

B(C₆F₅)₃-Catalyzed Divergent Cyanosilylations of Chromones Dependent on Temperature

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Supporting Information

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General consideration

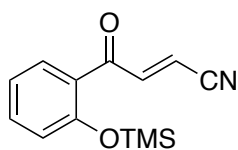
All air-sensitive compounds were handled under an atmosphere of argon or in a nitrogen-filled glovebox. ^1H NMR and ^{13}C NMR spectra were recorded on Bruker AV 500 at ambient temperature with CDCl_3 and acetone- d_6 as solvent and TMS as internal standard. Chemical shifts (δ) were given in ppm, referenced to the residual proton resonance of TMS (0) or to the carbon resonance of the CDCl_3 (77.23) and acetone- d_6 (205.45, 29.01). Coupling constants (J) were given in Hertz (Hz). All solvents were purified by conventional methods, distilled before use. Commercially available reagents were used without further purification. All the substrates were synthesized according to reported method.

General procedure for the 1,4-cyanosilylation chromones (Scheme 2): To a sealed-tube were added chromone **4** (0.3 mmol), $\text{B}(\text{C}_6\text{F}_5)_3$ (0.0077 g, 0.015 mmol), TMSCN (0.0714 g, 0.72 mmol, 0.096 mL) and dry toluene (1.5 mL) in a nitrogen atmosphere glovebox. After being sealed, the resulting mixture was stirred at 30 °C for 24 h. The reaction mixture was then cooled to room temperature, and the solvent was removed under vacuum. The crude residue was purified by flash chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as the eluent to give the desired product **5**.

General procedure for the C-O bond cyanosilylation (Scheme 3): To a sealed-tube were added chromones **4** (0.3 mmol), $\text{B}(\text{C}_6\text{F}_5)_3$ (0.0077 g, 0.015 mmol), TMSCN (0.0714 g, 0.72 mmol, 0.096 mL) and dry toluene (3.0 mL) in a nitrogen atmosphere glovebox. After being sealed, the resulting mixture was stirred at 80 °C for 24 h. The

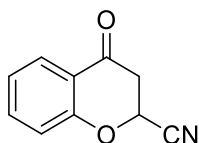
reaction mixture was cooled to room temperature, and the solvent was removed under vacuum. The crude residue was purified by flash chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as the eluent to give the desired product **6**.

Procedure for control experiments (Scheme 5): 1) **5a** (0.0173 g, 0.1 mmol) was dissolved in toluene (1.0 mL) and stirring at 80 °C for 48 h; 2) **5a** (0.0173 g, 0.1 mmol) and B(C₆F₅)₃ (0.0026 g, 0.025 mmol) were dissolved in toluene (1.0 mL), and the mixture was stirring at 80 °C for 24 h; 3) **5a** (0.0173 g, 0.1 mmol), B(C₆F₅)₃ (0.0026 g, 0.025 mmol), and TMSCN (0.0238 g, 0.24 mmol, 0.032 mL) were dissolved in toluene (1.0 mL), and the mixture was stirring at 80 °C for 24 h. All reactions were monitored by crude ¹H NMR.

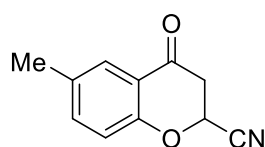


Intermediate of the C-O bond cyanosilylation: ¹H NMR (300 MHz, CDCl₃, ppm) δ 7.75 (d, *J* = 15.0 Hz, 1H), 7.77-7.73 (m, 1H), 7.55-7.45 (m, 1H), 7.09 (t, *J* = 9.0 Hz, 1H), 6.91 (d, *J* = 9.0 Hz, 1H), 6.41 (d, *J* = 15.0 Hz, 1H), 0.35 (s, 9H); HRMS (ESI) calcd. for C₁₃H₁₆O₂NSi [M+H]⁺: 246.0945, Found: 246.0943.

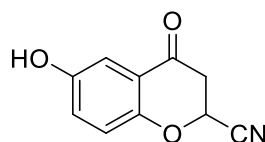
Characterization of products



4-Oxochromane-2-carbonitrile (5a): yellow solid, 0.0425 g, 82% yield, m.p. 86-91 °C; IR (film): 2919, 2849, 1691, 1461, 764 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.94 (d, $J = 7.5$ Hz, 1H), 7.59-7.56 (m, 1H), 7.18-7.15 (m, 1H), 7.07 (d, $J = 8.5$ Hz, 1H), 5.36 (t, $J = 5.0$ Hz, 1H), 3.09 (dd, $J = 17.0, 5.0$ Hz, 1H), 3.00 (dd, $J = 17.0, 7.0$ Hz, 1H).; ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 187.0, 158.7, 137.1, 127.4, 123.6, 120.9, 118.3, 115.9, 65.1, 40.5; HRMS (ESI) calcd. for $\text{C}_{10}\text{H}_8\text{NO}_2$ $[\text{M}+\text{H}]^+$: 174.0550, Found: 174.0548.

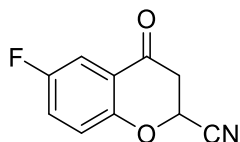


6-Methyl-4-oxochromane-2-carbonitrile (5b): yellow solid, 0.0458 g, 82% yield, m.p. 97-99 °C; IR (film): 3369, 2922, 1687, 1489, 837 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.73 (s, 1H), 7.38 (dd, $J = 8.5, 2.0$ Hz, 1H), 6.98 (d, $J = 8.5$ Hz, 1H), 5.39 (t, $J = 5.5$ Hz, 1H), 3.13 (dd, $J = 17.0, 5.0$ Hz, 1H), 3.04 (dd, $J = 17.0, 6.5$ Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 186.1, 155.7, 136.9, 132.2, 125.9, 119.4, 117.0, 114.9, 64.0, 39.5, 19.5; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_{10}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 188.0706, Found: 188.0709.

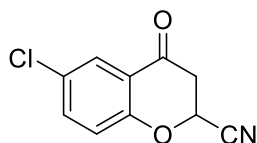


6-Hydroxy-4-oxochromane-2-carbonitrile (5c): brown solid, 0.0421 g, 75% yield, m.p. 145-147 °C; IR (film): 3195, 2921, 1687, 802 cm^{-1} ; ^1H NMR (500 MHz, acetone- d_6 , ppm) δ 8.59 (s, 1H), 7.28 (d, $J = 3.0$ Hz, 1H), 7.17 (dd, $J = 8.5, 3.0$ Hz, 1H), 7.02

(d, $J = 9.0$ Hz, 1H), 5.82 (t, $J = 5.5$ Hz, 1H), 3.31 (dd, $J = 17.5$, 5.0 Hz, 1H), 3.07 (dd, $J = 17.0$, 6.0 Hz, 1H); ^{13}C NMR (125 MHz, acetone- d_6 , ppm) δ 187.9, 153.4, 152.6, 125.1, 121.8, 119.7, 117.21, 110.9, 65.9, 40.5; HRMS (ESI) calcd. for $\text{C}_{10}\text{H}_6\text{NO}_3$ $[\text{M}-\text{H}]^-$: 188.0353, Found: 188.0348.

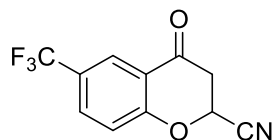


6-Fluoro-4-oxochromane-2-carbonitrile (5d): yellow solid, 0.0497 g, 87% yield, m.p. 79-83 °C; IR (film): 3391, 2920, 1698, 1484, 1165, 708 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.60 (dd, $J = 7.5$, 2.5 Hz, 1H), 7.33-7.29 (m, 1H), 7.09 (dd, $J = 9.0$, 4.0 Hz, 1H), 5.42 (t, $J = 6.0$ Hz, 1H), 3.17 (dd, $J = 17.5$, 5.0 Hz, 1H), 3.08 (dd, $J = 17.0$, 6.5 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 186.1, 158.3 (d, $J_{\text{C-F}} = 245.7$ Hz), 154.7, 124.5 (d, $J_{\text{C-F}} = 24.7$ Hz), 121.5 (d, $J_{\text{C-F}} = 6.8$ Hz), 120.2 (d, $J_{\text{C-F}} = 7.4$ Hz), 115.5, 112.6 (d, $J_{\text{C-F}} = 23.9$ Hz), 65.2, 40.2; ^{19}F NMR (376 MHz, CDCl_3 , ppm) δ -117.9; HRMS (ESI) calcd. for $\text{C}_{10}\text{H}_5\text{FNO}_2$ $[\text{M}-\text{H}]^-$: 190.0310, Found: 190.0305.

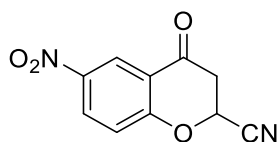


6-Chloro-4-oxochromane-2-carbonitrile (5e): yellow solid, 0.0554 g, 89% yield, m.p. 133-137 °C; IR (film): 3385, 3053, 1697, 1266, 739 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.91 (d, $J = 2.5$ Hz, 1H), 7.53 (dd, $J = 9.0$, 3.0 Hz, 1H), 7.06 (d, $J = 8.5$ Hz, 1H), 5.43 (t, $J = 6.5$ Hz, 1H), 3.17 (dd, $J = 17.5$, 5.0 Hz, 1H), 3.08 (dd, $J = 17.5$, 7.0 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 185.8, 157.0, 136.8, 129.3, 126.7, 121.6, 120.0,

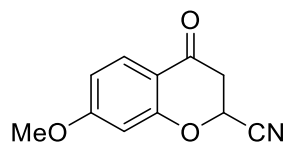
115.4, 65.1, 40.2; HRMS (ESI) calcd. for $C_{10}H_5ClNO_2$ $[M-H]^-$: 206.0014, Found: 206.0010.



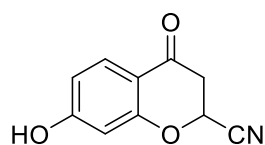
4-Oxo-6-(trifluoromethyl)chromane-2-carbonitrile (5f): yellow solid, 0.0662 g, 92% yield, m.p. 87-89 °C; IR (film): 2920, 1703, 1270, 836 cm^{-1} ; 1H NMR (500 MHz, $CDCl_3$, ppm) δ 8.23 (s, 1H), 7.82 (dd, J = 9.0, 2.0 Hz, 1H), 7.23 (d, J = 8.5 Hz, 1H), 5.52 (t, J = 6.5 Hz, 1H), 3.15 (dd, J = 17.5, 5.0 Hz, 1H), 3.06 (dd, J = 17.0, 6.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 184.7, 159.5, 132.3 (q, J_{C-F} = 3.8 Hz), 125.2 (q, J_{C-F} = 34.0 Hz), 124.1 (q, J_{C-F} = 5.0 Hz), 122.3 (d, J_{C-F} = 272.0 Hz), 119.5, 118.3, 114.2, 64.2, 39.1; ^{19}F NMR (376 MHz, $CDCl_3$, ppm) δ -62.5; HRMS (ESI) calcd. for $C_{11}H_5F_3NO_2$ $[M-H]^-$: 240.0278, Found: 240.0276.



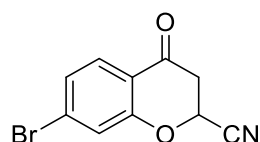
6-Nitro-4-oxochromane-2-carbonitrile (5g): yellow solid, 0.0497 g, 76% yield, m.p. 135-140 °C; IR (film): 3446, 2920, 1617, 747 cm^{-1} ; 1H NMR (500 MHz, acetone- d_6 , ppm) δ 8.64 (d, J = 2.5 Hz, 1H), 8.50 (dd, J = 9.0, 3.0 Hz, 1H), 7.44 (d, J = 9.0 Hz, 1H), 6.13 (t, J = 7.0 Hz, 1H), 3.53 (dd, J = 17.0, 5.0 Hz, 1H), 3.37 (dd, J = 17.5, 7.0 Hz, 1H); ^{13}C NMR (125 MHz, acetone- d_6 , ppm) δ 186.2, 162.7, 143.3, 130.9, 122.5, 120.8, 120.0, 115.9, 66.1, 39.6; HRMS (ESI) calcd. for $C_{10}H_5N_2O_4$ $[M-H]^-$: 217.0255, Found: 217.0254.



7-Methoxy-4-oxochromane-2-carbonitrile (5h): yellow solid, 0.0239 g, 43% yield, m.p. 137-139 °C; IR (film): 3059, 2919, 1672, 1266, 739 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.82-7.80 (m, 1H), 6.64-6.62 (m, 1H), 6.44 (s, 1H), 5.34-5.32 (m, 1H), 3.80 (s, 3H), 3.02 (dd, $J = 17.0, 5.0$ Hz, 1H), 2.93 (dd, $J = 17.0, 6.5$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 184.4, 165.6, 159.6, 128.1, 114.8, 113.6, 110.7, 100.4, 64.3, 54.9, 39.0; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_{10}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 204.0655, Found: 204.0657.

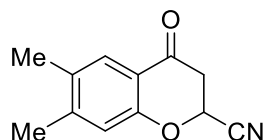


7-Hydroxy-4-oxochromane-2-carbonitrile (5i): brown solid, 0.0434 g, 77% yield, m.p. 159-163 °C; IR (film): 2955, 2849, 1260, 803 cm^{-1} ; ^1H NMR (500 MHz, acetone- d_6 , ppm) δ 7.77 (d, $J = 8.5$ Hz, 1H), 6.70 (dd, $J = 8.5, 2.0$ Hz, 1H), 6.51 (d, $J = 2.0$ Hz, 1H), 5.85 (t, $J = 6.0$ Hz, 1H), 3.25 (dd, $J = 17.0, 5.0$ Hz, 1H), 3.01 (dd, $J = 17.0, 6.0$ Hz, 1H); ^{13}C NMR (125 MHz, acetone- d_6 , ppm) δ 187.3, 166.7, 162.5, 130.7, 118.6, 115.9, 113.7, 105.0, 67.5, 41.5; HRMS (ESI) calcd. for $\text{C}_{10}\text{H}_6\text{NO}_3$ $[\text{M}-\text{H}]^-$: 188.0353, Found: 188.0349.

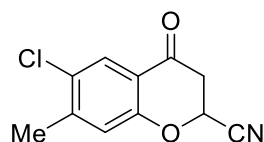


7-Bromo-4-oxochromane-2-carbonitrile (5j): yellow solid, 0.0603 g, 80% yield, m.p. 105-108 °C; IR (film): 3458, 1606, 977 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.97

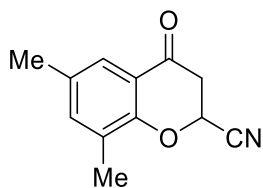
(d, $J = 2.5$ Hz, 1H), 7.59 (dd, $J = 9.0, 2.5$ Hz, 1H), 6.93 (d, $J = 8.5$ Hz, 1H), 5.37 (t, $J = 6.5$ Hz, 1H), 3.09 (dd, $J = 17.0, 5.0$ Hz, 1H), 3.00 (dd, $J = 17.5, 7.0$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 184.6, 156.4, 138.6, 128.8, 121.0, 119.3, 115.4, 114.4, 64.1, 39.1; HRMS (ESI) calcd. for $\text{C}_{10}\text{H}_5\text{BrNO}_2$ $[\text{M-H}]^-$: 249.9509, Found: 249.9508.



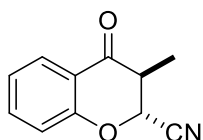
6,7-Dimethyl-4-oxochromane-2-carbonitrile (5k): brown solid, 0.0433g, 72% yield, m.p. 164-166 °C; IR (film): 2920, 1687, 1249, 869 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.59 (s, 1H), 6.78 (s, 1H), 5.30 (t, $J = 6.5$ Hz, 1H), 3.02 (dd, $J = 17.0, 5.0$ Hz, 1H), 2.92 (dd, $J = 17.0, 6.5$ Hz, 1H), 2.22 (s, 3H), 2.17 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 185.8, 155.9, 146.8, 131.4, 126.2, 117.6, 117.5, 115.0, 64.1, 39.4, 19.6, 17.9; HRMS (ESI) calcd. for $\text{C}_{12}\text{H}_{10}\text{NO}_2$ $[\text{M-H}]^-$: 200.0717, Found: 200.0713.



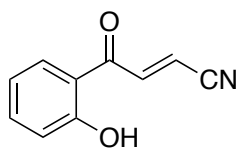
6-Chloro-7-methyl-4-oxochromane-2-carbonitrile (5l): gray solid, 0.0581 g, 88% yield, m.p. 122-126°C; IR (film): 3311, 2960, 1701, 1237, 909 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.87 (s, 1H), 6.98 (s, 1H), 5.42 (t, $J = 6.0$ Hz, 1H), 3.06 (dd, $J = 17.5, 5.0$ Hz, 1H), 2.96 (dd, $J = 17.5, 6.5$ Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 184.6, 155.7, 145.4, 128.8, 126.0, 119.3, 118.7, 114.6, 64.1, 39.1, 20.0; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_7\text{ClNO}_2$ $[\text{M-H}]^-$: 220.0171, Found: 220.0167.



6,8-Dimethyl-4-oxochromane-2-carbonitrile (5m): brown solid, 0.0491 g, 82% yield, m.p. 108-111 °C; IR (film): 2923, 1701, 872 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.57 (s, 1H), 7.24 (s, 1H), 5.42 (t, J = 6.5 Hz, 1H), 3.11 (dd, J = 17.0, 5.0 Hz, 1H), 3.02 (dd, J = 17.0, 7.0 Hz, 1H), 2.29 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 187.6, 155.0, 139.2, 132.4, 127.4, 124.5, 120.3, 116.1, 65.0, 40.4, 20.5, 15.4; HRMS (ESI) calcd. for $\text{C}_{12}\text{H}_{10}\text{NO}_2$ $[\text{M}-\text{H}]^-$: 200.0717, Found: 200.0713.

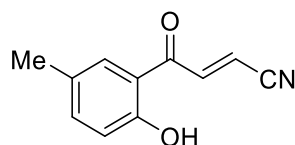


trans-3-Methyl-4-oxochromane-2-carbonitrile (5q): yellow solid, 0.0434 g, 77% yield, m.p. 140-142 °C; IR (film): 3392, 2919, 2848, 2428, 2437, 1688, 1126, 476 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.94 (dd, J = 7.6, 1.2 Hz, 1H), 7.57 (t, J = 7.6 Hz, 1H), 7.16 (t, J = 7.2 Hz, 1H), 7.07 (d, J = 8.4 Hz, 1H), 4.99 (d, J = 9.6 Hz, 1H), 3.11-3.03 (m, 1H), 1.44 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3 , ppm) δ 190.2, 158.7, 136.7, 127.7, 123.4, 112.0, 118.0, 115.4, 70.5, 44.1, 11.3; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_8\text{NO}_2$ $[\text{M}-\text{H}]^-$: 186.0561, Found: 186.0544.

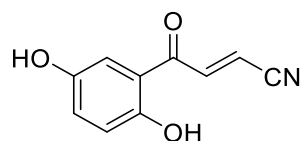


(E)-4-(2-hydroxyphenyl)-4-oxobut-2-enenitrile (6a): yellow solid, 0.0470 g, 91% yield, m.p. 121-125 °C; IR (film): 3045, 2919, 2226, 1592, 757 cm^{-1} ; ^1H NMR (500

MHz, CDCl₃, ppm) δ 12.01 (s, 1H), 7.89 (d, J = 16.0 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.58 (t, J = 8.5 Hz, 1H), 7.06 (d, J = 8.5 Hz, 1H), 6.99 (t, J = 8.0 Hz, 1H), 6.64 (d, J = 16.0 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃, ppm) δ 188.9, 163.0, 139.0, 137.2, 128.8, 118.6, 118.0, 117.6, 115.1, 111.5; HRMS (ESI) calcd. for C₁₀H₆NO₂ [M-H]⁻: 172.0404, Found: 172.0396.

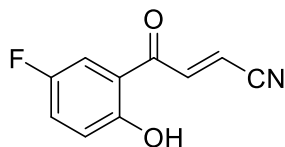


(E)-4-(2-hydroxy-5-methylphenyl)-4-oxobut-2-enenitrile (6b): orange solid, 0.0488 g, 87% yield, m.p. 86-89 °C; IR (film): 3393, 2919, 2229, 1644, 961, 528 cm⁻¹; ¹H NMR (500 MHz, acetone-*d*₆, ppm) δ 11.76 (s, 1H), 7.80 (d, J = 15.5 Hz, 1H), 7.40 (s, 1H), 7.29 (d, J = 8.5 Hz, 1H), 6.85 (d, J = 8.5 Hz, 1H), 6.51 (d, J = 15.5 Hz, 1H), 2.25 (s, 3H); ¹³C NMR (125 MHz, CDCl₃, ppm) δ 188.8, 161.0, 139.9, 138.4, 128.4, 127.9, 117.7, 117.3, 115.2, 111.2, 19.5; HRMS (ESI) calcd. for C₁₁H₁₀NO₂ [M+H]⁺: 188.0706, Found: 188.0706.

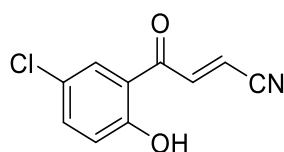


(E)-4-(2,5-dihydroxyphenyl)-4-oxobut-2-enenitrile (6c): orange solid, 0.0408 g, 72% yield, m.p. 128-135 °C; IR (film): 3370, 2920, 2849, 2241, 1647, 1181, 788 cm⁻¹; ¹H NMR (400 MHz, acetone-*d*₆, ppm) δ 11.43 (s, 1H), 8.36 (br s, 1H), 8.24 (d, J = 15.6 Hz, 1H), 7.47 (d, J = 2.8 Hz, 1H), 7.23 (dd, J = 9.2, 2.8 Hz, 1H), 6.92 (d, J = 8.8 Hz, 1H), 6.77 (d, J = 16.0 Hz, 1H); ¹³C NMR (100 MHz, acetone-*d*₆, ppm) δ 190.9, 157.0,

149.8, 142.3, 126.6, 118.9, 116.5, 114.9, 111.9; HRMS (ESI) calcd. for $C_{10}H_6NO_3$ $[M-H]^-$: 188.0353, Found: 188.0346.

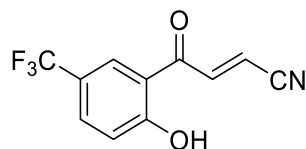


(E)-4-(5-fluoro-2-hydroxyphenyl)-4-oxobut-2-enenitrile (6d): yellow solid, 0.0518 g, 90% yield, m.p. 137-140 °C; IR (film): 3098, 2918, 2231, 1484, 1176, 781, 543 cm^{-1} ; 1H NMR (500 MHz, $CDCl_3$, ppm) δ 11.70 (s, 1H), 7.71 (d, J = 15.0 Hz, 1H), 7.33 (dd, J = 8.5, 2.5 Hz, 1H), 7.29-7.25 (m, 1H), 6.97 (dd, J = 9.5, 4.5 Hz, 1H), 6.60 (d, J = 15.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 188.3 (d, J_{C-F} = 2.9 Hz), 159.3, 154.0 (d, J_{C-F} = 241.0 Hz), 139.0, 125.1 (d, J_{C-F} = 23.8 Hz), 119.5 (d, J_{C-F} = 7.4 Hz), 116.9 (d, J_{C-F} = 6.4 Hz), 114.9, 113.4 (d, J_{C-F} = 23.6 Hz), 112.3; ^{19}F NMR (376 MHz, $CDCl_3$, ppm) δ -122.5; HRMS (ESI) calcd. for $C_{10}H_5FNO_2$ $[M-H]^-$: 190.0310, Found: 190.0303.

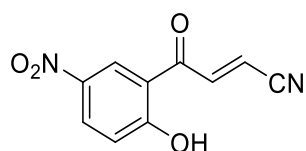


(E)-4-(5-chloro-2-hydroxyphenyl)-4-oxobut-2-enenitrile (6e): yellow solid, 0.0558 g, 90% yield, m.p. 131-133 °C; IR (film): 3086, 2919, 2228, 1641, 528 cm^{-1} ; 1H NMR (500 MHz, $CDCl_3$, ppm) δ 11.83 (s, 1H), 7.74 (d, J = 16.0 Hz, 1H), 7.62 (d, J = 2.5 Hz, 1H), 7.45 (dd, J = 9.0, 2.5 Hz, 1H), 6.95 (d, J = 9.0 Hz, 1H), 6.59 (d, J = 16.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 188.3, 161.4, 139.0, 137.1, 127.8, 123.4, 119.7,

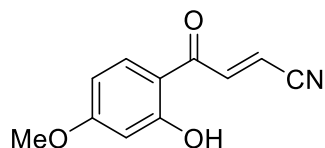
118.1, 114.9, 112.4; HRMS (ESI) calcd. for $C_{10}H_5ClNO_2$ $[M-H]^-$: 206.0014, Found: 206.0008.



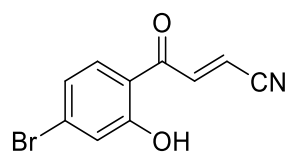
(E)-4-(2-hydroxy-5-(trifluoromethyl)phenyl)-4-oxobut-2-enenitrile (6f): yellow solid, 0.0671 g, 93% yield, m.p. 77-80 °C; IR (film): 3091, 2919, 2229, 1646, 1289, 624 cm^{-1} ; 1H NMR (500 MHz, $CDCl_3$, ppm) δ 12.27 (s, 1H), 8.01 (s, 1H), 7.91 (dd, J = 15.5, 2.5 Hz, 1H), 7.79 (d, J = 9.0 Hz, 1H), 7.16 (d, J = 8.0 Hz, 1H), 6.70 (dd, J = 16.0, 3.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 188.9, 165.0, 138.7, 133.3 (q, J_{C-F} = 3.8 Hz), 126.4 (q, J_{C-F} = 3.8 Hz), 123.6, 121.4, 121.1 (q, J_{C-F} = 34.0 Hz), 119.0, 115.9 (q, J_{C-F} = 268.4 Hz), 112.8; ^{19}F NMR (376 MHz, $CDCl_3$, ppm) δ -62.0; HRMS (ESI) calcd. for $C_{11}H_5F_3NO_2$ $[M-H]^-$: 240.0278, Found: 240.0275.



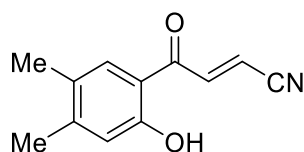
(E)-4-(2-hydroxy-5-nitrophenyl)-4-oxobut-2-enenitrile (6g): yellow solid, 0.0569 g, 87% yield, m.p. 152-157 °C; IR (film): 3079, 2916, 1643, 1332, 743 cm^{-1} ; 1H NMR (500 MHz, acetone- d_6 , ppm) δ 12.47 (s, 1H), 9.00 (s, 1H), 8.54-8.47 (m, 2H), 7.27 (d, J = 9.0 Hz, 1H), 6.88 (d, J = 15.5 Hz, 1H); ^{13}C NMR (125 MHz, acetone- d_6 , ppm) δ 190.9, 167.1, 141.8, 140.3, 131.8, 127.4, 119.4, 118.9, 116.3, 113.2; HRMS (ESI) calcd. for $C_{10}H_5N_2O_4$ $[M-H]^-$: 217.0255, Found: 217.0250.



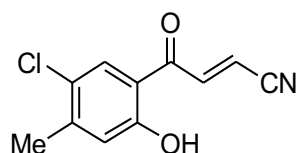
(E)-4-(2-hydroxy-4-methoxyphenyl)-4-oxobut-2-enenitrile (6h): yellow solid, 0.0569 g, 93% yield, m.p. 171-174 °C; IR (film): 3049, 2919, 2226, 1639, 1267, 786, 617 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 12.60 (s, 1H), 7.74 (dd, J = 16.0, 2.5 Hz, 1H), 7.56 (dd, J = 9.0, 3.0 Hz, 1H), 6.55 (dd, J = 16.0, 2.5 Hz, 1H), 6.42-6.41 (m, 1H), 3.81 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 186.4, 166.7, 166.4, 140.1, 130.4, 115.4, 111.9, 110.5, 108.0, 100.2, 54.8; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_8\text{NO}_3$ $[\text{M}-\text{H}]^-$: 202.0510, Found: 202.0503.



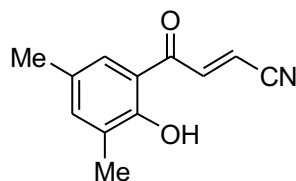
(E)-4-(4-bromo-2-hydroxyphenyl)-4-oxobut-2-enenitrile (6j): yellow solid, 0.0670 g, 89% yield, m.p. 173-175 °C; IR (film): 3079, 2919, 2320, 1592, 752 cm^{-1} ; ^1H NMR (500 MHz, acetone- d_6 , ppm) δ 11.86 (s, 1H), 8.36 (d, J = 16.0 Hz, 1H), 8.27 (d, J = 2.5 Hz, 1H), 7.74 (dd, J = 9.0, 2.0 Hz, 1H), 7.00 (d, J = 9.0 Hz, 1H), 6.80 (d, J = 16.0 Hz, 1H); ^{13}C NMR (125 MHz, acetone- d_6 , ppm) δ 191.0, 162.6, 142.2, 140.6, 133.4, 121.1, 120.8, 116.8, 113.0, 111.2; HRMS (ESI) calcd. for $\text{C}_{10}\text{H}_5\text{BrNO}_2$ $[\text{M}-\text{H}]^-$: 249.9509, Found: 249.9506.



(E)-4-(2-hydroxy-4,5-dimethylphenyl)-4-oxobut-2-enenitrile (6k): orange solid, 0.0565 g, 94% yield, m.p. 135-138 °C; IR (film): 3565, 3090, 2921, 2227, 1641, 1188, 768 cm⁻¹; ¹H NMR (500 MHz, acetone-*d*₆, ppm) δ 11.91 (s, 1H), 8.27 (d, *J* = 16.0 Hz, 1H), 7.86 (s, 1H), 6.80 (s, 1H), 6.73 (d, *J* = 16.0 Hz, 1H), 2.29 (s, 3H), 2.23 (s, 3H); ¹³C NMR (125 MHz, acetone-*d*₆, ppm) δ 190.2, 162.2, 149.2, 142.0, 130.7, 128.2, 118.7, 116.9, 116.6, 111.6, 19.8, 17.9; HRMS (ESI) calcd. for C₁₂H₁₀NO₂ [M-H]⁻: 200.0717, Found: 200.0710.

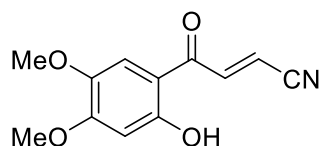


(E)-4-(5-chloro-2-hydroxy-4-methylphenyl)-4-oxobut-2-enenitrile (6l): orange solid, 0.0601 g, 91% yield, m.p. 158-160 °C; IR (film): 3089, 2921, 2227, 1641, 1172, 977, 700 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, ppm) δ 11.89 (s, 1H), 7.79 (d, *J* = 16.0 Hz, 1H), 7.68 (s, 1H), 6.95 (s, 1H), 6.65 (d, *J* = 16.0 Hz, 1H), 2.41 (s, 3H); ¹³C NMR (125 MHz, CDCl₃, ppm) δ 188.7, 162.4, 148.1, 140.2, 129.2, 125.2, 121.0, 117.6, 116.0, 113.0, 21.1; HRMS (ESI) calcd. for C₁₁H₇ClNO₂ [M-H]⁻: 220.0171, Found: 220.0167.

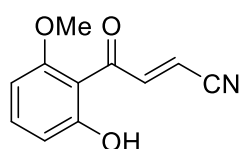


(E)-4-(2-hydroxy-3,5-dimethylphenyl)-4-oxobut-2-enenitrile (6m): red solid, 0.0533 g, 88% yield, m. p. 137-141 °C; IR (film): 3089, 2920, 2228, 1637, 1295, 767 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, ppm) δ 12.19 (s, 1H), 7.89 (d, *J* = 16.0 Hz, 1H), 7.33 (s, 1H), 7.27 (s, 1H), 6.60 (d, *J* = 16.0 Hz, 1H), 2.31 (s, 3H), 2.25 (s, 3H); ¹³C NMR

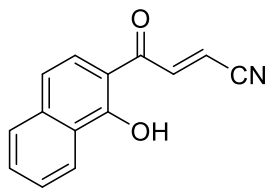
(125 MHz, CDCl₃, ppm) δ 189.9, 160.7, 141.3, 140.3, 128.1, 127.9, 126.8, 117.6, 116.3, 112.0, 20.5, 15.4; HRMS (ESI) calcd. for C₁₂H₁₂NO₂ [M+H]⁺: 202.0863, Found: 202.0865.



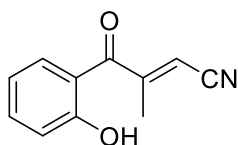
(E)-4-(2-hydroxy-4,5-dimethoxyphenyl)-4-oxobut-2-enenitrile (6n): orange solid, 0.0583 g, 83% yield, m.p. 190-193 °C; IR (film): 3392, 2919, 2848, 1519, 1208, 783, 442 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, ppm) δ 12.74 (s, 1H), 7.81 (d, *J* = 15.6 Hz, 1H), 6.99 (s, 1H), 6.64 (d, *J* = 16.0 Hz, 1H), 6.52 (s, 1H), 3.96 (s, 3H), 3.91 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, ppm) δ 186.9, 163.0, 158.7, 142.8, 141.2, 116.5, 111.5, 110.9, 109.4, 100.9, 56.7, 56.5; HRMS (ESI) calcd. for C₁₂H₁₀NO₄ [M-H]⁻: 232.0615, Found: 232.0615.



(E)-4-(2-hydroxy-6-methoxyphenyl)-4-oxobut-2-enenitrile (6o): orange solid, 0.0551 g, 90% yield, m.p. 107-110 °C; IR (film): 3392, 3065, 2919, 2225, 1583, 1088, 795, 444 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, ppm) δ 12.38 (s, 1H), 7.90 (d, *J* = 16.0 Hz, 1H), 7.36 (t, *J* = 8.4 Hz, 1H), 6.55 (d, *J* = 8.4 Hz, 1H), 6.36 (d, *J* = 16.0 Hz, 1H), 6.35 (d, *J* = 9.2 Hz, 1H), 3.87 (s, 3H); ¹³C NMR (125 MHz, CDCl₃, ppm) δ 189.9, 164.3, 160.1, 146.7, 137.0, 115.8, 110.1, 109.7, 108.0, 100.6, 55.1; HRMS (ESI) calcd. for C₁₁H₈NO₃ [M-H]⁻: 202.0499, Found: 202.0503.

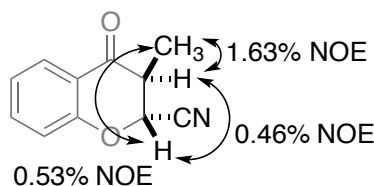


(E)-4-(1-hydroxynaphthalen-2-yl)-4-oxobut-2-enenitrile (6p): red solid, 0.0627 g, 94% yield, m.p. 192-195 °C; IR (film): 2955, 2918, 2230, 1259, 798 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3 , ppm) δ 14.10 (s, 1H), 8.49 (d, $J = 8.5$ Hz, 1H), 7.97 (d, $J = 16.0$ Hz, 1H), 7.79 (d, $J = 8.0$ Hz, 1H), 7.70 (t, $J = 7.5$ Hz, 1H), 7.60-7.56 (m, 2H), 7.33 (d, $J = 9.0$ Hz, 1H), 6.70 (d, $J = 16.0$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 188.0, 164.7, 140.1, 136.9, 130.4, 126.6, 125.6, 124.1, 123.8, 121.9, 118.3, 115.3, 111.4, 111.0; HRMS (ESI) calcd. for $\text{C}_{14}\text{H}_8\text{NO}_2$ $[\text{M}-\text{H}]^-$: 222.0561, Found: 222.0556.



(E)-4-(2-hydroxyphenyl)-3-methyl-4-oxobut-2-enenitrile (6q): yellow oil, 0.0408 g, 72% yield, IR (film): 3094, 2919, 2849, 2224, 1628, 1243, 761 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3 , ppm) δ 11.46 (s, 1H), 7.69-7.44 (m, 2H), 7.05 (d, $J = 8.4$ Hz, 1H), 6.95 (t, $J = 7.6$ Hz, 1H), 5.61 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , ppm) δ 199.7, 163.5, 157.0, 137.9, 131.9, 119.4, 119.0, 117.2, 114.78, 103.8, 19.0; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_8\text{NO}_2$ $[\text{M}-\text{H}]^-$: 186.0561, Found: 186.0552.

NOE studies to determine stereochemistry of 5q



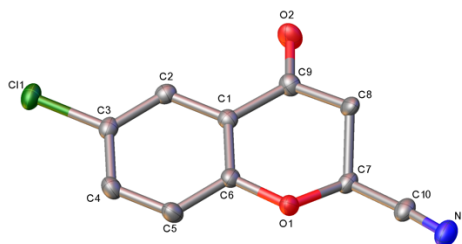


Table S1. Crystal data and structure refinement of **5e**

Identification code	mx7039	
Empirical formula	C ₁₀ H ₆ Cl N O ₂	
Formula weight	207.61	
Temperature	173.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 2 ₁ /c 1	
Unit cell dimensions	a = 8.082(4) Å	a = 90°.
	b = 5.884(2) Å	b = 101.210(6)°.
	c = 19.020(8) Å	g = 90°.
Volume	887.2(6) Å ³	
Z	4	
Density (calculated)	1.554 Mg/m ³	
Absorption coefficient	0.397 mm ⁻¹	
F(000)	424	
Crystal size	0.318 x 0.23 x 0.053 mm ³	
Theta range for data collection	2.569 to 27.465°.	
Index ranges	-10 ≤ h ≤ 10, -7 ≤ k ≤ 7, -24 ≤ l ≤ 24	
Reflections collected	6521	
Independent reflections	2009 [R(int) = 0.0360]	
Completeness to theta = 25.242°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.85027	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2009 / 60 / 155	
Goodness-of-fit on F ²	1.157	
Final R indices [I > 2σ(I)]	R1 = 0.0411, wR2 = 0.0934	
R indices (all data)	R1 = 0.0434, wR2 = 0.0947	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.244 and -0.172 e. Å ⁻³	

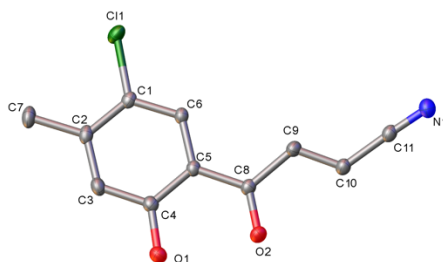


Table S2. Crystal data and structure refinement of **61**

Identification code	mx7044	
Empirical formula	C11 H8 Cl N O2	
Formula weight	221.63	
Temperature	173.15 K	
Wavelength	0.71073 $\approx$	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 10.406(3) $\approx$ b = 9.108(2) $\approx$ c = 10.949(3) $\approx$	a = 90 $^\circ$. b = 104.637(4) $^\circ$. g = 90 $^\circ$.
Volume	1004.0(4) $\approx^3$	
Z	4	
Density (calculated)	1.466 Mg/m ³	
Absorption coefficient	0.356 mm ⁻¹	
F(000)	456	
Crystal size	0.364 x 0.338 x 0.143 mm ³	
Theta range for data collection	2.023 to 27.491 $^\circ$.	
Index ranges	-11 $\leq$ h $\leq$ 13, -11 $\leq$ k $\leq$ 11, -14 $\leq$ l $\leq$ 14	
Reflections collected	6493	
Independent reflections	2272 [R(int) = 0.0263]	
Completeness to theta = 25.242 $^\circ$	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.81153	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2272 / 0 / 138	
Goodness-of-fit on F ²	1.101	
Final R indices [I > 2sigma(I)]	R1 = 0.0358, wR2 = 0.0943	
R indices (all data)	R1 = 0.0370, wR2 = 0.0954	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.314 and -0.258 e. $\approx^{-3}$	

Computational Details

All calculations were performed with the Gaussian 09 program.¹ Geometry optimizations of all stationary points were performed with the M06-2X functional², which has been proven to be suitable to describe the dispersion effects. The 6-31G(d) basis set was applied for all elements in substrates and the latent catalyst. Frequency calculations at the same level were performed to confirm each stationary point to be either a minimum or a transition structure. Intrinsic reaction coordinate (IRC)³ calculations were performed to confirm the connection of each transition state to its corresponding reactant and product. All figures of structures were prepared using CYLView.⁴

(1) Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.

(2) (a) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157. (b) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.

(3) (a) Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523. (b) Gonzalez, C.; Schlegel, H. B. *J. Chem. Phys.* **1989**, *90*, 2154.

(4) Legault, C. Y. CYLview, 1.0b; Université de Sherbrooke: Sherbrooke, Québec, Canada, 2009; <http://www.cylview.org>.

Calculated Energy Surface of the Cyanosilylation of Chromone.

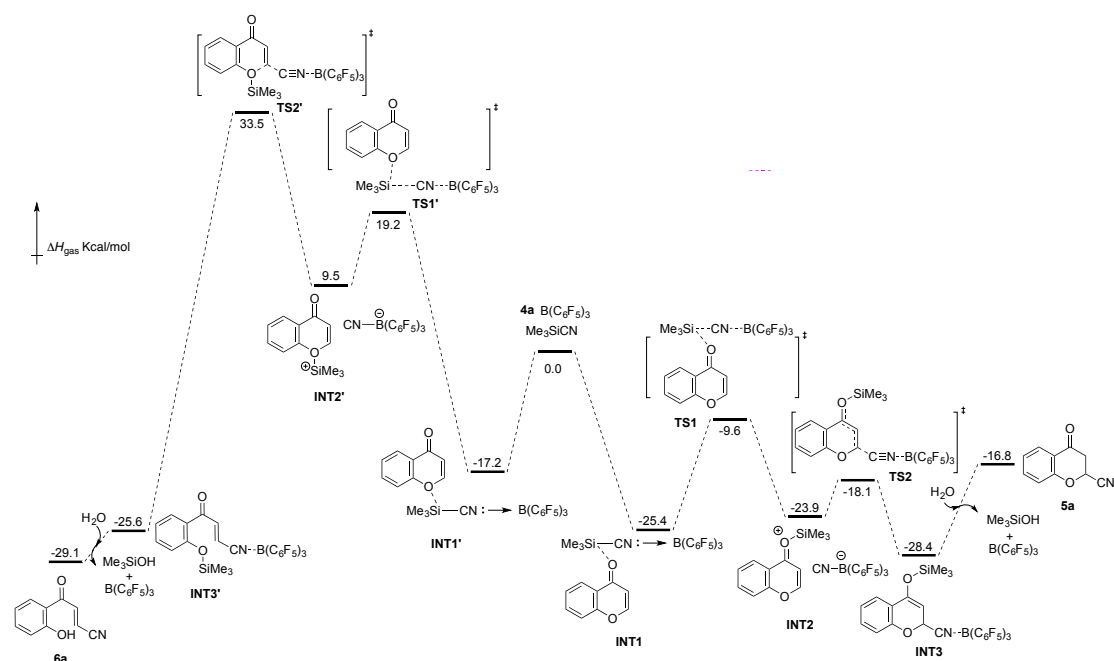
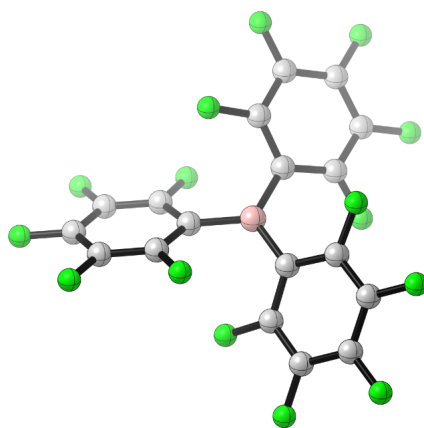


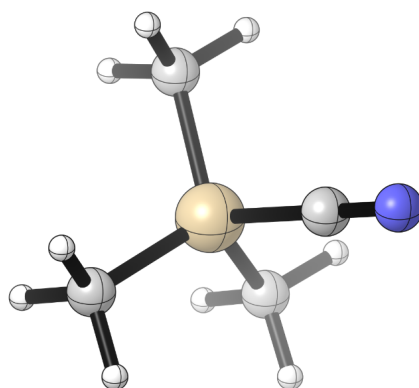
Figure S1. DFT-computed energy profile for the regeneration of cyanosilylation of Chromone. Enthalpies are calculated at 273.15 K and 1.0 atm in gas phase.

Coordinates of All Stationary Points



B(C₆F₅)₃

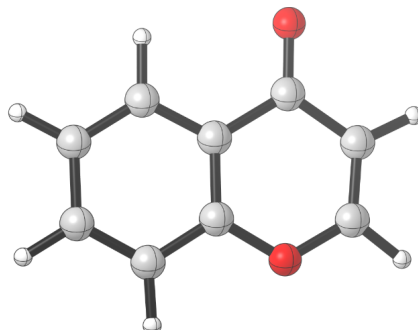
B	-0.00042800	0.00089200	0.00044700	F	-2.26164600	-1.33013200	1.27123600
C	-1.48188600	0.51279300	-0.00096400	F	2.28454900	-1.29247100	1.26790000
C	-1.85973000	1.70233900	-0.63152400	F	2.76912600	-3.91150400	1.26887400
C	-2.51457800	-0.18847200	0.62989400	F	1.07994600	-5.61376800	-0.00064100
C	-3.16507500	2.16762900	-0.64833400	F	-1.12163600	-4.65898700	-1.26897400
C	-3.82784600	0.25397900	0.64862300	F	-1.64168500	-2.04697800	-1.26854100
C	-4.15297900	1.43862600	0.00078200	C	1.18452100	1.02669300	-0.00098100
C	0.29574800	-1.53858600	0.00049700	C	1.09428900	2.27286500	0.62769500
C	-0.54688500	-2.46038700	-0.62882500	C	2.40445000	0.75672000	-0.62950700
C	1.41989500	-2.08223100	0.62981900	C	2.13524600	3.18738300	0.64670300
C	-0.29745100	-3.82353100	-0.64641000	C	3.46099500	1.65324600	-0.64635300
C	1.69318300	-3.44088600	0.64767000	C	3.32434000	2.87434700	0.00101500
C	0.82911400	-4.31453100	0.00051200	F	-0.02152100	2.62871500	1.26555100
F	-0.95546400	2.44434600	-1.27181300	F	2.00689500	4.35326500	1.27070000
F	-3.47737900	3.29838300	-1.27193300	F	4.32616300	3.73887900	0.00225900
F	-5.40267400	1.87349900	0.00264200	F	4.59672900	1.35659700	-1.26863500
F	-4.77208000	-0.44192100	1.27235400	F	2.59401600	-0.39708100	-1.27093900



TMSCN

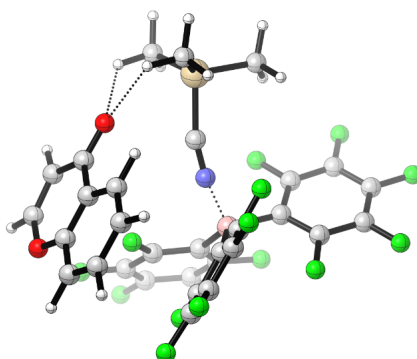
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C	0.85121400	-0.30728900	1.76641600	C	0.85020200	1.68441300	-0.61750400
H	0.47431100	-1.26794200	2.12829100	H	0.47265300	1.86994500	-1.62692200
H	1.94378800	-0.32190400	1.83452300	H	0.47740400	2.47725900	0.03693000

H 0.47868700	0.47689800	2.43136700	H 1.94271000	1.74933800	-0.64429000
C 0.84980500	-1.37729800	-1.14931000	C -1.56328400	0.00019000	0.00039400
H 0.47864100	-2.34444300	-0.79887000	N -2.72234100	-0.00005700	0.00081600
H 0.46999900	-1.21309900	-2.16155900			



4a

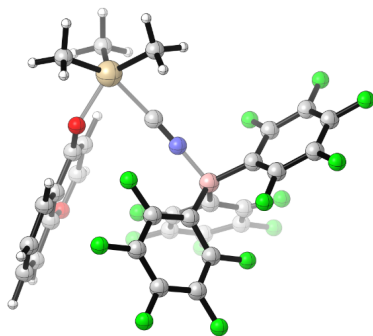
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C 0.33454300	-0.85862400	-0.00000400	C -1.93156700	-1.42539700	0.00000000
C 0.03093000	0.50475800	0.00000000	H -3.40514000	0.08187900	0.00002600
C 1.08422500	1.43008900	0.00000600	H -2.59523500	-2.28213300	0.00001500
C 2.39808000	0.99607300	0.00000400	O -0.64175200	-1.81601300	-0.00000600
H 3.70990300	-0.72051800	0.00000000	C -1.38175200	0.95338000	0.00000100
H 1.84725500	-2.38000100	-0.00000500	O -1.69960400	2.13299500	-0.00001200
H 0.82567500	2.48450200	0.00000700			



INT1

B 0.74590100	-0.04226800	-0.14480200	F -0.73671300	-2.12999900	-1.81396600
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C 3.08904400	-1.01649300	0.71148400	N 0.02479100	1.07342500	0.73270400
C 2.91792500	1.30705000	0.43294200	Si -0.42245600	3.26887500	2.79072800
C 4.39518000	-0.87674000	1.17137000	C -1.10622000	4.79373700	1.96918600
C 4.20854600	1.49454300	0.89877700	C 1.40085600	3.40625200	3.20671700
C 4.95706700	0.38605900	1.27148100	C -1.43412600	2.57036800	4.19047500
C 0.48790600	0.41385200	-1.68399300	H -2.12807000	4.60238100	1.63494100
C 1.46197400	0.72789900	-2.62373200	H -1.11099100	5.62655400	2.68028300
C -0.82293000	0.57866700	-2.11888800	H -0.49376100	5.08717700	1.11160100
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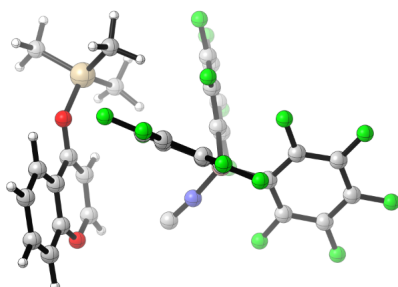
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F 2.62163100	-2.26907300	0.64530600	H -1.04402400	1.59678200	4.50393400
F 5.10611900	-1.94665300	1.52149900	H -1.39496100	3.24186500	5.05453700
F 6.20051000	0.53571400	1.71666000	H -2.47227900	2.45442200	3.87227000
F 4.72946300	2.71844100	0.98796300	C -4.26548500	-2.49657800	0.90408200
F 2.25257000	2.41542700	0.05544700	C -4.58575800	-1.82959600	-0.26493200
F -1.82468000	0.27268000	-1.27716400	C -4.37072000	-0.45155100	-0.32997400
F -2.45664000	1.15906100	-3.73187500	C -3.83157300	0.25584000	0.74686900
F -0.47313700	1.76713100	-5.50340700	C -3.50405900	-0.44470900	1.91668600
F 2.12887000	1.46770800	-4.76800700	C -3.72812900	-1.80566700	2.00225400
F 2.76388100	0.60747000	-2.34606700	C -4.02226700	2.27773200	0.63688500
C 0.00598400	-1.41432600	0.32891300	C -4.51991000	1.48970300	1.60865900
C -0.01432800	-1.72307000	1.68802200	O -4.69996500	0.16647300	-1.50069100
C -0.67664400	-2.30584300	-0.48917600	C -3.59044400	1.70432600	0.62690500
C -0.66416400	-2.82460500	2.21777500	O -3.06329700	2.36159700	1.52549500
C -1.35062600	-3.41828600	0.00327400	H -4.40330800	-3.57211800	0.96187000
C -1.34523100	-3.67618000	1.36194400	H -4.98575800	-2.34357900	-1.13177900
F 0.61160900	-0.91428800	2.56151300	H -3.07064400	0.11578200	2.73977200
F -0.70962600	-3.03385400	3.53466300	H -3.46413100	-2.35095100	2.90353700
F -2.06775800	-4.68133100	1.85555800	H -3.90690800	3.34118900	-0.80460400
F -2.05406300	-4.20177600	-0.81421400	H -4.82529700	1.84523800	-2.58521600



TS1

B 1.11386000	-0.06236400	-0.19096500	F 1.75132400	-2.55351800	-1.29311900
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C 3.55979500	-0.80102000	0.66626400	N 0.43299100	1.12000700	0.57093300
C 3.30558200	1.32846600	-0.28890500	Si -0.94135800	3.03785900	2.77469300
C 4.91378600	-0.55468700	0.87991800	C -1.28881800	4.68144600	1.93214900
C 4.64555500	1.61665900	-0.09417700	C 0.83953900	3.00247800	3.45001400
C 5.45892800	0.65987500	0.50006000	C -1.89377300	2.99904000	4.41583800
C 0.65912400	0.12699000	-1.75483600	H -2.35660800	4.83297600	1.74369400
C 1.49286100	0.24785400	-2.86103600	H -0.96979700	5.47152900	2.62125000
C -0.69992900	0.18969000	-2.03869600	H -0.73723800	4.81690300	0.99669800
C 1.01248800	0.45803500	-4.15089700	H 0.91987200	3.66070600	4.32239400
C -1.22250000	0.41584000	-3.30179000	H 1.11484000	1.99254300	3.77674200

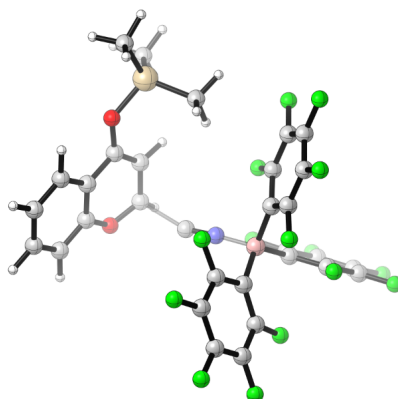
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F 3.11905800	-1.99670700	1.07728900	H -1.79517300	2.02247100	4.90363000
F 5.68416000	-1.47728800	1.45484200	H -1.47872500	3.74738900	5.09974800
F 6.74954700	0.91061200	0.69951400	H -2.96213100	3.19482700	4.28589700
F 5.15942600	2.78812900	-0.46742000	C -5.14588200	-1.97498500	0.48784400
F 2.56057800	2.27389200	-0.88432100	C -5.08071400	-1.03493300	-0.52269400
F -1.59505400	0.03060900	-1.04072600	C -4.35245400	0.13219900	-0.29264100
F -2.54562800	0.51091200	-3.48847900	C -3.71281000	0.37642800	0.92890200
F -0.82305800	0.76920200	-5.59846500	C -3.79488500	-0.59827700	1.94125400
F 1.85431600	0.57593800	-5.17488900	C -4.50046600	-1.76198600	1.71905000
F 2.81977700	0.16996100	-2.74029200	C -2.88595700	2.46256900	-0.05154200
C 0.47860600	-1.46178700	0.35525300	C -3.55372800	2.12100400	-1.18151300
C -0.44869200	-1.63313400	1.37405900	O -4.28345700	1.02303500	-1.31763800
C 0.83830300	-2.62734100	-0.31641000	C -2.94087500	1.59430500	1.08480100
C -0.99808000	-2.86831400	1.70094000	O -2.37339100	1.82822400	2.18952400
C 0.32057200	-3.87857700	-0.02229500	H -5.69525400	-2.89600900	0.32231800
C -0.61633800	-3.99773100	0.99713300	H -5.55478000	-1.17980800	-1.48656300
F -0.88051200	-0.59849500	2.12039000	H -3.27230300	-0.42061900	2.87365900
F -1.89426700	-2.96816200	2.68963600	H -4.54289300	-2.52335300	2.48929100
F -1.13644100	-5.18494500	1.29819500	H -2.31356600	3.37950500	-0.02624600
F 0.70406100	-4.95919500	-0.69927900	H -3.55865000	2.71654400	-2.08669200



INT2

B -0.80899300	0.25599100	-1.08700600	F -3.26691100	-1.02379800	-0.64185700
C -1.10216500	0.71218300	0.46461600	Si 3.17327300	-2.00636600	2.09781300
C -2.23960300	1.32776000	0.97031000	C 3.11807500	-2.47641800	0.29170400
C -0.10032200	0.50370100	1.40340000	C 1.59388500	-2.40953700	2.99023700
C -2.38163600	1.68307200	2.31177900	C 4.66776200	-2.72892600	2.95068600
C -0.19712200	0.82229200	2.74433600	H 2.36383900	-1.91087400	-0.26691600
C -1.35703400	1.42747100	3.20762400	H 4.08905100	-2.38808100	-0.20608600
C -0.32660300	-1.31754400	-1.18325200	H 2.82886000	-3.53418900	0.24458300
C -0.48701900	-2.29417200	-0.20610100	H 1.55227300	-3.49225300	3.15627000
C 0.29003000	-1.75543700	-2.35376300	H 1.54621600	-1.91330400	3.96346100
C -0.01268400	-3.59338300	-0.34028800	H 0.70734500	-2.13025800	2.41538000
C 0.76671800	-3.04884000	-2.53590100	H 4.71263200	-2.41709100	3.99864700
C 0.62020900	-3.97367500	-1.51277900	H 4.62426000	-3.82293300	2.92824600
F -3.27792300	1.62596100	0.18508300	H 5.59794000	-2.42087300	2.46321500
F -3.49624300	2.27391700	2.73873800	C 3.01784900	4.60561400	3.23491400

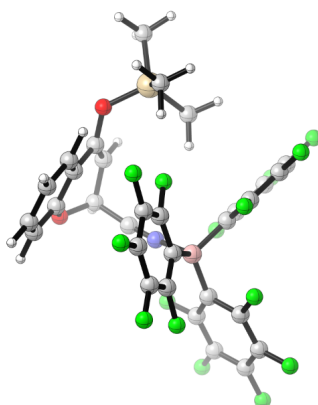
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F 1.05480500	-0.09155800	1.01661900	C 3.34916800	2.04679300	2.17389200
F 0.44496600	-0.91143000	-3.37955700	C 3.12283800	2.21257200	3.55536800
F 1.36874300	-3.40300600	-3.67138800	C 2.95930100	3.47732800	4.07513200
F 1.11699000	-5.20439900	-1.63604900	C 3.76449900	0.72612400	0.17215500
F -0.11586600	-4.46330000	0.66920100	C 3.79066900	1.90258000	-0.52933500
F -1.08552500	-2.01764800	0.96466000	O 3.65449500	3.08796400	0.02956200
C -2.07845500	0.40500200	-2.08864500	C 3.51174600	0.75576600	1.55353400
C -2.10862700	1.09804000	-3.29175500	O 3.44643700	-0.28712100	2.31515900
C -3.22932600	-0.31637200	-1.78394300	H 2.87983900	5.59544000	3.65699700
C -3.22015500	1.09264000	-4.13161300	H 3.29719500	5.32352100	1.20952400
C -4.35715800	-0.34408000	-2.58659100	H 3.07491800	1.33087000	4.18190200
C -4.34775200	0.37077700	-3.77777000	H 2.77970800	3.60781300	5.13630800
F -1.06125200	1.81329900	-3.71196800	H 3.88575700	-0.20154100	-0.36652900
F -3.20444300	1.77370500	-5.27882800	H 3.95731300	1.96705700	-1.59452300
F -5.41616700	0.35926300	-4.57305500	C 1.33891000	1.76597900	-1.71702000
F -5.43845200	-1.04325600	-2.23849700	N 0.38756900	1.12216800	-1.50865400



TS2

B -5.04921700	1.63689800	-1.83360800	F -9.32791200	2.20289000	-5.65926100
C -5.36033600	2.16778400	-0.31619000	F -9.69619300	0.85653700	-3.32320400
C -6.45372700	2.93004900	0.07955400	F -7.66974000	0.66167100	-1.55161600
C -4.47108300	1.85375100	0.70626700	Si -0.87384400	-0.67045700	1.02470900
C -6.66765000	3.32151100	1.39975400	C -1.21124700	-1.16178100	-0.74725700
C -4.66052000	2.18616300	2.03524600	C -2.31807100	-1.09737800	2.12830800
C -5.76891800	2.94590900	2.38397400	C 0.72057400	-1.40321600	1.66283000
C -4.67031600	0.04119400	-1.92313900	H -2.01053600	-0.55519300	-1.18869000
C -4.87848500	-0.92721300	-0.94682500	H -0.32665300	-1.10898000	-1.38932400
C -4.10495300	-0.42844800	-3.10767800	H -1.55068400	-2.20474600	-0.74690400
C -4.51480500	-2.25895600	-1.11130500	H -2.23393200	-2.13904200	2.45711400
C -3.74108000	-1.75123500	-3.31979100	H -2.33696500	-0.46287800	3.01937500
C -3.94546600	-2.67490000	-2.30469600	H -3.27603300	-0.98024600	1.61423500
F -7.37294500	3.33919900	-0.79889500	H 0.91135500	-1.08807200	2.69327800
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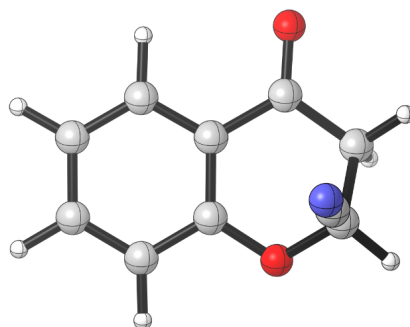
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F -3.36490800	1.13564300	0.40981000	C -1.23392900	3.29011700	0.93616600
F -3.87792600	0.43054800	-4.11275900	C -1.57376800	3.40155600	2.29112100
F -3.19067700	-2.13531800	-4.46999800	C -2.00708200	4.61365400	2.79945300
F -3.57122900	-3.94171100	-2.46265400	C -0.53094900	2.02472500	-1.00888200
F -4.68495000	-3.13227200	-0.11842800	C -0.85522600	3.18391600	-1.77880500
F -5.42213100	-0.61958100	0.23855900	O -0.96191100	4.37765100	-1.19402900
C -6.21827600	1.90871700	-2.91990100	C -0.78013100	2.04438100	0.33434500
C -6.07299900	2.57644000	-4.12644000	O -0.60874300	1.02849800	1.15685800
C -7.46349200	1.33028000	-2.69574800	H -2.42429200	6.68672800	2.37197000
C -7.10385100	2.68788600	-5.05466900	H -1.77732700	6.51134800	-0.03592000
C -8.51808900	1.41882500	-3.58895200	H -1.50216100	2.52041800	2.91594100
C -8.33166200	2.10584600	-4.78311300	H -2.28850800	4.69157700	3.84387000
F -4.90771300	3.15119100	-4.45287400	H -0.20820900	1.13592400	-1.53161900
F -6.91784800	3.34345400	-6.20009500	H -0.47133300	3.28066600	-2.78598500
H 1.57378800	-1.09357500	1.05157600	C -2.58472320	2.89798963	-2.32178521
C -2.08240200	5.73942600	1.96870200	N -3.66822000	2.39413000	-2.19914100



INT3

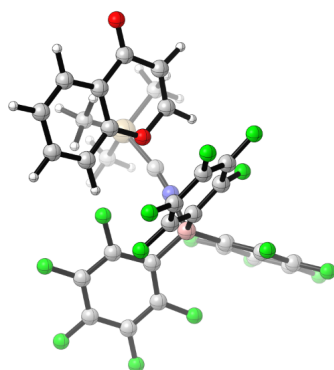
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C -2.14512000	1.62463700	1.03191500	C 2.95057900	-2.47972400	0.45115300
C -0.27375900	0.42273500	1.78040100	C 2.73491800	-2.14867700	3.52112300
C -2.39557700	2.06135400	2.33037300	C 5.45054500	-2.84346800	2.24026700
C -0.50449900	0.80648500	3.08893900	H 2.07399400	-1.85701200	0.24316500
C -1.57164800	1.65003400	3.36485100	H 3.60645200	-2.46098300	-0.42508200
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C -0.84960700	-2.33305200	0.06971500	H 2.43864300	-3.19560900	3.64857500
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C -0.57767800	-3.68900600	-0.07567100	H 1.82423500	-1.54930900	3.43702700
C 0.49856700	-3.22767300	-2.16799300	H 5.98277500	-2.47218500	3.12157700
C 0.10175200	-4.13809300	-1.19829800	H 5.28550900	-3.91763200	2.37513100
F -2.98596700	2.07562400	0.09683800	H 6.10114500	-2.70735600	1.37088800
F -3.41645400	2.87714500	2.58194200	C 1.77313800	3.96513900	2.93890100

F -1.79371300	2.05717400	4.61005400	C 2.15329200	4.02172800	1.60043900
F 0.28039500	0.38053900	4.08195000	C 2.76838200	2.91609700	1.03266600
F 0.79844800	-0.36818600	1.56497300	C 3.02852500	1.75954700	1.77945600
F 0.60555800	-1.03706600	-2.94874300	C 2.65071800	1.72703100	3.12179400
F 1.14937500	-3.64628700	-3.25157600	C 2.01375200	2.82029100	3.69789700
F 0.37557700	-5.43080300	-1.34123800	C 3.87951500	0.66361500	-0.21179500
F -0.96038900	-4.55935600	0.85619100	C 3.16062100	1.75663100	-0.95304400
F -1.50887700	-1.97894700	1.17694500	O 3.14485800	2.99508300	-0.29281100
C -1.77780900	0.60341500	-1.96200800	C 3.73495000	0.64648400	1.12588600
C -1.48599100	1.26042700	-3.14824100	O 4.24804900	-0.29546300	1.92637400
C -3.07841200	0.12375300	-1.84132500	H 1.27626500	4.81920900	3.38755200
C -2.43010600	1.45417200	-4.15210700	H 1.97150100	4.89789300	0.98795700
C -4.05034100	0.29818500	-2.81181000	H 2.85995000	0.83299800	3.69959500
C -3.71764200	0.97167200	-3.98162500	H 1.69826600	2.77641800	4.73500300
F -0.25750700	1.74540400	-3.38699200	H 4.41805400	-0.09576100	-0.76362700
F -2.10271000	2.09300900	-5.27447000	H 3.56882600	1.93016200	-1.94996800
F -4.63050000	1.14892200	-4.93148700	C 1.73322400	1.29898900	-1.10004900
F -5.28498200	-0.16947900	-2.64246700	N 0.66694400	0.88252700	-1.06112700



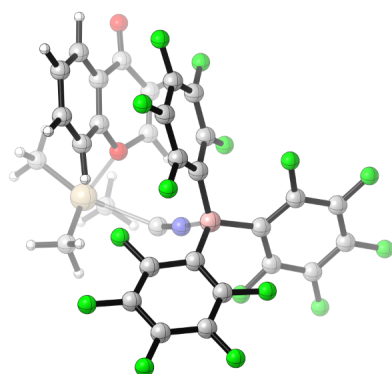
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C -2.85322600	-0.92164300	0.08629200	C 1.84818100	0.78081900	-0.87055600
C -1.68492300	-1.48652400	-0.40848000	C 1.82464100	-0.72044300	-0.58859800
C -0.53083000	-0.70776200	-0.47394800	H 1.76439000	0.92743800	-1.95418000
C -0.54454500	0.63019400	-0.05874600	O 0.59513300	-1.30778900	-0.97595800
C -1.73113400	1.17699600	0.44666400	C 0.66638900	1.47248500	-0.21229500
C -2.88191200	0.40897000	0.52233600	O 0.70898800	2.64032800	0.11056700
H -3.75214400	-1.52765200	0.14190800	H 2.77793500	1.23953800	-0.52755600
H -1.64012400	-2.51958000	-0.73504700	H 2.59213000	-1.23890000	-1.16741200
H -1.71475000	2.21570200	0.76235300	C 2.08500700	-0.99490200	0.84885300
H -3.79969700	0.83402400	0.91331100	N 2.30762900	-1.20286200	1.96294700



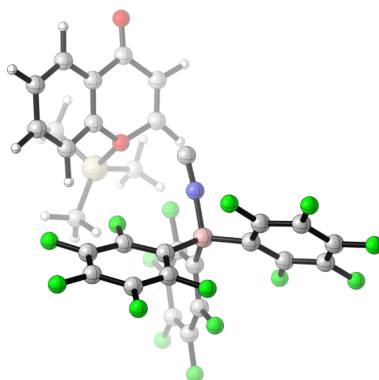
INT1'

B 0.06640700 -0.39138800 -1.00414600	F -2.40949100 -0.78386000 -2.65651200
C 0.00829100 -0.33646600 0.62184200	Si 4.22010800 1.43119600 -1.93737800
C -0.65247900 0.61618800 1.38644900	C 3.99020600 1.75608200 -3.76207700
C 0.80534400 -1.21474900 1.35114800	C 5.63950100 0.28875800 -1.53850600
C -0.53493800 0.69807000 2.77119500	C 4.13085500 2.96677200 -0.88188600
C 0.94622200 -1.17964400 2.72795400	H 3.87791000 0.82473100 -4.32447800
C 0.26581900 -0.20610900 3.44890400	H 3.10391600 2.37237700 -3.93956500
C -0.09694700 -1.86322900 -1.66910300	H 4.85884500 2.29139700 -4.15933800
C -0.67667800 -2.96348700 -1.04954800	H 6.58367900 0.76855200 -1.81691800
C 0.31545700 -2.06854400 -2.98192100	H 5.67961700 0.07384500 -0.46675600
C -0.82611000 -4.19359000 -1.67967100	H 5.56665800 -0.65512200 -2.08592500
C 0.18853500 -3.27801800 -3.64797000	H 4.48260800 2.77132600 0.13532800
C -0.38951200 -4.35237500 -2.98627300	H 4.76657100 3.74685400 -1.31379300
F -1.41763200 1.56318700 0.82389800	H 3.10799400 3.35215200 -0.82593300
F -1.16686800 1.66037700 3.43927800	C 1.33636600 4.63574800 2.61016900
F 0.39462400 -0.13619500 4.76815400	C 1.34463800 3.40612100 1.97274800
F 1.75381600 -2.03416100 3.35313200	C 2.46988400 2.59132800 2.11587400
F 1.55464300 -2.12071800 0.69548400	C 3.57087300 2.98962200 2.87760400
F 0.86087000 -1.05064700 -3.67286800	C 3.53731000 4.24024000 3.50872200
F 0.60858100 -3.41495200 -4.90483900	C 2.43068800 5.05870600 3.37884700
F -0.52342700 -5.52304300 -3.60044300	C 4.58989200 0.81007500 2.33925400
F -1.38556600 -5.21802900 -1.04008800	C 3.47792800 0.53489500 1.63638100
F -1.13234900 -2.88388300 0.20583200	O 2.44292300 1.38312100 1.46955500
C -0.81469500 0.74316300 -1.77410400	C 4.74750800 2.10032300 3.02008700
C -0.46904500 2.09059800 -1.71178900	O 5.74383100 2.41361500 3.64798000
C -1.94284300 0.46351200 -2.53860700	H 0.46569600 5.27568400 2.51148600
C -1.15479000 3.09914200 -2.36656100	H 0.50905600 3.06716500 1.37078500
C -2.66500800 1.44534200 -3.21233300	H 4.40317100 4.52801100 4.09632900
C -2.26606200 2.76933600 -3.13162500	H 2.40403000 6.02471900 3.87119900
F 0.57659600 2.47629500 -0.94994900	H 5.37498200 0.06918200 2.43045100
F -0.76634100 4.36979600 -2.26376500	H 3.29176800 -0.40932600 1.13233000
F -2.94315700 3.71720100 -3.76988800	N 1.57622400 0.02821700 -1.30246600
F -3.73529400 1.11909900 -3.93192700	C 2.61968000 0.46776600 -1.50122900



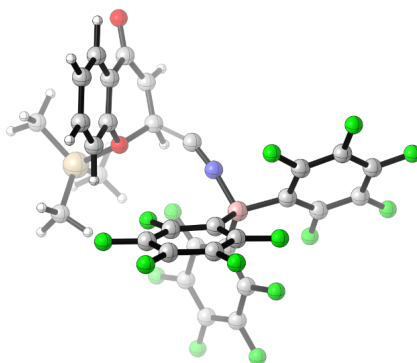
TS1'

B 0.13083100 0.18051800 -0.88264300	F -2.09573000 -0.79968200 -2.73560700
C 0.03404500 0.38996500 0.74602600	Si 4.09486600 3.23748300 -0.38990500
C -0.88966500 1.16590800 1.43491400	C 2.92079700 4.17046800 -1.49377000
C 1.02638300 -0.17886800 1.54506300	C 5.53868600 2.31294800 -1.11962100
C -0.82774700 1.38501000 2.81083500	C 4.82182400 4.43439200 0.86330400
C 1.11653200 0.00031000 2.91551500	H 3.11774800 3.87121200 -2.52793500
C 0.17941700 0.80107400 3.55628300	H 1.86813900 3.95545800 -1.30297600
C 0.20814900 -1.38026700 -1.34399800	H 3.09428200 5.24565600 -1.38122200
C -0.09079800 -2.48574500 -0.55911400	H 6.15033400 3.06370000 -1.63670100
C 0.61008200 -1.67089100 -2.64518300	H 6.17295700 1.87167200 -0.34480700
C 0.01522400 -3.79493700 -1.01872200	H 5.23935600 1.54813900 -1.83517700
C 0.72920700 -2.95763900 -3.14533600	H 5.41315600 3.92746400 1.63412000
C 0.43029900 -4.03253100 -2.31862200	H 5.49946400 5.10653800 0.32208300
F -1.90213700 1.77602800 0.80774000	H 4.07151800 5.05578300 1.36007600
F -1.70622100 2.19258600 3.40608800	C 0.92663500 4.15628500 2.89247000
F 0.26849300 1.02047700 4.86638900	C 1.57820200 3.53879500 1.82723000
F 2.10993700 -0.54700600 3.62460100	C 2.65784400 2.72566900 2.12190300
F 1.96815800 -0.95313200 0.97748700	C 3.10157700 2.48752500 3.41867500
F 0.87535700 -0.66488700 -3.49185900	C 2.43160100 3.11931900 4.46809700
F 1.11770000 -3.17320600 -4.40229900	C 1.35427700 3.95555200 4.20668900
F 0.53800600 -5.27823300 -2.77364500	C 4.50076500 0.64846600 2.51007400
F -0.27779400 -4.81943900 -0.21751800	C 4.06610600 0.94743300 1.29072600
F -0.50730900 -2.34579800 0.70792100	O 3.31877300 2.10770900 1.03548100
C -0.96663500 1.04331100 -1.73667100	C 4.16729300 1.48677600 3.68263800
C -0.94699800 2.43237100 -1.67845100	O 4.67406900 1.33189200 4.77177800
C -1.93108600 0.51955500 -2.59097400	H 0.05773300 4.77359100 2.69068800
C -1.77821500 3.26454200 -2.40613400	H 1.22120700 3.63706800 0.80871200
C -2.79368800 1.31374300 -3.34399200	H 2.76445400 2.90852900 5.47915200
C -2.71548600 2.69334000 -3.25658300	H 0.82431600 4.42983400 5.02498300
F -0.08537800 3.04846600 -0.83486500	H 5.07196500 -0.25840400 2.66778000
F -1.69430200 4.59120500 -2.29126600	H 4.20759700 0.38388900 0.37770400
F -3.53219200 3.46360000 -3.96915800	N 1.52530500 0.80567600 -1.22312700
F -3.69451600 0.75296500 -4.14829300	C 2.56366100 1.31341200 -1.34608600



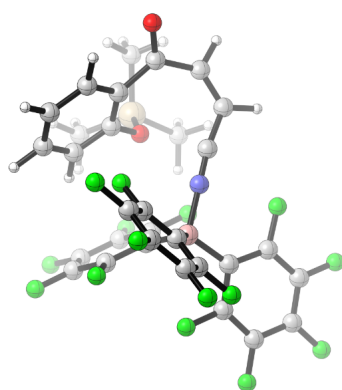
INT2'

B -1.37551800 0.08695100 0.28259700	F -3.21155700 -1.47422700 -1.20453100
C -1.27910500 0.88106800 -1.15846800	C 0.68918500 1.10573100 1.69874200
C -2.28182900 1.56763700 -1.83318000	N -0.21544800 0.63024300 1.13194800
C -0.05163400 0.87343700 -1.80539200	Si 4.03903200 -1.68754400 0.21897100
C -2.06208500 2.23857900 -3.03439600	C 3.23505100 -1.92742100 -1.43159900
C 0.22217000 1.53614500 -2.98872000	C 3.73950300 -3.01776500 1.47773000
C -0.80176800 2.23209000 -3.61419000	C 5.83234200 -1.19076200 0.16051000
C -2.74716700 0.36917300 1.11422300	H 2.18734200 -1.61946300 -1.42571000
C -3.12033600 1.68714300 1.36678200	H 3.75835400 -1.38195300 -2.22153400
C -3.58002400 -0.59289600 1.67005900	H 3.26524600 -2.99733300 -1.66645600
C -4.24615700 2.04349100 2.09239300	H 4.25529200 -2.81730200 2.42063200
C -4.72020700 -0.28181400 2.40506100	H 2.67936100 -3.19677900 1.65755700
C -5.05569400 1.04479600 2.61662300	H 4.15599600 -3.94307500 1.06006200
F -3.52498900 1.62276400 -1.35034200	H 6.02860200 -0.40008000 -0.56859100
F -3.05468000 2.89323100 -3.63380600	H 6.19286100 -0.85802400 1.13996500
F -0.57881400 2.87716800 -4.75692100	H 6.42314900 -2.06920800 -0.12461400
F 1.45455200 1.50314300 -3.51884500	C 4.17837000 2.59230600 -1.31399500
F 0.97484800 0.17059500 -1.26912900	C 3.58448800 1.43030900 -0.82887600
F -3.31942300 -1.90273800 1.53475700	C 3.80441800 1.10834600 0.49866200
F -5.48450900 -1.25085300 2.91172500	C 4.58447100 1.87897100 1.35169700
F -6.14268700 1.36078700 3.31735300	C 5.17304800 3.03597500 0.83741200
F -4.56032200 3.32438800 2.28865300	C 4.97600600 3.38937000 -0.49010900
F -2.37681200 2.68878400 0.87747600	C 3.79581300 0.47061900 3.24159800
C -1.12784300 -1.48713000 -0.11180000	C 3.06250700 -0.22929500 2.38383000
C 0.01572100 -2.23397300 0.11245300	O 3.26953200 -0.12325000 0.98381900
C -2.07971300 -2.12164800 -0.90871600	C 4.73311900 1.51725600 2.78586400
C 0.22466000 -3.50613800 -0.40733300	O 5.51322800 2.07649700 3.52641000
C -1.92722500 -3.39568400 -1.43500200	H 3.99219400 2.87769000 -2.34417200
C -0.75345900 -4.09767700 -1.18599100	H 2.93638000 0.82995800 -1.45251600
F 1.05218200 -1.74989200 0.84334000	H 5.77356800 3.63918800 1.51064200
F 1.38152600 -4.14719600 -0.16726700	H 5.42798200 4.29269600 -0.88471200
F -0.57074700 -5.31405000 -1.69348500	H 3.64238900 0.33928300 4.30616300
F -2.87606200 -3.94669500 -2.18795500	H 2.29614200 -0.96074900 2.59477300



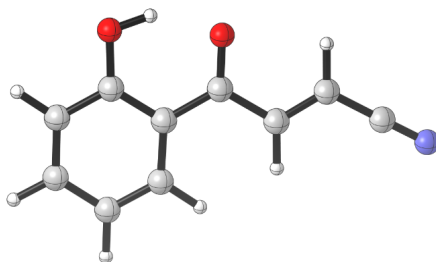
TS2'

B -1.29604900	0.03602800	0.16893000	F -3.44217900	-1.44104600	-0.86565000
C -1.01744200	0.48287800	-1.38239200	C 0.99926400	0.75791800	1.42362700
C -1.88704500	1.17355500	-2.21878700	N -0.02220100	0.49789600	0.95187300
C 0.19031800	0.12051800	-1.96782200	Si 4.25374500	-1.56125800	0.67454100
C -1.56106300	1.52218900	-3.52710700	C 3.91447200	-2.16670500	-1.04854200
C 0.56429900	0.46077900	-3.25699300	C 3.73509400	-2.76954600	1.98462500
C -0.32432400	1.17317400	-4.04881700	C 5.94295900	-0.83491000	0.94499300
C -2.54172100	0.77000600	0.90807000	H 2.83838500	-2.21315000	-1.24000400
C -2.62960000	2.15920800	0.85721200	H 4.37853100	-1.53880200	-1.81377800
C -3.51683600	0.14518200	1.67601000	H 4.32099900	-3.17902400	-1.15234900
C -3.62057300	2.89253700	1.48939500	H 3.83906600	-2.35529400	2.99123700
C -4.52952400	0.84152100	2.32897900	H 2.71603300	-3.13587800	1.83631800
C -4.58207400	2.22244700	2.23437100	H 4.40872700	-3.63237200	1.91375700
F -3.09532400	1.54757600	-1.79577600	H 6.20607800	-0.10949700	0.16955900
F -2.42698200	2.19296400	-4.28173000	H 6.00446500	-0.33838300	1.91882000
F 0.00513500	1.51132400	-5.29136100	H 6.68815900	-1.63829600	0.92435000
F 1.76790000	0.11125600	-3.73074000	C 3.95336800	2.38286300	-1.71507200
F 1.08722800	-0.60566600	-1.26100500	C 3.47033200	1.20872700	-1.14159000
F -3.52465500	-1.18391500	1.84434600	C 3.54725200	1.09761200	0.23634500
F -5.43683700	0.19009200	3.05506900	C 4.07409500	2.07784100	1.06845200
F -5.53916000	2.90282000	2.85701300	C 4.55561400	3.23821400	0.46352800
F -3.65704100	4.22066600	1.39661400	C 4.49675300	3.39097200	-0.91725300
F -1.71574600	2.85039100	0.15985500	C 3.31963800	0.82844200	3.06148000
C -1.33053200	-1.59770600	0.15782800	C 2.51537200	0.11419100	2.18874700
C -0.32130700	-2.47049300	0.53160700	O 3.10849000	-0.12225800	0.84600900
C -2.43333800	-2.20790800	-0.43745700	C 4.13041100	1.90584400	2.56723800
C -0.38878500	-3.84814000	0.36154800	O 4.82574700	2.65817600	3.23624700
C -2.55202700	-3.57632200	-0.62130900	H 3.88783900	2.50692600	-2.79107200
C -1.51497800	-4.40903500	-0.21541500	H 3.02357300	0.42454600	-1.73934500
F 0.83609600	-2.02883200	1.08273600	H 4.97715300	3.99905000	1.11300700
F 0.63252900	-4.61976900	0.74782500	H 4.87028200	4.29982200	-1.37711400
F -1.60304900	-5.72394100	-0.38672400	H 3.18744100	0.69578300	4.12747400
F -3.63535300	-4.10044400	-1.18788800	H 2.04107100	-0.80697800	2.51349100



INT3'

B -1.16939000 0.05074300 0.26012600	F -3.29255400 -0.50861500 -1.43602900
C -0.33659700 -0.37647600 -1.07964100	C 0.76320800 -0.10924500 2.16735600
C -0.34617500 0.29643500 -2.29693500	N -0.07290100 0.02609600 1.39453900
C 0.40662100 -1.55395700 -1.05522800	Si 4.13588000 -1.83401600 0.36517300
C 0.34321400 -0.15762900 -3.41760500	C 4.74718300 -1.86228800 -1.40351600
C 1.10265200 -2.04111500 -2.15010600	C 3.37103800 -3.44248100 0.91077300
C 1.07610700 -1.33373800 -3.34355800	C 5.51681800 -1.28362800 1.51130800
C -1.75238500 1.56544700 0.27310800	H 3.95306800 -2.14240200 -2.10218000
C -0.84986700 2.61026600 0.10014300	H 5.14730000 -0.88843800 -1.70389700
C -3.07675500 1.95047800 0.44596100	H 5.55226600 -2.59838500 -1.50672900
C -1.20269300 3.94823900 0.08292800	H 2.94103800 -3.34283100 1.91296300
C -3.47859400 3.28380500 0.43206900	H 2.57280900 -3.74384200 0.22863800
C -2.53926200 4.28644800 0.25033200	H 4.12012600 -4.24034700 0.94220600
F -1.03483500 1.42920800 -2.45258000	H 5.81822800 -0.24895900 1.31116500
F 0.30594200 0.52652700 -4.55922300	H 5.22465500 -1.35579600 2.56464600
F 1.75052900 -1.78096800 -4.39820600	H 6.40274700 -1.91350300 1.37439300
F 1.80995700 -3.17295700 -2.06363900	C 3.03795500 2.32498200 -1.51678600
F 0.46521100 -2.28704900 0.06843600	C 2.91585500 0.99125200 -1.15483900
F -4.04779000 1.05329000 0.64503500	C 3.02131400 0.60960200 0.18347300
F -4.76005800 3.60306300 0.60012300	C 3.26642000 1.58254900 1.16773200
F -2.91364900 5.56100100 0.23969500	C 3.40547200 2.92442600 0.77791700
F -0.28506000 4.89888700 -0.09120300	C 3.28081500 3.30115000 -0.54797300
F 0.44803000 2.31703000 -0.07563300	C 2.89302200 0.13333700 3.35584400
C -2.24552400 -1.12392900 0.57799500	C 1.68023900 -0.41218700 3.21751200
C -2.25398000 -2.01350900 1.64300900	O 2.87297600 -0.70152300 0.51567900
C -3.23546500 -1.33096100 -0.37996700	C 3.49918500 1.29191700 2.60681800
C -3.18495900 -3.04011000 1.76406700	O 4.16836800 2.03392300 3.30057500
C -4.18482500 -2.33564400 -0.29731600	H 2.93652900 2.60508200 -2.56095700
C -4.15455000 -3.20266600 0.78851300	H 2.72918700 0.21763300 -1.89240600
F -1.35007000 -1.92986700 2.63777900	H 3.61334400 3.65770600 1.55021900
F -3.14598100 -3.86628300 2.80888500	H 3.36713600 4.34469100 -0.82943000
F -5.05163000 -4.17774000 0.89089300	H 3.48700500 -0.16020700 4.21696900
F -5.11495400 -2.48176600 -1.23768800	H 1.29804300 -1.14824400 3.91940800



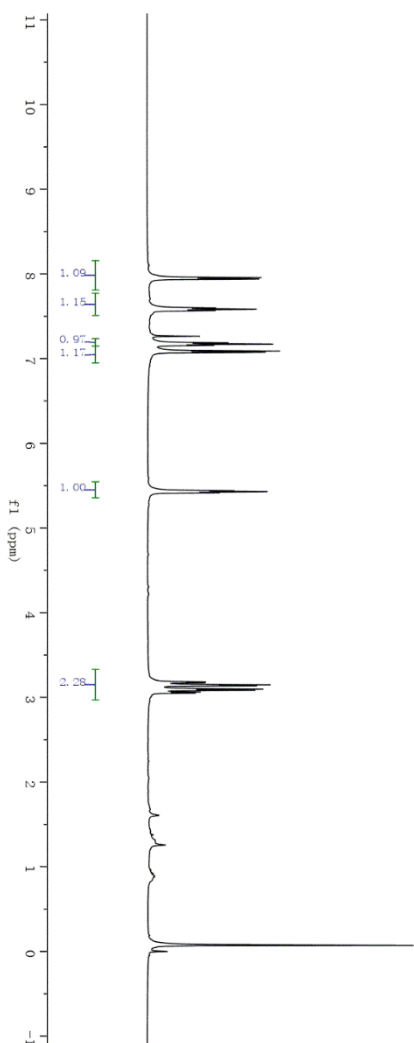
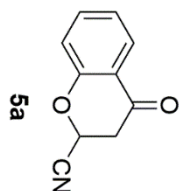
6a

C -3.35611200 -1.22051000 -0.00000500	C 1.76081800 -0.24218600 0.00011100
C -3.23600800 0.15630400 -0.00000200	C 2.94763000 0.37657400 -0.00006800
C -1.96670700 0.75412500 -0.00003400	H 1.71129600 -1.32345000 0.00029200
C -0.80381800 -0.06038200 0.00000100	O -1.91884900 2.08729500 0.00003700
C -0.96593200 -1.46212200 -0.00002100	C 0.51519400 0.58541700 0.00005700
C -2.21860300 -2.04295500 -0.00003200	O 0.63342900 1.81441000 -0.00003400
H -4.34518900 -1.66858400 0.00000800	H -0.97430300 2.36058700 0.00003000
H -4.10329100 0.80708300 0.00001300	H 3.00074900 1.46223100 -0.00023900
H -0.09669200 -2.10882400 -0.00002800	C 4.18090000 -0.35432300 -0.00002300
H -2.32061800 -3.12199600 -0.00004900	N 5.18103500 -0.93719200 0.00000800

7.96
7.94
7.60
7.58
7.57
7.19
7.17
7.16
7.09
7.07

5.44
5.43
5.42

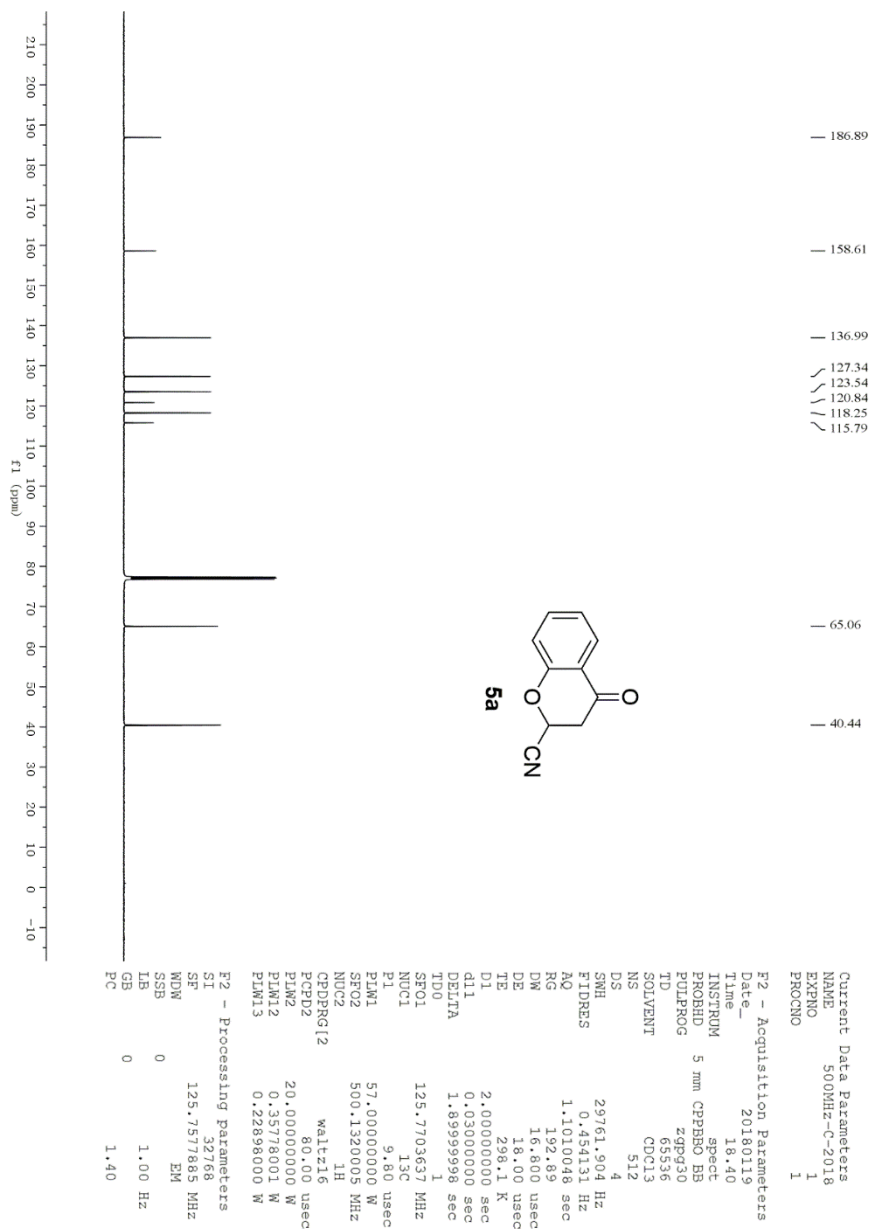
3.18
3.17
3.15
3.10
3.08
3.06
3.05



Current Data Parameters
NAME 500MHz-H-2018
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180209
Time 11.12
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SF01 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

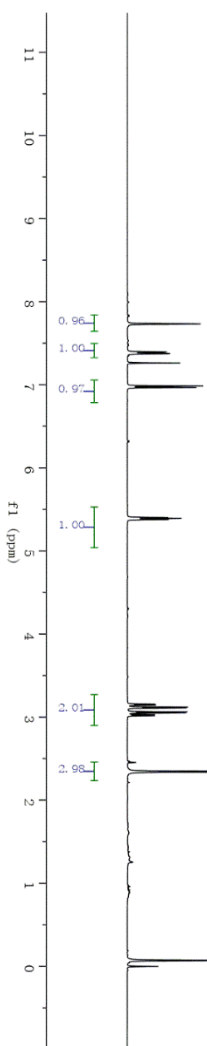
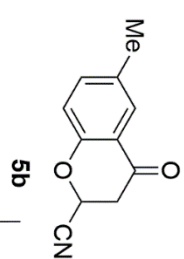
F2 - Processing parameters
SI 65536
SF 500.130093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.73
7.39
7.37
6.98
6.97

5.40
5.39
5.39
5.38

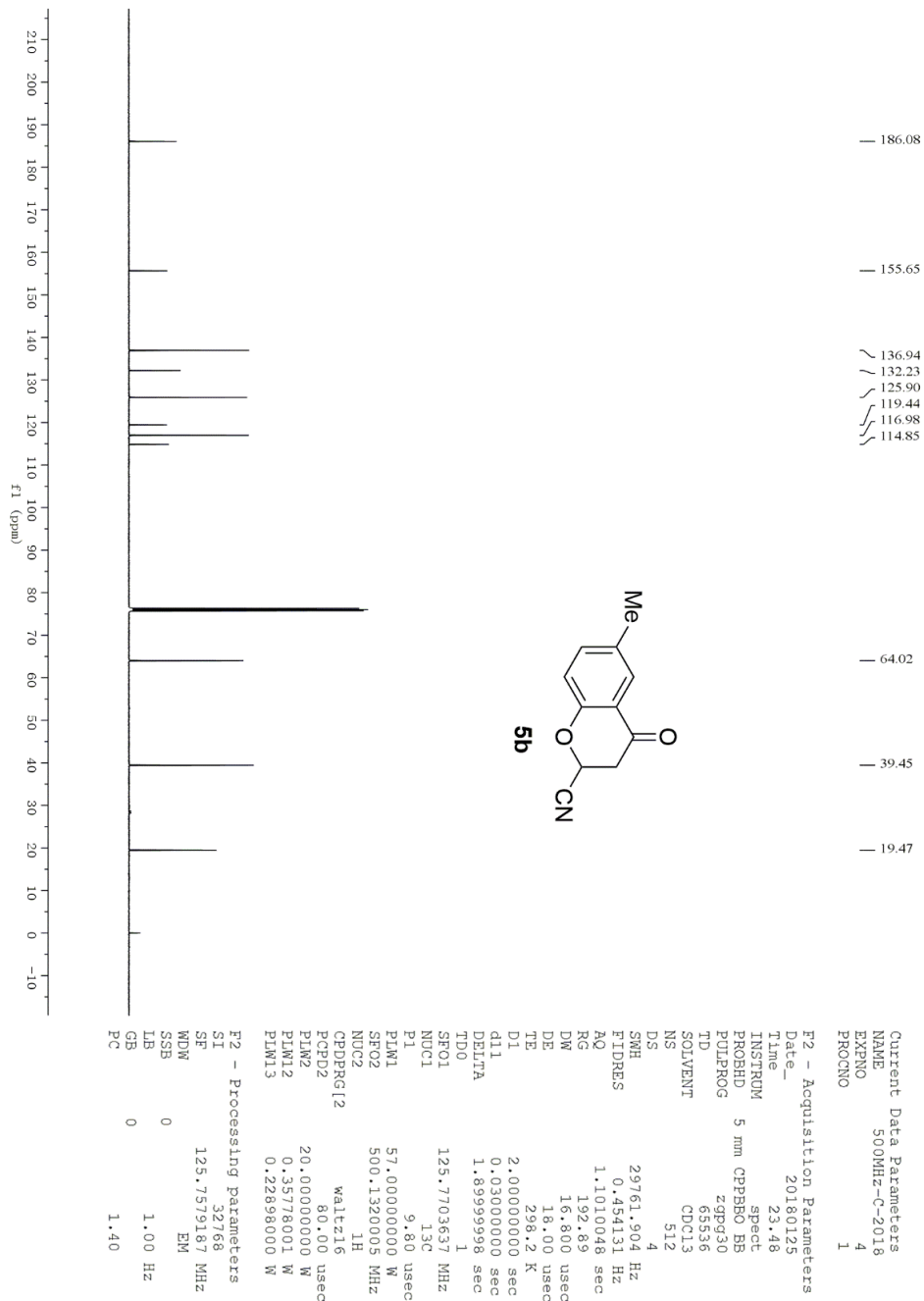
3.15
3.14
3.12
3.11
3.06
3.05
3.02

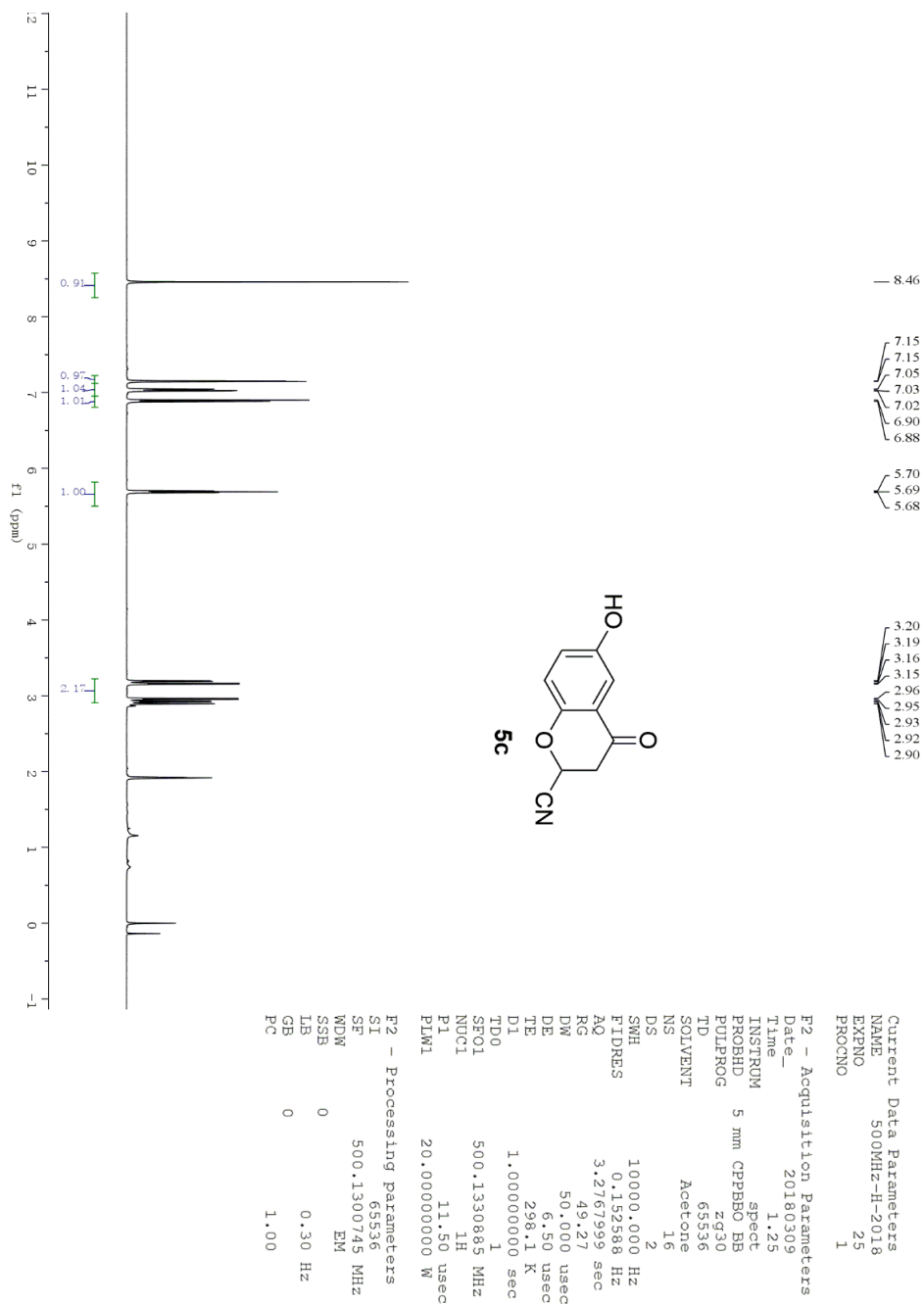


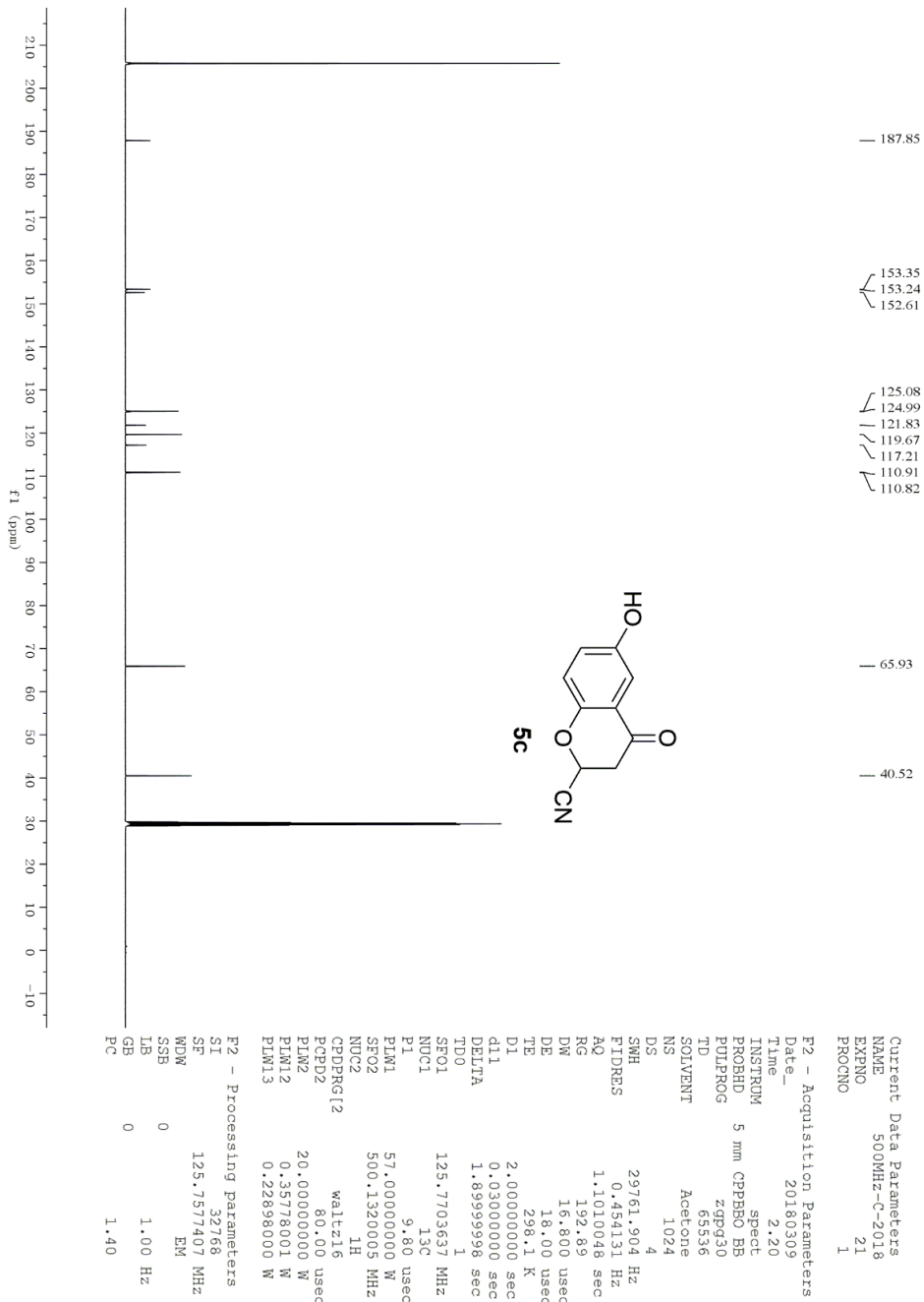
Current Data Parameters
NAME 500MHz-H-2018
EXPNO 15
PROCNO 1

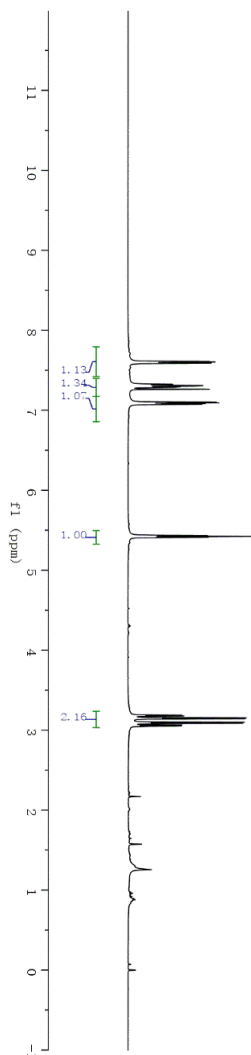
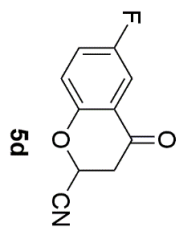
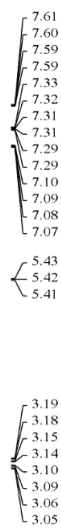
F2 - Acquisition Parameters
Date_ 20180208
Time 9.18
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 49.27
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





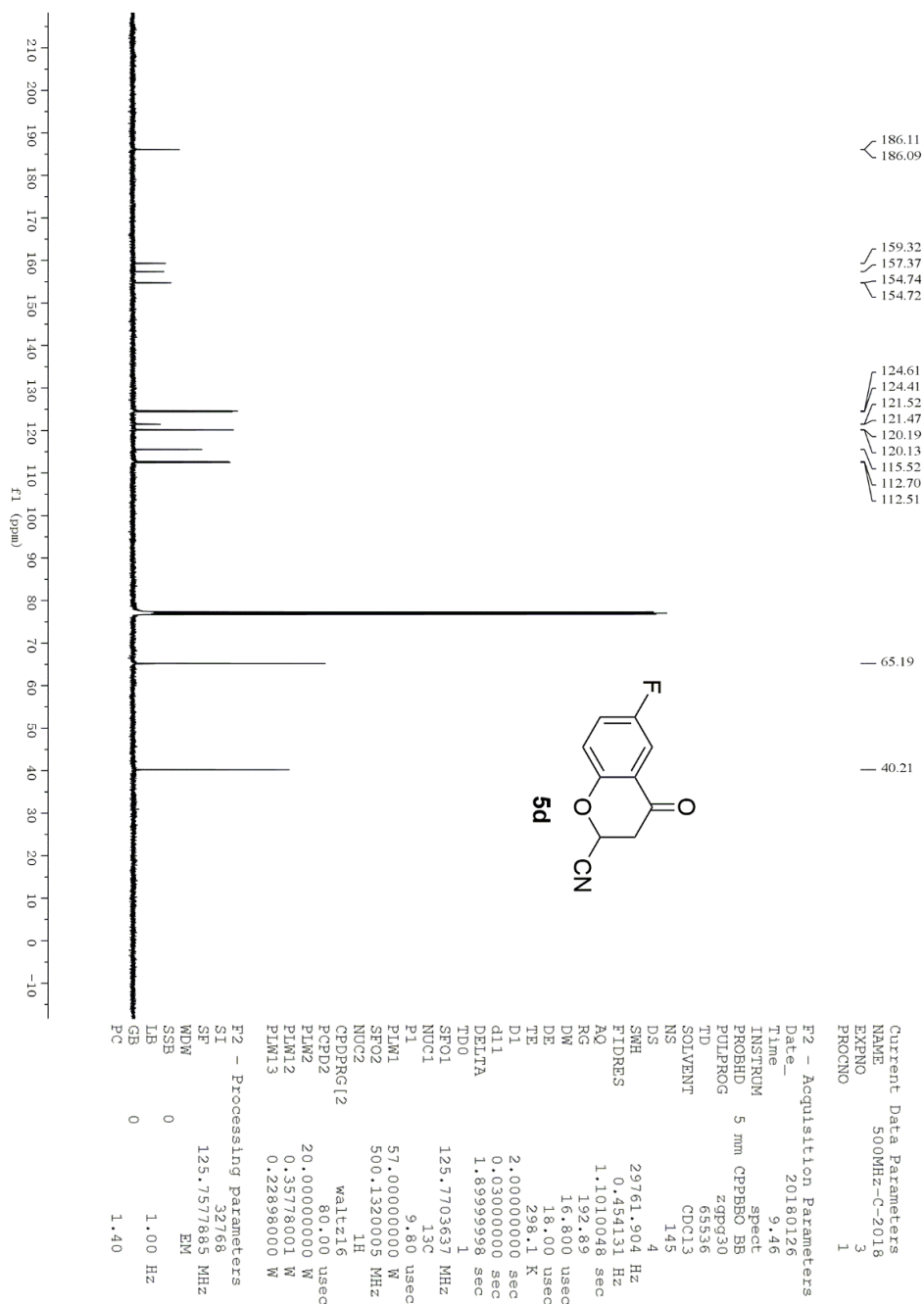


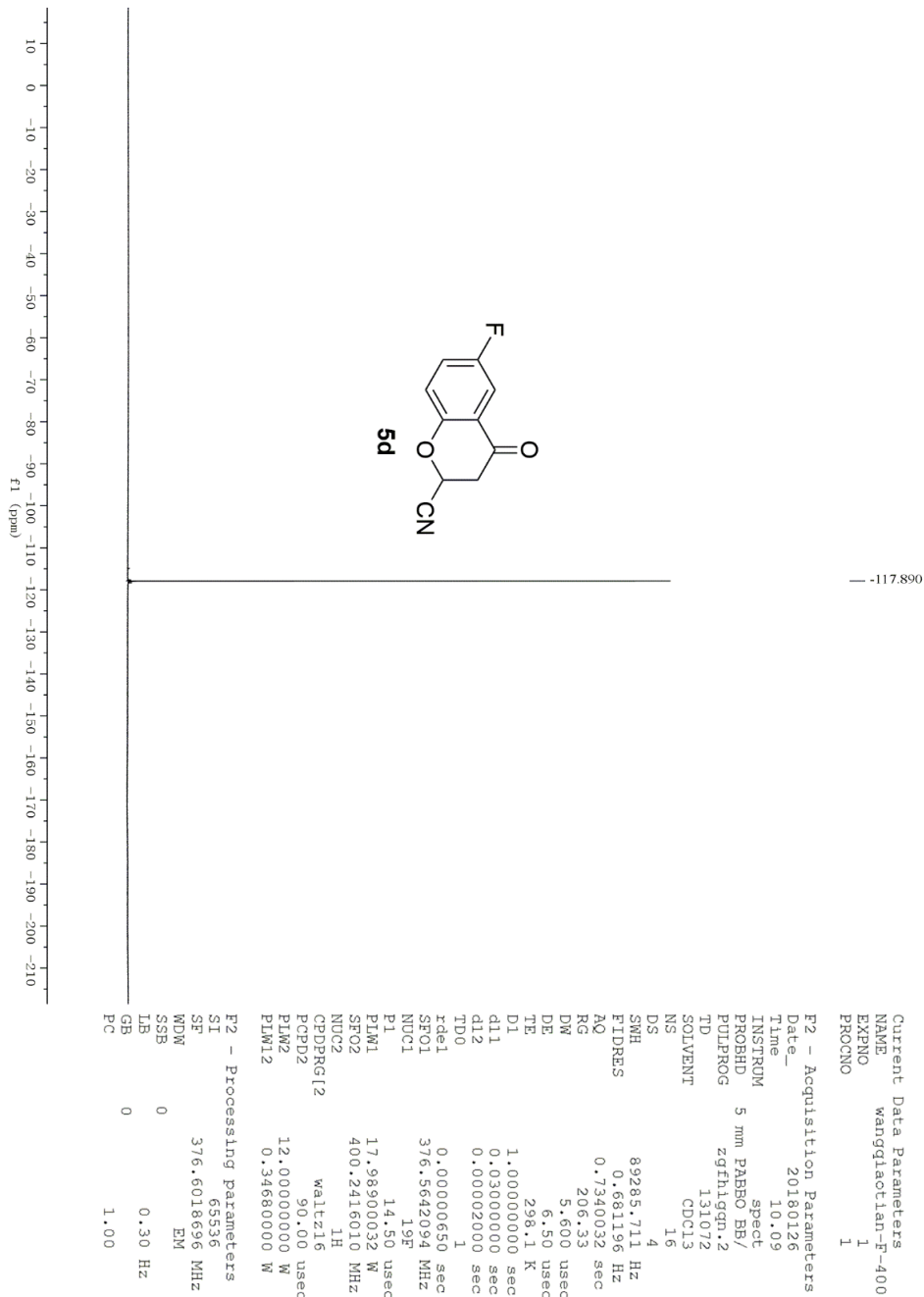
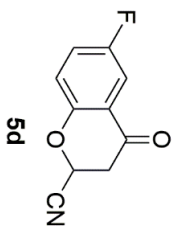


Current Data Parameters
NAME 500MHz-H-2018
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180125
Time 22.49
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 55.37
DM 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 500.130885 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





7.91
7.90
7.54
7.53
7.52
7.52
7.07
7.05

5.44
5.43
5.42

3.19
3.18
3.15
3.14
3.10
3.09
3.07
3.05

Current Data Parameters
NAME 500MHz-H-2018
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180119
Time 18.43

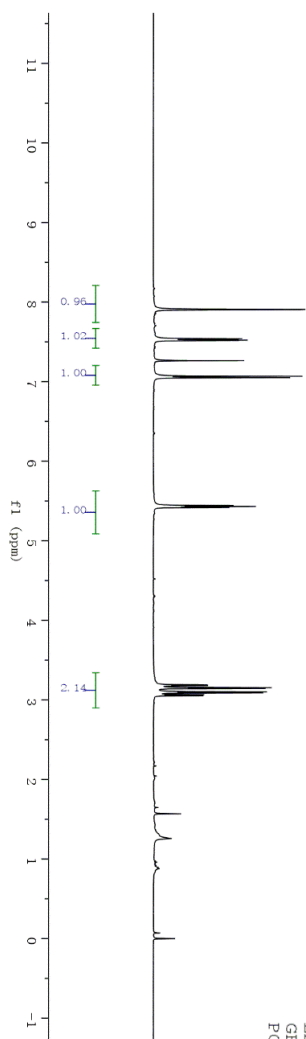
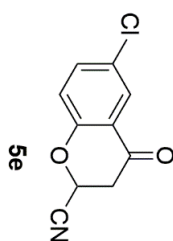
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2

SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 62.06

DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec

TD0 1
SFO1 500.133085 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

F2 - Processing Parameters
SI 65536
SF 500.1300108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

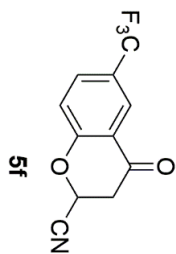




8.15
7.75
7.75
7.73
7.73
7.16
7.14

5.45
5.44
5.43

3.17
3.16
3.14
3.13
3.08
3.07
3.04
3.03



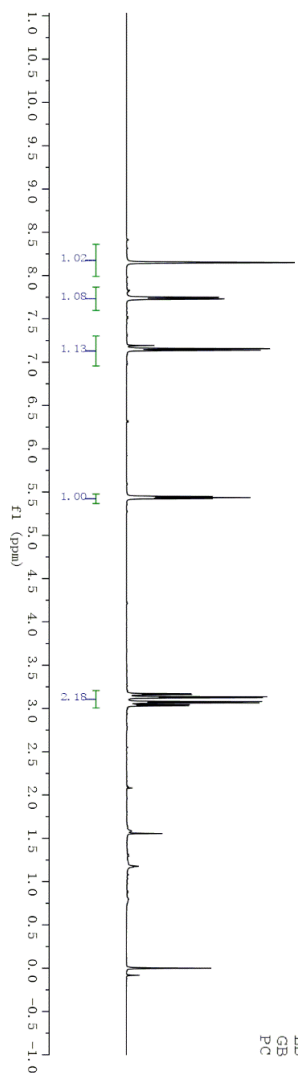
Current Data Parameters
NAME 500MHz-H-2018
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180328
Time 20.40
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 500.130085 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W

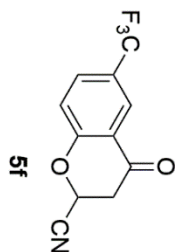
F2 - Processing Parameters

SI 65536
SF 500.1300463 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



184.66
184.65
159.46
132.35
132.33
132.30
132.28
125.57
125.54
125.30
125.03
124.76
124.17
124.14
124.10
124.07
123.38
121.22
119.52
118.33
114.19

64.22
39.09

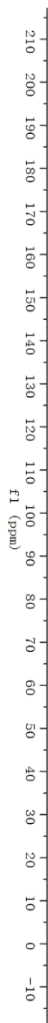


Current Data Parameters
NAME 500MHz-C-2018
EXPNO 28
PROCNO 1

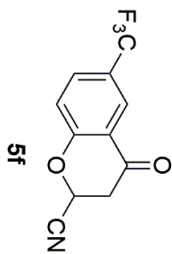
F2 - Acquisition Parameters
Date_ 20180328

Time 21.35
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SF01 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing Parameters
SI 32768
SF 125.7579166 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



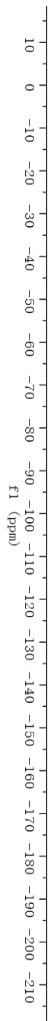
-62.492



Current Data Parameters
NAME wangliactlan-F-400
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180405
Time 14.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 206.33
DW 5.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
TD0 1
TD1 0.00000650 sec
rfdel 376.5642094 MHz
SFO1 19F
NUC1 19F
P1 14.50 usec
PLM1 17.98900032 W
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 90.00 usec
PLM2 12.00000000 W
PLM12 0.34680000 W

F2 - Processing parameters
SI 65536
SF 376.6018696 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

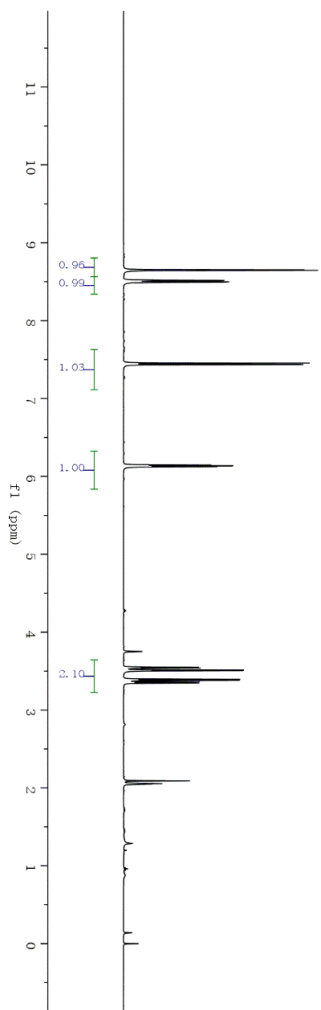
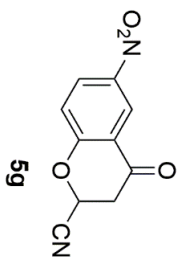


8.65
8.65
8.52
8.51
8.50
8.49

7.45
7.44

6.15
6.13
6.12

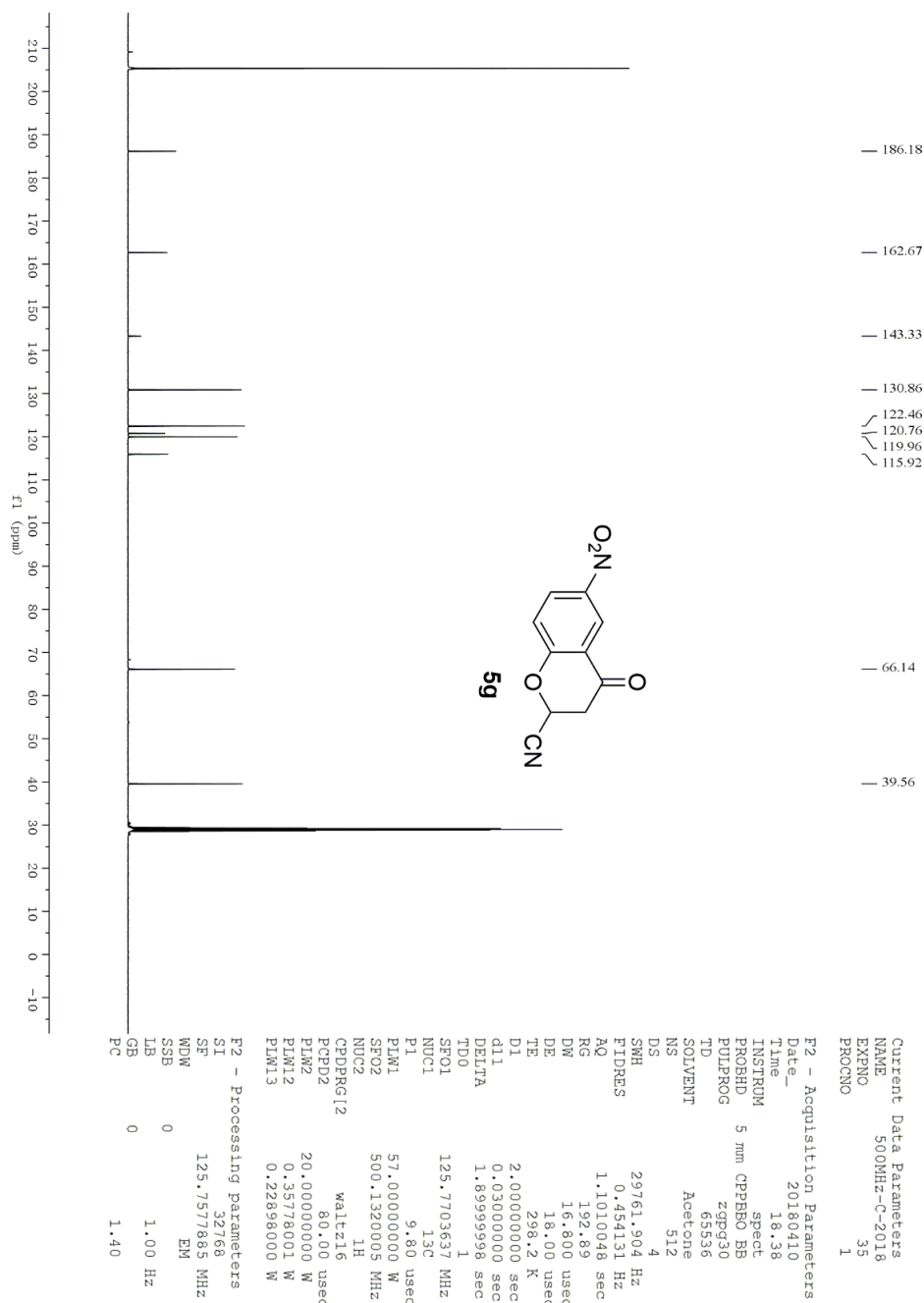
3.55
3.54
3.51
3.50
3.40
3.38
3.36
3.35



Current Data Parameters
NAME 500MHz-H-2018
EXPNO 39
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180410
Time 18.37
INSTRUM spect
PROBHD 5 mm CPBBO BS
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SMH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 55.37
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing Parameters
SI 65536
SF 500.130065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.82
7.80

6.64
6.62
6.43

5.34
5.32
5.32

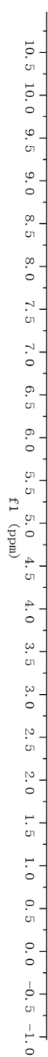
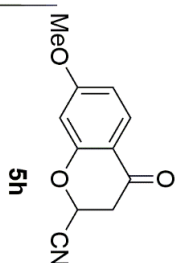
3.80
3.04
3.03
3.01
3.00
2.96
2.94
2.91

Current Data Parameters
NAME 500MHz-H-2018
EXPNO 21
PROCNO 1

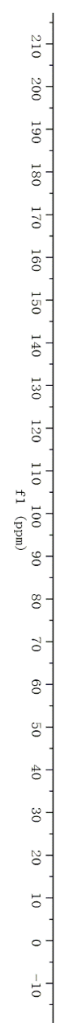
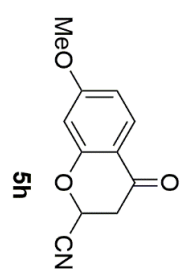
F2 - Acquisition Parameters
Date_ 20180301

Time 23.19
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152568 Hz
AQ 3.2767999 sec
RG 49.27
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.133085 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

F2 - Processing Parameters
SI 65536
SF 500.1300461 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



184.40
 165.63
 159.55
 130.39
 128.11
 114.81
 113.56
 110.70
 100.41
 64.28
 54.86
 38.99



Current Data Parameters
 NAME 500MHz-C-2018
 EXPNO 17
 PROCNO 1

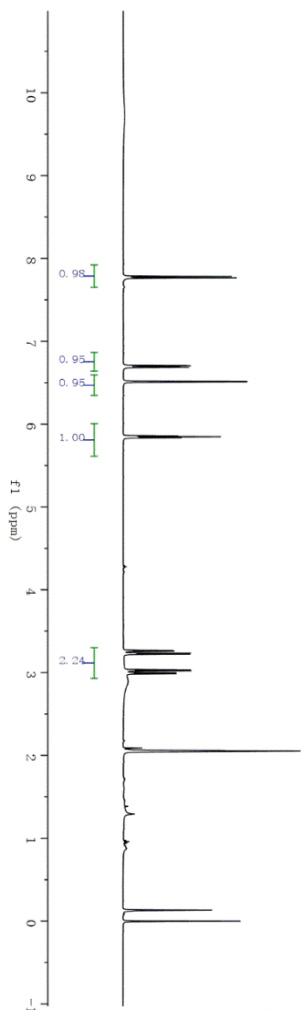
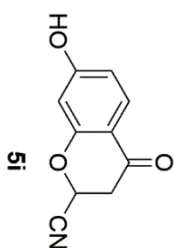
F2 - Acquisition Parameters
 Date_ 20180301
 Time 23:47

INSTRUM 5 mm CPPBBO BB
 PROBD zpgp30
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLM1 57.00000000 W
 SFO2 500.132005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLM2 20.00000000 W
 PLM12 0.35778001 W
 PLM13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7579186 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

7.78
7.77
6.71
6.70
6.69
6.52
6.51
5.86
5.85
5.84

3.27
3.26
3.23
3.22
3.03
3.02
3.00
2.99



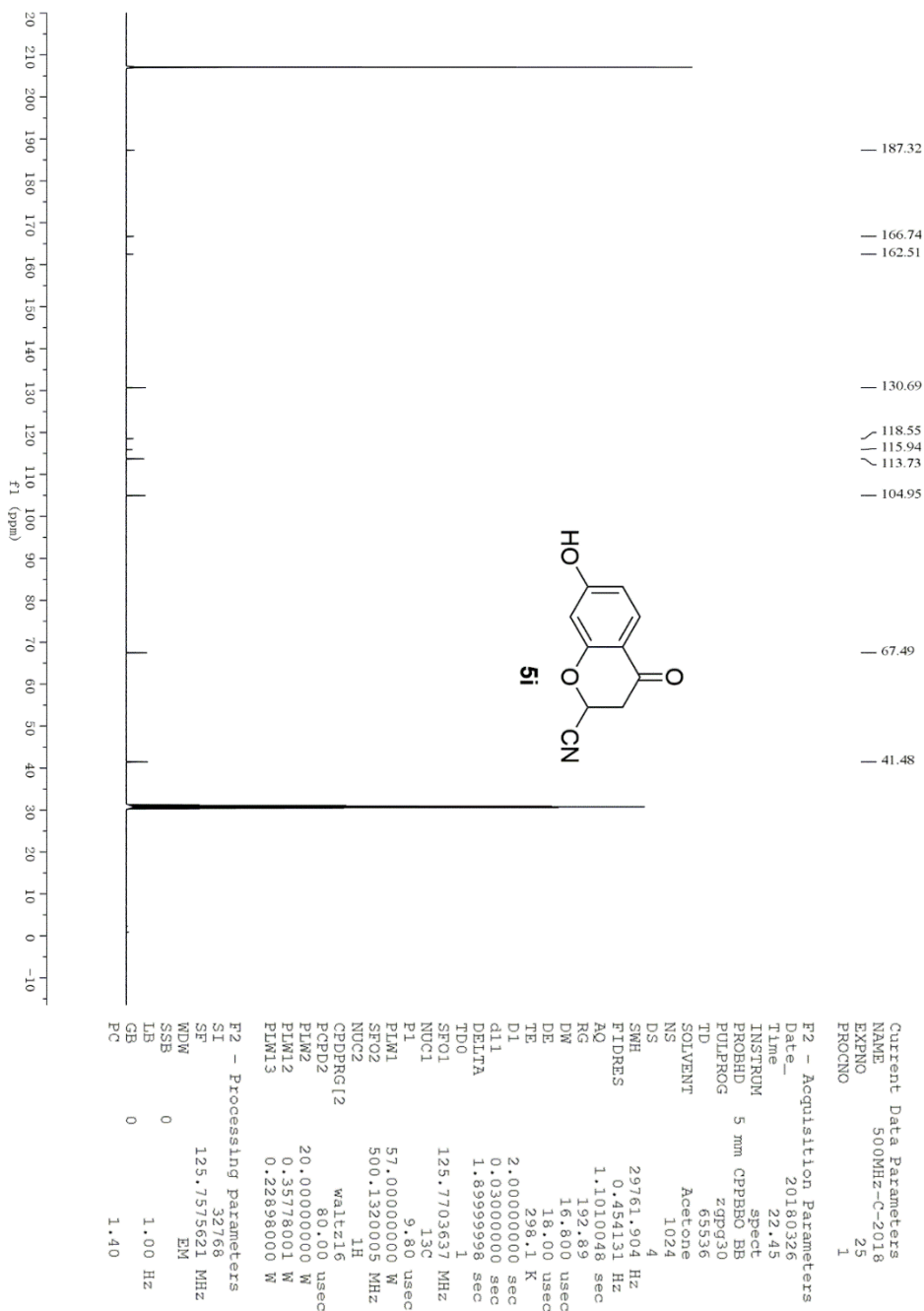
Current Data Parameters
NAME 500MHz-H-2018
EXPNO 29
PROCNO 1

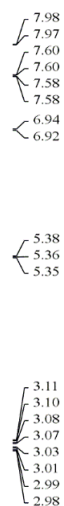
F2 - Acquisition Parameters

Date_ 20180326
Time_ 21.50
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 62.06
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing parameters

SI 65536
SF 500.130068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

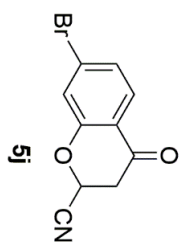




Current Data Parameters
 NAME 500MHz-H-2018
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters

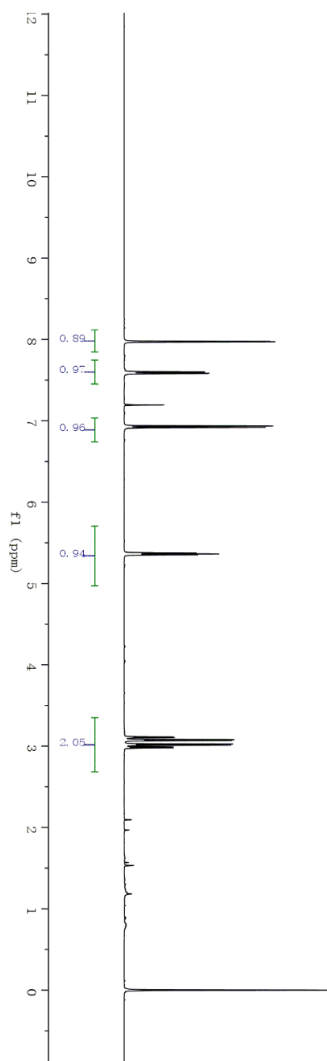
Date_ 20180301
 Time 23.50
 INSTRUM spect
 PROBHD 5 mm CPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃



NS 16
 DS 2
 SMH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.276799 sec
 RG 49.27
 DM 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.133085 MHz
 NUC1 ¹H
 P1 11.50 usec
 PLW1 20.00000000 W

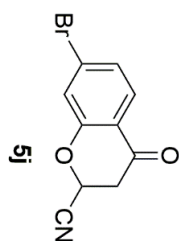
F2 - Processing Parameters

SI 65536
 SF 500.1300453 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



184.63
156.41
138.60
128.78
120.96
119.26
115.44
114.36

64.06
39.08



Current Data Parameters
NAME 500MHz-C-2018
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180302

Time 0.44

INSTRUM spect

PROBHD 5 mm CPBBO BB

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 1024

DS 4

SWH 29761.904 Hz

FIDRES 0.454131 Hz

AQ 1.1010048 sec

RG 192.89

DW 16.800 usec

DE 18.00 usec

TE 298.2 K

D1 2.00000000 sec

d11 0.03000000 sec

DELTA 1.89999996 sec

TD0 1

SFO1 125.7703637 MHz

NUC1 13C

P1 9.80 usec

PLM1 57.00000000 W

SFO2 500.1320005 MHz

NUC2 1H

CPDPRG12 waltz16

PCPD2 80.00 usec

PLW2 20.00000000 W

PLM12 0.35778001 W

PLM13 0.22898000 W

F2 - Processing Parameters

SI 32768

SF 125.7579192 MHz

WDW EM

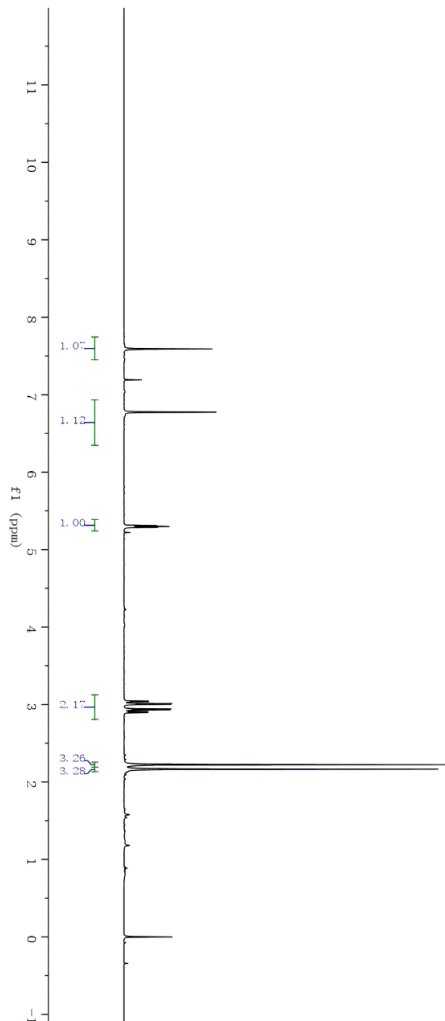
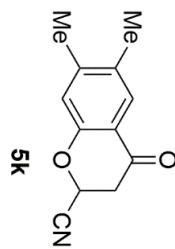
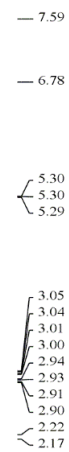
SSB 0

LB 1.00 Hz

GB 0

PC 1.40





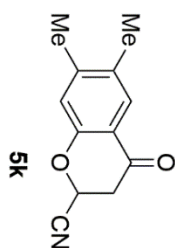
Current Data Parameters
NAME 500MHz-H-2018
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180326
Time 22.48
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 500.133085 MHz
NUC1 ¹H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300453 MHz
WDW EM
SSB 0
GB 0.30 Hz
PC 1.00

185.79
155.86
146.77
131.35
126.19
117.63
117.59
115.00

64.06
39.35
19.57
17.85



Current Data Parameters
NAME 500MHz-C-2018
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180326
Time 23.43

INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4

SMH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec

RG 192.89
DW 16.800 usec
DE 16.00 usec

TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec

DELTA 1.89999998 sec
TD0 1
SFO1 125.7703637 MHz

NUC1 13C
P1 9.80 usec
PLM1 57.00000000 W

SFO2 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16

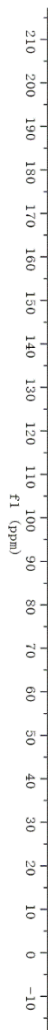
PCPD2 80.00 usec
PLW2 20.00000000 W

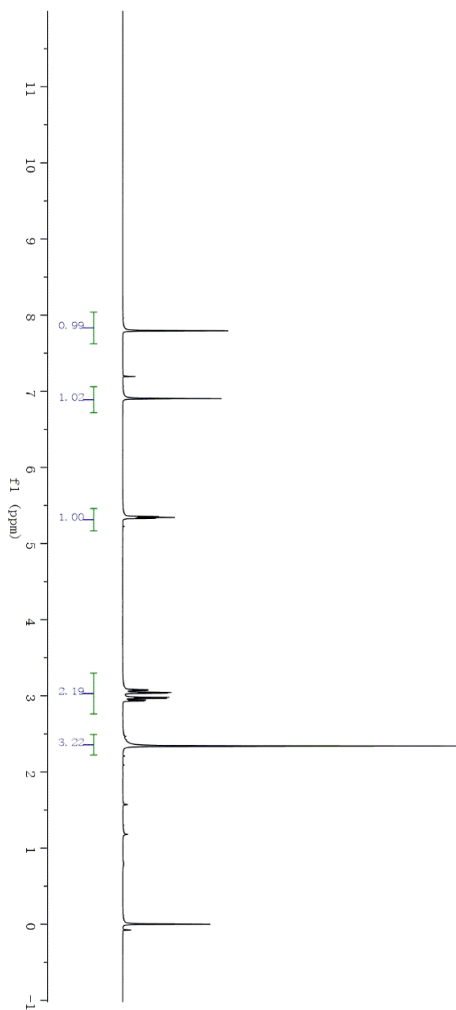
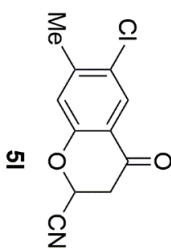
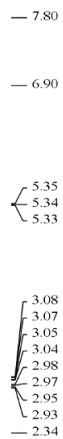
PLM12 0.35776001 W
PLM13 0.22896000 W

F2 - Processing parameters
SI 32768
SF 125.7579185 MHz

WDW EM
SSB 0
LB 1.00 Hz

GB 0
PC 1.40





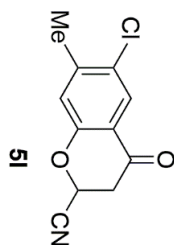
Current Data Parameters
NAME 500MHz-H-2018
EXPNO 36
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180407
Time 20.23
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing Parameters
SI 65536
SF 500.1300443 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

— 184.63
— 155.72
— 145.44
/ 128.83
/ 125.95
/ 119.28
/ 118.72
/ 114.57

— 64.13
— 39.08
— 19.95



Current Data Parameters
NAME 500MHz-C-2018
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180407

Time 20.31

INSTRUM spect

PROBHD 5 mm CPBBO BB

PULPROG zgpg30

TD 65536

SOLVENT CDC13

NS 1024

DS 4

SWH 29761.904 Hz

FIDRES 0.454131 Hz

AQ 1.1010048 sec

RG 192.89

DW 16.800 usec

DE 18.00 usec

TE 298.2 K

D1 2.00000000 sec

d11 0.03000000 sec

DELTA 1.89999998 sec

TD0 1

SFO1 125.7703637 MHz

NUC1 13C

P1 9.80 usec

PLM1 57.00000000 W

SFO2 500.1320005 MHz

NUC2 1H

CPDPRG12 waltz16

PCPD2 80.00 usec

PLM2 20.00000000 W

PLM12 0.35718001 W

PLM13 0.22898000 W

F2 - Processing Parameters

SI 32768

SF 125.7579187 MHz

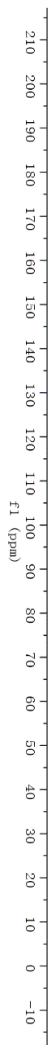
WDW 0 EM

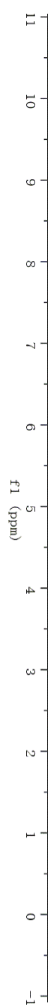
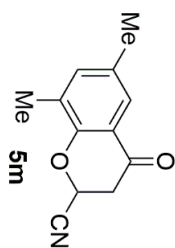
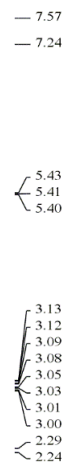
SSB 0

LB 1.00 Hz

GB 0

PC 1.40





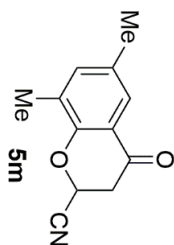
Current Data Parameters
 NAME 500MHz-H-2018
 EXPNO 37
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180409
 Time 9.22
 INSTRUM spect
 PROBHD 5 mm CPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.276799 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.50 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.130091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

187.55
154.96
139.16
132.44
127.41
124.48
120.29
116.11

64.98
40.37
20.45
15.40



Current Data Parameters
NAME 500MHz-C-2018
EXPNO 33
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180409
Time_ 9.24

INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 169
DS 4

SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec

RG 192.89
DW 16.800 usec
DE 18.00 usec

TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec

DELTA 1.89999998 sec
TD0 1
SF01 125.7703637 MHz

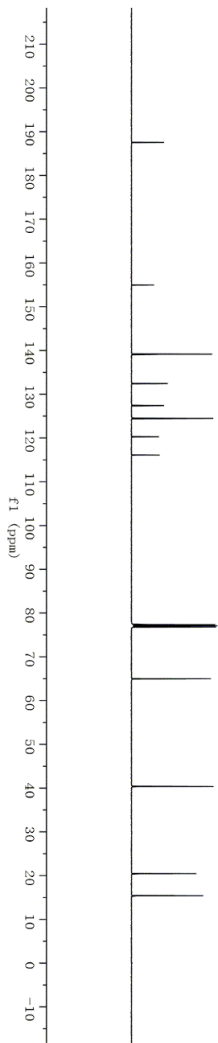
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

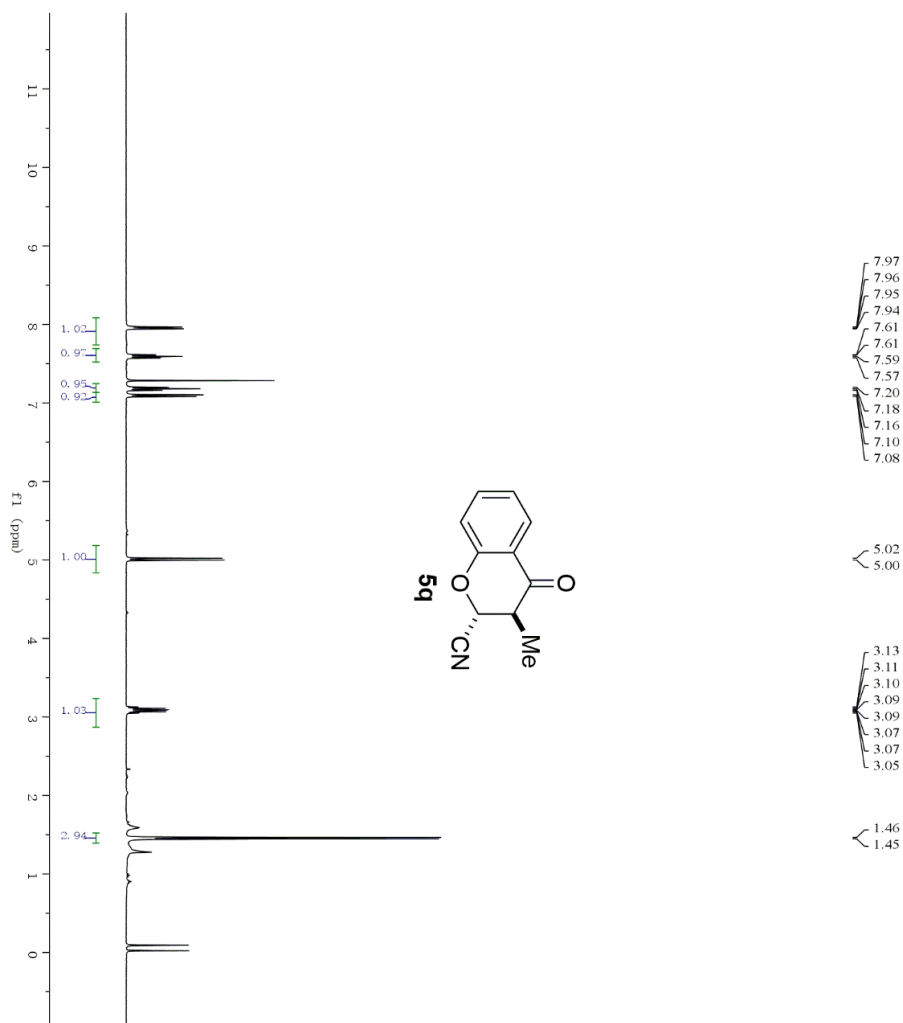
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16

PCPD2 80.00 usec
PLW2 20.00000000 W

PLW12 0.35778001 W
PLW13 0.22888000 W

F2 - Processing Parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

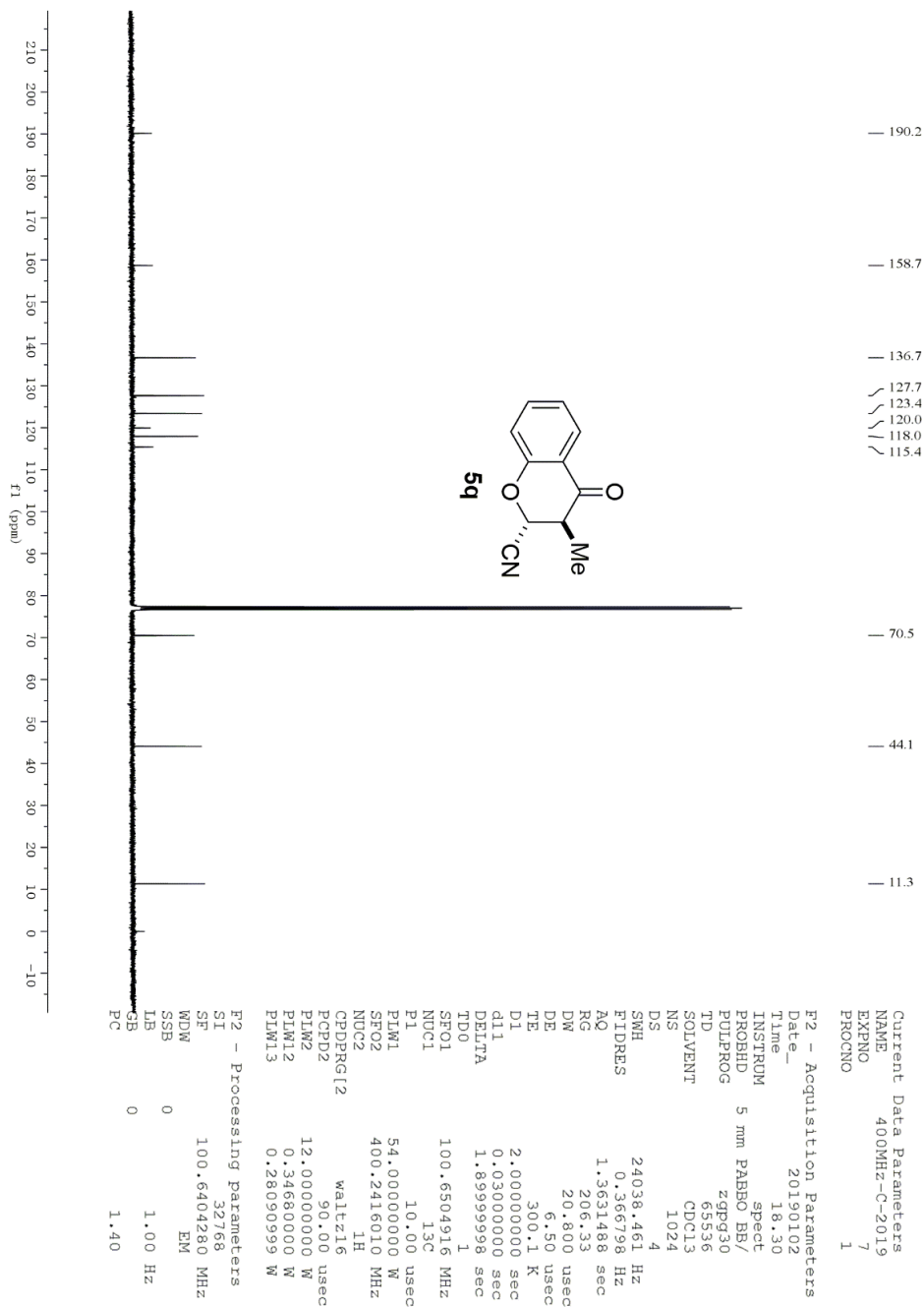


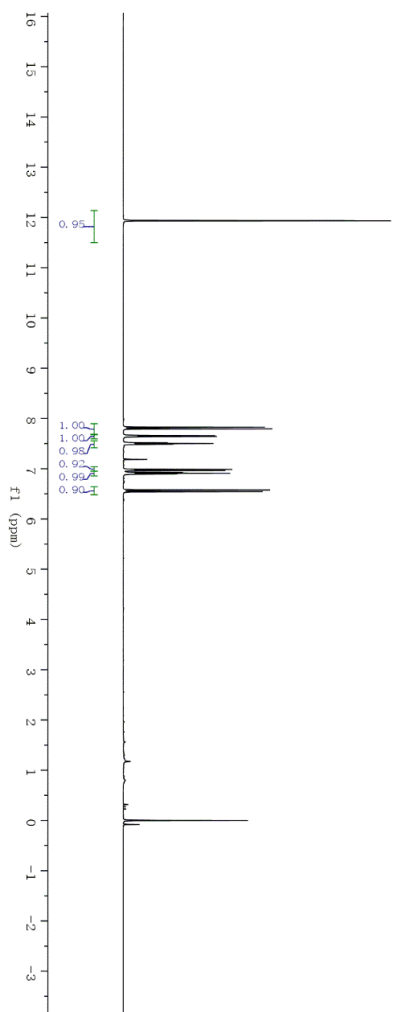
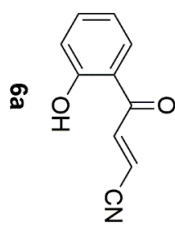
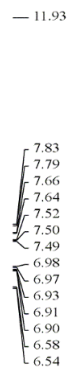


Current Data Parameters
NAME 400MHz-H-2019
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190107
Time 11.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 206.33
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TDO 1
SFO1 400.242416 MHz
NUC1 1H
P1 14.30 usec
PLM1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.240000 MHz
WDW EM
SSB 0
GB 0
PC 1.00



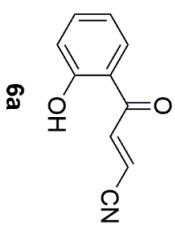


Current Data Parameters
NAME 500MHz-H-2018
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180202
Time 16.53
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 31.72
DM 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1
SFO1 500.133085 MHz
NUC1 ¹H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300493 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

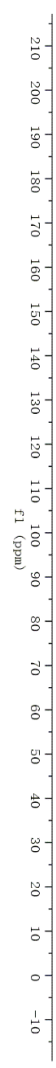
188.93
 162.97
 139.70
 137.19
 128.80
 118.63
 118.01
 117.59
 115.14
 111.51



Current Data Parameters
 NAME 500MHz-C-2018
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180202
 Time_ 17.21
 INSTRUM spect
 PROBD 5 mm CPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 ID0 1
 SF01 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W
 SE02 500.1320005 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing Parameters
 SI 32768
 SF 125.7579198 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



11.76
7.82
7.78
7.30
7.28
6.87
6.85
6.54
6.50

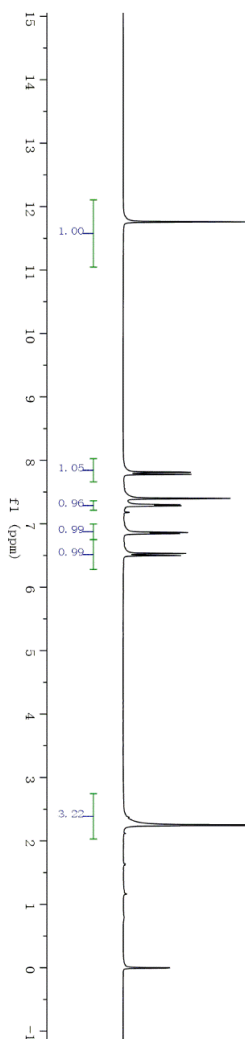
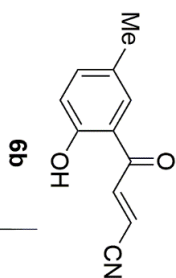
2.25

Current Data Parameters
NAME 500MHz-H-2018
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180308
Time 23.29

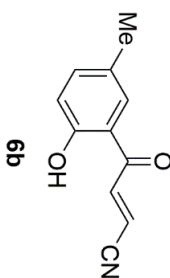
INSTRUM spect
PROBHD 5 mm CPEBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 31.72
DM 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TDO 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing Parameters
SI 65536
SF 500.1300526 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



188.77
160.96
139.90
138.37
128.37
127.87
117.71
117.26
115.24
111.19

19.47

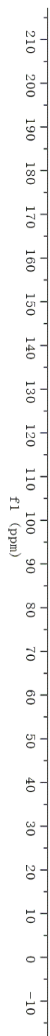


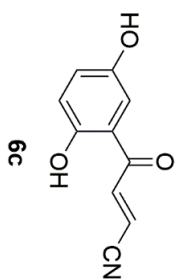
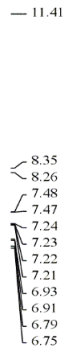
Current Data Parameters
NAME 500MHz-C-2018
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180309

Time 0.23
INSTRUM spect
PROBHD 5 mm CPBPB0 BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.8999996 sec
TD0 1
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLM1 57.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLM2 20.00000000 W
PLM12 0.35776001 W
PLM13 0.22896000 W

F2 - Processing Parameters
SI 32768
SF 125.7579204 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

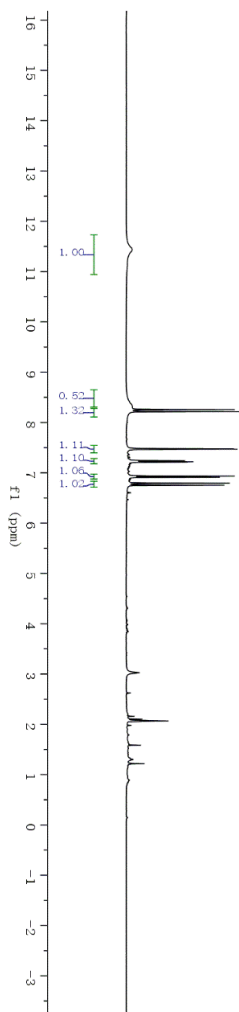




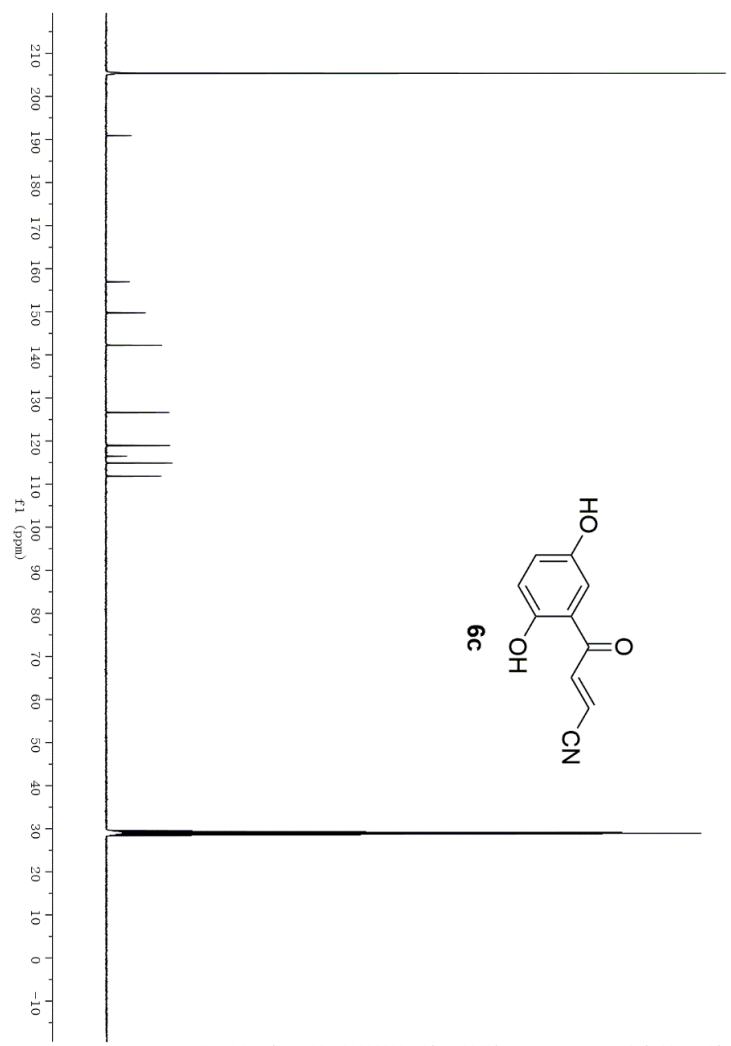
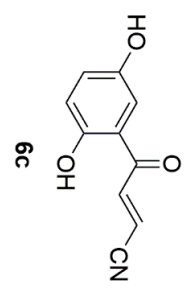
Current Data Parameters
NAME 45678
EXPNO 46
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181126
Time 21.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
FIDRES 0.244532 Hz
RG 2.044723 sec
DE 62.400 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
SF01 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLM1 12.00000000 W

F2 - Processing Parameters
SI 65536
SF 400.2400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



156.96
 149.77
 142.25
 126.63
 118.97
 116.49
 114.88
 111.86



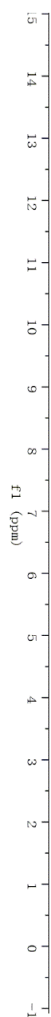
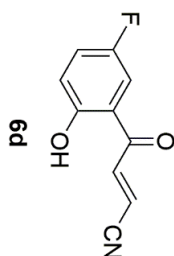
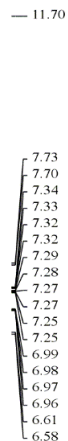
Current Data Parameters
 NAME 3467
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20181126
 Time 21:20
 INSTRUM spect
 PROBHD 5 mm PABBO BBI
 PULPROG zgpg30
 FIDPROC 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631468 sec
 RG 206.33
 IN 20.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1
 SFO1 100.6504916 MHz
 P1 150
 P11 10.00 usec
 SFO2 54.0000000 MHz
 SFO2 400.2416010 MHz
 NUC2 1H
 P2PRG12 waltz16
 PCPD2 30.00 usec
 PLM2 12.0000000 W
 PLM12 0.34680000 W
 PLM13 0.28090999 W

F2 - Processing parameters

SI 32768
 SF 100.6404280 MHz
 MDW 0 EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 500MHz-H-2018
 EXPNO 19
 PROCNO 1

F2 - Acquisition Parameters

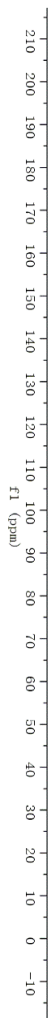
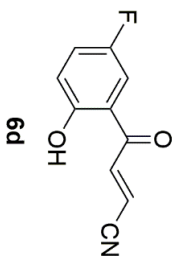
Date_ 20180301
 Time 22.18
 INSTRUM spect
 PROBHD 5 mm CPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.276799 sec
 RG 55.37
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1
 SFO1 500.1350889 MHz
 NUC1 1H
 P1 11.50 usec
 PL1 20.00000000 W

F2 - Processing Parameters

SI 65536
 SF 500.1300471 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

188.32
188.30
188.27

161.39
161.37
161.34
138.96
138.94
138.91
138.89
137.05
137.03
137.00
127.84
127.82
127.79
127.77
123.42
123.40
123.37
119.67
119.65
119.62
118.10
118.08
118.04
114.86
114.84
114.81
112.42
112.40
112.38
112.36

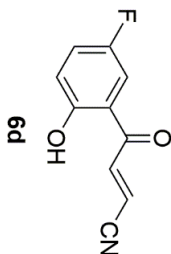


Current Data Parameters
NAME 500MHz-C-2018
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180301
Time 22.46
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLM1 57.00000000 W
SFO2 500.132005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLM2 20.00000000 W
PLM12 0.35778001 W
PLM13 0.22898000 W

F2 - Processing Parameters
SI 32768
SF 125.7579186 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

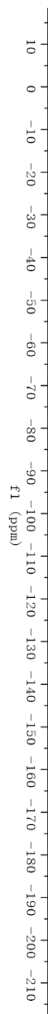
1 -122.454



Current Data Parameters
NAME wanglaotian-F-400
EXPNO 14
PROCNO 1

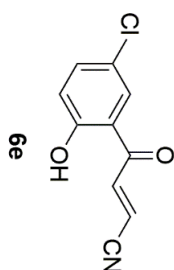
F2 - Acquisition Parameters
Date_ 20180628
Time 20.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 9
DS 4
SWH 89285.711 Hz
FIDRES 0.061196 Hz
AQ 0.7340032 sec
RG 206.33
DW 5.600 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec
TD0 1
rde1 0.00000650 sec
SF01 376.5642094 MHz
NUC1 19F
P1 14.50 usec
PLW1 17.98300032 W
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.34680000 W

F2 - Processing parameters
SI 65536
SF 376.6018696 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



11.83

7.76
7.73
7.62
7.46
7.45
7.44
7.44
6.96
6.94
6.61
6.57



Current Data Parameters
NAME 500MHz-H-2018
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180301

Time 21.47

INSTRUM spect

PROBHD 5 mm CPBBD BB

PULPROG zg30

TD 65536

SOLVENT CDCl3

NS 16

DS 2

SWH 10000.000 Hz

FIDRES 0.152588 Hz

AQ 3.276799 sec

RG 31.72

DM 50.000 usec

DE 6.50 usec

TE 298.1 K

DI 1.00000000 sec

TD0 1

SFO1 500.1330869 MHz

NUC1 1H

P1 11.50 usec

PLM1 20.00000000 W

F2 - Processing Parameters

SI 65536

SF 500.1300472 MHz

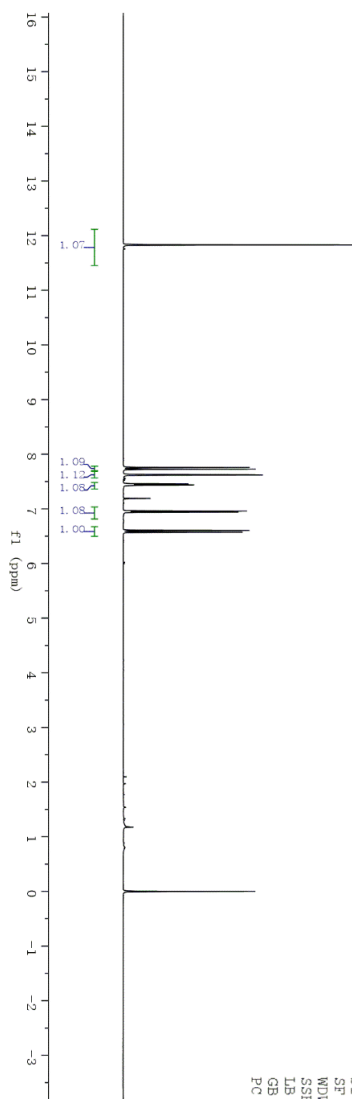
WDW EM

SSB 0

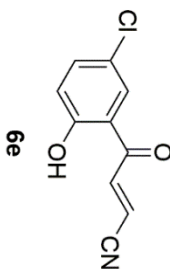
LB 0.30 Hz

GB 0

PC 1.00



188.32
161.40
138.95
138.72
137.05
127.83
123.42
119.67
118.09
114.85
112.42



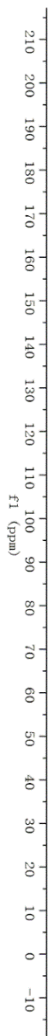
Current Data Parameters
NAME 500MHz-C-2018
EXPNO 13
PROCNO 1

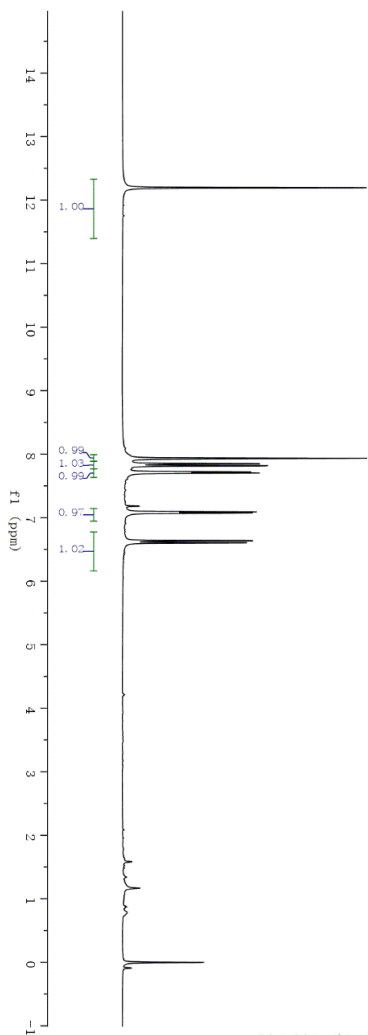
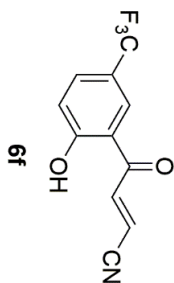
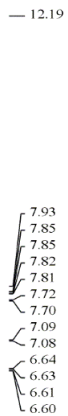
F2 - Acquisition Parameters

Date_ 20180501
Time 22.15
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999996 sec
TD0 1
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLM1 57.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLM2 20.00000000 W
PLM12 0.35776001 W
PLM13 0.22896000 W

F2 - Processing parameters

SI 32768
SF 125.7579193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
 NAME 500MHz-H-2018
 EXPNO 33
 PROCNO 1

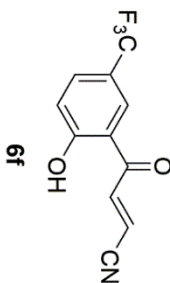
F2 - Acquisition Parameters

Date_ 20180328
 Time 21.37
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.276799 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.50 usec
 PLM1 20.00000000 W

F2 - Processing Parameters

SI 65536
 SF 500.1300519 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

188.88
165.04
138.73
133.32
133.29
133.26
133.24
126.43
126.40
126.36
126.33
123.55
121.50
121.39
121.23
120.96
120.69
118.99
116.94
114.81
112.84

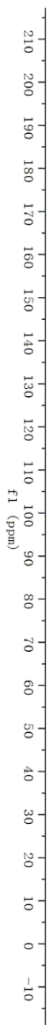


Current Data Parameters
NAME 500MHz-C-2018
EXPNO 29
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180328

Time 22.01
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SF01 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.3578001 W
PLW13 0.22898000 W

F2 - Processing Parameters
SI 32768
SF 125.7579167 MHz
WDW EM
SSB 0
IB 1.00 Hz
GB 0
PC 1.40



-62.021

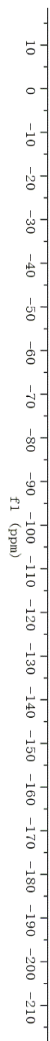
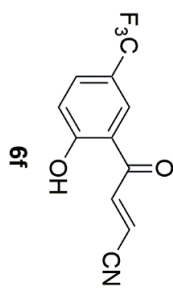
Current Data Parameters
NAME wangqiaotian-F-400
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

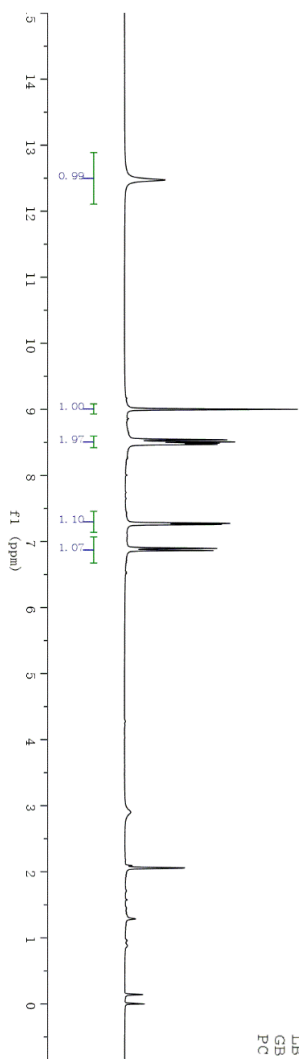
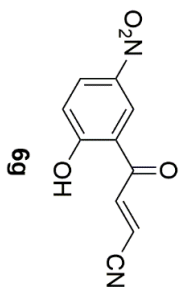
Date_ 20180405
Time 14.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30n.2
TD 131072
SOLVENT CDC13
NS 12
DS 4
SMH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 206.33
DW 5.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.0002000 sec
TD0 1
rdel 0.0000650 sec
SFO1 376.5642094 MHz
NUC1 19F
P1 14.50 usec
PLM1 17.98900032 W
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 90.00 usec
PLM2 12.00000000 W
PLM12 0.34680000 W

F2 - Processing Parameters

SI 65536
SF 376.6018696 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



12.47
9.00
8.54
8.54
8.51
8.51
8.49
8.47
7.27
7.26
6.90
6.86

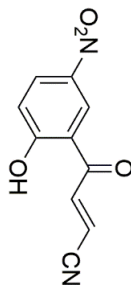


Current Data Parameters
NAME 500MHz-H-2018
EXPNO 27
PROCNO 1

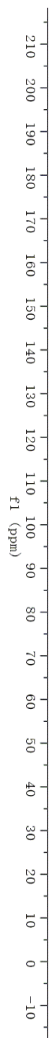
F2 - Acquisition Parameters
Date_ 20180309
Time 3.21
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 49.27
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing parameters
SI 65536
SF 500.130049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

190.92
167.13
141.76
140.34
131.78
127.36
119.37
118.94
116.28
113.20



6g



Current Data Parameters
NAME 500MHz-C-2018
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180309
Time 4.16

INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zgpg30
TD 65836
SOLVENT Acetone
NS 1024
DS 4

SMH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec

RG 192.89
DE 16.800 usec
TE 18.00 usec
D1 298.2 K

DELTA 2.00000000 sec
d11 0.03000000 sec
TD0 1.69999998 sec

SE01 125.7703637 MHz
NUC1 13C
P1 9.80 usec

PLM1 57.00000000 W
SE02 500.1320005 MHz
NUC2 1H

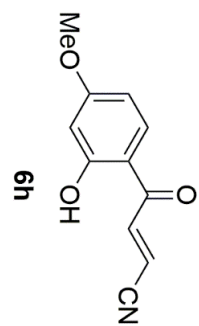
CPDPRG12 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W

PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz

WDW EM
SSB 0
LB 1.00 Hz

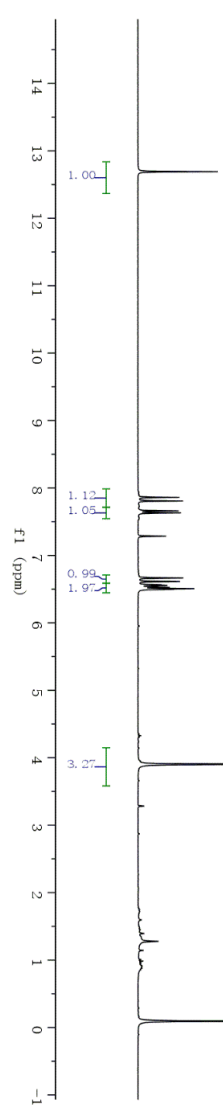
GB 0
PC 1.40



12.69

7.86
7.81
7.66
7.63
6.67
6.61
6.56
6.53

3.90



Current Data Parameters

NAME 300MHz-H-2018

EXPNO 166

PROCNO 1

F2 - Acquisition Parameters

Date_ 20180301

Time_ 16.12

INSTRUM spect

PROBHD 5 mm DUL 13C-1

PULPROG zg30

TD 65536

SOLVENT CDCl3

NS 4

DS 2

SWH 6009.615 Hz

FIDRES 0.091699 Hz

AO 5.4525952 sec

RG 209.09

DW 83.200 usec

DE 6.50 usec

TE 299.0 K

D1 1.00000000 sec

TD0 1

SFO1 300.1318534 MHz

NUC1 1H

P1 8.00 usec

PLW1 18.00000000 W

F2 - Processing parameters

SI 65536

SF 300.1300000 MHz

WDW EM

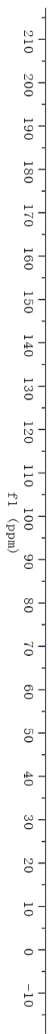
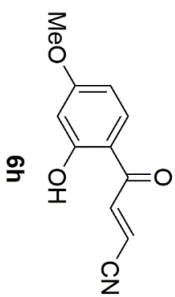
SSB 0

LB 0.30 Hz

GB 0

PC 1.00

186.36
 166.69
 166.40
 140.06
 130.37
 115.36
 111.88
 110.51
 108.01
 100.22
 54.84



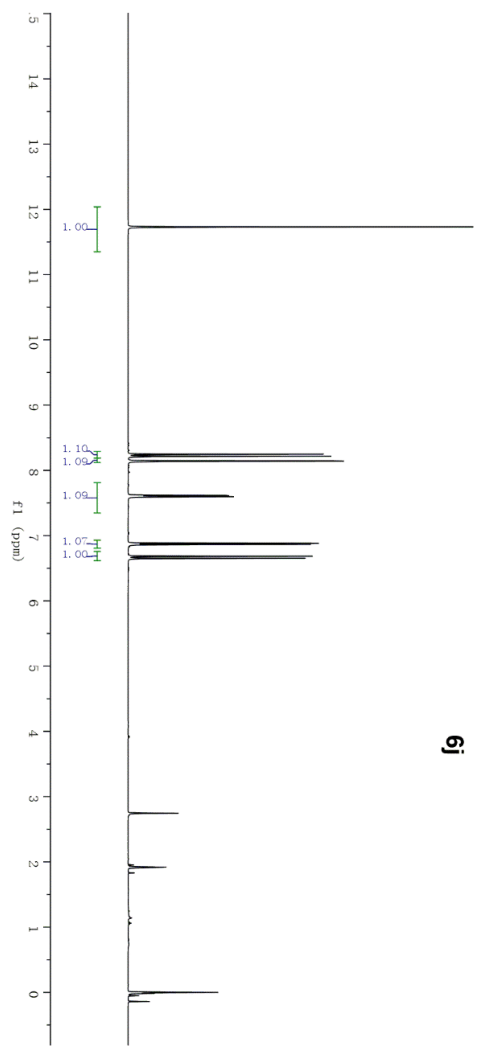
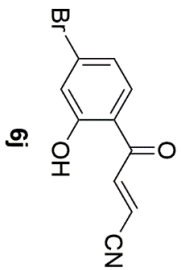
Current Data Parameters
 NAME 500MHz-H-2018
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180301
 Time 22.49
 INSTRUM spect
 PROBD 5 mm CPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 10000.000 Hz
 FIDRES 0.152568 Hz
 AQ 3.276799 sec
 RG 55.37
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.1330685 MHz
 NUC1 1H
 P1 11.50 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300458 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.25
8.22
8.15
8.14
7.62
7.60
6.88
6.86
6.68
6.65

11.73



Current Data Parameters
NAME 500MHz-H-2018
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180309
Time 2.23
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300743 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

190.99
162.56
142.21
140.60
133.43
121.06
120.84
116.78
113.04
111.19
111.16

Current Data Parameters
NAME 500MHz-C-2018
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180309
Time 3.17

INSTRUM spect
PROBHD 5 mm CPBBO BB

PULPROG zgpg30
TD 65536

SOLVENT Acetone
NS 1024

DS 4
SWH 29761.904 Hz

FIDRES 0.454131 Hz
AQ 1.1010048 sec

RG 192.89
DW 16.800 usec

DE 18.00 usec
TE 298.1 K

D1 2.00000000 sec
d11 0.03000000 sec

DELTA 1.89999998 sec
TD0 1

SFO1 125.7703637 MHz
NUC1 13C

P1 9.80 usec
PLW1 57.00000000 W

SFO2 500.1320005 MHz
NUC2 1H

CPDPRG12 waltz16
PCPD2 80.00 usec

PLW2 20.00000000 W
PLW12 0.35778001 W

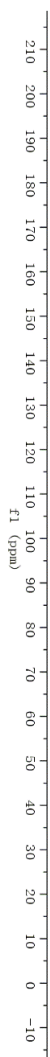
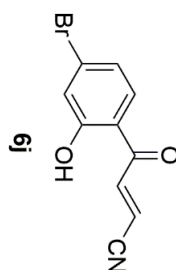
PLW13 0.22898000 W

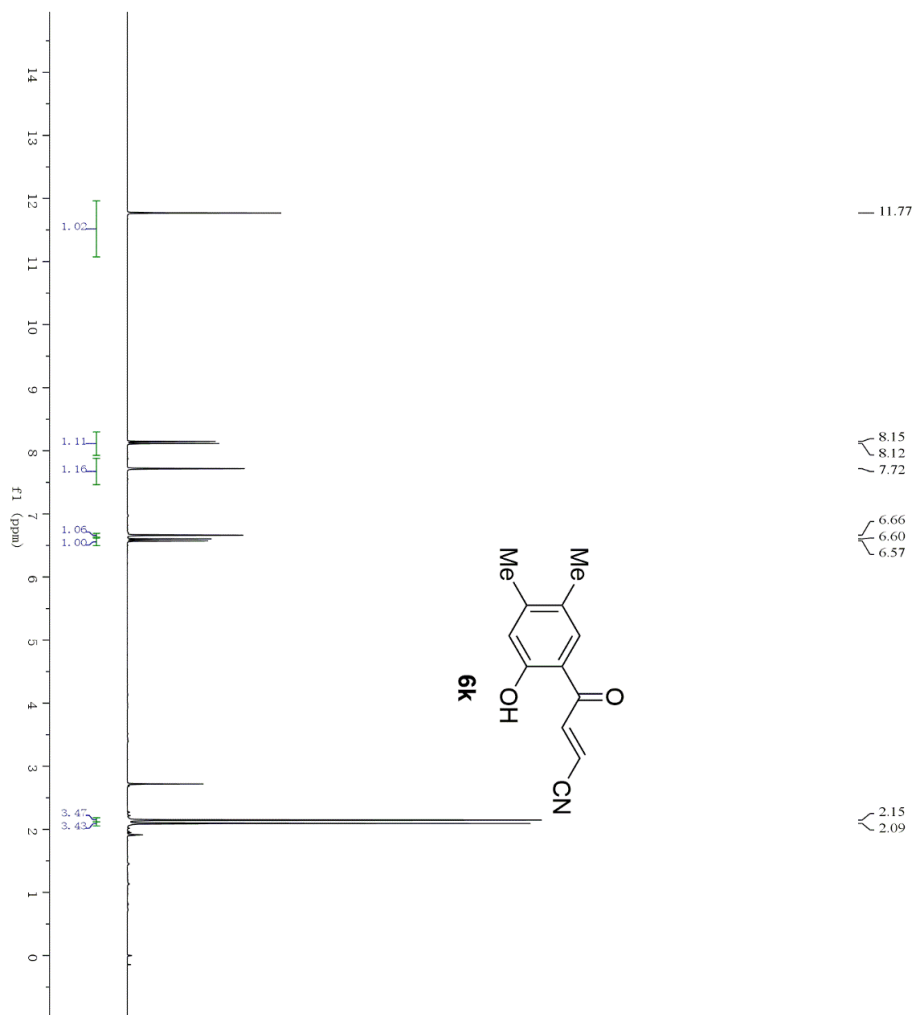
F2 - Processing Parameters
SI 32768

SF 125.7577420 MHz
WDW EM

SSB 0
LB 1.00 Hz

GB 0
PC 1.40





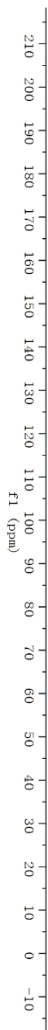
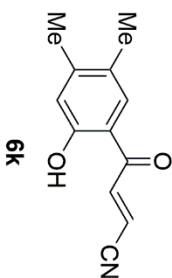
Current Data Parameters
NAME 500MHz-H-2018
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180326
Time 23.47
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLWL 20.00000000 W

F2 - Processing Parameters
SI 65536
SF 500.1300775 MHz
MDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

190.20
162.20
149.23
142.03
130.73
128.16
118.69
116.92
116.62
111.57

19.75
17.85



Current Data Parameters
NAME 500MHz-C-2018
EXPNO 27
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180327
Time 0.42
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.434131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22896000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

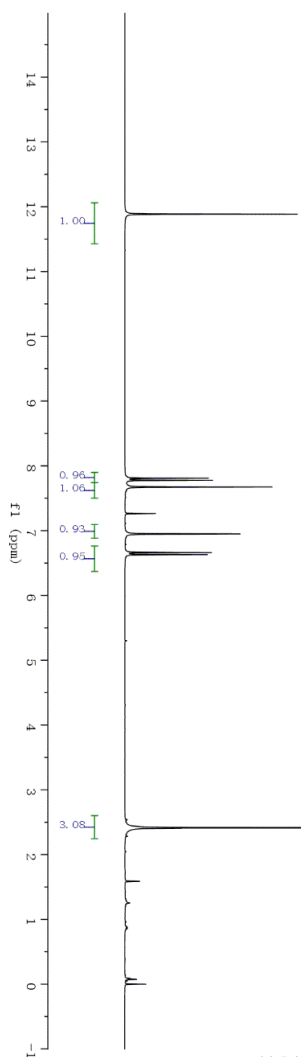
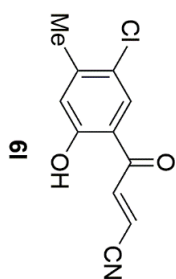
11.89
7.81
7.78
7.67
6.95
6.66
6.63

2.41

Current Data Parameters
NAME 500MHz-H-2018
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters

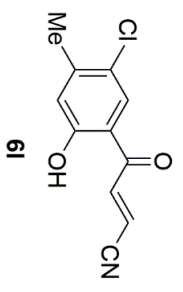
Date_ 20180407
Time 18.28
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SF01 500.1330685 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W



F2 - Processing Parameters
SI 65536
SF 500.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

188.65
 162.38
 148.05
 140.20
 129.18
 125.16
 120.95
 117.56
 115.98
 112.98

21.11



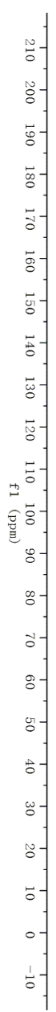
Current Data Parameters
 NAME 500MHz-C-2018
 EXPNO 30
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20180407
 Time 19:22
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SMH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

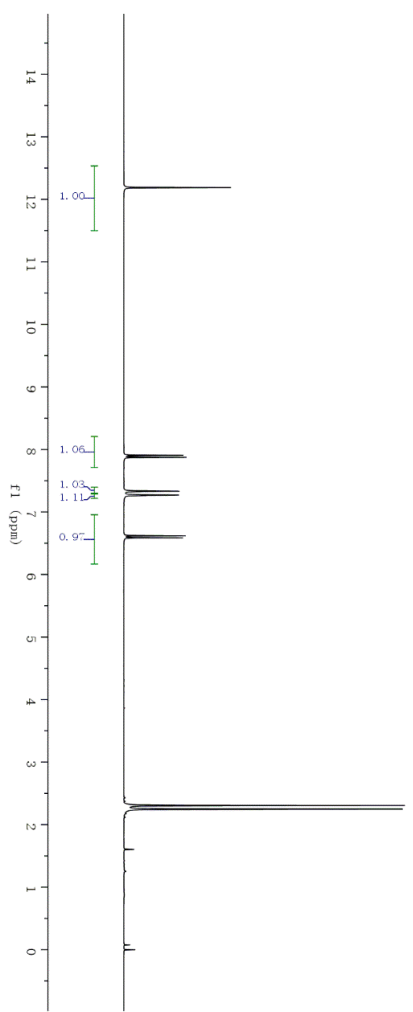
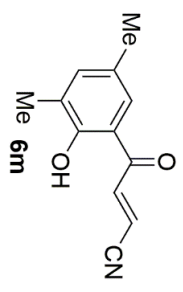
F2 - Processing parameters

SI 32768
 SF 125.757898 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



12.19
7.91
7.88
7.33
7.27
6.62
6.59

2.31
2.25



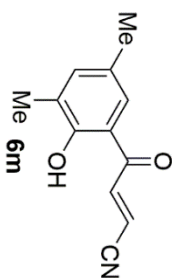
Current Data Parameters
NAME 500MHz-H-2018
EXPNO 38
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180410
Time 16.21
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276799 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TDO 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLM1 20.00000000 W

F2 - Processing Parameters
SI 65536
SF 500.1300114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

189.85
160.65
141.27
140.34
128.12
127.93
126.82
117.61
116.30
111.95

20.54
15.44



Current Data Parameters
NAME 500MHz-C-2018
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180410
Time 17.16
INSTRUM spect
PROBHD 5 mm CPBBO B5
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4

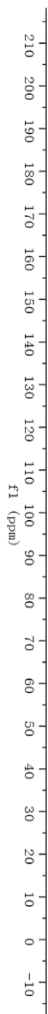
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89

DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLM1 57.00000000 W
SFO2 500.1320005 MHz
NUC2 1H

CPDPRG12 waltz16
PCPD2 80.00 usec
PLM2 20.00000000 W
PLM12 0.35778001 W
PLM13 0.22898000 W

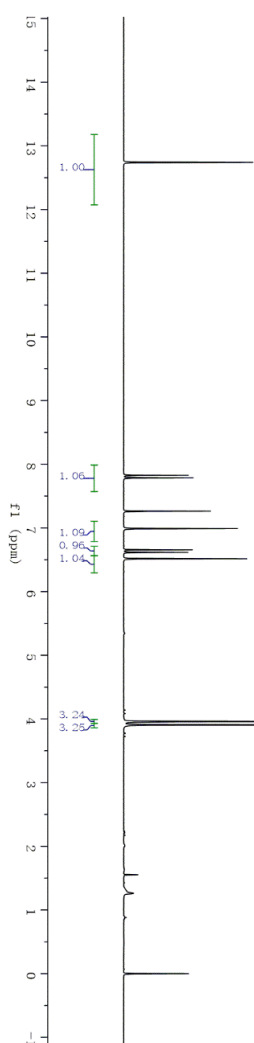
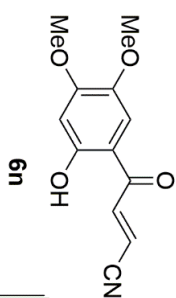
F2 - Processing parameters
SI 32768
SF 125.7577898 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



12.74

7.83
7.79
7.26
6.99
6.66
6.62
6.52

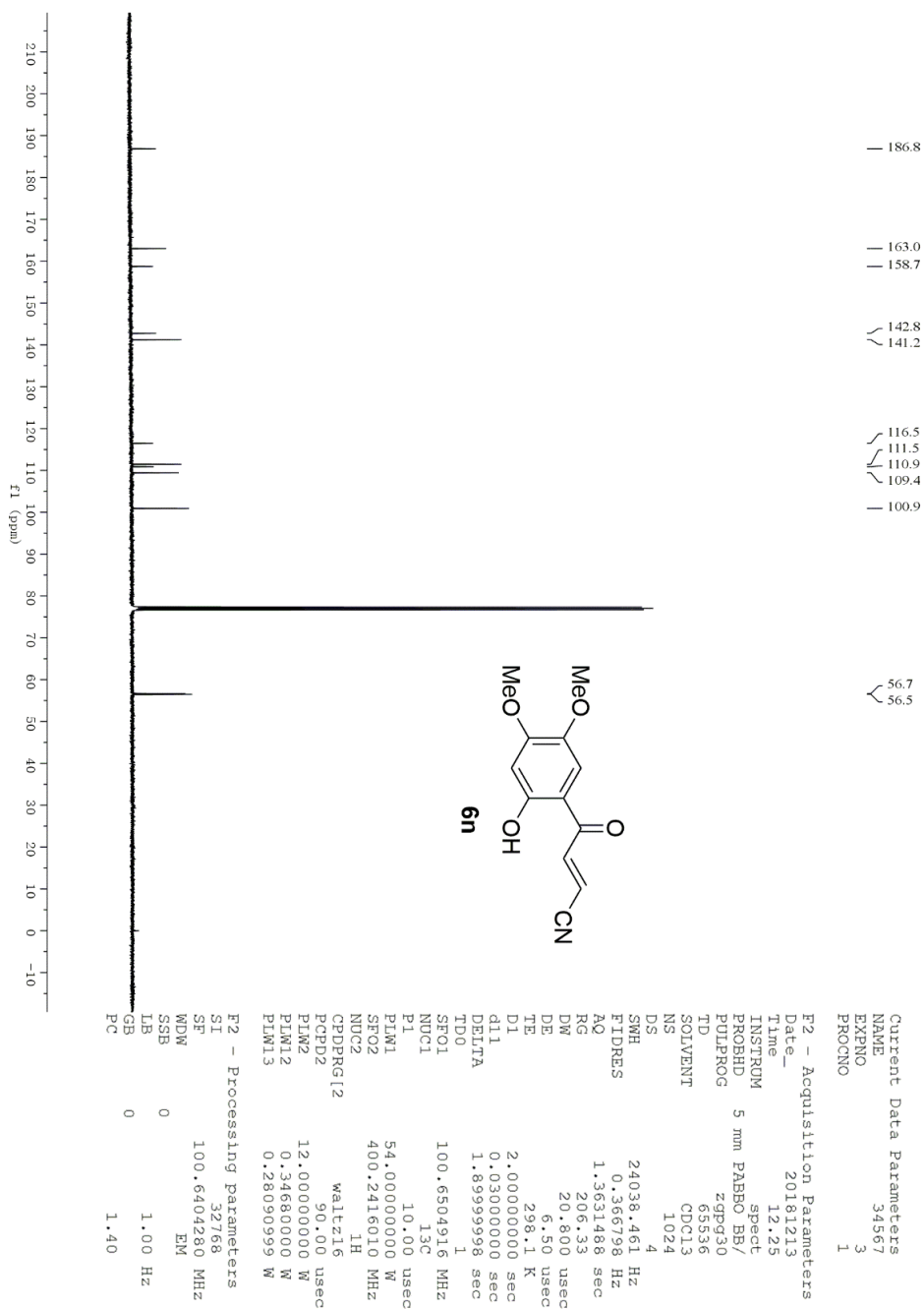
3.96
3.91



Current Data Parameters
NAME 45678
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181213
Time 11.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.047233 sec
RG 206.33
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
TDO 1
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

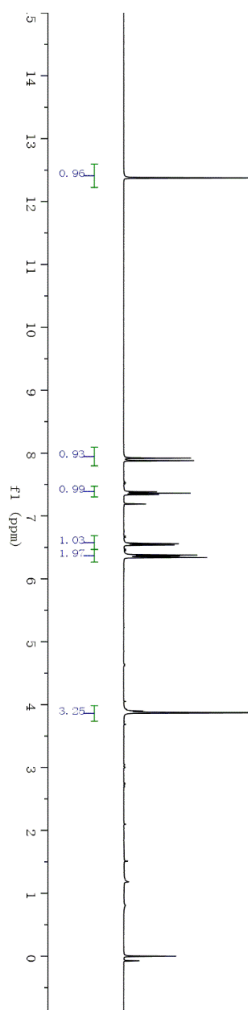
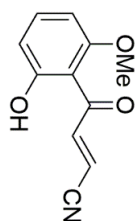
F2 - Processing parameters
SI 65536
SF 400.2400085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



12.38

7.92
7.88
7.38
7.36
7.34
6.56
6.54
6.38
6.36
6.34

3.87



Current Data Parameters
NAME 45678
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20181208
Time 21.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0

SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 206.33

DW 62.400 usec
DE 6.50 usec
TE 298.0 K

TD0 2.00000000 sec
D1 1

SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec

PLM1 12.00000000 W

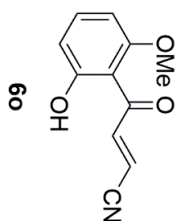
F2 - Processing parameters

SI 65536
SF 400.2400375 MHz

WDW EM
SSB 0

GB 0.30 Hz
PC 1.00

189.9
164.3
160.1
146.7
137.0
115.8
110.1
109.7
108.0
100.6
55.1



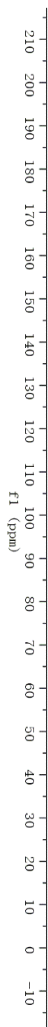
Current Data Parameters
NAME 34567
EXPNO 1
PROCNO 1

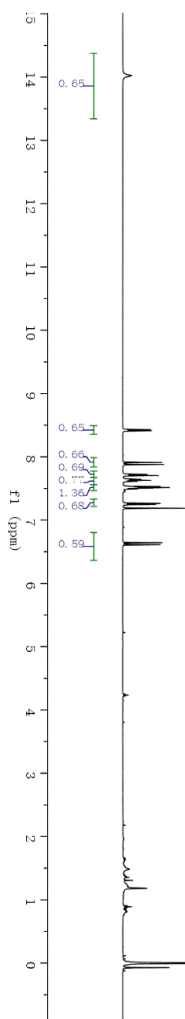
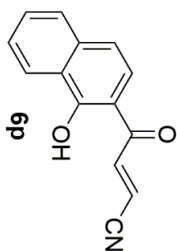
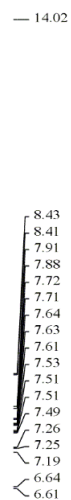
F2 - Acquisition Parameters

Date_ 20181208
Time 21:28
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 156
DS 4
SMH 29761.904 Hz
FIDRES 0.494131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLM1 57.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLM2 20.00000000 W
PLM12 0.35778001 W
PLM13 0.22898000 W

F2 - Processing parameters

SI 32768
SF 125.7579188 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME 500MHz-H-2018
EXPNO 35
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180407
Time 19.26
INSTRUM spect
PROBHD 5 mm CPEBBO BB
PULPROG zg30
TD 65536
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 62.06
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

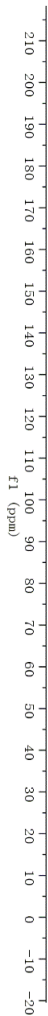
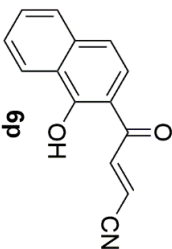
F2 - Processing parameters
SI 65536
SF 500.1300487 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

— 188.05
 — 164.70
 140.12
 136.94
 130.41
 126.63
 125.57
 124.10
 123.81
 121.95
 118.33
 115.33
 111.37
 110.99

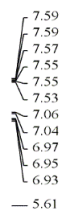
Current Data Parameters
 NAME 400MHz-C-2018
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20180405
 Time 15.02
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.36798 Hz
 AQ 1.363148 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W



F2 - Processing parameters
 SI 32768
 SF 100.6405328 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

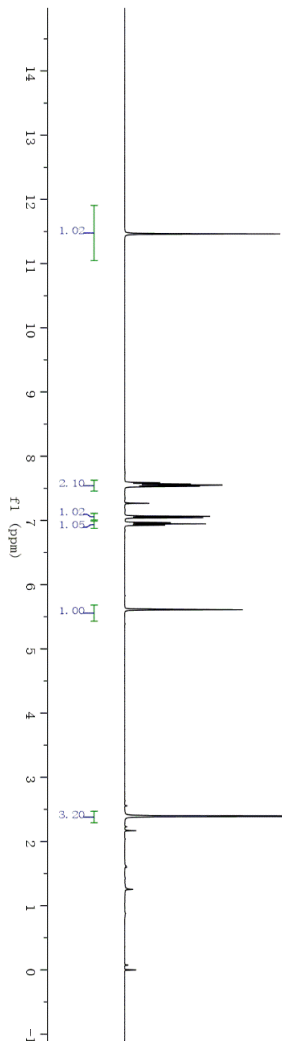
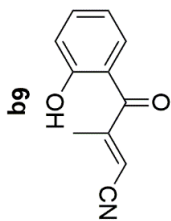


2.40

Current Data Parameters
NAME 400MHz-H-2019
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

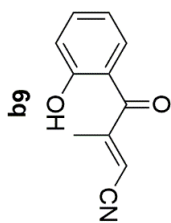
Date_ 20190106
Time 20.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
ID 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 73.9
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
SF01 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLM1 12.00000000 W



F2 - Processing parameters
SI 65536
SF 400.2400069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

199.7
163.5
157.0
137.9
131.9
119.4
119.0
117.2
114.8
103.8

19.0



Current Data Parameters
NAME 400MHz-C-2019
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190106
Time 20.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.36798 Hz
AQ 1.363148 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLM1 54.00000000 W
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLM2 12.00000000 W
PLM12 0.34680000 W
PLM13 0.28090999 W

F2 - Processing Parameters

SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

