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## General Considerations

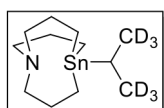
All reactions were carried out in oven or flame-dried glassware under dry nitrogen atmosphere using standard Schlenk techniques or in a glove box. 1,2-Dichloroethane and  $\text{CD}_2\text{Cl}_2$  were distilled over  $\text{CaH}_2$  and then degassed via 3 freeze-pump-thaw cycles following distillation. Reactions were monitored by thin-layer chromatography on commercially prepared plates with a particle size of 60 Å. Developed plates were visualized under a UV lamp (254 nm), or stained with ceric ammonium molybdate. Flash chromatography was performed using 230-400 mesh silica gel.

## Characterization

Unless otherwise noted,  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for all adduct products were obtained in  $\text{CDCl}_3$  at 300 and 75 MHz, respectively. Chemical shifts are reported in parts per million (ppm,  $\delta$ ) relative to tetramethylsilane (TMS) as an external standard. Proton and carbon spectra were calibrated against the solvent residual peak [ $\text{CHCl}_3$  (7.24 ppm) and  $\text{CDCl}_3$  (77.0 ppm)], [ $\text{CH}_2\text{Cl}_2$  (5.32 ppm) and  $\text{CD}_2\text{Cl}_2$  (53.8 ppm)], and in case of 1,2-dichloroethane against known solvent resonance [ $^1\text{H}$  (3.72 ppm) and  $^{13}\text{C}$  (43.6 ppm)].  $^{11}\text{B}$  and  $^{119}\text{Sn}$  NMR spectra of tricarbostannatranes were recorded on Bruker Avance-300 ( $^{11}\text{B}$ : 96 MHz,  $^{119}\text{Sn}$ : 112 MHz) with  $^1\text{H}$  decoupling in 1,2-dichloroethane calibrated against external  $\text{BF}_3\cdot\text{OEt}_2$  and  $\text{Me}_4\text{Sn}$ , respectively. The spectral references (sr) which were obtained from the external standards, were used to calibrate all  $^{119}\text{Sn}$  NMR and  $^{11}\text{B}$  NMR chemical shifts. Spectral reference values of  $-171.61$  Hz and  $-5.13$  Hz were used to calibrate  $^{119}\text{Sn}$  and  $^{11}\text{B}$  chemical shifts in 1,2-dichloroethane, respectively. Abbreviations used to define NMR spectral multiplicities are as follows: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; br = broad. High resolution mass spectra (ESI) were run at the University of Waterloo Mass Spectrometry facility. Fragment signals are given in mass per charge number (m/z).

The following compounds were prepared according to literature procedures: 5-(*iso*-propyl)-1-aza-5-stannabicyclo[3.3.3]undecane,<sup>1</sup> 5-benzylidene-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6a**),<sup>2</sup> 5-(4-methoxybenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6b**),<sup>3</sup> 5-(4-chlorobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6c**),<sup>4</sup> 1,3-dimethyl-5-(4-nitrobenzylidene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6m**),<sup>5</sup> Other reagents were purchased from commercial suppliers and used without further purification.

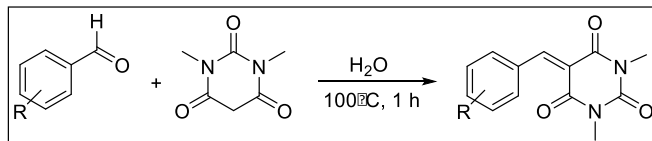
### 5-(Propan-2-yl-1,1,1,3,3,3-*d*<sub>6</sub>)-1-aza-5-stannabicyclo[3.3.3]undecane (2-*d*<sub>6</sub>)



(Propan-2-yl-1,1,1,3,3,3-*d*<sub>6</sub>)magnesium bromide reagent (2.0 M in diethyl ether) (2 equiv.) was synthesized from 2-bromopropane-1,1,1,3,3,3-*d*<sub>6</sub> (99% atom D),<sup>6</sup> and was added

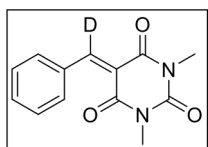
dropwise to a suspension of 5-chloro-1-aza-5-stannabicyclo[3.3.3]undecane (235 mg, 0.798 mmol) in anhydrous THF at  $-78^{\circ}\text{C}$ . The resulting mixture was stirred at  $-78^{\circ}\text{C}$  for 3 hours, allowed to warm to room temperature, and stirred overnight. The reaction mixture was poured into a separatory funnel containing a mixture of  $\text{Et}_2\text{O}$  and water. The layers were partitioned, and the organic layer was washed with brine, dried over  $\text{MgSO}_4$ , and filtered. Solvent was removed under reduced pressure to provide the crude product. A yellow oil (259 mg, 84 % yield) was isolated and was used without further purification;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.33 (t,  $J = 5.4$  Hz, 6H), 1.62 (m, 6H), 1.45 (m, 7H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  54.7, 23.4, 16.8, 4.4;  $^2\text{H}$  NMR ( $\text{CHCl}_3$ , 46 MHz)  $\delta$  1.00 (brd,  $J = 0.1$  Hz). HRMS (+ESI)  $m/z$  calcd. for  $\text{C}_{12}\text{H}_{19}^2\text{H}_6\text{NSn}$  (M) $^+$ : 309.13801. Found: 309.15384.

### General Experimental Procedure A - Synthesis of Benzylidene 1,3-Dimethylbarbituric Acids (6a-d<sub>1</sub>, 6d-6l)



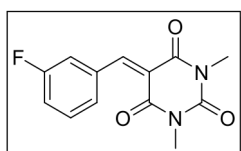
To a stirred solution of the 1,3-dimethylbarbituric acid (1.56 g, 10.0 mmol) in water (40 ml) was added the corresponding benzaldehyde (10.0 mmol) in one portion at ambient temperature. After refluxing for an hour, the resulting suspension was filtered and the solid was collected and was dried under vacuum. Products **6a-d<sub>1</sub>**, **6d-6l** were used without further purification unless otherwise noted.

#### 1,3-Dimethyl-5-(phenylmethylene-*d*)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (6a-d<sub>1</sub>)



Prepared according to General Procedure A from 1,3-dimethylbarbituric acid (454 mg, 2.90 mmol), water (12 ml), and benzaldehyde- $\alpha$ -*d*<sub>1</sub> (312 mg, 2.90 mmol); isolated as a yellow solid (636 mg, 89% yield);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.03 (d,  $J = 7.1$  Hz, 2H), 7.44 (m, 3H), 3.37 (s, 3H), 3.32 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  162.4, 160.3, 158.6 (t), 151.1, 133.4, 132.9, 132.4, 128.1, 117.3, 29.0, 28.3;  $^2\text{H}$  NMR ( $\text{CHCl}_3$ , 46 MHz)  $\delta$  8.61 (brs). HRMS (ESI)  $m/z$  calcd for  $\text{C}_{13}\text{H}_{12}^2\text{HN}_2\text{O}_3$  (M+H) $^+$ : 246.09835; Found: 246.09835.

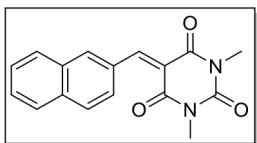
#### 5-(3-Fluorobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (6d).



Prepared according to General Procedure A from 4-fluorobenzaldehyde (1.24 g, 10.0 mmol); reaction was purified by recrystallization from MeOH and isolated as a white solid (2.12 g, 81% yield); M.p.  $143$ - $145^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.49 (s, 1H), 7.89 (d,  $J = 10.2$  Hz, 1H), 7.66 (d,  $J = 7.8$  Hz, 1H), 7.41 (q,  $J = 5.7$  Hz, 1H), 7.21 (td,  $J = 8.3, 2.7$  Hz, 1H), 3.41 (s, 3H), 3.36 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  162.1, 162.0 (d,  $J_{\text{C-F}} = 245.0$

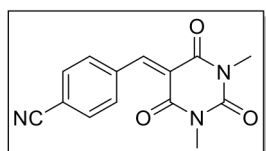
Hz), 160.0, 157.1 (d,  $J_{C-F}$  = 2.3 Hz), 151.0, 134.5 (d,  $J_{C-F}$  = 8.5 Hz), 129.6 (d,  $J_{C-F}$  = 8.0 Hz), 129.3 (d,  $J_{C-F}$  = 2.9 Hz), 119.4 (d,  $J_{C-F}$  = 5.7 Hz), 119.3 (d,  $J_{C-F}$  = 50.2 Hz), 118.6, 29.0, 28.4. HRMS (ESI)  $m/z$  calcd for  $C_{13}H_{12}O_3N_2F$  (M+H)<sup>+</sup>: 263.08320; Found: 263.08249.

### 1,3-Dimethyl-5-(naphthalen-2-ylmethylene)pyrimidine-2,4,6(1H,3H,5H)-trione (6e).



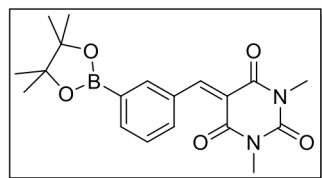
Prepared according to General Procedure A from 2-naphthaldehyde (1.56 g, 10.0 mmol); isolated as a pale yellow solid (2.56 g, 87% yield); M.p. 206-207 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.69 (s, 1H), 8.57 (s, 1H), 8.13 (d,  $J$  = 8.7 Hz, 1H), 7.92 (d,  $J$  = 7.8 Hz, 1H), 7.84 (d,  $J$  = 8.7 Hz, 2H), 3.41 (s, 3H), 3.38 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 162.6, 160.4, 159.2, 151.3, 136.4, 135.3, 132.5, 130.3, 129.6, 129.0, 128.7, 127.7, 127.6, 126.7, 117.2, 29.1, 28.4. HRMS (ESI)  $m/z$  calcd for  $C_{17}H_{15}N_2O_3$  (M+H)<sup>+</sup>: 295.10827; Found: 295.10764.

### 4-((1,3-Dimethyl-2,4,6-trioxotetrahydropyrimidin-5(2H)-ylidene)methyl)benzonitrile (6f).



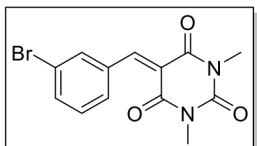
Prepared according to General Procedure A from 4-formylbenzonitrile (1.31 g, 10.0 mmol); isolated as a white solid (2.40 g, 89% yield). M.p. 185-186 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.50 (s, 1H), 7.91 (d,  $J$  = 8.1 Hz, 2H), 7.70 (d,  $J$  = 8.1 Hz, 2H), 3.41 (s, 3H), 3.33 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 161.5, 159.8, 155.8, 150.9, 137.1, 132.0, 131.7, 120.3, 118.1, 114.8, 29.2, 28.5. HRMS (ESI)  $m/z$  calcd for  $C_{14}H_{11}O_3N_3$  (M+H)<sup>+</sup>: 270.08787; Found: 270.08701.

### 1,3-Dimethyl-5-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (6g).



Prepared according to General Procedure A from 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde (2.32 g, 10.0 mmol); isolated as a white solid (2.36 g, 64% yield); M.p. 189-190 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.59 (s, 1H), 8.34 (d,  $J$  = 8.1 Hz, 1H), 8.19 (s, 1H), 7.92 (d,  $J$  = 7.2 Hz, 1H), 7.45 (t,  $J$  = 7.8 Hz, 1H), 3.39 (s, 3H), 3.34 (s, 3H), 1.33 (s, 12H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 162.4, 160.3, 159.5, 151.3, 140.5, 139.1, 135.0, 132.2, 127.6, 117.5, 84.1, 29.0, 28.4, 24.9. HRMS (ESI)  $m/z$  calcd for  $C_{19}H_{24}O_5N_2B$  (M+H)<sup>+</sup>: 371.17783. Found: 371.17722.

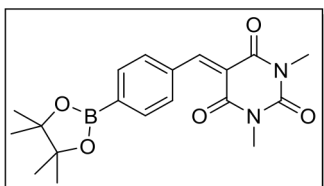
### 5-(3-Bromobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (6h).



Prepared according to General Procedure A from 3-bromobenzaldehyde (1.85 g, 10.0 mmol); recrystallized from MeOH and isolated as a white solid (2.77 g, 86% yield); M.p. 151-153 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.44 (s, 1H), 8.16 (s, 1H), 7.87 (d,  $J$

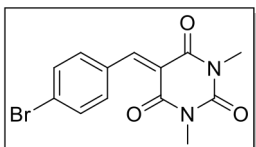
= 7.8 Hz, 1H), 7.62 (d,  $J$  = 8.1 Hz, 1H), 7.31 (t,  $J$  = 7.8 Hz, 1H), 3.40 (s, 3H), 3.35 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  162.0, 160.0, 157.0, 151.0, 135.2, 135.2, 134.5, 131.4, 129.6, 122.2, 118.8, 29.1, 28.5. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{13}\text{H}_{12}\text{O}_3\text{N}_2\text{Br}$  ( $\text{M}+\text{H}$ ) $^+$ : 323.00313; Found: 323.00320.

**1,3-Dimethyl-5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (6i).**



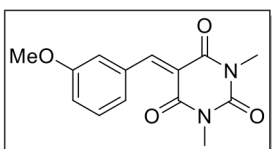
Prepared according to General Procedure A from 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde (2.32 g, 10.0 mmol); isolated as a white solid (1.96 g, 53% yield); M.p. 195-197 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.55 (s, 1H), 7.92 (d,  $J$  = 7.8 Hz, 2H), 7.86 (d,  $J$  = 7.8 Hz, 2H), 3.40 (s, 3H), 3.34 (s, 3H), 1.33 (s, 12H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  162.3, 160.1, 159.1, 151.2, 135.1, 134.3, 131.7, 118.2, 84.1, 29.0, 28.4, 24.8. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{19}\text{H}_{24}\text{O}_5\text{N}_2\text{B}$  ( $\text{M}+\text{H}$ ) $^+$ : 371.17783. Found: 371.17685.

**5-(4-Bromobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (6j).**



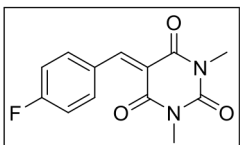
Prepared according to General Procedure A from 4-bromobenzaldehyde (1.85 g, 10.0 mmol); isolated as a white solid (2.77 g, 86% yield); M.p. 175-176 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.43 (s, 1H), 7.90 (d,  $J$  = 8.4 Hz, 2H), 7.56 (d,  $J$  = 8.7 Hz, 2H), 3.38 (s, 3H), 3.34 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  162.2, 160.3, 157.5, 151.1, 134.8, 131.6, 131.4, 128.0, 117.9, 29.1, 28.4. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{13}\text{H}_{12}\text{O}_3\text{N}_2\text{Br}$  ( $\text{M}+\text{H}$ ) $^+$ : 323.00313; Found: 323.00311.

**5-(3-Methoxybenzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (6k).**



Prepared according to General Procedure A from 3-methoxybenzaldehyde (1.36 mg, 10.0 mmol); isolated as a yellow solid (2.47 g, 90% yield); M.p. 139-141 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.52 (s, 1H), 7.76 (s, 1H), 7.55 (d,  $J$  = 7.6 Hz, 1H), 7.35 (t,  $J$  = 7.8 Hz, 1H), 7.06 (dd,  $J$  = 8.3, 2.7 Hz, 1H), 3.84 (s, 3H), 3.40 (s, 3H), 3.35 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  162.5, 160.3, 159.2, 159.1, 151.2, 133.8, 129.2, 126.6, 119.4, 117.7, 117.6, 55.4, 29.1, 28.5. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{14}\text{H}_{15}\text{O}_4\text{N}_2$  ( $\text{M}+\text{H}$ ) $^+$ : 275.10318; Found: 275.10260.

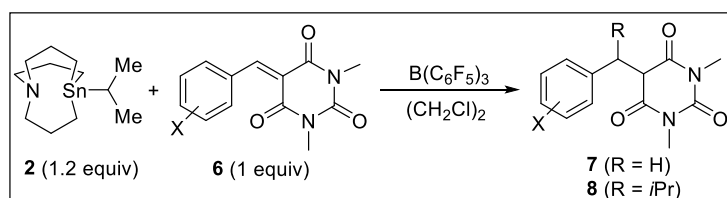
**5-(4-Fluorobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (6l).**



Prepared according to General Procedure A from 4-fluorobenzaldehyde (1.24 g, 10.0 mmol); isolated as a pale yellow solid (2.04 g, 78% yield). M.p. 169-171 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.50 (s, 1H), 8.20-8.15 (m, 2H), 7.16-7.09 (m, 2H), 3.40 (s, 3H),

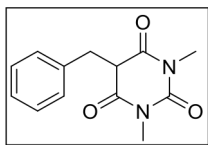
3.36 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  165.3 (d,  $^1J_{\text{C-F}} = 256.0$  Hz), 162.4, 160.4, 157.7, 151.1, 136.7 (d,  $^3J_{\text{C-F}} = 9.3$  Hz), 128.8 (d,  $^4J_{\text{C-F}} = 3.1$  Hz), 116.9, 115.5 (d,  $^2J_{\text{C-F}} = 21.6$  Hz), 29.0, 28.3. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{13}\text{H}_{12}\text{O}_3\text{N}_2\text{F}$  ( $\text{M}+\text{H}$ ) $^+$ : 263.08320; Found: 263.08237.

### General Experimental Procedure B - $\text{B}(\text{C}_6\text{F}_5)_3$ -Catalyzed Transfer 1,4-Hydrostannylation



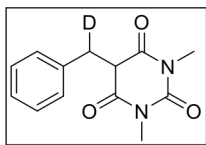
In a J. Young NMR tube, benzylidene 1,3-dimethylbarbituric acid (0.100 mmol) was added to a solution of 5-isopropyl-1-aza-5-stannabicyclo[3.3.3]undecane (36.2 mg, 0.120 mmol) and tris(pentafluorophenyl)borane (8.0 mg, 0.015 mmol) in 1 mL of 1,2-dichloroethane in a glove box and the mixture was put in a preheated oil bath at 95 °C for 36 h. All volatiles were evaporated under vacuum and the product was purified by flash chromatography (EtOAc:pentane) on silica gel. In these reactions, compounds **8a-I** were isolated as byproducts.

#### 5-Benzylidene-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7a**).



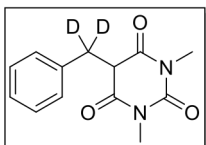
Prepared according to General Procedure B from **6a** (24.4 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:5 to 1:4) and the product was isolated as a white solid (22.4 mg, 91% yield); M.p. 115-116 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.23-7.21 (m, 3H), 7.03-6.99 (m, 2H), 3.75 (t,  $J = 4.8$  Hz, 1H), 3.45 (d,  $J = 4.5$  Hz, 2H), 3.10 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  168.3, 151.0, 135.1, 128.8, 128.6, 127.8, 50.7, 37.9, 28.2. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{13}\text{H}_{15}\text{O}_3\text{N}_2$  ( $\text{M}+\text{H}$ ) $^+$ : 247.10827; Found: 247.10773; 1,3-Dimethyl-5-(2-methyl-1-phenylpropyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8a**): Isolated as a white solid (2.3 mg, 8% yield); M.p. 88-89 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.22-7.19 (m, 3H), 6.91-6.88 (m, 2H), 3.91 (d,  $J = 3.6$  Hz, 1H), 3.06 (s, 3H), 3.00 (dd,  $J = 11.3, 3.6$  Hz, 2H), 2.94 (s, 3H), 2.53-2.41 (m, 1H), 1.31 (d,  $J = 6.6$  Hz, 3H), 0.72 (d,  $J = 6.6$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  169.5, 167.3, 150.9, 138.0, 128.4, 128.1, 127.6, 59.3, 52.0, 28.6, 28.0, 27.8, 21.5, 21.3. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{16}\text{H}_{21}\text{O}_3\text{N}_2$  ( $\text{M}+\text{H}$ ) $^+$ : 289.15522; Found: 289.15463.

### 1,3-Dimethyl-5-(phenylmethyl-*d*)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7a-*d*<sub>1</sub>).



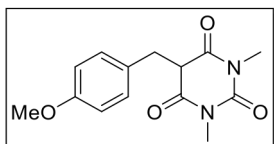
In a vial, **6a** (24.4 mg, 0.100 mmol) was added to a solution of 5-(propan-2-yl-1,1,1,3,3,3-*d*<sub>6</sub>)-1-aza-5-stannabicyclo[3.3.3]undecane (30.0 mg, 0.0974 mmol) and tris(pentafluorophenyl)borane (52.0 mg, 0.102 mmol) in 1,2-dichloroethane (1 ml). After stirring for 18 hours at room temperature, all volatiles were removed and the reaction was purified eluting with EtOAc:pentane (1:5 to 1:4) and the product was isolated as a white solid (22.0 mg, 92% yield, 54% D-incorporation); M.p. 115-116 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.23-7.20 (m, 3H), 7.02-6.99 (m, 2H), 3.76-3.74 (m, 1H), 3.45-3.44 (m, 1.46 H), 3.10 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 168.3, 151.0, 135.1, 135.0, 128.8, 128.6, 127.8, 50.7, 50.6, 37.6 (t), 28.2. <sup>2</sup>H NMR (CHCl<sub>3</sub>, 46 MHz) δ 3.45. HRMS (ESI) *m/z* calcd for C<sub>13</sub>H<sub>14</sub><sup>2</sup>HO<sub>3</sub>N<sub>2</sub> (M+H)<sup>+</sup>: 248.11400; Found: 248.11369.

### 1,3-Dimethyl-5-(phenylmethyl-*d*<sub>2</sub>)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7a-*d*<sub>2</sub>).



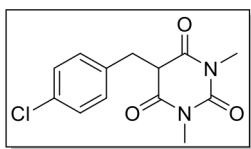
In a vial, **6a-*d*<sub>1</sub>** (24.5 mg, 0.100 mmol) was added to a solution of 5-(propan-2-yl-1,1,1,3,3,3-*d*<sub>6</sub>)-1-aza-5-stannabicyclo[3.3.3]undecane (30.0 mg, 0.0974 mmol) and tris(pentafluorophenyl)borane (52.0 mg, 0.102 mmol) in 1,2-dichloroethane (1 ml). After stirring for 18 hours at room temperature, all volatiles were removed and the reaction was purified eluting with EtOAc:pentane (1:5 to 1:4) and the product was isolated as a white solid (21.9 mg, 89% yield, 55% D-incorporation); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.24-7.21 (m, 3H), 7.03-7.00 (m, 2H), 3.76-3.75 (m, 1H), 3.44-3.41 (m, 0.45 H), 3.11 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 168.3, 151.0, 135.1, 135.0, 128.8, 128.6, 127.8, 50.62, 50.60, 37.8-36.9 (m), 28.2. <sup>2</sup>H NMR (CHCl<sub>3</sub>, 46 MHz) δ 3.44. HRMS (ESI) *m/z* calcd for C<sub>13</sub>H<sub>13</sub><sup>2</sup>H<sub>2</sub>N<sub>2</sub>O<sub>3</sub> (M+H)<sup>+</sup>: 249.12027; Found: 249.12036.

### 5-(4-Methoxybenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7b).



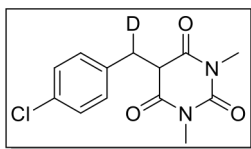
Prepared according to General Procedure B from **6b** (27.4 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a white solid (19.9 mg, 72% yield); M.p. 88-89 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 6.93 (d, *J* = 8.7 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 3.74-3.70 (m, 4H), 3.39 (d, *J* = 4.5 Hz, 2H), 3.12 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 168.4, 159.1, 151.0, 130.0, 127.0, 113.9, 55.2, 50.9, 37.1, 28.2. HRMS (ESI) *m/z* calcd for C<sub>14</sub>H<sub>17</sub>O<sub>4</sub>N<sub>2</sub> (M+H)<sup>+</sup>: 277.11883; Found: 277.11841; 5-(1-(4-Methoxyphenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8b**): Isolated as a colorless oil (6.7 mg, 21% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 6.82 (dt, *J* = 8.7, 2.7 Hz, 2H), 6.73 (dt, *J* = 9.0, 2.7 Hz, 2H), 3.88 (d, *J* = 3.6 Hz, 2H), 3.74 (s, 3H), 3.07 (s, 3H), 2.99-2.94 (m, 4H), 2.48-2.35 (m, 1H), 1.29 (d, *J* = 6.3 Hz, 3H), 0.70 (d, *J* = 6.6 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 169.7, 167.4, 159.2, 150.9, 129.9, 128.6, 113.8, 58.4, 55.2, 52.0, 28.8, 28.0, 27.9, 21.5, 21.4. HRMS (ESI) *m/z* calcd for C<sub>17</sub>H<sub>23</sub>O<sub>4</sub>N<sub>2</sub> (M+H)<sup>+</sup>: 319.16578; Found: 319.16525.

### 5-(4-Chlorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7c).<sup>7</sup>



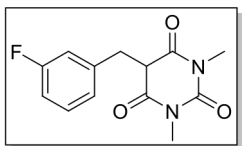
Prepared according to General Procedure B from **6c** (27.9 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a white solid (23.3 mg, 83% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.19 (d, *J* = 8.4 Hz, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 3.74 (t, *J* = 4.8 Hz, 1H), 3.44 (d, *J* = 4.8 Hz, 2H), 3.15 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 167.8, 150.9, 134.0, 133.7, 130.4, 128.8, 50.4, 36.0, 28.3; 5-(1-(4-Chlorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**8c**): Isolated as a colorless oil (4.5 mg, 14% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.19 (d, *J* = 8.1 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 3.89 (d, *J* = 3.6 Hz, 1H), 3.08-2.99 (m, 4H), 2.51-2.38 (m, 1H), 1.28 (d, *J* = 6.3 Hz, 3H), 0.69 (d, *J* = 6.6 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 169.2, 167.0, 150.7, 136.8, 133.8, 129.0, 128.7, 58.0, 51.6, 28.8, 28.1, 27.9, 21.4, 21.3. HRMS (ESI) *m/z* calcd for C<sub>16</sub>H<sub>20</sub>O<sub>3</sub>N<sub>2</sub>Cl (M+H)<sup>+</sup>: 323.11625; Found: 323.11572.

### 5-((4-Chlorophenyl)methyl-*d*)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7c-*d*<sub>1</sub>).



In a vial, **6c** (27.0 mg, 0.0969 mmol) was added to a solution of 5-(propan-2-yl-1,1,1,3,3,3-*d*<sub>6</sub>)-1-aza-5-stannabicyclo[3.3.3]undecane (30.0 mg, 0.0974 mmol) and tris(pentafluorophenyl)borane (52.0 mg, 0.102 mmol) in 1,2-dichloroethane (1 ml). After stirring for 18 hours at room temperature, all volatiles were removed and the reaction was purified eluting with EtOAc:pentane (1:5) and the product was isolated as a clear oil (23.3 mg, 86% yield, 59% D-incorporation); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.19 (d, *J* = 8.4 Hz, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 3.76-3.73 (m, 1H), 3.45-3.43 (m, 1.41H), 3.16 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 167.9, 150.9, 134.02, 133.98, 133.7, 130.5, 128.8, 50.4, 50.3, 35.7 (t), 28.3; <sup>2</sup>H NMR (CHCl<sub>3</sub>, 46 MHz) δ 3.44. HRMS (ESI) *m/z* calcd for C<sub>13</sub>H<sub>13</sub><sup>2</sup>HN<sub>2</sub>O<sub>3</sub>Cl (M+H)<sup>+</sup>: 282.07502; Found: 282.07504.

### 5-(3-Fluorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7d).

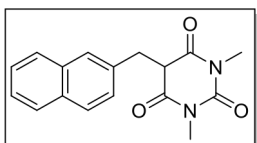


Prepared according to General Procedure B from **6d** (26.2 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a white solid (21.4 mg, 81% yield); M.p. 100-102 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.17 (q, *J* = 6.6 Hz, 1H), 6.89 (t, *J* = 8.4 Hz, 1H), 6.82-6.74 (m, 2H), 3.74 (t, *J* = 4.5 Hz, 1H), 3.43 (d, *J* = 4.8 Hz, 2H), 3.13 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 167.8, 162.6 (d, *J*<sub>C-F</sub> = 245.4 Hz), 150.9, 137.9 (d, *J*<sub>C-F</sub> = 7.4 Hz), 130.1 (d, *J*<sub>C-F</sub> = 8.3 Hz), 124.6 (d, *J*<sub>C-F</sub> = 2.9 Hz), 115.9 (d, *J*<sub>C-F</sub> = 21.5 Hz), 114.6 (d, *J*<sub>C-F</sub> = 20.8 Hz), 50.3, 36.5, 36.4, 28.2. HRMS (ESI) *m/z* calcd for C<sub>13</sub>H<sub>14</sub>O<sub>3</sub>N<sub>2</sub>F (M+H)<sup>+</sup>: 265.09885; Found: 265.09818; 5-(1-(3-Fluorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**8d**): Isolated as a white solid (5.2 mg, 17% yield); M.p. 68-70 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.19 (q, *J* = 6.0 Hz, 1H), 6.92 (td, *J* = 8.4, 2.4 Hz, 1H), 6.72-6.64 (m, 2H), 3.89 (d, *J* = 3.6 Hz, 3H), 3.10-2.99 (m, 4H), 2.51-2.38 (m, 1H), 1.30 (d, *J* = 6.3 Hz, 3H), 0.73 (d, *J* = 6.6 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 167.1(d,



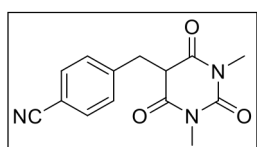
$J_{C-F} = 163.6$  Hz), 162.8 (d,  $J_{C-F} = 245.9$  Hz), 150.8, 140.9 (d,  $J_{C-F} = 6.8$  Hz), 130.0 (d,  $J_{C-F} = 8.3$  Hz), 123.4 (d,  $J_{C-F} = 2.7$  Hz), 115.1, 114.9, 114.5 (d,  $J_{C-F} = 21.5$  Hz), 58.5, 51.6, 28.7, 28.1, 27.9, 21.4, 21.2. HRMS (ESI)  $m/z$  calcd for  $C_{16}H_{20}O_3N_2F$  (M+H)<sup>+</sup>: 307.14580; Found: 307.14545.

### 1,3-Dimethyl-5-(naphthalen-2-ylmethyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7e).



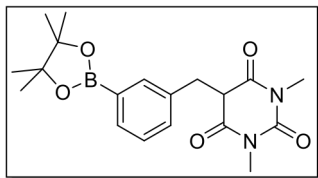
Prepared according to General Procedure B from **6e** (29.4 g, 0.100 mmol); reaction was purified by flash chromatography on silica gel with EtOAc:pentane (1:5) and the product was isolated as a yellow solid (25.5 mg, 86% yield); M.p. 126-128 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$  7.78-7.69 (m, 3H), 7.52 (s, 1H), 7.45-7.42 (m, 2H), 7.13 (d,  $J = 8.4$  Hz, 1H), 3.83 (t,  $J = 4.8$  Hz, 1H), 3.62 (d,  $J = 4.8$  Hz, 1H), 3.08 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  168.2, 150.5, 133.3, 132.7, 132.6, 128.3, 127.9, 127.7, 127.5, 126.7, 126.4, 126.1, 50.7, 37.6, 28.2. HRMS (ESI)  $m/z$  calcd for  $C_{17}H_{17}O_3N_2$  (M+H)<sup>+</sup>: 279.12392; Found: 279.12296; 1,3-Dimethyl-5-(2-methyl-1-(naphthalen-2-yl)propyl)pyrimidine-2,4,6(1H,3H,5H)-trione (**8e**): Isolated as a yellow oil (3.7 mg, 11% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$  7.77-7.69 (m, 3H), 7.45-7.40 (m, 3H), 7.02 (d,  $J = 8.4$  Hz, 1H), 3.98 (d,  $J = 3.6$  Hz, 1H), 3.20 (dd,  $J = 11.1, 3.6$  Hz, 1H), 3.05 (s, 3H), 2.85 (s, 3H), 2.67-2.55 (m, 1H), 1.36 (d,  $J = 6.3$  Hz, 3H), 0.74 (d,  $J = 6.6$  Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  169.5, 167.3, 150.7, 135.5, 133.2, 132.8, 128.2, 127.7, 127.5, 127.1, 126.5, 126.2, 124.8, 59.2, 52.0, 28.7, 28.0, 27.9, 21.6, 21.4. HRMS (ESI)  $m/z$  calcd for  $C_{20}H_{23}O_3N_2$  (M+H)<sup>+</sup>: 339.17087; Found: 339.17111.

### 4-((1,3-Dimethyl-2,4,6-trioxohexahydropyrimidin-5-yl)methyl)benzotrile (7f).<sup>8</sup>



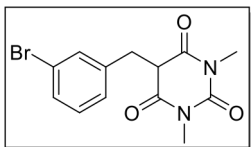
Prepared according to General Procedure B from **6f** (26.9 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a colorless oil (22.8 mg, 84% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$  7.53 (d,  $J = 8.1$  Hz, 2H), 7.24 (d,  $J = 8.1$  Hz, 2H), 3.79 (t,  $J = 4.8$  Hz, 1H), 3.52 (d,  $J = 4.8$  Hz, 2H), 3.18 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  167.3, 150.8, 141.6, 132.3, 130.1, 118.4, 111.6, 50.1, 35.3, 28.5. HRMS (ESI)  $m/z$  calcd for  $C_{14}H_{14}O_3N_3$  (M+H)<sup>+</sup>: 272.10297; Found: 272.10278; 4-(1-(1,3-Dimethyl-2,4,6-trioxohexahydropyrimidin-5-yl)-2-methylpropyl)benzotrile (**8f**): Isolated as a colorless oil (4.4 mg, 14% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$  7.53 (d,  $J = 8.1$  Hz, 2H), 7.09 (d,  $J = 8.4$  Hz, 2H), 3.92 (d,  $J = 3.6$  Hz, 1H), 3.17-3.10 (m, 4H), 3.00 (s, 3H), 2.59-2.45 (m, 1H), 1.29 (d,  $J = 6.6$  Hz, 2H), 0.69 (d,  $J = 6.6$  Hz, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  168.6, 166.6, 150.5, 144.2, 132.3, 128.7, 118.2, 112.1, 58.0, 51.3, 28.7, 28.2, 28.0, 21.4, 21.1. HRMS (ESI)  $m/z$  calcd for  $C_{17}H_{20}O_3N_3$  (M+H)<sup>+</sup>: 314.15047; Found: 314.15012.

**1,3-Dimethyl-5-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7g).**



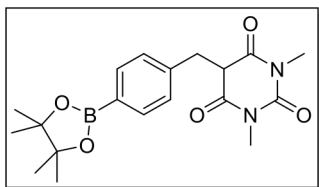
Prepared according to General Procedure B from **6g** (37.0 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a white solid (31.6 mg, 85% yield); M.p. 142-144 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) 7.65 (d, *J* = 7.2 Hz, 1H), 7.43 (s, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 7.5 Hz, 1H), 3.75 (t, *J* = 4.5 Hz, 1H), 3.43 (d, *J* = 4.5 Hz, 1H), 3.08 (s, 6H), 1.30 (s, 12H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 168.4, 150.9, 134.8, 134.2, 131.7, 127.9, 83.9, 50.8, 38.5, 28.5, 24.8. HRMS (ESI) *m/z* calcd for C<sub>19</sub>H<sub>26</sub>O<sub>5</sub>N<sub>2</sub>B (M+H)<sup>+</sup>: 373.19348. Found: 373.19266; 1,3-Dimethyl-5-(2-methyl-1-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)pyrimidine-2,4,6(1H,3H,5H)-trione (**8g**): Isolated as a white solid (5.4 mg, 13% yield); M.p. 161-163 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) 7.64 (d, *J* = 7.5 Hz, 1H), 7.32 (s, 1H), 7.21 (t, *J* = 7.8 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 3.90 (d, *J* = 3.6 Hz, 1H), 3.06 (s, 3H), 3.01 (dd, *J* = 19.1, 3.9 Hz, 1H), 2.89 (s, 3H), 2.54-2.41 (m, 1H), 1.33-1.30 (m, 15H), 0.72 (d, *J* = 6.6 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 169.6, 167.3, 150.8, 137.1, 134.5, 133.5, 130.9, 127.7, 83.9, 59.5, 52.1, 28.5, 27.9, 27.8, 24.9, 24.8, 21.7, 21.3. HRMS (ESI) *m/z* calcd for C<sub>22</sub>H<sub>32</sub>O<sub>5</sub>N<sub>2</sub>B (M+H)<sup>+</sup>: 415.24043. Found: 415.24023.

**5-(3-Bromobenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7h).**



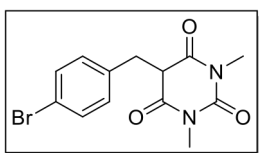
Prepared according to General Procedure B from **6h** (32.3 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a white solid (25.7 mg, 79% yield); M.p. 84-86 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.36 (d, *J* = 7.8 Hz, 1H), 7.22 (s, 1H), 7.09 (t, *J* = 7.8 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 3.74 (t, *J* = 4.8 Hz, 1H), 3.41 (d, *J* = 4.8 Hz, 2H), 3.15 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 167.8, 150.9, 137.7, 132.0, 130.9, 127.6, 122.6, 50.4, 36.6, 28.3. HRMS (ESI) *m/z* calcd for C<sub>13</sub>H<sub>14</sub>O<sub>3</sub>N<sub>2</sub>Br (M+H)<sup>+</sup>: 325.01878; Found: 325.01837; 5-(1-(3-Bromophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**8h**): Isolated as a white solid (7.3 mg, 20% yield); M.p. 121-124 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.36 (d, *J* = 8.7 Hz, 1H), 7.12-7.07 (m, 2H), 6.85 (d, *J* = 7.8 Hz, 1H), 3.90 (d, *J* = 3.9 Hz, 1H), 3.11 (s, 3H), 3.01-2.96 (m, 4H), 2.50-2.38 (m, 1H), 1.30 (d, *J* = 6.3 Hz, 3H), 0.73 (d, *J* = 6.6 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 169.2, 167.0, 150.8, 140.6, 131.2, 130.7, 130.0, 126.4, 122.7, 58.6, 51.7, 28.6, 28.1, 27.9, 21.5, 21.2. HRMS (ESI) *m/z* calcd for C<sub>16</sub>H<sub>20</sub>O<sub>3</sub>N<sub>2</sub>Br (M+H)<sup>+</sup>: 367.06573; Found: 367.06549.

**1,3-Dimethyl-5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7i).**



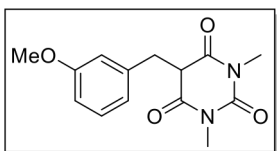
Prepared according to General Procedure B from **6i** (37.0 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:6 to 1:4) and the product was isolated as a white solid (30.5 mg, 82% yield); M.p. 131-133 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.64 (d, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 3.76 (t, *J* = 4.8 Hz, 1H), 3.46 (d, *J* = 4.8 Hz, 2H), 3.12 (s, 6H), 1.32 (s, 12H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 168.2, 150.9, 138.3, 135.1, 128.3, 83.9, 50.5, 37.7, 28.2, 24.9. HRMS (ESI) *m/z* calcd for C<sub>19</sub>H<sub>26</sub>O<sub>5</sub>N<sub>2</sub>B (M+H)<sup>+</sup>: 373.19348. Found: 373.19247; 1,3-Dimethyl-5-(2-methyl-1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)pyrimidine-2,4,6(1H,3H,5H)-trione (**8i**): Isolated as a colorless oil (5.8 mg, 14% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.63 (d, *J* = 7.8 Hz, 2H), 6.91 (d, *J* = 7.5 Hz, 2H), 3.91 (d, *J* = 3.6 Hz, 1H), 3.08-2.96 (m, 7H), 2.55-2.43 (m, 1H), 1.32-1.29 (m, 15H), 0.67 (d, *J* = 6.6 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 169.4, 167.3, 150.8, 141.3, 135.0, 127.1, 83.9, 59.1, 51.7, 28.7, 28.1, 27.9, 24.9, 21.5, 21.3. HRMS (ESI) *m/z* calcd for C<sub>22</sub>H<sub>32</sub>O<sub>5</sub>N<sub>2</sub>B (M+H)<sup>+</sup>: 415.24043. Found: 415.23969.

**5-(4-Bromobenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7j).**



Prepared according to General Procedure B from **6j** (32.3 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a white solid (24.1 mg, 74% yield); M.p. 85-87 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.35 (d, *J* = 8.4 Hz, 2H), 6.94 (d, *J* = 8.1 Hz, 2H), 3.74 (t, *J* = 4.8 Hz, 1H), 3.42 (d, *J* = 4.5 Hz, 2H), 3.16 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 167.8, 150.9, 134.6, 131.8, 130.8, 121.8, 50.3, 36.0, 28.4. HRMS (ESI) *m/z* calcd for C<sub>13</sub>H<sub>14</sub>O<sub>3</sub>N<sub>2</sub>Br (M+H)<sup>+</sup>: 325.01878. Found: 325.01831; 5-(1-(4-Bromophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**8j**): Isolated as a colorless oil (8.4 mg, 23% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.34 (d, *J* = 8.4 Hz, 2H), 6.80 (d, *J* = 8.1 Hz, 2H), 3.89 (d, *J* = 3.6 Hz, 2H), 3.09 (s, 3H), 3.04-3.00 (m, 4H), 2.51-2.39 (m, 1H), 1.28 (d, *J* = 6.3 Hz, 3H), 0.69 (d, *J* = 6.6 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 169.1, 167.0, 150.7, 137.4, 131.7, 129.4, 121.9, 58.0, 51.5, 28.8, 28.1, 27.9, 21.4, 21.3. HRMS (ESI) *m/z* calcd for C<sub>16</sub>H<sub>20</sub>O<sub>3</sub>N<sub>2</sub>Br (M+H)<sup>+</sup>: 367.06573. Found: 367.06542.

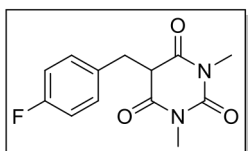
**5-(3-Methoxybenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7k).**



Prepared according to General Procedure B from **6k** (27.4 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a pale yellow solid (26.0 mg, 94% yield); M.p. 64-66 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.13 (t, *J* = 7.8 Hz, 1H), 6.75 (d, *J* = 8.1 Hz, 1H), 6.60-6.56 (m, 2H), 3.76-3.72 (m, 4H), 3.42 (d, *J* = 4.8 Hz, 2H), 3.12 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 168.2, 159.7, 151.0, 136.6, 129.6, 121.1, 114.4, 113.3, 55.1, 50.6, 37.7, 28.2. HRMS (ESI) *m/z* calcd for C<sub>14</sub>H<sub>17</sub>O<sub>4</sub>N<sub>2</sub>

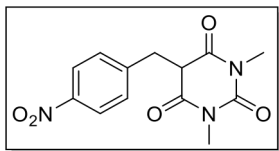
(M+H)<sup>+</sup>: 277.11883. Found: 277.11789; 5-(1-(3-Methoxyphenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8k**): Isolated as a white solid (1.6 mg, 5% yield); M.p. 100-102 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.12 (t, *J* = 7.8 Hz, 1H), 6.74 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.50-6.47 (m, 2H), 3.89 (d, *J* = 3.6 Hz, 2H), 3.72 (s, 3H), 3.08 (s, 3H), 3.00-3.95 (m, 4H), 2.50-2.38 (m, 1H), 1.30 (d, *J* = 6.3 Hz, 3H), 0.74 (d, *J* = 6.6 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 169.5, 167.3, 159.8, 139.6, 129.4, 119.8, 113.7, 113.0, 59.1, 55.2, 51.9, 28.6, 28.0, 27.9, 21.5, 21.3. HRMS (ESI) *m/z* calcd for C<sub>17</sub>H<sub>23</sub>O<sub>4</sub>N<sub>2</sub> (M+H)<sup>+</sup>: 319.16578. Found: 319.16437.

#### 5-(4-Fluorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7l**).



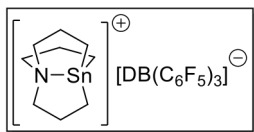
Prepared according to General Procedure B from **6l** (26.2 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a white solid (23.3 mg, 88% yield); M.p. 59-61 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.03-6.87 (m, 4H), 3.73 (t, *J* = 4.8 Hz, 1H), 3.43 (d, *J* = 4.8 Hz, 2H), 3.13 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 168.0, 162.6 (d, *J*<sub>C-F</sub> = 245.3 Hz), 150.9, 131.1, 130.6 (d, *J*<sub>C-F</sub> = 8.0 Hz), 115.5 (d, *J*<sub>C-F</sub> = 21.2 Hz), 50.6, 36.3, 28.3. HRMS (ESI) *m/z* calcd for C<sub>13</sub>H<sub>14</sub>O<sub>3</sub>N<sub>2</sub>F (M+H)<sup>+</sup>: 265.09885. Found: 265.09769; 5-(1-(4-Fluorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8l**): Isolated as a colorless oil (3.1 mg, 10% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 6.95-6.86 (m, 4H), 3.90 (d, *J* = 3.6 Hz, 1H), 3.09 (s, 3H), 3.05-2.99 (m, 4H), 2.50-2.38 (m, 1H), 1.30 (d, *J* = 6.3 Hz, 3H), 0.70 (d, *J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 169.3, 167.1, 162.2 (d, *J*<sub>C-F</sub> = 246.0 Hz), 150.8, 133.9 (d, *J*<sub>C-F</sub> = 3.8 Hz), 129.2 (d, *J*<sub>C-F</sub> = 7.8 Hz), 115.5 (d, *J*<sub>C-F</sub> = 21.1 Hz), 58.1, 51.8, 28.9, 28.1, 27.9, 21.4, 21.3. HRMS (ESI) *m/z* calcd for C<sub>16</sub>H<sub>20</sub>O<sub>3</sub>N<sub>2</sub>F (M+H)<sup>+</sup>: 307.14580. Found: 307.14517.

#### 1,3-Dimethyl-5-(4-nitrobenzyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7m**).<sup>9</sup>



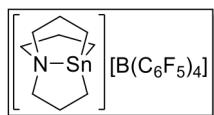
Prepared according to General Procedure B from **6m** (28.9 mg, 0.100 mmol); reaction was purified eluting with EtOAc:pentane (1:4) and the product was isolated as a white solid (7.0 mg, 24% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.10 (d, *J* = 8.7 Hz, 2H), 7.31 (d, *J* = 8.7 Hz, 2H), 3.82 (t, *J* = 4.8 Hz, 1H), 3.58 (d, *J* = 5.1 Hz, 2H), 3.20 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 167.2, 150.5, 147.4, 143.9, 130.3, 123.7, 50.0, 34.7, 28.5. 1,3-Dimethyl-5-(2-methyl-1-(4-nitrophenyl)propyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8m**): Isolated as a pale yellow oil (24.3 mg, 76% yield); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.10 (d, *J* = 8.7 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 3.94 (d, *J* = 3.3 Hz, 1H), 3.25 (d, *J* = 3.3 Hz, 1H), 3.21 (d, *J* = 3.3 Hz, 1H), 3.12 (s, 3H), 3.02 (s, 3H), 2.51 (m, 1H), 1.30 (d, *J* = 6.3 Hz, 3H), 0.70 (d, *J* = 6.6 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 168.5, 166.6, 150.5, 147.5, 146.4, 128.9, 123.7, 57.6, 51.2, 28.9, 28.3, 28.1, 21.4, 21.2. HRMS (ESI) *m/z* calcd for C<sub>16</sub>H<sub>20</sub>O<sub>5</sub>N<sub>3</sub> (M+H)<sup>+</sup>: 334.13975. Found: 334.13864.

**[N(CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>)<sub>3</sub>Sn][DB(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>] (9).**



To a solution of 5-(propan-2-yl-1,1,1,3,3,3-*d*<sub>6</sub>)-1-aza-5-stannabicyclo[3.3.3]undecane (30.1 mg, 0.100 mmol) in CD<sub>2</sub>Cl<sub>2</sub> (1 ml) in a vial, was added tris(pentafluorophenyl)borane (51.1 mg, 0.100 mmol). After stirring for 2 min, the solution was transferred to a J. Young NMR tube; <sup>1</sup>H NMR (CD<sub>2</sub>Cl<sub>2</sub>, 300 MHz) δ 2.66 (m, 6H, NCH<sub>2</sub>), 2.04 (m, 6H, CH<sub>2</sub>), 1.45 (t, *J* = 6.6, 6H, SnCH<sub>2</sub>); <sup>13</sup>C NMR (CD<sub>2</sub>Cl<sub>2</sub>, 75 MHz) δ 56.5 (NCH<sub>2</sub>), 25.2 (CH<sub>2</sub>), 15.4 (SnCH<sub>2</sub>); <sup>119</sup>Sn NMR (CD<sub>2</sub>Cl<sub>2</sub>, 112 MHz) δ 151.4; <sup>11</sup>B NMR (CDCl<sub>3</sub>, 96 MHz) δ -18.1; <sup>2</sup>H NMR (CHCl<sub>3</sub>, 46 MHz) δ 5.05 (d, *J* = 2.3 Hz), 4.95 (d, *J* = 1.5 Hz), 1.68 (brd, *J* = 0.1 Hz). HRMS (-ESI) *m/z* calcd. for C<sub>18</sub>H<sub>18</sub>BF<sub>15</sub> (M<sup>-</sup>): 512.99891. Found: 512.99935; (+ESI) *m/z* calcd. for C<sub>9</sub>H<sub>18</sub>NSn (M<sup>+</sup>): 260.04557. Found: 260.04538.

**[N(CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>)<sub>3</sub>Sn][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>] (13).**



To a solution of 5-methyl-1-aza-5-stannabicyclo[3.3.3]undecane (27.5 mg, 0.100 mmol) in 1,2-dichloroethane (1 ml) in a vial, was added trityl tetrakis(pentafluorophenyl)borate (92.2 mg, 0.100 mmol). After stirring for 2 min, the solution was transferred to a J. Young NMR tube; <sup>1</sup>H NMR ((CH<sub>2</sub>Cl)<sub>2</sub>, 300 MHz) δ 2.70 (t, 6H, NCH<sub>2</sub>), 2.10 (m, 6H, CH<sub>2</sub>), 1.71 (t, 6H, SnCH<sub>2</sub>); <sup>119</sup>Sn NMR (Cl(CH<sub>2</sub>)<sub>2</sub>Cl, 112 MHz) δ 251.1.

<sup>1</sup> Li, L.; Wang, C. Y.; Huang, R.; Biscoe, M. R. *Nat. Chem.* **2013**, *5*, 607–612.

<sup>2</sup> Deb, M. L.; Bhuyan, P. J. *Tetrahedron Lett.* **2005**, *46*, 6453–6456.

<sup>3</sup> Pałasz, A. *Synthesis* **2010**, 4021–4032.

<sup>4</sup> Deb, M. L.; Bhuyan, P. J. *Tetrahedron Lett.* **2005**, *46*, 6453–6456

<sup>5</sup> Mohammed Khan, K.; Khan, M.; Ali, M.; Taha, M.; Hameed, A. Ali, S. Perveen, S. Choudhary, M. I. *Med. Chem.* **2011**, *7*, 231–236.

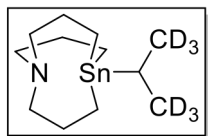
<sup>6</sup> McNallyla, J. P.; Cooper, N. J. *Organometallics* **1988**, *7*, 1704–1715.

<sup>7</sup> Löfberg, C.; Grigg, R.; Keep, A.; Derrick, A.; Sridharana, V.; Kilnera, C. *Chem. Commun.* **2006**, 5000–5002.

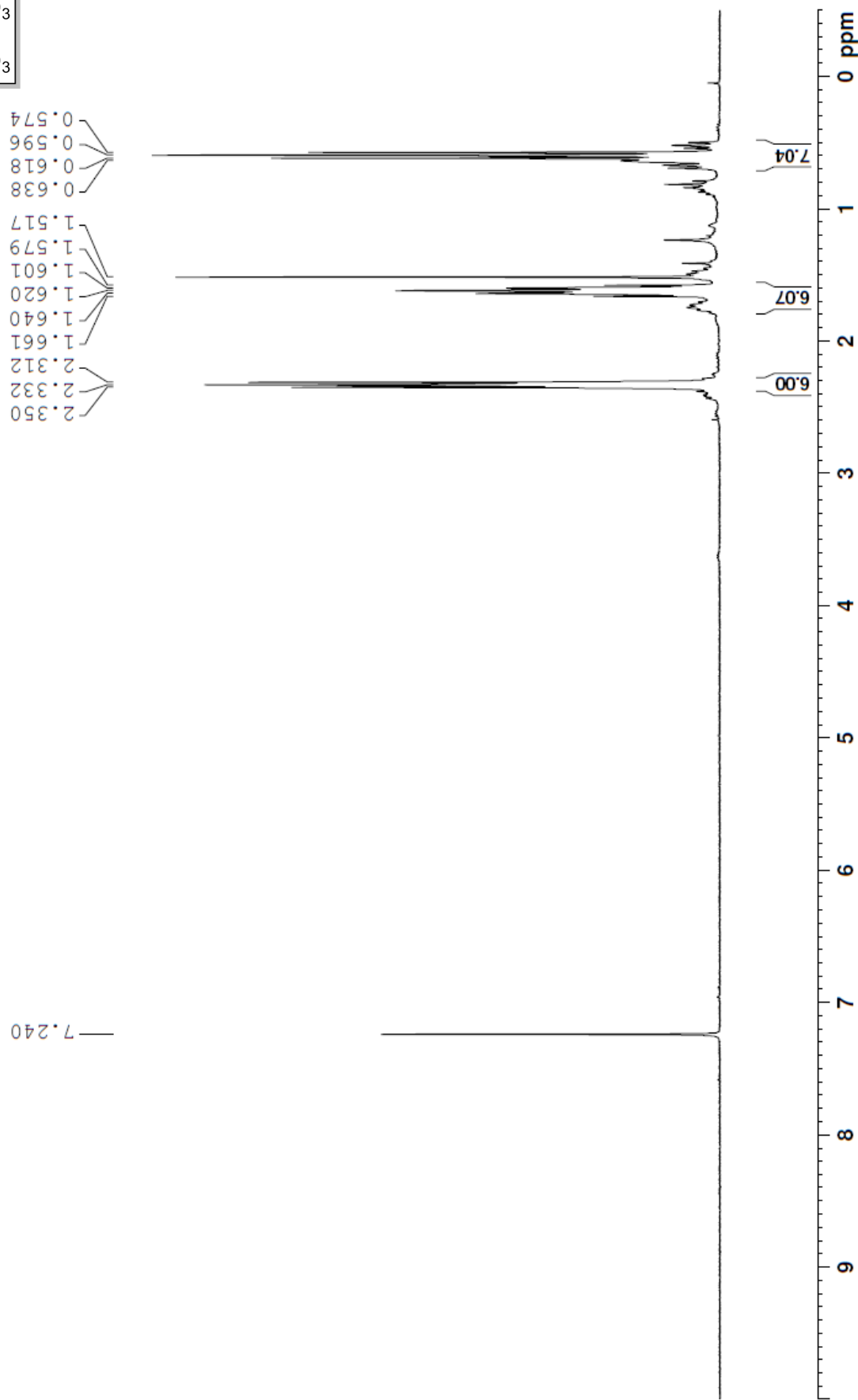
<sup>8</sup> Rehse, K.; Kapp, W-D. *Arch. Pharm.* **1982**, *4*, 346–353.

<sup>9</sup> Tanaka, K.; Chen, X.; Kimura, T.; Yoneda, F. *Chem. Pharm. Bull.* **1988**, *36*, 60–69.

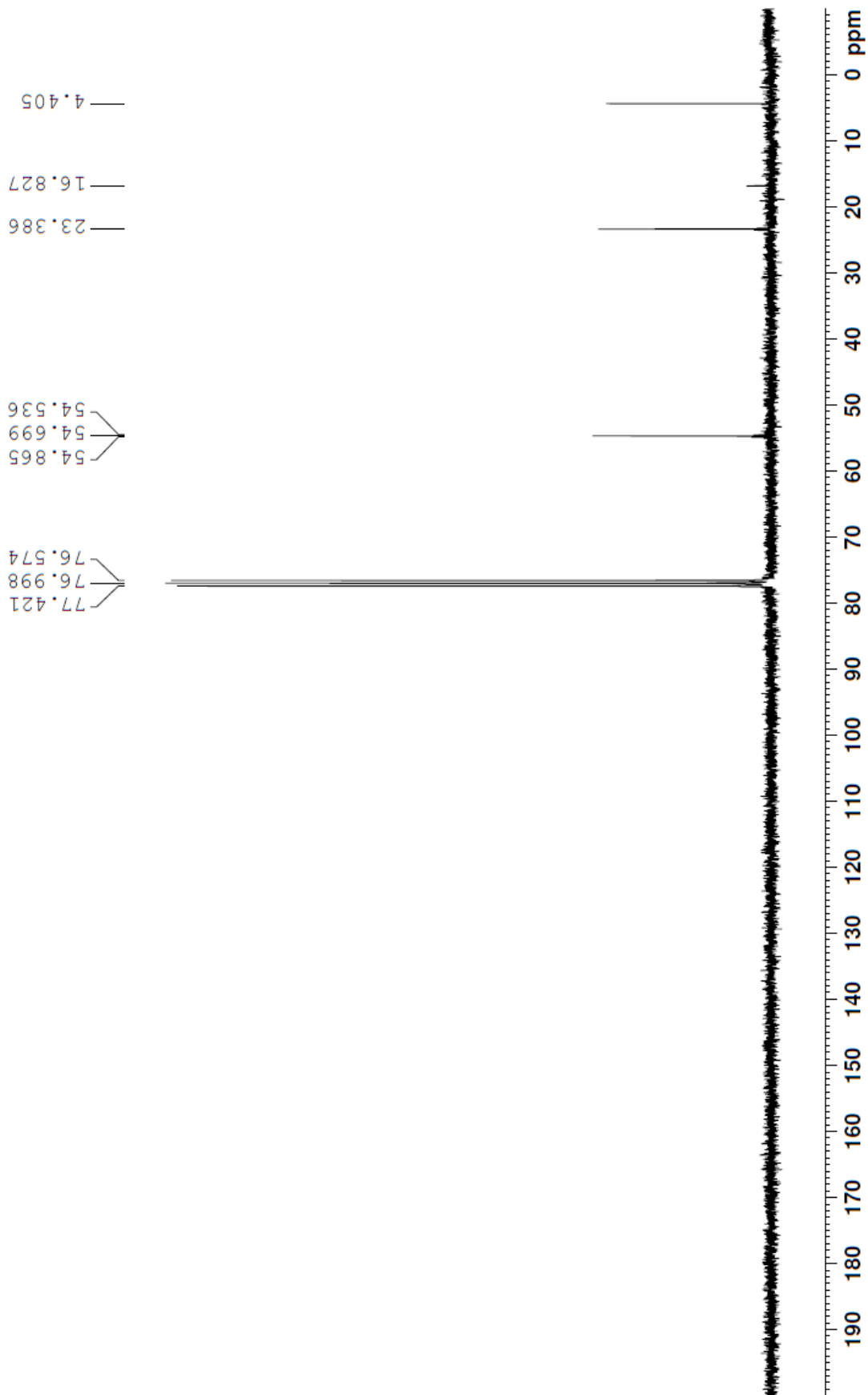
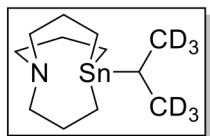
$^1\text{H}$  NMR Spectra of 5-(propan-2-yl-1,1,1,3,3,3- $d_6$ )-1-aza-5-stannabicyclo[3.3.3]undecane ( $2-d_6$ )



AK-3-232-cr  
proton, 16 scans  
AVANCE-300B

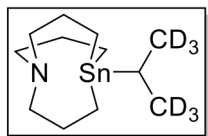


<sup>13</sup>C NMR Spectra of 5-(propan-2-yl-1,1,1,3,3,3-d<sub>6</sub>)-1-aza-5-stannabicyclo[3.3.3]undecane (2-d<sub>6</sub>)

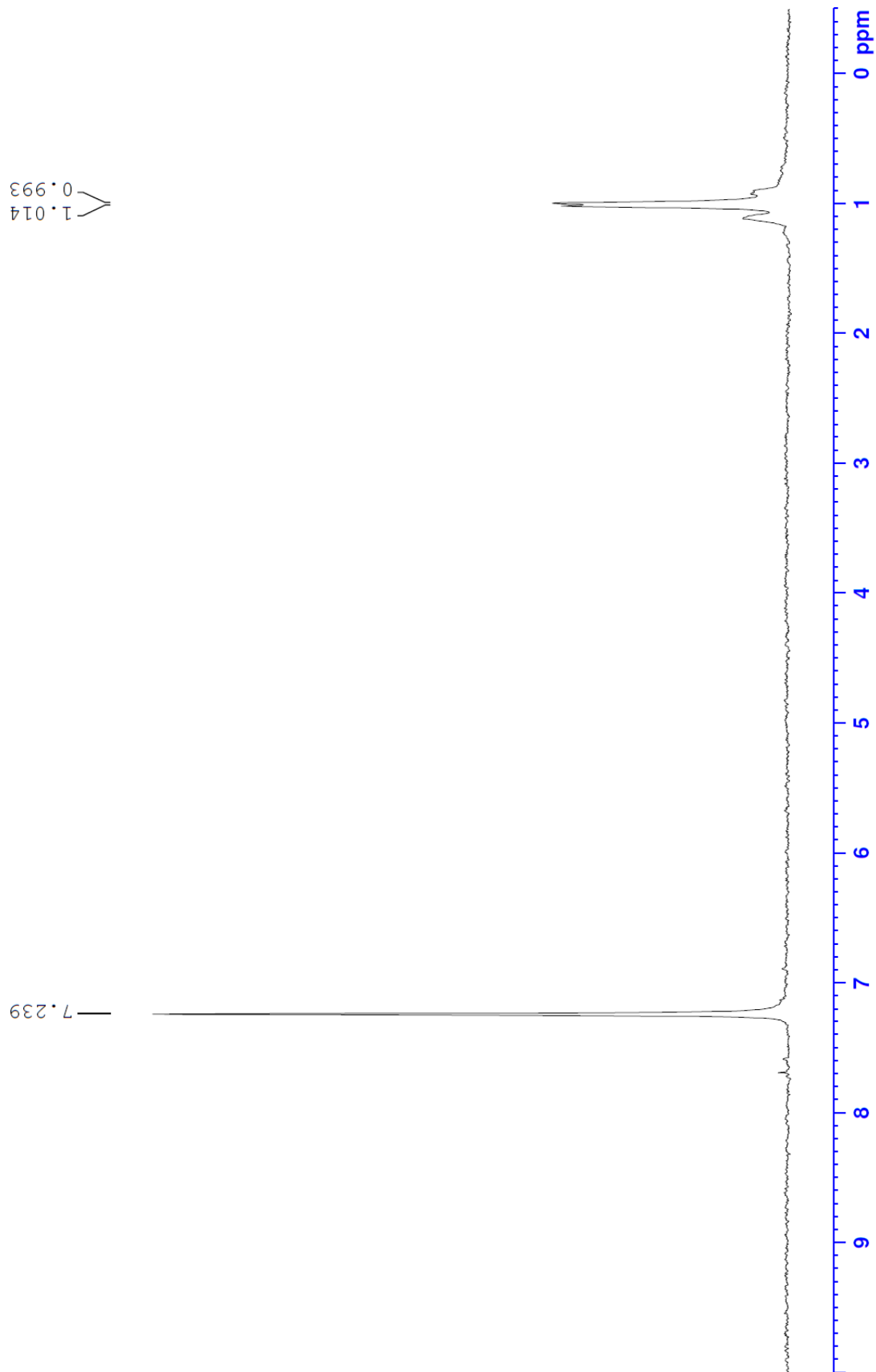


AK-3-232-Cr-C AVANCE-300B  
C-13 with Decoupling

$^2\text{H}$  NMR Spectra of 5-(propan-2-yl-1,1,1,3,3,3- $d_6$ )-1-aza-5-stannabicyclo[3.3.3]undecane ( $2-d_6$ )

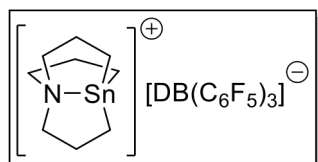


AK-3-232-D-in-CHCl3-2drops-CDCl3

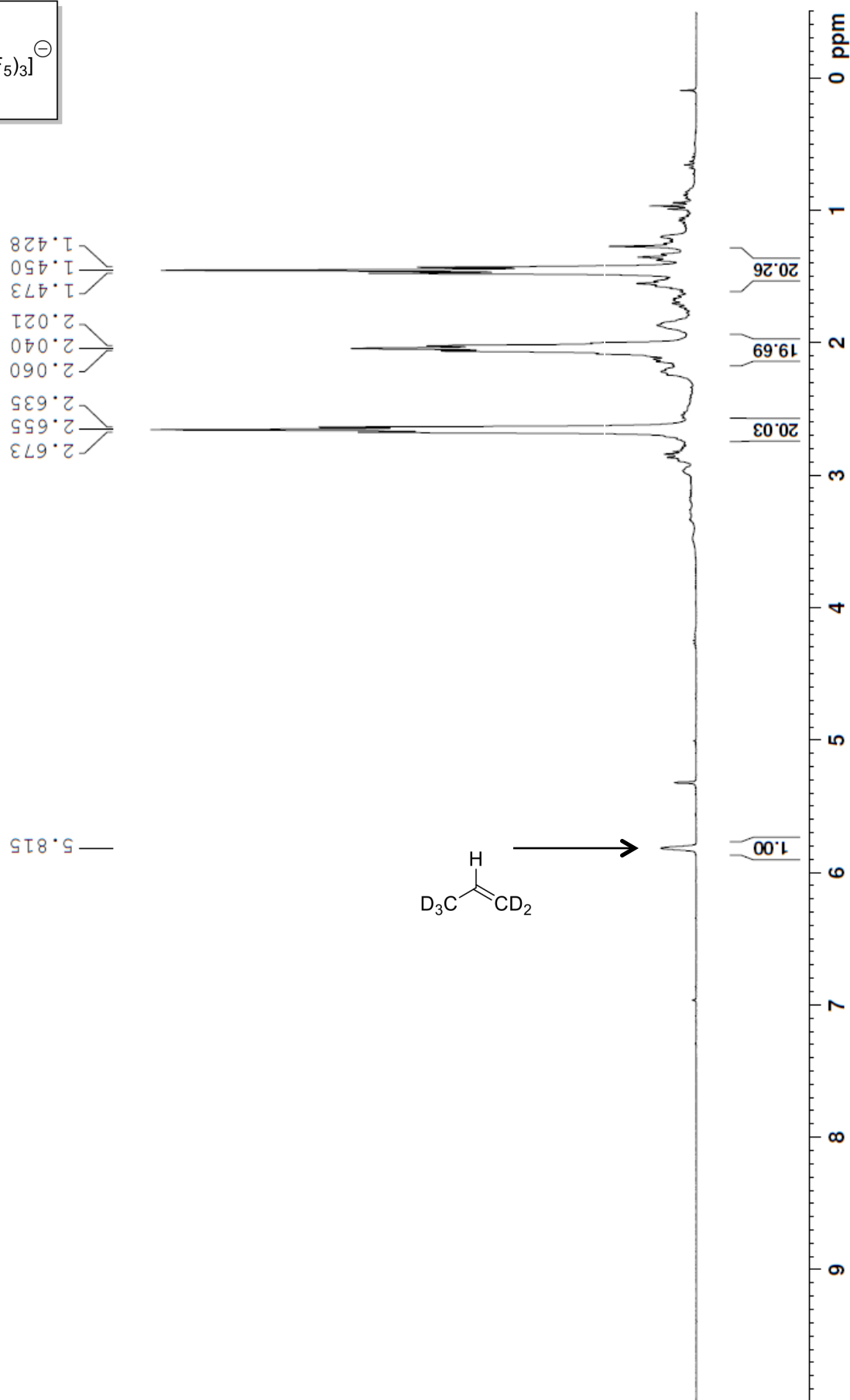




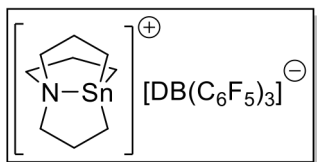
$^1\text{H}$  NMR spectra of  $[\text{N}(\text{CH}_2\text{CH}_2\text{CH}_2)_3\text{Sn}][\text{DB}(\text{C}_6\text{F}_5)_3]$  (**3-d<sub>1</sub>**)



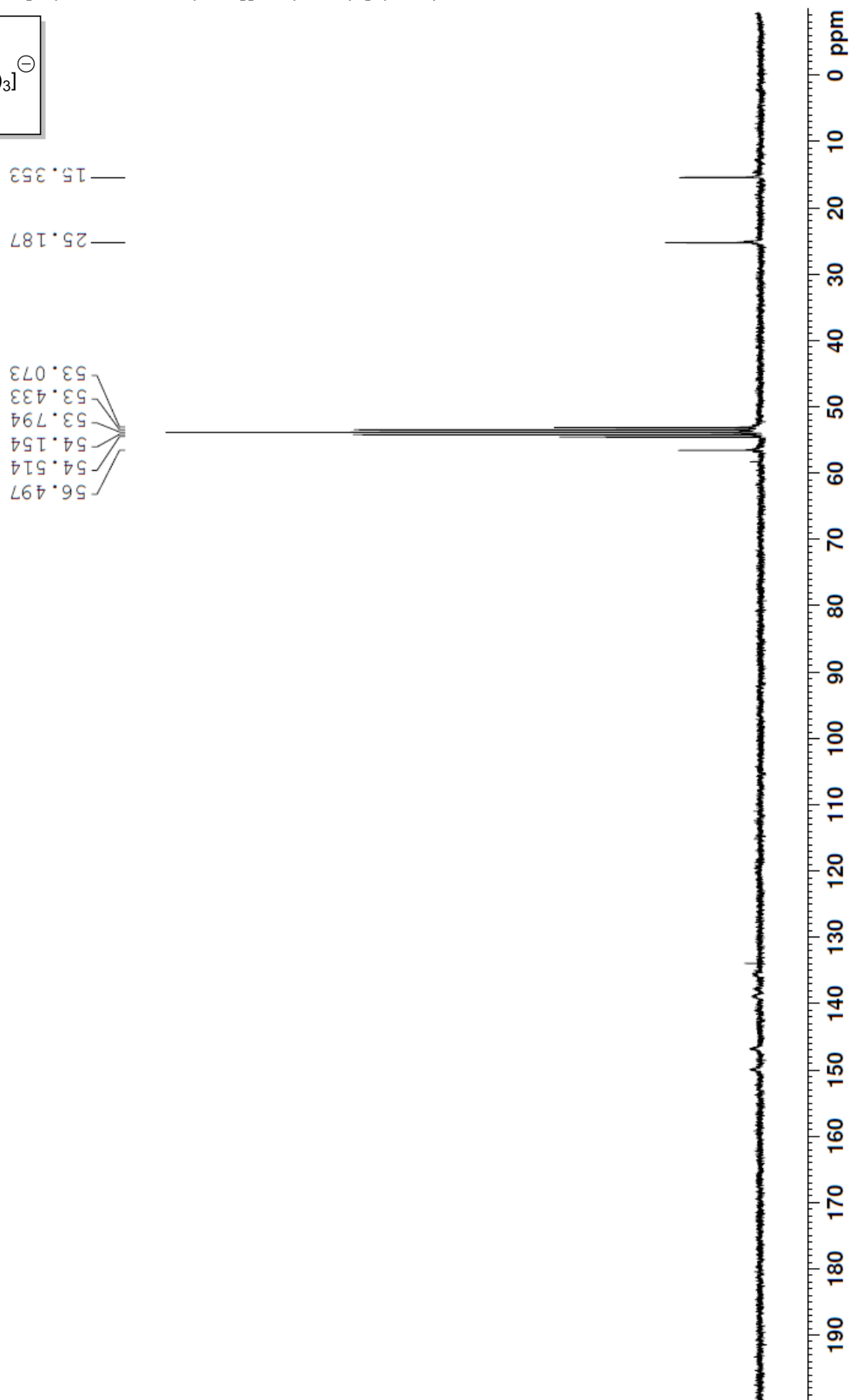
AK-3-244-H  
proton, 16 scans AVANCE-300E



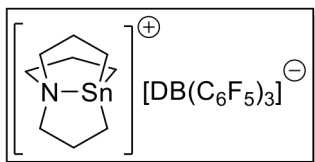
$^{13}\text{C}$  NMR spectra of  $[\text{N}(\text{CH}_2\text{CH}_2\text{CH}_2)_3\text{Sn}][\text{DB}(\text{C}_6\text{F}_5)_3]$  (**3-d<sub>1</sub>**)



AK-3-244-C  
C-13 with Decoupling AVANCE-300B



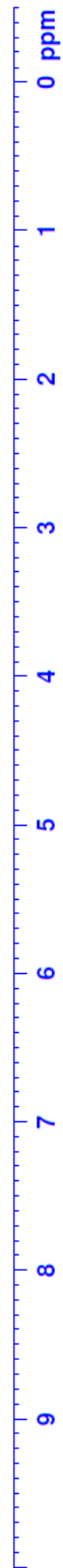
$^2\text{H}$  NMR spectra of  $[\text{N}(\text{CH}_2\text{CH}_2\text{CH}_2)_3\text{Sn}][\text{DB}(\text{C}_6\text{F}_5)_3]$  (**3-d<sub>1</sub>**)



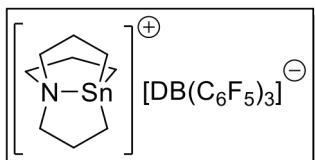
AK-2-244-D-in-CH<sub>2</sub>CL<sub>2</sub>-3drops-CD<sub>2</sub>CL<sub>2</sub>

1.687  
1.672

5.319  
5.081  
5.023  
4.971  
4.938

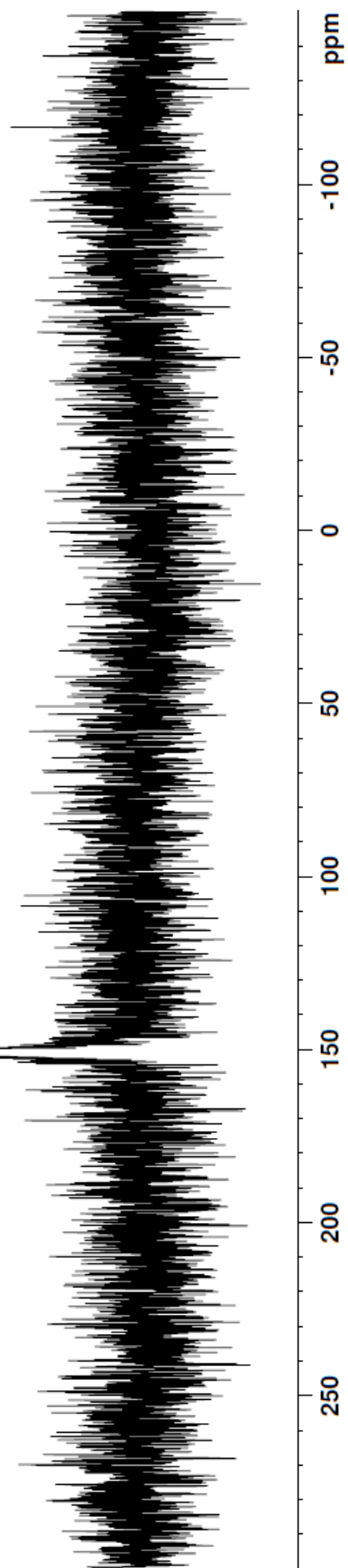


$^{119}\text{Sn}$  NMR spectra of  $[\text{N}(\text{CH}_2\text{CH}_2\text{CH}_2)_3\text{Sn}][\text{DB}(\text{C}_6\text{F}_5)_3]$  (**3-d<sub>1</sub>**)

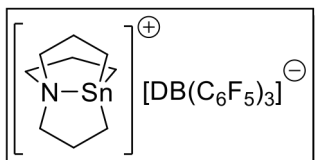


AK-3-244-Sn  
119Sn with decoupling 1k scans AVANCE 300B

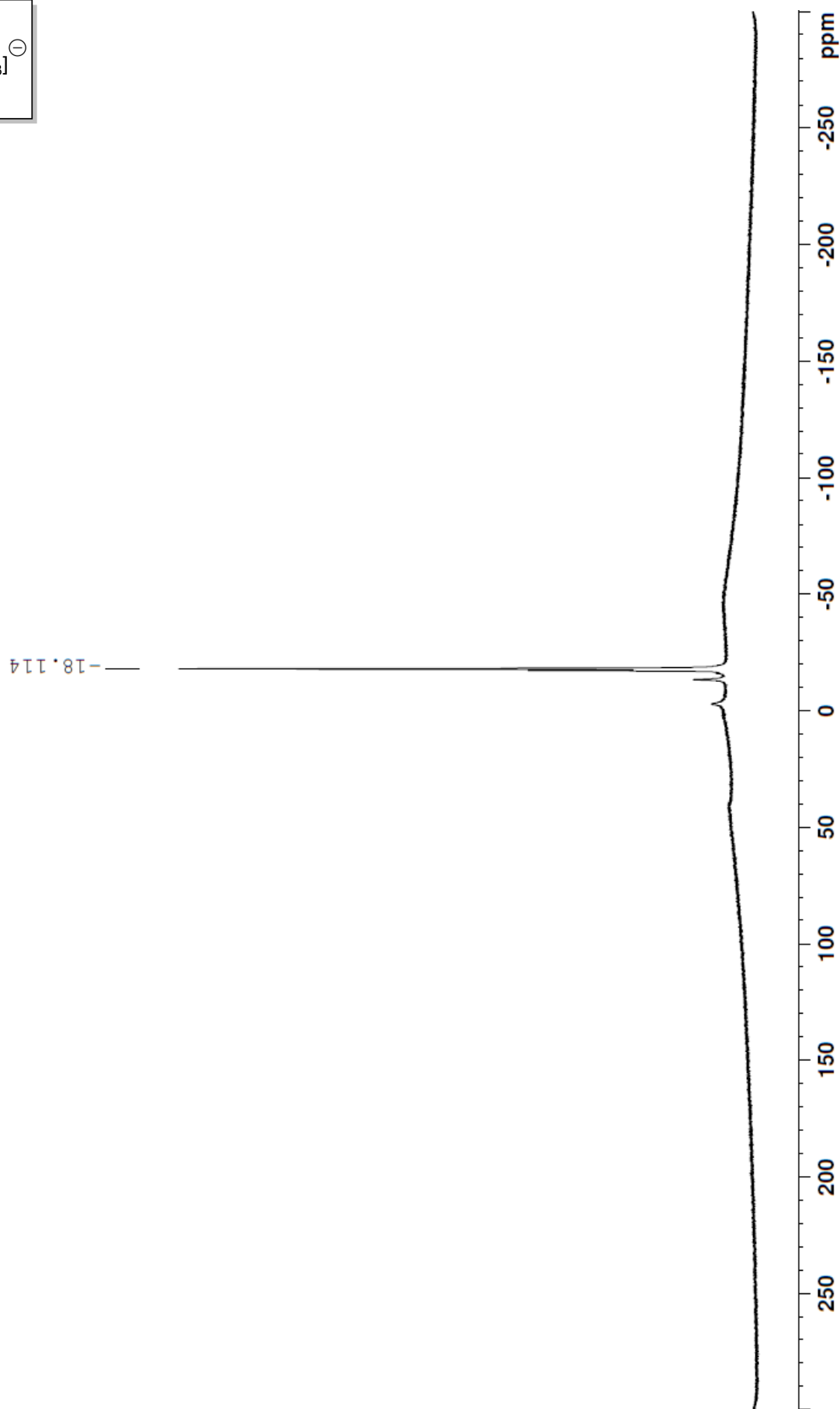
151.419



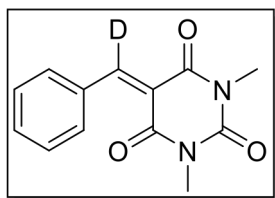
$^{11}\text{B}$  NMR spectra of  $[\text{N}(\text{CH}_2\text{CH}_2\text{CH}_2)_3\text{Sn}][\text{DB}(\text{C}_6\text{F}_5)_3]$  (**3-d<sub>1</sub>**)



AK-3-244-B  
B-11 128 scans No Decoupling AVANCE 300B



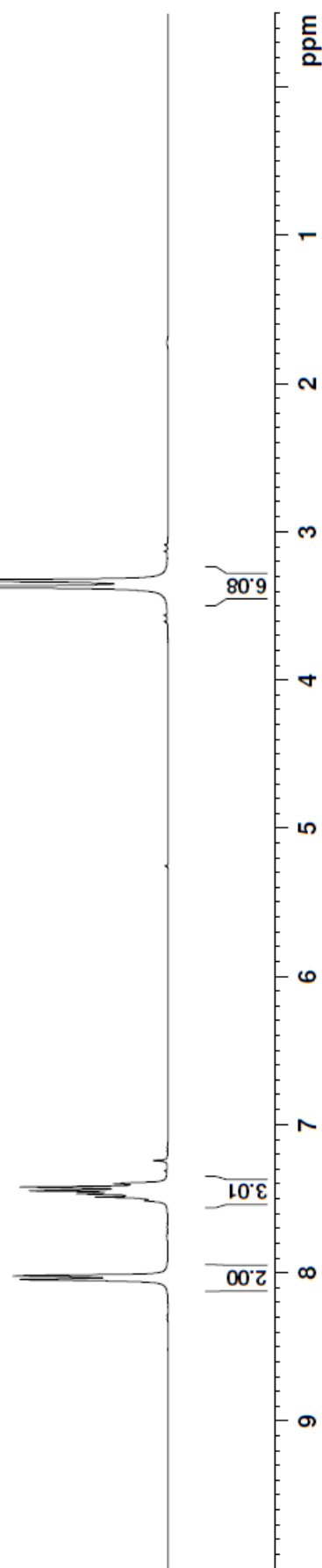
<sup>1</sup>H NMR Spectra of 1,3-Dimethyl-5-(phenylmethylene-d)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6a-d<sub>1</sub>**)



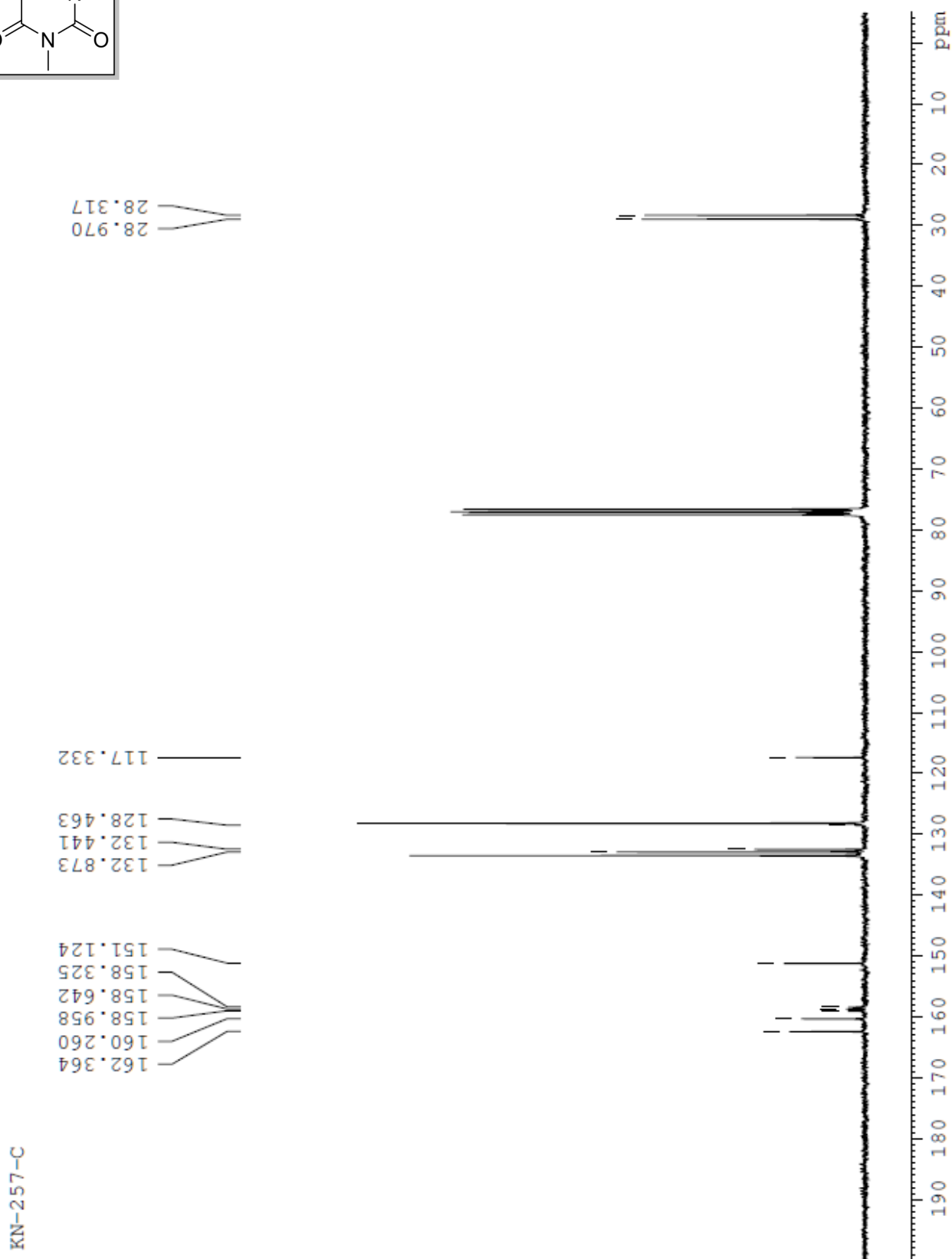
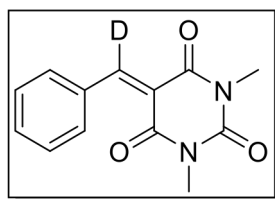
KN-1-257  
proton, 16 scans AVANCE-300B

8.042  
8.019  
7.463  
7.444  
7.418

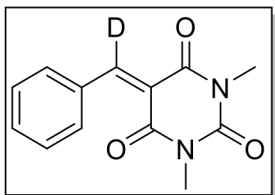
3.367  
3.324



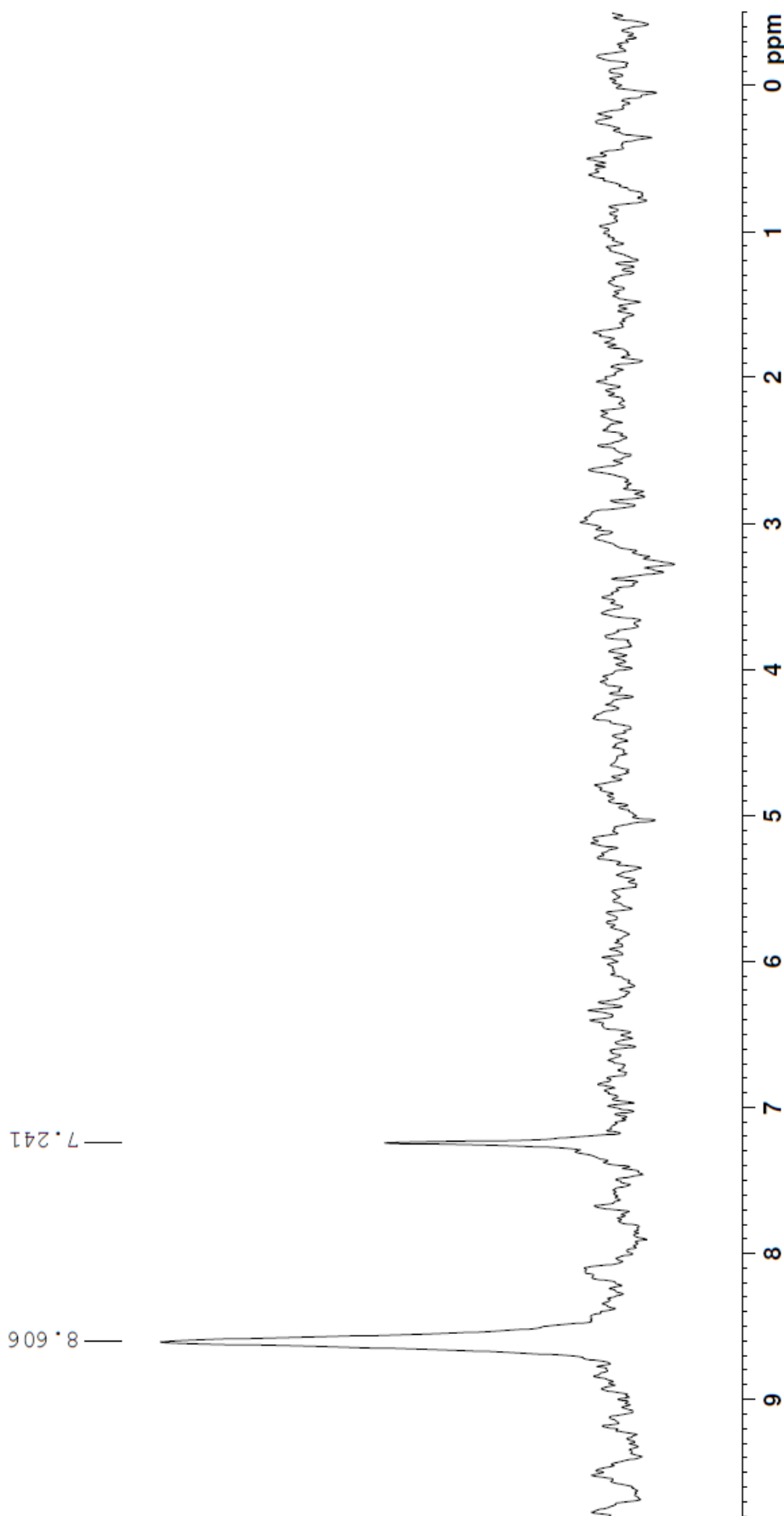
<sup>13</sup>C NMR Spectra of 1,3-Dimethyl-5-(phenylmethylene-d)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6a-d<sub>1</sub>**)



$^2\text{H}$  NMR Spectra of 1,3-Dimethyl-5-(phenylmethylene-d)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6a-d<sub>1</sub>**)

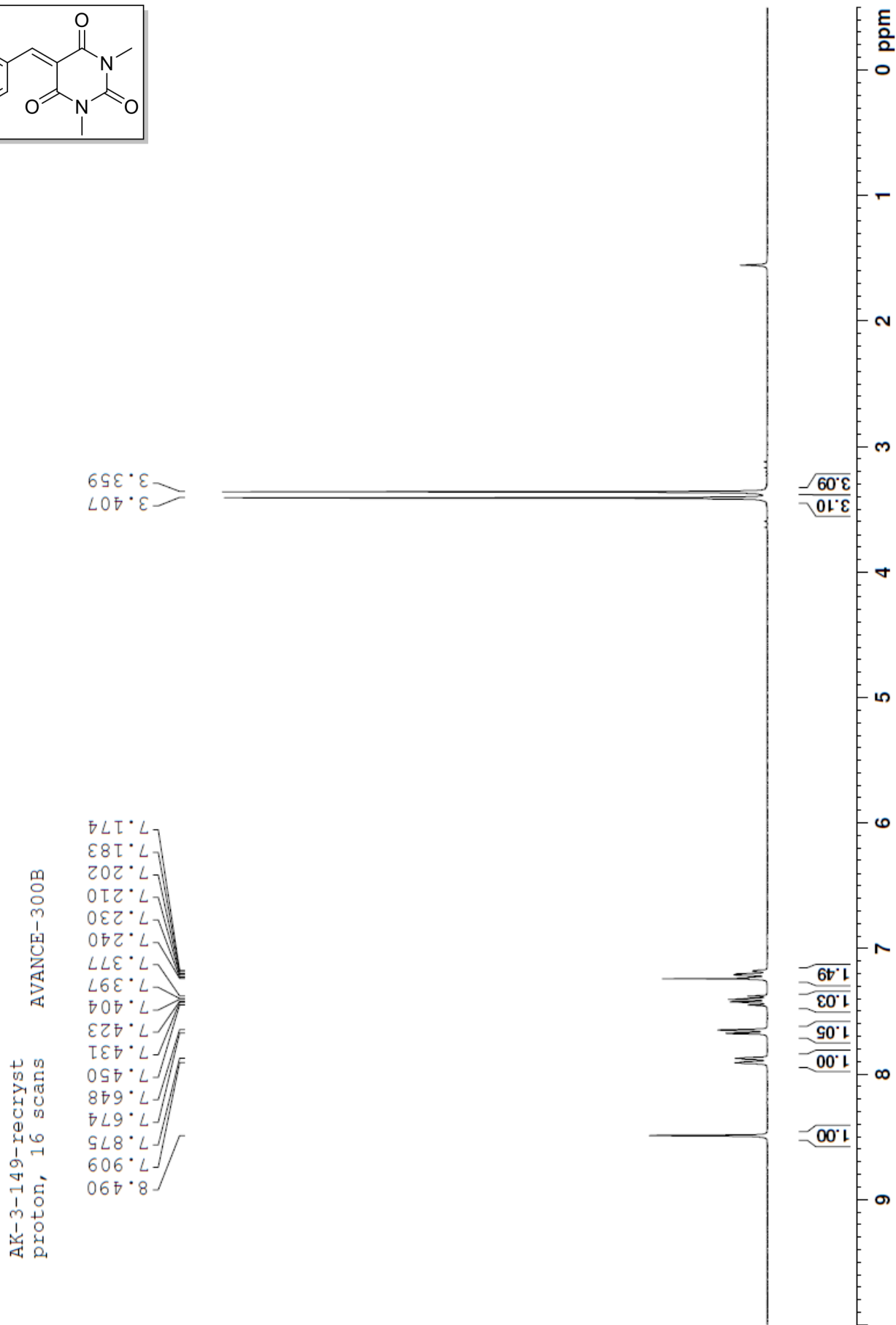
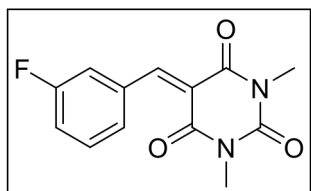


KN-1-257-D  
Deuterium

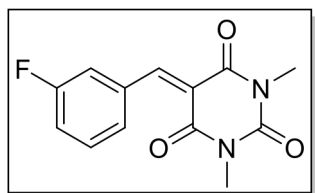




<sup>1</sup>H NMR Spectra of 5-(3-fluorobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6d**)



<sup>13</sup>C NMR Spectra of 5-(3-fluorobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6d**)

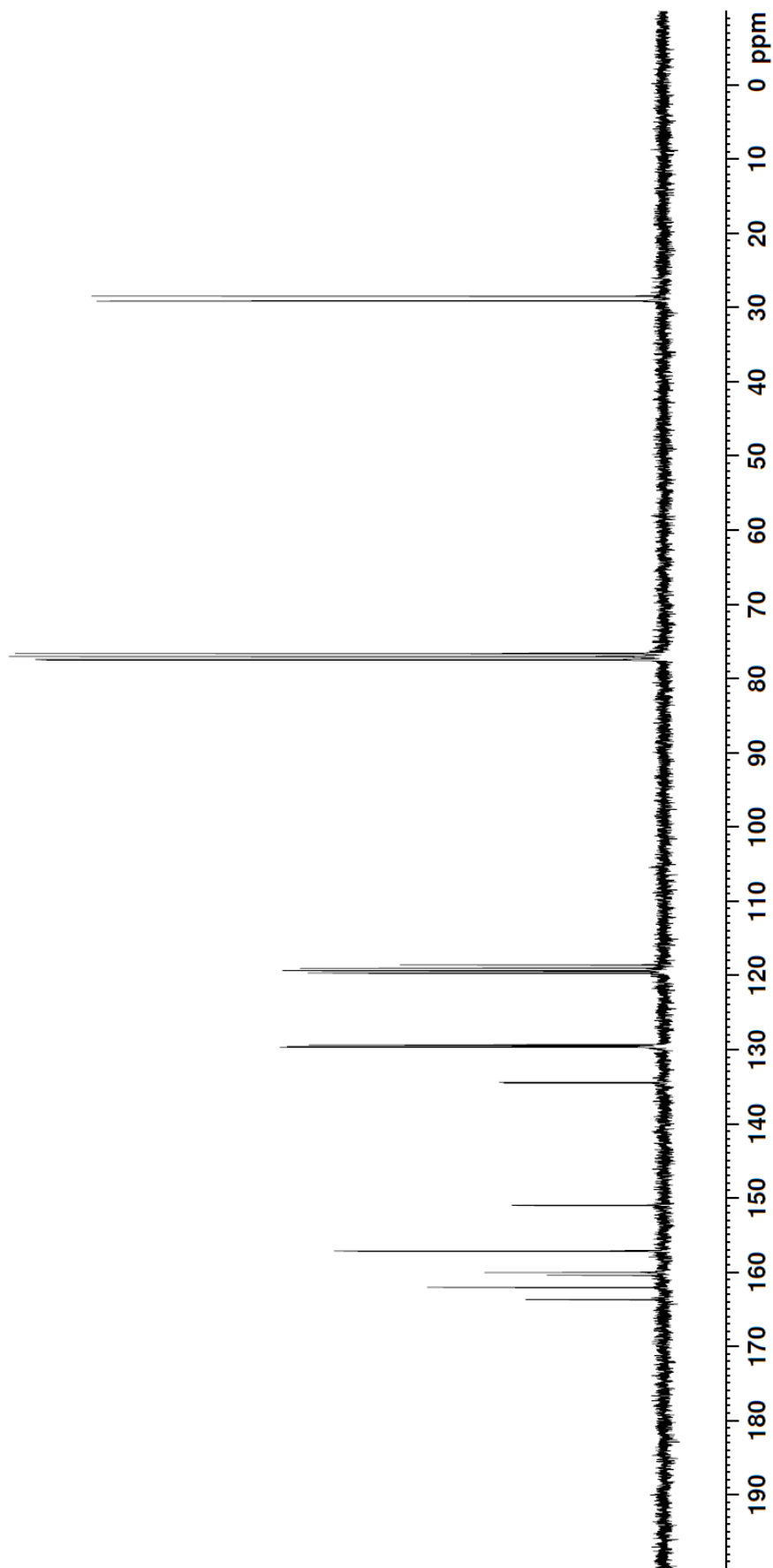


AK-3-149-C-2 AVANCE-300B  
C-13 with Decoupling

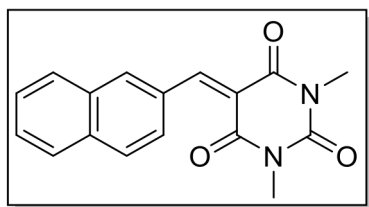
163.667  
162.045  
160.401  
160.040  
157.147  
157.116  
150.996  
134.511  
134.398  
129.652  
129.545  
129.350  
129.312  
119.672  
119.388  
119.312  
119.003  
118.547

77.422  
76.998  
76.574

29.043  
28.393



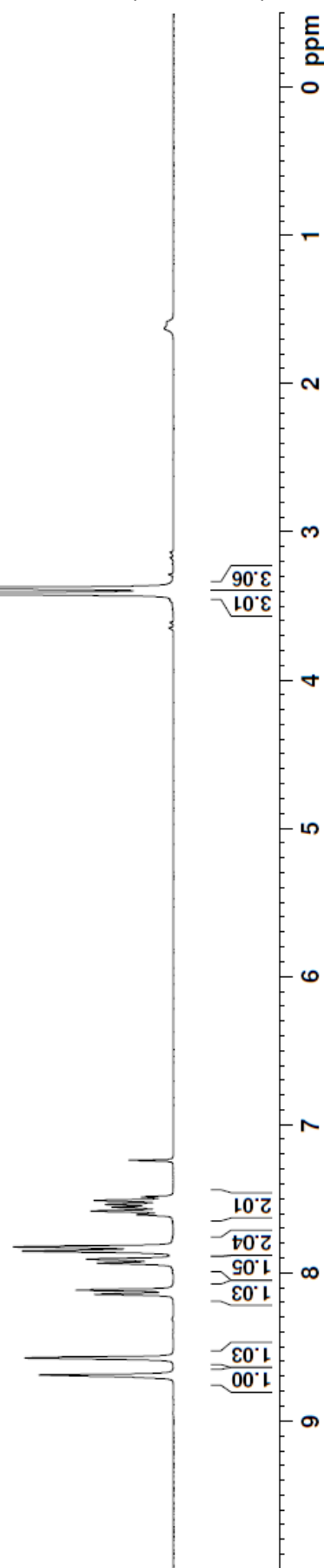
<sup>1</sup>H NMR Spectra of 1,3-dimethyl-5-(naphthalen-2-ylmethylene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6e**)



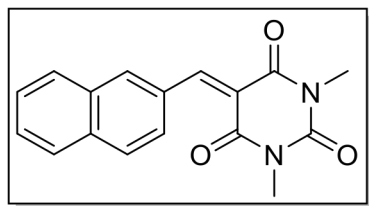
AK-3-166-cr AVANCE-300B  
proton, 16 scans

8.689  
8.574  
8.145  
8.116  
7.934  
7.908  
7.853  
7.824  
7.607  
7.583  
7.558  
7.538  
7.512  
7.488  
7.240

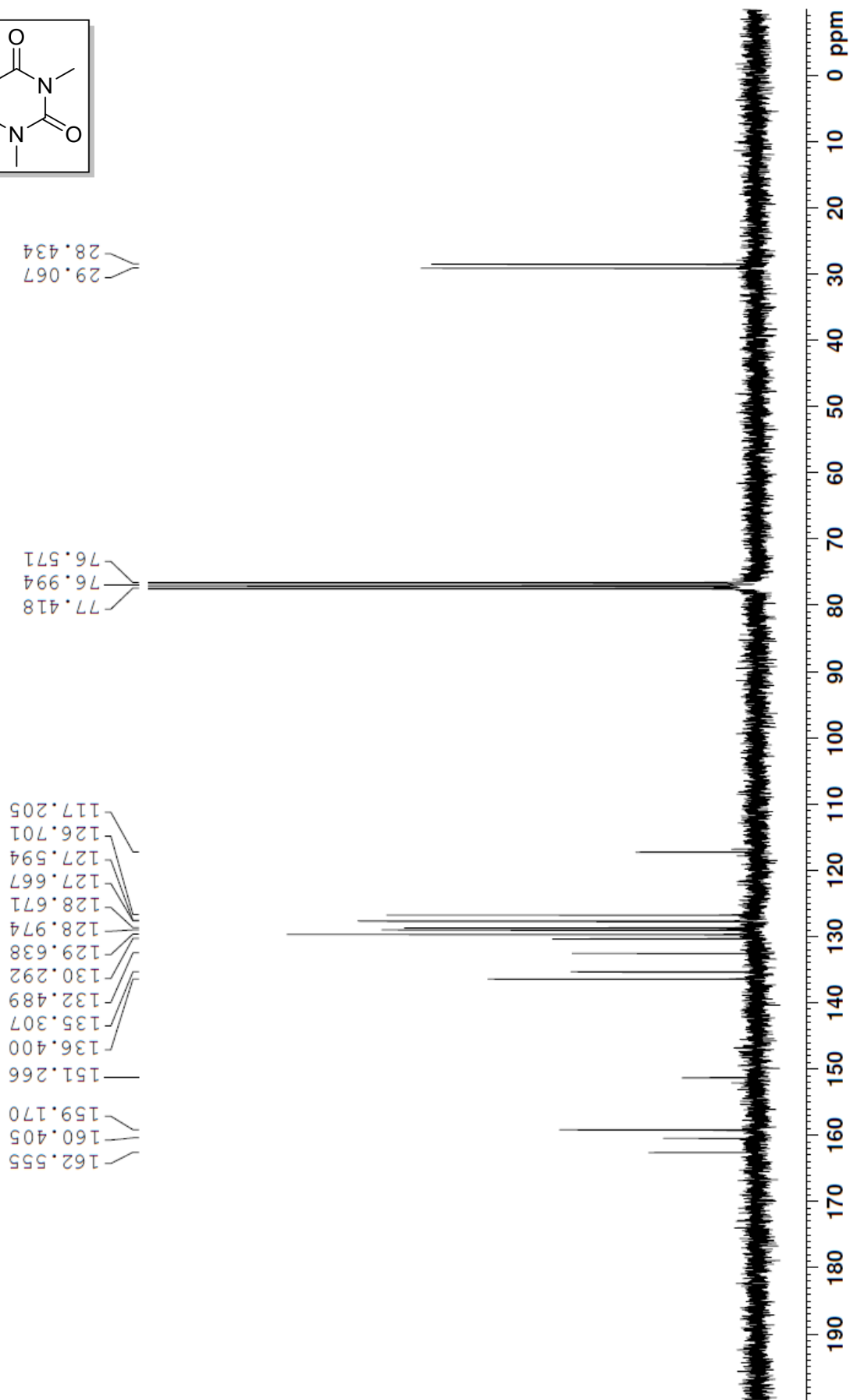
3.413  
3.376



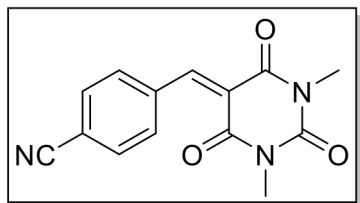
<sup>13</sup>C NMR Spectra of 1,3-dimethyl-5-(naphthalen-2-ylmethylene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (6e)



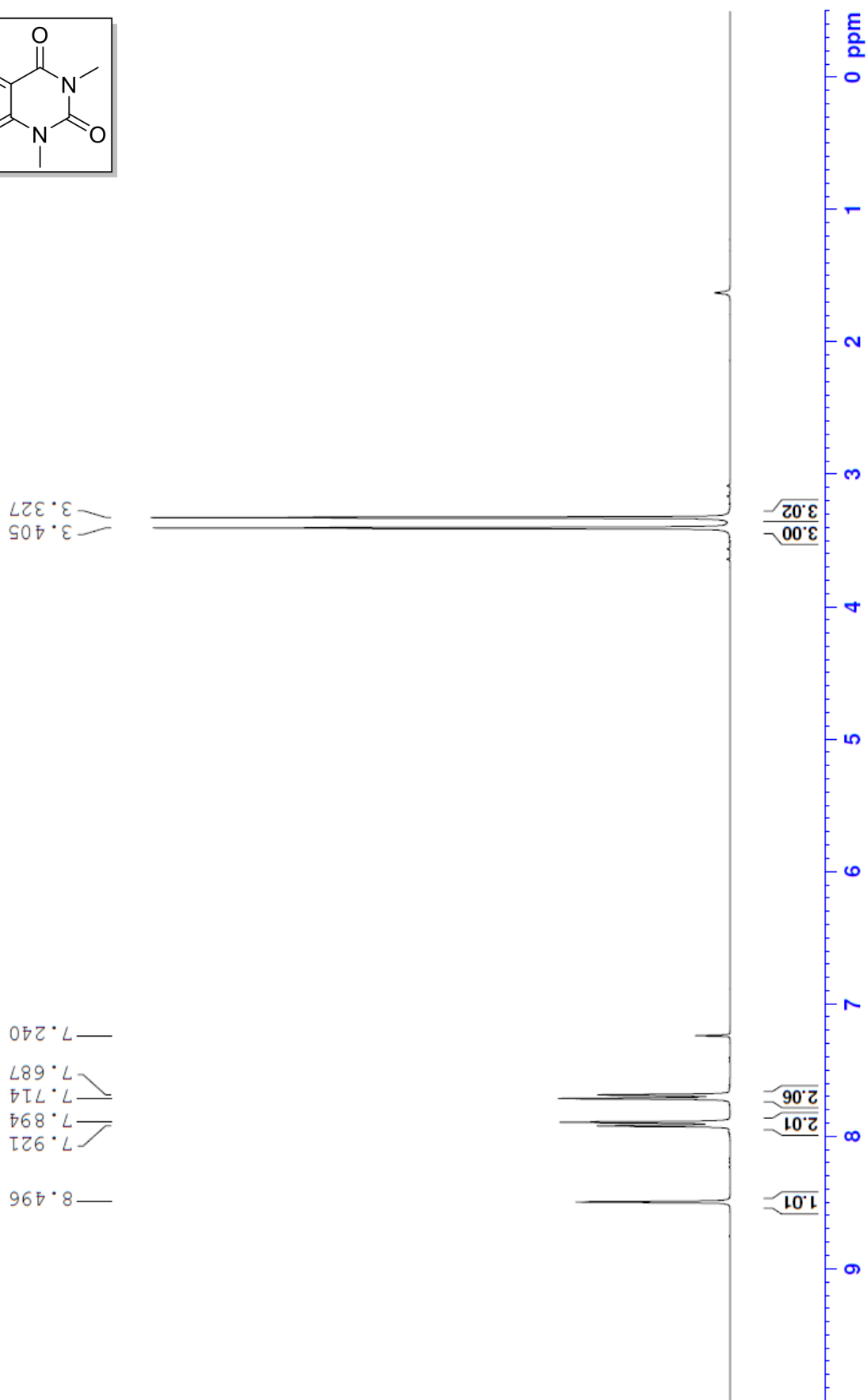
AK-3-166-C AVANCE-300B  
C-13 with Decoupling



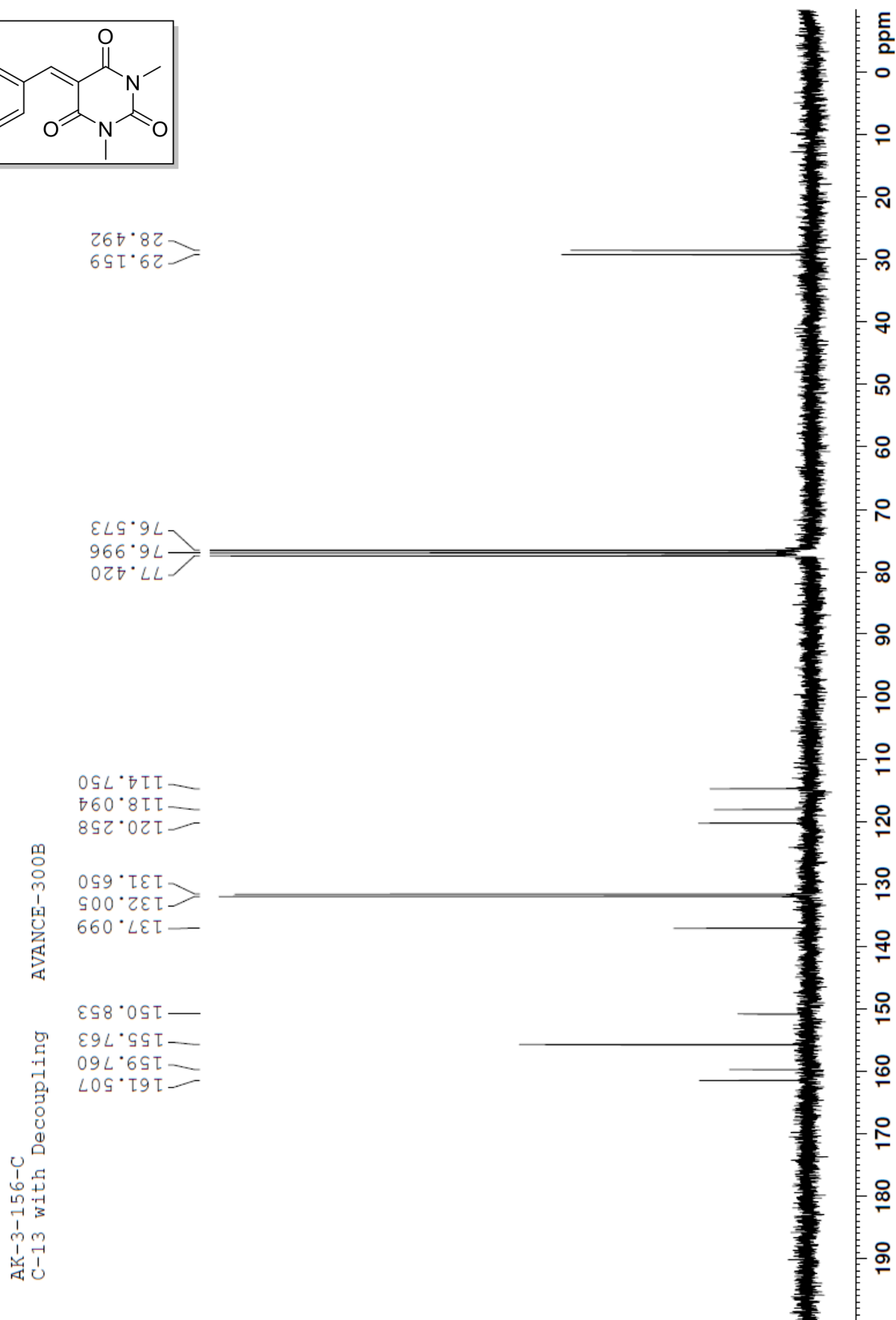
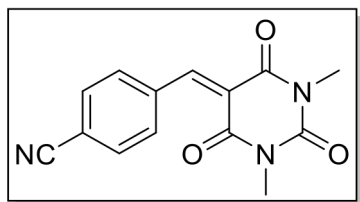
<sup>1</sup>H NMR spectra of 4-((1,3-dimethyl-2,4,6-trioxotetrahydropyrimidin-5(2H)-ylidene)methyl)benzonitrile (6f)



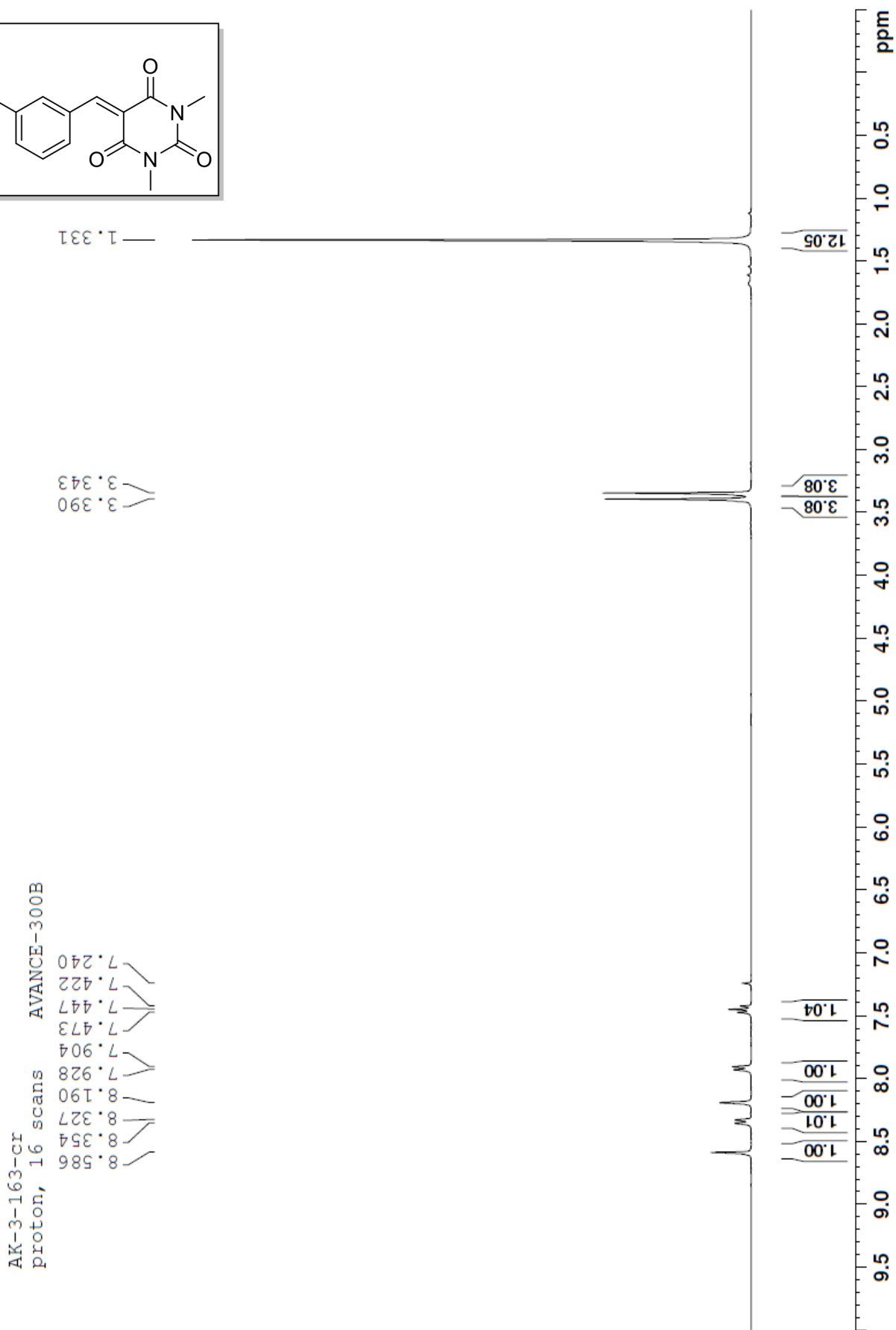
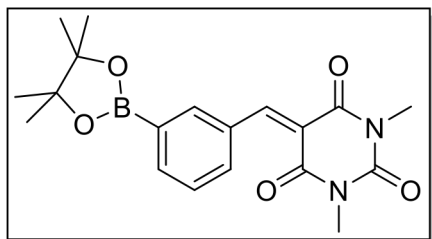
AK-3-156-H  
proton, 16 scans AVANCE-300B



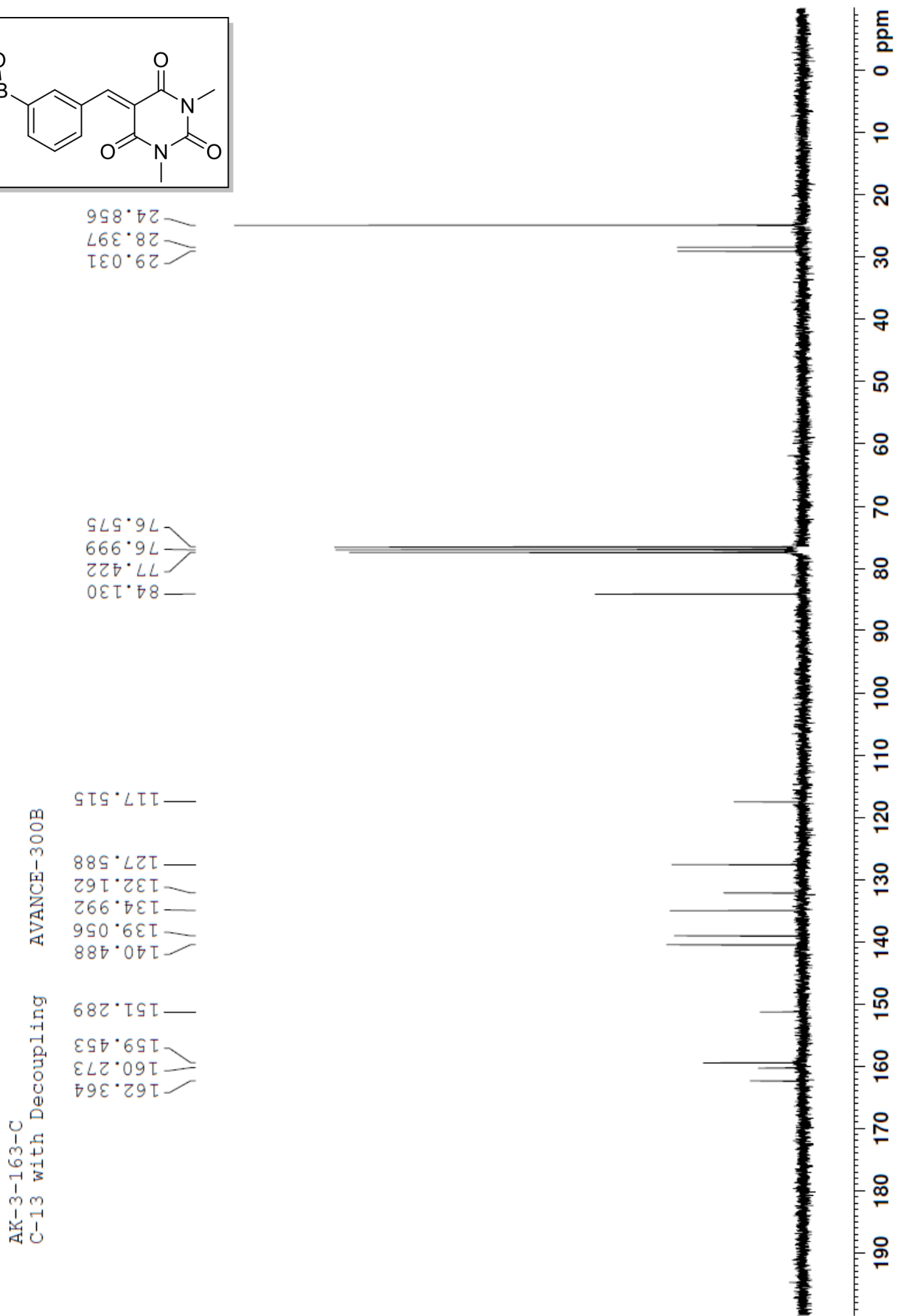
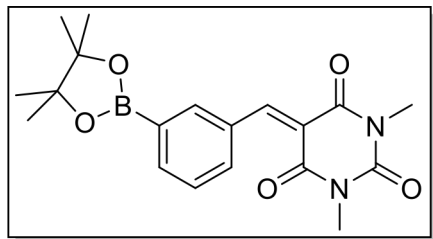
<sup>13</sup>C NMR spectra of 4-((1,3-dimethyl-2,4,6-trioxotetrahydropyrimidin-5(2H)-ylidene)methyl)benzonitrile (6f)



<sup>1</sup>H NMR Spectra of 1,3-dimethyl-5-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzylidene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6g**)

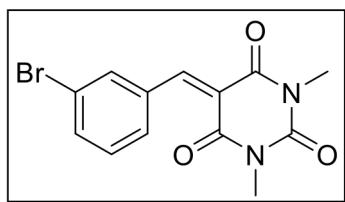


<sup>13</sup>C NMR Spectra of 1,3-dimethyl-5-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzylidene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6g**)





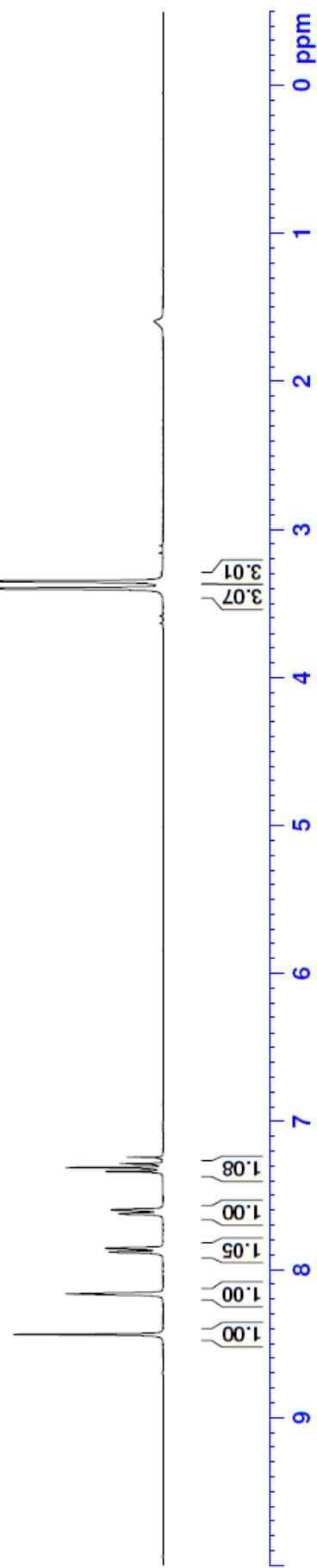
<sup>1</sup>H NMR Spectra of 5-(3-bromobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (6h)



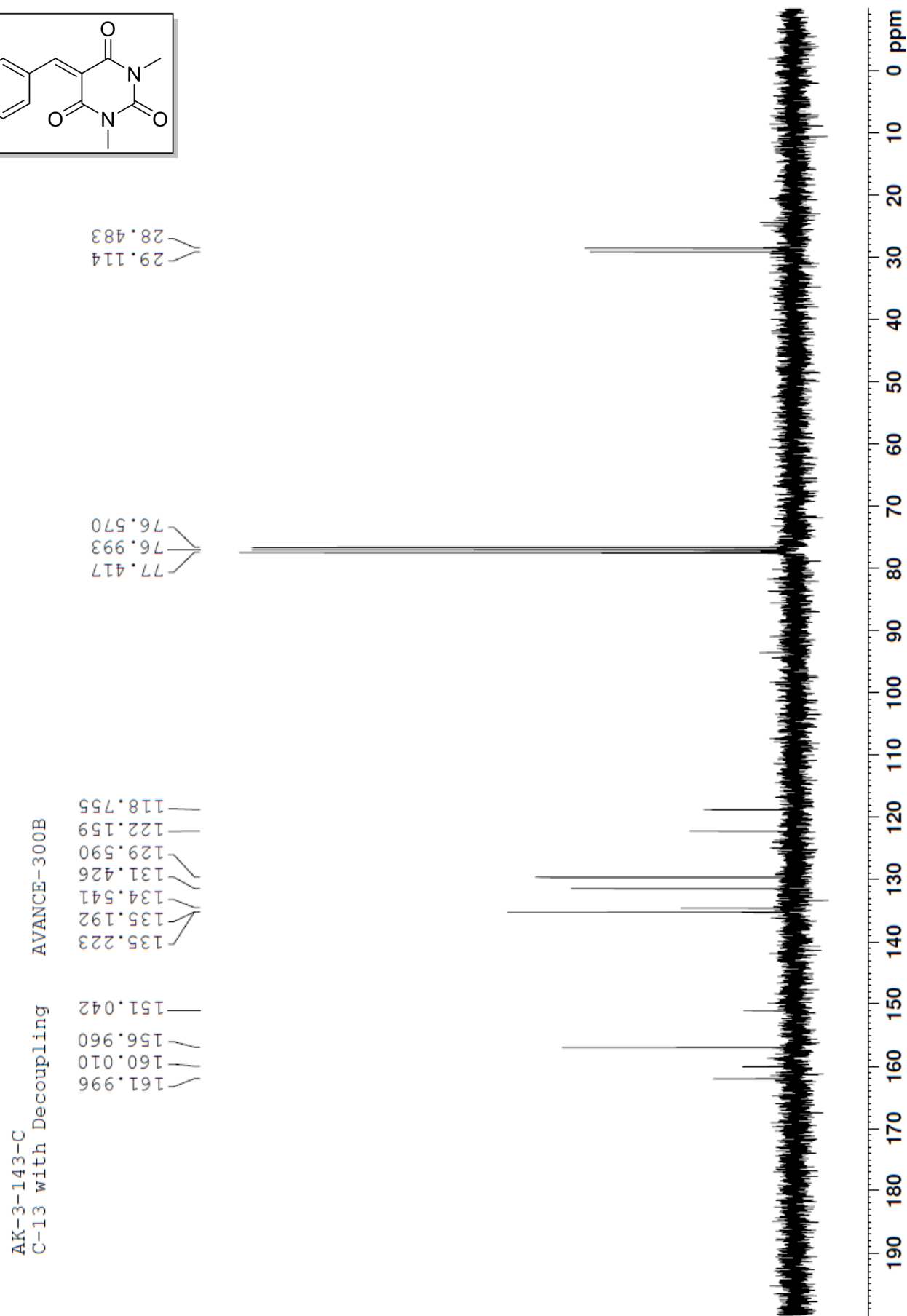
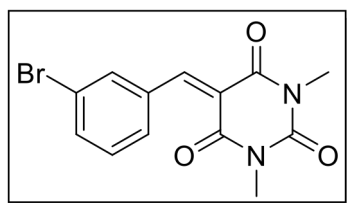
AK-3-143  
proton, 16 scans AVANCE-300B

8.438  
8.164  
7.882  
7.856  
7.624  
7.597  
7.337  
7.311  
7.285  
7.240

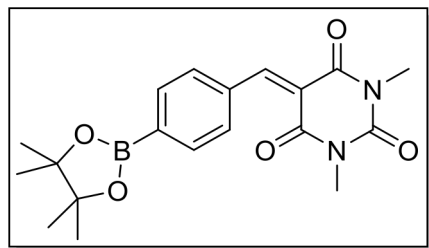
3.397  
3.348



<sup>13</sup>C NMR Spectra of 5-(3-bromobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6h**)



$^1\text{H}$  NMR spectra of 1,3-dimethyl-5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzylidene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6i**)



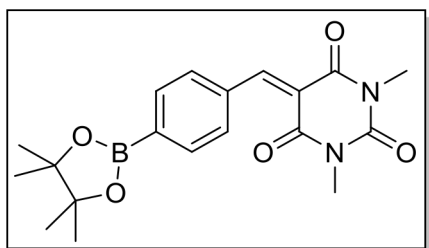
AK-3-162-recryst  
proton, 16 scans  
AVANCE-300B

8.554  
7.934  
7.908  
7.868  
7.842  
7.240  
3.395  
3.336  
1.328

1.00  
2.01  
2.02  
3.00  
3.02  
12.08

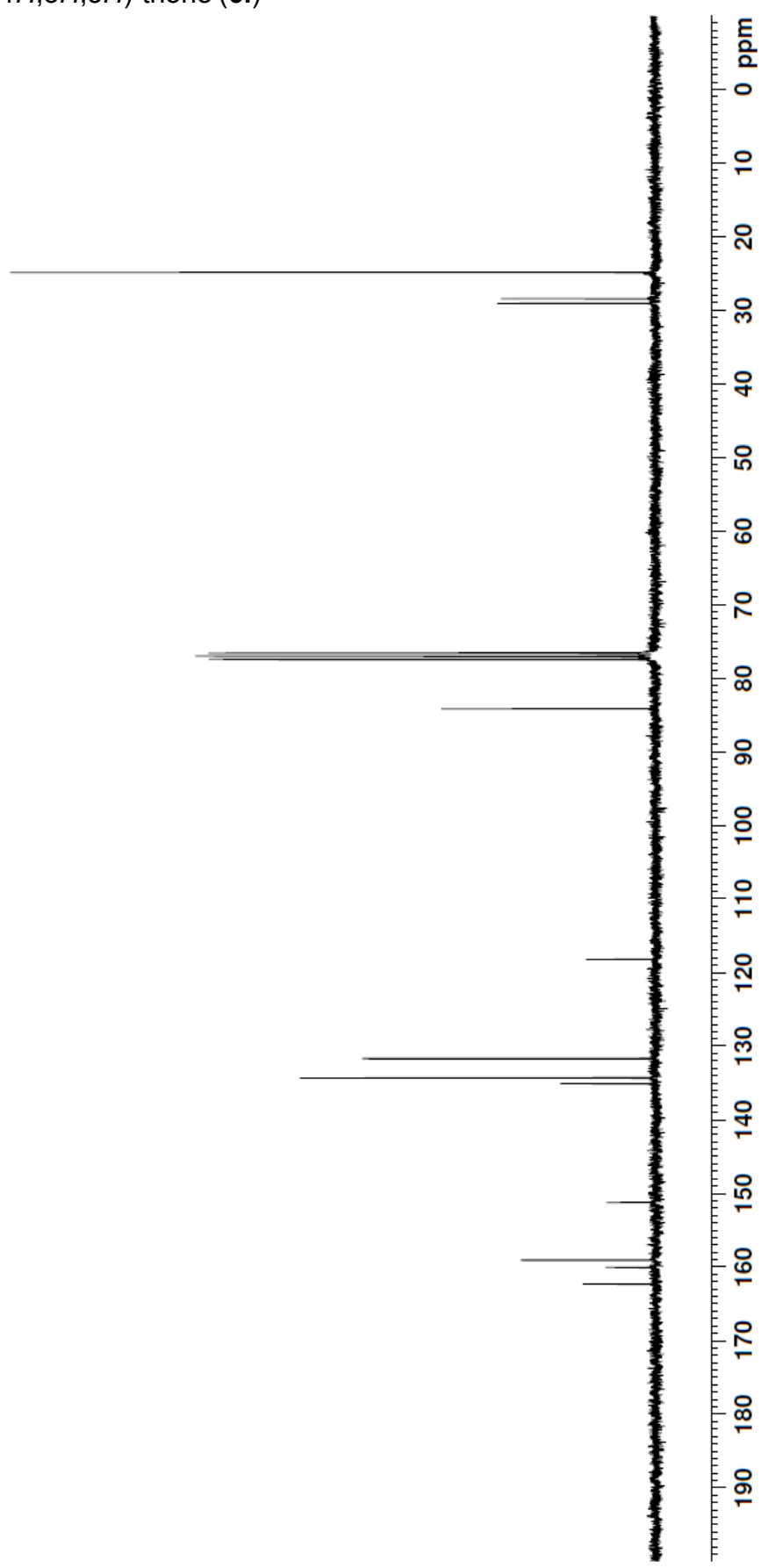


<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzylidene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6i**)

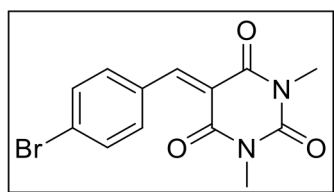


AK-3-162-C-2  
C-13 with Decoupling  
AVANCE-300B

- 29.037
- 28.393
- 24.821
- 84.129
- 77.417
- 76.994
- 76.570
- 162.297
- 160.067
- 159.052
- 151.219
- 135.073
- 134.312
- 131.684
- 118.200



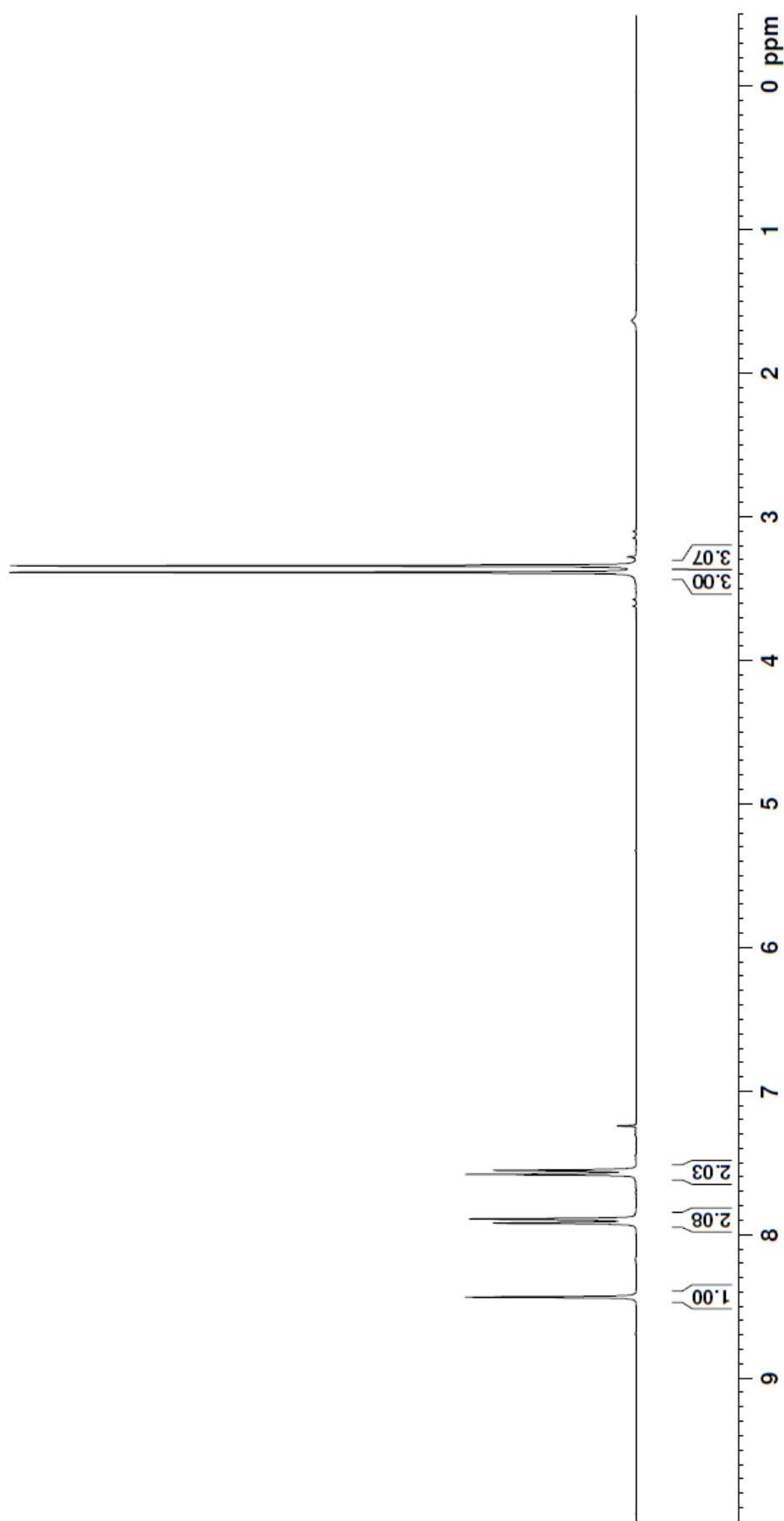
<sup>1</sup>H NMR spectra of 5-(4-bromobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6j**)



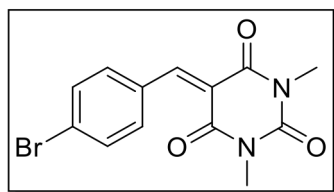
AK-3-160  
proton, 16 scans AVANCE-300B

8.433  
7.917  
7.889  
7.578  
7.549  
7.240

3.384  
3.337



<sup>13</sup>C NMR spectra of 5-(4-bromobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6j**)



AK-3-160-C  
C-13 with Decoupling

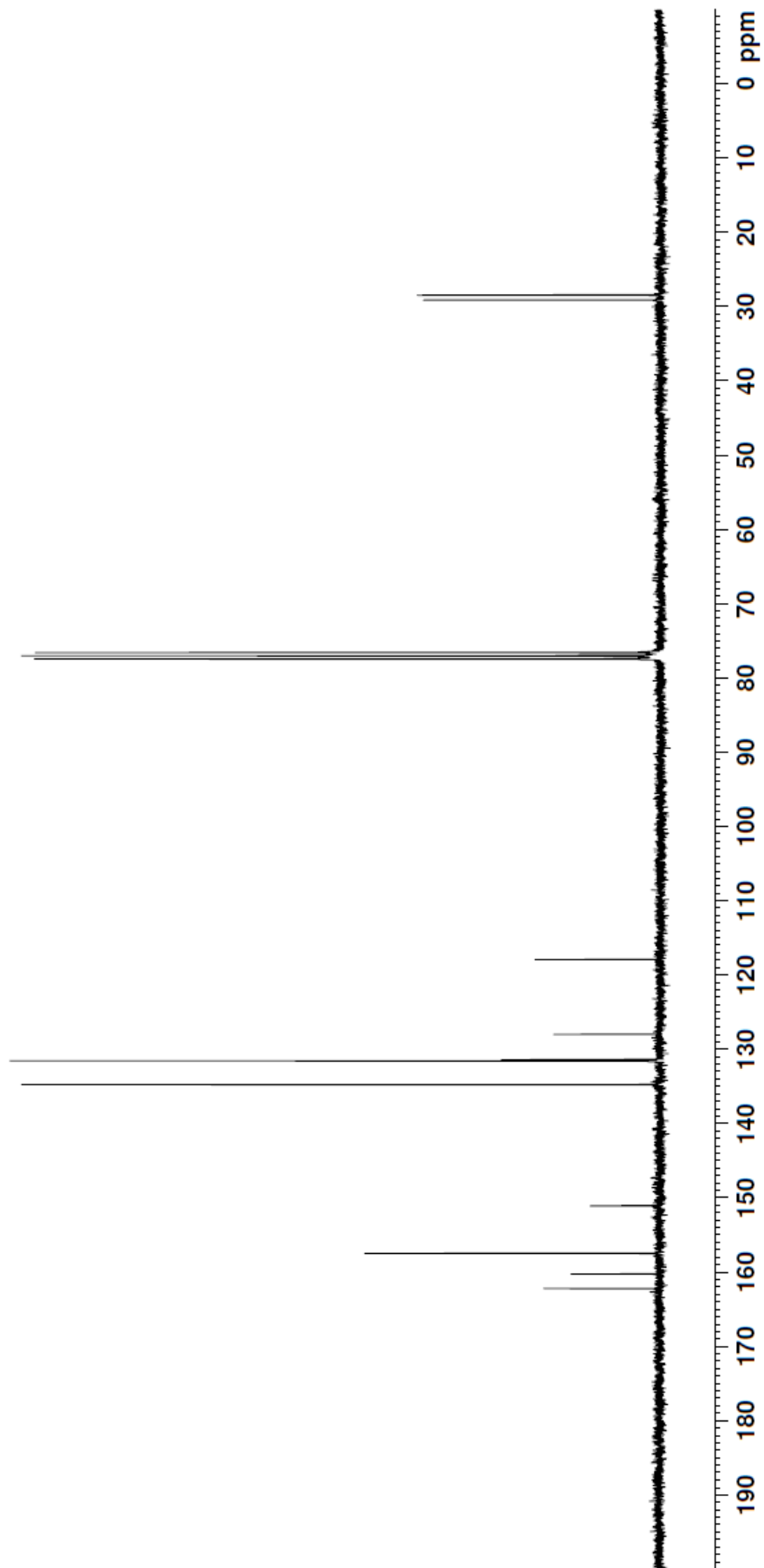
AVANCE-300B

162.210  
160.263  
157.462  
151.054

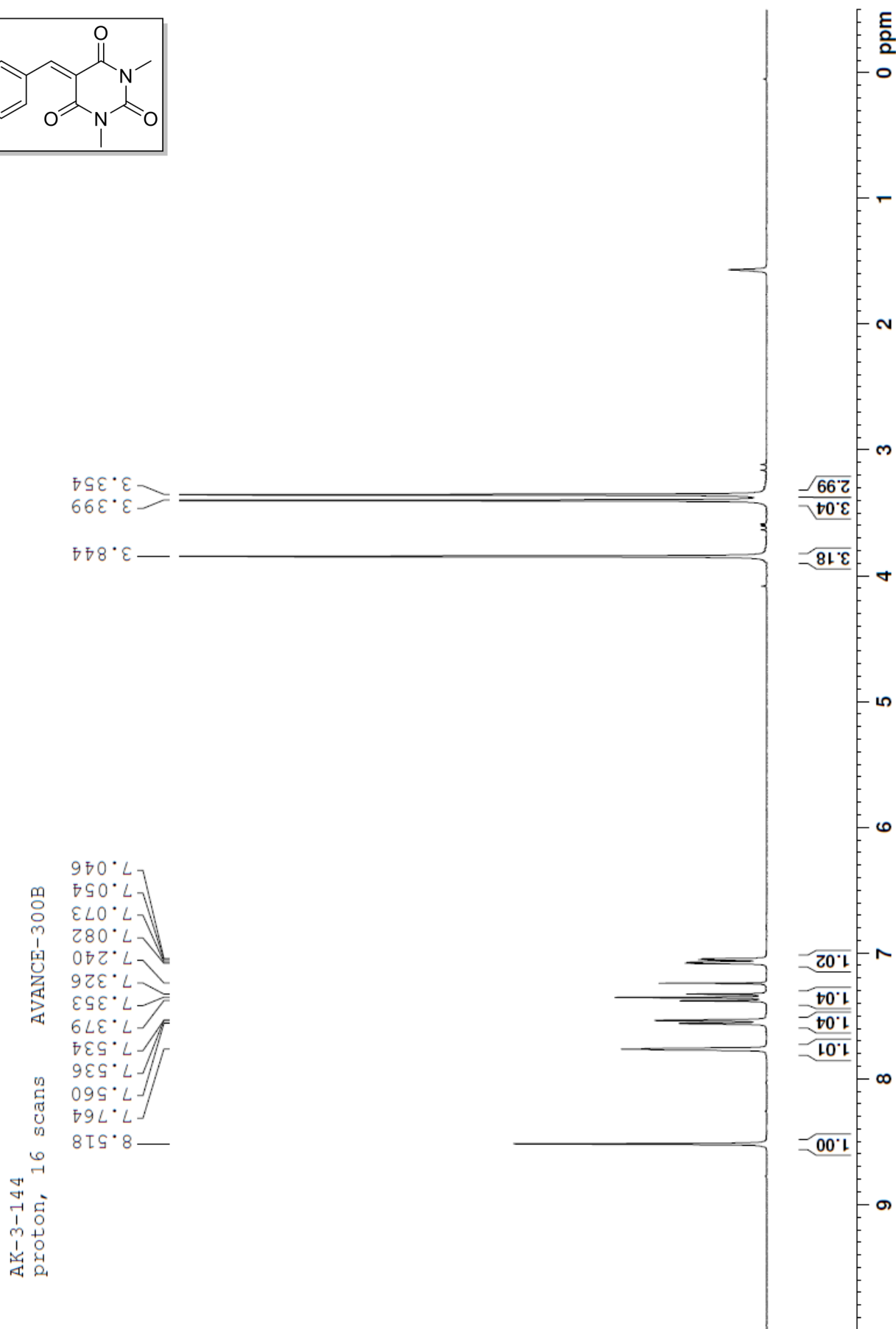
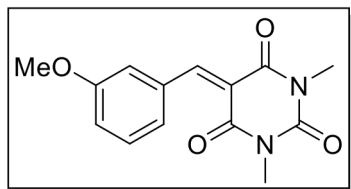
134.750  
131.552  
131.380  
127.963  
117.906

77.418  
76.995  
76.571

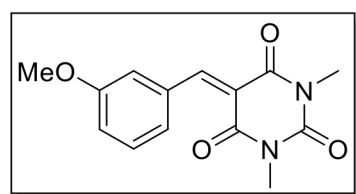
29.084  
28.419



<sup>1</sup>H NMR spectra of 5-(3-methoxybenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6k**)



<sup>13</sup>C NMR spectra of 5-(3-methoxybenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6k**)



AK-3-144-C  
C-13 with Decoupling

AVANCE-300B

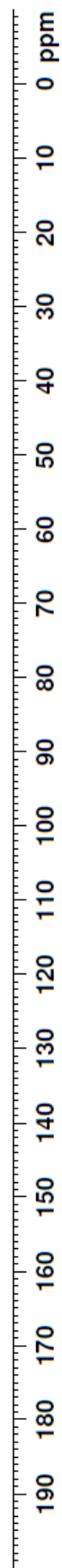
162.507  
160.281  
159.177  
159.118  
151.225

133.800  
129.160  
126.577  
119.385  
117.668  
117.636

77.420  
76.997  
76.573

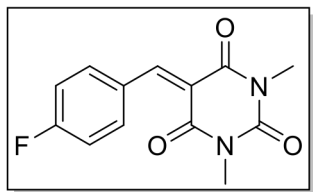
55.415

29.094  
28.454





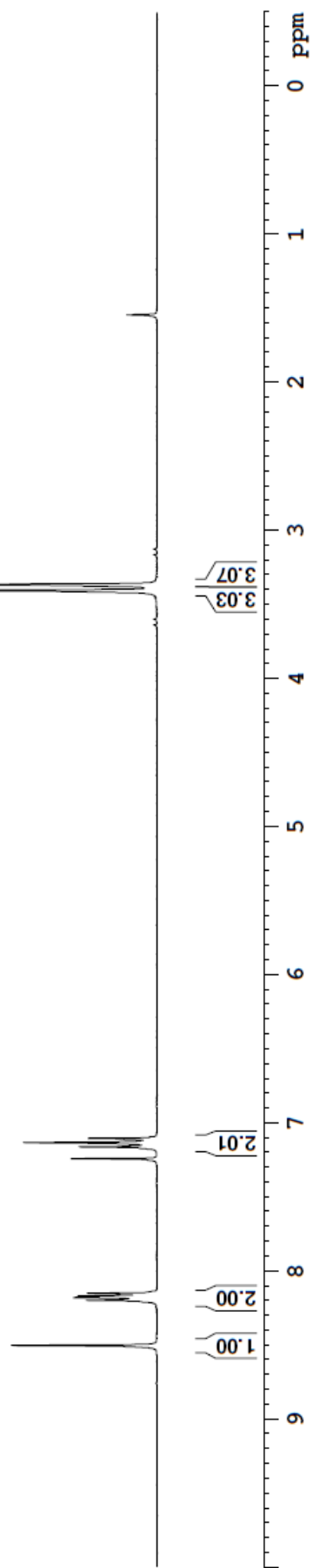
<sup>1</sup>H NMR spectra of 5-(4-fluorobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**61**)



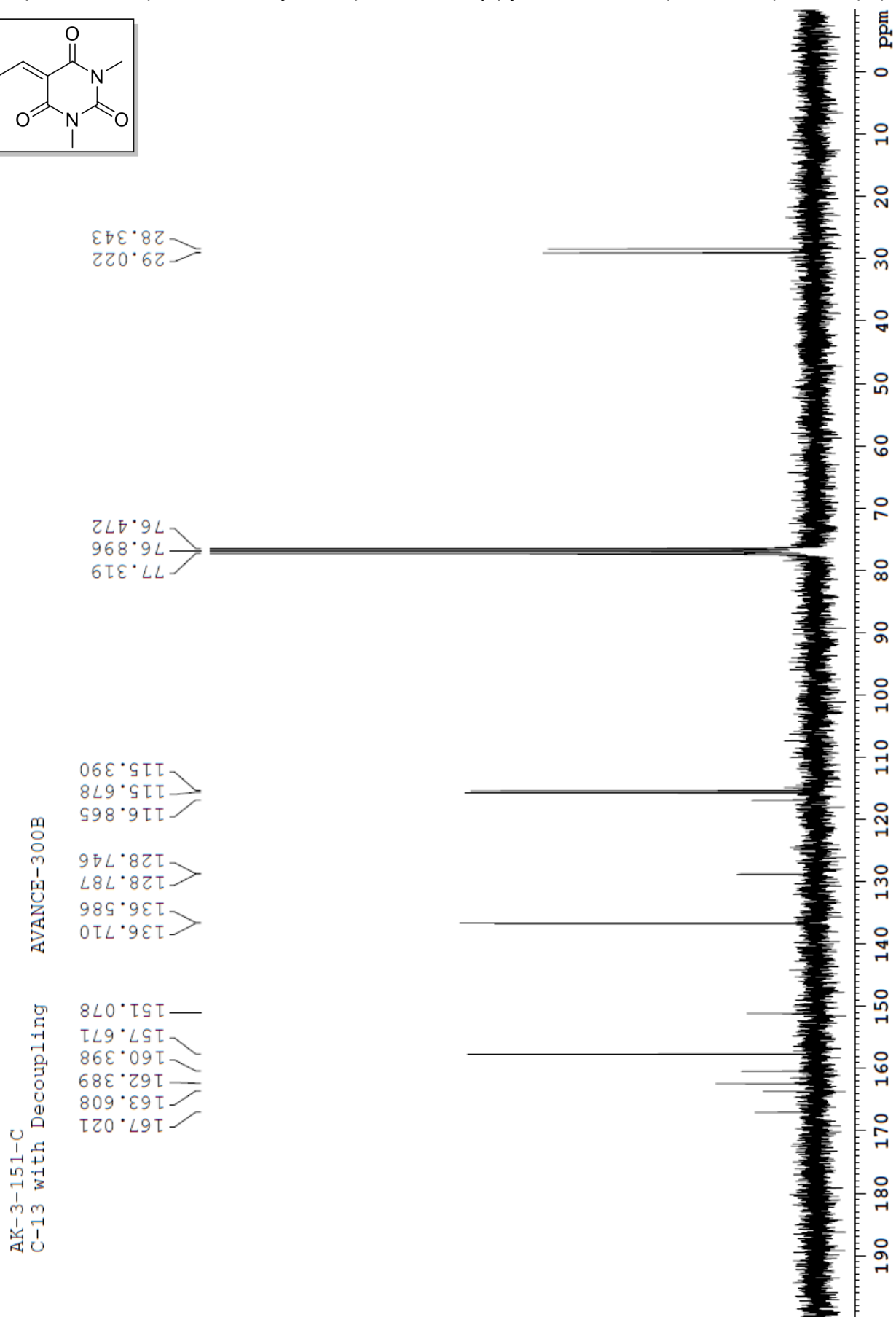
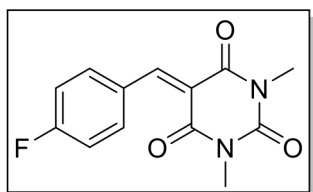
AK-3-151  
proton, 16 scans AVANCE-300B

8.501  
8.197  
8.190  
8.179  
8.168  
8.149  
7.240  
7.161  
7.154  
7.132  
7.103  
7.093

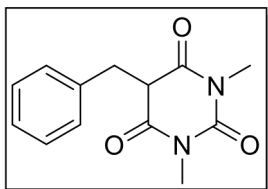
3.402  
3.362



<sup>13</sup>C NMR spectra of 5-(4-fluorobenzylidene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**6l**)



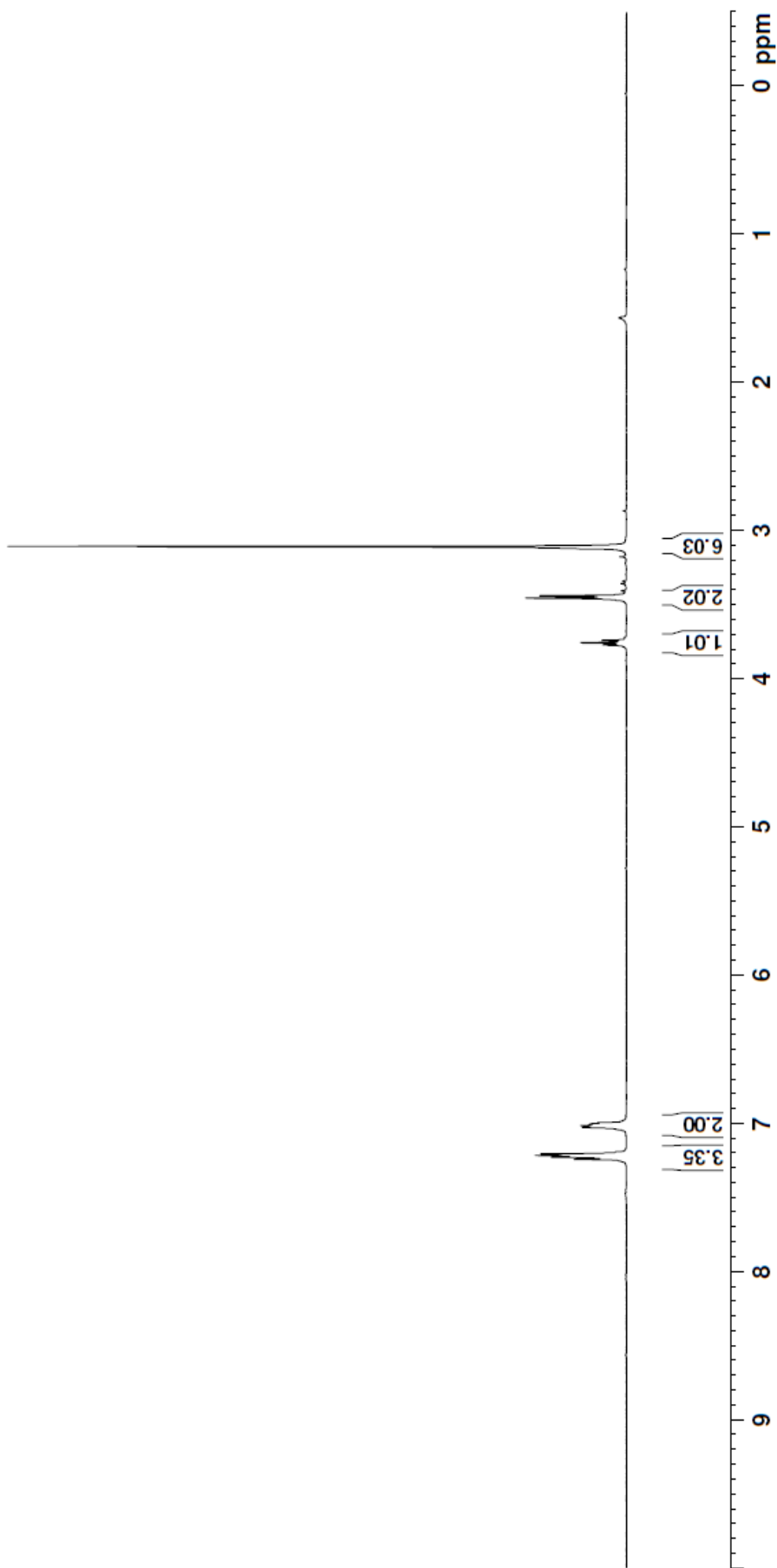
<sup>1</sup>H NMR spectra of 5-benzylidene-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7a**)



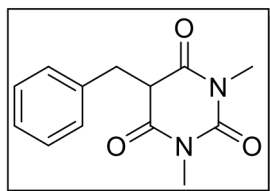
AK-3-155-F-H  
proton, 16 scans AVANCE-300B

7.240  
7.226  
7.214  
7.205  
7.025  
7.013  
7.002  
6.994

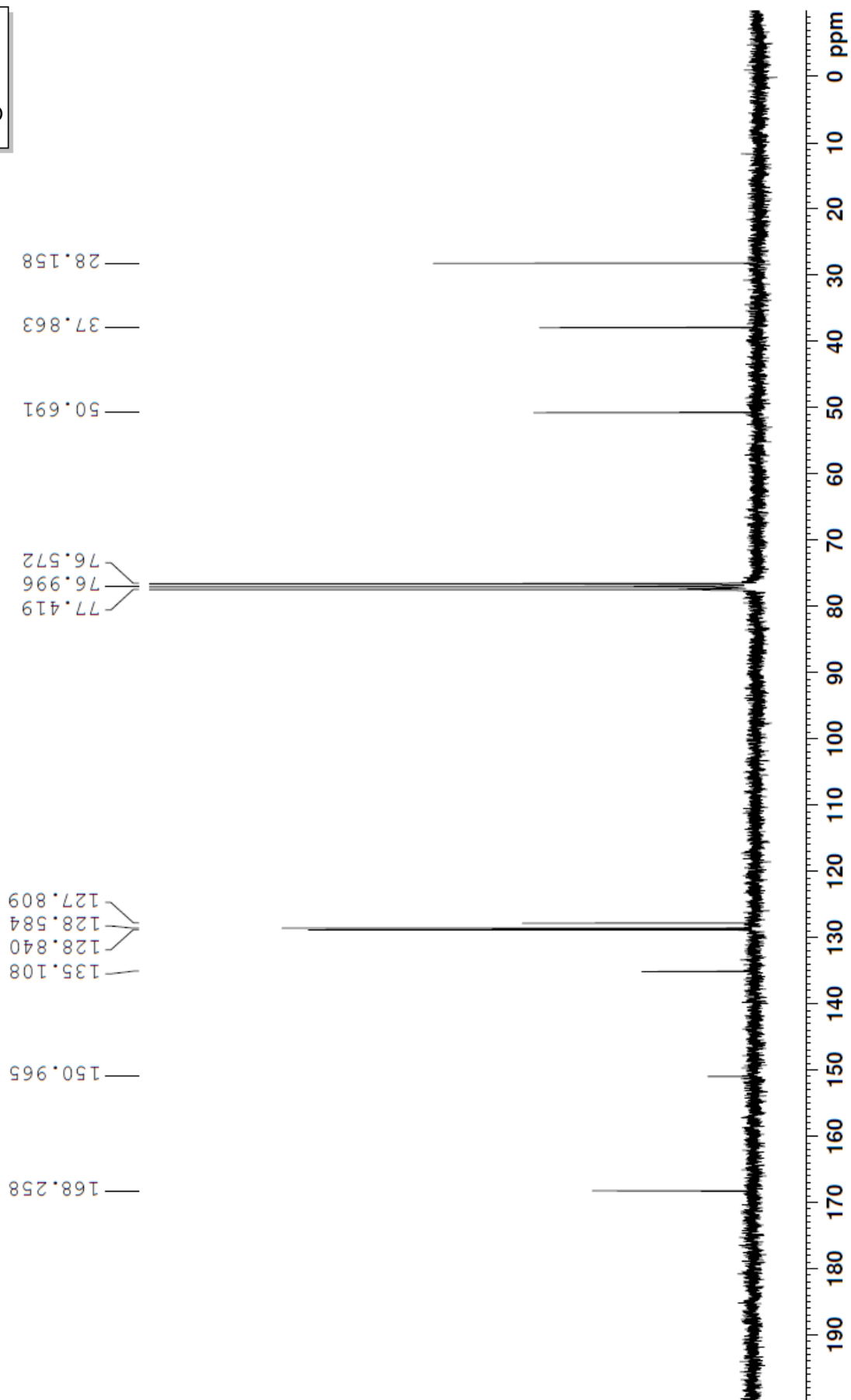
3.770  
3.754  
3.739  
3.453  
3.438  
3.174  
3.105



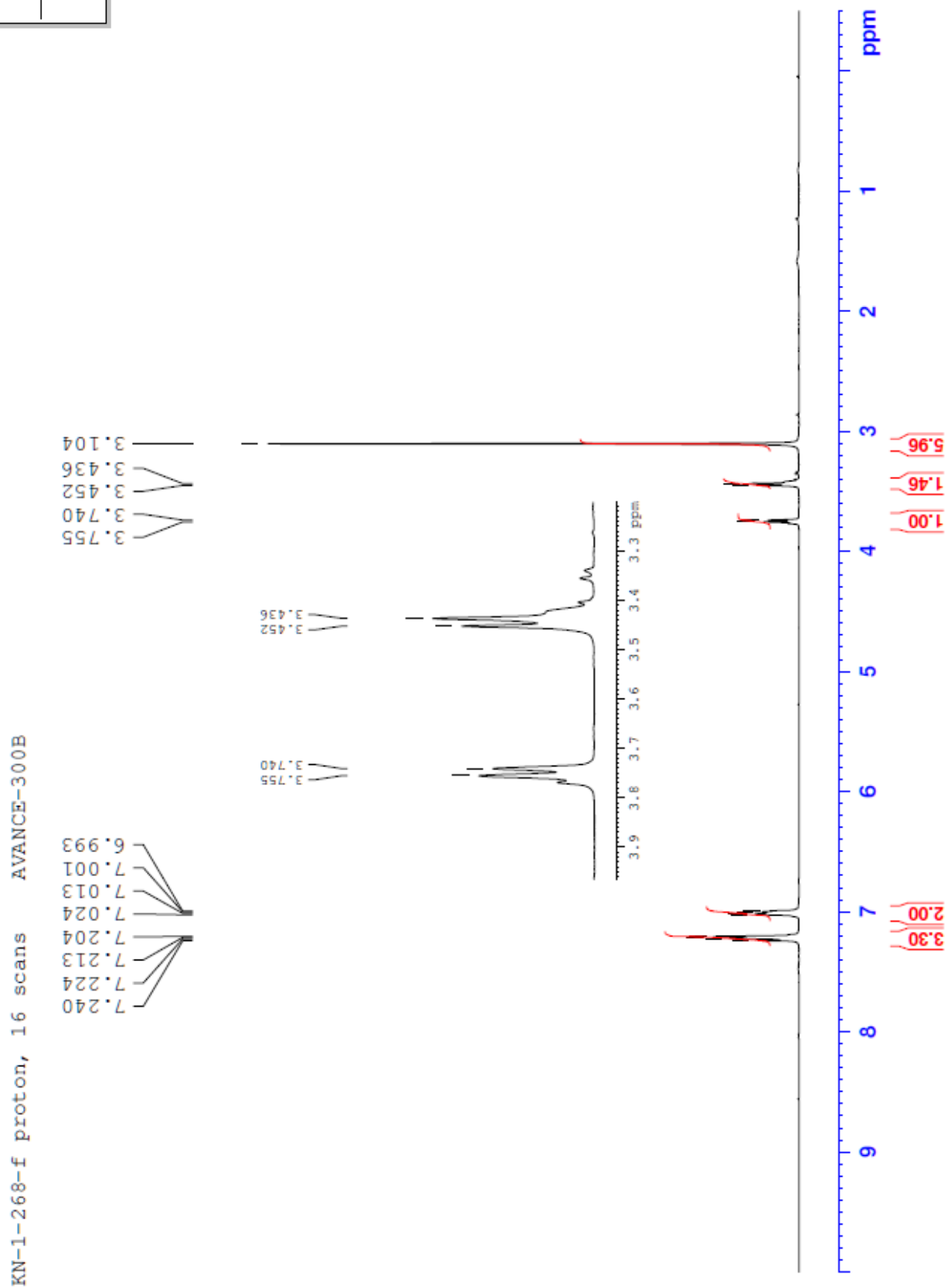
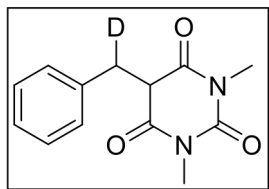
<sup>13</sup>C NMR spectra of 5-benzylidene-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7a)



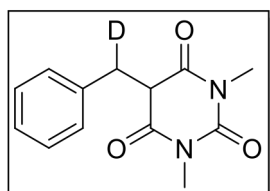
AK-3-155-F-C AVANCE-300B  
C-13 with Decoupling



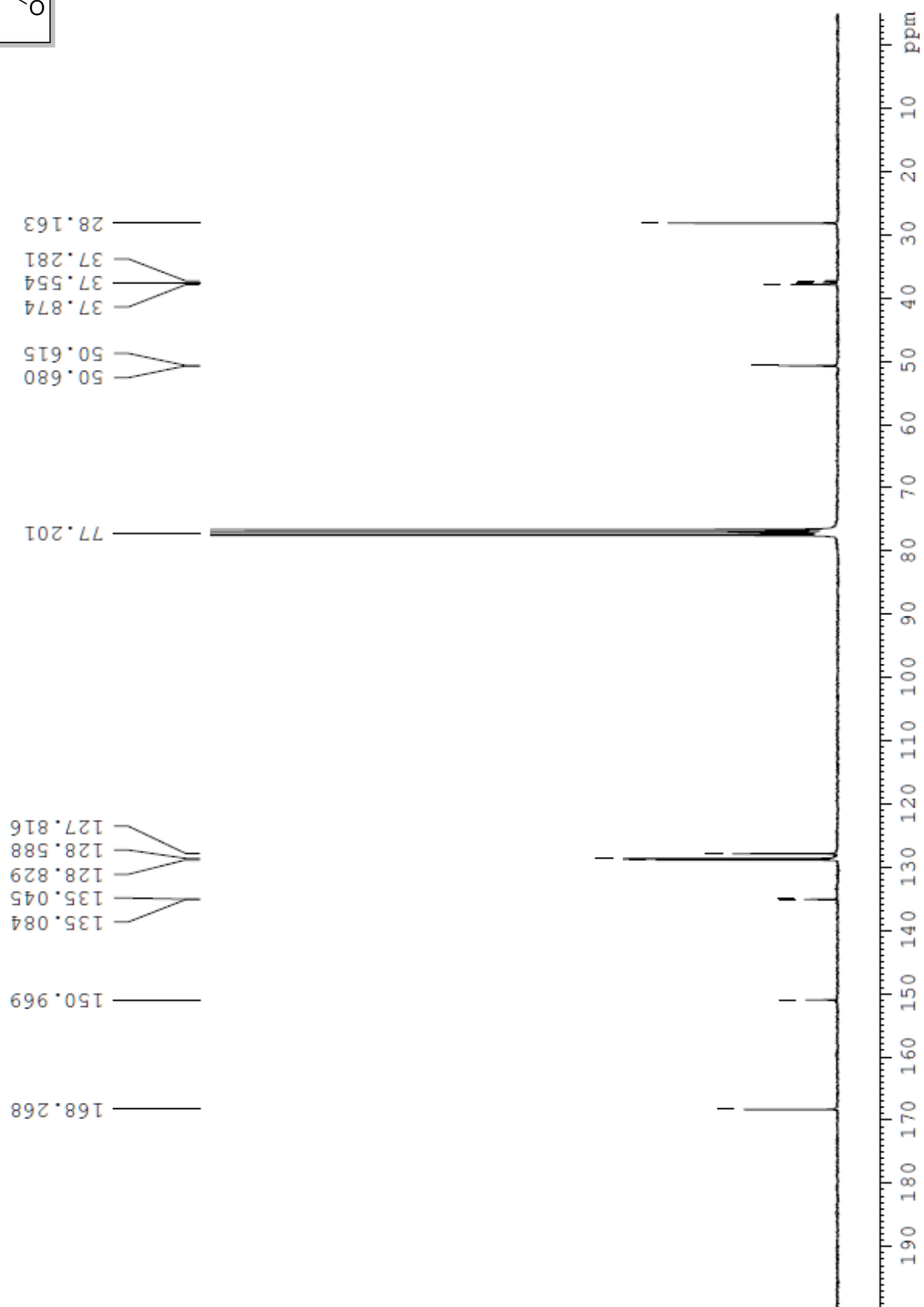
<sup>1</sup>H NMR spectra of 1,3-dimethyl-5-(phenylmethyl-d)pyrimidine--2,4,6(1H,3H,5H)-trione (**7a-d<sub>1</sub>**)



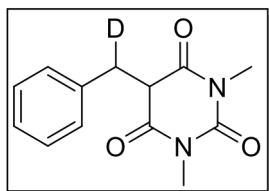
<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(phenylmethyl-*d*)pyrimidine--2,4,6(1*H*,3*H*,5*H*)-trione (**7a-d<sub>1</sub>**)



KN-268-C



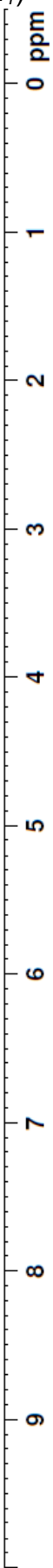
$^2\text{H}$  NMR spectra of 1,3-dimethyl-5-(phenylmethyl-*d*)pyrimidine--2,4,6(1*H*,3*H*,5*H*)-trione (**7a-*d***)



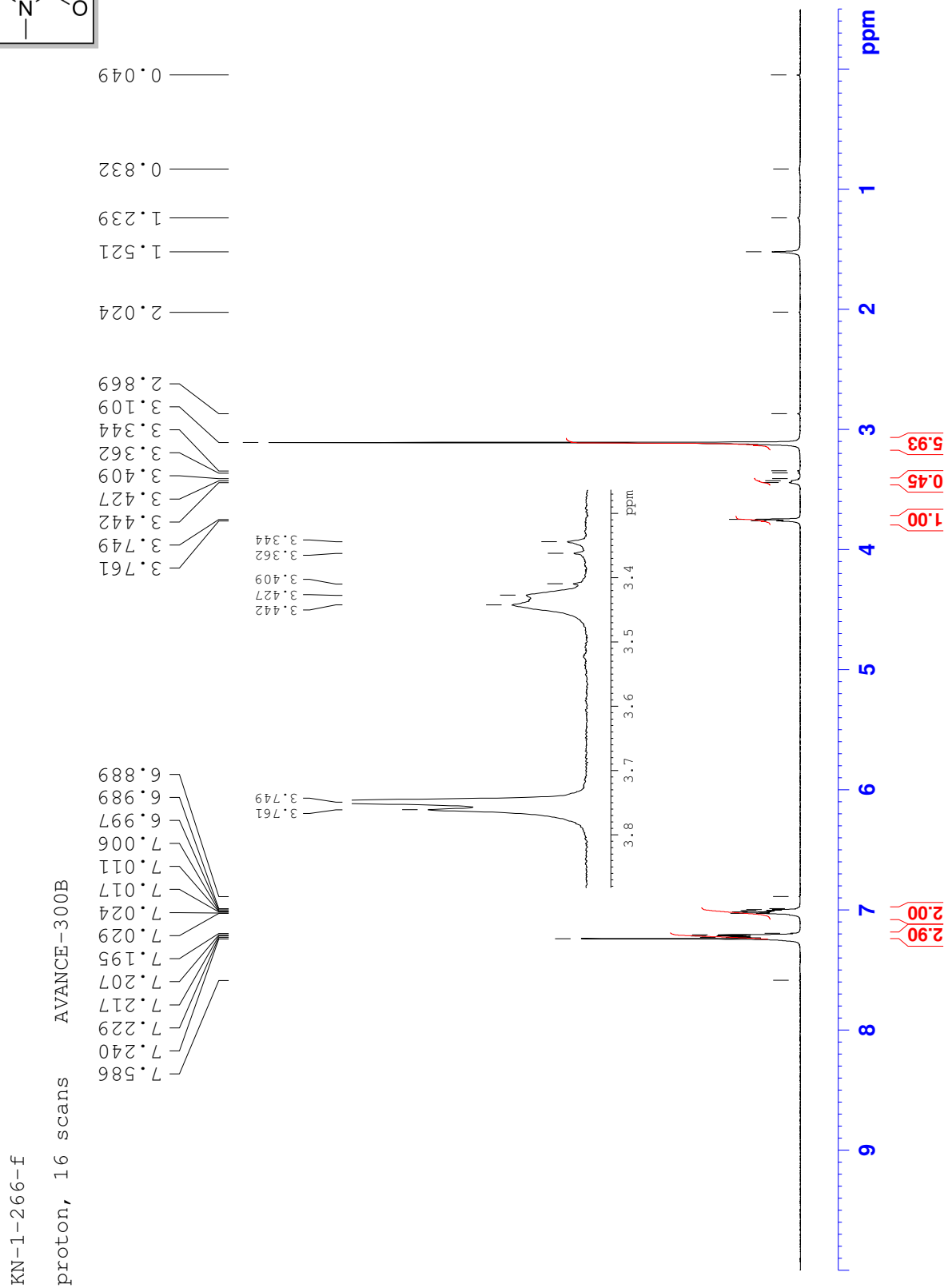
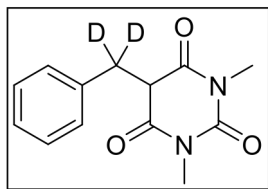
AK-3-286-D  
Deuterium, 300B

7.238

3.452

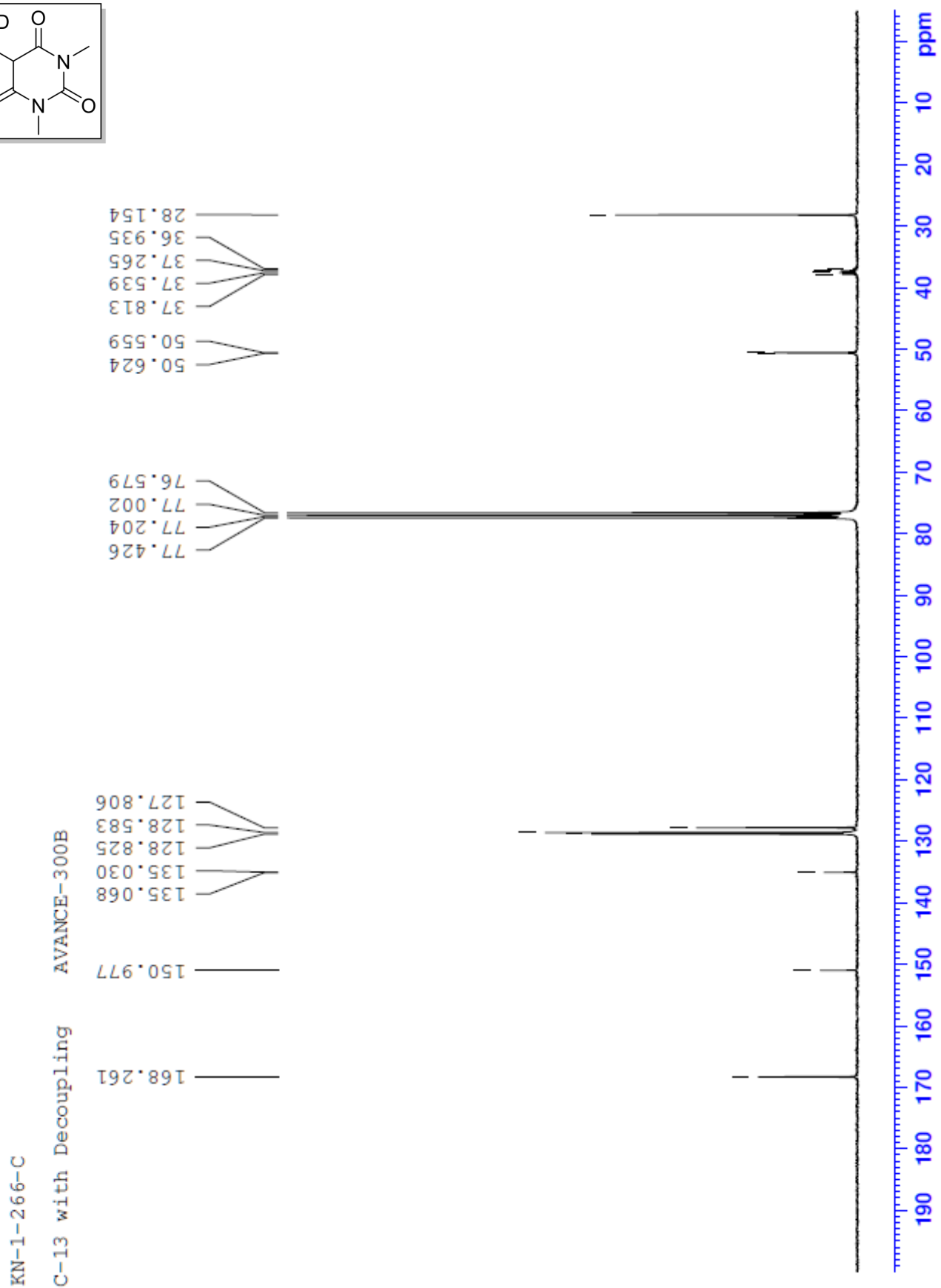
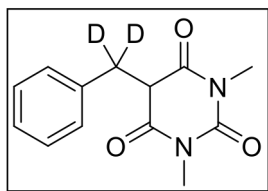


<sup>1</sup>H NMR spectra of 1,3-Dimethyl-5-(phenylmethyl-d<sub>2</sub>)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7a-d<sub>2</sub>**)

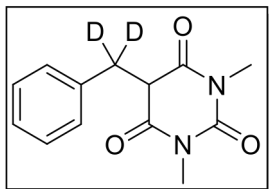




<sup>13</sup>C NMR spectra of 1,3-Dimethyl-5-(phenylmethyl-d<sub>2</sub>)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7a-d<sub>2</sub>**)



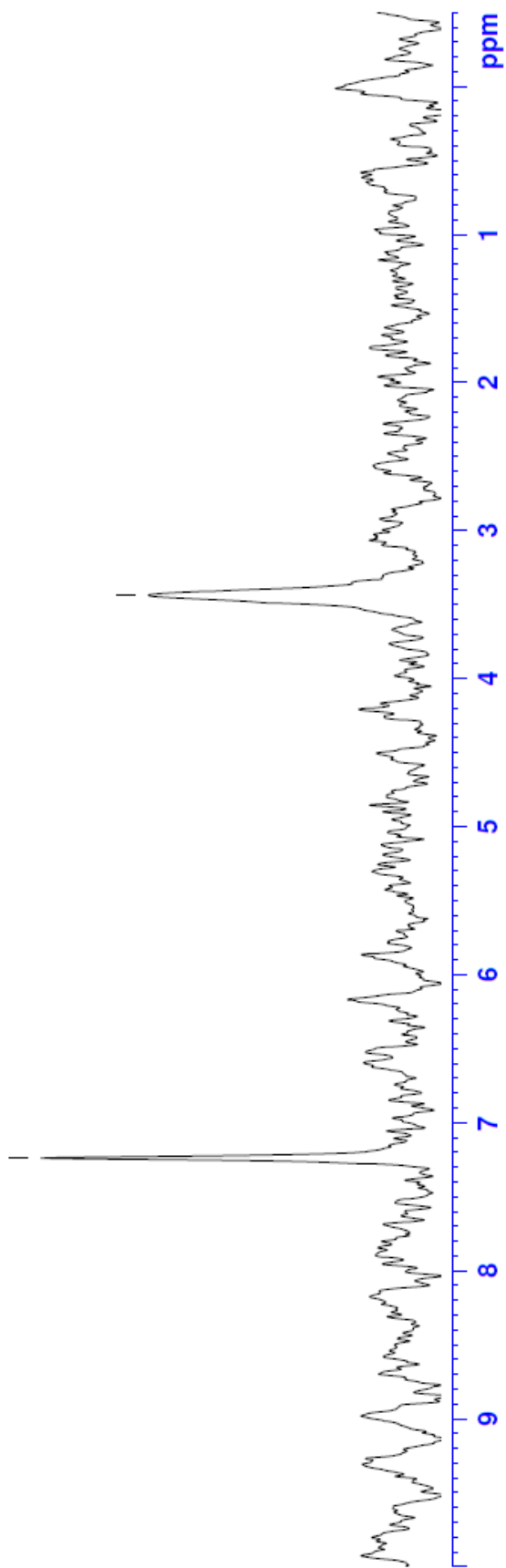
$^2\text{H}$  NMR spectra of 1,3-Dimethyl-5-(phenylmethyl- $d_2$ )pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7a- $d_2$** )



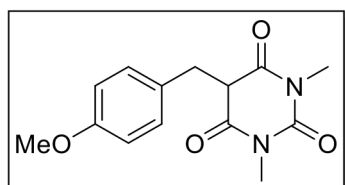
KN-1-259-D  
Deuterium

3.437

7.240



<sup>1</sup>H NMR spectra of 5-(4-methoxybenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7b**)



AK-3-173-F  
proton, 16 scans AVANCE-300B

7.240  
6.941  
6.912  
6.745  
6.716

3.736  
3.714  
3.699  
3.401  
3.386  
3.117

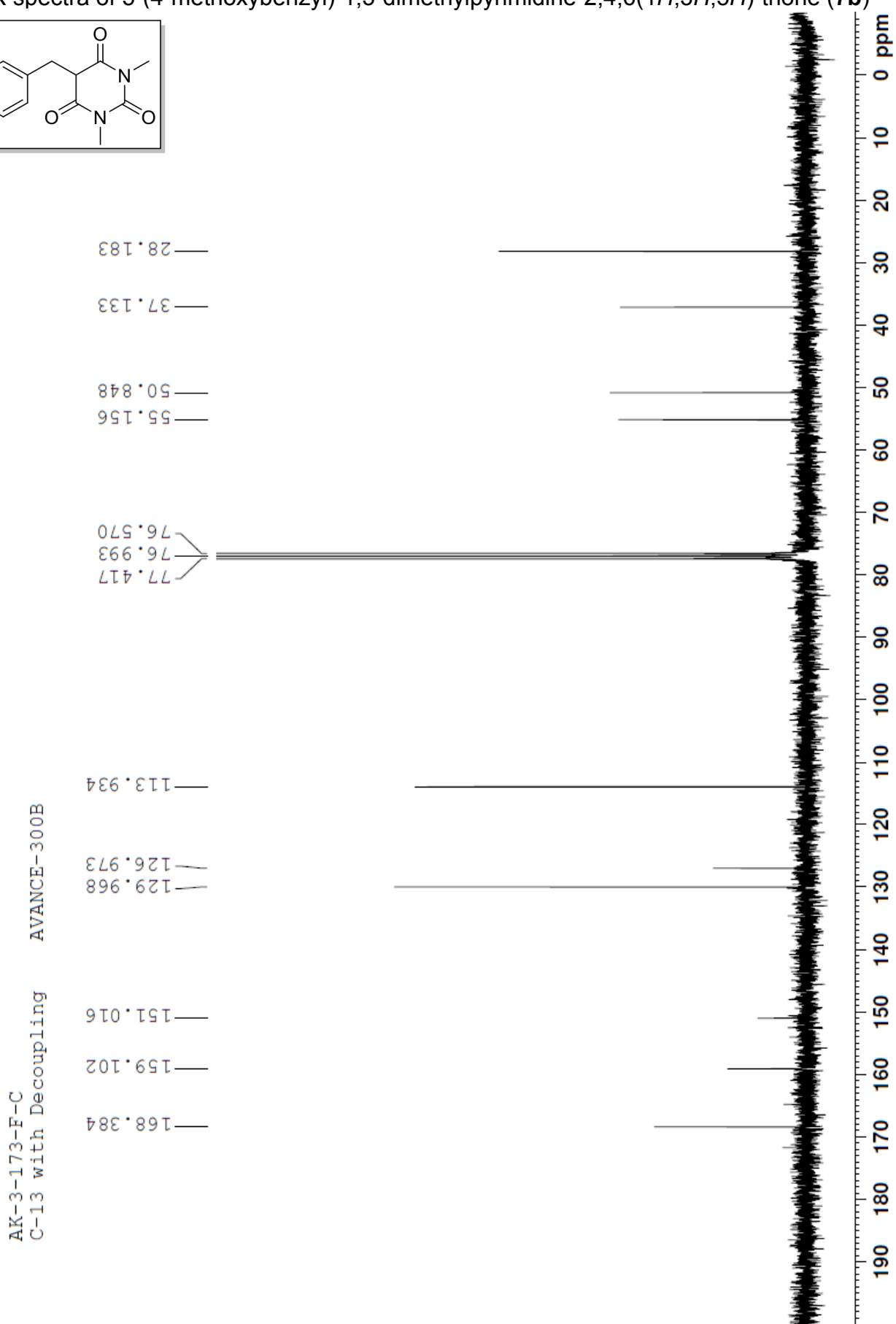
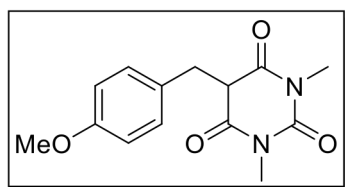
2.00  
2.02

4.02

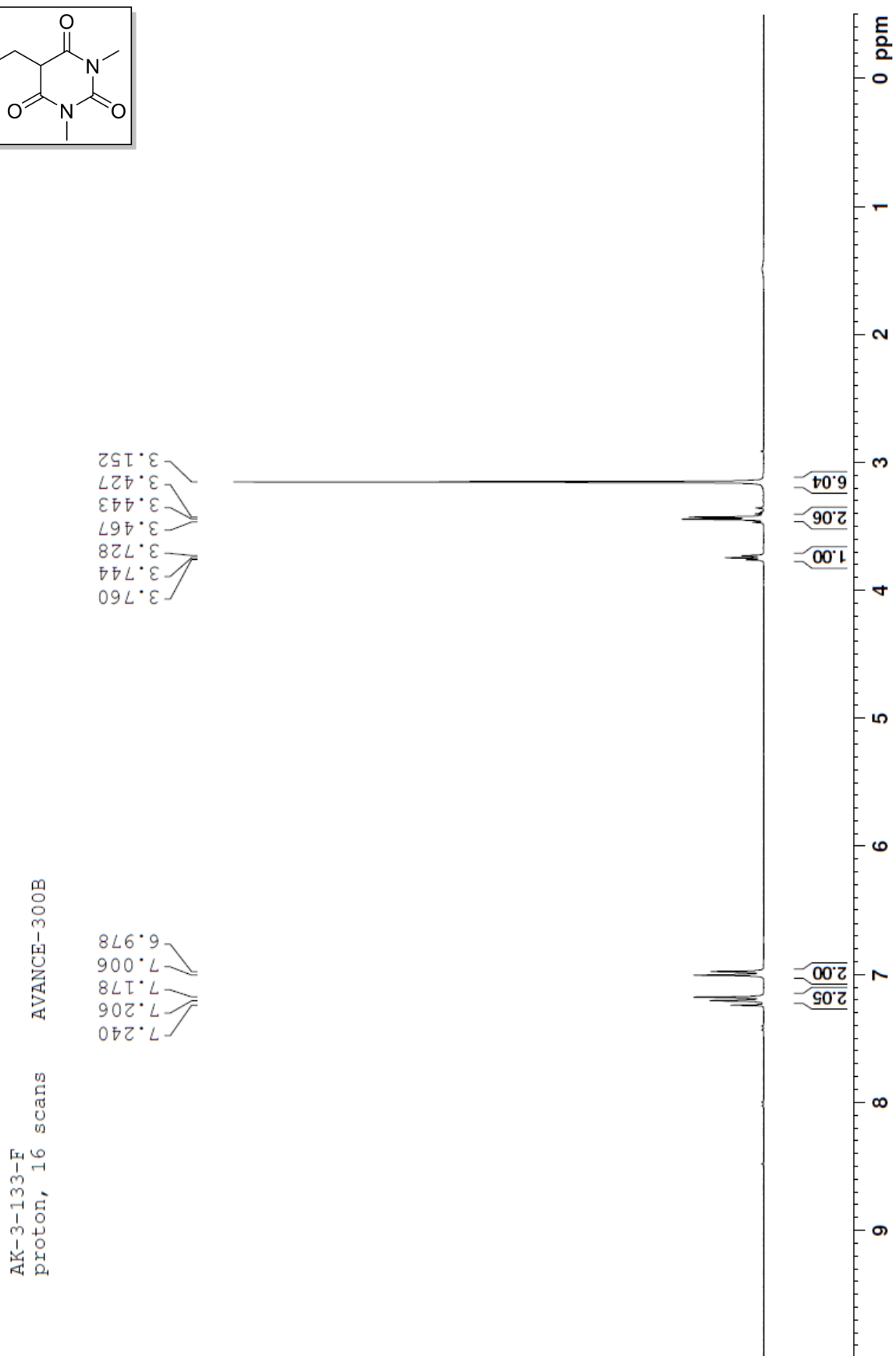
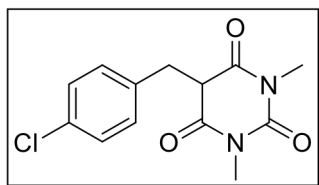
2.06  
6.02



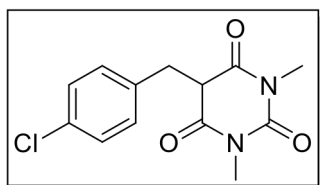
<sup>13</sup>C NMR spectra of 5-(4-methoxybenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7b)



<sup>1</sup>H NMR spectra of 5-(4-Chlorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7c**)

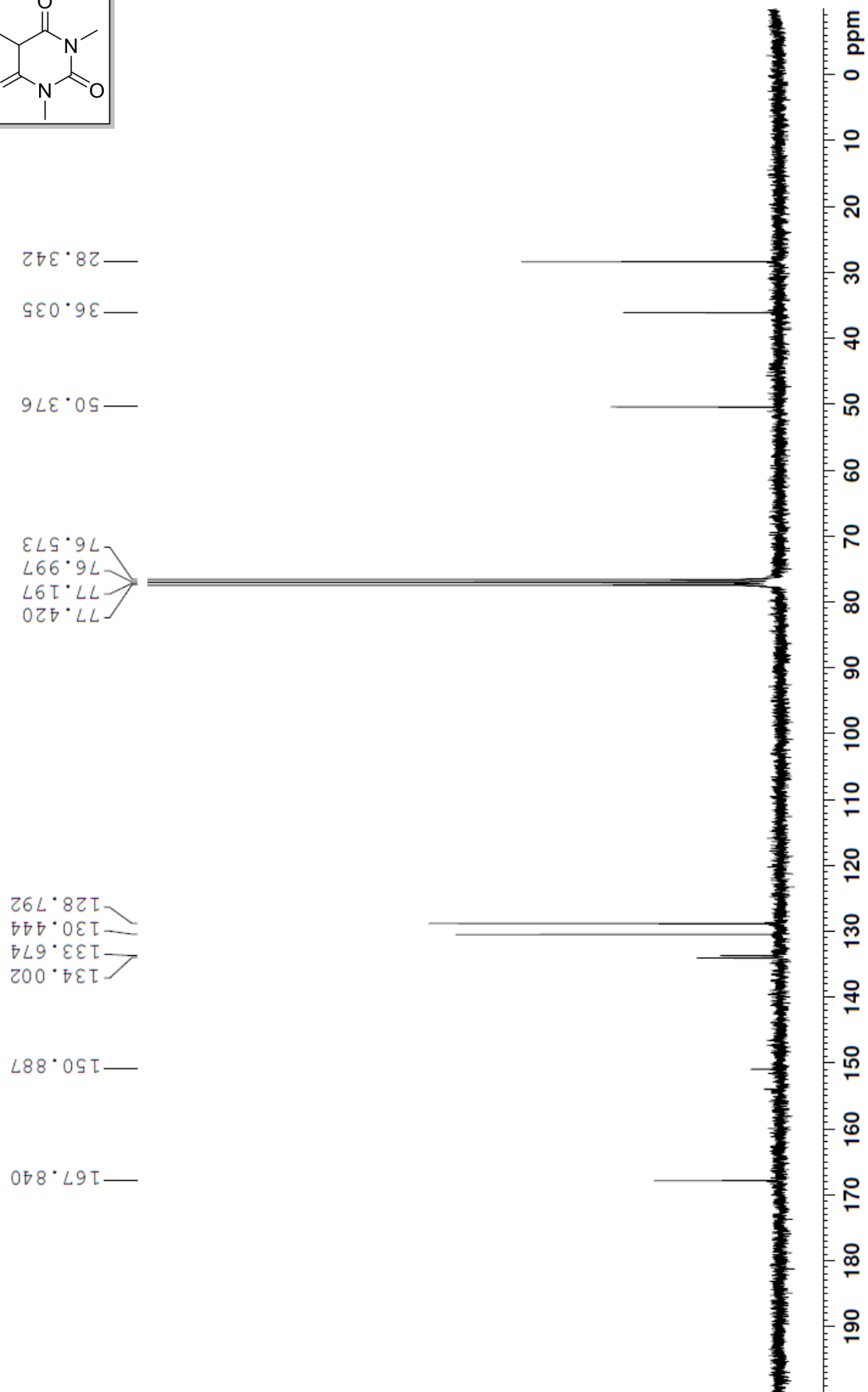


<sup>13</sup>C NMR spectra of 5-(4-Chlorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7c**)

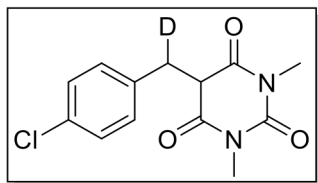


AK-3-133-F-C  
C-13 with Decoupling

AVANCE-300B

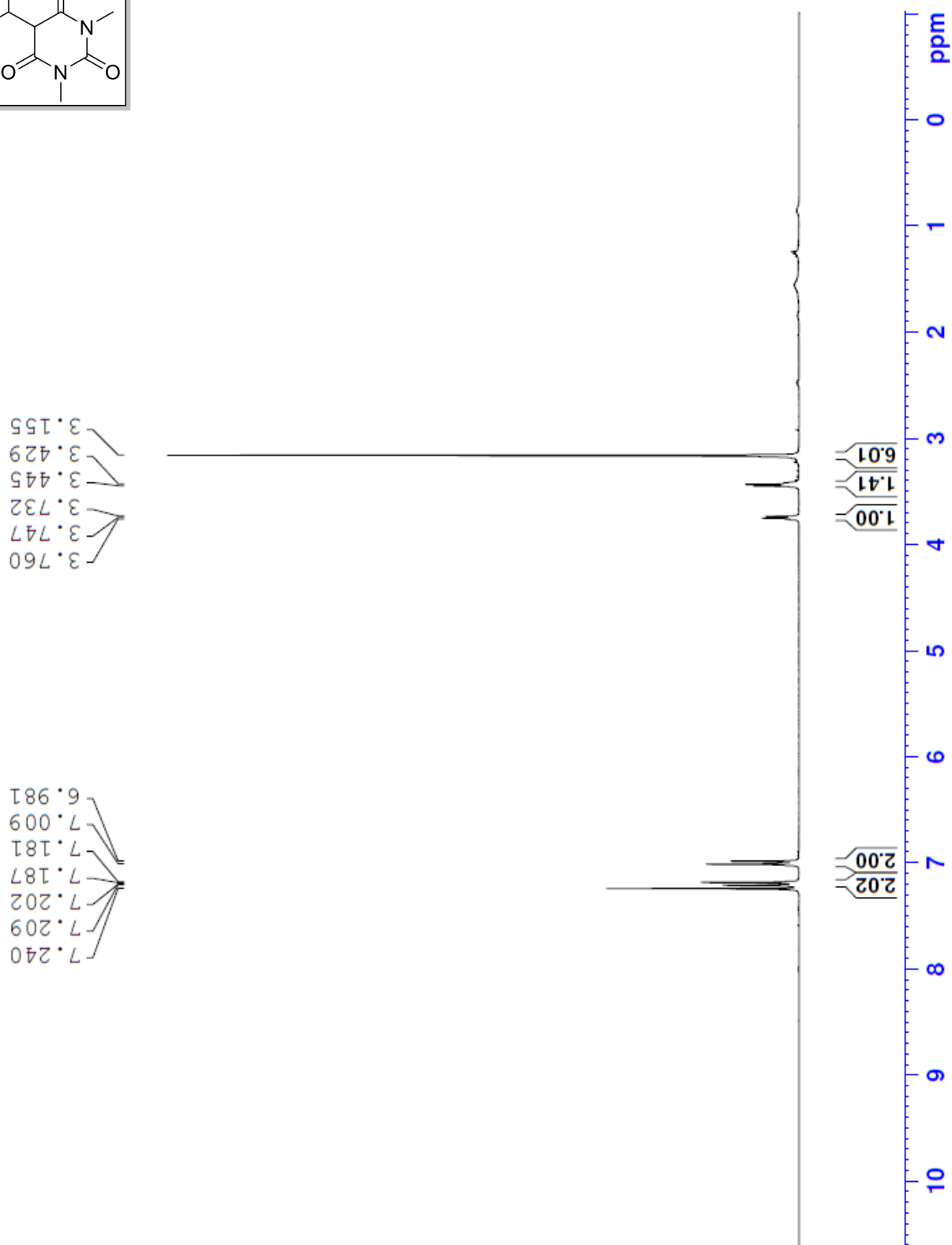


<sup>1</sup>H NMR spectra of 5-((4-Chlorophenyl)methyl-*d*)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7c-d<sub>1</sub>**)

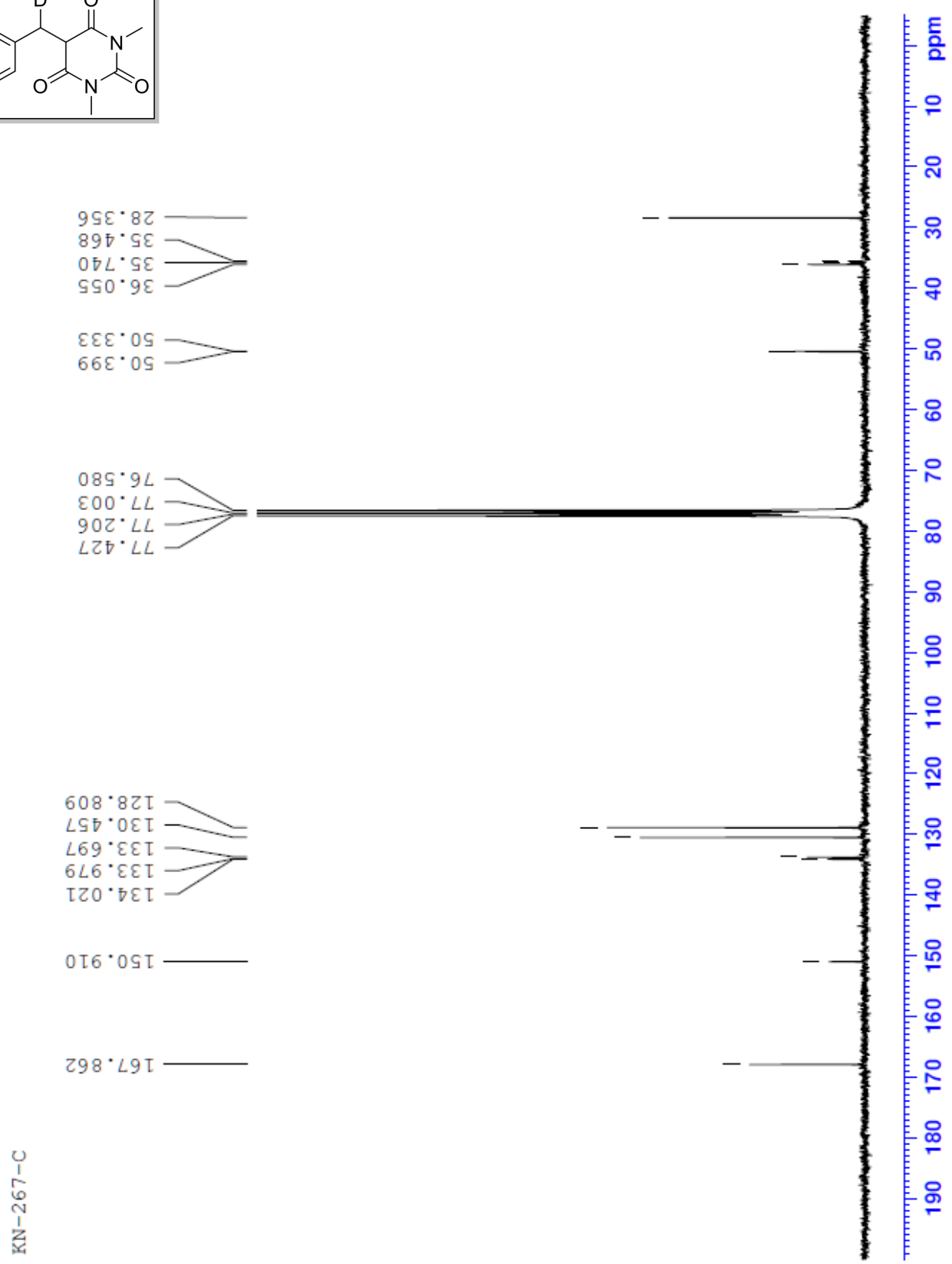
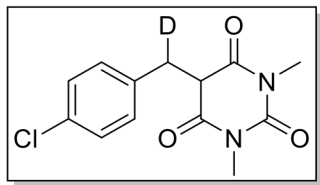


KN-1-267-f  
proton, 16 scans

AVANCE-300B



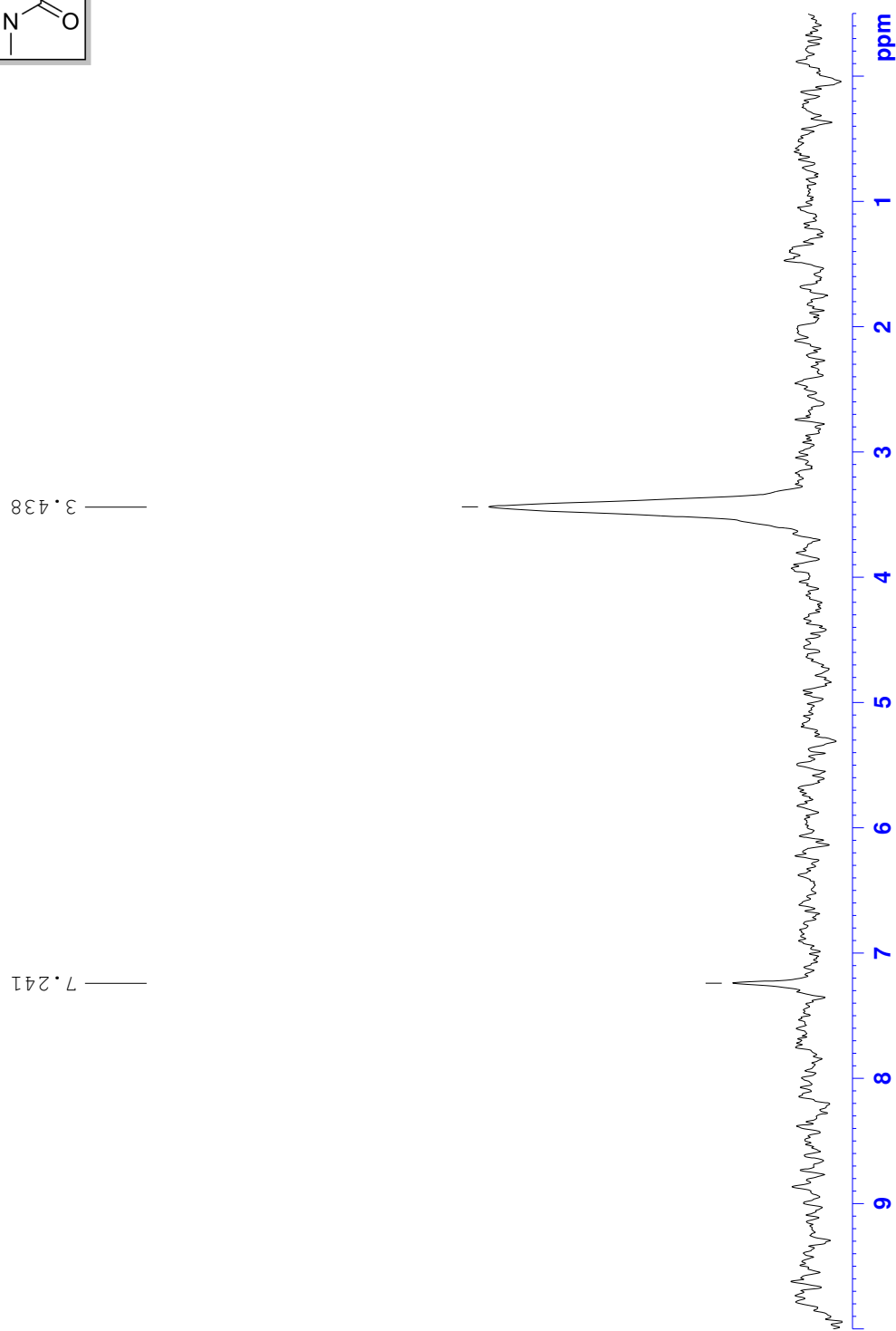
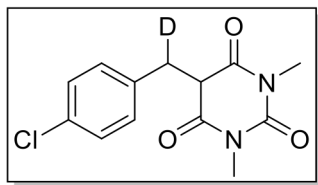
<sup>13</sup>C NMR spectra of 5-((4-Chlorophenyl)methyl-*d*)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7c-d<sub>1</sub>**)



KN-267-C

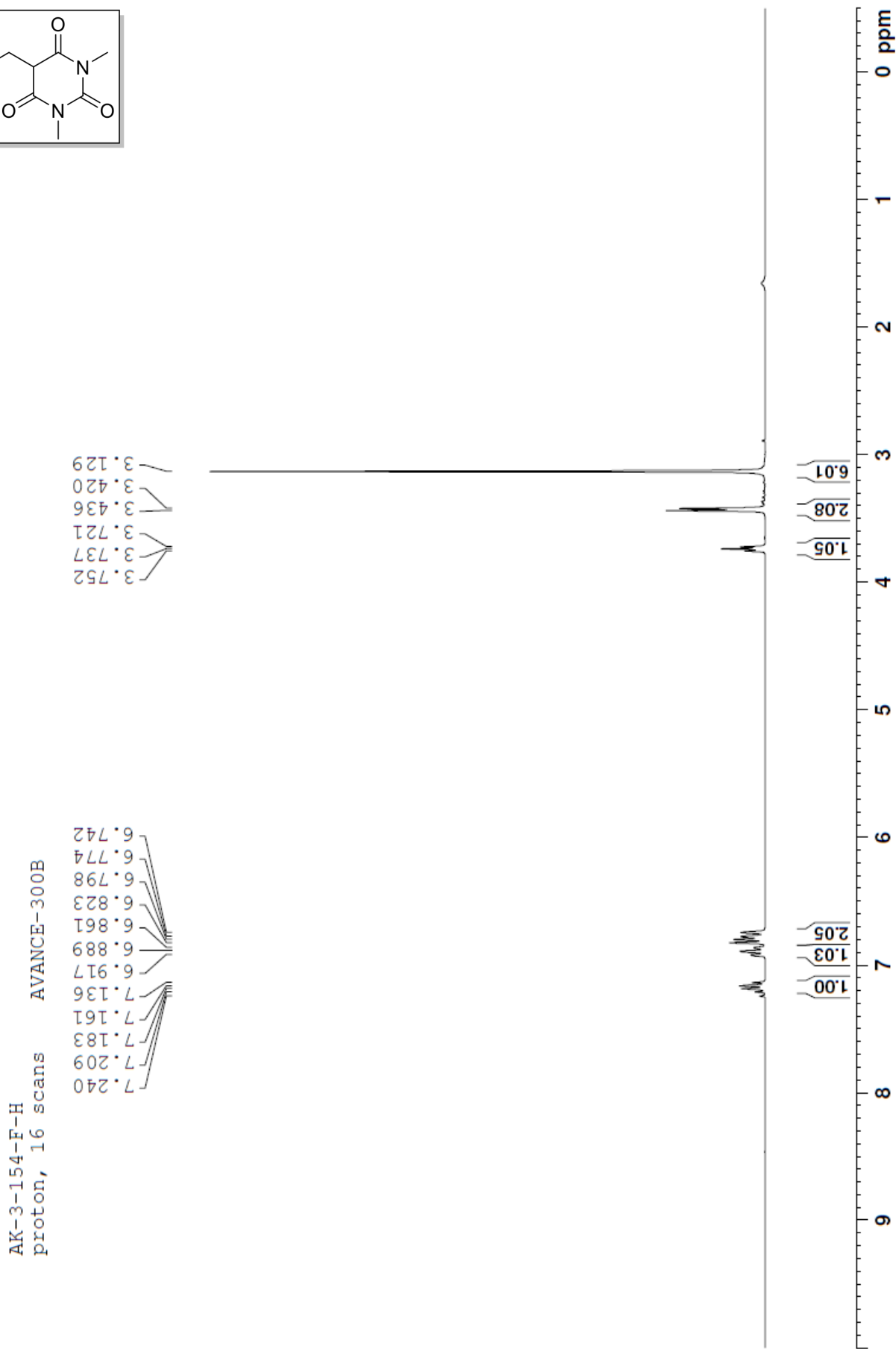
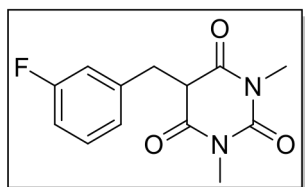


$^2\text{H}$  NMR spectra of 5-((4-Chlorophenyl)methyl-*d*)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7c-*d*<sub>1</sub>**)

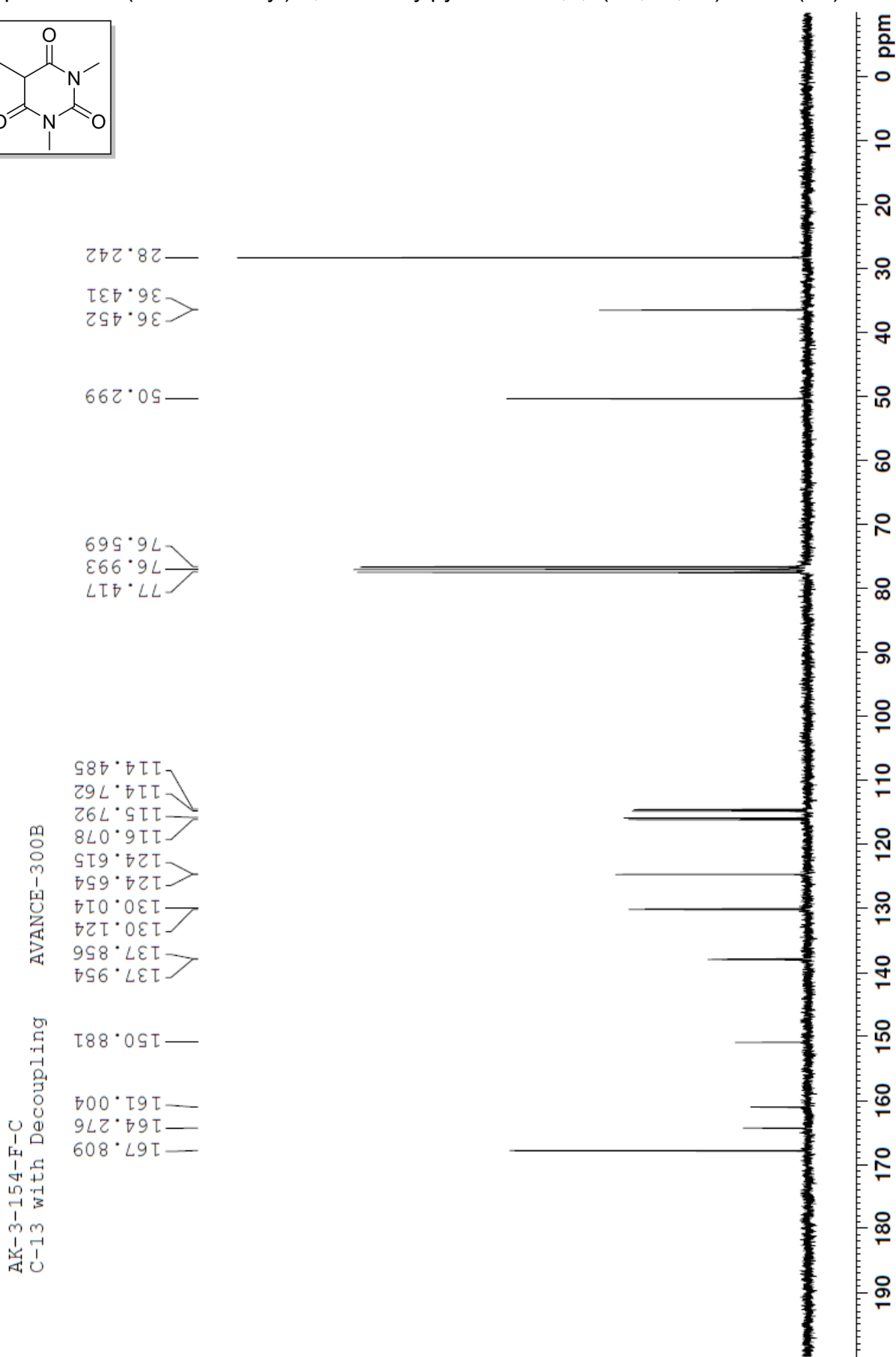
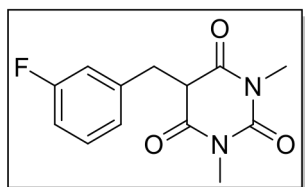


KN-1-262-D  
Deuterium

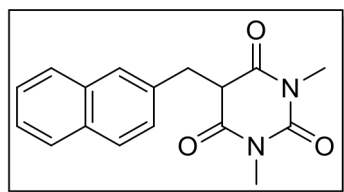
<sup>1</sup>H NMR spectra of 5-(3-fluorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7d**)



<sup>13</sup>C NMR spectra of 5-(3-fluorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7d)



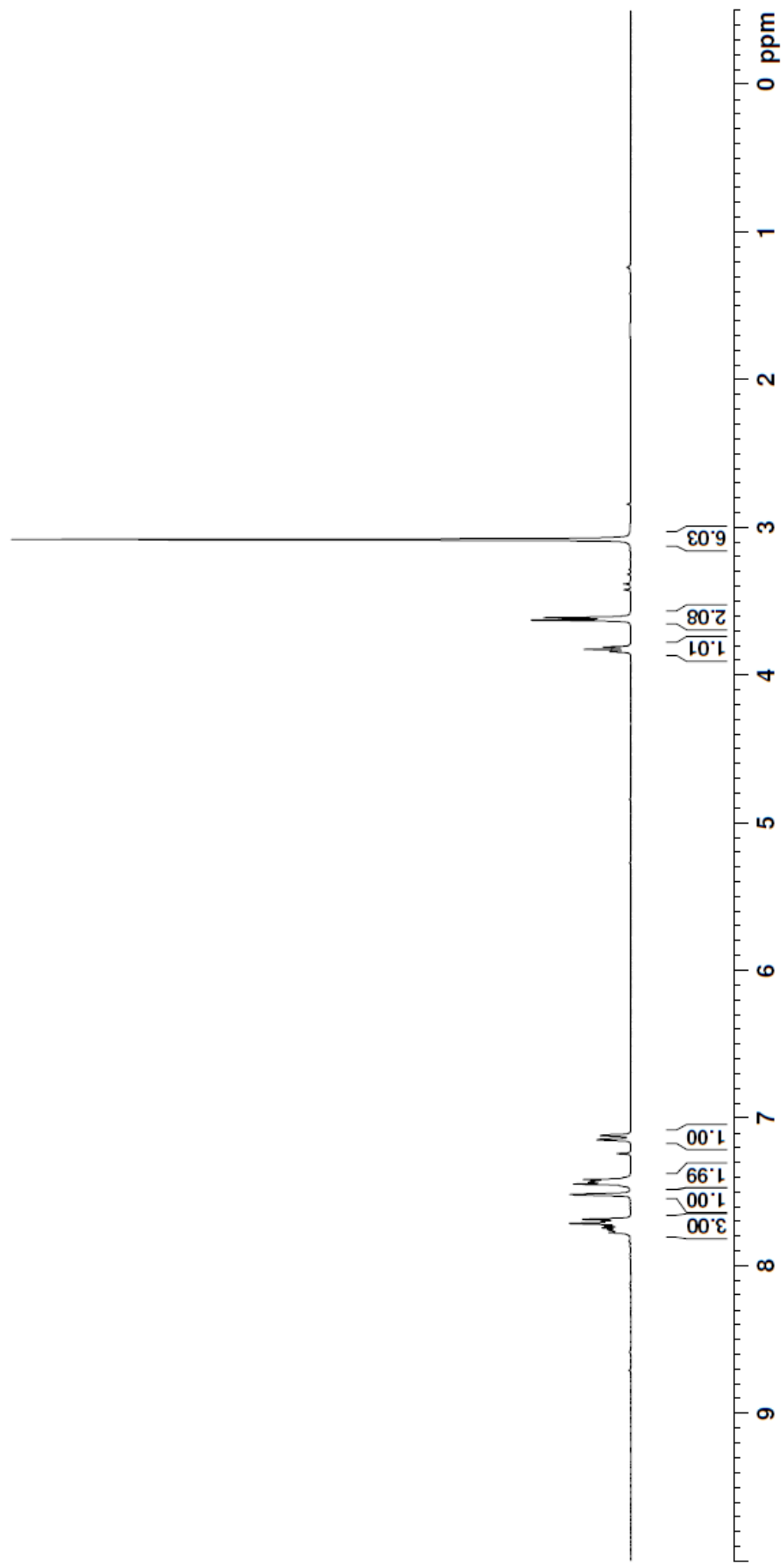
<sup>1</sup>H NMR spectra of 1,3-Dimethyl-5-(naphthalen-2-ylmethyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7e)



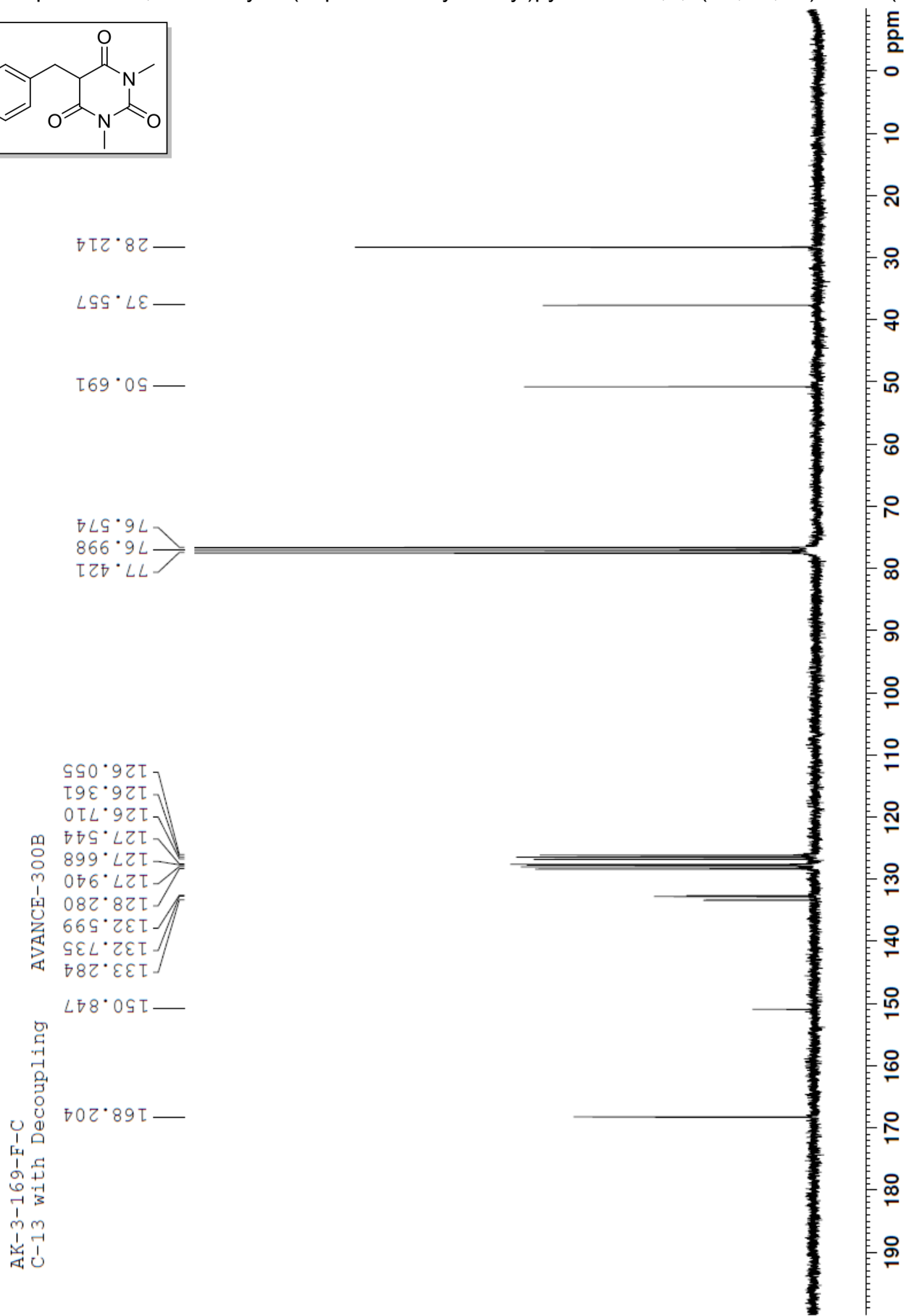
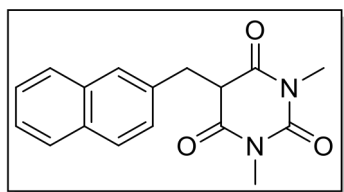
AK-3-169-F-H  
proton, 16 scans AVANCE-300B

7.775  
7.755  
7.744  
7.731  
7.713  
7.699  
7.685  
7.518  
7.447  
7.436  
7.427  
7.415  
7.240  
7.147  
7.119

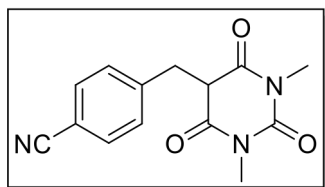
3.841  
3.825  
3.810  
3.627  
3.611  
3.081



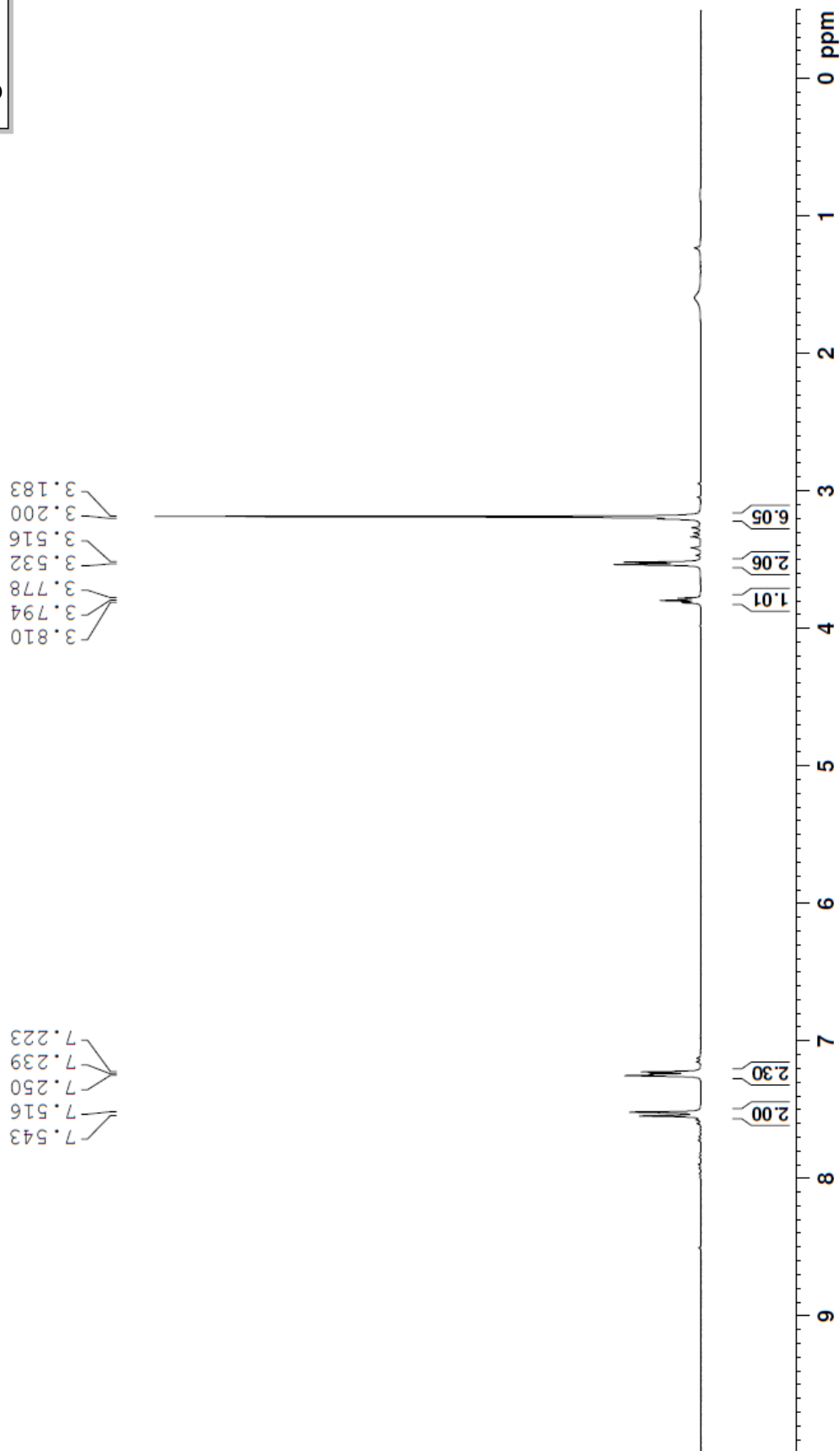
<sup>13</sup>C NMR spectra of 1,3-Dimethyl-5-(naphthalen-2-ylmethyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7e**)



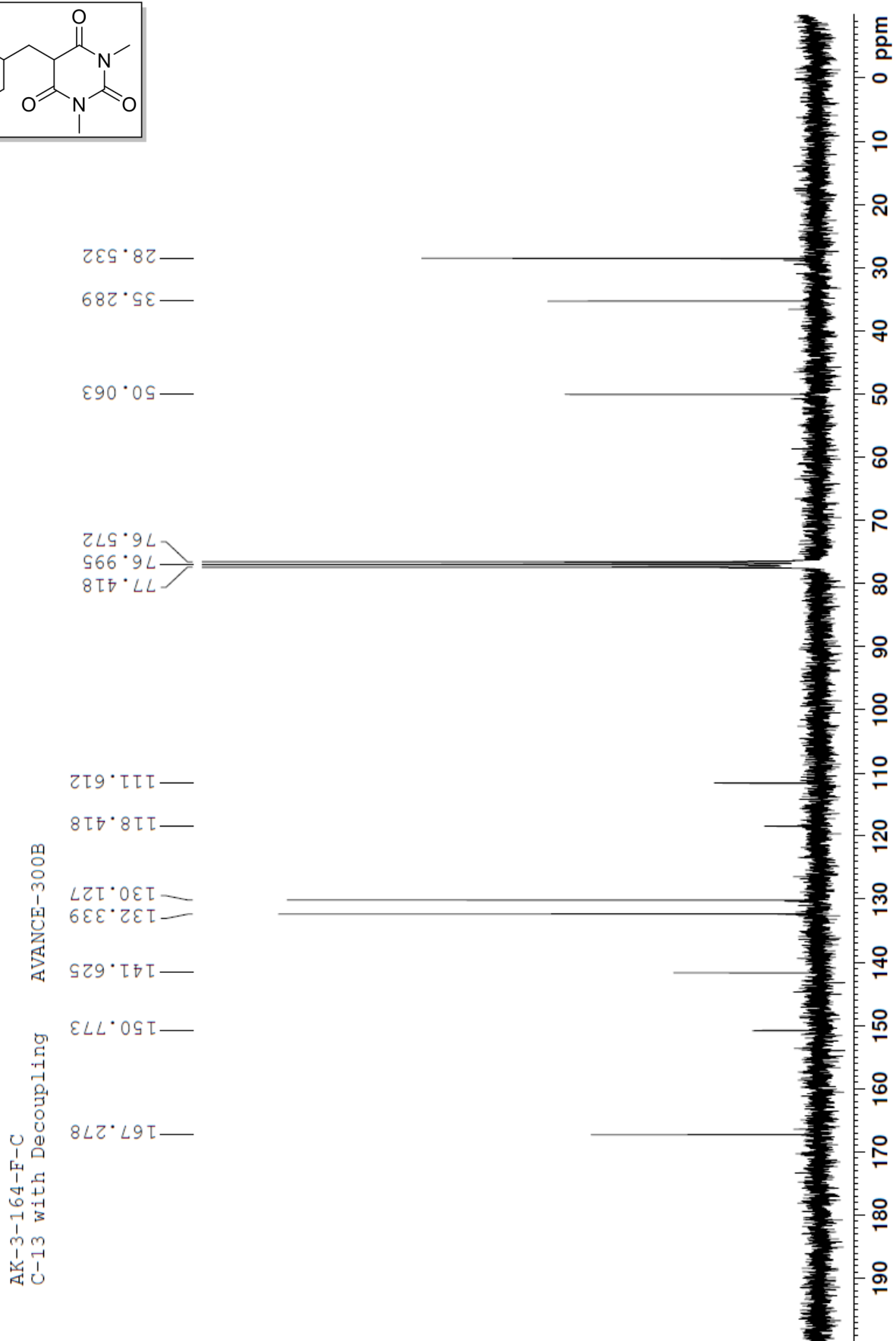
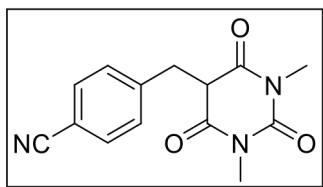
<sup>1</sup>H NMR spectra of 4-((1,3-Dimethyl-2,4,6-trioxohexahydropyrimidin-5-yl)methyl)benzonitrile (**7f**)



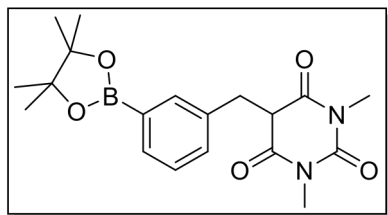
AK-3-164-F  
proton, 16 scans AVANCE-300B



<sup>13</sup>C NMR spectra of 4-((1,3-Dimethyl-2,4,6-trioxohexahydropyrimidin-5-yl)methyl)benzonitrile (7f)



<sup>1</sup>H NMR spectra of 1,3-dimethyl-5-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7g**)

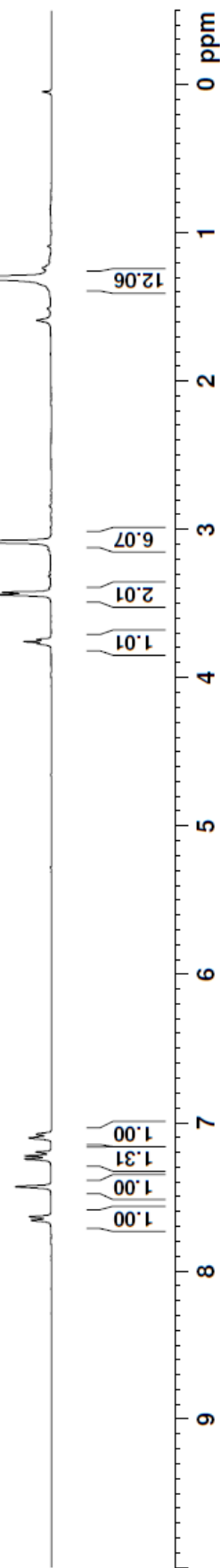


AK-3-167-F-H  
proton, 16 scans AVANCE-300B

7.657  
7.633  
7.430  
7.244  
7.240  
7.221  
7.196  
7.101  
7.076

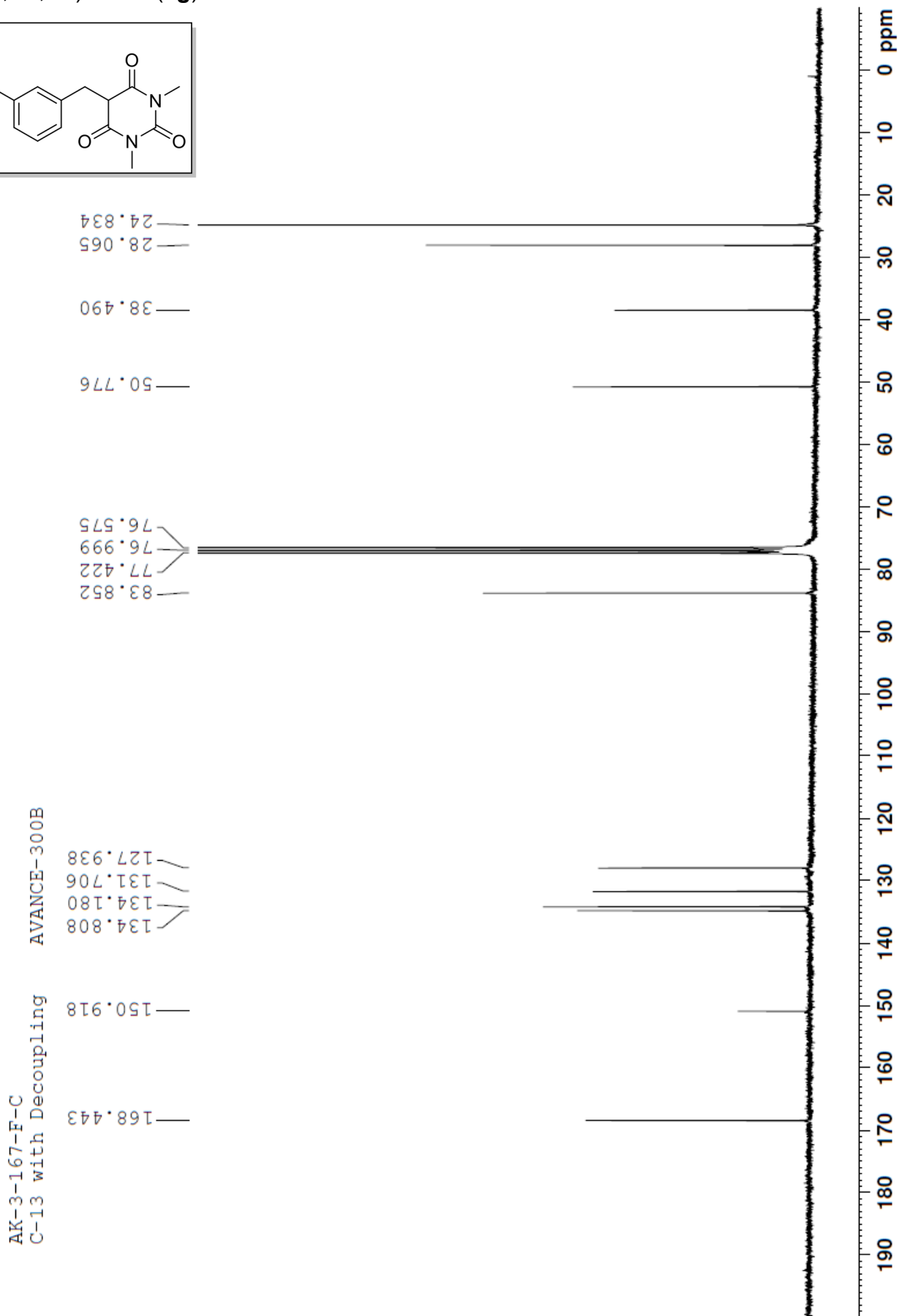
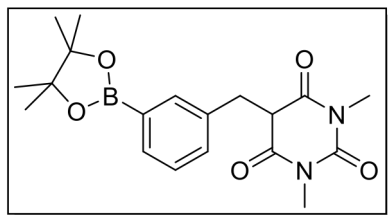
3.769  
3.754  
3.739  
3.437  
3.422  
3.078

1.299

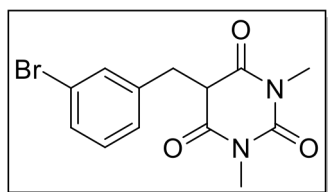




<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7g**)



<sup>1</sup>H NMR spectra of 5-(3-bromobenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**7h**)



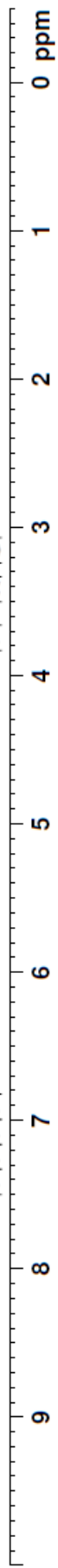
AK-3-158-F-H  
proton, 16 scans  
AVANCE-300B

7.362  
7.336  
7.240  
7.223  
7.118  
7.092  
7.066  
6.986  
6.960

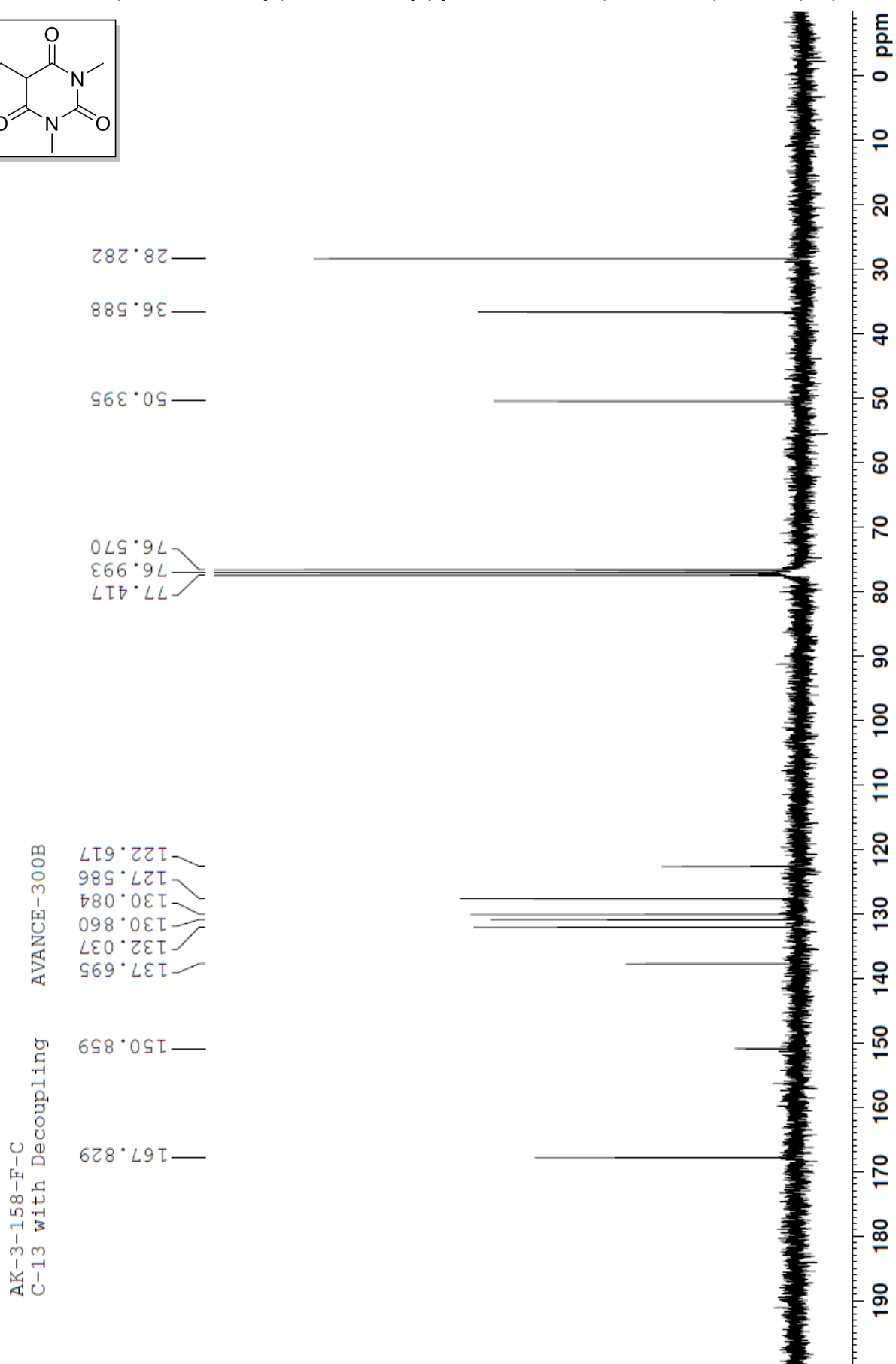
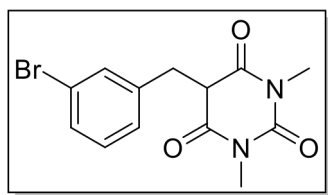
3.759  
3.743  
3.727  
3.418  
3.402  
3.148

1.00  
1.15  
1.04  
1.04

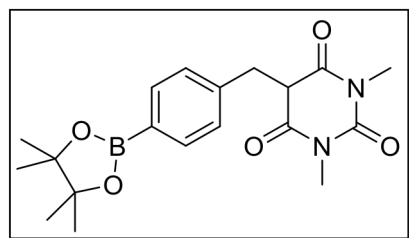
1.02  
2.02  
6.06



<sup>13</sup>C NMR spectra of 5-(3-bromobenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7h)



<sup>1</sup>H NMR spectra of 1,3-dimethyl-5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7i**)

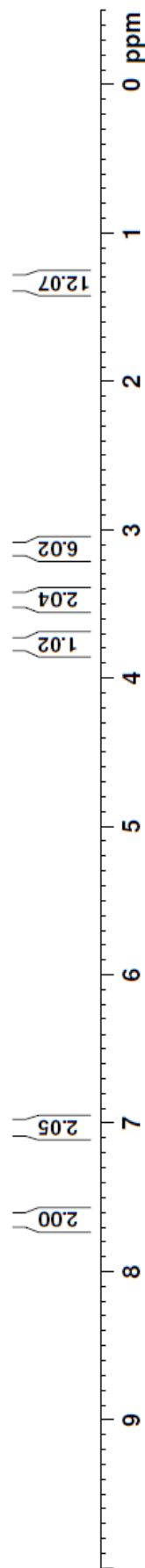


AK-3-168-F-H  
proton, 16 scans AVANCE-300B

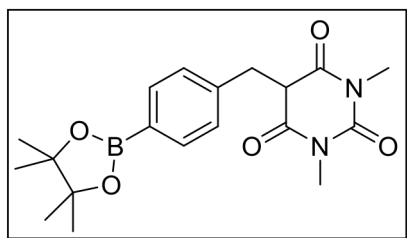
7.656  
7.630  
7.240  
7.034  
7.008

3.777  
3.761  
3.745  
3.472  
3.456  
3.115

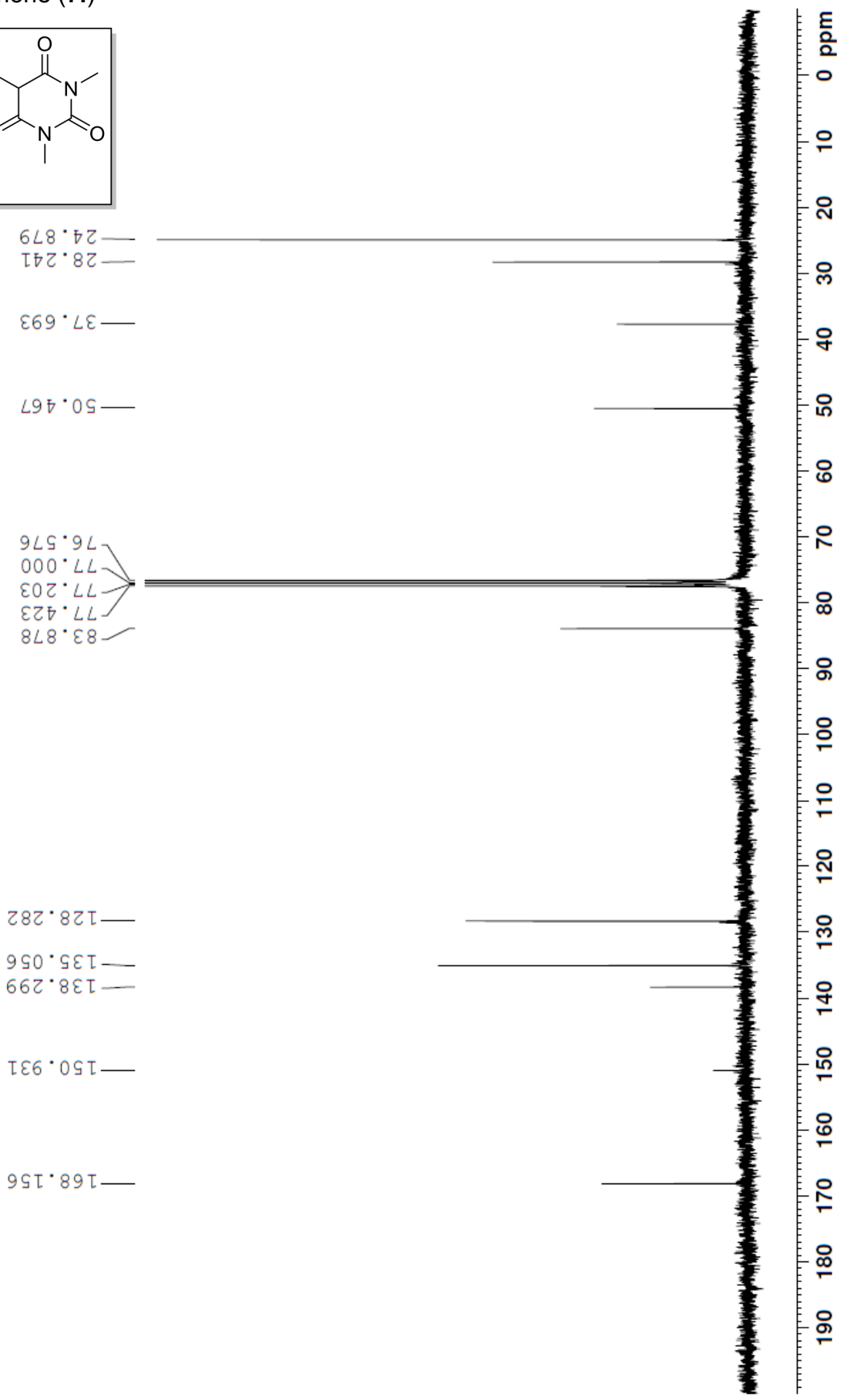
1.316



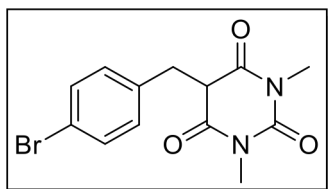
<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7i**)



AK-3-168-F-C  
C-13 with Decoupling AVANCE-300B



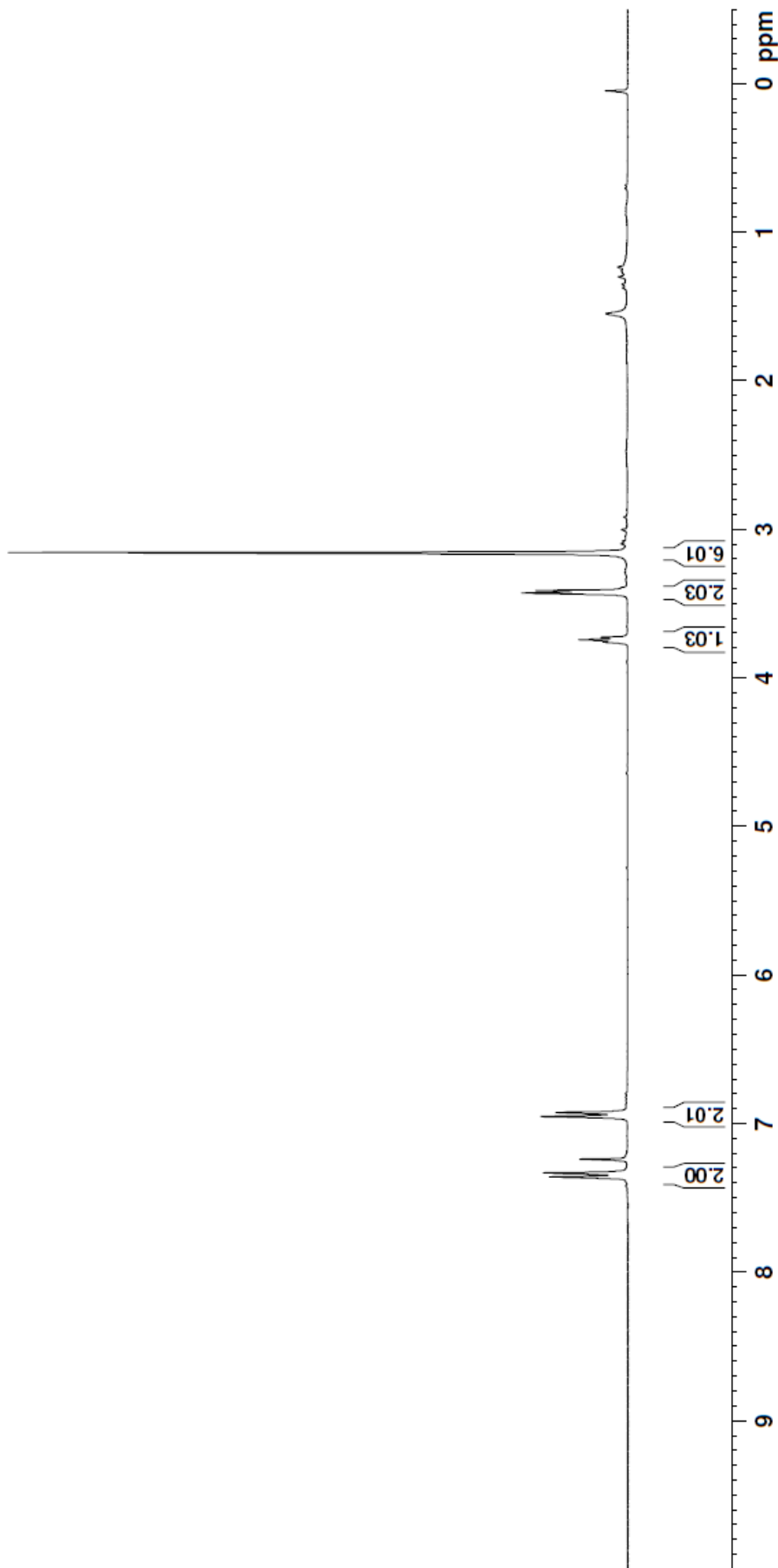
<sup>1</sup>H NMR spectra of 5-(4-Bromobenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7j)



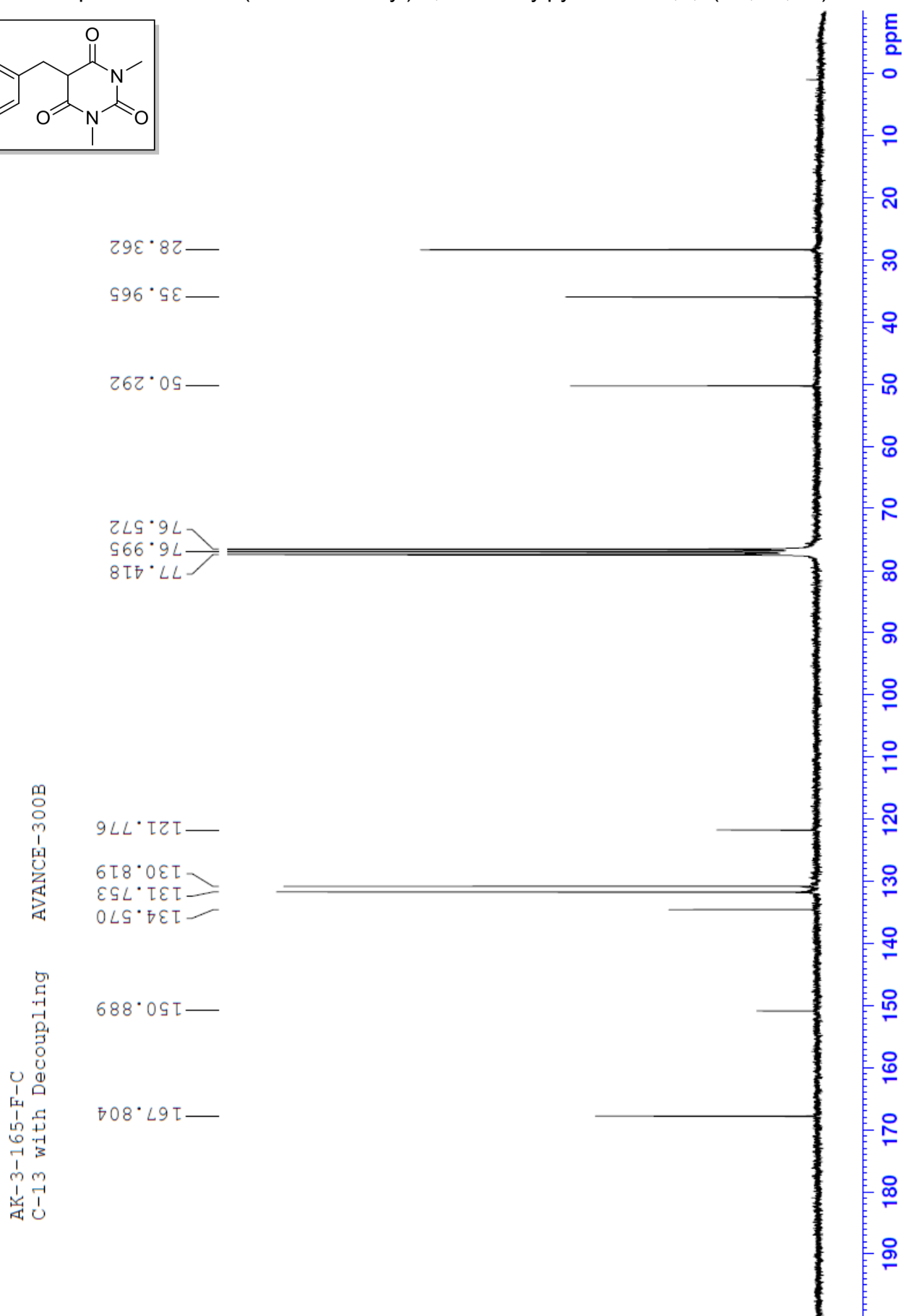
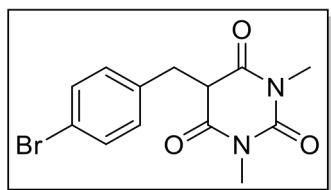
AK-3-165-F  
proton, 16 scans  
AVANCE-300B

7.359  
7.331  
7.240  
6.952  
6.925

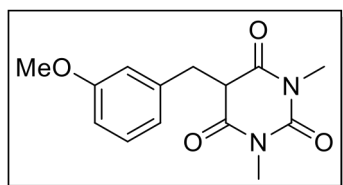
3.758  
3.742  
3.727  
3.428  
3.413  
3.156



<sup>13</sup>C NMR spectra of 5-(4-Bromobenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7j)



<sup>1</sup>H NMR spectra of 5-(3-methoxybenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**7k**)

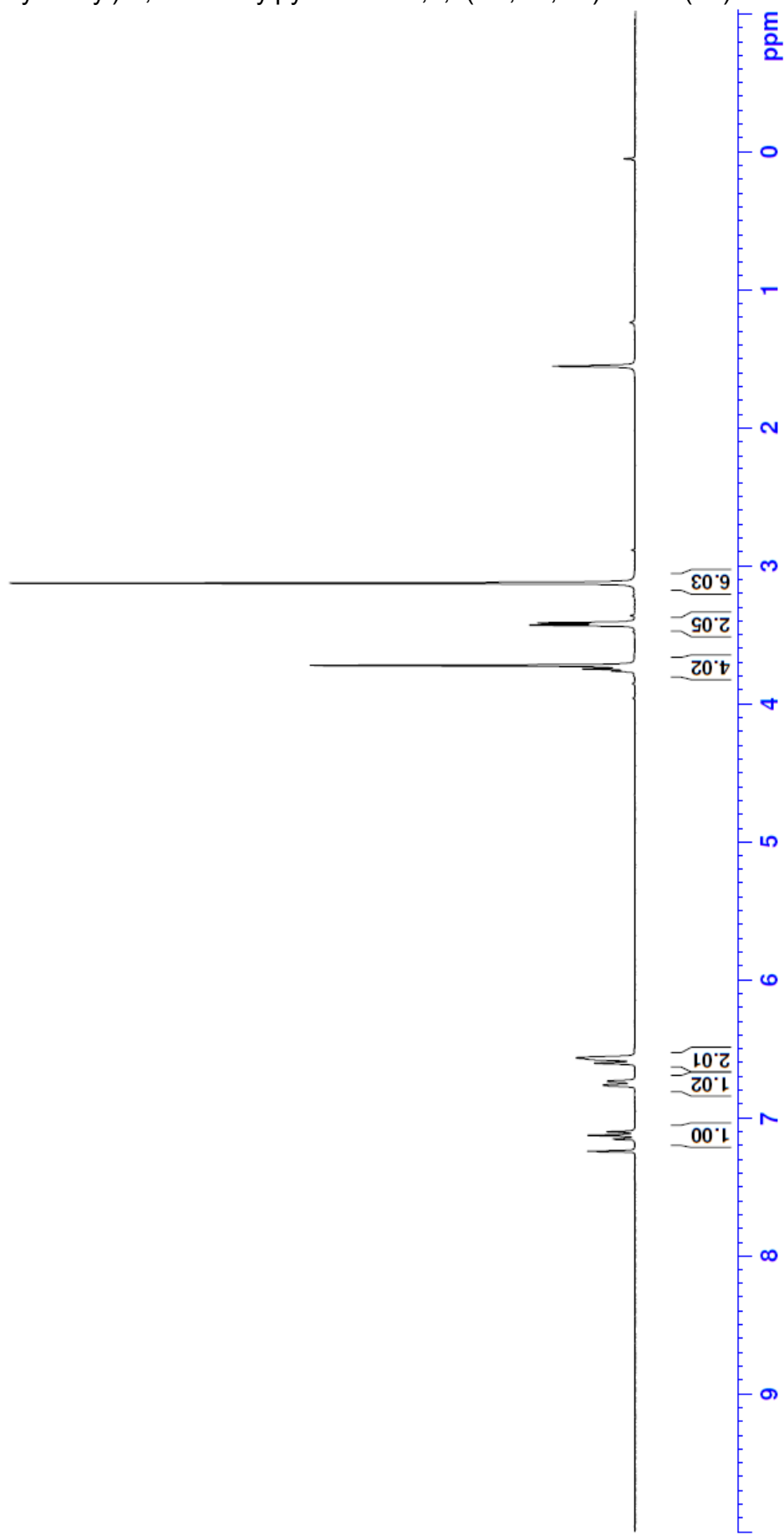


AK-3-153-F-H  
proton, 16 scans

AVANCE-300B

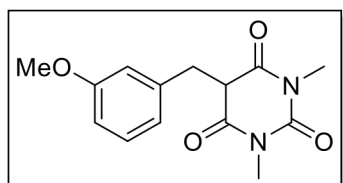
7.240  
7.151  
7.125  
7.099  
6.760  
6.733  
6.602  
6.562

3.760  
3.744  
3.719  
3.427  
3.411  
3.122

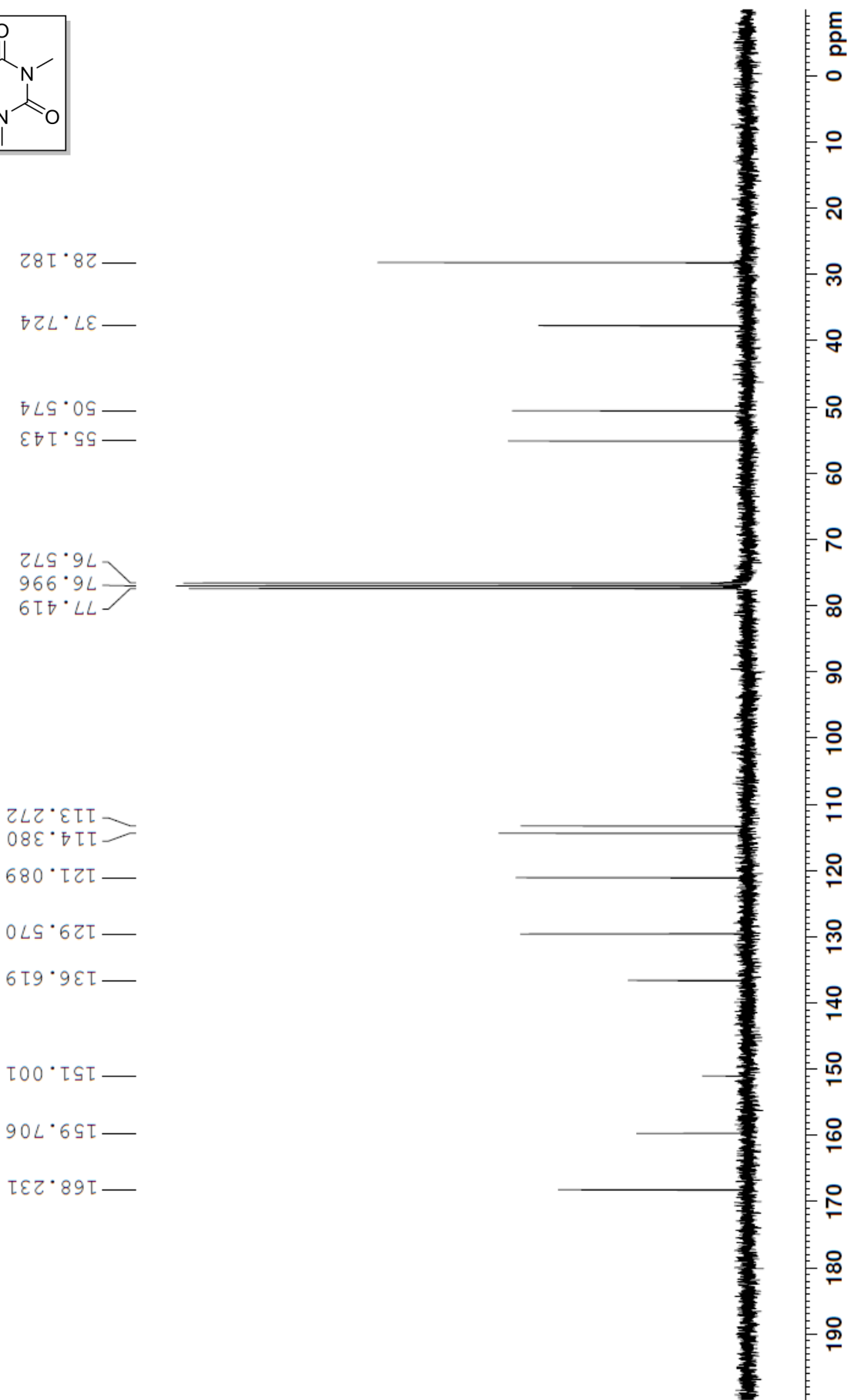




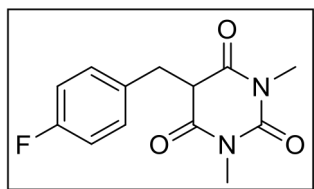
<sup>13</sup>C NMR spectra of 5-(3-methoxybenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7k)



AK-3-153-F-C  
C-13 with Decoupling AVANCE-300B



<sup>1</sup>H NMR spectra of 5-(4-fluorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (7I)

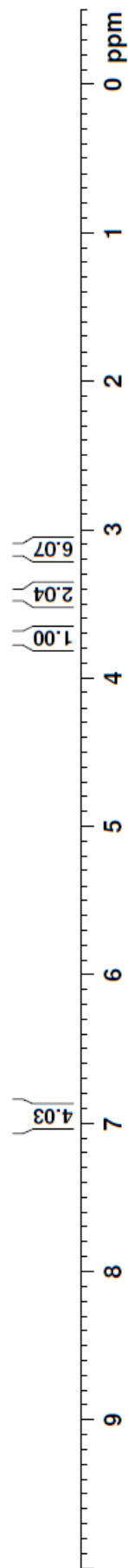


proton, 16 scans  
AK-3-159-F-H

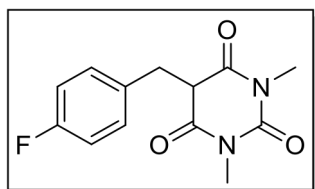
AVANCE-300B

7.240  
7.034  
7.015  
7.006  
6.988  
6.940  
6.930  
6.902  
6.873

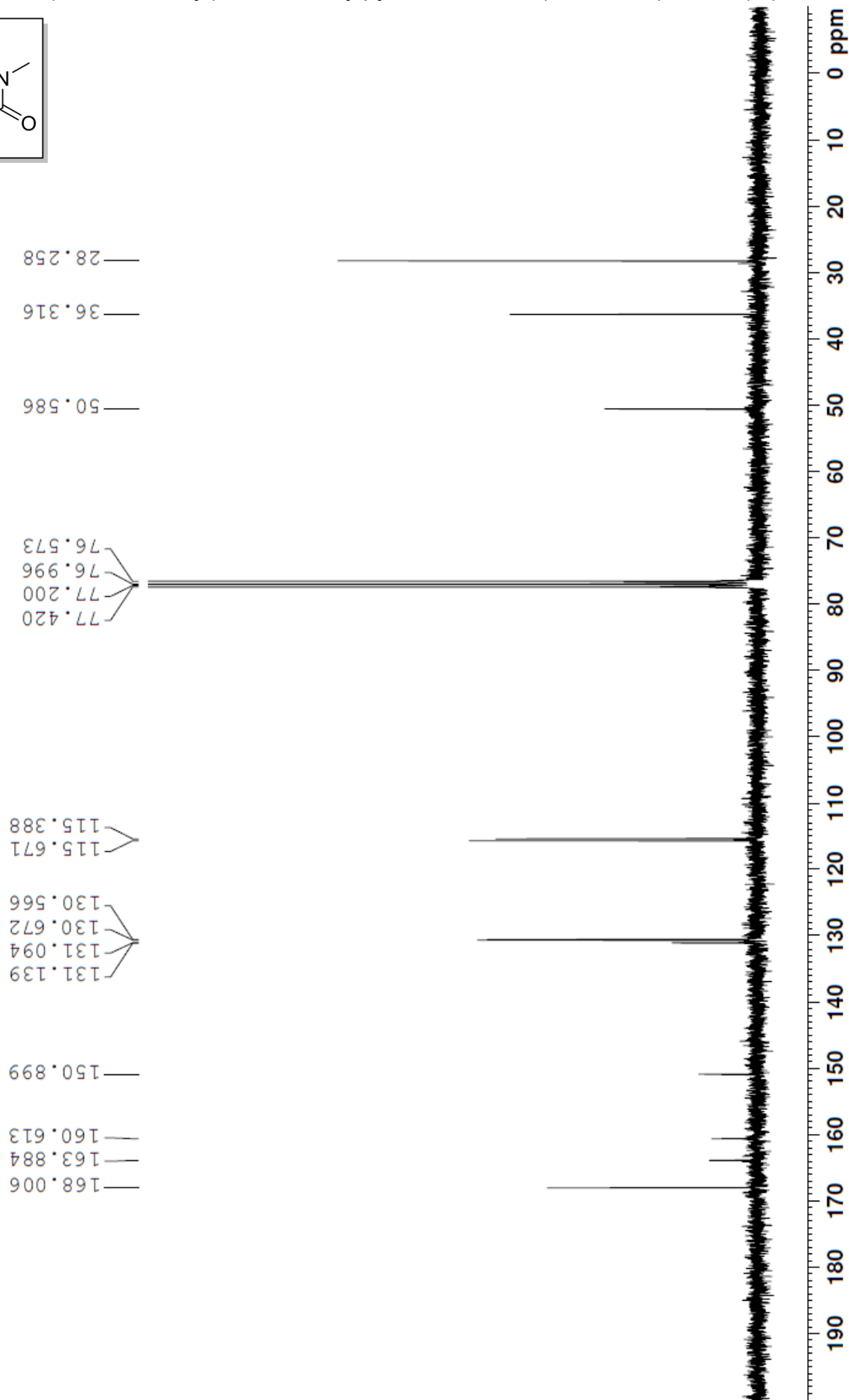
3.747  
3.731  
3.716  
3.438  
3.422  
3.134



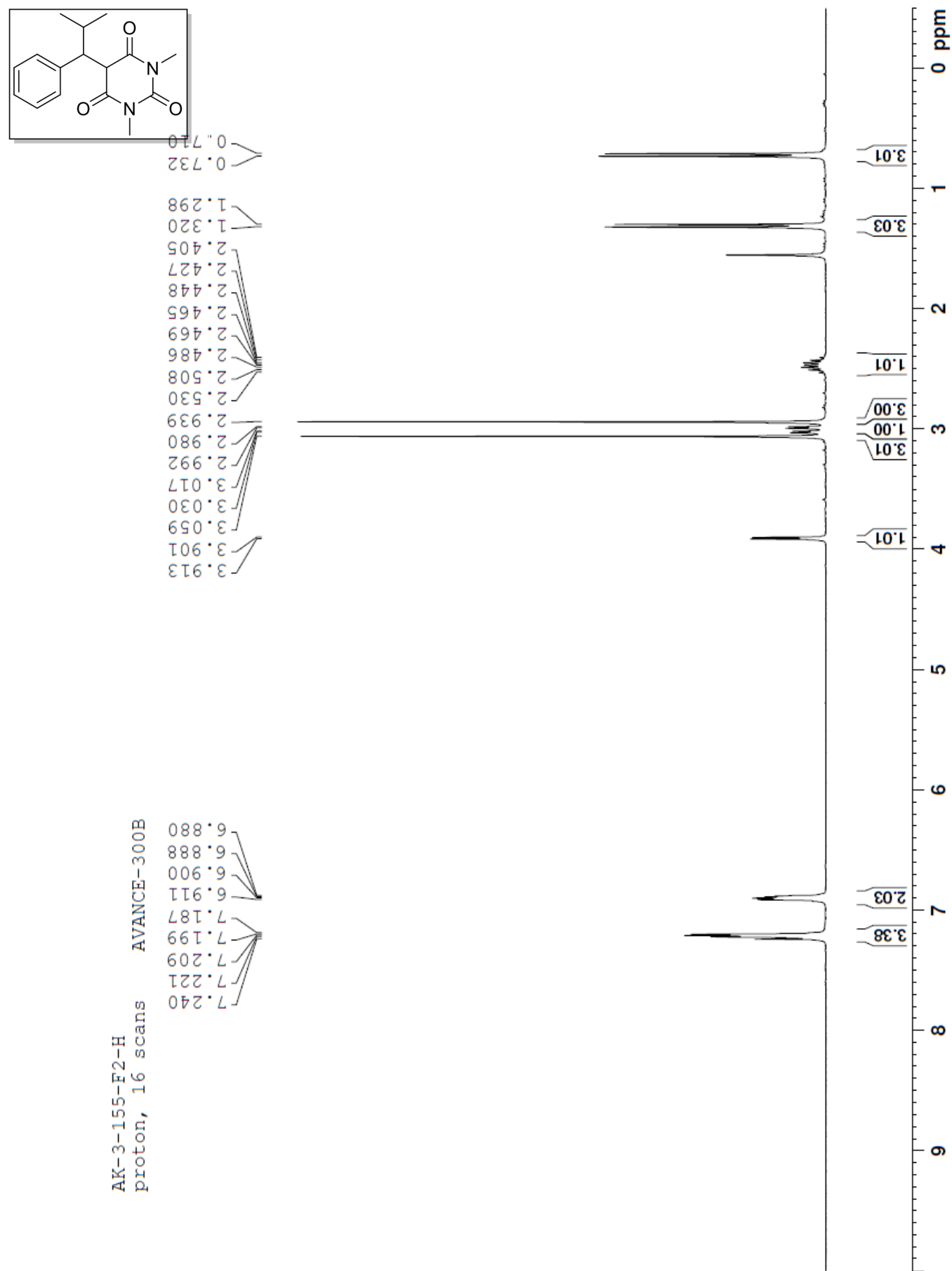
<sup>13</sup>C NMR spectra of 5-(4-fluorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (71)



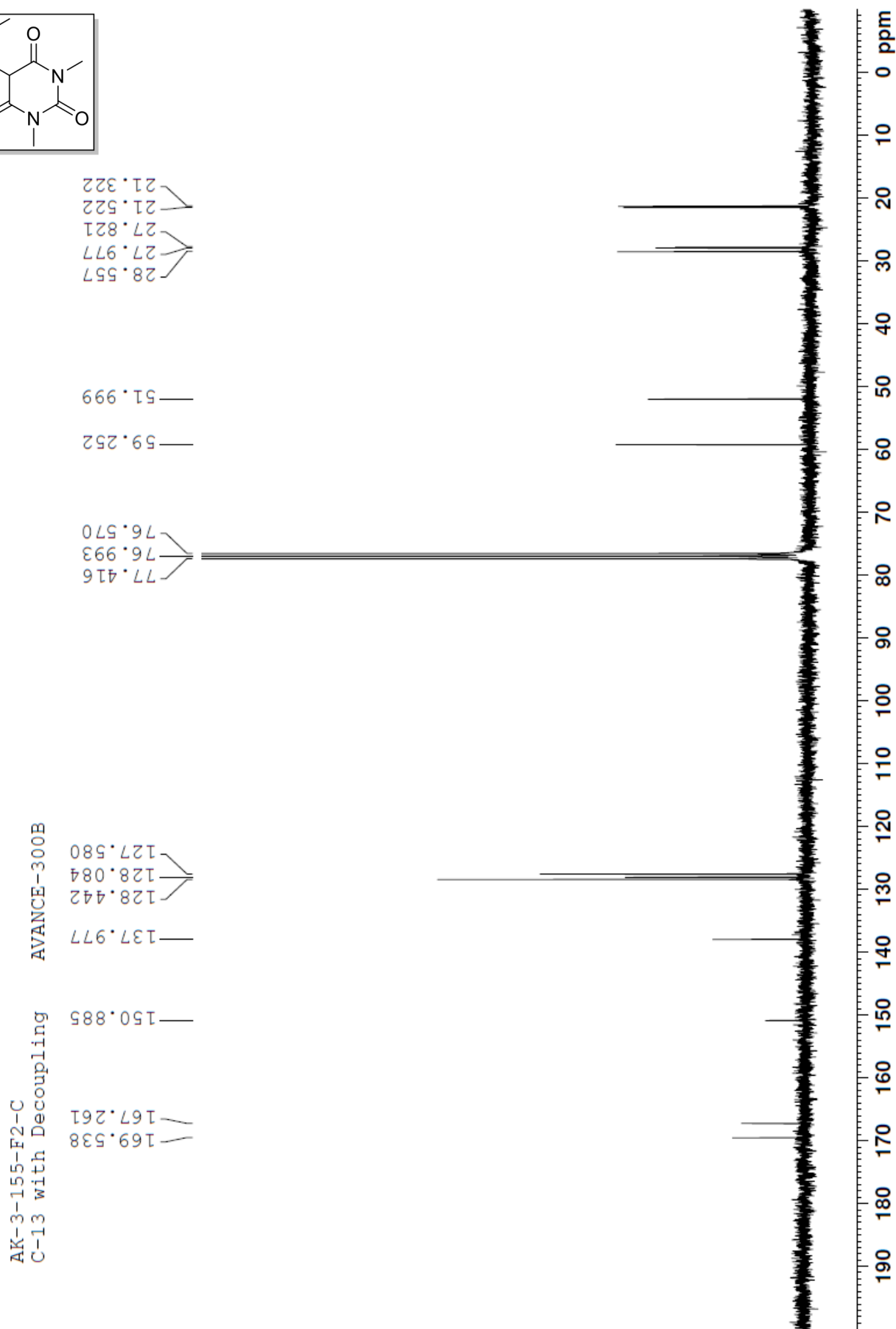
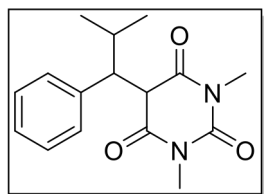
AK-3-159-F-C  
C-13 with Decoupling  
AVANCE-300B



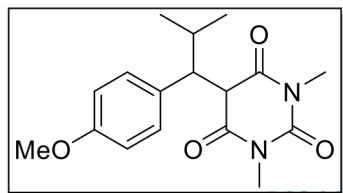
<sup>1</sup>H NMR spectra of 1,3-dimethyl-5-(2-methyl-1-phenylpropyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8a**)



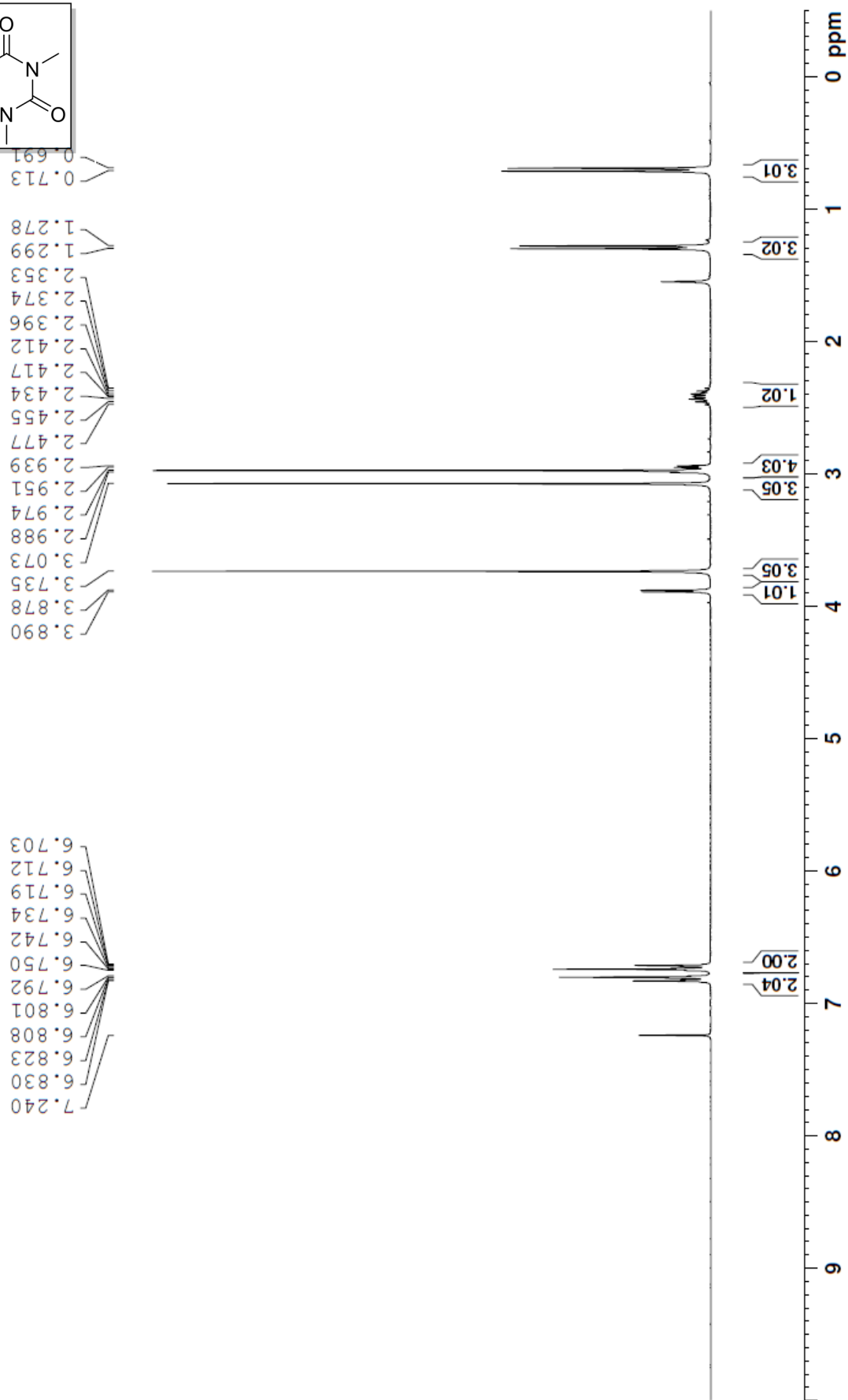
<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(2-methyl-1-phenylpropyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8a**)



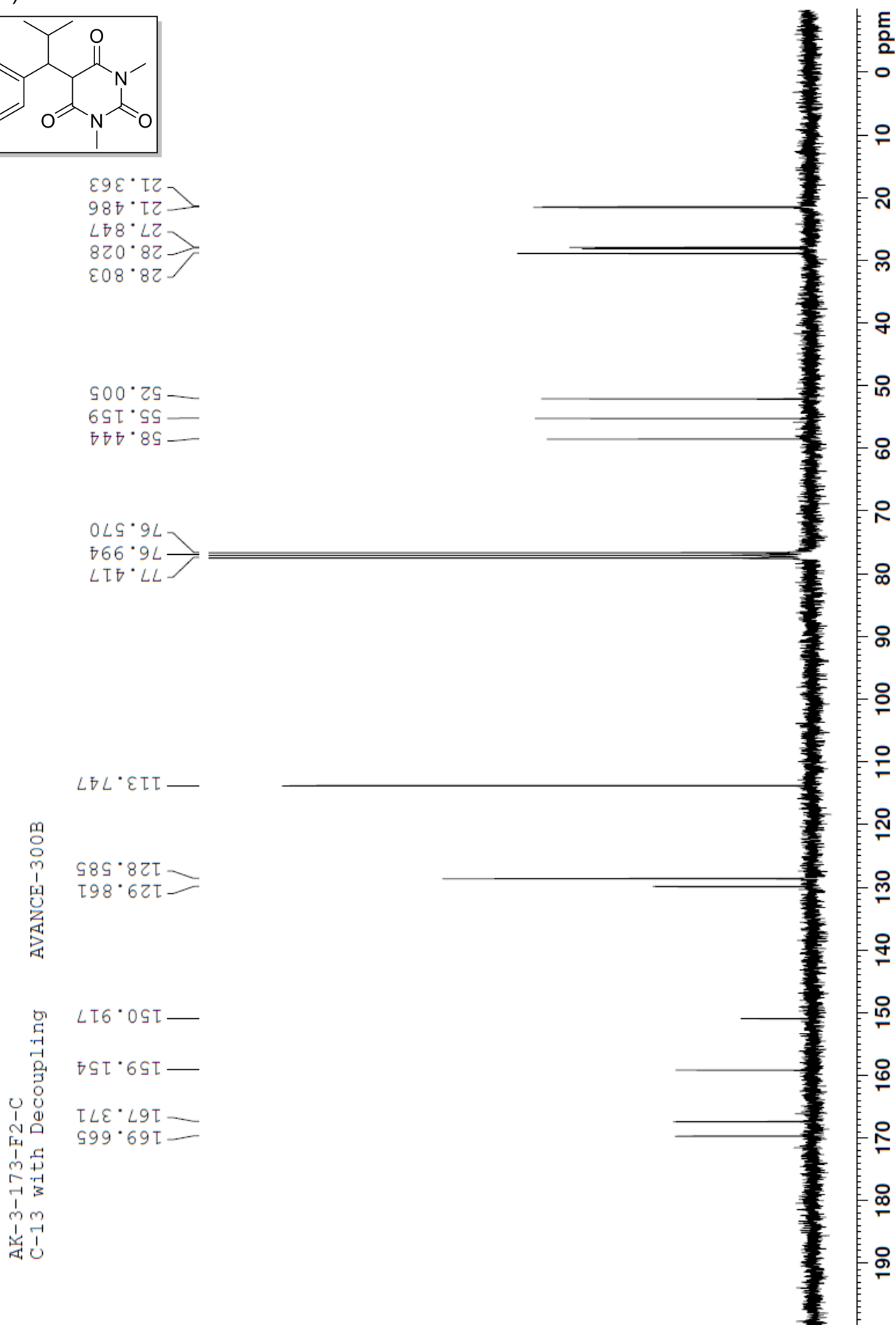
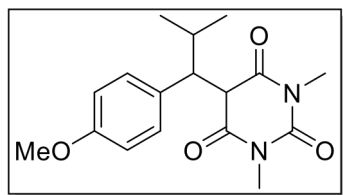
<sup>1</sup>H NMR spectra of 5-(1-(4-methoxyphenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8b**)



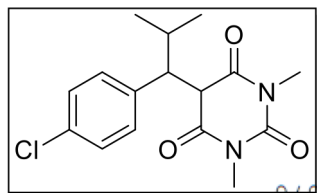
AK-3-173-F2-H  
proton, 16 scans  
AVANCE-300B



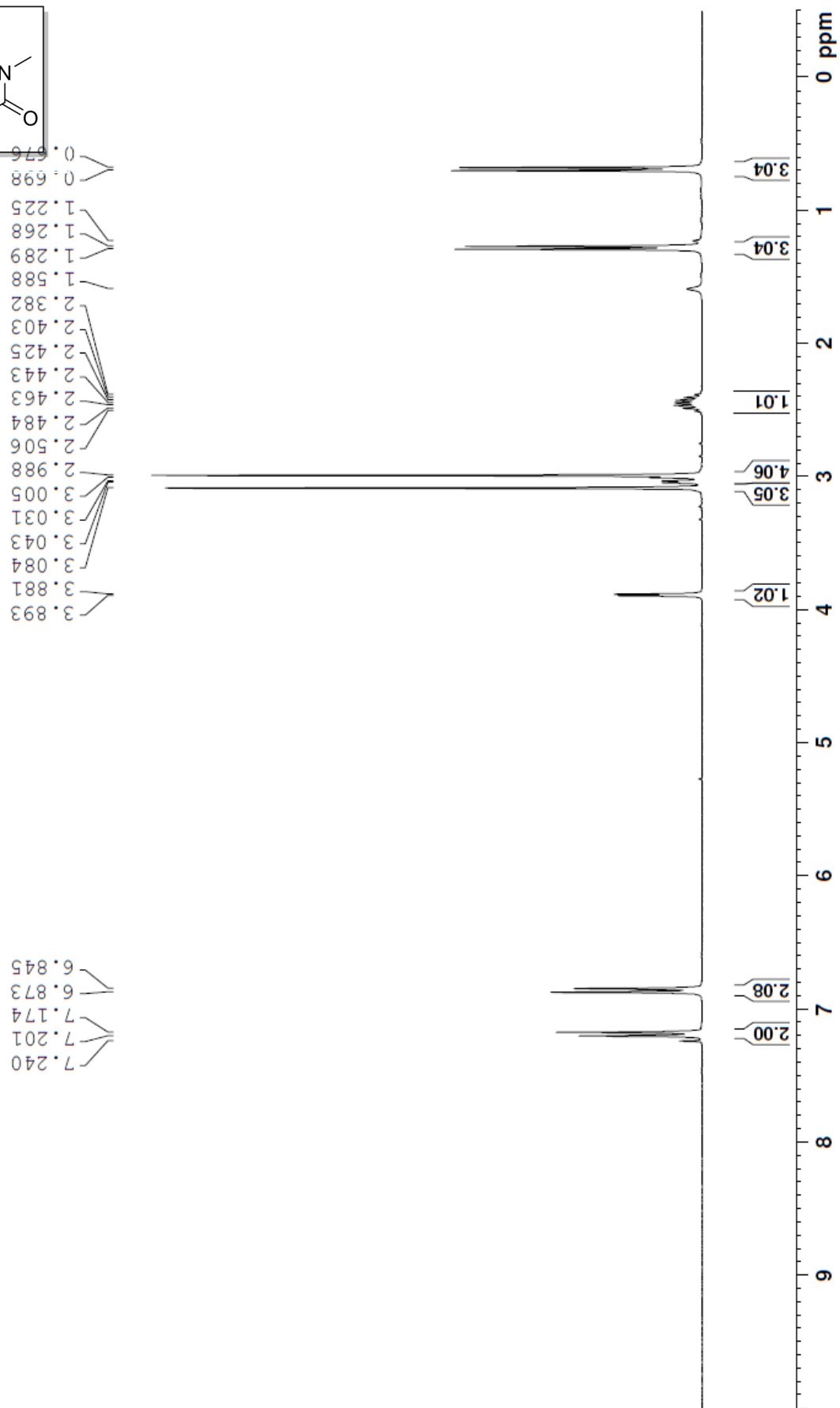
<sup>13</sup>C NMR spectra of 5-(1-(4-methoxyphenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8b**)



<sup>1</sup>H NMR spectra of 5-(1-(4-chlorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8c**)

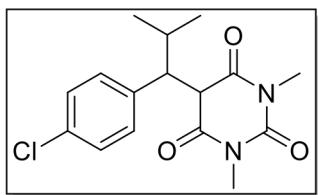


AK-3-133-F2-H  
proton, 16 scans  
AVANCE-300B

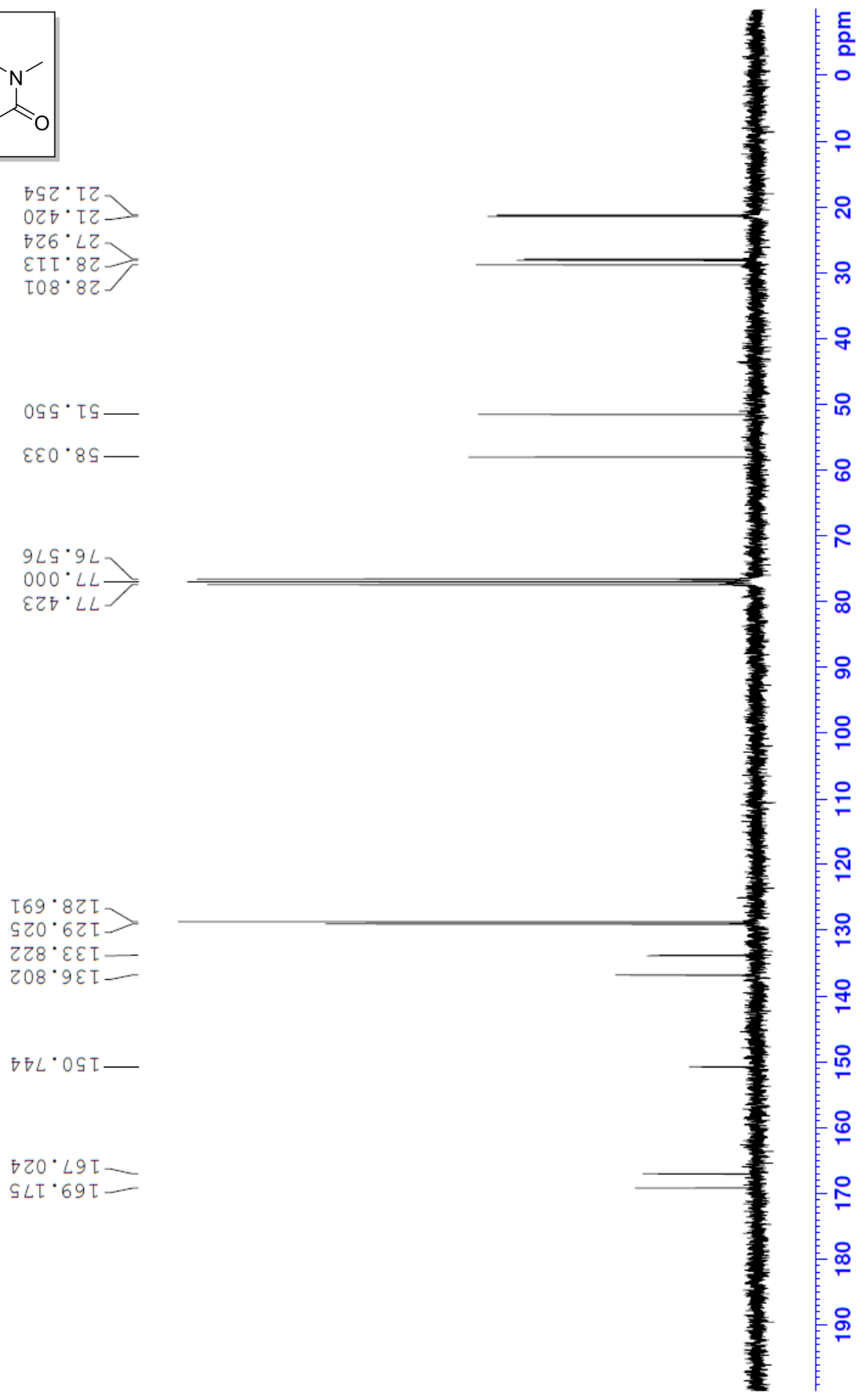




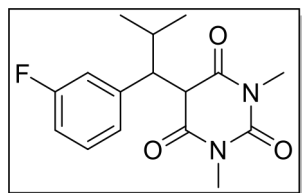
<sup>13</sup>C NMR spectra of 5-(1-(4-chlorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**8c**)



AK-3-133-F2-C  
C-13 with Decoupling  
AVANCE-300B



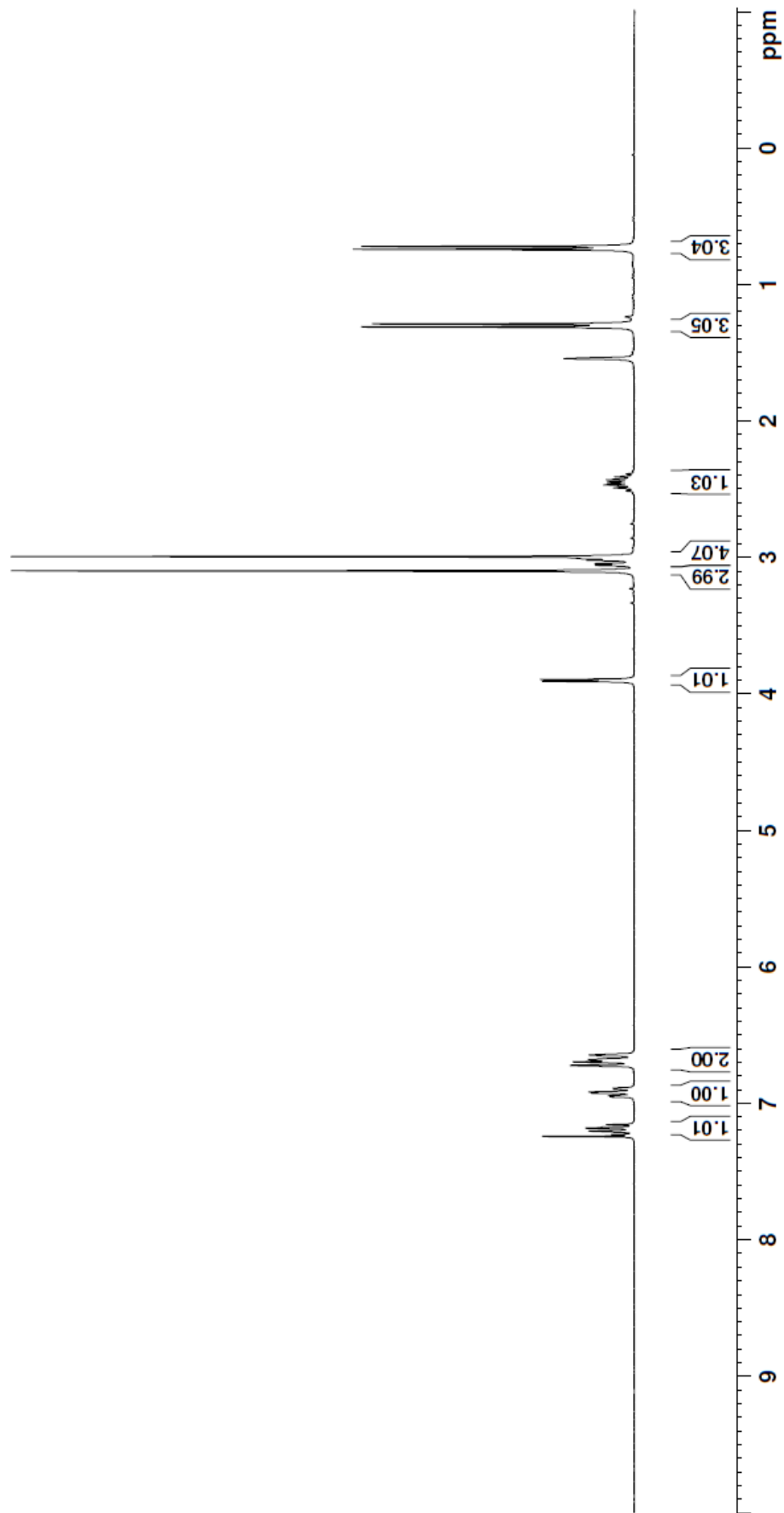
<sup>1</sup>H NMR spectra of 5-(1-(3-fluorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8d**)



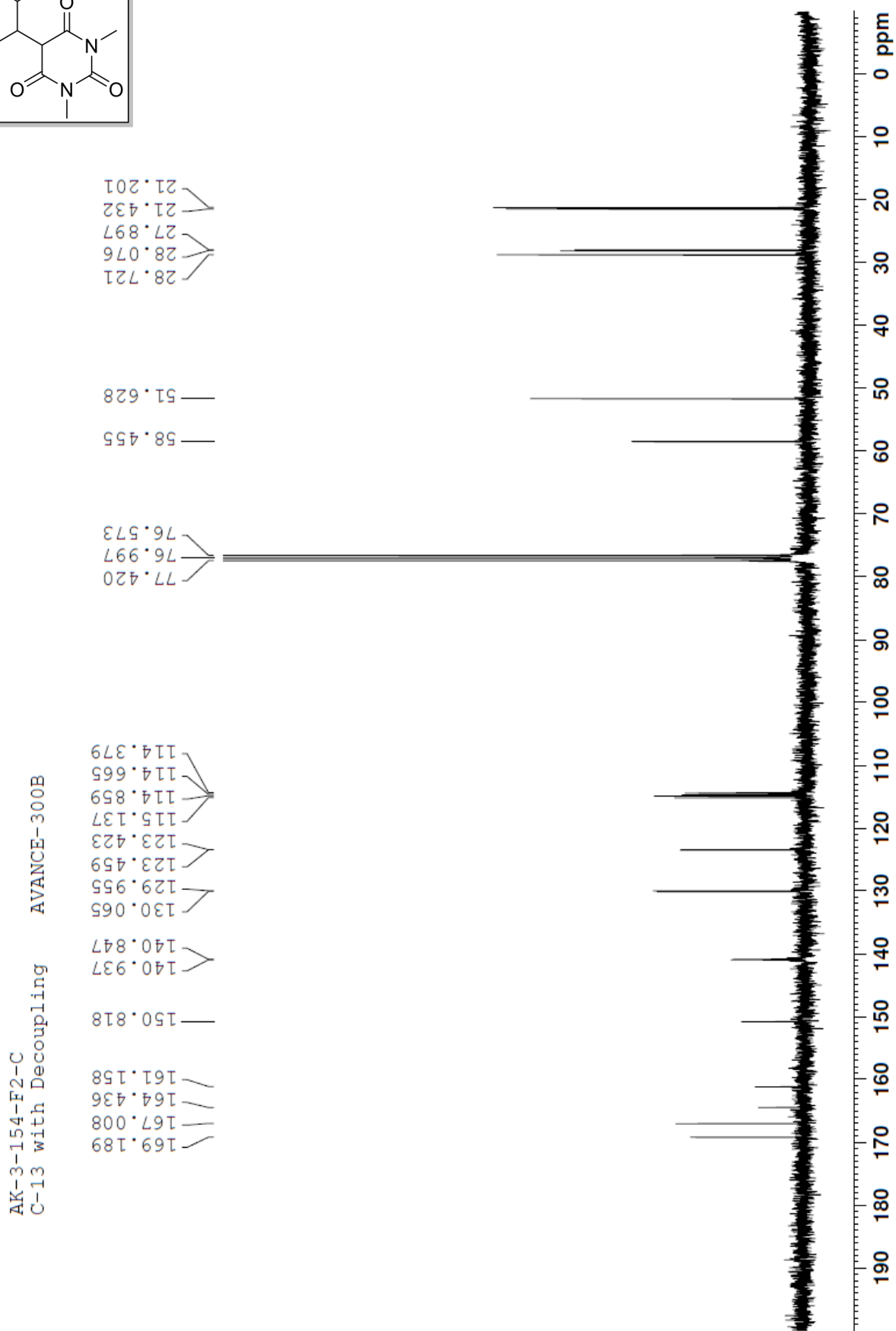
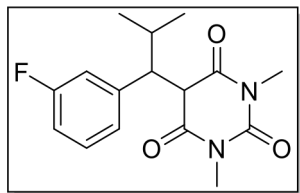
AK-3-154-F2-H  
proton, 16 scans AVANCE-300B

7.240  
7.226  
7.200  
7.180  
7.153  
6.950  
6.942  
6.922  
6.914  
6.895  
6.886  
6.866  
6.720  
6.694  
6.683  
6.676  
6.649  
6.643

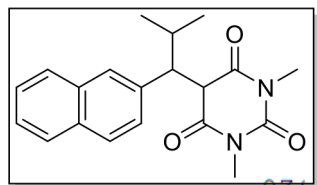
3.904  
3.892  
3.095  
3.055  
3.043  
3.017  
3.004  
2.990  
2.508  
2.487  
2.465  
2.444  
2.427  
2.406  
2.384  
1.541  
1.307  
1.286  
1.233  
0.739  
0.717



<sup>13</sup>C NMR spectra of 5-(1-(3-fluorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8d**)



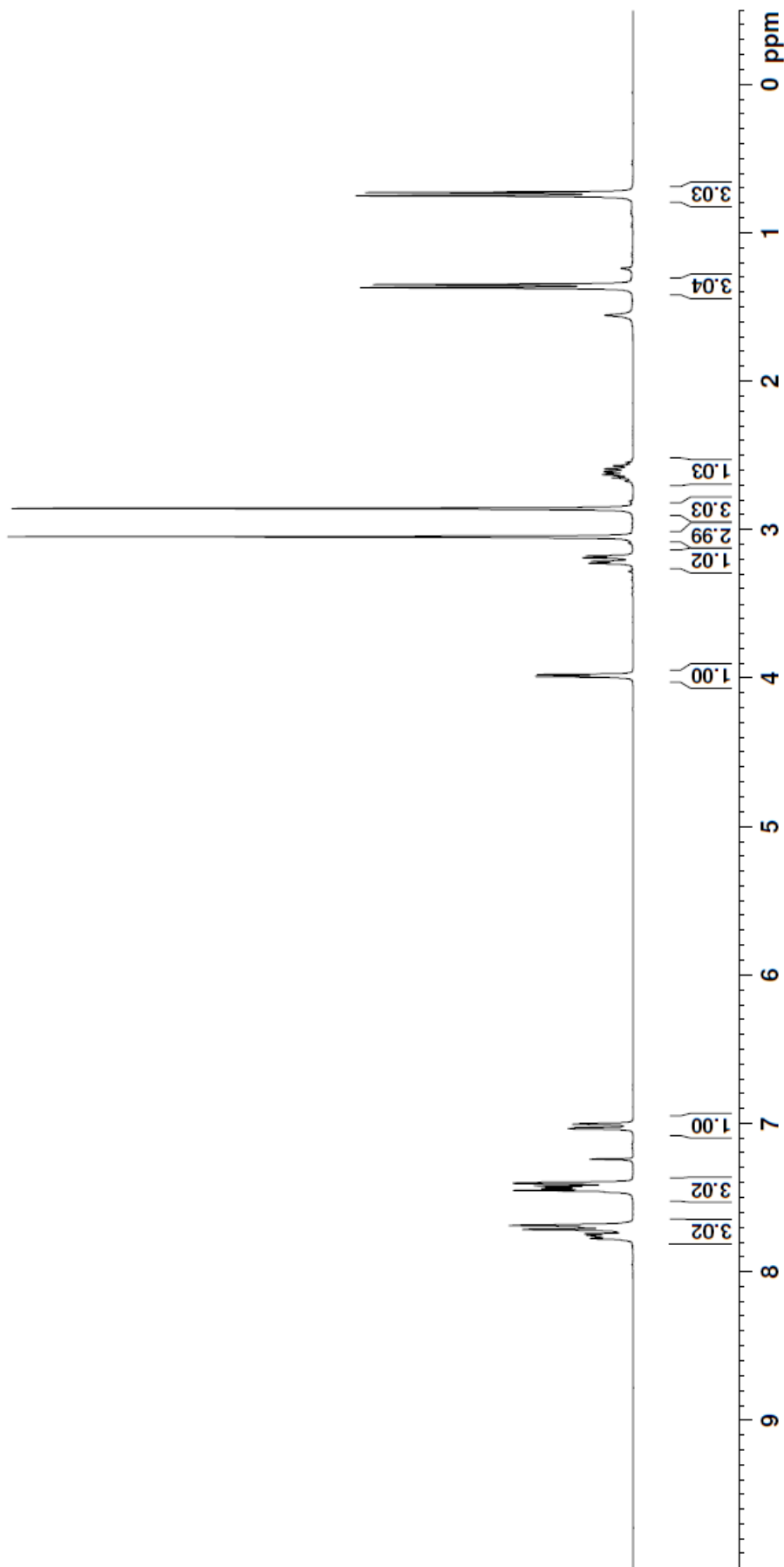
<sup>1</sup>H NMR spectra of 1,3-dimethyl-5-(2-methyl-1-(naphthalen-2-yl)propyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8e**)



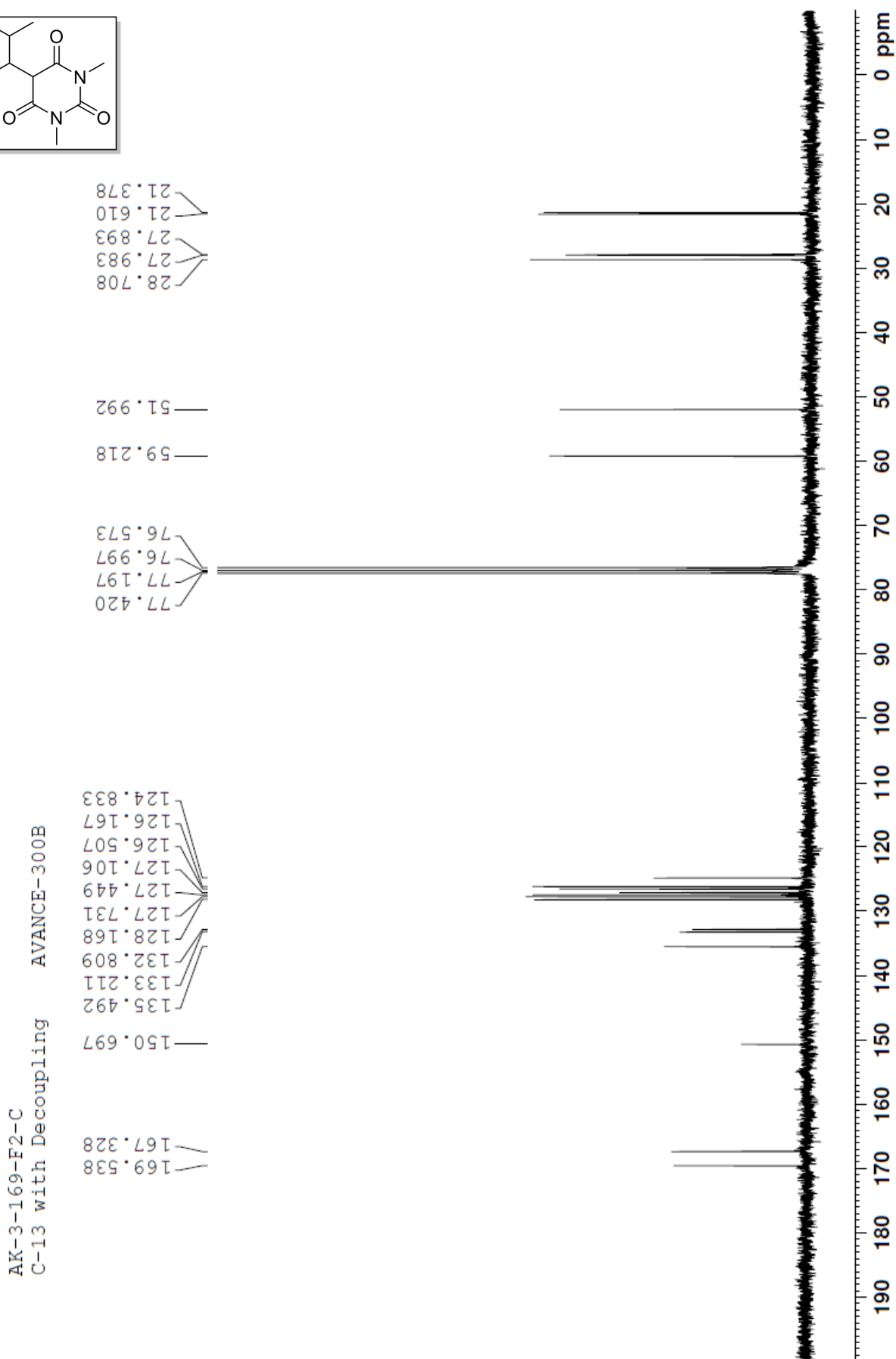
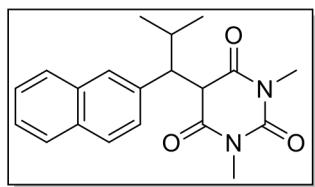
AK-3-169-F2-H  
proton, 16 scans AVANCE-300B

7.774  
7.762  
7.754  
7.743  
7.714  
7.699  
7.687  
7.450  
7.440  
7.429  
7.418  
7.401  
7.240  
7.033  
7.005

3.987  
3.975  
3.224  
3.212  
3.187  
3.174  
3.045  
2.854  
2.670  
2.648  
2.627  
2.610  
2.589  
2.567  
2.546  
1.554  
1.367  
1.346  
0.748  
0.726

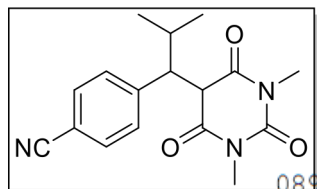


<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(2-methyl-1-(naphthalen-2-yl)propyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8e**)



<sup>1</sup>H NMR spectra of methylpropylbenzimidazole (8f)

of 4-(1-(1,3-dimethyl-2,4,6-trioxohexahydropyrimidin-5-yl)-2-

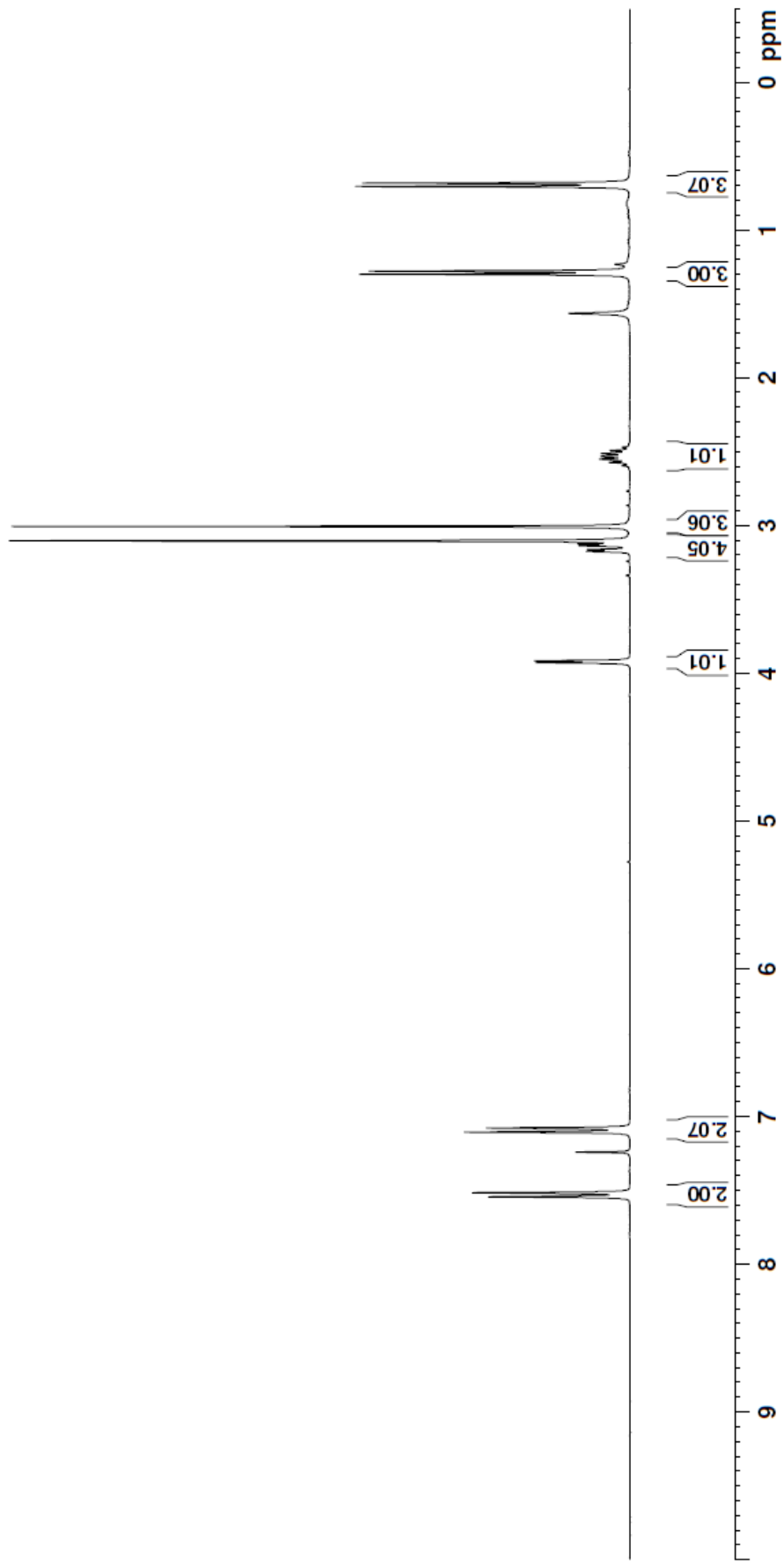


0.680  
0.702

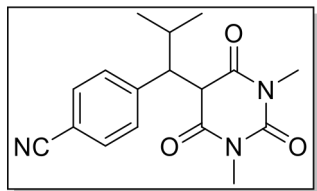
1.275  
1.297  
1.561  
2.468  
2.489  
2.511  
2.531  
2.549  
2.571  
2.592  
3.004  
3.101  
3.123  
3.135  
3.161  
3.173  
3.914  
3.926

7.077  
7.105  
7.240  
7.515  
7.542

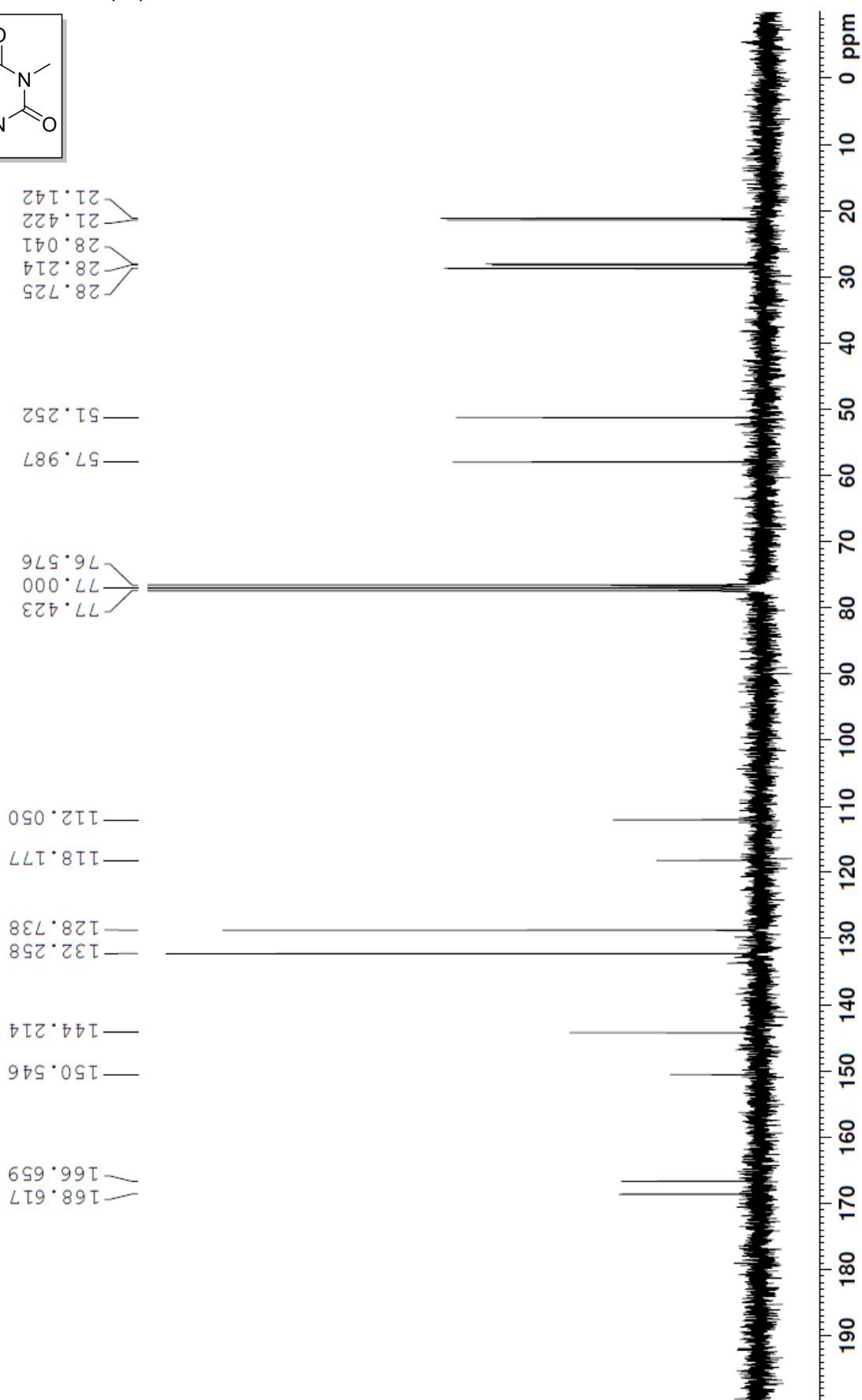
AK-3-164-F2-H  
proton, 16 scans  
AVANCE-300B



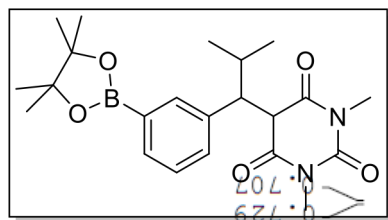
<sup>13</sup>C NMR spectra of methylpropyl(benzonitrile) (8f)



AK-3-164-F2-C  
C-13 with Decoupling  
AVANCE-300B



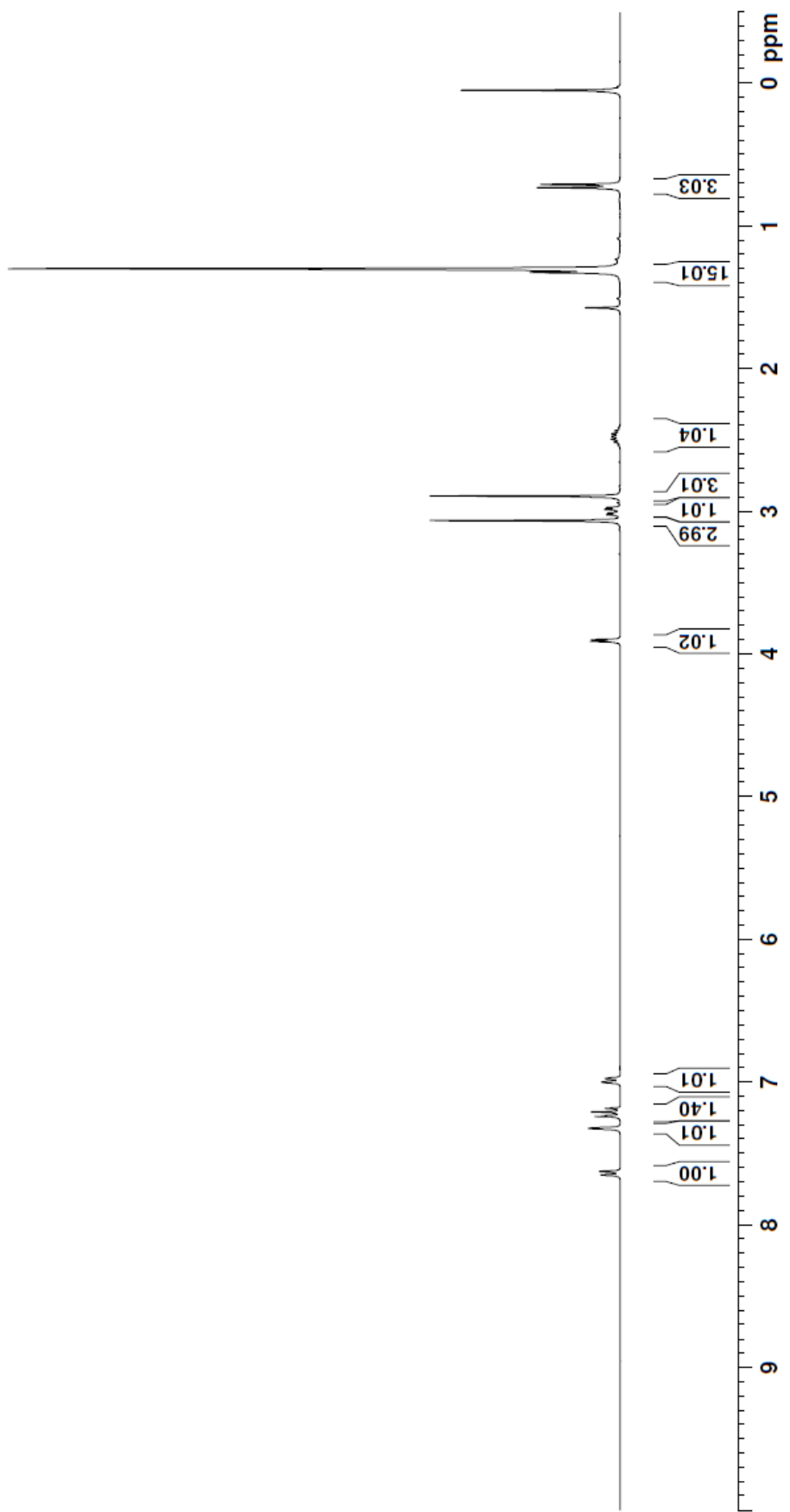
<sup>1</sup>H NMR spectra of 1,3-dimethyl-5-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8g**)



AK-3-167-F2-H  
proton, 16 scans AVANCE-300B

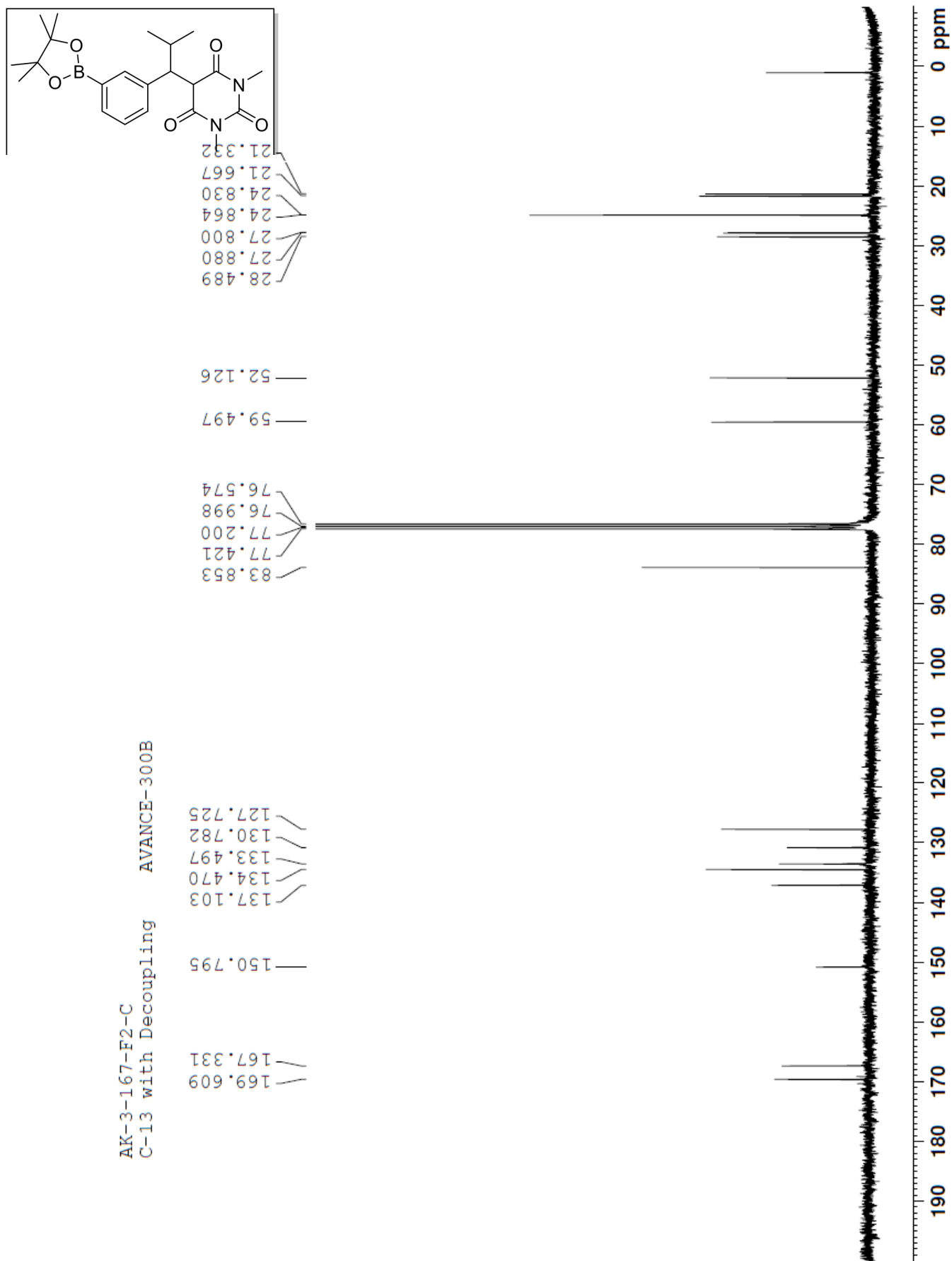
3.910  
3.898  
3.062  
3.022  
3.010  
2.985  
2.972  
2.891  
2.536  
2.514  
2.493  
2.472  
2.455  
2.434  
2.412  
1.325  
1.298

7.649  
7.624  
7.322  
7.240  
7.234  
7.208  
7.183  
6.999  
6.973

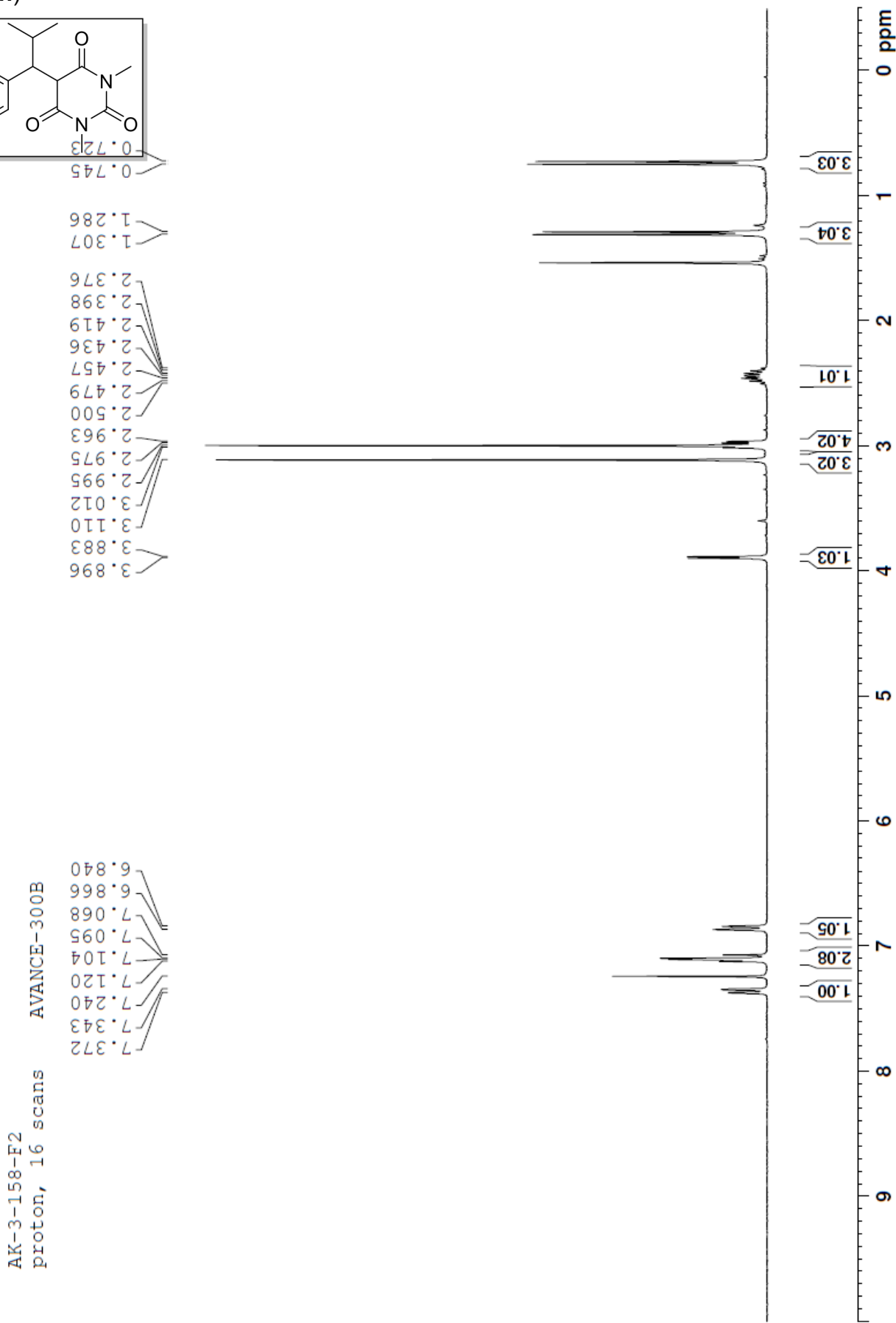
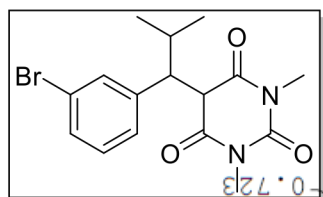




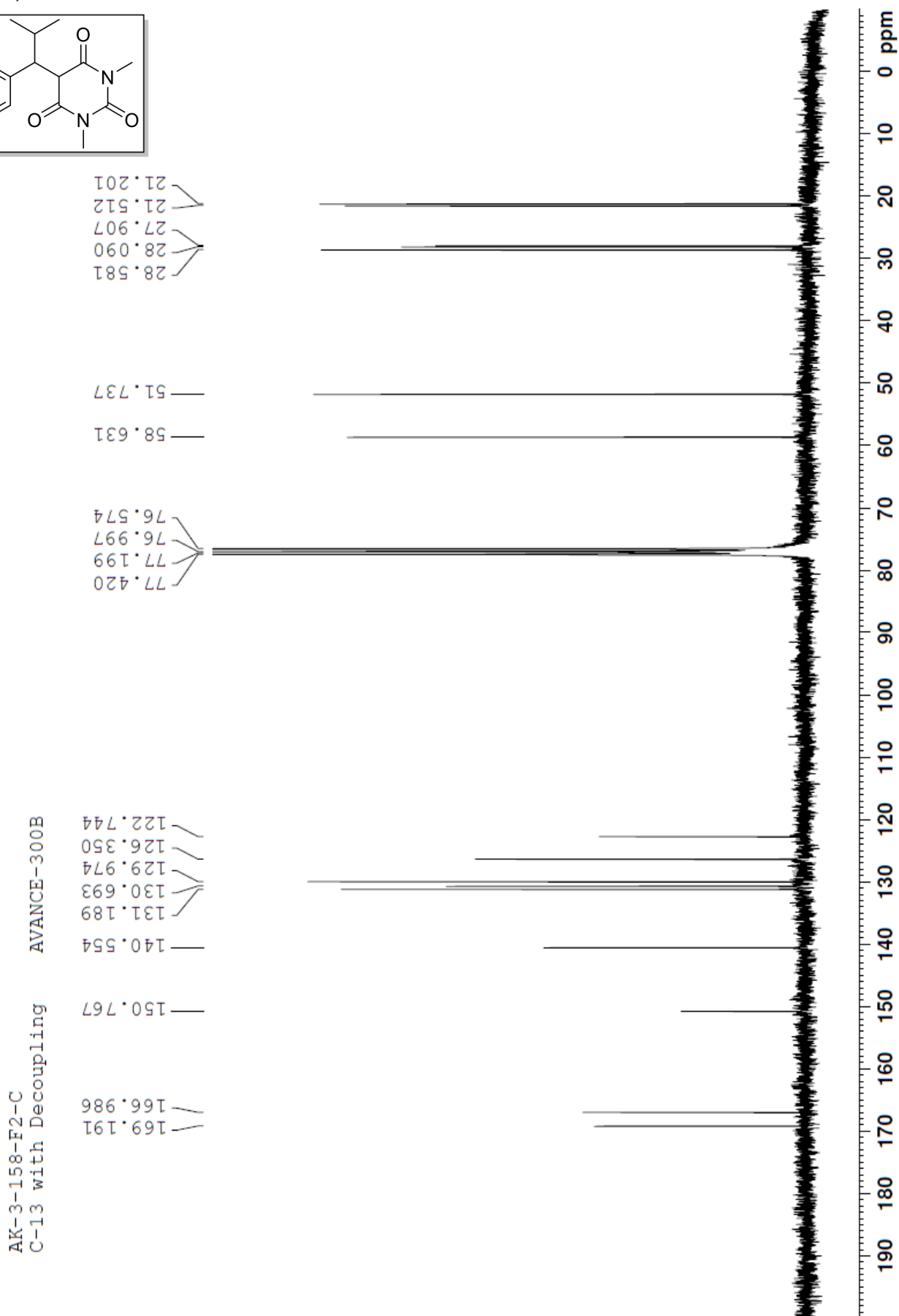
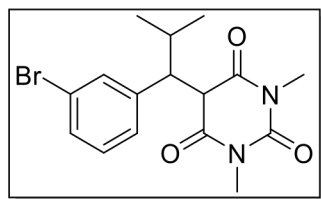
<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8g**)



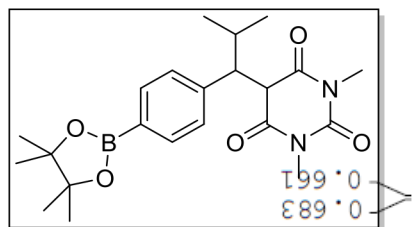
<sup>1</sup>H NMR spectra of 5-(1-(3-bromophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8h**)



<sup>13</sup>C NMR spectra of 5-(1-(3-bromophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8h**)



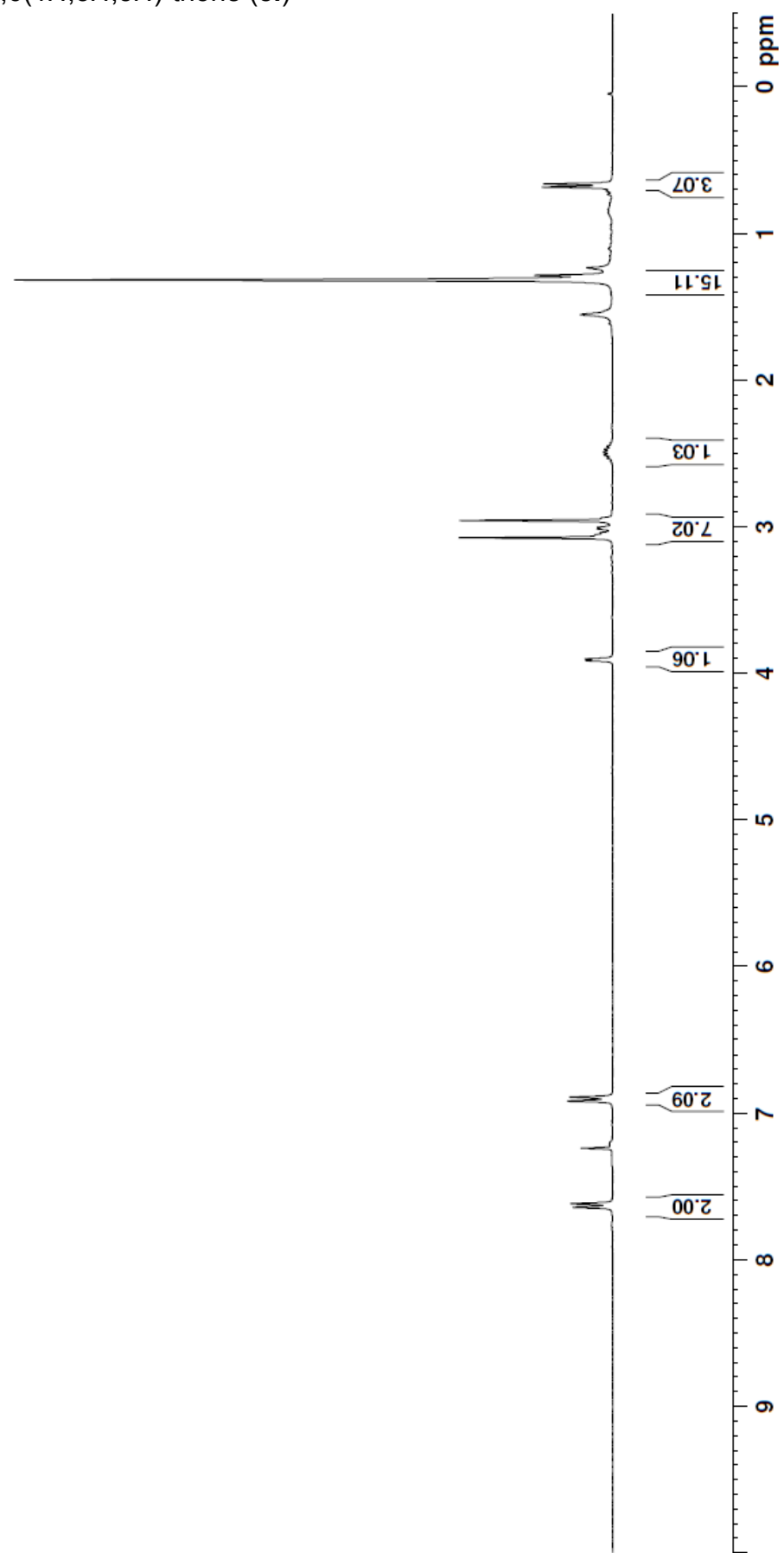
<sup>1</sup>H NMR spectra of 1,3-dimethyl-5-(2-methyl-1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8i**)



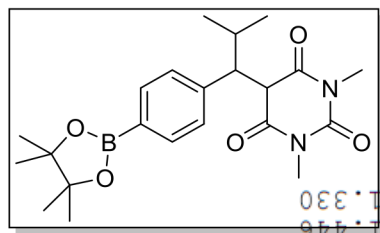
1.285  
1.317  
2.429  
2.451  
2.472  
2.490  
2.510  
2.532  
2.553  
2.958  
3.004  
3.015  
3.041  
3.075  
3.901  
3.913

AK-3-168-F2-H-2  
proton, 16 scans  
AVANCE-300B

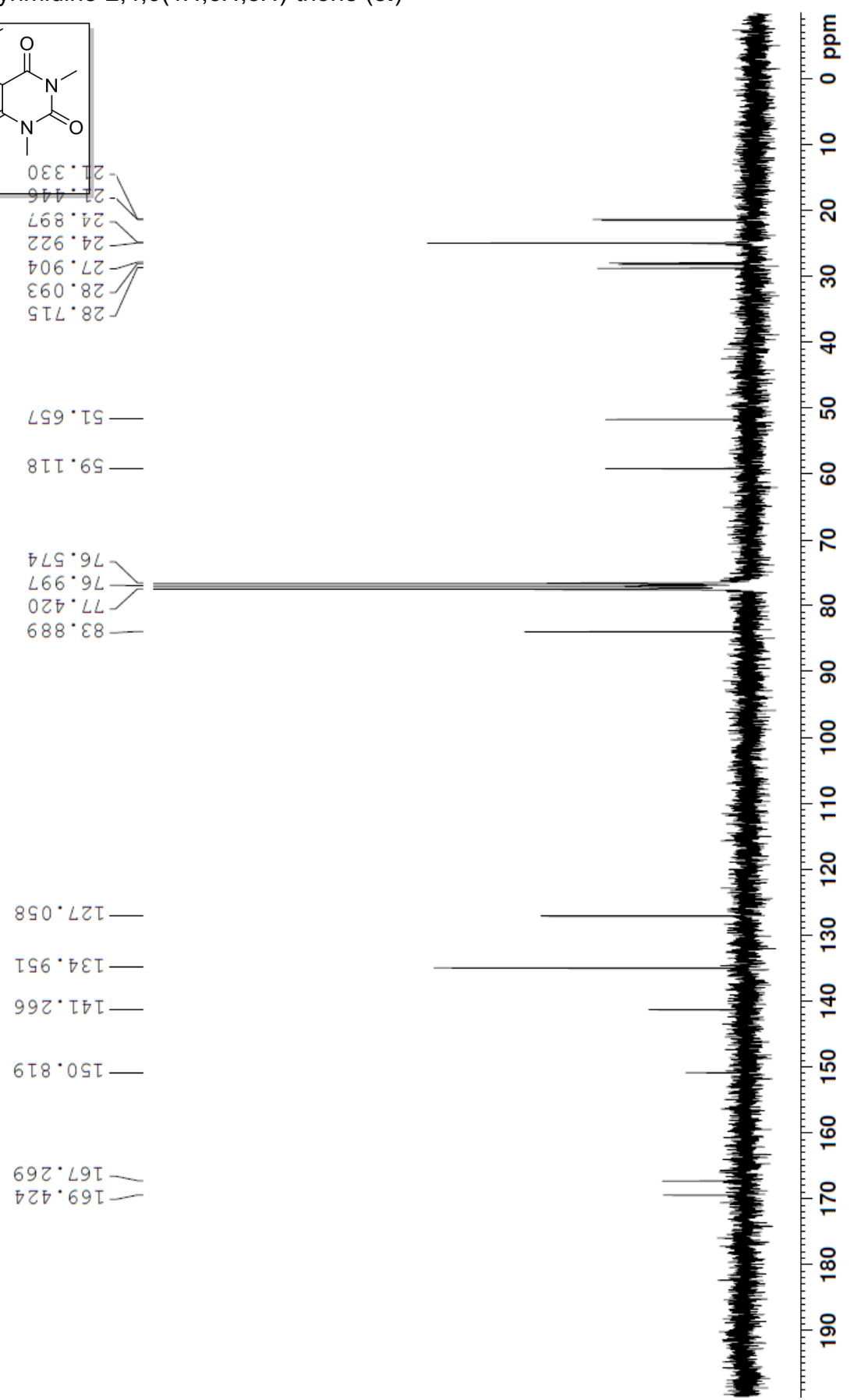
7.643  
7.617  
7.240  
6.917  
6.892



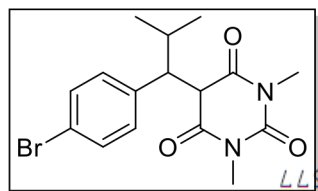
<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(2-methyl-1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8i**)



AK-3-168-F2-c  
C-13 with Decoupling  
AVANCE-300B



<sup>1</sup>H NMR spectra of 5-(1-(4-bromophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8j**)



0.677  
0.699

1.267  
1.288

1.571  
1.571

2.385  
2.407  
2.428

2.445  
2.466  
2.488

2.509  
2.995  
2.995

3.025  
3.037  
3.090

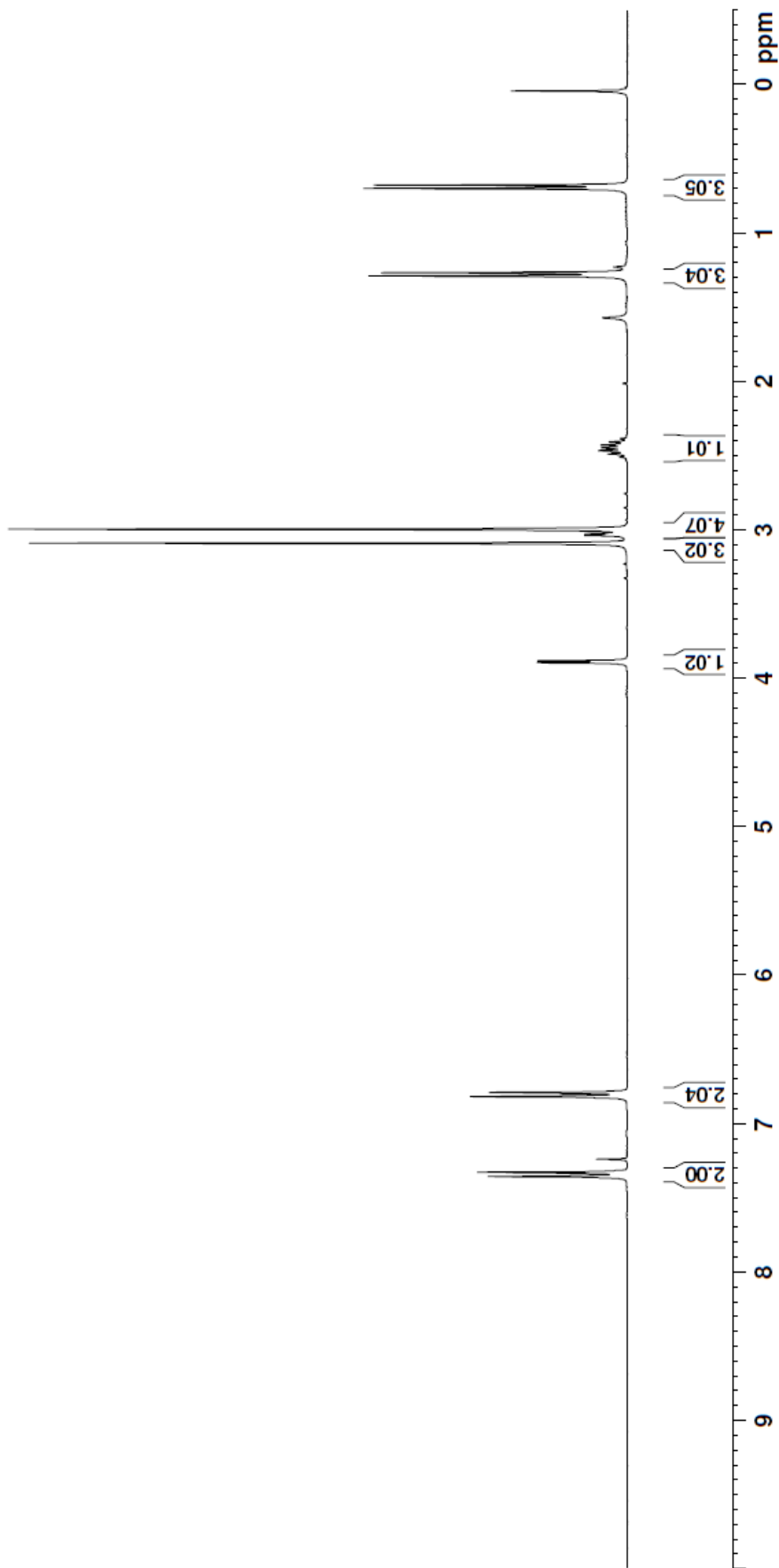
3.882  
3.894

6.790  
6.818

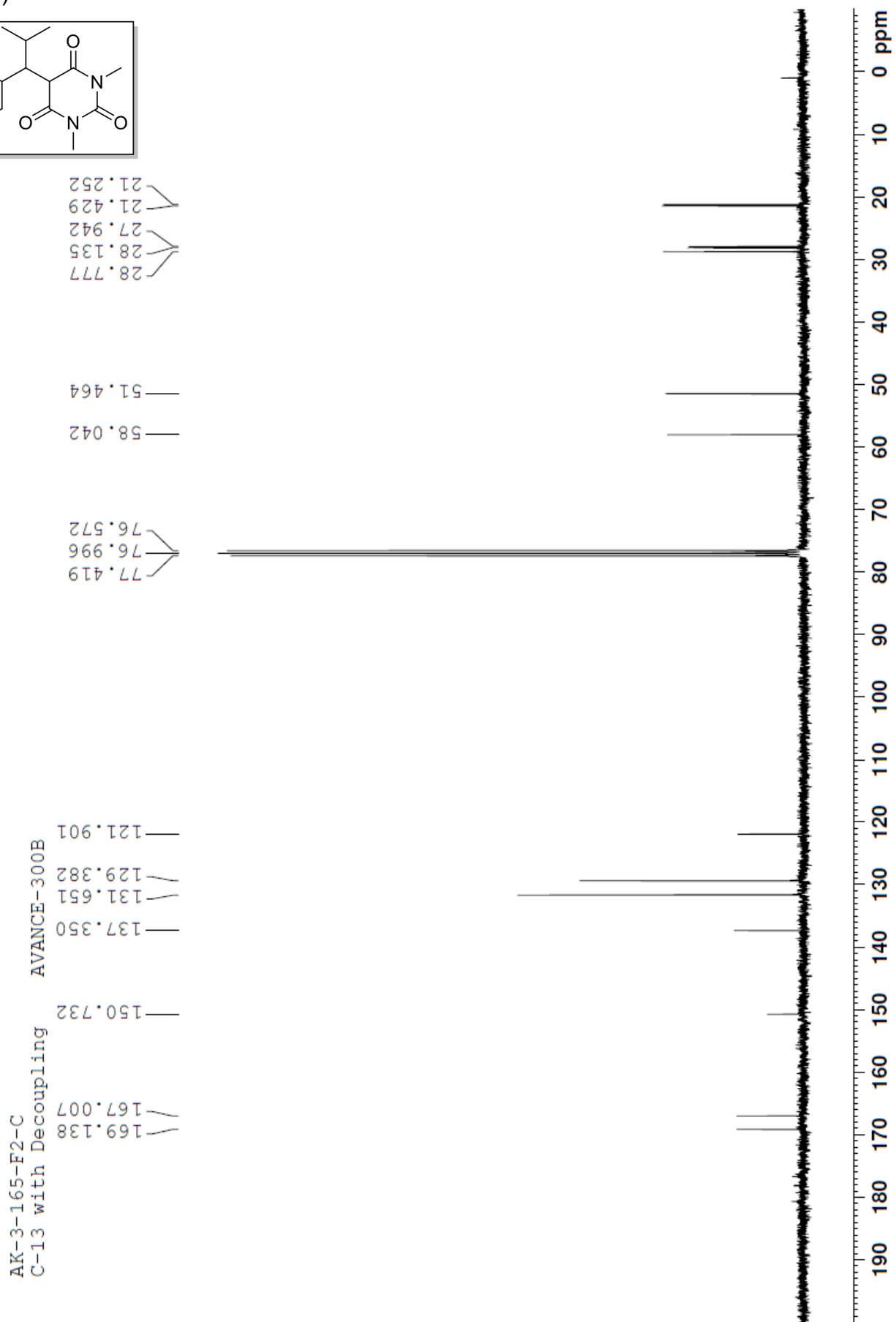
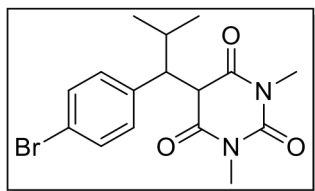
7.240  
7.328

7.356

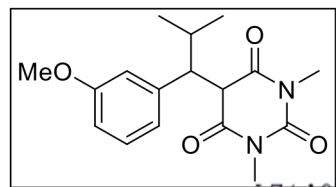
AK-3-165-F2-H  
proton, 16 scans AVANCE-300B



<sup>13</sup>C NMR spectra of 5-(1-(4-bromophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8j**)



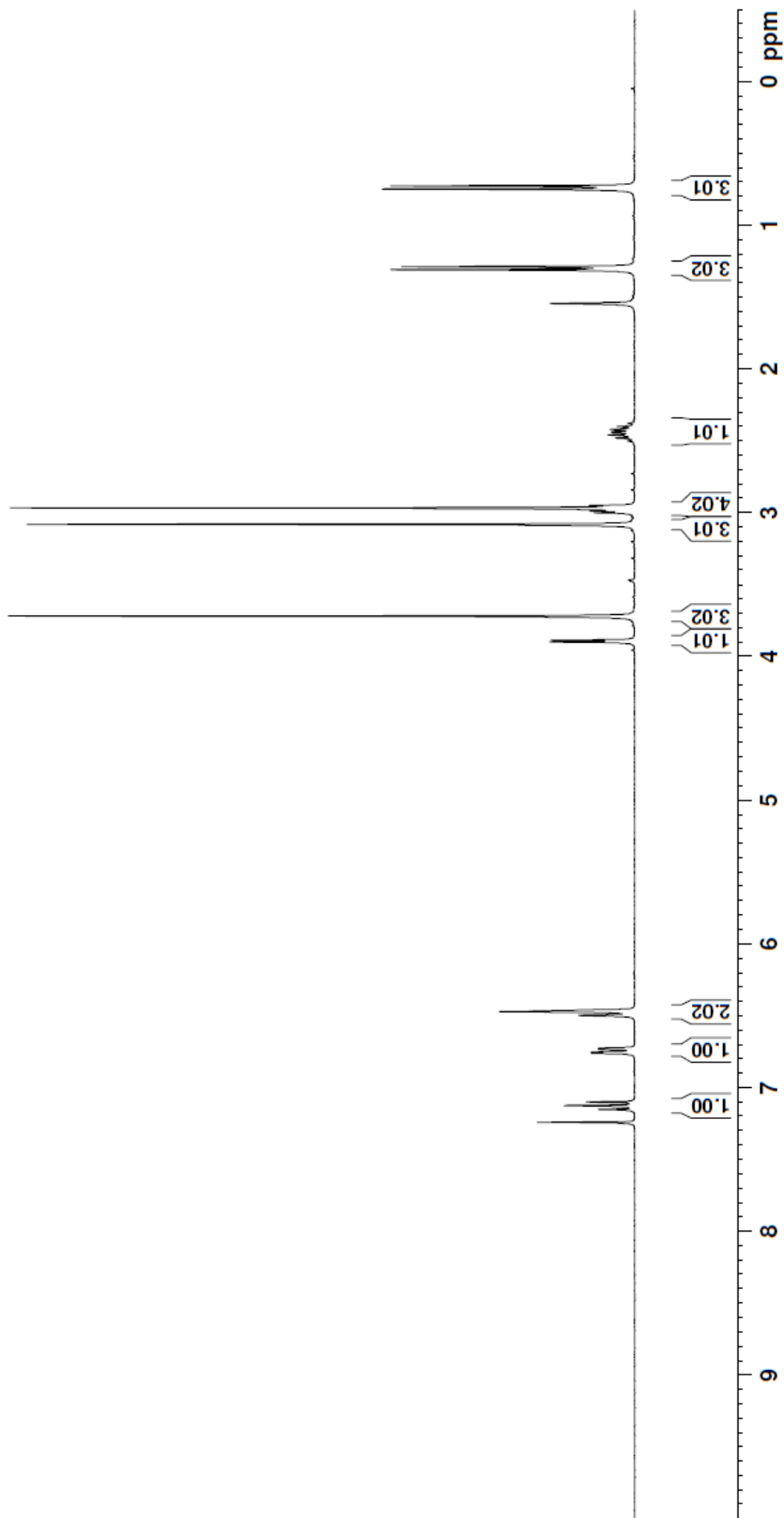
<sup>1</sup>H NMR spectra of 5-(1-(3-methoxyphenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8k**)



AK-3-153-F2-H  
proton, 16 scans  
AVANCE-300B

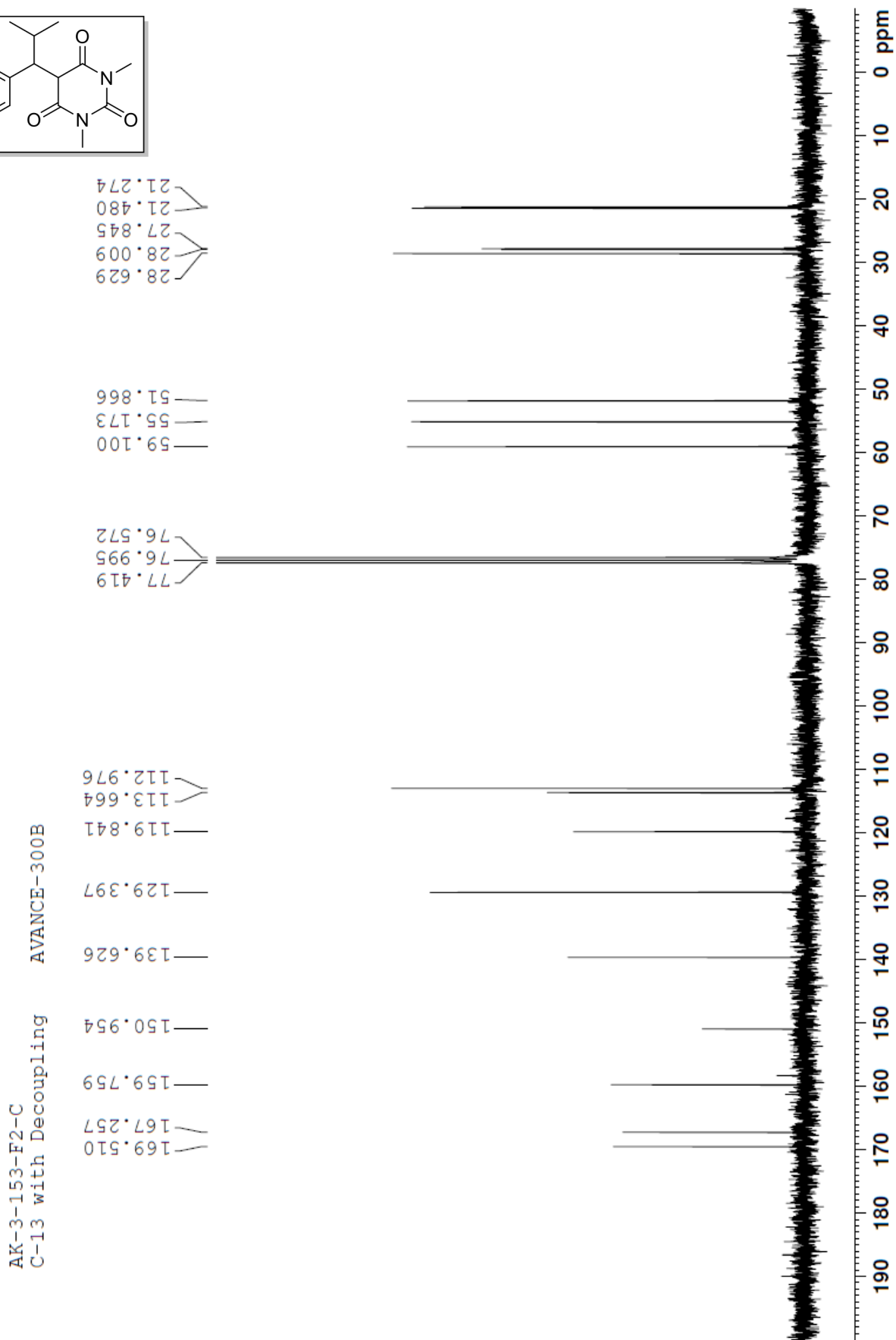
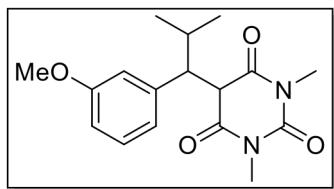
7.240  
7.150  
7.124  
7.098  
6.760  
6.752  
6.732  
6.729  
6.725  
6.495  
6.469

3.897  
3.885  
3.717  
3.079  
2.998  
2.986  
2.965  
2.949  
2.500  
2.478  
2.457  
2.440  
2.435  
2.419  
2.397  
2.376  
1.542  
1.307  
1.286  
0.746  
0.724

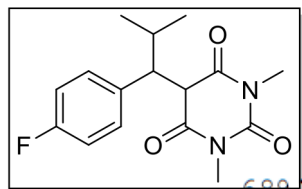




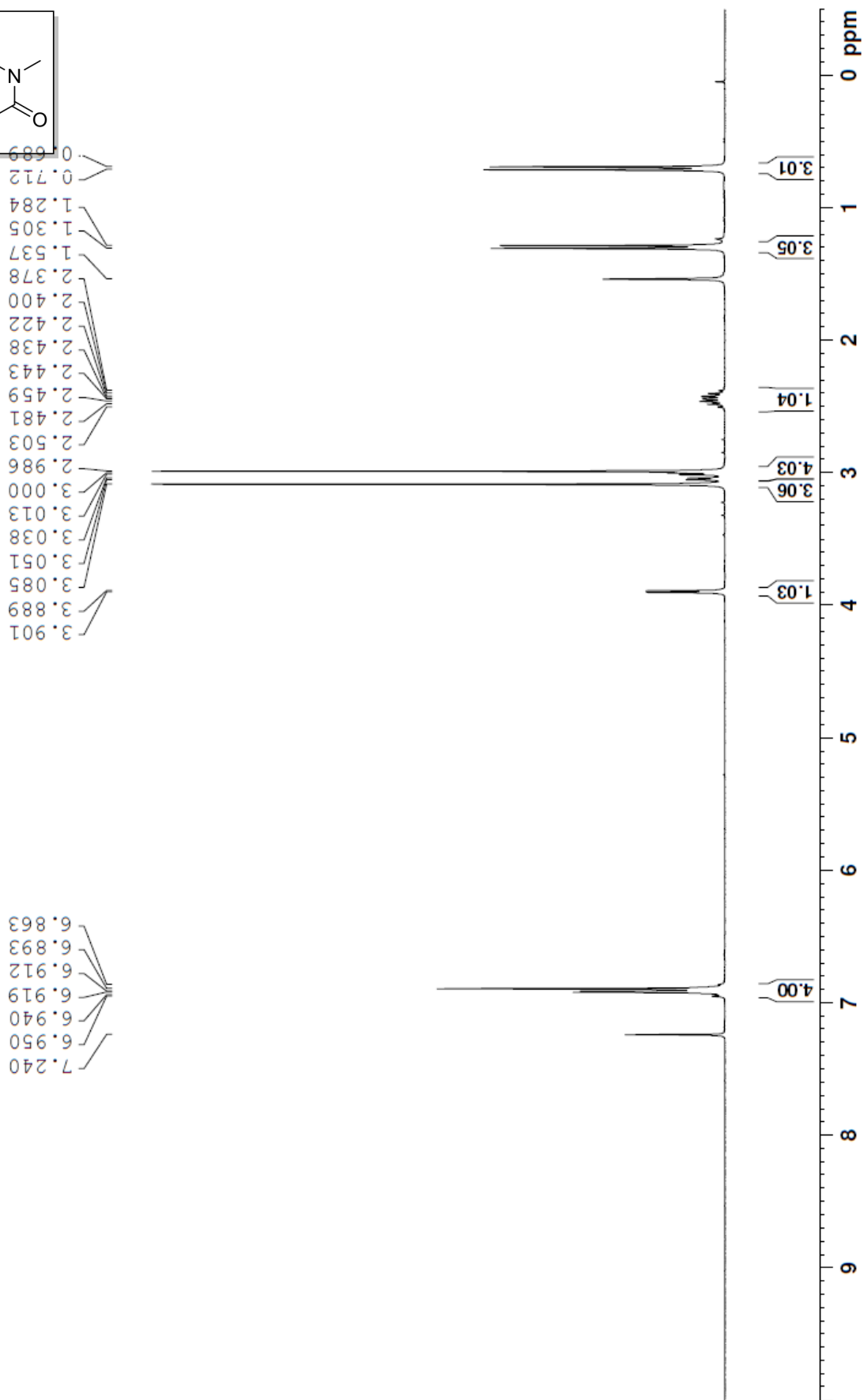
<sup>13</sup>C NMR spectra of 5-(1-(3-methoxyphenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8k**)



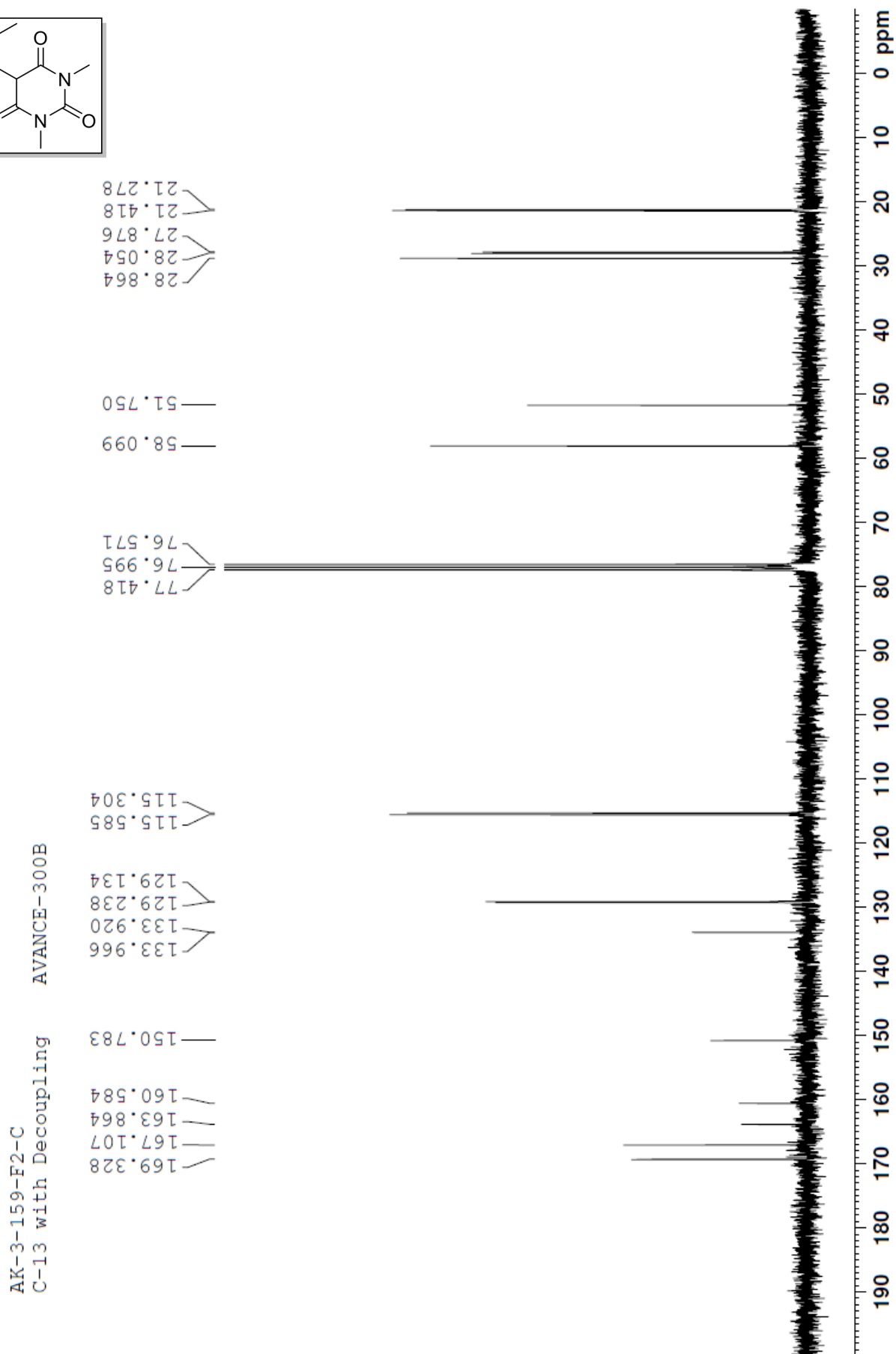
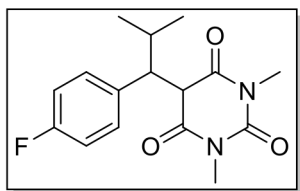
<sup>1</sup>H NMR spectra of 5-(1-(4-fluorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**8l**)



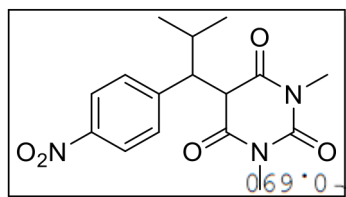
AK-3-159-F2-H  
proton, 16 scans  
AVANCE-300B



<sup>13</sup>C NMR spectra of 5-(1-(4-fluorophenyl)-2-methylpropyl)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8**)



<sup>1</sup>H NMR spectra of 1,3-dimethyl-5-(2-methyl-1-(4-nitrophenyl)propyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8m**)



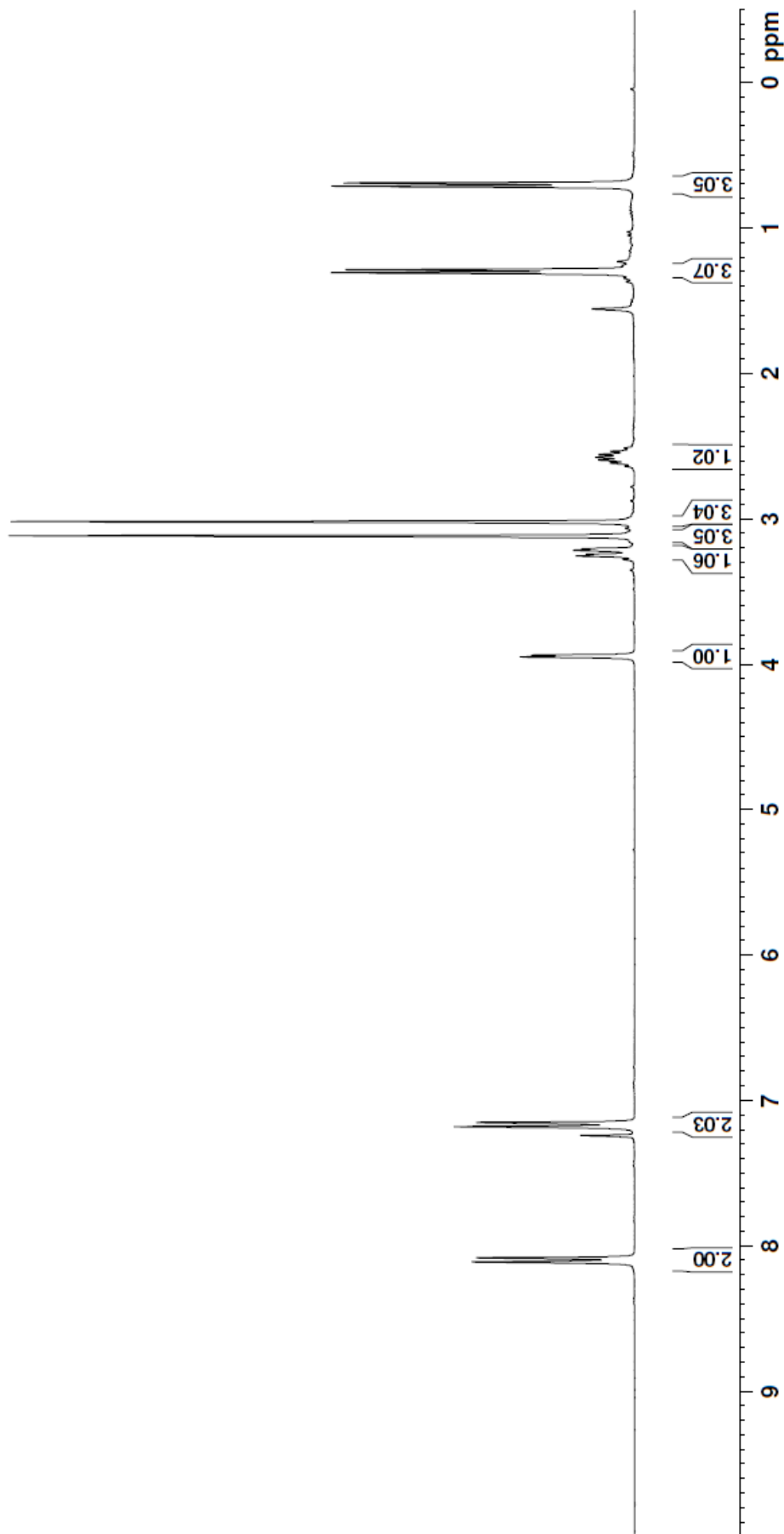
AK-3-157-F-H  
 proton, 16 scans  
 AVANCE-300B

8.111  
 8.082  
 7.240  
 7.180  
 7.152

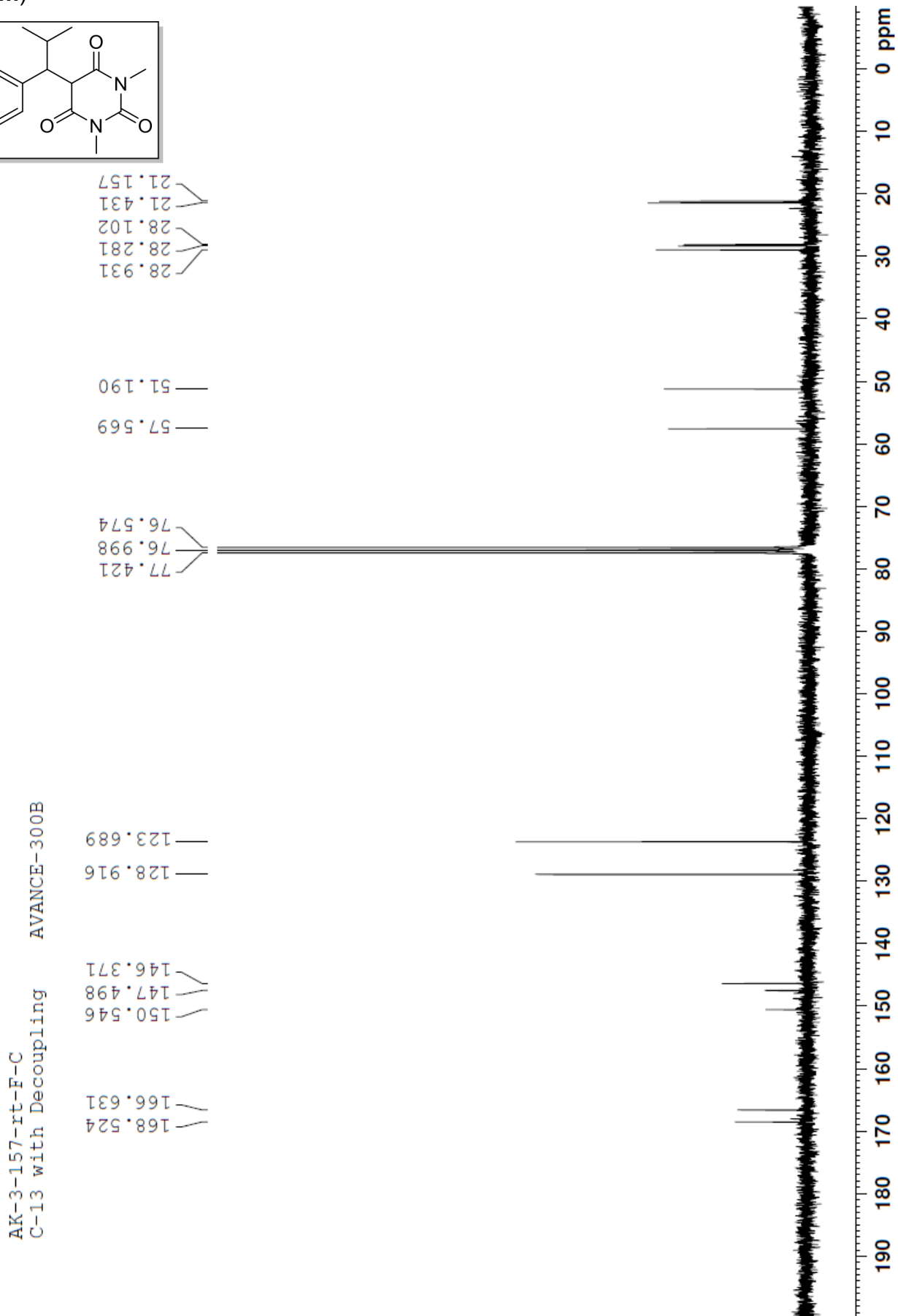
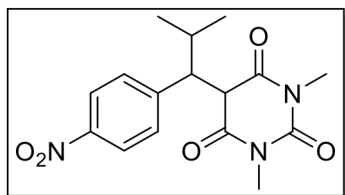
3.949  
 3.938  
 3.254  
 3.243  
 3.217  
 3.206  
 3.116  
 3.018  
 2.637  
 2.616  
 2.595  
 2.576  
 2.556  
 2.536  
 2.513

1.307  
 1.286

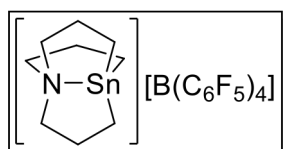
0.690  
 0.712



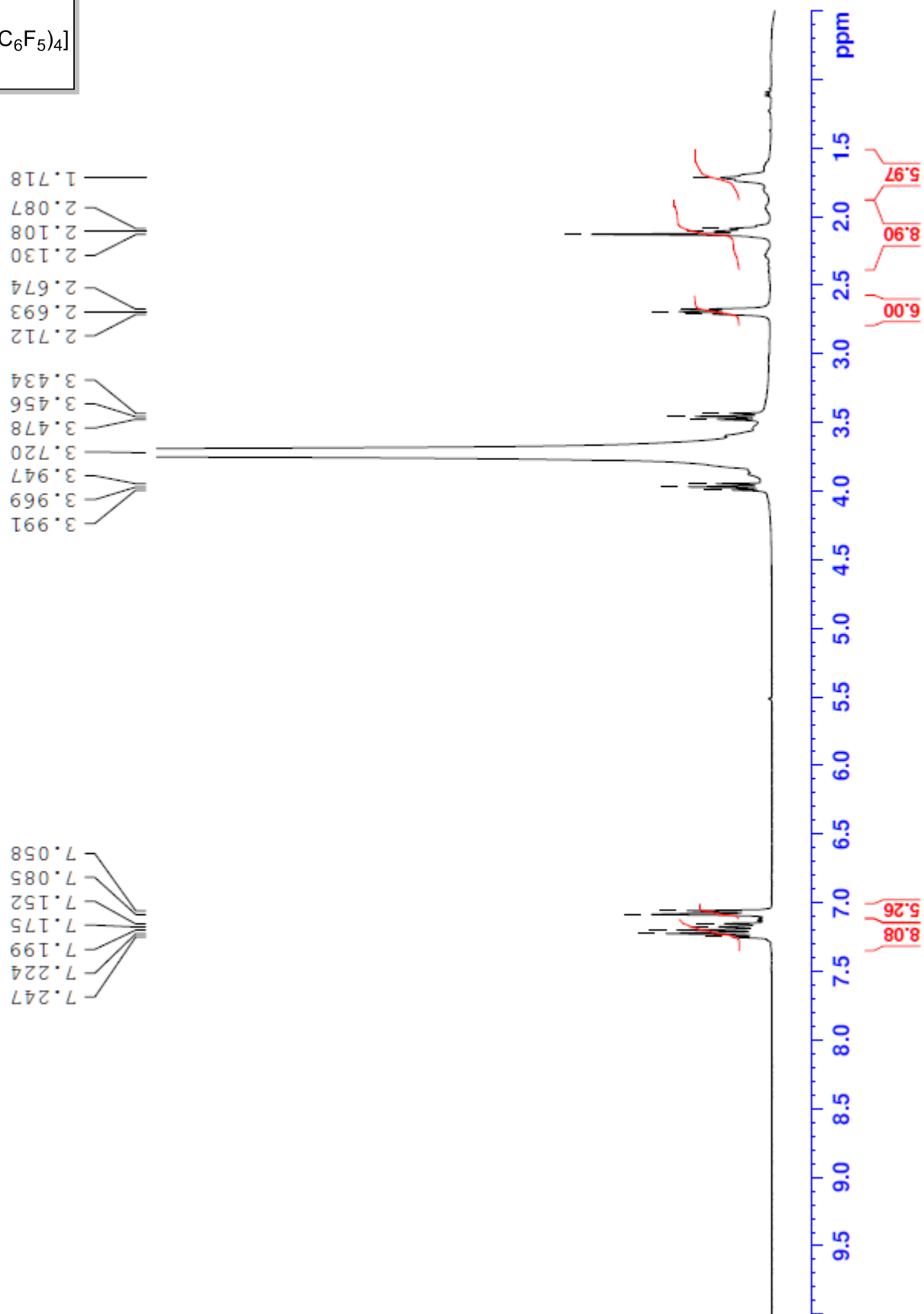
<sup>13</sup>C NMR spectra of 1,3-dimethyl-5-(2-methyl-1-(4-nitrophenyl)propyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8m**)



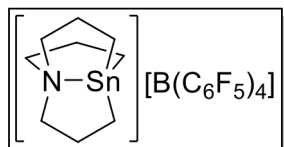
$^1\text{H}$  NMR spectra of  $[\text{N}(\text{CH}_2\text{CH}_2\text{CH}_2)_3\text{Sn}][\text{B}(\text{C}_6\text{F}_5)_4]$  (**13**)



CI-1-73-1H in ClCH2CH2Cl  
proton, 16 scans AVANCE-300B



$^{119}\text{Sn}$  NMR spectra of  $[\text{N}(\text{CH}_2\text{CH}_2\text{CH}_2)_3\text{Sn}][\text{B}(\text{C}_6\text{F}_5)_4]$  (**13**)



CI-1-73-119Sn in C1CH2CH2C1 [N(CH2CH2CH2)3Sn] [B(C6F5)4]  
119Sn with decoupling 1k scans AVANCE 300B

251.094

