

Expanding the Limit of Pd-Catalyzed Decarboxylative Benzylations

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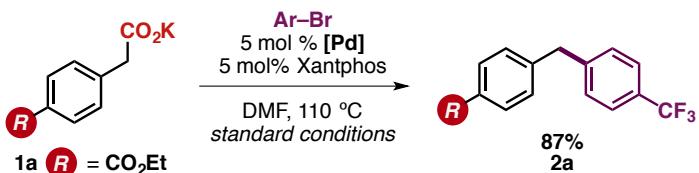
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I. General Considerations

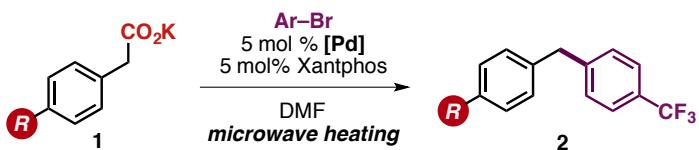
Unless noted, all reactions were conducted under inert atmosphere employing standard Schleck technique or by the use of a N₂-filled glovebox. All glassware was oven-dried prior to use. Flash chromatography was performed as described by Still and co-workers¹ (SiliaFlash P60, 40-63μm, 60A silica gel, Silicycle) or by automated flash chromatography (Ultra SNAP silica cartridges, Biotage). Analytical thin-layer chromatography was performed using glass plates pre-coated with silica (SiliaPlate G TLC - Glass-Backed, 250μm, Silicycle). TLC plates were visualized by UV light and/or staining with aqueous basic potassium permanganate. Unless otherwise noted, all reagents were obtained from commercial vendors and used as supplied. Potassium aryl acetate salts were synthesized from the corresponding aryl acetate acids as described by Liu and co-workers.²

II. Additional Optimization Data



entry	deviation from standard conditions	conv. 1a / Ar-Br (%)	2a (%)
1	XPhos instead of Xantphos	60	46
2	SPhos instead of Xantphos	32	32
3	DPPF instead of Xantphos	59	50
4	BINAP instead of Xantphos	64	44
5	DPPP instead of Xantphos	50	17
6	DPPB instead of Xantphos	52	21
7	DPEPhos instead of Xantphos	77	51
8	SPANPhos instead of Xantphos	50	28
9	IPr instead of Xantphos	31	23
10	Pd(OAc) ₂	101	82
11	Pd(dba) ₂	111	98
12	Pd(CH ₃ CN) ₂ Cl ₂	82	48
			11

1a (0.12 mmol), ArBr (0.1 mmol), DMF (0.5 mL), 2.5h, conv. and yield determined by calibrated NMR, conversion of **1a** is calculated out of 120%, [Pd] = Pd(cinnamyl)Cl, Ar = 4-CF₃C₆H₄



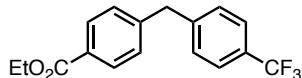
entry	R	temp.	conv. 1 / Ar-Br (%)	2 (%)
1	CN	100 °C	91	73
2	CN	130 °C	120	100
3 ^a	CF ₃	100 °C	32	28
4 ^a	CF ₃	130 °C	70	44
				43

1 (1.2 equiv), ArBr (1.0 equiv.), DMF (0.2 M), 1 h, conv. and yield determined by calibrated NMR, conversion of **1** is calculated out of 120%, [Pd] = Pd(cinnamyl)Cl; ^awith DEA-Xantphos

III Pd-Catalyzed Decarboxylative Benzylation of Aryl Bromides

General Procedure: Xantphos or DEA-Xantphos ligand (0.050 equiv.), potassium aryl acetate (1.2 equiv.) and aryl bromide (1.0 equiv.) were added sequentially to a 1-dram vial charged with a stir bar. [Pd(cinnamyl)Cl]₂ dimer (0.025 equiv.) was then added as a solution in anhydrous DMF (0.0050 M). The vial was sealed with a PTFE-lined cap under inert atmosphere, removed from the glovebox and heated while stirring. ¹H NMR analysis of small aliquots (~5 µL) was used to follow reactions to completion (1–24 hours), after which the mixture was

diluted in ethyl acetate (80 mL) and washed sequentially with saturated NH₄Cl (20 mL) and brine (20 mL). For reactions using heteroaryl bromides, Na₂CO₃ (1 M, 20 mL) was used instead of NH₄Cl. The organic layer was dried over Na₂SO₄, concentrated *in vacuo* and purified by flash column chromatography.



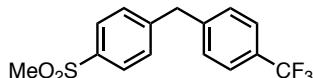
2a Prepared according to the General Procedure from the corresponding aryl bromide (113 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (148 mg, 0.60 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and XantPhos (14.5 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 110 °C. Isolated in 73% yield after purification by silica gel chromatography (20:1 hexane:EtOAc) as a light yellow solid.

¹H NMR (CDCl₃, 498 MHz) δ 7.99 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 2H), 7.24 (d, *J* = 8.3 Hz, 2H), 4.37 (q, *J* = 7.2 Hz, 2H), 4.09 (s, 2H), 1.38 (t, *J* = 7.2 Hz, 3H);

¹³C NMR (CDCl₃, 126 MHz) δ 166.4, 145.1, 144.3, 130.0, 129.3, 128.9 (2), 128.8 (q, *J* = 27.3 Hz) 127.4 (q, *J* = 272.6 Hz), 125.5 (q, *J* = 3.7 Hz), 60.9, 41.7, 14.4;

¹⁹F NMR (CDCl₃, 469 MHz) δ -62.4;

HRMS (EI): calcd for C₁₇H₁₅F₃O₂ [M]⁺: 308.1024. Found 308.1023.



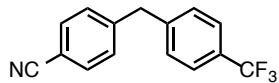
2b: Prepared according to the General Procedure from the corresponding aryl bromide (68 mg, 0.30 mmol, 1.0 equiv.), potassium aryl acetate (91 mg, 0.36 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (3.9 mg, 0.0075 mmol, 0.025 equiv.), and XantPhos (8.7 mg, 0.015 mmol, 0.050 equiv.) in 1.5 mL DMF, 90 °C. Isolated in 79% yield after purification by silica gel chromatography (4:1 hexane:EtOAc) as a light yellow solid.

¹H NMR (CDCl₃, 498 MHz) δ 7.89–7.87 (m, 2H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 4.13 (s, 2H), 3.04 (s, 3H);

¹³C NMR (CDCl₃, 126 MHz) δ 146.4, 143.4, 138.8, 129.8, 129.3, 129.1 (q, *J* = 32.5 Hz), 127.8, 126.2 (q, *J* = 272.7 Hz), 125.7 (q, *J* = 4.3 Hz), 44.5, 41.5;

¹⁹F NMR (CDCl₃, 469 MHz) δ -62.5;

HRMS (EI): calcd for C₁₅H₁₃F₃O₂S [M]⁺: 314.0588. Found 314.0586.

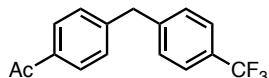


2c: Prepared according to the General Procedure from the corresponding aryl bromide (113 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (120 mg, 0.60 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and XantPhos (14.7 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 100 °C. Isolated in 76% yield after purification by silica gel chromatography (20:1 to 10:1 hexane:EtOAc) as a light yellow oil. Spectroscopic data agreed with that reported.³

¹H NMR (CDCl_3 , 500 MHz) δ 7.62–7.57 (m, 4H), 7.30–7.27 (m, 4H), 4.11 (s, 2H);

¹³C NMR (CDCl_3 , 126 MHz) δ 145.5, 143.3, 132.5, 129.6, 129.3, 129.1 (q, $J = 32.4$ Hz), 125.7 (q, $J = 3.8$ Hz), 124.1 (q, $J = 271.5$ Hz), 118.8, 110.6, 41.7;

¹⁹F NMR (CDCl_3 , 469 MHz) δ -62.5.

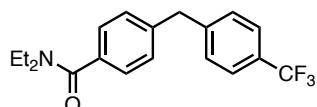


2d: Prepared according to the General Procedure from the corresponding aryl bromide (45 mg, 0.20 mmol, 1.0 equiv.), potassium aryl acetate (52 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and XantPhos (5.8 mg, 0.01 mmol, 0.050 equiv.) in 1.0 mL DMF, 110 °C. Isolated in 72% yield after purification by silica gel chromatography (8:1 hexane:EtOAc) as a light yellow oil. Spectroscopic data agreed with that reported.⁴

¹H NMR (CDCl_3 , 498 MHz) δ 7.91–7.89 (m, 2H), 7.55 (d, $J = 7.5$ Hz, 2H), 7.29–7.26 (m, 4H), 4.09 (s, 2H), 2.58 (s, 3H);

¹³C NMR (CDCl_3 , 126 MHz) δ 197.6, 145.5, 144.0, 135.6, 129.2, 129.1, 128.9 (q, $J = 32.6$ Hz), 128.7, 125.5 (q, $J = 3.9$ Hz), 124.2 (q, $J = 273.0$ Hz), 41.6, 26.6;

¹⁹F NMR (CDCl_3 , 469 MHz) δ -62.4.



2e: Prepared according to the General Procedure from the corresponding aryl bromide (45 mg, 0.20 mmol, 1.0 equiv.), potassium aryl acetate (66 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and DEA-XantPhos (5.6 mg, 0.01 mmol,

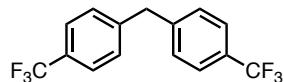
0.050 equiv.) in 1.0 mL DMF, 135 °C. Isolated in 60% yield after purification by silica gel chromatography (2:1 hexane:EtOAc) as a light yellow solid.

¹H NMR (CDCl₃, 498 MHz) δ 7.54 (d, *J* = 8.1 Hz, 2H), 7.32–7.26 (m, 4H), 7.19 (d, *J* = 8.1 Hz, 2H), 4.04 (s, 2H), 3.38 (br, 4H), 1.17 (br, 6H);

¹³C NMR (CDCl₃, 126 MHz) δ 171.1, 144.6, 141.0, 135.5, 129.2, 128.9, 128.7 (q, *J* = 33.8 Hz), 126.8, 125.4 (q, *J* = 4.2 Hz), 124.3 (q, *J* = 271.3 Hz), 43.3, 41.5, 39.3, 14.2, 12.9;

¹⁹F NMR (CDCl₃, 469 MHz) δ -62.3;

HRMS (ESI): calcd for C₁₉H₂₁F₃NO [M+H]⁺: 336.1570. Found 336.1571.

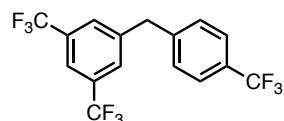


2f: Prepared according to the General Procedure from the corresponding aryl bromide (113 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (145 mg, 0.60 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂(6.5 mg, 0.0125 mmol, 0.025 equiv.), and DEA-XantPhos (14 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 125 °C. 66% yield by ¹H NMR using durene as internal standard (53% isolated yield). Spectroscopic data agreed with that reported.⁵

¹H NMR (CDCl₃, 498 MHz) δ 7.56 (d, *J* = 8.2 Hz, 4H), 7.29 (d, *J* = 8.2 Hz, 4H), 4.09 (s, 2H);

¹³C NMR (CDCl₃, 126 MHz) δ 143.9, 129.2, 128.9 (q, *J* = 33.8 Hz), 125.6 (q, *J* = 4.2 Hz), 124.1 (q, *J* = 271.3 Hz), 41.5;

¹⁹F NMR (CDCl₃, 469 MHz) δ -62.4.

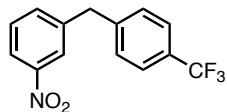


2g: Prepared according to the General Procedure from the corresponding aryl bromide (113 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (186 mg, 0.60 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂(6.5 mg, 0.0125 mmol, 0.025 equiv.), and DEA-XantPhos (14 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 110 °C. Isolated in 61% yield after purification by silica gel chromatography (40:1 hexane:EtOAc) as a white solid. Spectroscopic data agreed with that reported.⁶

¹H NMR (CDCl₃, 700 MHz) δ 7.77 (s, 1H), 7.62–7.59 (m, 4H), 7.29 (d, *J* = 7.5 Hz, 2H), 4.16 (s, 2H);

¹³C NMR (CDCl₃, 126 MHz) δ 142.7, 142.3, 132.0 (q, *J* = 39.2 Hz), 129.5 (q, *J* = 39.2 Hz), 129.1, 129.0-128.9 (m), 125.9 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 272.7 Hz), 123.2 (q, *J* = 272.7 Hz), 120.8-120.6 (m), 41.2;

¹⁹F NMR (CDCl₃, 469 MHz) δ -62.5, -62.8.



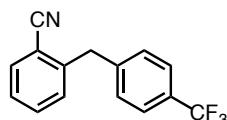
2h: Prepared according to the General Procedure from the corresponding aryl bromide (45 mg, 0.20 mmol, 1.0 equiv.), potassium aryl acetate (53 mg, 0.24 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (5.2 mg, 0.01 mmol, 0.05 equiv.), and DEA-XantPhos (11.2 mg, 0.02 mmol, 0.10 equiv.) in 1.0 mL DMF, 120 °C. Isolated in 48% yield after purification by silica gel chromatography (15:1 hexane:EtOAc) as a white solid.

¹H NMR (CDCl₃, 498 MHz) δ 8.12–8.09 (m, 1H), 8.06 (s, 1H), 7.58 (d, *J* = 6.8 Hz, 2H), 7.52–7.47 (m, 2H), 7.31 (d, *J* = 6.8 Hz, 2H), 4.17 (s, 2H);

¹³C NMR (CDCl₃, 176 MHz) δ 148.5, 143.3, 141.9, 134.9, 129.6, 129.2, 129.1 (q, *J* = 35.0 Hz), 125.7 (q, *J* = 2.3 Hz), 124.1 (q, *J* = 271.2 Hz), 123.7, 121.7, 41.2;

¹⁹F NMR (CDCl₃, 469 MHz) δ -62.5;

HRMS (EI): calcd for C₁₄H₁₀F₃NO₂ [M]⁺: 281.0664. Found 281.0666.

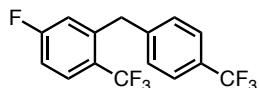


2i: Prepared according to the General Procedure from the corresponding aryl bromide (45 mg, 0.2 mmol, 1.0 equiv.), potassium aryl acetate (48 mg, 0.24 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (2.6 mg, 0.005 mmol, 0.025 equiv.), and XantPhos (5.8 mg, 0.010 mmol, 0.050 equiv.) in 1.0 mL DMF, 105 °C. Isolated in 80% yield after purification by silica gel chromatography (2% to 15% EtOAc in Hexane) as a yellow oil. Spectroscopic data agreed with that reported.⁷

¹H NMR (CDCl₃, 500 MHz) δ 7.67 (m, 1H), 7.66 (m, 2H), 7.57 (m, 1H), 7.36–7.33 (m, 3H), 7.27 (m, 1H), 4.26 (s, 2H);

¹³C NMR (CDCl₃, 126 MHz) δ 143.7, 142.8, 133.1, 130.1, 129.7, 129.3, 129.0 (q, *J* = 32.4 Hz), 127.3, 125.7 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 272.7 Hz), 118.0, 112.7, 41.6;

¹⁹F NMR (CDCl₃, 377 MHz) δ -62.6.



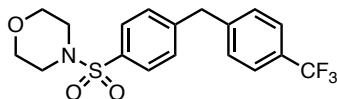
2j: Prepared according to the General Procedure from the corresponding aryl bromide (68 mg, 0.30 mmol, 1.0 equiv.), potassium aryl acetate (93 mg, 0.36 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (3.9 mg, 0.0075 mmol, 0.025 equiv.), and XantPhos (8.7 mg, 0.015 mmol, 0.050 equiv.) in 1.5 mL DMF, 110 °C. 65% yield by ¹H NMR using durene as internal standard.

¹H NMR (CDCl₃, 498 MHz) δ 7.73–7.68 (m, 1H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.26 (m, 2H), 7.05–7.01 (m, 1H), 6.82 (m, 1H), 4.25 (s, 2H);

¹³C NMR (CDCl₃, 126 MHz) δ 164.5 (d, *J* = 252.6 Hz), 142.9, 141.7 (d, *J* = 8.3 Hz), 129.4, 129.1 (q, *J* = 32.6 Hz), 128.6 (m), 127.6, 125.9 (q, *J* = 3.8 Hz), 125.6 (m), 125.0 (m), 124.1 (q, *J* = 232.6 Hz), 124.0 (q, *J* = 233.5 Hz), 118.7 (d, *J* = 22.8 Hz), 113.7 (d, *J* = 21.9 Hz), 37.6;

¹⁹F NMR (CDCl₃, 469 MHz) δ -58.9, -62.5, -107.4;

HRMS (EI): calcd for C₁₅H₉F₇ [M]⁺: 322.0592. Found 322.0589.



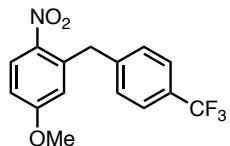
2k: Prepared according to the General Procedure from the corresponding aryl bromide (23 mg, 0.10 mmol, 1.0 equiv.), potassium aryl acetate (39 mg, 0.12 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (1.3 mg, 0.0025 mmol, 0.025 equiv.), and XantPhos (2.9 mg, 0.005 mmol, 0.050 equiv.) in 0.5 mL DMF, 100 °C. Isolated in 75% yield after purification by silica gel chromatography (8:1 to 2:1 hexane:EtOAc) as a yellow solid.

¹H NMR (CDCl₃, 700 MHz) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 4.12 (s, 2H), 3.74 (t, *J* = 4.8 Hz, 4H), 2.99 (m, 4H);

¹³C NMR (CDCl₃, 176 MHz) δ 145.7, 143.4, 133.3, 129.6, 129.3, 129.1 (q, *J* = 33.3 Hz), 128.3, 125.7 (q, *J* = 3.5 Hz), 124.0 (q, *J* = 271.3 Hz), 66.1, 45.9, 41.4;

¹⁹F NMR (CDCl₃, 469 MHz) δ -62.4;

HRMS (ESI): calcd for C₁₈H₁₈F₃NO₃SNa [M+Na]⁺: 408.0852. Found 408.0851.



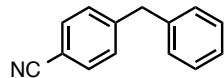
2l: Prepared according to the General Procedure from the corresponding aryl bromide (45 mg, 0.20 mmol, 1.0 equiv.), potassium aryl acetate (60 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and XPhos (7.2 mg, 0.015 mmol, 0.075 equiv.) in 1.0 mL DMF, 40 °C. Isolated in 82% yield after purification by silica gel chromatography (20:1 to 10:1 hexane:EtOAc) as a yellow solid.

$^1\text{H NMR}$ (CDCl_3 , 498 MHz) δ 8.13 (d, J = 9.2 Hz, 1H), 7.54 (d, J = 8.2 Hz, 2H), 7.28–7.25 (m, 2H), 6.88 (dd, J = 9.2 Hz, 2.8 Hz, 1H), 6.73 (d, J = 2.8 Hz, 1H), 4.41 (s, 2H), 3.86 (s, 3H);

$^{13}\text{C NMR}$ (CDCl_3 , 126 MHz) δ 163.3, 142.8, 142.0, 137.9, 129.1, 128.9 (q, J = 31.3 Hz), 128.7, 125.5 (q, J = 3.6 Hz), 124.2 (q, J = 271.3 Hz), 118.0, 112.2, 55.9, 39.2;

$^{19}\text{F NMR}$ (CDCl_3 , 469 MHz) δ -62.4;

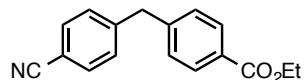
HRMS (ESI): calcd for $\text{C}_{15}\text{H}_{11}\text{F}_3\text{NO}_3$ [M-H] $^+$: 310.0697. Found 310.0690



3a: Prepared according to the General Procedure from the corresponding aryl bromide (79 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (120 mg, 0.60 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and XantPhos (14.7 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 100 °C. Isolated in 81% yield after purification by silica gel chromatography (20:1 to 10:1 Pentane:Et₂O) as a pale yellow oil. Spectroscopic data agreed with that reported.⁸

$^1\text{H NMR}$ (CDCl_3 , 500 MHz) δ 7.57 (m, 2H), 7.33–7.24 (m, 5H), 7.16 (m, 2H), 4.04 (s, 2H);

$^{13}\text{C NMR}$ (CDCl_3 , 126 MHz) δ 146.7, 139.3, 132.3, 129.6, 129.1, 128.8, 126.7, 119.0, 110.1, 42.0;



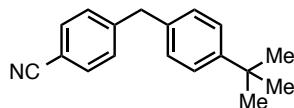
3b: Prepared according to the General Procedure from the corresponding aryl bromide (115 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (120 mg, 0.60 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and XantPhos (14.7 mg, 0.025 mmol,

0.050 equiv.) in 2.5 mL DMF, 100 °C. Isolated in 68% yield after purification by silica gel chromatography (15:1 to 8:1 hexane:EtOAc) as an off-white solid.

¹H NMR (CDCl₃, 500 MHz) δ 7.99 (m, 2H), 7.59 (m, 2H), 7.27 (m, 2H), 7.22 (m, 2H), 4.37 (q, J = 7.1 Hz, 2H), 4.08 (s, 2H), 1.38 (t, J = 7.1 Hz, 3H);

¹³C NMR (CDCl₃, 126 MHz) δ 166.3, 145.7, 144.4, 132.4, 130.1, 129.7, 129.1, 128.9, 118.8, 110.4, 61.0, 41.9, 14.3;

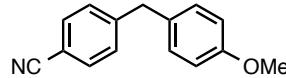
HRMS (EI): calcd for C₁₇H₁₅NO₂ [M]⁺: 265.1103. Found 265.1105.



3c: Prepared according to the General Procedure from the corresponding aryl bromide (107 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (120 mg, 0.60 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and XantPhos (14.7 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 100 °C. Isolated in 58% yield after purification by silica gel chromatography (20:1 to 10:1 Pentane:Et₂O) as a pale yellow oil. Spectroscopic data agreed with that reported.⁶

¹H NMR (CDCl₃, 500 MHz) δ 7.58 (m, 2H), 7.34 (m, 2H), 7.29 (m, 2H), 7.09 (m, 2H), 4.00 (s, 2H), 1.31 (s, 9H);

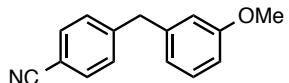
¹³C NMR (CDCl₃, 126 MHz) δ 149.6, 146.9, 136.3, 132.3, 129.7, 128.6, 128.6, 125.7, 119.0, 41.5, 34.4, 31.4.



3d: Prepared according to the General Procedure from the corresponding aryl bromide (94 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (120 mg, 0.60 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and XantPhos (14.7 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 100 °C. 75% yield by ¹H NMR using durene as internal standard. Spectroscopic data agreed with that reported.¹

¹H NMR (CDCl₃, 500 MHz) δ 7.56 (m, 2H), 7.26 (m, 2H), 7.07 (m, 2H), 6.85 (m, 2H), 3.97 (s, 2H), 3.79 (s, 3H);

¹³C NMR (CDCl₃, 126 MHz) δ 158.4, 147.2, 132.3, 131.4, 129.9, 129.5, 119.0, 114.2, 110.0, 55.3, 41.1.

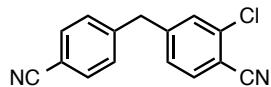


3e: Prepared according to the General Procedure from the corresponding aryl bromide (37 mg, 0.20 mmol, 1.0 equiv.), potassium aryl acetate (48 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.0050 mmol, 0.025 equiv.), and XantPhos (5.8 mg, 0.010 mmol, 0.050 equiv.) in 1.0 mL DMF, 100 °C. Isolated in 49% yield after purification by silica gel chromatography (50:1 to 4:1 hexane:EtOAc) as a colourless oil.

$^1\text{H NMR}$ (CDCl_3 , 498 MHz) δ 7.59–7.55 (m, 2H), 7.30–7.27 (m, 2H), 7.23 (t, J = 8.1 Hz, 1H), 6.78 (dd, J = 8.2, 2.6 Hz, 1H), 6.75 (d, J = 7.4 Hz, 1H), 6.69 (m, 1H), 4.00 (s, 2H), 3.78 (s, 3H);

$^{13}\text{C NMR}$ (CDCl_3 , 126 MHz) δ 160.1, 146.7, 141.0, 132.4, 129.9, 129.8, 121.5, 119.1, 115.1, 111.9, 110.3, 55.3, 42.1;

HRMS (EI): calcd for $\text{C}_{15}\text{H}_{13}\text{NO} [\text{M}]^+$: 223.0997. Found 223.0997.

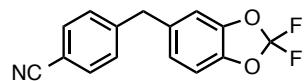


3f: Prepared according to the General Procedure from the corresponding aryl bromide (43 mg, 0.2 mmol, 1.0 equiv.), potassium aryl acetate (48 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and XantPhos (5.8 mg, 0.010 mmol, 0.050 equiv.) in 1.0 mL DMF, 100 °C. Isolated in 85% yield after purification by silica gel chromatography (8:1 to 4:1 Hexane:EtOAc) as a white solid.

$^1\text{H NMR}$ (CDCl_3 , 500 MHz) δ 7.64–7.60 (m, 3H), 7.31 (m, 1H), 7.27 (m, 2H), 7.16 (m, 1H), 4.07 (s, 2H);

$^{13}\text{C NMR}$ (CDCl_3 , 126 MHz) δ 146.4, 143.9, 137.1, 134.2, 132.7, 130.4, 129.7, 127.7, 118.5, 115.8, 111.8, 111.2, 41.6;

HRMS (EI): calcd for $\text{C}_{15}\text{H}_9^{35}\text{ClN}_2 [\text{M}]^+$: 252.0454. Found 252.0451.



3g: Prepared according to the General Procedure from the corresponding aryl bromide (59 mg, 0.25 mmol, 1.0 equiv.), potassium aryl acetate (60 mg, 0.30 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (3.2 mg, 0.00625 mmol, 0.025 equiv.), and XantPhos (7.2 mg, 0.0125 mmol,

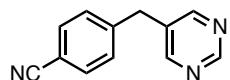
0.050 equiv.) in 1.25 mL DMF, 100 °C. Isolated in 83% yield after purification by silica gel chromatography (2% to 18% EtOAc in Hexane) as a white solid.

¹H NMR (CDCl₃, 700 MHz) δ 7.58 (m, 2H), 7.26 (m, 2H), 6.98 (m, 1H), 6.87 (m, 1H), 6.84 (m, 1H), 4.01 (s, 2H);

¹³C NMR (CDCl₃, 176 MHz) δ 145.8, 144.1, 142.5, 135.4, 132.4, 131.6 (t, *J* = 251.9 Hz), 129.5, 123.9, 118.8, 110.5, 110.1, 109.5, 41.6;

¹⁹F NMR (CDCl₃, 378 MHz) δ -50.1;

HRMS (EI): calcd for C₁₅H₉NO₂F² [M]⁺: 273.0602. Found 273.0606.

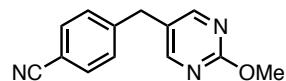


3h: Prepared according to the General Procedure from the corresponding aryl bromide (40 mg, 0.25 mmol, 1.0 equiv.), potassium aryl acetate (60 mg, 0.30 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (3.3 mg, 0.00625 mmol, 0.025 equiv.), and XantPhos (7.3 mg, 0.0125 mmol, 0.050 equiv.) in 1.25 mL DMF, 100 °C. Isolated in 87% yield after purification by silica gel chromatography (1:3 hexane:EtOAc) as a yellow solid.

¹H NMR (CDCl₃, 498 MHz) δ 9.12 (s, 1H), 8.57 (s, 2H), 7.63–7.62 (m, 2H), 7.30–7.28 (m, 2H), 4.04 (s, 2H);

¹³C NMR (CDCl₃, 176 MHz) δ 157.4, 157.0, 143.7, 132.8, 132.7, 129.5, 118.4, 111.2, 36.5;

HRMS (EI): calcd for C₁₂H₉N₃ [M]⁺: 195.0797. Found 195.0794.

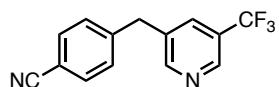


3i: Prepared according to the General Procedure from the corresponding aryl bromide (47 mg, 0.25 mmol, 1.0 equiv.), potassium aryl acetate (60 mg, 0.30 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂ (3.3 mg, 0.00625 mmol, 0.025 equiv.), and XantPhos (7.3 mg, 0.0125 mmol, 0.050 equiv.) in 1.25 mL DMF, 100 °C. Isolated in 83% yield after purification by silica gel chromatography (2:1 hexane:EtOAc) as a light yellow solid.

¹H NMR (CDCl₃, 498 MHz) δ 8.35 (s, 2H), 7.63–7.62 (m, 2H), 7.30–7.28 (m, 2H), 4.01 (s, 3H), 3.98 (s, 2H);

¹³C NMR (CDCl₃, 176 MHz) δ 164.8, 159.3, 144.6, 132.6, 129.4, 125.7, 118.6, 110.9, 54.9, 35.5;

HRMS (EI): calcd for C₁₃H₁₁N₃O [M]⁺: 225.0902. Found 225.0897.



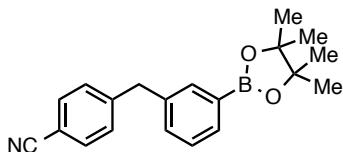
3j: Prepared according to the General Procedure from the corresponding aryl bromide (57 mg, 0.25 mmol, 1.0 equiv.), potassium aryl acetate (60 mg, 0.30 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (3.3 mg, 0.00625 mmol, 0.025 equiv.), and XantPhos (7.3 mg, 0.0125 mmol, 0.050 equiv.) in 1.25 mL DMF, 100 °C. Isolated in 76% yield after purification by silica gel chromatography (4:1 hexane:EtOAc) as a colourless oil;

$^1\text{H NMR}$ (CDCl_3 , 498 MHz) δ 8.78 (s, 1H), 8.66 (s, 1H), 7.68 (s, 1H), 7.63 (d, J = 8.3 Hz, 2H), 7.29 (d, J = 8.3 Hz, 2H), 4.12 (s, 2H);

$^{13}\text{C NMR}$ (CDCl_3 , 176 MHz) δ 153.3, 145.1 (q, J = 3.5 Hz), 143.9, 135.1, 133.1 (q, J = 3.5 Hz), 132.8, 129.6, 126.7 (q, J = 29.8 Hz), 123.3 (q, J = 271.3 Hz), 118.5, 111.2, 38.7;

$^{19}\text{F NMR}$ (CDCl_3 , 469 MHz) δ -62.4;

HRMS (EI): calcd for $\text{C}_{14}\text{H}_9\text{N}_2\text{F}_3$ [M] $^+$: 262.0718. Found 262.0714.

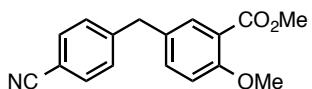


3k: Prepared according to the General Procedure from the corresponding aryl bromide (71 mg, 0.25 mmol, 1.0 equiv.), potassium aryl acetate (60 mg, 0.30 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (3.2 mg, 0.00625 mmol, 0.025 equiv.), and XantPhos (7.2 mg, 0.0125 mmol, 0.050 equiv.) in 1.25 mL DMF, 100 °C. 66% yield by $^1\text{H NMR}$ using durene as internal standard and isolated in 28% yield after purification by silica gel chromatography (2% to 18% EtOAc in Hexane) as a colourless oil.

$^1\text{H NMR}$ (CDCl_3 , 700 MHz) δ 7.69 (d, J = 7.3 Hz, 1H), 7.65 (s, 1H), 7.56 (m, 2H), 7.32 (t, J = 7.4 Hz, 1H), 7.27 (m, 2H), 7.23 (m, 1H), 4.03 (s, 2H), 1.34 (s, 12H);

$^{13}\text{C NMR}$ (CDCl_3 , 176 MHz) δ 146.8, 138.5, 135.3, 133.2, 132.3, 131.9, 129.6, 128.2, 119.0, 110.0, 83.9, 41.9, 24.9. The carbon directly attached to boron atom was not detected.

HRMS (EI): calcd for $\text{C}_{20}\text{H}_{22}\text{NO}_2\text{B}$ [M] $^+$: 319.1744. Found 319.1745.

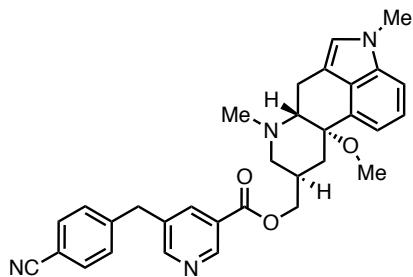


3l: Prepared according to the General Procedure from the corresponding aryl bromide (61 mg, 0.25 mmol, 1.0 equiv.), potassium aryl acetate (60 mg, 0.30 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (3.2 mg, 0.00625 mmol, 0.025 equiv.), and XantPhos (7.2 mg, 0.0125 mmol, 0.050 equiv.) in 1.25 mL DMF, 100 °C. Isolated in 58% yield after purification by silica gel chromatography (12:1 to 1:1 hexane/EtOAc) as a pale yellow oil.

^1H NMR (CDCl_3 , 500 MHz) δ 7.74 (m, 1H), 7.58 (m, 2H), 7.27 (m, 2H), 6.77 (m 1H), 6.74 (m, 1H), 4.04 (s, 2H), 3.87 (s, 3H), 3.85 (s, 3H);

^{13}C NMR (CDCl_3 , 126 MHz) δ 166.4, 159.5, 145.6, 145.4, 132.4, 132.2, 129.6, 120.8, 118.8, 118.5, 112.7, 111.5, 56.0, 52.0, 42.1;

HRMS (EI): calcd for $\text{C}_{17}\text{H}_{15}\text{NO}_3$ $[\text{M}]^+$: 281.1052. Found 281.1053.

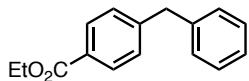


3m: Prepared according to the General Procedure from the corresponding aryl bromide (97 mg, 0.20 mmol, 1.0 equiv.), potassium aryl acetate (48 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and XantPhos (5.8 mg, 0.01 mmol, 0.050 equiv.) in 1.0 mL DMF, 100 °C. Isolated in 87% yield after purification by silica gel chromatography (10:1 DCM:MeOH) as a light yellow solid.

^1H NMR (CDCl_3 , 498 MHz) δ 9.13 (s, 1H), 8.65 (s, 1H), 8.07 (s, 1H), 8.07–8.06 (m, 2H), 7.29–7.18 (m, 4H), 7.03 (d, J = 7.0 Hz, 1H), 6.80 (s, 1H), 4.40–4.37 (m, 1H), 4.29–4.25 (m, 1H), 4.09 (s, 2H), 3.77 (s, 3H), 3.23–3.17 (m, 2H), 3.05–2.95 (m, 5H), 2.63–2.59 (m, 1H), 2.46 (s, 3H), 2.35–2.31 (m, 1H), 2.06 (t, J = 11.8 Hz, 1H), 1.36 (t, J = 13.3 Hz, 1H);

^{13}C NMR (CDCl_3 , 126 MHz) δ 165.0, 153.8, 149.2, 144.5, 137.2, 135.1, 135.0, 132.7, 129.7, 129.6, 126.3, 126.2, 123.3, 121.4, 118.6, 114.9, 110.9, 110.3, 109.0, 73.6, 70.1, 68.2, 60.7, 49.5, 43.9, 38.8, 32.8, 31.6, 30.2, 22.4;

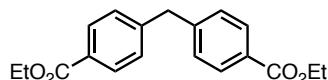
HRMS (ESI): calcd for $\text{C}_{32}\text{H}_{33}\text{N}_4\text{O}_3$ $[\text{M}+\text{H}]^+$: 521.2547. Found 521.2545.



4a: Prepared according to the General Procedure from the corresponding aryl bromide (79 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (148 mg, 0.60 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and XantPhos (14.5 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 110 °C. Isolated in 77% yield after purification by silica gel chromatography (30:1 hexane:EtOAc) as a colourless oil. Spectroscopic data agreed with that reported.⁹

¹H NMR (CDCl_3 , 498 MHz) δ 7.99 (m, 2H), 7.33–7.18 (m, 7H), 4.38 (q, J = 7.5 Hz, 2H), 4.05 (s, 2H), 1.40 (t, J = 7.5 Hz, 3H);

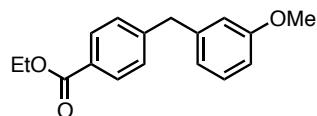
¹³C NMR (CDCl_3 , 126 MHz) δ 166.6, 146.4, 140.2, 129.8, 128.9, 128.8, 128.6, 128.4, 126.4, 60.8, 41.9, 14.4.



4b: Prepared according to the General Procedure from the corresponding aryl bromide (115 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (148 mg, 0.60 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and XantPhos (14.5 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 110 °C. Isolated in 71% yield after purification by silica gel chromatography (30:1 hexane:EtOAc) as a colourless oil. Spectroscopic data agreed with that reported.¹⁰

¹H NMR (CDCl_3 , 498 MHz) δ 7.98–7.96 (m, 4H), 7.25–7.23 (m, 4H), 4.36 (q, J = 7.0 Hz, 4H), 4.08 (s, 2H), 1.38 (t, J = 7.2 Hz, 6H);

¹³C NMR (CDCl_3 , 126 MHz) δ 166.4, 145.4, 129.9, 128.9, 128.8, 60.8, 41.8, 14.3.

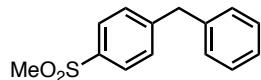


4c: Prepared according to the General Procedure from the corresponding aryl bromide (37 mg, 0.20 mmol, 1.0 equiv.), potassium aryl acetate (59 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and XantPhos (5.8 mg, 0.01 mmol, 0.05 equiv.), 110°C. Isolated in 56% yield after purification by silica gel chromatography (100:1 to 10:1 hexane:EtOAc) as a colorless oil.

¹H NMR (CDCl₃, 498 MHz) δ 7.98 - 7.95 (m, 2H), 7.27–7.24 (m, 2H), 7.21 (t, *J* = 7.8 Hz, 1H), 6.78–6.75 (m, 2H), 7.71 (m, 1H), 4.36 (q, *J* = 7.2 Hz, 2H), 4.00 (s, 2H), 3.77 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H);

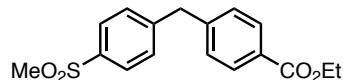
¹³C NMR (CDCl₃, 126 MHz) δ 166.7, 160.0, 146.3, 141.9, 129.9, 129.7, 129.0, 128.7, 121.5, 115.0, 111.7, 61.0, 55.3, 42.1, 14.5;

HRMS (EI): calcd for C₁₇H₁₈O₃ [M]⁺: 270.1256. Found 270.1255.



5a: Prepared according to the General Procedure from the corresponding aryl bromide (68 mg, 0.30 mmol, 1.0 equiv.), potassium aryl acetate (91 mg, 0.36 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂(3.9 mg, 0.0075 mmol, 0.025 equiv.), and XantPhos (8.7 mg, 0.015 mmol, 0.050 equiv.) in 1.5 mL DMF, 90 °C. 67% yield by ¹H NMR using durene as internal standard. Spectroscopic data agreed with that reported.¹¹

¹H NMR (CDCl₃, 498 MHz) δ 7.85 (m, 2H), 7.38 (d, *J* = 8.3 Hz, 2H), 7.32 (m, 2H), 7.23 (m, 1H), 7.18 (d, *J* = 6.8 Hz, 2H), 4.07 (s, 2H), 3.03 (t, *J* = 8.0 Hz, 3H).

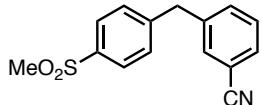


5b: Prepared according to the General Procedure from the corresponding aryl bromide (69 mg, 0.30 mmol, 1.0 equiv.), potassium aryl acetate (91 mg, 0.36 mmol, 1.2 equiv.), [Pd(cinnamyl)Cl]₂(3.9 mg, 0.0075 mmol, 0.025 equiv.), and XantPhos (8.7 mg, 0.015 mmol, 0.050 equiv.) in 1.5 mL DMF, 90 °C. Isolated in 83% yield after purification by silica gel chromatography (4:1 to 2:1 hexane:EtOAc) as a light yellow solid.

¹H NMR (CDCl₃, 498 MHz) δ 8.01 (m, 2H), 7.88 (m, 2H), 7.38 (d, *J* = 8.8 Hz, 2H), 7.27 (d, *J* = 8.8 Hz, 2H), 4.39 (q, *J* = 7.0 Hz, 2H), 4.14 (s, 2H), 3.05 (s, 3H), 1.40 (t, *J* = 7.5 Hz, 3H);

¹³C NMR (CDCl₃, 126 MHz) δ 166.3, 146.7, 144.4, 138.7, 130.1, 129.8, 129.0, 128.9, 127.8, 60.9, 44.6, 41.7, 14.3;

HRMS (EI): calcd for C₁₇H₁₈O₄S [M]⁺: 318.0926. Found 318.0924.

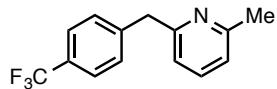


5c: Prepared according to the General Procedure from the corresponding aryl bromide (55 mg, 0.30 mmol, 1.0 equiv.), potassium aryl acetate (91 mg, 0.36 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (3.9 mg, 0.0075 mmol, 0.025 equiv.), and XantPhos (8.7 mg, 0.015 mmol, 0.050 equiv.) in 1.5 mL DMF, 90 °C. Isolated in 67% yield after purification by silica gel chromatography (2:1 hexane:EtOAc) as a white solid.

^1H NMR (CDCl_3 , 498 MHz) δ 7.93-7.91 (m, 2H), 7.58-7.56 (m, 1H), 7.47-7.43 (m, 3H), 7.39-7.37 (m, 2H), 4.13 (s, 2H), 3.07 (s, 3H);

^{13}C NMR (CDCl_3 , 126 MHz) δ 145.8, 140.9, 139.1, 133.4, 132.5, 130.5, 129.8, 129.6, 127.9, 118.6, 112.9, 44.6, 41.2;

HRMS (EI): calcd for $\text{C}_{15}\text{H}_{13}\text{O}_2\text{SN}$ [M] $^+$: 271.0667. Found 271.0667.

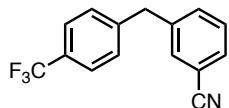


6a: Prepared according to the General Procedure from the corresponding aryl bromide (69 mg, 0.40 mmol, 2.0 equiv.), potassium aryl acetate (48 mg, 0.20 mmol, 1.0 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and DEA-XantPhos (5.6 mg, 0.01 mmol, 0.050 equiv.) in 1.0 mL DMF, 125 °C. Isolated in 52% yield after purification by silica gel chromatography (4:1 to 2:1 hexane:EtOAc) as a colourless oil. Spectroscopic data agreed with that reported.¹²

^1H NMR (CDCl_3 , 498 MHz) δ 7.54 (d, J = 8.4 Hz, 2H), 7.47 (t, J = 7.7 Hz, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.01 (d, J = 8.0 Hz, 1H), 6.87 (d, J = 8.0 Hz, 1H), 4.17 (s, 2H), 2.55 (s, 3H);

^{13}C NMR (CDCl_3 , 126 MHz) δ 159.2, 158.3, 143.8, 136.9, 129.4, 128.7 (q, J = 31.3 Hz), 125.4 (q, J = 3.8 Hz), 124.3 (q, J = 271.3 Hz), 121.1, 120.1, 44.5, 24.6;

^{19}F NMR (CDCl_3 , 469 MHz) δ -62.4.



6b: Prepared according to the General Procedure from the corresponding aryl bromide (91 mg, 0.50 mmol, 1.0 equiv.), potassium aryl acetate (145 mg, 0.60 mmol, 1.2 equiv.),

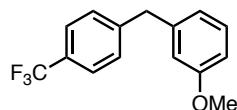
$[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and DEA-XantPhos (14 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 125 °C. Isolated in 60% yield after purification by silica gel chromatography (10:1 hexane:EtOAc) as a yellow solid.

^1H NMR (CDCl_3 , 498 MHz) δ 7.59 (d, J = 8.0 Hz, 2H), 7.55–7.53 (m, 1H), 7.48–7.43 (m, 1H), 7.43–7.42 (m, 2H), 7.29–7.28 (m, 2H), 4.08 (s, 2H);

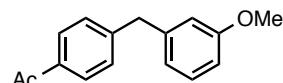
^{13}C NMR (CDCl_3 , 126 MHz) δ 143.4, 141.5, 133.4, 132.4, 130.3, 129.5, 129.2, 129.1 (q, J = 32.5 Hz), 125.7 (q, J = 3.8 Hz), 124.1 (q, J = 272.8 Hz), 118.7, 112.8, 41.1;

^{19}F NMR (CDCl_3 , 469 MHz) δ -62.5;

HRMS (EI): calcd for $\text{C}_{15}\text{H}_{10}\text{NF}_3$ [M] $^+$: 261.0765. Found 261.0767.



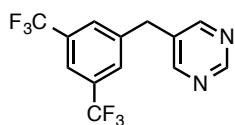
6c: Prepared according to the General Procedure from the corresponding aryl bromide (18.7 mg, 0.10 mmol, 1.0 equiv.), potassium aryl acetate (29 mg, 0.12 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (1.3 mg, 0.0025 mmol, 0.025 equiv.), and DEA-XantPhos (2.8 mg, 0.005 mmol, 0.050 equiv.) in 0.5 mL DMF, 125 °C. 11% yield by ^1H NMR using durene as internal standard. Spectroscopic data agreed with that reported.¹³



7a: Prepared according to the General Procedure from the corresponding aryl bromide (37 mg, 0.2 mmol, 1.0 equiv.), potassium aryl acetate (52 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and XantPhos (5.8 mg, 0.010 mmol, 0.050 equiv.) in 1.0 mL DMF, 110 °C. Isolated in 55% yield after purification by silica gel chromatography (2% to 15% EtOAc in Hexane) as a colourless oil. Spectroscopic data agreed with that reported.¹⁴

^1H NMR (CDCl_3 , 500 MHz) δ 7.88 (m, 2H), 7.28 (m, 2H), 7.21 (t, J = 8.0 Hz, 1H), 6.77 (m, 2H), 6.72 (m, 1H), 4.00 (s, 2H), 3.77 (s, 3H), 2.58 (s, 3H);

^{13}C NMR (CDCl_3 , 126 MHz) δ 197.8, 159.8, 146.6, 141.6, 135.3, 129.6, 129.1, 128.6, 121.3, 114.9, 111.6, 55.2, 41.9, 26.6.



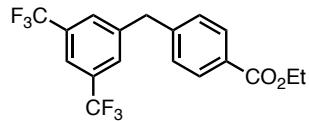
7b: Prepared according to the General Procedure from the corresponding aryl bromide (32 mg, 0.2 mmol, 1.0 equiv.), potassium aryl acetate (74 mg, 0.24 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (2.6 mg, 0.005 mmol, 0.025 equiv.), and DEA-XantPhos (5.6 mg, 0.010 mmol, 0.050 equiv.) in 1.0 mL DMF, 110 °C. Isolated in 64% yield after purification by silica gel chromatography (16% to 100% EtOAc in Hexane) as an orange solid.

$^1\text{H NMR}$ (CDCl_3 , 700 MHz) δ 9.16 (s, 1H), 8.61 (s, 2H), 7.80 (s, 1H), 7.64 (s, 2H), 4.12 (s, 2H);

$^{13}\text{C NMR}$ (CDCl_3 , 176 MHz) δ 157.7, 157.0, 140.1, 132.4 (q, $J = 34.7$ Hz), 132.2, 128.8 (m), 123.0 (q, $J = 271.6$ Hz), 121.3 (quint, $J = 3.63$ Hz), 36.1;

$^{19}\text{F NMR}$ (CDCl_3 , 378 MHz) δ -63.0;

HRMS (EI): calcd for $\text{C}_{13}\text{H}_8\text{N}_2\text{F}_6$ [M] $^+$: 306.0592. Found 306.0591.



7c: Prepared according to the General Procedure from the corresponding aryl bromide (115 mg, 0.50 mmol, 1 equiv.), potassium aryl acetate (186 mg, 0.60 mmol, 1.2 equiv.), $[\text{Pd}(\text{cinnamyl})\text{Cl}]_2$ (6.5 mg, 0.0125 mmol, 0.025 equiv.), and DEA-XantPhos (14 mg, 0.025 mmol, 0.050 equiv.) in 2.5 mL DMF, 110 °C. Isolated in 70% yield after purification by silica gel chromatography (12:1 hexane:EtOAc) as a light yellow oil.

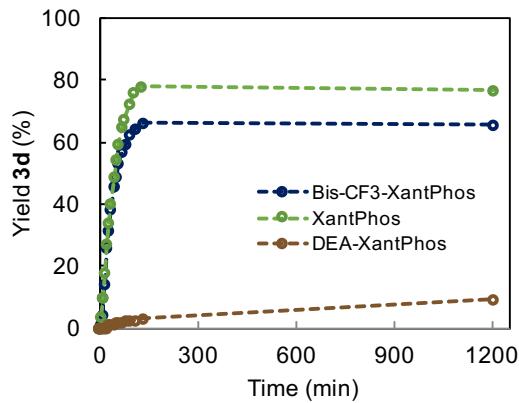
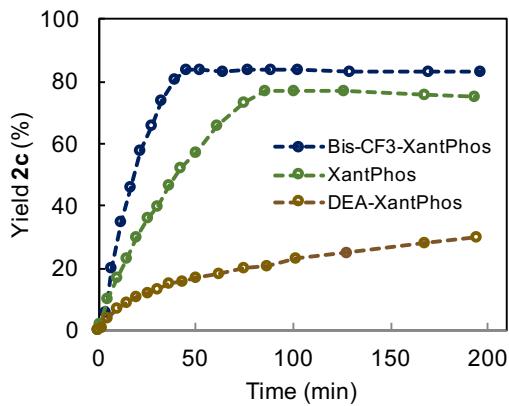
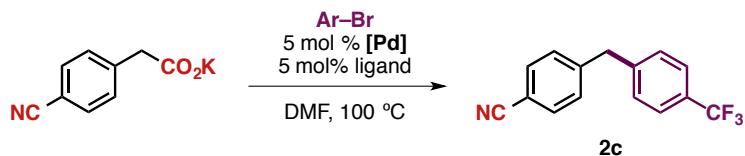
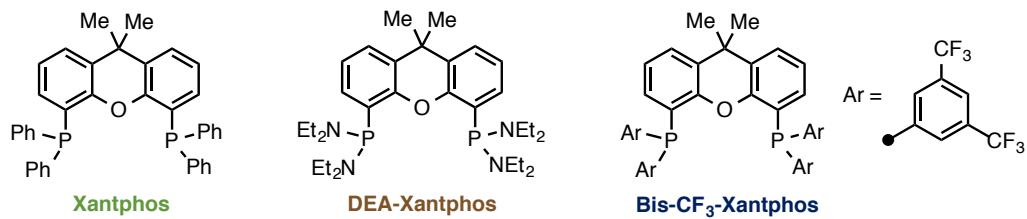
$^1\text{H NMR}$ (CDCl_3 , 498 MHz) δ 8.02 (m, 2H), 7.75 (s, 1H), 7.61 (s, 2H), 7.24 (m, 2H), 4.38(q, $J = 7.3$ Hz, 2H), 4.16 (s, 2H), 1.39 (t, $J = 7.3$ Hz, 3H).

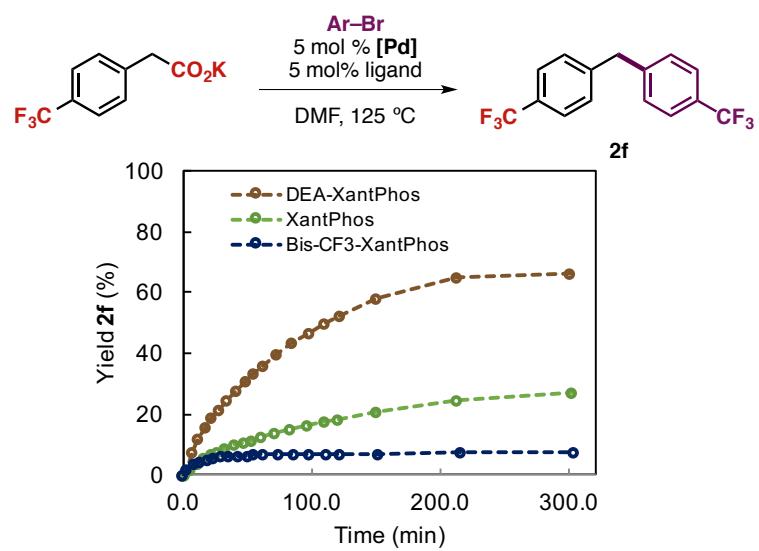
$^{13}\text{C NMR}$ (CDCl_3 , 126 MHz) δ 166.3, 143.8, 142.6, 131.9 (q, $J = 32.5$ Hz), 130.2, 129.3, 128.9, 128.8, 123.3 (d, $J = 271.3$ Hz), 120.6 (m), 61.0, 41.4, 14.3.

$^{19}\text{F NMR}$ (CDCl_3 , 469 MHz) δ -62.8.

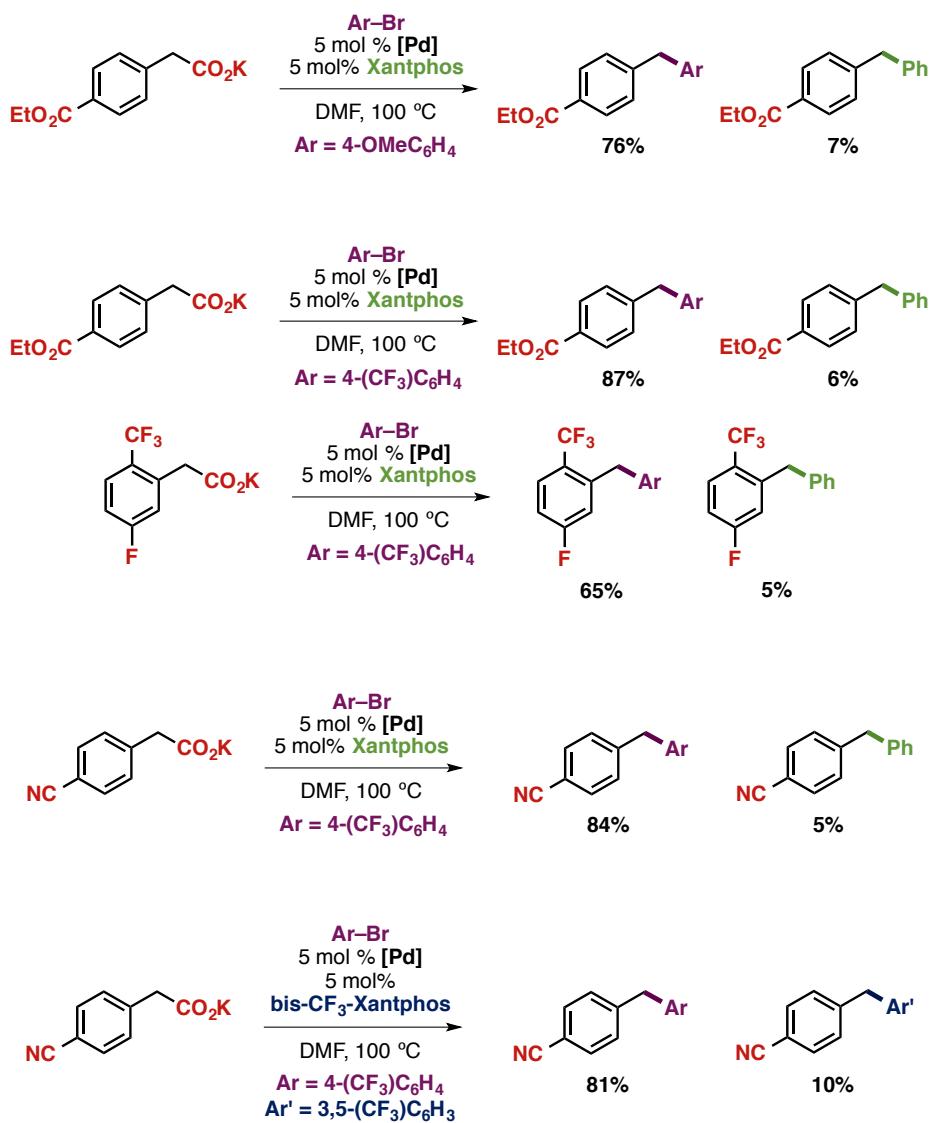
HRMS (EI): calcd for $\text{C}_{18}\text{H}_{14}\text{O}_2\text{F}_6$ [M] $^+$: 376.0898. Found 376.0899.

IV. Reaction Kinetics with Different Xantphos Derivatives





V. Diarylmethane Products Arising from Ligand Aryl Exchange



VI. References

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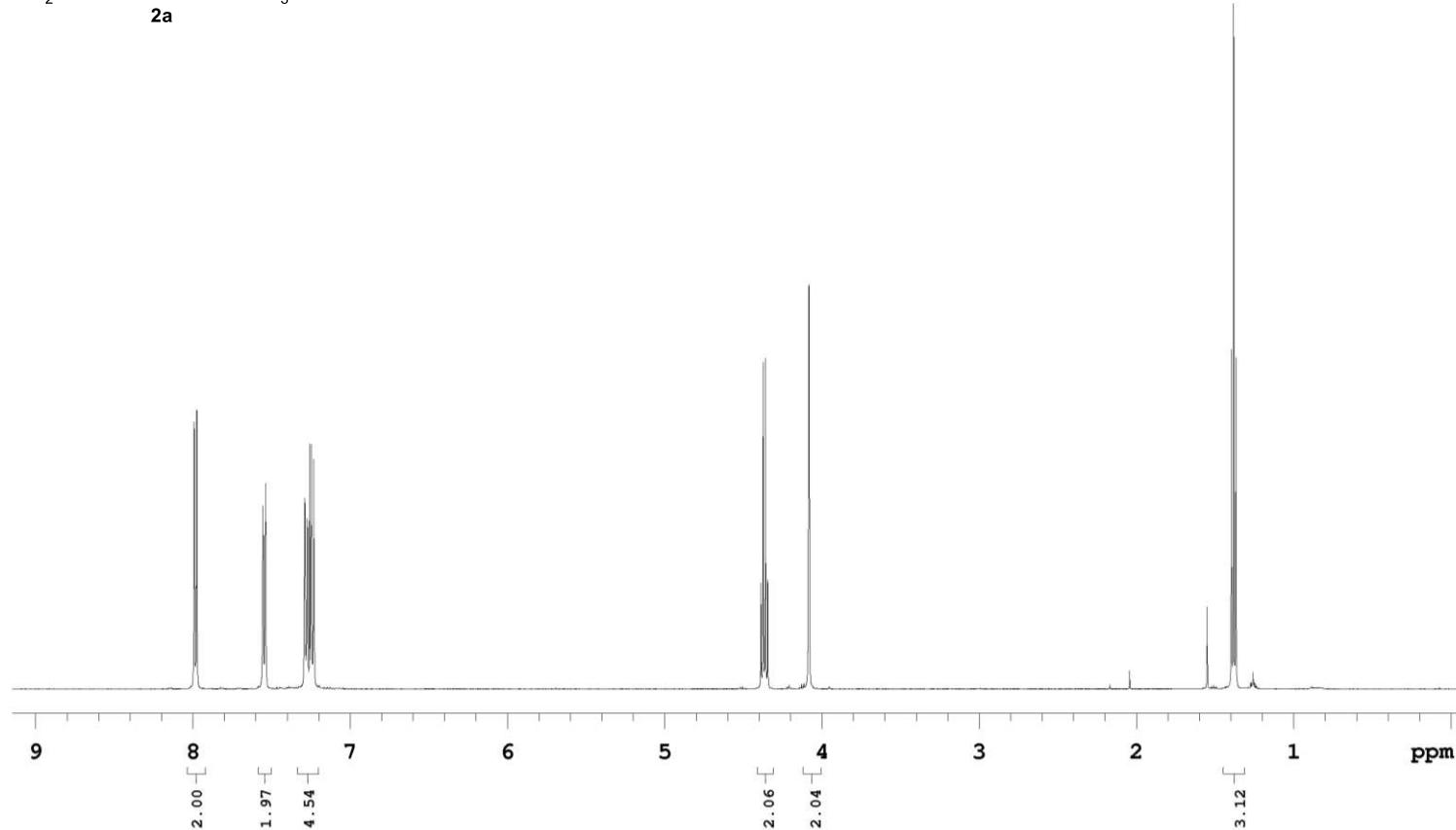
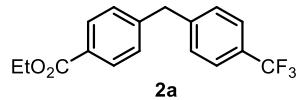
Recorded on: **iBD5, Feb 23 2018**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **6000.6**
Digital Res.(Hz/pt): **0.09**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **19.14**

Relaxation Delay(s): **0.1**
Completed Scans **16**

DK-3-103-B
498.118 MHz H1 1D in CDCl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe





Department of Chemistry, University of Alberta

Recorded on: u500, Feb 24 2018

Sweep Width(Hz): 33783.8

Acquisition Time(s): 1

Relaxation Delay(s): 1

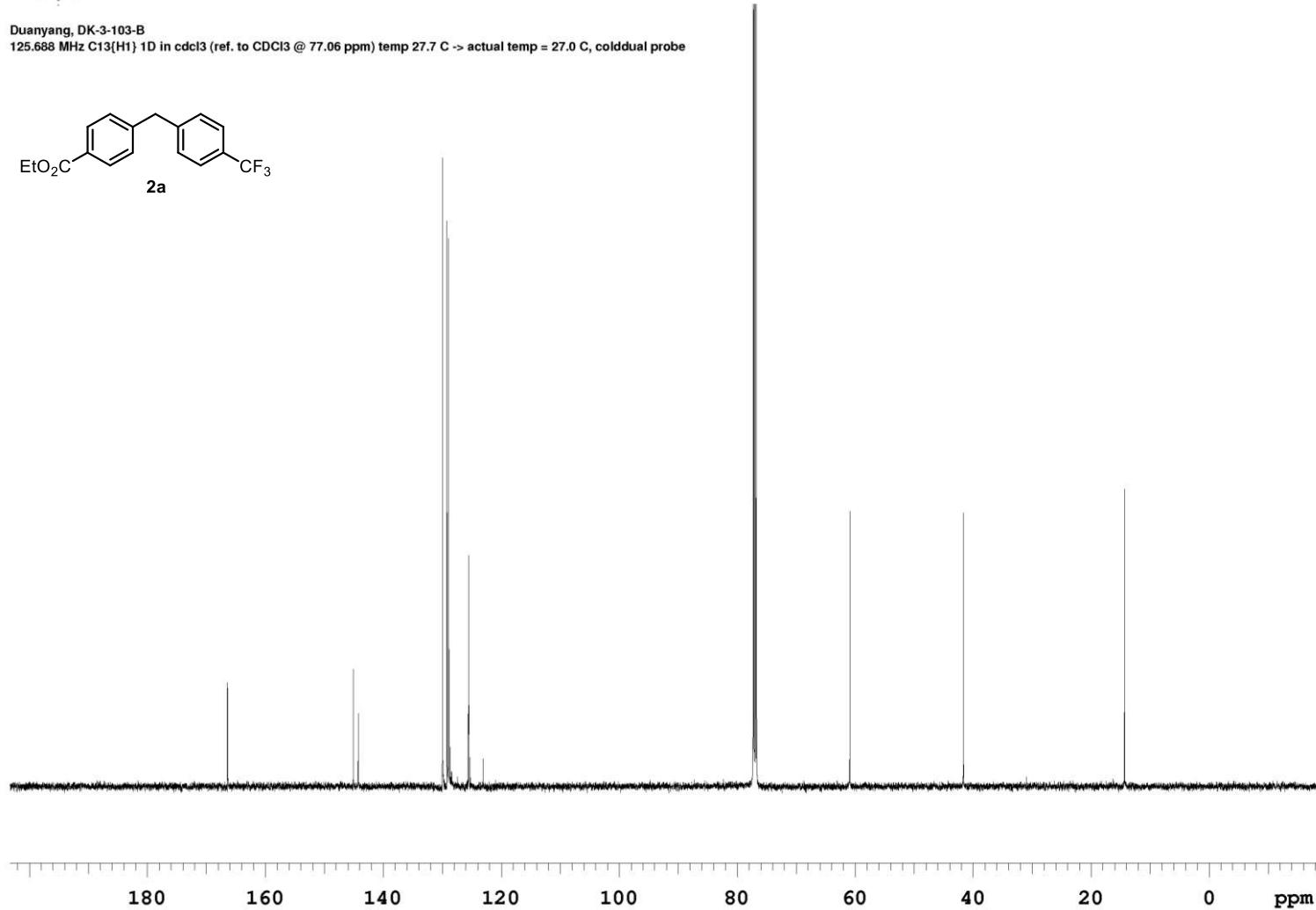
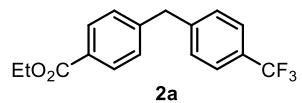
Pulse Sequence: s2pul

Digital Res.(Hz/pt): 0.26

Hz per mm(Hz/mm): 116.41

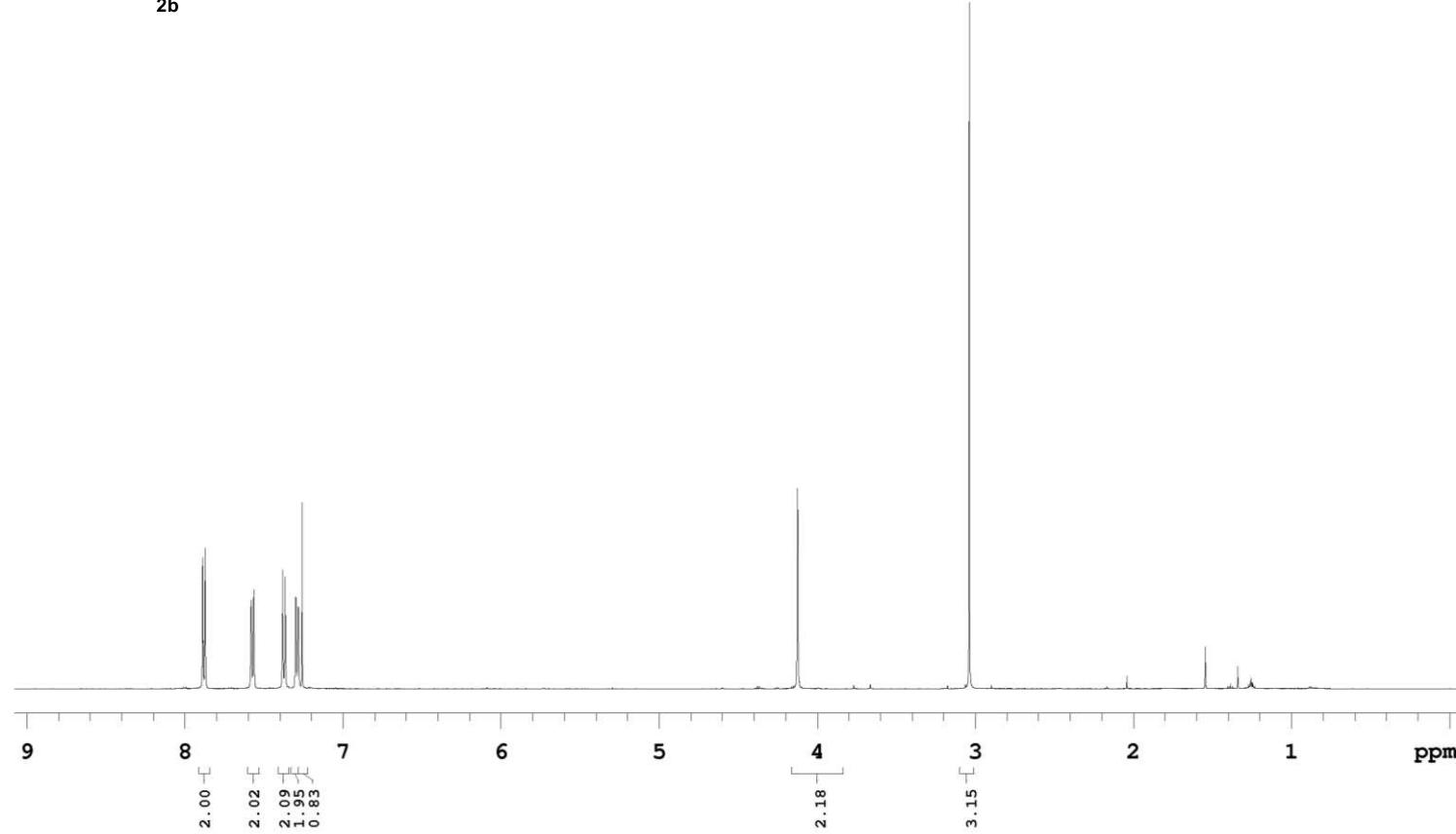
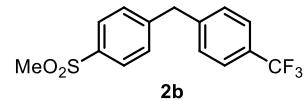
Completed Scans 144

Duanyang, DK-3-103-B
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, colddual probe





Department of Chemistry, University of Alberta

Recorded on: ibd5, Mar 1 2018
Pulse Sequence: s2pulSweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.06Relaxation Delay(s): 0.1
Completed Scans 16DK-3-127-A
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe



Department of Chemistry, University of Alberta

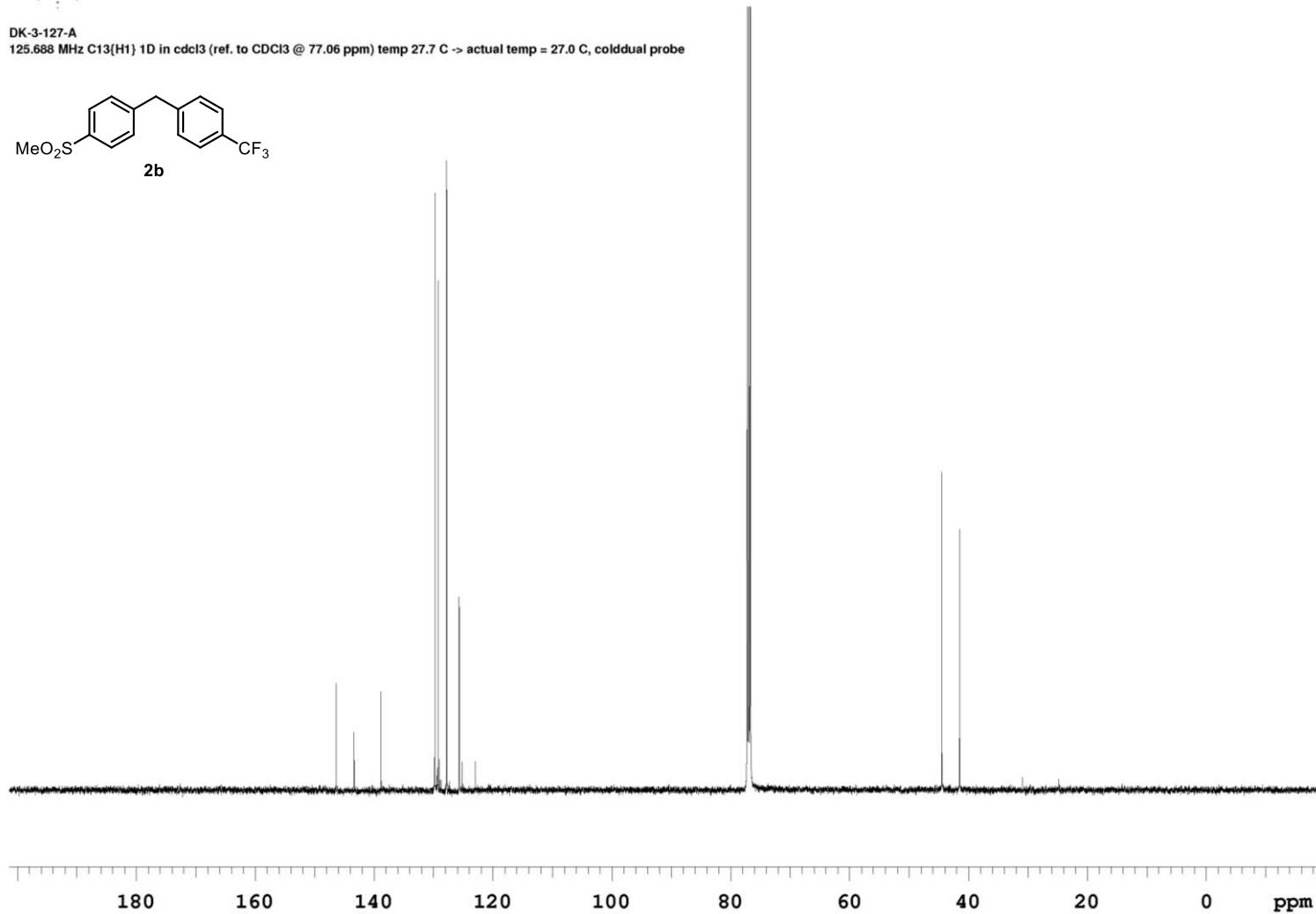
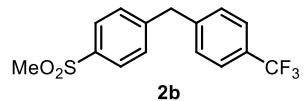
Recorded on: u500, Mar 1 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26

Acquisition Time(s): 1
Hz per mm(Hz/mm): 115.52

Relaxation Delay(s): 1
Completed Scans: 280

DK-3-127-A
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, cold dual probe





Department of Chemistry, University of Alberta

Recorded on: u500, Feb 25 2018

Sweep Width(Hz): 6009.62

Acquisition Time(s): 5

Relaxation Delay(s): 0.1

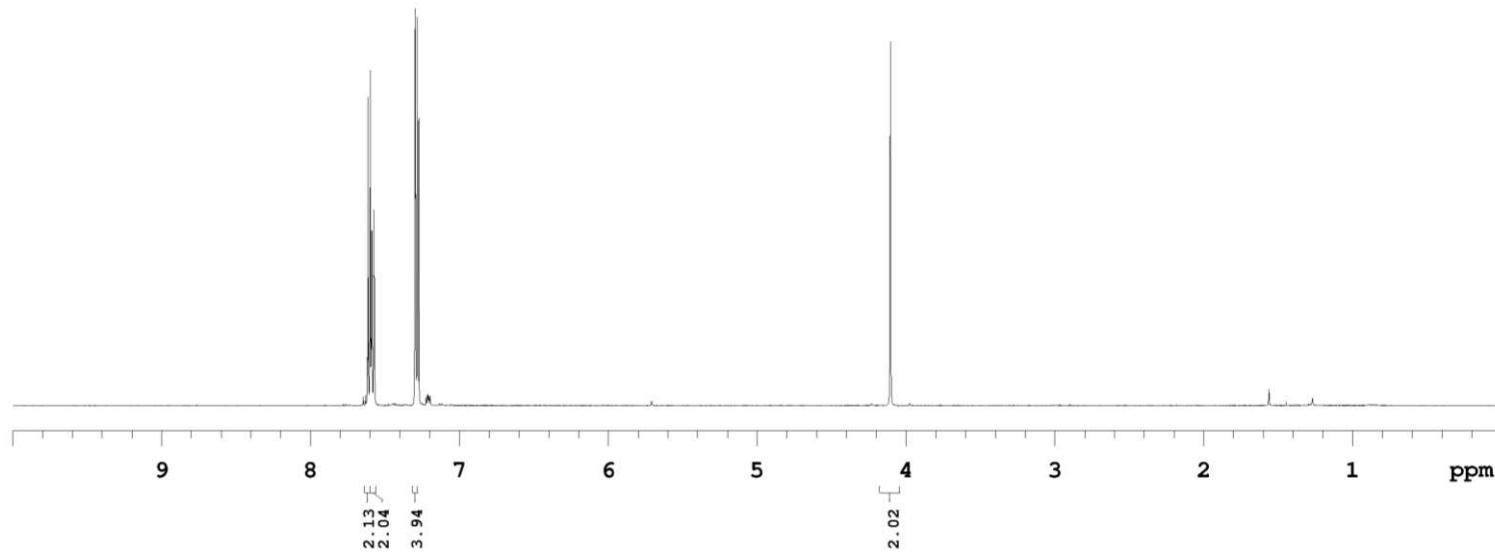
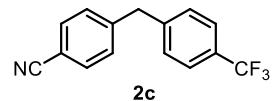
Pulse Sequence: PRESAT

Digital Res.(Hz/pt): 0.09

Hz per mm(Hz/mm): 20.85

Completed Scans: 1

WQ-03-186-A
499.797 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe





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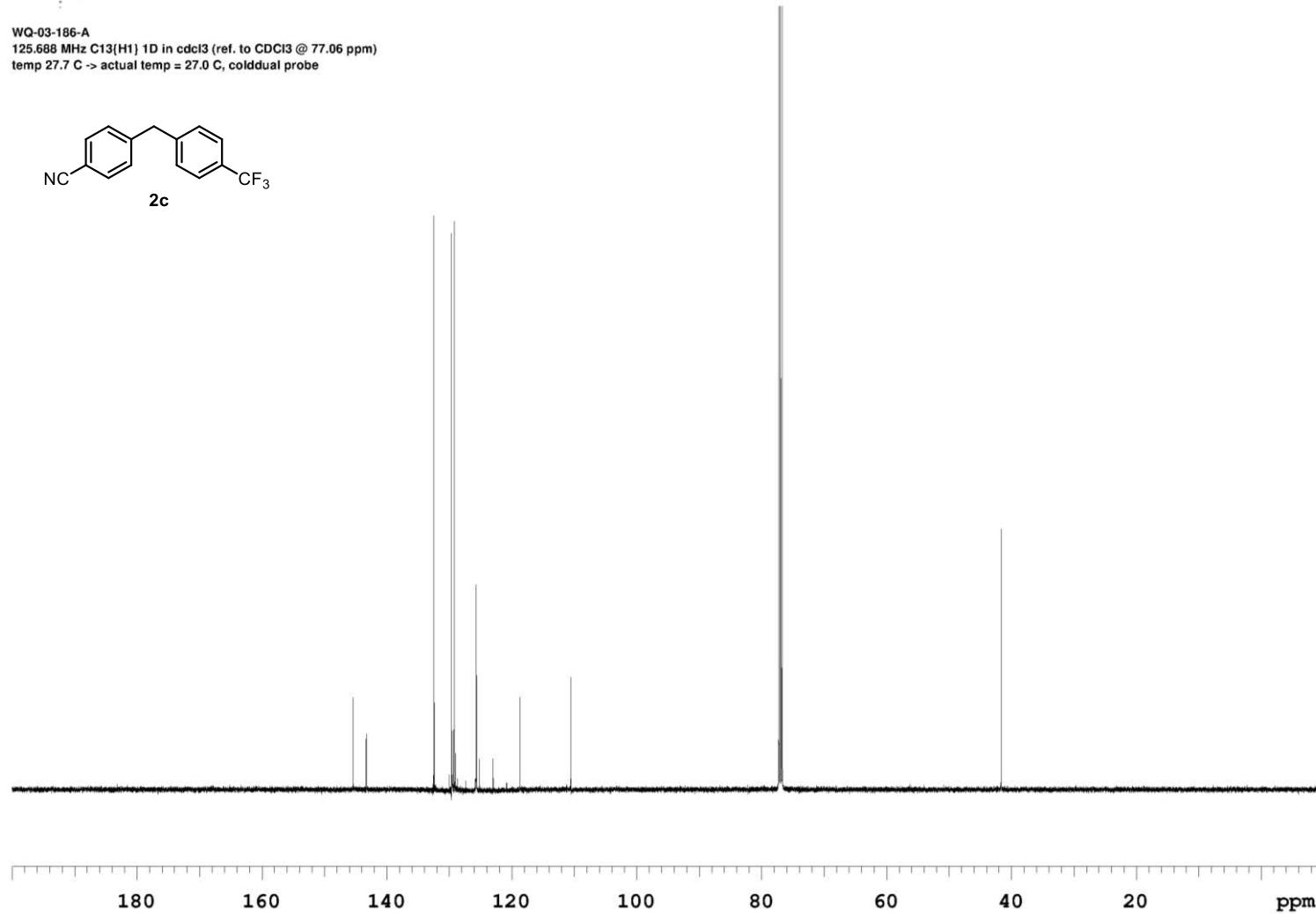
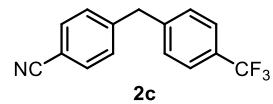
Recorded on: **u500, Feb 25 2018**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **33783.8**
Digital Res.(Hz/pt): **0.26**

Acquisition Time(s): **1**
Hz per mm(Hz/mm): **109.95**

Relaxation Delay(s): **1**
Completed Scans: **80**

WQ-03-186-A
125.688 MHz C13(H1) 1D in *cdcl*3 (ref. to *CDCl*3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe





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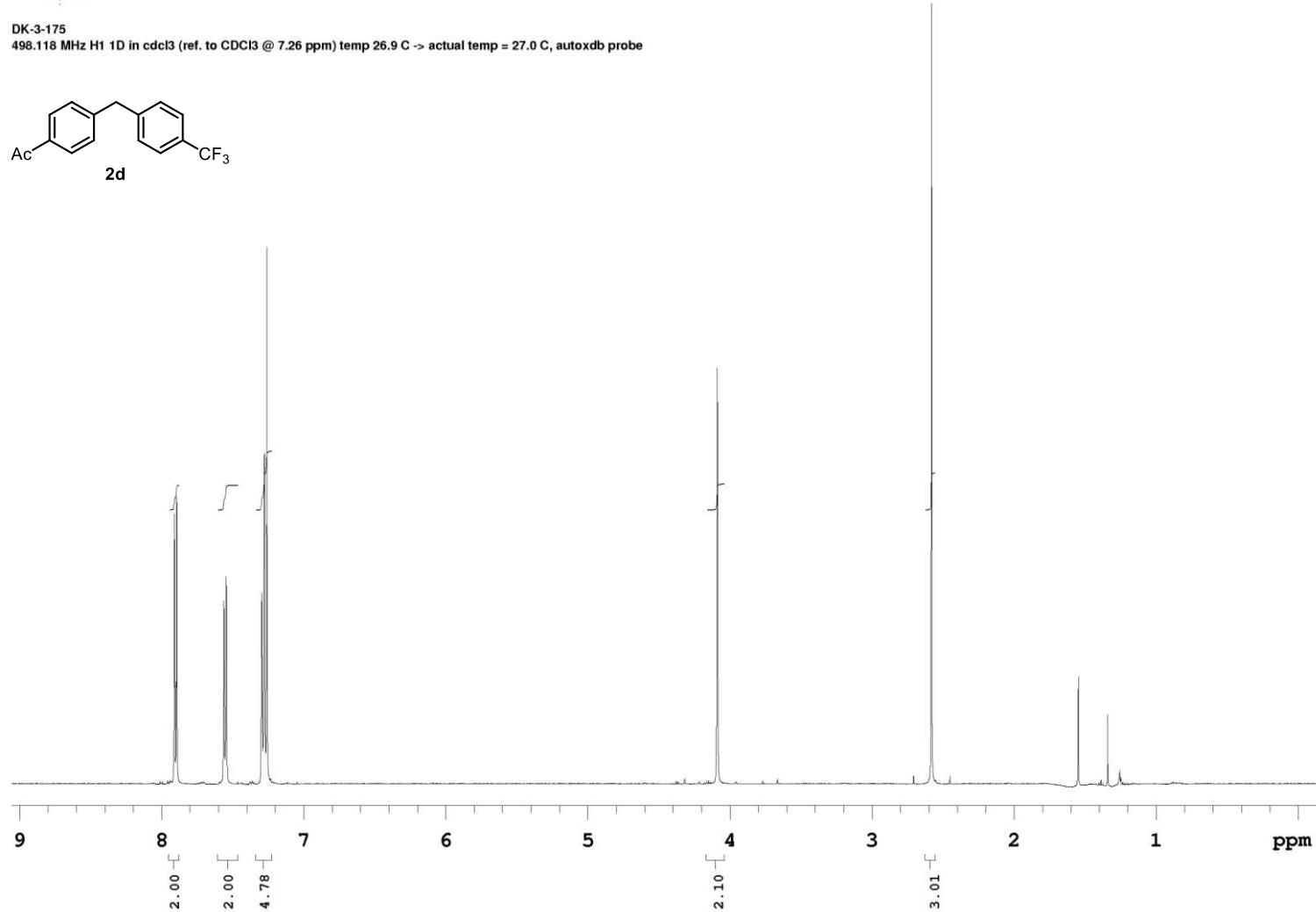
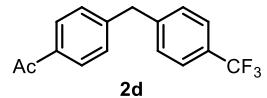
Recorded on: ibd5, Mar 11 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.1

Relaxation Delay(s): 0.1
Completed Scans 16

DK-3-175
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe





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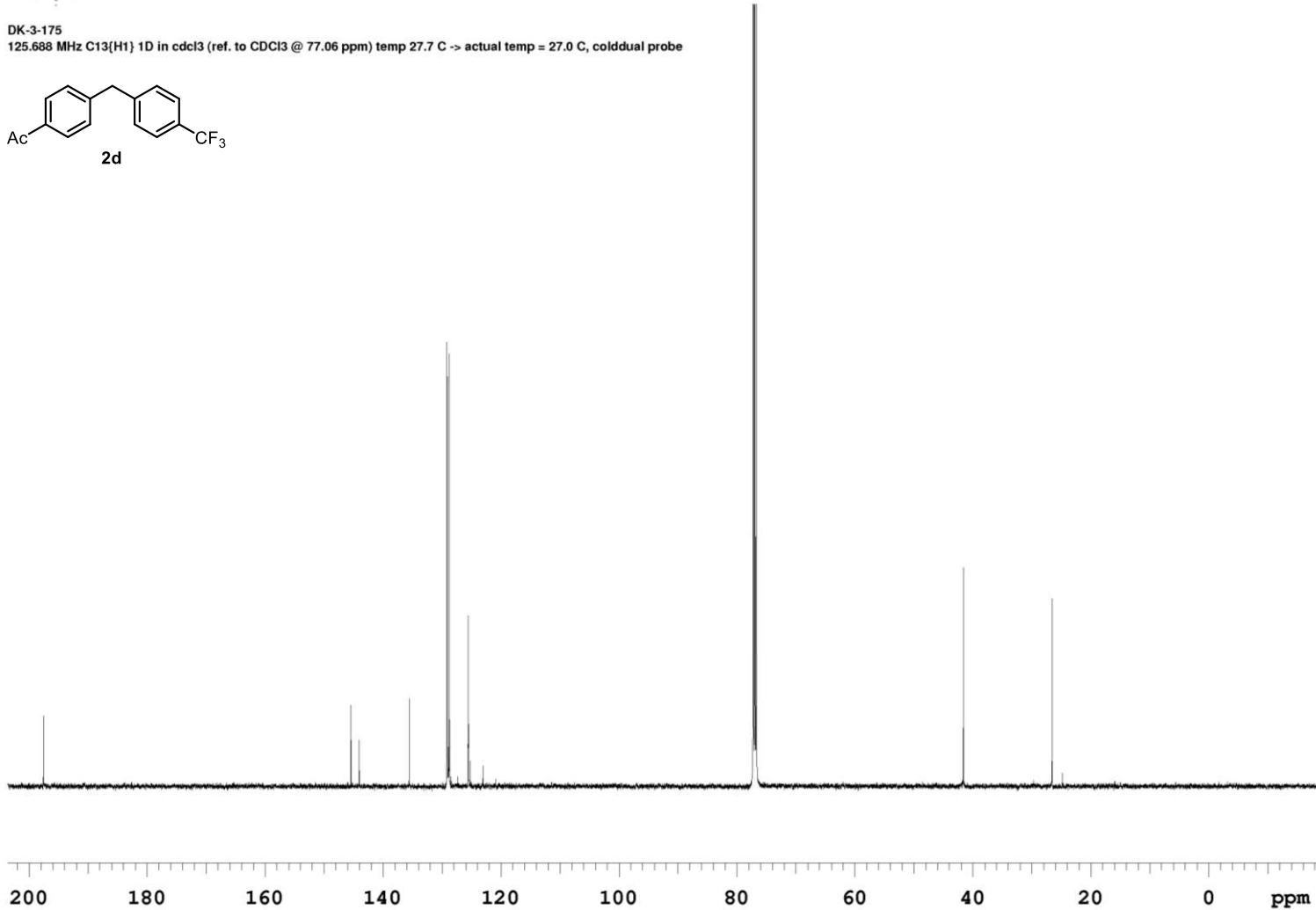
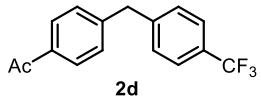
Recorded on: **u500, Mar 11 2018**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **33783.8**
Digital Res.(Hz/pt): **0.26**

Acquisition Time(s): **1**
Hz per mm(Hz/mm): **116.34**

Relaxation Delay(s): **1**
Completed Scans: **420**

DK-3-175
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, cold dual probe





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Recorded on: ibd5, Mar 20 2018
Pulse Sequence: s2pul

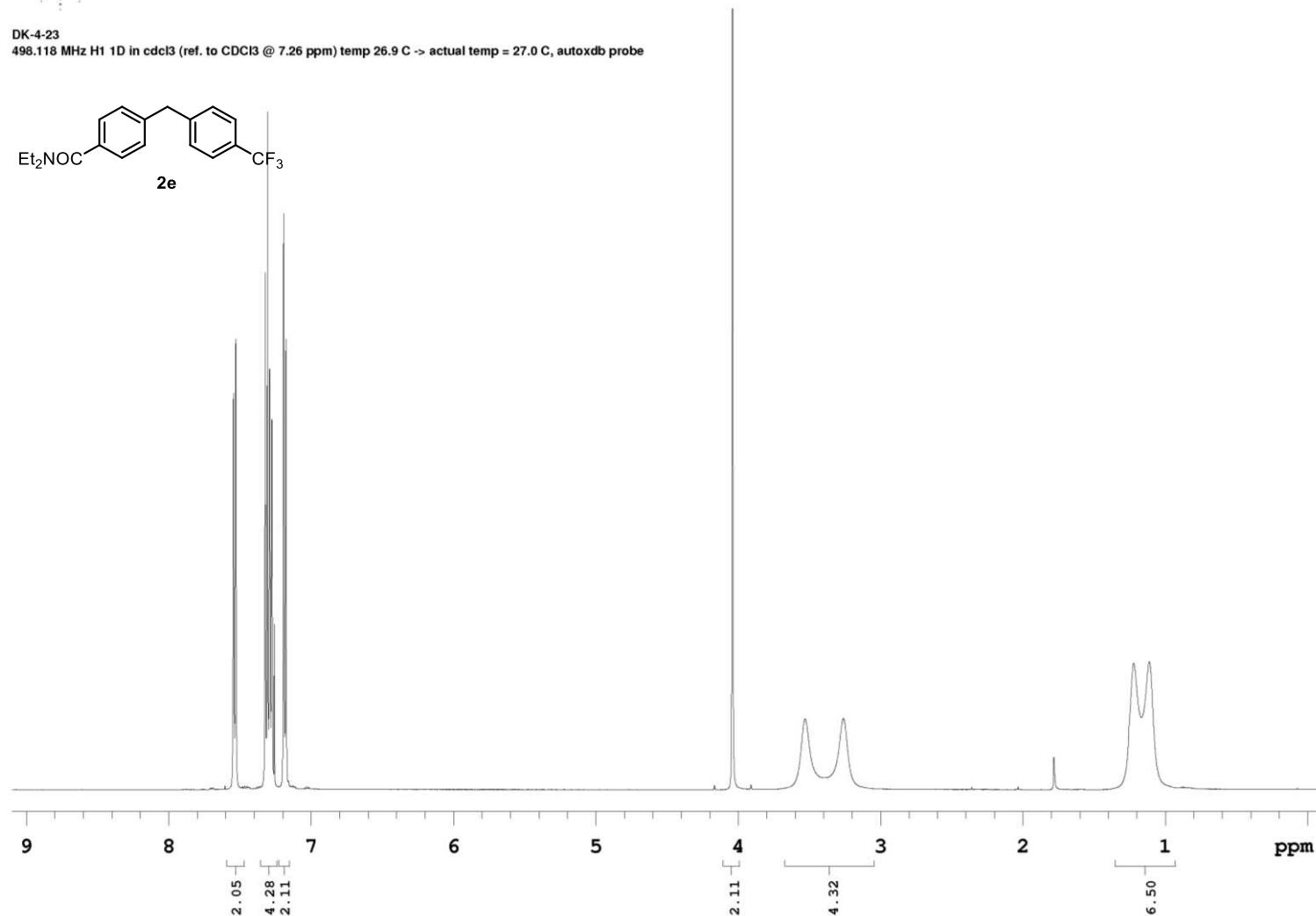
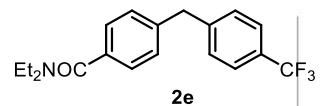
Sweep Width(Hz): **6000.6**
Digital Res.(Hz/pt): **0.09**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **19.09**

Relaxation Delay(s): **0.1**
Completed Scans **16**

DK-4-23

498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe





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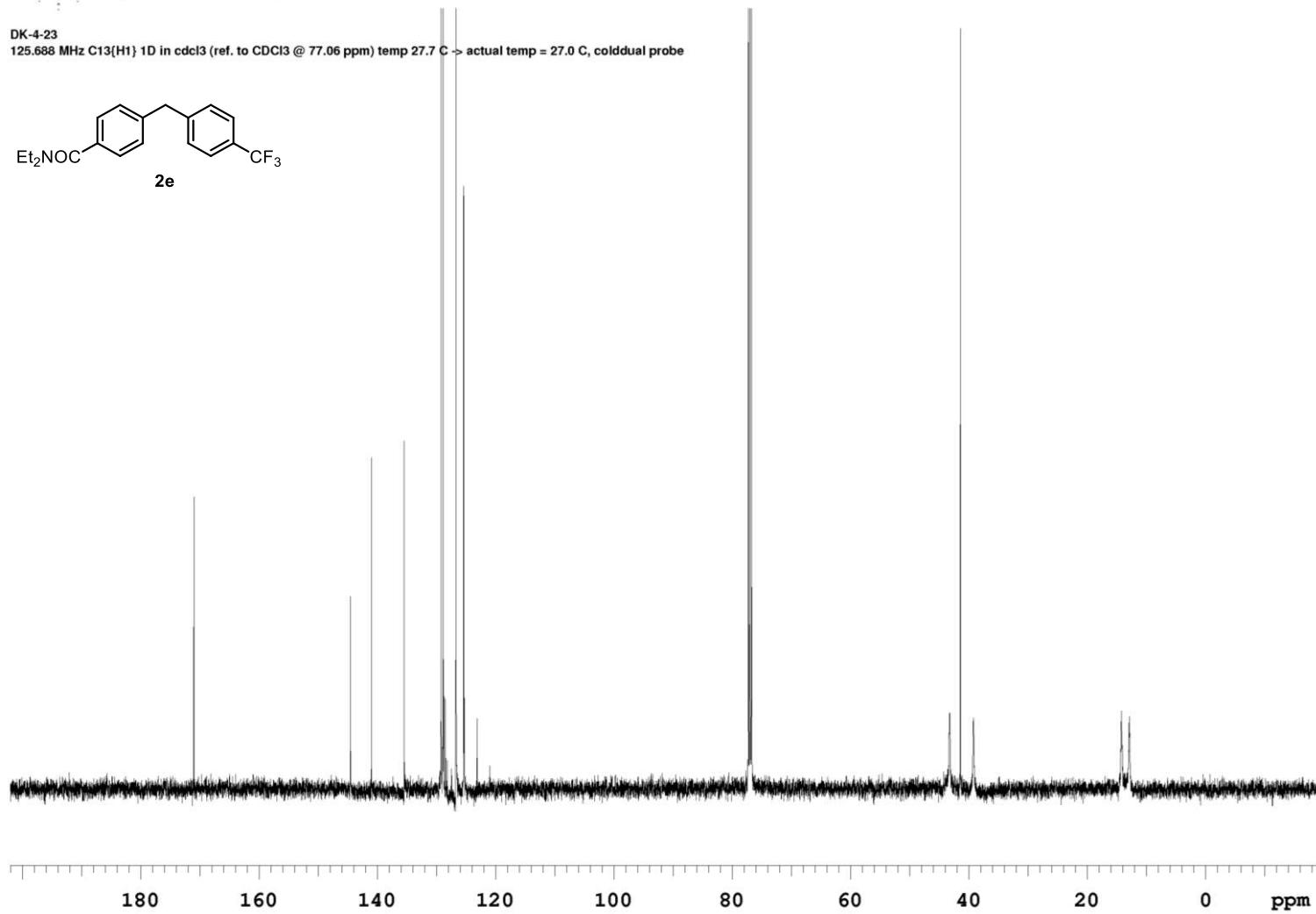
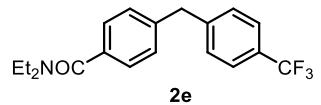
Recorded on: u500, Mar 20 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26

Acquisition Time(s): 1
Hz per mm(Hz/mm): 115.79

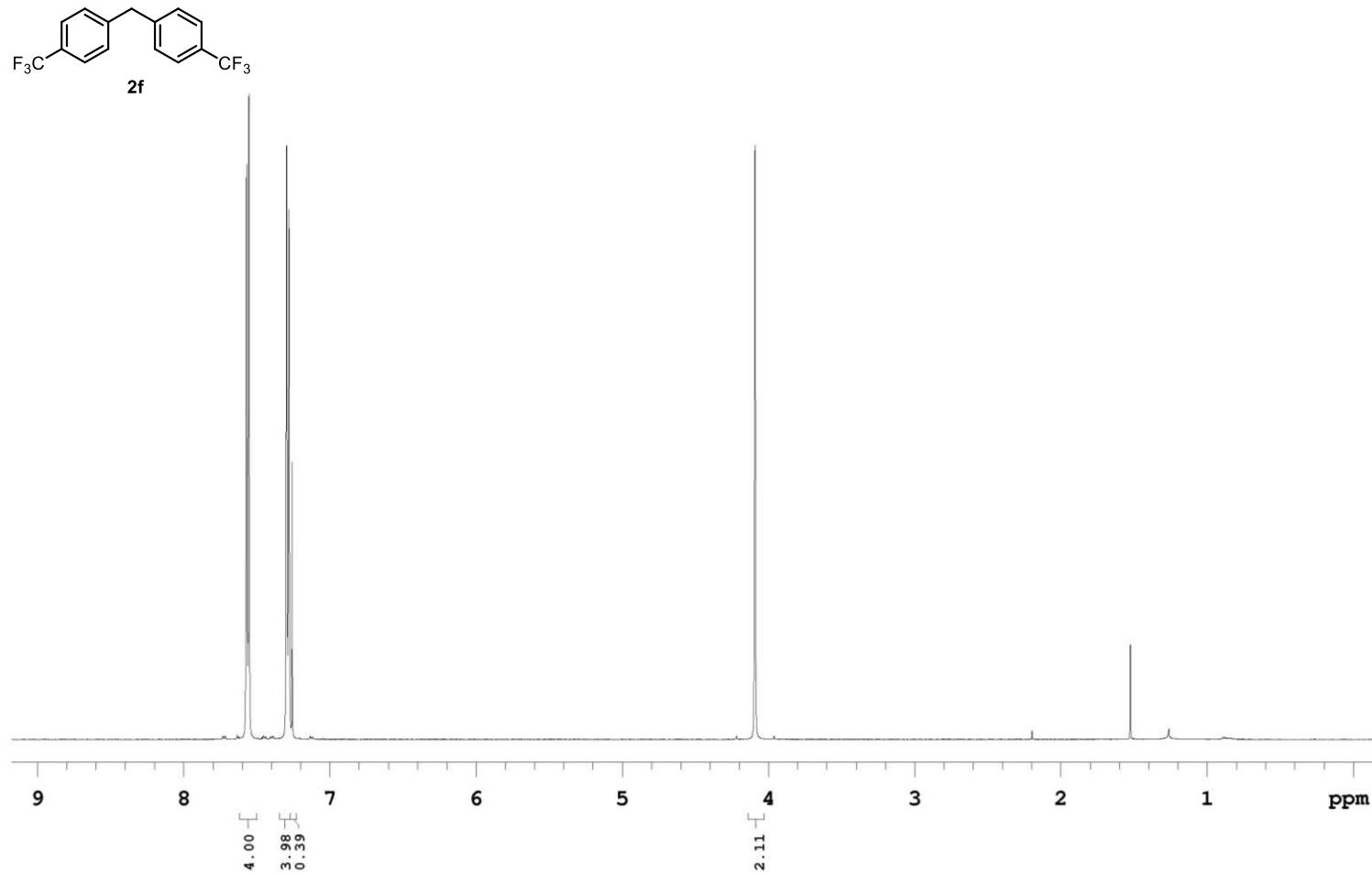
Relaxation Delay(s): 1
Completed Scans 20

DK-4-23
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, cold dual probe





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Recorded on: ibd5, Mar 8 2018
Pulse Sequence: s2pulSweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.39Relaxation Delay(s): 0.1
Completed Scans 16DK-3-151-A
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe



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Recorded on: u500, Mar 9 2018

Sweep Width(Hz): 33783.8

Acquisition Time(s): 1

Relaxation Delay(s): 1

Pulse Sequence: s2pul

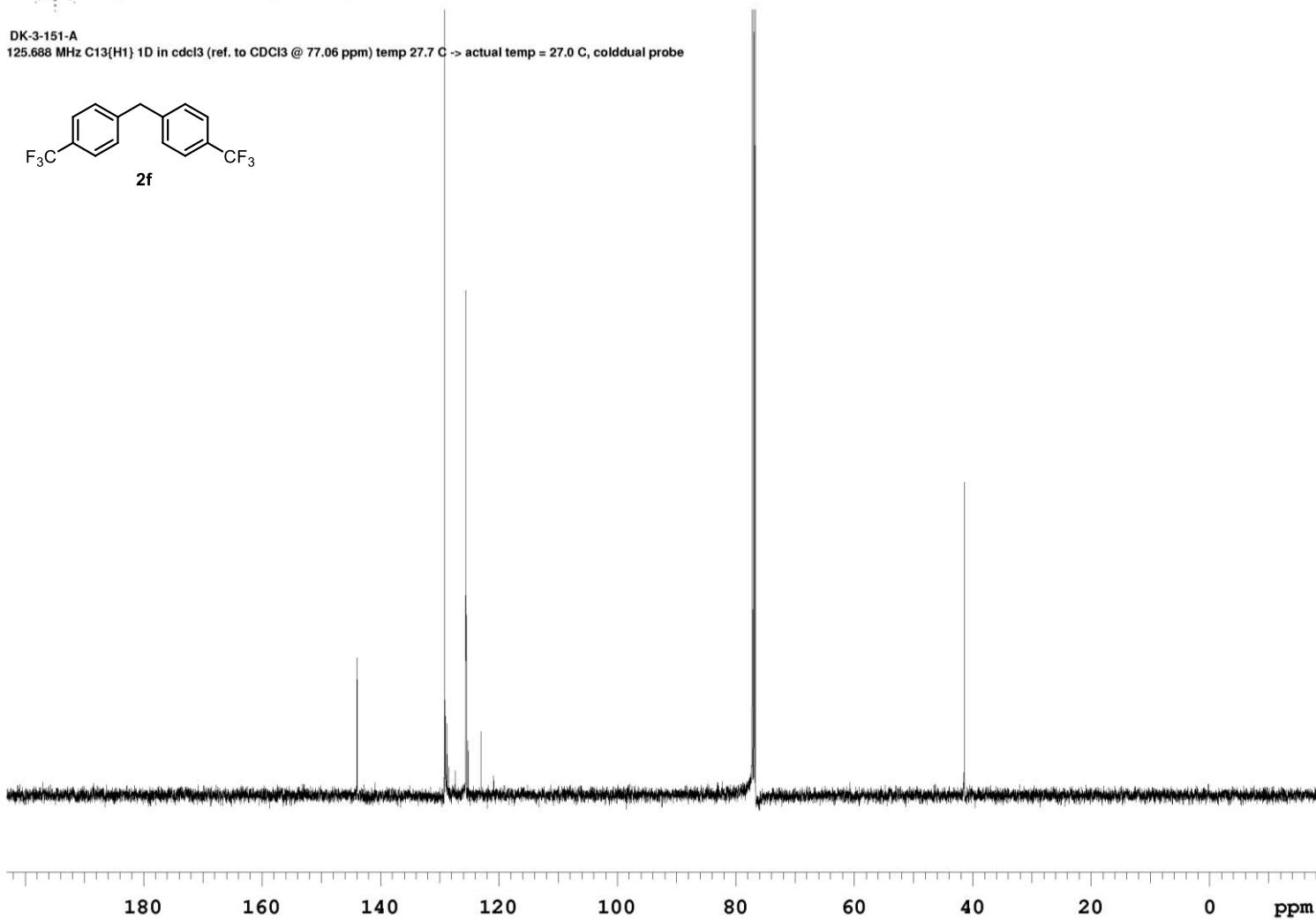
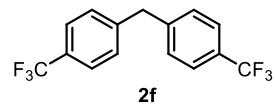
Digital Res.(Hz/pt): 0.26

Hz per mm(Hz/mm): 116.25

Completed Scans 28

DK-3-151-A

125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, coldlual probe





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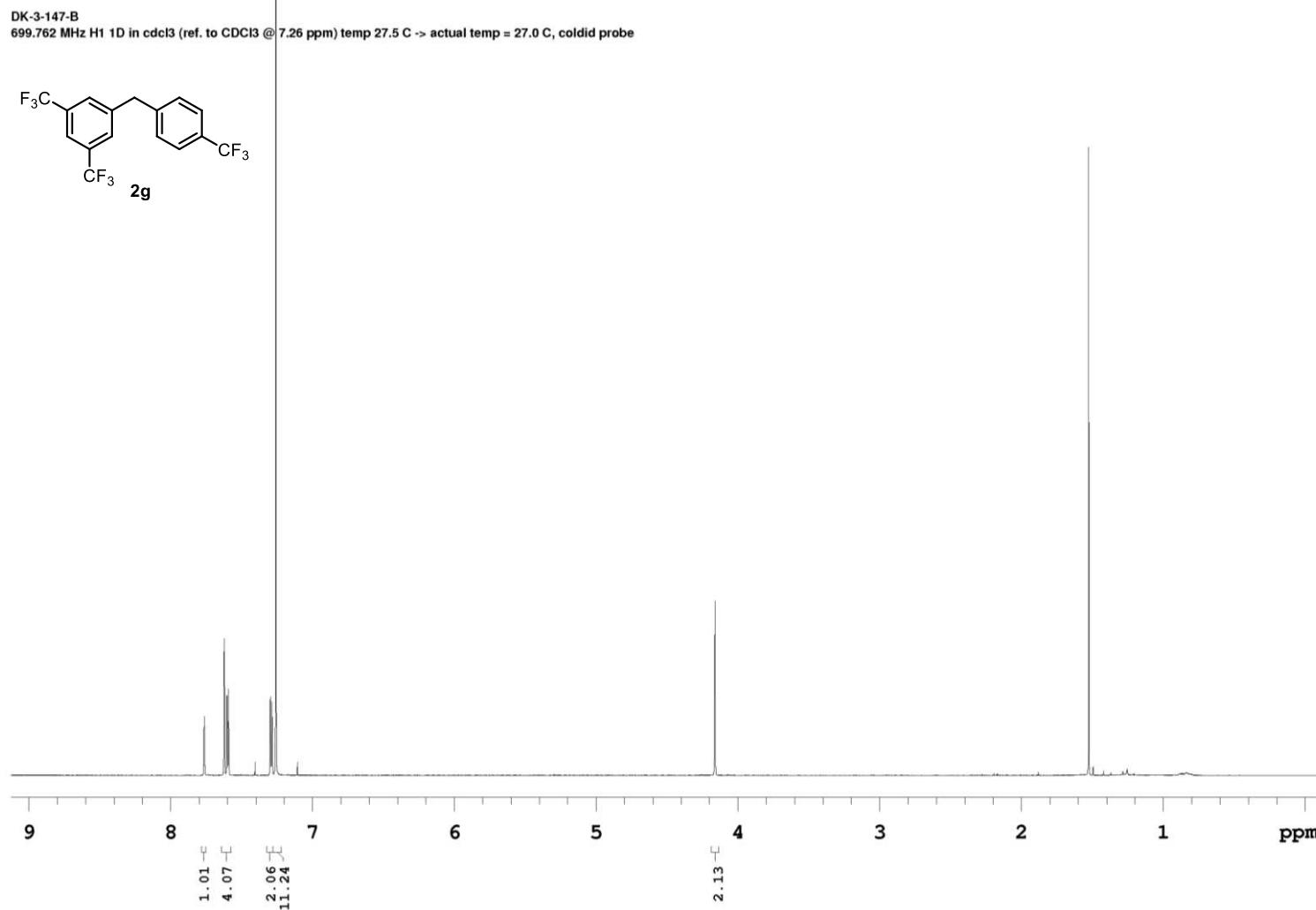
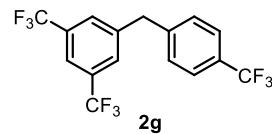
Recorded on: v700, Mar 6 2018
Pulse Sequence: PRESAT

Sweep Width(Hz): 8389.26
Digital Res.(Hz/pt): 0.13

Acquisition Time(s): 5
Hz per mm(Hz/mm): 27.05

Relaxation Delay(s): 0.1
Completed Scans 8

DK-3-147-B
699.762 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 27.5 C -> actual temp = 27.0 C, coldid probe





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Recorded on: u500, Mar 6 2018

Sweep Width(Hz): 33783.8

Acquisition Time(s): 1

Relaxation Delay(s): 1

Pulse Sequence: s2pul

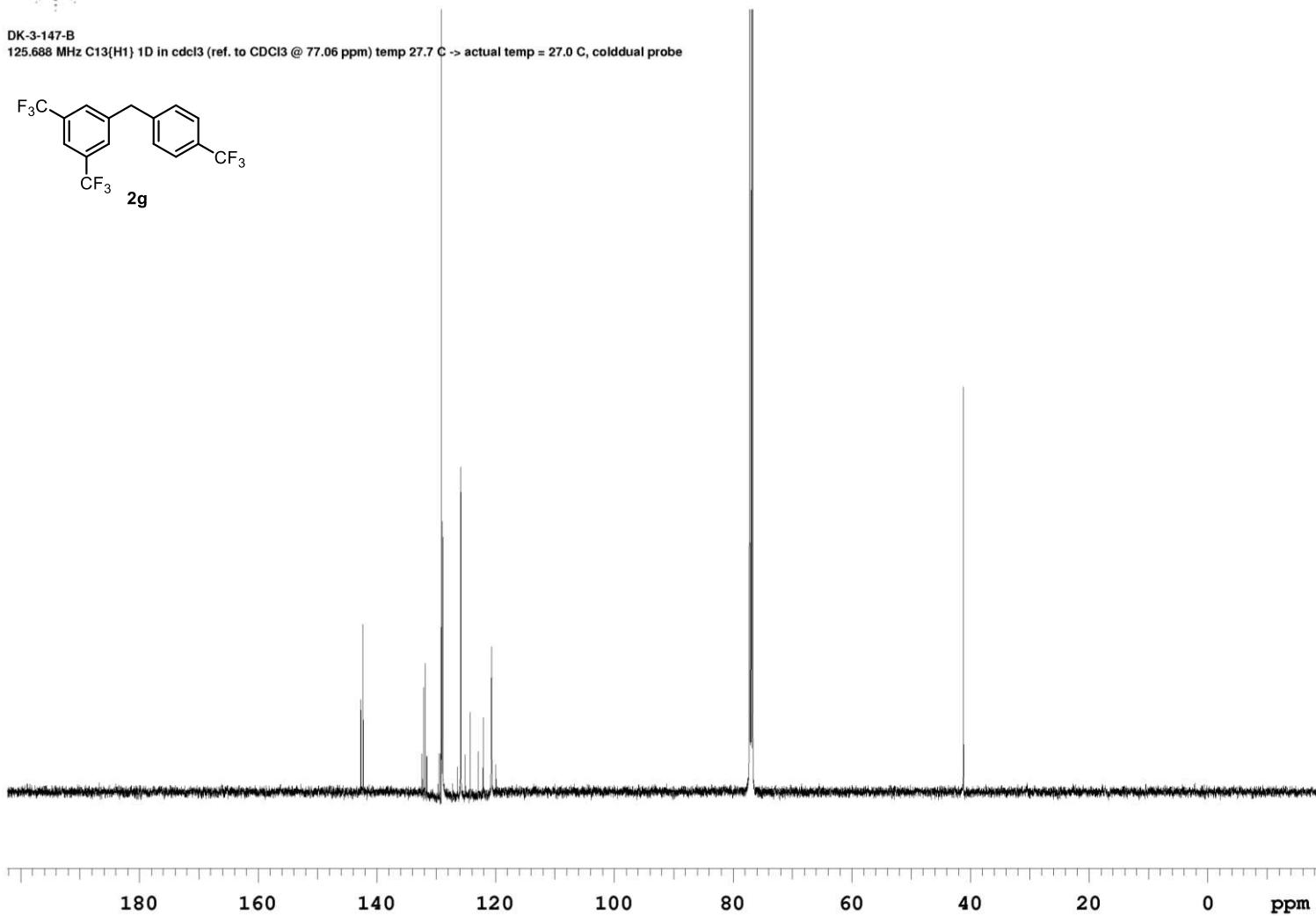
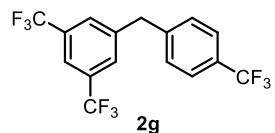
Digital Res.(Hz/pt): 0.26

Hz per mm(Hz/mm): 115.61

Completed Scans 168

DK-3-147-B

125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, coldlual probe





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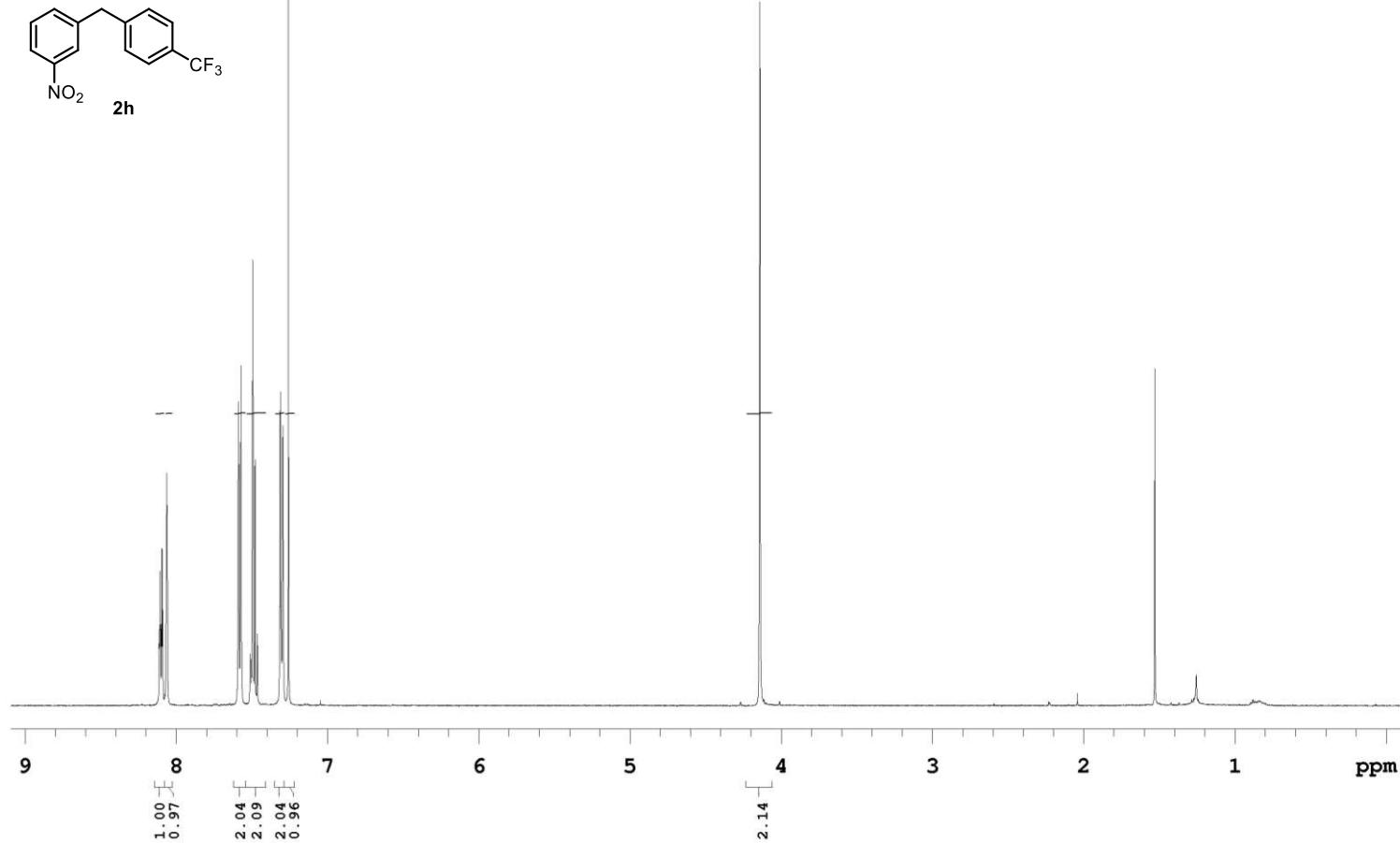
Recorded on: ibd5, Mar 16 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.14

Relaxation Delay(s): 0.1
Completed Scans 16

DK-3-193-C
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe





Agilent Technologies

Department of Chemistry, University of Alberta

Recorded on: v700, Mar 16 2018
Pulse Sequence: s2pul

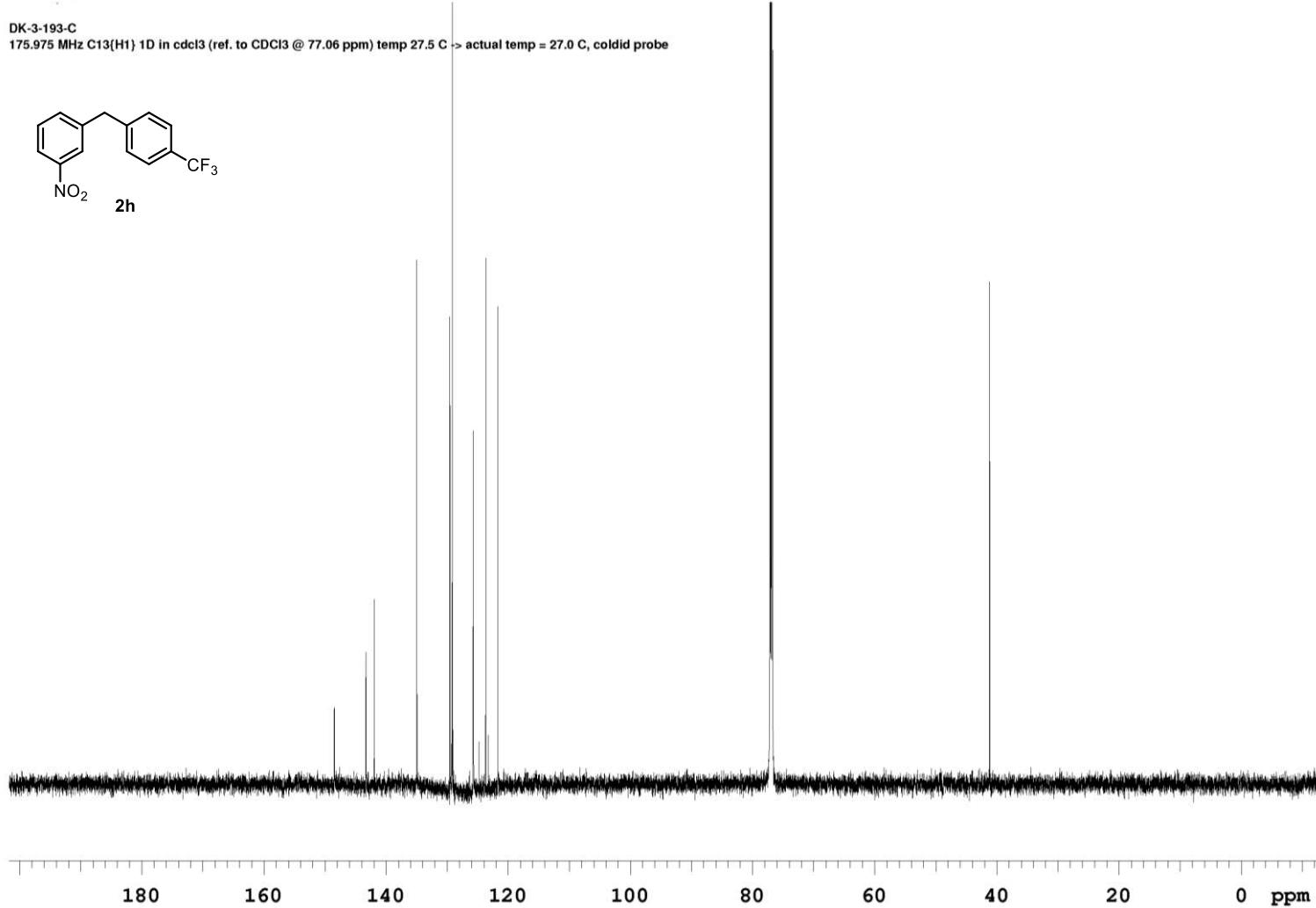
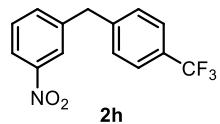
Sweep Width(Hz): 48076.9
Digital Res.(Hz/pt): 0.37

Acquisition Time(s): 1
Hz per mm(Hz/mm): 157.1

Relaxation Delay(s): 1
Completed Scans 512

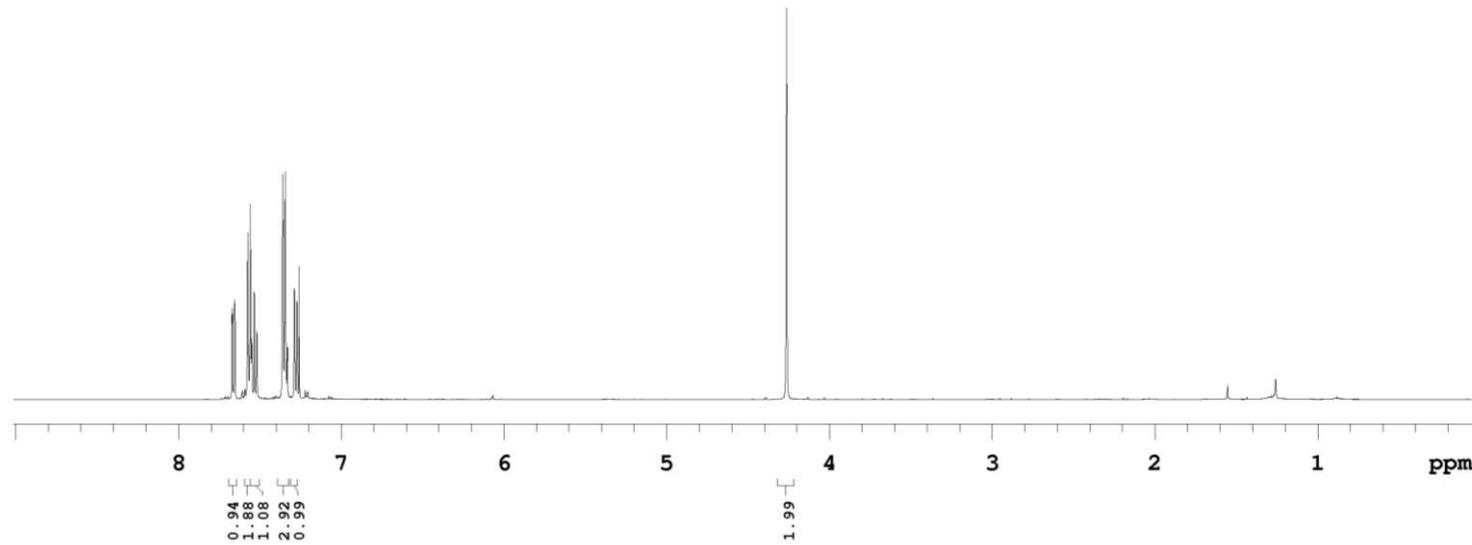
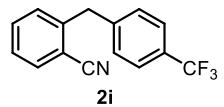
DK-3-193-C

175.975 MHz C13(H1) 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.5 C -> actual temp = 27.0 C, coldid probe



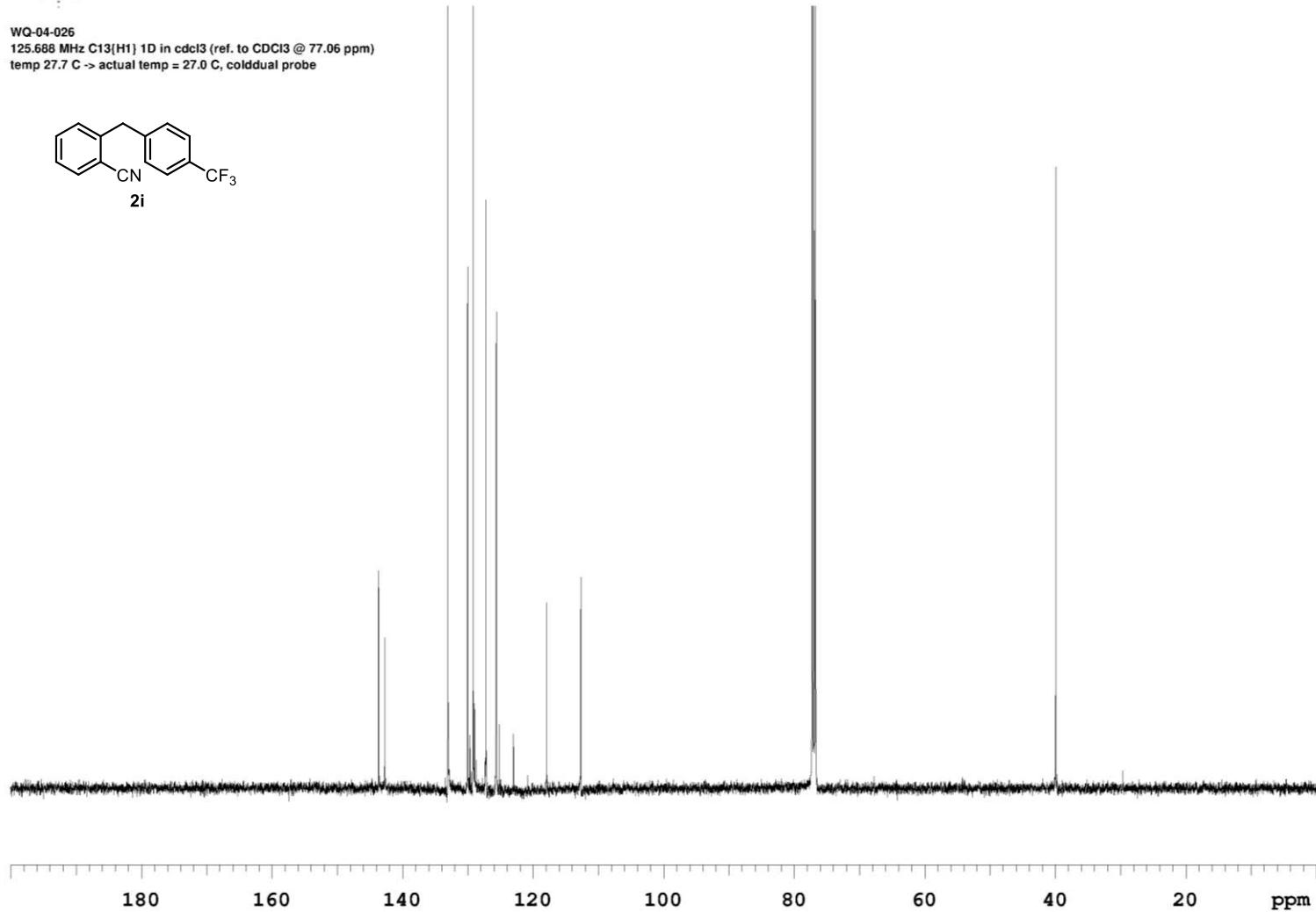
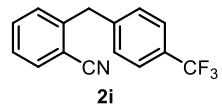


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Recorded on: u500, Mar 10 2018
Pulse Sequence: PRESATSweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 18.78Relaxation Delay(s): 0.1
Completed Scans 8WQ-04-026
499.797 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe



Department of Chemistry, University of Alberta

Recorded on: u500, Mar 10 2018
Pulse Sequence: s2pulSweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26Acquisition Time(s): 1
Hz per mm(Hz/mm): 104.92Relaxation Delay(s): 1
Completed Scans 60WQ-04-026
125.688 MHz C13(H1) 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe



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Recorded on: ibd5, Mar 12 2018
Pulse Sequence: s2pul

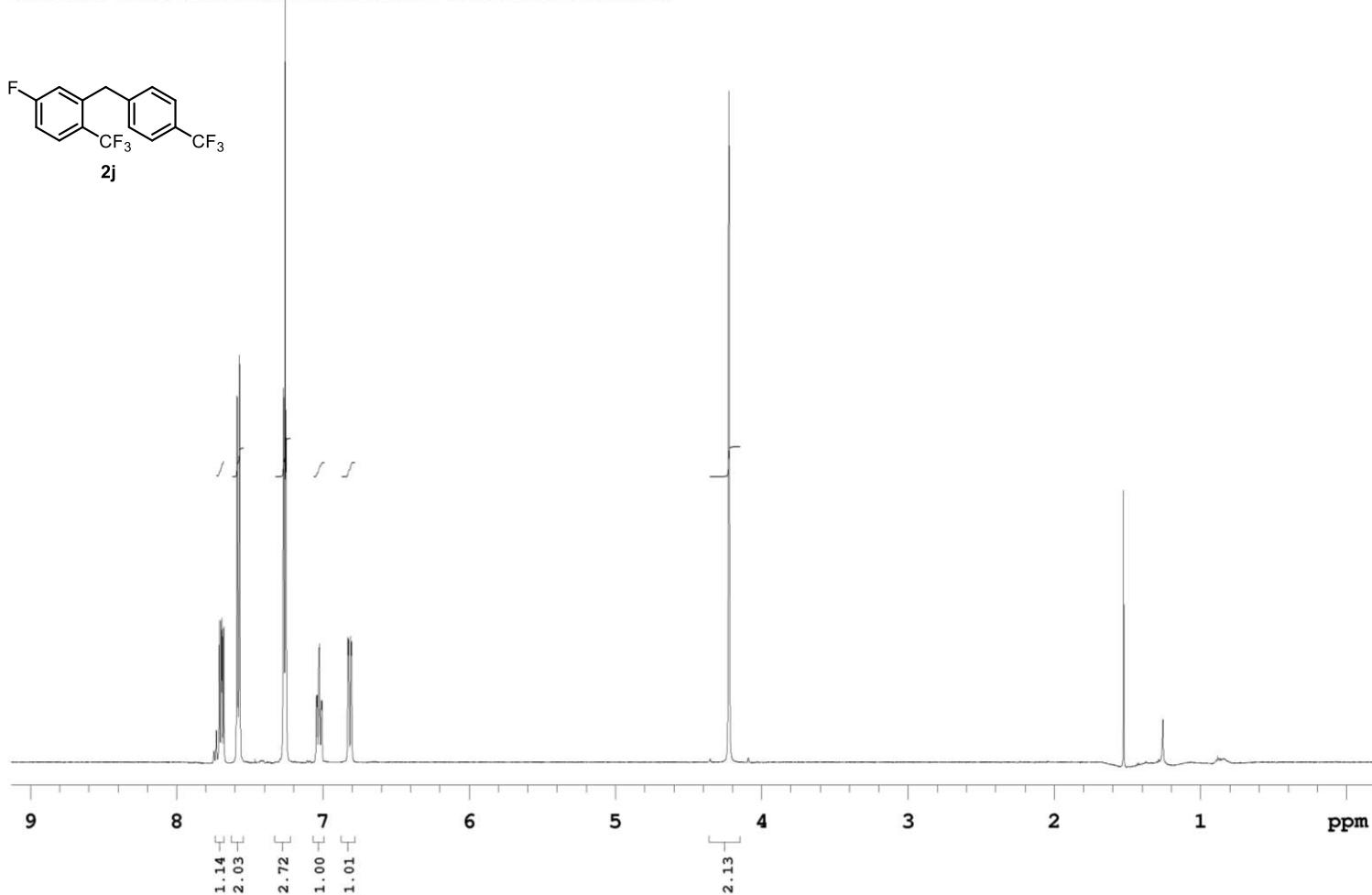
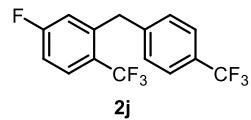
Sweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.37

Relaxation Delay(s): 0.1
Completed Scans: 16

DK-3-171

498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe





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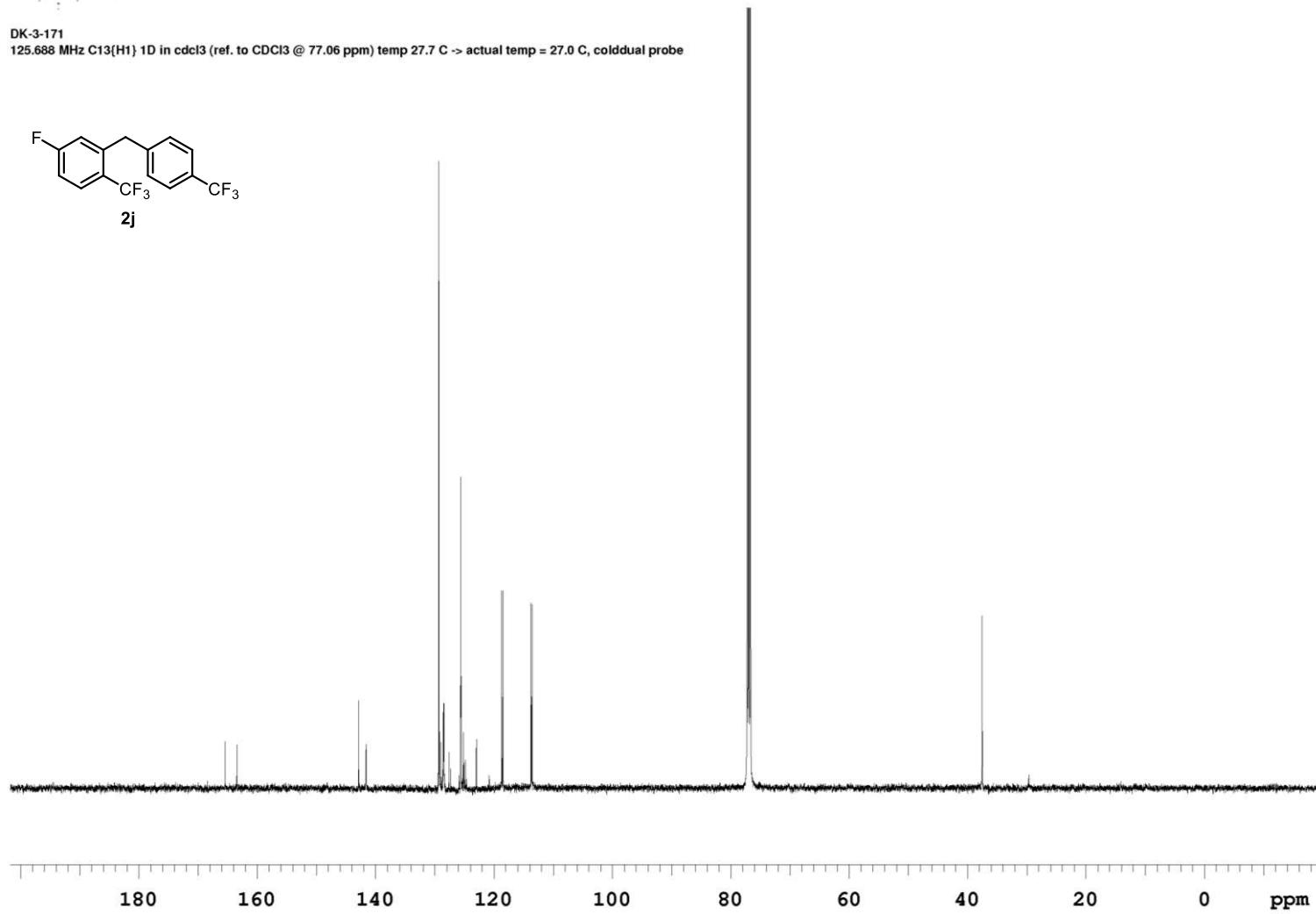
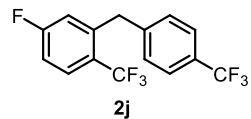
Recorded on: **u500, Mar 13 2018**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **33783.8**
Digital Res.(Hz/pt): **0.26**

Acquisition Time(s): **1**
Hz per mm(Hz/mm): **115.61**

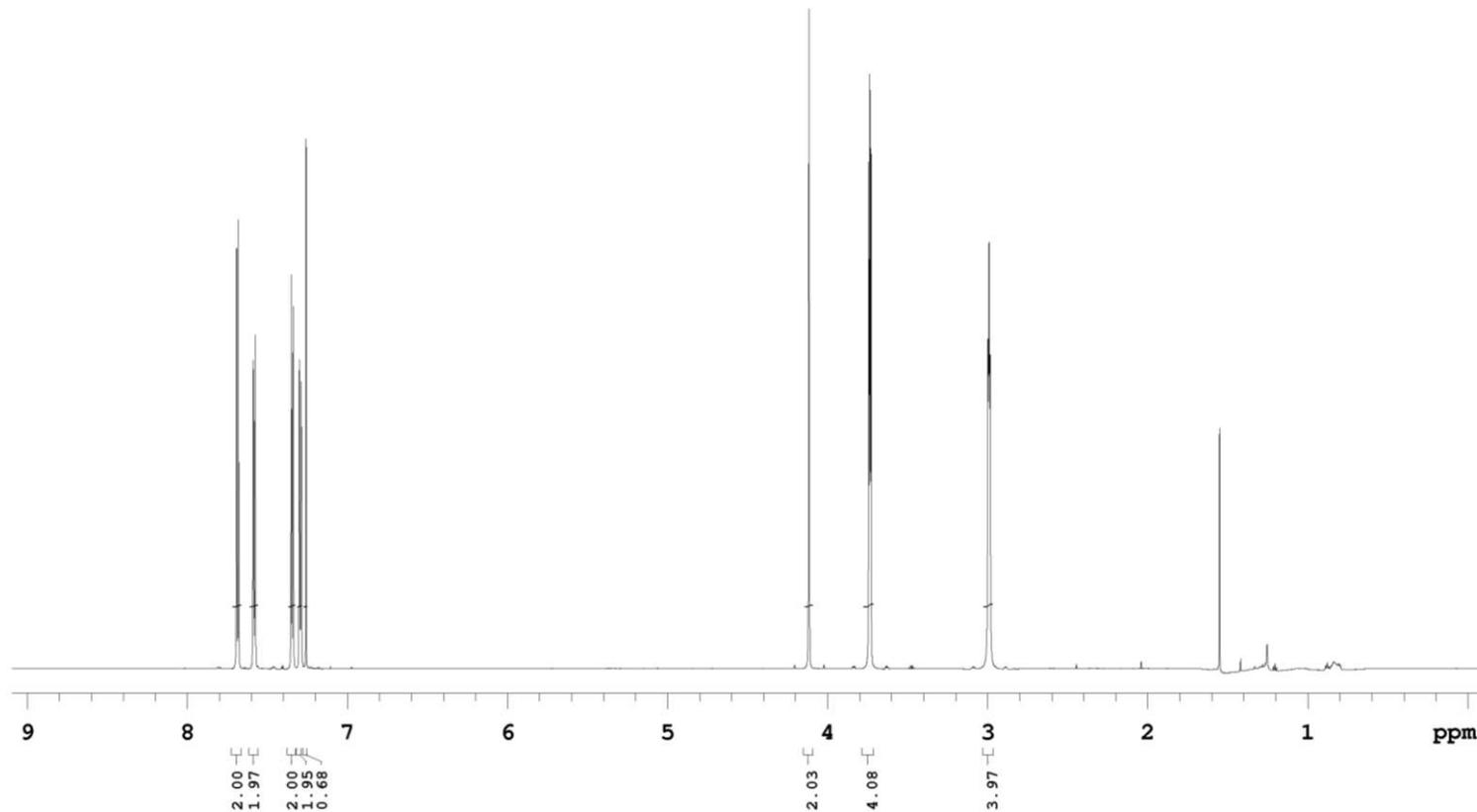
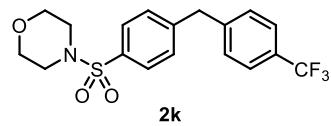
Relaxation Delay(s): **1**
Completed Scans **576**

DK-3-171
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, colddual probe





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Recorded on: v700, Mar 22 2018
Pulse Sequence: PRESATSweep Width(Hz): 8389.26
Digital Res.(Hz/pt): 0.13Acquisition Time(s): 5
Hz per mm(Hz/mm): 26.84Relaxation Delay(s): 0.1
Completed Scans 8DK-4-33-P
699.762 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 27.5 C -> actual temp = 27.0 C, coldid probe



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Recorded on: v700, Mar 22 2018
Pulse Sequence: s2pul

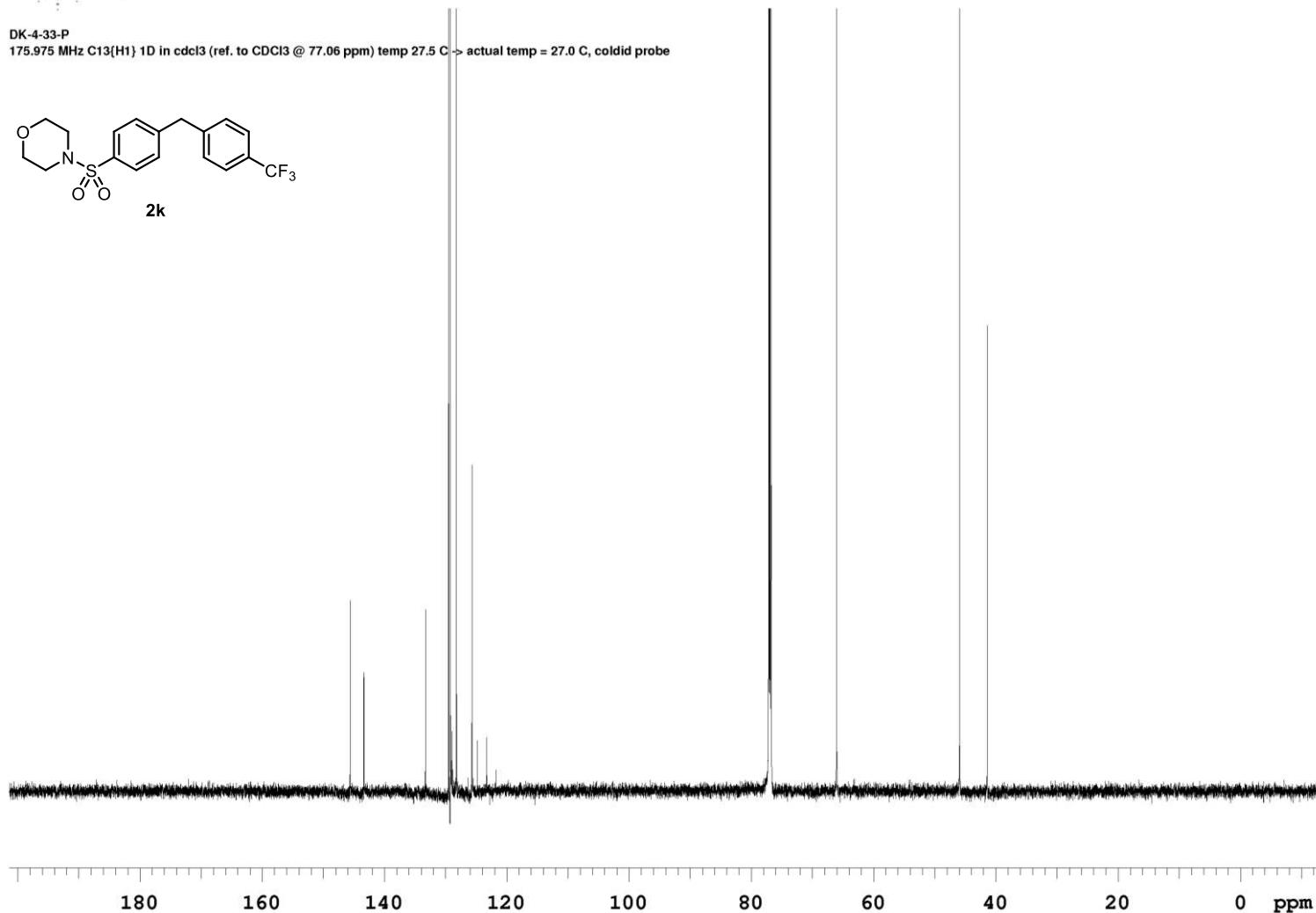
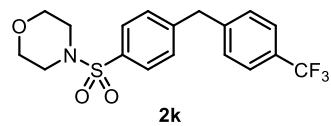
Sweep Width(Hz): 48076.9
Digital Res.(Hz/pt): 0.37

Acquisition Time(s): 1
Hz per mm(Hz/mm): 157.23

Relaxation Delay(s): 1
Completed Scans 512

DK-4-33-P

175.975 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.5 C -> actual temp = 27.0 C, coldid probe





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Recorded on: **iBD5, Mar 22 2018**
Pulse Sequence: **s2pul**

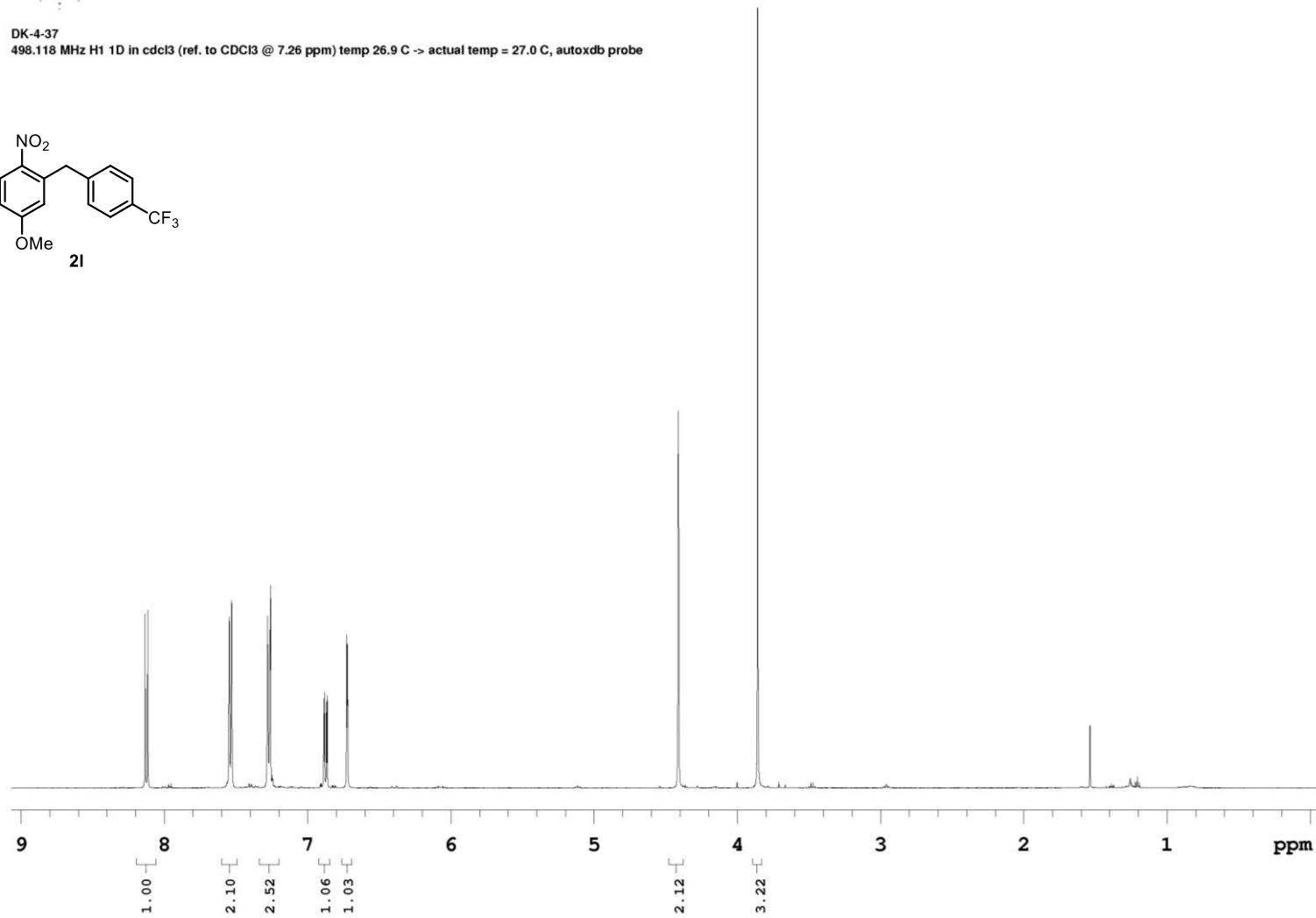
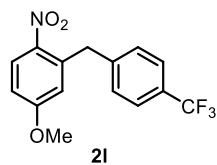
Sweep Width(Hz): **6000.6**
Digital Res.(Hz/pt): **0.09**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **18.97**

Relaxation Delay(s): **0.1**
Completed Scans: **16**

DK-4-37

498.118 MHz H1 1D in CDCl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe





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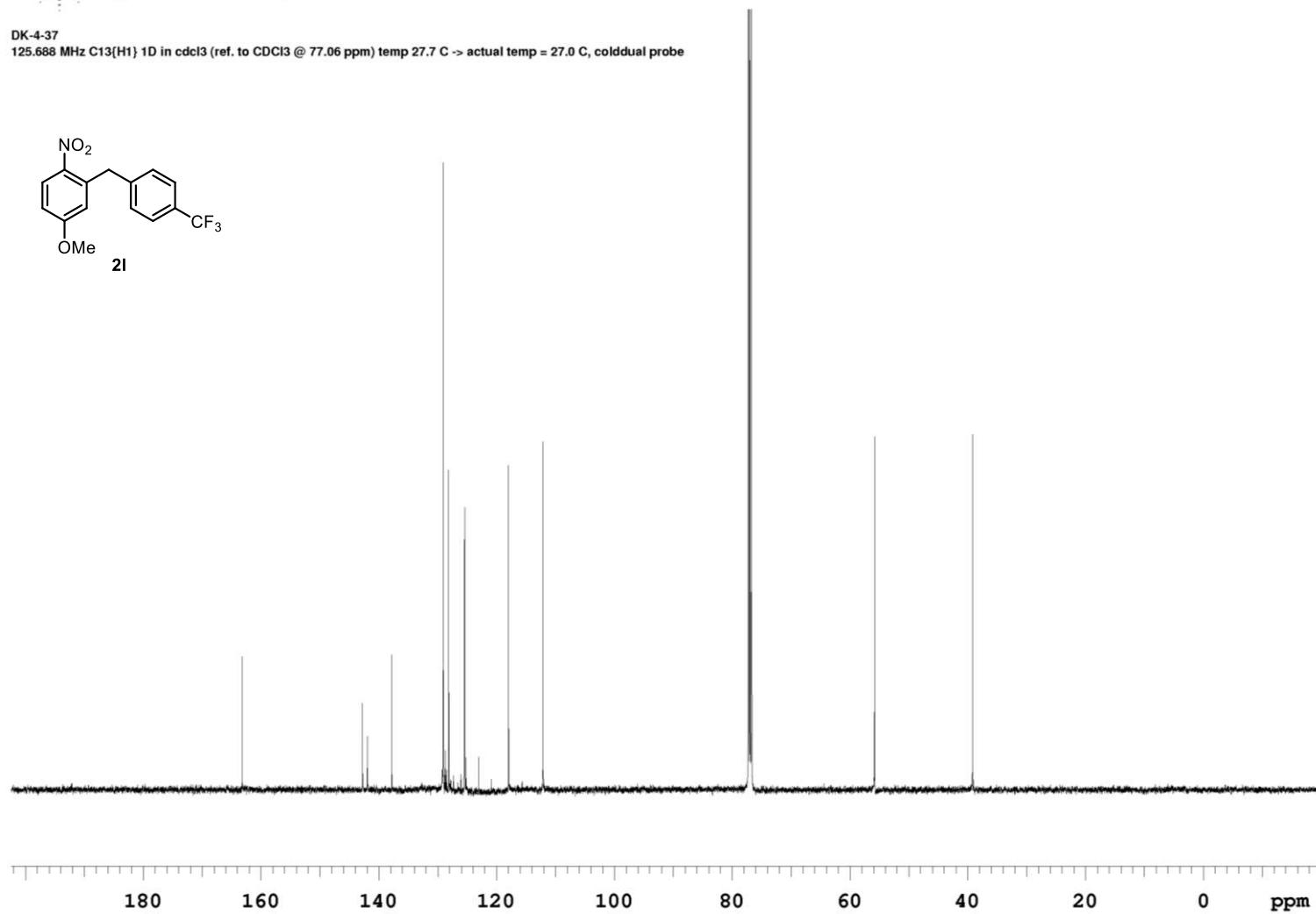
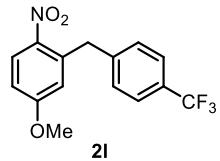
Recorded on: u500, Mar 22 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26

Acquisition Time(s): 1
Hz per mm(Hz/mm): 116.16

Relaxation Delay(s): 1
Completed Scans 152

DK-4-37
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, cold dual probe





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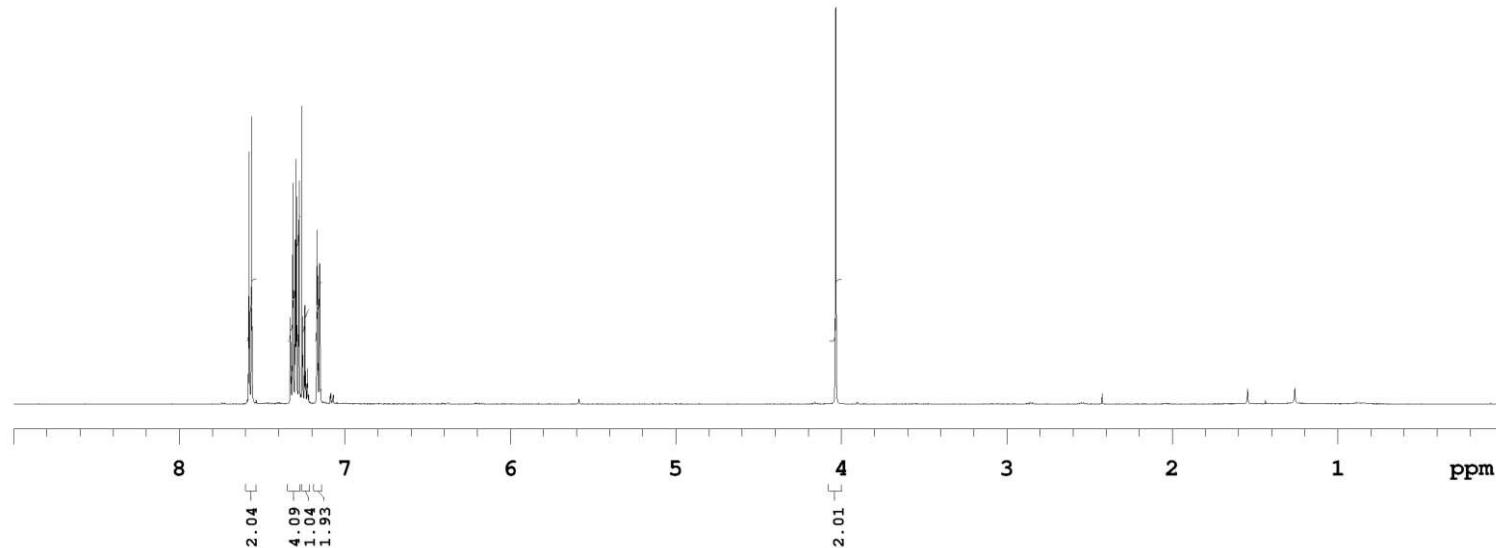
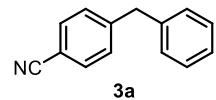
Recorded on: u500, Mar 5 2018
Pulse Sequence: PRESAT

Sweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 18.74

Relaxation Delay(s): 0.1
Completed Scans 2

WQ-03-196-B
499.797 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, cold dual probe





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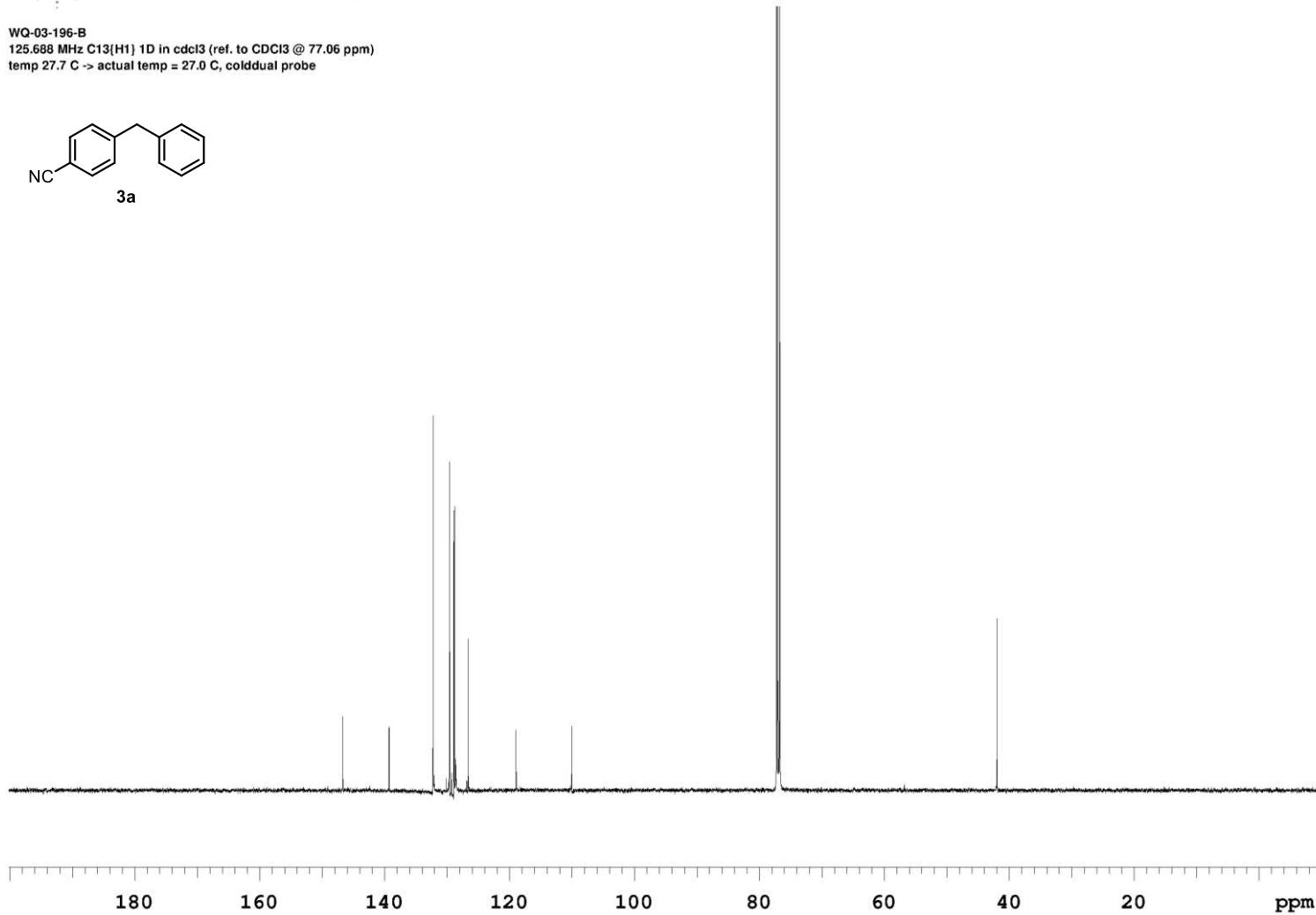
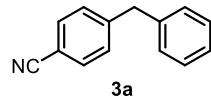
Recorded on: **u500, Mar 5 2018**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **33783.8**
Digital Res.(Hz/pt): **0.26**

Acquisition Time(s): **1**
Hz per mm(Hz/mm): **110.14**

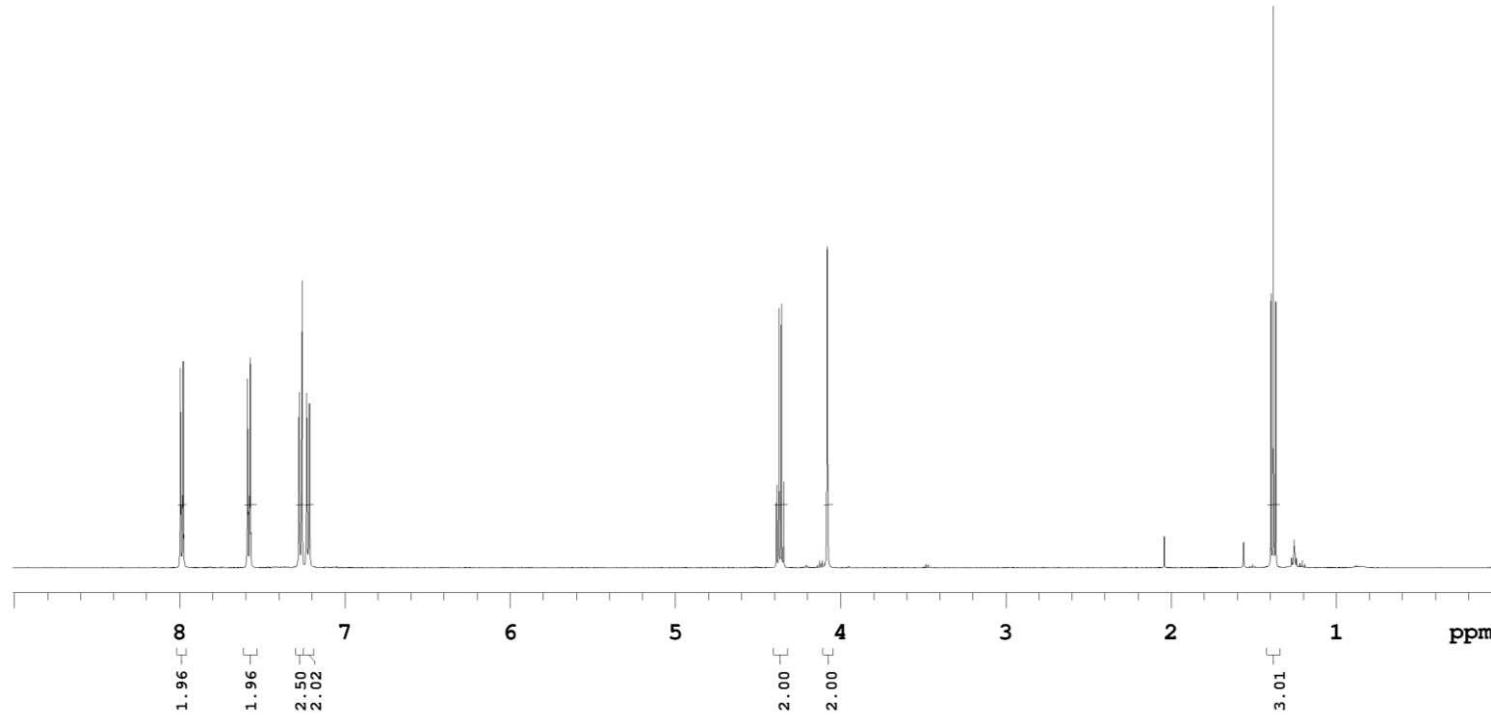
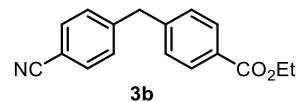
Relaxation Delay(s): **1**
Completed Scans **100**

WQ-03-196-B
125.688 MHz C13(H1) 1D in *cdcl*3 (ref. to CDCl₃ @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe



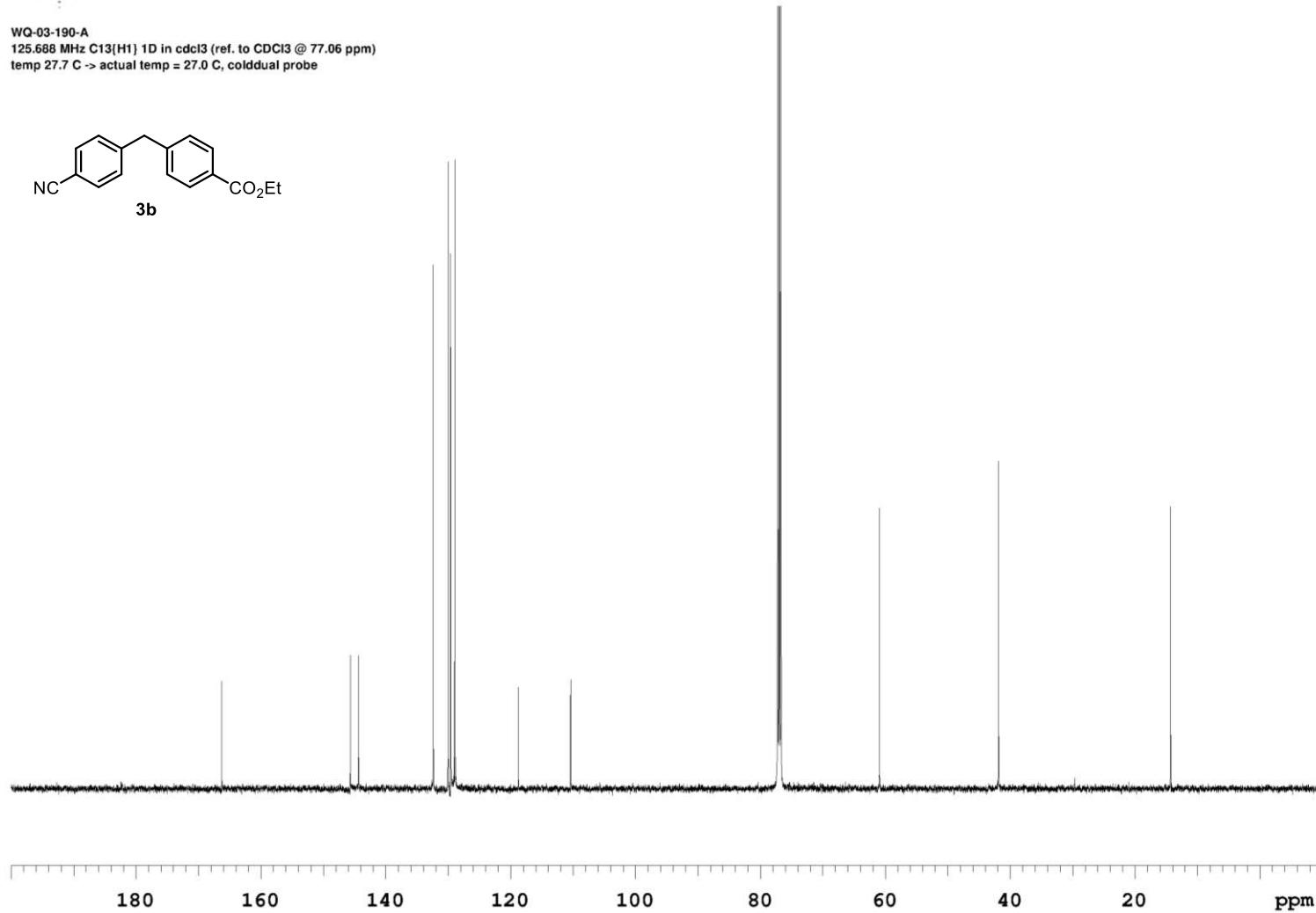
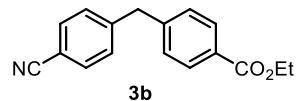


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Recorded on: u500, Mar 1 2018
Pulse Sequence: PRESATSweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 18.78Relaxation Delay(s): 0.1
Completed Scans 2WQ-03-190-A
499.797 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, cold dual probe



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Recorded on: u500, Mar 1 2018
Pulse Sequence: s2pulSweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26Acquisition Time(s): 1
Hz per mm(Hz/mm): 109.95Relaxation Delay(s): 1
Completed Scans 220WQ-03-190-A
125.688 MHz C13{H1} 1D in CDCl_3 (ref. to CDCl_3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, cooldual probe



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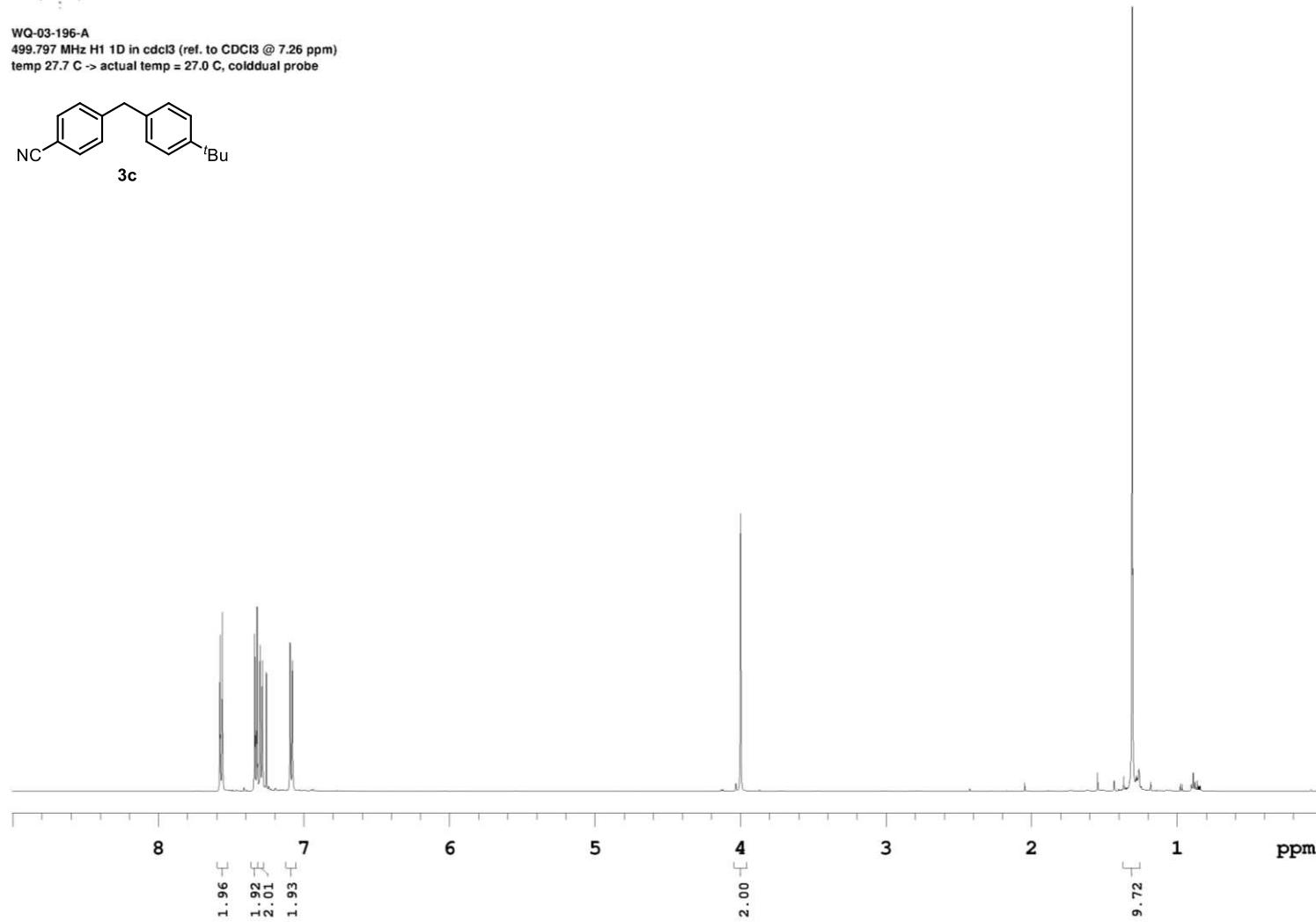
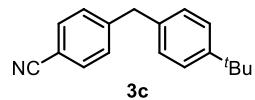
Recorded on: u500, Mar 8 2018
Pulse Sequence: PRESAT

Sweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 18.78

Relaxation Delay(s): 0.1
Completed Scans 4

WQ-03-196-A
499.797 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, cold dual probe





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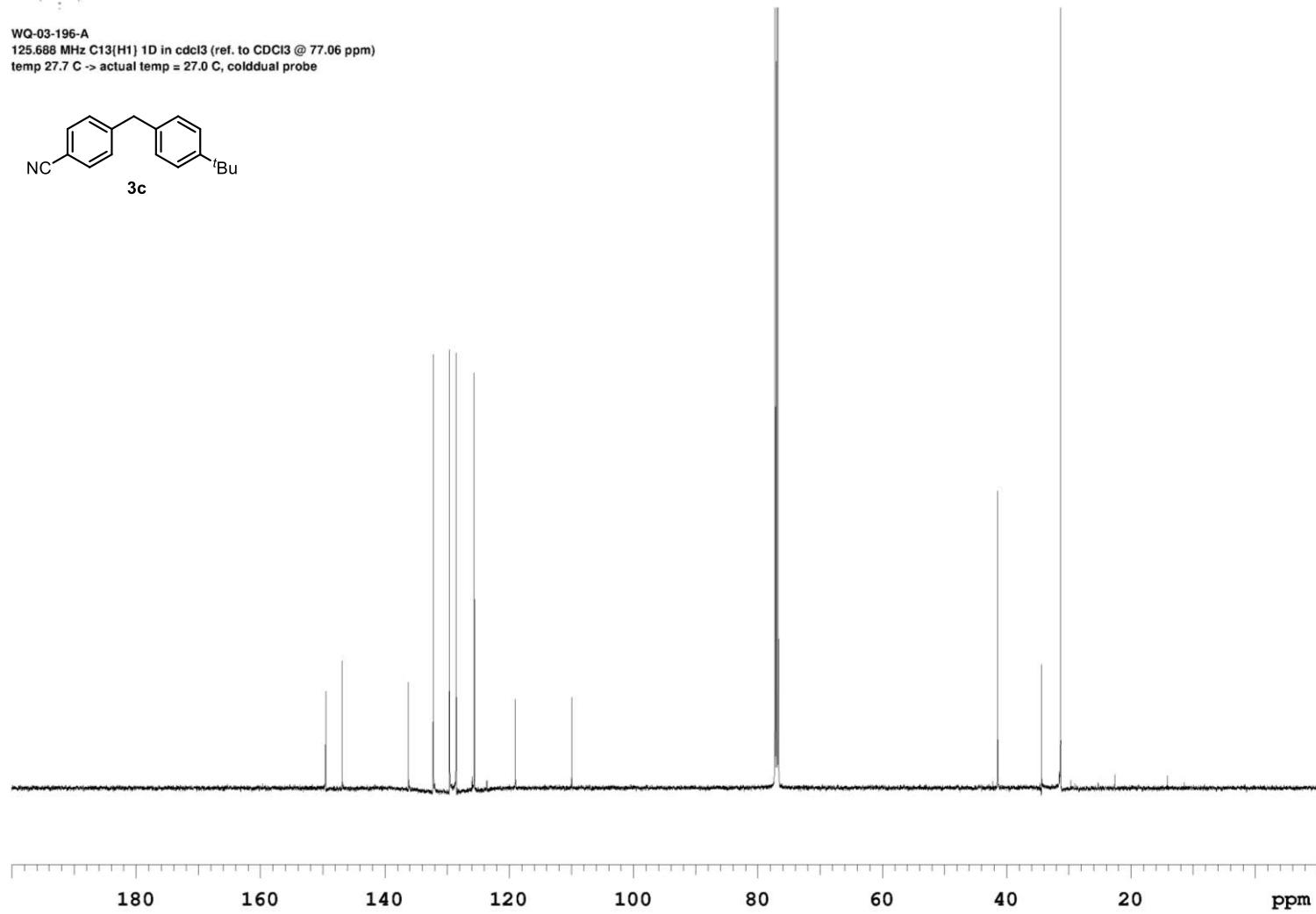
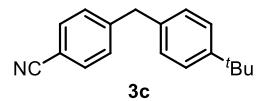
Recorded on: u500, Mar 8 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26

Acquisition Time(s): 1
Hz per mm(Hz/mm): 110.11

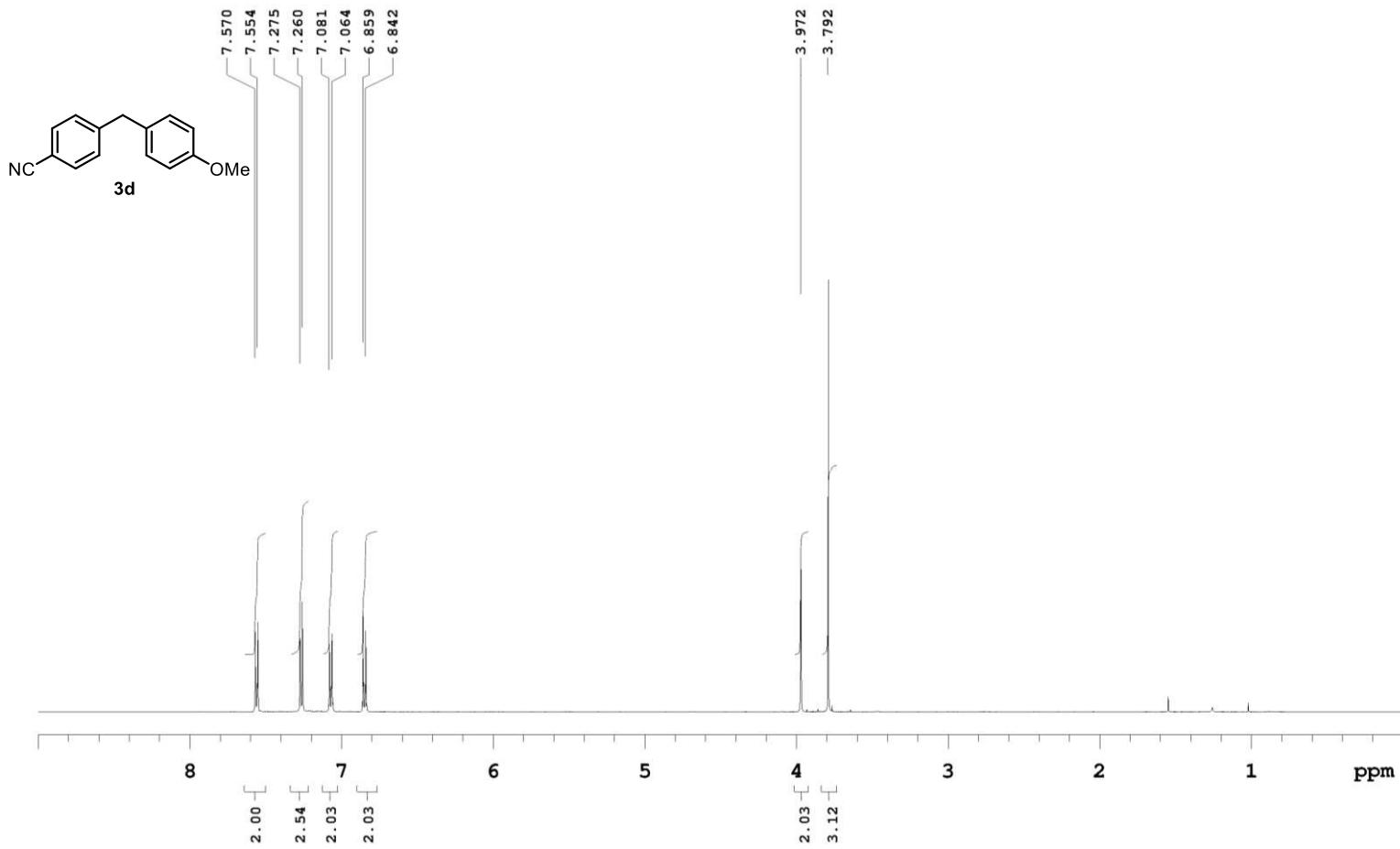
Relaxation Delay(s): 1
Completed Scans 140

WQ-03-196-A
125.688 MHz C13(H1) 1D in CDCl_3 (ref. to CDCl_3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe





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Recorded on: u500, Feb 25 2018
Pulse Sequence: PRESATSweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 18.74Relaxation Delay(s): 0.1
Completed Scans 1WQ-03-186-B
499.797 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe



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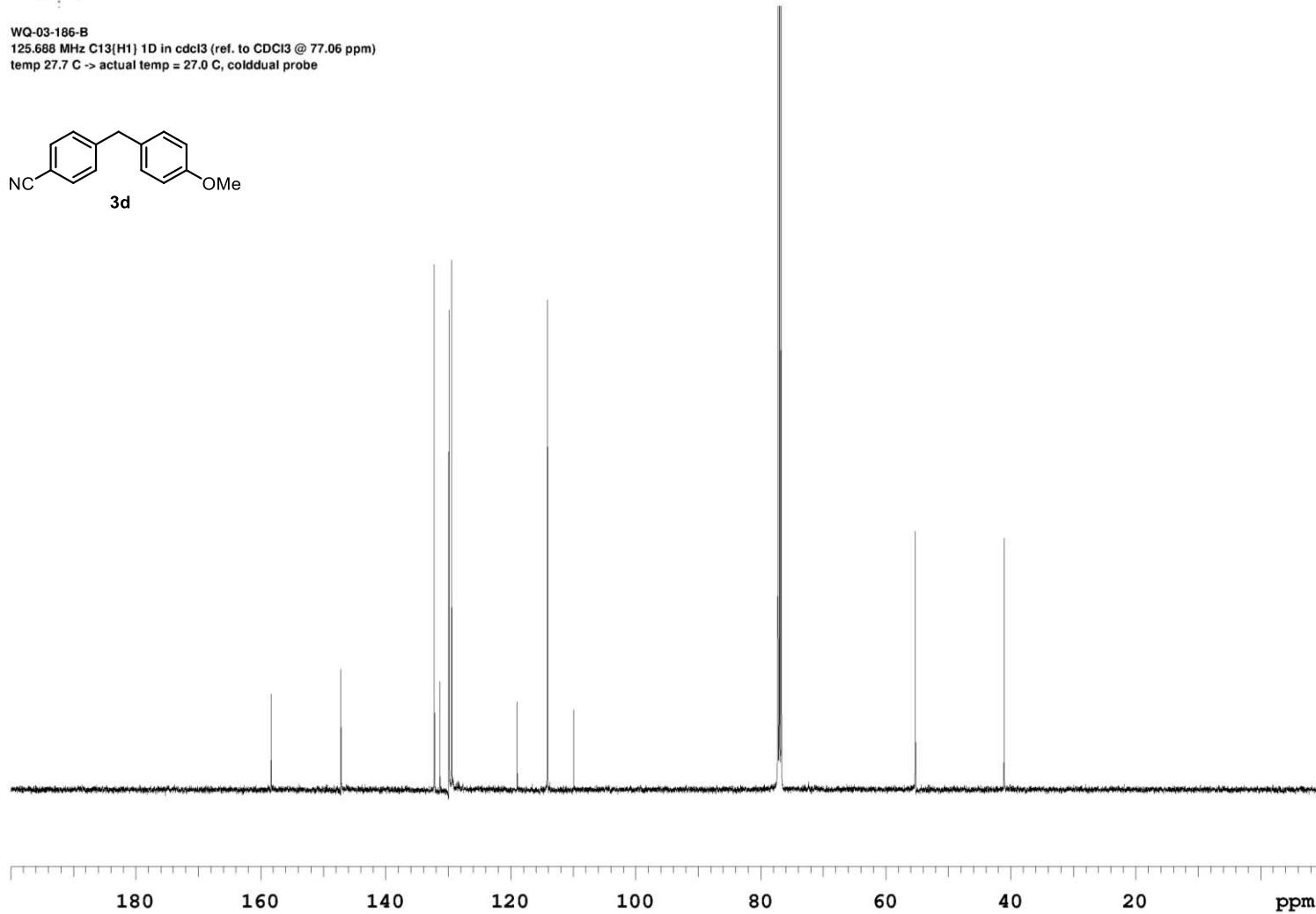
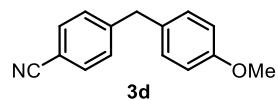
Recorded on: u500, Feb 25 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 33763.8
Digital Res.(Hz/pt): 0.26

Acquisition Time(s): 1
Hz per mm(Hz/mm): 109.95

Relaxation Delay(s): 1
Completed Scans 128

WQ-03-186-B
125.688 MHz C13(H1) 1D in CDCl_3 (ref. to CDCl_3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, cold dual probe





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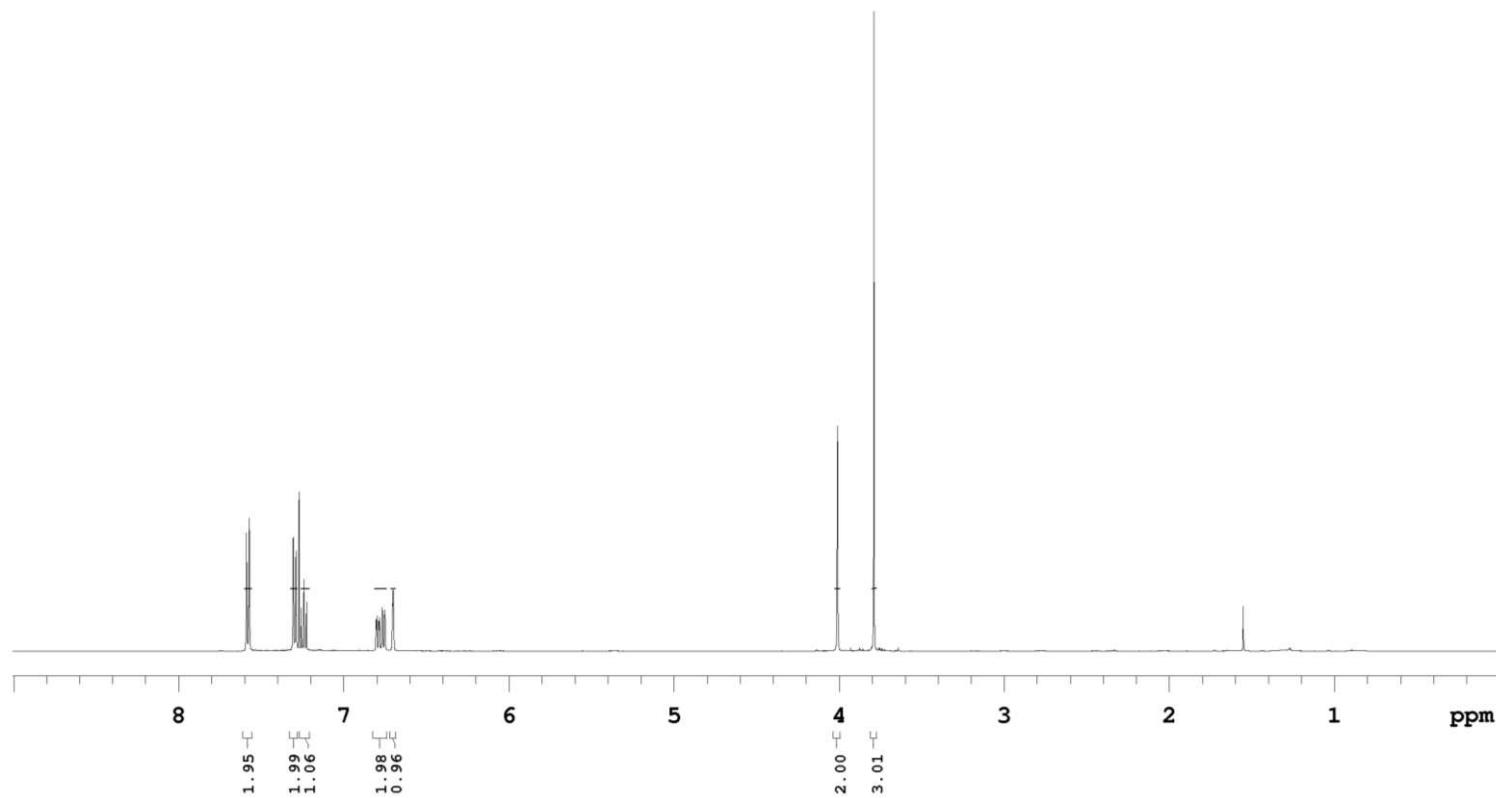
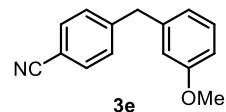
Recorded on: u500, Mar 14 2018
Pulse Sequence: PRESAT

Sweep Width(Hz): **6009.62**
Digital Res.(Hz/pt): **0.09**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **18.8**

Relaxation Delay(s): **0.1**
Completed Scans **8**

Patrick, PM-14-153-A
499.797 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, coldl dual probe

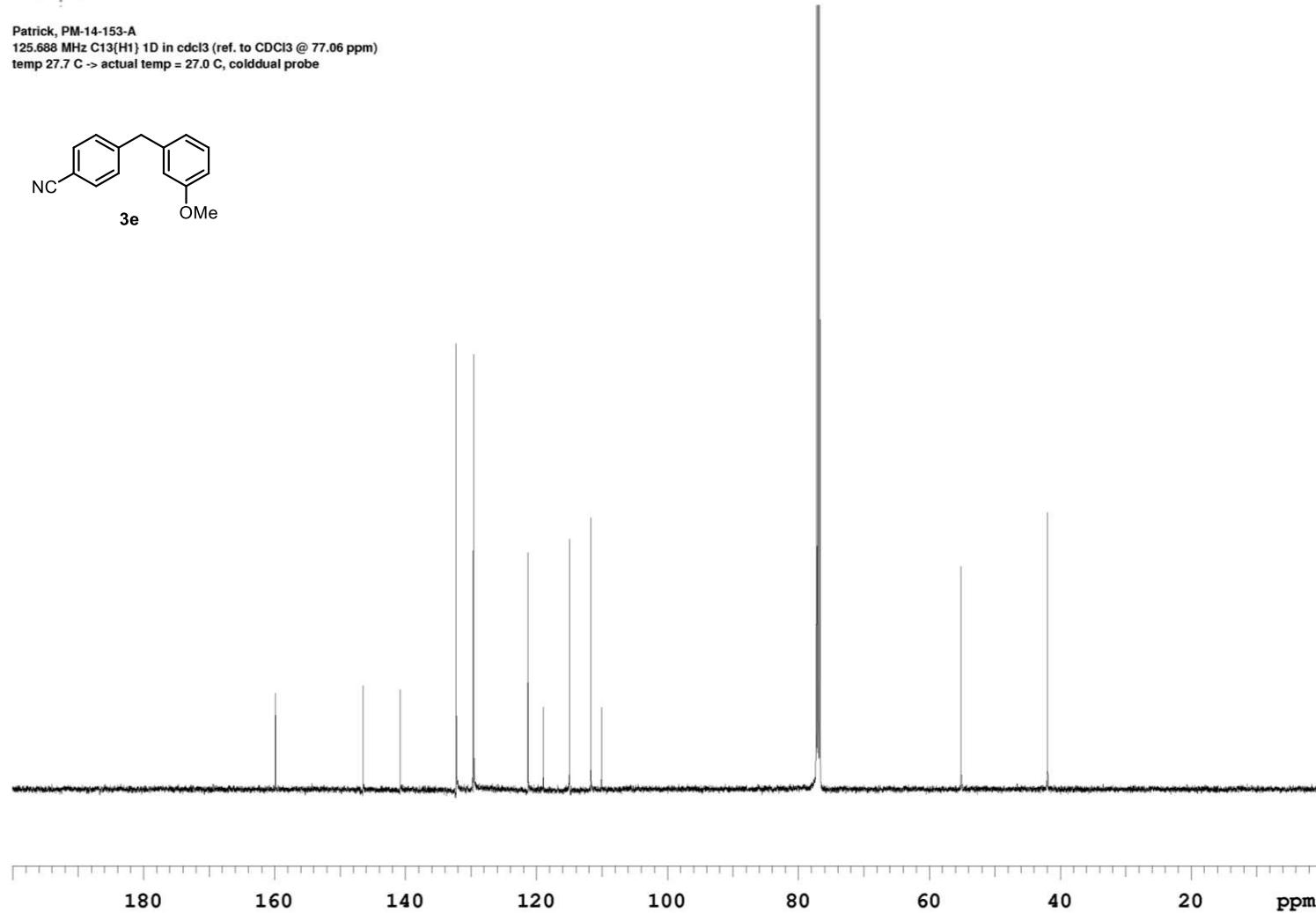
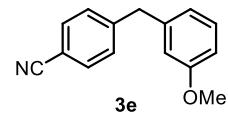




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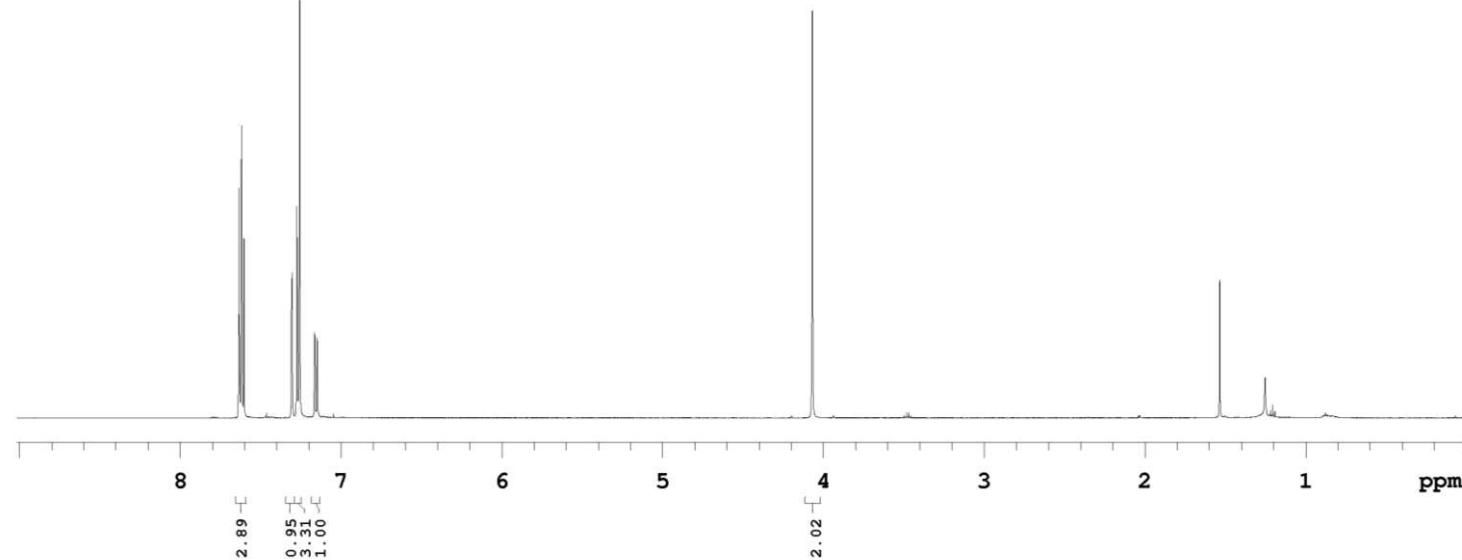
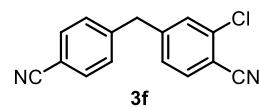
Recorded on: u500, Mar 14 2018
Pulse Sequence: s2pulSweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26Acquisition Time(s): 1
Hz per mm(Hz/mm): 104.88Relaxation Delay(s): 1
Completed Scans 256

Patrick, PM-14-153-A
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe





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Recorded on: u500, Mar 8 2018
Pulse Sequence: PRESATSweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 18.84Relaxation Delay(s): 0.1
Completed Scans: 4WQ-04-024
499.797 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, cold dual probe



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Recorded on: u500, Mar 8 2018
Pulse Sequence: s2pul

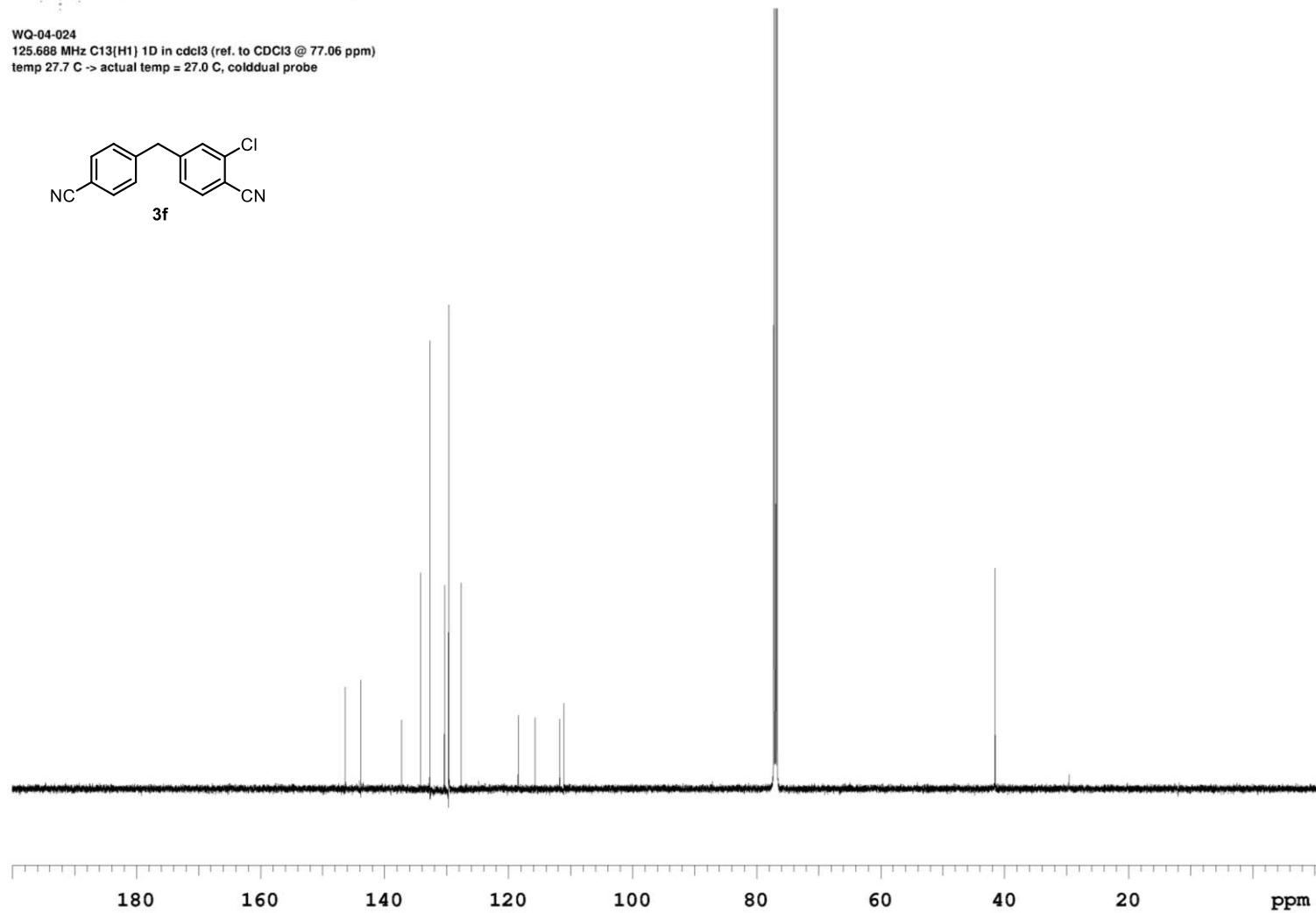
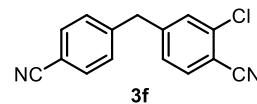
Sweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26

Acquisition Time(s): 1
Hz per mm(Hz/mm): 110.29

Relaxation Delay(s): 1
Completed Scans 512

WQ-04-024

125.688 MHz C13(H1) 1D in CDCl_3 (ref. to CDCl_3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe





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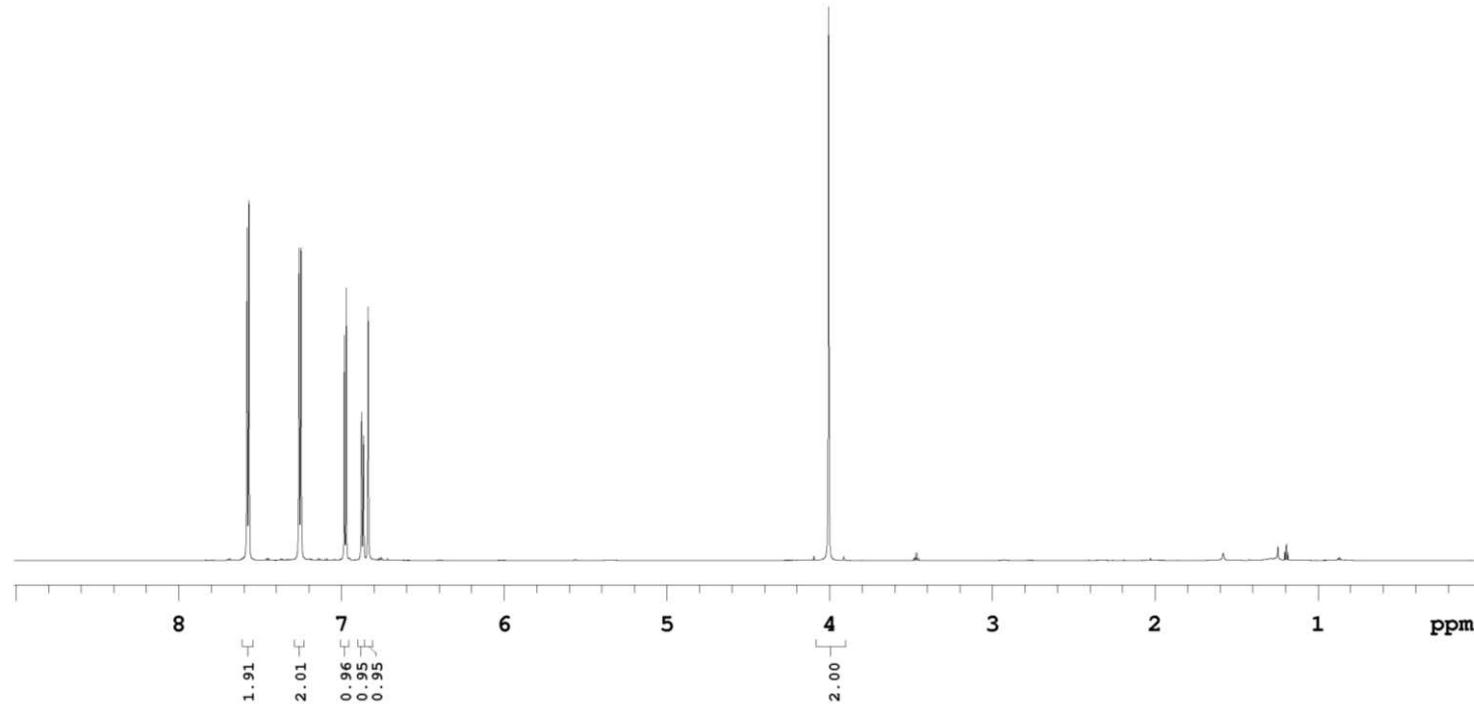
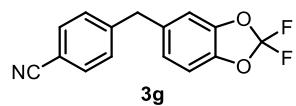
Recorded on: v700, Mar 22 2018
Pulse Sequence: PRESAT

Sweep Width(Hz): 8389.26
Digital Res.(Hz/pt): 0.13

Acquisition Time(s): 5
Hz per mm(Hz/mm): 26.31

Relaxation Delay(s): 0.1
Completed Scans 8

PM-14-165-A
699.762 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.5 C -> actual temp = 27.0 C, coldid probe





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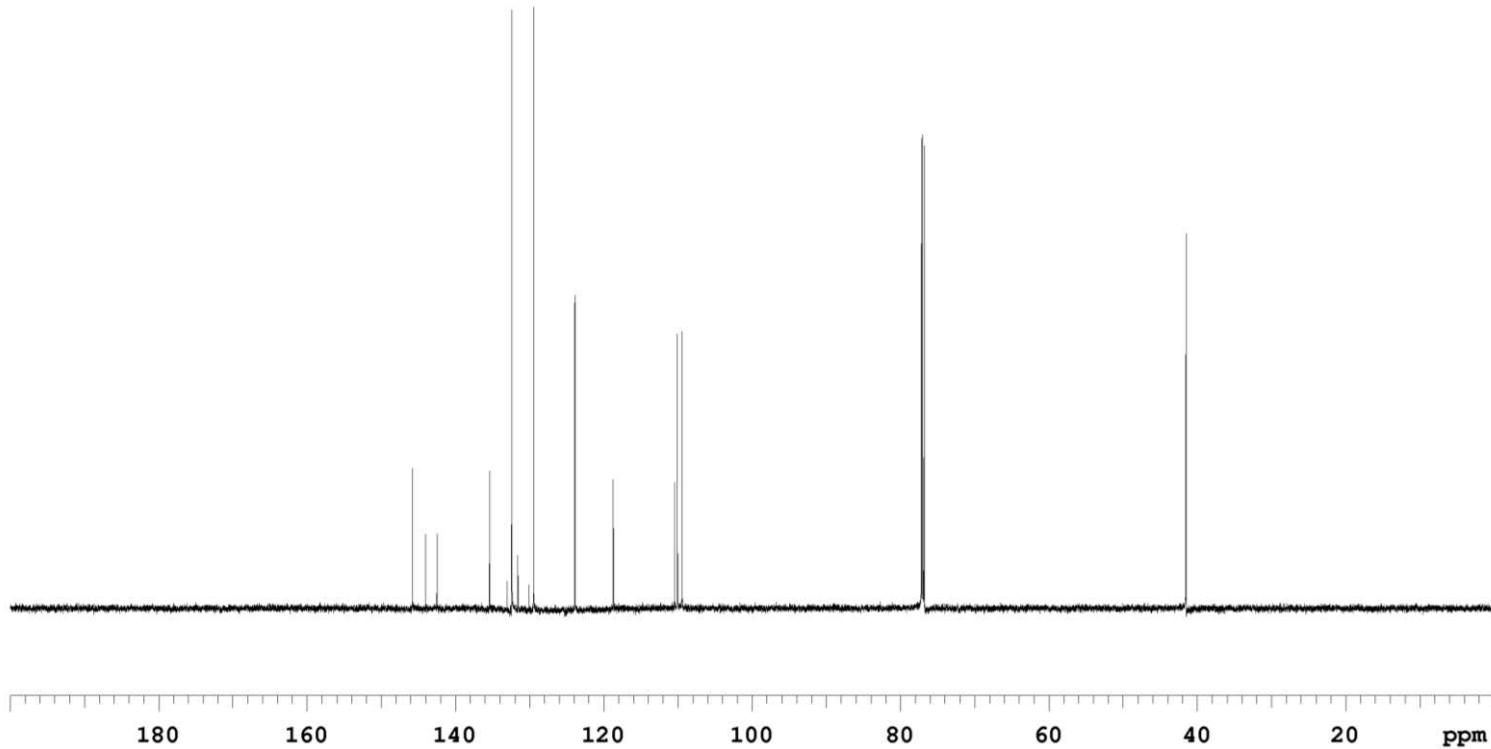
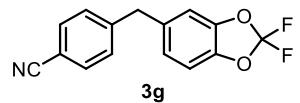
Recorded on: v700, Mar 22 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 48076.9
Digital Res.(Hz/pt): 0.37

Acquisition Time(s): 1
Hz per mm(Hz/mm): 146.81

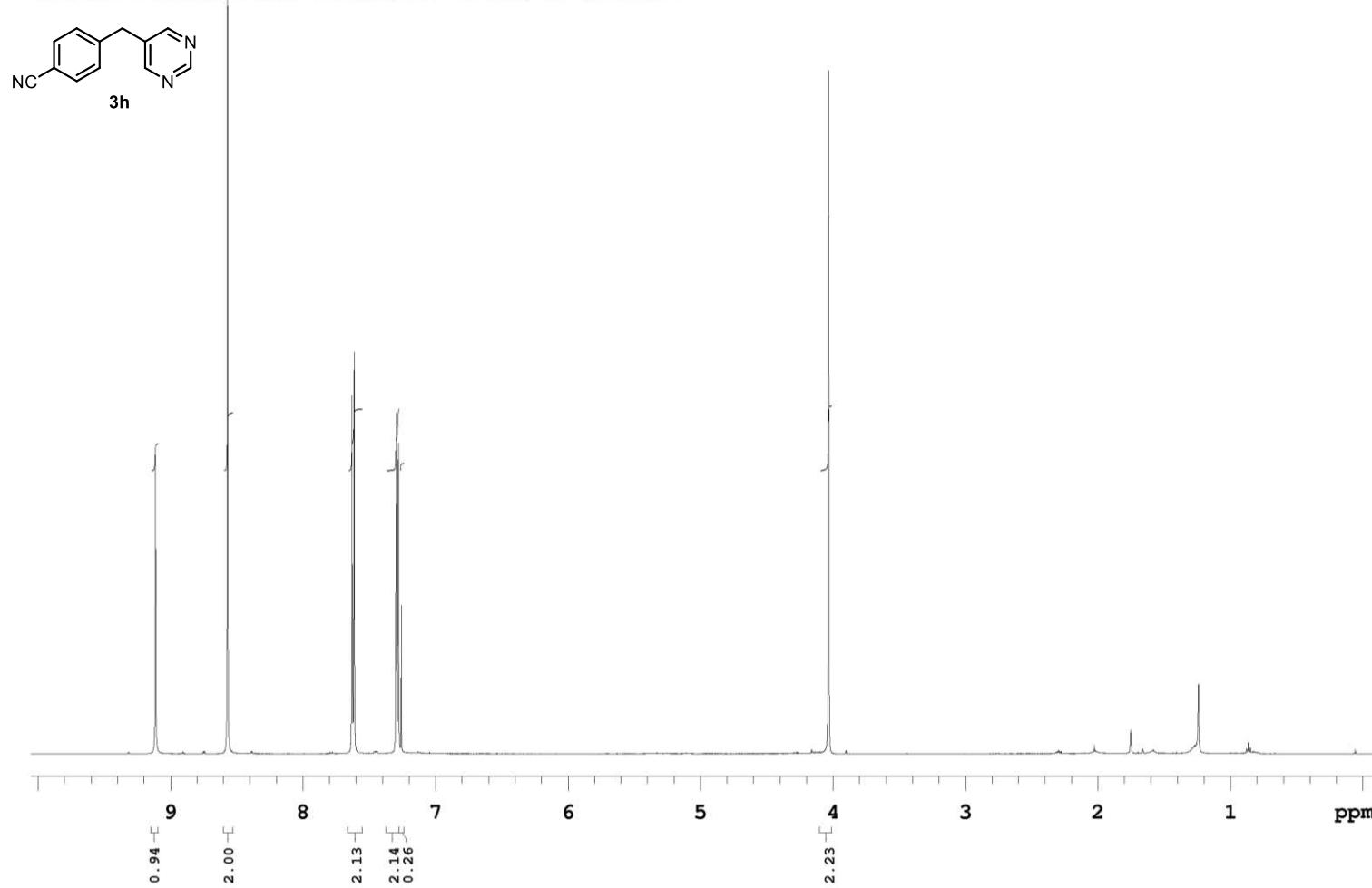
Relaxation Delay(s): 1
Completed Scans 24

PM-14-165-A
175.975 MHz C13{H1} 1D in CDCl_3 (ref. to CDCl_3 @ 77.06 ppm)
temp 27.5 C -> actual temp = 27.0 C, coldid probe





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Recorded on: **ibd5, Mar 18 2018**
Pulse Sequence: **s2pul**Sweep Width(Hz): **6000.6**
Digital Res.(Hz/pt): **0.09**Acquisition Time(s): **5**
Hz per mm(Hz/mm): **21.18**Relaxation Delay(s): **0.1**
Completed Scans: **16**DK-3-201-B
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe



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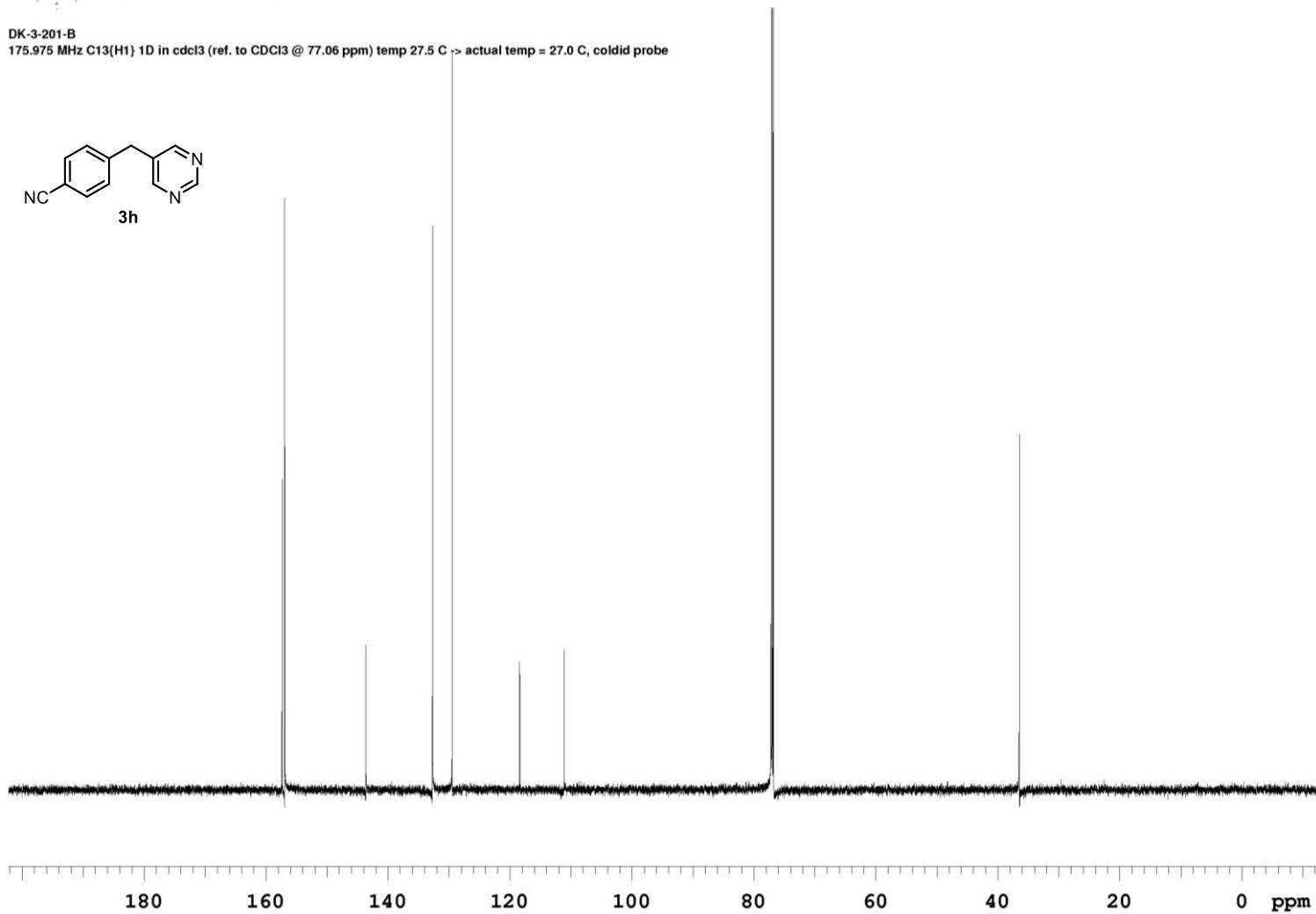
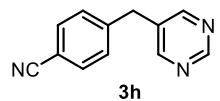
Recorded on: v700, Mar 18 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 48076.9
Digital Res.(Hz/pt): 0.37

Acquisition Time(s): 1
Hz per mm(Hz/mm): 157.5

Relaxation Delay(s): 1
Completed Scans 60

DK-3-201-B
175.975 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.5 C -> actual temp = 27.0 C, coldid probe





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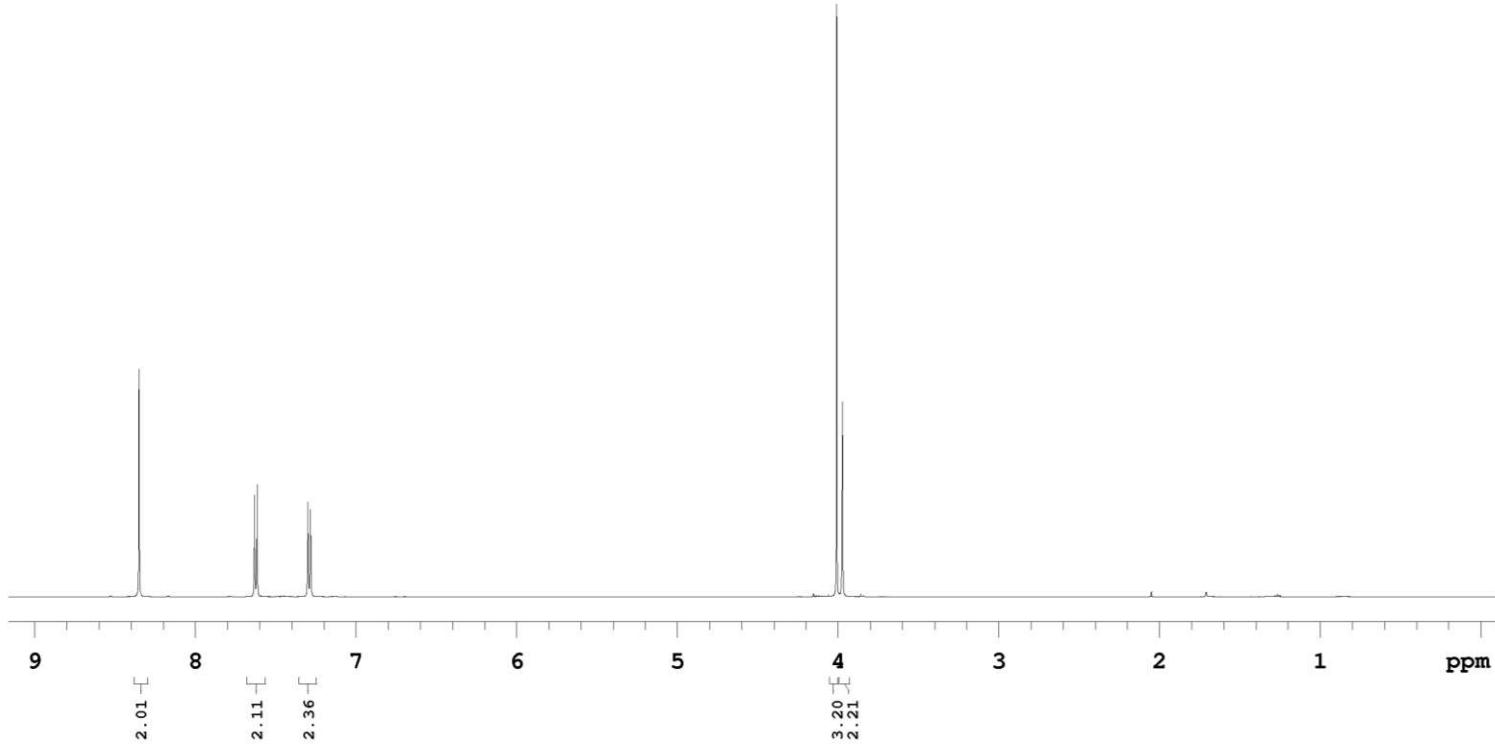
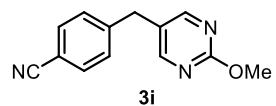
Recorded on: ibd5, Mar 17 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09

Acquisiton Time(s): 5
Hz per mm(Hz/mm): 19.25

Relaxation Delay(s): 0.1
Completed Scans: 16

DK-3-201-D
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe





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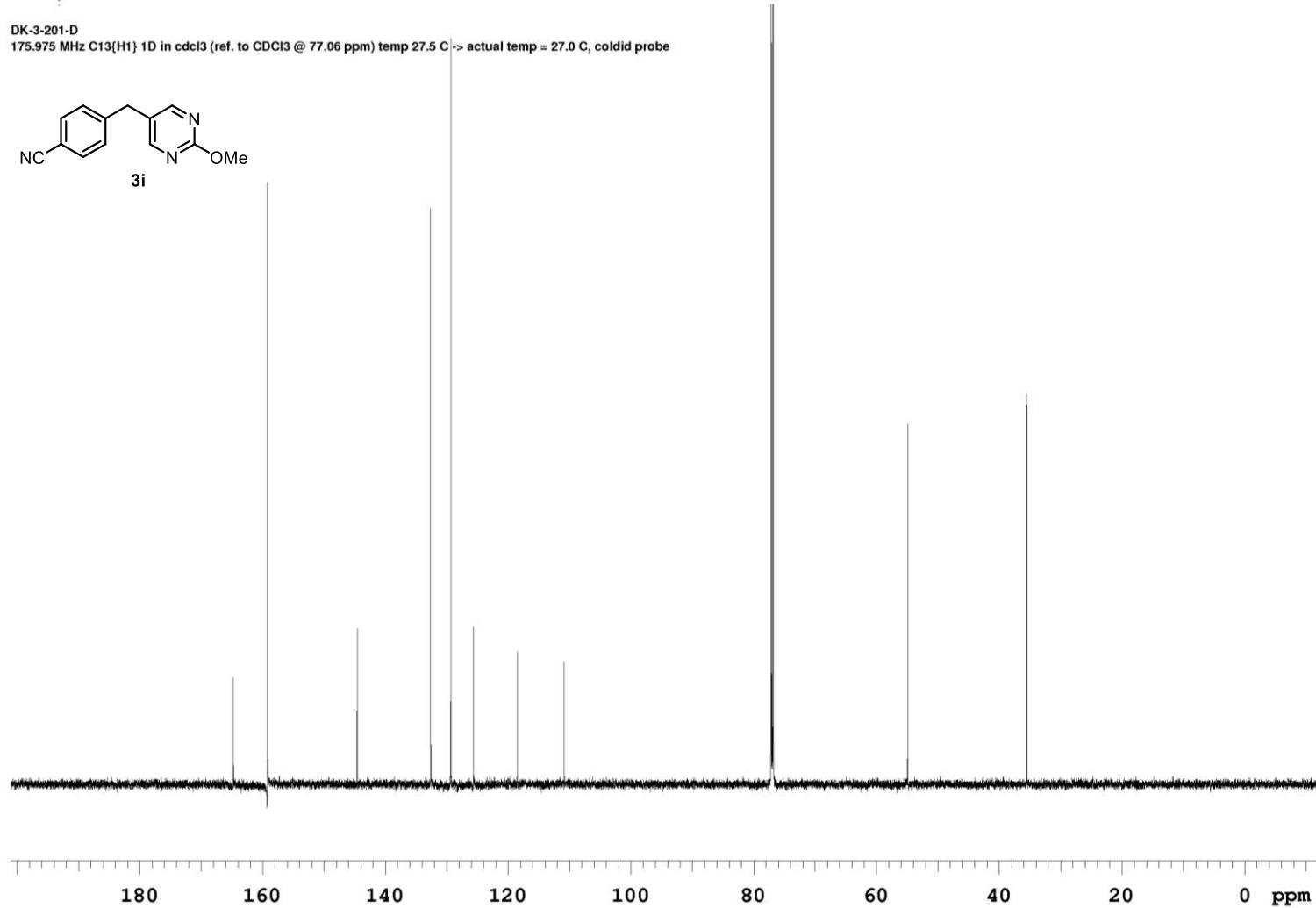
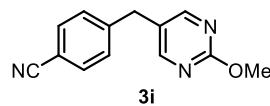
Recorded on: v700, Mar 17 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 48076.9
Digital Res.(Hz/pt): 0.37

Acquisition Time(s): 1
Hz per mm(Hz/mm): 156.19

Relaxation Delay(s): 1
Completed Scans 80

DK-3-201-D
175.975 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.5 C -> actual temp = 27.0 C, coldid probe





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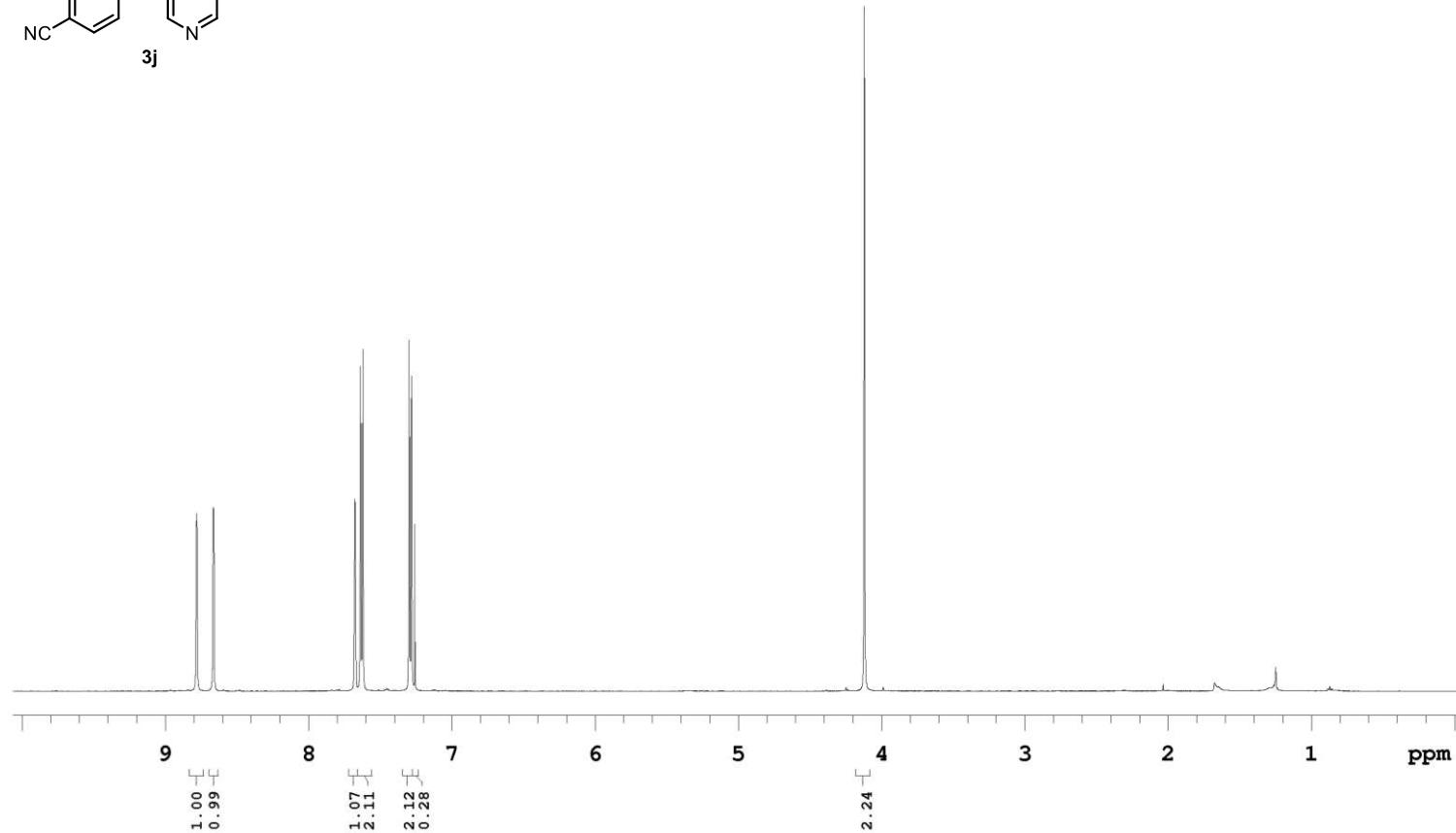
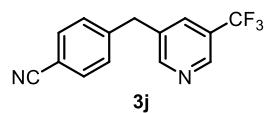
Recorded on: ibd5, Mar 17 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 20.96

Relaxation Delay(s): 0.1
Completed Scans 16

DK-3-201-C
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe





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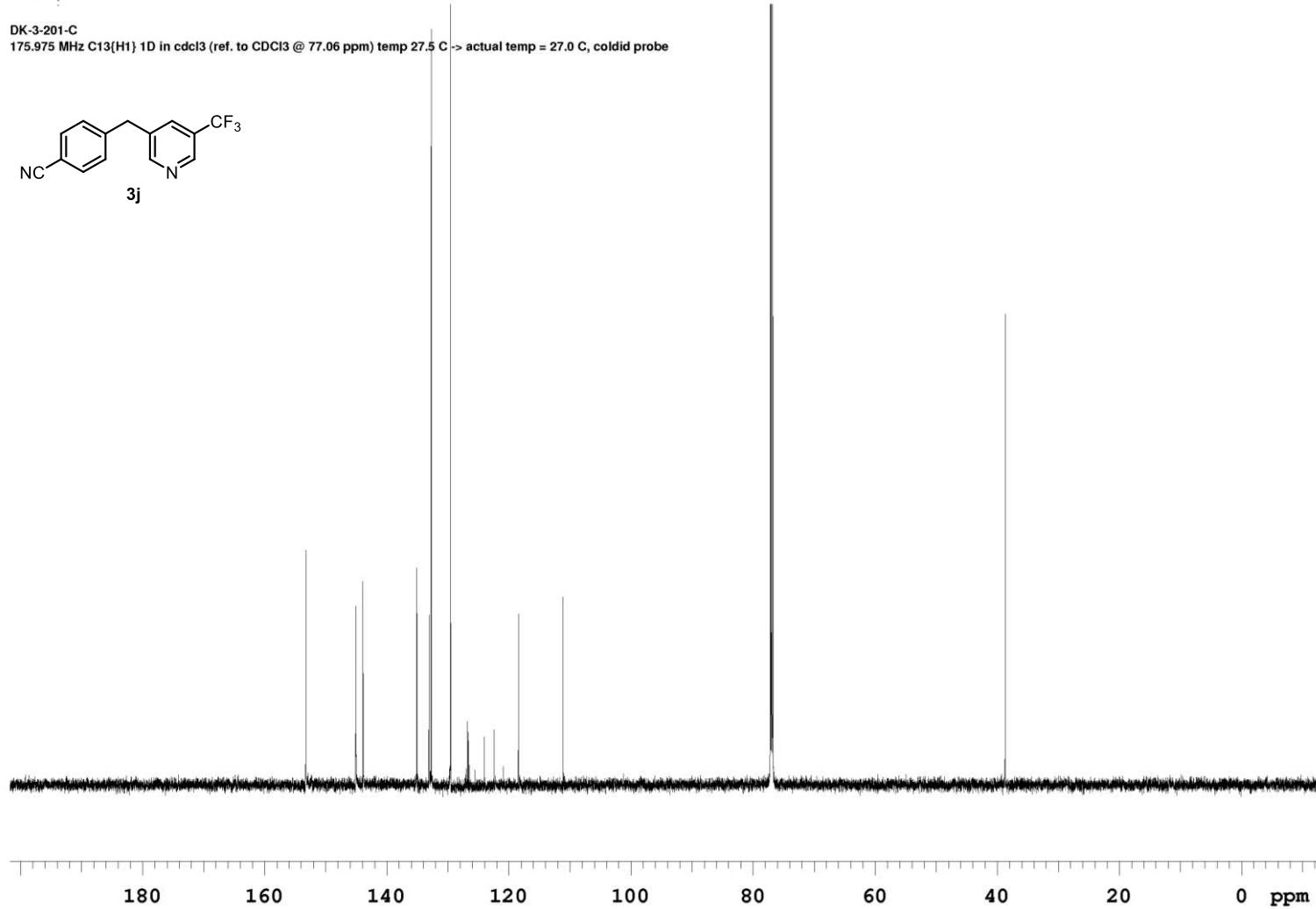
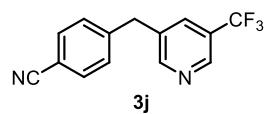
Recorded on: v700, Mar 17 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 48076.9
Digital Res.(Hz/pt): 0.37

Acquisition Time(s): 1
Hz per mm(Hz/mm): 156.97

Relaxation Delay(s): 1
Completed Scans 80

DK-3-201-C
175.975 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.5 C -> actual temp = 27.0 C, coldid probe





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Recorded on: v700, Mar 23 2018

Pulse Sequence: PRESAT

Sweep Width(Hz): 8389.26

Digital Res.(Hz/pt): 0.13

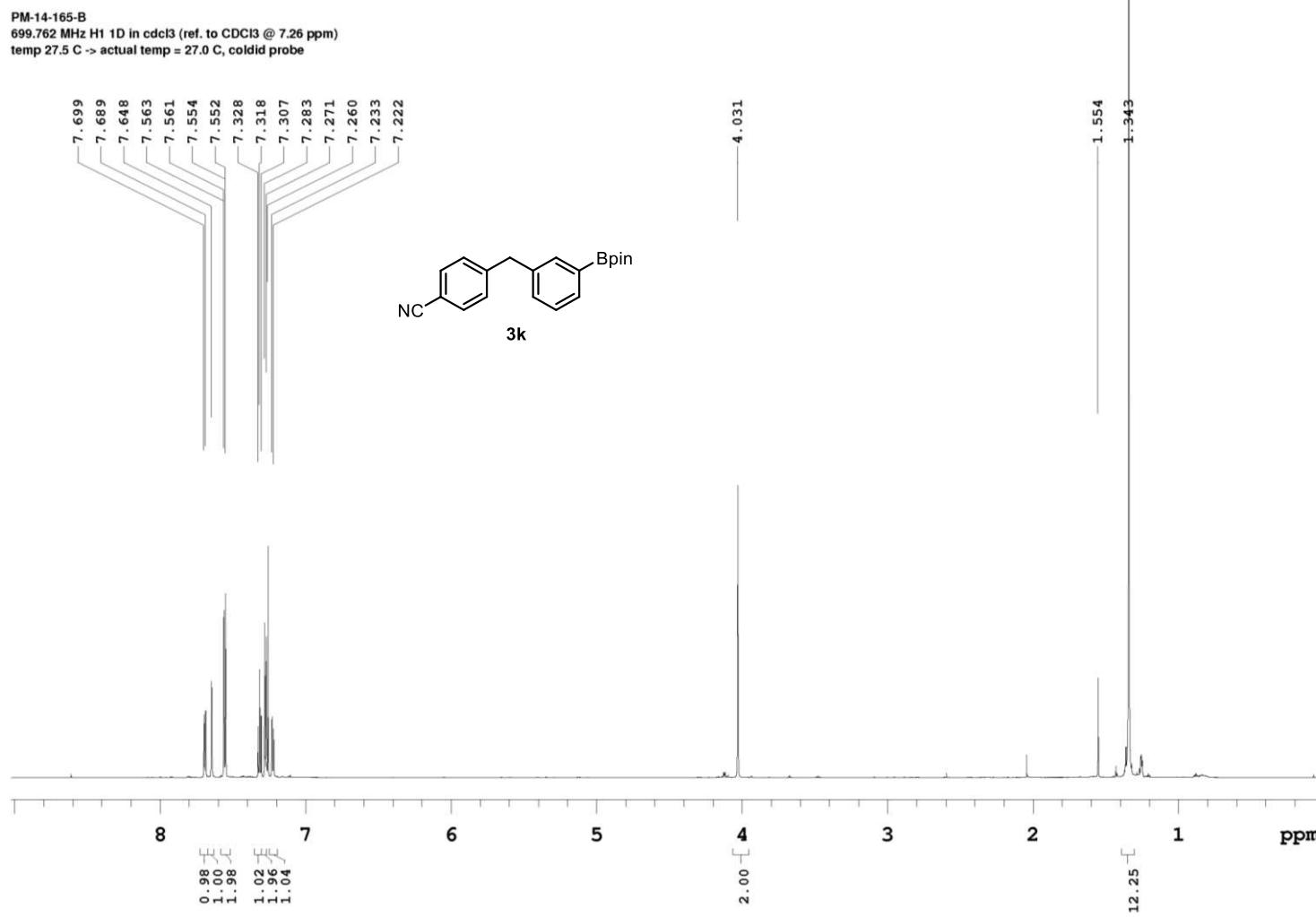
Acquisition Time(s): 5

Hz per mm(Hz/mm): 26.37

Relaxation Delay(s): 0.1

Completed Scans 8

PM-14-165-B
699.762 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.5 C -> actual temp = 27.0 C, coldid probe





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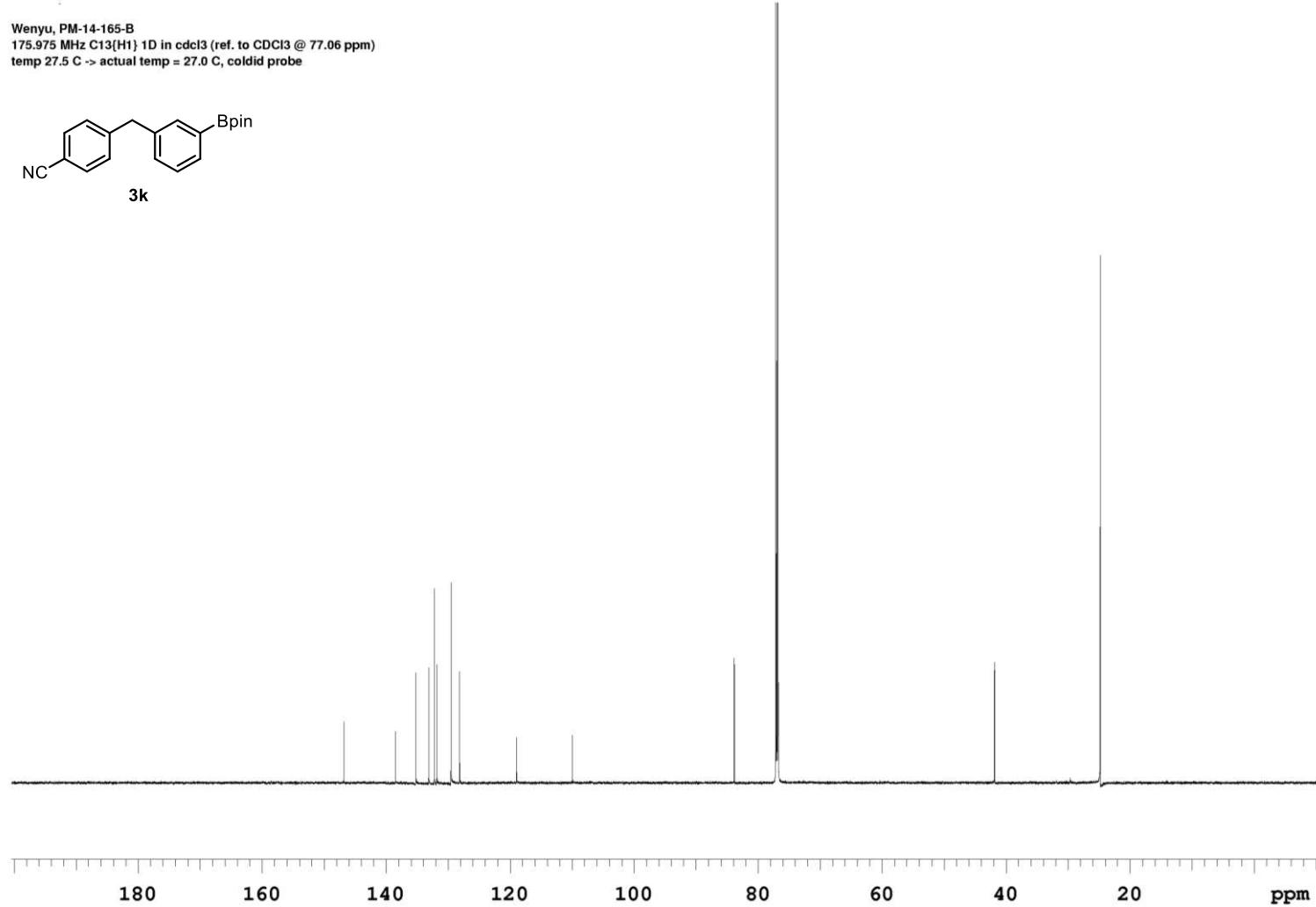
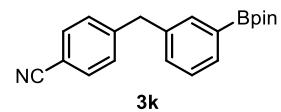
Recorded on: v700, Mar 23 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 48076.9
Digital Res.(Hz/pt): 0.37

Acquisition Time(s): 1
Hz per mm(Hz/mm): 154.46

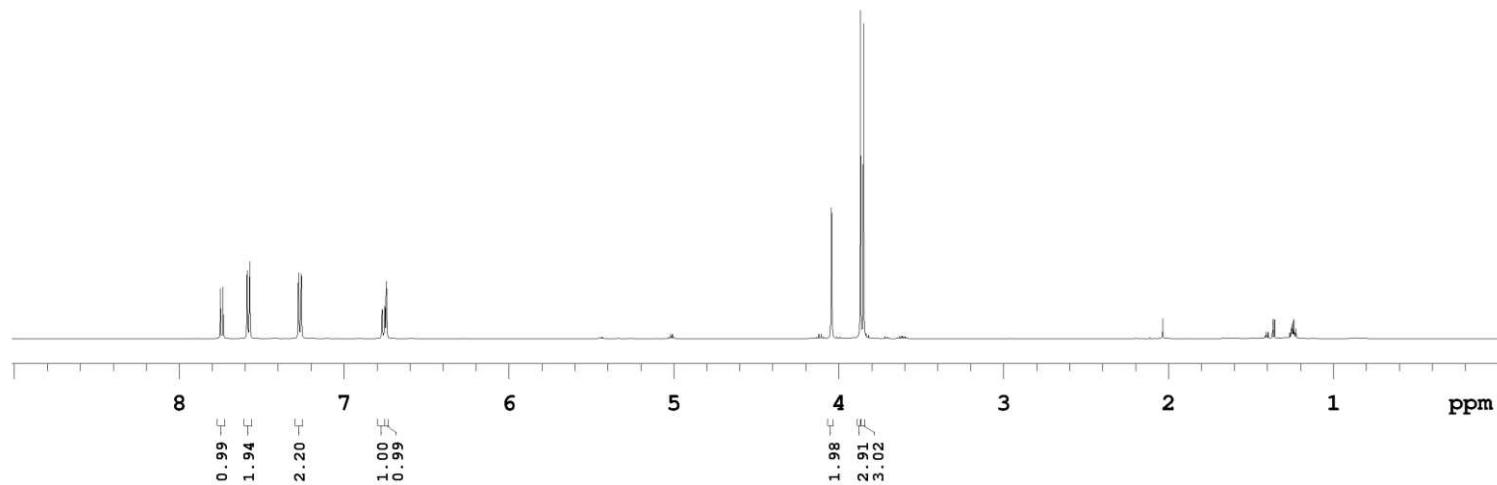
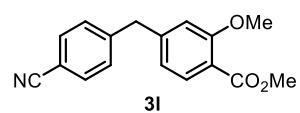
Relaxation Delay(s): 1
Completed Scans 1188

Wenyu, PM-14-165-B
175.975 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm)
temp 27.5 C -> actual temp = 27.0 C, coldid probe





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Recorded on: u500, Mar 22 2018
Pulse Sequence: PRESATSweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 18.82Relaxation Delay(s): 0.1
Completed Scans 4PM-14-165-C
499.797 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe



Department of Chemistry, University of Alberta

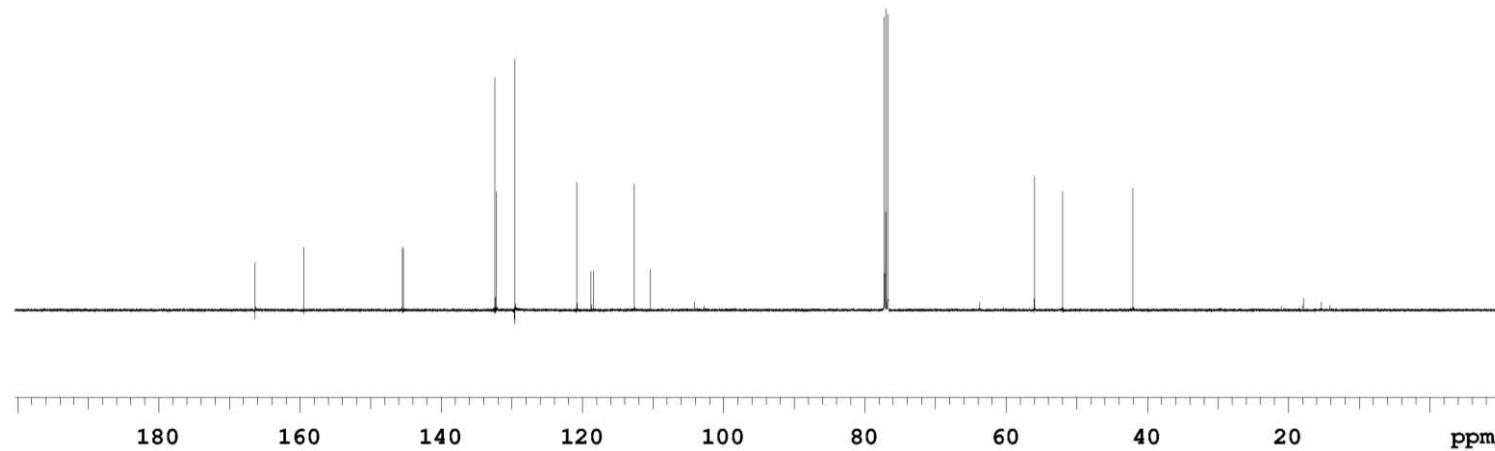
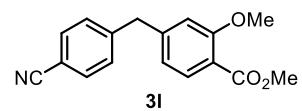
Recorded on: **u500, Mar 22 2018**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **33783.8**
Digital Res.(Hz/pt): **0.26**

Acquisition Time(s): **1**
Hz per mm(Hz/mm): **110.47**

Relaxation Delay(s): **1**
Completed Scans: **64**

PM-14-165-C
125.688 MHz C13(H1) 1D in CDCl_3 (ref. to CDCl_3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, cold dual probe



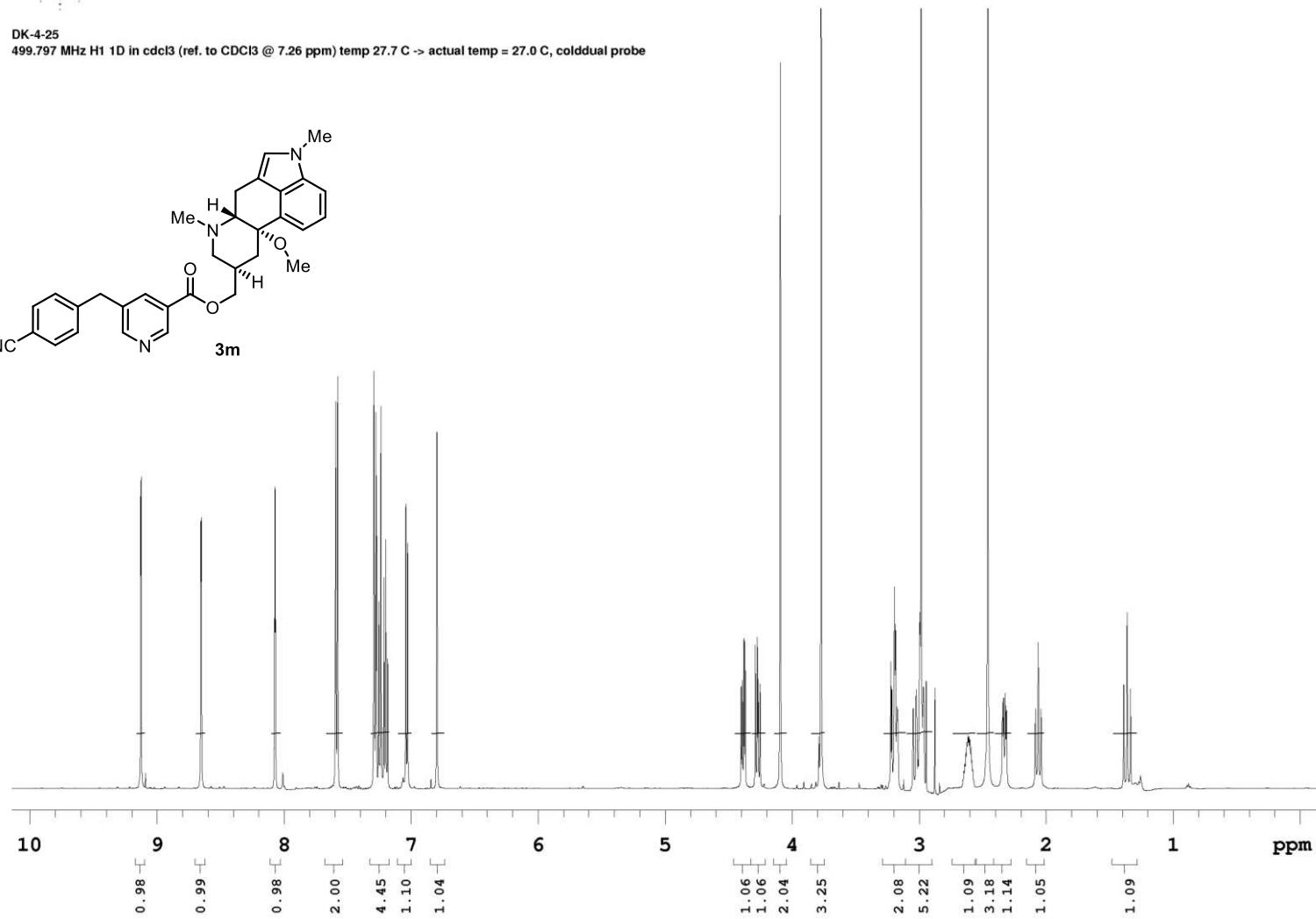
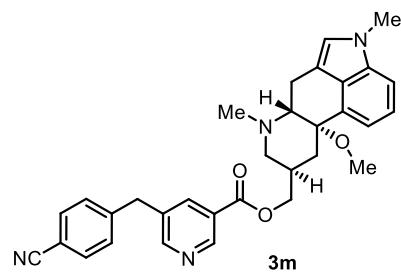


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Recorded on: u500, Mar 20 2018
Pulse Sequence: PRESATSweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 21.44Relaxation Delay(s): 0.1
Completed Scans: 8

DK-4-25

499.797 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 27.7 C -> actual temp = 27.0 C, colddual probe





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Recorded on: u500, Mar 20 2018

Sweep Width(Hz): 33783.8

Acquisition Time(s): 1

Relaxation Delay(s): 1

Pulse Sequence: s2pul

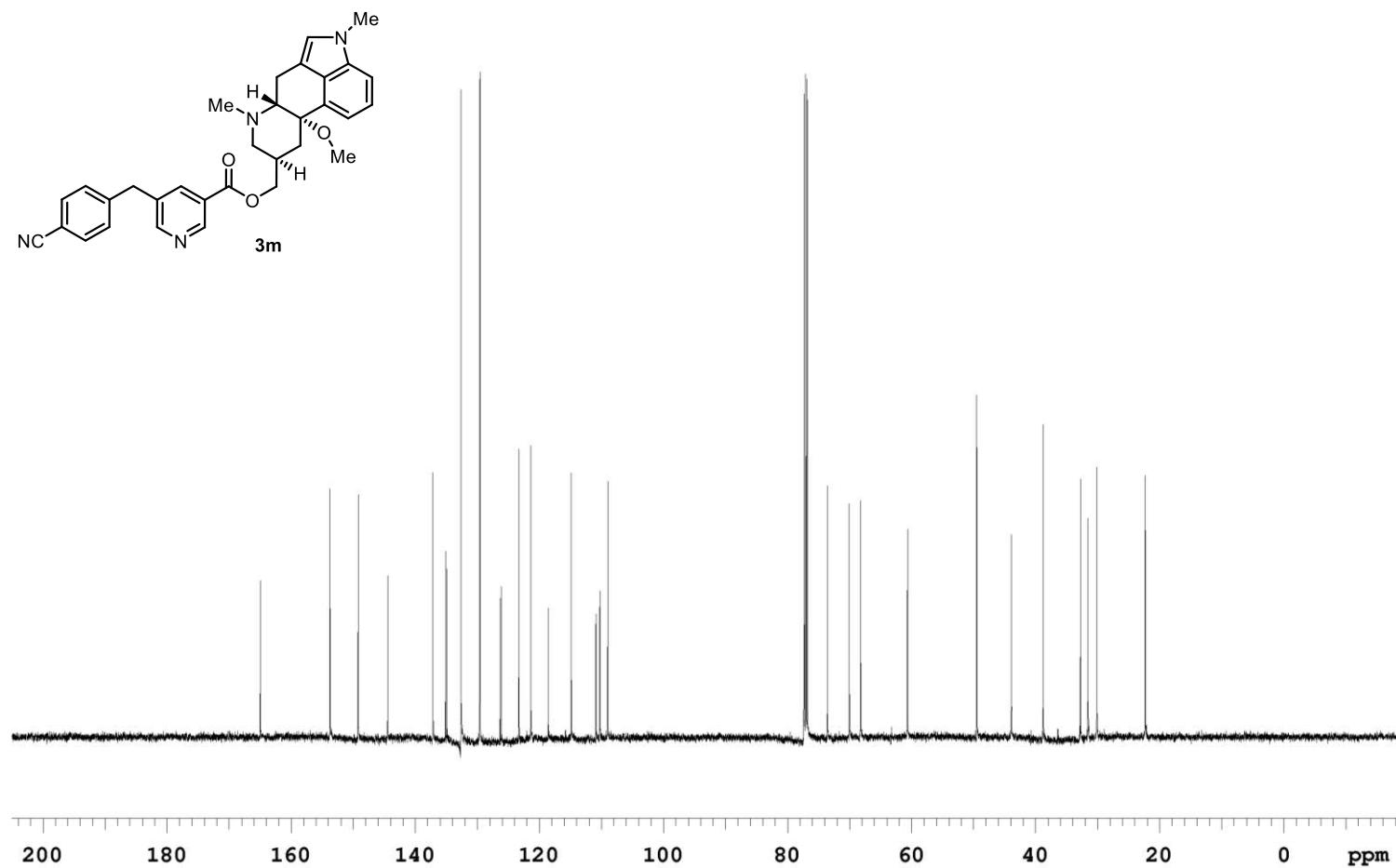
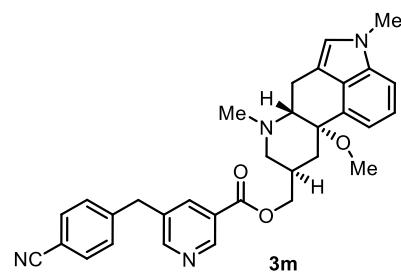
Digital Res.(Hz/pt): 0.26

Hz per mm(Hz/mm): 116.98

Completed Scans 48

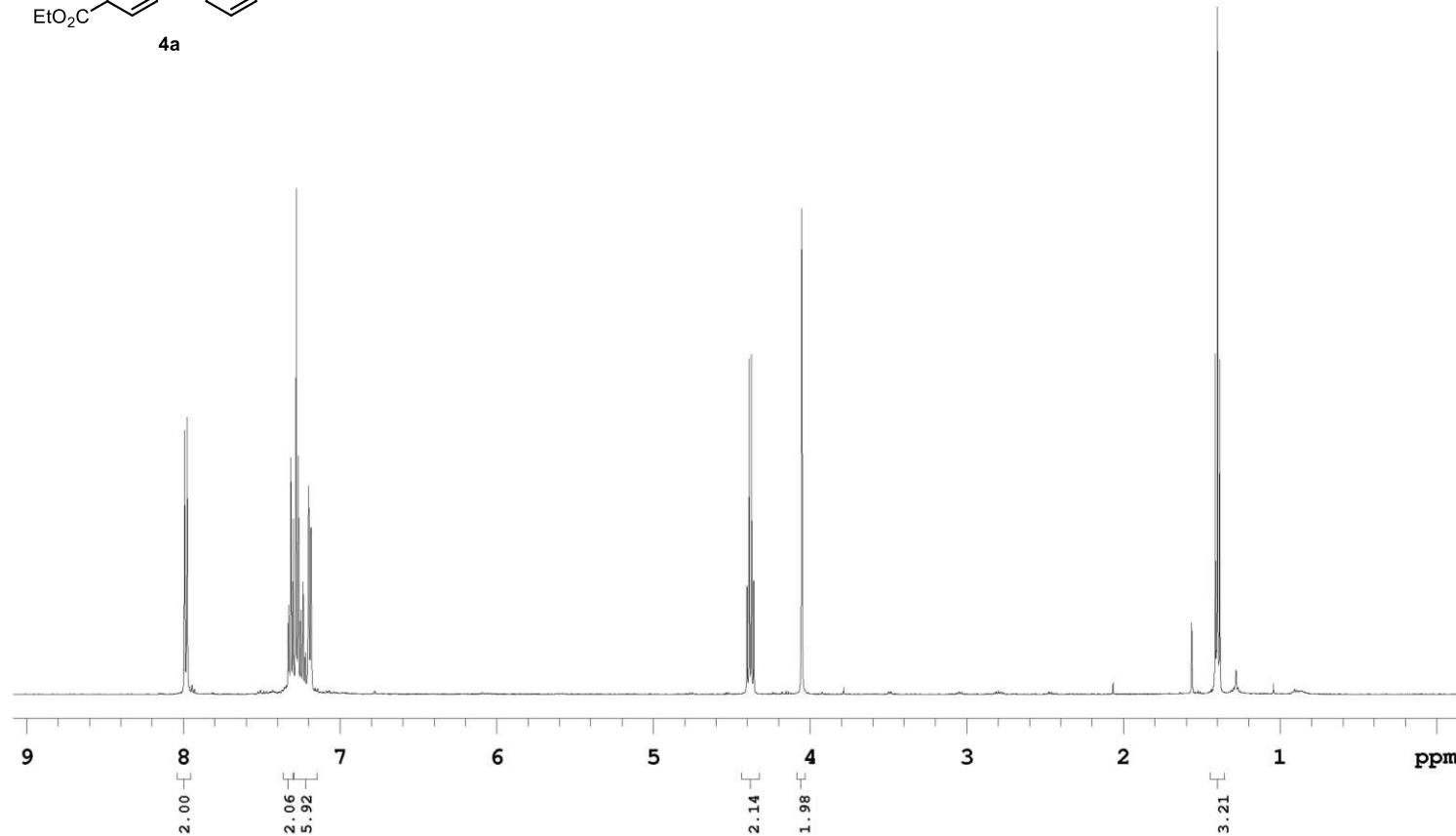
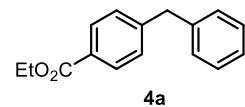
DK-4-25

125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, cold dual probe



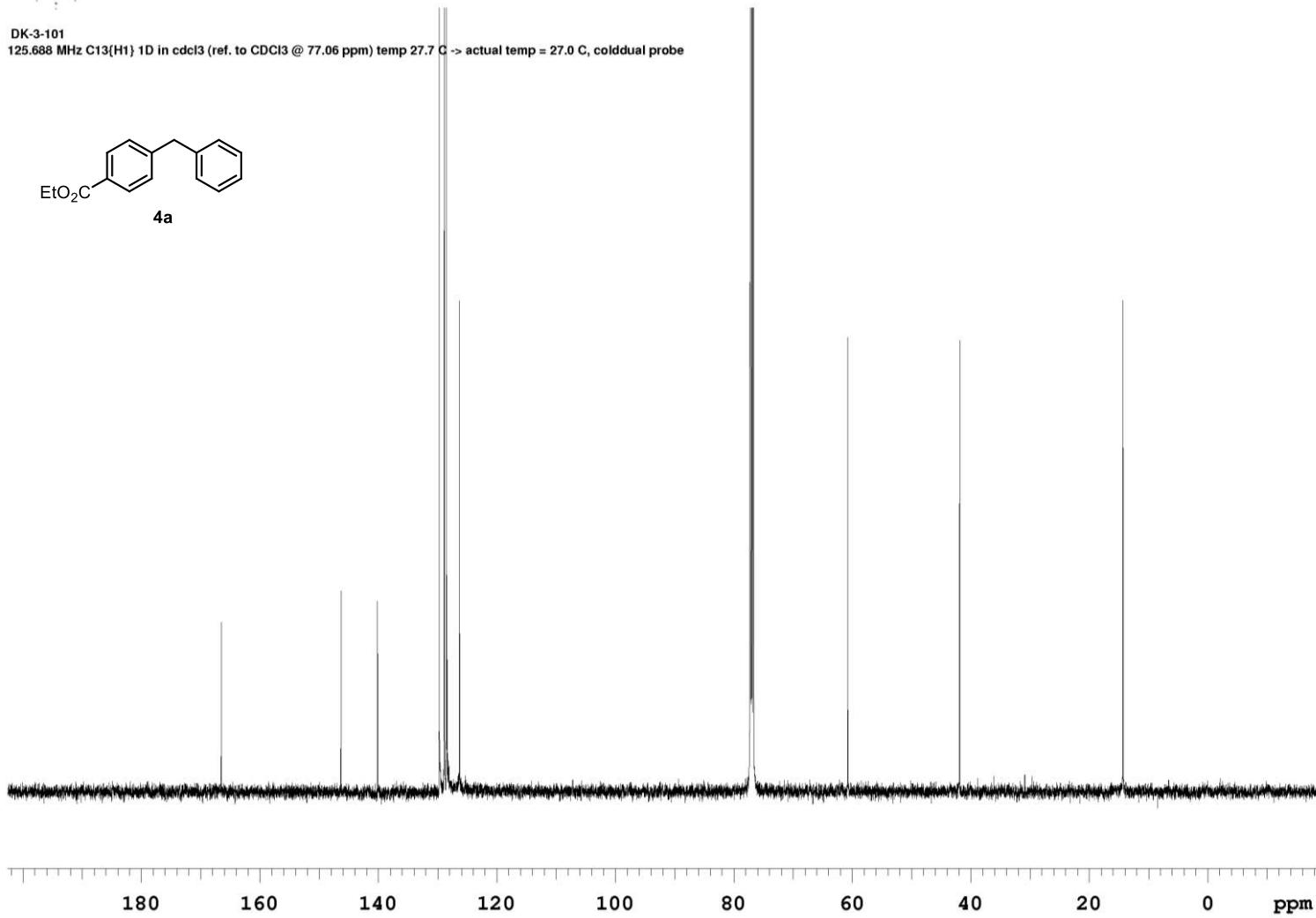
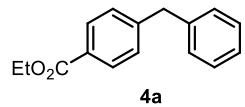


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Recorded on: ibd5, Feb 23 2018
Pulse Sequence: s2pulSweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.25Relaxation Delay(s): 0.1
Completed Scans 16DK-3-101
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe

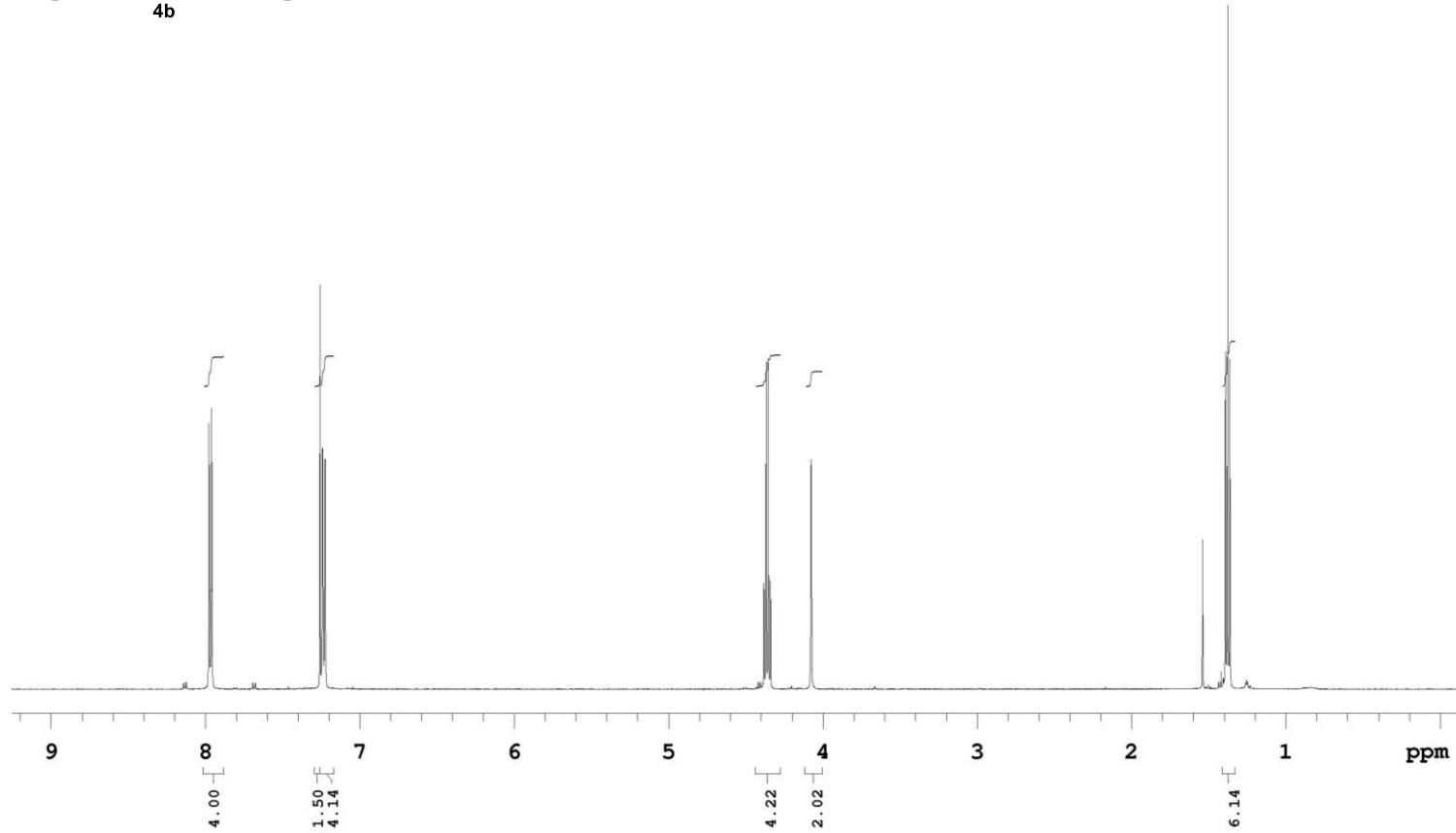
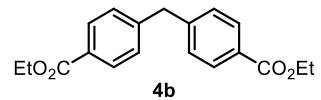


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Recorded on: **u500, Feb 23 2018**
Pulse Sequence: **s2pul**Sweep Width(Hz): **33783.8**
Digital Res.(Hz/pt): **0.26**Acquisition Time(s): **1**
Hz per mm(Hz/mm): **116.07**Relaxation Delay(s): **1**
Completed Scans: **256**DK-3-101
125.688 MHz C13(H1) 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, cold dual probe



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Recorded on: ibd5, Feb 23 2018
Pulse Sequence: s2pulSweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.44Relaxation Delay(s): 0.1
Completed Scans 16D-3-103-A
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe



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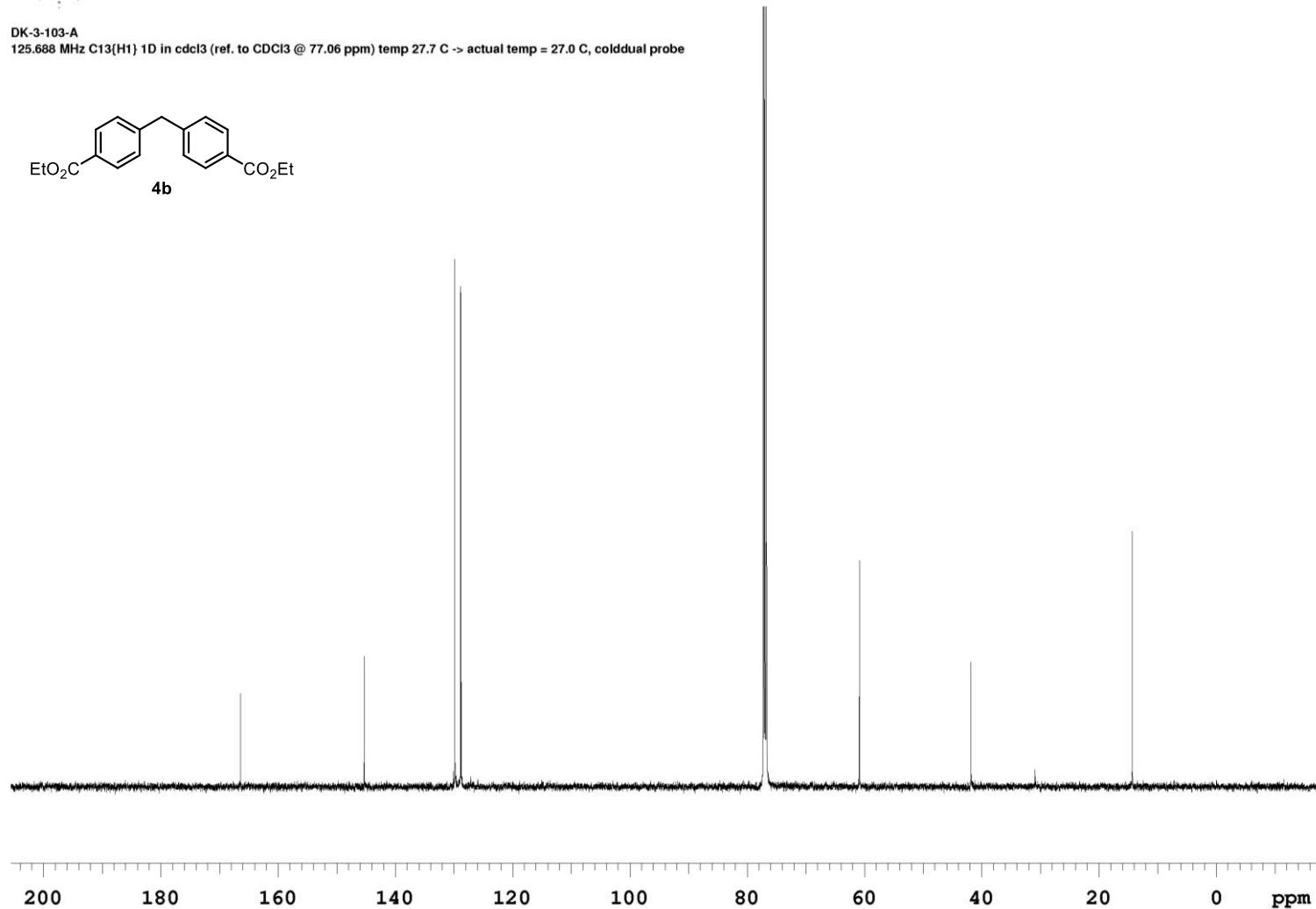
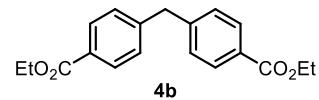
Recorded on: u500, Feb 24 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26

Acquisition Time(s): 1
Hz per mm(Hz/mm): 116.8

Relaxation Delay(s): 1
Completed Scans 256

DK-3-103-A
125.688 MHz C13(H1) 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, colddual probe

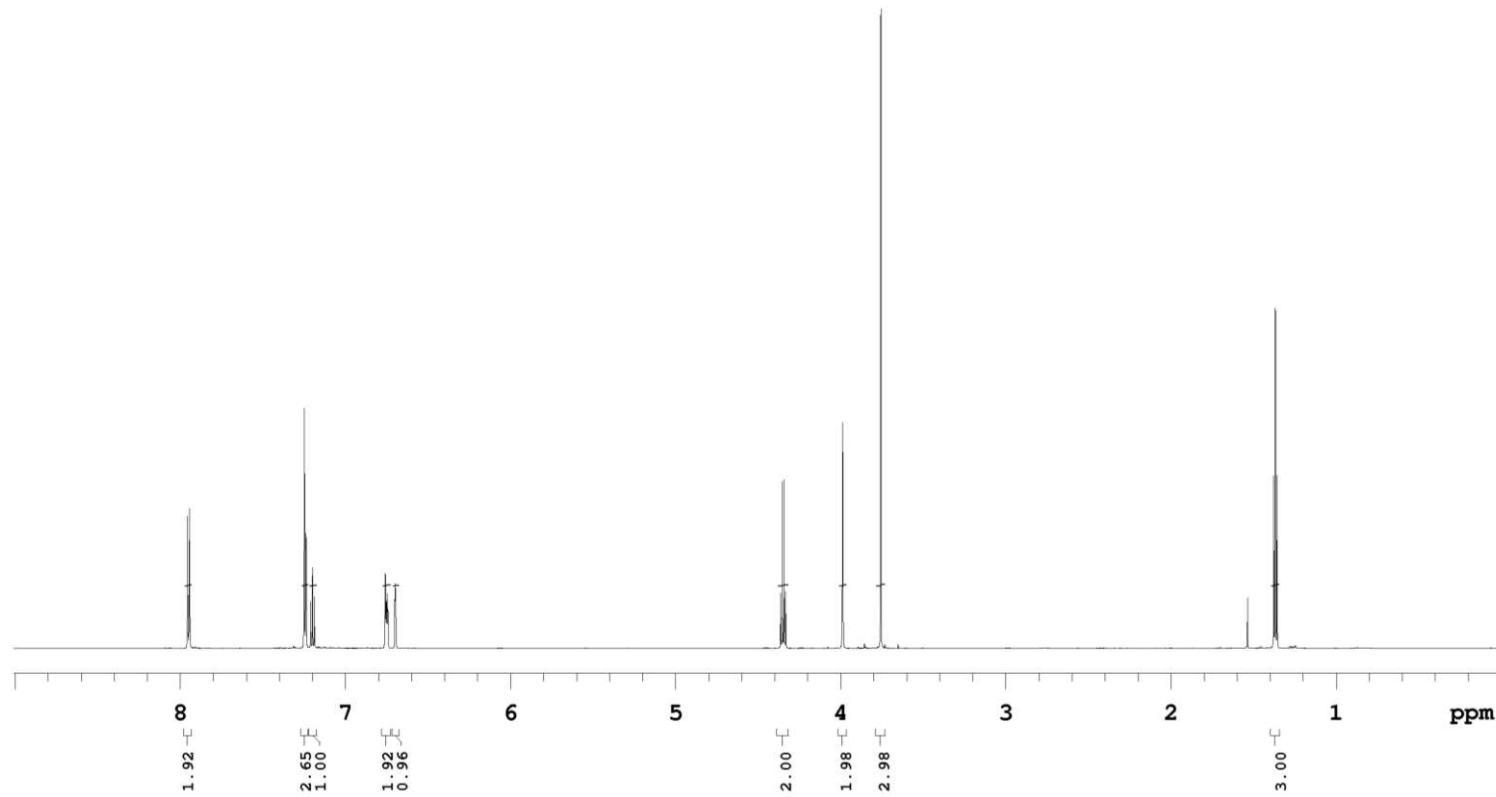
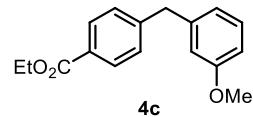




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Recorded on: v700, Mar 14 2018
Pulse Sequence: PRESATSweep Width(Hz): 8389.26
Digital Res.(Hz/pt): 0.13Acquisition Time(s): 5
Hz per mm(Hz/mm): 26.3Relaxation Delay(s): 0.1
Completed Scans 8

Patrick, PM-14-153-B
699.762 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
temp 27.5 C -> actual temp = 27.0 C, coldid probe

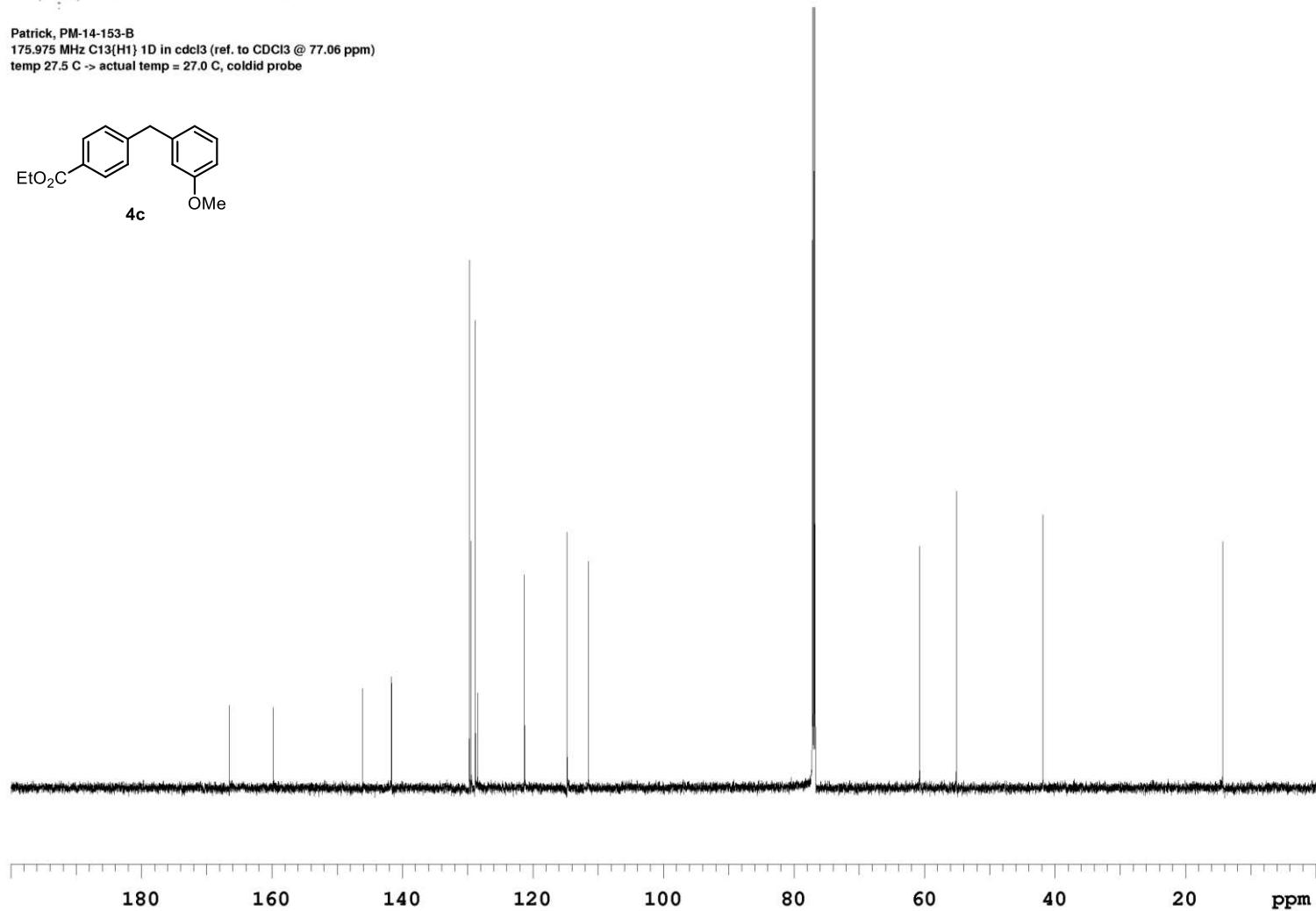
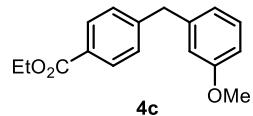




Department of Chemistry, University of Alberta

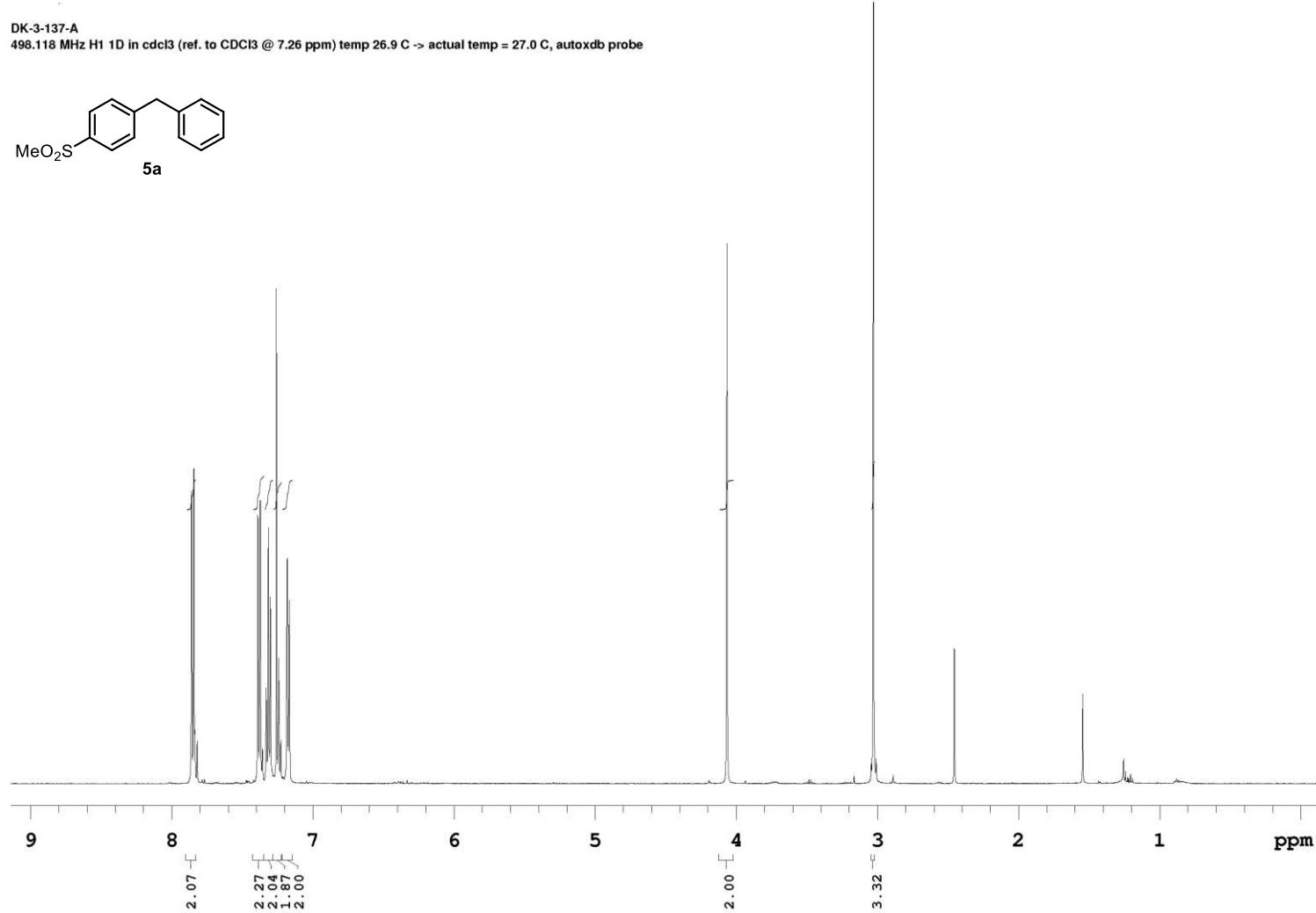
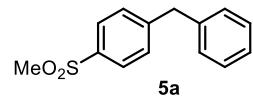
Recorded on: v700, Mar 14 2018
Pulse Sequence: s2pulSweep Width(Hz): 48076.9
Digital Res.(Hz/pt): 0.37Acquisition Time(s): 1
Hz per mm(Hz/mm): 146.92Relaxation Delay(s): 1
Completed Scans 256

Patrick, PM-14-153-B
175.975 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm)
temp 27.5 C -> actual temp = 27.0 C, coldid probe





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Recorded on: ibd5, Mar 4 2018
Pulse Sequence: s2pulSweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.27Relaxation Delay(s): 0.1
Completed Scans 16DK-3-137-A
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe



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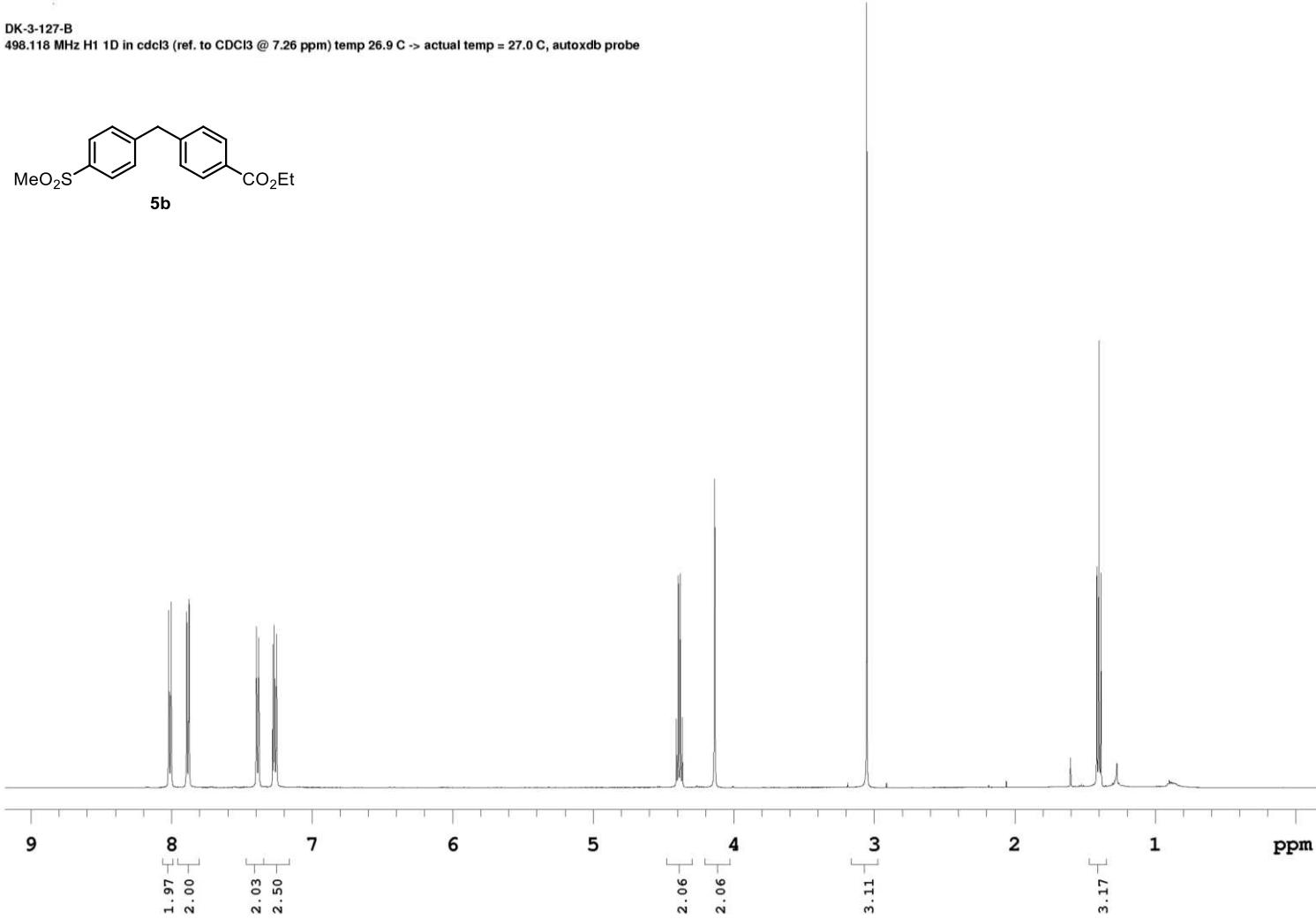
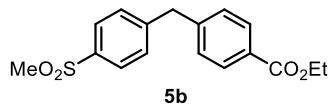
Recorded on: ibd5, Mar 1 2018
Pulse Sequence: s2pul

Sweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.43

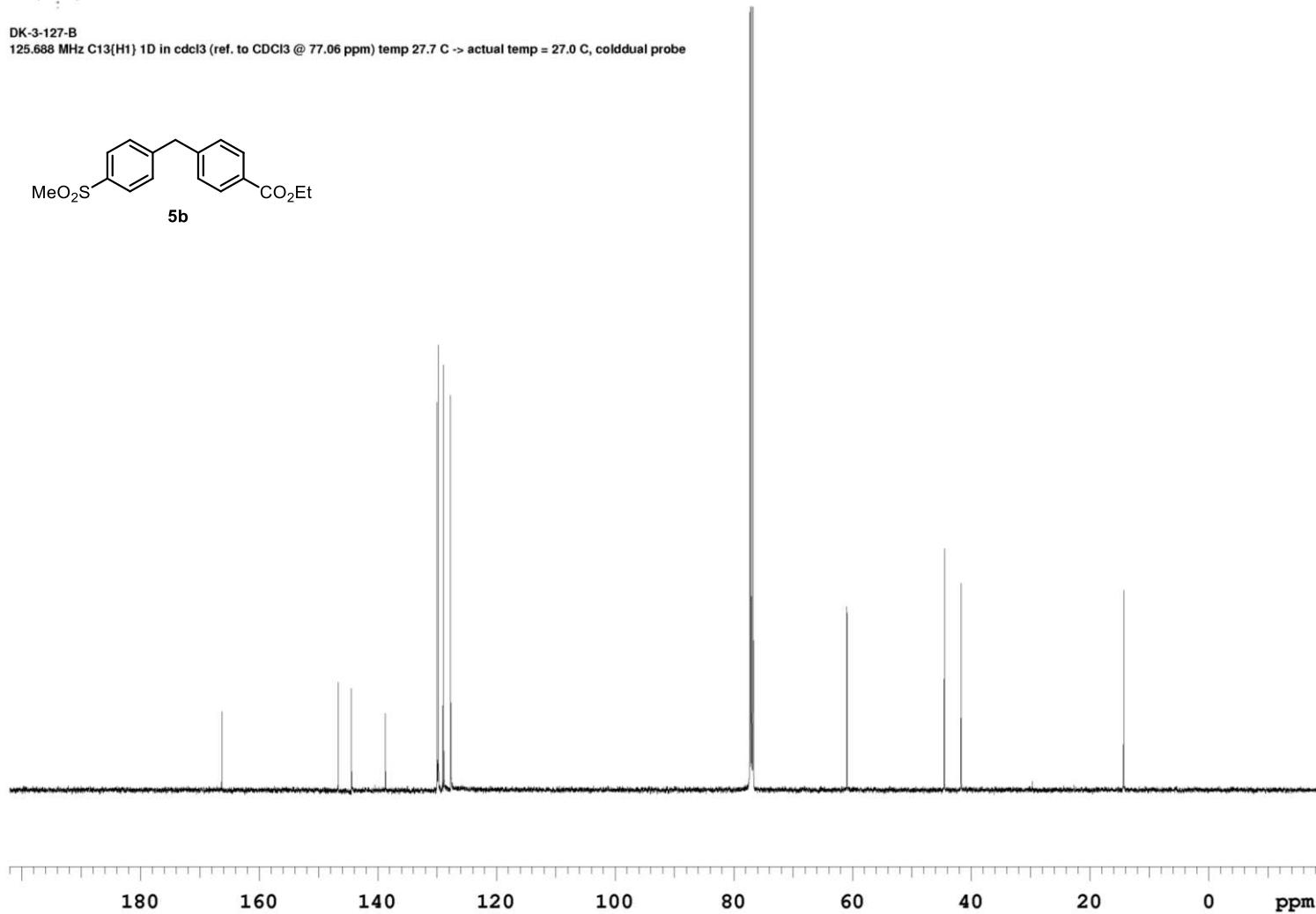
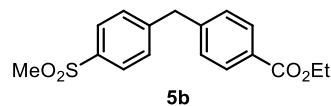
Relaxation Delay(s): 0.1
Completed Scans 16

DK-3-127-B
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe



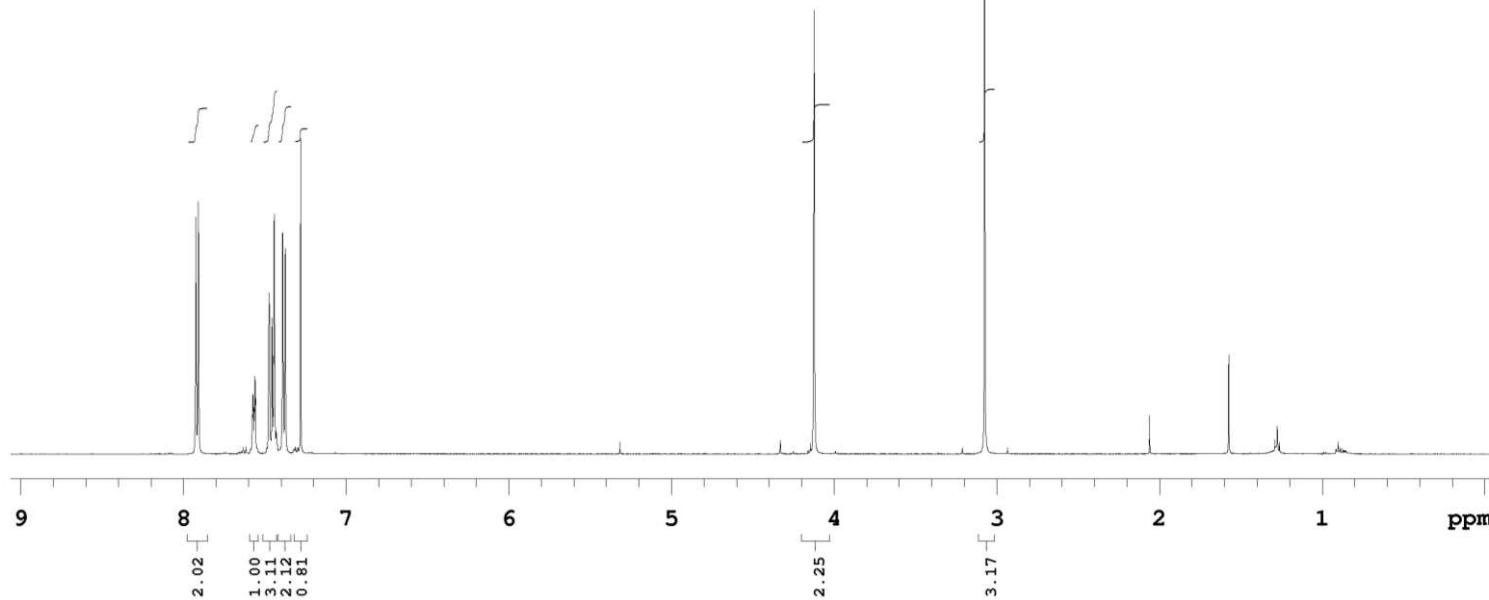
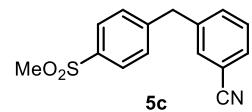


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Recorded on: u500, Mar 1 2018
Pulse Sequence: s2pulSweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26Acquisition Time(s): 1
Hz per mm(Hz/mm): 115.89Relaxation Delay(s): 1
Completed Scans 120DK-3-127-B
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, coldlual probe

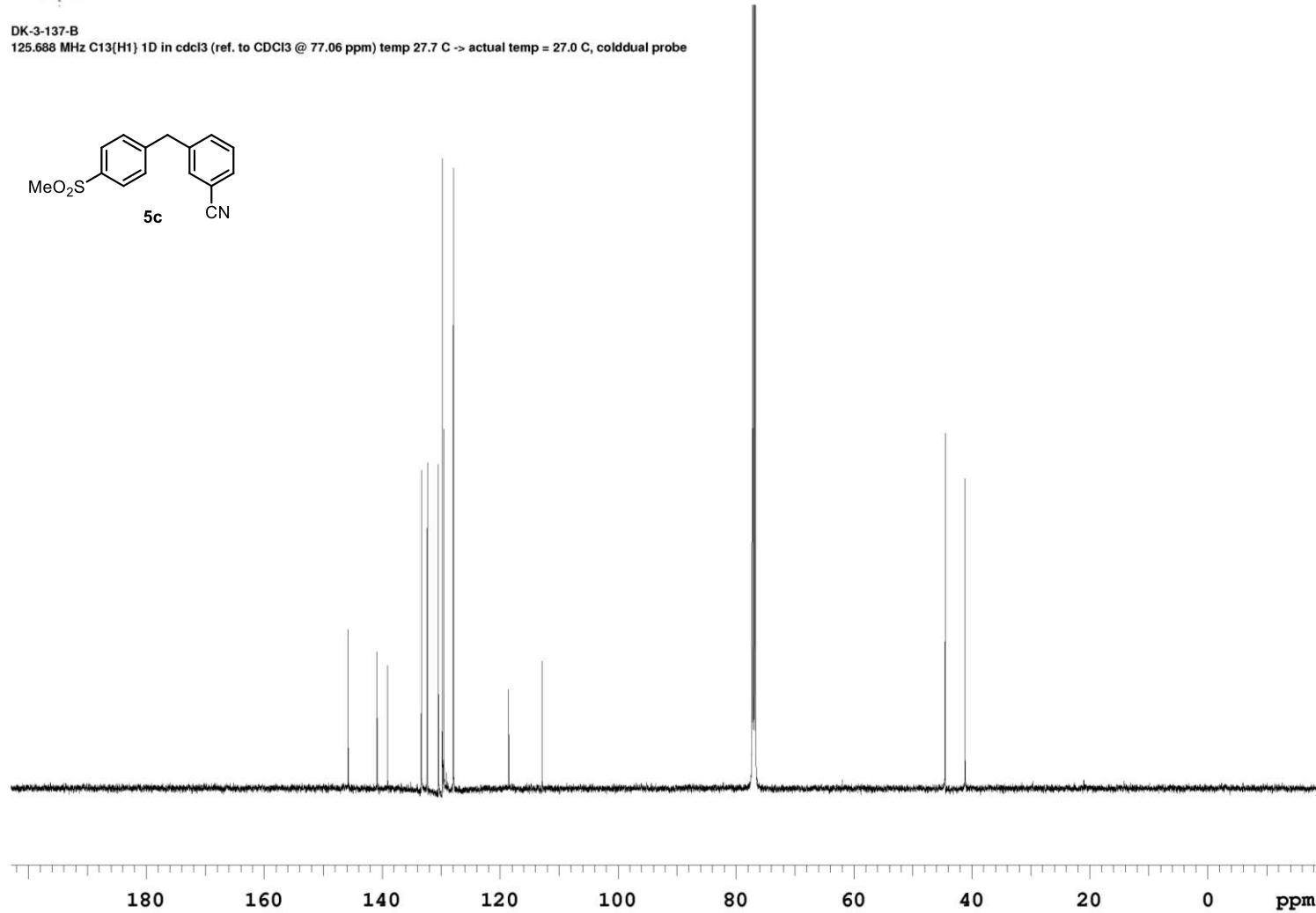
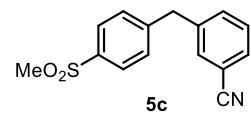


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Recorded on: ibd5, Mar 3 2018
Pulse Sequence: s2pulSweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.02Relaxation Delay(s): 0.1
Completed Scans: 16DK-3-137-B
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe

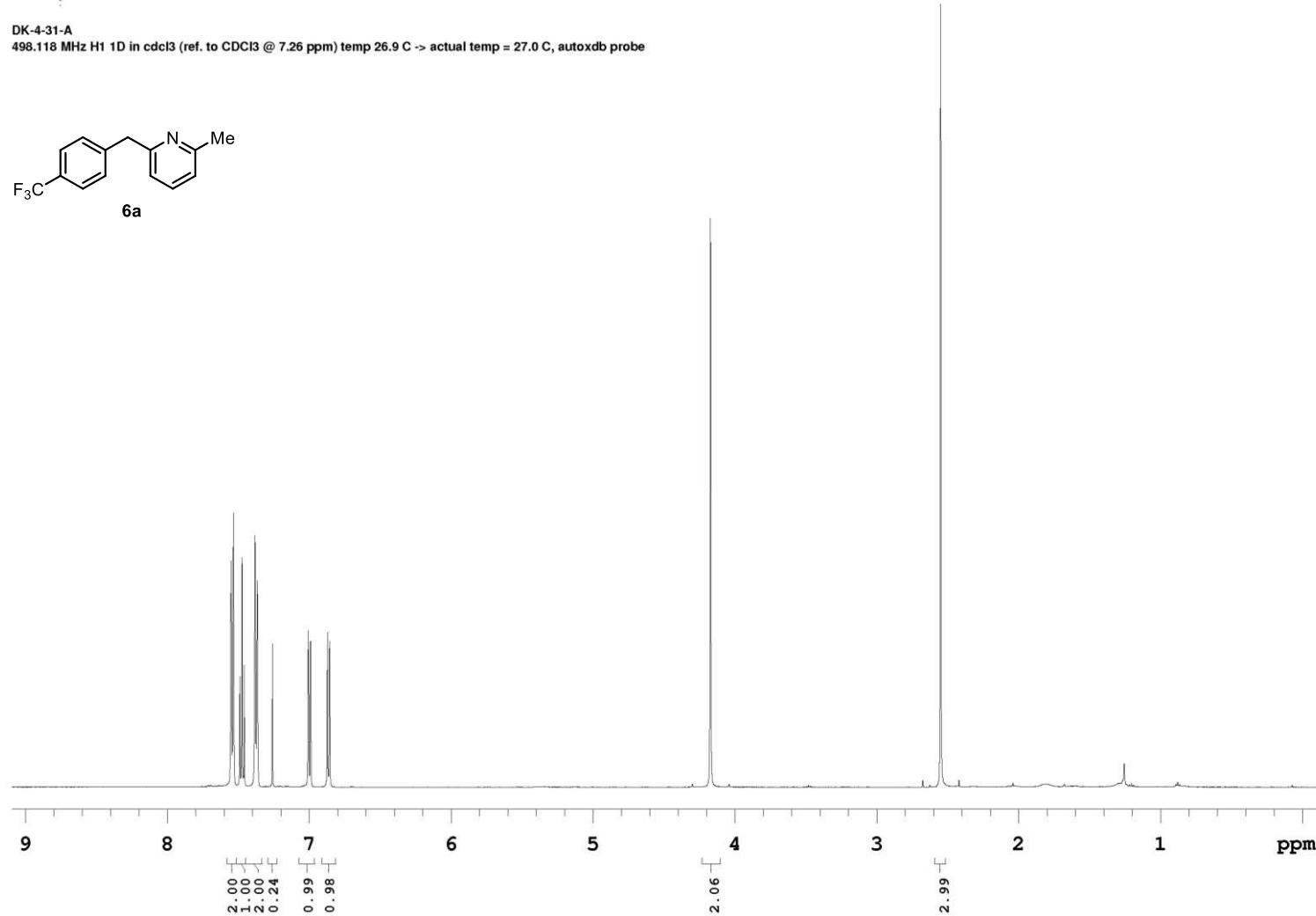
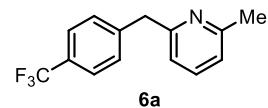


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Recorded on: u500, Mar 3 2018
Pulse Sequence: s2pulSweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26Acquisition Time(s): 1
Hz per mm(Hz/mm): 116.53Relaxation Delay(s): 1
Completed Scans 472DK-3-137-B
125.688 MHz C13(H1) 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, cold dual probe



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Recorded on: ibd5, Mar 21 2018
Pulse Sequence: s2pulSweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.19Relaxation Delay(s): 0.1
Completed Scans 16DK-4-31-A
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe



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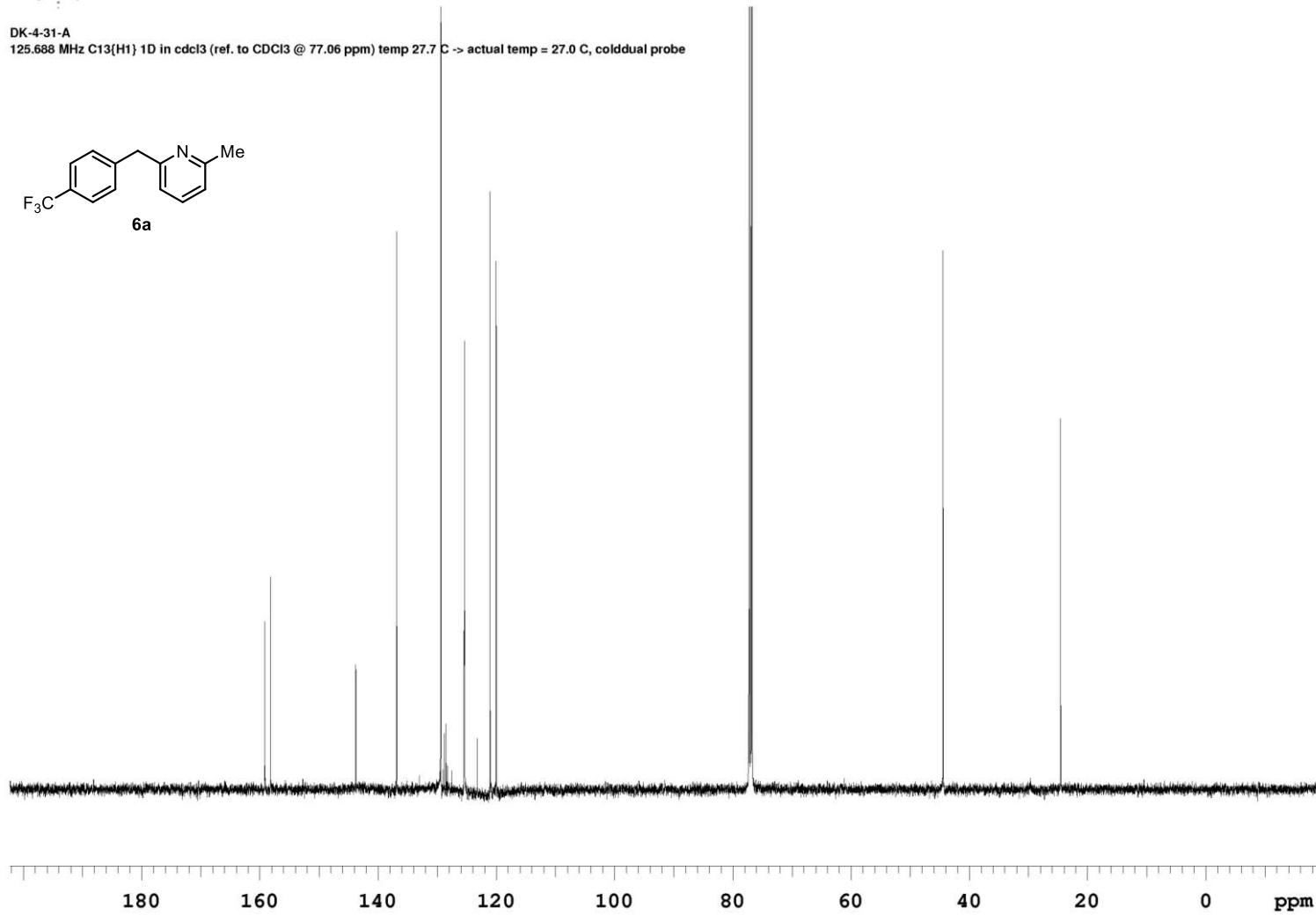
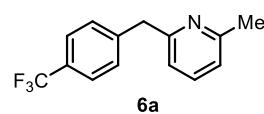
Recorded on: **u500, Mar 21 2018**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **33783.8**
Digital Res.(Hz/pt): **0.26**

Acquisition Time(s): **1**
Hz per mm(Hz/mm): **116.14**

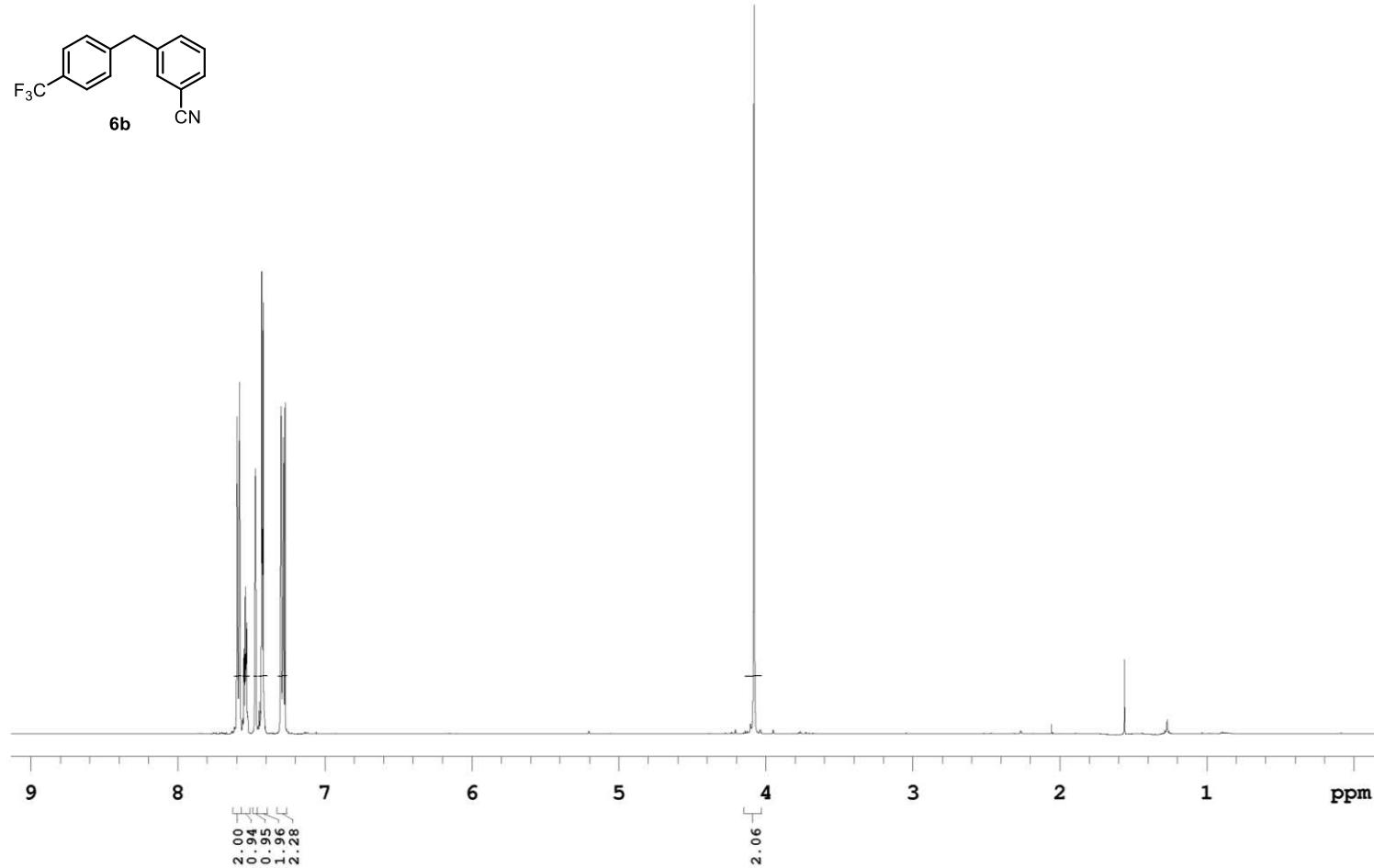
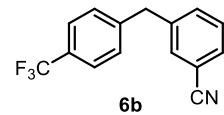
Relaxation Delay(s): **1**
Completed Scans: **68**

DK-4-31-A
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, cold dual probe





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Recorded on: u500, Mar 8 2018
Pulse Sequence: PRESATSweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.39Relaxation Delay(s): 0.1
Completed Scans: 8DK-3-151-B
499.797 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 27.7 C -> actual temp = 27.0 C, coldual probe



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Recorded on: u500, Mar 8 2018

Sweep Width(Hz): 33783.8

1

Relaxation Delay(s): 1

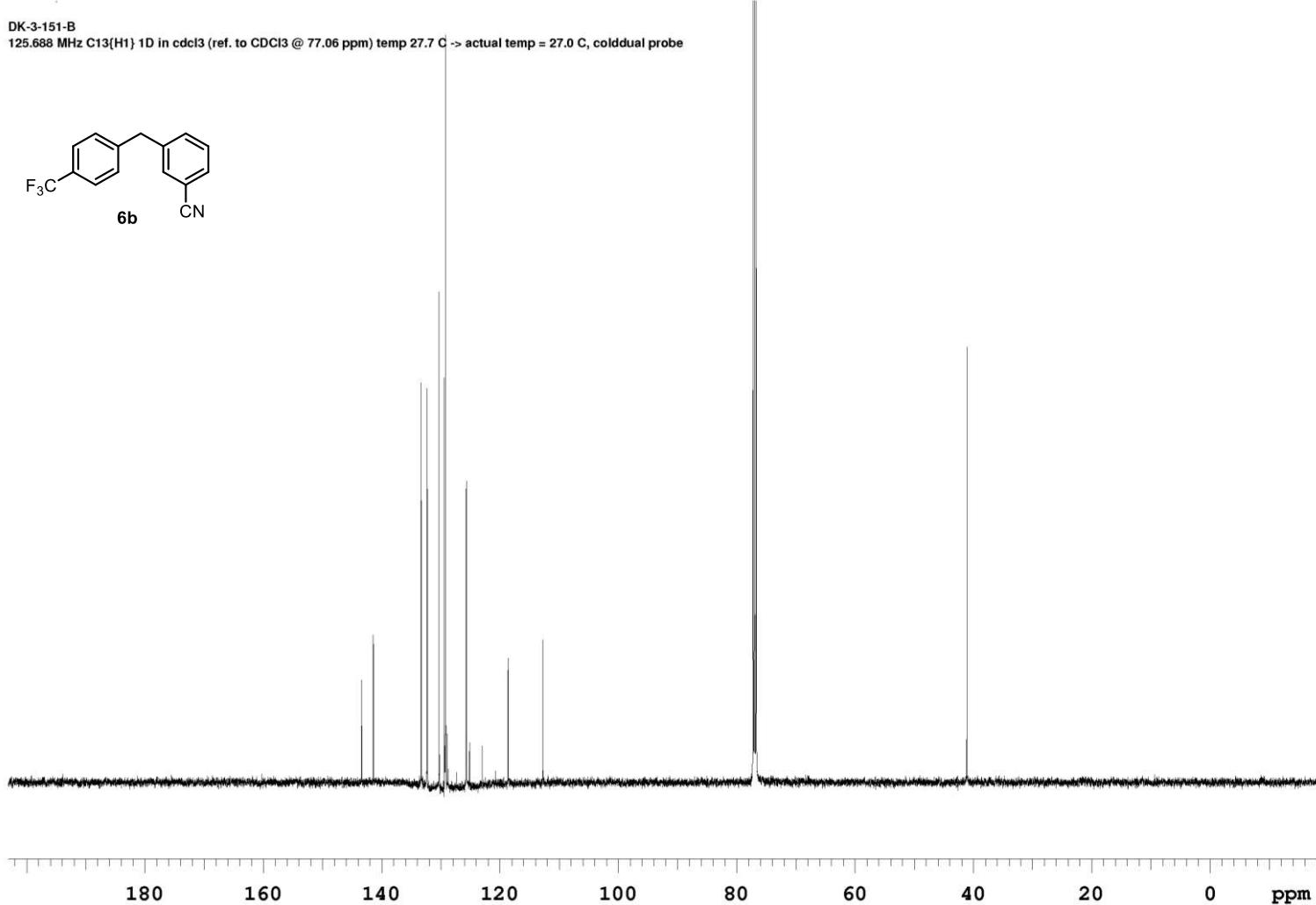
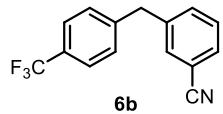
Pulse Sequence: s2pul

Digital Res.(Hz/pt): 0.26

Acquisition Time(s): Hz per mm(Hz/mm): 115.98

Completed Scans 92

DK-3-151-B
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, colddual probe





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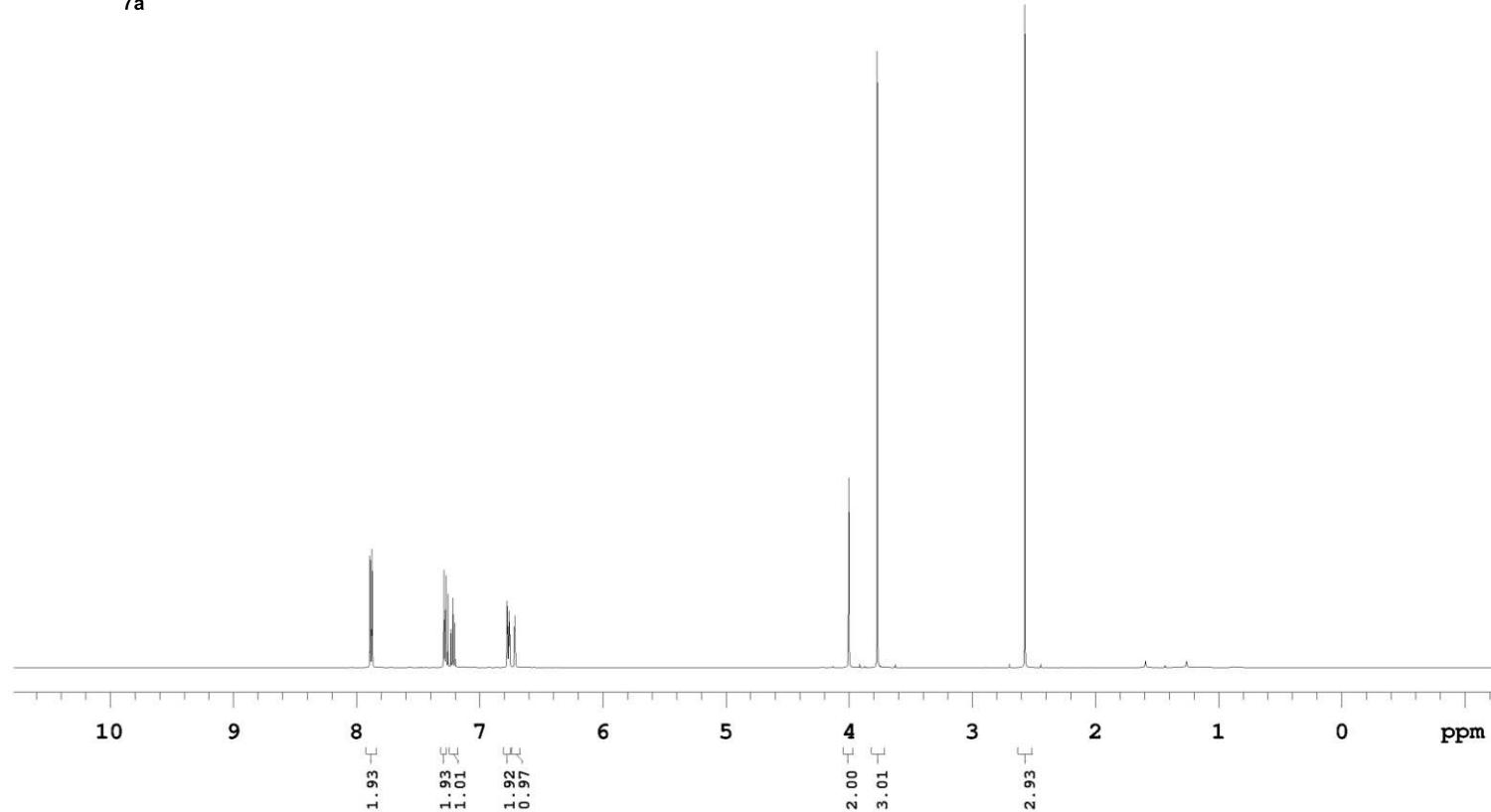
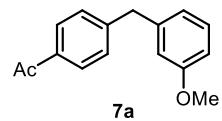
Recorded on: u500, Mar 22 2018
Pulse Sequence: PRESAT

Sweep Width(Hz): 6009.62
Digital Res.(Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 25.04

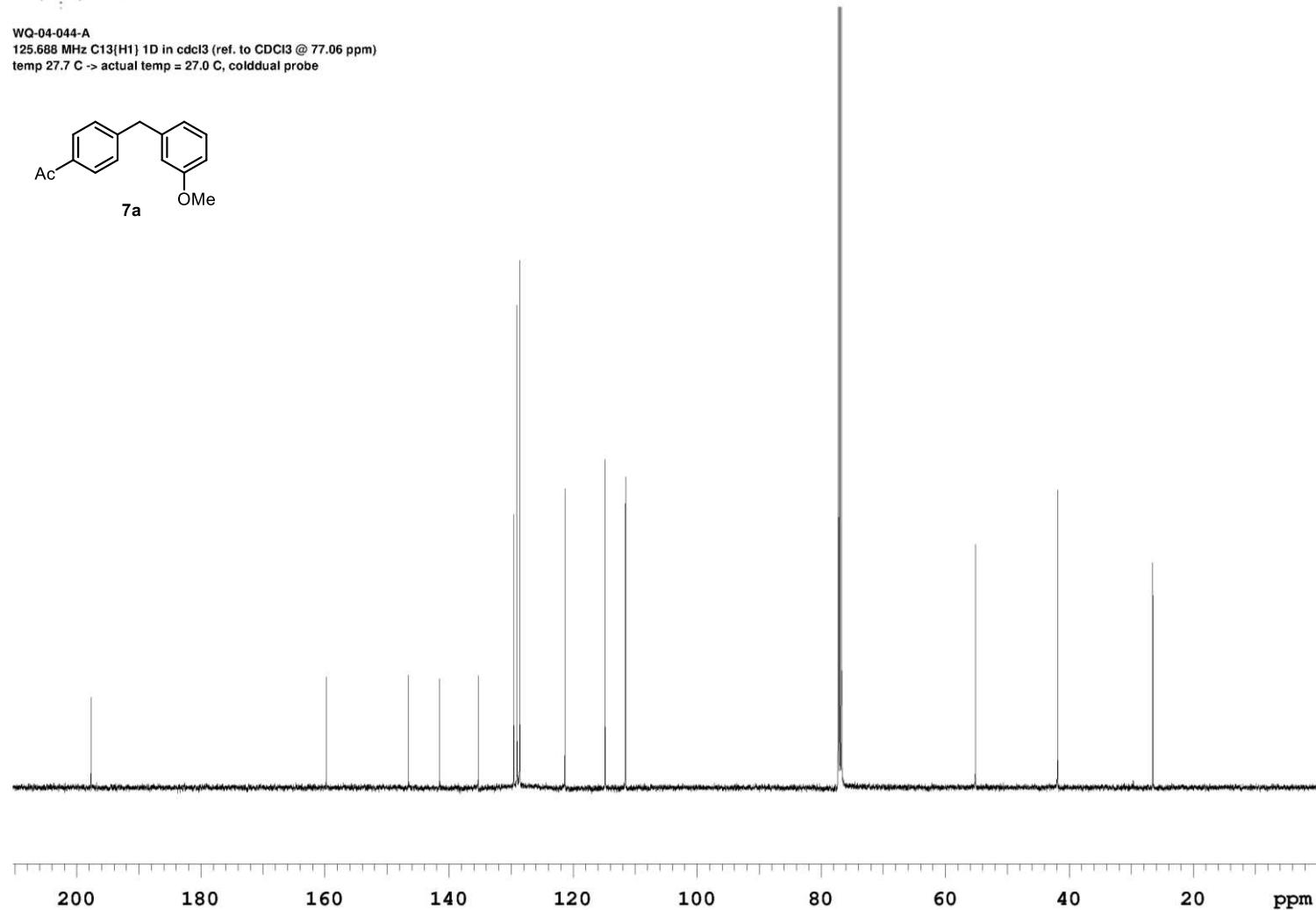
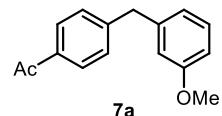
Relaxation Delay(s): 0.1
Completed Scans 4

WQ-04-044-A
499.797 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe





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Recorded on: u500, Mar 22 2018
Pulse Sequence: s2pulSweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26Acquisition Time(s): 1
Hz per mm(Hz/mm): 110.41Relaxation Delay(s): 1
Completed Scans 76WQ-04-044-A
125.688 MHz C13{H1} 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm)
temp 27.7 C -> actual temp = 27.0 C, colddual probe



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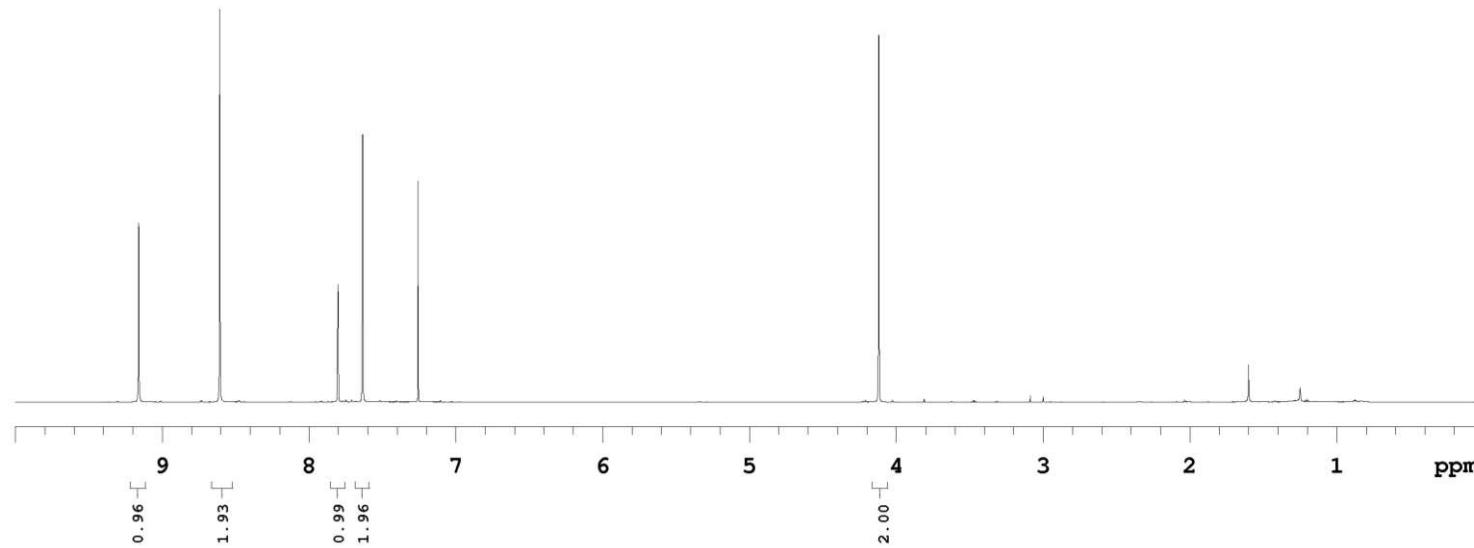
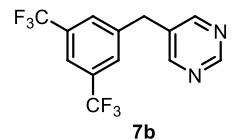
Recorded on: v700, Mar 22 2018
Pulse Sequence: PRESAT

Sweep Width(Hz): 8389.26
Digital Res.(Hz/pt): 0.13

Acquisition Time(s): 5
Hz per mm(Hz/mm): 29.23

Relaxation Delay(s): 0.1
Completed Scans 8

Wenyu, WQ-04-044-F
699.762 MHz H1 1D in *cdcl*3 (ref. to *CDCI*3 @ 7.26 ppm)
temp 27.5 C -> actual temp = 27.0 C, coldid probe





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Recorded on: v700, Mar 22 2018

Sweep Width(Hz): 48076.9

Acquisition Time(s): 1

Relaxation Delay(s): 1

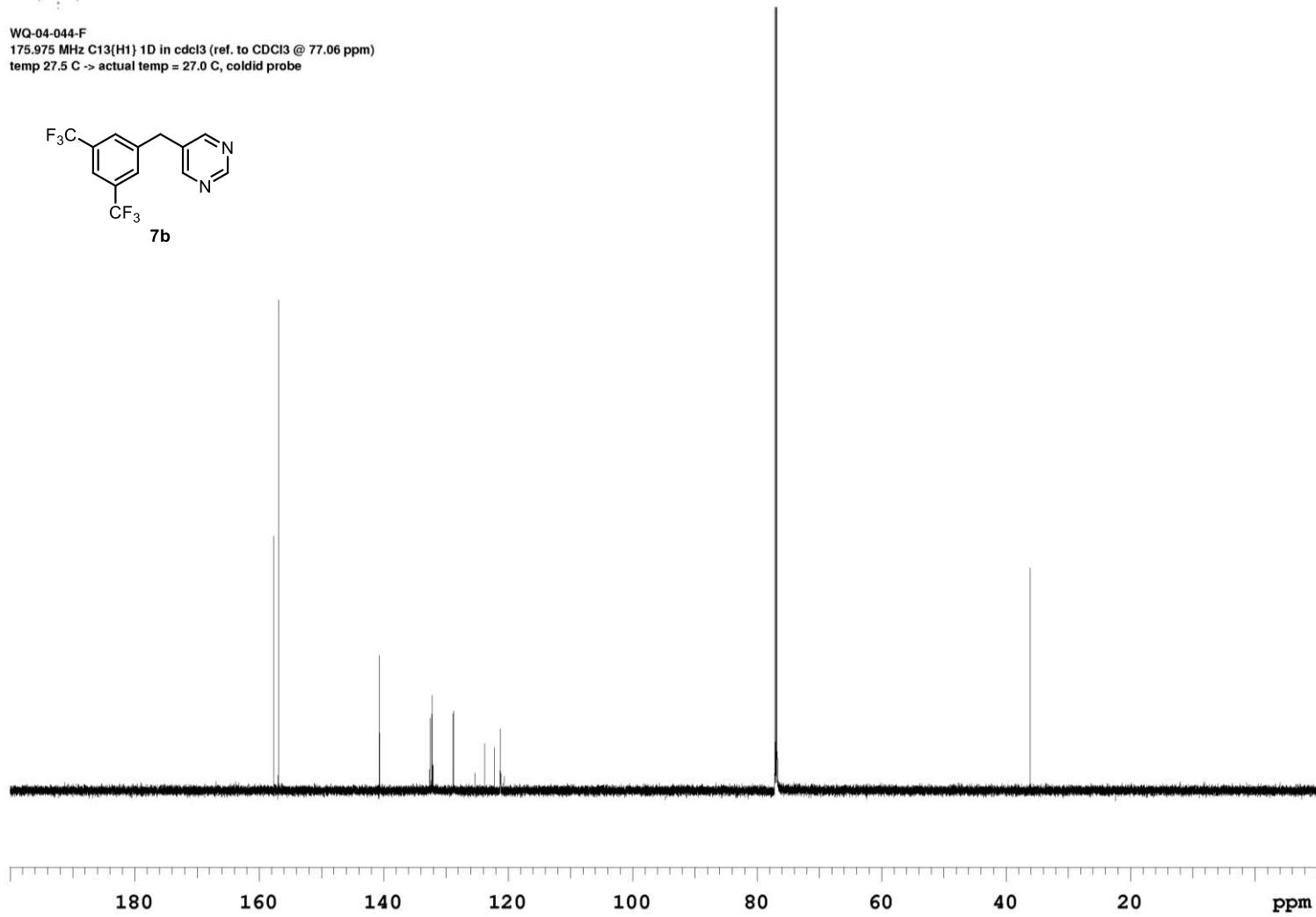
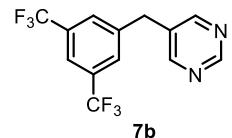
Pulse Sequence: s2pul

Digital Res.(Hz/pt): 0.37

Hz per mm(Hz/mm): 154.27

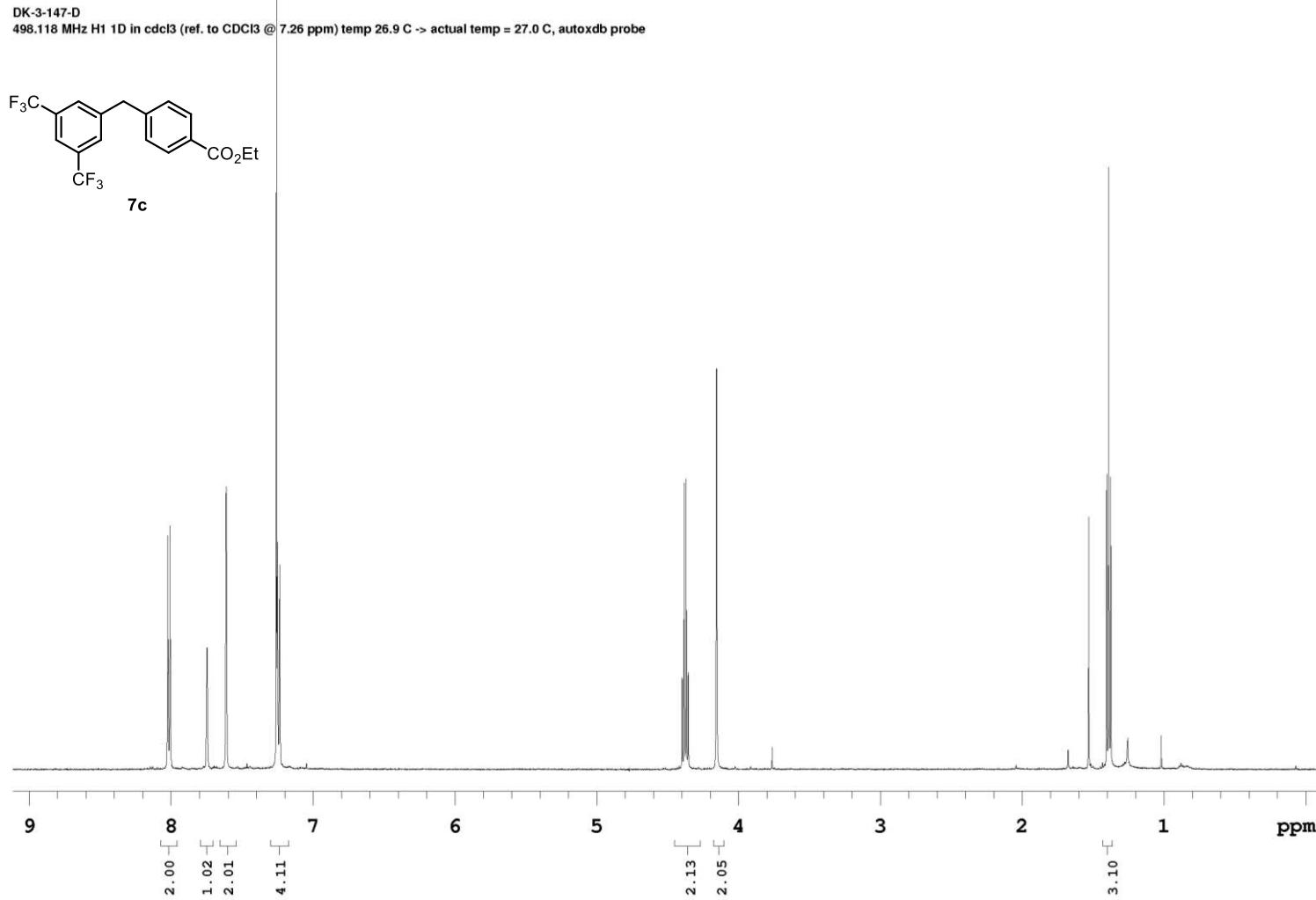
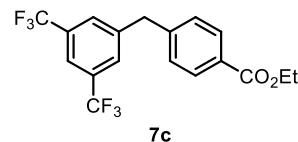
Completed Scans 256

WQ-04-044-F
175.975 MHz C13(H1) 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm)
temp 27.5 C -> actual temp = 27.0 C, coldid probe





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Recorded on: ibd5, Mar 6 2018
Pulse Sequence: s2pulSweep Width(Hz): 6000.6
Digital Res.(Hz/pt): 0.09Acquisition Time(s): 5
Hz per mm(Hz/mm): 19.19Relaxation Delay(s): 0.1
Completed Scans 8DK-3-147-D
498.118 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm) temp 26.9 C -> actual temp = 27.0 C, autoxdb probe



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Recorded on: u500, Mar 6 2018
Pulse Sequence: s2pulSweep Width(Hz): 33783.8
Digital Res.(Hz/pt): 0.26Acquisition Time(s): 1
Hz per mm(Hz/mm): 115.43Relaxation Delay(s): 1
Completed Scans: 256DK-3-147-D
125.688 MHz C13(H1) 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm) temp 27.7 C -> actual temp = 27.0 C, coldual probe