

# Mechanism of Cobalt Oxazoline Palladacycle-Catalyzed Asymmetric Synthesis of Allylic Esters and Aryl Ethers

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## **Part 1. Experimental Procedures**

**General Procedures.** All reactions were carried out using oven-dried glassware under an atmosphere of Ar or N<sub>2</sub> unless otherwise indicated. [(*R*<sub>p</sub>,*S*)-COP-OAc]<sub>2</sub> (**4**), [(*R*<sub>p</sub>,*S*)-COP-NHCOCCl<sub>3</sub>]<sub>2</sub> (**6**) and [(*R*<sub>p</sub>,*S*)-COP-Cl]<sub>2</sub> (**5**) and their enantiomers were prepared according to published procedures.<sup>1</sup> Currently, both enantiomers of [(*R*<sub>p</sub>,*S*)-COP-OAc]<sub>2</sub> are commercially available from Aldrich Chemical Co. (661716 and 661708). Solid carboxylic acids were recrystallized from methanol. Acetic acid was distilled from acetic anhydride and CrO<sub>3</sub>. Tributyltin hydride was synthesized from lithium aluminum hydride and tributyltin chloride. Dichloromethane and diethyl ether were dried by passage through activated alumina using a GlassContour solvent purification system. Tetrahydrofuran (THF) was purified by distillation from sodium metal. Ethyl acetate was used without further purification from EMD Chemicals, Inc. All other commercial reagents were used as received unless otherwise noted. Analytical thin layer chromatography (TLC) was carried out using 0.25 mm silica plates purchased from Merck. Eluted plates were visualized using UV light and anisaldehyde stain. Silica gel chromatography was performed using 230–400 mesh silica gel purchased from Merck. Enantiomeric excess was determined by SFC analysis using columns with enantioselective stationary phases (Chiralcel<sup>®</sup> type columns) using a Mettler Toledo SFC. Racemic samples were used to calibrate enantioselective chromatographic analysis. Racemic mixtures of esters and aryl ethers were obtained by reaction of trichloroacetimidates with acids or phenols in the presence of palladium(II) acetate [0.5 M CH<sub>2</sub>Cl<sub>2</sub>, rt, 5 mol% Pd(OAc)<sub>2</sub>]. <sup>1</sup>H NMR (500 MHz) and <sup>13</sup>C NMR (125 MHz) spectra were obtained on Bruker FT NMR instruments. NMR spectra were reported

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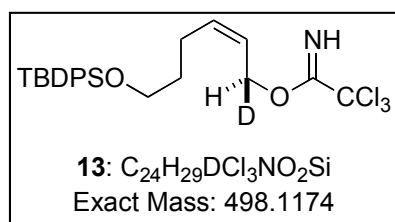
<sup>1</sup> (a) Anderson, C. E.; Kirsch, S. F.; Overman, L. E.; Richards, C. J.; Watson, M. P. *Org. Synth.* **2007**, *84*, 148–155 (b) Anderson, C. E.; Overman, L. E.; Richards, C. J.; Watson, M. P.; White, N. S. *Org. Synth.* **2007**, *84*, 139–147.

as  $\delta$  values in ppm relative to  $\text{CDCl}_3$  calibrated to 7.27 ppm in  $^1\text{H}$  NMR and 77.23 in  $^{13}\text{C}$  NMR. Splitting patterns are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), broad (b), apparent (app) and combinations thereof. Infrared (IR) spectra were obtained using a Varian 640-IR FT-IR spectrometer as thin films from  $\text{CHCl}_3$ . Optical rotations were obtained using a JASCO J-1010 digital polarimeter. High-resolution mass spectra (HRMS) were obtained using a Waters-MicroMass Analytical LCT (ESI) spectrometer.

Experimental details and spectral data for the preparation of imidates **1** ( $\text{R} = \text{Bn}$ ) can be found in the Supplementary Information that accompanies the article concerning scope and limitations.<sup>2</sup> (*Z*)-6-(*tert*-Butyldiphenylsilyloxy)-2-hexen-1-ol was synthesized according to the procedure of Baltas et al.<sup>3</sup> 4-(*tert*-Butyldiphenylsilyloxy)-butanoic acid was synthesized according to the procedure of Meyer et al.<sup>4</sup> Alkynoate **15** was synthesized according to the procedure of Deslongchamps et al.<sup>5</sup>

### General Procedure for Preparation of Allylic Trichloroacetimidates.

(*S*)-(Z)-6-(*tert*-Butyldiphenylsilyloxy)-1-deutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (**13**).



Allylic alcohol **21** (50 mg, 0.141 mmol) and trichloroacetonitrile (20  $\mu\text{L}$ , 0.169 mmol) were dissolved in dichloromethane (0.6 mL). 1,8-Diazabicyclo[5.4.0]undec-7-ene (1.2  $\mu\text{L}$ , 0.0085

<sup>2</sup> Cannon, J. S.; Kirsch, S. F.; Overman, L. E., previous paper in this issue.

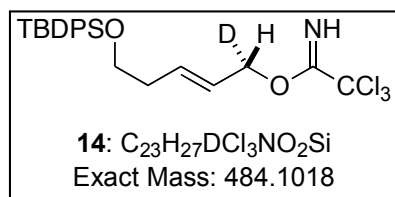
<sup>3</sup> Nacro, K.; Baltas, M.; Gorrichon, L. *Tetrahedron* **1999**, *55*, 14013–14030.

<sup>4</sup> Salit, A.-F.; Meyer, C.; Cossy, J.; Delouvrié, B.; Hennequin, L. *Tetrahedron* **2008**, *64*, 6684–6697.

<sup>5</sup> Hall, D. G.; Deslongchamps, P. *J. Org. Chem.* **1995**, *60*, 7796–7814.

mmol) was added, and the reaction mixture was maintained at room temperature for 1 h. The solution was then concentrated and the residue was purified by silica gel chromatography (1:4:95 triethylamine:ether:pentane) to provide 58 mg (82%) of **13** as a clear, colorless oil:  $R_f$  0.54 (25% EtOAc/hexanes);  $^1\text{H}$  NMR (500 MHz  $\text{CDCl}_3$ )  $\delta$  8.31 (s, 1H), 7.70 (d,  $J = 7.8$  Hz, 4H), 7.47–7.39 (m, 6H), 5.75–5.69 (m, 2H), 4.86 (d,  $J = 6.1$  Hz, 1H), 3.71 (t,  $J = 6.3$  Hz, 2H), 2.29 (q,  $J = 6.9$  Hz, 2H), 1.68 (quintet,  $J = 6.4$  Hz, 2H), 1.09 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  162.8, 135.9, 135.8, 134.1, 129.8, 127.8, 127.6, 123.2, 91.7, 65.1 (t,  $J_{\text{CD}} = 22.5$  Hz), 63.3, 32.5, 27.1, 24.3, 19.4;  $[\alpha]_{\text{D}}^{24} -0.11$ ,  $[\alpha]_{577}^{24} -0.29$ ,  $[\alpha]_{546}^{24} -0.27$ ,  $[\alpha]_{435}^{24} -0.58$ ,  $[\alpha]_{405}^{24} -0.56$  (c 3.33,  $\text{CHCl}_3$ ); IR (thin film) 3343, 3070, 2931, 2857, 1661  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{29}\text{DCl}_3\text{NO}_2\text{SiNa}$  ( $\text{M} + \text{Na}^+$ ) 521.1072, found 521.1066.

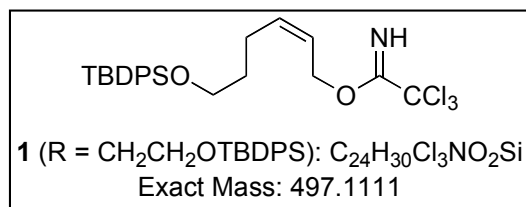
**(S)-(E)-6-(tert-Butyldiphenylsilyloxy)-1-deutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (14).**



Following the general procedure, **14** (113 mg, 82%) was obtained as a clear, colorless oil from **22** (101 mg, 0.284 mmol).  $R_f$  0.54 (25% EtOAc/hexanes);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$

8.28 (s, 1H), 7.68 (dd,  $J = 7.8, 1.3$  Hz, 4H), 7.44–7.37 (m, 6H), 5.86 (dt,  $J = 15.4, 6.7$  Hz, 1H), 5.68 (dd,  $J = 15.4, 6.2$  Hz, 1H), 4.71 (d,  $J = 6.1$  Hz, 1H), 3.69 (t,  $J = 6.3$  Hz, 2H), 2.21 (q,  $J = 7.1$  Hz, 2H), 1.68 (quintet,  $J = 6.4$  Hz, 2H), 1.06 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz  $\text{CDCl}_3$ )  $\delta$  162.8, 136.7, 135.8, 134.2, 129.8, 127.8, 123.5, 91.7, 69.9 (t,  $J_{\text{CD}} = 22.5$  Hz), 63.3, 31.9, 28.8, 27.1, 19.4;  $[\alpha]_{\text{D}}^{24} -0.09$ ,  $[\alpha]_{577}^{24} -0.25$ ,  $[\alpha]_{546}^{24} -0.34$ ,  $[\alpha]_{435}^{24} -0.53$ ,  $[\alpha]_{405}^{24} -0.88$  (c 1.03,  $\text{CHCl}_3$ ); IR (thin film) 3344, 3070, 2935, 1661  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{29}\text{Cl}_3\text{DO}_2\text{NSiNa}$  ( $\text{M} + \text{Na}^+$ ) 521.1072, found 521.1076.

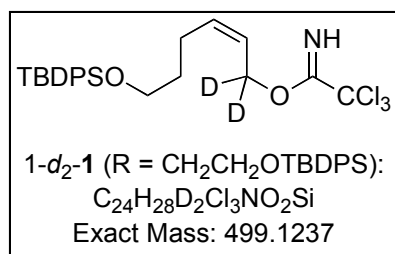
**(Z)-6-(tert-Butyldiphenylsilyloxy)-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (1 (R = CH<sub>2</sub>CH<sub>2</sub>OTBDPS)).**



Following the general procedure, **1** (R = CH<sub>2</sub>CH<sub>2</sub>OTBDPS) (1.07 g, 88%) was obtained as a clear, colorless oil from (Z)-6-(tert-

Butyldiphenylsilyloxy)-2-hexen-1-ol (865 mg, 2.44 mmol): R<sub>f</sub> 0.54 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 8.33 (s, 1H), 7.73 (d, *J* = 7.8 Hz, 4H), 7.48–7.41 (m, 6H), 5.76–5.69 (m, 2H), 4.90 (d, *J* = 6.1 Hz, 2H), 3.74 (t, *J* = 6.3 Hz), 2.30 (q, *J* = 6.9 Hz, 2H), 1.70 (quintet, *J* = 6.4 Hz, 2H), 1.12 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 162.8, 135.9, 135.8, 134.1, 129.8, 127.8, 123.2, 91.7, 65.3, 63.3, 32.5, 27.1, 24.3, 19.4; IR (thin film) 3343, 3070, 2931, 2857, 1661 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>24</sub>H<sub>30</sub>Cl<sub>3</sub>NO<sub>2</sub>SiNa (M + Na<sup>+</sup>) 520.1009, found 520.1003.

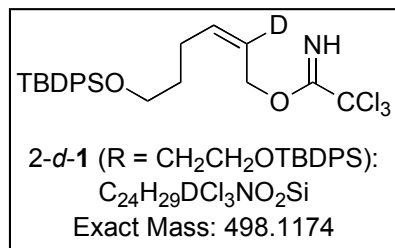
**(Z)-6-(tert-Butyldiphenylsilyloxy)-1,1-dideutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (1-*d*<sub>2</sub>-1 (R = CH<sub>2</sub>CH<sub>2</sub>OTBDPS)).**



Following the general procedure, 1-*d*<sub>2</sub>-1 (R = CH<sub>2</sub>CH<sub>2</sub>OTBDPS) (555 mg, 87%) was obtained as a clear, colorless oil from **17** (454 mg, 1.27 mmol): R<sub>f</sub> 0.54 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 8.37 (s, 1H), 7.77 (d, *J* = 7.8 Hz, 4H), 7.51–

7.45 (m, 6H), 5.82–5.74 (m, 2H, C<sub>2</sub>H, C<sub>3</sub>H), 3.78 (t, *J* = 6.3 Hz, 2H), 2.35 (q, *J* = 6.9 Hz, 2H), 1.75 (quintet, *J* = 6.4 Hz, 2H), 1.17 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 162.9, 135.9, 135.9, 134.1, 129.8, 127.8, 123.1, 91.7, 64.6 (quintet, *J*<sub>CD</sub> = 22.6 Hz), 63.3, 32.4, 27.1, 24.3, 19.4; IR (thin film) 3345, 3071, 2933, 2859, 1665 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>24</sub>H<sub>28</sub>D<sub>2</sub>Cl<sub>3</sub>NO<sub>2</sub>SiNa (M + Na<sup>+</sup>) 522.1135, found 522.1124.

**(Z)-6-(tert-Butyldiphenylsilyloxy)-2-deutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (2-d-1 (R=CH<sub>2</sub>CH<sub>2</sub>OTBDPS)).**

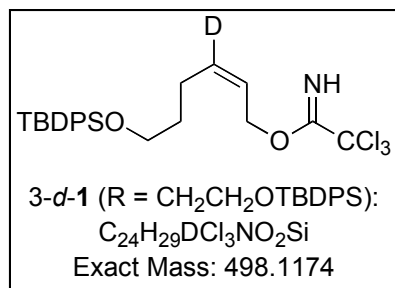


Following the general procedure, 2-d-1 (R = CH<sub>2</sub>CH<sub>2</sub>OTBDPS)

(64 mg, 91%) was obtained as a clear, colorless oil from **S12** (50 mg, 0.141 mmol): R<sub>f</sub> 0.54 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 8.29 (s, 1H), 7.68 (d, *J* = 7.8 Hz, 4H), 7.46–7.38

(m, 6H), 5.72 (t, *J* = 7.6 Hz, 1H), 4.86 (s, 2H), 3.70 (t, *J* = 6.3 Hz, 2H), 2.27 (q, *J* = 6.9 Hz, 2H), 1.66 (quintet, *J* = 6.4 Hz, 2H), 1.07 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 162.9, 135.8, 135.7, 134.1, 129.8, 127.8, 122.9 (t, *J*<sub>CD</sub> = 23.8 Hz), 91.7, 65.3, 63.4, 32.5, 27.1, 24.3, 19.4; IR (thin film) 3344, 3071, 2932, 2858, 1664 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>24</sub>H<sub>29</sub>DCl<sub>3</sub>NO<sub>2</sub>SiNa (M + Na<sup>+</sup>) 521.1072, found 521.1089.

**(Z)-6-(tert-Butyldiphenylsilyloxy)-3-deutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (3-d-1 (R = CH<sub>2</sub>CH<sub>2</sub>OTBDPS)).**



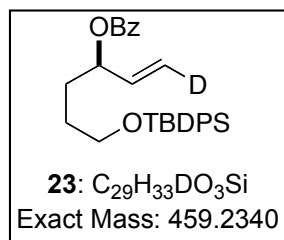
Following the general procedure, 3-d-1 (R = CH<sub>2</sub>CH<sub>2</sub>OTBDPS)

(469 mg, 80%) was obtained as a clear, colorless oil from **S8** (415 mg, 1.17 mmol): R<sub>f</sub> 0.54 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 8.29 (s, 1H), 7.68 (d, *J* = 7.8 Hz, 4H), 7.46–

7.38 (m, 6H), 5.68 (t, *J* = 6.7 Hz, 1H), 4.86 (d, *J* = 6.1 Hz, 2H), 3.70 (t, *J* = 6.3 Hz, 2H), 2.27 (q, *J* = 6.9 Hz, 2H), 1.67 (quintet, *J* = 6.4 Hz, 2H), 1.07 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 162.9, 135.8, 135.5 (t, *J*<sub>CD</sub> = 23.8 Hz), 134.1, 129.8, 127.8, 123.1, 91.7, 65.4, 63.4, 32.5, 27.1, 24.3, 19.4; IR (thin film) 3344, 3071, 2932, 2858, 1664 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>24</sub>H<sub>29</sub>DCl<sub>3</sub>NO<sub>2</sub>SiNa (M + Na<sup>+</sup>) 521.1072, found 521.1068.

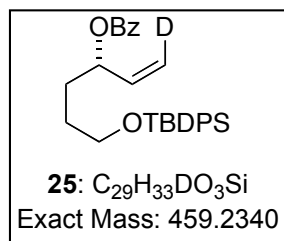
## General Procedure for Preparation of Enantioenriched Allylic Esters.

### (*R*)-(*E*)-6-(*tert*-Butyldiphenylsilyloxy)-1-deutero-1-hexen-3-yl Benzoate (**23**).



Imidate **13** (20 mg, 0.040 mmol) and benzoic acid (15 mg, 0.120 mmol) were dissolved in dichloromethane (0.1 mL). The flask was protected from light, and [(*R<sub>p</sub>*,*S*)-COP-OAc]<sub>2</sub> (0.6 mg, 0.00040 mmol) was added. After 17 h, ethylenediamine (0.1 mL) was added. The crude reaction mixture was concentrated under reduced pressure, and the residue was purified by silica gel chromatography (10% ether/hexanes) to give 16 mg (89%) of **23** as a clear, colorless oil. The *E*:*Z*-ratio was calculated as 83:17 using <sup>1</sup>H NMR spectroscopy: R<sub>f</sub> = 0.49 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.07 (d, *J* = 7.2 Hz, 2H), 7.67 (d, *J* = 6.9 Hz, 4H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.47–7.36 (m, 8H), 5.89 (dd, *J* = 17.2, 6.1 Hz, 1H), 5.52 (q, *J* = 6.3 Hz, 1H), 5.31 (d, *J* = 17.2 Hz, 1H), 3.72 (t, *J* = 6.3 Hz, 2H), 1.88 (q, *J* = 7.4 Hz, 2H), 1.74–1.65 (m, 2H), 1.06 (s, 9H); <sup>13</sup>C NMR (125 MHz CDCl<sub>3</sub>) δ 166.0, 136.6, 135.8, 134.1, 133.1, 130.7, 129.81, 129.78, 128.5, 127.8, 116.6 (t, *J*<sub>CD</sub> = 23.8 Hz), 75.3, 63.7, 30.9, 28.4, 27.1, 19.4; [α]<sub>D</sub><sup>24</sup> -14.3, [α]<sub>577</sub><sup>24</sup> -15.0, [α]<sub>546</sub><sup>24</sup> -16.8, [α]<sub>435</sub><sup>24</sup> -34.1, [α]<sub>405</sub><sup>24</sup> -44.3 (*c* 0.81, CHCl<sub>3</sub>); IR (thin film) 3070, 2930, 2857, 1720, 1601 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>29</sub>H<sub>33</sub>O<sub>3</sub>DSiNa (M + Na<sup>+</sup>) 482.2238, found 482.2240.

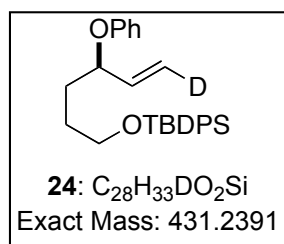
### (*S*)-(*Z*)-6-(*tert*-Butyldiphenylsilyloxy)-1-deutero-1-hexen-3-yl Benzoate (**25**).



Following the general procedure, **25** (16 mg, 89%) was obtained as a clear, colorless oil when **13** (20 mg, 0.040 mmol) was allowed to react with benzoic acid (15 mg, 0.120 mmol) and [(*S<sub>p</sub>*,*R*)-COP-OAc]<sub>2</sub>. The *E*:*Z*-ratio was calculated as 17:83 using <sup>1</sup>H NMR spectroscopy: R<sub>f</sub> = 0.49

(25% EtOAc/hexanes);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 7.2$  Hz, 2H), 7.67 (d,  $J = 6.9$  Hz, 4H), 7.57 (t,  $J = 7.4$  Hz, 1H), 7.47–7.36 (m, 8H), 5.91–5.87 (m, 1H), 5.53 (q,  $J = 6.3$  Hz, 1H), 5.20 (d,  $J = 10.6$  Hz, 1H), 3.72 (t,  $J = 6.3$  Hz, 2H), 1.88 (q,  $J = 7.4$  Hz, 2H), 1.74–1.65 (m, 2H), 1.06 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz  $\text{CDCl}_3$ )  $\delta$  166.0, 136.6, 135.8, 134.1, 133.1, 130.7, 129.81, 129.78, 128.6, 127.8, 116.6 (t,  $J_{\text{CD}} = 23.8$  Hz), 75.3, 63.7, 30.9, 28.4, 27.1, 19.4;  $[\alpha]_{\text{D}}^{24}$  17.1,  $[\alpha]_{577}^{24}$  17.9,  $[\alpha]_{546}^{24}$  22.3,  $[\alpha]_{435}^{24}$  29.8 ( $c$  1.62,  $\text{CHCl}_3$ ); IR (thin film) 3070, 2930, 2857, 1720, 1601  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{29}\text{H}_{33}\text{O}_3\text{DSiNa}$  ( $\text{M} + \text{Na}^+$ ) 482.2238, found 482.2231.

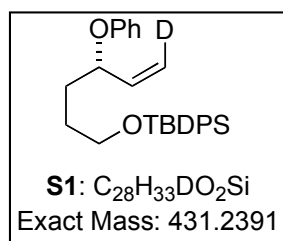
**(*R*)-Phenyl (*E*)-6-(*tert*-Butyldiphenylsilyloxy)-1-deutero-1-hexen-3-yl Ether (**24**).**



Following the general procedure, **24** (13 mg, 50%) was obtained as a clear, colorless oil when **13** (30 mg, 0.060 mmol) was allowed to react with phenol (17 mg, 0.18 mmol) and  $[(R_p, S)\text{-COP-OAc}]_2$ . The *E*:*Z*-ratio was calculated as 92:6 using  $^1\text{H}$  NMR spectroscopy:  $R_f$  0.64 (25% EtOAc/hexanes);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J = 7.9$  Hz, 4 H), 7.43 (t,  $J = 7.2$  Hz, 2H), 7.38 (t,  $J = 8.1$  Hz, 4H), 7.25 (t,  $J = 8.4$  Hz, 2H), 6.92 (t,  $J = 7.3$  Hz, 1H), 6.88 (d,  $J = 8.1$  Hz, 2H), 5.84 (dd,  $J = 17.3, 6.1$  Hz, 1H), 5.23 (d,  $J = 17.3$  Hz, 1H), 4.61 (q,  $J = 6.1$  Hz, 1H), 3.71 (t,  $J = 6.2$  Hz, 2H), 1.89–1.68 (m, 4H), 1.06 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz  $\text{CDCl}_3$ )  $\delta$  158.5, 138.1, 135.8, 134.2, 129.8, 129.5, 127.8, 120.9, 116.3 (t,  $J_{\text{CD}} = 23.8$  Hz), 116.2, 78.7, 63.8, 32.1, 28.5, 27.1, 19.4;  $[\alpha]_{\text{D}}^{25}$  1.20,  $[\alpha]_{435}^{25}$  5.81 ( $c$  0.89,  $\text{CHCl}_3$ ) IR (thin film) 3068, 2935, 1962, 1595  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{28}\text{H}_{33}\text{O}_2\text{DSiNa}$  ( $\text{M} + \text{Na}^+$ ) 454.2289, found 454.2279.

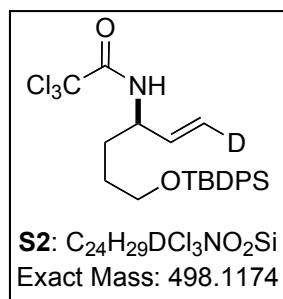


**(S)-Phenyl (Z)-6-(tert-butyldiphenylsilyloxy)-1-deutero-1-hexen-3-yl Ether (S1).**



Following the general procedure, **S1** (19 mg, 73%) was obtained as a clear, colorless oil when **13** (30 mg, 0.060 mmol) was allowed to react with phenol (17 mg, 0.18 mmol) and [(Sp,R)-COP-OAc]<sub>2</sub>. The *E*:*Z*-ratio was calculated as 7:92 using <sup>1</sup>H NMR spectroscopy: R<sub>f</sub> 0.64 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.69 (d, *J* = 7.8 Hz, 4H), 7.45 (t, *J* = 6.1 Hz, 2H), 7.40 (t, *J* = 8.2 Hz, 4H), 7.27 (t, *J* = 6.0 Hz, 2H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 2H), 5.86 (m, 1H), 5.20 (d, *J* = 10.6 Hz, 1H), 4.64 (q, *J* = 6.1 Hz, 1H), 3.74 (t, *J* = 6.2 Hz, 2H), 1.91–1.69 (m, 4H), 1.08 (s, 9H); <sup>13</sup>C NMR (125 MHz CDCl<sub>3</sub>) δ 158.5, 138.1, 135.8, 134.2, 129.8, 129.5, 127.8, 120.9, 116.3 (t, *J*<sub>CD</sub> = 23.8 Hz), 116.2, 78.7, 63.8, 32.1, 28.5, 27.1, 19.4; [α]<sub>D</sub><sup>25</sup> -1.53, [α]<sub>435</sub><sup>25</sup> -3.60 (*c* 0.89, CHCl<sub>3</sub>); IR (thin film) 3068, 2935, 1962, 1595 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>28</sub>H<sub>33</sub>O<sub>2</sub>DSiNa (M + Na<sup>+</sup>) 454.2289, found 454.2294.

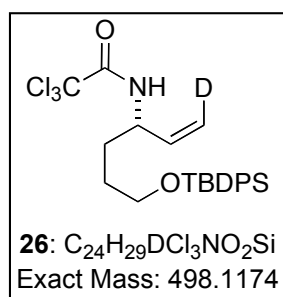
**(R)-2',2',2'-Trichloro-N-((E)-6-(tert-butyldiphenylsilyloxy)-1-deutero-hex-1-en-3-yl)acetamide (S2).**



Following the general procedure, **S2** (38 mg, 76%) was obtained as a clear, colorless oil when **14** (50 mg, 0.10 mmol) was allowed to react with [(Sp,R)-COP-Cl]<sub>2</sub>. The *E*:*Z*-ratio was calculated as 89:11 using <sup>1</sup>H NMR spectroscopy. Enantioselective SFC analysis indicated a 96% enantiomeric excess [ODH column; flow: 0.8 mL/min; 10% isopropanol/90% CO<sub>2</sub>; 230 nm; major enantiomer, *t*<sub>R</sub> = 19.5 min, minor enantiomer, *t*<sub>R</sub> = 20.4 min]; R<sub>f</sub> 0.46 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.67 (d, *J* = 6.6 Hz, 4H), 7.46–7.38 (m, 6H), 6.54 (d, *J* = 8.1 Hz, 1H), 5.81 (dd, *J* = 17.2, 7.8 Hz, 1H), 5.23 (d, *J* = 17.2

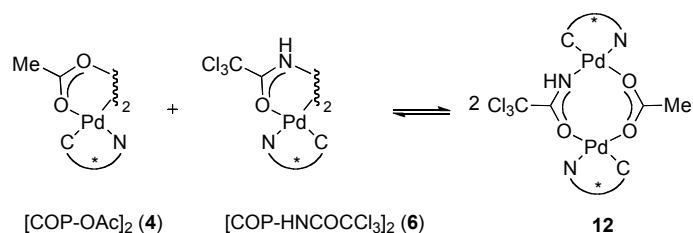
Hz, 1H), 4.44 (q,  $J = 7.0$  Hz, 1H), 3.74–3.70 (m, 2H), 1.85–1.80 (m, 1H), 1.71–1.61 (m, 3H), 1.07 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz  $\text{CDCl}_3$ )  $\delta$  161.4, 136.7, 135.7, 133.9, 129.9, 127.9, 116.1 (t,  $J_{\text{CD}} = 25.0$  Hz), 93.0, 63.3, 53.5, 31.0, 28.8, 27.1, 19.4;  $[\alpha]_{\text{D}}^{24} -8.40$ ,  $[\alpha]_{577}^{24} -8.54$ ,  $[\alpha]_{546}^{24} -9.73$ ,  $[\alpha]_{435}^{24} -16.0$ ,  $[\alpha]_{405}^{24} -18.9$  ( $c$  2.04,  $\text{CHCl}_3$ ); IR (thin film) 3421, 3327, 3070, 2930, 2857, 1695, 1514  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{29}\text{DCl}_3\text{NO}_2\text{SiNa}$  ( $\text{M} + \text{Na}^+$ ) 521.1072, found 521.1063.

**(S)-2',2',2'-Trichloro-N-((Z)-6-(*tert*-butyldiphenylsilyloxy)-1-deutero-hex-1-en-3-yl)acetamide (26).**

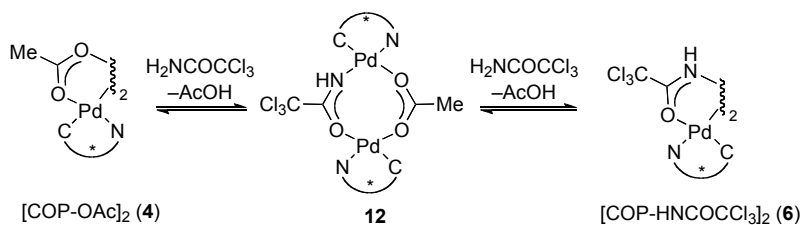


Following the general procedure, **26** (43 mg, 86%) was obtained as a clear, colorless oil when **14** (50 mg, 0.10 mmol) was allowed to react with  $[(R_p,S)\text{-COP-HNCOCCl}_3]_2$ . The *E:Z*-ratio was calculated as 7:93 using  $^1\text{H}$  NMR spectroscopy. Enantioselective SFC analysis indicated a 96% enantiomeric excess [ODH column; flow: 0.8 mL/min; 10% isopropanol/90%  $\text{CO}_2$ ; 230 nm; minor enantiomer,  $t_{\text{R}} = 19.5$  min, major enantiomer,  $t_{\text{R}} = 20.4$  min]:  $R_{\text{f}}$  0.46 (25% EtOAc/hexanes);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J = 6.5$  Hz, 4H), 7.47–7.38 (m, 6H), 6.55 (d,  $J = 7.8$  Hz, 1H), 5.82–5.79 (m, 1H), 5.20 (d,  $J = 10.5$  Hz, 1H), 4.45 (q,  $J = 7.0$  Hz, 1H), 3.74–3.71 (m, 2H), 1.84–1.80 (m, 1H), 1.71–1.62 (m, 3H), 1.08 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz  $\text{CDCl}_3$ )  $\delta$  161.4, 136.7, 135.7, 133.9, 129.9, 127.9, 116.1 (t,  $J_{\text{CD}} = 23.8$  Hz), 93.0, 63.3, 53.5, 31.0, 28.8, 27.1, 19.4;  $[\alpha]_{\text{D}}^{24} 8.34$ ,  $[\alpha]_{577}^{24} 9.07$ ,  $[\alpha]_{546}^{24} 10.4$ ,  $[\alpha]_{435}^{24} 16.2$  ( $c$  2.44,  $\text{CHCl}_3$ ); IR (thin film) 3421, 3328, 3070, 2931, 2857, 1694, 1514  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{29}\text{DCl}_3\text{NO}_2\text{SiNa}$  ( $\text{M} + \text{Na}^+$ ) 521.1072, found 521.1066.

## Representative Experimental Procedures Employed to Explore Catalyst Equilibria.

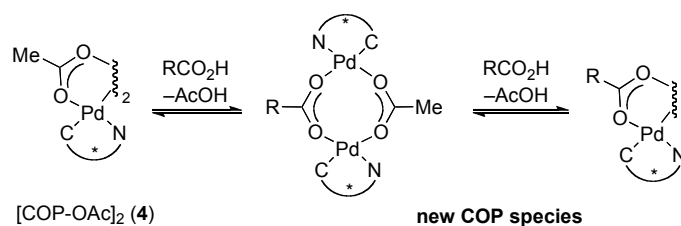


A solution of palladacycles **4** (4.2 mg,  $2.8 \times 10^{-3}$  mmol) and **6** (4.9 mg,  $2.8 \times 10^{-3}$  mmol) in  $\text{CD}_2\text{Cl}_2$  (0.6 mL) in an NMR tube was maintained at room temperature for 4 h. Integrations of the acetate peaks of **4** and **12** and the amidate peak of **6** using  $^1\text{H}$  NMR spectroscopy found the concentrations of **4**, **12**, and **6** to be  $2.07 \times 10^{-3}$  M,  $4.55 \times 10^{-3}$  M, and  $2.69 \times 10^{-3}$  M respectively. See page S93 for a representative spectrum.



In a separate experiment, a solution of palladacycle **4** (8.4 mg,  $5.6 \times 10^{-3}$  mmol) and trichloroacetamide (1.8 mg,  $1.1 \times 10^{-3}$  mmol) in  $\text{CD}_2\text{Cl}_2$  (0.6 mL) in an NMR tube was maintained at room temperature for 15 h. Integrations of the acetate peaks of **4** and **12** and the amidate peak of **6** using  $^1\text{H}$  NMR spectroscopy found the concentrations of **4**, **12**, and **6** to be  $2.16 \times 10^{-3}$  M,  $2.81 \times 10^{-3}$  M, and  $4.32 \times 10^{-3}$  M respectively. See page S94 for a representative spectrum.

**Representative Experimental Procedure for the Investigation of New Palladium Species Formed by the Reaction of [COP-OAc]<sub>2</sub> with Carboxylic Acids.**



Palladacycle **4** (8.4 mg,  $5.6 \times 10^{-3}$  mmol) was added to a solution of benzoic acid (1.3 mg, 0.011 mmol) in CD<sub>2</sub>Cl<sub>2</sub> (0.6 mL) in an NMR tube. <sup>1</sup>H NMR spectroscopy determined the ratio of **4** to other COP species to be 1:10.8. See spectra on pages S95–S97 for an explanation of how these ratios were calculated.

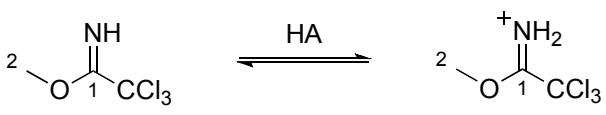
**Determination of Enantiomeric Excess as a Function of Time .**

[(*R<sub>p</sub>*,*S*)-COP-OAc]<sub>2</sub> (**4**) (10 mg, 0.0065 mmol) was added to a solution of **1** (R = Bn) (200 mg, 0.65 mmol) and benzoic acid (0.24 g, 2.0 mmol) in dichloromethane (1.3 mL). At reaction times of 1, 2, 3, 5, 10, and 25 h, a 0.08 mL aliquot was removed, diluted with pentane, treated with ethylenediamine (0.1 mL), and passed through a short plug of silica gel. The eluent was concentrated and % conversion and enantiomeric excess of was determined by enantioselective HPLC against methoxynaphthalene as an internal standard [OJ column, 0.1% isopropanol in heptanes, major enantiomer  $t_R = 40.9$  min, minor enantiomer  $t_R = 25.1$  min, internal standard  $t_R = 72.7$  min].

## Estimation of the $pK_a$ of Methyl Trichloroacetimidate Conjugate Acid

Four samples of methyl trichloroacetimidate (30 mg, 0.17 mmol) were each dissolved in  $CD_2Cl_2$  (0.7 mL) in an NMR tube. To each sample was added one of the following carboxylic acids: acetic acid (0.01 mL, 0.17 mmol), chloroacetic acid (16 mg, 0.17 mmol), dichloroacetic acid (0.014 mL, 0.17 mmol), trifluoroacetic acid (0.013 mL, 0.17 mmol). A  $^1H$  NMR and  $^{13}C$  NMR spectrum was obtained for each. Key peaks are compiled in Table S 1

**Table S 1** Chemical Shifts of Key Peaks of Methyl Trichloroacetimidate When Mixed with Carboxylic Acids in  $CD_2Cl_2$

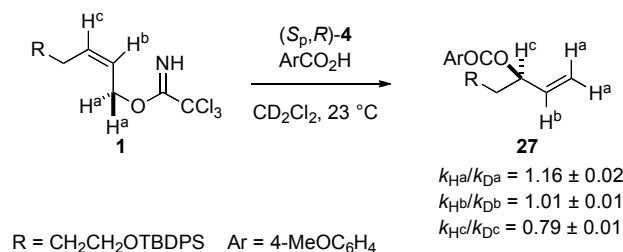


Acid ( $pK_a$ )	Carbon 1		Carbon 2
	$^{13}C$ NMR	$^1H$ NMR	$^{13}C$ NMR
no acid	163.9	3.93	57.0
Acetic acid (4.8)	164.0	3.93	57.0
Chloroacetic acid (2.9)	164.4	3.94	57.2
Dichloroacetic acid (1.3)	165.2	3.99	57.6
Trifluoroacetic acid (-0.3)	167.1	4.10	59.1

Assuming that trifluoroacetic acid fully protonates methyl trichloroacetimidate, dichloroacetic acid provides a 60:40 ratio of methyl imidate to its conjugate acid. Therefore, the  $pK_a$  should be

defined as:  $\frac{40}{60} = 10^{pK_a-1.3}$ . As a result, the  $pK_a$  is estimated to be  $\sim 1.1$ .

## Representative Experimental Procedure for Measuring Kinetic Isotope Effects.

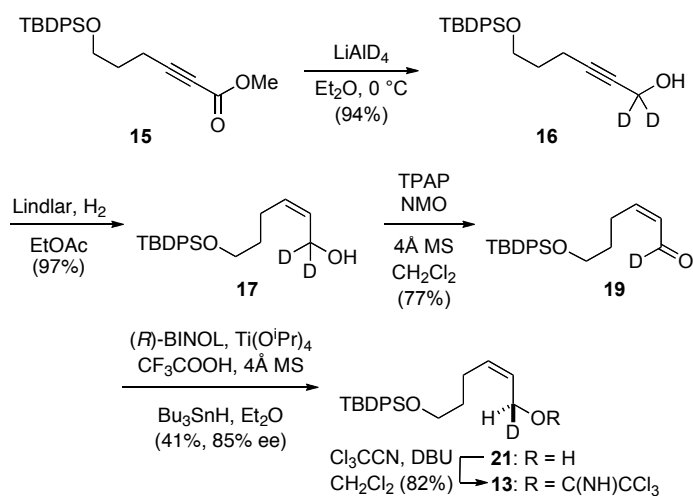


Allylic imidates **1** ( $\text{R} = \text{CH}_2\text{CH}_2\text{OTBDPS}$ ) (5 mg, 0.010 mmol) and 1- $d_2$ -**1** (5 mg, 0.010 mmol) were dissolved in  $\text{CD}_2\text{Cl}_2$  (0.6 mL) in an NMR tube. A  $^1\text{H}$  NMR spectrum was obtained and the  $d_0:d_1$  ratio was determined to be 1.15:1.00. To this solution was added *para*-methoxybenzoic acid (0.6 mg, 0.004 mmol) and [( $R_p, S$ )-COP-OAc]<sub>2</sub> (**4**) (1.5 mg, 0.001 mmol). The solution was protected from light and maintained at room temperature for 15 h. The solution was then treated with ethylenediamine (0.1 mL), concentrated and the residue was chromatographed ( $\text{SiO}_2$ , 5%  $\text{Et}_2\text{O}/95\%$  pentane) to produce 1.5 mg (77%) of **27** as a clear, colorless oil.  $^1\text{H}$  NMR analysis of **27** showed a  $d_0:d_2$  ratio of 1.27:1.00 or a  $k_{\text{H}}/k_{\text{D}}$  of 1.10. Data for all KIE determination experiments are summarized in Table S 2. Representative spectra for determination of KIE's can be found on pages S97–S102. Characterization data for non-deuterated **27**:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02 (d,  $J = 8.8$  Hz, 2H), 7.68 (d,  $J = 7.7$  Hz, 4H), 7.45–7.36 (m, 6H), 6.93 (d,  $J = 8.8$  Hz, 2H), 5.90 (ddd,  $J = 16.8, 10.6, 6.1$  Hz, 1H), 5.50 (q,  $J = 6.2$  Hz, 1H), 5.32 (d,  $J = 17.3$  Hz, 1H), 5.21 (d,  $J = 10.6$  Hz, 1H), 3.88 (s, 3H), 3.72 (t,  $J = 6.3$  Hz, 2H), 1.87 (q,  $J = 6.9$  Hz, 2H), 1.73–1.65 (m, 2H), 1.07 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz  $\text{CDCl}_3$ )  $\delta$  165.8, 163.5, 136.9, 135.8, 134.1, 131.8, 129.8, 127.8, 123.2, 116.7, 113.8, 74.9, 63.7, 55.6, 30.9, 28.4, 27.1, 19.4;  $[\alpha]_{\text{D}}^{24} -14.7$ ,  $[\alpha]_{577}^{24} -16.2$ ,  $[\alpha]_{546}^{24} -18.8$ ,  $[\alpha]_{435}^{24} -36.7$ ,  $[\alpha]_{405}^{24} -46.1$  ( $c$  2.70,  $\text{CHCl}_3$ ); IR (thin film) 3070, 3049, 2955, 2931, 2041, 1713  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{30}\text{H}_{36}\text{O}_4\text{SiNa}$  ( $\text{M} + \text{Na}^+$ ) 511.2281, found 511.2275.

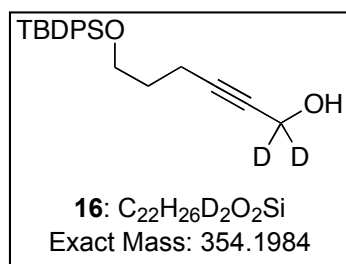
**Table S 2.** Collected Data for Determination of Secondary Kinetic Isotope Effects

entry	site	1: <i>d</i> -1	27: <i>d</i> -27	$k_H/k_D$	Average	Standard Deviation	Standard Error
1	H <sup>a</sup>	1.15:1.00	1.27:1.00	1.10	1.16	0.04	±0.02
		1.00:1.01	1.18:1.00	1.19			
		1.04:1.00	1.18:1.00	1.13			
		1.00:1.19	1.00:1.04	1.14			
		3.39:1.00	4.08:1.00	1.20			
2	H <sup>b</sup>	1.34:1.00	1.36:1.00	1.01	1.01	0.01	±0.01
		1.00:1.17	1.00:1.14	1.03			
		1.15:1.00	1.14:1.00	0.99			
		1.36:1.00	1.39:1.00	1.02			
		10.6:1.00	10.6:1.00	1.00			
3	H <sup>c</sup>	1.12:1.00	1.00:1.14	0.78	0.79	0.02	±0.01
		1.31:1.00	1.01:1.00	0.77			
		1.04:1.00	1.00:1.19	0.81			
		1.16:1.00	1.00:1.09	0.79			
		1.00:4.38	1.00:5.41	0.81			

**Synthesis of (S)-(Z)-6-(*tert*-Butyldiphenylsilyloxy)-1-deutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (13).**

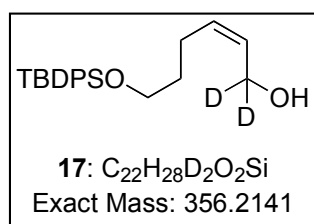


### 6-(*tert*-Butyldiphenylsilyloxy)-1,1-bis-deutero-2-hexyn-1-ol (**16**).



A solution of alkyne **15** (2.0 g, 5.3 mmol) in diethyl ether (26 mL) was cooled to  $-20\text{ }^{\circ}\text{C}$ . Lithium aluminum deuteride (330 mg, 7.9 mmol) was added portionwise, and the reaction mixture was stirred and maintained at  $-20\text{ }^{\circ}\text{C}$  for 30 min before addition of water (0.33 mL). After stirring for 5 min, 15% aqueous NaOH (0.33 mL) was added, followed by additional water (1 mL). The mixture was filtered through a short plug of silica gel with excess ether and the eluent was concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (25% ether/hexanes) to give 1.75 g (94%) of **16** as a clear, colorless oil:  $R_f$  0.29 (25% EtOAc/hexanes);  $^1\text{H}$  NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.68 (dd,  $J = 7.9, 1.6$  Hz, 4H), 7.46–7.38 (m, 6H), 3.75 (t,  $J = 6.0$  Hz, 2H), 2.38 (t,  $J = 7.1$  Hz, 2H), 1.77 (quintet,  $J = 6.1$  Hz, 2H), 1.42 (s, 1H), 1.07 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  135.8, 134.0, 129.8, 127.8, 86.3, 78.6, 62.5, 51.0 (quintet,  $J_{\text{CD}} = 6.0$  Hz), 31.7, 27.1, 19.4, 15.5; IR (thin film) 3351, 3069, 2935, 2246  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for C<sub>22</sub>H<sub>26</sub>O<sub>2</sub>SiD<sub>2</sub>Na ( $M + \text{Na}^+$ ) 377.1882, found 377.1876.

### (*Z*)-6-(*tert*-Butyldiphenylsilyloxy)-1,1-bis-deutero-2-hexen-1-ol (**17**).

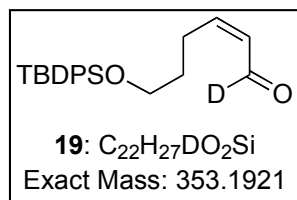


A flask charged with propargyl alcohol **16** (600 mg, 1.69 mmol), was evacuated and refilled with nitrogen five times. The alcohol was dissolved in ethyl acetate (3.4 mL) and Lindlar's catalyst (34 mg) was added to the solution. The flask was then evacuated and refilled with hydrogen three times. After 2 h, the reaction mixture was filtered through a short plug of silica gel with extra ethyl acetate and concentrated to give 585 mg (97%) of **17** as a clear colorless oil:  $R_f$  0.29 (25% EtOAc/hexanes);  $^1\text{H}$  NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.67 (dd,  $J = 7.8, 1.2$  Hz, 4H),



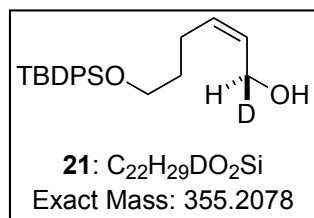
7.45–7.38 (m, 6H), 5.64 (d,  $J = 10.8$  Hz, 1H), 5.53 (dt,  $J = 10.8, 7.2$  Hz, 1H), 3.68 (t,  $J = 6$  Hz, 2H), 2.21 (q,  $J = 7.2$  Hz, 2H), 1.60 (quintet,  $J = 6.6$  Hz, 2H), 1.34 (bs, 1H), 1.07 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  135.8, 134.1, 132.9, 129.8, 129.1, 127.9, 63.2, 57.9 (quintet,  $J_{\text{CD}} = 21.5$  Hz), 32.4, 27.1, 23.8, 19.4; IR (thin film) 3334, 3069, 2934  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{28}\text{O}_2\text{D}_2\text{SiNa}$  ( $\text{M} + \text{Na}^+$ ) 379.2038, found 379.2036.

**(Z)-6-(tert-Butyldiphenylsilyloxy)-1-deutero-2-hexenal (19).**



(Z)-Allylic alcohol **17** (5.2 g, 14 mmol) was dissolved in dichloromethane (73 mL). To this solution was added molecular sieves (4 Å, 10 g) and 4-methylmorpholine *N*-oxide monohydrate (2.9 g, 21.9 mmol). Tetrapropylammonium perruthenate (76 mg, 0.22 mmol) was added, and the reaction mixture was stirred for 3 h. The crude reaction mixture was passed through a short plug of silica gel with extra dichloromethane, concentrated, and the residue was purified by silica gel chromatography (10% ether/hexanes) to provide 4.0 g (77%) of **19** as a clear, colorless oil:  $R_f$  0.47 (25% EtOAc/hexanes);  $^1\text{H}$  NMR (500 MHz  $\text{CDCl}_3$ )  $\delta$  7.66 (dd,  $J = 7.9, 1.4$  Hz, 4H), 7.45–7.38 (m, 6H), 6.63 (dt,  $J = 11.2, 8.1$  Hz, 1H), 5.96 (d, 11.2 Hz), 3.72 (t,  $J = 6.0$  Hz, 2H), 2.74 (q,  $J = 8.1$  Hz, 2H), 1.75 (quintet,  $J = 7.4$  Hz, 2H), 1.07 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.7 (t,  $J_{\text{CD}} = 6.0$  Hz), 153.1, 135.7, 133.8, 130.6, 129.9, 127.9, 62.8, 32.2, 27.1, 24.8, 19.4; IR (thin film) 3069, 2934, 1668  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{27}\text{O}_2\text{SiDNa}$  ( $\text{M} + \text{Na}^+$ ) 376.1819, found 376.1824.

**(S)-(Z)-6-(tert-Butyldiphenylsilyloxy)-1-deutero-2-hexen-1-ol (21).**

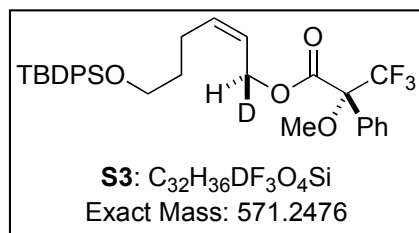


The general procedure of Keck was followed.<sup>6</sup> Titanium isopropoxide (81 mg, 0.283 mmol) was added to a stirring mixture of (*R*)-BINOL (0.16 g, 0.566 mmol), trifluoroacetic acid (85  $\mu$ L, 0.5M in CH<sub>2</sub>Cl<sub>2</sub>, 0.043 mmol), molecular sieves (4 Å, 1.4 g) and diethyl ether (11 mL).

The red-orange mixture was heated to reflux for 1 h, cooled to room temperature, and  $\alpha,\beta$ -unsaturated aldehyde **19** (1.0 g, 2.83 mmol) was added. The resulting mixture was stirred at room temperature for 10 min, then cooled to  $-78$  °C and tributyltin hydride (0.99 g, 3.40 mmol) was added dropwise. The reaction was stirred at  $-78$  °C for 20 min, then transferred to a  $-20$  °C freezer, without stirring. After 23 h, the mixture was removed from the freezer and saturated aqueous NaHCO<sub>3</sub> (10 mL) was added. The mixture was stirred for 1 h at room temperature, and then filtered through a pad of celite. The layers were separated, and the organic layer was dried with MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (25% ether/hexanes) to give 0.42 g (41%) of **21** as a clear colorless oil. Mosher's ester analysis of the product, found it to be of 85% enantiomeric excess and predominantly the (*S*) enantiomer: R<sub>f</sub> 0.26 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>)  $\delta$  7.70 (d,  $J = 6.6$  Hz, 4H), 7.47–7.40 (m, 6H), 5.65 (app t,  $J = 8.9$  Hz, 1H), 5.54 (dd,  $J = 15.8, 7.4$  Hz, 1H), 4.19 (s, 1H), 3.71 (t,  $J = 6.2$  Hz, 2H), 2.23 (q,  $J = 7.3$  Hz, 2H), 1.63 (quintet,  $J = 6.2$  Hz, 2H), 1.10 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  135.7, 134.0, 132.6, 129.8, 129.1, 127.8, 63.2, 58.2 (t,  $J_{CD} = 22.5$  Hz), 32.4, 27.1, 23.8, 19.4;  $[\alpha]_D^{24}$  0.41,  $[\alpha]_{546}^{24}$  0.29,  $[\alpha]_{435}^{24}$  0.71 (*c* 1.01, CHCl<sub>3</sub>); IR (thin film) 3325, 3070, 2931, 2857 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>22</sub>H<sub>29</sub>O<sub>2</sub>SiDNa (M + Na<sup>+</sup>) 378.1975, found 378.1971.

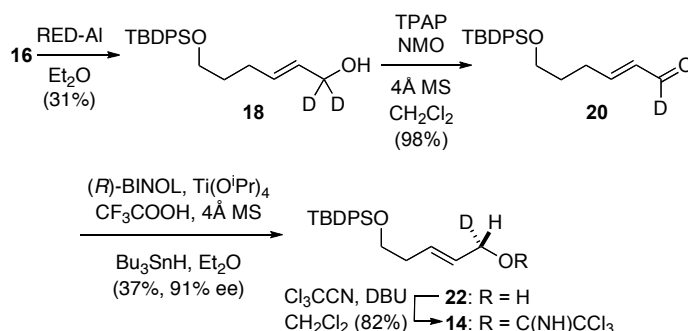
<sup>6</sup> Keck, G. E.; Krishnamurthy, D. *J. Org. Chem.* **1996**, *61*, 7638–7639.

**(S)-(Z)-6-(tert-Butyldiphenylsilyloxy)-1-deutero-hex-2-en-1-yl (R)-3',3',3'-Trifluoro-2'-methoxy-2'-phenylpropanoate (S3).**

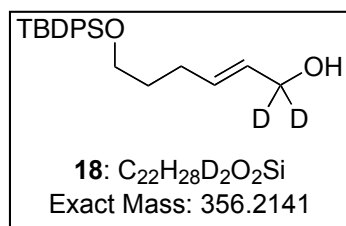


(Z)-Allylic alcohol **21** (10 mg, 0.028 mmol), 4-(dimethylamino)pyridine (0.3 mg, 0.0028 mmol), and (R)-2-trifluoromethyl-2-methoxy-2-phenyl acetic acid (9 mg, 0.0366 mmol) were dissolved in CH<sub>2</sub>Cl<sub>2</sub> (0.6 mL). *N,N'*-Dicyclohexylcarbodiimide (8 mg, 0.0366 mmol) was added at room temperature and the solution was stirred overnight. The solution was then diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 ml) and washed with a saturated solution of NaHCO<sub>3</sub> (5 mL). The aqueous layer was back extracted three times with CH<sub>2</sub>Cl<sub>2</sub> (5 mL). The combined aqueous layers were dried over MgSO<sub>4</sub>, filtered and concentrated. The crude oil was purified by silica gel chromatography (25% ether/hexanes) to give 8 mg (50%) of a 92:8 mixture of (1*S*,2'*R*)-**S3**:(1*R*,2'*R*)-**S3** as a clear colorless oil: Major diastereomer (1*S*,2'*R*): <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 7.67 (dd, *J* = 7.9, 1.4 Hz, 4H), 7.52 (t, *J* = 3.0 Hz, 2 H), 7.45–7.37 (m, 9H), 5.71 (dt, *J* = 10.9, 7.6 Hz, 1H), 5.56 (dd, *J* = 10.9, 7.2 Hz, 1H), 4.82 (d, *J* = 7.0 Hz, 1H), 3.67 (t, *J* = 6.2 Hz, 2H), 3.55 (s, 3H), 2.24 (q, *J* = 7.2 Hz, 2H), 1.62 (quintet, *J* = 7.5 Hz, 2H), 1.06 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 166.6, 136.8, 135.8, 134.1, 132.6, 129.81, 129.78, 128.6, 127.9, 127.5, 124.6, 122.4, 63.2, 61.9 (t, *J*<sub>CD</sub> = 23.1 Hz), 55.7, 32.4, 27.1, 24.2, 19.4; [α]<sub>D</sub><sup>24</sup> 34.1, [α]<sub>577</sub><sup>24</sup> 33.1, [α]<sub>546</sub><sup>24</sup> 36.0, [α]<sub>435</sub><sup>24</sup> 63.0 (*c* 1.1, CHCl<sub>3</sub>); IR (thin film) 2931, 2858, 1745, 1183, 1106 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>32</sub>H<sub>36</sub>O<sub>4</sub>SiDF<sub>3</sub>Na (M + Na<sup>+</sup>) 594.2374, found 594.2369.

**Synthetic Scheme for the Synthesis of (*S*)-(*E*)-6-(*tert*-Butyldiphenylsilyloxy)-1-deutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (**14**).**



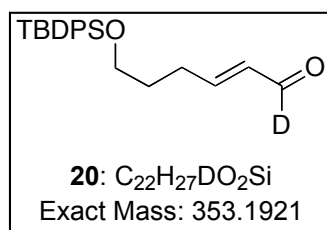
**(*E*)-6-(*tert*-Butyldiphenylsilyloxy)-1,1-bis-deutero-2-hexen-1-ol (**18**).**



A solution of propargyl alcohol **16** (1.0 g, 2.82 mmol) and ether (1.5 mL) was added dropwise to a stirring solution of sodium bis(2-methoxyethoxy)aluminum hydride (RED-Al, 65% solution in toluene, 1.7 mL, 5.64 mmol) in ether (2 mL) at 0 °C. The solution was maintained at 0 °C for 10 min, then allowed to warm to room temperature. After 4 h, 10 mL of 3.6 M H<sub>2</sub>SO<sub>4</sub> was added very slowly. The layers were separated and the aqueous layer was washed with ether (3 x 5 mL). The combined organic layers were then washed with water (2 x 5 mL), and brine (5 mL). The ether solution was dried with MgSO<sub>4</sub>, filtered and concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (25% ether/hexanes) to provide 310 mg (31%) of **18** as a clear colorless oil: R<sub>f</sub> 0.29 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 6.6 Hz, 4H), 7.46–7.39 (m, 6H), 5.70–5.62 (m, 2H), 3.70 (t, *J* = 6.3 Hz, 2H), 2.17 (q, *J* = 6.5 Hz, 2H), 1.68 (quintet, *J* = 6.4 Hz, 2H), 1.38 (bs, 1H), 1.08 (s, 9H); <sup>13</sup>C NMR (125 MHz CDCl<sub>3</sub>) δ 135.8, 134.18, 133.14, 129.7, 129.3, 127.8, 63.33, 63.26 (quintet, *J*<sub>CD</sub> = 21.6 Hz), 32.1, 28.7, 27.1, 19.4; IR (thin film) 3342, 3068, 2932, 1665 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>22</sub>H<sub>28</sub>O<sub>2</sub>D<sub>2</sub>SiNa (M + Na<sup>+</sup>) 379.2038, found

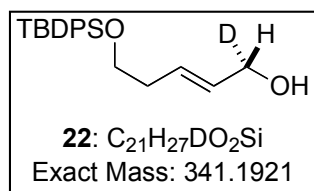
379.2038.

**(E)-6-(tert-Butyldiphenylsilyloxy)-1-deutero-2-hexenal (20).**



(Z)-Allylic alcohol **18** (0.310 g, 0.869 mmol) was dissolved in dichloromethane (4.3 mL). Molecular sieves (4 Å, 0.61 g), 4-methylmorpholine *N*-oxide monohydrate (0.175 g, 1.30 mmol), and tetrapropylammonium perruthenate (15 mg, 0.0435 mmol) was added to the reaction mixture. After 3 h, the crude reaction mixture was passed through a short plug of silica gel with extra dichloromethane, concentrated, and the residue was purified by silica gel chromatography (10% ether/hexanes) to provide 0.300 g (98%) of **20** as a clear, colorless oil: R<sub>f</sub> 0.47 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.67 (d, *J* = 7.9 Hz, 4H), 7.47–7.39 (m, 6H), 6.84 (dt, *J* = 15.6, 6.7 Hz, 1H), 6.12 (d, *J* = 15.6 Hz, 1H), 3.72 (t, *J* = 6.0 Hz, 2H), 2.47 (q, *J* = 6.8 Hz, 2H), 1.77 (quintet, *J* = 7.2 Hz, 2H), 1.08 (s, 9H); <sup>13</sup>C NMR (125 MHz CDCl<sub>3</sub>) δ 194.0 (t, *J*<sub>CD</sub> = 26.3 Hz), 158.7, 135.7, 133.8, 133.2, 129.9, 127.8, 63.0, 30.9, 29.5, 27.1, 19.4; IR (thin film) 3069, 2935, 2070, 1678 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>22</sub>H<sub>27</sub>O<sub>2</sub>DSiNa (M + Na<sup>+</sup>) 376.1819, found 376.1815.

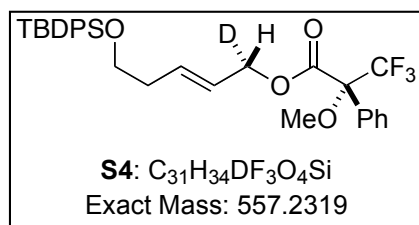
**(S)-(E)-6-(tert-Butyldiphenylsilyloxy)-1-deutero-2-hexen-1-ol (22).**



The general procedure of Keck was followed.<sup>6</sup> Titanium isopropoxide (24 mg, 0.085 mmol) was added to a stirring mixture of (*R*)-BINOL (49 mg, 0.169 mmol), trifluoroacetic acid (25 μL, 0.5M in CH<sub>2</sub>Cl<sub>2</sub>, 0.013 mmol), and molecular sieves (4 Å, 0.5 g) in ether (3.4 mL). The red-orange mixture was heated to reflux for 1 h, cooled to room temperature, and α,β-

unsaturated aldehyde **20** (0.300 g, 0.848 mmol) was added. The mixture was stirred at room temperature for 10 min, then cooled to  $-78\text{ }^{\circ}\text{C}$  and tributyltin hydride (93 mg, 1.02 mmol) was added dropwise. The reaction was stirred at  $-78\text{ }^{\circ}\text{C}$  for 20 min then transferred to a  $-20\text{ }^{\circ}\text{C}$  freezer, without stirring. After 23 h the mixture was removed from the freezer and saturated aqueous  $\text{NaHCO}_3$  (1 mL) was added. The mixture was stirred for 1 h at room temperature. The slurry was then filtered through a pad of celite. The layers were separated, and the organic layer was dried with  $\text{MgSO}_4$ , filtered, and concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (25% ether/hexanes) to give 0.11 g (37%) of **22** as a clear colorless oil. Mosher's ester analysis of the product (see procedure below) found it to be 91% enantiomeric excess and predominantly the *S* enantiomer:  $R_f$  0.26 (25% EtOAc/hexanes);  $^1\text{H}$  NMR (500 MHz  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 6.7$  Hz, 4H), 7.46–7.38 (m, 6H), 5.69–6.63 (m, 2H), 4.05 (bs, 1H), 3.69 (t,  $J = 6.3$  Hz, 2H), 2.17 (q,  $J = 6.8$  Hz, 2H), 1.67 (quintet,  $J = 6.6$  Hz, 2H), 1.27 (s, 1H), 1.07 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  135.8, 134.2, 133.1, 129.8, 129.4, 127.8, 63.6 (t,  $J_{\text{CD}} = 21.3$  Hz), 63.3, 32.1, 28.7, 27.1, 19.4;  $[\alpha]_{\text{D}}^{24}$  0.16,  $[\alpha]_{405}^{24}$  1.07 ( $c$  0.95,  $\text{CHCl}_3$ ); IR (thin film) 3309, 3048, 2932, 1963, 1667  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{29}\text{O}_2\text{DSiNa}$  ( $\text{M} + \text{Na}^+$ ) 378.1975, found 378.1971.

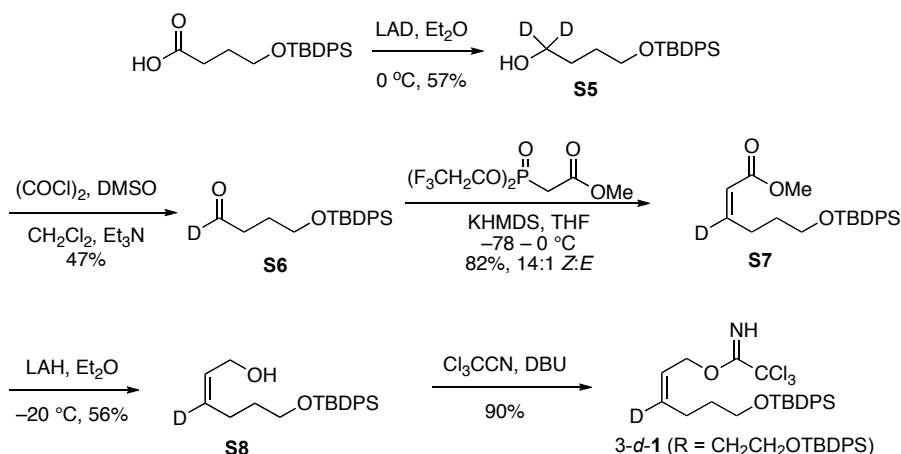
**(S)-(E)-6-(tert-Butyldiphenylsilyloxy)-1-deutero-hex-2-en-1-yl (R)-3',3',3'-Trifluoro-2'-methoxy-2'-phenylpropanoate (S4).**



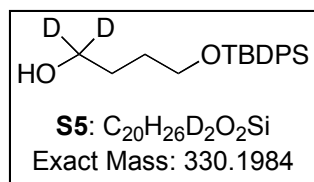
(*E*)-Allylic alcohol **22** (10 mg, 0.028 mmol), 4-(dimethylamino)pyridine (0.3 mg, 0.0028 mmol), and (*R*)-2-trifluoromethyl-2-methoxy-2-phenyl acetic acid (8.6 mg, 0.037 mmol) were dissolved in dichloromethane (0.6 mL). *N,N'*-

Dicyclohexylcarbodiimide (7.5 mg, 0.037 mmol) was added at room temperature and the solution was stirred overnight. The solution was then diluted with dichloromethane (5 mL) and washed with a saturated solution of NaHCO<sub>3</sub> (5 mL). The aqueous layer was back extracted three times with dichloromethane (5 mL). The combined aqueous layers were dried over MgSO<sub>4</sub>, filtered and concentrated. The crude oil was purified by silica gel chromatography (25% ether/hexanes) to give 8 mg (51%) of a 96:4 mixture of (1*S*,2'*R*)-**S4** (1*R*,2'*R*)-**S4** as a clear colorless oil: Major diastereomer (1*S*,2'*R*): <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 7.66 (d, *J* = 6.7 Hz, 4H), 7.53 (t, *J* = 1.2 Hz, 2 H), 7.45–7.37 (m, 9H), 5.82 (dt, *J* = 15.3, 6.7 Hz, 1H), 5.57 (dd, *J* = 15.3, 6.4 Hz, 1H), 4.69 (d, *J* = 6.5 Hz, 1H), 3.66 (t, *J* = 6.2 Hz, 2H), 3.56 (s, 3H), 2.15 (q, *J* = 7.3 Hz, 2H), 1.63 (quintet, *J* = 7.4 Hz, 2H), 1.06 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 166.6, 138.1, 135.7, 134.1, 132.6, 129.8, 128.6, 127.8, 127.5, 124.6, 122.8, 66.9 (t, *J*<sub>CD</sub> = 22.6 Hz), 63.3, 55.7, 31.9, 31.9, 28.8, 27.1, 19.4; [α]<sub>D</sub><sup>24</sup> 16.7, [α]<sub>577</sub><sup>24</sup> 16.5, [α]<sub>546</sub><sup>24</sup> 18.9, [α]<sub>435</sub><sup>24</sup> 36.0 (*c* 1.13, CHCl<sub>3</sub>); IR (thin film) 2937, 2853, 1742, 1265, 1109 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>32</sub>H<sub>36</sub>O<sub>4</sub>SiDF<sub>3</sub>Na (M + Na<sup>+</sup>) 594.2374, found 594.2357.

**Synthetic scheme for the synthesis of (Z)-6-(*tert*-butyldiphenylsilyloxy)-3-deutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (3-*d*-1).**

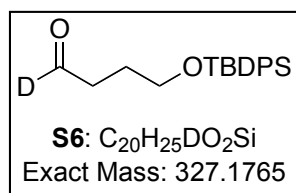


#### 4-(*tert*-Butyldiphenylsilyloxy)-1-dideutero-1-butanol (**S5**).



4-(*tert*-Butyldiphenylsilyloxy)-butanoic acid (87 mg, 0.25 mmol) was added dropwise to a 0 °C mixture of LiAlD<sub>4</sub> (13 mg, .31 mmol) in ether (1.3 mL). The mixture was stirred for 0.5 h, then 0.1 mL of water was added. After 5 min 0.1 mL of 15% aqueous NaOH was added followed by 0.3 mL water. The resulting slurry was filtered through a short pad of silica gel with extra ether. The solution was then concentrated under reduced pressure, and purified by silica gel chromatography (3:1 hexane:ether) to provide 48 mg (57%) of alcohol **S5** as a clear, colorless oil: <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 7.70 (dd, *J* = 7.9, 1.3 Hz, 4H), 7.47–7.40 (m, 6H), 3.72 (t, *J* = 5.6 Hz, 2H), 2.19 (bs, 1H), 1.71–1.65 (m, 4H), 1.08 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 135.8, 133.8, 129.9, 127.9, 64.2, 62.2 (quintet, *J*<sub>CD</sub> = 21.6 Hz), 29.8, 29.4, 27.0, 19.4; IR (thin film) 3354, 3069, 2935, 2862, 1962, 1894 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>20</sub>H<sub>26</sub>O<sub>2</sub>D<sub>2</sub>SiNa (M + Na)<sup>+</sup> 353.1882, found 353.1884.

#### 4-(*tert*-Butyldiphenylsilyloxy)-1-deuterobutanal (**S6**).

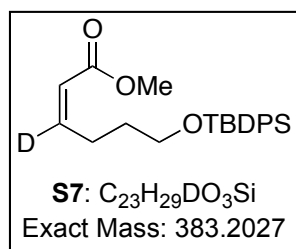


Oxalyl chloride (0.067 mL, 0.77 mmol) was dissolved in dichloromethane (1.5 mL) and cooled to -78 °C. Dimethyl sulfoxide (0.12 mL, 1.7 mmol) was added to the oxalyl chloride solution dropwise. After stirring for 5 min, alcohol **S5** (232 mg, 0.70 mmol) dissolved in dichloromethane (0.6 mL) was added to the dimethyl sulfoxide solution dropwise. The solution was maintained at -78 °C for 30 min then triethylamine (0.49 mL, 3.5 mmol) was added dropwise, and the solution was allowed to warm to room temperature. After 15 min water (2 mL) was added. The layers were separated and the aqueous layer was extracted with dichloromethane (2 x 5 mL). The combined



organic layers were washed sequentially with 1M HCl (1 x 5 mL), water (1 x 5 mL), saturated aqueous NaHCO<sub>3</sub> (1 x 5 mL), then brine (1 x 5 mL). The organic layer was then dried over MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (5:1 hexanes:ether) to provide 107 mg (47%) of **S6** as a clear, colorless oil: <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 7.66 (dd, *J* = 7.9, 1.4 Hz, 4H), 7.45–7.38 (m, 6H), 3.70 (t, *J* = 6.0 Hz, 2H), 2.56 (t, *J* = 7.2 Hz, 2H), 1.90 (quintet, *J* = 7.0 Hz, 2H), 1.06 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 202.5 (t, *J*<sub>CD</sub> = 26.4 Hz), 135.8, 133.8, 129.9, 127.9, 63.1, 40.8, 27.0, 25.4, 19.4; IR (thin film) 2932, 2858, 1711, 1107 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>20</sub>H<sub>25</sub>O<sub>2</sub>DSiCH<sub>3</sub>OHNa (M + CH<sub>3</sub>OH + Na<sup>+</sup>) 382.1925, found 382.1917.

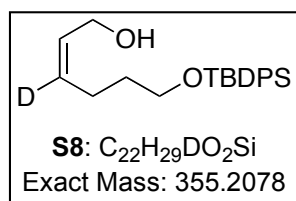
#### Methyl (Z)-6-(*tert*-Butyldiphenylsilyloxy)-3-deutero-2-hexenoate (**S7**).



Potassium bis(trimethylsilyl)amide (6.0 mL, 3.0 mmol, 0.5M in toluene) was added to a solution of 18-crown-6 (2.7 g, 10 mmol) and bis(2,2,2-trifluoroethyl) (methoxycarbonylmethyl)phosphonate (0.70 mL, 3.3 mmol) in THF (13 mL) at -78 °C. After 10 min at -78 °C, aldehyde **S6** (829 mg, 2.5 mmol) was added. The solution was maintained at -78 °C for 1 h then allowed to warm to room temperature for 2 h. The solution was diluted with EtOAc (20 mL), and washed with saturated aqueous NH<sub>4</sub>Cl (1 x 20 mL). The aqueous layer was then extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine (1 x 20 mL), dried over MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (9:1 hexanes:ether) to provide 794 mg (82%) of ester **S7** as a clear, colorless oil as a 14:1 mixture of *Z*:*E* stereoisomers: <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 7.70 (dd, *J* = 7.7, 1.0 Hz, 4H), 7.46–7.40 (m, 6H), 5.79 (s, 1H), 3.74 (t, *J* = 5.0, 2H), 3.72 (s, 3H), 2.79 (t, *J* = 7.3 Hz, 2H),

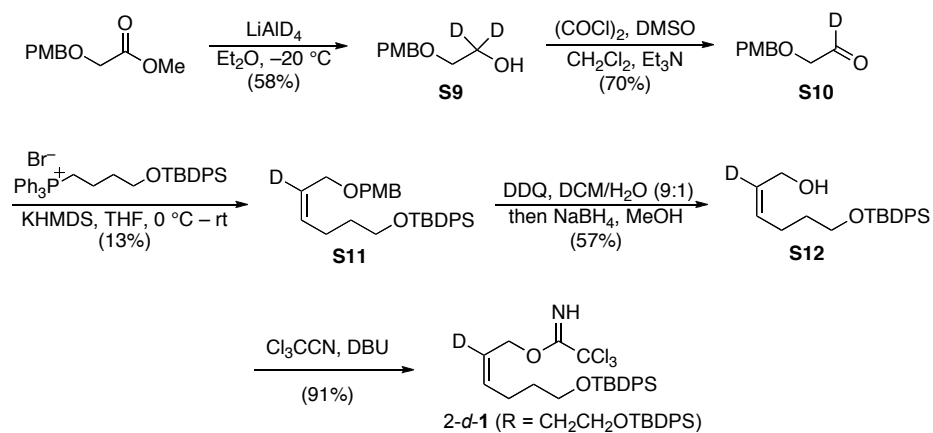
1.75 (quintet,  $J = 6.8$  Hz, 2H), 1.09 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  167.0, 150.2 (t,  $J_{\text{CD}} = 23.9$  Hz), 135.8, 134.1, 129.8, 127.8, 119.5, 63.6, 51.2, 32.1, 27.0, 25.8, 19.4; IR (thin film) 3069, 2941, 2862, 1723  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{29}\text{O}_3\text{DSiNa}$  ( $\text{M} + \text{Na}^+$ ) 406.1925, found 406.1911.

**(Z)-6-(tert-Butyldiphenylsilyloxy)-3-deutero-2-hexenol (S8).**

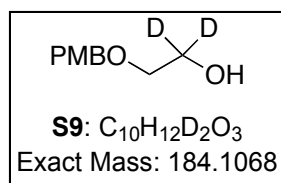


Lithium aluminum hydride (94 mg, 2.5 mmol) was added to a solution of methyl ester **S7** (794 mg, 2.1 mmol) in ether (10 mL) at  $-20$  °C. The mixture was stirred for 2 h, then 0.1 mL of water was added. After 5 min 0.1 mL of 15% aqueous NaOH was added followed by 0.3 mL water. The resulting slurry was filtered through a short pad of silica gel with extra ether. The solution was then concentrated under reduced pressure, and the residue was purified by silica gel chromatography (3:1 pentane:ether) to provide 415 mg (56%) of alcohol **S8** as a clear, colorless oil:  $^1\text{H}$  NMR (500 MHz  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 6.8$  Hz, 4H), 7.44–7.38 (m, 6H), 5.64 (t,  $J = 7.0$  Hz, 1H), 4.20 (t,  $J = 5.5$  Hz, 2H), 3.69 (t,  $J = 6.1$  Hz, 2H), 2.21 (t,  $J = 7.3$  Hz, 2H), 1.60 (quintet,  $J = 7.0$  Hz, 2H), 1.41 (s, 1H), 1.07 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  135.8, 134.1, 132.4 (t,  $J_{\text{CD}} = 22.6$ ), 129.8, 129.1, 127.9, 63.2, 58.6, 32.4, 27.1, 23.7, 19.4; IR (thin film) 3340, 3069, 2934, 2861, 1428  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{29}\text{O}_2\text{DSiNa}$  ( $\text{M} + \text{Na}^+$ ) 378.1975, found 378.1978.

**Synthetic Scheme for the Synthesis of (Z)-6-(*tert*-Butyldiphenylsilyloxy)-2-deutero-hex-2-en-1-yl-2',2',2'-trichloroacetimidate (2-*d*-1).**

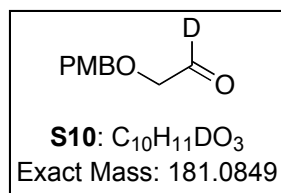


***p*-Methoxybenzyl 2-Dideutero-2-hydroxyethyl ether (S9).**



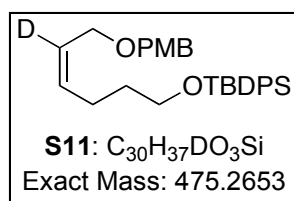
Lithium aluminum deuteride (78 mg, 1.9 mmol) was added to a solution of methyl glycoate PMB ether (327 mg, 1.6 mmol) in ether (7.8 mL) at – 20 °C. The mixture was stirred for 2 h then 0.1 mL of water was added. After 5 min 0.1 mL of 15% aqueous NaOH was added followed by 0.3 mL water. The resulting slurry was filtered through a short pad of silica gel with extra ether. The solution was then concentrated under reduced pressure, and the residue was purified by silica gel chromatography (3:1 dichloromethane:EtOAc) to provide 168 mg (58%) of alcohol **S9** as a clear, colorless oil: *R*<sub>f</sub> 0.09 (25% EtOAc/hexanes); <sup>1</sup>H NMR (500 MHz CDCl<sub>3</sub>) δ 7.27 (d, *J* = 8.9 Hz, 2H), 6.89 (d, *J* = 8.5 Hz, 2H), 4.50 (s, 2H), 3.82 (s, 3H), 3.57 (s, 2H), 2.04 (s, 1H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 159.5, 130.3, 129.7, 114.1, 73.2, 71.1, 61.4 (quintet, *J*<sub>CD</sub> = 21.0 Hz), 55.5; IR (thin film) 3403, 2900, 2857 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>10</sub>H<sub>12</sub>O<sub>3</sub>D<sub>2</sub>Na (M + Na<sup>+</sup>) 207.0966, found 207.0966.

### ***p*-Methoxybenzyl 2-Deutero-2-oxoethyl Ether (S10).**



Oxalyl chloride (0.7 mL, 8.3 mmol) was dissolved in dichloromethane (40 mL) and cooled to  $-78$  °C. Dimethyl sulfoxide (1.1 mL, 16 mmol) was added to the oxalyl chloride solution dropwise. After stirring for 5 min, alcohol **S9** (1.2 g, 6.4 mmol) dissolved in dichloromethane (13 mL) was added to the dimethyl sulfoxide solution dropwise. The solution was maintained at  $-78$  °C for 30 min then triethylamine (4.5 mL, 32 mmol) was added dropwise, and the solution was allowed to warm to room temperature. After 15 min water (30 mL) was added. The layers were separated and the aqueous layer was extracted with dichloromethane (2 x 40 mL). The combined organic layers were washed sequentially with 1M HCl (1 x 40 mL), water (1 x 40 mL), saturated aqueous NaHCO<sub>3</sub> (1 x 40 mL), then brine (1 x 40 mL). The organic layer was then dried over MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (5:1 hexanes:ether) to provide 804 mg (70%) of **S10** as a clear, colorless oil: Spectral data is consistent with those reported in the literature.<sup>7</sup>

### ***p*-Methoxybenzyl 6-(*tert*-Butyldiphenylsilyloxy)-2-deutero-2-hexenyl Ether (S11).**

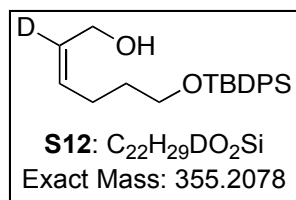


Potassium bis(trimethylsilyl)amide (6.1 mL, 3.1 mmol, 0.5 M in toluene) was added to a mixture of 4-(*tert*-butyldiphenylsilyloxy)butyl-1-phosphonium bromide (2 g, 3.06 mmol) in THF (20 mL) at 0 °C. The orange mixture was stirred at room temperature for 2 h. Aldehyde **S10** (428 mg, 2.4 mmol) dissolved in THF (4 mL) was then added. The mixture was stirred for 2 h. The resulting mixture was concentrated under reduced pressure, dissolved in ether and filtered to remove

<sup>7</sup> Yang, F.; Newsome, J. J.; Curran, D. P. *J. Am. Chem. Soc.* **2006**, *128*, 14200–14205.

triphenylphosphine oxide and remaining phosphonium salts. The ether solution was then concentrated under reduced pressure, and the crude oil was purified by silica gel chromatography (9:1 hexanes:EtOAc) to provide 150 mg (13%) of **S11** as a clear, colorless oil:  $^1\text{H}$  NMR (500 MHz  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J = 6.6$  Hz, 4H), 7.44–7.36 (m, 6H), 7.27 (m, 2H), 6.88 (dd,  $J = 13.0, 8.5$  Hz, 2H), 5.57 (t,  $J = 7.5$  Hz, 1H), 4.05 (s, 2H), 3.81 (s, 2H), 3.80 (s, 2H), 3.66 (t,  $J = 6.2$  Hz, 2H), 2.15 (q,  $J = 7.5$  Hz, 2H), 1.62 (quintet,  $J = 6.8$  Hz, 2H), 1.06 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  159.4, 135.8, 134.2, 133.2, 130.7, 129.8, 129.6, 127.8, 126.5 (t,  $J_{\text{CD}} = 21.0$  Hz), 117.2, 114.0, 72.0, 65.6, 63.4, 55.5, 32.6, 27.1, 24.2, 19.4; IR (thin film) 2932, 2857, 1613, 1513  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{30}\text{H}_{37}\text{O}_3\text{DSiNa}$  ( $\text{M} + \text{Na}^+$ ) 498.2551, found 498.2552.

**(Z)-6-(tert-Butyldiphenylsilyloxy)-2-deutero-2-hexen-1-ol (S12).**



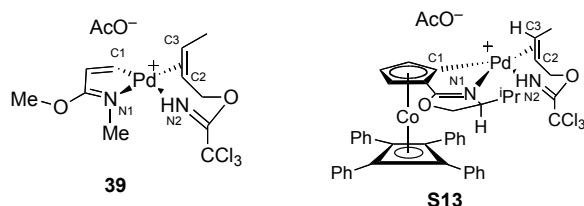
2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (96 mg, 0.35 mmol) was added to a mixture of PMB ether **S11** (150 mg, 0.32 mmol) in dichloromethane/water (9:1, 6.3 mL) at 0 °C. After stirring for 1 h, the blue-green mixture was allowed to warm to room temperature and stirred for an additional 1 h. The mixture was then diluted with dichloromethane and the organic phase was washed with saturated aqueous  $\text{NaHCO}_3$  (1 x 3 mL) and brine (1 x 3 mL) and dried over  $\text{MgSO}_4$ , filtered and concentrated under reduced pressure. The crude oil was dissolved in MeOH (6 mL), treated with  $\text{NaBH}_4$  (80 mg, 2.1 mmol), and the resulting slurry was stirred for 15 min. The MeOH mixture was diluted with EtOAc and washed with saturated aqueous  $\text{NH}_4\text{Cl}$  (1 x 3 mL) and concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (3:1 hexanes:EtOAc) to provide 64 mg (57%) of **S12** as a clear, colorless oil:  $^1\text{H}$  NMR (500 MHz  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J = 6.5$  Hz, 4H), 7.44–7.37 (m, 6H), 5.52 (t,  $J = 7.5$  Hz, 1H),

4.19 (d,  $J = 5.0$  Hz, 2H), 3.68 (t,  $J = 6.1$  Hz, 2H), 2.21 (q,  $J = 7.4$  Hz, 2H), 1.60 (quintet,  $J = 6.4$  Hz, 2H), 1.37 (t,  $J = 5.5$  Hz, 1H), 1.07 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  135.8, 134.1, 132.6, 129.8, 129.1 (t,  $J_{\text{CD}} = 21.0$  Hz), 127.9, 63.2, 58.6, 32.4, 27.1, 23.8, 19.4; IR (thin film) 3354, 2930, 1472  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{29}\text{O}_2\text{DSiNa}$  ( $\text{M} + \text{Na}^+$ ) 378.1975, found 378.1978.

### Part 3. Computational Results

#### NPA of Palladacycles **39** and **S13**

Natural population analysis was used to determine whether the model palladacycle **28** was a sufficient electronic model for [COP-OAc]<sub>2</sub> (**4**). For the analysis the imidate complex **39** was compared to the imidate complex of [COP-OAc]<sub>2</sub> **S13**. Table S 3 shows the similarity of some key atoms in the two complexes.



**Table S 3.** Natural charge of important atoms in complexes **39** and **S13**

Atom	<b>39</b>	<b>S13</b>
Pd	0.65954	0.69637
N1	-0.51670	-0.53991
C1	-0.19803	-0.16461
N2	-0.71743	-0.71596
C2	-0.28441	-0.29871
C3	-0.11598	-0.07817

The energy and XYZ coordinates for complex **39** are listed in the section for computational data for Figure 6 (page S45)

#### Natural Population Analysis of complex **39**

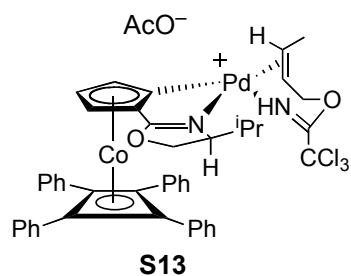
Atom No	Natural Population				
	Charge	Core	Valence	Rydberg	Total
1 pd	0.65954	7.98798	9.33445	0.01804	17.34046
2 c	-0.19803	1.99899	4.17191	0.02714	6.19803
3 n	-0.71743	1.99925	5.68448	0.03370	7.71743
4 c	0.55424	1.99900	3.40841	0.03834	5.44576
5 c	-0.16371	1.99927	4.10893	0.05550	6.16371

6 o	-0.44573	1.99968	6.42505	0.02101	8.44573
7 c	-0.10613	1.99908	4.08834	0.01871	6.10613
8 c	-0.28441	1.99913	4.26011	0.02518	6.28441
9 c	-0.11598	1.99917	4.09195	0.02486	6.11598
10 c	-0.65301	1.99939	4.64180	0.01182	6.65301
11 cl	0.05624	9.99960	6.92787	0.01629	16.94376
12 cl	0.04971	9.99959	6.93318	0.01751	16.95029
13 cl	0.06016	9.99960	6.92365	0.01659	16.93984
14 n	-0.51670	1.99926	5.48027	0.03716	7.51670
15 h	0.25530	0.00000	0.74281	0.00189	0.74470
16 h	0.20817	0.00000	0.79008	0.00176	0.79183
17 h	0.25082	0.00000	0.74723	0.00194	0.74918
18 h	0.23408	0.00000	0.76461	0.00130	0.76592
19 h	0.23677	0.00000	0.76113	0.00210	0.76323
20 h	0.21592	0.00000	0.78214	0.00195	0.78408
21 h	0.40060	0.00000	0.59682	0.00258	0.59940
22 h	0.22765	0.00000	0.76920	0.00315	0.77235
23 c	-0.40981	1.99899	4.39011	0.02071	6.40981
24 h	0.23160	0.00000	0.76595	0.00245	0.76840
25 c	0.58082	1.99907	3.39421	0.02590	5.41918
26 c	-0.43210	1.99937	4.41707	0.01566	6.43210
27 h	0.20485	0.00000	0.79338	0.00176	0.79515
28 h	0.22008	0.00000	0.77803	0.00189	0.77992
29 h	0.20694	0.00000	0.79138	0.00169	0.79306
30 o	-0.45884	1.99970	6.43735	0.02179	8.45884
31 c	-0.25726	1.99926	4.24383	0.01416	6.25726
32 h	0.19415	0.00000	0.80421	0.00164	0.80585
33 h	0.21052	0.00000	0.78821	0.00127	0.78948
34 h	0.19482	0.00000	0.80355	0.00164	0.80518
35 o	-0.79347	1.99977	6.77376	0.01994	8.79347
36 c	0.74778	1.99961	3.20323	0.04939	5.25222
37 c	-0.72158	1.99936	4.70953	0.01269	6.72158
38 h	0.20255	0.00000	0.79572	0.00173	0.79745
39 h	0.21176	0.00000	0.78698	0.00126	0.78824
40 h	0.21115	0.00000	0.78736	0.00150	0.78885
41 o	-0.82346	1.99975	6.80478	0.01892	8.82346
42 h	0.27144	0.00000	0.72329	0.00527	0.72856

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\* Total \*      0.00000    75.97388    135.42634    0.59978    212.00000



### Computational Data for Complex S13



SCF Energy = -5117.1219030400 hartree

Heat Capacity at 298K = 0.716192811 hartree

G<sub>tot</sub> = -5116.405710229 hartree

#### XYZ Coordinates

Pd	0.0069577	-1.0610360	1.2513649
N	2.1107545	-1.2424698	0.8624548
C	-0.0617867	-1.7905965	-0.6060784
C	1.2345485	-1.9647307	-1.1999824
C	2.3350672	-1.5777662	-0.3711702
C	1.0885335	-2.4944604	-2.5189950
C	-1.0147343	-2.1978652	-1.5712248
C	-0.3043510	-2.6419667	-2.7347042
Co	0.1693567	-0.6281327	-2.3906432
C	-0.5901623	1.2234233	-2.4980319
C	-0.5166045	0.5873673	-3.8104575
C	0.9392733	0.6067328	-3.7411167
C	0.8659273	1.2478467	-2.4281662
O	3.5959961	-1.5242530	-0.7876164
C	4.3451516	-0.8767014	0.2915940
C	3.4149255	-0.9957728	1.5172682
C	2.0099533	0.3561612	-4.7063213
C	3.2576340	-0.1925392	-4.3133087
C	4.2838169	-0.4002308	-5.2528994
C	4.0832093	-0.0613664	-6.6138328
C	2.8438114	0.4893482	-7.0153012
C	1.8208494	0.6946515	-6.0694796
C	-1.4752379	0.2927671	-4.8730767
C	-1.2545466	-0.7733647	-5.7834126
C	-2.1678576	-1.0399771	-6.8187848
C	-3.3274324	-0.2391719	-6.9694999
C	-3.5518694	0.8311968	-6.0724786
C	-2.6333348	1.0926931	-5.0373026
C	-1.6753030	1.8459602	-1.7439611
C	-2.9548662	1.2408024	-1.6511397
C	-4.0108436	1.8811386	-0.9741898

C	-3.8082051	3.1437982	-0.3653382
C	-2.5345727	3.7549740	-0.4501359
C	-1.4841679	3.1118510	-1.1352659
C	1.8350343	1.8535597	-1.5225600
C	3.0778153	2.3327557	-2.0070211
C	4.0077824	2.9419137	-1.1421683
C	3.7102359	3.0931380	0.2344620
C	2.4677728	2.6250499	0.7280795
C	1.5478534	2.0132248	-0.1420488
C	3.8412963	-2.1340367	2.4725397
C	5.1653582	-1.7803309	3.1597913
C	2.7833810	-2.4773471	3.5214678
H	2.6368605	-1.6471536	4.2189553
H	1.8241445	-2.7327584	3.0712184
H	3.1093354	-3.3330089	4.1159239
H	3.9972036	-3.0238089	1.8507319
H	5.0468373	-0.8968797	3.7940640
H	5.4930912	-2.6051857	3.7951651
H	5.9675783	-1.5756168	2.4486576
H	3.3799637	-0.0490785	2.0614654
H	5.2877813	-1.4055345	0.3918466
H	4.5220651	0.1548021	-0.0116787
H	1.8769565	-2.7263120	-3.2164818
H	-0.7627004	-3.0076817	-3.6402001
H	-2.0913575	-2.1975369	-1.4639127
H	0.5998551	1.6522965	0.2550394
H	2.2228405	2.7505142	1.7846243
H	4.4261704	3.5734560	0.9049759
H	4.9565742	3.3116221	-1.5362905
H	3.3175770	2.2492647	-3.0657805
H	3.4255936	-0.4705626	-3.2725070
H	0.8765860	1.1309944	-6.3932549
H	2.6813009	0.7584074	-8.0610813
H	4.8782350	-0.2237717	-7.3451765
H	5.2367724	-0.8277736	-4.9347161
H	-0.3719634	-1.4031255	-5.6767426
H	-1.9864439	-1.8679809	-7.5069185
H	-4.0399684	-0.4465783	-7.7710783
H	-4.4389378	1.4577811	-6.1848338
H	-2.8160784	1.9295909	-4.3652065
H	-4.9892561	1.3987719	-0.9162269
H	-3.1302201	0.2619350	-2.0992111
H	-0.5190397	3.6109365	-1.2127210
H	-2.3691735	4.7331868	0.0060231
H	-4.6269075	3.6413037	0.1590494
N	0.2104823	-0.1231420	3.1952248

C	-0.6706523	0.4080936	3.9413275
C	-0.4187365	0.9007089	5.3849024
O	-1.9255273	0.6032379	3.6097843
C	-2.3468398	0.6525281	2.2177726
C	-2.0961705	-0.5420744	1.3458052
C	-2.0814910	-1.8851948	1.6686104
C	-2.2199132	-2.5374162	3.0043044
Cl	-0.7370620	2.6589283	5.4321287
Cl	1.2621097	0.6037761	5.8986288
Cl	-1.5257896	0.0390338	6.4857354
H	-2.3353026	-0.2955255	0.3177801
H	-2.0834050	-1.8755213	3.8539684
H	-3.2410772	-2.9317464	3.0354119
H	-1.5448632	-3.3899029	3.0964166
H	-3.4208818	0.8214588	2.2966051
H	-1.8959218	1.5434394	1.7778577
H	1.1182762	-0.1833513	3.6427074
O	-5.0944258	-2.3977997	1.1682876
C	-5.0330521	-2.1910067	-0.0701977
C	-6.1752646	-1.3746518	-0.6947009
H	-6.4826083	-0.5668453	-0.0285387
H	-5.8955953	-0.9711445	-1.6678372
H	-7.0402409	-2.0301635	-0.8331374
O	-4.1339384	-2.6111934	-0.8469921
H	-2.2447571	-2.5529055	0.8331881

### Natural Population Analysis of complex S13

Atom No	Natural Population				
	Charge	Core	Valence	Rydberg	Total
1 pd	0.69637	7.98557	9.29470	0.02337	17.30363
2 n	-0.53991	1.99923	5.50433	0.03635	7.53991
3 c	-0.16461	1.99880	4.12714	0.03867	6.16461
4 c	-0.28294	1.99891	4.25072	0.03330	6.28294
5 c	0.59394	1.99891	3.37668	0.03047	5.40606
6 c	-0.25769	1.99911	4.23330	0.02528	6.25769
7 c	-0.33895	1.99913	4.31004	0.02977	6.33895
8 c	-0.27350	1.99922	4.24839	0.02590	6.27350
9 co	0.49066	17.99314	8.46608	0.05013	26.50934
10 c	-0.19671	1.99895	4.15511	0.04265	6.19671
11 c	-0.18175	1.99895	4.13995	0.04285	6.18175
12 c	-0.19456	1.99895	4.15214	0.04347	6.19456
13 c	-0.19241	1.99896	4.15164	0.04181	6.19241
14 o	-0.44313	1.99974	6.42262	0.02077	8.44313
15 c	-0.08803	1.99924	4.07277	0.01601	6.08803

16 c	-0.08085	1.99933	4.06120	0.02033	6.08085
17 c	0.10791	1.99925	3.88736	0.00547	5.89209
18 c	-0.18035	1.99972	4.17359	0.00705	6.18035
19 c	-0.19599	1.99975	4.18960	0.00665	6.19599
20 c	-0.19219	1.99977	4.18541	0.00702	6.19219
21 c	-0.19450	1.99975	4.18813	0.00662	6.19450
22 c	-0.17369	1.99974	4.16660	0.00735	6.17369
23 c	0.10786	1.99925	3.88749	0.00540	5.89214
24 c	-0.17443	1.99972	4.16768	0.00703	6.17443
25 c	-0.19591	1.99975	4.18960	0.00657	6.19591
26 c	-0.19124	1.99977	4.18451	0.00697	6.19124
27 c	-0.19436	1.99975	4.18801	0.00660	6.19436
28 c	-0.17369	1.99974	4.16672	0.00723	6.17369
29 c	0.11071	1.99924	3.88479	0.00526	5.88929
30 c	-0.18493	1.99971	4.17845	0.00676	6.18493
31 c	-0.19304	1.99973	4.18697	0.00634	6.19304
32 c	-0.19597	1.99976	4.18934	0.00688	6.19597
33 c	-0.19658	1.99974	4.19029	0.00654	6.19658
34 c	-0.17902	1.99973	4.17197	0.00731	6.17902
35 c	0.11281	1.99923	3.88293	0.00503	5.88719
36 c	-0.17094	1.99973	4.16406	0.00715	6.17094
37 c	-0.19902	1.99974	4.19273	0.00654	6.19902
38 c	-0.19549	1.99976	4.18880	0.00693	6.19549
39 c	-0.20247	1.99972	4.19620	0.00655	6.20247
40 c	-0.16964	1.99969	4.16306	0.00690	6.16964
41 c	-0.21281	1.99940	4.19953	0.01389	6.21281
42 c	-0.59617	1.99943	4.58724	0.00950	6.59617
43 c	-0.59389	1.99942	4.58468	0.00979	6.59389
44 h	0.18366	0.00000	0.81451	0.00182	0.81634
45 h	0.21296	0.00000	0.78573	0.00131	0.78704
46 h	0.21985	0.00000	0.77883	0.00131	0.78015
47 h	0.20178	0.00000	0.79588	0.00234	0.79822
48 h	0.20088	0.00000	0.79747	0.00165	0.79912
49 h	0.21577	0.00000	0.78296	0.00127	0.78423
50 h	0.20616	0.00000	0.79252	0.00132	0.79384
51 h	0.20725	0.00000	0.78932	0.00343	0.79275
52 h	0.20897	0.00000	0.78925	0.00178	0.79103
53 h	0.20103	0.00000	0.79562	0.00335	0.79897
54 h	0.24982	0.00000	0.74772	0.00246	0.75018
55 h	0.24456	0.00000	0.75323	0.00221	0.75544
56 h	0.28152	0.00000	0.71608	0.00240	0.71848
57 h	0.19087	0.00000	0.80913	0.00000	0.80913
58 h	0.19740	0.00000	0.80260	0.00000	0.80260
59 h	0.20203	0.00000	0.79797	0.00000	0.79797
60 h	0.20211	0.00000	0.79789	0.00000	0.79789
61 h	0.19870	0.00000	0.80130	0.00000	0.80130

62 h	0.19617	0.00000	0.80383	0.00000	0.80383
63 h	0.19761	0.00000	0.80239	0.00000	0.80239
64 h	0.19979	0.00000	0.80021	0.00000	0.80021
65 h	0.19934	0.00000	0.80066	0.00000	0.80066
66 h	0.19939	0.00000	0.80061	0.00000	0.80061
67 h	0.19510	0.00000	0.80490	0.00000	0.80490
68 h	0.19977	0.00000	0.80023	0.00000	0.80023
69 h	0.19934	0.00000	0.80066	0.00000	0.80066
70 h	0.19957	0.00000	0.80043	0.00000	0.80043
71 h	0.19656	0.00000	0.80344	0.00000	0.80344
72 h	0.20131	0.00000	0.79869	0.00000	0.79869
73 h	0.20382	0.00000	0.79618	0.00000	0.79618
74 h	0.19807	0.00000	0.80193	0.00000	0.80193
75 h	0.20160	0.00000	0.79840	0.00000	0.79840
76 h	0.20251	0.00000	0.79749	0.00000	0.79749
77 n	-0.71596	1.99925	5.68405	0.03265	7.71596
78 c	0.55279	1.99900	3.41000	0.03821	5.44721
79 c	-0.16565	1.99927	4.11067	0.05571	6.16565
80 o	-0.44413	1.99968	6.42335	0.02110	8.44413
81 c	-0.10585	1.99907	4.08651	0.02026	6.10585
82 c	-0.29871	1.99912	4.27119	0.02841	6.29871
83 c	-0.07817	1.99919	4.05261	0.02637	6.07817
84 c	-0.65523	1.99938	4.64393	0.01193	6.65523
85 cl	0.05770	9.99960	6.92637	0.01632	16.94230
86 cl	0.04772	9.99959	6.93486	0.01783	16.95228
87 cl	0.06585	9.99959	6.91784	0.01671	16.93415
88 h	0.26047	0.00000	0.73488	0.00465	0.73953
89 h	0.20514	0.00000	0.79312	0.00174	0.79486
90 h	0.26468	0.00000	0.73327	0.00205	0.73532
91 h	0.23098	0.00000	0.76772	0.00130	0.76902
92 h	0.23818	0.00000	0.75915	0.00267	0.76182
93 h	0.20733	0.00000	0.78949	0.00319	0.79267
94 h	0.39907	0.00000	0.59802	0.00290	0.60093
95 o	-0.80241	1.99977	6.78276	0.01988	8.80241
96 c	0.74973	1.99961	3.20069	0.04997	5.25027
97 c	-0.72399	1.99936	4.71112	0.01351	6.72399
98 h	0.20405	0.00000	0.79411	0.00185	0.79595
99 h	0.20043	0.00000	0.79760	0.00197	0.79957
100 h	0.21702	0.00000	0.78184	0.00114	0.78298
101 o	-0.81213	1.99975	6.79355	0.01883	8.81213
102 h	0.25692	0.00000	0.73887	0.00421	0.74308

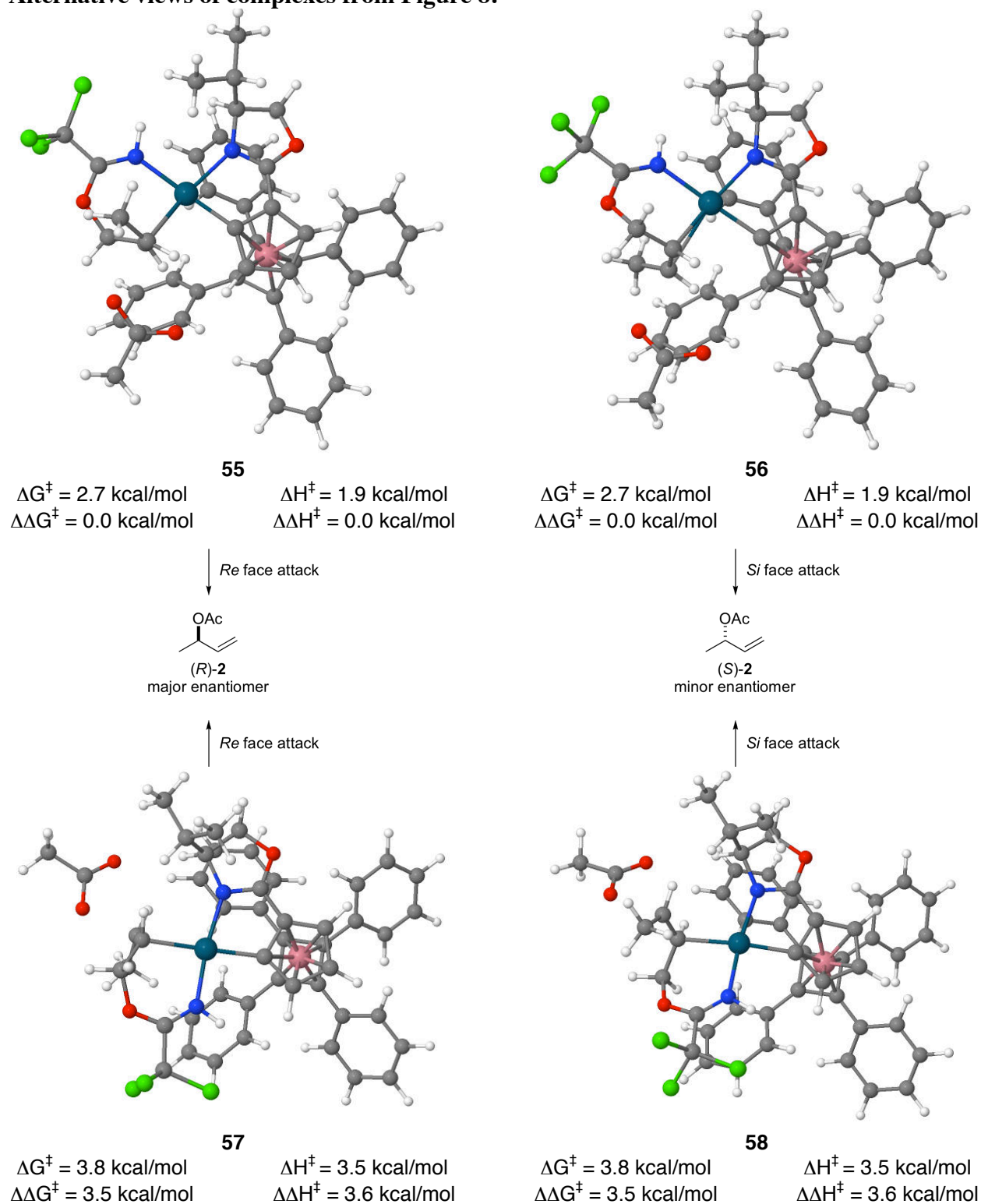
-----  
\* Total \*      0.00000   161.94736   304.89814   1.15450   468.00000

Table S 4 shows the small contributions of the entropy to the relative energies of the complexes calculated in each pathway for Figure 7.

**Table S 4.** T $\Delta$ S values calculated for palladium complexes in Figure 7

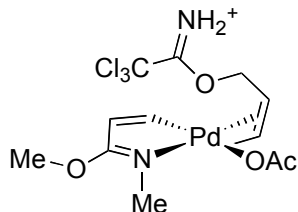
T $\Delta$ S relative to imidate-bound complex (kcal/mol) at 298 K					
Pathway	imidate-bound ( <b>42/39/33</b> )	oxypalladation TS ( <b>43/47/51</b> )	oxypalladate ( <b>44/48/52</b> )	deoxypalladation TS ( <b>45/49/53</b> )	ester-bound ( <b>46/50/54</b> )
I	0.0	-3.0	-3.82	-6.47	8.1
II	0.0	-1.5	-3.3	-2.66	-1.1
III	0.0	-3.0	-2.5	-1.5	0.0

### Alternative views of complexes from Figure 8.



### Computational Data for Figure 5

### Intermediate 29



SCF Energy = -2425.8517773250 hartree

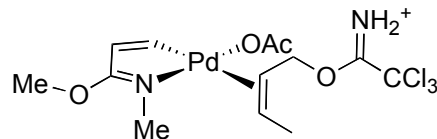
Zero-Point Energy = 0.3259914 hartree

$E_{\text{tot}} = -2425.52578593$  hartree

#### XYZ Coordinates

Pd	1.0233894	0.0162102	0.3208891
C	0.8964300	-1.8154295	1.0760552
H	0.8260242	-2.0453534	2.1359061
C	0.8659652	-2.8116373	0.1789843
H	0.7820263	-3.8582274	0.4409655
C	0.9486996	-2.3815696	-1.2136392
O	0.9312063	-3.2079826	-2.2523982
N	1.0448804	-1.1060307	-1.4319624
C	1.1399056	-0.5907772	-2.7919025
H	1.9413284	-1.0873568	-3.3437294
H	0.2035124	-0.7448293	-3.3349690
H	1.3486283	0.4734465	-2.7423520
C	0.8335917	-4.6339205	-2.0496393
H	-0.1000358	-4.8847537	-1.5473574
H	0.8431875	-5.0646171	-3.0464417
H	1.6883135	-4.9985715	-1.4809019
O	1.2879609	1.8799213	-0.6683875
C	0.2669022	2.5921432	-1.0089171
O	-0.9085228	2.3015695	-0.7558288
C	0.6082152	3.8621064	-1.7705395
H	1.3066432	4.4681346	-1.1904372
H	1.1036872	3.6053564	-2.7094174
H	-0.2900545	4.4386216	-1.9820722
C	0.2162170	1.0693340	2.1512517
H	-0.2731119	1.8607506	1.5952533
C	1.5943832	1.0945407	2.1696814
H	2.0972275	1.9303594	1.6967145
C	-0.6871363	0.2851043	3.0487372
H	-0.2051548	-0.5557705	3.5442306
H	-1.0632358	0.9589922	3.8265306
H	-1.5562892	-0.0790775	2.4996094
C	2.4283038	0.3603429	3.1636753

### Intermediate 30



SCF Energy = -2425.84476741070 hartree

Zero-Point Energy = 0.3259282 hartree

$E_{\text{tot}} = -2425.51883921$  hartree

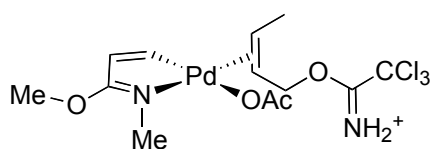
#### XYZ Coordinates

Pd	1.2463412	0.0065903	0.6202165
C	1.2799491	-1.8109945	1.3924126
H	1.4860348	-1.9745946	2.4441733
C	1.0180910	-2.8101947	0.5407832
H	0.9906752	-3.8546498	0.8232850
C	0.7631478	-2.3833225	-0.8294784
O	0.4631563	-3.2122936	-1.8238861
N	0.8379117	-1.1094136	-1.0798428
C	0.5986785	-0.6346957	-2.4379592
H	1.1433363	-1.2360400	-3.1680362
H	-0.4651689	-0.6743831	-2.6887482
H	0.9334392	0.3953574	-2.5284895
C	0.4052251	-4.6359312	-1.5922330
H	-0.3715363	-4.8727680	-0.8662940
H	0.1554188	-5.0710226	-2.5554255
H	1.3724741	-5.0083066	-1.2571159
C	0.4639179	2.2009042	-0.2732321
H	-0.1272409	1.7975884	-1.0884823
C	1.8099963	2.1541615	-0.4198141
H	2.2337158	1.7640063	-1.3380941
C	-0.3255939	2.9127023	0.7776682
H	0.2667516	3.2209720	1.6364973
H	-0.7731558	3.8078622	0.3330549
H	-1.1484762	2.2873190	1.1274008
C	2.7756355	2.8569018	0.4707161
H	3.1312400	3.7934168	0.0385917
H	2.3731413	3.0045234	1.4679188
O	3.9699894	1.9858201	0.5819883
C	4.8013590	2.1008142	1.5433071
N	4.7450758	2.9865770	2.4841244
H	4.0321663	3.7043763	2.5095939
C	5.9638363	1.0878185	1.4851324
Cl	6.9586513	1.1553195	2.9589363
Cl	5.2952183	-0.5405176	1.2922916



H	2.6343274	0.9936994	4.0303570
H	2.0109085	-0.5918180	3.4839467
O	3.7295997	0.0816340	2.5203898
C	4.6992830	-0.4311076	3.1803161
N	4.6522457	-0.7758125	4.4241932
C	5.9865105	-0.6105620	2.3522863
Cl	7.2757408	-1.3729144	3.3101356
Cl	5.5906663	-1.6355831	0.9564078
Cl	6.5016229	1.0111733	1.8337602
H	5.4666901	-1.1767011	4.8753060
H	3.8200167	-0.6613332	4.9898320

### Intermediate 31



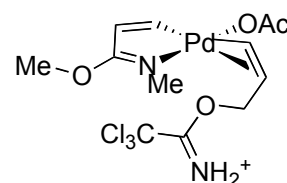
SCF Energy = -2425.8528262510 hartree  
 Zero-Point Energy = 0.3261788 hartree  
 $E_{\text{tot}} = -2425.52664745$  hartree

#### XYZ Coordinates

Pd	1.1888332	0.1648671	0.6603062
C	1.5044871	-1.6539308	1.3696138
H	1.8041217	-1.8534720	2.3960529
C	1.3406037	-2.6574492	0.4972217
H	1.4908589	-3.7002861	0.7441226
C	0.9301973	-2.2437500	-0.8423011
O	0.7317015	-3.0864159	-1.8494381
N	0.7513192	-0.9735153	-1.0400981
C	0.3193075	-0.4779705	-2.3402664
H	1.1571394	-0.4374873	-3.0410484
H	-0.4578554	-1.1156398	-2.7655537
H	-0.0734717	0.5266520	-2.2146531
C	0.8893429	-4.5082226	-1.6552798
H	0.1875310	-4.8719939	-0.9057567
H	0.6631014	-4.9535688	-2.6195706
H	1.9141980	-4.7431266	-1.3706868
O	0.6653587	2.0672711	-0.1843567
C	1.4302932	2.5580451	-1.1026307
O	2.4854122	2.0443361	-1.4840135
C	0.9423275	3.8685144	-1.7007376
H	-0.1022736	3.7824961	-2.0037603
H	1.0010611	4.6571580	-0.9460698
H	1.5527295	4.1536993	-2.5552209

Cl	6.9488603	1.5507646	0.0713687
H	5.4518240	3.0099497	3.2097342
O	1.7892295	0.8885598	2.3970852
C	1.0618207	0.7463342	3.4634933
O	-0.0277954	0.1797215	3.5074309
C	1.6841494	1.3509372	4.7119451
H	0.9840990	1.3117812	5.5435250
H	2.5855856	0.7925790	4.9745603
H	1.9791920	2.3861350	4.5316372

### Intermediate 32



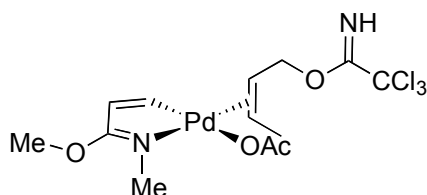
SCF Energy = -2425.84377543480 hartree  
 Zero-Point Energy = 0.3252919 hartree  
 $E_{\text{tot}} = -2425.51848353$  hartree

#### XYZ Coordinates

Pd	1.3273616	-0.3174310	0.5631862
C	1.8698647	-1.9847669	1.4468707
H	2.1497381	-1.9850164	2.4950787
C	1.8661313	-3.0873490	0.6885731
H	2.1437430	-4.0695199	1.0481773
C	1.4397091	-2.8659327	-0.6869595
O	1.3185666	-3.8349315	-1.5891069
N	1.1483910	-1.6449591	-1.0273075
C	0.6889296	-1.3639477	-2.3798976
H	1.1732900	-2.0099216	-3.1123021
H	-0.3931212	-1.5098401	-2.4632423
H	0.9212099	-0.3332789	-2.6298528
C	1.7070811	-5.1858062	-1.2606572
H	1.0828241	-5.5780170	-0.4586208
H	1.5436450	-5.7579138	-2.1691443
H	2.7596985	-5.2243178	-0.9831782
C	1.4771503	1.9899396	-0.5783247
H	2.2002015	2.2026368	0.2017801
C	0.1929006	1.8313482	-0.1898258
H	-0.0593941	1.9760657	0.8540430
C	2.0194296	2.0682913	-1.9677843
H	1.2924013	1.8446991	-2.7466669

C	2.3828000	1.0438303	2.3612974
H	2.9427068	0.1755993	2.6894304
C	1.0380728	1.0522019	2.6739142
H	0.6345492	0.2363192	3.2627540
C	3.2323993	2.2058056	1.9530167
H	2.6682623	3.0394308	1.5418879
H	3.7745539	2.5603582	2.8366886
H	3.9772499	1.8973757	1.2199630
C	0.2064746	2.2904819	2.6630711
H	0.0956147	2.7154917	3.6616118
H	0.5830064	3.0209893	1.9553723
O	-1.1556532	1.8957175	2.2375606
C	-1.9648023	2.7261446	1.7037887
N	-1.7437546	3.9877721	1.5278285
H	-0.8919383	4.4365152	1.8390872
C	-3.3185553	2.1031228	1.3038278
Cl	-4.2998580	3.2395181	0.3494407
Cl	-3.0220870	0.6347976	0.3588745
Cl	-4.1533801	1.7229470	2.8342499
H	-2.4456612	4.5756519	1.0943954

### Intermediate 33



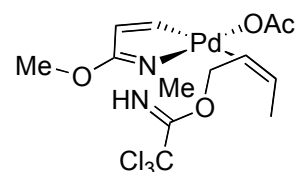
SCF Energy = -2425.4266592080 hartree  
 Zero-Point Energy = 0.3126270 hartree  
 $E_{\text{tot}} = -2425.11403221$  hartree

#### XYZ Coordinates

Pd	-0.4684601	2.7247164	-2.0657450
N	-1.8555306	1.1879803	-1.7366924
C	-0.0637481	1.5576187	-3.6102357
C	-0.7819500	0.4281542	-3.6913780
C	-1.7692315	0.2510850	-2.6295368
O	-2.5715120	-0.8054316	-2.5314055
C	-2.5328511	-1.8445347	-3.5306472
C	-2.8271059	1.0947508	-0.6556261
C	1.5045902	3.8138427	-2.2904863
C	0.5295083	4.4412551	-3.0367884
O	-1.0929087	3.9220776	-0.4161075
C	-0.7761895	3.5489638	0.7764777

H	2.3854266	3.0858885	-2.1380610
H	2.8819679	1.4085158	-2.0826534
C	-0.9749363	1.7623016	-1.1106867
H	-1.4768849	2.7313889	-1.1640446
H	-0.7416572	1.4033661	-2.1110223
O	-1.9488888	0.8126930	-0.5197105
C	-3.1365594	0.7054098	-0.9856975
N	-3.5938939	1.3447773	-2.0105319
H	-3.0299984	1.9975249	-2.5414336
C	-4.0267892	-0.2759424	-0.1984337
Cl	-5.6405813	-0.4220368	-0.9296291
Cl	-3.2206124	-1.8600343	-0.2052586
Cl	-4.1708281	0.3644799	1.4543758
H	-4.5504071	1.2053702	-2.3158183
O	1.4522422	0.7017973	2.3401207
C	2.5822562	1.2098023	2.7214891
O	3.6135237	1.2198442	2.0460408
C	2.5555597	1.8023480	4.1191790
H	2.7094718	0.9963102	4.8415777
H	3.3570795	2.5291155	4.2379770
H	1.5919632	2.2627917	4.3350453

### Intermediate 34



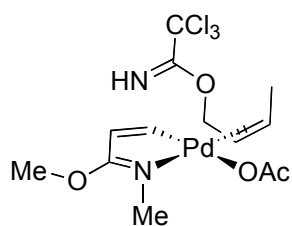
SCF Energy = -2425.4184830940 hartree  
 Zero-Point Energy = 0.3123160 hartree  
 $E_{\text{tot}} = -2425.10616709$  hartree

#### XYZ Coordinates

Pd	0.1257817	-1.3865918	-2.1032775
N	1.1850834	-1.9951818	-3.7887782
C	-1.2854660	-2.3613306	-3.0621246
C	-0.9301411	-2.9356923	-4.2179534
C	0.4628163	-2.7224882	-4.5883350
O	1.0230637	-3.2333338	-5.6826017
C	0.2303442	-3.9984871	-6.6129861
C	2.5834354	-1.7419407	-4.1104136
C	1.5803634	0.4685890	-1.0491626
C	1.9040505	-0.7074985	-0.4680936
H	2.8882691	-0.8005542	-3.6628687
H	3.2242867	-2.5382310	-3.7194237
H	2.7416121	-1.6774721	-5.1869489

O	-0.0934886	2.5543085	1.0467575
C	-1.3109386	4.4473037	1.8814299
H	-0.9081925	5.4557658	1.7630861
H	-2.3976773	4.5231515	1.8086051
H	-1.0362506	4.0609875	2.8610124
H	-2.5057334	0.3710196	0.0981812
H	-2.9152617	2.0692933	-0.1851204
H	-3.8058070	0.7893217	-1.0315016
H	-1.5529442	-2.3205329	-3.5501880
H	-3.2856390	-2.5644584	-3.2229656
H	-2.7851453	-1.4426567	-4.5114079
H	-0.6570572	-0.3107690	-4.4723970
H	0.6999213	1.7808603	-4.3517840
H	2.0800532	3.0441448	-2.7939833
H	0.4382455	4.1788649	-4.0844475
C	-0.1454641	5.7272437	-2.6598551
H	-0.1944067	5.8698431	-1.5826920
H	-1.1559007	5.7632157	-3.0715303
C	2.0929410	4.2790316	-0.9960873
H	2.2227307	3.4465978	-0.3043021
H	3.0882239	4.6863654	-1.2047446
H	1.5030769	5.0493977	-0.5056266
O	0.6386180	6.7918023	-3.2581176
C	0.1852100	8.0448082	-3.1348515
C	1.1617131	9.0085368	-3.8374533
Cl	2.7759104	8.8630311	-3.0623254
Cl	1.2911542	8.5465180	-5.5686886
Cl	0.6240444	10.6937132	-3.7324215
N	-0.8469803	8.4853336	-2.5638251
H	-1.4120102	7.7561671	-2.1341917

### Intermediate 35



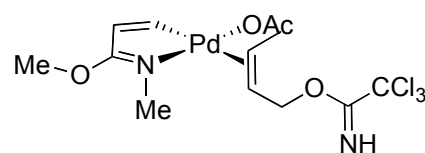
SCF Energy = -2425.4266351450 hartree  
 Zero-Point Energy = 0.3127287 hartree  
 $E_{\text{tot}}$  = -2425.11390645 hartree

#### XYZ Coordinates

Pd	-0.5230630	2.8347975	-1.9219314
N	-1.9320374	1.3082912	-1.7275617

H	-0.5806656	-3.3924103	-7.0155399
H	0.9144419	-4.2751319	-7.4100024
H	-0.1613902	-4.8954770	-6.1343482
H	-1.6024269	-3.5128932	-4.8392621
H	-2.2868884	-2.4345798	-2.6506900
H	0.6447968	0.9235845	-0.7420640
H	1.2462942	-1.1007833	0.2983709
C	3.2007801	-1.4407436	-0.6154362
H	3.8225284	-1.0522001	-1.4217292
H	3.0264578	-2.5074394	-0.7769835
C	2.4083843	1.3081553	-1.9672091
H	1.8664145	1.5280405	-2.8902357
H	2.5941434	2.2716497	-1.4826203
H	3.3715421	0.8690256	-2.2200126
O	3.9083871	-1.2769214	0.6387297
C	5.0776914	-1.9111513	0.7883665
C	5.6464943	-1.5988420	2.1864328
Cl	5.8699465	0.1768172	2.3381036
Cl	4.4744605	-2.1582431	3.4267205
Cl	7.2030874	-2.3993161	2.4639291
N	5.7063547	-2.6595226	-0.0053599
H	5.2318824	-2.7916401	-0.8956694
O	-1.1226738	-1.0558403	-0.5116227
C	-2.0109413	-0.1146486	-0.5633645
O	-2.1411383	0.6862839	-1.4908771
C	-2.9395328	-0.0726154	0.6384509
H	-2.4397323	-0.4233799	1.5403133
H	-3.3207601	0.9367995	0.7849568
H	-3.7880642	-0.7342569	0.4439618

### Intermediate 36



SCF Energy = -2425.4214340870 hartree  
 Zero-Point Energy = 0.3121016 hartree  
 $E_{\text{tot}}$  = -2425.10933249 hartree

#### XYZ Coordinates

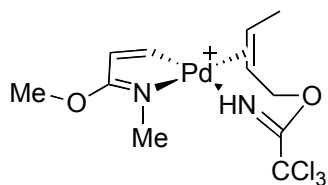
Pd	-0.3715952	-1.8264817	-1.5221673
N	1.1764621	-1.9113071	-2.9065751
C	-1.3648401	-2.4779851	-3.0990081
C	-0.6393377	-2.6618244	-4.2100028

C 0.0947893 1.6040715 -3.3506748  
C -0.6343082 0.4893040 -3.5109756  
C -1.7561650 0.3534689 -2.5876129  
O -2.5957612 -0.6773135 -2.5806670  
C -2.4118678 -1.7700831 -3.5040868  
C -3.0217665 1.2482535 -0.7628034  
C 0.5670477 4.6710487 -2.6916460  
C 1.3292856 4.0369554 -1.7347053  
O -1.2691705 3.9799105 -0.2892199  
C -2.2182413 4.8275454 -0.4955968  
O -2.7313563 5.0559002 -1.5982935  
C -2.6739414 5.5899276 0.7386531  
H -2.6832600 4.9447899 1.6172204  
H -1.9658225 6.4004492 0.9307848  
H -3.6602392 6.0224588 0.5789652  
H -3.0265893 0.2923651 -0.2338910  
H -2.8896697 2.0516927 -0.0444508  
H -3.9895582 1.3711996 -1.2569064  
H -1.4453170 -2.2470768 -3.3450700  
H -3.2103116 -2.4711068 -3.2792820  
H -2.5045866 -1.4216109 -4.5321650  
H -0.4299434 -0.2618112 -4.2629346  
H 0.9400172 1.7906681 -4.0057996  
H -0.1674264 5.3843650 -2.3341995  
H 1.1883881 4.3312121 -0.7009611  
C 2.5926731 3.2721673 -1.9943132  
H 2.6569229 2.8843557 -3.0099655  
H 2.6959808 2.4479689 -1.2860979  
C 0.8231129 4.7276927 -4.1642595  
H -0.1053885 4.6199292 -4.7269202  
H 1.2224204 5.7197450 -4.4015614  
H 1.5379121 3.9875308 -4.5176758  
O 3.6822180 4.2056621 -1.7848054  
C 4.9340239 3.7355695 -1.8615368  
C 5.9244369 4.8877147 -1.6019480  
Cl 5.6717572 6.1567644 -2.8480654  
Cl 5.6018658 5.5782876 0.0237507  
Cl 7.6095347 4.3431422 -1.6704436  
N 5.3539258 2.5733475 -2.1020856  
H 4.6089352 1.8984060 -2.2601170

**Intermediate 37**

C 0.7756599 -2.3434831 -4.0647579  
O 1.6715643 -2.4699390 -5.0409340  
C 1.2629724 -2.9322456 -6.3444452  
C 2.5866166 -1.5854691 -2.7242827  
C 1.0290232 -1.7074677 0.5562447  
C 0.7276985 -0.4442397 0.1731142  
H 2.9160747 -0.8383192 -3.4503267  
H 2.7419562 -1.1838719 -1.7272929  
H 3.2155008 -2.4722577 -2.8399101  
H 0.5362456 -2.2488275 -6.7826065  
H 2.1697397 -2.9389324 -6.9422978  
H 0.8535363 -3.9399790 -6.2821902  
H -1.0458257 -3.0188676 -5.1475224  
H -2.4301682 -2.6769908 -3.0580661  
H 1.9025039 -2.1647380 0.1020691  
H 1.3858857 0.0634123 -0.5234718  
C -0.3175941 0.4342334 0.7886755  
H -1.0113015 -0.1186031 1.4177891  
H -0.8825443 0.9630031 0.0182466  
C 0.4089173 -2.5099521 1.6547600  
H 0.1314792 -3.5035306 1.2984081  
H 1.1533319 -2.6519705 2.4449760  
H -0.4700587 -2.0411809 2.0901627  
O 0.3908407 1.4119292 1.5937257  
C -0.3296904 2.3682144 2.1905328  
C 0.6159095 3.3018933 2.9715625  
Cl 1.5065565 2.3354673 4.1958772  
Cl 1.7898182 4.0298705 1.8224143  
Cl -0.2624884 4.6020066 3.7948370  
N -1.5719495 2.5745970 2.1891384  
H -2.0928038 1.8948508 1.6395148  
O -2.0678934 -1.7122603 -0.3868307  
C -2.7493659 -2.7730796 -0.0881902  
O -2.4354239 -3.9273841 -0.3797619  
C -4.0321586 -2.4765926 0.6716341  
H -3.8506525 -1.7564288 1.4701645  
H -4.7574646 -2.0302911 -0.0132324  
H -4.4513646 -3.3924844 1.0833851

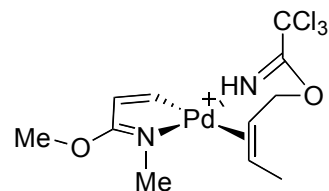
**Intermediate 38**



SCF Energy = -2196.7949511650 hartree  
 Zero-Point Energy = 0.2635880 hartree  
 $E_{\text{tot}} = -2196.53136317$  hartree

XYZ Coordinates

Pd	0.7969874	0.3521723	0.1634235
C	0.2054693	1.5625070	-1.2875241
N	1.2924811	-0.9496214	1.8216998
C	2.0856633	-1.9395207	1.8735452
C	2.5382916	-2.6315243	3.1777304
O	2.6516814	-2.5042365	0.8285721
C	2.0855042	-2.3489837	-0.4982577
C	2.0290882	-0.9702799	-1.0902378
C	2.8239930	0.1298280	-0.8568341
C	3.9913144	0.2793282	0.0689375
Cl	1.9946382	-4.3308639	3.1236243
Cl	1.8428243	-1.8378683	4.6121788
Cl	4.3197657	-2.5523180	3.2730626
N	-0.7806678	1.3262488	1.1245353
H	1.4572804	-0.9816603	-2.0137295
H	4.0936900	-0.5180200	0.7981669
H	4.8980190	0.2850317	-0.5457755
H	3.9589185	1.2403800	0.5846272
H	2.7218082	-2.9828544	-1.1165843
H	1.0855214	-2.7847918	-0.4789185
H	0.9533563	-0.6717676	2.7370998
H	0.6665309	1.5833771	-2.2710194
C	-0.8359240	2.3497707	-0.9929938
H	-1.2755528	3.0459772	-1.6950922
C	-1.3626871	2.2045828	0.3631699
C	-1.2018994	1.0868460	2.4971119
H	-0.3867454	1.3351484	3.1819268
H	-2.0698474	1.6846521	2.7673925
H	-1.4534619	0.0320705	2.6242889
O	-2.3796123	2.9100996	0.8335590
C	-3.0408931	3.8921338	0.0043716
H	-3.4911863	3.4145477	-0.8647343
H	-3.8153137	4.3183268	0.6348630
H	-2.3400531	4.6687440	-0.2984413
H	2.7556098	0.9177352	-1.5979705

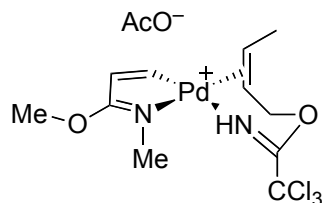


SCF Energy = -2196.7914988860 hartree  
 Zero-Point Energy = 0.2637272 hartree  
 $E_{\text{tot}} = -2196.52777169$  hartree

XYZ Coordinates

Pd	0.9768369	0.3898169	0.1144746
C	-0.4567104	1.2885757	1.1597322
N	1.0926944	-1.1163445	1.5104731
C	1.6478897	-2.2621661	1.5009077
C	1.7637391	-3.1648694	2.7484770
O	2.2093648	-2.8357538	0.4631883
C	1.8778691	-2.4404060	-0.8958152
C	2.2224720	-1.0419749	-1.3145305
C	3.1945758	-0.2076944	-0.8712217
C	4.2330501	-0.4282666	0.1827411
Cl	0.8703492	-4.6757802	2.4196379
Cl	1.0824322	-2.3838100	4.1949715
Cl	3.4911496	-3.5159348	3.0342679
N	0.6377407	2.0352471	-1.0871721
H	1.7053204	-0.7761430	-2.2321856
H	4.1561367	-1.3866205	0.6871962
H	5.2141538	-0.3799901	-0.2999075
H	4.2168460	0.3743186	0.9239086
H	2.4244310	-3.1615865	-1.5035777
H	0.8104875	-2.6177733	-1.0331928
H	0.7055553	-0.8773928	2.4180446
H	-0.8520076	0.8796057	2.0854296
C	-0.8963897	2.4447573	0.6537693
H	-1.6615114	3.0540905	1.1170579
C	-0.2591549	2.8420106	-0.5992450
C	1.3042740	2.3548227	-2.3444457
H	1.6271799	1.4352509	-2.8276397
H	0.6336123	2.8807455	-3.0234956
H	2.1825136	2.9830517	-2.1711409
O	-0.5417500	3.9596775	-1.2496306
C	-1.5743205	4.8487869	-0.7664385
H	-1.3081795	5.2409631	0.2140087
H	-1.6126986	5.6569892	-1.4903156
H	-2.5338515	4.3349002	-0.7322444
H	3.3328384	0.7028429	-1.4438669

**Computational Data for Figure 6**  
**Intermediate 39**

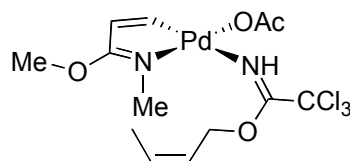


SCF Energy = -2425.4099840110 hartree  
 Zero-Point Energy = 0.3124629 hartree  
 $E_{\text{tot}} = -2425.09752111$  hartree

XYZ Coordinates

Pd	0.7807801	0.3415584	0.1736358
C	0.2060151	1.5570614	-1.2779179
N	1.2803646	-0.9731304	1.8330359
C	2.0886440	-1.9508770	1.8791136
C	2.5512312	-2.6442608	3.1798941
O	2.6612631	-2.5052796	0.8337231
C	2.0945509	-2.3471642	-0.4965692
C	2.0213961	-0.9655511	-1.0797361
C	2.8213827	0.1342983	-0.8695556
C	3.9911245	0.2887895	0.0491126
Cl	2.0224246	-4.3500783	3.1213134
Cl	1.8509081	-1.8654217	4.6215056
Cl	4.3317781	-2.5527030	3.2764185
N	-0.7980782	1.3277683	1.1361503
H	1.4496435	-0.9798641	-2.0036490
H	4.1025273	-0.4997928	0.7875549
H	4.8868498	0.2905446	-0.5815332
H	3.9654171	1.2564868	0.5533927
H	2.7424714	-2.9694261	-1.1144531
H	1.1014859	-2.7985462	-0.4781242
H	0.9381672	-0.7045129	2.7496828
H	0.6997503	1.5723805	-2.2470762
C	-0.8333796	2.3493970	-0.9823507
H	-1.2606019	3.0538609	-1.6844488
C	-1.3675962	2.2082462	0.3684555
C	-1.2290083	1.0954208	2.5056959
H	-0.4222739	1.3551283	3.1967780
H	-2.1059565	1.6850586	2.7661639
H	-1.4698011	0.0386500	2.6395086
O	-2.3843948	2.9247589	0.8344675
C	-3.0332932	3.9036325	-0.0045978
H	-3.4747337	3.4256491	-0.8782648

**Intermediate 40**



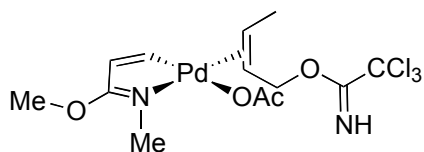
SCF Energy = -2425.4360712300 hartree  
 Zero-Point Energy = 0.3128604 hartree  
 $E_{\text{tot}} = -2425.12321083$  hartree

XYZ Coordinates

Pd	0.7124935	0.8434959	-0.0955601
C	0.2111460	2.0285958	-1.5716730
N	1.3062487	-0.4398148	1.5992323
C	1.1973326	-1.6105908	2.0700532
C	1.9551824	-2.1161968	3.3229582
O	0.4438134	-2.5831003	1.5965839
C	-0.2646042	-2.4221908	0.3244314
C	-0.6846975	-3.7796643	-0.1226111
C	-1.9334086	-4.1827495	-0.3587137
C	-3.2068586	-3.4116042	-0.2081653
Cl	2.9727737	-0.8474882	4.0412182
Cl	2.9948779	-3.4941817	2.8476674
Cl	0.7537567	-2.6516775	4.5397307
N	-1.2274855	1.2958396	0.4570352
H	0.1300379	-4.4767251	-0.2919713
H	-3.9096128	-3.9682518	0.4183183
H	-3.0686667	-2.4243610	0.2312011
H	-3.6913935	-3.2841606	-1.1811533
H	-1.0985653	-1.7440284	0.4863034
H	2.0073497	0.1276695	2.0729423
H	0.9024451	2.2596527	-2.3778556
C	-1.0371354	2.5246989	-1.5404969
H	-1.4549836	3.1800761	-2.2936630
C	-1.8052801	2.1097092	-0.3755913
C	-1.9202420	0.9038219	1.6784149
H	-1.2766168	0.2458514	2.2545548
H	-2.1617621	1.7754187	2.2927420
H	-2.8554833	0.3812444	1.4582759
O	-3.0439465	2.5213033	-0.1060015
C	-3.7098845	3.4339392	-1.0003948
H	-3.8359230	2.9830627	-1.9844276
H	-4.6822615	3.6167792	-0.5518782
H	-3.1563429	4.3693704	-1.0763194

H	-3.8145723	4.3347681	0.6145276
H	-2.3283327	4.6781647	-0.3039253
O	4.1983782	0.3936417	-3.7640494
C	3.1184949	0.8005174	-4.2572967
C	2.6706554	0.2066441	-5.6003322
H	3.4573278	-0.3925646	-6.0584920
H	1.7941118	-0.4273845	-5.4387919
H	2.3706991	1.0034694	-6.2839242
O	2.3441745	1.6510621	-3.7338616
H	2.7483721	0.9026759	-1.6329764

### Intermediate 41



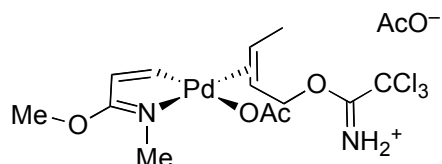
SCF Energy = -2654.4679647350 hartree  
 Zero-Point Energy = 0.3750372 hartree  
 $E_{\text{tot}} = -2654.09292754$  hartree

#### XYZ Coordinates

Pd	0.9542581	-0.0213654	0.3791321
C	0.8422814	-1.8680696	1.0736938
H	0.8041176	-2.1123920	2.1331683
C	0.7770483	-2.8380170	0.1498993
H	0.6867309	-3.8902381	0.3863030
C	0.8369078	-2.3733688	-1.2336630
O	0.7713953	-3.1823464	-2.2891734
N	0.9616729	-1.0971761	-1.4263837
C	1.0537356	-0.5541972	-2.7748691
H	1.6866976	-1.1781506	-3.4085281
H	0.0648833	-0.4815038	-3.2347577
H	1.4798389	0.4433486	-2.7179168
C	0.6778262	-4.6095959	-2.1077784
H	-0.2382957	-4.8692604	-1.5778950
H	0.6517697	-5.0239873	-3.1115163
H	1.5501036	-4.9872169	-1.5750564
O	1.1461389	1.9100780	-0.5088562
C	0.1521610	2.3685067	-1.1936681
O	-0.9383719	1.8030035	-1.3152847
C	0.4141230	3.7072816	-1.8679176
H	0.7190658	4.4479454	-1.1258945
H	1.2363681	3.6066348	-2.5799018
H	-0.4747532	4.0576467	-2.3890457
C	1.8434304	0.7049739	2.2995399

O	2.5948360	0.5935383	-0.8855745
C	3.6127402	0.9243524	-0.1646369
C	4.9638137	0.7198162	-0.8287521
H	4.8676815	0.4312411	-1.8734916
H	5.5465341	1.6388500	-0.7507288
H	5.5073000	-0.0588414	-0.2887687
O	3.5546071	1.3672490	0.9897713
H	-2.0580600	-5.2012414	-0.7173603
H	0.4293759	-1.9661542	-0.3843687

### Intermediate 42



SCF Energy = -2654.4679647350 hartree  
 Zero-Point Energy = 0.3750372 hartree  
 $E_{\text{tot}} = -2654.09292754$  hartree

#### XYZ Coordinates

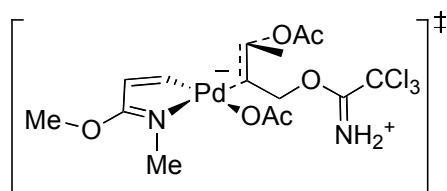
Pd	1.1896326	0.1580405	0.6570329
C	1.4906731	-1.6540326	1.3738619
H	1.7696832	-1.8201963	2.4133199
C	1.3260775	-2.6586333	0.5001109
H	1.4620470	-3.7014773	0.7567224
C	0.9306492	-2.2514486	-0.8422527
O	0.7293919	-3.1023091	-1.8477330
N	0.7650567	-0.9817281	-1.0536837
C	0.3472156	-0.4941180	-2.3600894
H	1.1876731	-0.4738255	-3.0594767
H	-0.4391739	-1.1218900	-2.7844496
H	-0.0282034	0.5187091	-2.2468733
C	0.8717443	-4.5210747	-1.6356519
H	0.1614259	-4.8707566	-0.8871000
H	0.6494994	-4.9774373	-2.5961231
H	1.8913964	-4.7639530	-1.3384968
O	0.6597180	2.0784824	-0.1938437
C	1.3926676	2.5964609	-1.1174666
O	2.4532315	2.1187370	-1.5341116
C	0.8606583	3.9044550	-1.6900994
H	-0.1792233	3.7864896	-1.9994885
H	0.8865439	4.6784432	-0.9186167
H	1.4620469	4.2301522	-2.5367268
C	2.3821852	1.0235006	2.3743303

H	2.2836456	-0.2187581	2.6582267
C	0.4722419	0.8148500	2.3890927
H	-0.0839952	-0.0024238	2.8342091
C	2.8061882	1.8379123	2.1164258
H	2.3701964	2.6792442	1.5833851
H	3.1337593	2.1796945	3.1050592
H	3.6963805	1.5088511	1.5789274
C	-0.2697908	2.1162951	2.3784269
H	-0.1045835	2.6404240	3.3273091
H	0.0412162	2.7614961	1.5573726
O	-1.6715161	1.8121916	2.2637698
C	-2.5369634	2.8309640	2.2917533
N	-2.3314054	4.0716374	2.3636194
H	-1.3442441	4.3140030	2.4025525
C	-3.9749481	2.2783732	2.2393930
Cl	-5.1837293	3.5765590	2.2445236
Cl	-4.1799935	1.2960996	0.7583242
Cl	-4.2369941	1.2394670	3.6869066

H	2.9231670	0.1514832	2.7257391
C	1.0390299	1.0356455	2.6872506
H	0.6467715	0.2221969	3.3021141
C	3.2428965	2.1757390	1.9570187
H	2.6871337	3.0087605	1.5317414
H	3.7839331	2.5382195	2.8383814
H	3.9903233	1.8556430	1.2308712
C	0.2171633	2.2770801	2.6624730
H	0.0920089	2.7006845	3.6602202
H	0.5939375	3.0109551	1.9577436
O	-1.1489889	1.8889700	2.2205677
C	-1.9476255	2.7292045	1.6954277
N	-1.7232592	3.9961574	1.5503259
H	-0.8736864	4.4319174	1.8841646
C	-3.2987055	2.1196991	1.2653571
Cl	-4.2543743	3.2740602	0.3004549
Cl	-3.0013237	0.6571232	0.3148128
Cl	-4.1669419	1.7369907	2.7762680
O	2.2617267	-1.7730791	4.5868173
C	1.1377056	-1.8126439	5.1532946
O	0.1388665	-1.1017612	4.8621093
C	0.9525427	-2.8434504	6.2769013
H	0.2527798	-2.4805612	7.0309490
H	0.5322307	-3.7578481	5.8470221
H	1.9049537	-3.0979013	6.7430666
H	-2.4166197	4.5950613	1.1202469

### Computational Data for Figure 7

#### Transition State 43

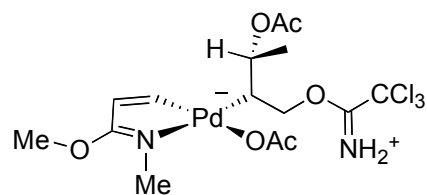


SCF Energy = -2654.4540131090 hartree  
 Zero-Point Energy = 0.3750575 hartree  
 $E_{\text{tot}}$  = -2654.07895561 hartree

#### XYZ Coordinates

Pd	-0.9756113	-0.6739601	0.1770421
C	-2.3829856	-1.0871077	-1.1326998
H	-2.9905218	-0.3334572	-1.6302123
C	-2.5908877	-2.3911796	-1.3875492

#### Intermediate 44



SCF Energy = -2654.4711466270 hartree  
 Zero-Point Energy = 0.3770468 hartree  
 $E_{\text{tot}}$  = -2654.09409983 hartree

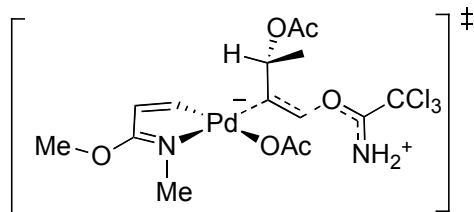
#### XYZ Coordinates

Pd	0.1885986	0.2173607	-0.1431458
C	-1.6757597	0.1993322	-0.7585426
H	-2.4076278	0.9860621	-0.5761200
C	-2.0660440	-0.8903300	-1.4537317



H	-3.3420227	-2.7581729	-2.0754854	H	-3.0675179	-1.0313401	-1.8421155
C	-1.7196945	-3.3083437	-0.6598817	C	-1.0378783	-1.9058573	-1.6609933
O	-1.7815223	-4.6402179	-0.7820663	O	-1.2575938	-3.0484259	-2.3407645
N	-0.8468050	-2.7892024	0.1420876	N	0.1344781	-1.6909594	-1.1657733
C	0.0790428	-3.6270831	0.8874823	C	1.2017937	-2.6579984	-1.3574140
H	0.9428274	-3.0262355	1.1622050	H	2.1345187	-2.2124258	-1.0216100
H	-0.3830142	-3.9983284	1.8068499	H	1.0263586	-3.5687625	-0.7753154
H	0.4116031	-4.4847515	0.2989166	H	1.3037438	-2.9490010	-2.4073393
C	-2.7127855	-5.2377254	-1.7017956	C	-2.5369435	-3.2922837	-2.9447407
H	-2.5156176	-4.9081882	-2.7218535	H	-2.7743688	-2.5230934	-3.6802545
H	-2.5467102	-6.3088245	-1.6241627	H	-2.4445699	-4.2551765	-3.4410552
H	-3.7390150	-5.0038972	-1.4186532	H	-3.3219341	-3.3453684	-2.1895705
O	0.6874067	-0.3433337	1.5279839	O	2.2990642	0.1663801	0.3891712
C	0.6150460	-0.6811137	2.7656886	C	2.7532314	-0.6433290	1.2706912
O	-0.4032066	-1.0919907	3.3372629	O	2.0731482	-1.3984336	1.9813861
C	1.9093390	-0.5144549	3.5549814	C	4.2699619	-0.6198755	1.4551043
H	2.7731489	-0.8073294	2.9573835	H	4.7805908	-0.3698237	0.5251447
H	2.0305646	0.5389104	3.8236000	H	4.5242100	0.1421881	2.1980518
H	1.8767583	-1.0974472	4.4737433	H	4.6246366	-1.5796156	1.8291330
C	-2.2742832	1.5310858	0.6773509	C	-0.7859291	2.0422106	2.0192480
H	-3.2065351	1.1746943	0.2699983	H	-1.7508349	1.5659034	1.8701598
C	-1.1660630	1.4432067	-0.1874341	C	-0.0747722	2.1180111	0.6777690
H	-1.4150003	1.5024508	-1.2428095	H	-0.7224011	2.6760188	-0.0041652
C	-2.2170382	1.7144813	2.1636219	C	-0.0404470	1.3741970	3.1631231
H	-1.8511106	0.8010736	2.6402119	H	0.2808544	0.3760566	2.8648788
H	-1.5606085	2.5351505	2.4534895	H	0.8447907	1.9434182	3.4564013
H	-3.2125768	1.9277349	2.5473649	H	-0.6869436	1.2932831	4.0387020
C	0.0741864	2.1972399	0.1636825	C	1.2342688	2.8566616	0.7909796
H	0.0684067	3.2322859	-0.1803477	H	1.1562709	3.9156403	1.0485322
H	0.2931511	2.1371862	1.2252141	H	1.9241281	2.3463015	1.4583085
O	1.2093774	1.5593672	-0.5688237	O	1.8575229	2.8611725	-0.5711678
C	2.3887546	1.5398562	-0.0993597	C	3.1135149	2.8806361	-0.7388991
N	2.7963630	2.1755408	0.9548371	N	4.0043998	3.0105917	0.1956348
H	2.1853494	2.7872502	1.4783177	H	3.7401332	3.1214961	1.1644472
C	3.4025143	0.7506322	-0.9564823	C	3.5538134	2.8263177	-2.2181479
Cl	2.6592057	-0.7082438	-1.6115976	Cl	2.6050505	1.6208477	-3.0889098
Cl	3.8693874	1.8699759	-2.2756522	Cl	3.2487393	4.4681566	-2.8681659
Cl	4.8445289	0.3141325	-0.0032715	Cl	5.2900628	2.4438715	-2.3656650
O	-3.0162329	3.5044552	0.3654676	O	-1.0824498	3.4251990	2.5138010
C	-3.9189533	3.5984305	-0.5325465	C	-2.2787678	3.9626411	2.2682680
O	-4.4275725	2.6471094	-1.1547754	O	-3.1831833	3.3920323	1.6927145
C	-4.4095444	5.0130280	-0.8450648	C	-2.3681114	5.3795407	2.7730082
H	-5.4723758	5.0820634	-0.6016648	H	-3.4117716	5.6619905	2.8923870
H	-3.8631842	5.7697733	-0.2839888	H	-1.8305931	5.4980079	3.7128900
H	-4.3073995	5.2049386	-1.9151748	H	-1.9087080	6.0434210	2.0360155
H	3.7517146	2.0855408	1.2736588	H	4.9907389	3.0024493	-0.0254168

### Transition State 45

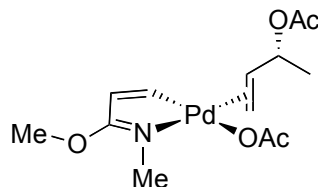


SCF Energy = -2654.4689445840 hartree  
Zero-Point Energy = 0.3760328 hartree  
 $E_{\text{tot}} = -2654.09291178$  hartree

#### XYZ Coordinates

Pd	0.3698607	-1.4008432	0.0050981
C	0.8556540	-1.9887842	-1.8083895
H	0.2195064	-1.9038594	-2.6884752
C	2.0761504	-2.5413778	-1.9450640
H	2.4679184	-2.9062267	-2.8861173
C	2.8689258	-2.6224902	-0.7208352
O	4.1168042	-3.1185360	-0.6901862
N	2.3258695	-2.1829021	0.3662307
C	3.0197919	-2.2060891	1.6430596
H	2.3497106	-2.6151618	2.3993093
H	3.9336245	-2.7985281	1.6112903
H	3.2743597	-1.1856263	1.9441652
C	4.7092828	-3.6556408	-1.8843101
H	4.8116196	-2.8846886	-2.6485486
H	5.6940001	-4.0051981	-1.5852599
H	4.1245936	-4.4925263	-2.2670343
O	0.0320166	-0.6027811	1.9826234
C	-0.0959310	-1.2728763	3.0836538
O	-0.1505979	-2.5001794	3.1454852
C	-0.1594889	-0.4239290	4.3430611
H	0.7984862	0.0813745	4.4878511
H	-0.9251838	0.3487955	4.2486057
H	-0.3725049	-1.0422616	5.2124615
C	-2.7199829	-0.8855641	0.2710701
H	-2.6334473	-1.8314423	0.7999767
C	-1.5259439	-0.7282090	-0.6694569
H	-1.6263541	-1.5115383	-1.4243917
C	-3.0299006	0.2341847	1.2479419
H	-2.2312805	0.3293126	1.9780343
H	-3.1606979	1.1934845	0.7432539
H	-3.9541244	0.0104288	1.7820681

### Intermediate 46



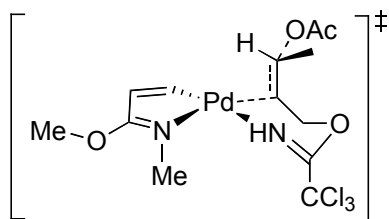
SCF Energy = -2654.5328074670 hartree  
Zero-Point Energy = 0.3751883 hartree  
 $E_{\text{tot}} = -2654.09292754$  hartree

#### XYZ Coordinates

Pd	1.0567107	-0.2478983	-0.1867989
C	1.0917878	0.4038761	-2.0530248
H	1.5525939	1.3417431	-2.3526912
C	0.4756025	-0.3768930	-2.9530532
H	0.4024747	-0.1389740	-4.0062472
C	-0.1140731	-1.5955616	-2.4082858
O	-0.7791592	-2.4885148	-3.1377717
N	0.0239498	-1.8035044	-1.1352496
C	-0.5199397	-3.0021592	-0.5124485
H	-0.3406632	-3.8845171	-1.1299145
H	-0.0383218	-3.1388868	0.4515438
H	-1.5971375	-2.9048403	-0.3520730
C	-0.9055227	-2.3124478	-4.5632306
H	0.0758586	-2.2944118	-5.0361221
H	-1.4653865	-3.1765970	-4.9091435
H	-1.4575638	-1.4006129	-4.7892078
O	1.0520340	-1.1559610	1.7451759
C	-0.0443912	-1.1798072	2.4214221
O	-1.0928067	-0.6163370	2.0841936
C	0.0044267	-1.9941872	3.7053964
H	-0.3014205	-3.0196078	3.4785803
H	1.0110416	-2.0285136	4.1205732
H	-0.6931610	-1.5897058	4.4377542
C	0.9461721	2.1833912	1.8617458
H	-0.0414119	1.7240887	1.9117332
C	1.6311445	1.8134360	0.5633161
H	1.3341171	2.4411340	-0.2691847
C	1.7266577	1.8823230	3.1286628
H	1.9072150	0.8111962	3.2099567
H	2.6858766	2.4027702	3.1248328
H	1.1542096	2.1994333	4.0003894
C	2.7470795	1.0296890	0.4244471

C	-1.4863317	0.5242845	-1.4332468
H	-1.1206173	0.4143368	-2.4455678
H	-2.3690280	1.1587245	-1.4013429
O	-0.3998727	1.7237099	-1.0617695
C	-0.0910756	2.3492625	-0.0087176
N	-0.0431687	1.9158000	1.2107969
H	-0.1161968	0.9029311	1.5111735
C	0.2926725	3.8344626	-0.2962691
Cl	1.6287519	3.8424971	-1.4744755
Cl	-1.1512268	4.6291827	-0.9829480
Cl	0.8025509	4.7217998	1.1650474
O	-3.9569366	-0.9812515	-0.5544203
C	-4.3395397	-2.1777968	-1.0122735
O	-3.7477765	-3.2133790	-0.7899775
C	-5.5905504	-2.0740193	-1.8433775
H	-5.9332354	-3.0676314	-2.1209384
H	-6.3700932	-1.5492728	-1.2897096
H	-5.3801571	-1.4951066	-2.7451917
H	0.2355524	2.5725879	1.9278735

#### Transition State 47



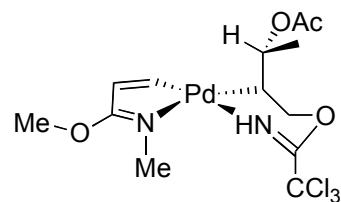
SCF Energy = -2425.4024311240 hartree  
 Zero-Point Energy = 0.3119580 hartree  
 $E_{\text{tot}}$  = -2425.090447312 hartree

#### XYZ Coordinates

Pd	-0.2486590	0.4825243	-1.0819138
N	-0.0194813	2.4670210	-1.7793502
C	-0.2566510	0.1693718	-3.0359897
C	-0.1244630	1.2649073	-3.8008110
C	0.0118622	2.5251825	-3.0739973
O	0.1652673	3.7049540	-3.6771557
C	0.1799607	3.7914494	-5.1155725
H	-0.7649297	3.4433193	-5.5317248
H	1.0126566	3.2215641	-5.5267607
C	0.1017068	3.6526373	-0.9472143
H	0.0627163	4.5735761	-1.5266468
C	-1.3819577	-1.6497774	0.7898148
O	-0.6407181	-1.1224342	1.9383687

H	3.3360576	1.0709531	-0.4822546
H	3.2055683	0.5438347	1.2755593
O	1.9616822	3.8910881	-2.4267779
C	1.4294273	4.9742862	-2.5651432
N	1.7051484	6.0679155	-1.8509223
H	2.4230797	6.0105284	-1.1447940
C	0.2701839	5.1130909	-3.6166382
Cl	-0.0867719	6.8096432	-4.0771715
Cl	0.6991141	4.2027181	-5.0808145
Cl	-1.1894267	4.4008663	-2.8576008
O	0.7561180	3.6312030	1.7511565
C	-0.3394995	4.1765295	2.3110699
O	-1.1832144	3.5399759	2.8983805
C	-0.3633783	5.6663764	2.1111992
H	-1.2852818	6.0770247	2.5142085
H	0.4928788	6.1163033	2.6171384
H	-0.2813553	5.9032519	1.0495614
H	1.2803992	6.9611809	-2.0347607

#### Intermediate 48



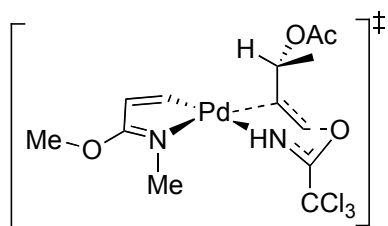
SCF Energy = -2425.4272827580 hartree  
 Zero-Point Energy = 0.3150313 hartree  
 $E_{\text{tot}}$  = -2425.11225146 hartree

#### XYZ Coordinates

Pd	-0.1823845	2.1945844	-1.1046399
N	0.5776437	3.8798764	-2.2504613
C	0.0409494	1.3475214	-2.8834027
C	0.5383621	2.1411747	-3.8523519
C	0.8355312	3.5189303	-3.4646159
O	1.3665782	4.4152056	-4.3125400
C	1.6090773	4.0634102	-5.6852512
H	0.6815842	3.7828535	-6.1848315
H	2.3366267	3.2547885	-5.7564742
C	0.8506801	5.2388115	-1.8125470
H	0.6638091	5.9736271	-2.5979689
C	-1.7193667	0.7406484	0.9959118
O	-0.9943192	1.4192405	2.0939703
C	-0.4977655	2.6169774	1.9174559

C	-0.2875616	0.1382686	2.0043378
N	-0.2194815	0.9372220	1.0182941
C	0.0509878	0.5253293	3.4623480
Cl	1.3293098	-0.5650555	4.0672739
Cl	-1.4301204	0.3437292	4.4481427
Cl	0.6245677	2.2091045	3.5814435
C	-0.7361034	-1.5424755	-0.5645246
C	0.5644863	-1.9540617	-0.8592076
C	1.7162658	-2.0362281	0.0910877
O	0.3369318	-4.2288626	-0.9068251
C	0.2526514	-4.6761627	-2.0924268
O	0.4418379	-4.0165210	-3.1383243
C	-0.0948193	-6.1607152	-2.2393148
H	0.3124860	4.8468308	-5.3363616
H	-0.7124618	3.6689222	-0.2191506
H	1.0481578	3.6287443	-0.3991991
H	-0.3656700	-0.8101422	-3.4952340
H	-0.1179913	1.2426945	-4.8829581
H	0.0572459	1.8748871	1.2889291
H	-0.8842609	-6.2852451	-2.9828529
H	0.7857359	-6.6952392	-2.6051229
H	-0.4064139	-6.6002420	-1.2925768
H	1.4161535	-2.3949489	1.0740224
H	2.4721317	-2.7057936	-0.3128369
H	2.1786174	-1.0522887	0.2134040
H	0.7954942	-2.0872529	-1.9051080
H	-1.5211800	-2.6945445	1.0679759
H	-2.3516202	-1.1517259	0.7876290
H	-1.4703632	-1.7606110	-1.3366603

#### Transition State 49



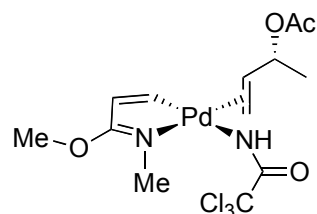
SCF Energy = -2425.4069625700 hartree  
 Zero-Point Energy = 0.3122428 hartree  
 $E_{\text{tot}}$  = -2654.09471977 hartree

#### XYZ Coordinates

Pd	-0.2259162	0.6361316	-0.8674273
N	0.0950368	2.7155606	-0.8434210
C	-0.4515315	1.0513166	-2.7968493

N	-0.3003433	3.1704313	0.7896579
C	-0.1817116	3.2782161	3.2779690
Cl	0.9396176	2.2266419	4.1906042
Cl	-1.7139493	3.4662553	4.1859292
Cl	0.5694706	4.8834775	3.0792555
C	-0.9385790	0.4564441	-0.2671778
C	0.0782153	-0.6693116	-0.1747794
C	1.2497973	-0.4757586	0.7759339
O	-0.6520359	-1.8884501	0.2674350
C	-0.3000070	-3.0739883	-0.2352192
O	0.5851275	-3.2351526	-1.0509898
C	-1.1239736	-4.1905854	0.3493691
H	2.0146229	4.9609943	-6.1447731
H	0.2080428	5.4772143	-0.9648620
H	1.8915761	5.3473468	-1.4891290
H	-0.1971119	0.3154827	-3.1374542
H	0.7183811	1.8100982	-4.8677994
H	0.0686820	4.1113837	0.8687007
H	-1.0004649	-5.0916464	-0.2467134
H	-0.7804194	-4.3874088	1.3679585
H	-2.1756114	-3.9100105	0.4018699
H	0.9116592	-0.3481203	1.8047558
H	1.9175638	-1.3378657	0.7349737
H	1.8174431	0.4096960	0.4856017
H	0.4545333	-0.8880711	-1.1712585
H	-1.7028002	0.1399842	-0.9857105
H	-2.0573438	-0.1645364	1.5006562
H	-2.5828184	1.3688732	0.7744111

#### Intermediate 50



SCF Energy = -2425.4447965660 hartree  
 Zero-Point Energy = 0.3126645 hartree  
 $E_{\text{tot}}$  = -2425.13213207 hartree

#### XYZ Coordinates

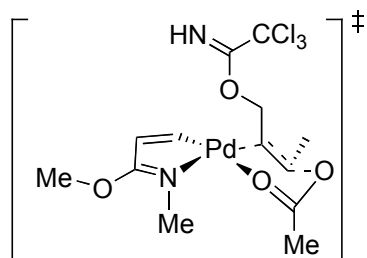
Pd	0.3980017	2.0107247	-1.2185745
N	1.0927338	3.6932911	-2.2566531
C	0.3778223	1.3083704	-3.0809841

C	-0.2768542	2.3414573	-3.1377691
C	0.0342359	3.2364133	-2.0299132
O	0.2641687	4.5445528	-2.1837715
C	0.1337788	5.1524643	-3.4822693
H	-0.8780786	5.0277499	-3.8674921
H	0.8607025	4.7343718	-4.1784677
C	0.4023008	3.5181926	0.3294425
H	0.2662726	4.5831488	0.1454262
C	-1.2597607	-2.1417826	-0.2348860
O	-1.1031105	-1.4939127	1.6497660
C	-0.3302571	-0.5526236	1.9746835
N	0.1454172	0.3627122	1.1957345
C	0.0518174	-0.5828269	3.4956696
Cl	0.9695369	-2.0902616	3.8112222
Cl	-1.4472699	-0.5766655	4.4735322
Cl	1.0599154	0.8083139	4.0129071
C	-0.5635286	-1.4969126	-1.2712361
C	0.7297881	-2.1156227	-1.7679077
C	1.7986378	-2.3458551	-0.7153897
O	0.4545747	-3.4590731	-2.3367459
C	0.0296725	-3.5378239	-3.6032485
O	-0.1227190	-2.5767244	-4.3281737
C	-0.2577473	-4.9589020	-4.0056465
H	0.3399635	6.2078415	-3.3268635
H	-0.2503929	3.2185470	1.1496397
H	1.4383886	3.3529030	0.6415635
H	-0.6748018	0.3247820	-3.5758980
H	-0.3477006	2.7152909	-4.1511952
H	0.7577327	1.0160968	1.6653322
H	-0.2822699	-5.0356669	-5.0901832
H	0.4823639	-5.6417735	-3.5904037
H	-1.2359267	-5.2434383	-3.6096176
H	1.4329319	-2.9726724	0.1002126
H	2.6662838	-2.8348590	-1.1598421
H	2.1134580	-1.3907101	-0.2956037
H	1.1268156	-1.5173651	-2.5842841
H	-1.2495155	-1.2181111	-2.0693229
H	-0.8937574	-3.0643376	0.1932318
H	-2.3275948	-1.9977381	-0.1623091

**Transition State 51**

C	0.7754874	2.1683039	-4.0297154
C	1.1651465	3.4862084	-3.5364535
O	1.5817794	4.4776828	-4.3178437
C	1.6775313	4.2913533	-5.7453222
H	0.6984854	4.0690462	-6.1684878
H	2.0399271	5.2391088	-6.1325544
C	1.4580454	4.9948650	-1.7102321
H	1.2959753	4.9785764	-0.6373103
O	-1.7757098	3.3275265	0.9881145
C	-0.5932652	3.4088475	1.3341686
N	0.4555495	2.9383039	0.7026270
H	1.3393713	3.1281504	1.1542170
C	-0.3670660	4.1711299	2.7065667
Cl	-1.2671972	3.2986887	3.9899818
Cl	-1.0241764	5.8314471	2.5431424
Cl	1.3511094	4.3049683	3.2307223
C	-0.8861886	0.3738294	-0.4582982
H	-1.5203175	0.1899893	-1.3160715
C	0.3927467	-0.1168285	-0.4296472
H	0.7647414	-0.6585800	-1.2910756
C	1.2645938	-0.2860794	0.7970151
H	2.0297968	0.4897169	0.8285447
H	-1.3790901	0.7444609	0.4293120
O	1.9506891	-1.5562326	0.5820984
C	3.2231574	-1.6725340	1.0111941
O	3.8353198	-0.7731728	1.5398794
C	3.7575710	-3.0531006	0.7612960
H	3.5262592	-3.3762369	-0.2535135
H	4.8314712	-3.0669740	0.9290933
H	3.2755512	-3.7505023	1.4502866
C	0.5257418	-0.3425258	2.1227637
H	-0.2014827	-1.1559772	2.1244735
H	1.2349014	-0.4965958	2.9359520
H	0.0020268	0.5948826	2.3041397
H	2.3874732	3.4994710	-5.9809464
H	0.8491310	5.7904207	-2.1473351
H	0.0562471	0.3049986	-3.3522584
H	2.5088873	5.2227969	-1.9076970
H	0.8073990	1.9335608	-5.0858674

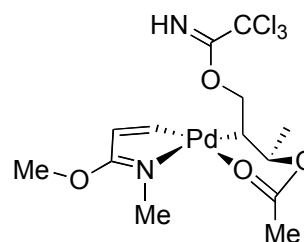
**Intermediate 52**



SCF Energy = -2425.3930211520 hartree  
 Zero-Point Energy = 0.3123850 hartree  
 $E_{\text{tot}} = -2425.08063615$  hartree

XYZ Coordinates

Pd	0.0850095	-2.0958273	0.0856121
N	-0.5935654	-4.0190247	-0.4272686
C	0.8432999	-2.2532461	-1.7289450
C	0.5960587	-3.4131646	-2.3659972
C	-0.2071163	-4.3698364	-1.6121216
O	-0.5654276	-5.5719681	-2.0741937
C	-0.1421122	-5.9999063	-3.3821735
C	-1.4106836	-4.9133982	0.3801818
C	1.3772075	0.1254067	1.6292898
C	0.8304411	-0.0739975	0.3271511
O	-0.8608405	-2.1471699	2.0018292
C	-0.1962148	-1.8642569	3.0347864
O	0.9176963	-1.2665741	3.0373667
C	-0.7717872	-2.2488736	4.3811185
H	-1.1723762	-1.3502306	4.8570380
H	-1.5708472	-2.9788904	4.2713128
H	0.0136478	-2.6415187	5.0265605
H	-0.8836873	-5.8478399	0.5949969
H	-1.6418816	-4.4150968	1.3174871
H	-2.3458025	-5.1642850	-0.1289821
H	0.9453283	-6.0453637	-3.4396806
H	-0.5578605	-6.9960407	-3.5068763
H	-0.5371619	-5.3374154	-4.1522459
H	0.9511473	-3.6440938	-3.3623089
H	1.4345453	-1.4888797	-2.2301132
H	2.3953299	-0.2174284	1.7526640
H	1.6339113	-0.1701871	-0.4007723
C	-0.2997053	0.7963907	-0.1437085
H	-1.1390161	0.8011231	0.5542949
H	-0.6563982	0.4749729	-1.1217203
C	0.9729287	1.2407383	2.5328101
H	1.3816579	1.1205907	3.5322058
H	1.3767831	2.1618009	2.0987807



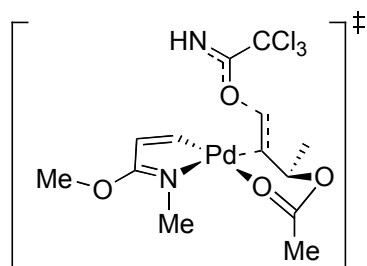
SCF Energy = -2425.4133719460 hartree  
 Zero-Point Energy = 0.3147379 hartree  
 $E_{\text{tot}} = -2425.09863405$  hartree

XYZ Coordinates

Pd	0.1038599	2.3686500	-2.0899257
N	-1.8482459	1.4675781	-2.3036220
C	0.6151108	0.4978400	-2.4623854
C	-0.4063367	-0.3603521	-2.6545919
C	-1.7494029	0.2077291	-2.5626661
O	-2.8686848	-0.5123936	-2.7358363
C	-2.7880256	-1.9195079	-3.0216804
H	-2.3053873	-2.4547543	-2.2037232
H	-2.2552452	-2.0961093	-3.9562929
C	-3.1532328	2.1010013	-2.2028293
H	-3.7597928	1.6505891	-1.4108363
C	3.1289224	2.3482648	-2.3827078
H	3.1524904	1.3845773	-1.8769259
H	3.0807428	2.1873812	-3.4617902
O	4.4160607	3.0102897	-2.0976041
C	5.5379893	2.3944249	-2.4619869
N	5.7159552	1.2879675	-3.0430113
H	4.8419583	0.8123003	-3.2554806
C	6.7531605	3.2561788	-2.0584681
Cl	6.7371482	3.4806914	-0.2757806
Cl	6.6211410	4.8612925	-2.8574171
Cl	8.2921501	2.5104909	-2.5275788
C	1.9988883	3.1944446	-1.8635541
C	2.0408687	4.6014790	-2.4602434
C	1.6684409	4.7427228	-3.9276629
H	2.3522322	4.1473420	-4.5353925
H	0.6544910	4.3941762	-4.1242700
H	1.7613432	5.7829467	-4.2452258
O	-0.6665750	4.3475382	-1.6272869
C	-0.0316232	5.3708683	-1.3811706
O	1.2383846	5.5612370	-1.6624577
C	-0.6681579	6.5608227	-0.7293520
H	-1.6048195	6.2719969	-0.2596696
H	0.0079526	7.0027645	0.0015871

H	-0.1090840	1.3608628	2.5912935
O	0.1676116	2.1852805	-0.2921699
C	-0.6957263	3.0868552	-0.7595957
C	0.0038475	4.4572410	-0.8807989
Cl	0.5914860	4.9583651	0.7428500
Cl	1.4056795	4.2994761	-1.9930816
Cl	-1.0829926	5.7118938	-1.5041588
N	-1.9078881	2.9681260	-1.0891187
H	-2.2607746	2.0215998	-0.9664755

### Transition State 53



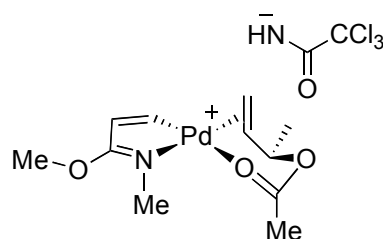
SCF Energy = -2425.3950919570 hartree  
 Zero-Point Energy = 0.3121878 hartree  
 $E_{\text{tot}}$  = -2425.08290416 hartree

#### XYZ Coordinates

Pd	-2.0861857	-0.1042640	0.0277261
N	-4.0424331	-0.7281014	-0.4841793
C	-2.1421319	-1.8515427	0.9358255
C	-3.2955395	-2.5294493	0.8272473
C	-4.3251460	-1.8875329	0.0145681
O	-5.5199753	-2.4254402	-0.2332291
C	-5.8613101	-3.7164087	0.3098170
H	-5.8603530	-3.6868400	1.3991808
H	-5.1744646	-4.4803672	-0.0533930
C	-5.0052131	-0.0242183	-1.3189802
H	-5.9559777	0.1178197	-0.7979012
C	0.4739549	-0.5928723	0.0513287
H	0.4129344	-1.5601392	0.5178410
H	0.6642981	-0.5931429	-1.0106862
O	2.4182896	-0.4582432	0.5062663
C	3.3193026	-0.7884337	-0.3447528
N	3.2808389	-1.5182129	-1.4002932
H	2.3442815	-1.9012859	-1.5211120
C	4.7082685	-0.1639343	0.0173498
Cl	5.2131396	-0.7902836	1.6299761
Cl	4.5407155	1.6278862	0.1220837
Cl	6.0005825	-0.5310470	-1.1534108

H	-0.8682742	7.3126762	-1.4967072
H	2.1337482	3.2945047	-0.7794019
H	3.0346961	5.0273566	-2.3122259
H	1.6238569	0.0981978	-2.5257060
H	-3.7142947	2.0177165	-3.1388165
H	-0.2663087	-1.4132439	-2.8661756
H	-3.0097133	3.1548708	-1.9750294
H	-3.8176635	-2.2534677	-3.1196503

### Intermediate 54



SCF Energy = -2425.4074997690 hartree  
 Zero-Point Energy = 0.3126157 hartree  
 $E_{\text{tot}}$  = -2425.09488407 hartree

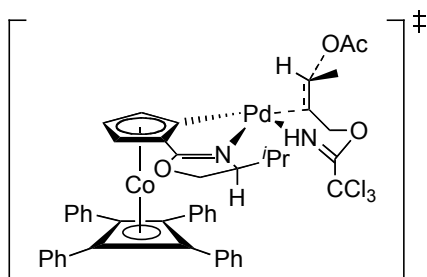
#### XYZ Coordinates

Pd	-1.5947667	-0.3333400	-0.7008802
N	-3.6053570	-0.7354980	-0.3062847
C	-1.5086284	-2.2836050	-0.4163540
C	-2.6655161	-2.8771560	-0.1042358
C	-3.8251729	-1.9919065	-0.0700391
O	-5.0626473	-2.3917354	0.1824312
C	-5.3409666	-3.7870292	0.4369617
H	-4.8175641	-4.1213706	1.3317583
H	-5.0632697	-4.3932698	-0.4241437
C	-4.7073547	0.2185913	-0.3208431
H	-5.2151900	0.2438281	0.6466183
C	0.3453392	-0.5470355	-1.7916038
H	0.5598091	-1.6042455	-1.7633582
H	0.2048074	-0.1232934	-2.7775963
O	3.7620444	1.4710633	0.4695660
C	3.5433192	0.5412719	1.2846213
N	2.6681600	0.4087580	2.2360714
H	2.1231302	1.2724156	2.2669758
C	4.5020253	-0.6961993	1.0928456
Cl	6.2093544	-0.1406821	1.2496511
Cl	4.2691378	-1.3517795	-0.5763481
Cl	4.2560585	-2.0431247	2.2456478
C	0.5639513	0.2509203	-0.6987254

C	-0.1334383	0.5201350	0.6576894
C	0.2505520	1.8903844	0.1272338
C	0.6224691	1.9894211	-1.3441073
H	1.5649937	1.4708630	-1.5147841
H	-0.1353535	1.5633189	-2.0010239
H	0.7717565	3.0360684	-1.6119265
O	-2.4181016	1.9345134	-0.7010656
C	-1.9518352	2.9049234	-0.1020405
O	-0.7579301	2.9315172	0.4496719
C	-2.7060824	4.1897549	0.0367230
H	-3.7715292	3.9862293	0.1200611
H	-2.3513480	4.7628362	0.8905028
H	-2.5383346	4.7798036	-0.8684434
H	-0.1859168	0.4888641	1.7446512
H	1.0907647	2.2497959	0.7215430
H	-1.3341838	-2.2456207	1.5457370
H	-5.2054152	-0.5768558	-2.2416294
H	-3.4730992	-3.4803180	1.3130976
H	-4.5956575	0.9494257	-1.5748359
H	-6.8648857	-3.9226423	-0.0511498

C	0.8060860	1.7376244	-0.8144847
C	0.6419038	2.3729925	-2.1837742
H	1.3796554	1.9529365	-2.8680540
H	-0.3509764	2.2290882	-2.6102040
H	0.8379374	3.4424446	-2.1051049
O	-1.9538590	1.8340815	-0.5238029
C	-1.2472428	2.5925131	0.1438244
O	0.0655564	2.5224845	0.1941325
C	-1.8148339	3.7065684	0.9616553
H	-2.8577930	3.5083822	1.1943123
H	-1.2323299	3.8460699	1.8709332
H	-1.7487088	4.6281764	0.3770545
H	0.9121567	-0.1885060	0.2315616
H	1.8364811	1.8746499	-0.4697784
H	-0.5757320	-2.8354083	-0.4463600
H	-5.4410187	-0.0453538	-1.0865965
H	-2.7443488	-3.9323529	0.1218288
H	-4.3097463	1.2060347	-0.5345780
H	-6.4139307	-3.8381039	0.5952498

**Computational Data for Figure 8**  
**Transition State 55**

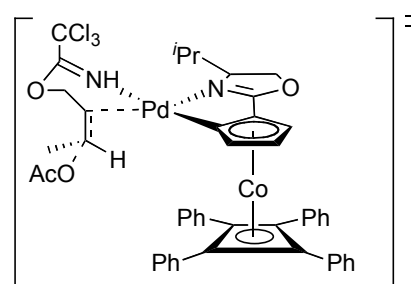


SCF Energy = -5117.1171909120 hartree  
Heat Capacity at 298K = 0.715711132 hartree  
 $G_{\text{tot}}$  = -5116.40147978 hartree

XYZ Coordinates

Pd	0.0507650	-0.9057408	1.4252447
N	2.1433611	-1.2350871	0.9435335
C	-0.1437286	-1.6869348	-0.4065585
C	1.1124447	-1.9439435	-1.0558652
C	2.2751399	-1.5982314	-0.2924157
C	0.8846666	-2.5036529	-2.3515176
C	-1.1537596	-2.0752496	-1.3233580
C	-0.5223031	-2.5894653	-2.5036573

**Transition State 56**



SCF Energy = -5117.1143859220 hartree  
Heat Capacity at 298K = 0.715252804 hartree  
 $G_{\text{tot}}$  = -5116.399133118 hartree

XYZ Coordinates

Pd	0.1305585	-0.9897365	1.5346677
N	2.2340168	-0.9882827	1.0122168
C	0.0053529	-1.6617931	-0.3481857
C	1.2846145	-1.8129581	-0.9854886
C	2.4049858	-1.3513160	-0.2190243
C	1.1180697	-2.4061288	-2.2765173
C	-0.9595931	-2.1368853	-1.2725810

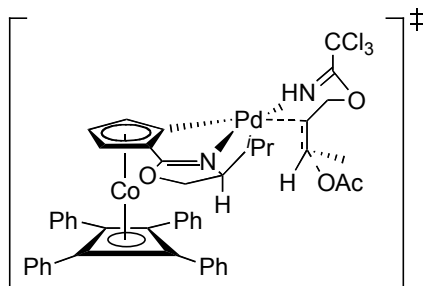


Co	0.0583276	-0.5958919	-2.2471744	C	-0.2758629	-2.6092744	-2.4414884
C	-0.6584766	1.2670187	-2.3821935	Co	0.1475760	-0.5741753	-2.2183375
C	-0.6246194	0.6003744	-3.6819865	C	-0.7210679	1.2168000	-2.4827189
C	0.8327359	0.5880448	-3.6404725	C	-0.5293285	0.5103460	-3.7456488
C	0.7986291	1.2611633	-2.3419603	C	0.9156064	0.6296103	-3.5977158
O	3.5129459	-1.6113766	-0.7897784	C	0.7226903	1.3376727	-2.3301422
C	4.3527138	-0.9745726	0.2247662	O	3.6411681	-1.2468012	-0.7105731
C	3.4951263	-1.0269440	1.5068189	C	4.4031272	-0.5061534	0.2945379
C	1.8802712	0.2986546	-4.6208218	C	3.5582942	-0.6443271	1.5776234
C	3.1159626	-0.2870896	-4.2440501	C	2.0454941	0.4234398	-4.5058878
C	4.1221055	-0.5285718	-5.1972663	C	3.3047097	-0.0429266	-4.0506157
C	3.9129929	-0.1880215	-6.5563850	C	4.3830782	-0.2000140	-4.9409849
C	2.6851030	0.3984542	-6.9422236	C	4.2248299	0.1080668	-6.3143797
C	1.6824725	0.6379640	-5.9826938	C	2.9735296	0.5763832	-6.7788352
C	-1.6076438	0.2974973	-4.7190165	C	1.8987752	0.7311650	-5.8823244
C	-1.4080594	-0.7789529	-5.6226724	C	-1.3959011	0.0856856	-4.8403461
C	-2.3429050	-1.0547781	-6.6361408	C	-1.0339043	-1.0030399	-5.6761215
C	-3.5046166	-0.2541629	-6.7709111	C	-1.8546220	-1.3970527	-6.7472989
C	-3.7094800	0.8247608	-5.8794874	C	-3.0632641	-0.7056511	-7.0101376
C	-2.7690874	1.0959344	-4.8665606	C	-3.4301754	0.3844159	-6.1873535
C	-1.7146787	1.9210042	-1.6130445	C	-2.6033054	0.7737045	-5.1158740
C	-2.9917310	1.3253645	-1.4531560	C	-1.8875115	1.8429275	-1.8632993
C	-4.0188243	1.9909951	-0.7574381	C	-3.1249588	1.1616575	-1.7528087
C	-3.7890228	3.2710728	-0.1963779	C	-4.2634437	1.8113230	-1.2412537
C	-2.5174527	3.8732743	-0.3486279	C	-4.1855549	3.1616690	-0.8191401
C	-1.4960190	3.2040733	-1.0520593	C	-2.9511496	3.8475561	-0.9162934
C	1.7999962	1.8606189	-1.4680508	C	-1.8176598	3.1926003	-1.4338082
C	3.0455552	2.2966174	-1.9853814	C	1.5889146	2.0479920	-1.3983641
C	4.0093407	2.8944186	-1.1499419	C	2.8445440	2.5572846	-1.8131783
C	3.7439580	3.0776761	0.2290765	C	3.6738983	3.2615200	-0.9175485
C	2.4991903	2.6531914	0.7550062	C	3.2586058	3.4794799	0.4187510
C	1.5446708	2.0531244	-0.0856449	C	2.0017115	2.9812981	0.8417010
C	3.9307399	-2.1581881	2.4661969	C	1.1821367	2.2750199	-0.0575249
C	5.3133126	-1.8559150	3.0556078	C	4.1215589	-1.7206496	2.5347123
C	2.9277870	-2.4146536	3.5909754	C	5.4581092	-1.2543423	3.1245663
C	-2.2701655	0.7664187	2.4840382	C	3.1612610	-2.1046882	3.6598805
O	-1.7596721	0.7438849	3.8570148	H	2.9732289	-1.2560163	4.3237987
C	-0.4945147	0.5372737	4.1270407	H	2.2051189	-2.4626119	3.2795412
N	0.3553953	0.0134674	3.3397302	H	3.5992045	-2.8982478	4.2692508
C	-0.1750863	1.0140666	5.5631907	H	4.3029619	-2.6161280	1.9275172
Cl	-1.2343844	0.1477743	6.7084471	H	5.3163805	-0.3659709	3.7472266
Cl	-0.4815244	2.7740928	5.6471205	H	5.8864673	-2.0365130	3.7544116
Cl	1.5261987	0.7054350	6.0016525	H	6.1955067	-1.0103243	2.3580025
C	-2.0158978	-0.4312306	1.6117169	H	3.4961049	0.3145224	2.0985258
C	-2.2981198	-1.7525390	1.9726746	H	5.3878819	-0.9591732	0.3535760
C	-2.3316762	-2.3310670	3.3503554	H	4.4813039	0.5238305	-0.0531359

O	-4.5996358	-1.7225012	1.8600200	H	1.8930693	-2.6435960	-2.9872239
C	-5.0404563	-1.8289096	0.6734517	H	-0.7493689	-3.0224679	-3.3186091
O	-4.3730842	-2.1664091	-0.3279350	H	-2.0316810	-2.1429725	-1.1319928
C	-6.5181735	-1.4799567	0.4700575	H	0.2229828	1.8887715	0.2856587
H	1.2805368	-0.0525382	3.7481344	H	1.6664095	3.1546586	1.8663189
H	-6.5908415	-0.4267315	0.1833607	H	3.8959664	4.0322333	1.1124004
H	-6.9459399	-2.0752104	-0.3369575	H	4.6346014	3.6527486	-1.2584506
H	-7.0931210	-1.6199720	1.3852374	H	3.1733814	2.4213823	-2.8423448
H	-2.6654258	-1.6136844	4.0973438	H	3.4418468	-0.2986419	-3.0000351
H	-3.0023002	-3.1876232	3.3610611	H	0.9449379	1.1036899	-6.2541649
H	-1.3387895	-2.6894647	3.6357348	H	2.8421209	0.8212287	-7.8348278
H	-2.3657189	-2.4554432	1.1579325	H	5.0605348	-0.0145472	-7.0070558
H	-3.3406046	0.8969868	2.6407172	H	5.3446959	-0.5643321	-4.5739084
H	-1.8729161	1.6682250	2.0176992	H	-0.1113105	-1.5499596	-5.4833124
H	-2.2735282	-0.1797805	0.5885004	H	-1.5628560	-2.2396633	-7.3774935
H	2.8648833	-1.5537431	4.2637933	H	-3.7039241	-1.0113124	-7.8404293
H	1.9311005	-2.6338981	3.2087291	H	-4.3566170	0.9273722	-6.3854576
H	3.2496731	-3.2650346	4.1955203	H	-2.8970682	1.6227089	-4.5005192
H	3.9999869	-3.0719636	1.8634620	H	-5.2066726	1.2679592	-1.1590898
H	5.2825706	-0.9493463	3.6672959	H	-3.2034123	0.1161131	-2.0506670
H	5.6393354	-2.6782340	3.6954262	H	-0.8803190	3.7409024	-1.5220378
H	6.0769419	-1.7147981	2.2886168	H	-2.8814102	4.8893887	-0.5969517
H	3.5313438	-0.0675271	2.0289575	H	-5.0685656	3.6666135	-0.4215493
H	5.2784084	-1.5391624	0.2798818	C	-2.0067489	-1.7936143	3.5252687
H	4.5524511	0.0429760	-0.1114169	O	-1.6668977	-0.7256248	4.4686240
H	1.6300851	-2.7940911	-3.0740450	C	-0.4911005	-0.1473634	4.4591982
H	-1.0369177	-2.9545943	-3.3789692	N	0.3556034	-0.2138533	3.5140054
H	-2.2215501	-2.0078023	-1.1687007	C	-0.2719616	0.6467890	5.7669198
H	0.5975437	1.7201732	0.3374983	Cl	-0.2795565	-0.5070921	7.1318661
H	2.2796592	2.7992063	1.8145947	Cl	-1.5915154	1.8331192	5.9576714
H	4.4869185	3.5476594	0.8771186	Cl	1.2867325	1.5169407	5.7527589
H	4.9603579	3.2294728	-1.5689424	C	-1.8775776	-1.4987682	2.0560982
H	3.2621058	2.1862672	-3.0467148	C	-2.3722800	-0.3558220	1.4279008
H	3.2890706	-0.5676788	-3.2047752	C	-2.6143445	0.9831534	2.0463883
H	0.7471334	1.1015302	-6.2943355	O	-4.6349761	-0.7947844	1.4029799
H	2.5159769	0.6689346	-7.9865597	C	-4.9927309	-1.5427014	0.4426287
H	4.6925073	-0.3763505	-7.2981083	C	-6.4822154	-1.9005676	0.3756029
H	5.0661392	-0.9835677	-4.8908190	O	-4.2471452	-2.0020924	-0.4499059
H	-0.5242752	-1.4088229	-5.5272907	H	-3.0467760	-2.0005170	3.7784835
H	-2.1764010	-1.8896911	-7.3197467	H	-1.3990547	-2.6568133	3.7973530
H	-4.2334310	-0.4682823	-7.5558842	H	1.2085756	0.2960072	3.7125976
H	-4.5984580	1.4508423	-5.9792712	H	-2.0064893	-2.4166350	1.4897511
H	-2.9371954	1.9390982	-4.1983898	H	-1.6912257	1.5678392	2.0686143
H	-4.9953727	1.5135625	-0.6450358	H	-3.3308655	1.5305470	1.4403219
H	-3.1858655	0.3322287	-1.8586585	H	-2.9930785	0.9057456	3.0635437
H	-0.5307145	3.6931961	-1.1779305	H	-6.9196029	-1.4379176	-0.5129572

H -2.3308213 4.8633780 0.0722834  
H -4.5846310 3.7876213 0.3449668

### Transition State 57



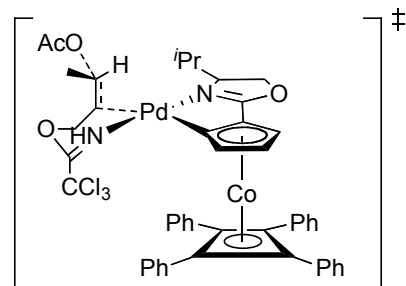
SCF Energy = -5117.1066540870 hartree  
Heat Capacity at 298K = 0.717157219 hartree  
G<sub>tot</sub> = -5116.389496868 hartree

#### XYZ Coordinates

Pd	0.4013332	-0.9950022	1.5799546
N	2.2993860	-1.2955378	0.7512161
C	-0.1354422	-1.7577132	-0.2314149
C	0.9944514	-1.9936356	-1.0827535
C	2.2566629	-1.6419718	-0.4992906
C	0.5707841	-2.5701962	-2.3201511
C	-1.2722379	-2.1621897	-0.9738000
C	-0.8400264	-2.6790581	-2.2418105
Co	-0.2650430	-0.6764885	-2.1124733
C	-0.8939314	1.2289933	-2.1325017
C	-1.2758083	0.5057064	-3.3444908
C	0.1314798	0.4089794	-3.7260117
C	0.5064564	1.1336389	-2.5157126
O	3.4119917	-1.6428931	-1.1576021
C	4.3765422	-1.0061011	-0.2507275
C	3.7283926	-1.1575739	1.1366472
C	0.8547018	0.0015925	-4.9290061
C	2.1657093	-0.5371456	-4.8522936
C	2.8684469	-0.8977405	-6.0158142
C	2.2722876	-0.7266112	-7.2899820
C	0.9681257	-0.1866140	-7.3774249
C	0.2701560	0.1734654	-6.2080753
C	-2.5348977	0.2390188	-4.0341216
C	-2.6855810	-0.8881851	-4.8831446
C	-3.8910025	-1.1241570	-5.5670202
C	-4.9805448	-0.2303288	-5.4199770
C	-4.8389439	0.9006026	-4.5827891

H -6.5984014 -2.9810586 0.2694903  
H -7.0240151 -1.5582258 1.2565889  
H -2.4632436 -0.4066879 0.3559212

### Transition State 58



SCF Energy = -5117.1085233970 hartree  
Heat Capacity at 298K = 0.716014672 hartree  
G<sub>tot</sub> = -5116.392508725 hartree

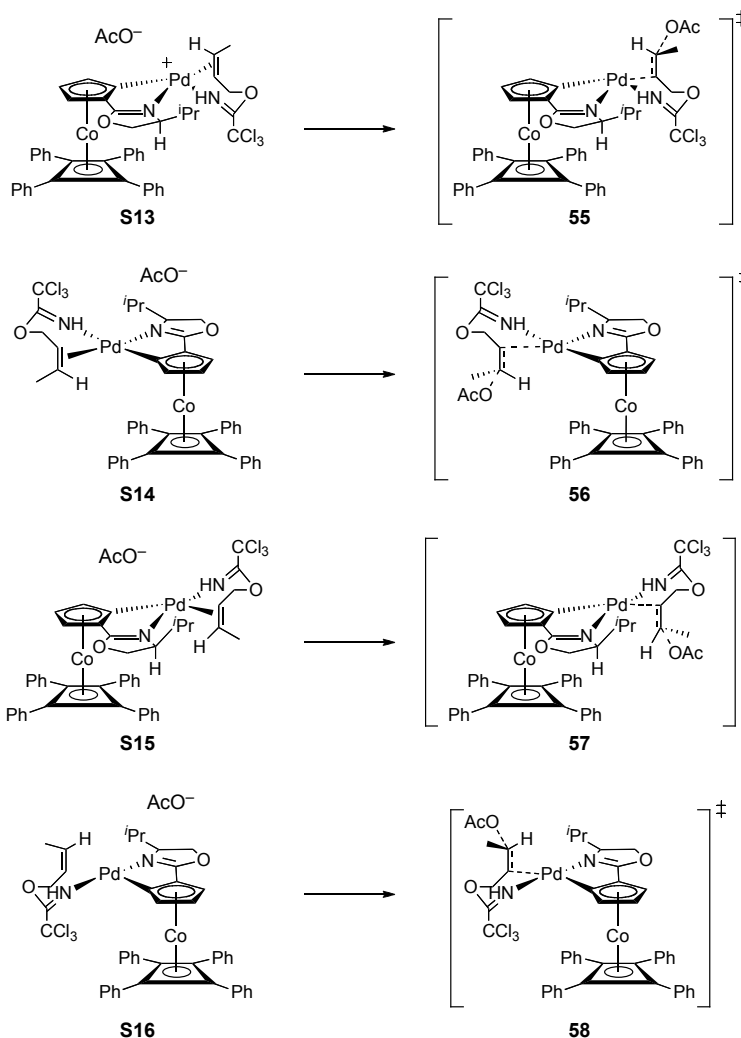
#### XYZ Coordinates

Pd	0.3428140	-0.8079783	1.4635241
N	2.2542801	-1.1157679	0.6836543
C	-0.1396697	-1.7120447	-0.2941323
C	1.0059268	-1.9663196	-1.1200708
C	2.2519018	-1.5752672	-0.5289785
C	0.6024894	-2.5588011	-2.3564483
C	-1.2647008	-2.1222595	-1.0516715
C	-0.8100166	-2.6594850	-2.3034761
Co	-0.2309913	-0.6543059	-2.1769162
C	-0.8724212	1.2429454	-2.1668910
C	-1.2168241	0.5507673	-3.4075849
C	0.1988206	0.4702041	-3.7550501
C	0.5403214	1.1692058	-2.5184594
O	3.4301371	-1.6584847	-1.1411707
C	4.3902657	-1.0026120	-0.2446322
C	3.6605706	-0.9430128	1.1104788
C	0.9440258	0.0936541	-4.9557531
C	2.2305287	-0.4994498	-4.8722896
C	2.9489822	-0.8348051	-6.0339064
C	2.3932601	-0.5825608	-7.3127784
C	1.1137228	0.0124289	-7.4069163
C	0.3998678	0.3462817	-6.2393275
C	-2.4513163	0.2928335	-4.1432300
C	-2.5660346	-0.8200350	-5.0162639
C	-3.7450754	-1.0486922	-5.7469617
C	-4.8430129	-0.1615525	-5.6235380
C	-4.7366535	0.9553041	-4.7625339

C	-3.6286986	1.1303341	-3.9005181	C	-3.5526025	1.1779565	-4.0333286
C	-1.6344410	1.9996300	-1.1368459	C	-1.6543822	1.9355262	-1.1458284
C	-2.8661759	1.5384636	-0.6076444	C	-2.9008386	1.4219526	-0.7046552
C	-3.6003009	2.3207849	0.3024283	C	-3.6686752	2.1081528	0.2530257
C	-3.1133839	3.5871622	0.7099894	C	-3.2034495	3.3305723	0.7984318
C	-1.8842711	4.0559200	0.1893498	C	-1.9632688	3.8544346	0.3617302
C	-1.1574870	3.2694092	-0.7258979	C	-1.2037296	3.1644642	-0.6046851
C	1.7388886	1.7437595	-2.0260671	C	1.7640298	1.7513618	-1.9763662
C	2.7129381	2.2191712	-2.9397473	C	2.8076878	2.1694423	-2.8400838
C	3.8849315	2.8505861	-2.4832078	C	3.9794786	2.7572670	-2.3271624
C	4.1087932	3.0188136	-1.0952918	C	4.1335859	2.9433165	-0.9313333
C	3.1417743	2.5490138	-0.1726655	C	3.0955218	2.5344226	-0.0589424
C	1.9719402	1.9213989	-0.6387750	C	1.9285857	1.9484959	-0.5814473
C	4.2941946	-2.3977267	1.8765500	C	4.1031814	-2.0241714	2.1238472
C	5.7274424	-2.1063402	2.3389598	C	4.0666884	-3.4518564	1.5702858
C	3.4571273	-2.8833042	3.0603720	C	5.4805710	-1.6722427	2.6958023
H	3.4750283	-2.1619633	3.8817273	H	6.2564357	-1.7079208	1.9250451
H	2.4194044	-3.0696627	2.7821127	H	5.4781833	-0.6704787	3.1304045
H	3.8730803	-3.8173884	3.4443528	H	5.7627914	-2.3837835	3.4745140
H	4.3248289	-3.2121782	1.1417250	H	3.3823405	-1.9817522	2.9448878
H	5.7330274	-1.2925968	3.0696468	H	4.7942052	-3.5991205	0.7677338
H	6.1604103	-2.9891604	2.8135371	H	4.3102503	-4.1628364	2.3625354
H	6.3855174	-1.8191816	1.5166561	H	3.0778614	-3.7133576	1.1879665
H	3.8691230	-0.2602602	1.7420591	H	3.7838272	0.0349473	1.5760616
H	5.3200281	-1.5303102	-0.3668121	H	5.2975318	-1.5996720	-0.2460440
H	4.4772567	0.0316724	-0.5648700	H	4.5921755	-0.0149734	-0.6567351
H	1.1912629	-2.8523497	-3.1551850	H	1.2367159	-2.8569903	-3.1753488
H	-1.4852863	-3.0650753	-3.0152209	H	-1.4417150	-3.0544420	-3.0838458
H	-2.3060232	-2.1119151	-0.6646475	H	-2.3034910	-2.0527509	-0.7655566
H	1.2372532	1.5564895	0.0778198	H	1.1425405	1.6265085	0.0992491
H	3.3187966	2.6617288	0.9005739	H	3.2089923	2.6673710	1.0205363
H	5.0171250	3.5090107	-0.7385840	H	5.0415405	3.4009095	-0.5326369
H	4.6208053	3.2186075	-3.2011641	H	4.7699364	3.0795286	-3.0080341
H	2.5497575	2.1130595	-4.0112250	H	2.7021527	2.0526236	-3.9174639
H	2.6361589	-0.6824095	-3.8796058	H	2.6685538	-0.7085604	-3.8960718
H	-0.7268187	0.6030556	-6.2950699	H	-0.5782622	0.8168073	-6.3298578
H	0.5031040	-0.0440809	-8.3550602	H	0.6800914	0.2169534	-8.3879729
H	2.8161757	-1.0064886	-8.1949861	H	2.9489738	-0.8434934	-8.2162730
H	3.8756062	-1.3123617	-5.9387155	H	3.9364990	-1.2934238	-5.9517179
H	-1.8596154	-1.5881777	-5.0057605	H	-1.7327001	-1.5144602	-5.1201114
H	-3.9895221	-1.9986984	-6.2134319	H	-3.8166403	-1.9123526	-6.4112961
H	-5.9180680	-0.4114824	-5.9504934	H	-5.7603238	-0.3373207	-6.1900188
H	-5.6692961	1.6007181	-4.4695522	H	-5.5739485	1.6497843	-4.6671179
H	-3.5334601	2.0161283	-3.2740950	H	-3.4835323	2.0529634	-3.3883414
H	-4.5490249	1.9527192	0.6970874	H	-4.6270846	1.6996607	0.5790129
H	-3.2506992	0.5633904	-0.9063298	H	-3.2667465	0.4761285	-1.1030749

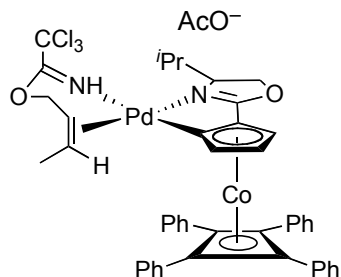
H	-0.2236714	3.6551971	-1.1321153	H	-0.2638853	3.5961047	-0.9455107
H	-1.5022670	5.0329760	0.4917402	H	-1.5997681	4.8012096	0.7662612
H	-3.6820941	4.1956796	1.4163714	H	-3.7971198	3.8643030	1.5437795
C	0.0651782	-0.5394592	4.6609058	C	-0.4373944	1.4735972	3.3924679
O	-1.3520030	-0.1944987	4.4213163	O	-1.6102332	0.6984238	3.8438124
C	-2.0104138	-0.5538274	3.3532509	C	-2.1356196	-0.2359402	3.1002120
N	-1.5191226	-0.8915235	2.2262570	N	-1.5919449	-0.7876343	2.0878516
C	-3.5310185	-0.5101003	3.6284214	C	-3.5222593	-0.6491904	3.6437175
Cl	-3.9757275	1.1321642	4.1673102	Cl	-4.5596623	0.7922277	3.8087716
Cl	-3.8905720	-1.6963556	4.9204576	Cl	-3.2721773	-1.4044777	5.2476982
Cl	-4.4914139	-0.9279619	2.1859015	Cl	-4.3338750	-1.8223560	2.5722381
C	1.0436619	-0.1966661	3.5815048	C	0.8041960	0.6899368	3.0863748
C	1.2775482	1.1018956	3.1419855	C	1.4656808	-0.0802714	4.0381411
C	0.2826074	2.2159011	3.1822569	C	0.8194877	-0.8063447	5.1730749
O	2.5705685	1.9996779	4.6567068	O	2.5007512	1.2920730	5.3260999
C	3.7919257	2.0413440	4.2960966	C	3.4581630	1.9020910	4.7388835
O	4.2264270	1.7744325	3.1567086	C	4.1249411	3.0219090	5.5415297
C	4.7967054	2.4361398	5.3798259	O	3.8719286	1.6729557	3.5874554
H	0.2584109	0.0018859	5.5873384	H	-0.2987102	2.1570242	4.2304003
H	0.0807594	-1.6092206	4.8688386	H	-0.7647414	2.0424784	2.5217743
H	-2.2254765	-1.1476870	1.5475213	H	-2.1857685	-1.4755579	1.6411322
H	1.9205639	-0.8289302	3.6407319	H	1.4721480	1.2593328	2.4463824
H	-0.2859493	2.2251768	4.1121352	H	0.3445619	-1.7206082	4.8038773
H	0.7862416	3.1733874	3.0695103	H	1.5667047	-1.0928042	5.9101202
H	-0.4270272	2.1158024	2.3550740	H	0.0536278	-0.2056083	5.6625263
H	4.3066519	2.8952128	6.2374733	H	5.2099970	2.9181864	5.4873587
H	5.3186409	1.5361951	5.7166617	H	3.8642821	3.9826354	5.0895675
H	5.5438891	3.1162471	4.9684319	H	3.8060821	3.0246490	6.5829493
H	2.1312266	1.2424912	2.4968473	H	2.4492403	-0.4140570	3.7559158

## Computational Data for Imidates that Lead to COP Transition States 55–58



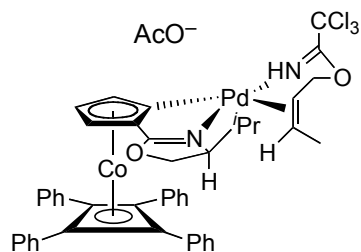
Computational data for intermediate **S13** are listed on page S33.

### Intermediate S14



SCF Energy =  $-5117.1240385550$  hartree  
 Heat Capacity at 298K =  $0.71504999$  hartree  
 $G_{\text{tot}} = -5116.408988565$  hartree

### Intermediate S15



SCF Energy =  $-5117.1185277660$  hartree  
 Heat Capacity at 298K =  $0.718680817$  hartree  
 $G_{\text{tot}} = -5116.399846949$  hartree

XYZ Coordinates

Pd	0.0185851	-0.9392318	1.3238306
N	2.1059302	-1.1741566	0.8913756
C	-0.1058039	-1.5733971	-0.5662225
C	1.1724092	-1.8130687	-1.1742651
C	2.2983684	-1.4730509	-0.3574832
C	0.9867378	-2.4025846	-2.4628258
C	-1.0871448	-2.0013275	-1.4925634
C	-0.4138334	-2.5218691	-2.6458686
Co	0.1277076	-0.5082596	-2.4175161
C	-0.5944808	1.3469735	-2.6591291
C	-0.4948181	0.6304002	-3.9276911
C	0.9583627	0.6292899	-3.8160081
C	0.8586808	1.3472971	-2.5445384
O	3.5512573	-1.4243942	-0.7978794
C	4.3244848	-0.7969959	0.2767902
C	3.4299457	-0.9618465	1.5219523
C	2.0485448	0.3055479	-4.7363886
C	3.2850572	-0.2180047	-4.2790445
C	4.3309902	-0.4919180	-5.1792602
C	4.1616748	-0.2481052	-6.5645897
C	2.9328395	0.2746152	-7.0306931
C	1.8903660	0.5474571	-6.1241331
C	-1.4283826	0.2892367	-4.9991996
C	-1.2218002	-0.8533461	-5.8153354
C	-2.1109215	-1.1663890	-6.8588388
C	-3.2306850	-0.3361157	-7.1138537
C	-3.4399912	0.8102804	-6.3122323
C	-2.5464437	1.1173532	-5.2676029
C	-1.6913455	2.0456733	-1.9945455
C	-2.9895124	1.4795830	-1.9163241
C	-4.0582116	2.1961998	-1.3455246
C	-3.8489362	3.4990473	-0.8297647
C	-2.5566996	4.0711916	-0.8997982
C	-1.4928225	3.3502759	-1.4769537
C	1.8144722	1.9753109	-1.6387002
C	3.0732785	2.4232005	-2.1107740
C	3.9951507	3.0413630	-1.2432270
C	3.6731908	3.2321703	0.1227416
C	2.4133056	2.7969071	0.6031724
C	1.5005982	2.1774559	-0.2695125
C	3.8833158	-2.1403079	2.4145644
C	5.2226404	-1.8079353	3.0830582
C	2.8573834	-2.5401125	3.4743946
H	2.7104490	-1.7375544	4.2026511
H	1.8918511	-2.7941617	3.0384510

XYZ Coordinates

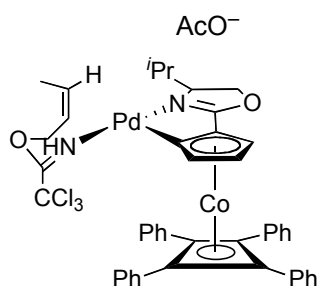
Pd	0.1837451	-0.8279667	1.4655264
N	2.1770329	-1.0487384	0.8436644
C	-0.1225593	-1.5958268	-0.3706100
C	1.0977912	-1.9391213	-1.0456350
C	2.2832140	-1.5510985	-0.3501809
C	0.7953639	-2.5493795	-2.3016598
C	-1.1862345	-1.9805735	-1.2211975
C	-0.6177700	-2.5740598	-2.3970414
Co	0.0691868	-0.5941126	-2.2525408
C	-0.5538018	1.2978592	-2.4744607
C	-0.5979376	0.5623145	-3.7335410
C	0.8565782	0.4652925	-3.7337191
C	0.9006724	1.2118218	-2.4750242
O	3.5067958	-1.6409845	-0.8572289
C	4.3910368	-0.9477401	0.0787696
C	3.5337002	-0.7442355	1.3490859
C	1.8511530	0.0731084	-4.7345733
C	3.0555005	-0.5866877	-4.3803411
C	4.0102661	-0.9229047	-5.3577088
C	3.7801328	-0.6037501	-6.7185097
C	2.5833916	0.0566980	-7.0821655
C	1.6317143	0.3893022	-6.0988124
C	-1.6280709	0.2604319	-4.7223399
C	-1.4989714	-0.8535217	-5.5920903
C	-2.4775878	-1.1293094	-6.5630001
C	-3.6125094	-0.2904706	-6.6880512
C	-3.7480568	0.8258157	-5.8283128
C	-2.7633477	1.0963200	-4.8576040
C	-1.5505220	2.0591315	-1.7218621
C	-2.8256521	1.5146227	-1.4297911
C	-3.8006332	2.2799245	-0.7636522
C	-3.5149967	3.6092046	-0.3669098
C	-2.2434100	4.1607367	-0.6518410
C	-1.2747444	3.3922024	-1.3263227
C	1.9509758	1.8110144	-1.6643901
C	3.2301312	2.0849690	-2.2106098
C	4.2370982	2.6911324	-1.4336842
C	3.9827468	3.0489626	-0.0869825
C	2.7041241	2.7895440	0.4658270
C	1.7074663	2.1758757	-0.3146759
C	3.9592624	-1.6112626	2.5533100
C	3.9360591	-3.1138206	2.2632976
C	5.3253157	-1.1535270	3.0771199
H	6.1200793	-1.3343852	2.3486276
H	5.3240319	-0.0872503	3.3166222

H	3.2141271	-3.4118428	4.0266400	H	5.5857795	-1.7005239	3.9852422
H	4.0300764	-2.9990897	1.7483715	H	3.2340151	-1.4146198	3.3469777
H	5.1162092	-0.9526083	3.7569226	H	4.6698281	-3.3922632	1.5024856
H	5.5687025	-2.6568342	3.6756006	H	4.1801626	-3.6732672	3.1686026
H	6.0068863	-1.5693263	2.3626286	H	2.9526984	-3.4440687	1.9239059
H	3.4162706	-0.0388115	2.1067343	H	3.5753921	0.3053532	1.6459796
H	5.2765111	-1.3146004	0.3350601	H	5.2665979	-1.5737062	0.2244455
H	4.4770628	0.2451761	-0.0034044	H	4.6801724	-0.0076159	-0.3875208
H	1.7559485	-2.6943424	-3.1594371	H	1.4985889	-2.9053689	-3.0368244
H	-0.9000805	-2.9195619	-3.5228498	H	-1.1862418	-2.9486521	-3.2339114
H	-2.1587353	-1.9881192	-1.3529284	H	-2.2525554	-1.8628931	-1.0762536
H	0.5399304	1.8392893	0.1170928	H	0.7307485	1.9790512	0.1251290
H	2.1498052	2.9511968	1.6517388	H	2.4914264	3.0801133	1.4973192
H	4.3841964	3.7170797	0.7953521	H	4.7579543	3.5304045	0.5132709
H	4.9575853	3.3856796	-1.6272249	H	5.2134122	2.9002419	-1.8756843
H	3.3331105	2.3063835	-3.1616680	H	3.4413611	1.8437425	-3.2510944
H	3.4292095	-0.4250487	-3.2184158	H	3.2456258	-0.8499132	-3.3396882
H	0.9550199	0.9616912	-6.4988189	H	0.7198187	0.9070780	-6.3940979
H	2.7938854	0.4701520	-8.0960243	H	2.3986846	0.3114795	-8.1278256
H	4.9720668	-0.4618325	-7.2652973	H	4.5197819	-0.8649607	-7.4787435
H	5.2757784	-0.8971350	-4.8112987	H	4.9305209	-1.4344273	-5.0686300
H	-0.3693451	-1.5056629	-5.6292194	H	-0.6370715	-1.5138355	-5.5024765
H	-1.9417195	-2.0533926	-7.4725760	H	-2.3664727	-1.9942156	-7.2199551
H	-3.9241610	-0.5789603	-7.9222575	H	-4.3765577	-0.5045052	-7.4387723
H	-4.2959756	1.4599132	-6.5059211	H	-4.6182166	1.4789828	-5.9187189
H	-2.7163877	2.0113506	-4.6695443	H	-2.8806578	1.9646713	-4.2113558
H	-5.0531442	1.7464690	-1.3003368	H	-4.7746666	1.8324028	-0.5547171
H	-3.1686838	0.4763280	-2.3042519	H	-3.0642292	0.4882917	-1.7125361
H	-0.5103465	3.8166726	-1.5441332	H	-0.3083145	3.8385509	-1.5592920
H	-2.3862979	5.0783246	-0.5139449	H	-2.0163600	5.1870935	-0.3560919
H	-4.6769799	4.0566741	-0.3868401	H	-4.2700871	4.2029854	0.1529271
O	-4.9904546	-2.5198962	1.7516578	O	-5.9745221	-0.5382495	-0.9611393
C	-4.9550206	-2.3900784	0.5007545	C	-5.3721247	-1.3044618	-1.7636649
C	-6.1015281	-1.6160828	-0.1643402	C	-5.9283822	-1.4013757	-3.1903615
H	-6.9921161	-1.5998502	0.4639475	H	-6.9441204	-1.0104071	-3.2555317
H	-5.7785377	-0.5829878	-0.3236999	H	-5.2859239	-0.8219424	-3.8583503
H	-6.3409943	-2.0385582	-1.1412700	H	-5.9065406	-2.4359884	-3.5373564
O	-4.0387723	-2.8104166	-0.2565101	O	-4.3453663	-1.9794322	-1.5066548
C	-2.2412822	-1.6880114	3.2416171	N	-1.8420076	-0.7704699	1.8423893
O	-1.8124192	-0.7435757	4.2689595	C	-2.5015069	-0.6386699	2.9259112
C	-0.5776539	-0.3079525	4.3326405	C	-4.0330150	-0.4801724	2.9794360
N	0.2657570	-0.3419028	3.3821107	O	-1.9865772	-0.5906194	4.1363278
C	-0.2874869	0.2832738	5.7314159	C	-0.6995465	-1.1755785	4.4377251
Cl	-0.4659261	-1.0228887	6.9356759	C	0.4985795	-0.5750433	3.7715840
Cl	-1.4576647	1.5900744	6.0578843	C	0.7091764	0.6862452	3.3124899
Cl	1.3661568	0.9460254	5.8343260	C	-0.1983603	1.8774399	3.3552509



C	-2.0824175	-1.3032830	1.8055763	Cl	-4.6801321	-1.8074355	4.0066458
C	-2.0487944	-0.0518626	1.2228806	Cl	-4.7846320	-0.5448019	1.3760210
C	-2.1963566	1.2959640	1.8611783	Cl	-4.3824982	1.1049315	3.7599984
H	-3.3033326	-1.8293105	3.4398321	H	1.3587701	-1.2264958	3.8705899
H	-1.7252722	-2.6282648	3.4409013	H	-1.1914960	1.6618690	3.7372690
H	1.1660821	0.0419182	3.6454888	H	0.2588073	2.6235996	4.0127684
H	-2.3671970	-2.1308107	1.1604220	H	-0.2894993	2.3466350	2.3735894
H	-1.5415587	2.0312107	1.3929428	H	-0.6199660	-1.0683994	5.5201884
H	-3.2191403	1.6347750	1.6663119	H	-0.7587058	-2.2404695	4.2063564
H	-2.0450555	1.3112242	2.9349163	H	-2.4450109	-0.8030883	1.0239554
H	-2.2167480	-0.0368512	0.1544201	H	1.7279670	0.9143763	3.0180142

### Intermediate S16



SCF Energy = -5117.1171309270 hartree  
 Heat Capacity at 298K = 0.716638917 hartree  
 $G_{\text{tot}} = -5116.40049201$  hartree

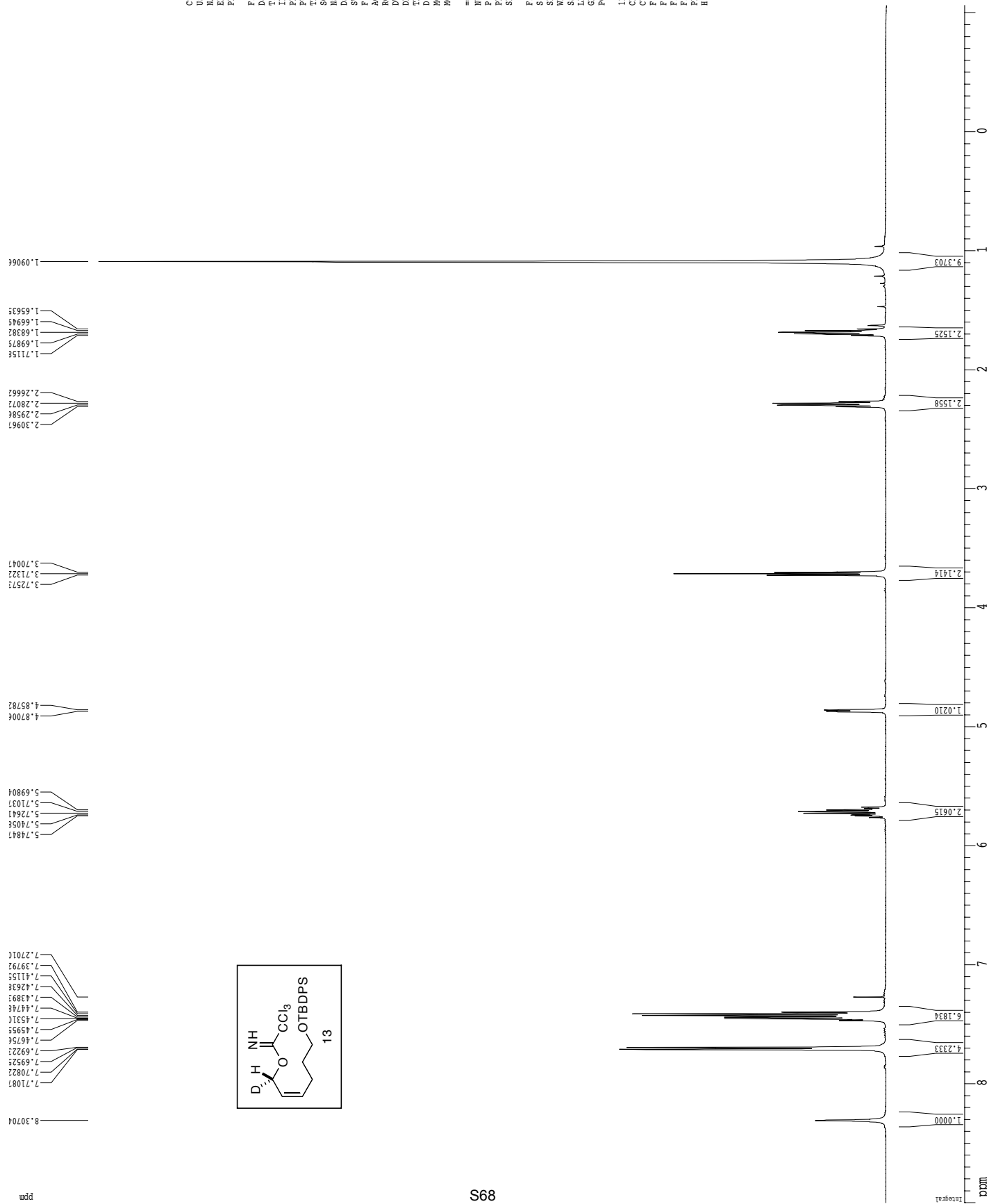
### XYZ Coordinates

Pd	0.0377022	-0.8336033	1.3791791
N	2.0617084	-1.1346973	0.9506486
C	-0.1189484	-1.6198736	-0.4666568
C	1.1542617	-1.8875637	-1.0762179
C	2.2763885	-1.5400581	-0.2651931
C	0.9550173	-2.4612398	-2.3688177
C	-1.1110263	-2.0143904	-1.3943393
C	-0.4471755	-2.5409183	-2.5516413
Co	0.1378887	-0.5400228	-2.2911517
C	-0.4885587	1.3571163	-2.3756597
C	-0.5909681	0.6940432	-3.6725923
C	0.8628465	0.6028277	-3.7432551
C	0.9657213	1.2755091	-2.4486900
O	3.5424681	-1.6056836	-0.6581277
C	4.3292804	-0.9975785	0.4183005
C	3.3680122	-0.9760679	1.6240817
C	1.8170843	0.2459018	-4.7936442
C	3.0503389	-0.3890493	-4.4958026
C	3.9681276	-0.7000626	-5.5152956
C	3.6708803	-0.3809200	-6.8633272

C	2.4453243	0.2545940	-7.1705536
C	1.5310806	0.5633791	-6.1446086
C	-1.6698022	0.4499130	-4.6249372
C	-1.6088480	-0.6332052	-5.5391569
C	-2.6415131	-0.8550531	-6.4665924
C	-3.7636777	0.0095430	-6.5031913
C	-3.8297156	1.0982723	-5.6019080
C	-2.7911960	1.3143606	-4.6753183
C	-1.4523130	2.0363879	-1.5126955
C	-2.7384891	1.4874269	-1.2770181
C	-3.6768190	2.1620989	-0.4754454
C	-3.3479907	3.4075690	0.1148682
C	-2.0685774	3.9665904	-0.1175837
C	-1.1360613	3.2876375	-0.9283255
C	2.0603025	1.8254974	-1.6588211
C	3.2910015	2.1795032	-2.2667256
C	4.3409817	2.7337323	-1.5099185
C	4.1806667	2.9568198	-0.1203814
C	2.9514768	2.6165699	0.4953676
C	1.9117682	2.0564882	-0.2668934
C	3.6366199	-2.0752952	2.6776501
C	3.6850791	-3.4905197	2.0945733
C	4.9061543	-1.7454057	3.4698114
H	5.7960145	-1.7734073	2.8347620
H	4.8474641	-0.7520865	3.9216993
H	5.0539818	-2.4719851	4.2706748
H	2.7956992	-2.0468947	3.3760347
H	4.5308102	-3.6253306	1.4158585
H	3.7968270	-4.2183567	2.9005546
H	2.7694790	-3.7368955	1.5539328
H	3.4112186	-0.0023243	2.1143705
H	5.2168924	-1.6073284	0.5588435
H	4.6111890	0.0008174	0.0874670
H	1.7151670	-2.7643678	-3.0702093
H	-0.9479730	-2.9163641	-3.4301334
H	-2.1879274	-1.9761201	-1.3019433
H	0.9743832	1.7914638	0.2186921
H	2.8129221	2.8017874	1.5633843
H	4.9907843	3.3955055	0.4660963
H	5.2792450	3.0052796	-1.9980860
H	3.4294527	2.0402466	-3.3375717
H	3.2914068	-0.6514995	-3.4654807
H	0.5968676	1.0634754	-6.3973160
H	2.2089293	0.5086325	-8.2059608
H	4.3815934	-0.6231969	-7.6567436
H	4.9111218	-1.1924226	-5.2692917

H	-0.7588046	-1.3144353	-5.5163051
H	-2.5839485	-1.6993884	-7.1563207
H	-4.5702382	-0.1642301	-7.2190684
H	-4.6879560	1.7727086	-5.6261471
H	-2.8537469	2.1648713	-3.9982251
H	-4.6638998	1.7256041	-0.3095554
H	-3.0054157	0.5229952	-1.7103914
H	-0.1669346	3.7470819	-1.1191968
H	-1.8091931	4.9325040	0.3204078
H	-4.0764353	3.9324258	0.7367836
O	-6.1931629	-2.2681673	-0.8654037
C	-5.3091232	-2.4682408	-1.7444642
C	-5.7097529	-2.2426024	-3.2083717
H	-6.7927839	-2.2231692	-3.3320625
H	-5.3027322	-1.2839889	-3.5415723
H	-5.2740009	-3.0134254	-3.8455755
O	-4.1223531	-2.8116960	-1.5243050
C	-1.1157114	1.5510455	3.0087303
O	-2.3342162	0.8133173	3.2593261
C	-2.7492737	-0.1117816	2.4219384
N	-2.0152264	-0.7195063	1.5748663
C	-4.2384019	-0.4492731	2.6511155
Cl	-5.1734769	1.0455644	2.9565720
Cl	-4.2886979	-1.4845411	4.1308869
Cl	-4.9478253	-1.3131896	1.2741342
C	0.1657467	0.7793847	3.0842432
C	0.4673840	-0.3469009	3.7785774
C	-0.3804105	-1.1796182	4.6883436
H	-1.1290150	2.3284921	3.7736156
H	-1.2142955	2.0346928	2.0349701
H	-2.5408054	-1.3665041	0.9928162
H	0.9949064	1.3467878	2.6729908
H	-0.3163974	-2.2372232	4.4227623
H	0.0256372	-1.0898378	5.7012419
H	-1.4232935	-0.8835860	4.7195085
H	1.5202513	-0.5970887	3.8078438

<sup>1</sup>H spectrum



Current Data Parameters  
 USER cannon  
 NAME JSC2050  
 EXPNO 1  
 PROCNO 1

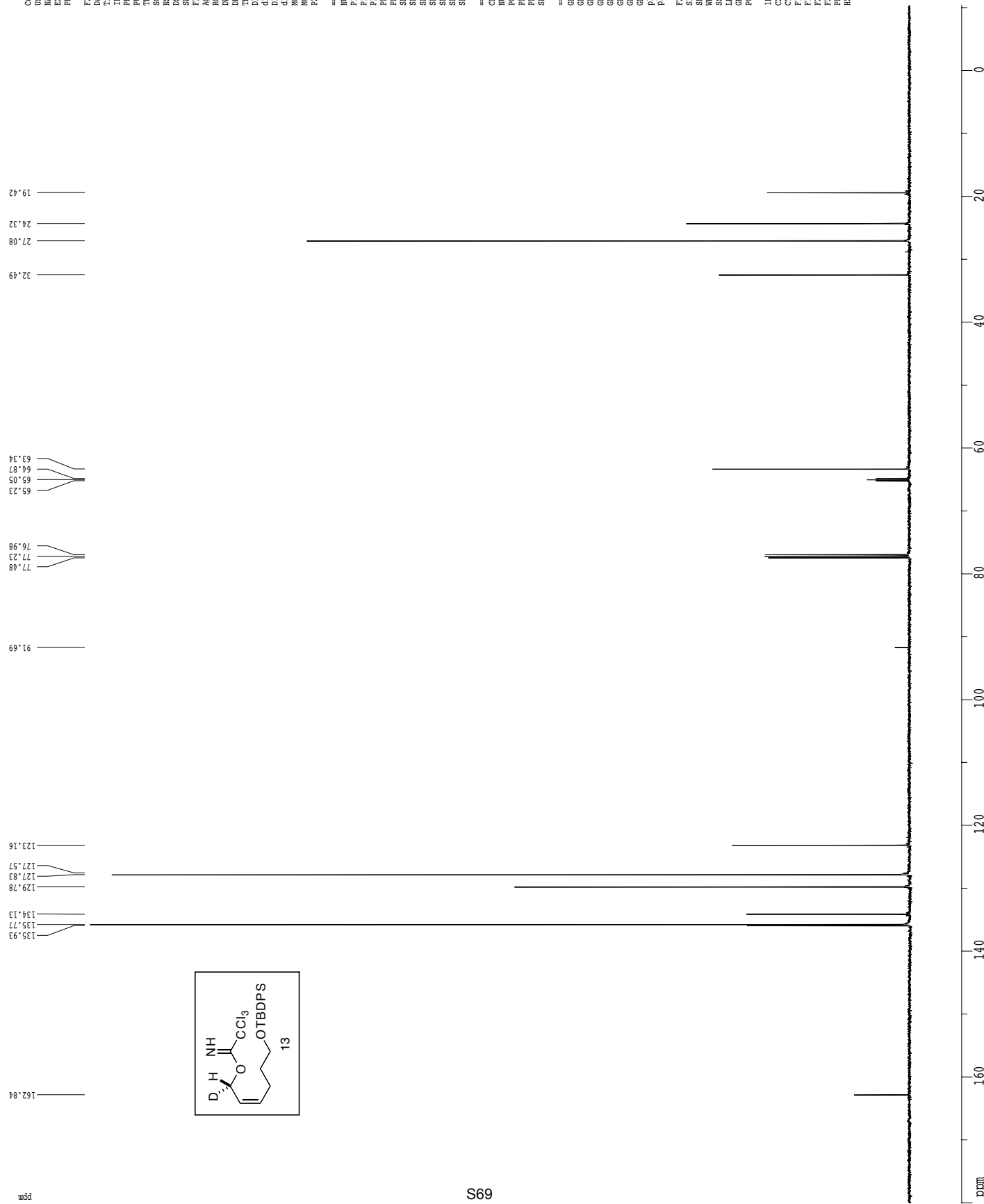
F2 - Acquisition Parameters  
 Date\_ 20081023  
 Time 13:02  
 INSTRUM crys000  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHF 801.280 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 3.2  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6536  
 SF 500.220263 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.062 ppm  
 F3 1.121 Hz  
 FWHM 0.483 ppm/cm  
 HECW 220.73375 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USR cannon  
 NAME JSZ2050  
 EXPNO 2  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20081023  
 Time 10.05  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI IH-  
 PULPROG SpinEchoSqr-prd  
 PRG02 0.0.0.0  
 SOLVENT CDCl3  
 NS 89  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0613840 sec  
 RG 7296.2  
 DW 16.500 usec  
 DE 16.000 usec  
 TE 298.2 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0020000 sec  
 d17 0.0001960 sec  
 d17 0.0001960 sec  
 MCRBST 0.0000000 sec  
 MCRPK 0.0150000 sec  
 F2 29.70 usec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 14.85 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SFO1 125.7942548 MHz  
 SF02 500.1363011 MHz  
 SP1 3.60 dB  
 SP2 3.60 dB  
 SPNAM1 Ctp60.0.5.20.1  
 SPNAM2 Ctp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

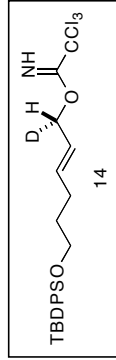
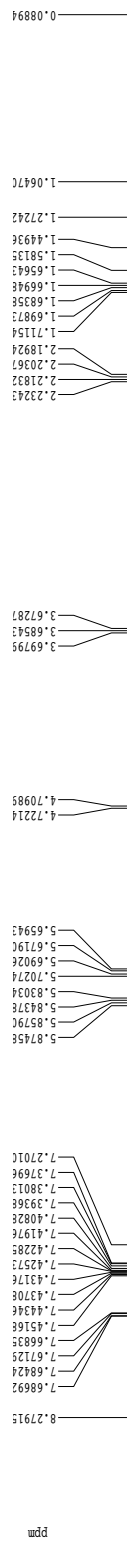
==== CHANNEL f2 =====  
 NUC2 13C  
 P1 14.85 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SFO1 125.7942548 MHz  
 SF02 500.2225011 MHz

==== GRADIENT CHANNEL =====  
 GPRAM1 SINE.100  
 GPRAM2 SINE.100  
 GRZ1 0.00 %  
 GRZ2 0.00 %  
 GRZ3 0.00 %  
 GRZ4 0.00 %  
 GRZ5 0.00 %  
 GRZ6 0.00 %  
 GRZ7 0.00 %  
 GRZ8 0.00 %  
 GRZ9 0.00 %  
 GRZ10 0.00 %  
 GRZ11 30.00 %  
 GRZ12 50.00 %  
 GRZ13 50.00 %  
 GRZ14 50.00 %  
 GRZ15 500.00 usec  
 GRZ16 1000.00 usec

F2 - Processing parameters  
 SI 65636  
 SF 125.7804043 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

1D NMR plot parameters  
 CX 22.80 cm  
 CT 15.65 cm  
 F1P 180.000 PPM  
 F1 22640.47 Hz  
 F2P -10.343 PPM  
 F2 -1300.59 Hz  
 PPMCM 8.34839 PPM/cm  
 HZCM 1030.06049 Hz/cm

**<sup>1</sup>H spectrum**



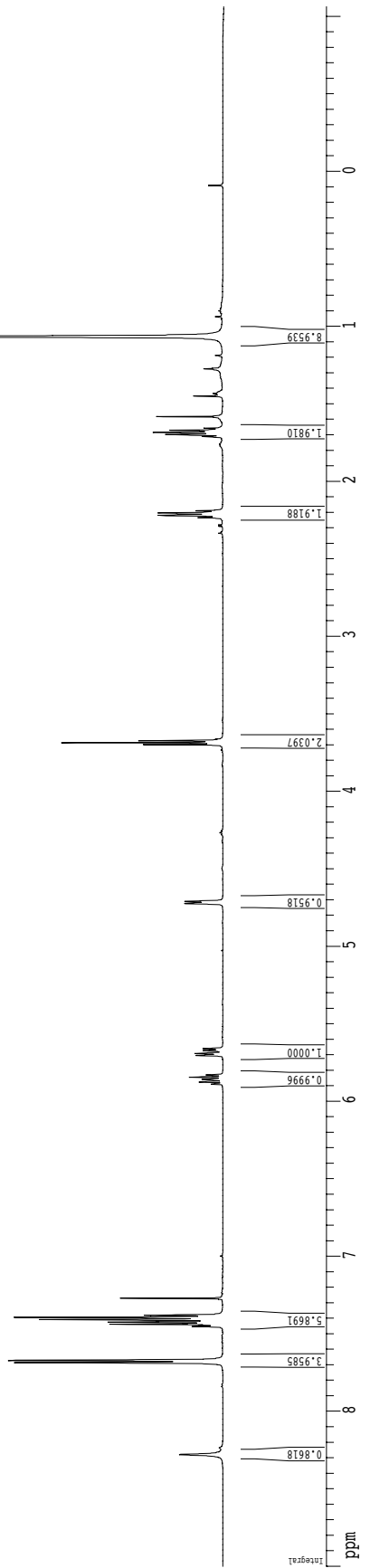
Current Data Parameters  
 USER cannon  
 NAME JSCI251  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080923  
 Time 13:53  
 INSTRUM cxtv6500  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHF 801.2820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWBK 0.01500000 sec

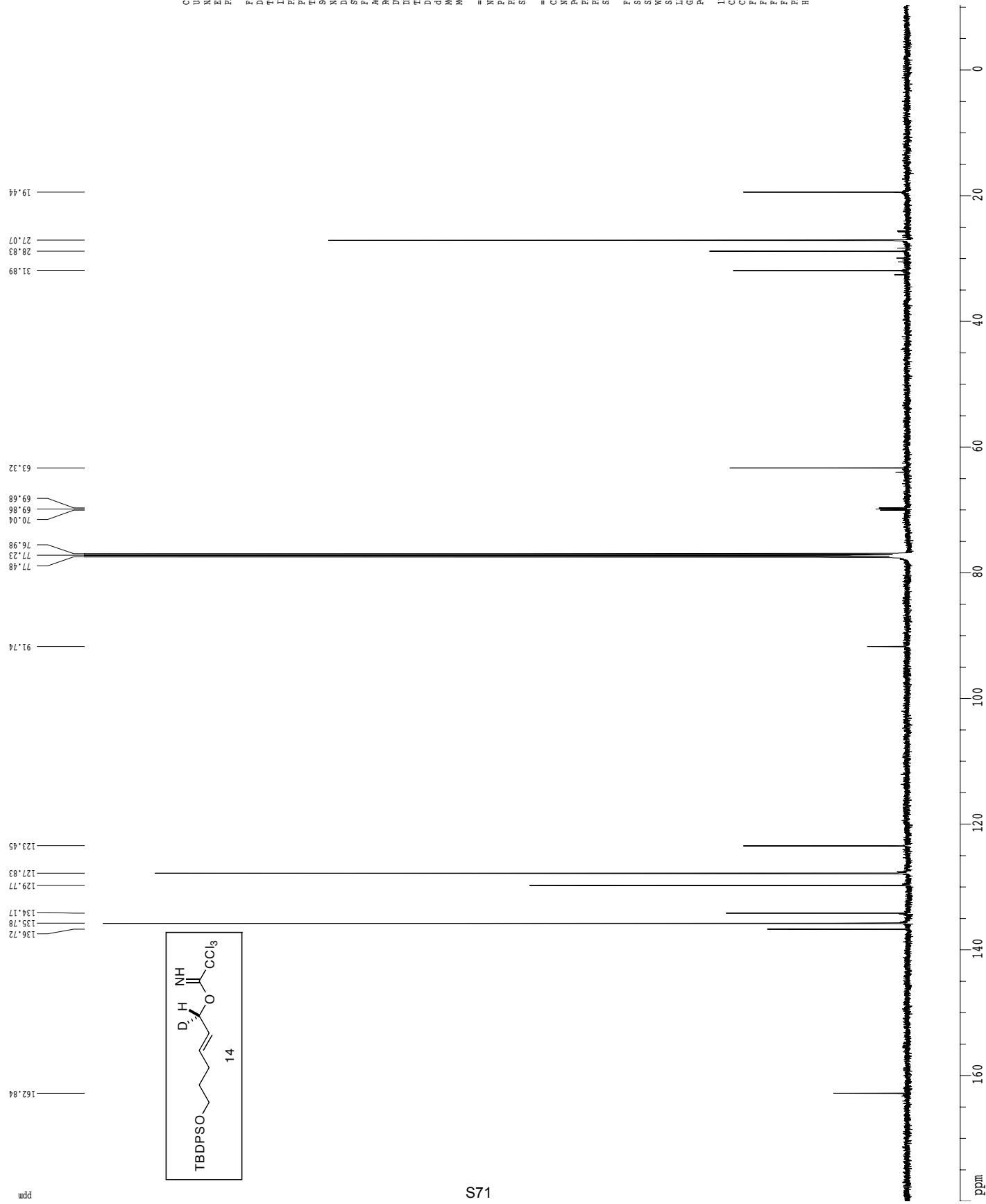
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.38 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2202280 MHz  
 EQ 2  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 45001.98 Hz  
 F2 -11.061 ppm  
 F3 45001.98 Hz  
 F4 0.482 ppm/cm  
 F5 220.73753 Hz/cm



**<sup>13</sup>C spectrum with <sup>1</sup>H decoupling**



```

Current Data Parameters
USER          camon
NAME         JSC1251
EXPNO        5
PROCNO       1

F2 - Acquisition Parameters
Date_        20080923
Time         15.01
INSTRUM      cryo00
PROBHD       5 mm CPCLP1H-
PULPROG      zgpg30
AQ           6.5418
RG           654.8
SOLVENT      CDCl3
NS           176
DS           4
SWH          30303.031 Hz
FIDRES       0.463222 Hz
AQ           1.0794470 sec
RG           91.95.2
DW           16.500 usec
DE           6.00 usec
TE           298.0 K
D1           2.0000000 sec
d11          0.0300000 sec
MCREST       0.0000000 sec
MCPRK        0.0150000 sec

===== CHANNEL f1 =====
NUC1          13C
P1           14.75 usec
PL1          -1.00 dB
SFO1         125.7942548 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2          1.60 dB
PL12         24.80 dB
SFO2         500.2225011 MHz

F2 - Processing parameters
SI           65536
SF           125.7804002 MHz
EN
SSB          0
GB           1.00 Hz
AG          2.00
PC

ID NMR plot parameters
CX           22.80 cm
CY           15.65 cm
F1P          180.000 ppm
F1           22640.47 Hz
F2P          -10.310 ppm
F2           -1296.82 Hz
PFMCH        8.34694 ppm/cm
HZCM         1049.88147 Hz/cm
    
```



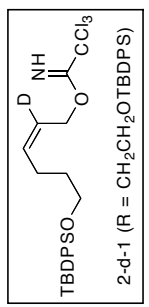
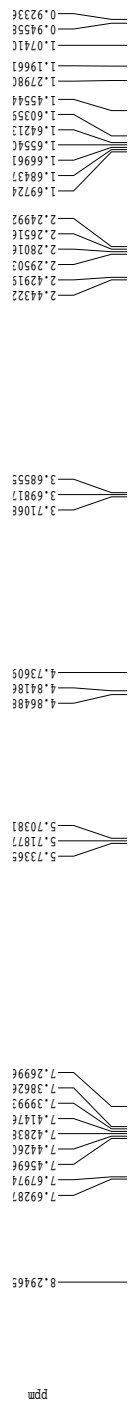








<sup>1</sup>H spectrum



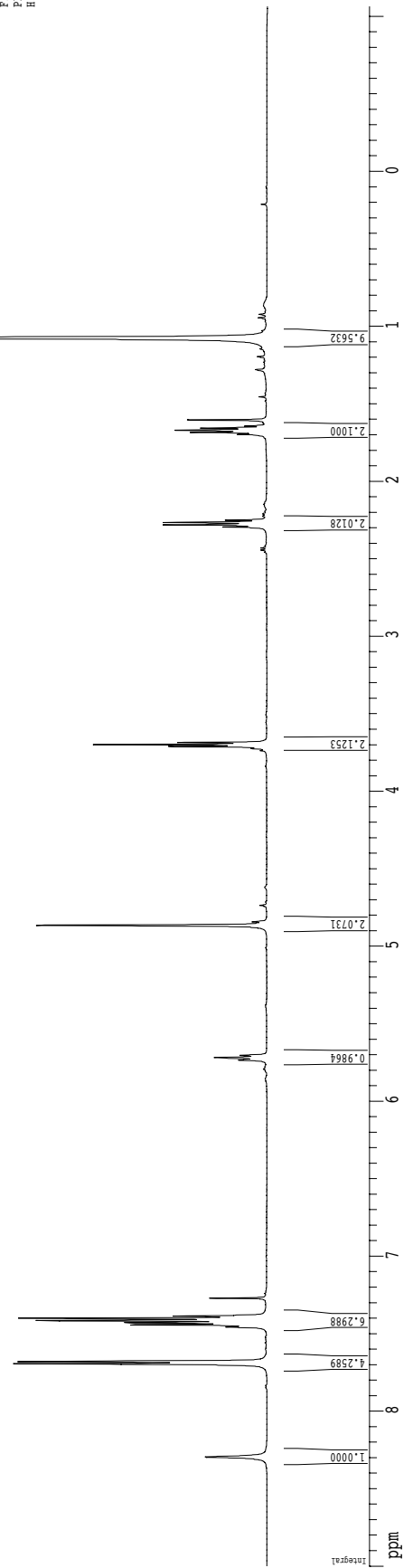
Current Data Parameters  
 USER cannon  
 NAME JS62170-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090422  
 Time 15:01:11  
 INSTRUM cxtv650  
 PROBRW 5 mm CPACT IH-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHF 801.2820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6536  
 SF 500.220262 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.062 ppm  
 FWHM 0.483 ppm/cm  
 FREQH 220.74829 Hz/cm

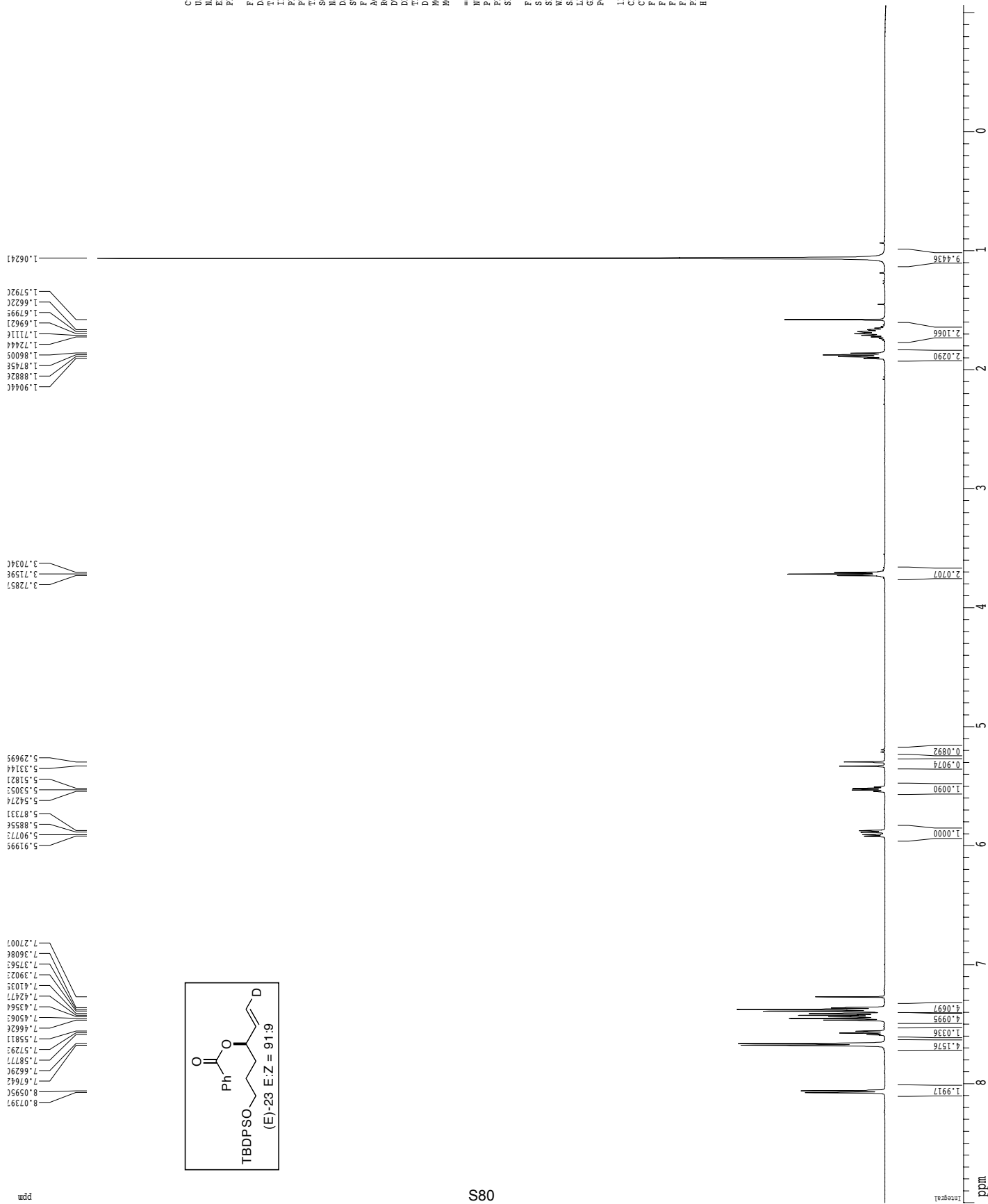








<sup>1</sup>H spectrum



Current Data Parameters  
 USER cannon  
 NAME JS62055-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081023  
 Time 15:02:00  
 INSTRUM cpc1500  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHR 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 5.7  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

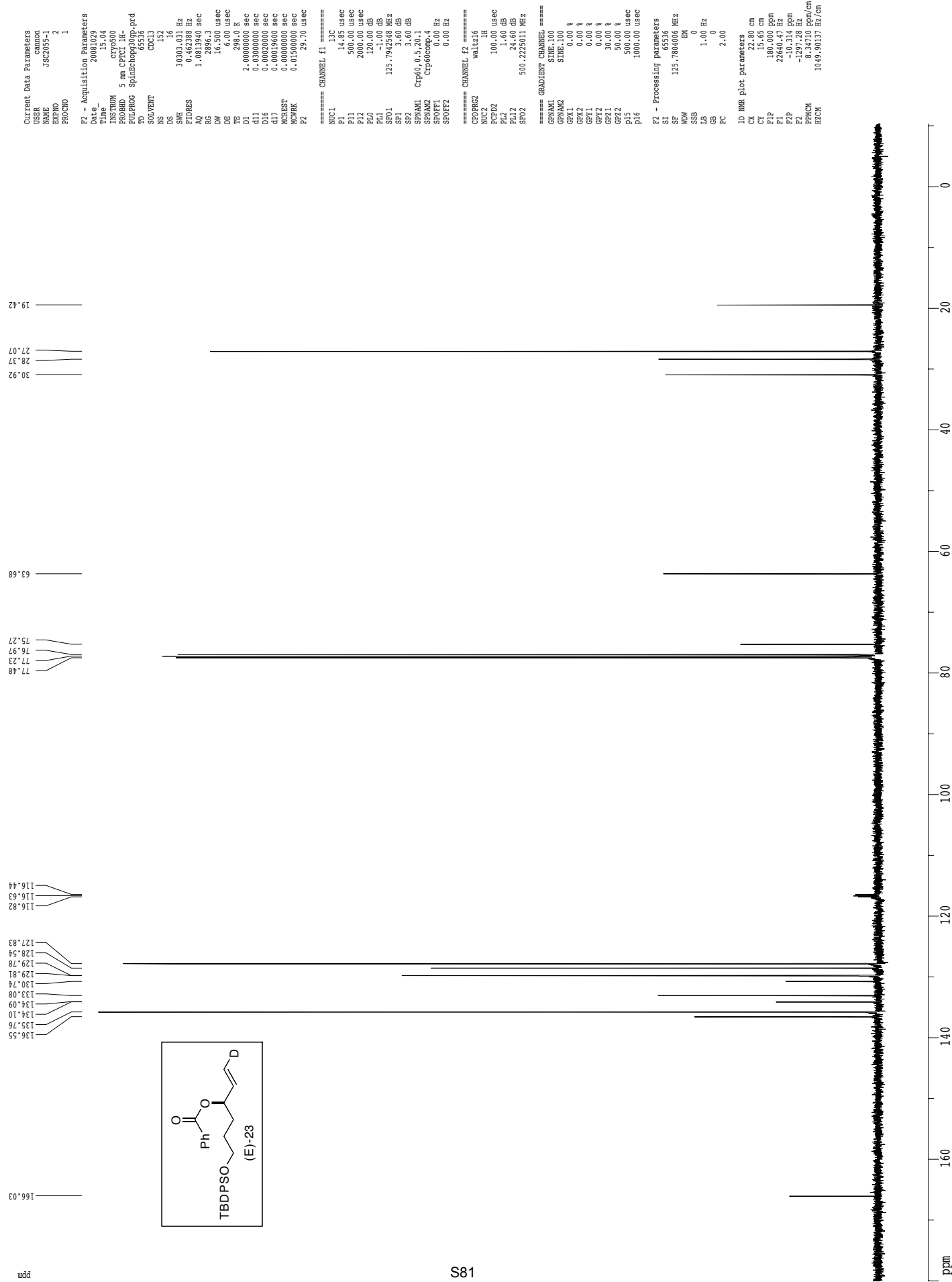
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6536  
 SF 500.220260 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

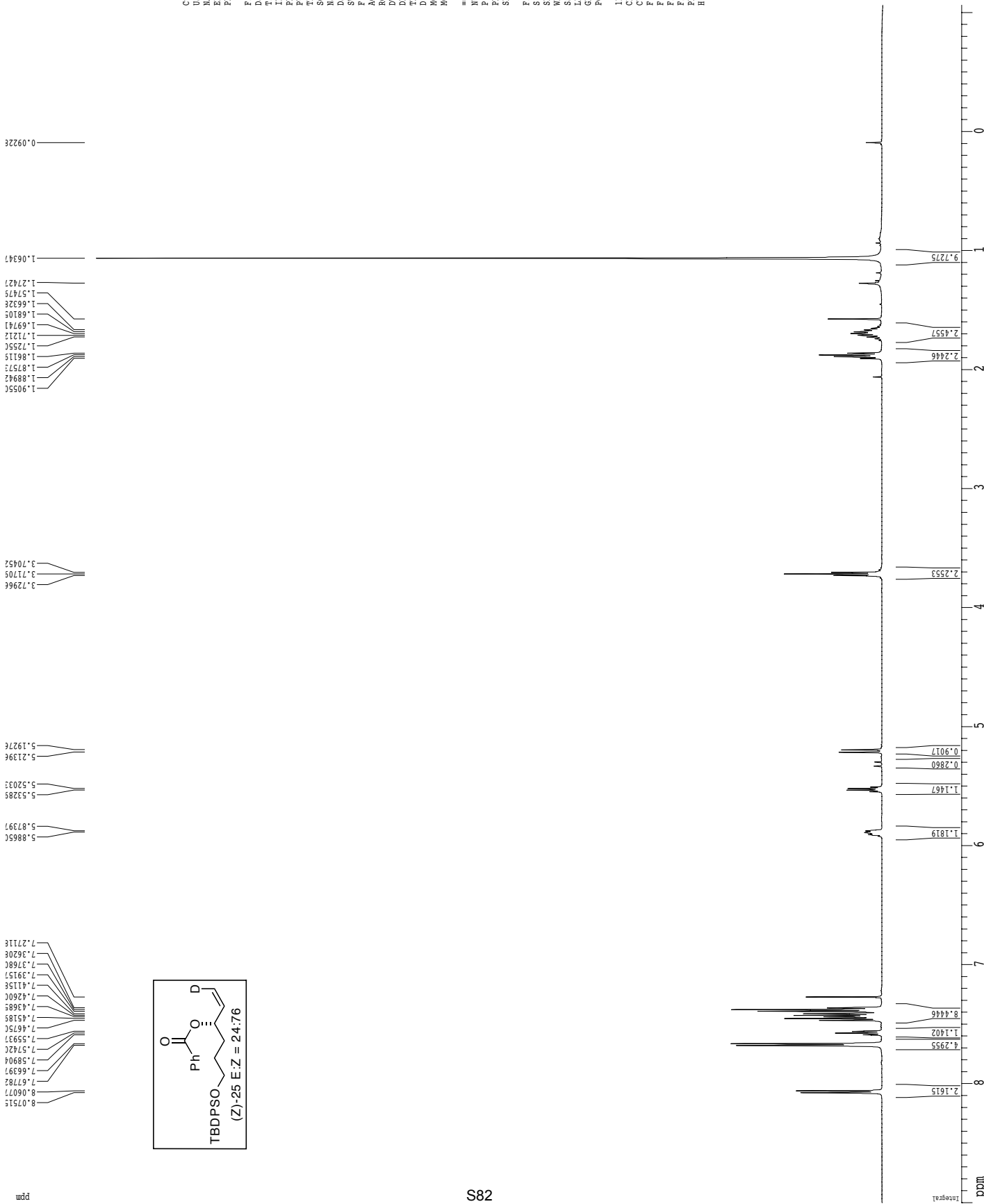
1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.062 ppm  
 F3 4.843 ppm/cm  
 F4 0.000 ppm/cm  
 HECN 220.76430 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



1H spectrum



Current Data Parameters  
 USER cannon  
 NAME JSC1166-1  
 EXPNO 1  
 PROCNO 1

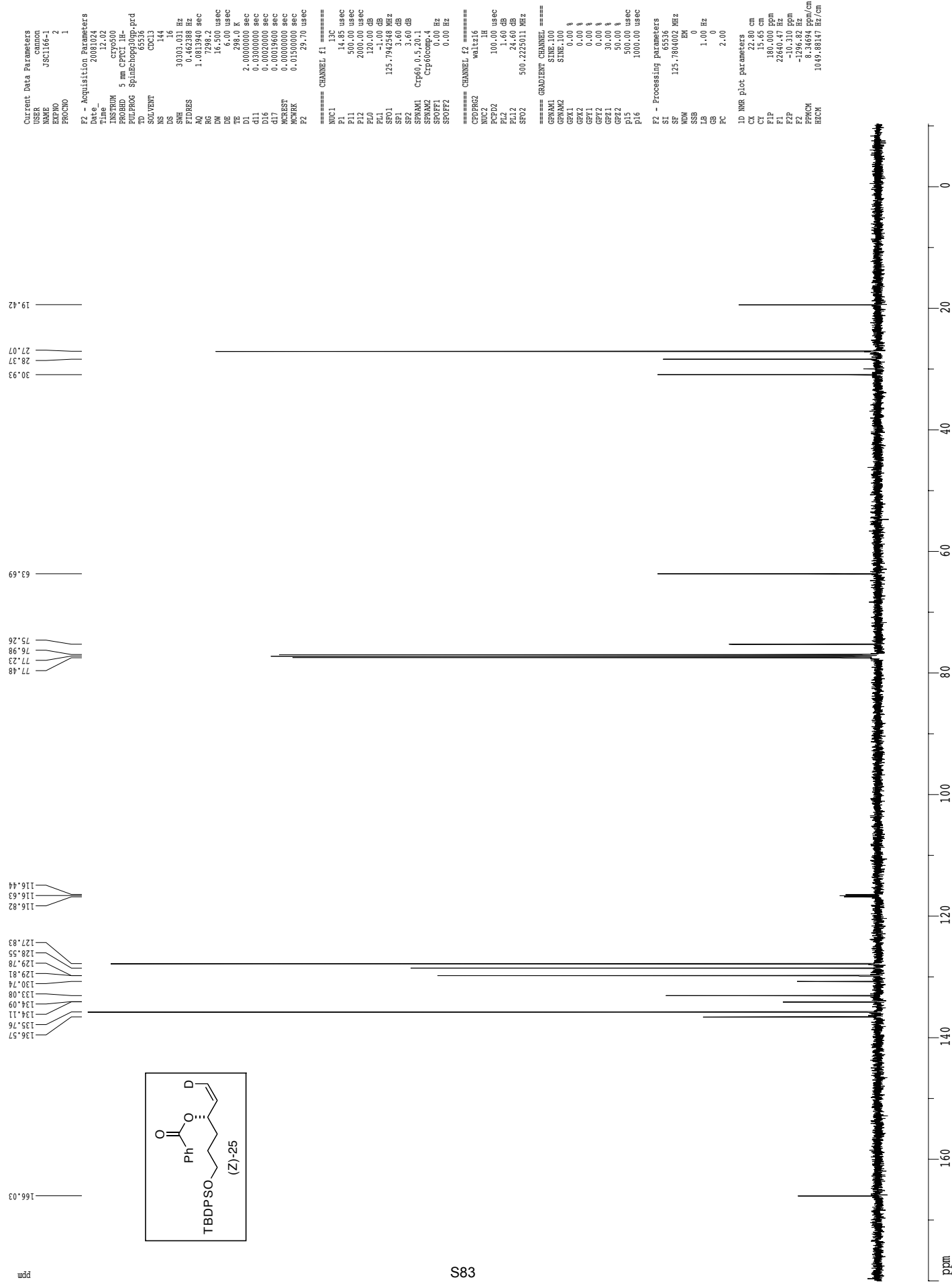
F2 - Acquisition Parameters  
 Date\_ 20081024  
 Time 13:05:33  
 INSTRUM cxts600  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHW 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 4.5  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWBK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6536  
 SF 500.2202626 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.061 ppm  
 F3 0.482 ppm/cm  
 FWHM 0.482 ppm/cm  
 HECW 220.73753 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USBR cannon  
 NAME JSC116-1  
 EXPNO 2  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20081024  
 Time\_ 12.02  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG SpinEchoSqr-prd  
 D1 2.00000000 sec  
 SOLVENT CDCl3  
 NS 144  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.061390 sec  
 RG 7296.2  
 DW 16.500 usec  
 DE 16.000 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00200000 sec  
 d17 0.00019600 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec  
 F2 29.70 usec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 14.85 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SFO1 125.7942548 MHz  
 SF02 500.1362973 MHz  
 SP2 3.60 dB  
 SPNAM1 Ctp60.0.5.20.1  
 SPNAM2 Ctp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

==== CHANNEL f2 =====  
 CDP6GZ waitz16  
 P1 100.00 usec  
 P12 1.60 dB  
 PL1 24.60 dB  
 SFO2 500.2225011 MHz

==== GRADIENT CHANNEL =====  
 GPRAM1 SINE.100  
 GPRAM2 SINE.100  
 GRZ1 0.00 %  
 GRZ2 0.00 %  
 GRZ3 0.00 %  
 GRZ4 0.00 %  
 GRZ5 0.00 %  
 GRZ6 0.00 %  
 GRZ7 0.00 %  
 GRZ8 0.00 %  
 GRZ9 0.00 %  
 GRZ10 0.00 %  
 GRZ11 30.00 %  
 GRZ12 50.00 %  
 GRZ13 50.00 usec  
 GRZ14 1000.00 usec  
 GRZ15 1000.00 usec  
 GRZ16 1000.00 usec

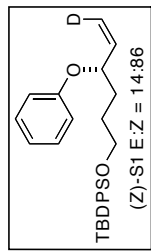
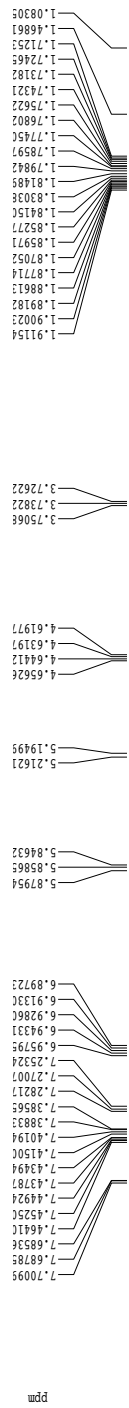
F2 - Processing parameters  
 SI 46356  
 SF 125.7804002 MHz  
 MDW EN  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

1D NMR plot parameters  
 CX 22.80 cm  
 CT 15.65 cm  
 F1P 180.000 PPM  
 F1 22640.47 Hz  
 F2P -10.310 PPM  
 F2 -1296.82 Hz  
 PPRCM 8.34694 PPM/cm  
 HZCM 1049.48147 Hz/cm





<sup>1</sup>H spectrum



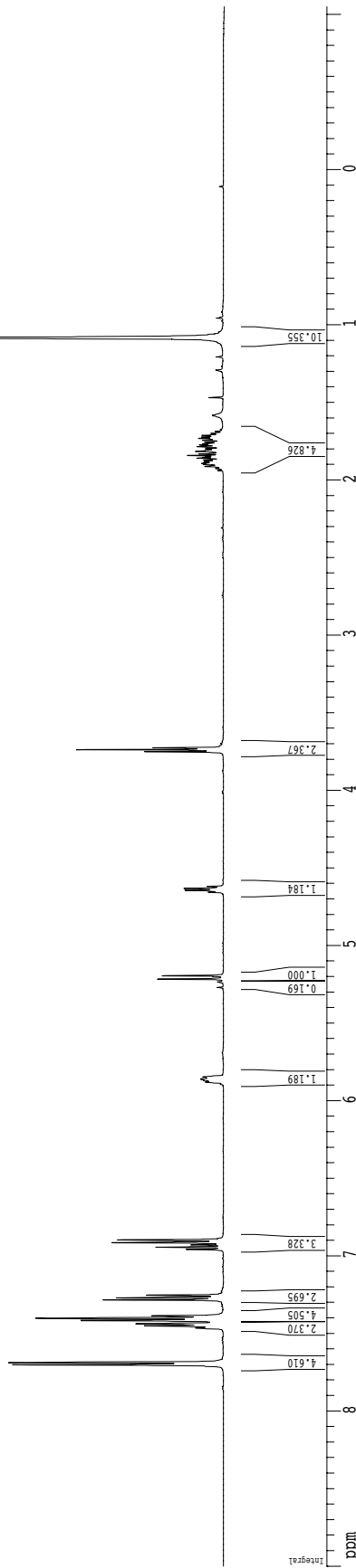
Current Data Parameters  
 USER cannon  
 NAME JSC1210  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180923  
 Time 11:01:11  
 INSTRUM spect  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHF 801.2820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 8  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 D11 0.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRE 0.01500000 sec

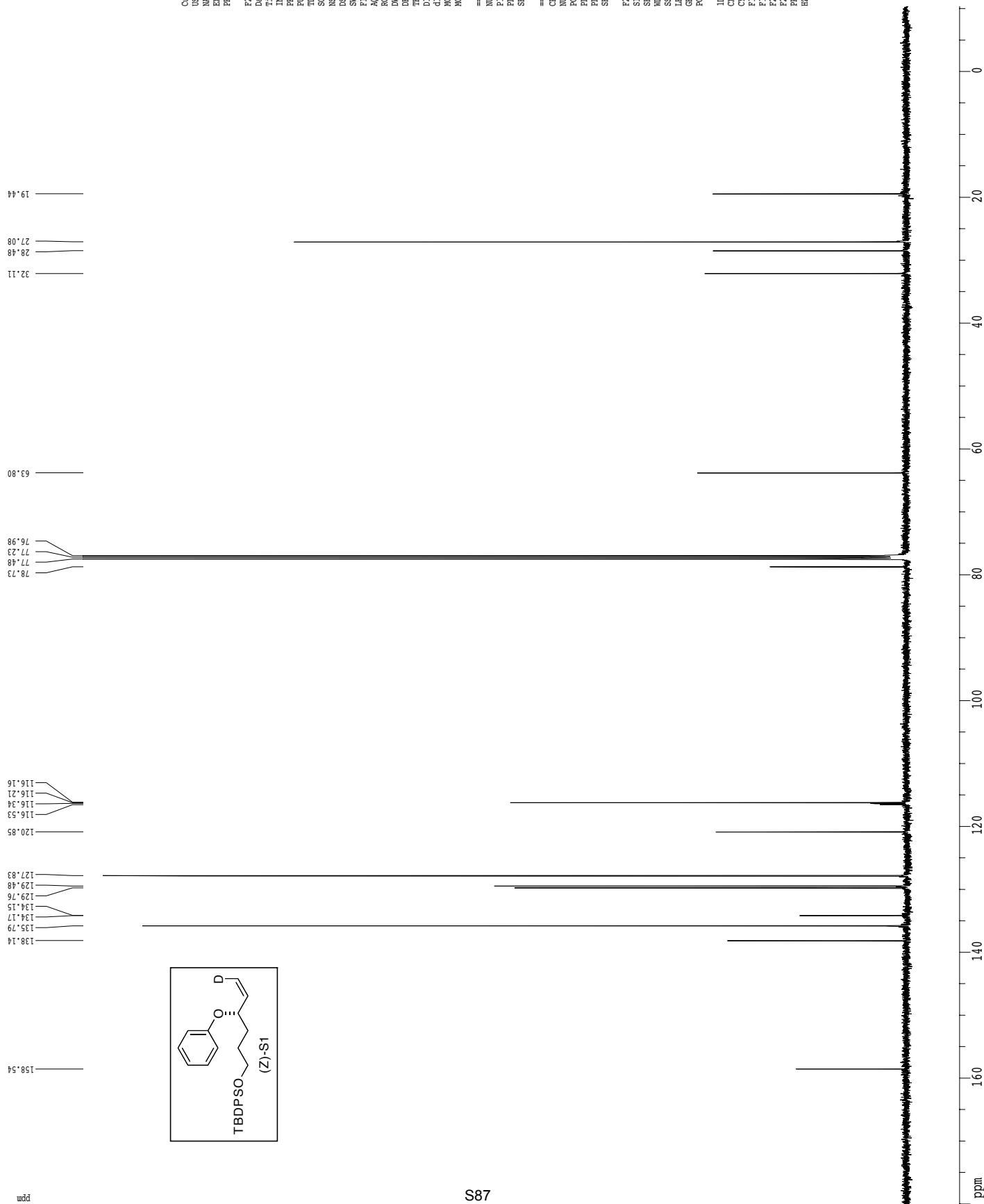
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.38 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2200139 MHz  
 EQ 2  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4500.98 Hz  
 F2 -1.069 ppm  
 F2F -524.72 Hz  
 FWHM 0.4841 ppm/cm  
 HECW 220.4694 Hz/cm



<sup>13</sup>C spectrum with <sup>1</sup>H decoupling



Current Data Parameters  
 USER camon  
 NAME JSC1210  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080923  
 Time 15.15  
 INSTRUM cryo00  
 PROBHD 5 mm CPCLP1H-  
 PULPROG zgpg30  
 TO 654.8  
 SOLVENT CDCl3  
 NS 160  
 DS 4  
 SPH 30303.031 Hz  
 FIDRES 0.463222 Hz  
 AQ 1.0794470 sec  
 RG 13004  
 DW 16.500 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 MCREST 0.0000000 sec  
 MCPRK 0.0150000 sec

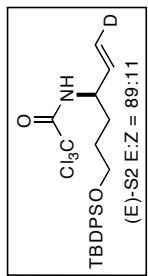
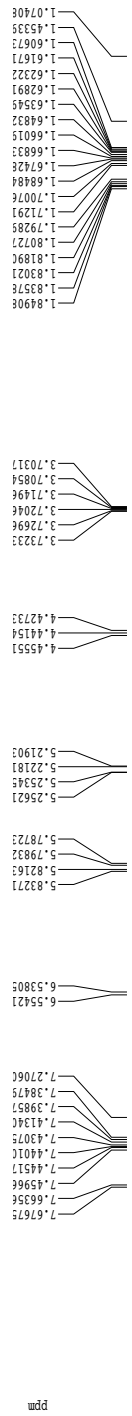
==== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 14.75 usec  
 PL1 -1.00 dB  
 SFO1 125.7942548 MHz

==== CHANNEL f2 =====  
 CPDPRG2 walz16  
 NUC2 <sup>1</sup>H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.80 dB  
 SFO2 500.2225011 MHz

F2 - Processing parameters  
 SI 65536  
 SF 125.7804006 MHz  
 EN  
 SSB 0  
 AB 1.00 Hz  
 GB  
 PC 2.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.65 cm  
 F1P 180.000 ppm  
 F1 22640.47 Hz  
 F2P -10.314 ppm  
 F2 -1297.28 Hz  
 PPMCH 8.34710 ppm/cm  
 HZCH 1049.90137 Hz/cm

1H spectrum



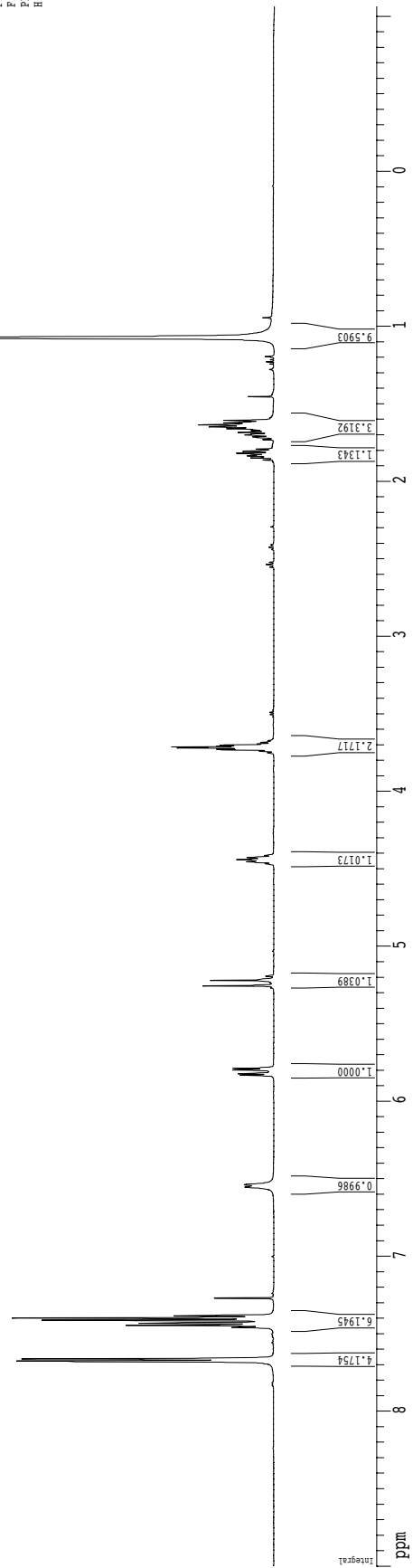
Current Data Parameters  
 USER cannon  
 NAME JSC2047R-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081023  
 Time 15:03  
 INSTRUM cp13500  
 PROBRD 5 mm CPACT IH-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 4  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWBK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

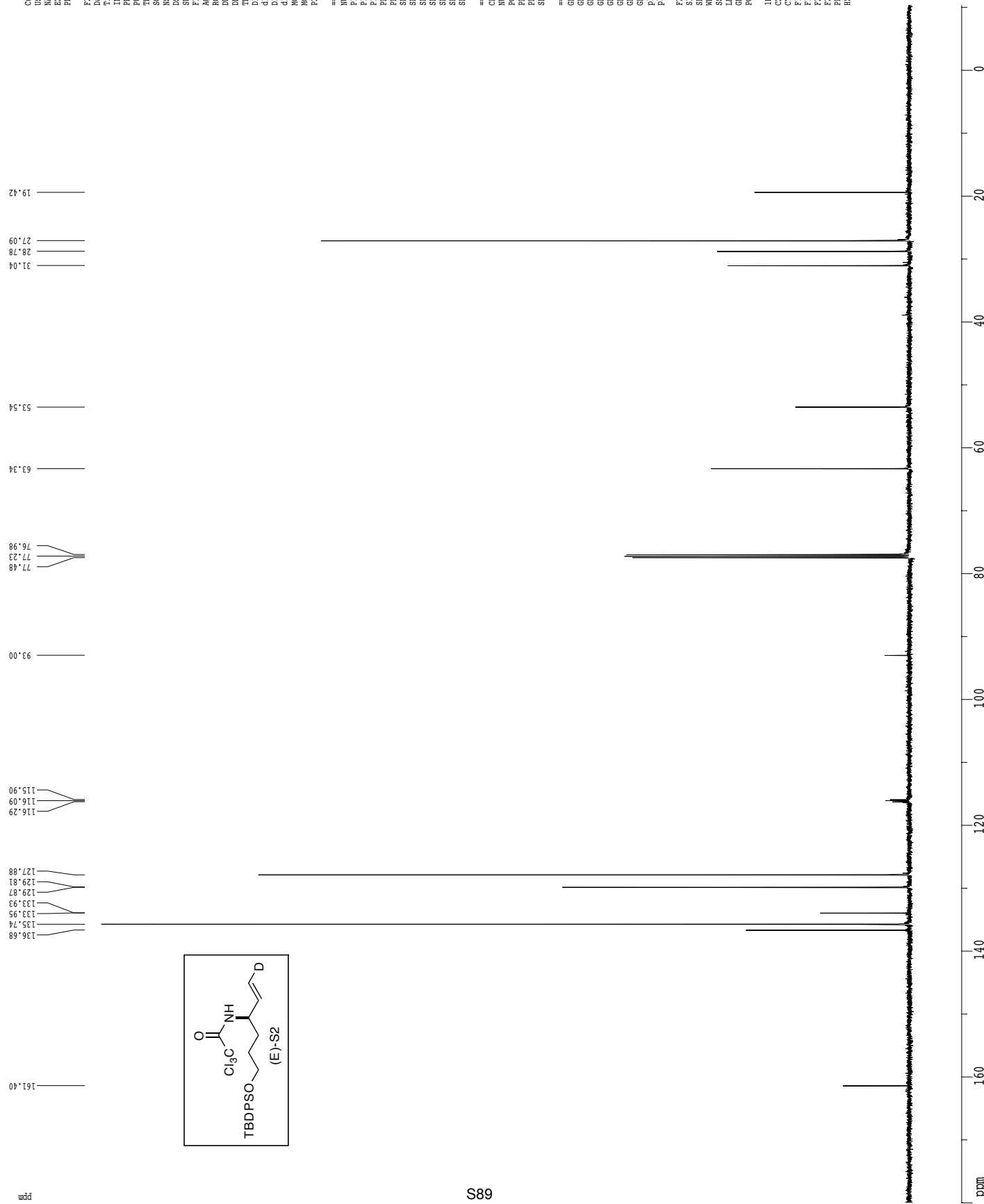
F2 - Processing parameters  
 SI 6536  
 SF 500.220261 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.061 ppm  
 F3 0.53056 Hz  
 FWHM 0.482 ppm/cm  
 HECW 220.74300 Hz/cm





Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USBR canon  
 NAME JSC2047R-1  
 EXPNO 2  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 200811023  
 Time\_ 12.05  
 INSTRUM cryo500  
 PROBDH 5 mm CPXI 1H-  
 PULPROG SpinEcho13cp-  
 13c-13c  
 SOLVENT CDCl3  
 NS 96  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0613840 sec  
 RG 5792.6  
 DW 16.500 usec  
 DE 1.000 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00019600 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec  
 F2 29.70 usec

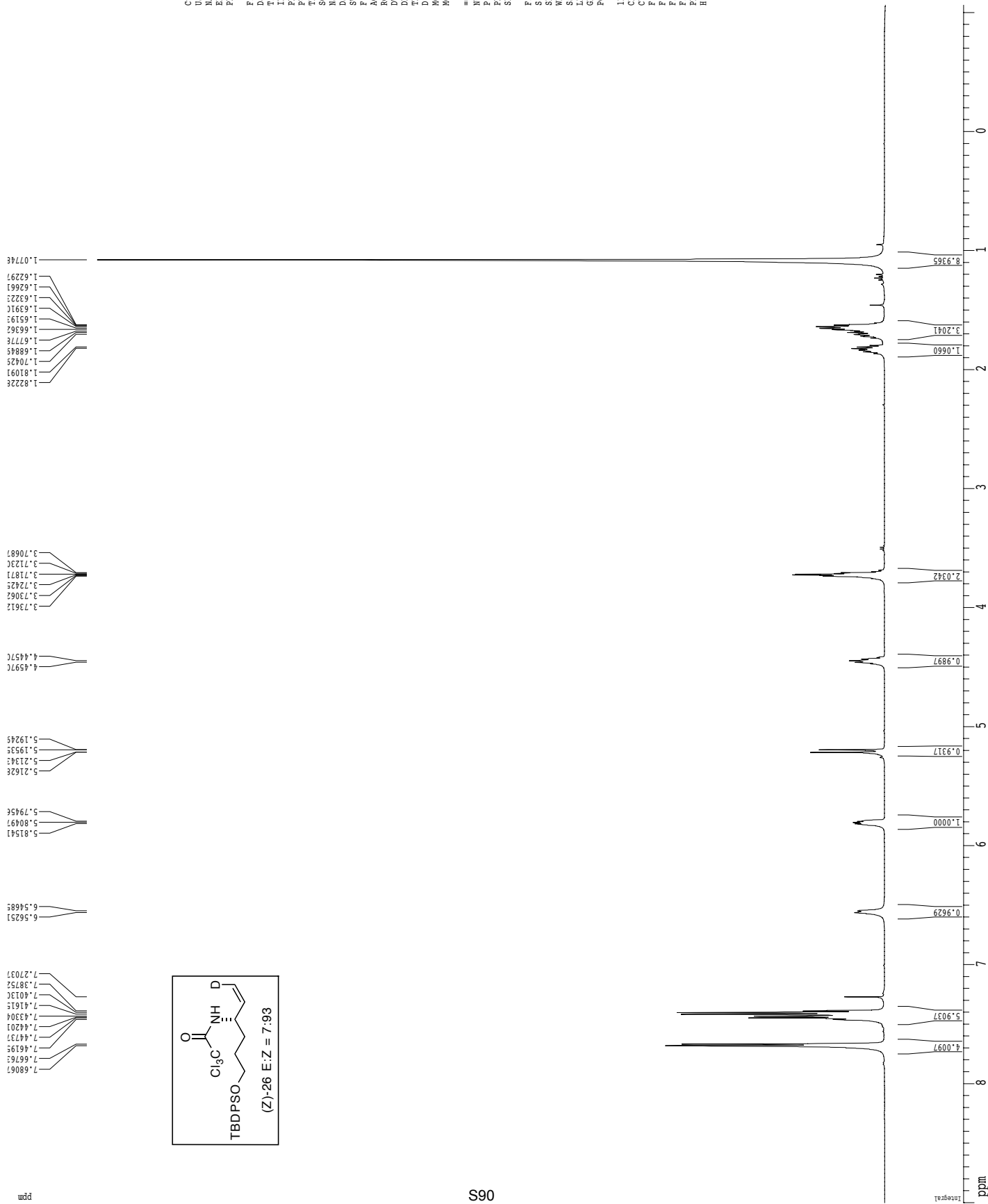
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 14.85 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SFO1 125.7942548 MHz  
 SF02 500.1362974 MHz  
 SP2 3.60 dB  
 SPANM1 Ctp60,0.5,20.1  
 SPANM2 Ctp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

==== CHANNEL f2 =====  
 CDPGZ wait216  
 P1 1.00 usec  
 P11 100.00 usec  
 P12 1.60 dB  
 PL1 24.60 dB  
 SFO2 500.2225011 MHz

==== GRADIENT CHANNEL =====  
 GPRM1 SINE,100  
 GPRM2 SINE,100  
 GRZ1 0.00 %  
 GRZ2 0.00 %  
 GRZ3 0.00 %  
 GRZ4 0.00 %  
 GRZ5 0.00 %  
 GRZ6 0.00 %  
 GRZ7 0.00 %  
 GRZ8 0.00 %  
 GRZ9 0.00 %  
 GRZ10 0.00 %  
 GRZ11 30.00 %  
 GRZ12 50.00 %  
 GRZ13 50.00 %  
 GRZ14 50.00 %  
 GRZ15 500.00 usec  
 GRZ16 1000.00 usec

F2 - Processing parameters  
 SI 46536  
 SF 125.7804025 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00  
 ID\_NMR plot parameters  
 CX 22.80 cm  
 CT 15.65 cm  
 F1P 180.000 PPM  
 F1 22640.47 Hz  
 F2P -10.329 PPM  
 F2 -1299.13 Hz  
 PPMCM 8.3474 PPM/cm  
 HZCM 1049.98254 Hz/cm

1H spectrum



Current Data Parameters  
 USER cannon  
 NAME JSC20475-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081023  
 Time 16:22  
 INSTRUM cxts600  
 PROBRD 5 mm CPCTC 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHW 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 5  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 296.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWREK 0.01500000 sec

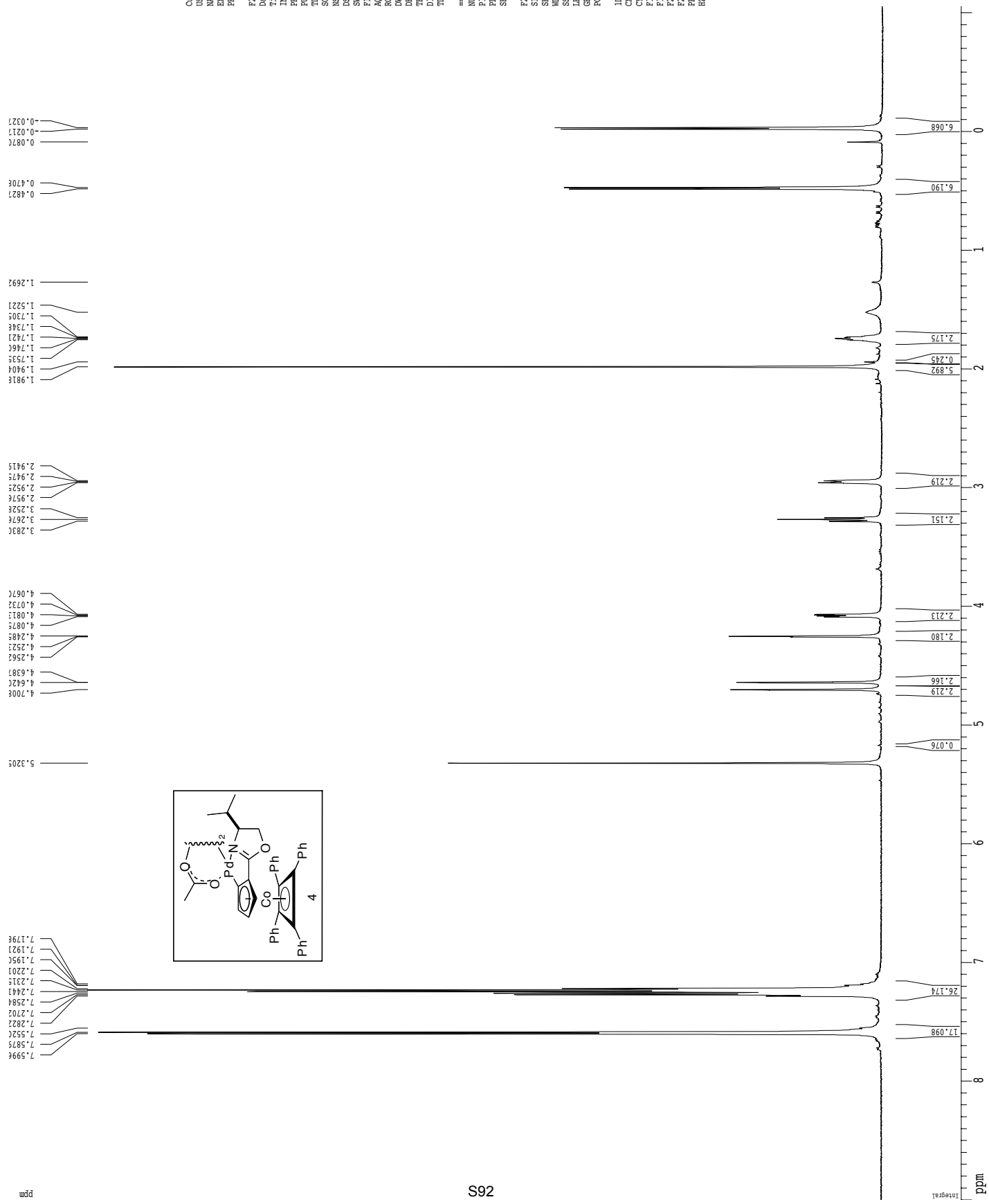
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2200220 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4500.98 Hz  
 F2 -1.061 ppm  
 F3 0.000 ppm  
 FWHM 0.4822 Hz/cm  
 HECW 220.73225 Hz/cm



1H spectrum



Current Data Parameters  
 USER camon  
 NAME JSC1040  
 EXPNO 101  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080311  
 Time 16.55  
 INSTRUM av600  
 PROBHD 5 mm BBO BB-HF  
 PULPROG zgpg30  
 TO 9.938  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 9615.385 Hz  
 FIDRES 0.098178 Hz  
 AQ 5.0928259 sec  
 RG 512  
 DW 52.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 TDO 1

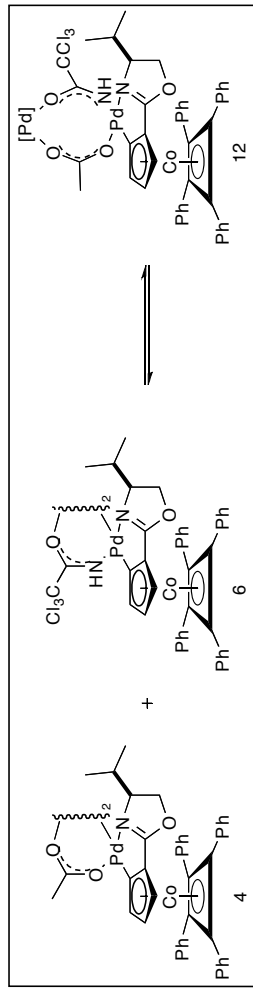
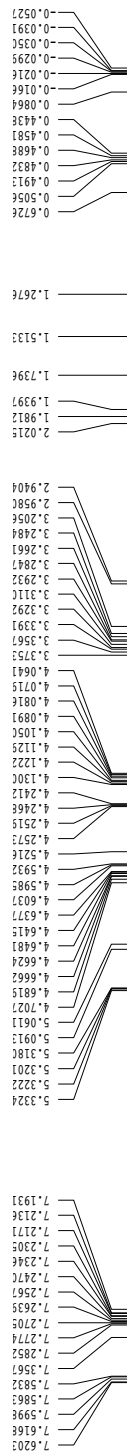
==== CHANNEL f1 =====  
 NUCL1 1H  
 P1 9.00 usec  
 PL1 -5.00 dB  
 SFO1 600.1342005 MHz

F2 - Processing Parameters  
 SI 65536  
 SF 600.1300246 MHz  
 MDW 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 CB 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CZ 15.00 cm  
 FID 9.000 ppm  
 F1 5401.17 Hz  
 F2 -1.052 ppm  
 F3 0.01488 Hz  
 FREQM 0.01488 ppm/cm  
 FREQN 264.58752 Hz/cm



<sup>1</sup>H spectrum



Current Data Parameters  
 USER cannon  
 NAME JSC1061  
 EXPNO 6  
 PROCNO 1

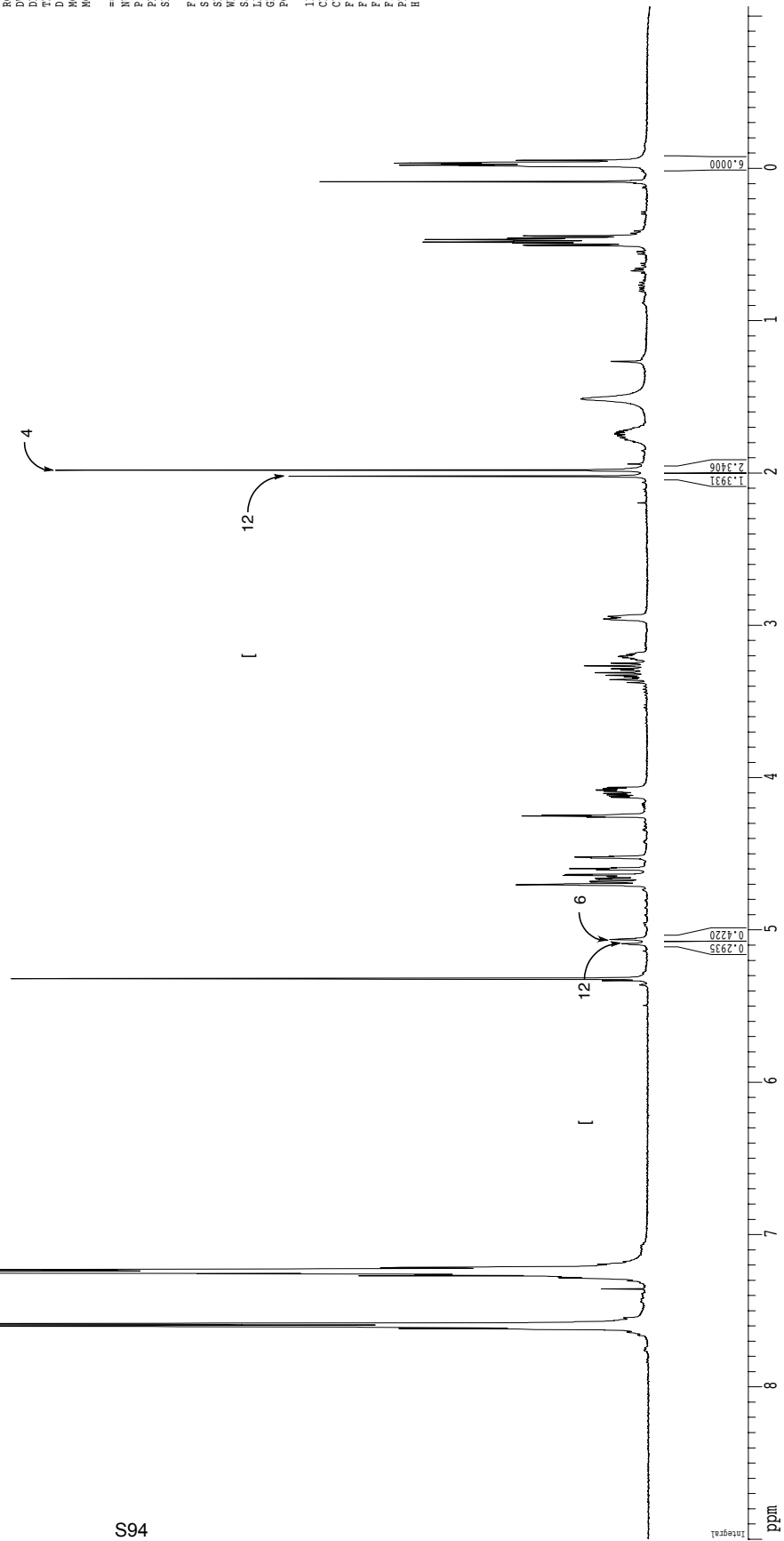
F2 - Acquisition Parameters

Date\_ 20100402  
 Time 11:05:00  
 INSTRUM spect  
 PULPROG 5 mm broadband  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 8  
 DS 2  
 SHF 801.2820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 912.3  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWBK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -3.00 dB  
 SFO1 499.8284988 MHz

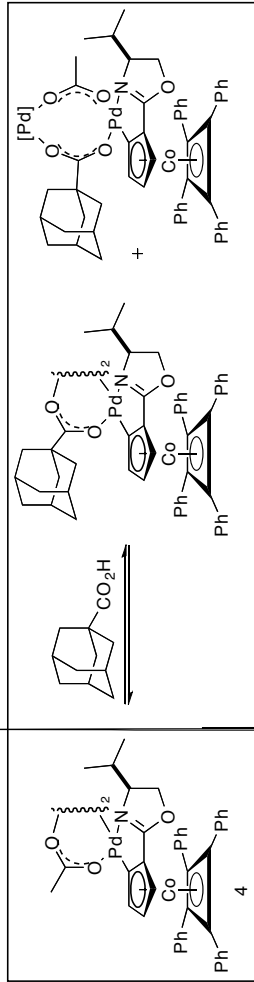
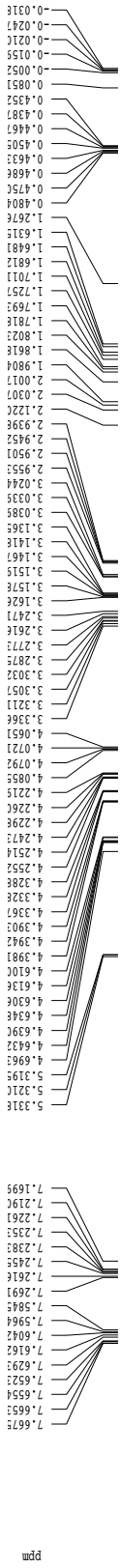
F2 - Processing parameters  
 SI 65536  
 SF 499.8284988 MHz  
 HF 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4498.43 Hz  
 F2 -11.061 ppm  
 F3 0.00000000 Hz  
 FWHM 0.4825 ppm/cm  
 HECN 220.56625 Hz/cm





1H spectrum



Current Data Parameters  
 USER camon  
 NAME JSC1109  
 EXPNO 101  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080523  
 Time 15.11  
 INSTRUM av600  
 PROBD 5 mm TBI 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SFO 9615.385 Hz  
 FIDRES 0.098178 Hz  
 AQ 5.0928259 sec  
 RG 512  
 DW 52.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 TD0 1

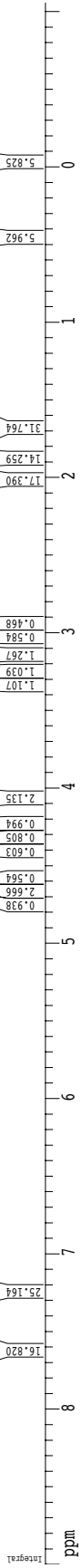
==== CHANNEL f1 =====  
 NUCL1 1H  
 P1 8.00 usec  
 PL1 -1.00 dB  
 SFO1 600.1342009 MHz

F2 - Processing Parameters  
 SI 65536  
 SF 600.1300259 MHz  
 MDW 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 FL 5401.17 Hz  
 FZ -1.054 ppm  
 G 0.0000 Hz  
 H 0.0000 Hz  
 HPCN 264.64261 Hz/cm

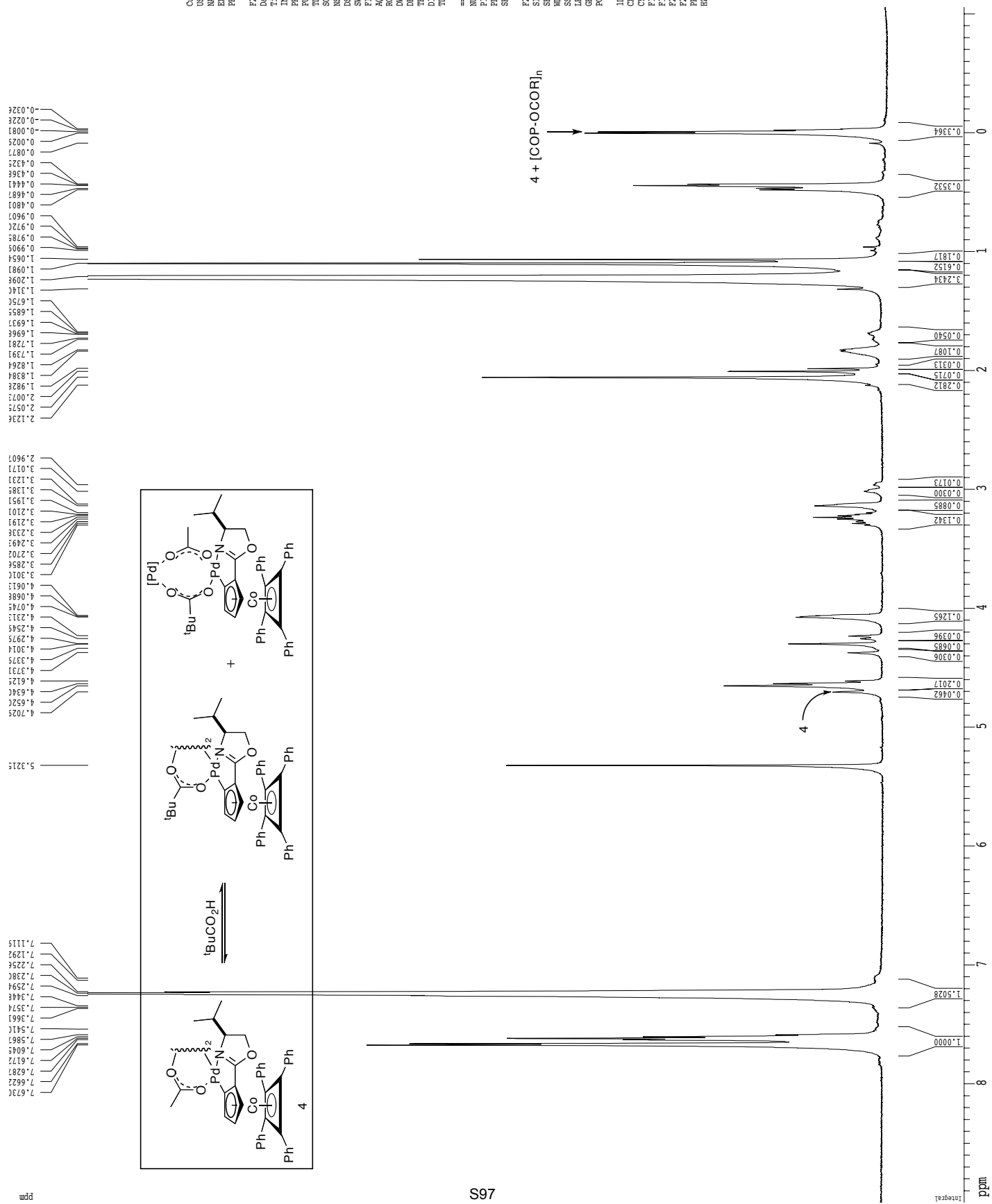
4 + [COP-OCOR]<sub>n</sub>

4

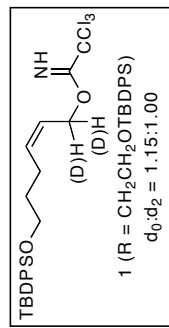
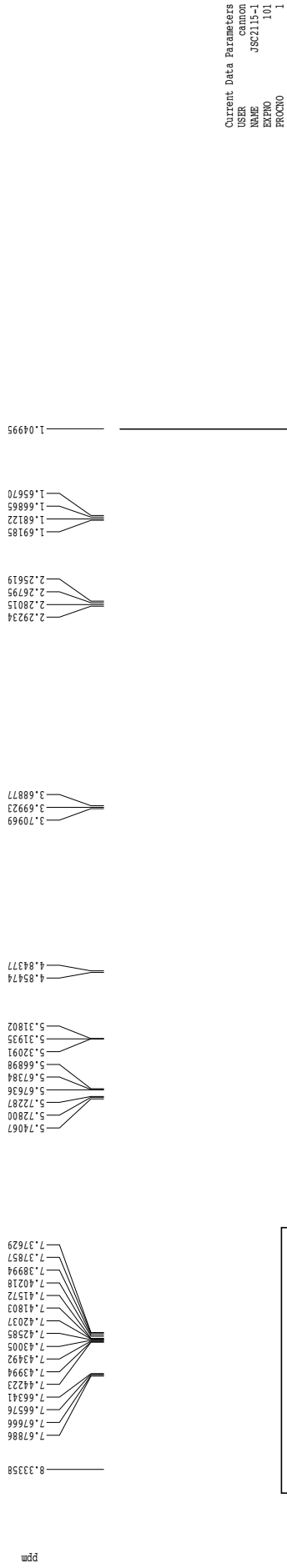




1H spectrum



1H spectrum



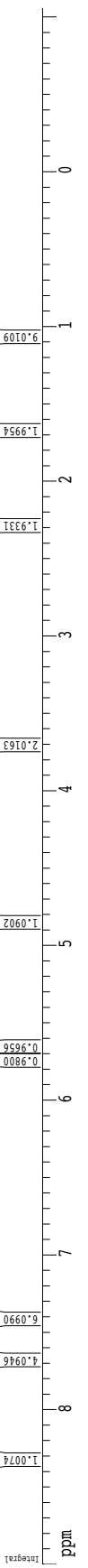
Current Data Parameters  
 USER camon  
 NAME JSC2115-1  
 EXPNO 101  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20/09/18  
 Time 19.07  
 INSTRUM av600  
 PROBD 5 mm TBI 1H/13  
 PULPROG zg30  
 AQ 17.236  
 RG 16  
 NS 2  
 DS 2  
 SWH 9615.385 Hz  
 FIDRES 0.055600 Hz  
 EQ 8.9928265 sec  
 RG 287  
 DW 52.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 21.0000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.00 usec  
 PL1 -1.00 dB  
 SFO1 600.1342019 MHz

F2 - Processing Parameters  
 SF 600.1300260 MHz  
 ST 65536  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

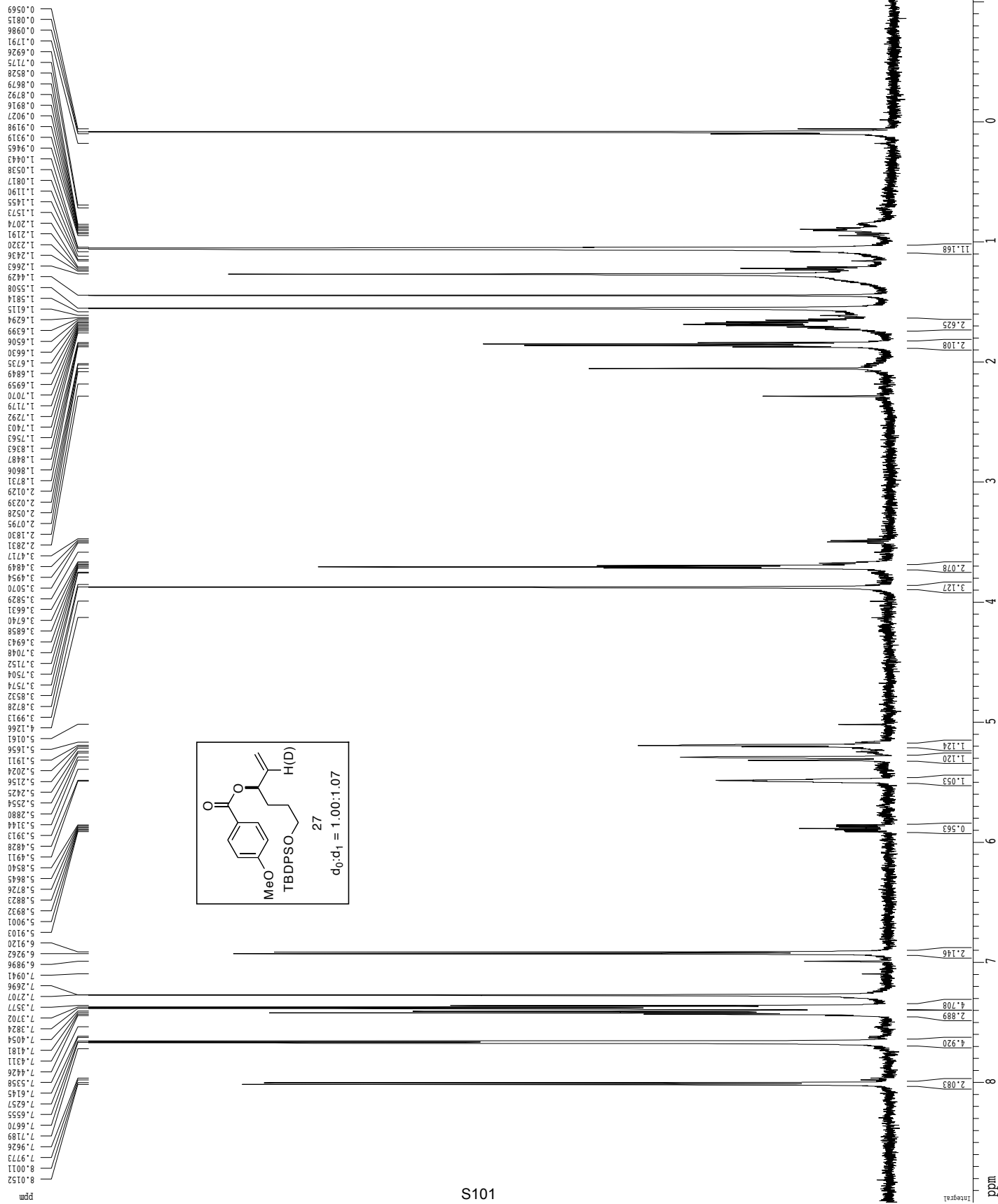
ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 5401.17 Hz  
 F2 -1.054 ppm  
 FZ 0.63275 Hz  
 PPMXCH 0.44098 ppm/cm  
 PPMYCH 264.64575 Hz/cm







2-chromatographed  
1H spectrum



Current Data Parameters  
 USER camon  
 NAME JS62171-2  
 EXPNO 103  
 PROCNO 1

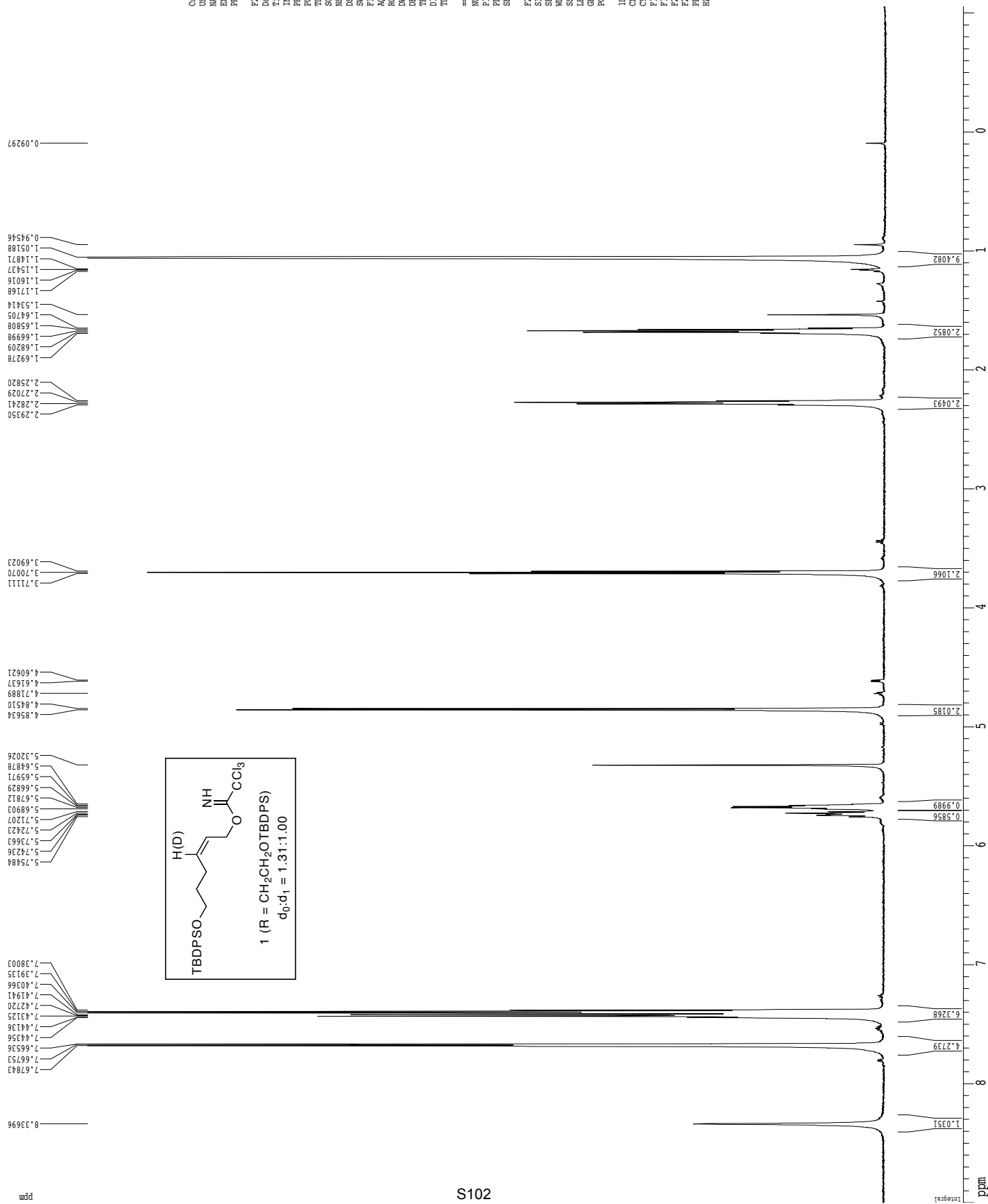
F2 - Acquisition Parameters  
 Date\_ 20/09/07  
 Time 14.46  
 INSTRUM av600  
 PROBHD 5 mm TBI H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 9615.385 Hz  
 FIDRES 0.055600 Hz  
 AQ 8.9928265 sec  
 RG 2050  
 DW 52.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 21.0000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.00 usec  
 PL1 0.00 dB  
 SFO1 600.1342009 MHz

F2 - Processing parameters  
 SI 65536  
 SF 600.1300287 MHz  
 MDW 0  
 EN 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Id NMR plot parameters  
 CX 22.80 cm  
 CT 120.00 cm  
 FIP 9.000 ppm  
 F1 5401.17 Hz  
 F2 41.029 ppm  
 F3 68.813 Hz  
 FWHM 0.4418 ppm/cm  
 HZCM 264.76624 Hz/cm

SM  
1H spectrum



Current Data Parameters  
 USER camon  
 NAME JS62112-1  
 EXPNO 101  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20/09/14  
 Time 18.41  
 INSTRUM av600  
 PROBHD 5 mm TBI 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 2  
 SWH 9615.385 Hz  
 FIDRES 0.055600 Hz  
 AQ 8.9928265 sec  
 RG 1150  
 DW 52.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 21.0000000 sec  
 TDO 1

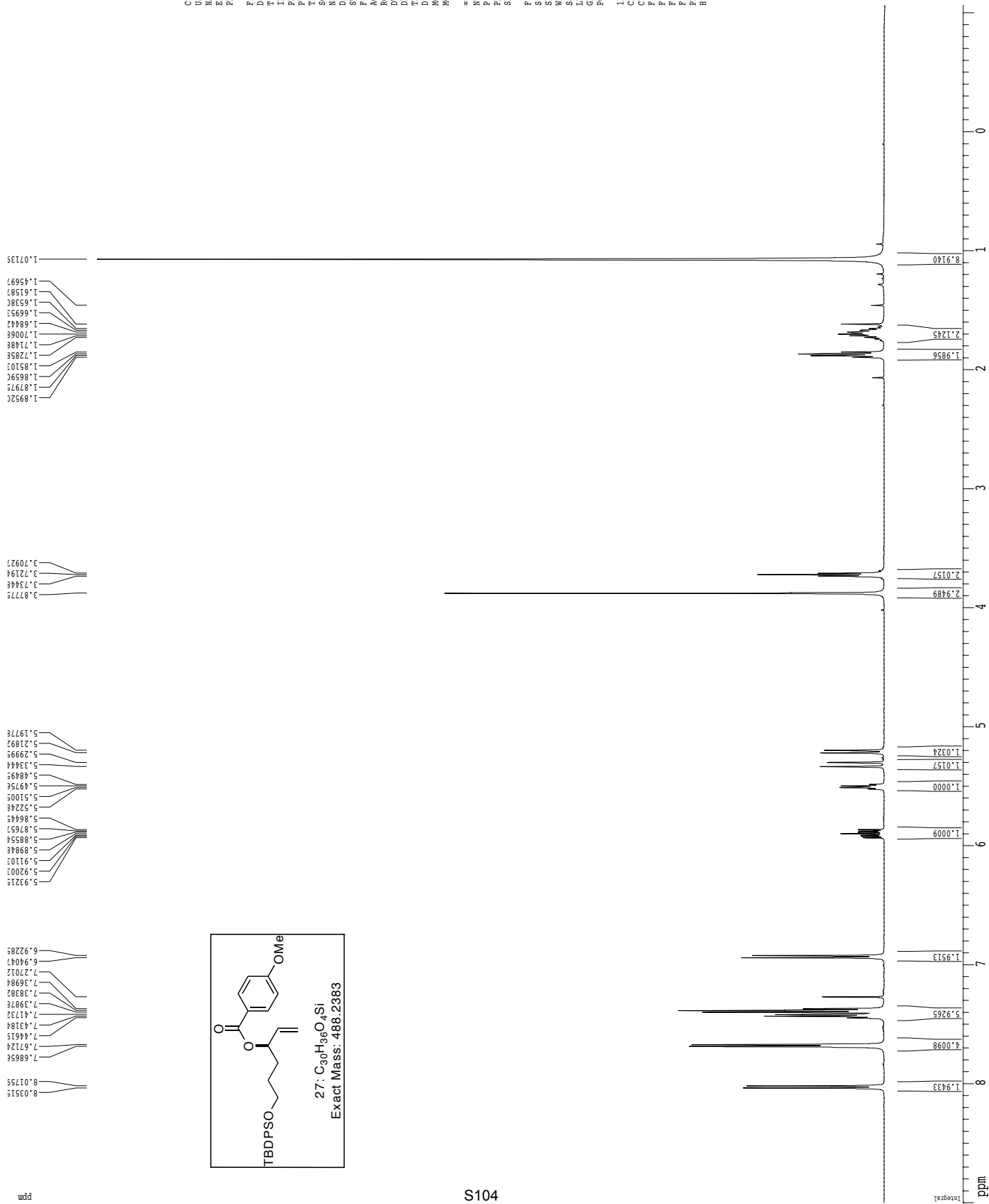
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.00 usec  
 PL1 0.00 dB  
 SFO1 600.134209 MHz

F2 - Processing parameters  
 SI 65536  
 SF 600.130255 MHz  
 MDW 0  
 EM 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Id NMR plot parameters  
 CX 22.80 cm  
 CT 120.00 cm  
 FIP 9.000 ppm  
 F1 5401.17 Hz  
 F2 41.55 ppm  
 F3 41.55 ppm  
 FWHM 0.84095 ppm/cm  
 HZCM 264.62521 Hz/cm



1H spectrum



Current Data Parameters  
 USER cannon  
 NAME JSC2186-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090330  
 Time 15:05:00  
 INSTRUM cxtv600  
 PROBRD 5 mm CPACT IH-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 5.7  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

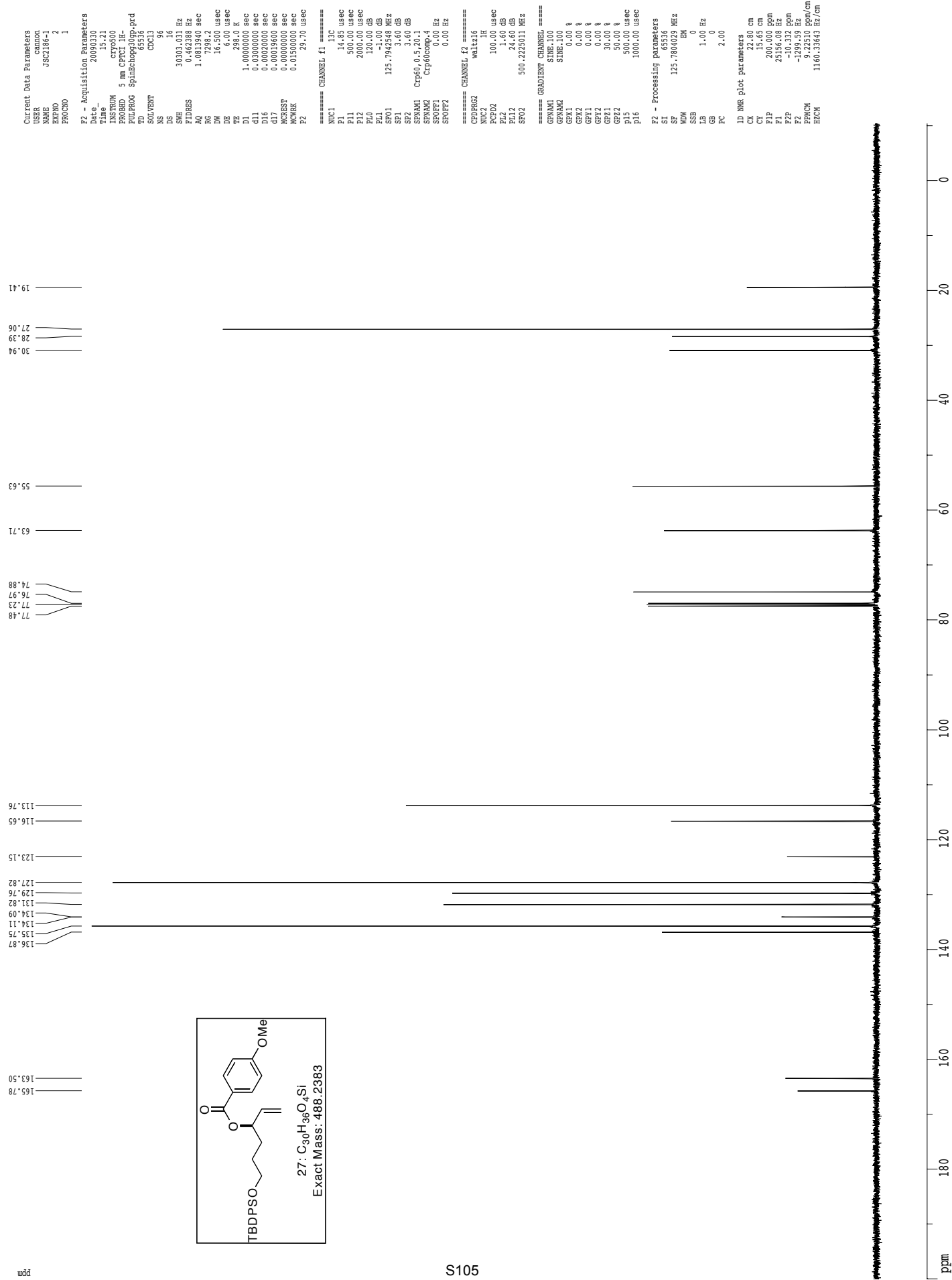
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6536  
 SF 500.220260 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

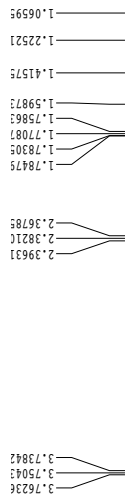
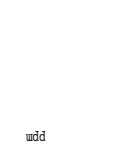
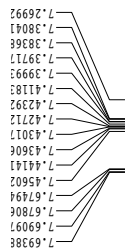
1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.062 ppm  
 F3 531.45 Hz  
 FWHM 0.483 ppm/cm  
 HECW 220.76451 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



1H spectrum



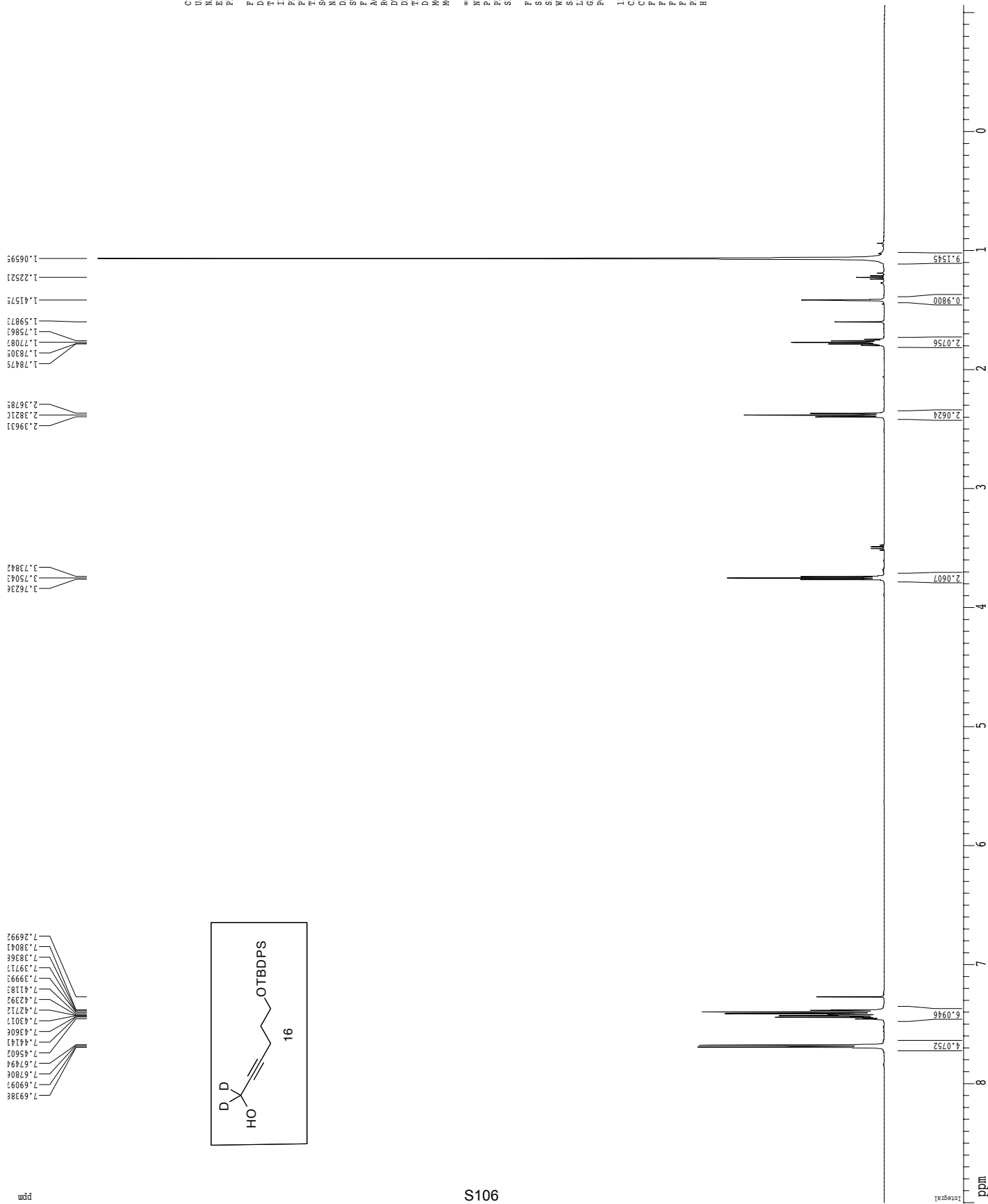
Current Data Parameters  
 USER cannon  
 NAME JSCI150  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080620  
 Time 11:41:01  
 INSTRUM cxts600  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHF 801.280 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 5.7  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.38 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

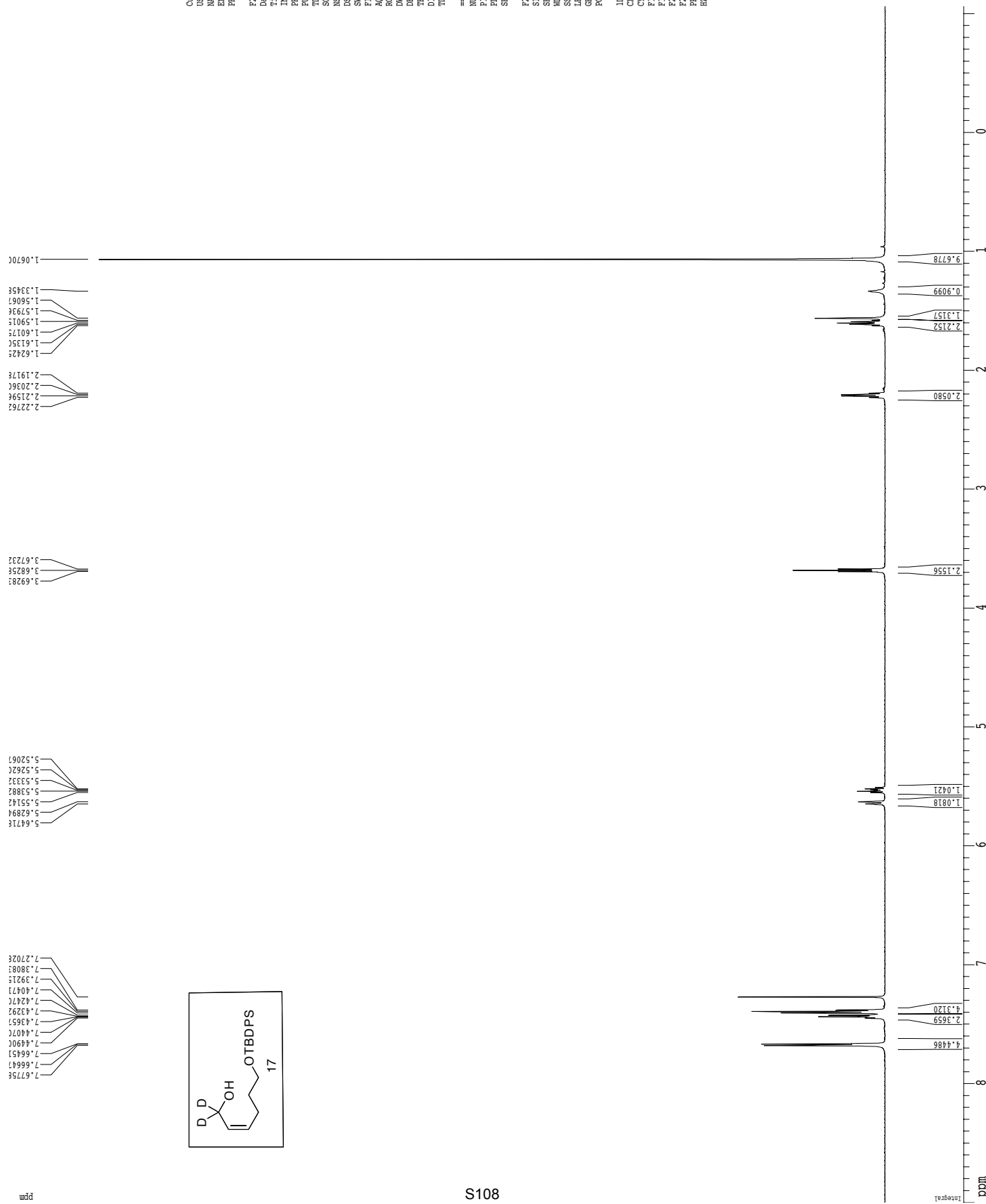
F2 - Processing parameters  
 SI 6536  
 SF 500.2200250 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.061 ppm  
 F3 0.71 Hz  
 FWHM 0.482 ppm/cm  
 HECN 220.73225 Hz/cm





1H spectrum



Current Data Parameters  
 USER camon  
 NAME JSC1175  
 EXPNO 101  
 PROCNO 1

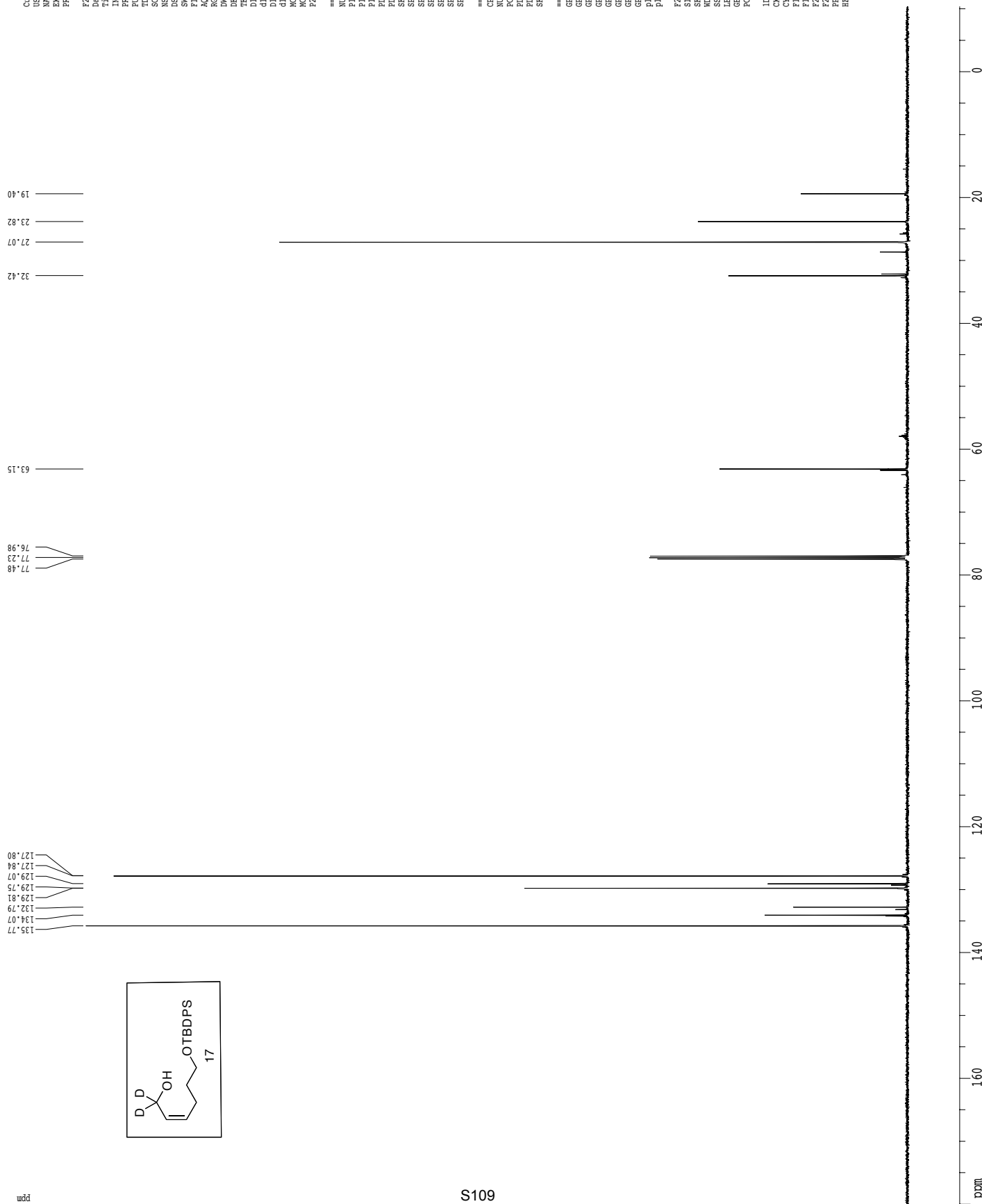
F2 - Acquisition Parameters  
 Date\_ 20080630  
 Time\_ 9.56  
 INSTRUM av600  
 PROBED 5 mm TBI 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 9615.385 Hz  
 FIDRES 0.098178 Hz  
 AQ 5.0928259 sec  
 RG 1620  
 DW 52.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUCL1 1H  
 P1 8.00 usec  
 PL1 -1.00 dB  
 SFO1 600.1362009 MHz

F2 - Processing parameters  
 SI 65536  
 SF 600.1300291 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 FI 5401.17 Hz  
 FZP -1.060 ppm  
 F1 0.3155 Hz  
 FREQCN 264.78156 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER cannon  
 NAME JSC1037  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081014  
 Time\_ 11:11  
 INSTRUM crys500  
 PROBHD 5 mm CPXI IH-  
 PULPROG SpinEchoSqr-prd  
 F2 125.76  
 SOLVENT CDCl3  
 NS 313  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0613940 sec  
 RG 832  
 DW 16.500 usec  
 DE 16.000 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00200000 sec  
 d17 0.00019600 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec  
 F2 29.70 usec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 14.85 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SFO1 125.7642548 MHz  
 SF02 500.1363000 MHz  
 SP1 3.60 dB  
 SP2 3.60 dB  
 SPNAM1 Ctp60.0.5.20.1  
 SPNAM2 Ctp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

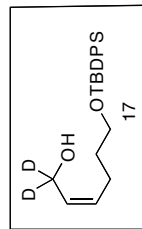
==== CHANNEL f2 =====  
 CDP6GZ waitz16  
 NUC2 13C  
 P2 14.85 usec  
 P21 500.00 usec  
 P22 2000.00 usec  
 PL2 120.00 dB  
 SFO2 500.2225011 MHz

==== GRADIENT CHANNEL =====  
 GPRAM1 SINE.100  
 GPRAM2 SINE.100  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC5 0.00 %  
 GPC6 0.00 %  
 GPC7 0.00 %  
 GPC8 0.00 %  
 GPC9 0.00 %  
 GPC10 0.00 %  
 GPC11 0.00 %  
 GPC12 0.00 %  
 GPC13 0.00 %  
 GPC14 0.00 %  
 GPC15 0.00 %  
 GPC16 0.00 %

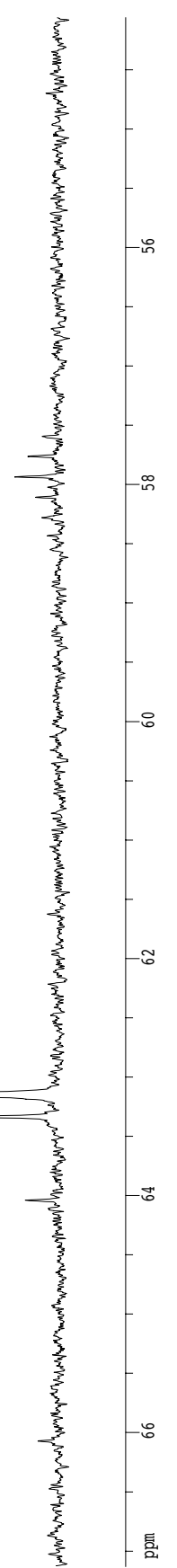
F2 - Processing parameters  
 SI 65536  
 SF 125.7604025 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

1D NMR plot parameters  
 CX 22.80 cm  
 CT 15.65 cm  
 F1P 180.000 PPM  
 F1 22640.47 Hz  
 F2P -10.329 PPM  
 F2 -1299.13 Hz  
 PPMCM 8.34774 PPM/cm  
 HZCM 1049.56254 Hz/cm

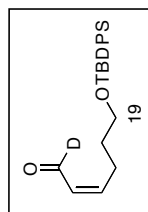
Z-restored spin-echo <sup>13</sup>C spectrum with <sup>1</sup>H decoupling



```
Current Data Parameters
USER          cannon
NAME         JSC1037
EXPNO        4
PROCNO       1
F2 - Acquisition Parameters
Date_        20081014
Time         11.11
INSTRUM     crys000
PROBHD      5 mm CPXI IH-
PULPROG     zgpg30
SOLVENT     CDCl3
NS          313
DS          16
SWH         30303.031 Hz
FIDRES     0.462388 Hz
AQ         1.0613940 sec
RG         832
AQ         16.500 usec
TE         298.2 K
D1         2.0000000 sec
d11        0.0300000 sec
D16        0.0002000 sec
d17        0.0001960 sec
MCREST     0.0000000 sec
MCPRK      0.0150000 sec
F2         29.70 usec
===== CHANNEL f1 =====
NUC1        13C
P1          14.85 usec
P11         500.00 usec
P12         2000.00 usec
PL0         120.00 dB
PL1         -1.00 dB
SFO1        125.7942548 MHz
P2          3.60 usec
SFO2        500.1362610 MHz
SFO3        500.1362610 MHz
SFO4        500.1362610 MHz
SFO5        500.1362610 MHz
SFO6        500.1362610 MHz
SFO7        500.1362610 MHz
SFO8        500.1362610 MHz
SFO9        500.1362610 MHz
SFO10       500.1362610 MHz
SFO11       500.1362610 MHz
SFO12       500.1362610 MHz
SFO13       500.1362610 MHz
SFO14       500.1362610 MHz
SFO15       500.1362610 MHz
SFO16       500.1362610 MHz
SFO17       500.1362610 MHz
SFO18       500.1362610 MHz
SFO19       500.1362610 MHz
SFO20       500.1362610 MHz
===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         13C
P2          14.85 usec
P21         500.00 usec
P22         2000.00 usec
PL0         120.00 dB
PL1         -1.00 dB
SFO1        125.7942548 MHz
SFO2        500.1362610 MHz
===== GRADIENT CHANNEL =====
GPRAM1      SINE.100
GPRAM2      SINE.100
GPRAM3      SINE.100
GPRAM4      SINE.100
GPRAM5      SINE.100
GPRAM6      SINE.100
GPRAM7      SINE.100
GPRAM8      SINE.100
GPRAM9      SINE.100
GPRAM10     SINE.100
GPRAM11     SINE.100
GPRAM12     SINE.100
GPRAM13     SINE.100
GPRAM14     SINE.100
GPRAM15     SINE.100
GPRAM16     SINE.100
GPRAM17     SINE.100
GPRAM18     SINE.100
GPRAM19     SINE.100
GPRAM20     SINE.100
===== Processing parameters =====
SI          65536
SF          125.7804025 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          2.00
ID, NMR plot parameters
CX          22.80 cm
CY          15.65 cm
F1P         67.129 ppm
F1          8443.46 Hz
F2P         54.061 ppm
F2          6799.84 Hz
PPHMCN     0.57313 ppm/cm
HSCN       72.08830 Hz/cm
```



1H spectrum



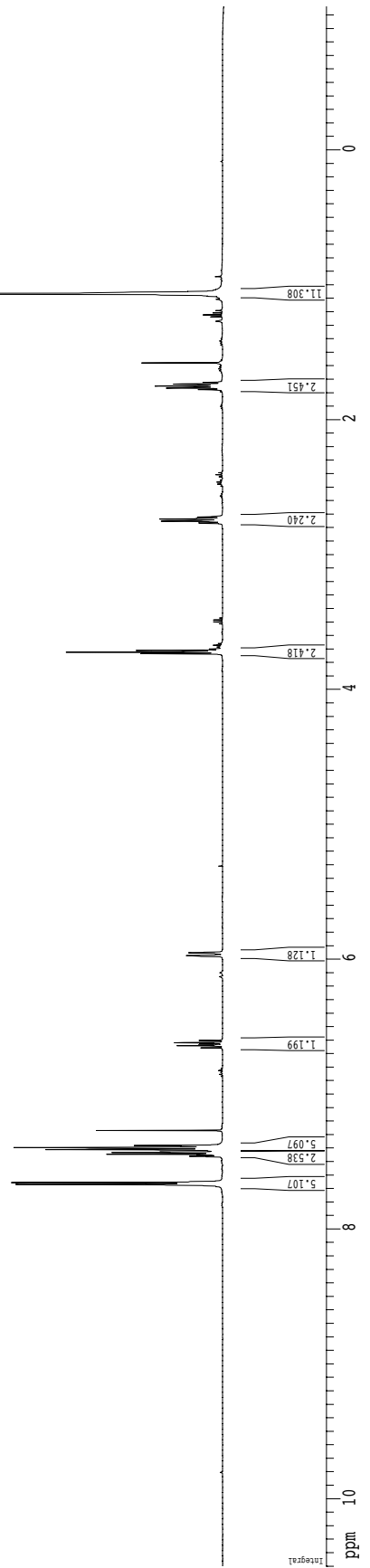
Current Data Parameters  
 USER cannon  
 NAME JSC1155  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180620  
 Time 13:02:03  
 INSTRUM cfd500  
 PROBRW 5 mm CPDCT IH-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHW 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 4.5  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWBK 0.01500000 sec

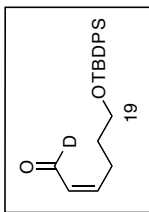
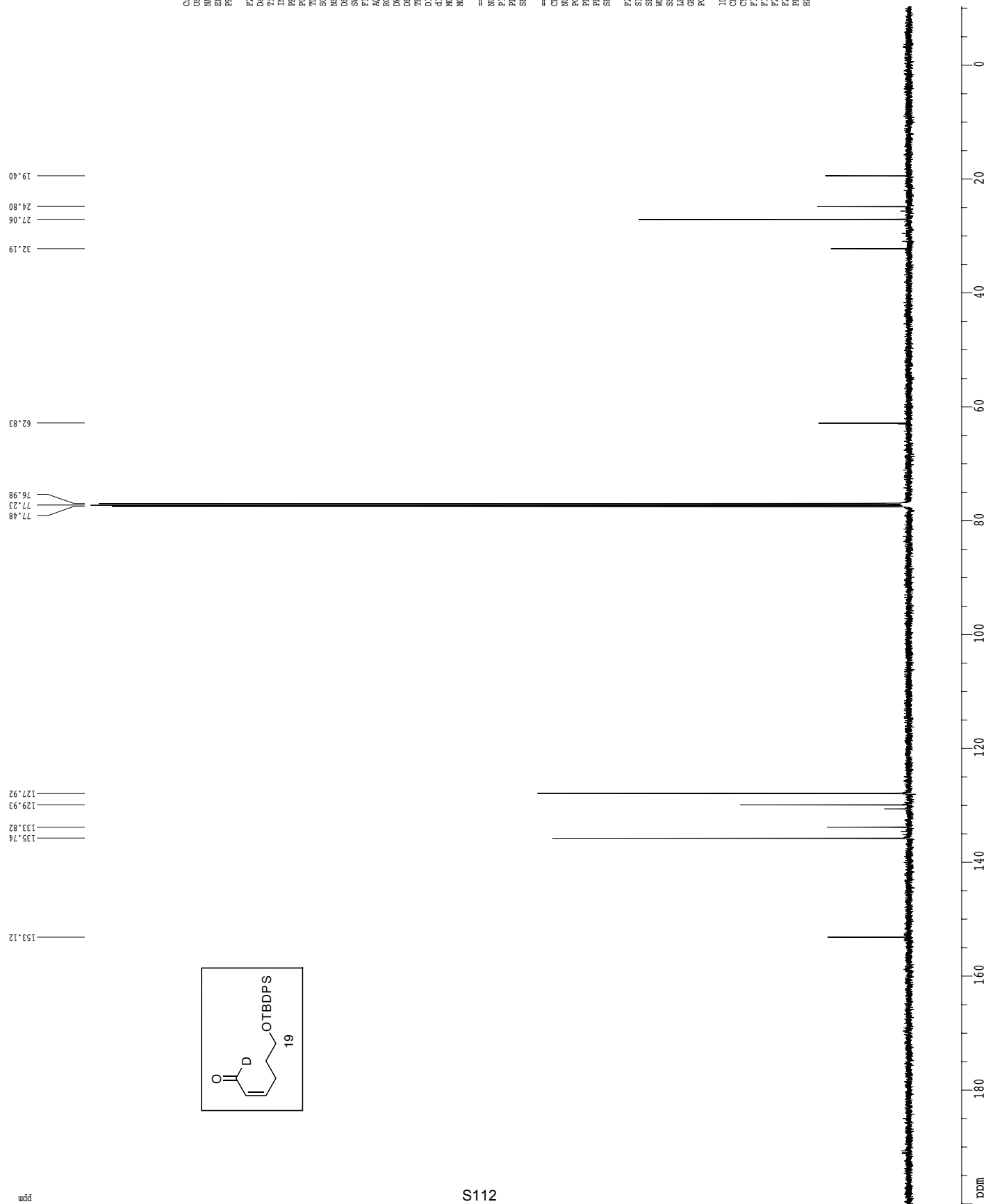
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.38 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6556  
 SF 500.2202250 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 10.500 ppm  
 F1 5252.31 Hz  
 F2 -1.061 ppm  
 F3 0.71 Hz  
 FREQ0 0.3071 Hz  
 FREQ1 253.6416 Hz/cm



13C spectrum with 1H decoupling



```

Current Data Parameters
USER camon
NAME JSC1155
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080620
Time 18.44
INSTRUM cryo00
PROBHD 5 mm CPCL1H-
PULPROG zgpg30
AQ 1.0794470 sec
RG 91.95.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 4.0000000 sec
d11 0.0300000 sec
MCREST 0.0000000 sec
MCPRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 14.75 usec
PL1 -1.00 dB
SFO1 125.7942548 MHz

===== CHANNEL f2 =====
CPDPRG2 walz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.80 dB
SFO2 500.2225011 MHz

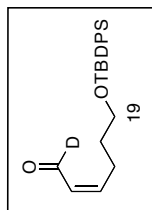
F2 - Processing parameters
SI 65536
SF 125.780397 MHz
WDW EM
SSB 0
GB 1.00 Hz
CB 2.00
PC

ID NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -10.307 ppm
F2 -1296.36 Hz
PFMCH 9.22397 ppm/cm
HZCM 1160.19458 Hz/cm
    
```



13C spectrum with 1H decoupling

ppm



Current Data Parameters  
USER camon  
NAME JSC1155  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080620  
Time 18.44  
INSTRUM cryo500  
PROBHD 5 mm CPCL1H-  
ZGR30  
PULPROG zgpg30  
TD 65438  
SOLVENT CDCl3  
NS 56  
DS 4  
SWH 30303.031 Hz  
FIDRES 0.463222 Hz  
AQ 1.0794470 sec  
RG 91.95.2  
DW 16.500 usec  
DE 6.00 usec  
TE 298.0 K  
D1 4.0000000 sec  
d11 0.0300000 sec  
MCREST 0.0000000 sec  
MCPRK 0.0150000 sec

==== CHANNEL f1 =====  
NUC1 13C  
P1 14.75 usec  
PL1 -1.00 dB  
SFO1 125.7942548 MHz

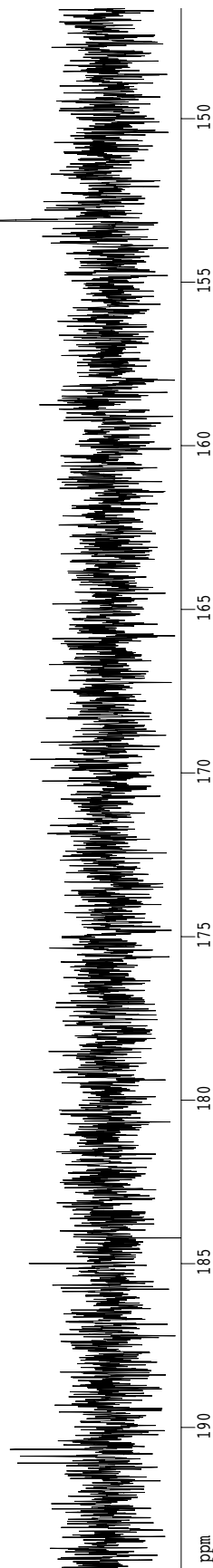
==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 1.60 dB  
PL12 24.80 dB  
SFO2 500.2225011 MHz

F2 - Processing parameters  
SI 65536  
SF 125.780397 MHz  
EN  
SSB 0  
GB 1.00 Hz  
CB 0  
PC 2.00

ID NMR plot parameters  
CX 22.80 cm  
CY 15.65 cm  
F1P 194.350 ppm  
F1 24445.42 Hz  
F2P 146.639 ppm  
F2 18444.27 Hz  
PFMCH 2.09260 ppm/cm  
HZCN 263.20837 Hz/cm

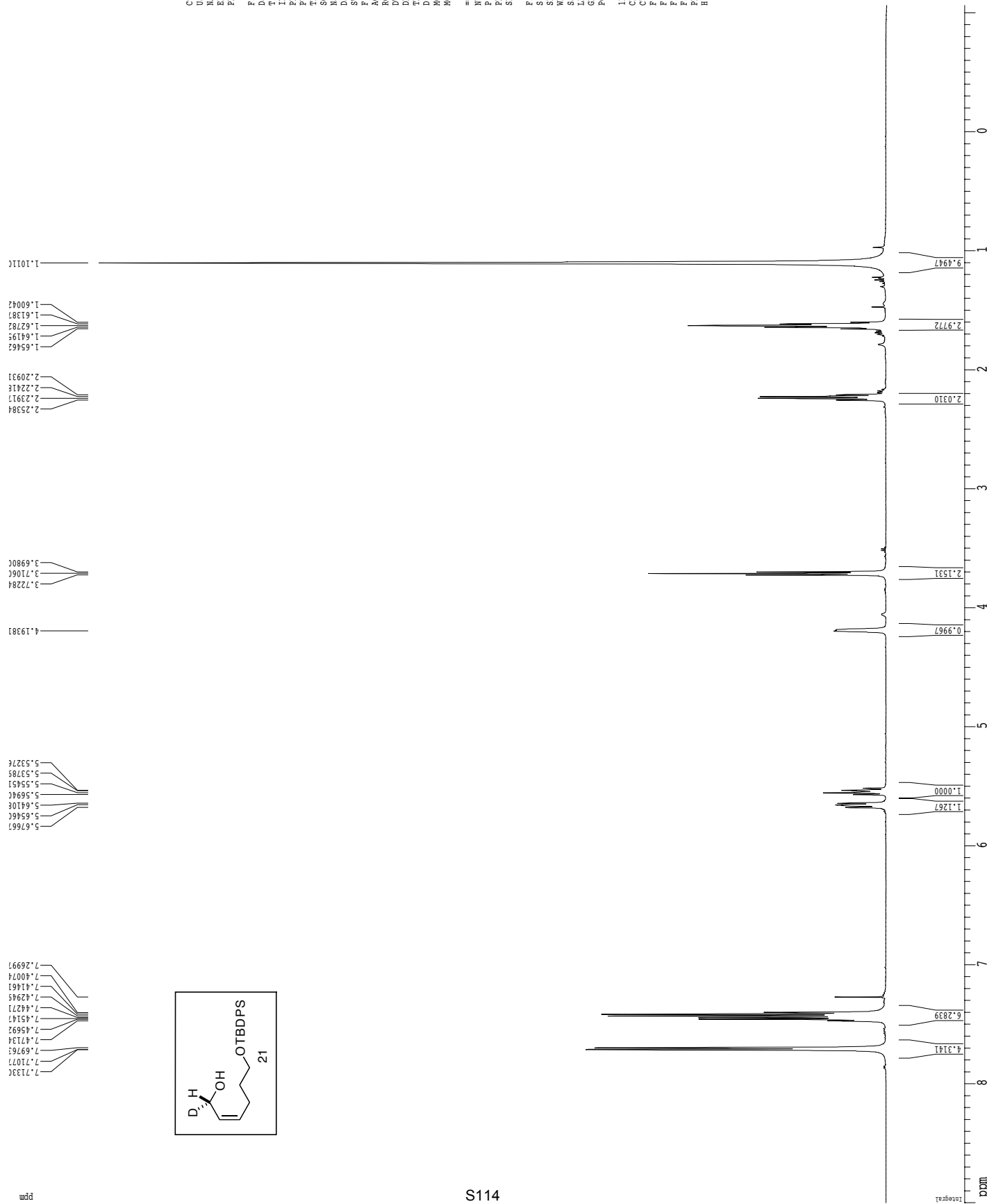
153.12

S113



ppm

<sup>1</sup>H spectrum



Current Data Parameters  
 USER cannon  
 NAME JS62043-3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081022  
 Time 15:05  
 INSTRUM cgy6500  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHF 801.280 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 3.2  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

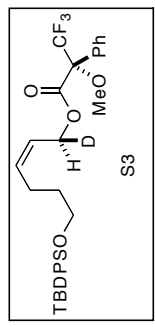
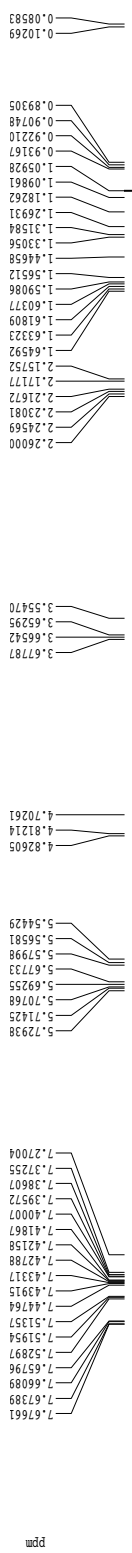
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6536  
 SF 500.220263 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.062 ppm  
 F3 11.21 Hz  
 FWHM 0.4833 ppm/cm  
 HECW 220.73375 Hz/cm



**<sup>1</sup>H spectrum**



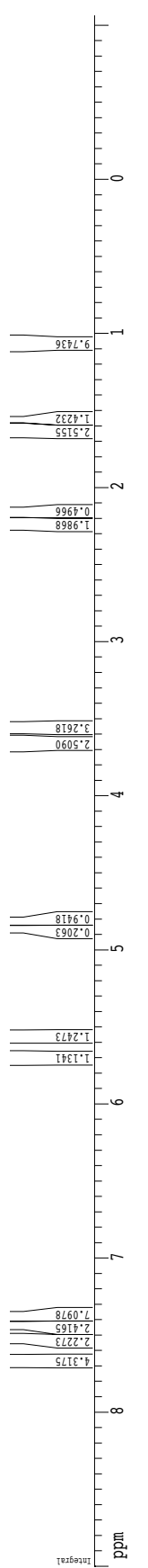
Current Data Parameters  
 USER cannon  
 NAME JSCI191  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080710  
 Time 12.31  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 32  
 DR 62.40 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.38 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220258 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

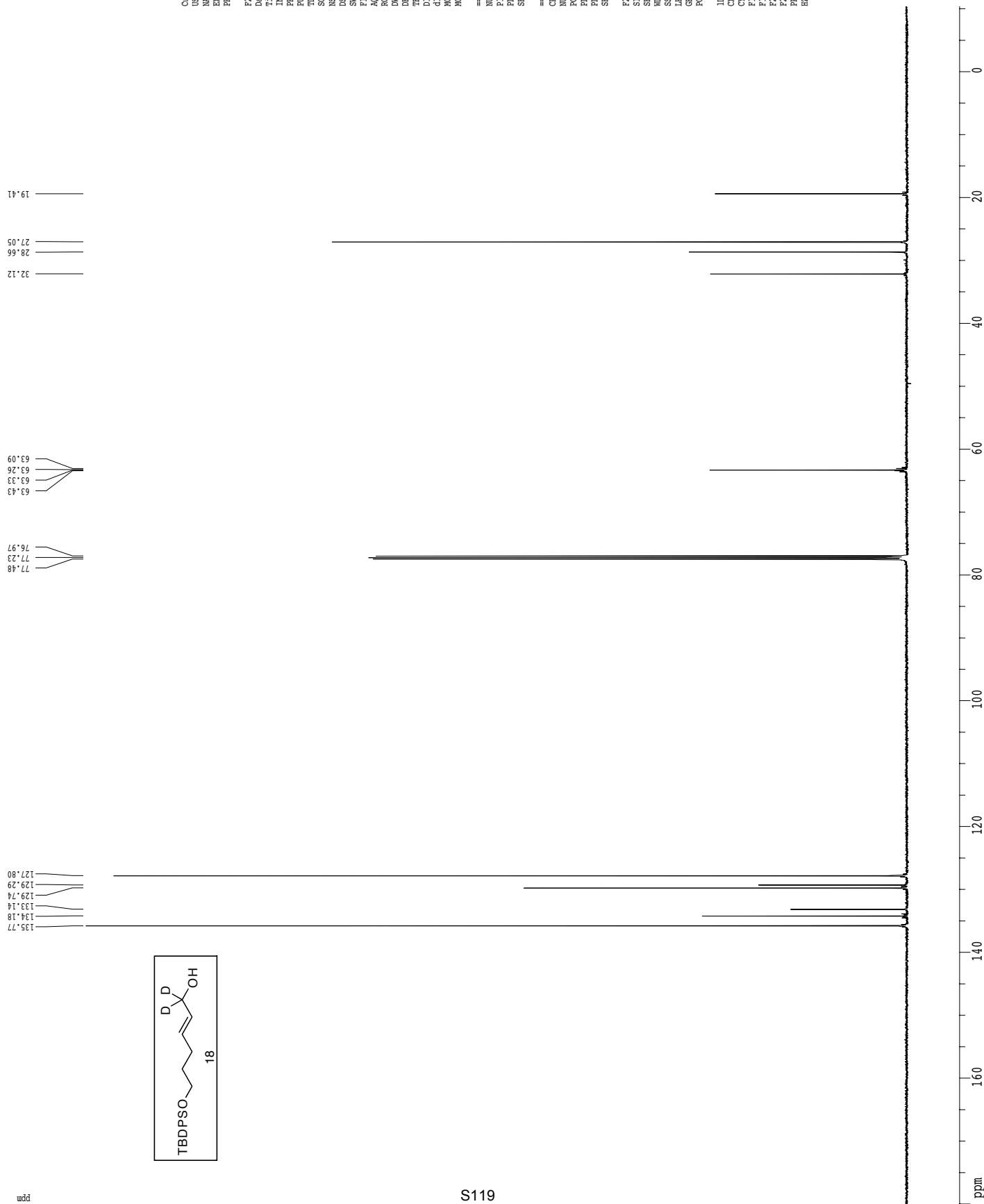
1D NMR plot parameters  
 CX 22.80 cm  
 CY 30.00 cm  
 FIP 9.000 ppm  
 F2 4501.38 Hz  
 F3 13.10 ppm  
 F4 -530.91 ppm  
 PRMCM 0.44127 ppm/cm  
 HZCM 220.73225 Hz/cm







<sup>13</sup>C spectrum with <sup>1</sup>H decoupling



Current Data Parameters  
 USER camon  
 NAME JSC1223  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080731  
 Time 14.15  
 INSTRUM cryo500  
 PROBED 5 mm CPCLH-  
 PULPROG zgpg30  
 TO 65438  
 SOLVENT CDCl3  
 CDC13  
 NS 144  
 DS 4  
 SWH 30303.031 Hz  
 FIDRES 0.463222 Hz  
 AQ 1.0794470 sec  
 RG 8192  
 DW 16.500 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 5.0000000 sec  
 d11 0.0300000 sec  
 MCREST 0.0000000 sec  
 MCPRK 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 14.75 usec  
 PL1 -1.00 dB  
 SFO1 125.7942548 MHz

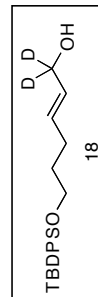
==== CHANNEL f2 =====  
 CPDPRG2 walz16  
 NUC2 <sup>1</sup>H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.80 dB  
 SFO2 500.2225011 MHz

F2 - Processing parameters  
 SI 65536  
 SF 125.7804048 MHz  
 EN  
 SSB 0  
 AB 1.00 Hz  
 GB  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.65 cm  
 F1P 180.000 ppm  
 F1 22640.47 Hz  
 F2P -10.347 ppm  
 F2 -1301.44 Hz  
 PPMCH 8.34855 ppm/cm  
 HZCH 1050.08386 Hz/cm

13C spectrum with 1H decoupling

62.913  
63.086  
63.258  
63.328  
63.431  
63.603



```

Current Data Parameters
USER camon
NAME JSC1223
EXPNO 4
PROCNO 1

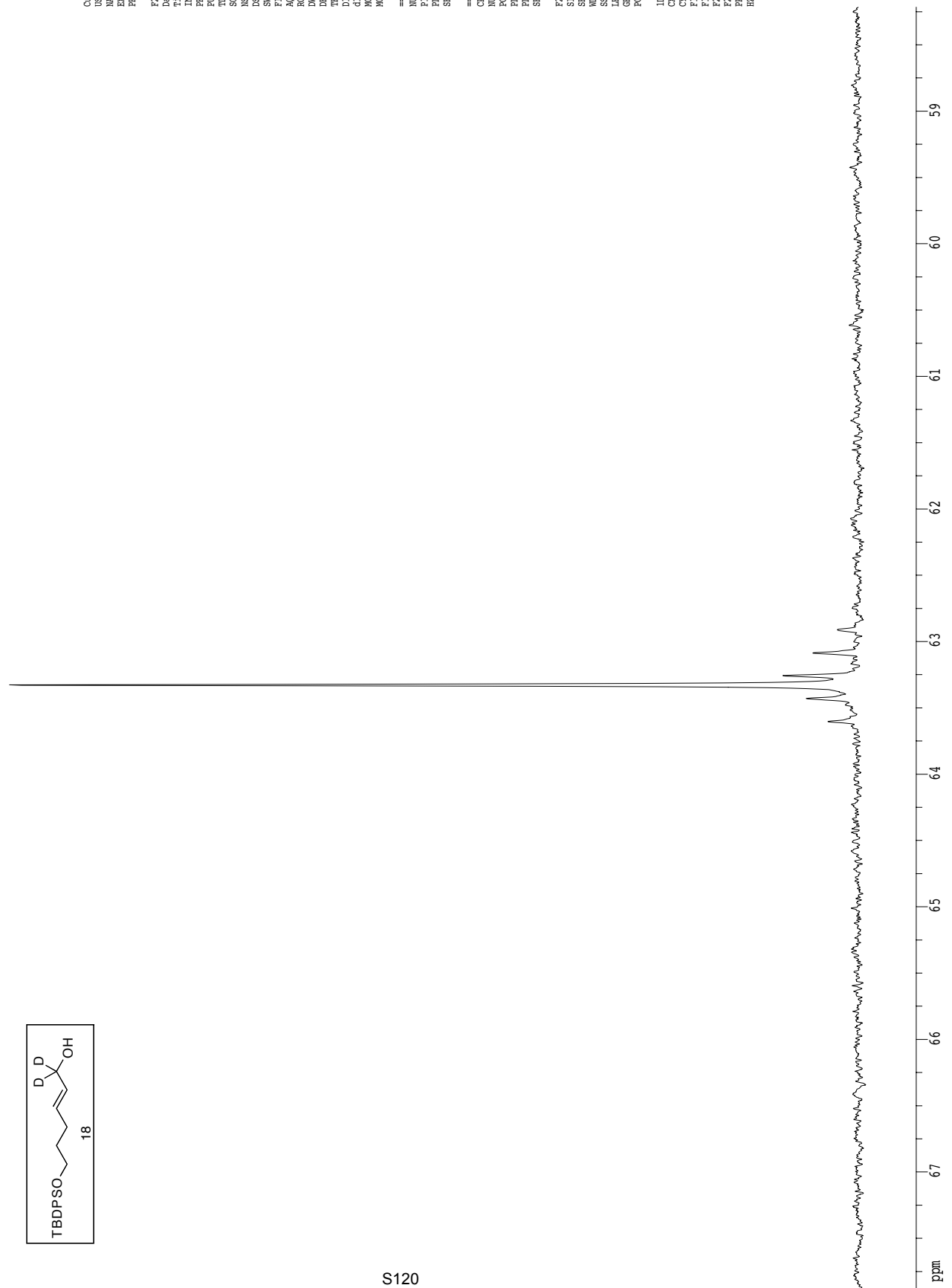
F2 - Acquisition Parameters
Date_ 20080731
Time 14.15
INSTRUM cryo500
PROBHD 5 mm CPCL1H-
PULPROG zgpg30
AQ 0.0513
RG 654.8
SOLVENT CDCl3
NS 144
DS 4
SWH 30303.031 Hz
FIDRES 0.463222 Hz
AQ 1.0794470 sec
RG 81.92
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 5.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 14.75 usec
PL1 -1.00 dB
SFO1 125.7942548 MHz

===== CHANNEL f2 =====
CPDPRG2 walz216
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.80 dB
SFO2 500.2225011 MHz

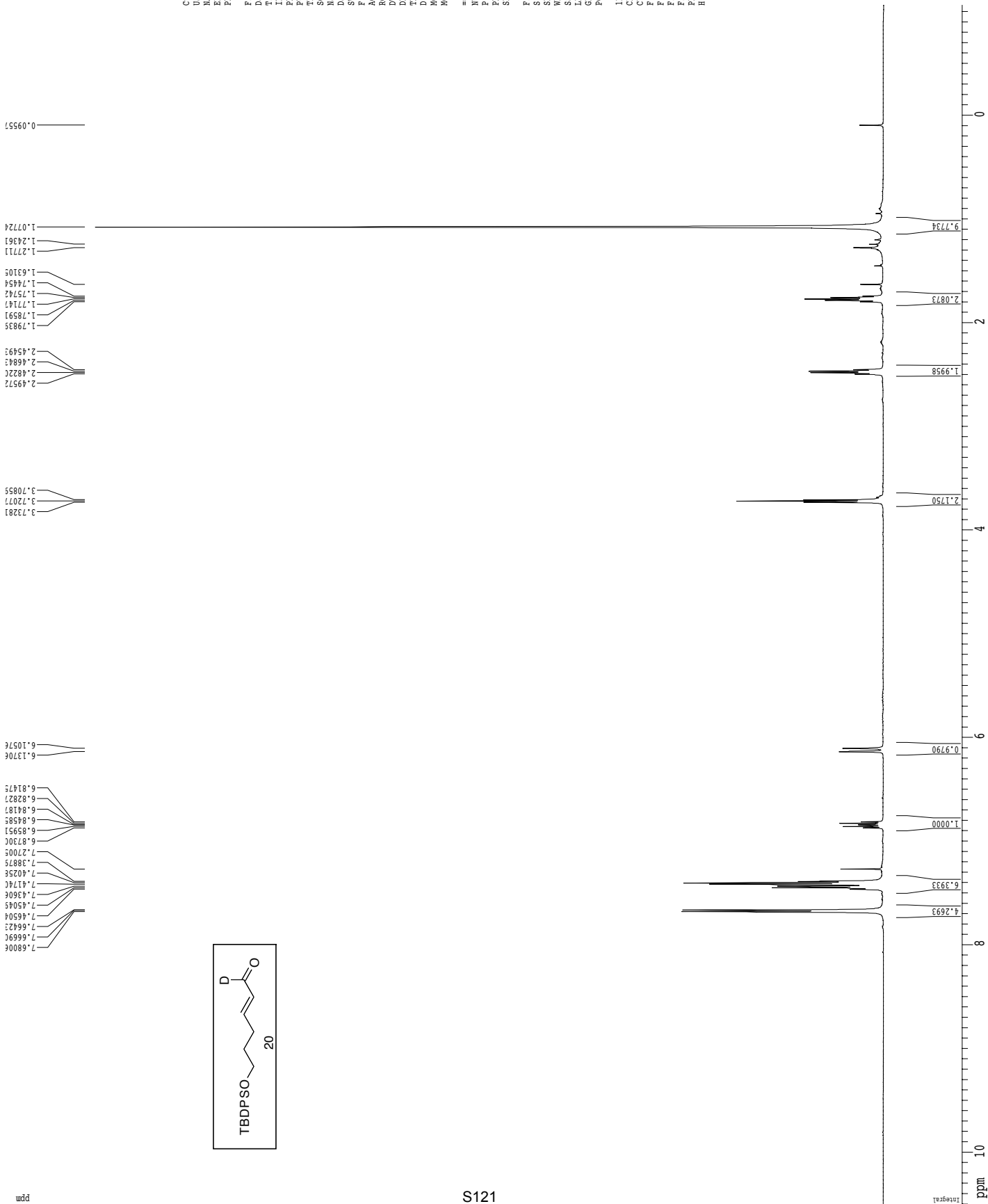
F2 - Processing parameters
SI 65536
SF 125.7804048 MHz
EN
SSB 0
GB 1.00 Hz
AG 2.00
PC

ID NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 67.875 ppm
F1 8537.38 Hz
F2P 58.216 ppm
F2 7322.41 Hz
PFMCH 0.42366 ppm/cm
HZCH 53.28785 Hz/cm
    
```

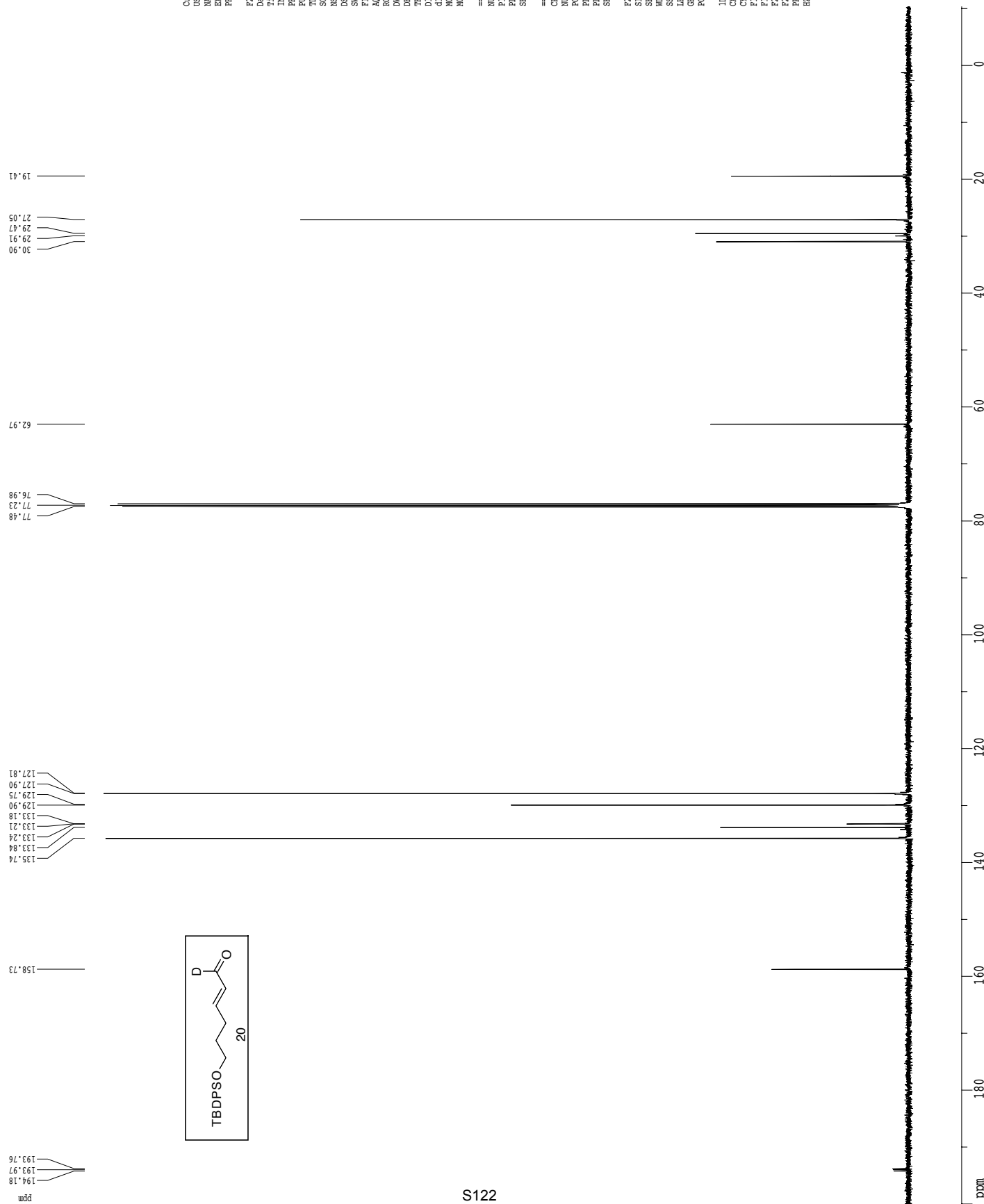




1H spectrum



13C spectrum with 1H decoupling



Current Data Parameters  
 USER camon  
 NAME JSC1221  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20/08/09 22  
 Time 15.34  
 INSTRUM cryo500  
 PROBED 5 mm CPCL1H-  
 PULPROG zgpg30  
 TO 65418  
 SOLVENT CDCl3  
 NS 80  
 DS 4  
 SPH 30303.031 Hz  
 FIDRES 0.463222 Hz  
 AQ 1.0794470 sec  
 RG 13004  
 DW 16.500 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 MCREST 0.0000000 sec  
 MCPRK 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 14.75 usec  
 PL1 -1.00 dB  
 SF01 125.7942548 MHz

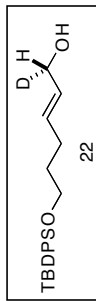
==== CHANNEL f2 =====  
 CPDPRG2 walz316  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.80 dB  
 SF02 500.2225011 MHz

F2 - Processing parameters  
 SI 65536  
 SF 125.7804025 MHz  
 EN  
 SSB 0  
 AB 1.00 Hz  
 GB  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.65 cm  
 F1P 200.000 ppm  
 F1 25156.08 Hz  
 F2P -10.329 ppm  
 F2 -1299.13 Hz  
 PPMCH 9.22494 ppm/cm  
 HZCH 1160.31628 Hz/cm



13C spectrum with 1H decoupling



```

Current Data Parameters
USER camon
NAME JSC2044
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081021
Time 11.06
INSTRUM cryo500
PROBHD 5 mm CPCLP1H-
PULPROG zgpg30
AQ 0.0310
RG 654.8
SOLVENT CDCl3
NS 56
DS 4
SWH 30303.031 Hz
FIDRES 0.463222 Hz
AQ 1.0794470 sec
RG 81.92
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
ICREST 0.0000000 sec
MCPRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 14.85 usec
PL1 -1.00 dB
SFO1 125.7942548 MHz

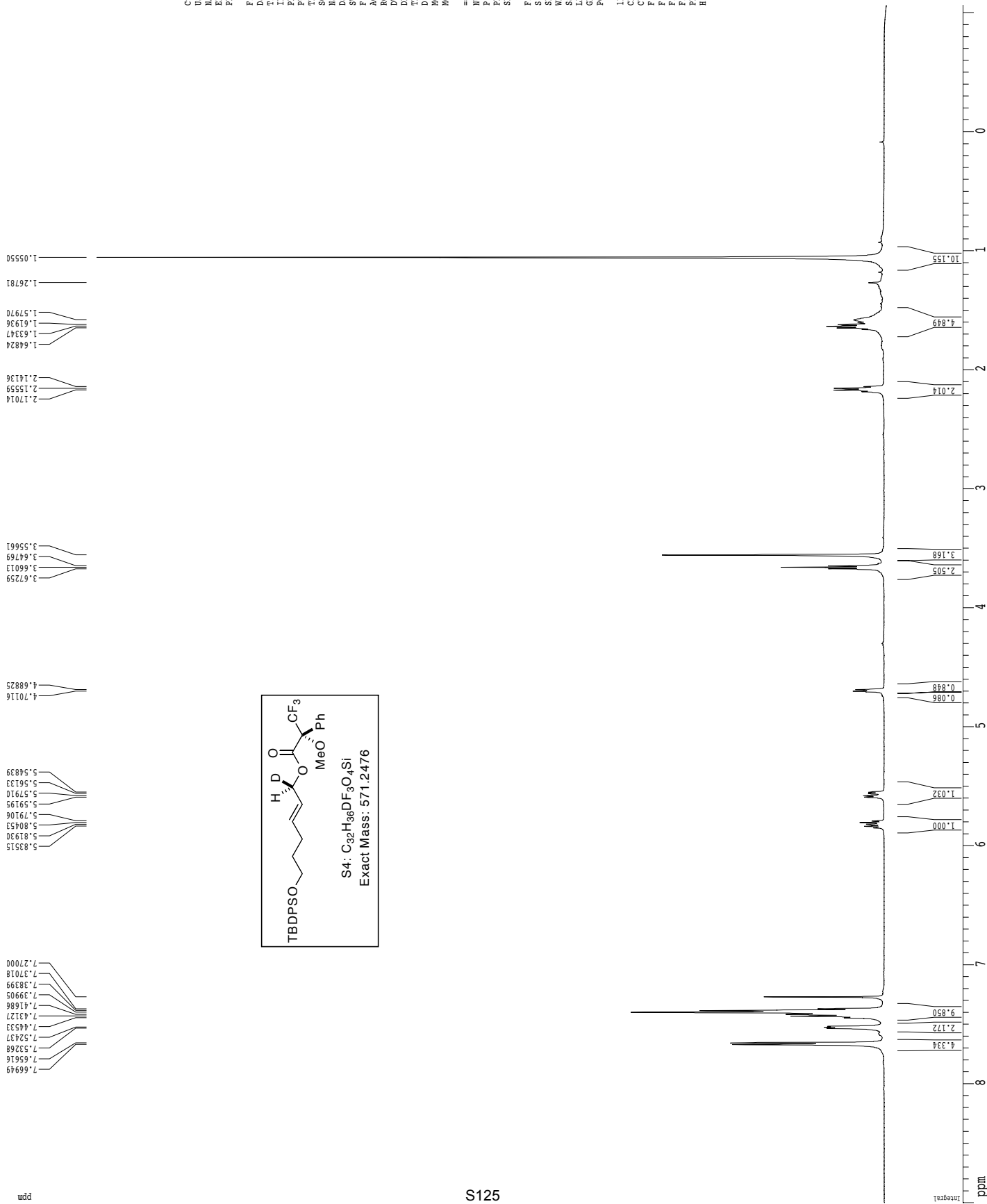
===== CHANNEL f2 =====
CPDPRG2 walz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz

F2 - Processing parameters
SI 65536
SF 125.7804025 MHz
WDW EM
SSB 0
GB 1.00 Hz
CB 2.00
PC

ID NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 180.000 ppm
F1 22640.47 Hz
F2P -10.329 ppm
F2 -1299.13 Hz
PFMCH 8.34774 ppm/cm
HZCM 1049.98254 Hz/cm
    
```



<sup>1</sup>H spectrum



Current Data Parameters  
 USER cannon  
 NAME JSC132R-1  
 EXPNO 1  
 PROCNO 1

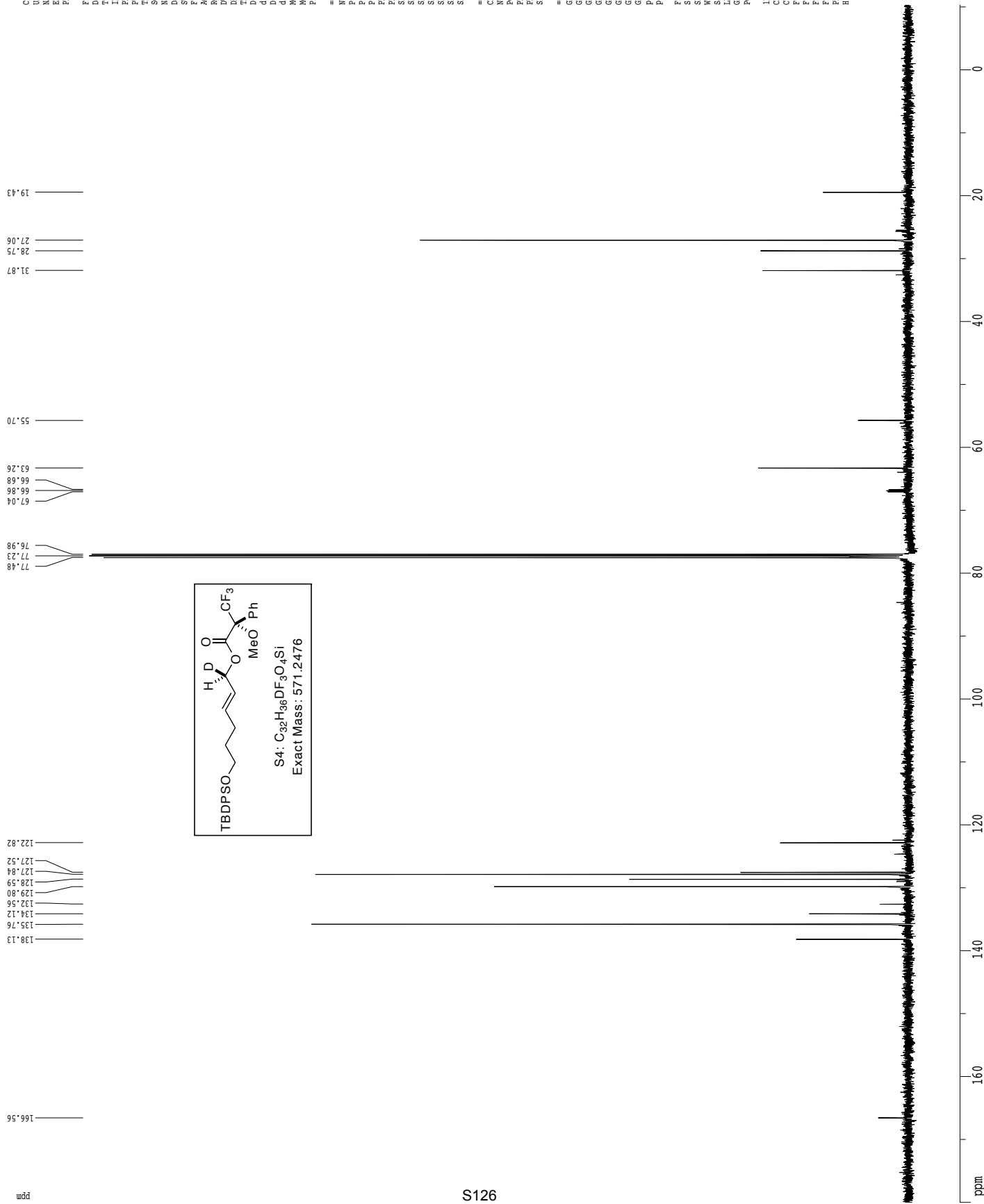
F2 - Acquisition Parameters  
 Date\_ 20100712  
 Time 17.01  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.098774 sec  
 RG 307  
 DW 62.00 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRK 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2202266 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F2 4501.39 Hz  
 F3 11.06 ppm  
 F4 -51.65 ppm  
 PRMCM 0.44133 ppm/cm  
 HZCM 220.76428 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER camon  
 NAME JSC122A-2  
 EXPRNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20100712  
 Time 17.04  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 421  
 DS 16  
 SHR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 4376  
 DW 6.00 usec  
 DE 16.00 usec  
 TE 298.2 K  
 D1 0.25000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 D17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 31.80 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.7947648 dB  
 PL2 125.7947648 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Ccp60.0.5.20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPRMR 1  
 GSPRMR2 1  
 GSPRMR3 1  
 GSPRMR4 1  
 GSPRMR5 1  
 GSPRMR6 1  
 GSPRMR7 1  
 GSPRMR8 1  
 GSPRMR9 1  
 GSPRMR10 1  
 GSPRMR11 1  
 GSPRMR12 1  
 GSPRMR13 1  
 GSPRMR14 1  
 GSPRMR15 1  
 GSPRMR16 1  
 GSPRMR17 1  
 GSPRMR18 1  
 GSPRMR19 1  
 GSPRMR20 1  
 GSPRMR21 1  
 GSPRMR22 1  
 GSPRMR23 1  
 GSPRMR24 1  
 GSPRMR25 1  
 GSPRMR26 1  
 GSPRMR27 1  
 GSPRMR28 1  
 GSPRMR29 1  
 GSPRMR30 1  
 GSPRMR31 1  
 GSPRMR32 1  
 GSPRMR33 1  
 GSPRMR34 1  
 GSPRMR35 1  
 GSPRMR36 1  
 GSPRMR37 1  
 GSPRMR38 1  
 GSPRMR39 1  
 GSPRMR40 1  
 GSPRMR41 1  
 GSPRMR42 1  
 GSPRMR43 1  
 GSPRMR44 1  
 GSPRMR45 1  
 GSPRMR46 1  
 GSPRMR47 1  
 GSPRMR48 1  
 GSPRMR49 1  
 GSPRMR50 1  
 GSPRMR51 1  
 GSPRMR52 1  
 GSPRMR53 1  
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 GSPRMR60 1  
 GSPRMR61 1  
 GSPRMR62 1  
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 GSPRMR73 1  
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 GSPRMR77 1  
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 GSPRMR82 1  
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 GSPRMR88 1  
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 GSPRMR90 1  
 GSPRMR91 1  
 GSPRMR92 1  
 GSPRMR93 1  
 GSPRMR94 1  
 GSPRMR95 1  
 GSPRMR96 1  
 GSPRMR97 1  
 GSPRMR98 1  
 GSPRMR99 1  
 GSPRMR100 1

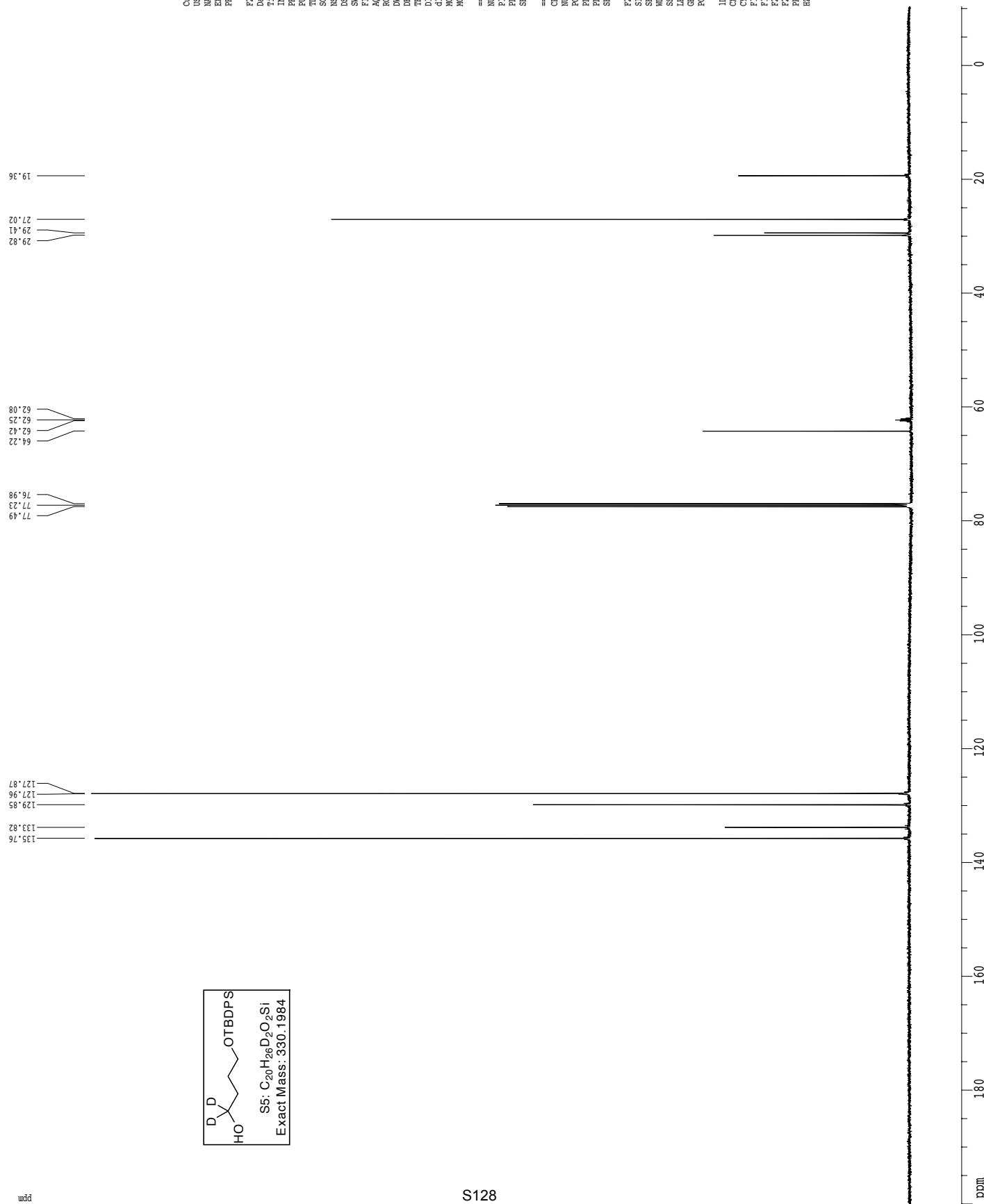
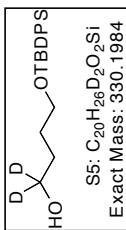
F2 - Processing parameters  
 SI 65536  
 SF 125.7803992 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.65 cm  
 FIP 180.000 ppm  
 F1 22640.47 Hz  
 F2 -10.303 ppm  
 F2 -1295.89 Hz  
 F2 15.648 ppm/cm  
 HECKN 1049.30049 Hz/cm



13C spectrum with 1H decoupling

ppm



```

Current Data Parameters
USER camron
NAME JSC1247
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080916
Time_ 15.12
INSTRUM cryo500
PROBHD 5 mm CPCL1H-
PULPROG zgpg30
AQ 0.0536
RG 655.6
SOLVENT CDCl3
NS 80
DS 4
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 11585.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
INCREMENT 0.0000000 sec
SCANS 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 14.75 usec
PL1 -1.00 dB
SFO1 125.7942548 MHz

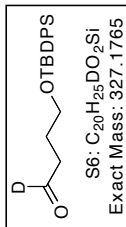
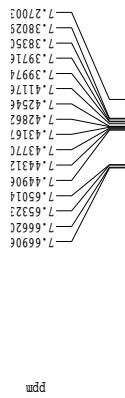
===== CHANNEL f2 =====
CPDPRG2 walz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.80 dB
SFO2 500.2225011 MHz

F2 - Processing parameters
SI 65536
SF 125.7804039 MHz
EN
SSB 0
GB 1.00 Hz
AB 2.00
PC

ID NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -10.340 ppm
F2 -1300.52 Hz
PFMCH 9.22542 ppm/cm
HZCM 1160.37732 Hz/cm
    
```



1H spectrum



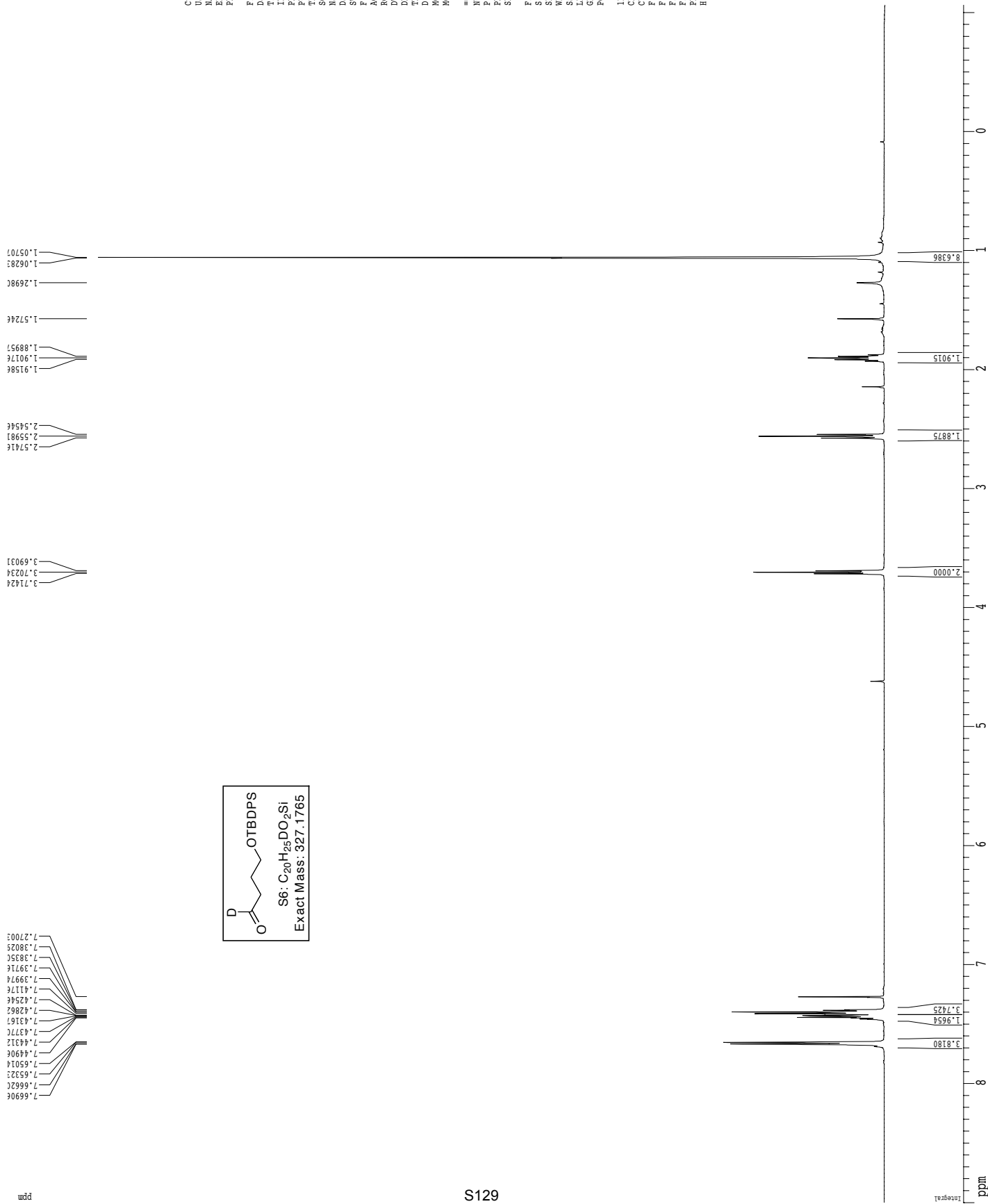
Current Data Parameters  
 USER cannon  
 NAME JSCI254  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080904  
 Time 13:05:03  
 INSTRUM cryo600  
 PROBRD 5 mm CPYCT 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHW 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 14.3  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCYCLE 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.38 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

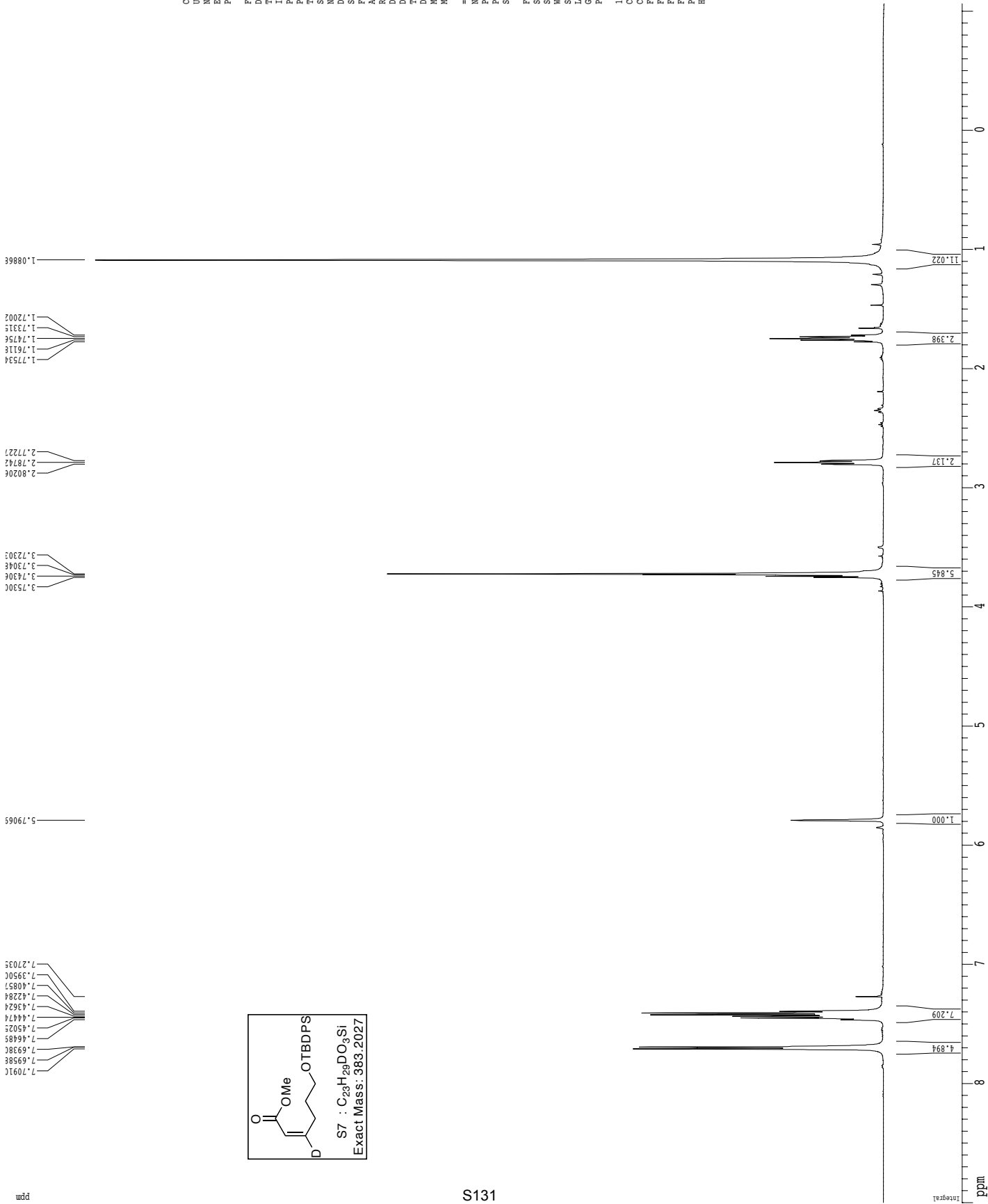
F2 - Processing parameters  
 SI 6536  
 SF 500.220262 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.062 ppm  
 F3 11.08 Hz  
 FWHM 0.483 ppm/cm  
 HECW 220.74829 Hz/cm





1H spectrum



Current Data Parameters  
 USER cannon  
 NAME JSCI268  
 EXPNO 4  
 PROCNO 1

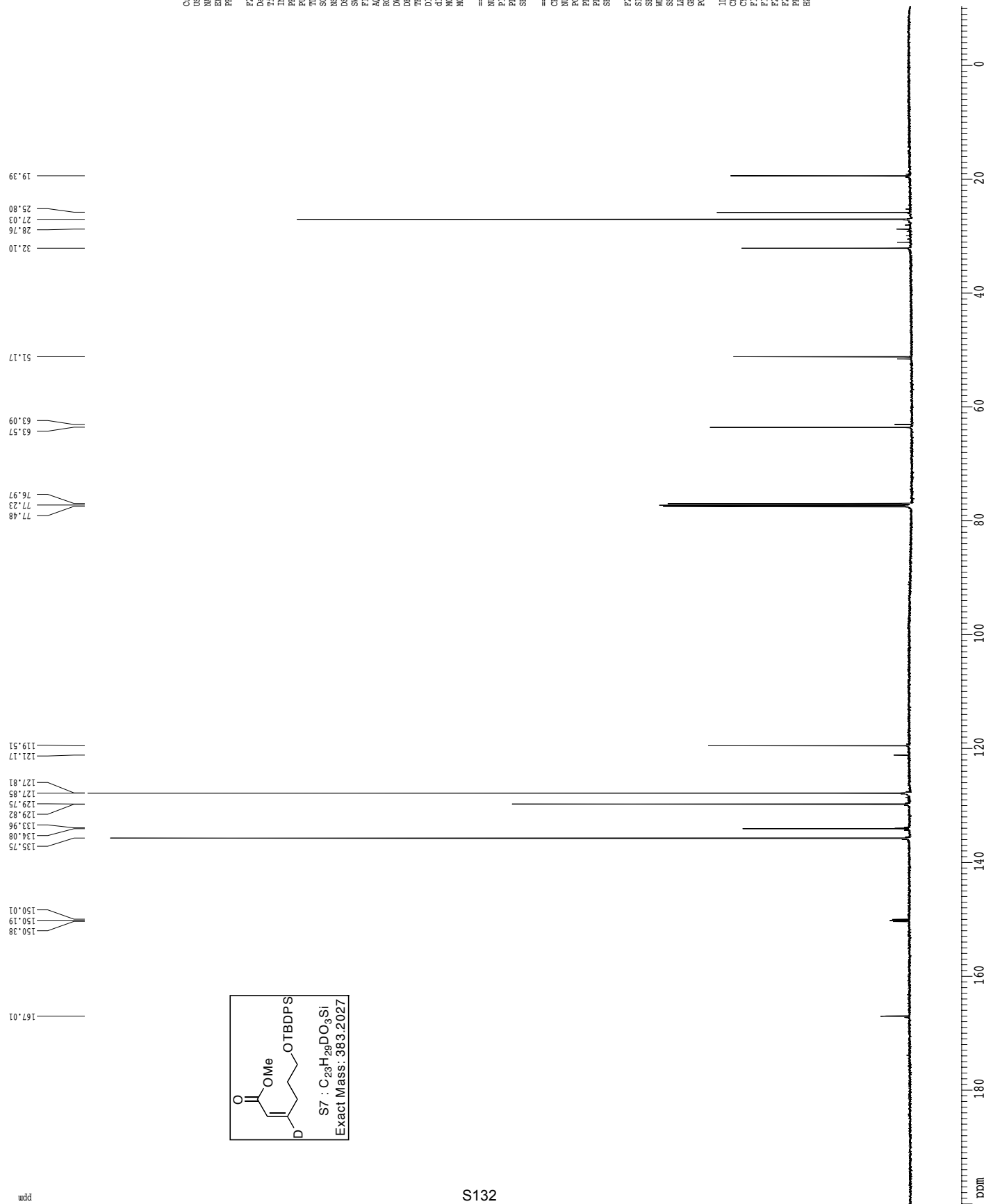
F2 - Acquisition Parameters  
 Date\_ 20080917  
 Time 13:05:33  
 INSTRUM spect  
 PROBRD 5 mm CPACT IH-  
 PULPROG zgpg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 5.7  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWBK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.38 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

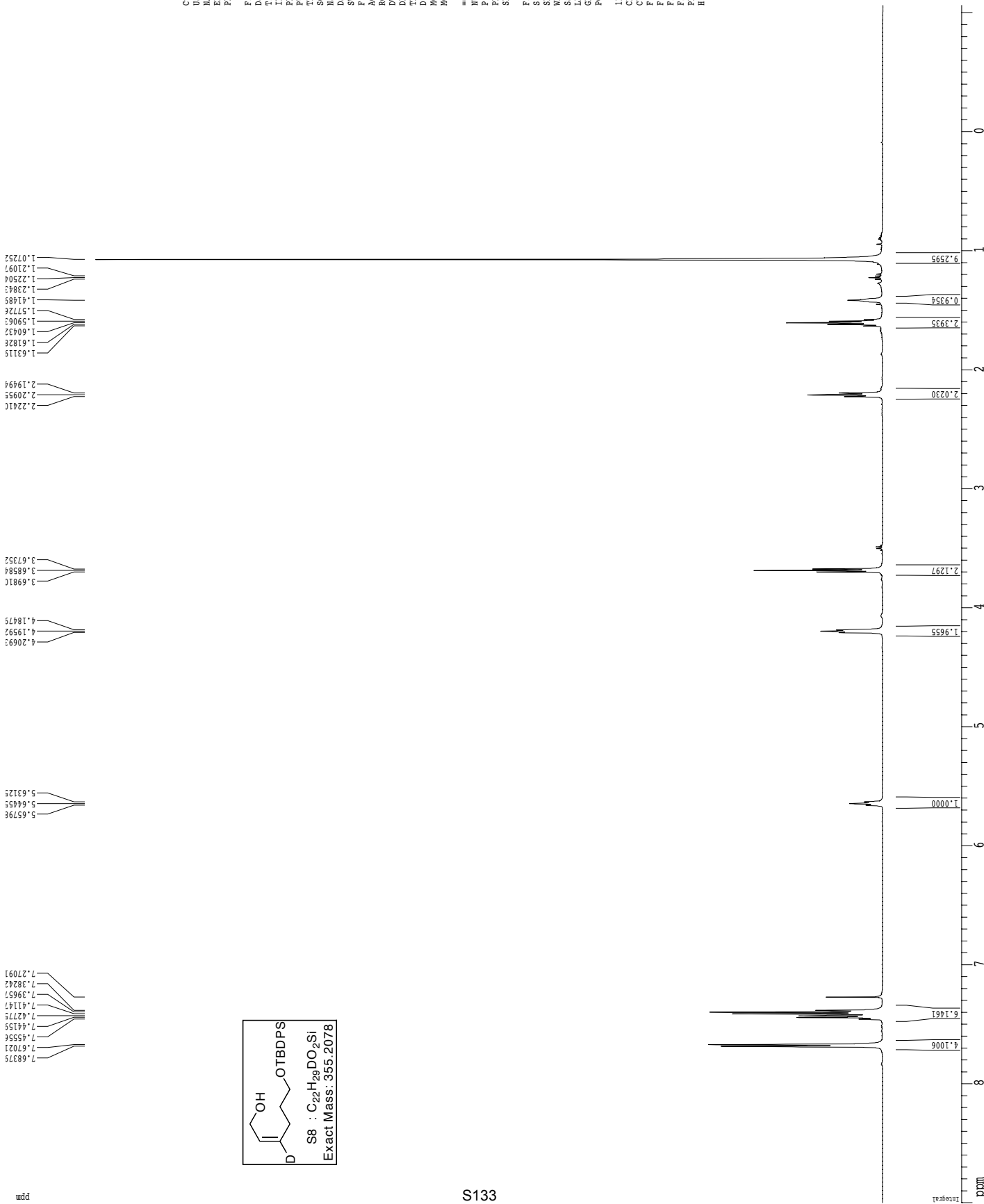
F2 - Processing parameters  
 SI 65536  
 SF 500.2200225 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.061 ppm  
 F3 0.000 Hz  
 FWHM 0.482 ppm/cm  
 HECW 220.72657 Hz/cm

**<sup>13</sup>C spectrum with <sup>1</sup>H decoupling**



1H spectrum



Current Data Parameters  
 USER cannon  
 NAME JSC1271  
 EXPNO 2  
 PROCNO 1

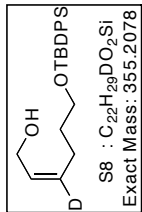
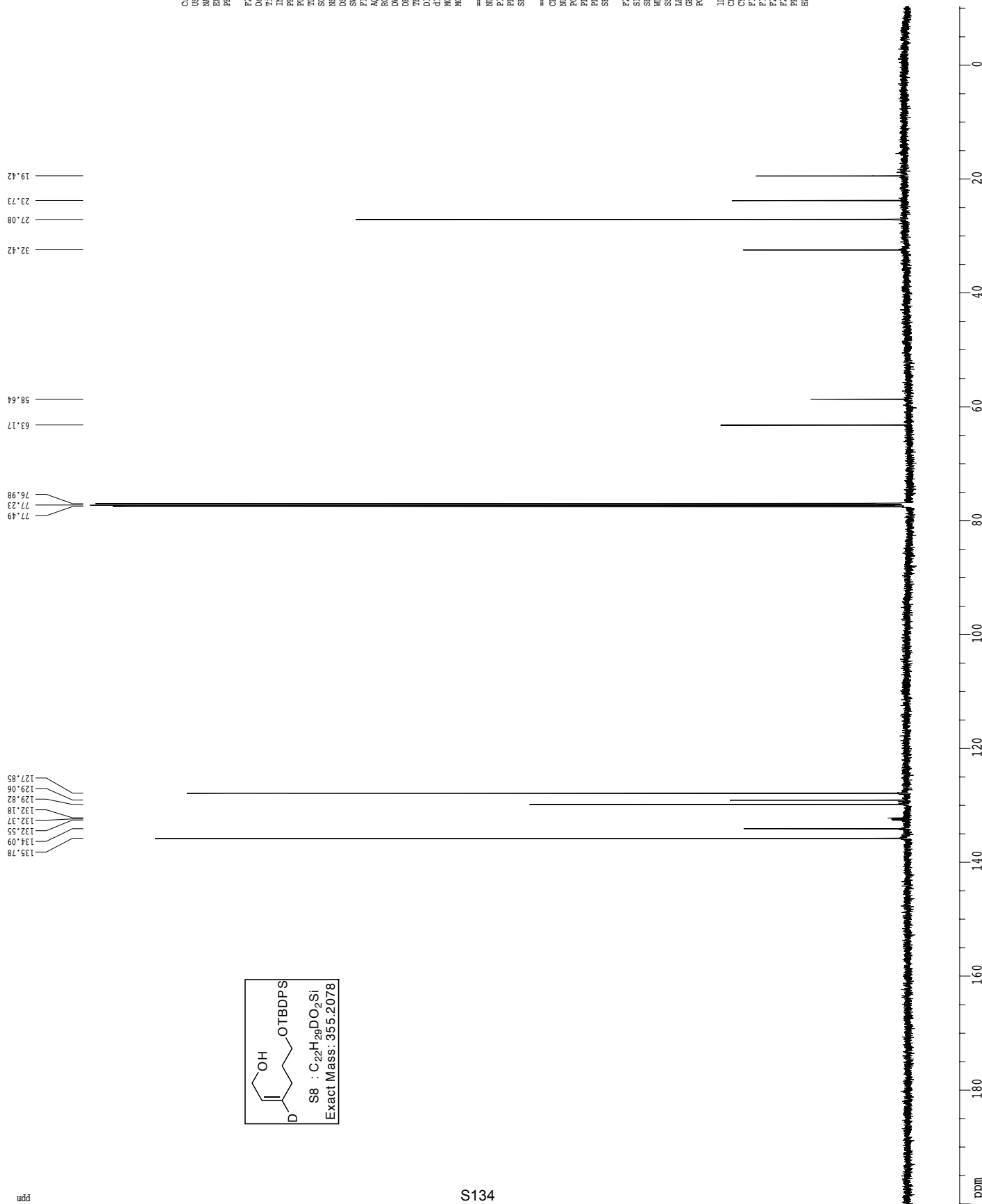
F2 - Acquisition Parameters  
 Date\_ 20100902  
 Time 14:04:00  
 INSTRUM cty6500  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 16  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.38 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6536  
 SF 500.2202653 MHz  
 RG 16  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -11.062 ppm  
 F3 11.21 Hz  
 FWHM 0.483 ppm/cm  
 HECN 220.73375 Hz/cm

13C spectrum with 1H decoupling



```

Current Data Parameters
USER camon
NAME JSC1271
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080902
Time 17.38
INSTRUM cryo500
PROBHD 5 mm CPCLP1H-
PULPROG zgpg30
AQ 4.9536
RG 65536
SOLVENT CDCl3
NS 170
DS 4
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 16384
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
ICREST 0.0000000 sec
MCPRK 0.0150000 sec

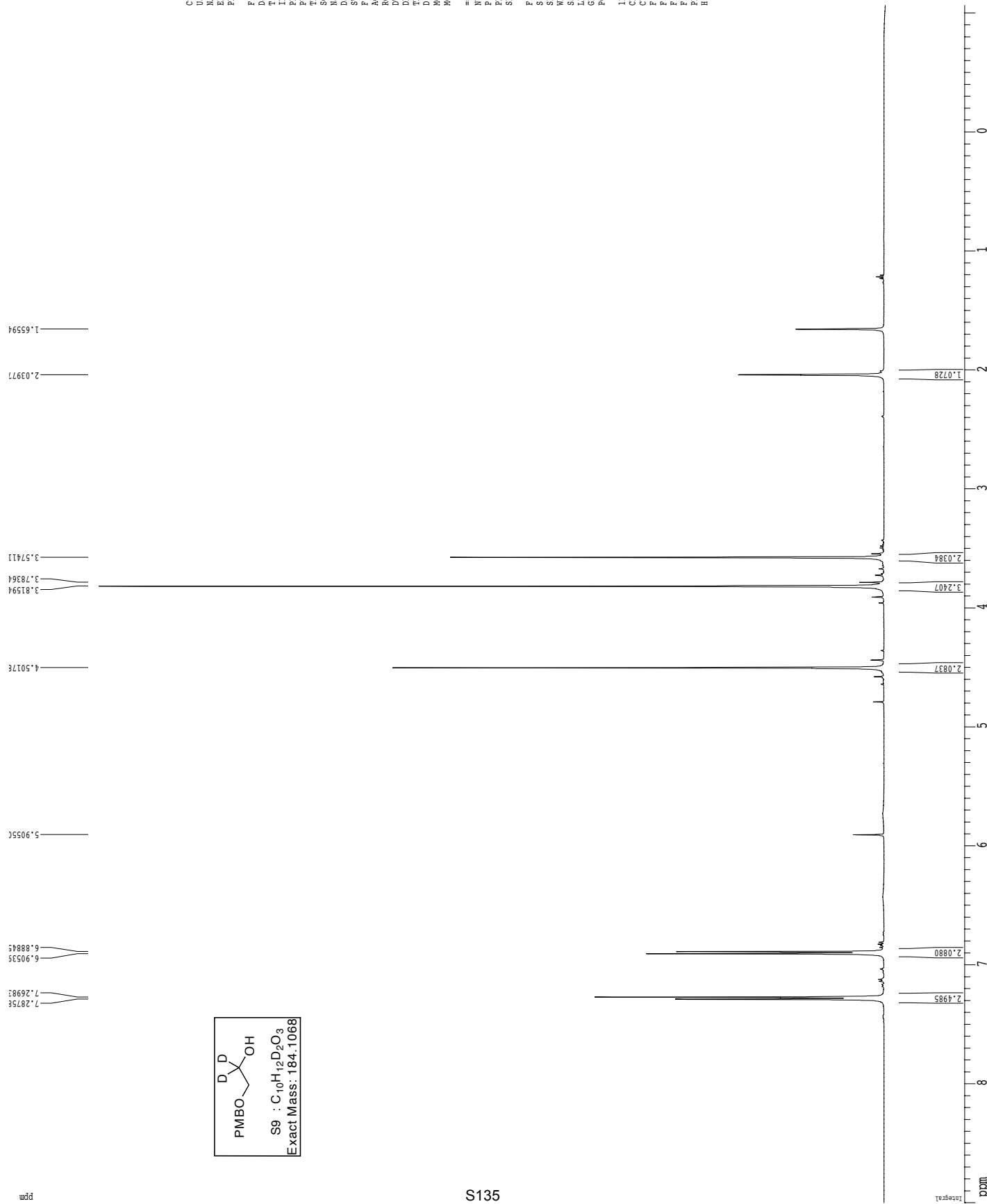
===== CHANNEL f1 =====
NUC1 13C
P1 14.75 usec
PL1 -1.00 dB
SFO1 125.7942548 MHz

===== CHANNEL f2 =====
CPDPRG2 walz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.80 dB
SFO2 500.2225011 MHz

F2 - Processing parameters
SI 65536
SF 125.7803997 MHz
EN
SSB 0
GB 1.00 Hz
AB 2.00
PC

ID NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -10.307 ppm
F2 -1296.36 Hz
PFMCH 9.22397 ppm/cm
HZCH 1160.19458 Hz/cm
  
```

1H spectrum



Current Data Parameters  
 USER cannon  
 NAME JS62146-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190219  
 Time 15:01  
 INSTRUM cryo500  
 PROBRD 5 mm CPACT RF-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHR 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6556  
 SF 500.2235015 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.88 Hz  
 F2 -1.064 ppm  
 F3 432.31 Hz  
 FWHM 0.486 ppm/cm  
 HECW 220.80200 Hz/cm





Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USBR canon  
 NAME JSCZ146-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090219  
 Time\_ 15:03  
 INSTRUM crys000  
 PROBHD 5 mm CPXI IH-  
 PULPROG Spinecho90pr-d  
 D1 1.0000000 sec  
 SOLVENT CDCl3  
 NS 264  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.061390 sec  
 RG 2048  
 DW 16.500 usec  
 DE 1.000 usec  
 TE 298.2 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0020000 sec  
 d17 0.0001960 sec  
 MCREST 0.0000000 sec  
 MCPRK 0.0150000 sec  
 F2 29.70 usec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 14.85 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SFO1 125.7942548 MHz  
 SF02 500.1363000 MHz  
 SP2 3.60 dB  
 SPNAM1 Ctp60\_0.5.20.1  
 SPNAM2 Ctp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

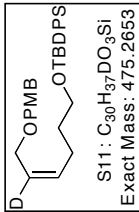
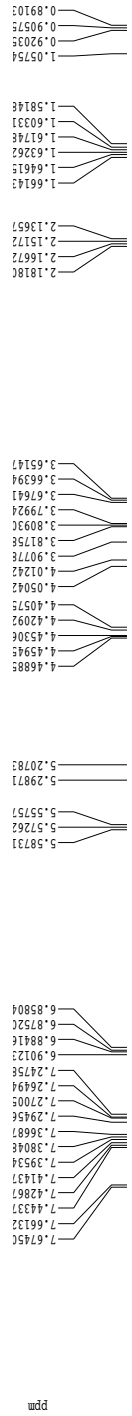
==== CHANNEL f2 =====  
 CDP6GZ waitz10  
 NUC2 13C  
 P2 100.00 usec  
 P21 1.60 dB  
 P22 24.60 dB  
 SFO2 500.2225011 MHz

==== GRADIENT CHANNEL =====  
 GPRAM1 SINE.100  
 GPRAM2 SINE.100  
 GPZ1 0.00 %  
 GPZ2 0.00 %  
 GPY1 0.00 %  
 GPY2 0.00 %  
 GPE1 30.00 %  
 GPE2 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 6556  
 SF 125.7804016 MHz  
 MDW EN  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID\_NMR plot parameters  
 CX 22.80 cm  
 CY 15.65 cm  
 F1P 72.210 ppm  
 F1 9082.58 Hz  
 F2P 57.743 ppm  
 F2 7262.50 Hz  
 PPRCM 0.43352 ppm/cm  
 HZCM 79.81046 Hz/cm

1H spectrum



Current Data Parameters  
 USER cannon  
 NAME JS62167-1  
 EXPNO 1  
 PROCNO 1

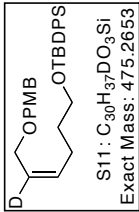
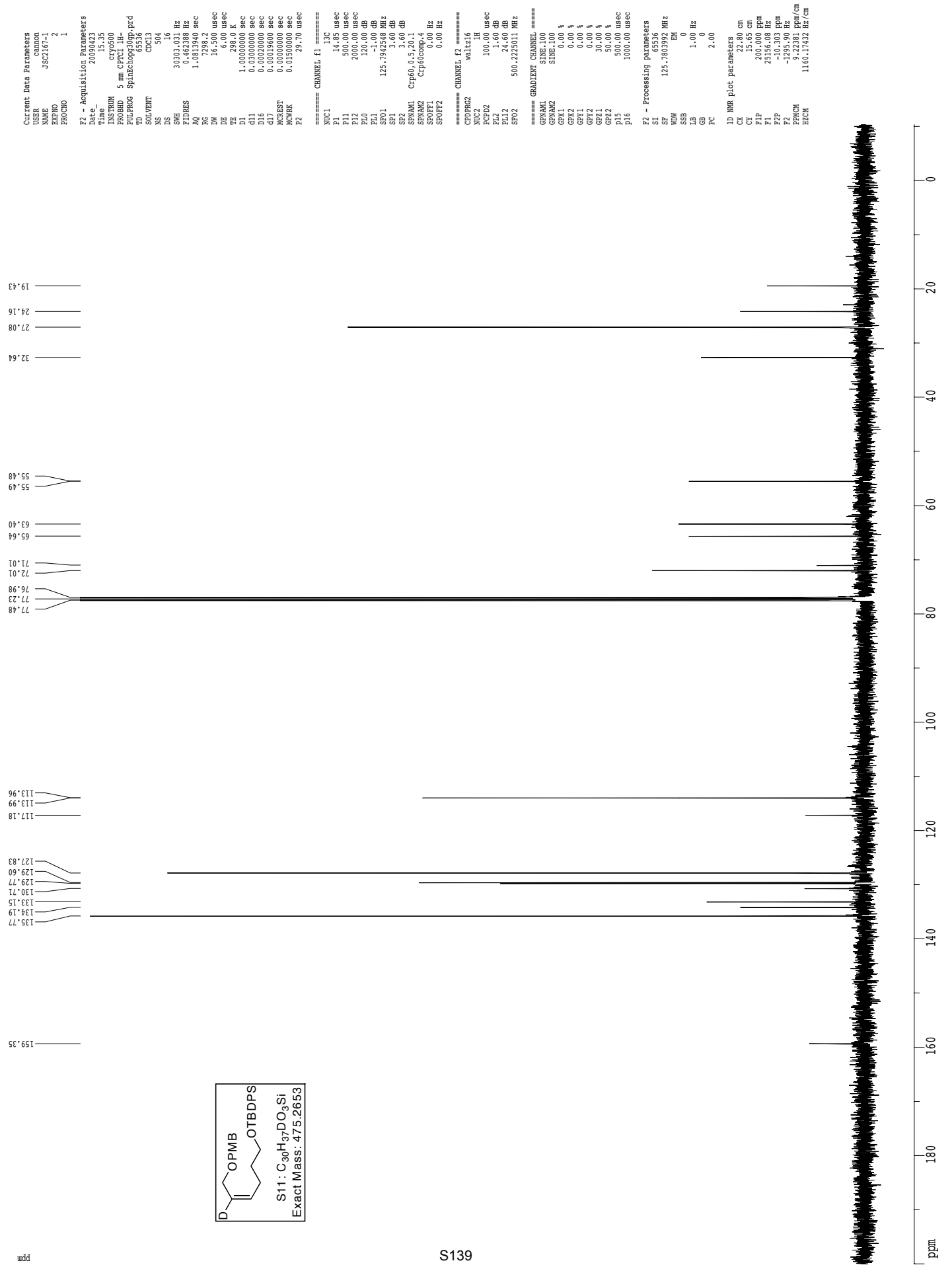
F2 - Acquisition Parameters  
 Date\_ 20090423  
 Time\_ 13:13:13  
 INSTRUM cxts600  
 PROBRD 5 mm CPACT IP-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHF 801.280 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRE 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6536  
 SF 500.220263 MHz  
 EQ 2  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 4501.98 Hz  
 F2 -1.062 ppm  
 F3 11.21 Hz  
 FWHM 0.483 ppm/cm  
 HECN 220.73375 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USBR canon  
 NAME JSCZ167-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090423  
 Time\_ 15:35  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG SpinEchoSqr.prd  
 D1 1.0000000 sec  
 SOLVENT CDCl3  
 NS 504  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.061390 sec  
 RG 7296.2  
 DW 16.500 usec  
 DE 16.000 usec  
 TE 298.2 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0020000 sec  
 d17 0.0001960 sec  
 MCREST 0.0000000 sec  
 MCPRK 0.0150000 sec  
 F2 29.70 usec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 14.85 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SFO1 125.7942548 MHz  
 SF02 500.2225011 MHz  
 SP1 3.60 dB  
 SP2 3.60 dB  
 SPNAM1 Ctp60,0.5,20.1  
 SPNAM2 Ctp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

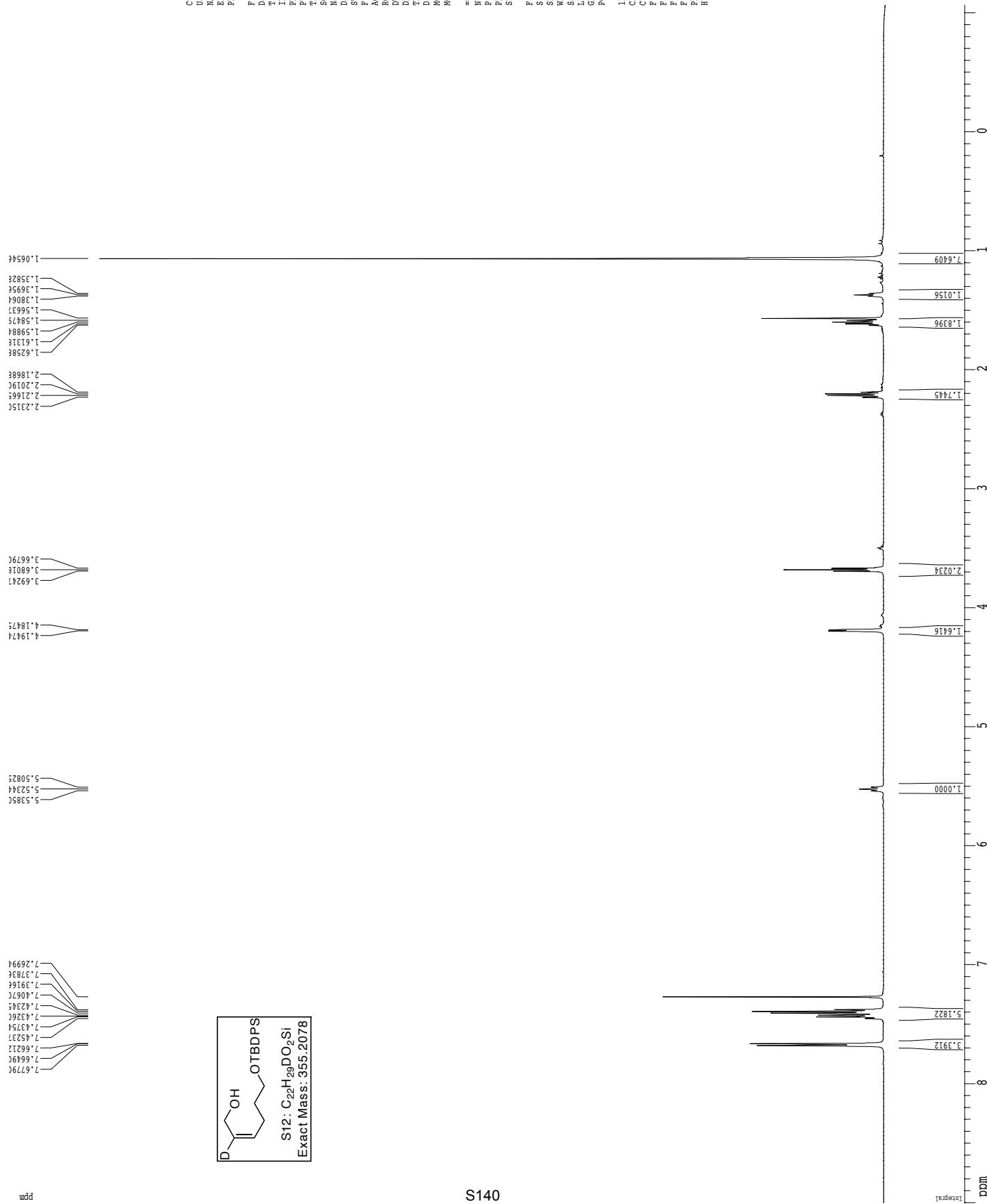
==== CHANNEL f2 =====  
 CDP6GZ waitZ16  
 NUC2 13C  
 P2 100.00 usec  
 P21 1.60 dB  
 P22 24.60 dB  
 SFO2 500.2225011 MHz

==== GRADIENT CHANNEL =====  
 GPRAM1 SINE,100  
 GPRAM2 SINE,100  
 GPRM1 0.00 %  
 GPRM2 0.00 %  
 GPRM3 0.00 %  
 GPRM4 0.00 %  
 GPRM5 30.00 %  
 GPRM6 50.00 %  
 GPRM7 500.00 usec  
 GPRM8 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803892 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID, NMR plot parameters  
 CX 22.80 cm  
 CT 15.65 cm  
 F1P 200.000 ppm  
 F1 25156.08 Hz  
 F2P -10.303 ppm  
 F2 -1295.50 Hz  
 PPRMCH 9.22381 ppm/cm  
 HZCN 1160.17432 Hz/cm

1H spectrum



Current Data Parameters  
 USER cannon  
 NAME JS02169-1  
 EXPNO 1  
 PROCNO 1

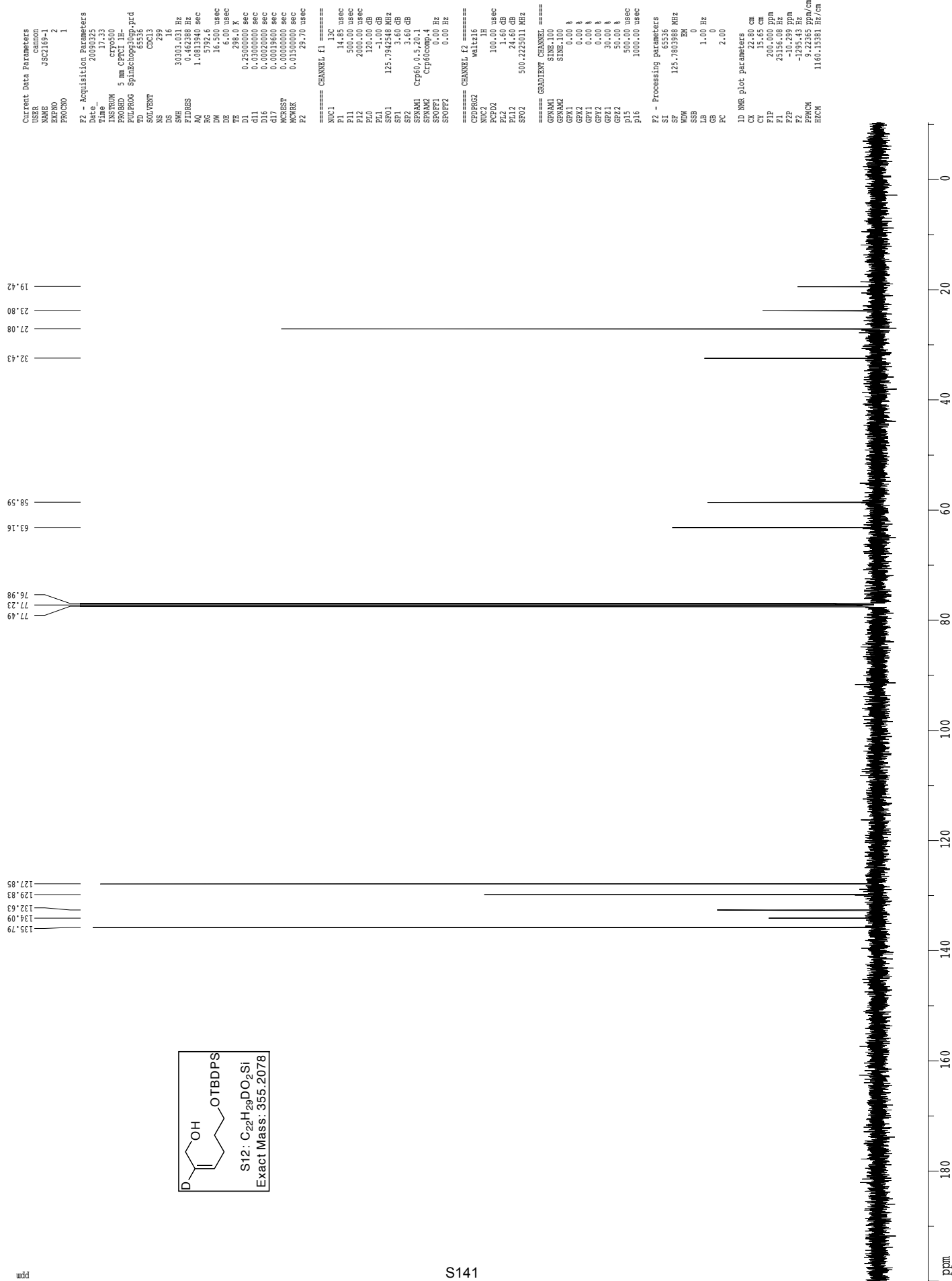
F2 - Acquisition Parameters  
 Date\_ 20190323  
 Time 15:22  
 INSTRUM cryo600  
 PROBRD 5 mm CPYCT-1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SHW 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 8.00 usec  
 TE 300.2 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRE 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

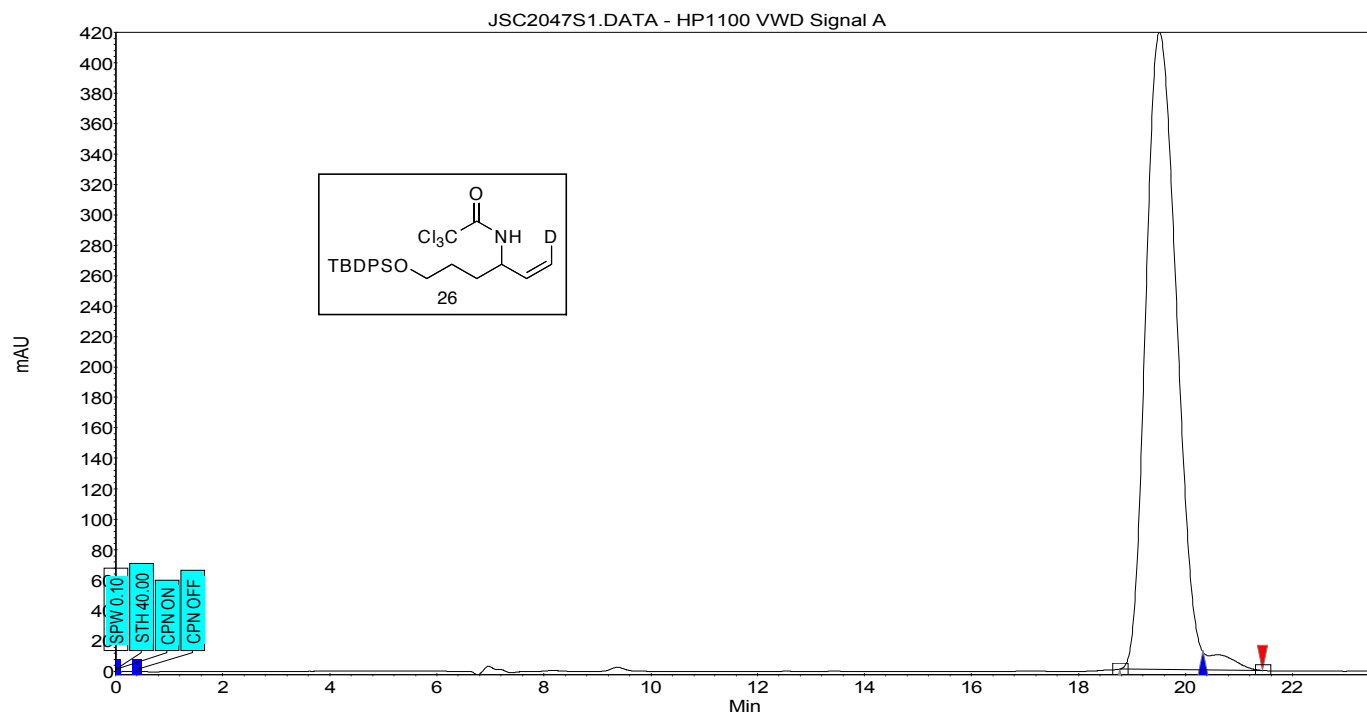
F2 - Processing parameters  
 SI 65536  
 SF 500.2200273 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 9.000 ppm  
 F1 45001.98 Hz  
 F2 -11.063 ppm  
 F3 0.483 ppm/cm  
 F4 220.78580 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling

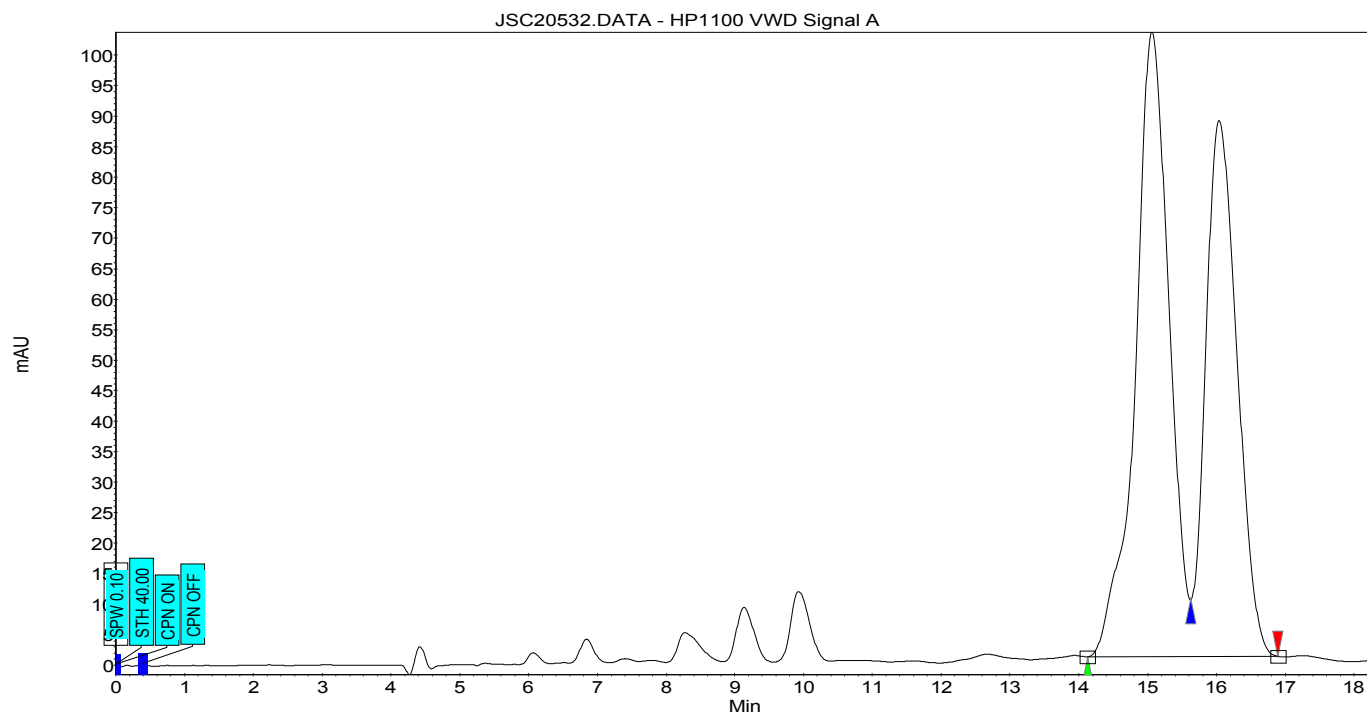


Runinfo: 10% IPA, ODH column, 230nm .8 ml/min, 35 degrees deprotected TBDPS benzoate



Index	Name	Time [Min]	Area [mAU*min]	Height [mAU]	Width [Min]	Area [%]
1	UNKNOWN	19.5058	276.3442	418.96	0.64	97.658
2	UNKNOWN	20.3198	6.6271	11.80	0.60	2.342
Total			282.9713			100.000

Runinfo: 10% IPA, ODH column, 230nm 1 ml/min, 35 degrees deprotected TBDPS benzoate



Index	Name	Time [Min]	Area [mAU*min]	Height [mAU]	Width [Min]	Area [%]
1	UNKNOWN	15.0581	58.0004	102.39	0.50	55.611
2	UNKNOWN	16.0368	46.2953	87.85	0.50	44.389
Total			104.2957			100.000