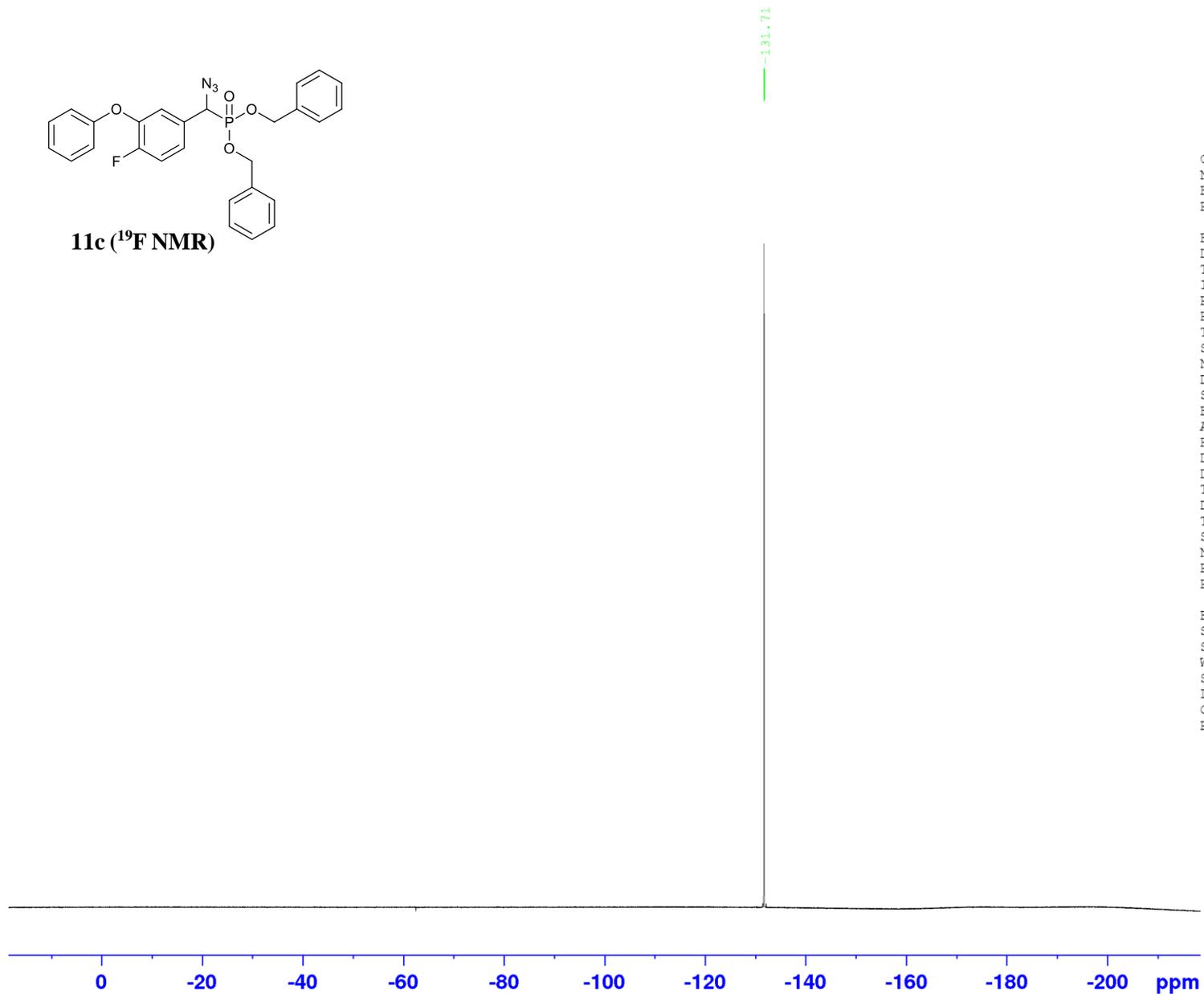
Current Data Parameters
 NAME CD58
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180427
 Time 11.27 h
 INSTRUM CAB AV4 500 MHZ BASIC
 PROBHD Z150364_0005 {
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 4
 SWH 81967.211 Hz
 FIDRES 2.501441 Hz
 AQ 0.3997696 sec
 RG 101
 DW 6.100 usec
 DE 18.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1
 SFO1 202.2899643 MHz
 NUC1 31P
 P1 12.00 usec
 PLW1 45.76100159 W
 SFO2 499.7459990 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 15.53100014 W
 PLW12 0.34306911 W
 PLW13 0.17194620 W

F2 - Processing parameters
 SI 32768
 SF 202.3000793 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



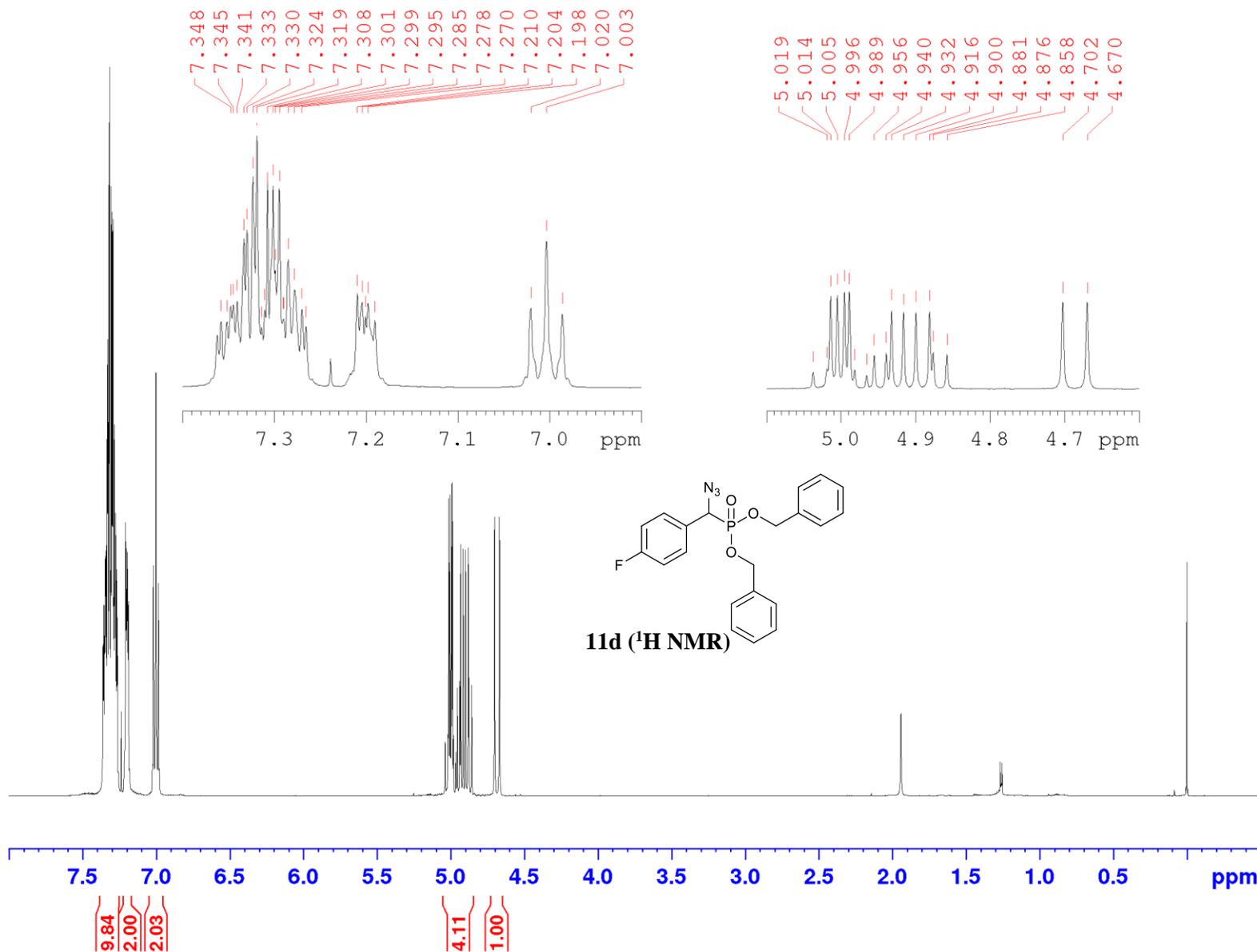
11c (¹⁹F NMR)



Current Data Parameters
NAME 19F
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180413
Time 22.41 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 sec
RG 196.38
DW 5.600 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1
SFO1 376.4889418 MHz
NUC1 19F
P1 15.00 usec
PLW1 17.75399971 W

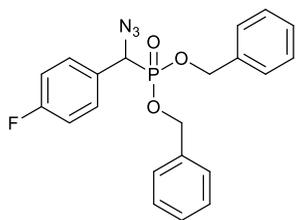
F2 - Processing parameters
SI 65536
SF 376.5265944 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



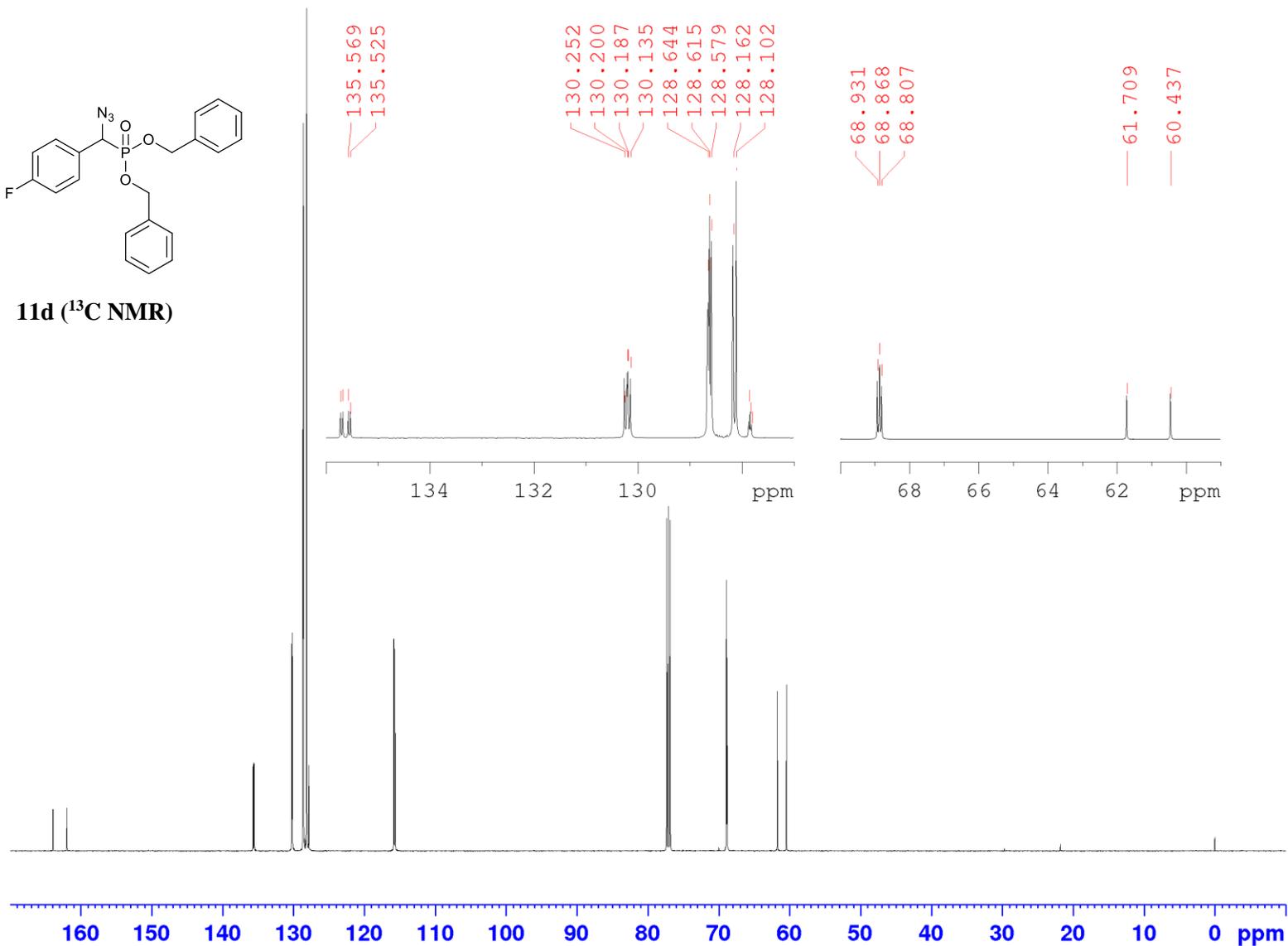
Current Data Parameters
NAME CD84
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190411
Time 17.07 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (zg30)
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 14.6484
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7440222 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



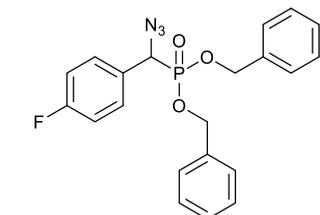
11d (¹³C NMR)



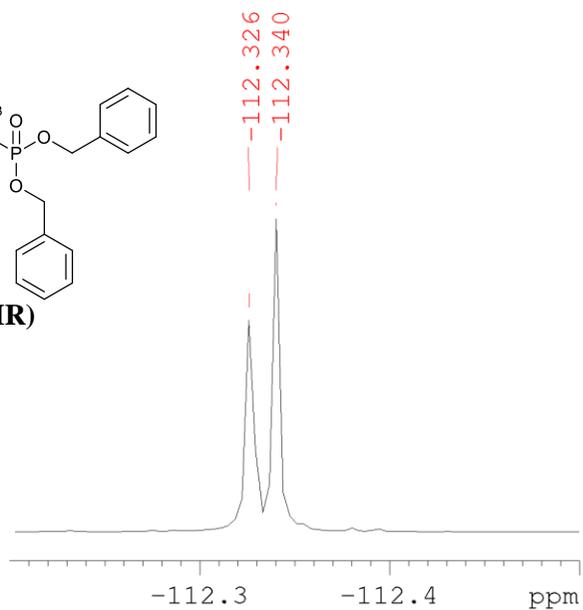
Current Data Parameters
NAME CD84
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190412
Time 0.52 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6607342 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



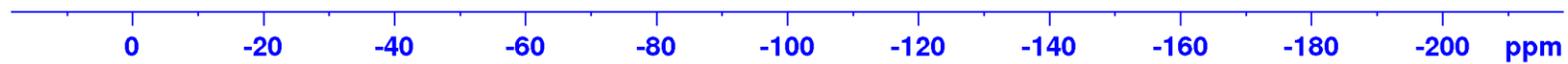
11d (¹⁹F NMR)

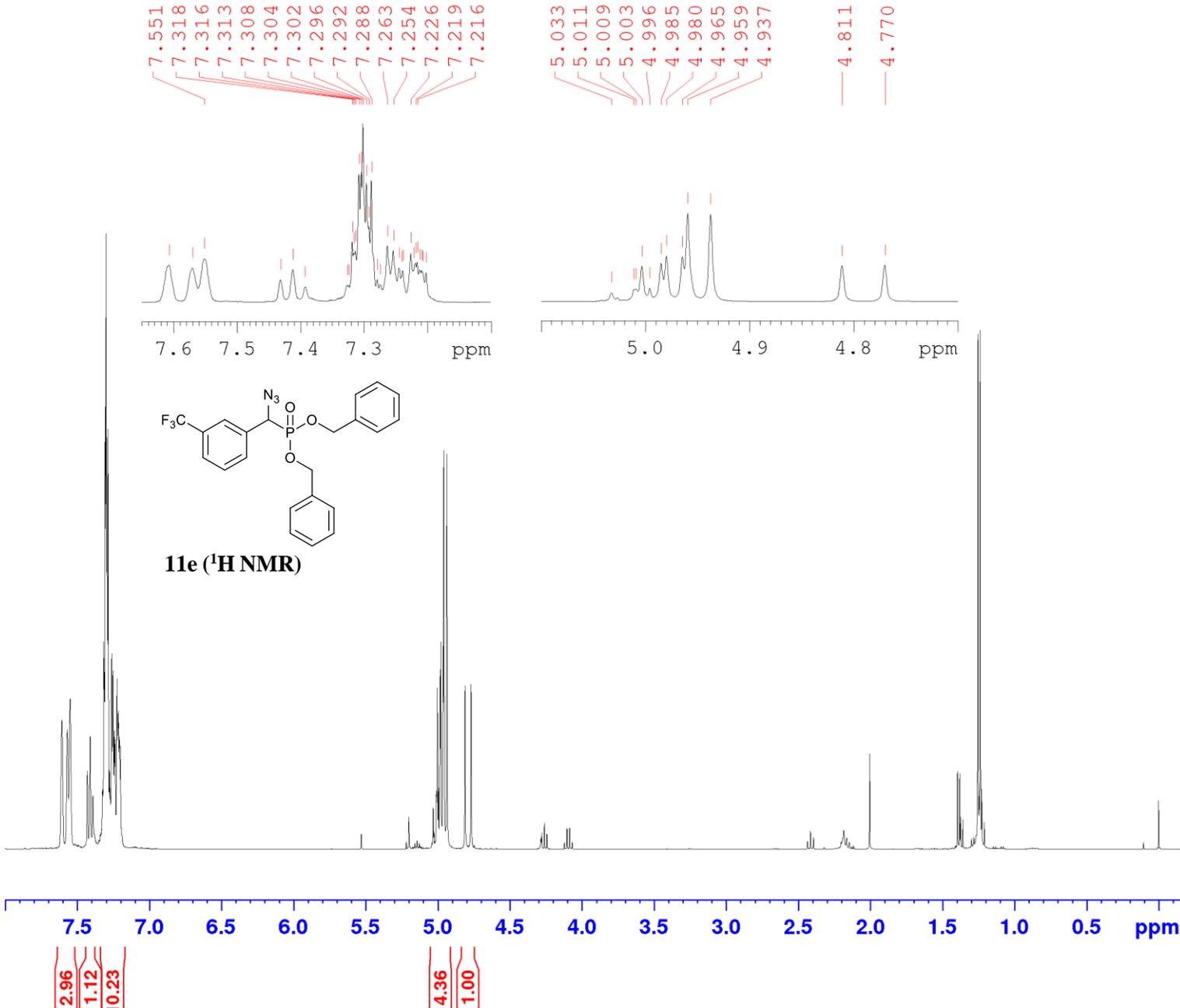


Current Data Parameters
NAME CD84 19F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190412
Time 11.30 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgfgqgn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 sec
RG 196.38
DW 5.600 usec
DE 120.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 376.4889418 MHz
NUC1 19F
P1 15.00 usec
PLW1 17.75399971 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W

F2 - Processing parameters
SI 65536
SF 376.5265944 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

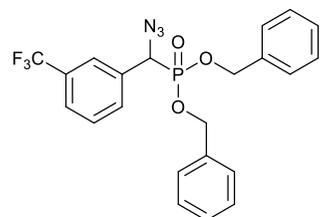




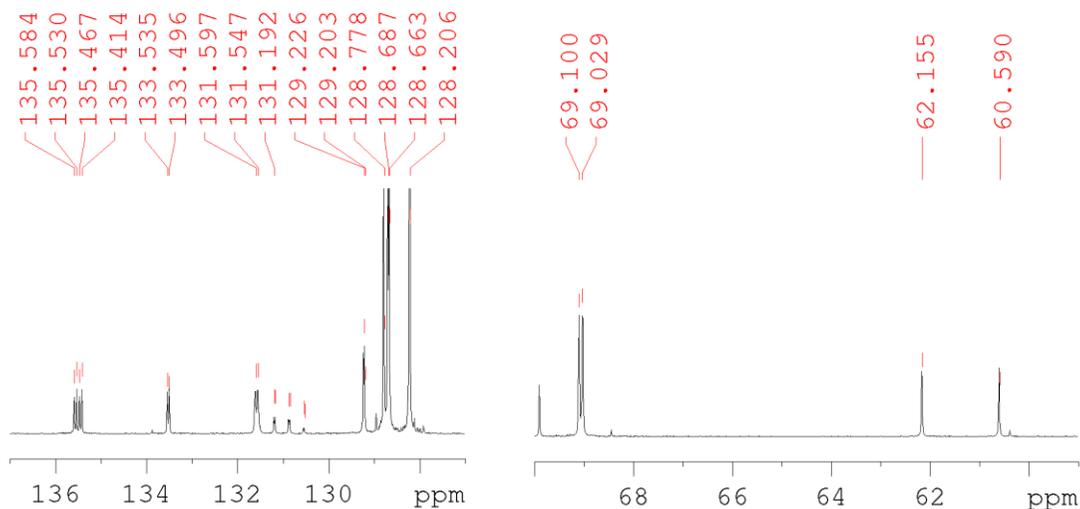
Current Data Parameters
NAME CD77
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180705
Time 15.54 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 20.22
DW 62.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters
SI 65536
SF 400.1600168 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



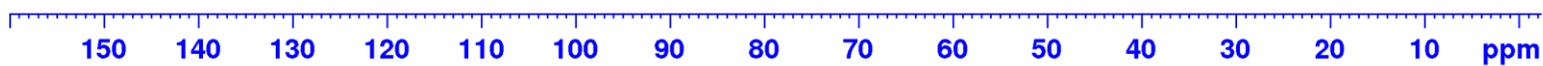
11e (¹³C NMR)

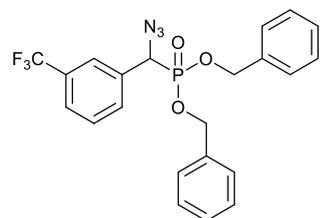


Current Data Parameters
NAME CD77
EXPNO 2
PROCNO 1

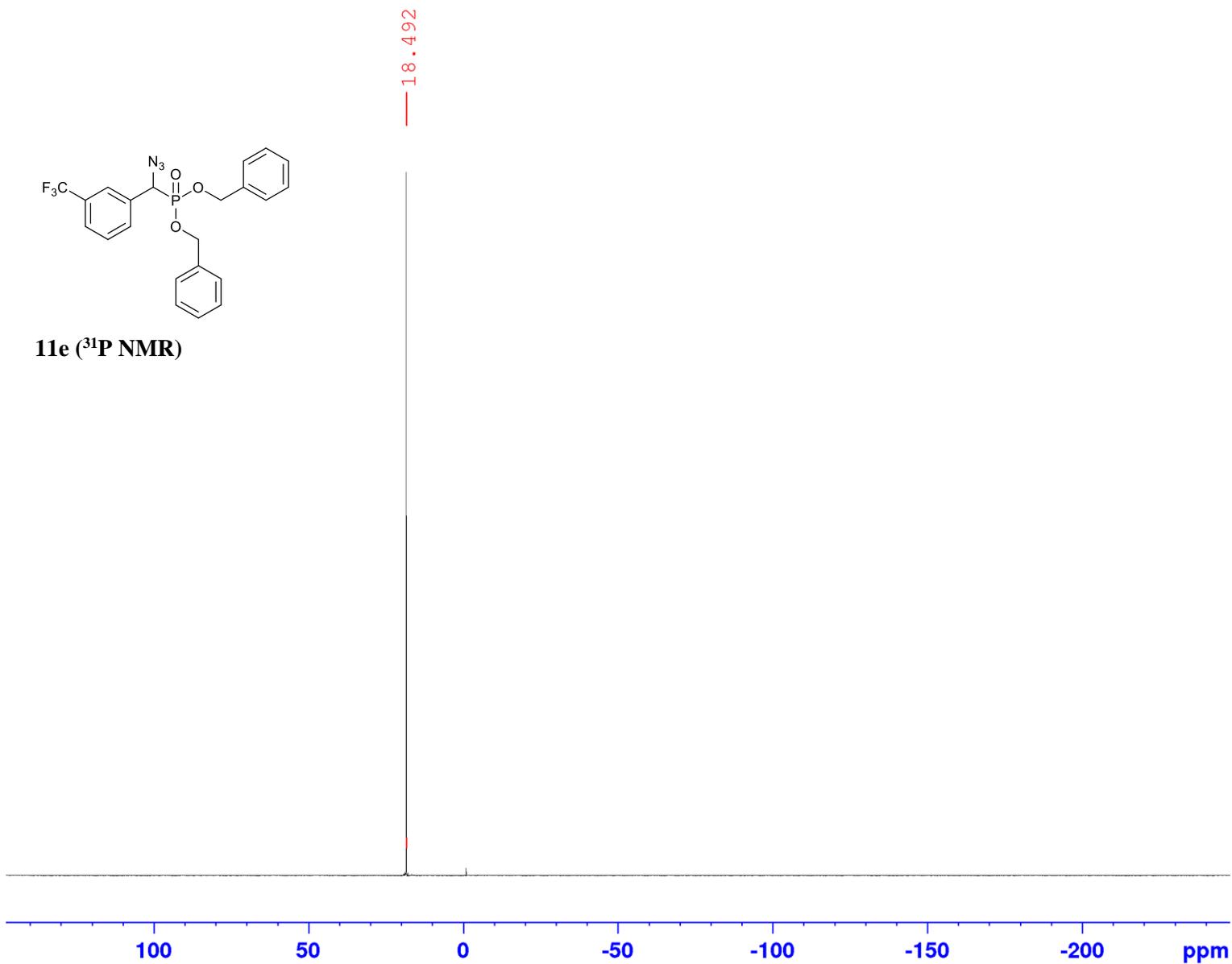
F2 - Acquisition Parameters
Date_ 20180705
Time 23.27 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 196.38
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6303741 MHz
NUC1 13C
P1 10.00 usec
PLW1 55.50099945 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

F2 - Processing parameters
SI 32768
SF 100.6203114 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





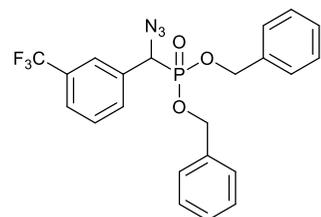
11e (³¹P NMR)



Current Data Parameters
NAME CD77
EXPNO 6
PROCNO 1

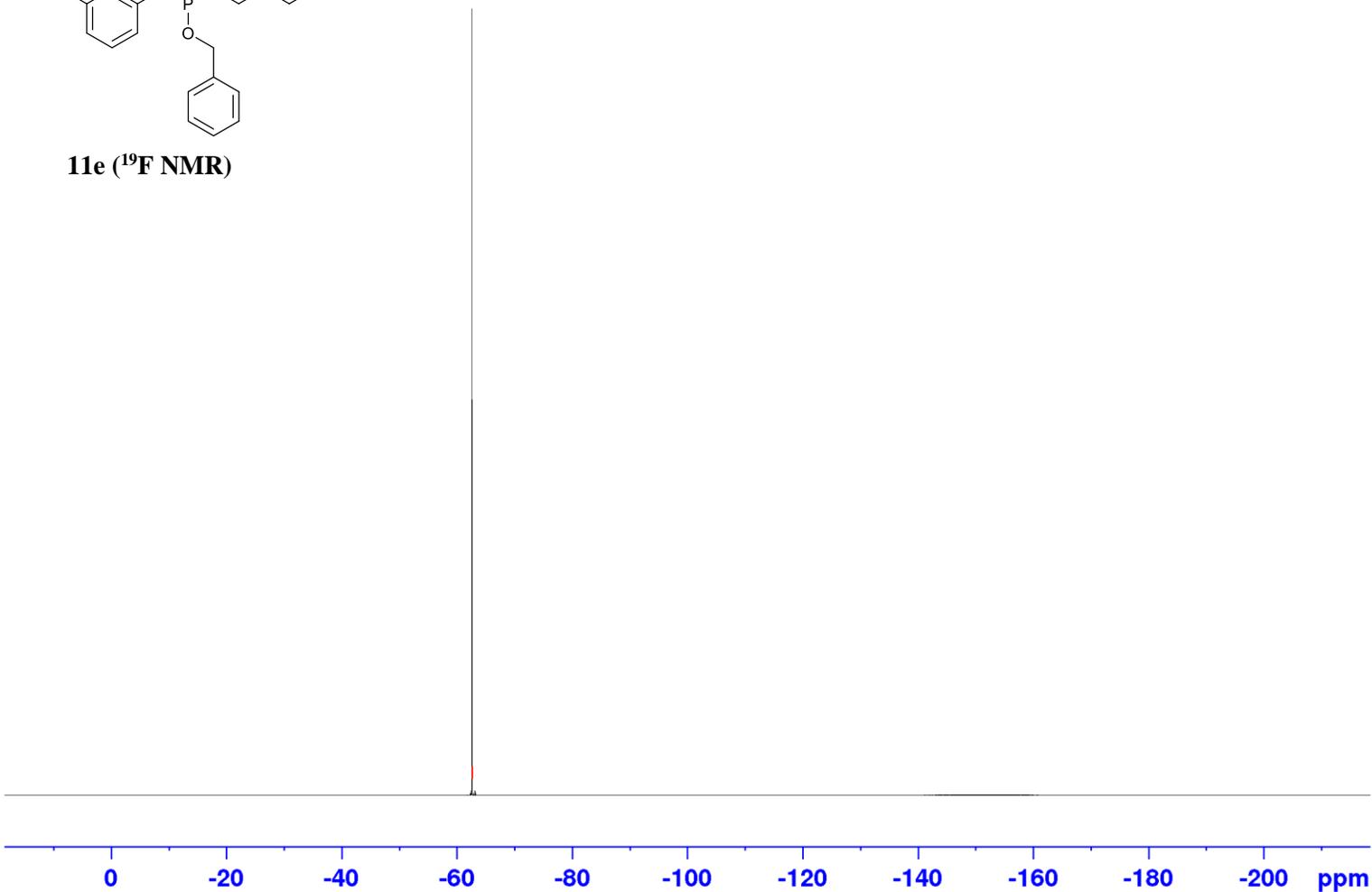
F2 - Acquisition Parameters
Date_ 20180706
Time 1.13 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 usec
PLW1 11.77099991 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

F2 - Processing parameters
SI 32768
SF 161.9877372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



11e (¹⁹F NMR)

--62.571



```
Current Data Parameters
NAME          CD77
EXPNO         7
PROCNO        1

F2 - Acquisition Parameters
Date_         20180706
Time          1.16 h
INSTRUM       spect
PROBHD        Z108618_0921 (
PULPROG       zgfhigqn.2
TD            131072
SOLVENT       CDC13
NS            16
DS            4
SWH           89285.711 Hz
FIDRES        1.362392 Hz
AQ            0.7340032 sec
RG            196.38
DW            5.600 usec
DE            6.50 usec
TE            298.8 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0           1
SFO1          376.4889418 MHz
NUC1          19F
P1            15.00 usec
PLW1          17.75399971 W
SFO2          400.1616006 MHz
NUC2          1H
CPDPRG[2]    waltz16
PCPD2        90.00 usec
PLW2          11.52400017 W
PLW12         0.27886000 W

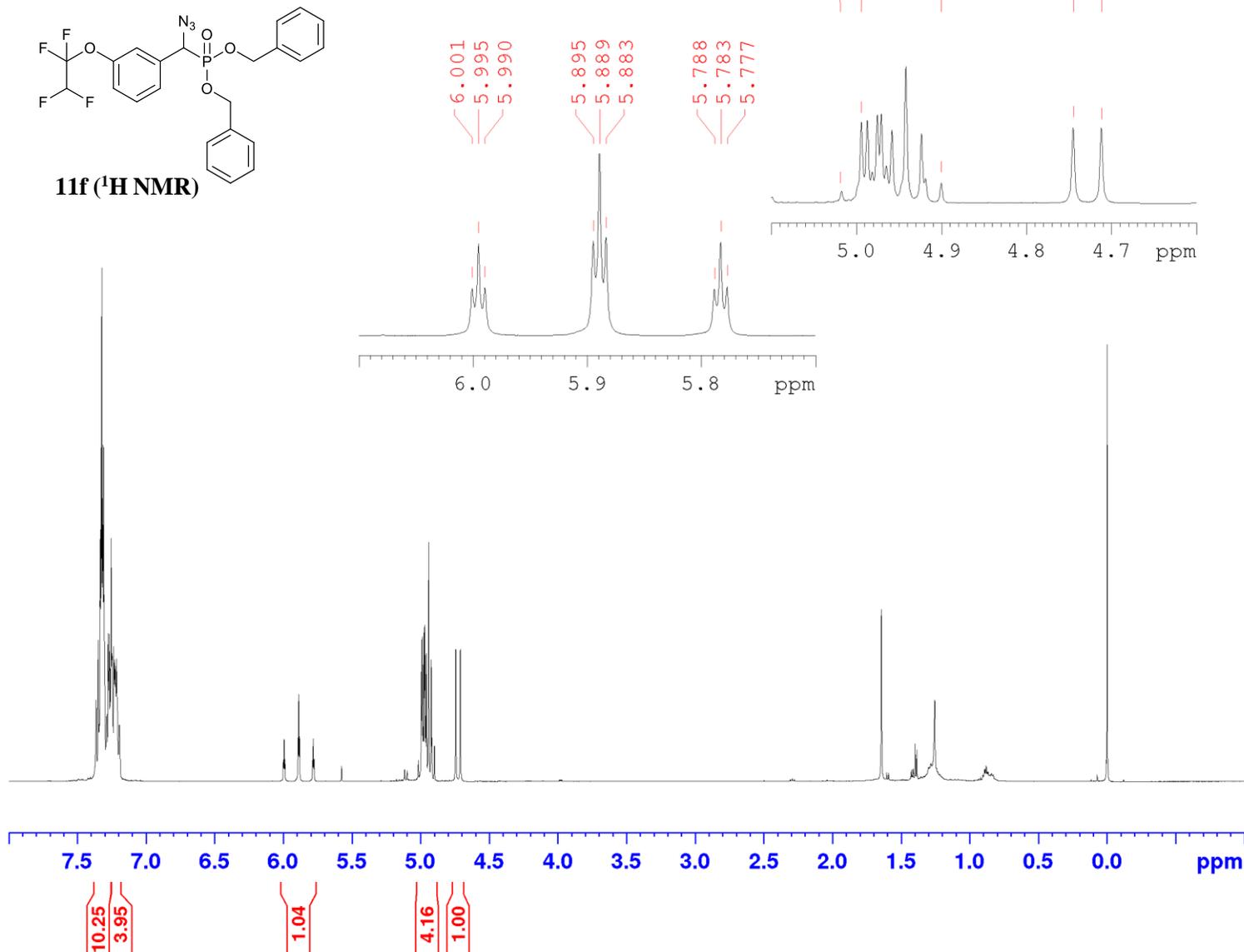
F2 - Processing parameters
SI            65536
SF            376.5265944 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
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Current Data Parameters
NAME CD54 B3P39
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190730
Time 17.22 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 50
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7440152 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

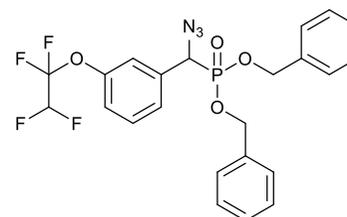




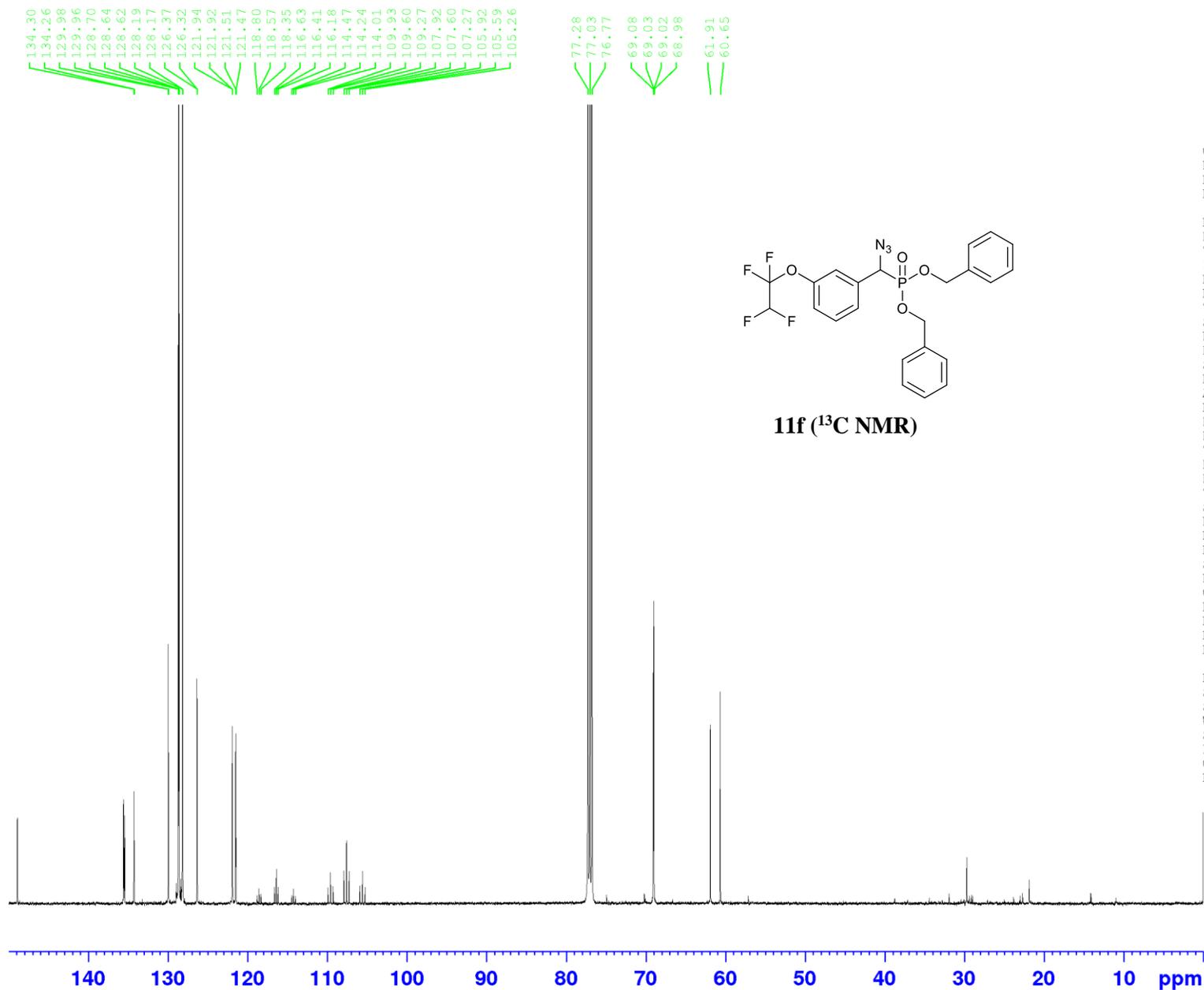
Current Data Parameters
NAME CD54 B3P39
EXPNO 2
PROCNO 1

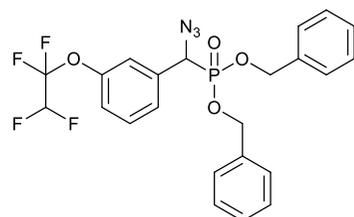
F2 - Acquisition Parameters
Date_ 20190731
Time 3.46 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2800
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SF02 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6607302 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

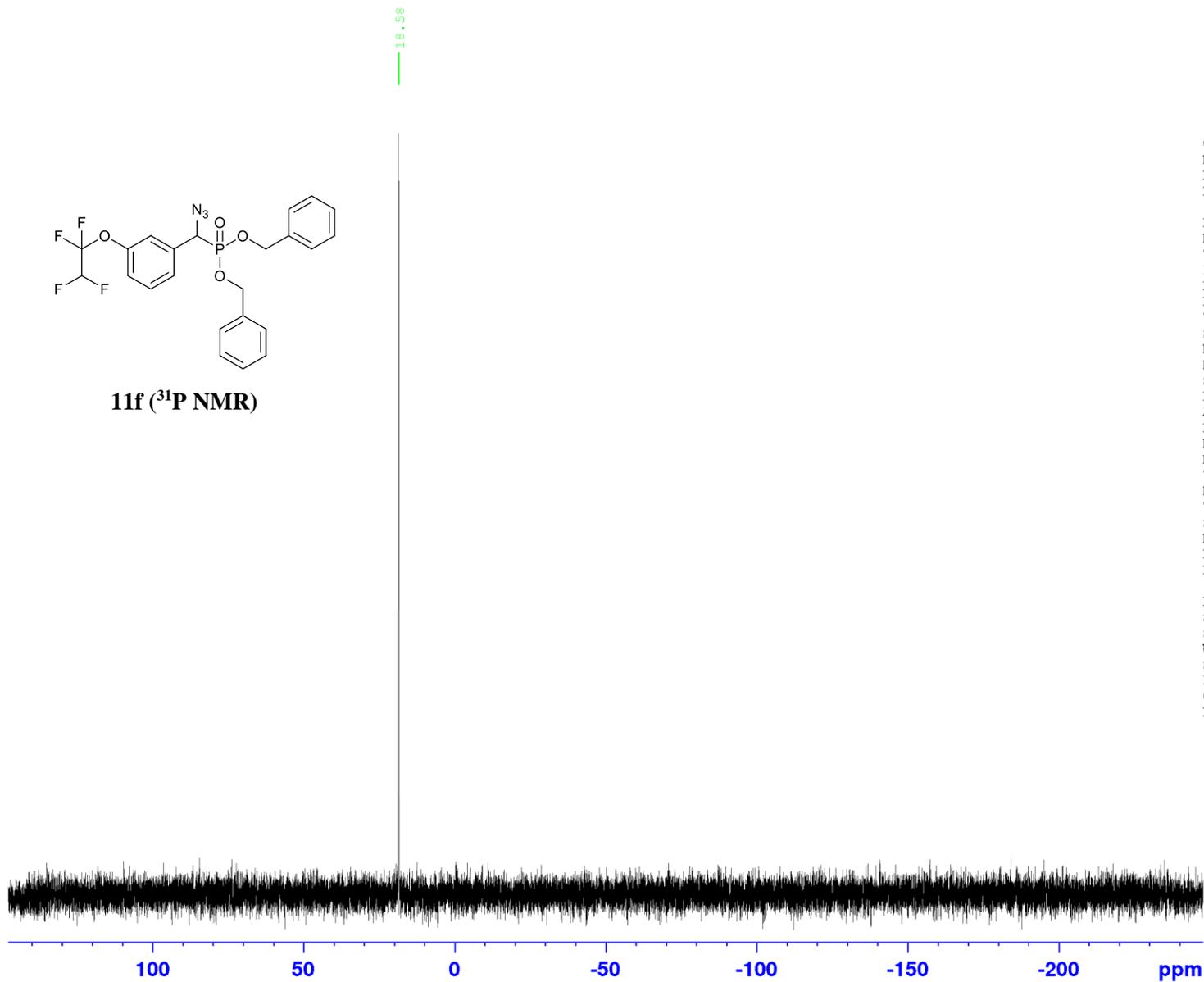


11f (¹³C NMR)





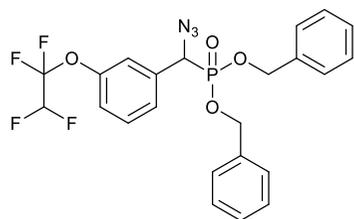
11f (³¹P NMR)



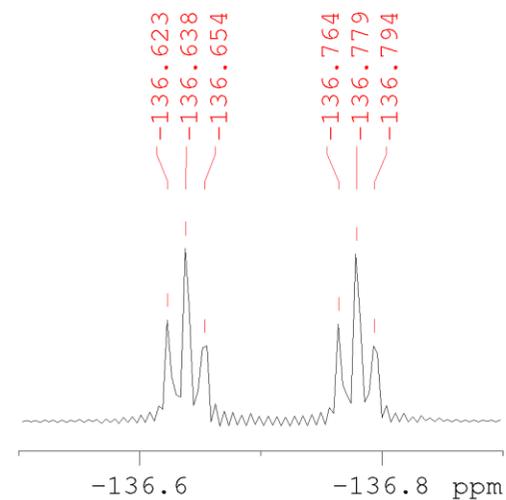
Current Data Parameters
NAME CD54 B3P39 P+F
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190801
Time_ 10.03 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 usec
DE 50.00 usec
TE 298.8 K
D1 2.00000000 sec
TD0 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 usec
PLW1 11.77099991 W

F2 - Processing parameters
SI 32768
SF 161.9877372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



11f (¹⁹F NMR)



Current Data Parameters
 NAME CD54 B3P39 P+F
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190801
 Time 10.02 h
 INSTRUM spect
 PROBHD Z108618_0921 (
 PULPROG zgflgn
 TD 65536
 SOLVENT CDCl3
 NS 4
 DS 0
 SWH 89285.711 Hz
 FIDRES 2.724784 Hz
 AQ 0.3670016 sec
 RG 196.38
 DW 5.600 usec
 DE 120.00 usec
 TE 298.8 K
 D1 1.0000000 sec
 TD0 1
 SFO1 376.4889413 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 17.75399971 W

F2 - Processing parameters
 SI 65536
 SF 376.5265940 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

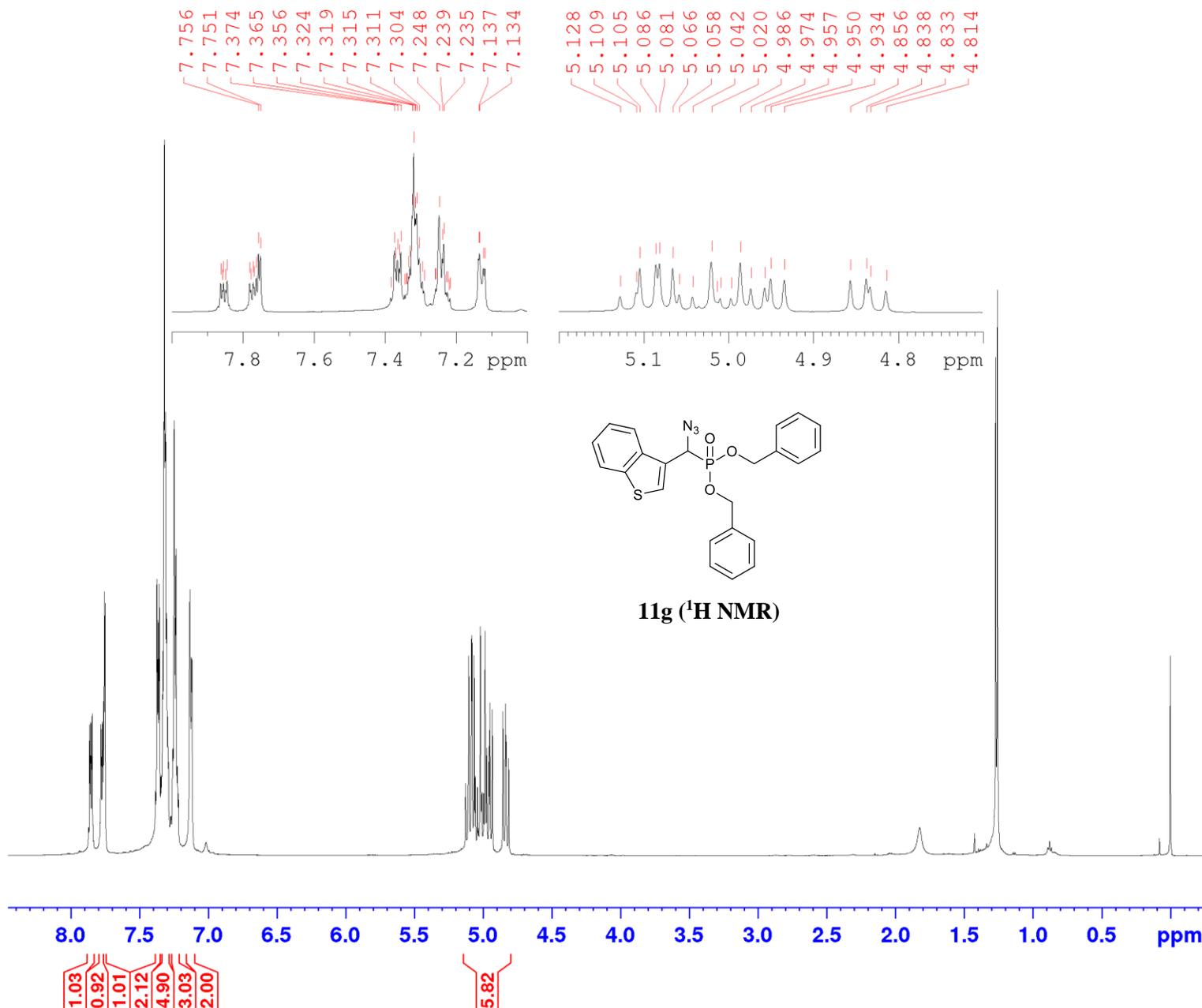


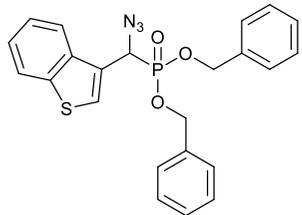


Current Data Parameters
NAME CD78
EXPNO 1
PROCNO 1

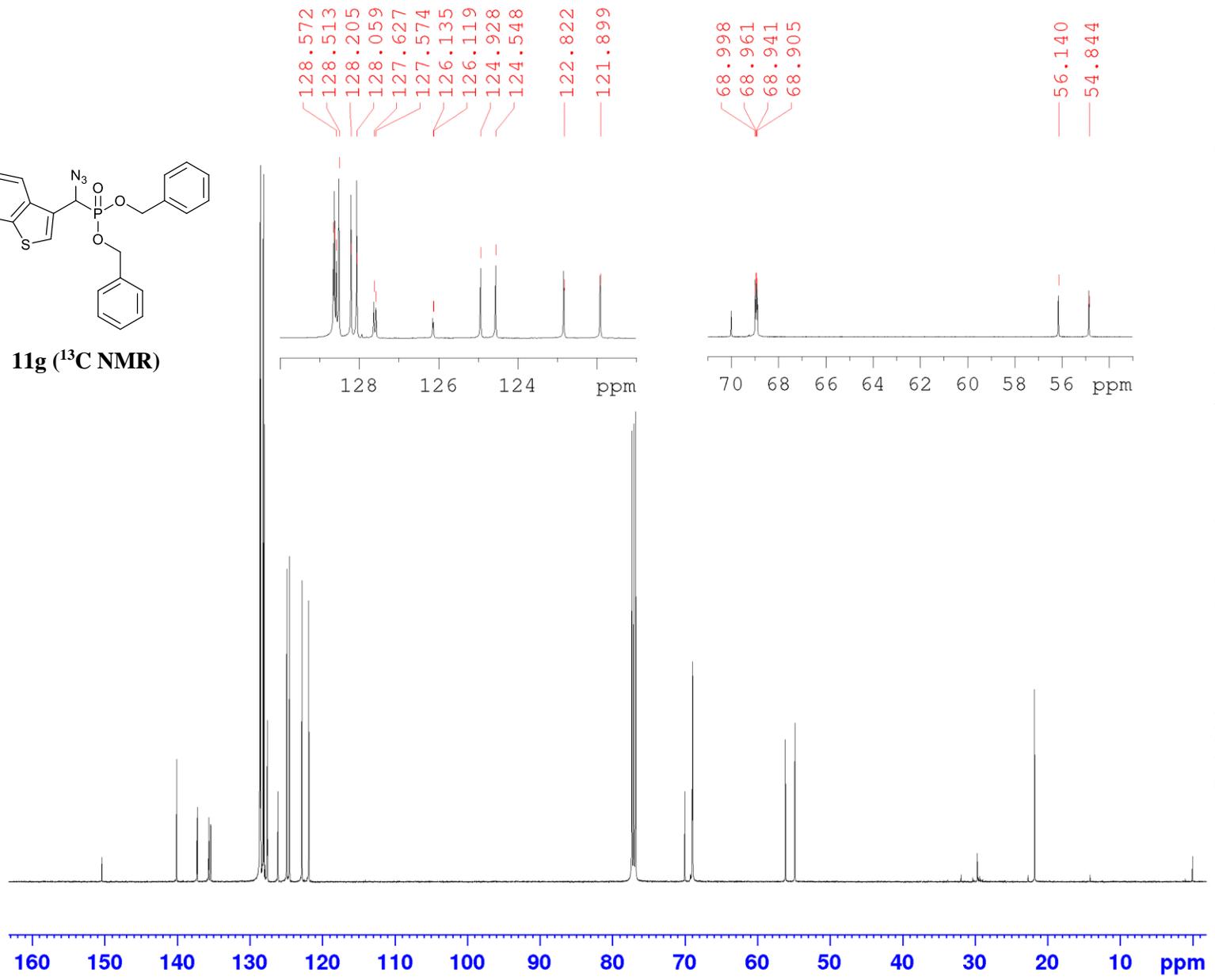
F2 - Acquisition Parameters
Date_ 20190321
Time 12.48 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 32
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7440226 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





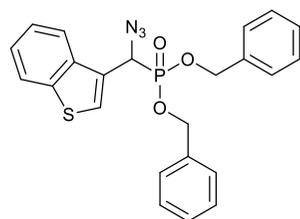
11g (¹³C NMR)



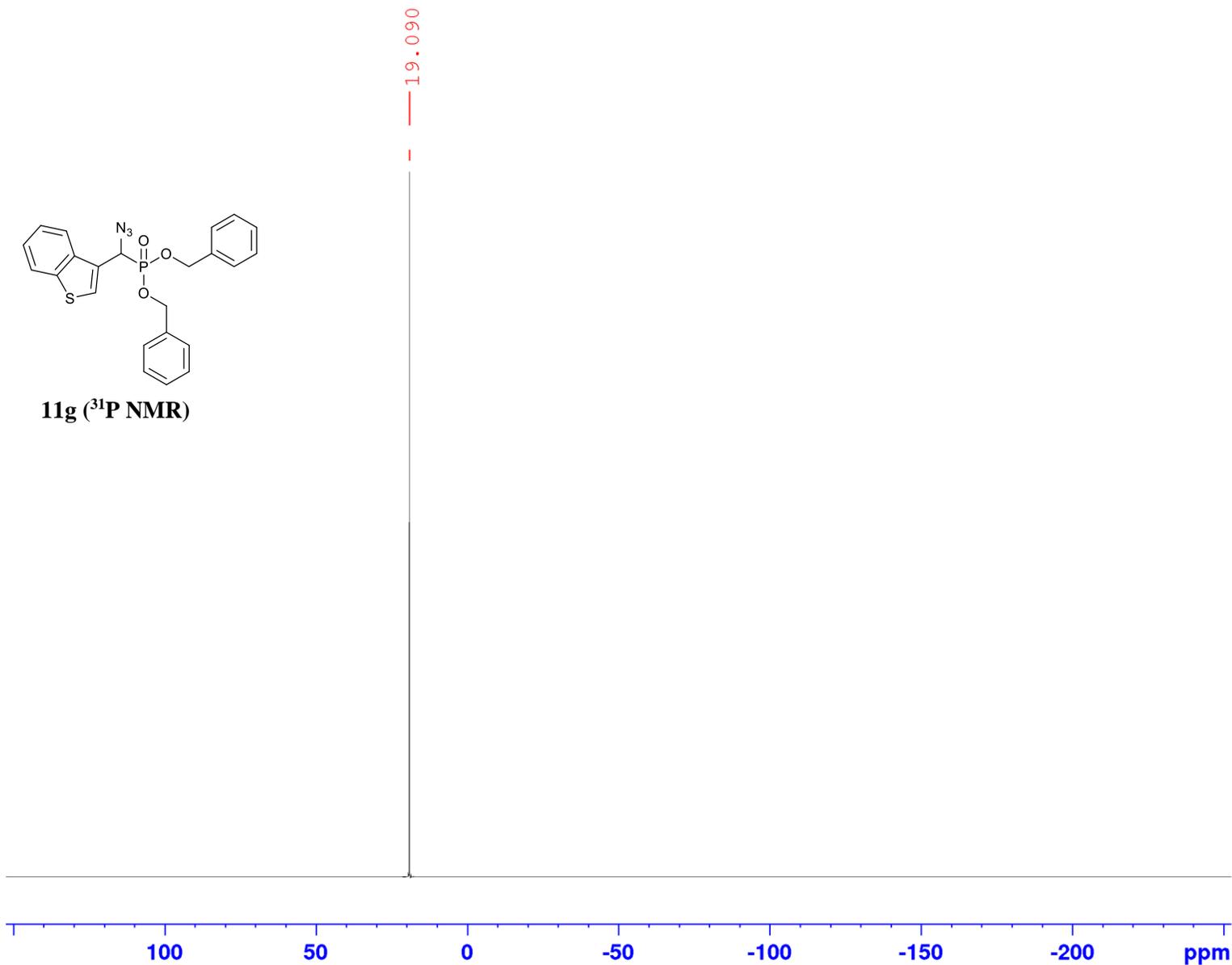
Current Data Parameters
NAME CD78
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190321
Time 19.53 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6607349 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



11g (³¹P NMR)



Current Data Parameters
NAME CD78
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180711
Time 0.42 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34306911 W
PLW13 0.17194620 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



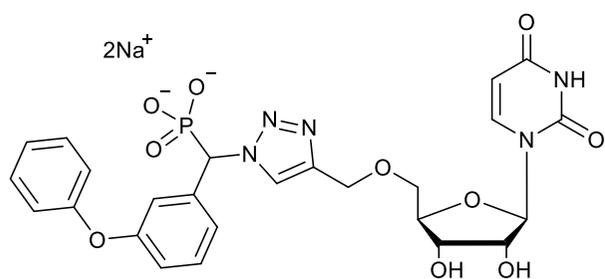
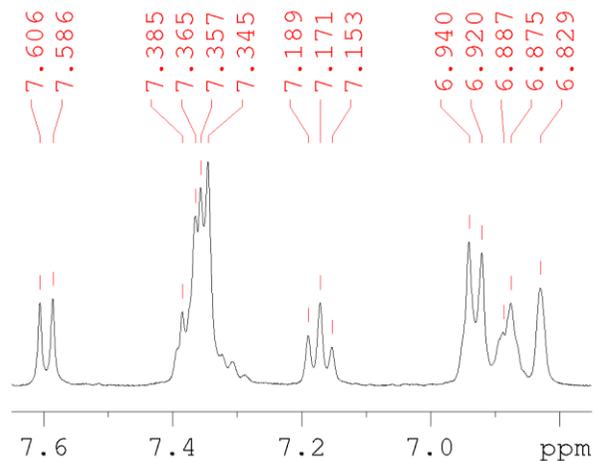
Current Data Parameters
NAME CD107s
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

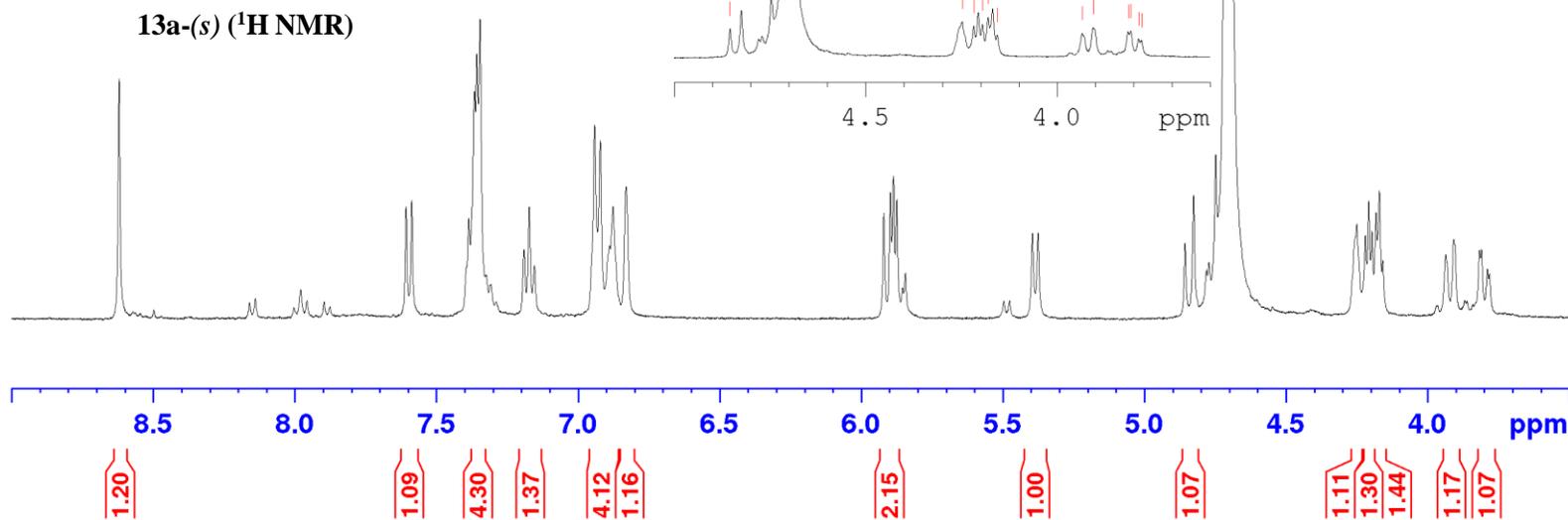
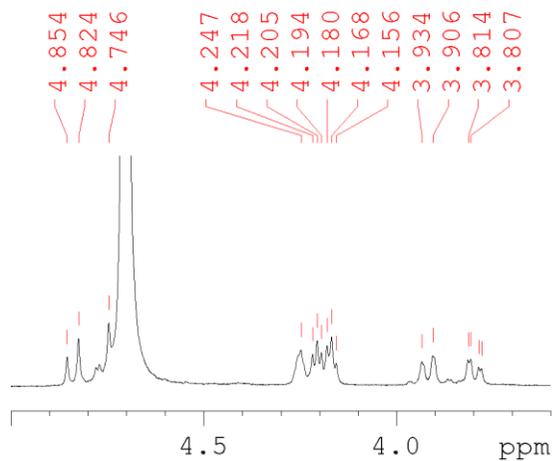
Date_ 20191213
Time 15.52 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 28
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 196.38
DW 62.400 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters

SI 65536
SF 400.1600000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13a-(s) (1H NMR)

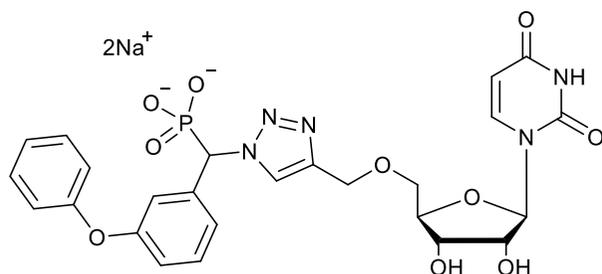
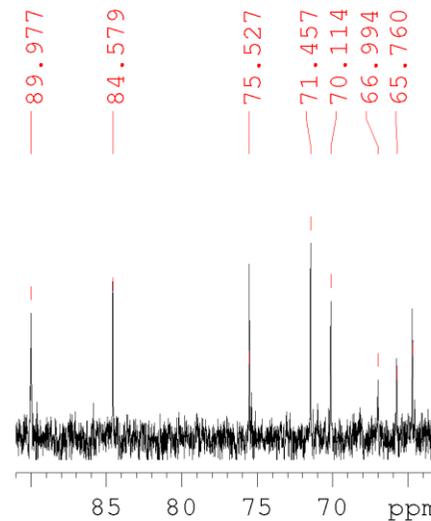
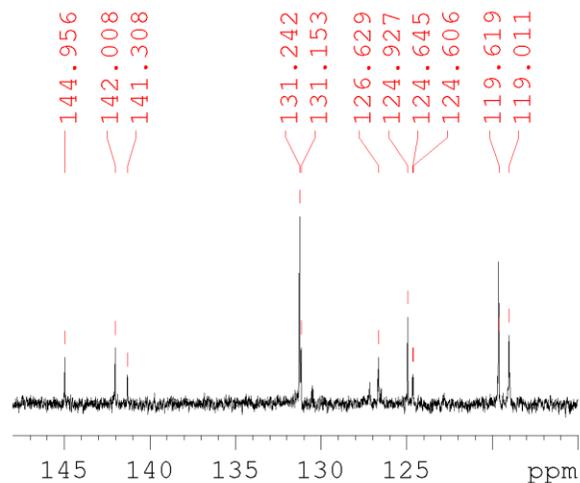




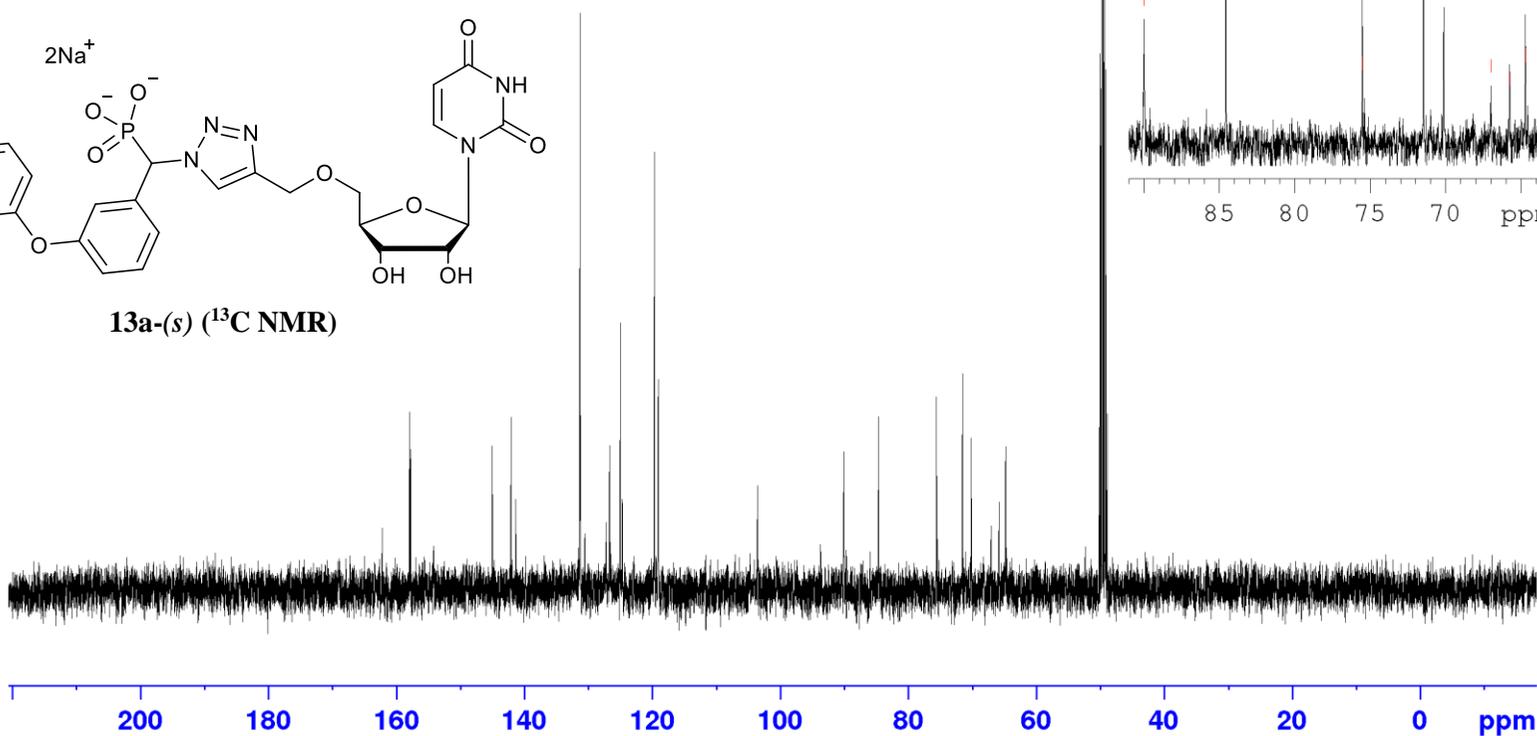
Current Data Parameters
NAME CD107s
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 2.34 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 3650
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 196.38
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6303741 MHz
NUC1 13C
P1 10.00 usec
PLW1 55.5009945 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

F2 - Processing parameters
SI 32768
SF 100.6201957 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13a-(s) (13C NMR)

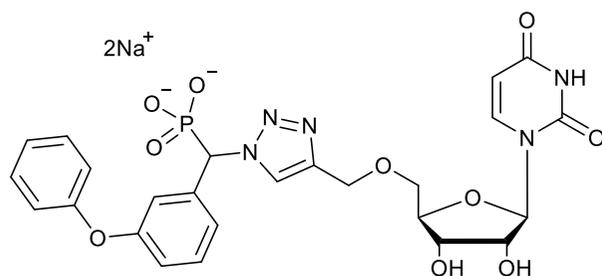




Current Data Parameters
NAME CD107s
EXPNO 5
PROCNO 1

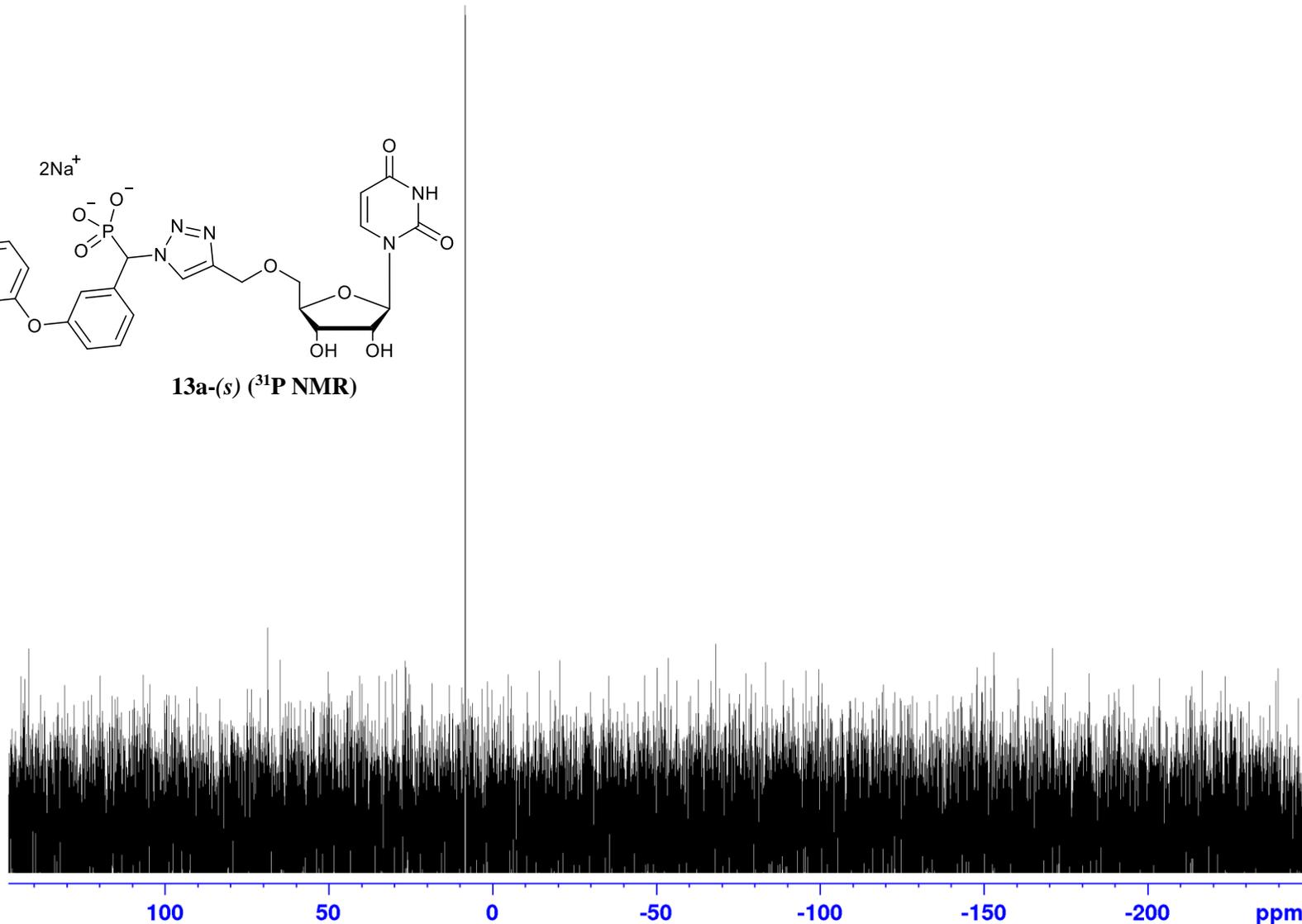
F2 - Acquisition Parameters
Date_ 20191214
Time 3.07 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 4
DS 0
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 usec
DE 50.00 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 usec
PLW1 11.77099991 W

F2 - Processing parameters
SI 32768
SF 161.9877372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13a-(s) (³¹P NMR)

8.36

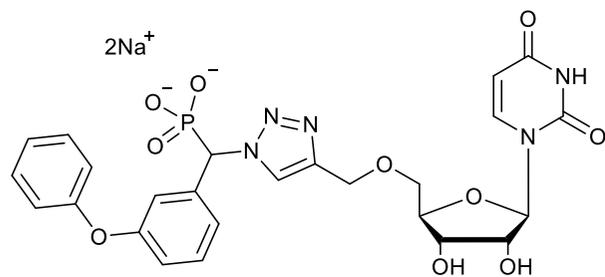




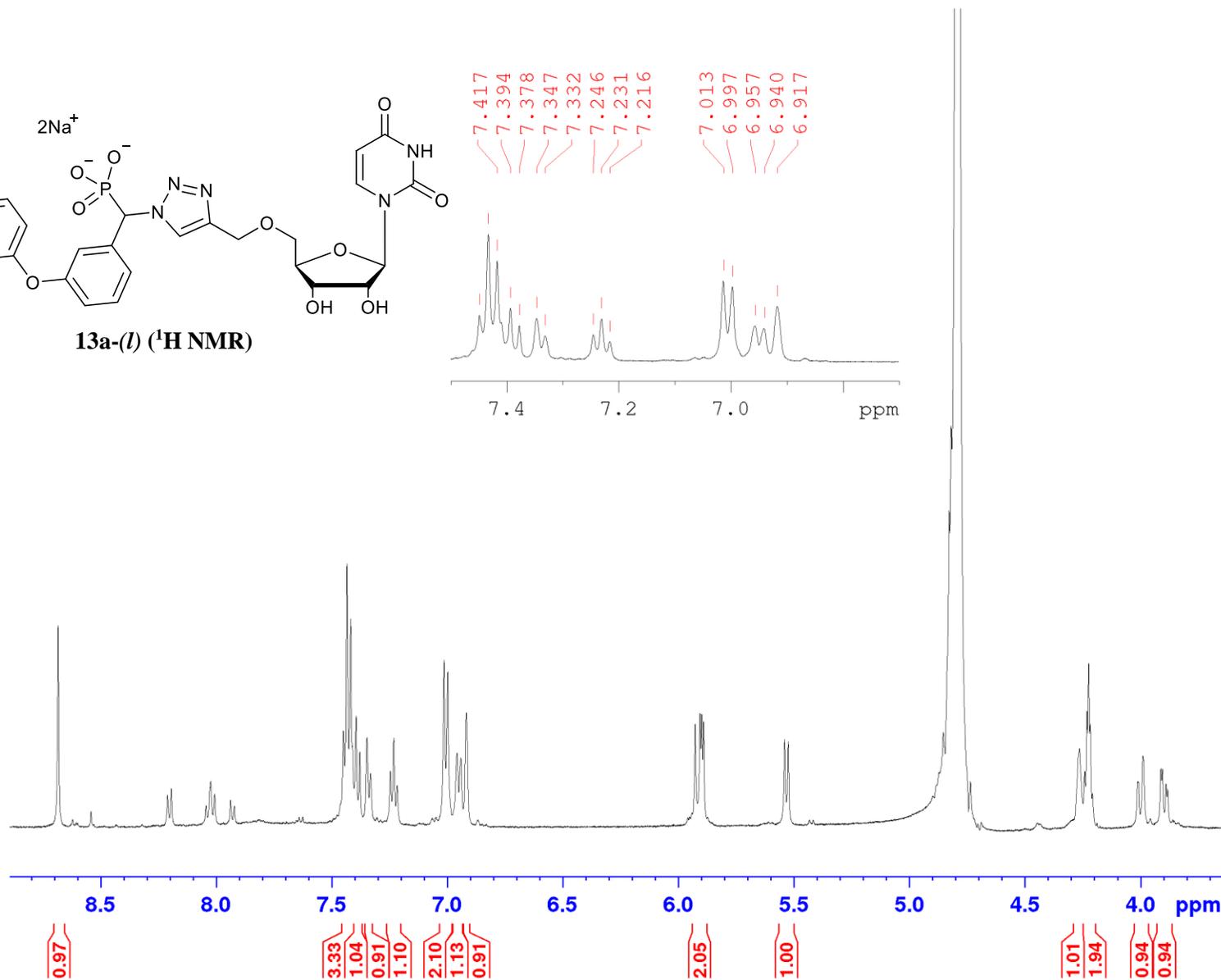
Current Data Parameters
NAME CD1071
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191213
Time_ 15.54 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 20
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7452260 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13a-(l) (¹H NMR)

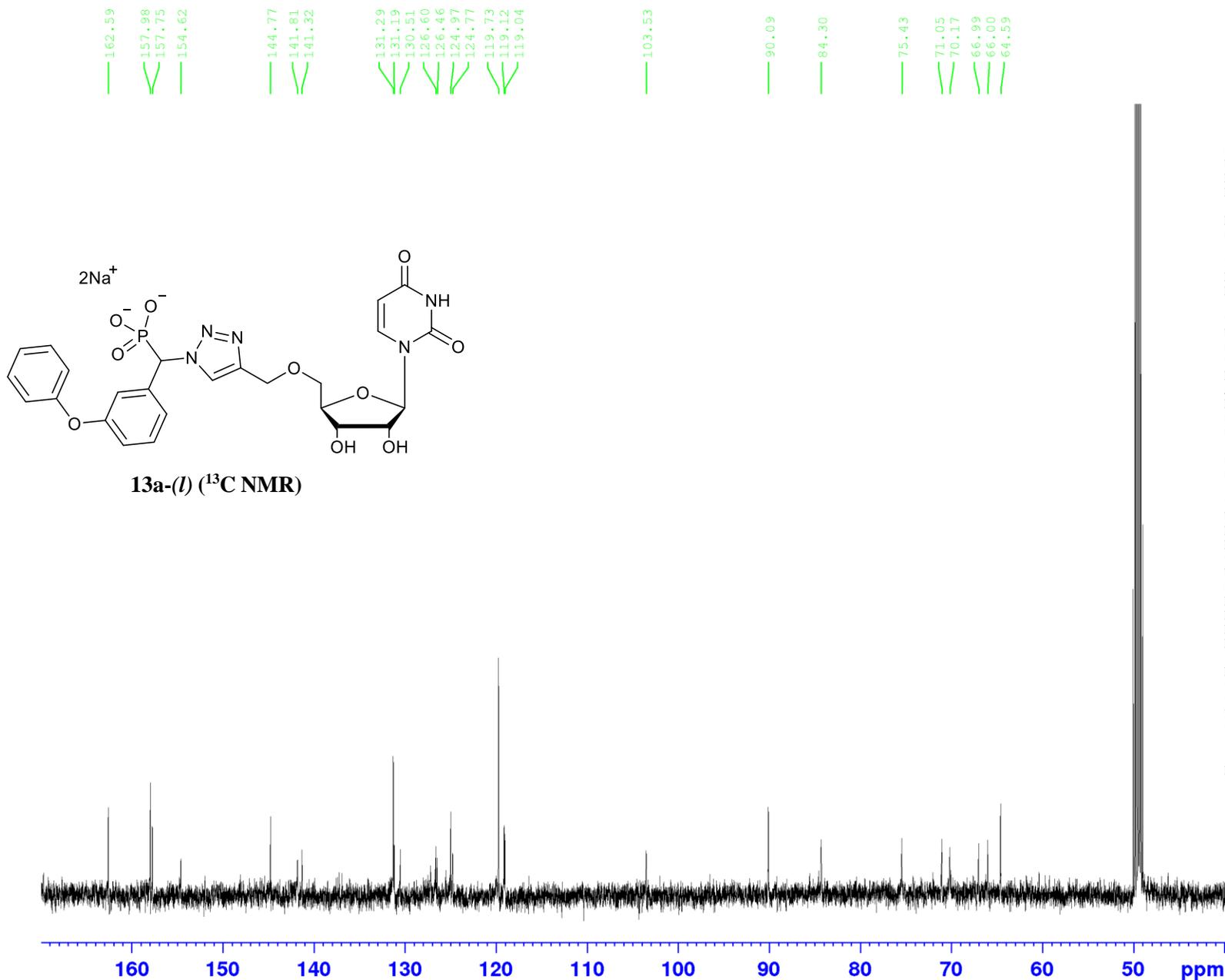




Current Data Parameters
NAME CD1071
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 17.41 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3800
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6608898 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

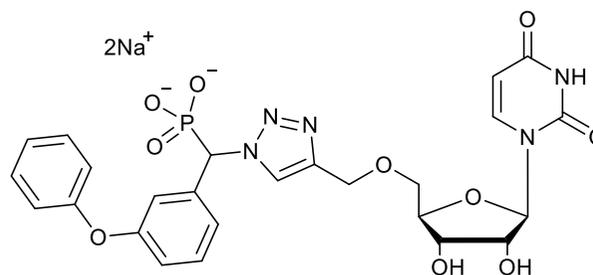




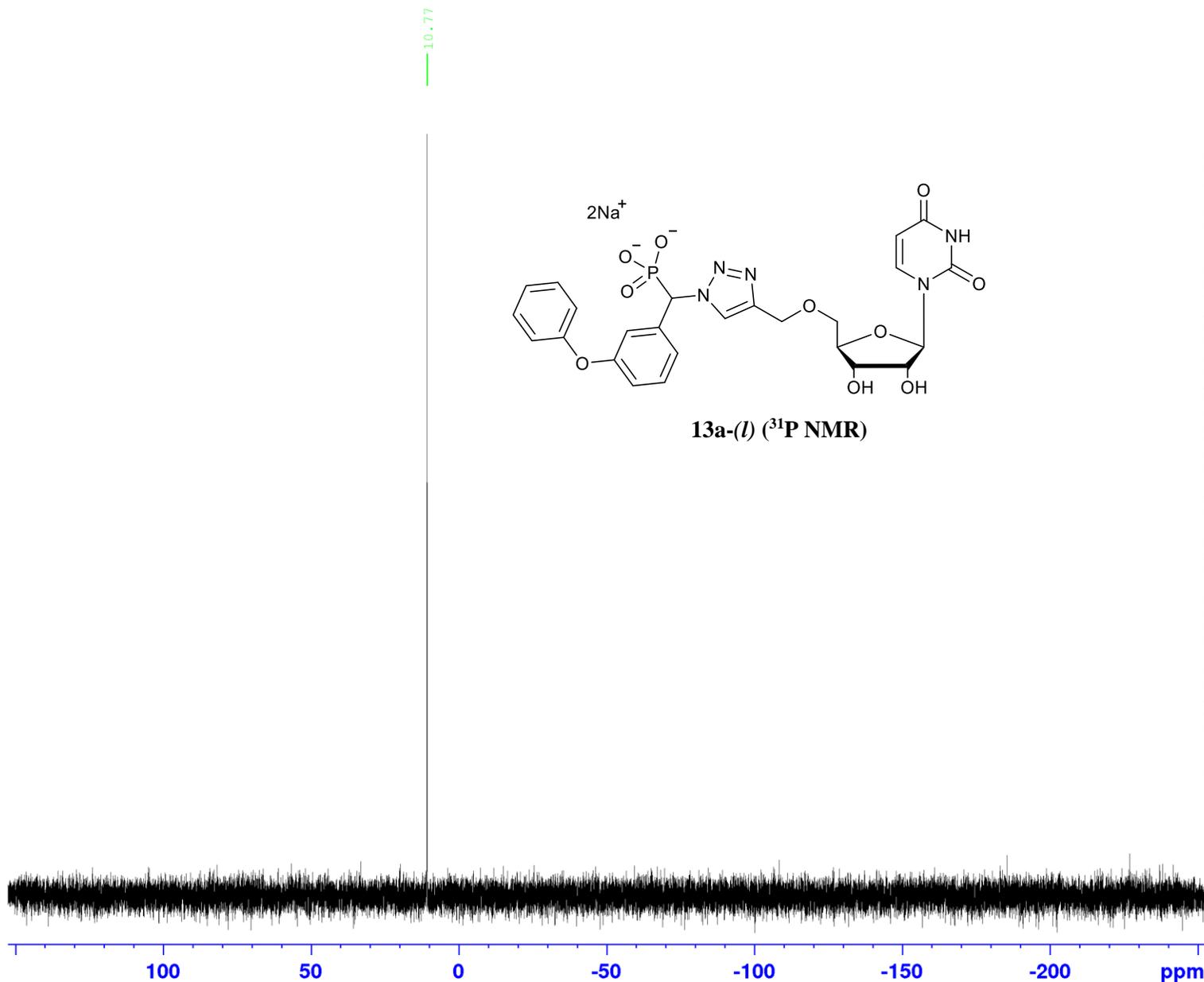
Current Data Parameters
NAME CD1071
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 18.13 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13a-(l) (³¹P NMR)

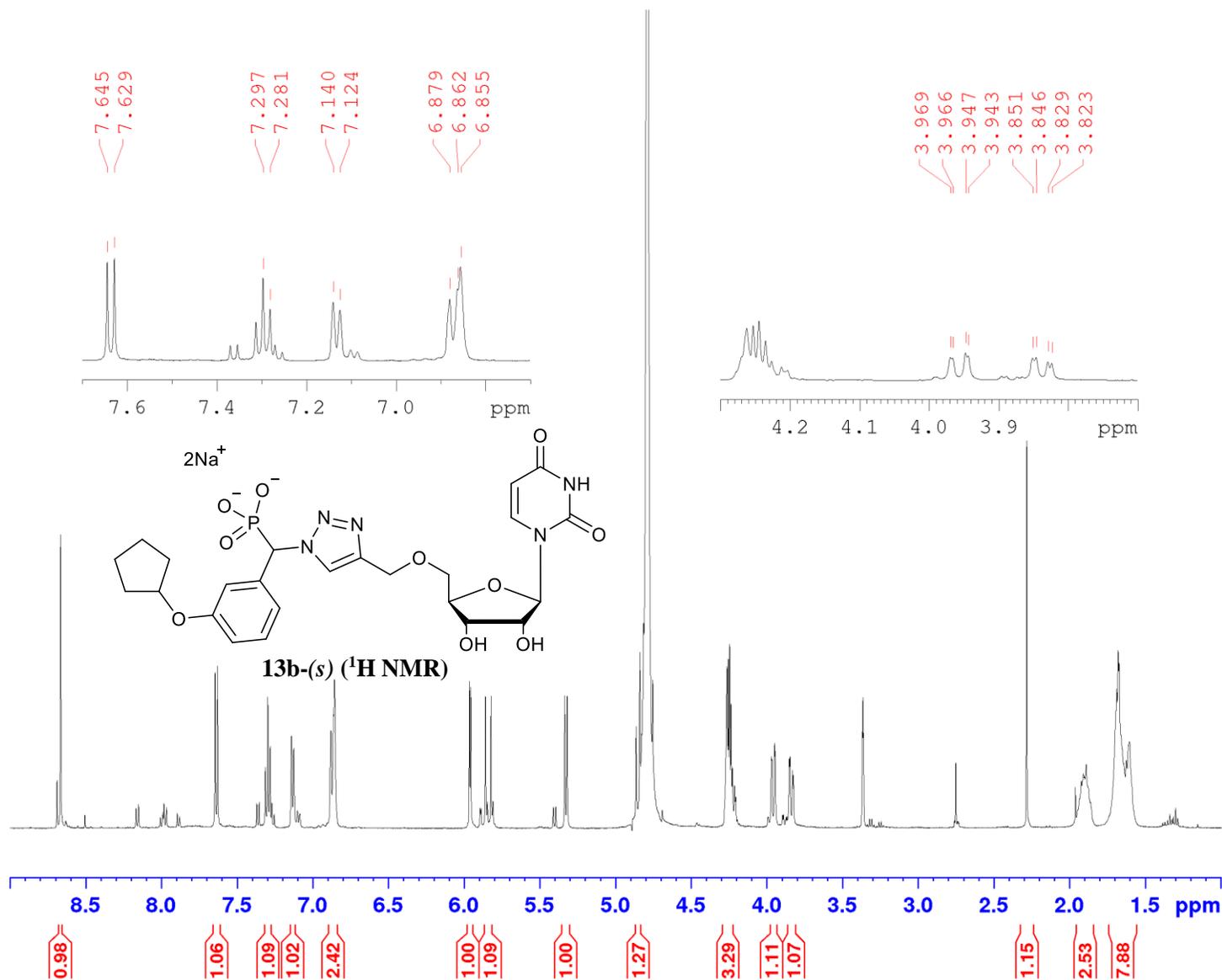




Current Data Parameters
NAME CD106s
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191212
Time 16.00 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7452261 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

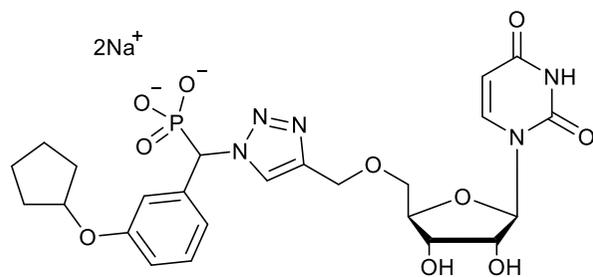
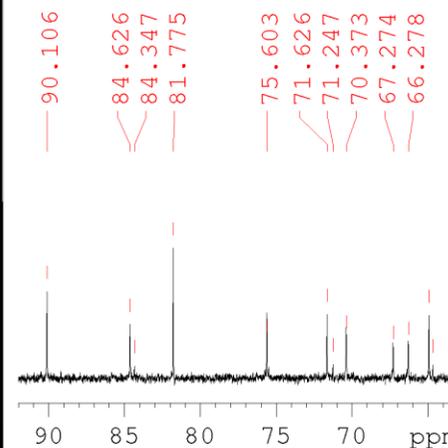
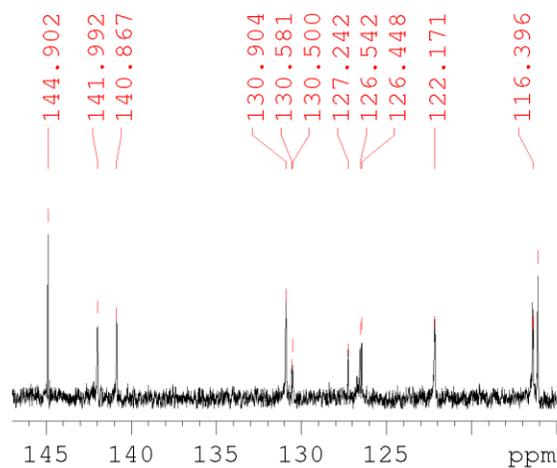




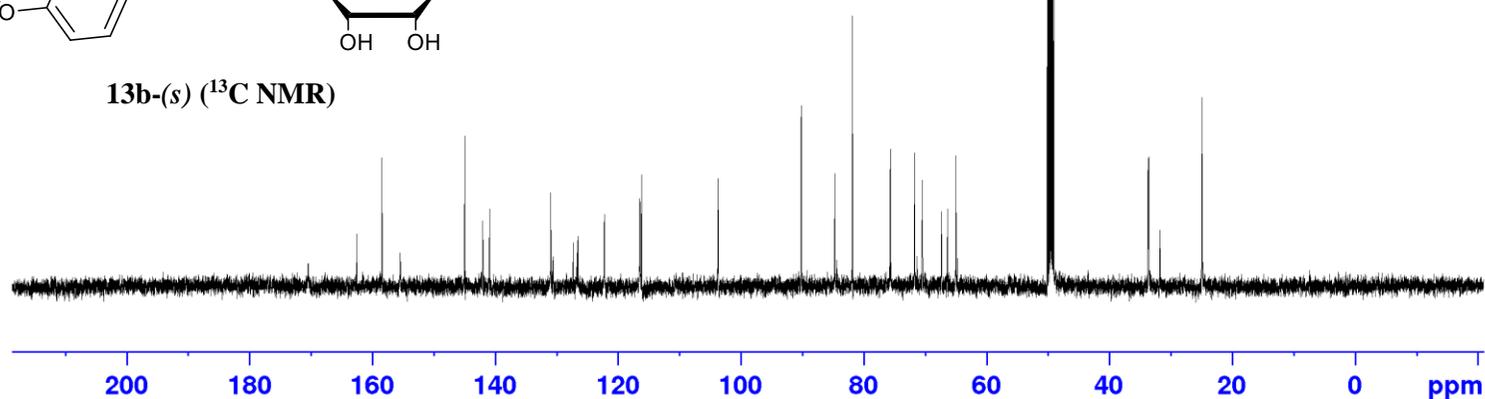
Current Data Parameters
NAME CD106s
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191213
Time 6.01 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3000
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.2360006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6608789 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13b-(s) (¹³C NMR)



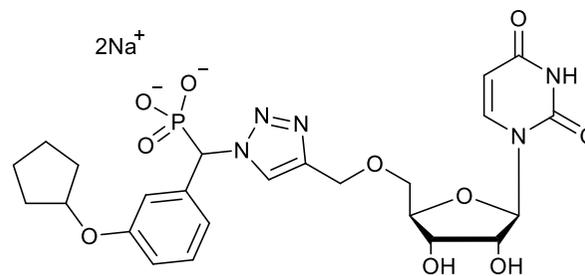


Current Data Parameters
NAME CD106s
EXPNO 5
PROCNO 1

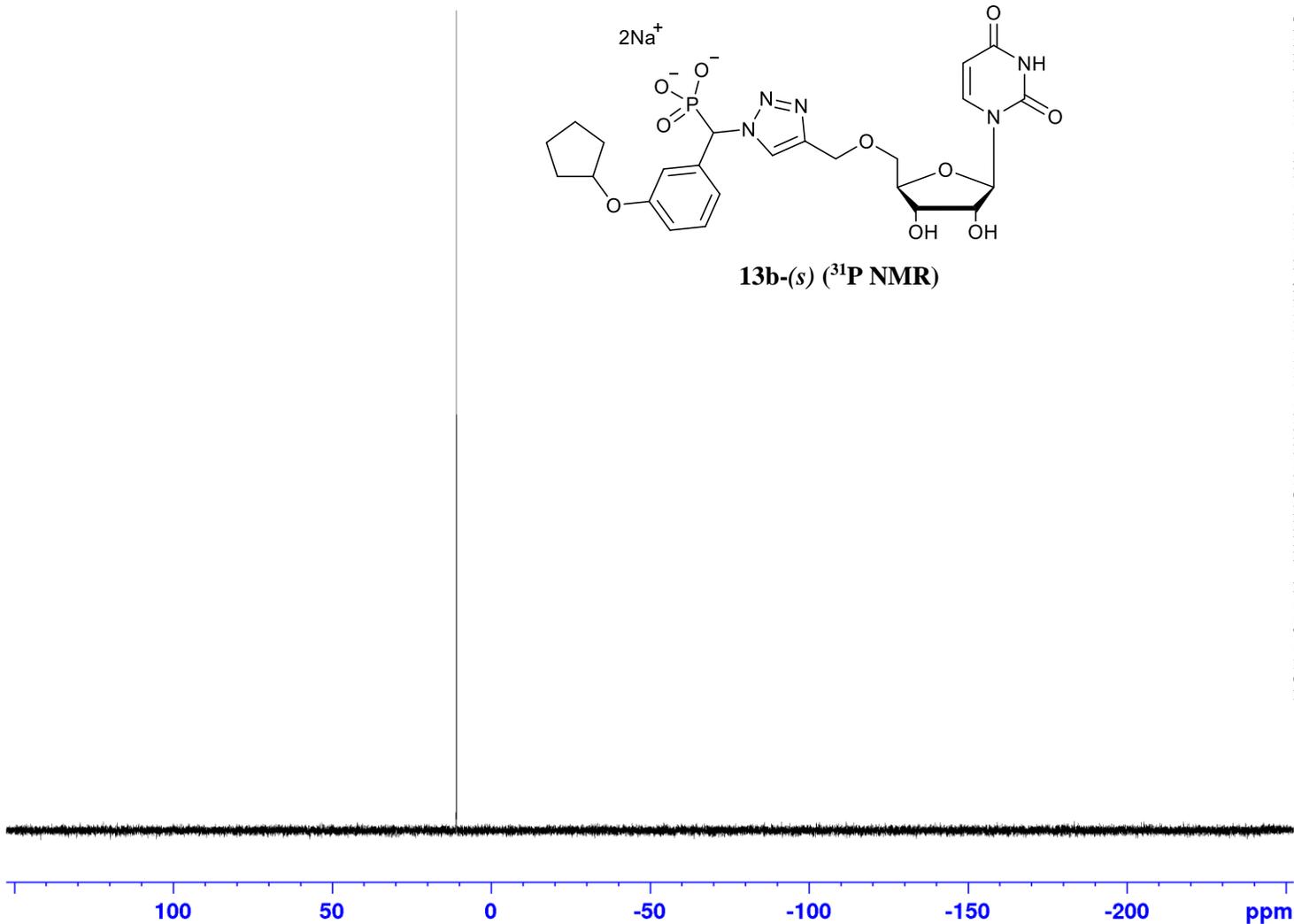
F2 - Acquisition Parameters
Date_ 20191213
Time 6.23 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCL3
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SF02 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10.94



13b-(s) (³¹P NMR)

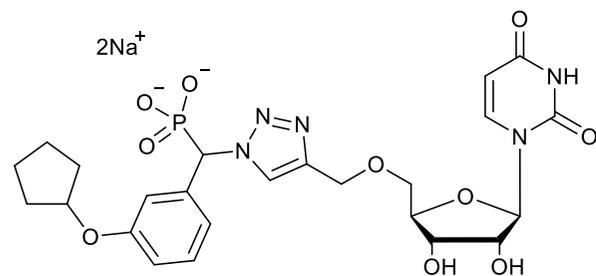




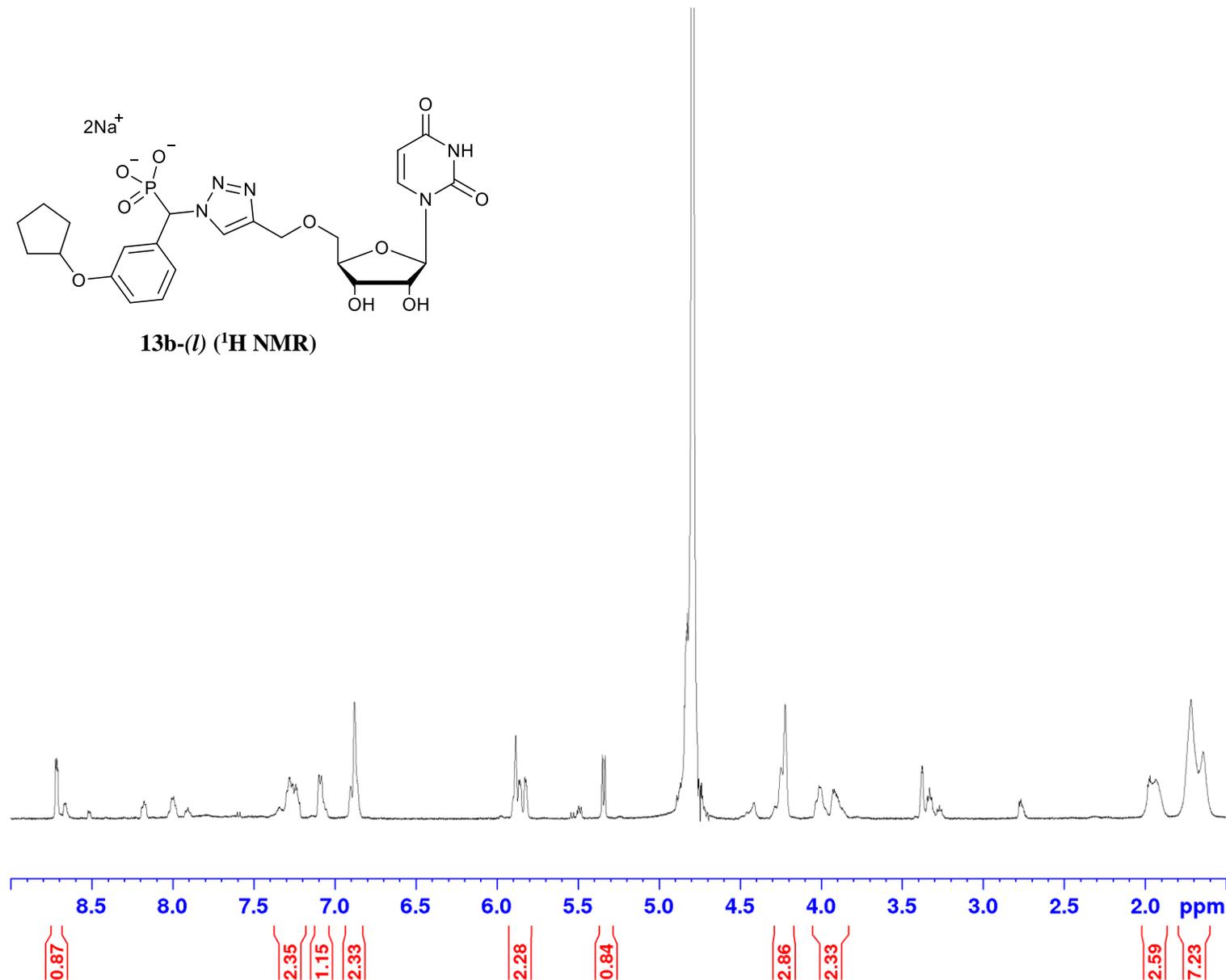
Current Data Parameters
NAME cd9_191211_16
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191211
Time 10.01 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7439563 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13b-(l) (¹H NMR)

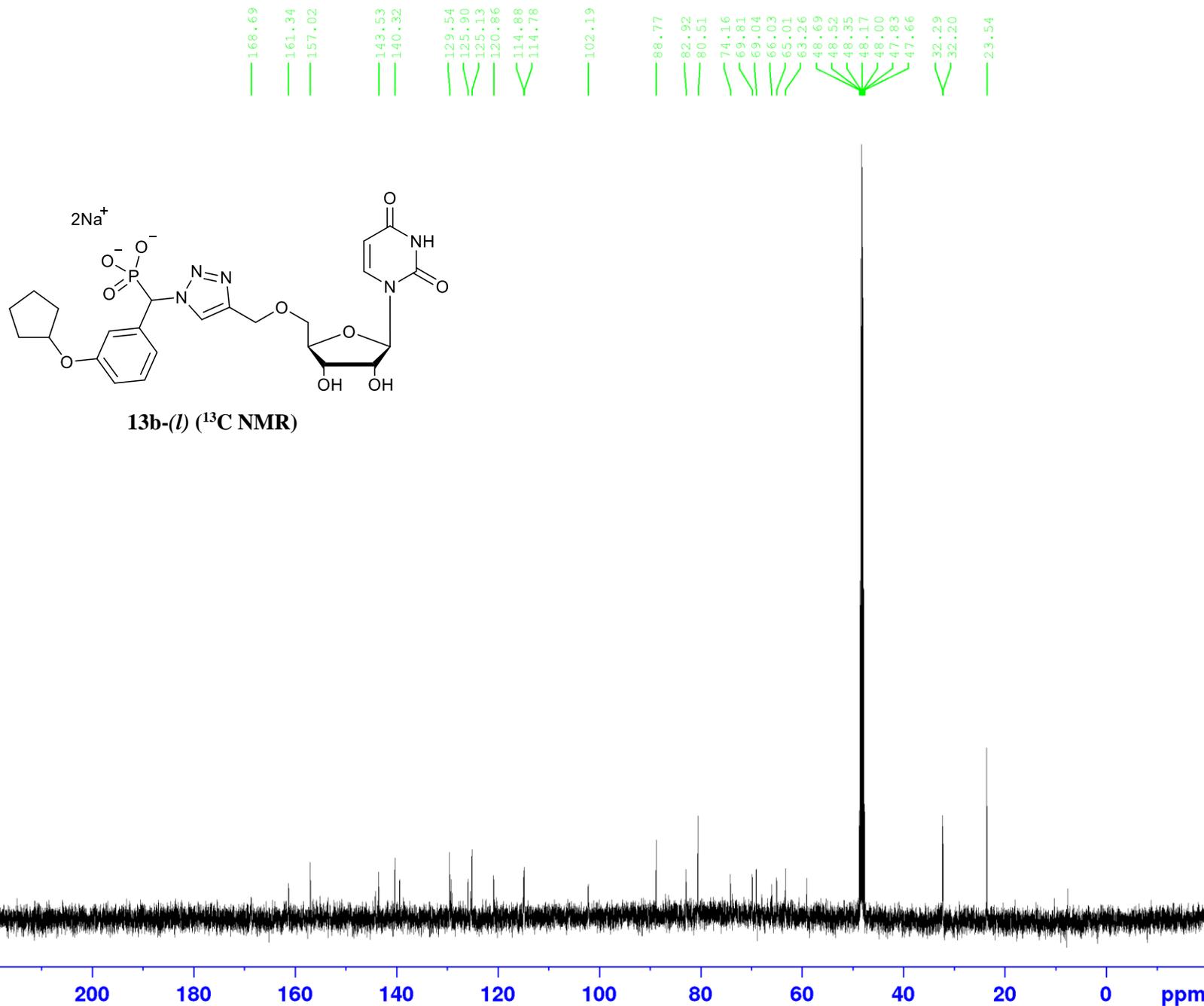




Current Data Parameters
NAME cd9_191211_16
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191212
Time 1.03 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 3000
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6607287 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

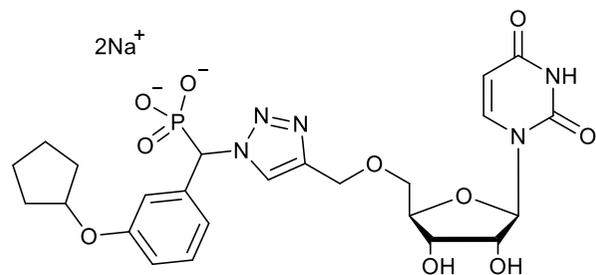




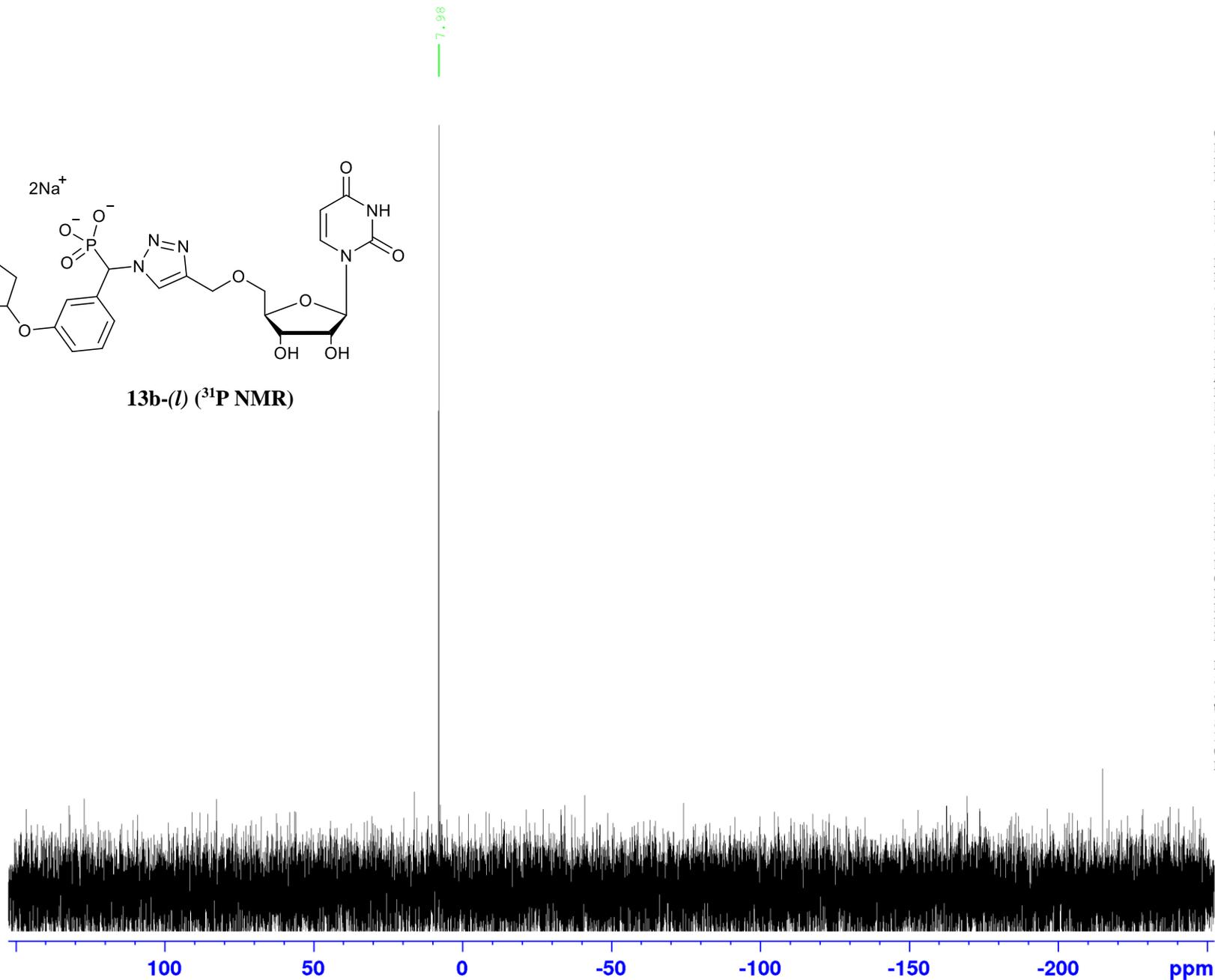
Current Data Parameters
NAME cd9_200213_53
EXPNO 6
PROCNO 1

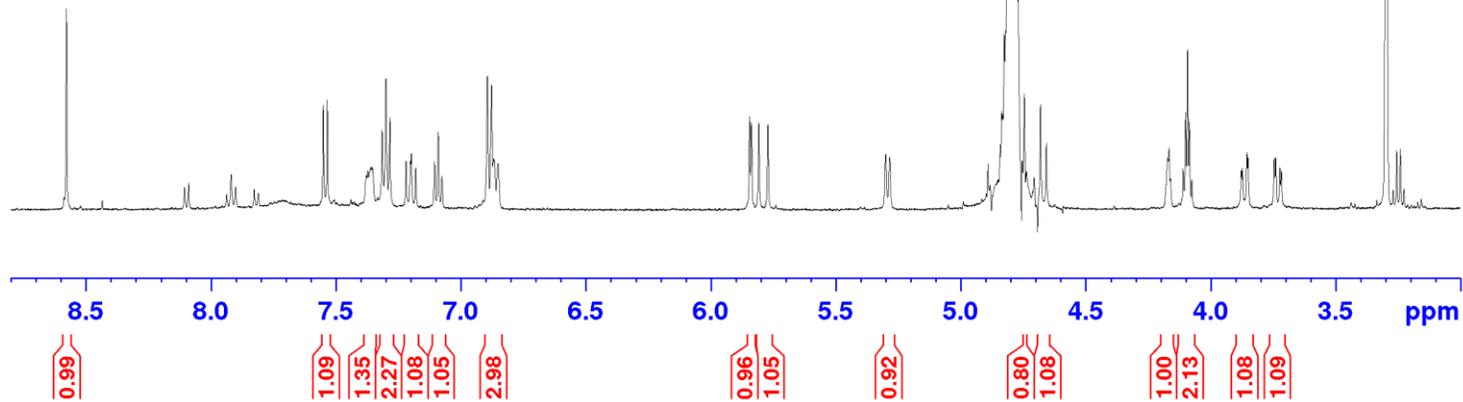
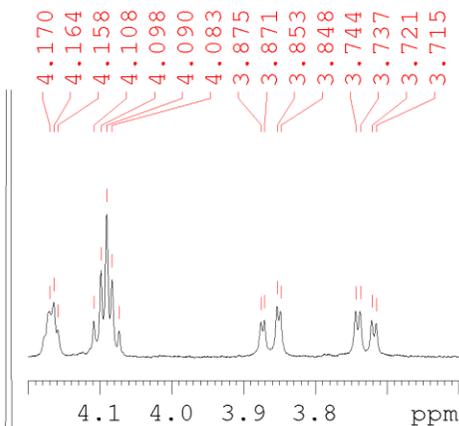
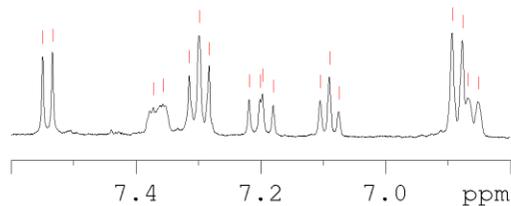
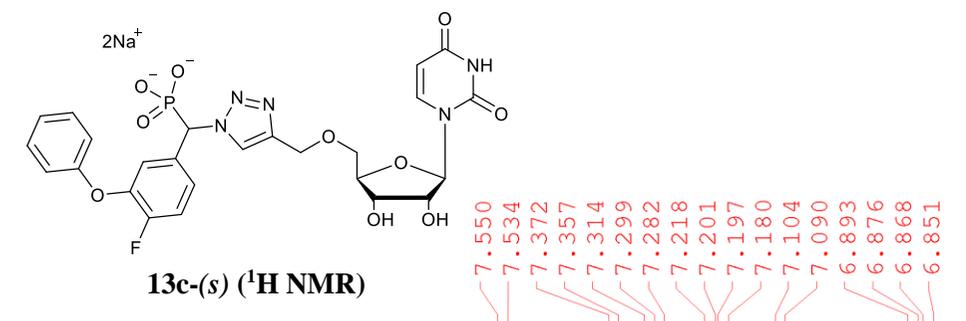
F2 - Acquisition Parameters
Date_ 20200213
Time 22.04 h
INSTRUM CAB AV4 500 MHz BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 286.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SF01 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SF02 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13b-(l) (³¹P NMR)





Current Data Parameters
 NAME CD67_s
 EXPNO 5
 PROCNO 1

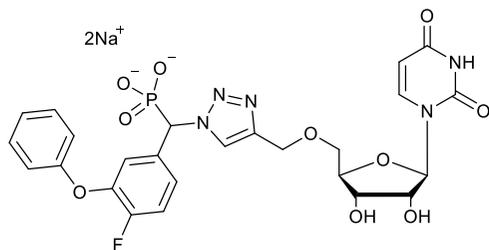
F2 - Acquisition Parameters
 Date_ 20181011
 Time_ 15.27 h
 INSTRUM CAB AV4 500 MHZ BASIC
 PROBHD Z150364_0005 ()
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 92.3077
 DW 50.000 usec
 DE 16.23 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 499.7470859 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 15.53100014 W

F2 - Processing parameters
 SI 65536
 SF 499.7439580 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

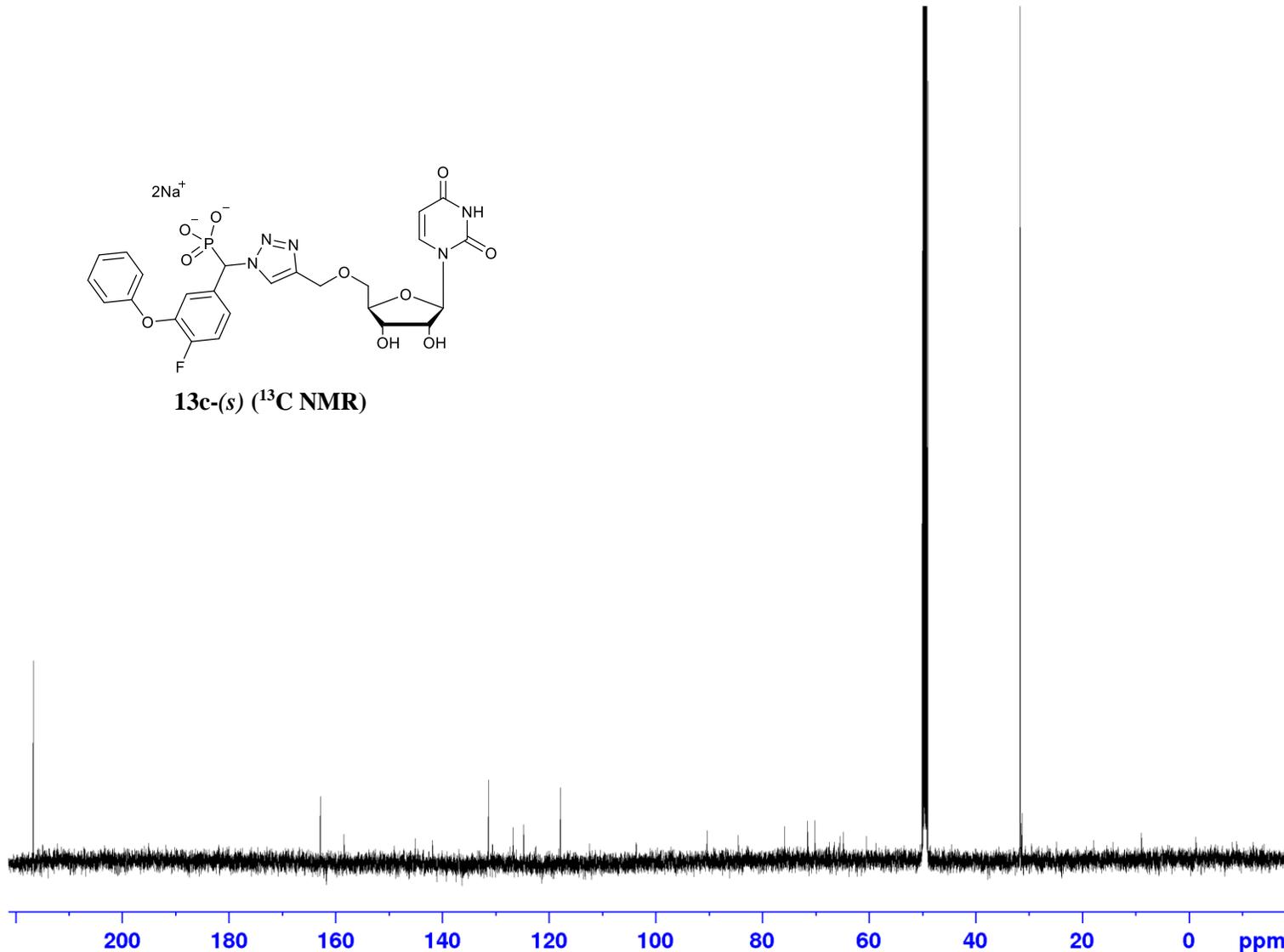
216.72

162.88
158.43
155.80
145.09
141.88
139.17
136.91
131.34
127.31
126.75
126.07
124.76
122.51
118.25
117.87
116.38
115.86
103.70

90.36
84.52
75.78
71.54
70.18
66.47
65.47
64.87
60.48
49.50



13c-(s) (¹³C NMR)



Current Data Parameters
NAME CD67_s
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181012
Time 0.17 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 2056
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

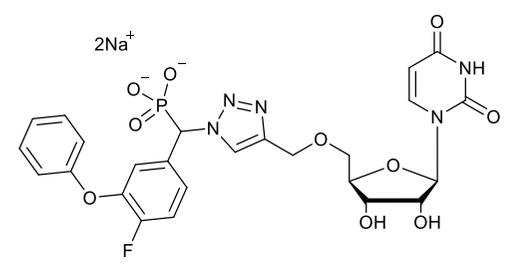
F2 - Processing parameters
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SF 125.6605389 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



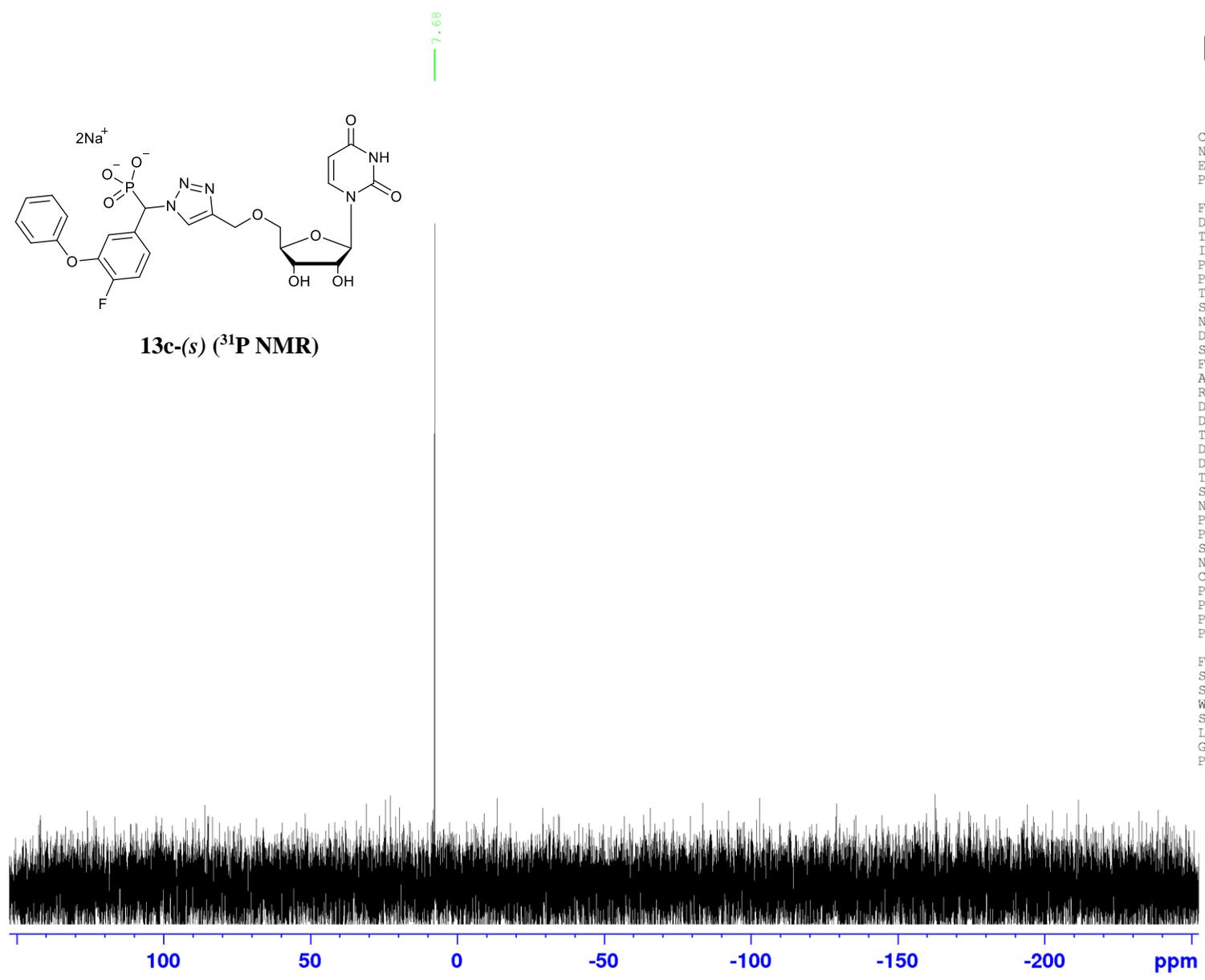
Current Data Parameters
NAME CD67_s
EXPNO 10
PROCNO 1

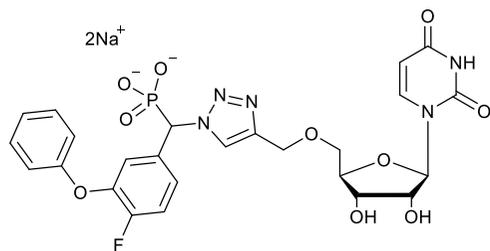
F2 - Acquisition Parameters
Date_ 20181012
Time 0.21 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13c-(s) (³¹P NMR)





13c-(s) (¹⁹F NMR)

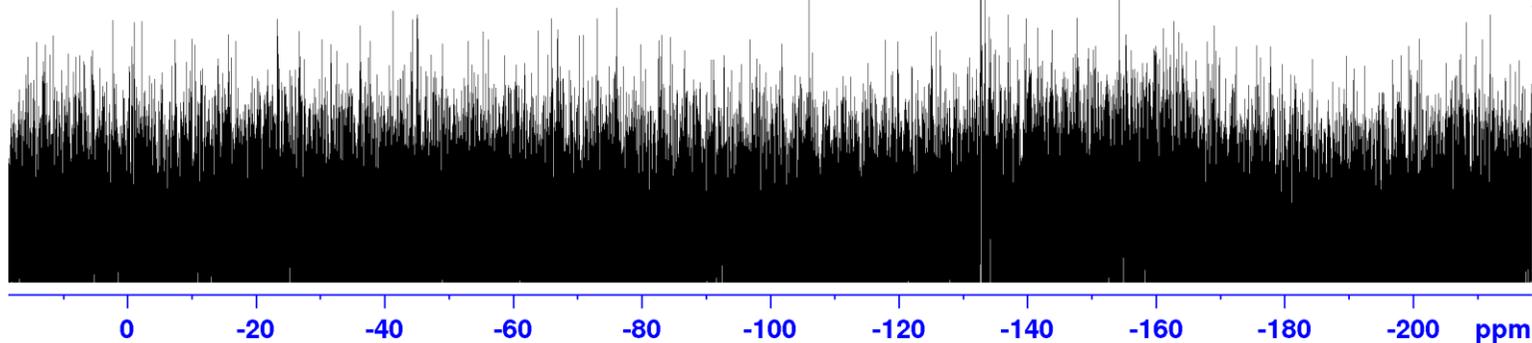
-132.78

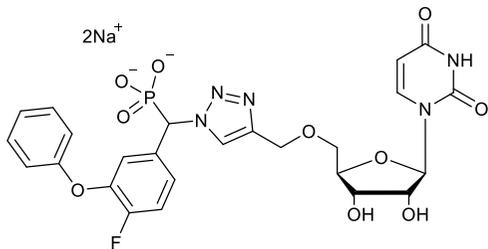


Current Data Parameters
 NAME cd2_200107_17
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200107
 Time 9.47 h
 INSTRUM spect
 PROBHD Z108618_0921 (
 PULPROG zgflqn
 TD 65536
 SOLVENT D2O
 NS 64
 DS 0
 SWH 89285.711 Hz
 FIDRES 2.724784 Hz
 AQ 0.3670016 sec
 RG 196.38
 DW 5.600 usec
 DE 120.00 usec
 TE 298.7 K
 D1 1.00000000 sec
 TD0 1
 SF01 376.4889413 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 17.75399971 W

F2 - Processing parameters
 SI 65536
 SF 376.5265940 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





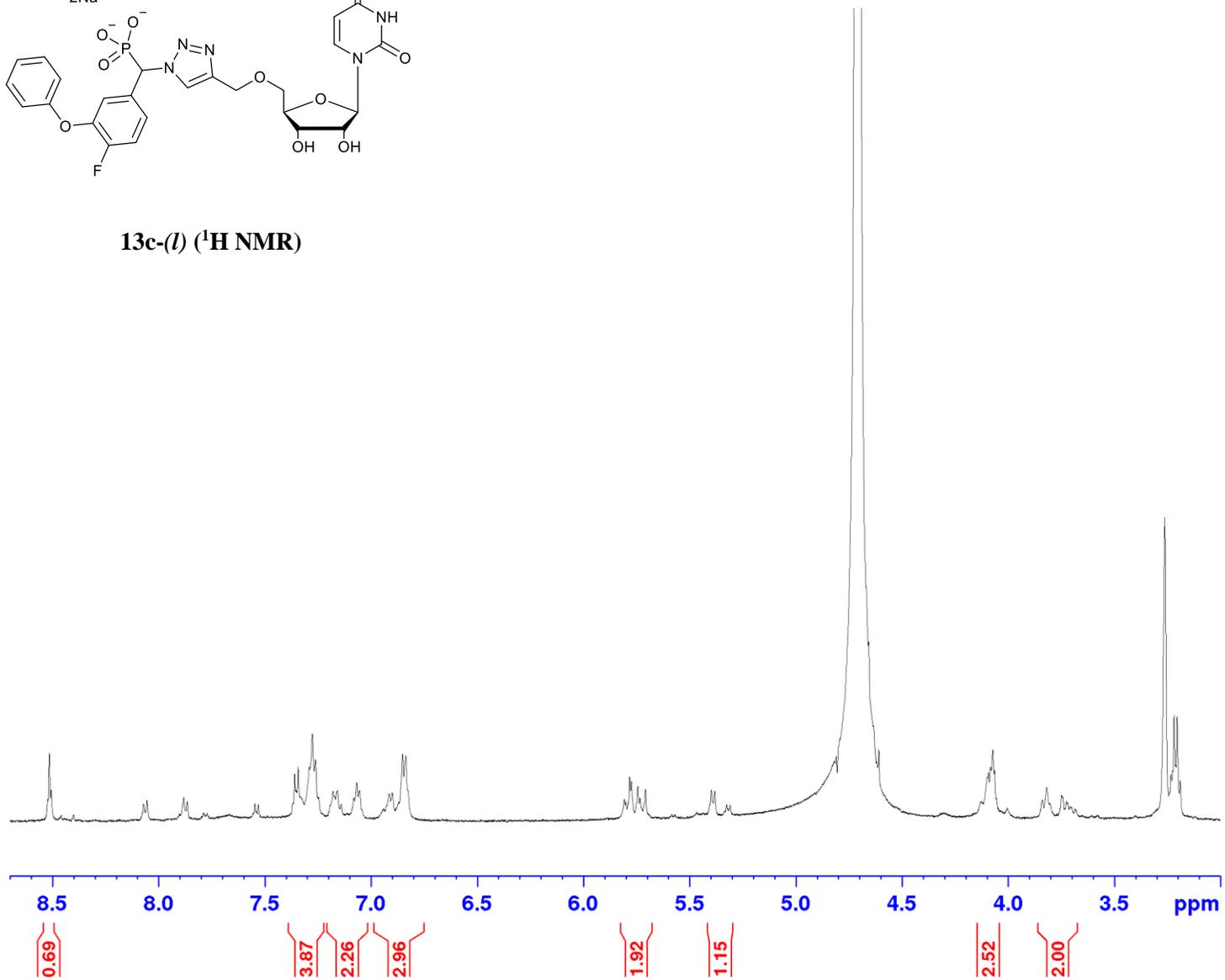
13c-(I) (¹H NMR)

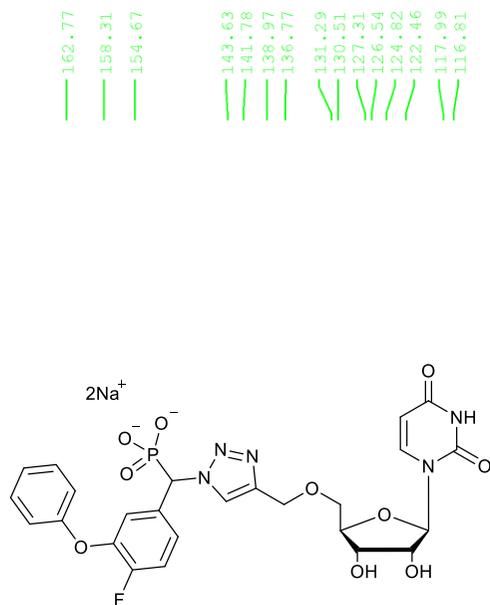


Current Data Parameters
 NAME CD67_1
 EXPNO 5
 PROCNO 1

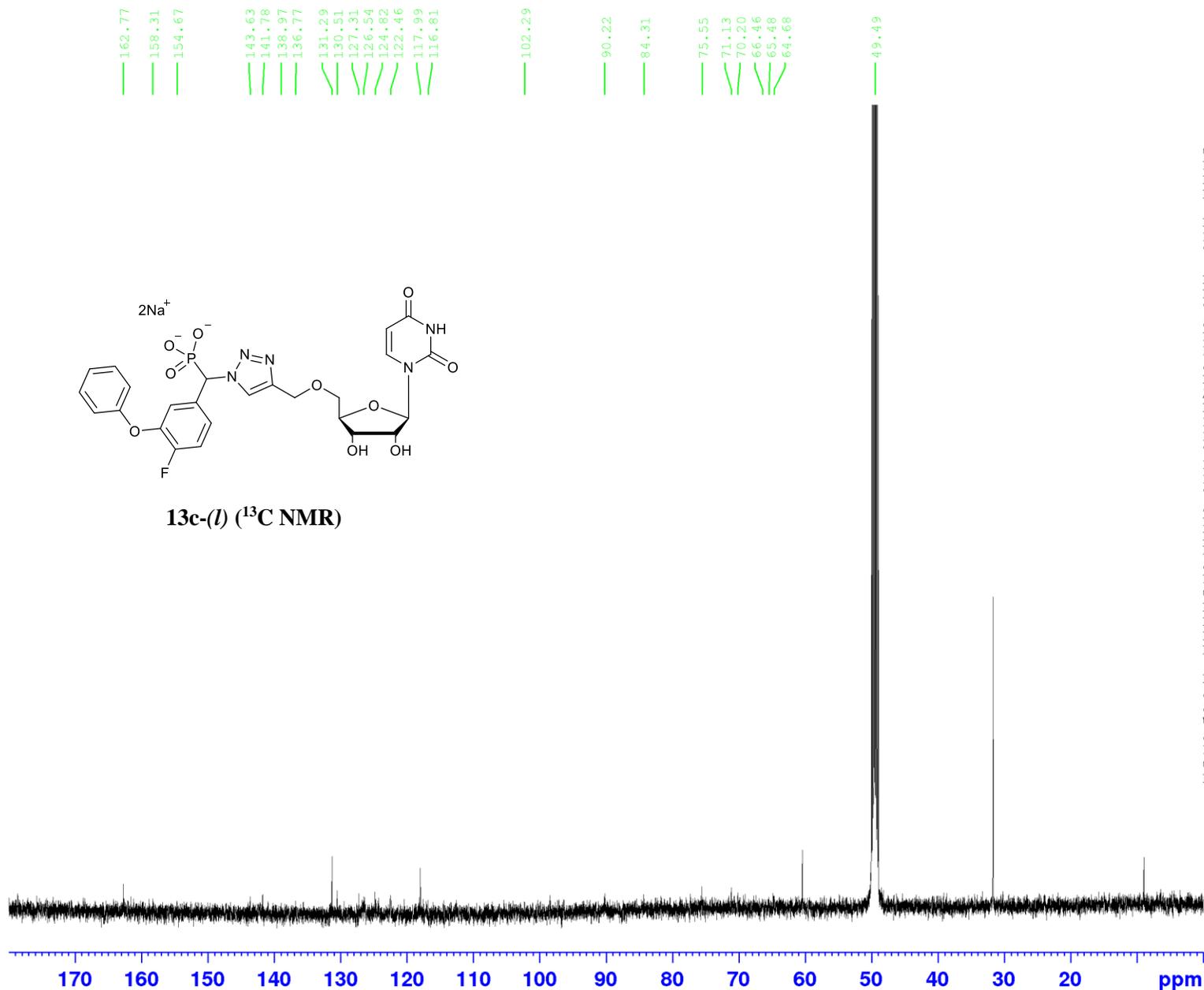
F2 - Acquisition Parameters
 Date_ 20181011
 Time 19.52 h
 INSTRUM CAB AV4 500 MHZ BASIC
 PROBHD Z150364_0005 (
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 101
 DW 50.000 usec
 DE 16.23 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 499.7470859 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 15.53100014 W

F2 - Processing parameters
 SI 65536
 SF 499.7440000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





13c-(I) (¹³C NMR)



Current Data Parameters
 NAME CD67_1
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181011
 Time 19.49 h
 INSTRUM CAB AV4 500 MHZ BASIC
 PROBHD Z150364_0005 (
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 2000
 DS 4
 SWH 30120.482 Hz
 FIDRES 0.919204 Hz
 AQ 1.0878977 sec
 RG 101
 DW 16.600 usec
 DE 18.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SF01 125.6732948 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 51.23600006 W
 SF02 499.7459990 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 15.53100014 W
 PLW12 0.34944999 W
 PLW13 0.17549001 W

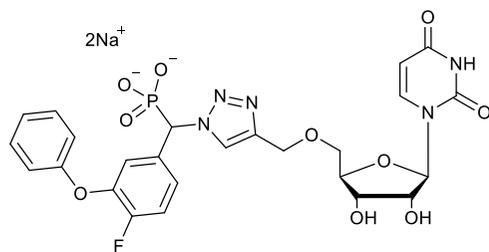
F2 - Processing parameters
 SI 32768
 SF 125.6605531 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME CD67_1
EXPNO 10
PROCNO 1

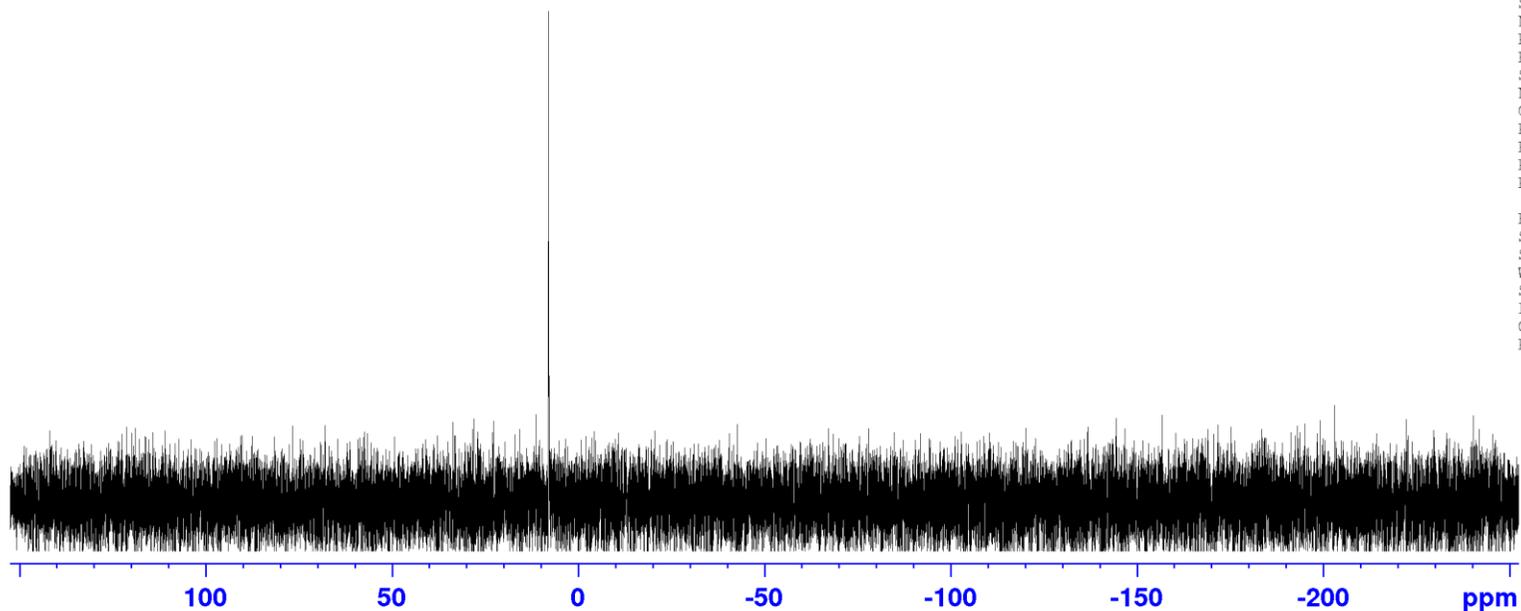
F2 - Acquisition Parameters
Date_ 20181011
Time 21.53 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 ()
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13c-(I) (³¹P NMR)

7.93





Current Data Parameters
NAME CD104s
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191219
Time 13.50 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7439590 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.68
8.67

7.51
7.49
7.48

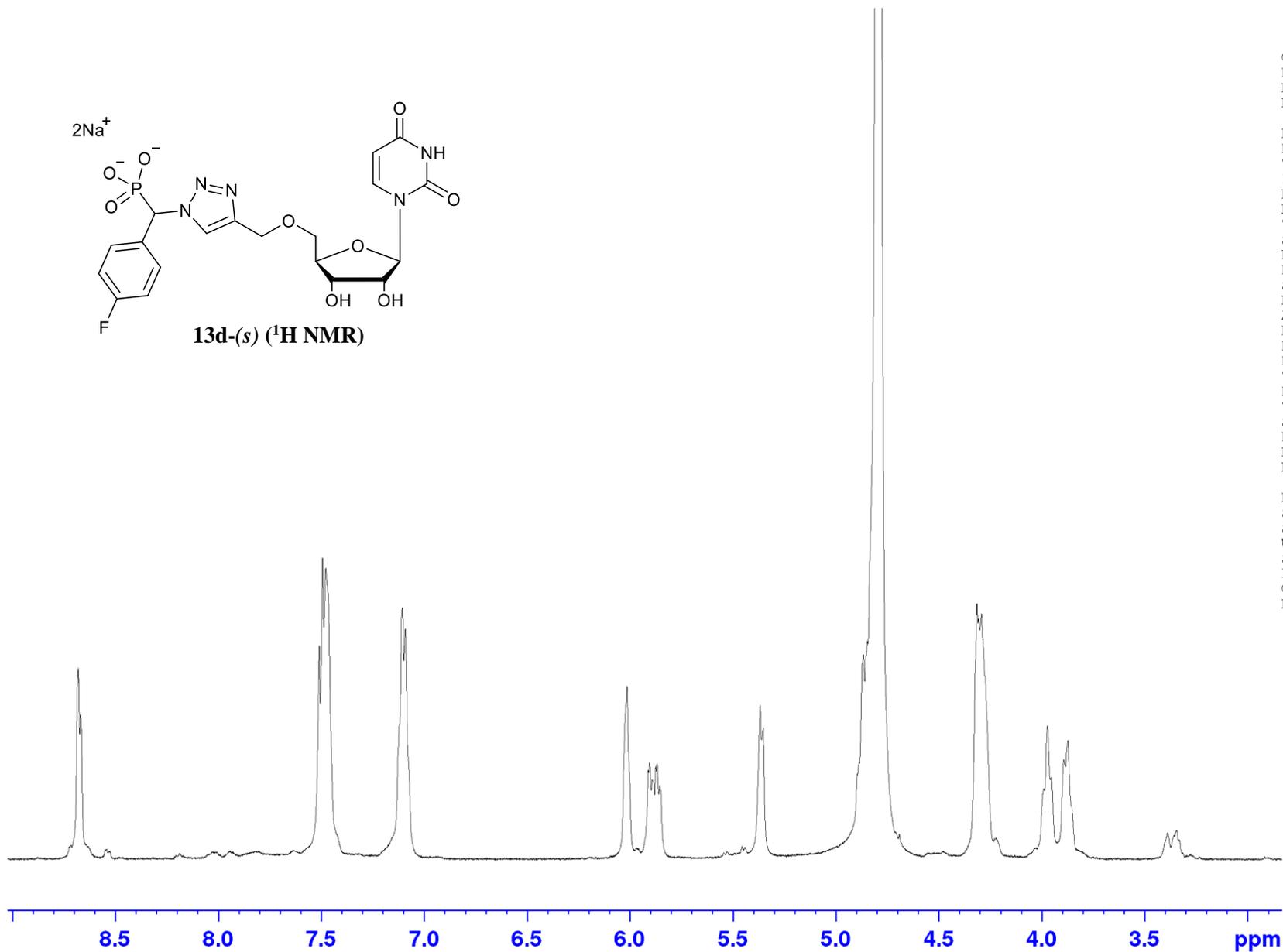
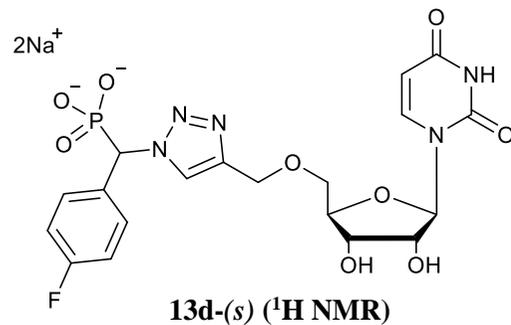
7.11
7.09

6.01
5.91
5.90
5.89
5.87
5.85

5.37
5.35

4.31
4.31
4.29

3.99
3.97
3.95
3.89
3.87

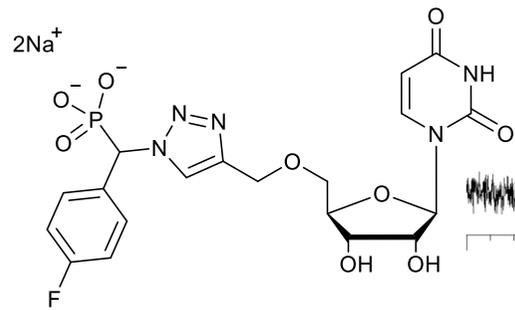




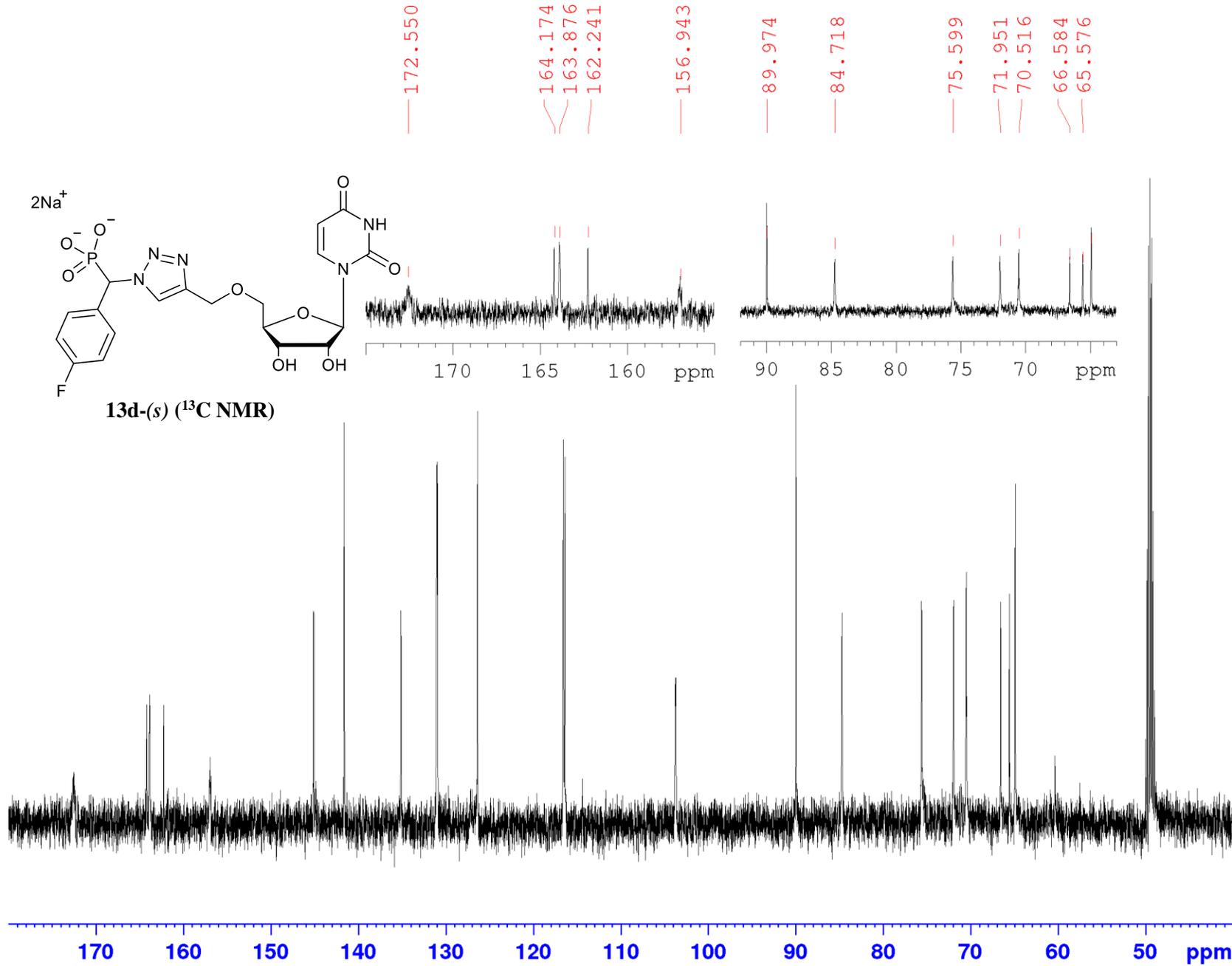
Current Data Parameters
NAME CD104s
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191220
Time 5.58 h
INSTRUM CAB AV4 500 MHz BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 3200
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6605690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13d-(s) (¹³C NMR)



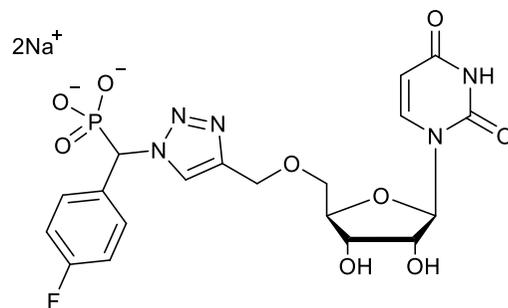


Current Data Parameters
NAME CD104s
EXPNO 5
PROCNO 1

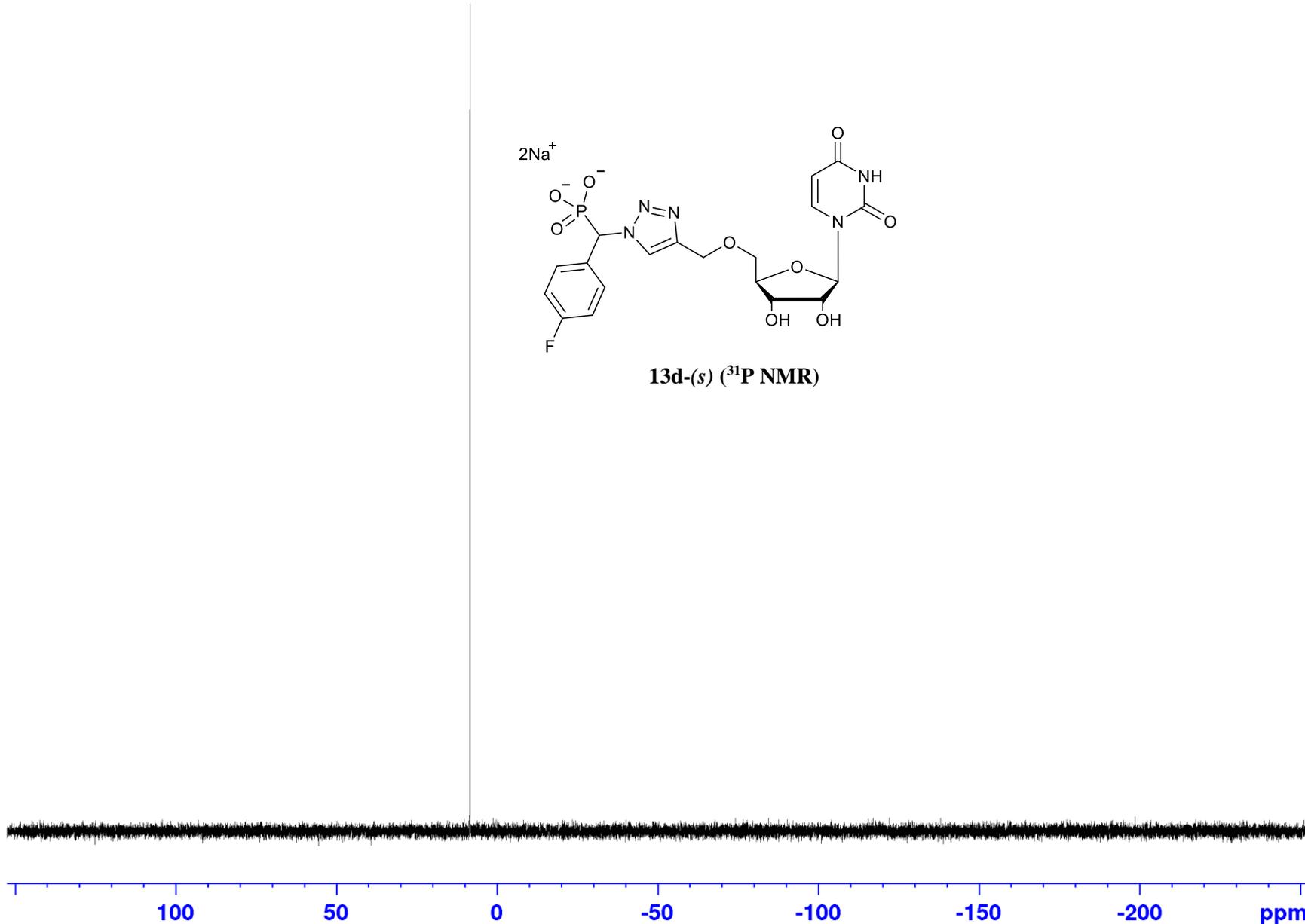
F2 - Acquisition Parameters
Date_ 20191220
Time 6.23 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 ()
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

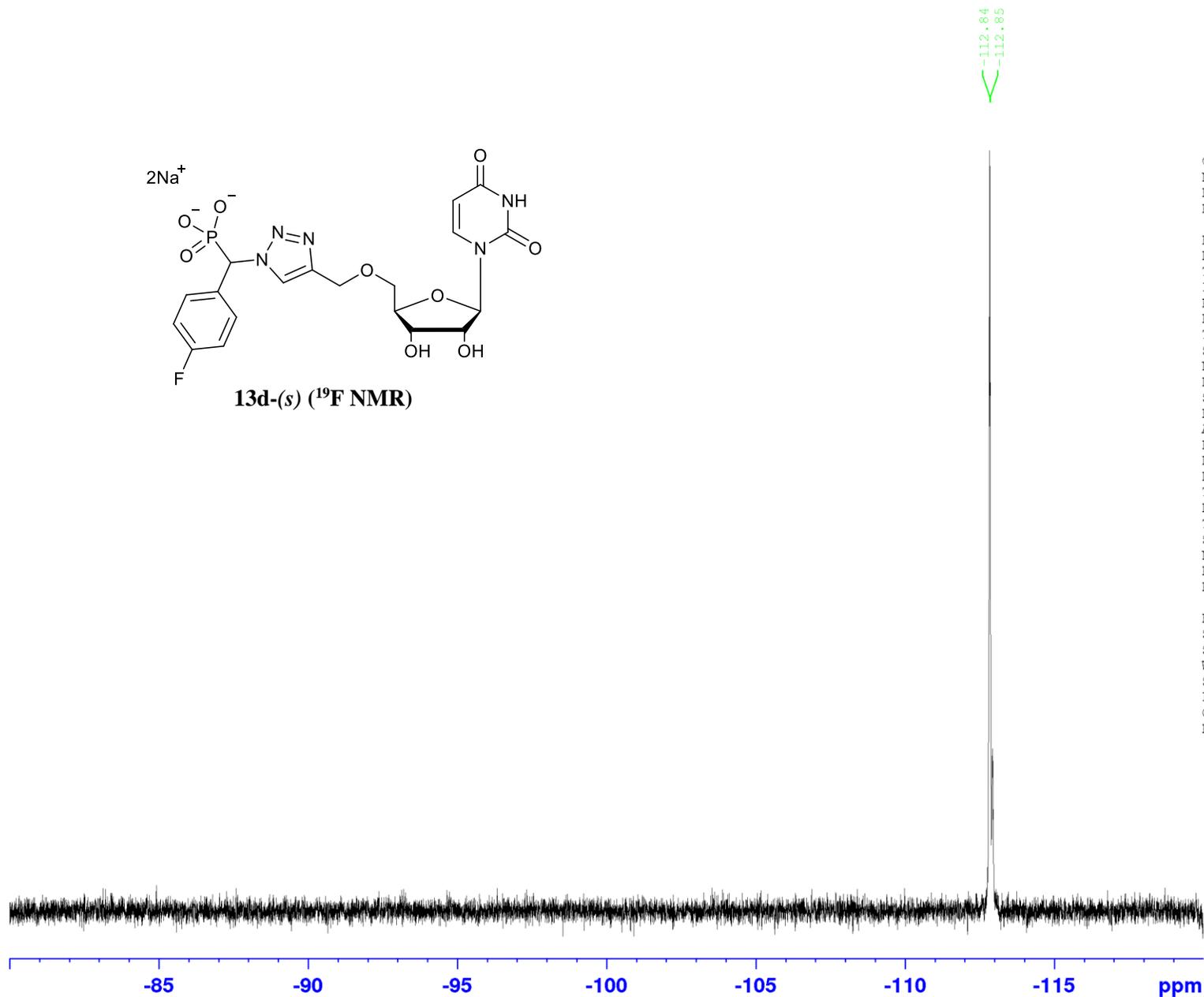
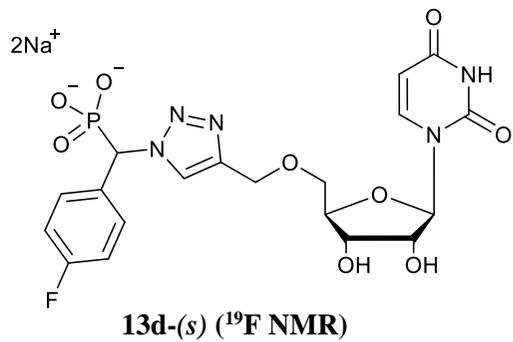
F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

8.44



13d-(s) (³¹P NMR)





Current Data Parameters
 NAME 19F
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200303
 Time 14.25 h
 INSTRUM spect
 PROBHD Z108618_0921 (
 PULPROG zgfglqn
 ID 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 89285.711 Hz
 FIDRES 2.724784 Hz
 AQ 0.3670016 sec
 RG 196.38
 DW 5.600 usec
 DE 120.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 376.4889413 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 17.75399971 W

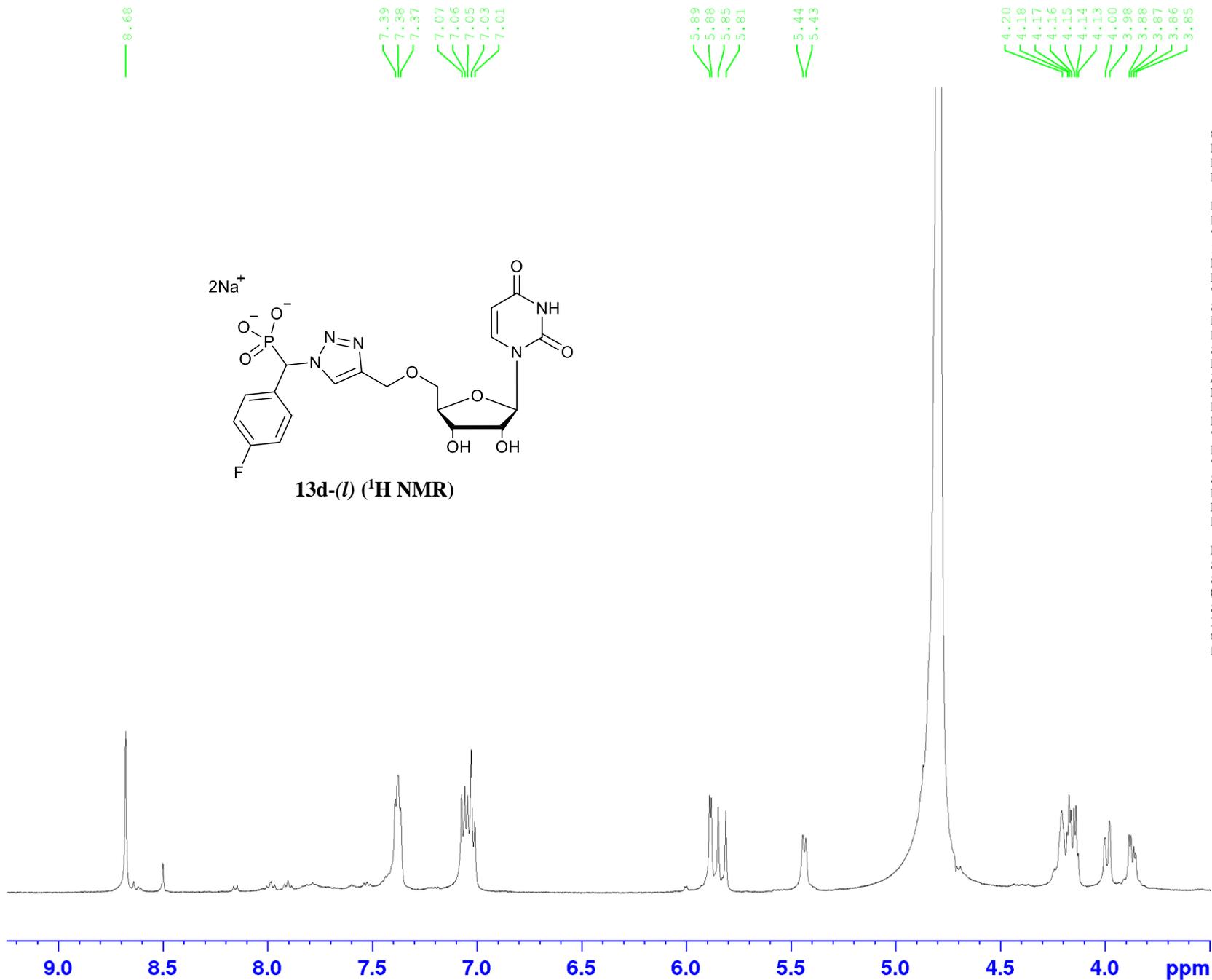
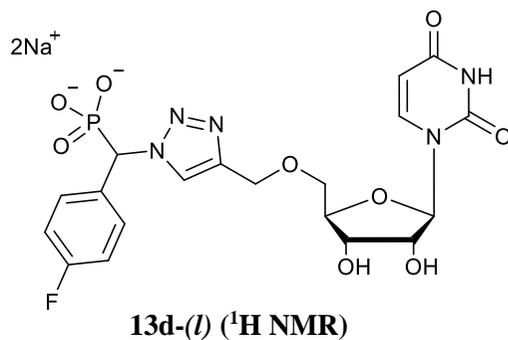
F2 - Processing parameters
 SI 65536
 SF 376.5265940 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME CD1041
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191219
Time 11.46 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 92.3077
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7439587 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

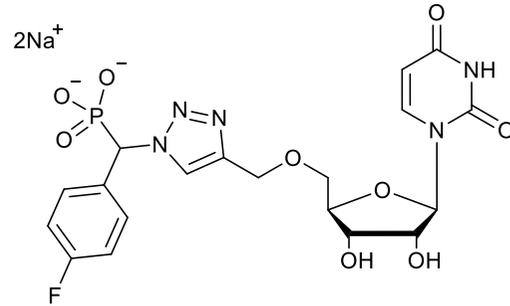




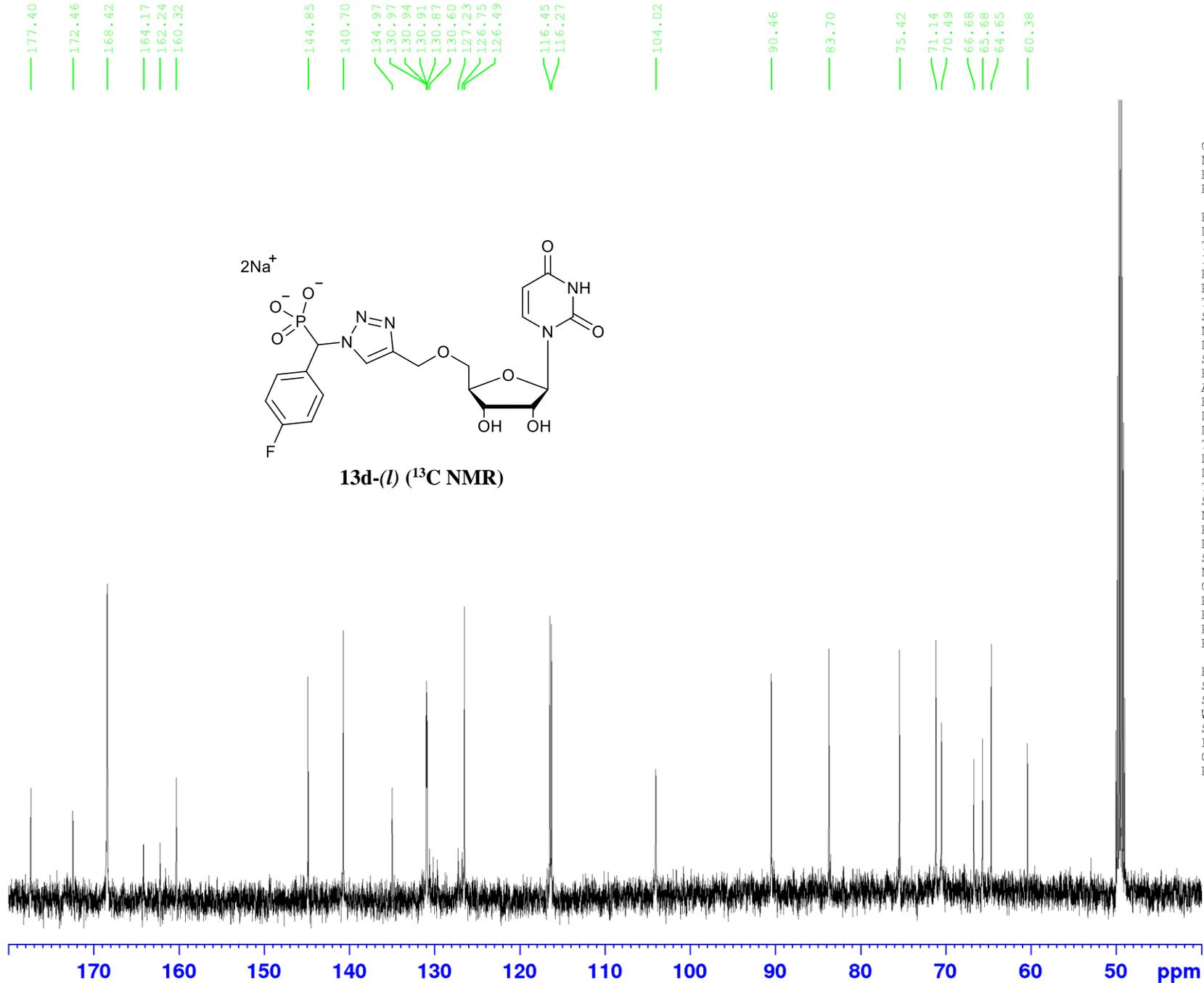
Current Data Parameters
NAME CD1041
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191220
Time 1.46 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 3000
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6605569 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13d-(I) (13C NMR)



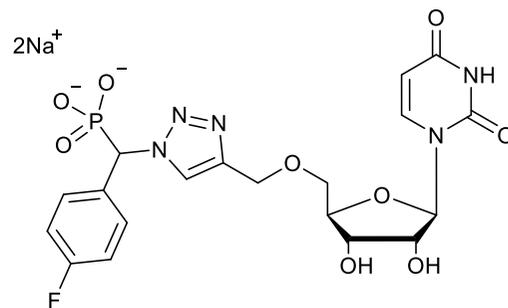


Current Data Parameters
NAME CD1041
EXPNO 5
PROCNO 1

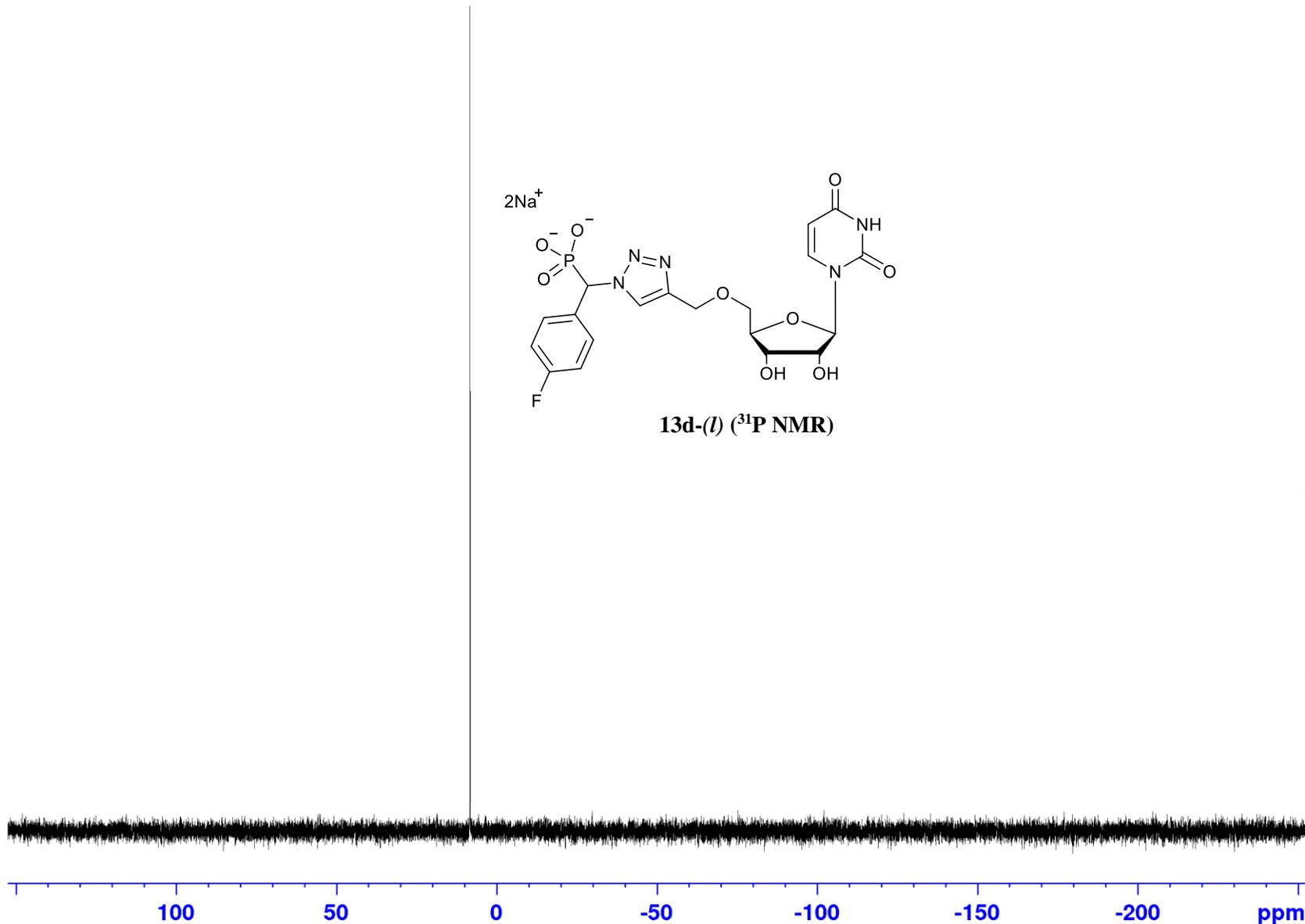
F2 - Acquisition Parameters
Date_ 20191220
Time 2.18 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

8.33



13d-(I) (³¹P NMR)

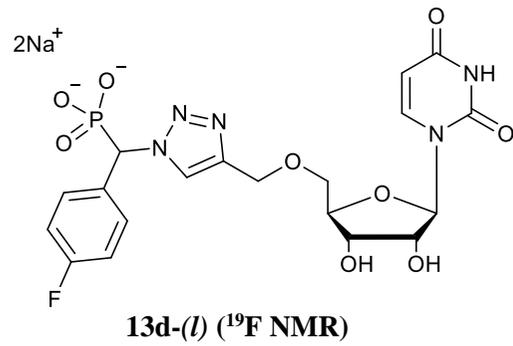




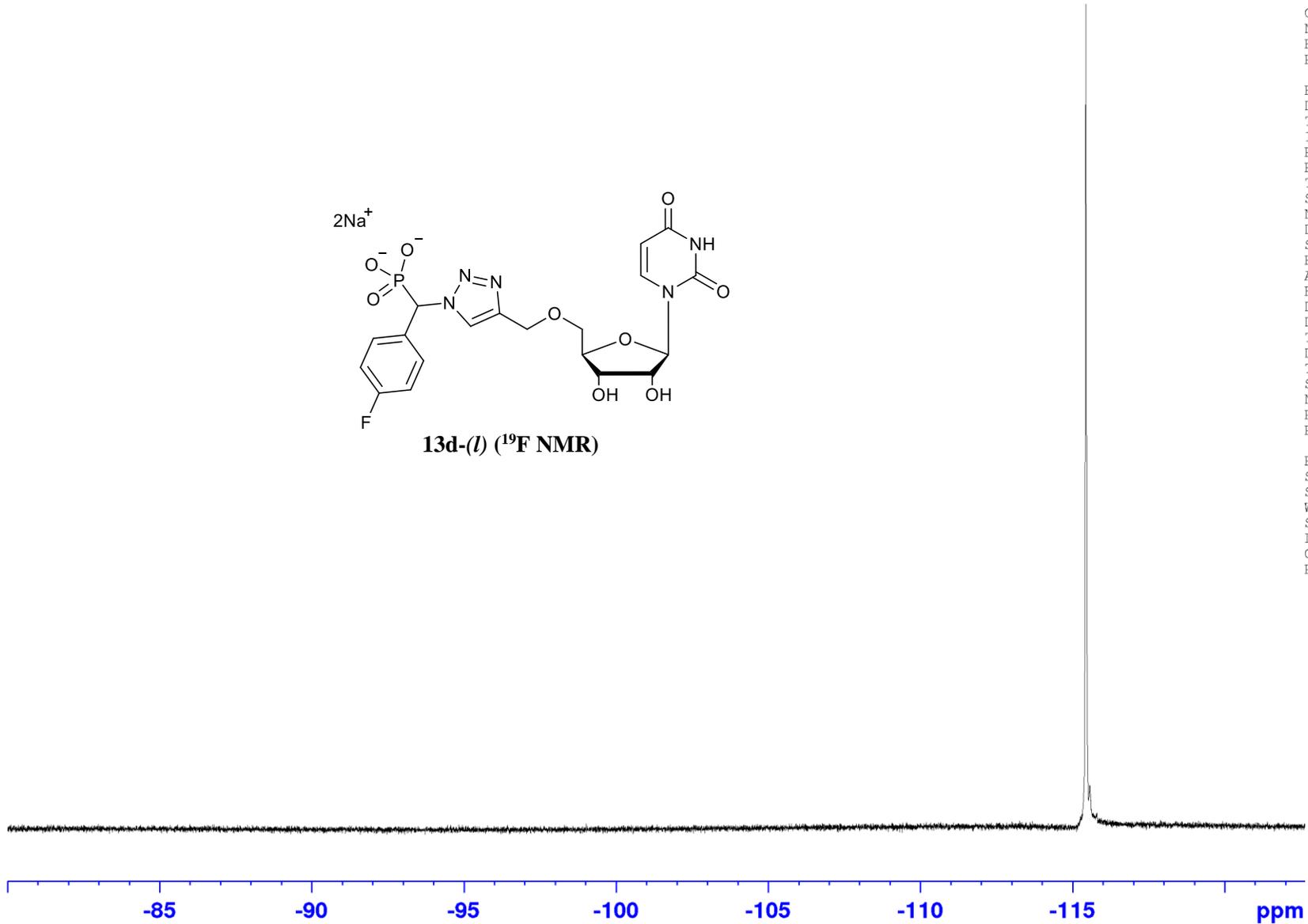
Current Data Parameters
NAME CD1041
EXPNO 6
PROCNO 1

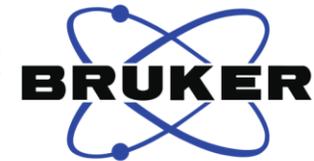
F2 - Acquisition Parameters
Date_ 20191220
Time 2.21 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg
TD 131072
SOLVENT D2O
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 1.733953 Hz
AQ 0.5767168 sec
RG 101
DW 4.400 usec
DE 180.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 470.1821514 MHz
NUC1 19F
P1 15.00 usec
PLW1 12.56499958 W

F2 - Processing parameters
SI 65536
SF 470.2291743 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



-115.43
-115.45

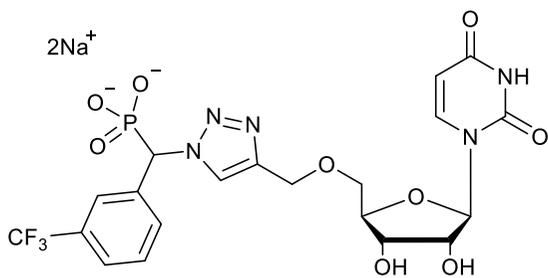




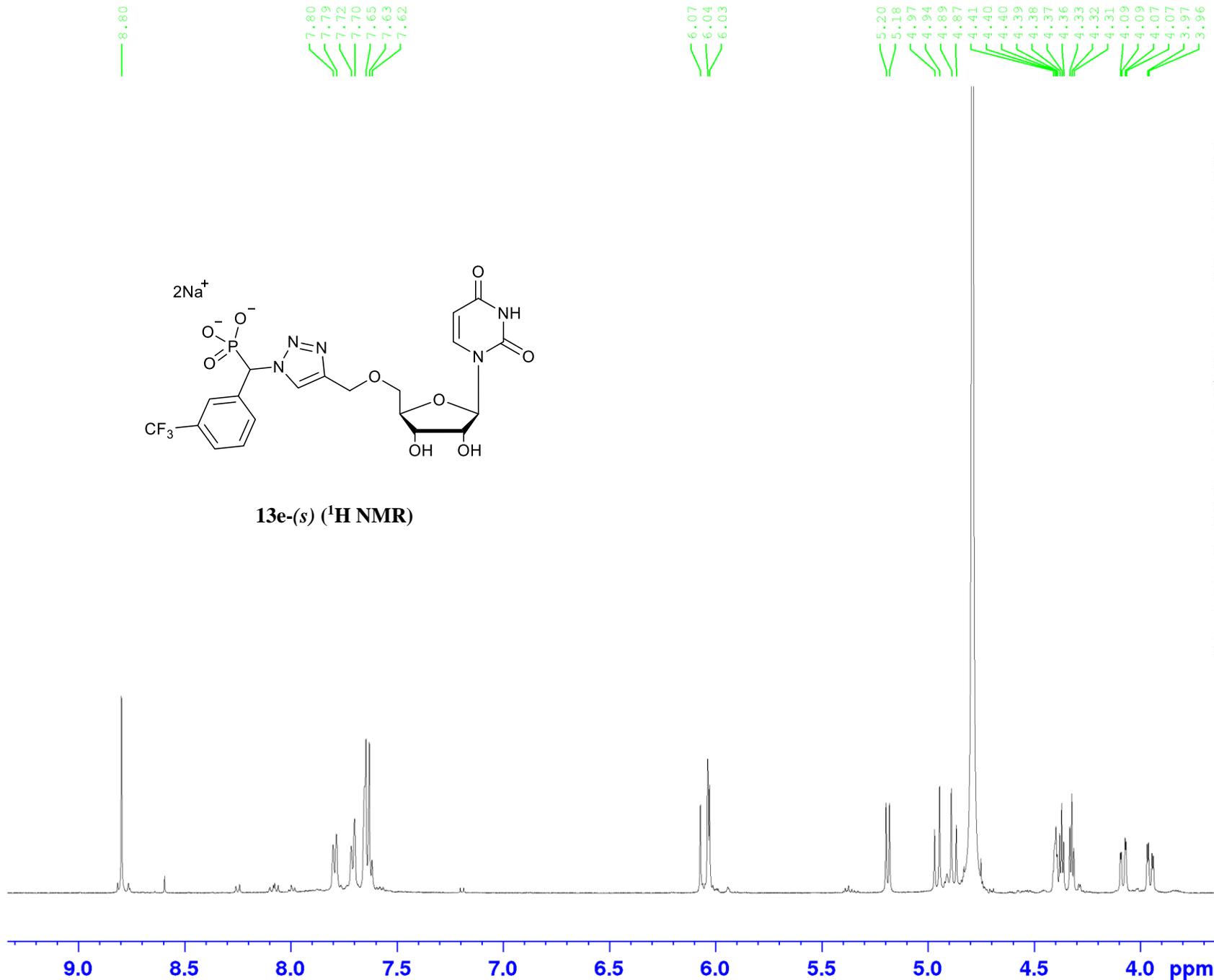
Current Data Parameters
NAME cd9_191219_8
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191219
Time 12.40 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7439583 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13e-(s) (1H NMR)

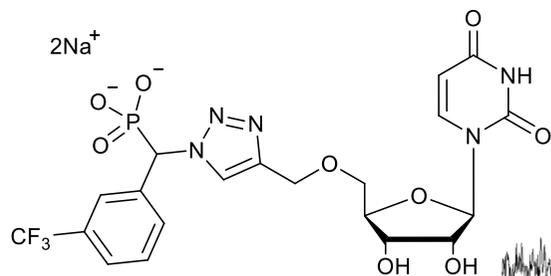




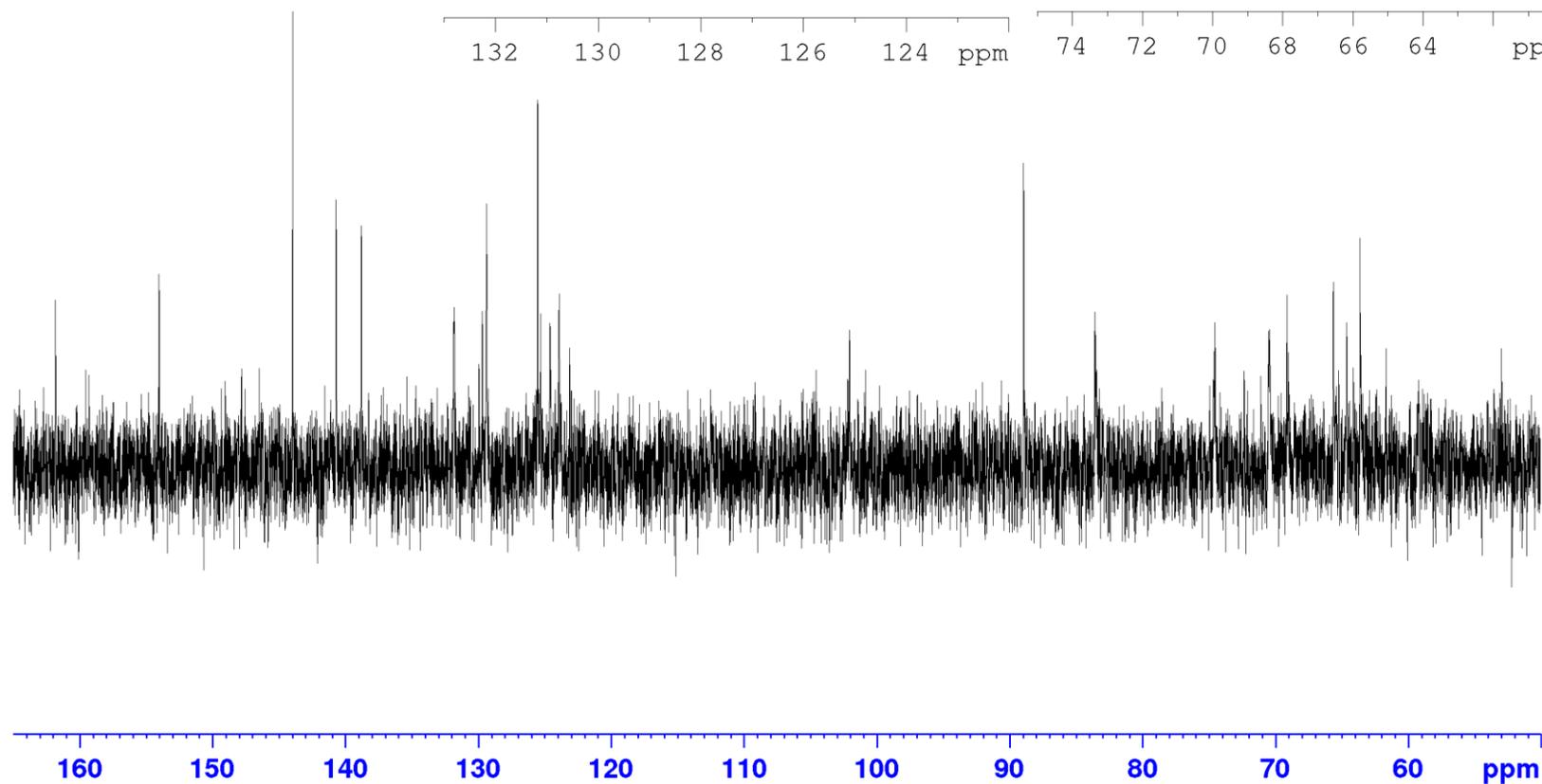
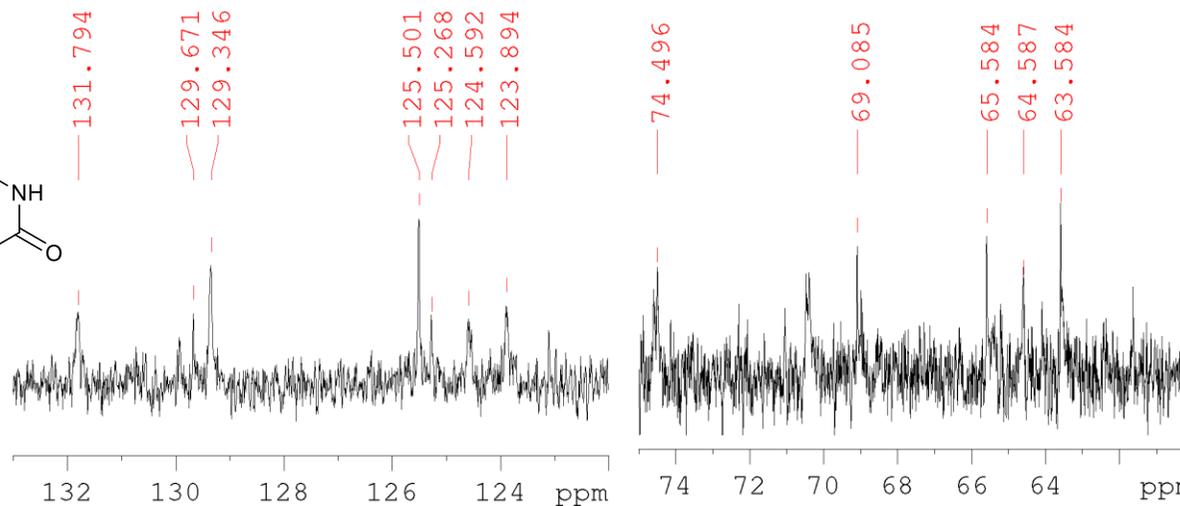
Current Data Parameters
NAME cd9_191219_8
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191219
Time 13.34 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 ()
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 1000
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6607287 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13e-(s) (¹³C NMR)

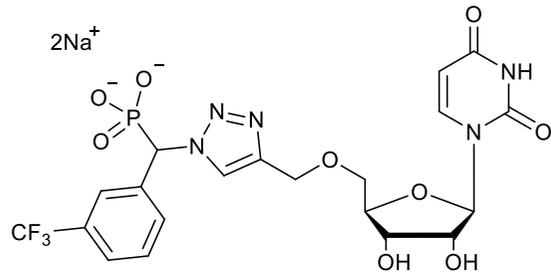




Current Data Parameters
NAME CD108s
EXPNO 5
PROCNO 1

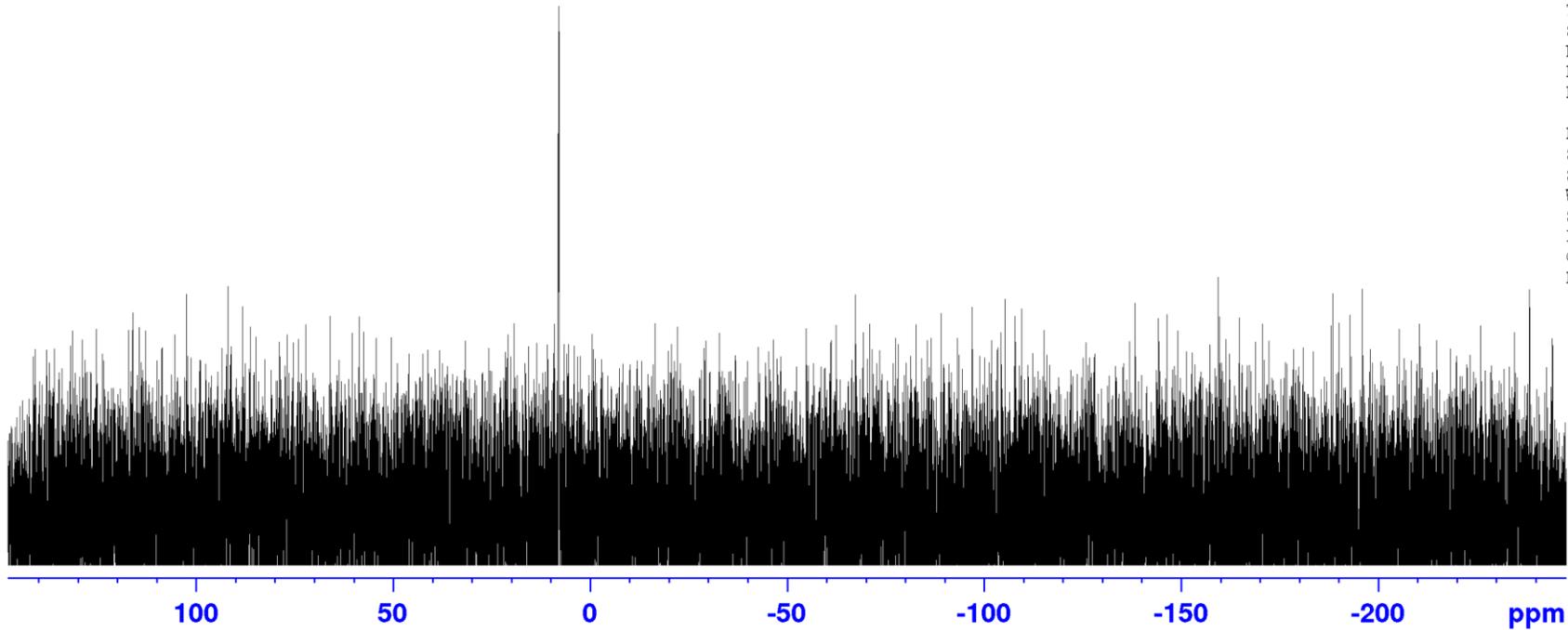
F2 - Acquisition Parameters
Date_ 20191217
Time 3.42 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 4
DS 0
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 usec
DE 50.00 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 usec
PLW1 11.77099991 W

F2 - Processing parameters
SI 32768
SF 161.9877372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13e-(s) (³¹P NMR)

8.01

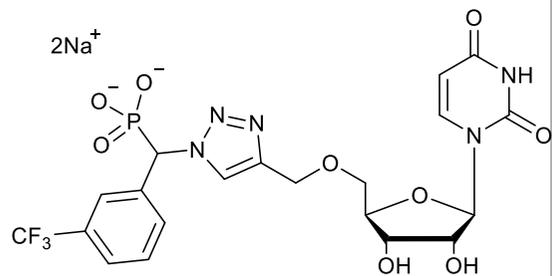




Current Data Parameters
NAME CD108s
EXPNO 6
PROCNO 1

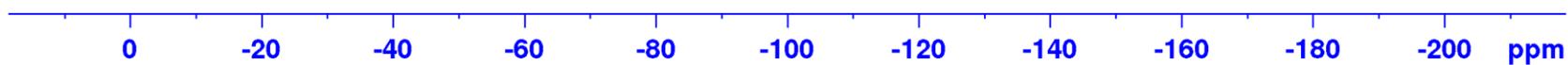
F2 - Acquisition Parameters
Date_ 20191217
Time 3.43 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zgflqn
TD 65536
SOLVENT D2O
NS 4
DS 0
SWH 89285.711 Hz
FIDRES 2.724784 Hz
AQ 0.3670016 sec
RG 196.38
DW 5.600 usec
DE 120.00 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1
SFO1 376.4889413 MHz
NUC1 19F
P1 15.00 usec
PLW1 17.75399971 W

F2 - Processing parameters
SI 65536
SF 376.5265940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13e-(s) (¹⁹F NMR)

-62.22

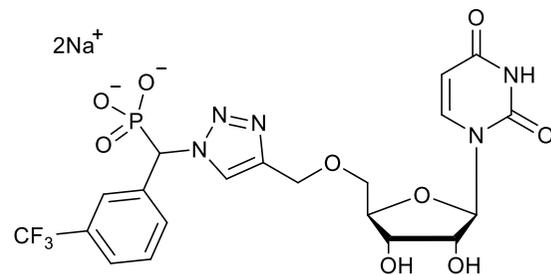




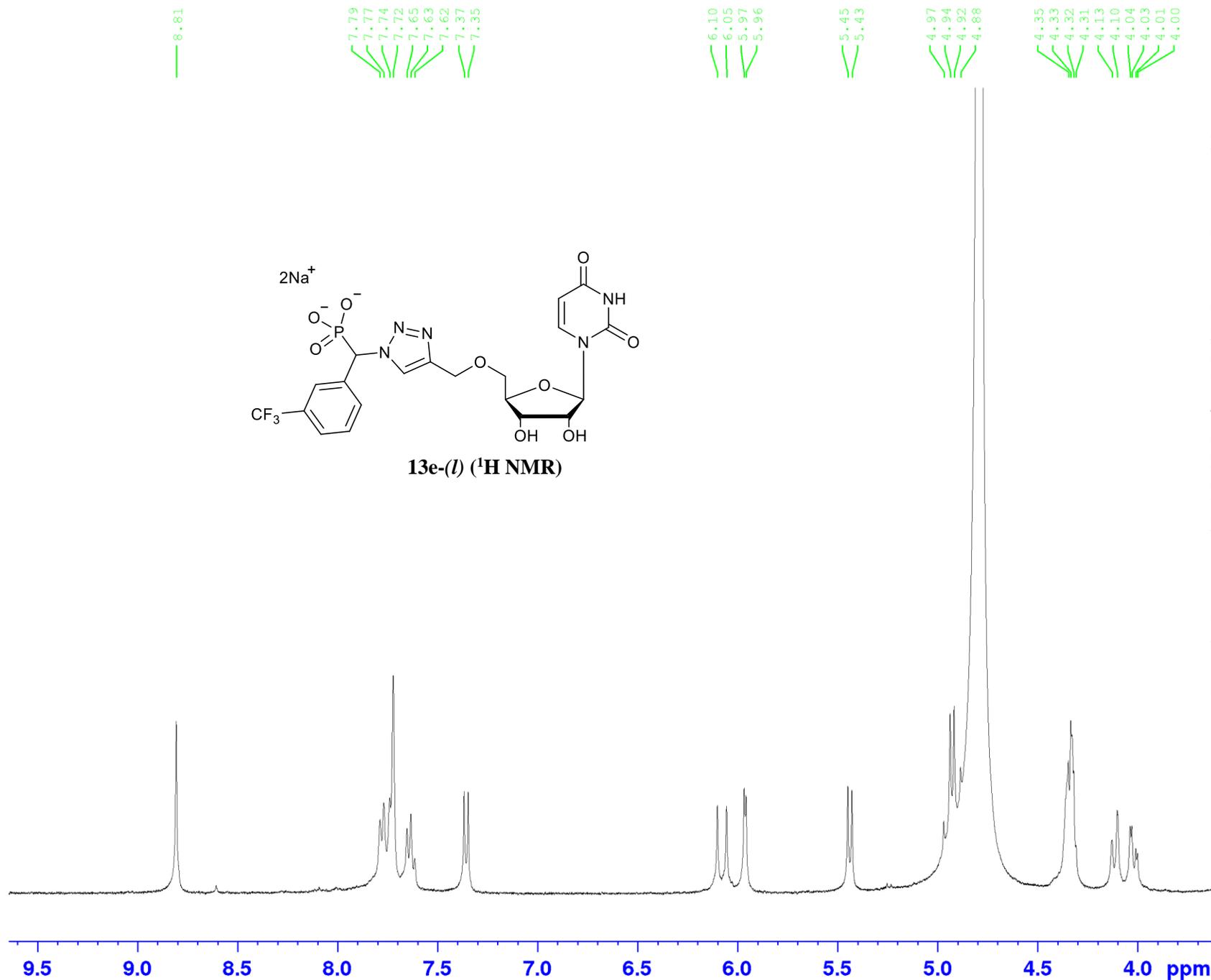
Current Data Parameters
NAME cd2_191217_55
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191217
Time 12.07 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 196.38
DW 62.400 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters
SI 65536
SF 400.1599647 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13e-(I) (¹H NMR)



166.78

152.78

148.17

145.20

142.27

139.76

133.03

130.80

130.51

126.59

125.79

125.02

102.95

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97.11

90.01

84.91

75.72

71.56

70.18

66.75

65.50

64.71

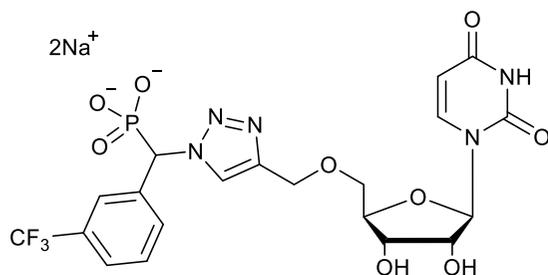
49.71



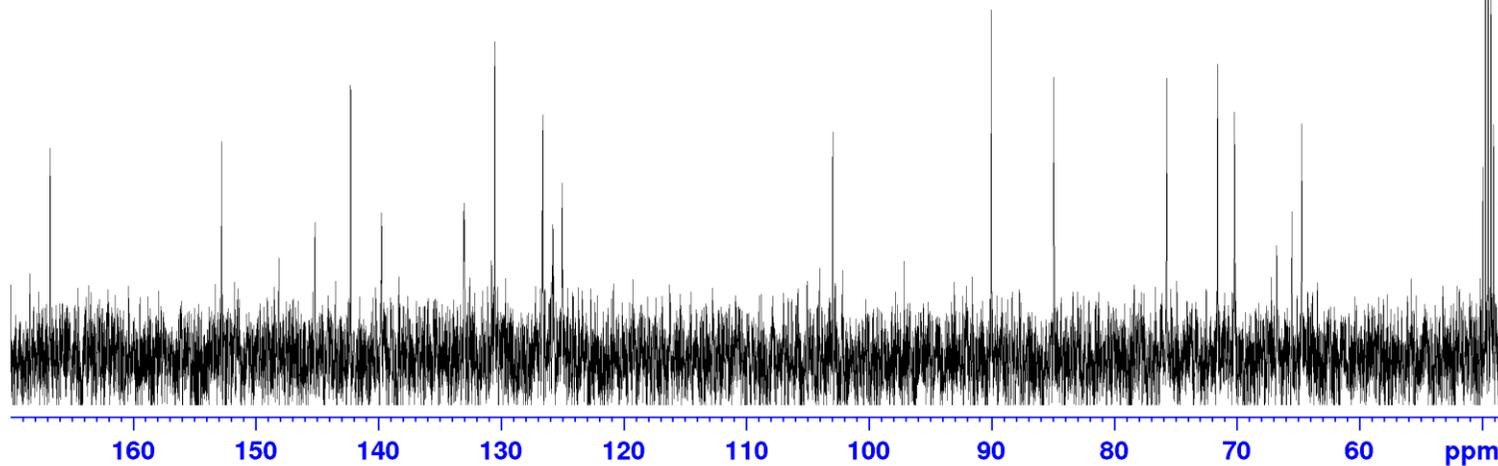
Current Data Parameters
 NAME CD108s
 EXPNO 3
 PROCNO 1

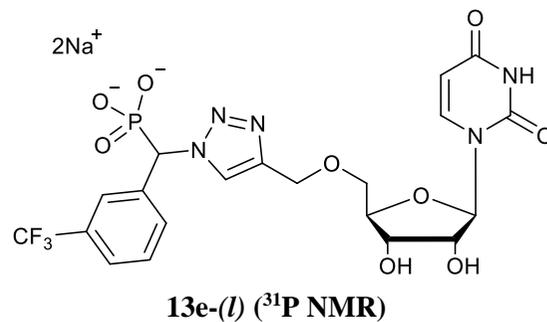
F2 - Acquisition Parameters
 Date_ 20191217
 Time 3.09 h
 INSTRUM spect
 PROBHD Z108618_0921 (
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 2500
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 196.38
 DW 20.800 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6303741 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 55.50099945 W
 SFO2 400.1616006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 11.52400017 W
 PLW12 0.27886000 W
 PLW13 0.14026000 W

F2 - Processing parameters
 SI 32768
 SF 100.6202010 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



13e-(I) (¹³C NMR)

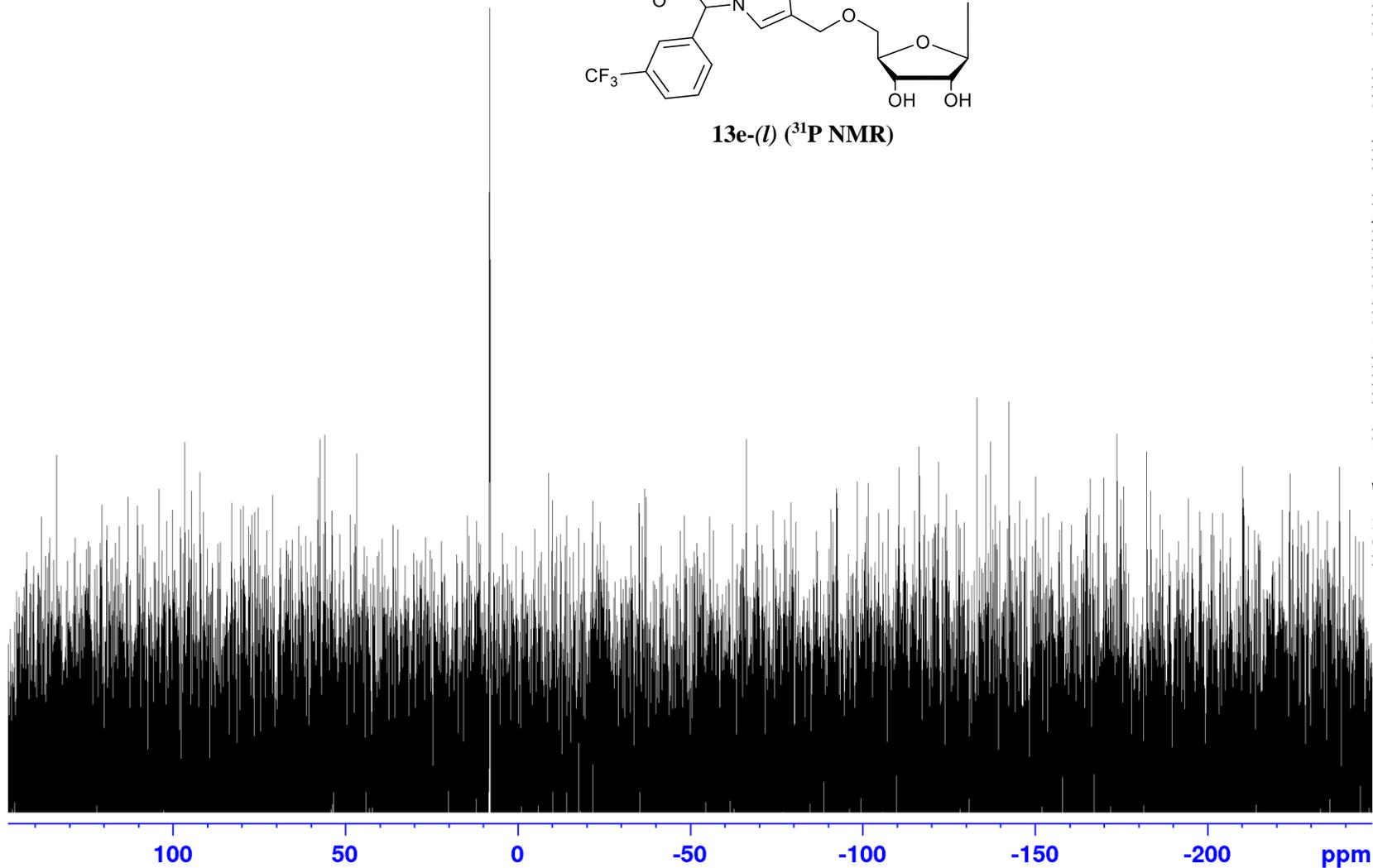




Current Data Parameters
NAME CD1081
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191217
Time 4.47 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 4
DS 0
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 usec
DE 50.00 usec
TE 299.1 K
D1 2.00000000 sec
TDO 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 usec
PLW1 11.77099991 W

F2 - Processing parameters
SI 32768
SF 161.9877372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

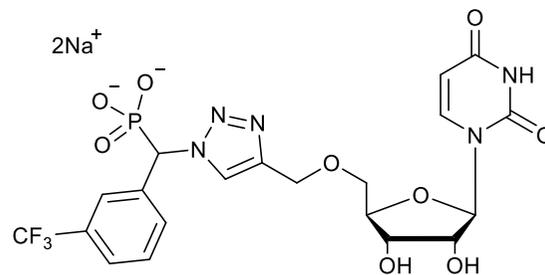




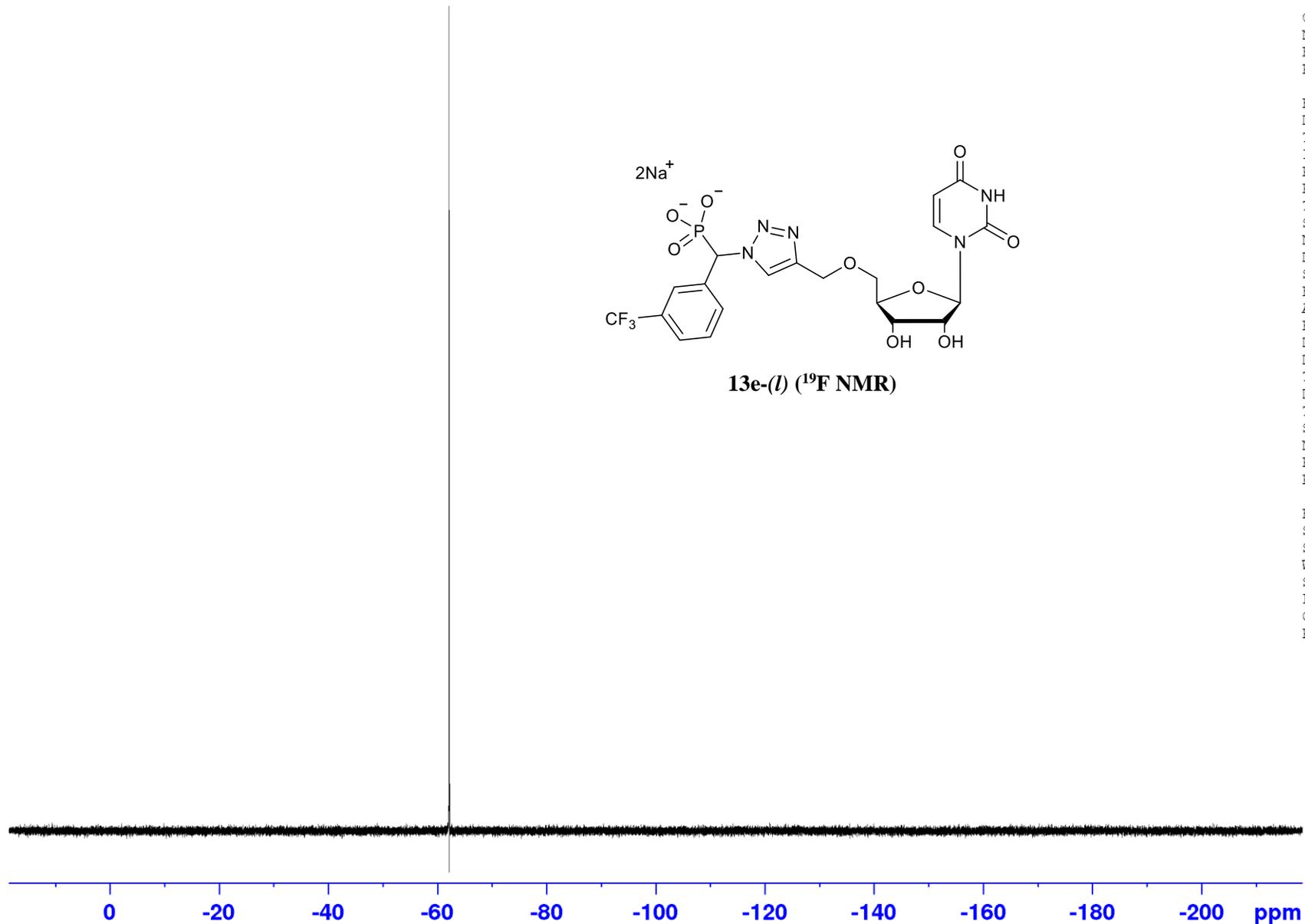
Current Data Parameters
NAME CD1081
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191217
Time 4.48 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zgflqn
TD 65536
SOLVENT D2O
NS 4
DS 0
SWH 89285.711 Hz
FIDRES 2.724784 Hz
AQ 0.3670016 sec
RG 196.38
DW 5.600 usec
DE 120.00 usec
TE 299.1 K
D1 1.00000000 sec
TDO 1
SFO1 376.4889413 MHz
NUC1 19F
P1 15.00 usec
PLW1 17.75399971 W

F2 - Processing parameters
SI 65536
SF 376.5265940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13e-(I) (¹⁹F NMR)

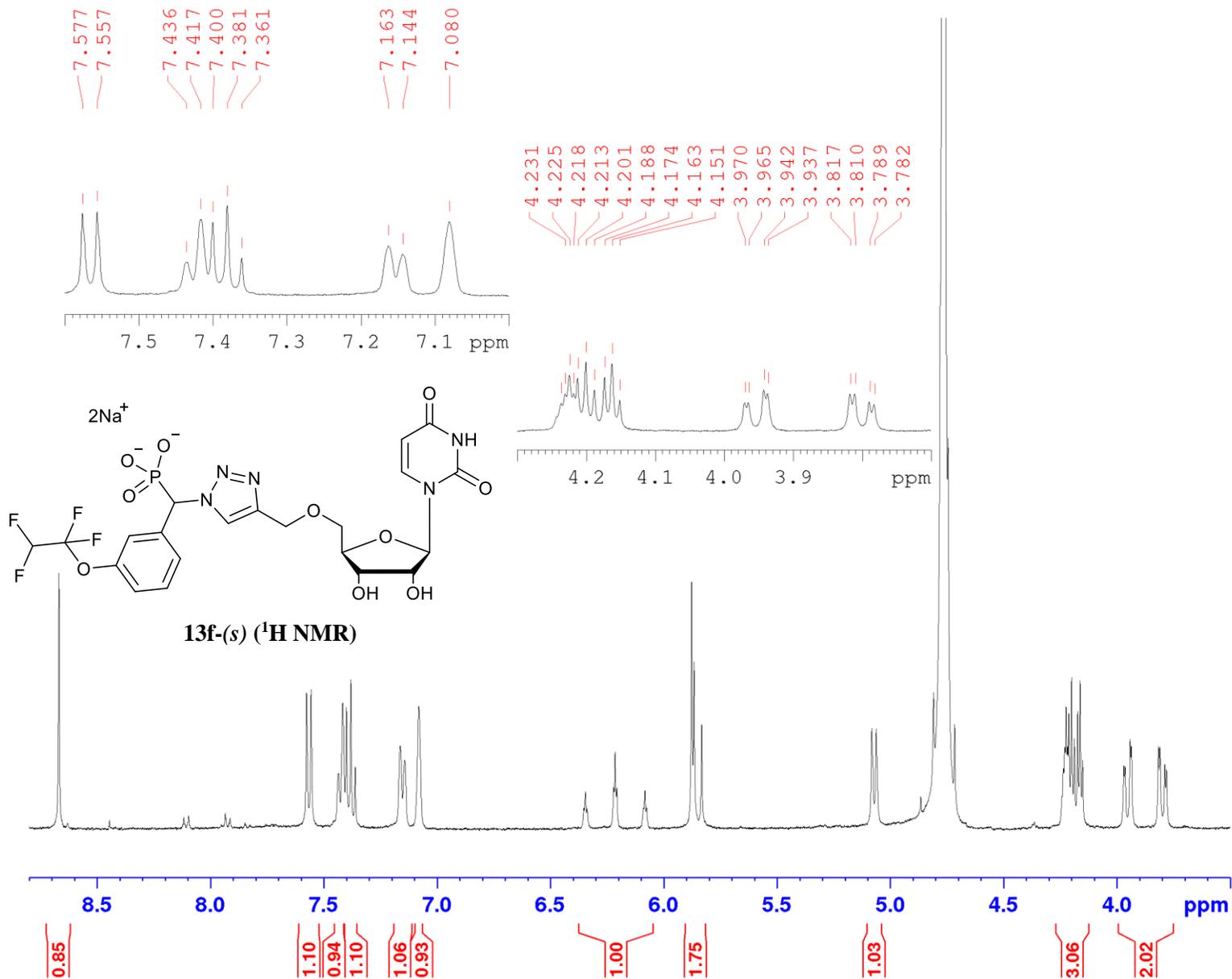




Current Data Parameters
NAME CD66_s
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180604
Time 13.37 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 158.68
DW 62.400 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters
SI 65536
SF 400.1599746 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

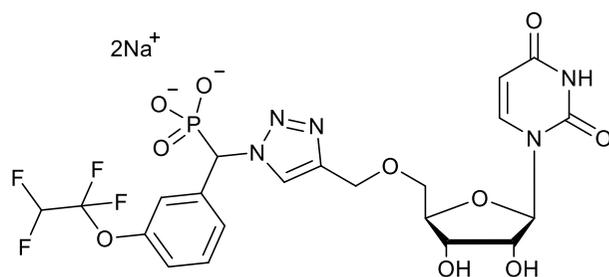




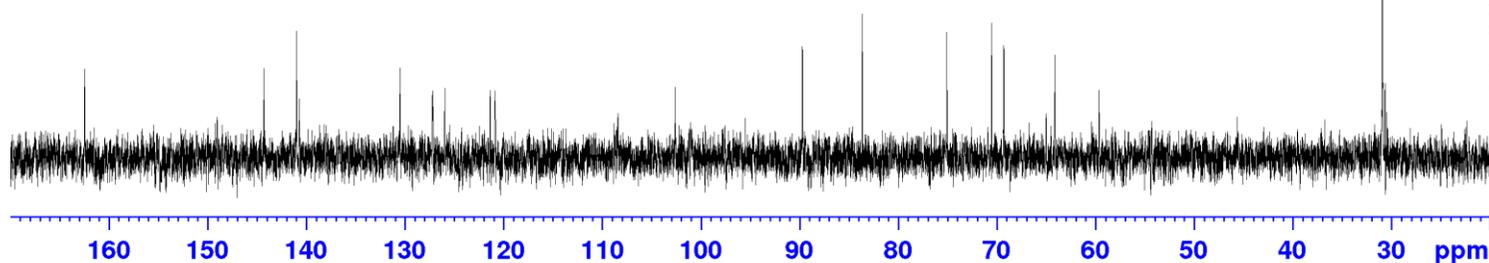
Current Data Parameters
NAME CD66_s
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180604
Time 20.00 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 196.38
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6303741 MHz
NUC1 13C
P1 10.00 usec
PLW1 55.50099945 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

F2 - Processing parameters
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SF 100.6202477 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13f-(s) (¹³C NMR)

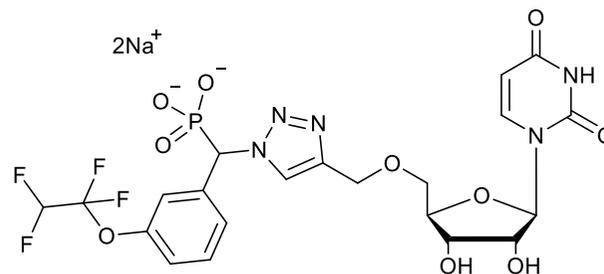




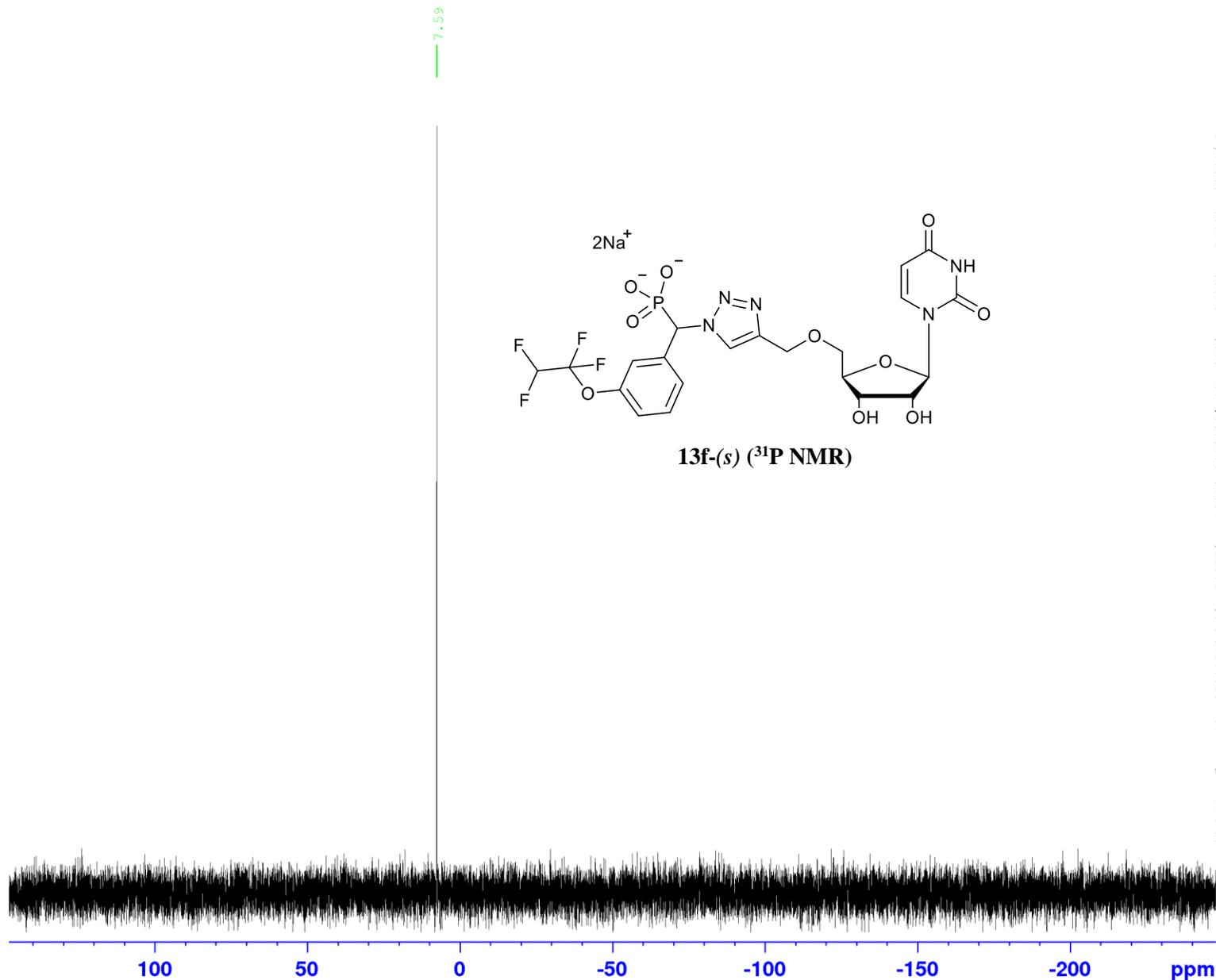
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NAME CD66_s
EXPNO 7
PROCNO 1

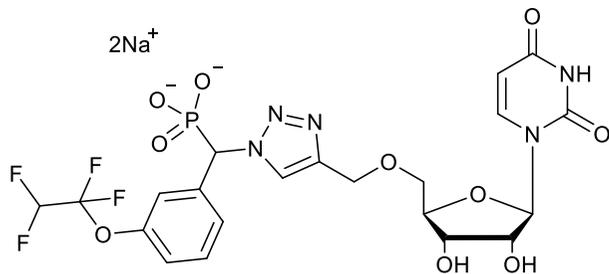
F2 - Acquisition Parameters
Date_ 20180604
Time 22.12 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 usec
PLW1 11.77099991 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

F2 - Processing parameters
SI 32768
SF 161.9877372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13f-(s) (³¹P NMR)

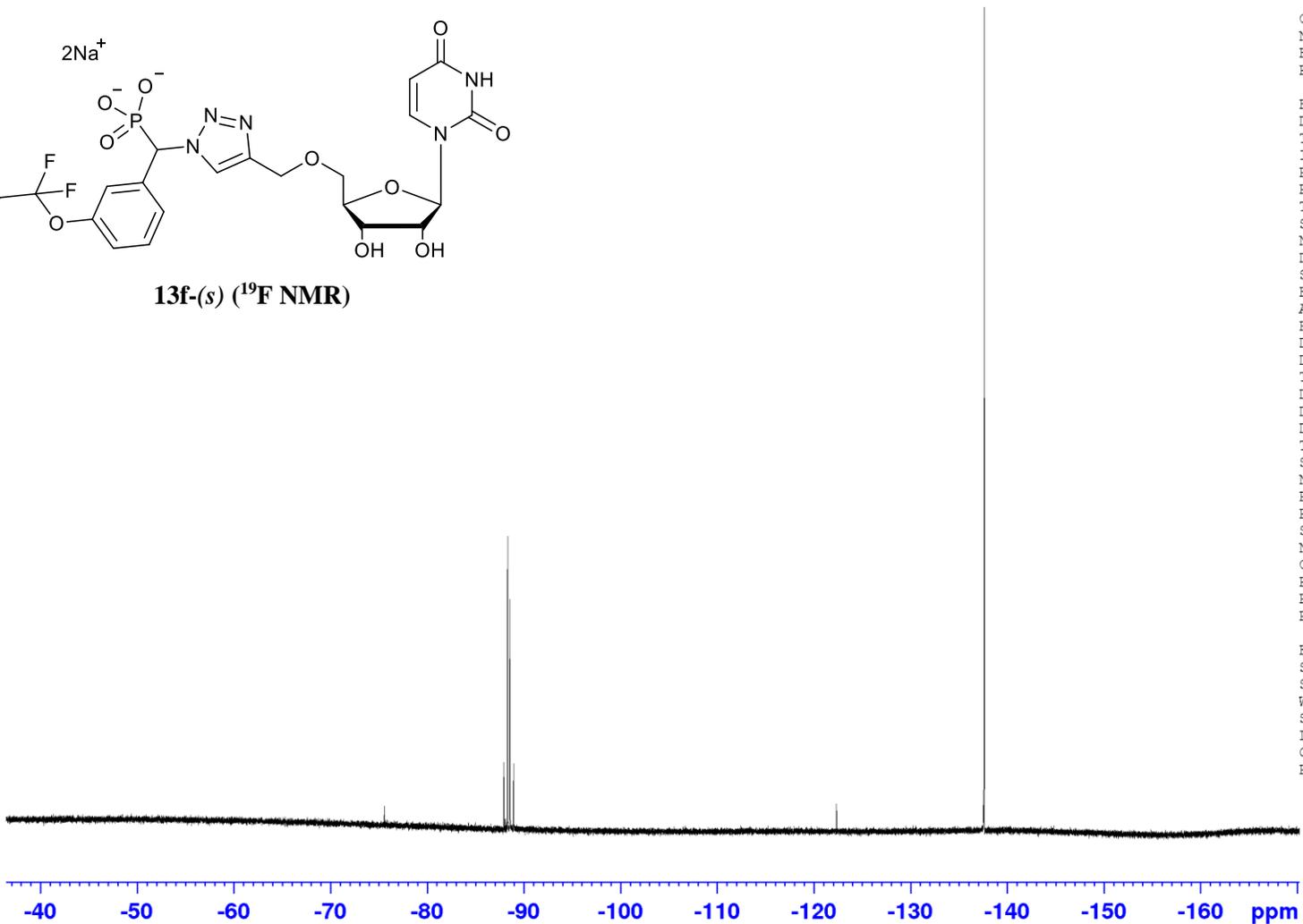




13f-(s) (¹⁹F NMR)

-87.93
-88.31
-88.56
-88.95

-137.61
-137.63
-137.65



Current Data Parameters
NAME CD66_s
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180604
Time 22.10 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT D2O
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 sec
RG 196.38
DW 5.600 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 376.4889418 MHz
NUC1 19F
P1 15.00 usec
PLW1 17.75399971 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W

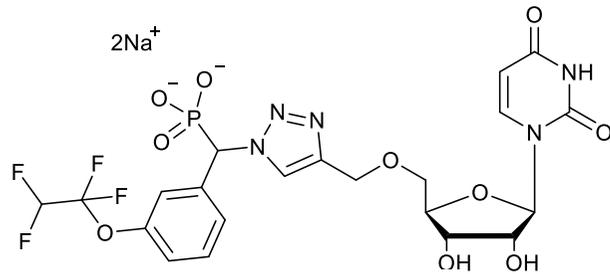
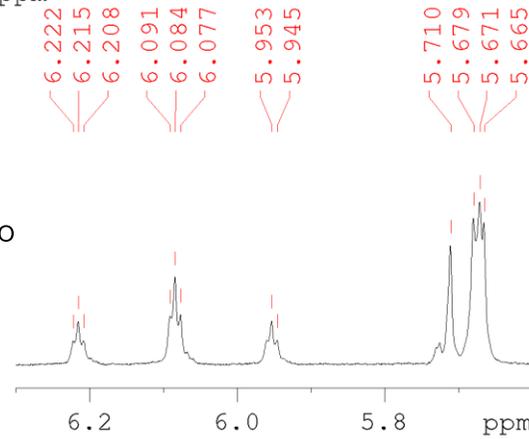
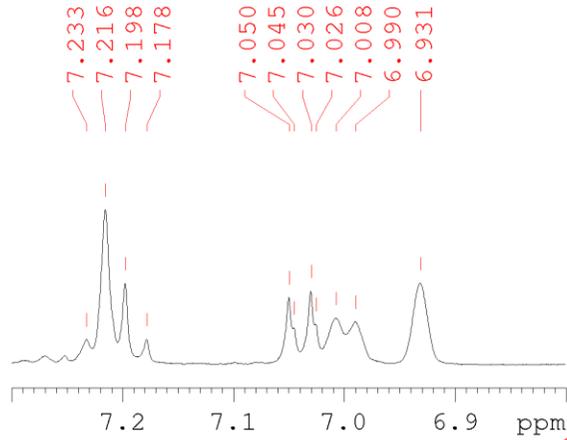
F2 - Processing parameters
SI 65536
SF 376.5265944 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



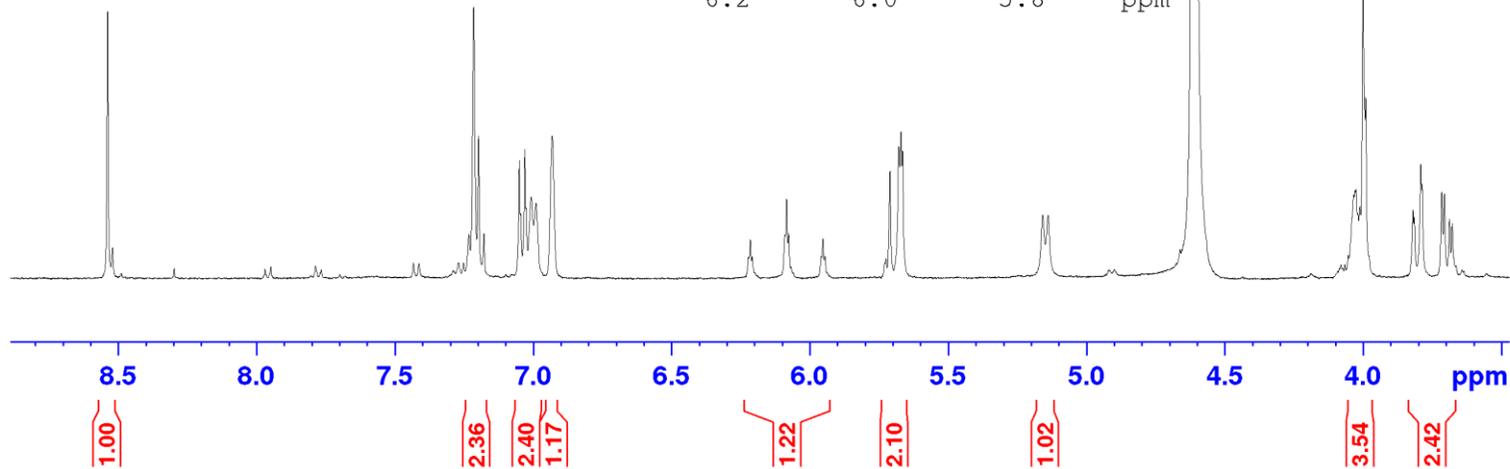
Current Data Parameters
NAME CD66_1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180605
Time 0.19 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 196.38
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P1 14.00 usec
PLW1 11.52400017 W

F2 - Processing parameters
SI 65536
SF 400.1600367 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13f-(I) (1H NMR)



161.66

156.77

148.37

143.49

140.90

140.13

129.72

126.34

125.34

120.51

120.42

110.28

107.84

105.42

102.16

88.89

82.66

74.14

69.70

68.87

65.64

64.39

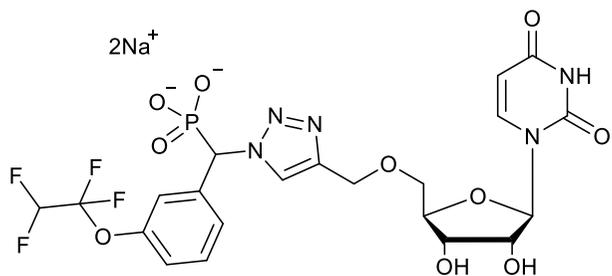
63.14



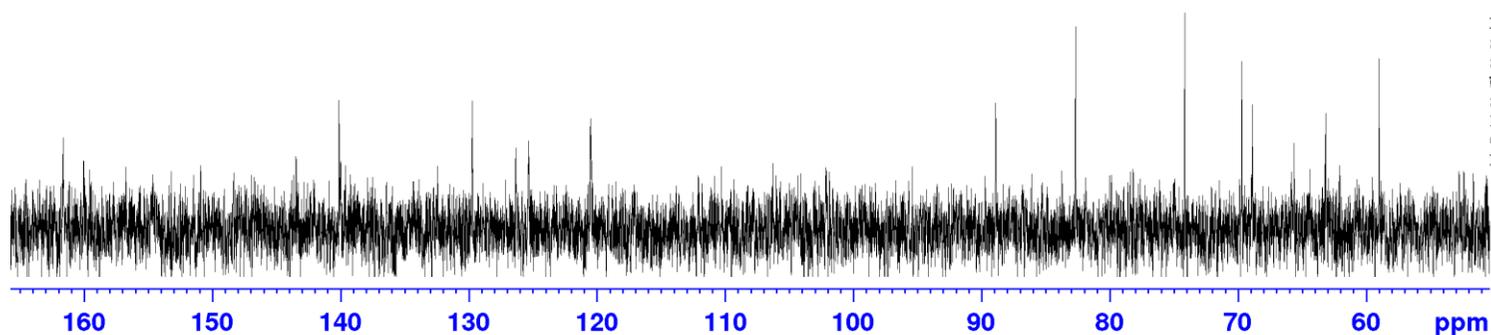
Current Data Parameters
 NAME CD66_1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180605
 Time 0.13 h
 INSTRUM spect
 PROBHD Z108618_0921 (
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 2048
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 196.38
 DW 20.800 usec
 DE 6.50 usec
 TE 299.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6303741 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 55.50099945 W
 SFO2 400.1616006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 11.52400017 W
 PLW12 0.27886000 W
 PLW13 0.14026000 W

F2 - Processing parameters
 SI 32768
 SF 100.6203120 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GE 0
 PC 1.40



13f-(l) (¹³C NMR)

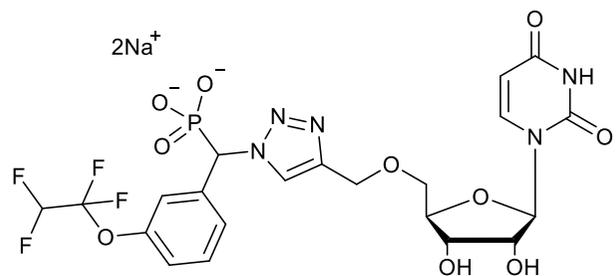




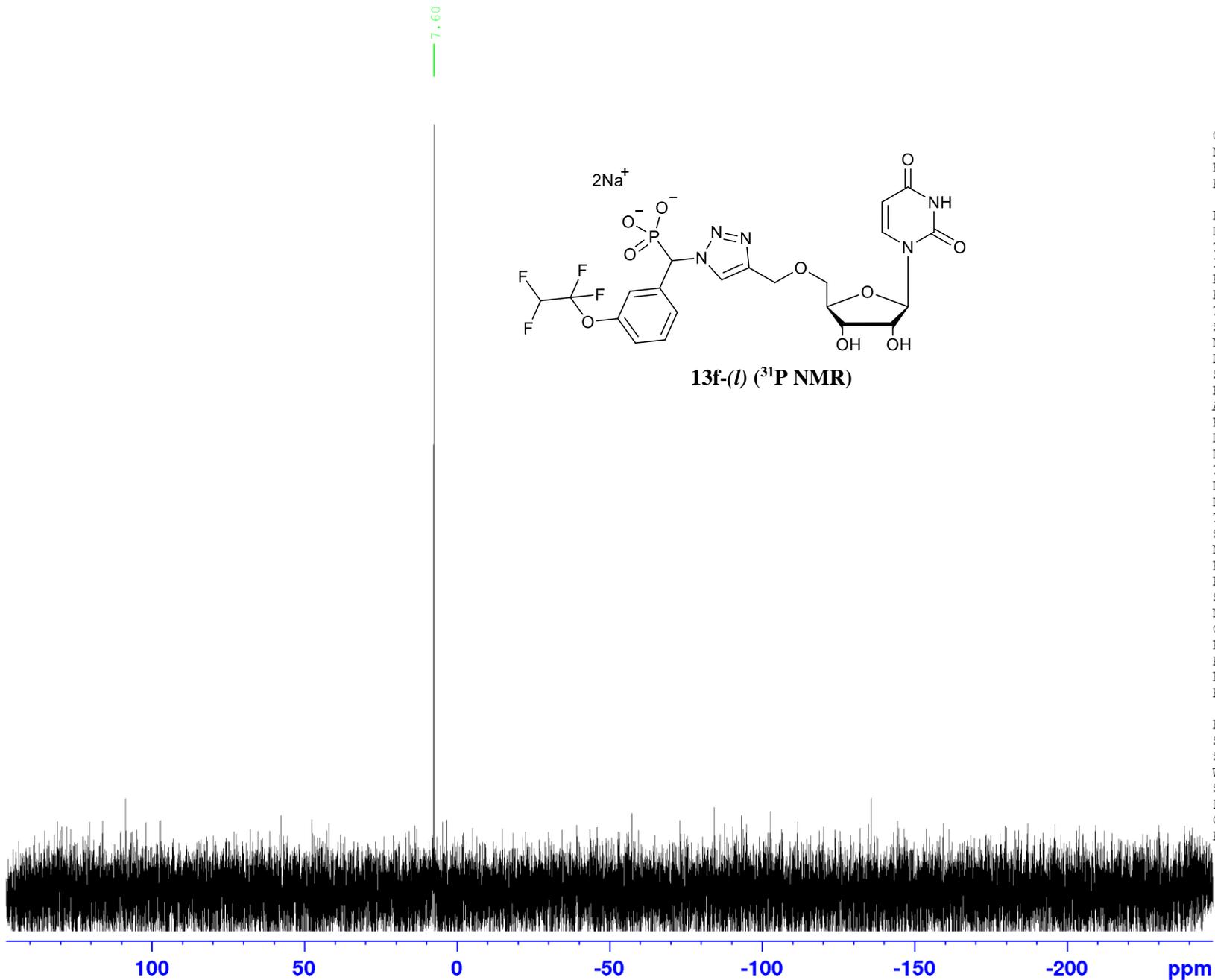
Current Data Parameters
NAME CD66_1
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180605
Time 2.24 h
INSTRUM spect
PROBHD z108618_0921 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 196.38
DW 7.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 161.9796378 MHz
NUC1 31P
P1 15.00 usec
PLW1 11.77099991 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W
PLW13 0.14026000 W

F2 - Processing parameters
SI 32768
SF 161.9877372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13f-(I) (³¹P NMR)



-87.78
-88.17
-88.52
-88.71

-137.59



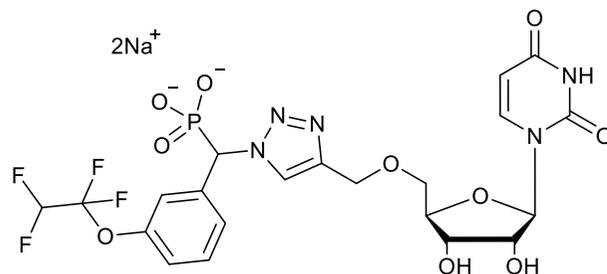
Current Data Parameters
NAME CD66_1
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters

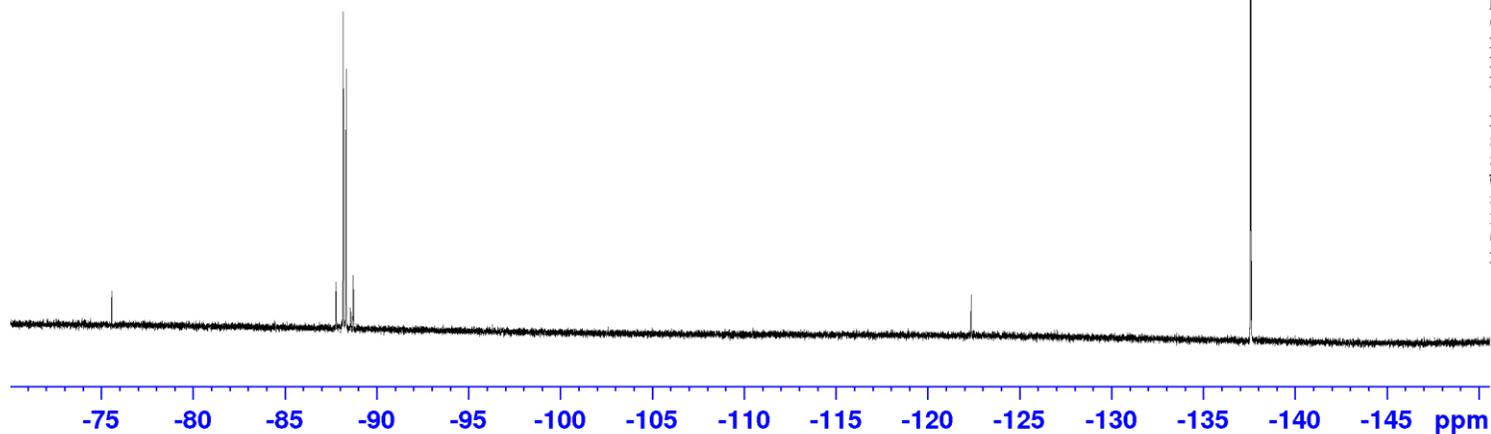
Date_ 20180605
Time 2.21 h
INSTRUM spect
PROBHD Z108618_0921 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT D2O
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 sec
RG 196.38
DW 5.600 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 376.4889418 MHz
NUC1 19F
P1 15.00 usec
PLW1 17.75399971 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.52400017 W
PLW12 0.27886000 W

F2 - Processing parameters

SI 65536
SF 376.5265944 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13f-(I) (¹⁹F NMR)

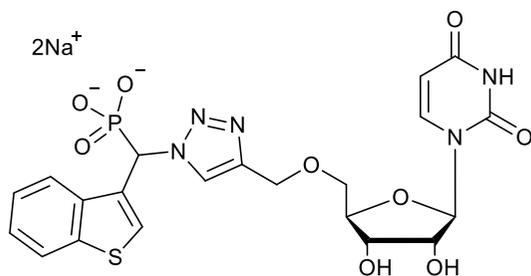
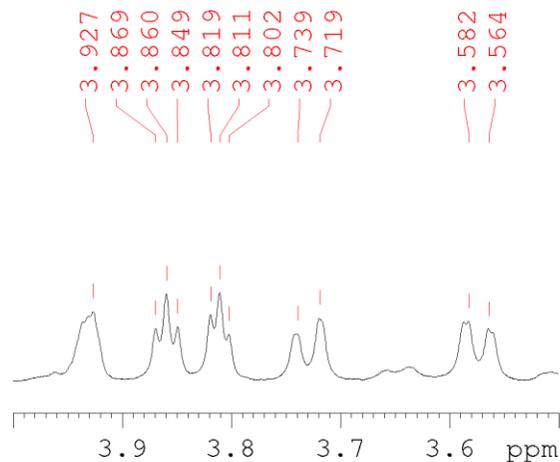




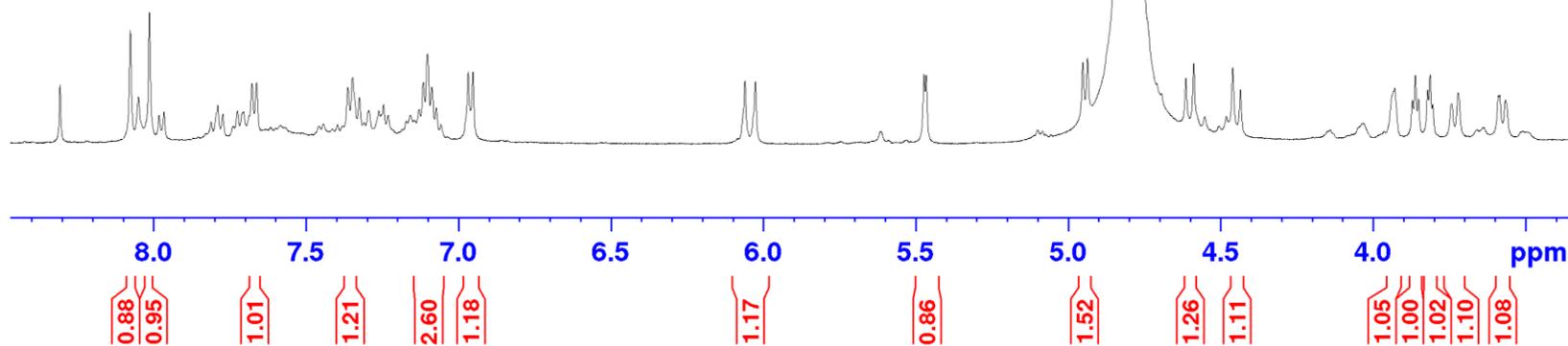
Current Data Parameters
NAME CD105s
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200228
Time 10.51 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zg30
TD 65536
SOLVENT D2O
NS 64
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 85.7143
DW 50.000 usec
DE 16.23 usec
TE 286.4 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7439537 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13g-(s) (1H NMR)



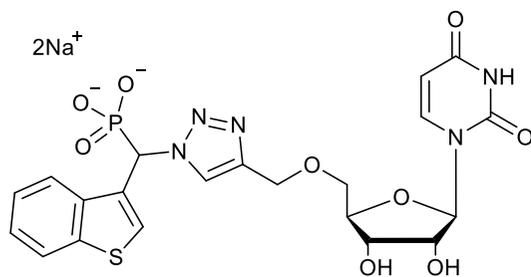


Current Data Parameters
NAME CD105s
EXPNO 5
PROCNO 1

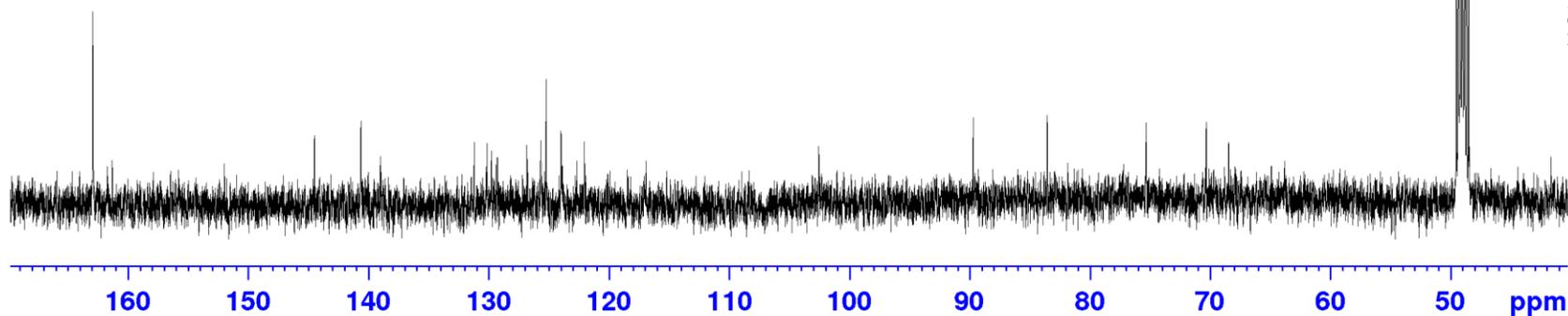
F2 - Acquisition Parameters
Date_ 20200228
Time 21.00 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 2500
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 285.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6605781 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

162.95
161.33
144.50
140.63
138.98
131.20
130.15
126.82
125.68
125.22
123.98
122.06
102.54
89.70
83.54
75.31
70.30
68.44
63.79
59.77
58.79



13g-(s) (13C NMR)

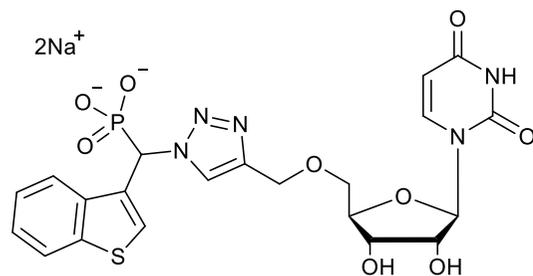




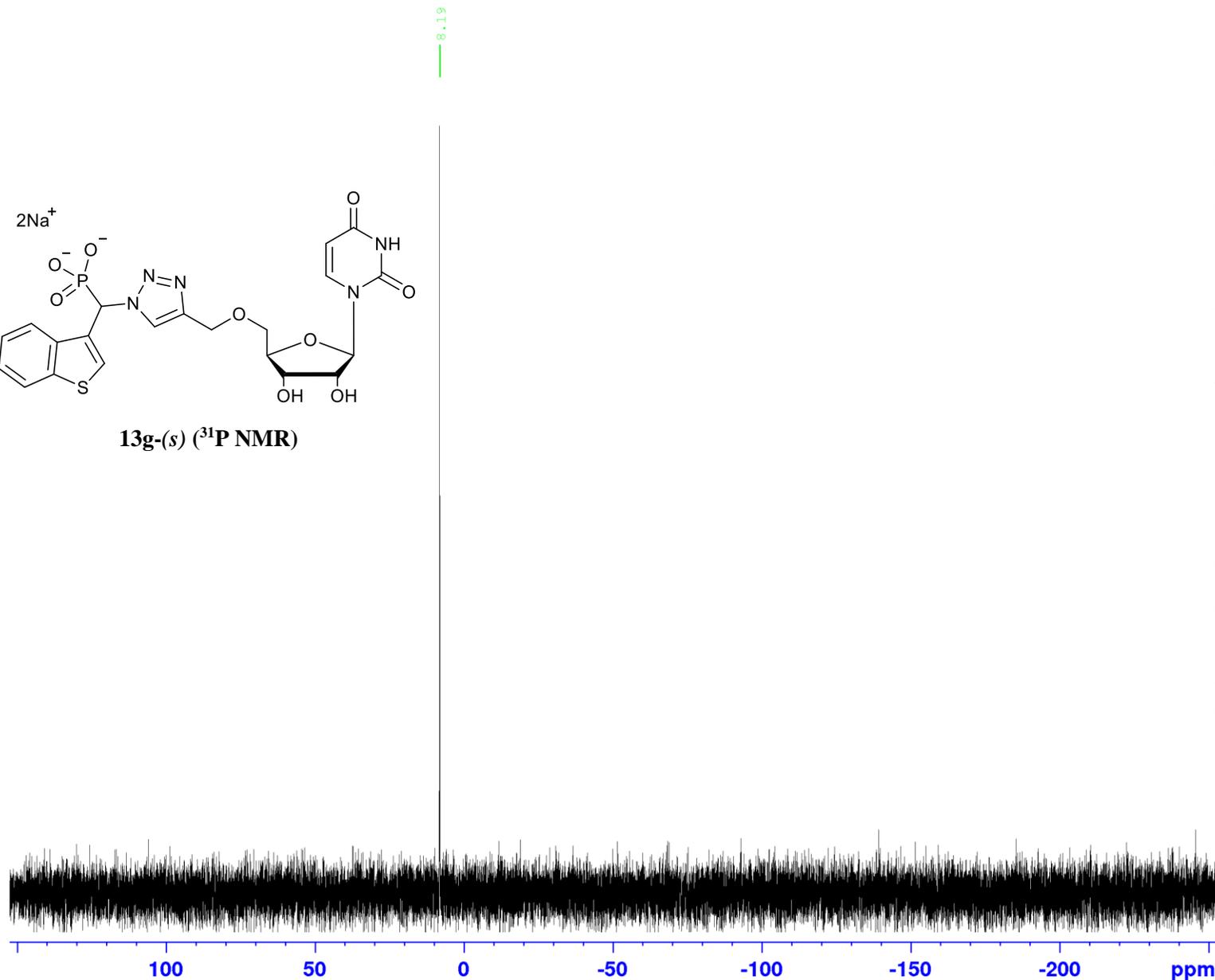
Current Data Parameters
NAME CD105s
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200228
Time 10.53 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 286.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SF01 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SF02 499.7459990 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13g-(s) (³¹P NMR)



8.28
8.17

7.85

7.57
7.56

7.29
7.28
7.28

6.93
6.92

6.22
6.18

5.72
5.71

5.07
5.06

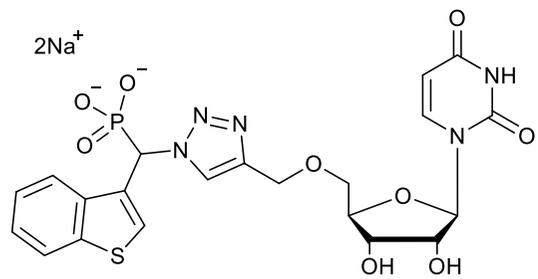
4.11
3.99
3.98
3.97
3.94
3.93
3.92
3.85
3.83
3.76
3.75
3.74
3.73



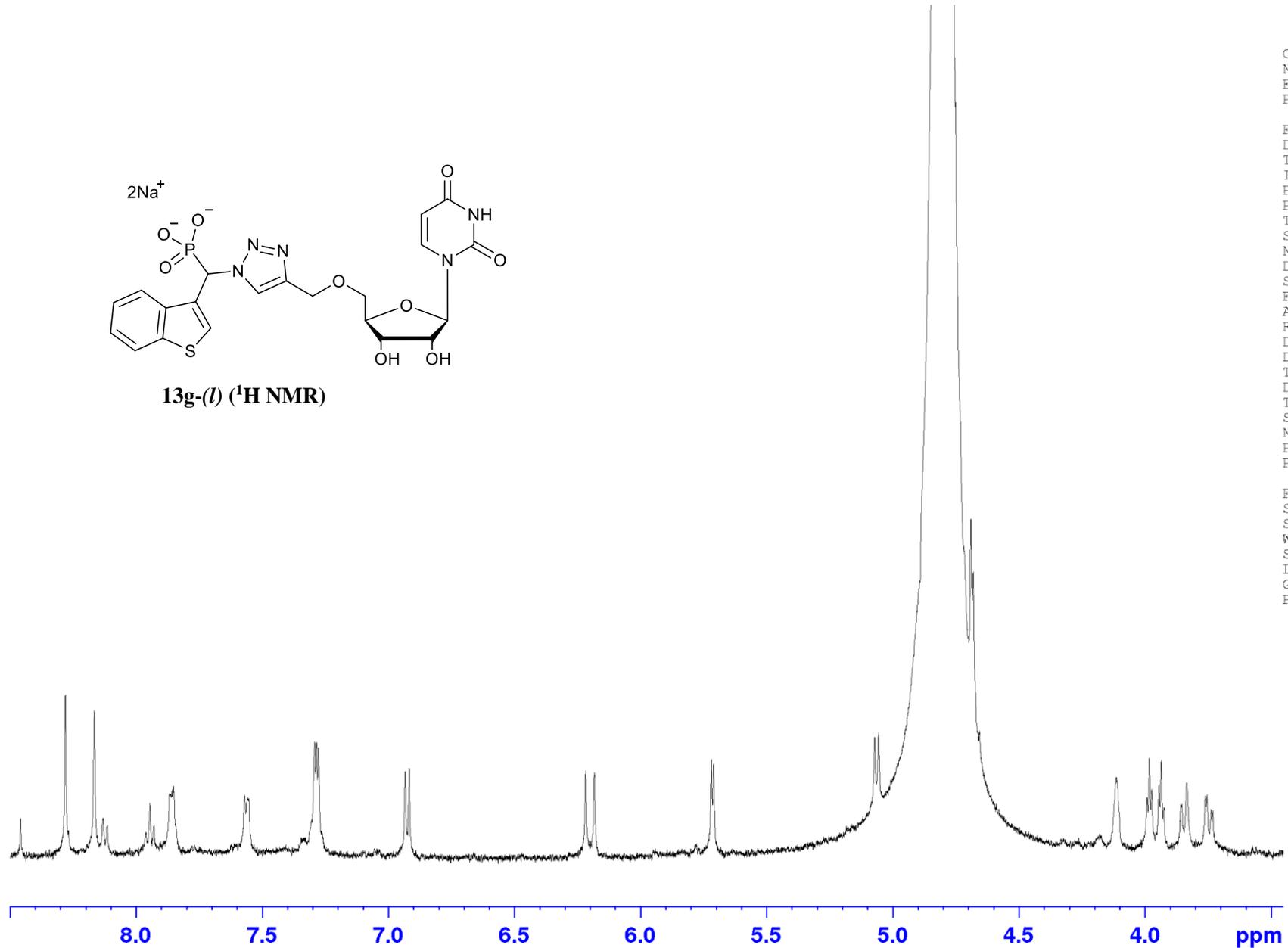
Current Data Parameters
NAME cd9_191210_29
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191210
Time 12.51 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 ()
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 80
DW 50.000 usec
DE 16.23 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 499.7470859 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.53100014 W

F2 - Processing parameters
SI 65536
SF 499.7439556 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13g-(l) (¹H NMR)

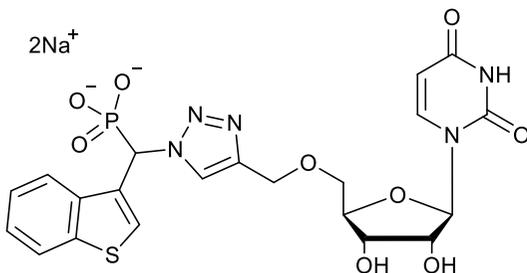




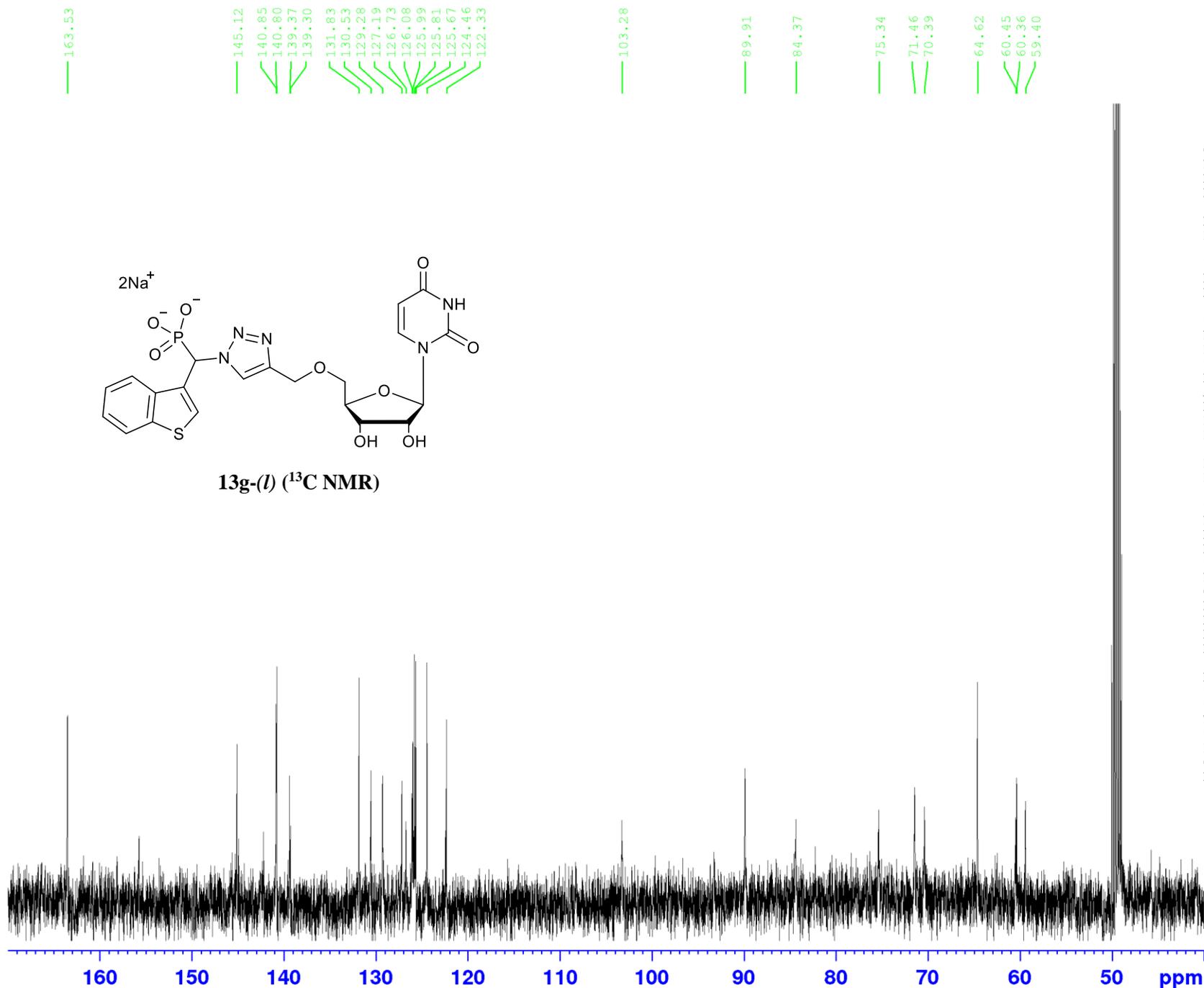
Current Data Parameters
NAME CD1051
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191213
Time 2.21 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 4500
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.6732948 MHz
NUC1 13C
P1 10.00 usec
PLW1 51.23600006 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 125.6605694 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13g-(I) (13C NMR)

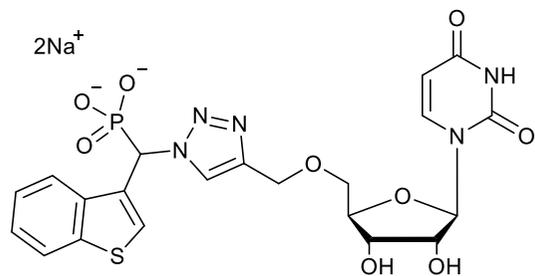




Current Data Parameters
NAME cd9_191210_29
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191211
Time 1.23 h
INSTRUM CAB AV4 500 MHZ BASIC
PROBHD Z150364_0005 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 4
SWH 81967.211 Hz
FIDRES 2.501441 Hz
AQ 0.3997696 sec
RG 101
DW 6.100 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 202.2899643 MHz
NUC1 31P
P1 12.00 usec
PLW1 45.76100159 W
SFO2 499.7459990 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.53100014 W
PLW12 0.34944999 W
PLW13 0.17549001 W

F2 - Processing parameters
SI 32768
SF 202.3000793 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13g-(I) (³¹P NMR)

