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## Chemical Materials and Methods.

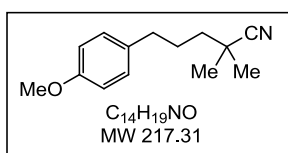
Unless stated otherwise, reactions were conducted in oven-dried glassware under an atmosphere of nitrogen or argon using anhydrous solvents (either freshly distilled (THF, Na/benzophenone) or passed through activated alumina columns). TMSCl was purified by distillation under a nitrogen atmosphere over CaH<sub>2</sub>. TBSCl, titanium chloride, and methyl vinyl ketone were purified by vacuum distillation from neat solutions. All other commercially obtained reagents were used as received. Reaction temperatures were controlled using an IKAmag temperature modulator. Thin-layer chromatography (TLC) was conducted with E. Merck silica gel 60 F254 pre-coated plates, (0.25 mm) and visualized by exposure to UV light (254 nm) or stained with anisaldehyde, ceric ammonium molybdate, or potassium permanganate. Flash column chromatography was performed using normal phase silica gel (60 Å, 230-240 mesh, Merck KGA) with a Biotage Isolera One chromatography system. <sup>1</sup>H NMR spectra were recorded on Bruker spectrometers (at 500 or 600 MHz) and are reported relative to deuterated solvent signals. Data for <sup>1</sup>H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. <sup>13</sup>C NMR spectra were recorded on Bruker Spectrometers (at 125 or 150 MHz). Data for <sup>13</sup>C NMR spectra are reported in terms of chemical shift. IR spectra were recorded on a Varian 640-IR spectrometer and are reported in terms of frequency of absorption (cm<sup>-1</sup>). Optical rotations were measured with a Jasco P-1010 polarimeter. High resolution mass spectra were obtained from the UC Irvine Mass Spectrometry Facility with a Micromass LCT spectrometer. See *JOC Standard Abbreviations and Acronyms* for abbreviations (available at

[http://pubs.acs.org/userimages/ContentEditor/1218717864819/jocea\\_h\\_abbreviations.pdf](http://pubs.acs.org/userimages/ContentEditor/1218717864819/jocea_h_abbreviations.pdf).

LiDDB was prepared by a slight modification of the literature method.<sup>1</sup> To a solution of 4,4'-di-(*tert*-butyl)biphenyl (3.0 g, 11 mmol) in THF (28 mL) at RT was added Li (0.40 g, ~55 mmol) that had been flattened and scraped with a razor. After ~ 3 min, significant dark green color appeared and the mixture was cooled to 0 °C and stirred vigorously for 3 h and then used within 1 h.

A 0.5 M solution of TMSCH<sub>2</sub>CuCNLi was prepared by a modification of the literature method.<sup>2</sup> CuCN (180 mg, 2.0 mmol) and THF (2 mL) were added to round-bottom flask and cooled to -78 °C. A pentane solution of TMSCH<sub>2</sub>Li (1 M, 2 mL, 2 mmol) was added slowly to the stirred mixture. The mixture was allowed to warm to 0 °C as a pale tan solution was formed; this reagent was used within 15 min.

### Experimental Procedures

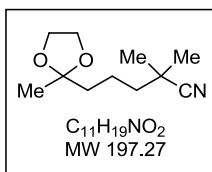


**5-(4-Methoxyphenyl)-2,2-dimethylpentanenitrile (S1):** A round-bottom flask was charged with *i*Pr<sub>2</sub>NH (2.0 mL, 14 mmol), THF (19 mL), and benzene (7 mL) and cooled to 0 °C in an ice-water bath. A solution of *n*BuLi in hexane (2.5 M, 6.0 mL, 15 mmol) was added dropwise to the cooled solution. After 30 min, isobutyronitrile (1.2 mL, 13 mmol) was added dropwise to the solution. The reaction was then stirred for an additional 75 min at 0 °C, after which 1-(3-bromopropyl)-4-methoxybenzene<sup>3</sup> (2.9 g, 13 mmol) was added to the reaction solution and the reaction was allowed to warm to RT overnight. The reaction was then quenched by pouring it into H<sub>2</sub>O (50 mL) and the layers were separated. The aqueous phase was extracted with Et<sub>2</sub>O (3 x 25 mL) and the organic layers were combined and washed with saturated aqueous NaCl solution, dried over Na<sub>2</sub>SO<sub>4</sub>, and concentrated *in vacuo* to produce a red-brown liquid. The red-brown liquid was purified by flash column chromatography (2% ethyl acetate/hexanes to 20% ethyl acetate/hexanes) to obtain **S1** as a clear colorless oil (2.50 g, 11.5 mmol, 92% yield). R<sub>f</sub>: 0.34 (14% ethyl acetate/hexanes); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.11 (d, *J* = 8.4 Hz, 2H), 6.84 (d, *J* = 8.4 Hz, 2H), 3.80 (s, 3H), 2.61 (t, *J* = 7.5 Hz, 2H), 1.77–1.82 (m, 2H), 1.54 (t, *J* = 4.6 Hz, 2H), 1.33 (s, 6H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 158.1, 133.7, 129.5, 125.3, 114.0, 55.5, 40.7, 35.0, 32.5, 27.4, 26.9; IR (thin film) 2976, 2940, 2862, 2233, 1612, 1513, 1463, 1246, 1036, 832 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>15</sub>H<sub>22</sub>O<sub>2</sub>, (M + Na)<sup>+</sup> 240.1364, found 240.1360.

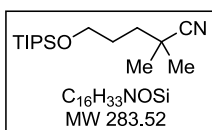
<sup>1</sup> B. Mudryk, T. Cohen, *Org. Synth.* **1995**, 72, 173.

<sup>2</sup> S. H. Bertz, M. Eriksson, G. B. Miao, J. P. Snyder, *J. Am. Chem. Soc.* **1996**, 118, 10906.

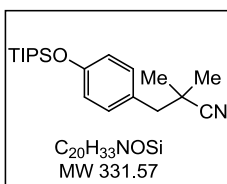
<sup>3</sup> C. Dai, J. M. R. Narayanam, C. R. J. Stephenson, *Nature Chem.* **2011**, 3, 140.



**2,2-Dimethyl-5-(2-methyl-1,3-dioxolan-2-yl)pentanenitrile (S2):** Following the procedure described for preparing **S1**, isobutyronitrile (3.8 mL, 41 mmol) was lithiated and alkylated with 2-(3-chloropropyl)-2-methyl-1,3-dioxolane<sup>4</sup> (6.8 g, 41 mmol) to produce a clear yellow liquid. The clear yellow liquid was purified by flash column chromatography (2% ethyl acetate/hexanes to 20% ethyl acetate/hexanes) to obtain **S2** as a clear colorless oil (4.0 g, 20 mmol, 50% yield). R<sub>f</sub>: 0.33 (20% ethyl acetate/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 3.91–3.96 (m, 4H), 1.65–1.68 (m, 2H), 1.51–1.60 (m, 4H), 1.34 (s, 6H), 1.32 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 125.3, 109.9, 64.9, 41.3, 39.1, 32.5, 26.8, 24.0, 20.0; IR (thin film) 2980, 2954, 2879, 2234, 1471, 1377, 1211, 1061, 871 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>15</sub>H<sub>22</sub>O<sub>2</sub>, (M + Na)<sup>+</sup> 220.1313, found 220.1319.



**2,2-Dimethyl-5-(triisopropylsilyloxy)pentanenitrile (S3):** Following the procedure described for preparing **S1**, isobutyronitrile (1.8 mL, 20 mmol) was lithiated and alkylated with (3-bromopropoxy)triisopropylsilane<sup>5</sup> (16.2 mL, 20.0 mmol) to produce a clear colorless liquid. The clear colorless liquid was purified by flash column chromatography (100% hexanes to 10% ethyl acetate/hexanes to 20% ethyl acetate/hexanes) to give **S3** as a clear colorless oil (5.1 g, 18 mmol, 89% yield). R<sub>f</sub>: 0.66 (20% ethyl acetate/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 1.08–1.12 (m, 21H), 3.73 (t, *J* = 5.8 Hz, 2H), 1.71–1.73 (m, 2H), 1.63–1.65 (m, 2H), 1.36 (s, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 125.4, 63.0, 37.8, 32.4, 29.0, 26.9, 18.2, 12.1; IR (thin film) 2943, 2866, 2235, 1463, 1107, 882 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>15</sub>H<sub>22</sub>O<sub>2</sub>, (M + Na)<sup>+</sup> 306.2229, found 306.2228.



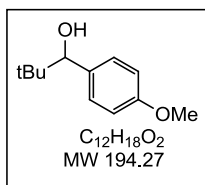
**2,2-Dimethyl-3-(4-(triisopropylsilyloxy)phenyl)propanenitrile (S4).** Following the procedure described for preparing **S1**, isobutyronitrile (0.89 g, 13.0 mmol) was lithiated and alkylated with (4-(bromomethyl)phenoxy)triisopropylsilane<sup>6</sup> (5.30 g, 15.4 mmol) to give a residue, which was purified by silica gel chromatography (33% Et<sub>2</sub>O/hexanes) to afford **S4** (4.10 g,

<sup>4</sup> M. C. Gutierrez, A. Slegers, H. D. Simpson, V. Alphand, R. Furstoss, *Org. Biomol. Chem.* **2003**, *1*, 3500.

<sup>5</sup> J. Clayden, F. E. Knowles, I. R. Baldwin, *J. Am. Chem. Soc.* **2005**, *127*, 2412.

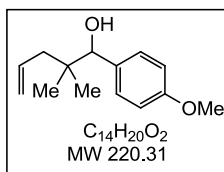
<sup>6</sup> T. Ohshima, V. Gnanadesikan, T. Shibuguchi, Y. Fukuta, T. Nemoto, M. Shibasaki, *J. Am. Chem. Soc.* **2003**, *125*, 11206.

12.4 mmol, 95%) as a colorless oil.  $R_f$ : 0.33 (33% Et<sub>2</sub>O/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.12 (d,  $J$  = 8.5 Hz, 2H), 6.85 (d,  $J$  = 8.5 Hz, 2H), 2.75 (s, 2H), 1.33 (s, 6H), 1.26 (dq,  $J$  = 14.9, 7.4 Hz, 3H), 1.11 (s, 9H), 1.10 (s, 9H); <sup>13</sup>C NMR (125 MHz; CDCl<sub>3</sub>)  $\delta$  155.6, 131.3, 128.3, 125.2, 119.9, 46.1, 33.8, 26.6, 18.1, 12.8; IR (thin film) 2944, 2867, 1609, 1511, 1465, 1268, 914 cm<sup>-1</sup>; HRMS-ESI ( $m/z$ ) (M+Na)<sup>+</sup> calculated for C<sub>20</sub>H<sub>33</sub>NOSiNa 354.2220; observed 354.2224.



**General procedure for generating a tertiary lithium reagent from a nitrile precursor. Preparation of 1-(4-methoxyphenyl)-2,2-dimethylpropan-1-ol (Table 1 Entry 1):**

A round-bottom flask with a glass-coated stir bar was cooled to -78 °C in a dry ice-acetone bath and LiDBB (0.4 M in THF, 4.0 mL, 1.6 mmol) was transferred via syringe. A THF solution (0.2 mL) of trimethylacetone nitrile (67 mg, 0.80 mmol) was then added over 30 sec down the side of the flask to the cooled solution, which changed from a dark green to a dark red color. After 30 sec, a solution of *p*-anisaldehyde (72 mg, 0.53 mmol) in THF (0.2 mL) was added slowly down the side of the flask to the cooled solution, which changed from a dark red to a clear yellow color. The reaction was then warmed to 0 °C in an ice-water bath for 30 min and quenched with a saturated aqueous solution of NH<sub>4</sub>Cl. The reaction mixture was extracted with Et<sub>2</sub>O (3 x 10 ml), and the combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The resultant residue was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (73 mg, 0.38 mmol, 71% yield).  $R_f$ : 0.33 (20% ethyl acetate/hexanes); spectral data were consistent with previously reported data.<sup>7</sup>



**1-(4-Methoxyphenyl)-2,2-dimethylpent-4-en-1-ol (Table 1 Entry 2):**

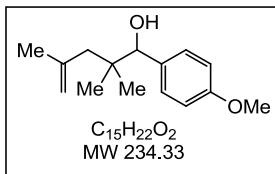
Following the general procedure, 2,2-dimethylpent-4-enenitrile<sup>8</sup> (175 mg, 1.60 mmol) gave a nearly colorless residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (171 mg, 0.780 mmol, 73% yield).  $R_f$ : 0.33 (20% ethyl acetate/hexanes); spectral data were consistent with previously reported data.<sup>9</sup>

<sup>7</sup> I. N. Lykakis, C. Tanielian, M. Orfanopoulos, *Org. Lett.* **2003**, *5*, 2875.

<sup>8</sup> G. A. Molander, E. G. Doedy, *J. Org. Chem.* **1998**, *63*, 8983.

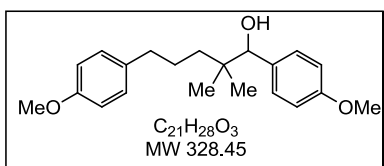
<sup>9</sup> A. Srikrishna, G. Satyanarayana, *Synth. Commun.* **2004**, *34*, 3847.





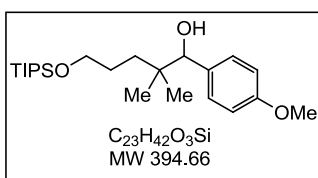
**1-(4-Methoxyphenyl)-2,2,4-trimethylpent-4-en-1-ol (Table 1 Entry 3):**

Following the general procedure, 2,2,4-trimethylpent-4-enitrile<sup>8</sup> (203 mg, 1.66 mmol) gave a crude residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (170 mg, 0.73 mmol, 66% yield).  $R_f$ : 0.33 (20% ethyl acetate/hexanes);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.24 (d,  $J = 8.7$  Hz, 2H), 6.86 (d,  $J = 8.7$  Hz, 2H), 4.91 (s, 1H), 4.73 (s, 1H), 4.45 (s, 1H), 3.82 (s, 3H), 2.21 (d,  $J = 12.9$  Hz, 1H), 2.02 (d,  $J = 12.9$  Hz, 1H), 1.89 (br s, 1H), 1.83 (s, 3H), 0.92 (s, 3H), 0.84 (s, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  159.0, 144.0, 134.3, 129.1, 114.8, 113.2, 81.1, 55.4, 46.6, 39.3, 25.8, 24.5, 22.7; IR (thin film) 3466, 3072, 2964, 1611, 1513, 1247, 1173, 1036, 835  $cm^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $C_{15}H_{22}O_2$ , (M + Na)<sup>+</sup> 257.1518, found 257.1527.



**1,5-Bis(4-methoxyphenyl)-2,2-dimethylpentan-1-ol (Table 1 Entry 4):**

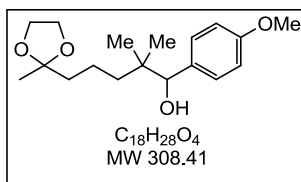
Following the general procedure, **S1** (219 mg, 1.01 mmol) gave a crude residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (158 mg, 0.480 mmol, 71% yield).  $R_f$ : 0.28 (20% ethyl acetate/hexanes);  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  7.21 (d,  $J = 8.5$  Hz, 2H), 7.11 (d,  $J = 8.3$  Hz, 2H), 6.85 (apt t,  $J = 8.3$  Hz, 4H), 4.42 (s, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 2.53 (m, 2H), 1.62 (br m, 3H), 1.41 (m, 1H), 1.27 (m, 1H), 0.89 (s, 3H), 0.82 (s, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  159.0, 157.9, 135.2, 134.5, 129.5, 129.0, 113.9, 113.2, 81.0, 55.5, 55.4, 38.7, 38.3, 36.2, 26.6, 23.3, 22.9; IR (thin film) 3494, 2936, 1736, 1612, 1513, 1245, 1034, 833  $cm^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $C_{21}H_{28}O_3$ , (M + Na)<sup>+</sup> 351.1936, found 351.1934.



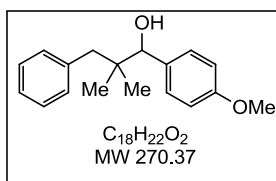
**1-(4-Methoxyphenyl)-2,2-dimethyl-5-(triisopropylsilyloxy)pentan-1-ol (Table 1 Entry 5):**

Following the general procedure, **S3** (467 mg, 1.65 mmol) gave a crude residue which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (264 mg, 0.670 mmol, 61% yield).  $R_f$ : 0.43 (20% ethyl acetate/hexanes);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.23 (d,  $J = 8.7$  Hz, 2H), 6.85 (d,  $J = 8.7$  Hz, 2H), 4.45 (m, 1H), 3.81 (s, 3H), 3.66 (t,  $J = 6.6$  Hz, 2H), 1.81 (s, 1H), 1.56 (m, 2H), 1.40 (m, 1H), 1.25 (m, 1H), 1.06 (br m, 21H), 0.90 (s, 3H), 0.84 (s, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  159.0, 134.4, 129.0, 113.1, 81.0, 64.4, 55.5, 38.2, 34.8, 27.7, 23.2,

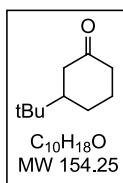
23.0, 18.3, 12.2; IR (thin film) 3492, 2944, 2725, 1614, 1514, 1247, 1175, 833, 883  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{42}\text{O}_3\text{Si}$ ,  $(\text{M} + \text{Na})^+$  417.2801, found 417.2815.



**1-(4-Methoxyphenyl)-2,2-dimethyl-5-(2-methyl-1,3-dioxolan-2-yl)pentan-1-ol (Table 1 Entry 6):** Following the general procedure, **S2** (316 mg, 1.60 mmol) gave a residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (193 mg, 0.630 mmol, 59% yield).  $R_f$ : 0.19 (20% ethyl acetate/hexanes);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.23 (d,  $J = 8.6$  Hz, 2H), 6.85 (d,  $J = 8.7$  Hz, 2H), 4.44 (s, 1H), 3.93 (m, 4H), 3.81 (s, 3H), 1.79 (br s, 1H), 1.61 (br m, 3H), 1.40 (br m, 3H), 1.33 (s, 3H), 0.90 (s, 3H), 0.83 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 134.4, 129.0, 113.1, 110.4, 81.0, 64.8, 55.5, 40.2, 39.1, 38.4, 24.0, 23.2, 22.8, 18.7; IR (thin film) 3478, 2955, 2876, 1611, 1512, 1247, 1175, 1034, 835  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{18}\text{H}_{28}\text{O}_4$ ,  $(\text{M} + \text{Na})^+$  331.1885, found 331.1877.



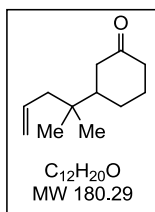
**1-(4-Methoxyphenyl)-2,2-dimethyl-3-phenylpropan-1-ol (Table 1 Entry 7):** Following the general procedure, 2,2-dimethyl-3-phenylpropanenitrile<sup>10</sup> (255 mg, 1.60 mmol) gave a residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (100 mg, 0.4 mmol, 70% yield).  $R_f$ : 0.28 (20% ethyl acetate/hexanes);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.35–7.24 (m, 7H), 6.91 (d,  $J = 8.7$  Hz, 2H), 4.45 (s, 1H), 3.86 (s, 3H), 2.89 (d,  $J = 12.8$  Hz, 1H), 2.62 (d,  $J = 12.8$  Hz, 1H), 2.05 (br s, 1H), 0.93 (s, 3H), 0.80 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 139.1, 134.3, 131.1, 129.1, 127.9, 126.0, 113.2, 80.3, 55.4, 44.8, 39.5, 23.7, 22.1; IR (thin film) 3417, 3071, 2962, 1681, 1607, 1514, 1174, 1030, 833  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{18}\text{H}_{22}\text{O}_2$ ,  $(\text{M} + \text{Na})^+$  293.1518, found 293.1516.



**General procedure for preparing 3-substituted cyclohexanones 6. Preparation of 3-tert-Butylcyclohexanone (Table 2 Entry 1):** A round-bottom flask with a glass-coated stir bar was cooled to  $-78$   $^{\circ}\text{C}$  in a dry ice-acetone bath and LiDBB (0.4 M in THF, 8.0 mL, 3.2 mmol) was transferred via syringe. Trimethylacetone nitrile (130 mg,

<sup>10</sup> G. A. Molander, E. M. Sommers, S. R. Baker, *J. Org. Chem.* **2008**, *71*, 1563.

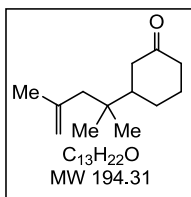
1.6 mmol) was then added in THF (0.2 mL) over 30 sec down the side of the flask to the cooled solution, which changed from a dark green to a dark red color. After 5 min, a solution of TMSCH<sub>2</sub>CuLiCN (0.5 M in 1:1 THF-pentane, 5.0 mL, 2.5 mmol) was added and the reaction was allowed to stir at -78 °C for 15 min at which point TMSCl (0.50 mL, 4.0 mmol) was added slowly, followed by 2-cyclohexen-1-one (77 mg, 0.80 mmol) in THF (0.2 mL). The reaction was then stirred for an additional 5 min at -78 °C and quenched with a saturated aqueous solution of 10:1 NH<sub>4</sub>Cl-NH<sub>4</sub>OH (10 mL) at -78 °C. The reaction mixture was extracted with Et<sub>2</sub>O (3 x 10 mL), and the combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The crude mixture was then dissolved in a 1:1 THF-1 N HCl solution (10 mL) and allowed to stir for 15 min at RT. The reaction was then extracted with ethyl acetate (3 x 10 mL), and the combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The resultant residue was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to give the title compound as a clear colorless oil (87 mg, 0.56 mmol, 71% yield). R<sub>f</sub>: 0.50 (20% ethyl acetate/hexanes); spectral data matched previously reported data.<sup>11</sup>



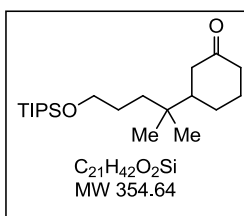
**3-(2-Methylpent-4-en-2-yl)cyclohexanone (Table 2 Entry 2):** Following the general procedure, 2,2-dimethylpent-4-enitrile<sup>8</sup> (175 mg, 1.60 mmol) gave a residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to give the title compound as a clear colorless oil (90 mg, 0.50 mmol, 63% yield). R<sub>f</sub>: 0.50 (20% ethyl acetate/hexanes); <sup>1</sup>H NMR (600

MHz, CDCl<sub>3</sub>) δ 5.74–5.82 (m, 1H), 5.00–5.05 (m, 2H), 2.41–2.44 (m, 1H), 2.34–2.37 (m, 1H), 2.20–2.25 (ddd, *J* = 6.5, 13.8, 13.8 Hz, 1H), 1.89–2.12 (m, 5H), 1.77 (s, 3H), 1.51–1.64 (m, 2H), 1.31–1.38 (dddd, *J* = 3.5, 12.3, 12.3, 12.3 Hz, 1H), 0.88 (s, 3H), 0.86 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 212.9, 134.9, 117.5, 47.2, 44.8, 43.4, 41.5, 25.9, 25.7, 24.40, 24.36; IR (thin film) 3074, 2961, 2867, 1718, 1469, 1368, 1233, 997, 913 cm<sup>-1</sup>; HRMS (ESI) *m/z* calcd for C<sub>12</sub>H<sub>20</sub>O, (M + Na)<sup>+</sup> 203.1412, found 203.1409.

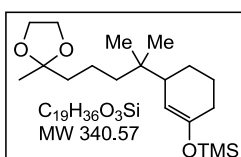
<sup>11</sup> S. Cren, P. Schair, P. Renaud, K. Schenk, *J. Org. Chem.* **2009**, *74*, 2942.



**3-(2,4-Dimethylpent-4-en-2-yl)cyclohexanone (Table 2 Entry 3):** Following the general procedure, 2,2,4-trimethylpent-4-enitrile<sup>8</sup> (197 mg, 1.60 mmol) gave a residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (87 mg, 0.45 mmol, 56% yield).  $R_f$ : 0.50 (20% ethyl acetate/hexanes);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  4.87 (s, 1H), 4.65 (s, 1H), 2.44–2.48 (m, 1H), 2.35–2.39 (m, 1H), 2.20–2.27 (ddd,  $J = 6.5, 13.7, 13.7$  Hz, 1H), 1.95–2.13 (m, 5H), 1.77 (s, 3H), 1.51–1.65 (m, 2H), 1.31–1.39 (dddd,  $J = 3.4, 12.8, 12.8, 12.8$  Hz, 1H), 0.90 (s, 3H), 0.89 (s, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  213.3, 143.3, 115.0, 48.1, 47.4, 43.7, 41.6, 36.3, 26.1, 25.8, 25.7, 25.2, 24.9; IR (thin film) 3073, 2964, 2866, 1714, 1641, 1449, 1232, 892  $cm^{-1}$ ; HRMS (GC)  $m/z$  calcd for  $C_{13}H_{22}O$ , (M + H)<sup>+</sup> 195.1749, found 195.1745.

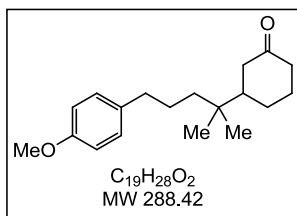


**3-(2-Methyl-5-(triisopropylsilyloxy)pentan-2-yl)cyclohexanone (Table 2 Entry 4):** Following the general procedure, **S3** (454 mg, 1.60 mmol) gave a residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (210 mg, 0.59 mmol, 75% yield).  $R_f$ : 0.52 (20% ethyl acetate/hexanes);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  3.63–3.66 (m, 2H), 2.41–2.35 (m, 2H), 2.27–2.20 (ddd,  $J = 6.4, 13.7, 13.7$  Hz, 1H), 2.05–2.12 (m, 2H), 1.91 (d,  $J = 13.0$  Hz, 1H), 1.45–1.65 (m, 4H), 1.21–1.38 (m, 3H), 1.05–1.09 (m, 21H), 0.87 (s, 3H), 0.86 (s, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  213.3, 64.2, 47.4, 43.5, 41.7, 36.3, 35.0, 27.5, 26.0, 25.9, 24.8, 24.6, 18.3, 12.2; IR (thin film) 2943, 2885, 1714, 1469, 1387, 1231, 1107, 883  $cm^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $C_{21}H_{42}O_2Si$ , (M + Na)<sup>+</sup> 377.2852, found 377.2853.



**Trimethyl(3-(2-methyl-5-(2-methyl-1,3-dioxolan-2-yl)pentan-2-yl)cyclohex-1-enyloxy)silane (Table 2 Entry 5):** Following the general procedure, **S2** (316 mg, 1.60 mmol) was converted to the corresponding cuprate and allowed to react with cyclohexenone. In this case, the product was isolated after the reaction was quenched with a saturated aqueous solution of 10:1  $NH_4Cl-NH_4OH$  at  $-78$  °C (not a 1:1 1 N HCl-THF solution). The resultant residue was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (190 mg, 0.56 mmol, 70% yield).  $R_f$ : 0.62 (20% ethyl acetate/hexanes);  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  4.89 (s, 1H), 3.93–3.96 (m, 4H), 1.82–2.07 (m, 4H), 1.48–1.68 (m, 4H), 1.33 (br s, 4H), 1.20–1.24 (m, 2H), 1.06–1.14 (m, 1H), 0.82 (appt d, 6H), 0.19 (s, 9H);  $^{13}C$  NMR

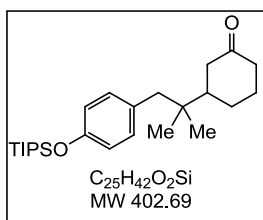
(125 MHz, CDCl<sub>3</sub>)  $\delta$  151.5, 110.4, 106.9, 64.8, 43.6, 40.7, 40.4, 35.5, 30.1, 24.9, 24.8, 24.0, 23.9, 23.2, 18.6, 0.63; IR (thin film) 2954, 2874, 1663, 1373, 1252, 2195, 1064, 916, 846 cm<sup>-1</sup>; HRMS (ESI)  $m/z$  calcd for C<sub>19</sub>H<sub>36</sub>O<sub>3</sub>Si, (M + Na)<sup>+</sup> 363.2332, found 363.2318.



### 3-(5-(4-Methoxyphenyl)-2-methylpentan-2-yl)cyclohexanone

**(Table 2 Entry 6):** Following the general procedure, **S1** (174 mg, 0.80 mmol) gave a residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (82 mg, 0.28 mmol,

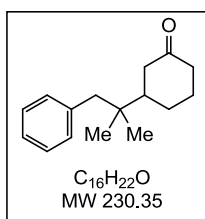
72% yield).  $R_f$ : 0.28 (20% ethyl acetate/hexanes); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.08 (d,  $J$  = 8.5 Hz, 1H), 6.83 (d,  $J$  = 8.6 Hz, 1H), 3.78 (s, 3H), 2.47–2.55 (m, 2H), 2.33–2.38 (m, 2H), 2.18–2.24 (ddd,  $J$  = 7.2, 14.4, 14.4 Hz, 1H), 2.03–2.10 (m, 2H), 1.84 (d,  $J$  = 13.1 Hz, 1H), 1.50–1.57 (m, 4H), 1.24–1.32 (m, 3H), 0.85 (s, 3H), 0.83 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  213.0, 157.8, 134.7, 129.3, 113.8, 55.3, 47.2, 43.3, 41.5, 39.9, 35.9, 35.1, 25.9, 25.84, 25.77, 24.6, 24.4; IR (thin film) 2938, 2864, 1710, 1512, 1246, 1177, 1037, 829 cm<sup>-1</sup>; HRMS (ESI)  $m/z$  calcd for C<sub>27</sub>H<sub>52</sub>O<sub>4</sub>Si<sub>2</sub>, (M + Na)<sup>+</sup> 311.1987, found 311.1982.



### 3-(2-Methyl-1-(4-(triisopropylsilyloxy)phenyl)propan-2-yl)cyclohexanone

**(Table 2 Entry 7):** Following the general procedure, **S4** (265 mg, 0.80 mmol) gave a residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (96 mg, 0.24 mmol, 60%

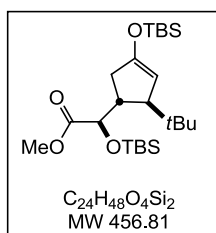
yield).  $R_f$ : 0.50 (20% ethyl acetate/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  6.94 (d,  $J$  = 8.3 Hz, 1H), 6.78 (d,  $J$  = 8.2 Hz, 1H), 2.48–2.52 (m, 1H), 2.36–2.39 (m, 1H), 2.22–2.29 (ddd,  $J$  = 6.4, 13.7, 13.7 Hz, 1H), 2.11–2.17 (m, 2H), 2.01–2.05 (m, 1H), 1.54–1.61 (m, 2H), 1.37–1.44 (m, 1H), 1.21–1.28 (m, 3H), 1.09 (d,  $J$  = 7.5 Hz, 18H), 0.83 (s, 3H), 0.81 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  213.0, 154.5, 131.6, 131.1, 119.4, 47.6, 45.0, 43.7, 41.6, 36.6, 26.4, 25.7, 24.4, 24.3, 18.1, 12.8; IR (thin film) 3030, 2945, 2867, 1714, 1608, 1514, 1470, 1265, 1171, 914, 883, 678 cm<sup>-1</sup>; HRMS (ESI)  $m/z$  calcd for C<sub>27</sub>H<sub>52</sub>O<sub>4</sub>Si<sub>2</sub>, (M + Na)<sup>+</sup> 425.2852, found 425.2846.



### 3-(2-Methyl-1-phenylpropan-2-yl)cyclohexanone

**(Table 2 Entry 8):** Following the general procedure, 2,2-dimethyl-3-phenylpropanenitrile<sup>10</sup> (130 mg, 0.80 mmol) gave a residue, which was purified by flash column chromatography (100% hexanes to 20% ethyl acetate/hexanes) to obtain the

title compound as a clear colorless oil (62 mg, 0.27 mmol, 67% yield).  $R_f$ : 0.40 (20% ethyl acetate/hexanes)  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.26–7.29 (m, 2H), 7.20–7.23 (m, 2H), 7.12 (d,  $J$  = 7.1 Hz, 1H), 2.52–2.57 (m, 3H), 2.38–2.41 (m, 1H), 2.24–2.31 (ddd,  $J$  = 6.4, 13.7, 13.7 Hz, 1H), 2.12–2.16 (m, 2H), 2.05–2.07 (m, 1H), 1.56–1.60 (m, 2H), 1.40–1.48 (dddd,  $J$  = 3.2, 12.6, 12.6, 12.6 Hz, 1H), 0.87 (s, 3H), 0.85 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  212.9, 138.8, 130.9, 128.0, 126.2, 47.6, 45.9, 43.7, 41.6, 36.7, 26.3, 25.7, 24.5, 24.3; IR (thin film) 3061, 3027, 2962, 2866, 1714, 1602, 1453, 1367, 1232, 732, 703  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{27}\text{H}_{52}\text{O}_4\text{Si}_2$ , ( $\text{M} + \text{Na}$ ) $^+$  253.1568, found 253.1562.



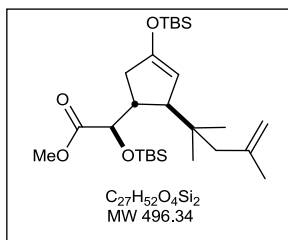
**(R)-Methyl 2-(tert-butyl dimethylsilyloxy)-2-((1R,2S)-4-(tert-butyl dimethylsilyloxy)-2-(2,4-dimethylpent-4-en-2-yl)cyclopent-3-enyl)acetate (Table 2 Entry 1B)** A round-bottom flask with a glass-coated stir bar was cooled to  $-78$   $^{\circ}\text{C}$  in a dry ice-acetone bath and LiDBB (0.4 M in THF, 3.5 mL, 1.4 mmol) was transferred via syringe. Trimethylacetoneitrile

(170 mg, 0.7 mmol) in THF (0.2 mL) was then added slowly down the side of the flask to the cooled solution, which changed from a dark green to a dark red color. After 5 min, a solution of  $\text{TMSCH}_2\text{CuLiCN}$  (0.5 M in 1:1 THF-pentane, 1.8 mL, 0.9 mmol) was added and the reaction was allowed to stir at  $-78$   $^{\circ}\text{C}$  for 15 min, after which a solution of TBSCl (100 mg, 0.70 mmol) and enone **2**<sup>12</sup> (100 mg, 0.35 mmol) in THF (0.2 mL) was added dropwise to the reaction. The reaction was then stirred for an additional 5 min and quenched with a saturated aqueous solution of 10:1  $\text{NH}_4\text{OH-NH}_4\text{Cl}$  at  $-78$   $^{\circ}\text{C}$ . The reaction mixture was extracted three times with  $\text{Et}_2\text{O}$ , and the combined organic layers were dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated *in vacuo*. The resultant residue was purified by flash column chromatography (100% hexanes to 0.2% ethyl acetate/hexanes to 1% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (110 mg, 0.27 mmol, 78% yield). Spectral data matched that previously reported.<sup>13</sup>

<sup>12</sup> See, M. J. Schnermann, C. M. Beaudry, N. E. Genung, S. M. Canham, N. L. Untiedt, B. D. W. Karanikolas, C. Sutterlin, L. E. Overman, *J. Am. Chem. Soc.* **2011**, *133*, 17494 and reference 16.

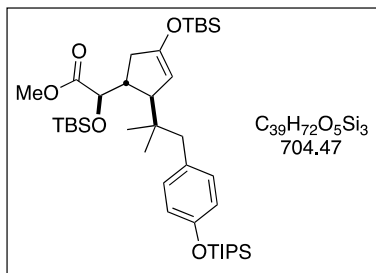
<sup>13</sup> M. J. Schnermann, L. E. Overman, *J. Am. Chem. Soc.* **2011**, *133*, 16425.

**(R)-methyl 2-(tert-butyldimethylsilyloxy)-2-((1R,2S)-4-(tert-butyldimethylsilyloxy)-2-(2,4-dimethylpent-4-en-2-yl)cyclopent-3-enyl)acetate (Table 2 Entry 3B)**



A round-bottom flask with a glass-coated stir bar was cooled to  $-78\text{ }^{\circ}\text{C}$  in a dry ice-acetone bath and LiDBB (0.4 M in THF, 3.5 mL, 1.4 mmol) was transferred via syringe. 2,2,4-Trimethylpent-4-enenitrile<sup>8</sup> (86 mg, 0.7 mmol) was then added in THF (0.2 mL) slowly down the side of the flask the cooled solution which changed from a dark green to a dark red color. After 5 min a solution of  $TMSCH_2CuLiCN$  (0.5 M in 1:1 THF-pentane, 1.8 mL, 0.9 mmol) was added and the reaction was allowed to stir at  $-78\text{ }^{\circ}\text{C}$  for 15 min, after which a solution of TBSCl (100 mg, 0.70 mmol) and enone **2** (100 mg, 0.35 mmol) in THF (0.2 mL) was added dropwise to the reaction. The reaction was then stirred for an additional 5 min and quenched with a saturated aqueous solution of 10:1  $NH_4OH/NH_4Cl$  at  $-78\text{ }^{\circ}\text{C}$ . The reaction mixture was extracted three times with  $Et_2O$ , and the combined organic layers were dried over  $Na_2SO_4$ , filtered, and concentrated *in vacuo*. The resultant residue was purified by flash column chromatography (100% hexanes to 0.2% ethyl acetate/hexanes to 1% ethyl acetate/hexanes) to obtain the title compound as a clear colorless oil (90 mg, 0.18 mmol, 51% yield).  $R_f$ : 0.42 (5% ethyl acetate/hexanes);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  4.85 (s, 1H), 4.63 (s, 1H), 4.56 (s, 1H), 4.00 (d,  $J = 6.6$  Hz, 1H), 3.70 (s, 3H), 2.44 (s, 1H), 2.30–2.42 (m, 2H), 2.00 (d,  $J = 12.6$  Hz, 1H), 1.98 (d,  $J = 13.7$  Hz, 1H), 1.83 (d,  $J = 12.9$  Hz, 1H), 1.78 (s, 3H), 0.92 (s, 9H), 0.90 (s, 9H), 0.84 (s, 3H), 0.81 (s, 3H), 0.16 (s, 3H), 0.05 (s, 3H), 0.04 (s, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  173.7, 154.4, 144.1, 114.4, 103.0, 76.3, 54.5, 51.8, 47.1, 40.7, 38.1, 36.5, 31.6, 26.2, 26.0, 25.9, 25.8, 24.5, 18.4, 18.3,  $-4.2$ ,  $-4.5$ ,  $-4.8$ ,  $-4.9$ ; IR (thin film) 3073, 2956, 2858, 1757, 1653, 1254  $cm^{-1}$ ; HRMS (ESI)  $m/z$  calcd for  $C_{27}H_{52}O_4Si_2$ ,  $(M + Na)^+$  519.3302, found 519.3287;  $[\alpha]_D^{24} -8.5^{\circ}$ ,  $[\alpha]_{577}^{24} -8.1^{\circ}$ ,  $[\alpha]_{546}^{24} -7.3^{\circ}$ ,  $[\alpha]_{435}^{24} -9.5^{\circ}$ , ( $c = 0.3$ ,  $CH_2Cl_2$ ).

**(R)-Methyl 2-(tert-butyldimethylsilyloxy)-2-((1R,2S)-4-(tert-butyldimethylsilyloxy)-2-(2-methyl-1-(4-(triisopropylsilyloxy)phenyl)propan-2-yl)cyclopent-3-enyl)acetate (Table 2 Entry 7B)**



A flame-dried round-bottom flask containing a glass-coated stir bar was cooled to  $-78\text{ }^{\circ}\text{C}$  in a dry ice-acetone bath and a solution of LiDBB (0.4 M in THF, 8.8 mL, 3.5 mmol) was transferred via syringe. A solution of nitrile **S4** (582 mg, 1.8 mmol) in THF (1.0 mL) was then added slowly down the side of

the flask to the cooled LiDBB solution, which changed from dark green to a dark red color. After 5 min, a solution of TMSCH<sub>2</sub>CuLiCN (0.5 M in 1:1 THF-pentane, 3.6 mL, 1.8 mmol) was added and the mixture was allowed to stir at -78 °C for 15 min, at which point a solution of TBSCl (500 mg, 3.5 mmol) and enone **2** (200 mg, 0.7 mmol) in THF (0.5 mL) was added to the reaction. The bright yellow mixture was then stirred for an additional 5 min and quenched with a saturated aqueous solution of 10:1 NH<sub>4</sub>Cl:NH<sub>4</sub>OH (50 mL) at -78 °C. The reaction mixture was extracted with Et<sub>2</sub>O (3 × 25 mL) and the combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. Purification of the residue by silica gel chromatography (5% Et<sub>2</sub>O/hexanes) gave the title compound (403 mg, 0.570 mmol, 81%) as a yellow oil: R<sub>f</sub>: 0.41 (5% Et<sub>2</sub>O/hexanes); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 6.94 (d, *J* = 8.4 Hz, 2H), 6.77 (d, *J* = 8.3 Hz, 2H), 4.64 (s, 1H), 4.02 (d, *J* = 6.4 Hz, 1H), 3.69 (s, 3H), 2.50–2.42 (m, 4H), 2.31 (d, *J* = 13.1 Hz, 1H), 2.00 (d, *J* = 14.3 Hz, 1H), 1.25 (dq, *J* = 15.0, 7.5 Hz, 3H), 1.11–1.09 (m, 18H), 0.94 (s, 9H), 0.88 (s, 9H), 0.73–0.70 (m, 6H), 0.18 (s, 6H), 0.03 (s, 3H), 0.02 (s, 3H); <sup>13</sup>C NMR (125 MHz; CDCl<sub>3</sub>) δ 173.7, 154.48, 154.28, 132.0, 131.7, 119.2, 103.0, 76.3, 54.2, 51.8, 44.7, 40.8, 38.5, 36.5, 26.0, 25.9, 24.0, 23.7, 18.4, 18.3, 18.2, 12.9, -4.2, -4.5, -4.87, -4.91; IR (thin film) 2951, 2930, 2893, 2865, 1756, 1737, 1652, 1608, 1509, 1464, 1258, 1201, 1169, 1133, 916, 838, 779, 678 cm<sup>-1</sup>; HRMS-ESI (*m/z*) (M+Na)<sup>+</sup> calculated for C<sub>39</sub>H<sub>72</sub>O<sub>5</sub>Si<sub>3</sub>Na 727.4586; observed 727.4585; [α]<sub>D</sub><sup>24</sup>-11.0, [α]<sub>577</sub><sup>24</sup>-13.1, [α]<sub>546</sub><sup>24</sup>-15.8, [α]<sub>435</sub><sup>24</sup>-31.8, [α]<sub>405</sub><sup>24</sup>-38.6 (*c* = 0.6, CH<sub>2</sub>Cl<sub>2</sub>).

### Preparation of Hydroazulene Nitriles **8** and **9**.

These precursors were synthesized from enantiomerically pure hydroazulenone **S5**<sup>14</sup> by the sequence summarized in Scheme S1. Addition of the Nagata reagent, Et<sub>2</sub>AlCN, to enone **8** and extended heating at elevated temperature provided two separable crystalline adducts, **S6** and **S7**, in a 1:2 ratio and high yield.<sup>15,16</sup> Consistent with a thermodynamically controlled process, resubjecting the minor epimer **S6** to the reaction conditions produced the initial 2:1 epimeric mixture. Direct methylenation of ketones **S6** and **S7** was unsuccessful under a variety of conditions, see Table S3 for details. As an alternative methylenation approach, ketones **S6** and **S7** were converted first to allylsilanes **S8** and **S9** by kinetic enol triflation and Negishi cross coupling. Subsequent acid-promoted allylic desilylation provided nitriles **8** and **9** in 30 and 18% overall yields from **S5**.<sup>17</sup>

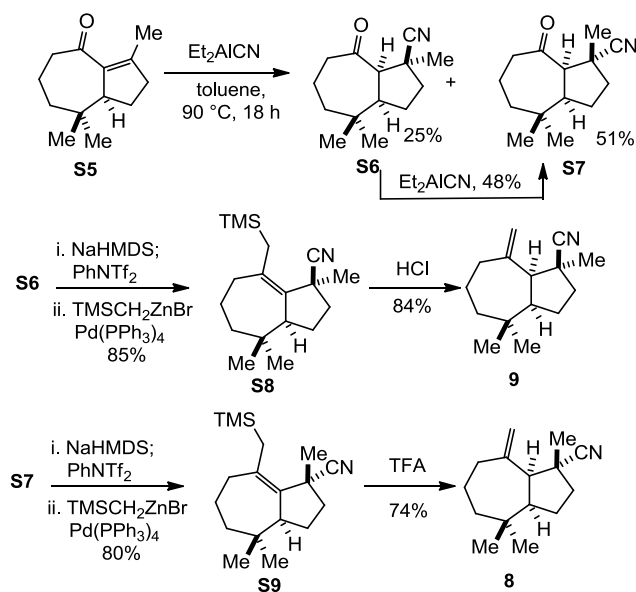
<sup>14</sup> M. J. Schnermann, L. E. Overman, following paper in this issue.

<sup>15</sup> W. Nagata, M. Yoshioka *Org. React.* **1997**, *25*, 255.

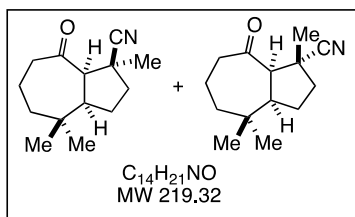
<sup>16</sup> The relative configuration of **S6** and **S7** was secured by X-ray crystallographic analysis: CDCC 885479 and CDCC 885480.

<sup>17</sup> For the development of this strategy to form related sesquiterpenes, see: M. S. Dowling, C. D. Vanderwal, *J. Am. Chem. Soc.* **2009**, *131*, 15090.





**Scheme S1:** Synthesis of **8** and **9**.

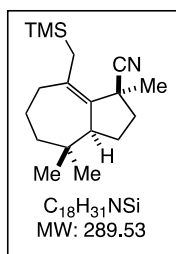


**(1R,3aR,8aR)-1,4,4-Trimethyl-8-oxodecahydroazulene-1-carbonitrile (S6)** and **(1S,3aR,8aR)-1,4,4-trimethyl-8-oxodecahydroazulene-1-carbonitrile (S7)**. To a solution of **S5** (1.6 g, 8.4 mmol)<sup>18</sup> in toluene (60 mL) was added  $Et_2AlCN$  (16.8 mL of a 1M solution in toluene, 16.8 mmol) and the solution was

heated to 100 °C. After 18 h, the tan solution was cooled to 0 °C and a 10% aqueous solution of sodium potassium tartrate (100 mL) was slowly added. After 30 min at 0 °C, the mixture was allowed to warm to RT, the layers were separated, and the aqueous layer was extracted with  $Et_2O$  (100 mL). The combined organic layers were dried with  $Na_2SO_4$  and concentrated. The residue was purified by column chromatography ( $SiO_2$ , 10–20% ethyl acetate/hexanes) to afford the more non-polar **S7** as white solid (931 mg, 51%) and the more polar **S6** as a colorless solid (460 mg, 25%). Data for **S7**:  $R_f$ : 0.35 (20% ethyl acetate/hexanes);  $^1H$  NMR ( $C_6D_6$ , 500 MHz)  $\delta$  2.90 (d,  $J = 8.2$  Hz, 1H), 2.14 (apt q,  $J = 9$  Hz, 1H), 2.02 (m, 1H), 1.82 (m, 1H), 1.73 (m, 1H), 1.51 (m, 1H), 1.35 (m, 1H), 1.27 (m, 4H), 1.13 (s, 3H), 0.85 (m, 1H), 0.57 (s, 3H), 0.54 (s, 3H);  $^{13}C$  NMR ( $C_6D_6$ , 125 MHz)  $\delta$  208.8, 125.3, 63.0, 49.9, 44.9, 41.8, 38.1, 37.9, 35.6, 29.5, 27.7, 24.7, 21.4, 21.3; IR (thin film) 2961.4, 2228, 1687, 1474, 1453; HRMS (ESI/TOF) calculated for  $C_{14}H_{21}NO$  ( $M+Na$ )<sup>+</sup> 242.1521, observed 242.1516;  $[\alpha]_D^{24} +3.3^\circ$ ,  $[\alpha]_{577}^{24} +3.8^\circ$ ,  $[\alpha]_{546}^{24} +3.9^\circ$ ,  $[\alpha]_{435}^{24} +19.1^\circ$ ,  $[\alpha]_{405}^{24} +32.1^\circ$  ( $c = 1.0$ ,  $CH_2Cl_2$ ); this product was recrystallized (m.p. 73–74°C) from ether/hexane to afford thin needles suitable for X-ray crystallography. Data for **S6**:  $R_f$ : 0.21 (20% ethyl acetate/hexanes);  $^1H$

<sup>18</sup> See the following communication in this issue.

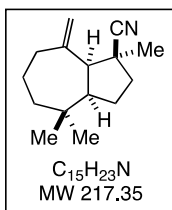
NMR (CDCl<sub>3</sub>, 500 MHz)  $\delta$  2.69 (d,  $J$  = 11.5 Hz, 1H), 2.55 (m, 1H), 2.43 (m, 2H), 2.21 (dd,  $J$  = 12.5, 6.4 Hz, 1H), 1.91 (m, 2H), 1.69 (m, 3H), 1.58 (m, 2H), 1.43 (s, 3H), 0.88 (s, 3H), 0.85 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$  209.1, 124.1, 65.7, 48.8, 44.7, 43.9, 40.5, 39.6, 36.4, 31.3, 27.5, 25.2, 22.0, 21.3; IR (thin film) 2959, 2231, 1704, 1454 cm<sup>-1</sup>; HRMS (ESI/TOF) calculated for C<sub>14</sub>H<sub>21</sub>NO (M+Na) 242.1521, observed 242.1517; [ $\alpha$ ]<sub>D</sub><sup>24</sup> +27.3°, [ $\alpha$ ]<sub>577</sub><sup>24</sup> +28.4°, [ $\alpha$ ]<sub>546</sub><sup>24</sup> +32.2°, [ $\alpha$ ]<sub>435</sub><sup>24</sup> +73.7°, [ $\alpha$ ]<sub>405</sub><sup>24</sup> +92.7°, ( $c$  = 1.0, CH<sub>2</sub>Cl<sub>2</sub>); this product was recrystallized (m.p. 58–60 °C) from ether/hexane to afford thin needles suitable for X-ray crystallography.



**(1S,3aS)-1,4,4-Trimethyl-8-((trimethylsilyl)methyl)-1,2,3,3a,4,5,6,7-octahydroazulene-1-carbonitrile (S8):** To a solution of **S6** (340 mg, 1.6 mmol) in THF (8 mL) at -78 °C was added 1 M NaHMDS in THF (2.0 mL, 2.0 mmol). After 10 min, a solution of PhNTf<sub>2</sub> (830 mg, 2.3 mmol) in THF (2 mL) was added. The dry ice bath was removed and the solution was allowed to warm to RT. After 30 min, saturated aqueous NH<sub>4</sub>Cl (20 mL) was added and the mixture

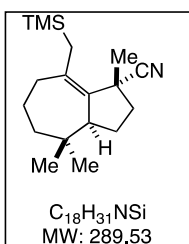
was extracted with Et<sub>2</sub>O (3 × 10 mL).<sup>a</sup> The combined organic extracts were dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated to yield the vinyl triflate as mixture containing impurities derived from PhNTf<sub>2</sub> that could be used without purification. The cross coupling was completed along the lines of the procedure reported by Corey.<sup>19</sup> To a solution of ZnBr<sub>2</sub> (1.03 g, 4.75 mmol) in THF at RT was added a solution of freshly prepared 1 M TMSCH<sub>2</sub>MgBr in Et<sub>2</sub>O (4.7 mL) to form a mixture containing white precipitate. After 1 h, the vinyl triflate from above in THF (2 mL) and Pd(PPh<sub>3</sub>)<sub>4</sub> (89 mg, 0.077 mmol) was added and the mixture was heated to reflux. After 18 h, the mixture was allowed to cool to RT, and saturated aqueous NH<sub>4</sub>Cl (50 mL) and Et<sub>2</sub>O (50 mL) was added and the layers were separated. The aqueous layer was extracted with Et<sub>2</sub>O (2 × 50 mL) and the combined organic layers were dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated. The residue was purified by column chromatography (SiO<sub>2</sub>, 1–3% ethyl acetate/hexanes) to afford **S8** as a clear oil (380 mg, 85%); R<sub>f</sub>: 0.56 (5% ethyl acetate/hexanes); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz)  $\delta$  2.67 (d,  $J$  = 8.0 Hz, 1H), 2.33 (m, 1H), 2.15 (m, 1H), 1.95 (m, 2H), 1.85 (m, 1H), 1.73 (m, 2H), 1.53 (m, 1H), 1.48 (m, 3H), 1.40 (s, 3H), 0.90 (s, 3H), 0.87 (s, 3H), 0.05 (s, 9H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$  138.9, 136.2, 125.5, 52.7, 48.4, 41.7, 39.4, 37.3, 34.0, 31.3, 27.5, 26.2, 25.7, 22.8, 22.1, 0.4; IR (thin film) 2953, 2228, 1450, 1248, 851 cm<sup>-1</sup>; HRMS (ESI/TOF) calculated for C<sub>18</sub>H<sub>31</sub>SiN (M+Na)<sup>+</sup> 312.2123, observed 312.2130; [ $\alpha$ ]<sub>D</sub><sup>24</sup> +42.6°, [ $\alpha$ ]<sub>577</sub><sup>24</sup> +41.4°, [ $\alpha$ ]<sub>546</sub><sup>24</sup> +45.5°, [ $\alpha$ ]<sub>435</sub><sup>24</sup> +98.2°, [ $\alpha$ ]<sub>405</sub><sup>24</sup> +122.4°, ( $c$  = 1.0, CH<sub>2</sub>Cl<sub>2</sub>).

<sup>19</sup> Y. Mi, J. V. Schreiber, E. J. Corey, *J. Am. Chem. Soc.* **2002**, *124*, 11290.



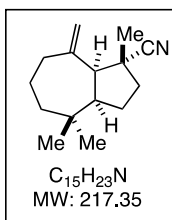
**(1*S*,3*aR*,8*aS*)-1,4,4-Trimethyl-8-methylenedecahydroazulene-1-carbonitrile**

**(9):** To a solution of **S8** (40 mg, 0.04 mmol) in MeOH (0.40 mL) was added AcCl (19  $\mu$ L, 0.082 mmol) and the solution was heated to 50 °C in a sealed vial. After 36 h, the solution was allowed to cool to RT and was concentrated. The residue was purified by column chromatography (SiO<sub>2</sub>, 2% ethyl acetate/hexanes) to afford **9** as a clear oil (25 mg, 84%):  $R_f$ : 0.53 (5% ethyl acetate/hexanes); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz)  $\delta$  4.93 (s, 1H), 4.82 (s, 1H), 2.63 (d,  $J$  = 9.4 Hz, 1H), 2.39 (dd,  $J$  = 5.5, 12.7 Hz, 1H), 2.28 (dq,  $J$  = 2.5, 6.7 Hz, 1H), 2.15 (apt t,  $J$  = 12.6 Hz, 1H), 2.01 (m, 1H), 1.89 (m, 1H), 1.84 (m, 1H), 1.76 (m, 1H), 1.65 (m, 2H), 1.49 (s, 3H), 1.40 (m, 1H), 1.32 (td,  $J$  = 3.9, 14.2 Hz, 1H), 0.96 (s, 3H), 0.95 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$  151.7, 125.2, 115.2, 59.1, 53.0, 45.1, 39.7, 38.7, 36.4, 36.1, 28.0, 27.7, 27.4, 26.6; IR (thin film) 2854, 2229, 1463, 1378 cm<sup>-1</sup>; HRMS (ESI/TOF) calculated for C<sub>15</sub>H<sub>23</sub>N (M+Na)<sup>+</sup> 240.1728, observed 240.1731;  $[\alpha]_D^{24}$  -3.9,  $[\alpha]_{577}^{24}$  -7.6,  $[\alpha]_{546}^{24}$  -20.3,  $[\alpha]_{435}^{24}$  -6.5°,  $[\alpha]_{405}^{24}$  -17.6°, ( $c$  = 0.1, CH<sub>2</sub>Cl<sub>2</sub>).



**(1*R*,3*aS*,*Z*)-1,4,4-Trimethyl-8-((trimethylsilyl)methyl)-1,2,3,3*a*,4,5,6,7-octahydroazulene-1-carbonitrile (S9):**

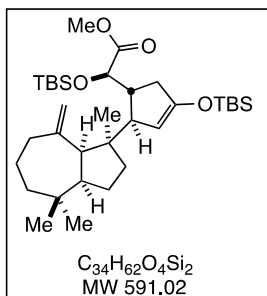
Compound **S7** (931 mg, 4.25 mmol) was subjected to identical procedure used for the synthesis of **S8** to afford **S9** as a clear oil (980 mg, 80%);  $R_f$ : 0.35 (5% ethyl acetate/hexanes); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz)  $\delta$  2.67 (m, 1H), 2.03 (m, 4H), 1.83 (m, 3H), 1.43 (m, 5H), 1.36 (s, 3H), 0.87 (s, 3H), 0.76 (s, 3H), 0.12 (s, 9H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$  137.8, 134.9, 125.8, 53.3, 47.7, 40.3, 37.1, 33.7, 31.3, 28.0, 26.9, 24.2, 21.8, 20.9, 0.2; IR (thin film) 2951, 2229, 1725, 1453, 1247 cm<sup>-1</sup>; HRMS (ESI/TOF) calculated for C<sub>18</sub>H<sub>31</sub>NSi (M+Na)<sup>+</sup> 312.2123, observed 312.2126;  $[\alpha]_D^{24}$  -9.5°,  $[\alpha]_{577}^{24}$  -8.7°,  $[\alpha]_{546}^{24}$  -9.4°,  $[\alpha]_{435}^{24}$  -14.5°,  $[\alpha]_{405}^{24}$  -18.6°, ( $c$  = 1.0, CH<sub>2</sub>Cl<sub>2</sub>).



**(1*R*,3*aR*,8*aS*)-1,4,4-Trimethyl-8-methylenedecahydroazulene-1-carbonitrile**

**(8)** A round-bottom flask was charged with **S9** (980 mg, 3.4 mmol) and placed in an ice bath. TFA (9 mL) was slowly added as a yellow solution was formed. The solution was allowed to warm to RT. After 2 h, the solution was concentrated and the residue was passed through a short plug of silica gel (20% ethyl acetate/hexanes). The resulting residue was purified by column chromatography (1% ethyl acetate/hexanes) to afford **8** (550 mg, 74%) as a clear oil:  $R_f$ : 0.33 (5% ethyl acetate/hexanes); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz)  $\delta$  4.95 (s, 1H), 4.73 (s, 1H), 2.99 (d,  $J$  = 7.5 Hz, 1H), 2.53 (m, 1H), 2.33

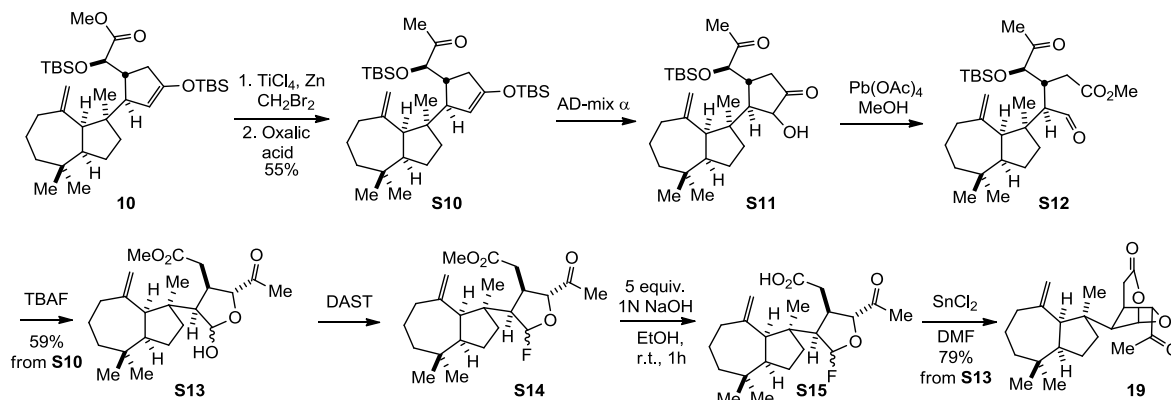
(dd,  $J = 5.6, 12.7$  Hz, 1H), 2.22 (m, 1H), 1.98 (m, 1H), 1.86 (m, 1H), 1.77 (m, 1H), 1.66 (m, 3H), 1.44 (m, 1H), 1.26 (m, 1H), 1.24 (s, 3H), 1.01 (s, 3H), 0.94 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  149.2, 127.3, 117.3, 57.4, 52.3, 43.3, 37.6, 37.5, 36.6, 36.2, 33.6, 28.6, 25.9, 24.6, 23.0; IR (thin film) 2954, 2229, 1630, 1453, 897  $\text{cm}^{-1}$ ; HRMS (ESI/TOF) calculated for  $\text{C}_{15}\text{H}_{23}\text{N}$  ( $\text{M}+\text{Na}$ ) $^+$  240.1728, observed 240.1728;  $[\alpha]_{\text{D}}^{24} -3.2^\circ$ ,  $[\alpha]_{577}^{24} -2.6^\circ$ ,  $[\alpha]_{546}^{24} -2.4^\circ$ ,  $[\alpha]_{435}^{24} -1.11^\circ$ ,  $[\alpha]_{405}^{24} +1.6^\circ$ , ( $c = 1.0, \text{CH}_2\text{Cl}_2$ ).



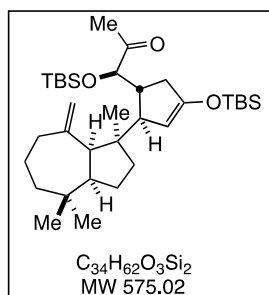
**(R)-Methyl 2-(tert-butyldimethylsilyloxy)-2-((1R,2S)-4-(tert-butyldimethylsilyloxy)-2-((1R,3aR,8aS)-1,4,4-trimethyl-8-methylenedecahydroazulen-1-yl)cyclopent-3-enyl)acetate (10):**

A solution of LiDDB (0.4 M in THF, 7.0 ml, 2.8 mmol) was added to a three-necked round-bottom flask with a glass-stir bar, and the dark green solution was cooled to  $-78^\circ\text{C}$  and maintained within  $3^\circ\text{C}$  of that temperature (by internal monitoring of the reaction temperature). Nitrile **8** (305 mg, 1.40 mmol) in THF (300  $\mu\text{L}$ ) was added to the solution slowly as a dark red solution was formed. After 30 sec.,  $\text{TMSCH}_2\text{CuLiCN}$  (0.5 M in 1:1 THF-pentane, 2.8 mL, 1.4 mmol) was added slowly. After 5 min, a solution of the enone **2** (200 mg, 0.70 mmol)<sup>12</sup> TBSCl (525 mg, 3.5 mmol) and THF (300  $\mu\text{L}$ ) was added as a bright yellow/orange solution was formed. After 30 min, complete conversion of starting material to product was observed by TLC and 10:1 saturated aqueous  $\text{NH}_4\text{Cl}$  to  $\text{NH}_4\text{OH}$  was added (30 mL) and the mixture was allowed to warm to RT.  $\text{Et}_2\text{O}$  was added (50 mL) and the layers were separated. The aqueous layer was extracted with  $\text{Et}_2\text{O}$  (2 x 50 mL) and the combined organic layers were dried ( $\text{Na}_2\text{SO}_4$ ) and concentrated. The residue was purified by column chromatography ( $\text{SiO}_2$ , 2% ethyl acetate/hexanes) to afford **10** as a clear oil (290 mg, 70%);  $R_f$ : 0.52 (5% ethyl acetate/hexanes);  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 500 MHz)  $\delta$  4.94 (d,  $J = 2.2$  Hz, 1H), 4.91 (s, 1H), 4.77 (s, 1H), 4.22 (d,  $J = 2.2$  Hz, 1H), 3.37 (s, 3H), 2.89 (bs, 1H), 2.73 (m, 1H), 2.46 (m, 4H), 2.32 (m, 1H), 1.76 (m, 5H), 1.6 (m, 1H), 1.4 (m, 1H), 1.16 (m, 1H), 1.09 (s, 3H), 1.03 (s, 9H), 0.99 (s, 9H), 0.97 (m, 4H), 0.90 (s, 3H), 0.19 (s, 6H), 0.12 (s, 3H), 0.06 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  173.1, 154.1, 154.0, 115.4, 105.0, 76.5, 60.2, 52.7, 51.5, 51.2, 50.7, 42.4, 37.7, 37.6, 36.9, 36.7, 36.5, 30.3, 26.3, 26.2, 26.1, 24.8, 23.8, 18.6, 18.4,  $-4.1$ ,  $-4.3$ ,  $-4.7$ ,  $-4.8$ ; IR (thin film) 2952, 1756, 1653, 1252, 839  $\text{cm}^{-1}$ ; HRMS (ESI/TOF) calculated for  $\text{C}_{34}\text{H}_{62}\text{O}_4\text{Si}_2$  ( $\text{M}+\text{Na}$ ) $^+$  613.4084, observed 613.4085;  $[\alpha]_{\text{D}}^{24} -3.9$ ,  $[\alpha]_{577}^{24} -4.9$ ,  $[\alpha]_{546}^{24} -6.3$ ,  $[\alpha]_{435}^{24} -9.1^\circ$ ,  $[\alpha]_{405}^{24} -7.5^\circ$ , ( $c = 0.5, \text{CH}_2\text{Cl}_2$ ).

The relative stereochemistry of **10** was unambiguously determined by conversion to crystalline **19**, whose structure was confirmed by single-crystal X-ray diffraction. This sequence is outlined in Scheme S2 and was completed in analogous fashion to that employed in our recent synthesis of aplyviolene.<sup>20</sup>



Scheme S2: Conversion of **10** to **19**

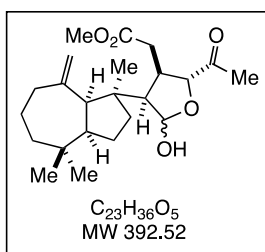


**(R)-1-(tert-Butyldimethylsilyloxy)-1-((1R,2S)-4-(tert-butylidimethylsilyloxy)-2-((1R,3aR,8aS)-1,4,4-trimethyl-8-methylenedecahydroazulen-1-yl)cyclopent-3-enyl)propan-2-one (S10)**

A stirring solution of  $TiCl_4$  (0.23 mL, 2.0 mmol) in  $CH_2Cl_2$  (6 mL) was cooled to 0 °C and THF (0.6 mL) was added dropwise to generate a yellow solution. After 5 min, TMEDA (2.0 mL, 12 mmol) was added dropwise to form a red solution. After 15 min, the solution was allowed to warm to RT and Zn (270 mg, 4.2 mmol) and  $PbCl_2$  (66 mg, 0.24 mmol) was added. The initial mixture became a blue solution over this time. After 15 min, a solution of **10** (180 mg, 0.30 mmol) and  $CH_2Br_2$  (0.14 mL, 2.0 mmol) in  $CH_2Cl_2$  (0.5 mL) was added. The solution became a dark mixture as it was refluxed for 1.5 h. The reaction mixture was cooled to RT and saturated aqueous  $K_2CO_3$  (0.5 mL) was added very slowly. The dark colored heterogenous mixture was filtered through a pad of silica with  $Et_2O$  and the eluent was concentrated *in vacuo*. The residue was passed through a second plug of silica with 5% ethyl acetate/hexanes to afford the enol ether as a clear oil that could be used without further purification. To a solution of enol ether (0.3 mmol) in *i*PrOH (1 mL) and  $H_2O$  (0.15 mL) at 0 °C was added oxalic acid (41 mg, 0.37 mmol) and the solution was allowed to warm to RT. After 2 h, saturated aqueous  $NaHCO_3$  (10 mL) and  $Et_2O$  (10 mL) were

<sup>20</sup> M. J. Schnermann, L. E. Overman, *J. Am. Chem. Soc.* **2011**, *133*, 16425.

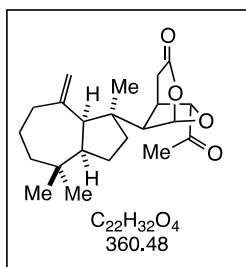
added to the solution. The layers were separated and the aqueous layer was washed with additional Et<sub>2</sub>O (10 mL). The organic phases were combined, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated. The residue was purified by column chromatography (SiO<sub>2</sub>, 1–2% ethyl acetate/hexanes) to afford ketone **S10** (95 mg, 55%) as a colorless oil: R<sub>f</sub>: 0.52 (5% ethyl acetate/hexanes); <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 500 MHz) δ 4.95 (apt s, 2H), 4.77 (s, 1H), 3.87 (d, *J* = 8.1 Hz, 1H), 2.75 (bs, 1H), 2.54 (qt, *J* = 7.9, 2.3 Hz, 1H), 2.46 (d, *J* = 7.7 Hz, 1H), 2.35 (m, 3H), 2.16 (apt t, *J* = 8.4 Hz, 1H), 2.02 (s, 3H), 1.80 (m, 5H), 1.58 (m, 2H), 1.42 (m, 1H), 1.07 (m, 4H), 0.97 (m, 24H), 0.20 (m, 6H), 0.02 (s, 3H) –0.02 (s, 3H); <sup>13</sup>C NMR (C<sub>6</sub>D<sub>6</sub>, 125 MHz) δ 209.1, 154.1, 153.9, 115.5, 105.0, 82.8, 59.8, 52.9, 51.4, 50.9, 41.4, 37.6, 37.0, 36.95, 36.7, 36.5, 34.6, 30.2, 26.2, 26.1, 25.2, 24.6, 23.8, 18.3, –4.3, –4.4, –4.7, –4.8 □ IR (thin film) 2954, 2931, 1714, 1652, 1253 cm<sup>-1</sup>; HRMS (ESI/TOF) calculated for C<sub>13</sub>H<sub>22</sub>O-NH<sub>4</sub> (M+Na)<sup>+</sup> C<sub>34</sub>H<sub>62</sub>O<sub>3</sub>Si<sub>2</sub> 597.4135, observed 597.4137; [α]<sub>D</sub><sup>24</sup> +16.5°, [α]<sub>577</sub><sup>24</sup> +16.9°, [α]<sub>546</sub><sup>24</sup> +19.7°, [α]<sub>435</sub><sup>24</sup> +47.4°, [α]<sub>405</sub><sup>24</sup> +63.7°, (*c* = 1.0, CH<sub>2</sub>Cl<sub>2</sub>).



**Methyl 2-((2R,3R,4R)-2-acetyl-5-hydroxy-4-((1S,3aR,8aS)-1,4,4-trimethyl-8-methylenedecahydroazulen-1-yl)tetrahydrofuran-3-yl)acetate (**S13**):** To a mixture of **S10** (35 mg, 0.060 mmol) in *t*BuOH (0.3 mL) and H<sub>2</sub>O (0.3 mL) at 0 °C was added commercial AD-mix α (85 mg), CH<sub>3</sub>SO<sub>2</sub>NH<sub>3</sub> (12 mg, 0.12 mmol) K<sub>2</sub>OsO<sub>4</sub>•(H<sub>2</sub>O)<sub>2</sub> (0.5 mg, 0.0006 mmol), and DHQ-PHAL (2.3 mg, 0.003 mmol). The mixture was

maintained at 0 °C and was stirred for 18 h and solid sodium sulfite (5 mg) was added and the mixture was stirred for an additional 5 min. The mixture was diluted with H<sub>2</sub>O (2 mL) and Et<sub>2</sub>O (2 mL). The layers were separated and the aqueous layer was washed with additional Et<sub>2</sub>O (2 mL). The organic phases were combined, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated. Rapid chromatography of the residue (SiO<sub>2</sub>, 1–2% ethyl acetate/hexanes) gave **S11** as a ~3:1 mixture of diastereomeric alcohols that could be used with further purification. To a solution of **S11** in MeOH (0.4 mL) and benzene (0.4 mL) at 0 °C was added Pb(OAc)<sub>4</sub> (31 mg, 0.070 mmol). After 10 min, saturated aqueous NaHCO<sub>3</sub> (0.3 mL) was added to the yellow solution and a brown precipitate was formed. After being stirred for 5 min, the mixture was diluted with Et<sub>2</sub>O (2 mL) and passed through a glass pipette contained Na<sub>2</sub>SO<sub>4</sub> on top of a short layer (~1 cm) of SiO<sub>2</sub> using Et<sub>2</sub>O as an eluent. The resulting clear solution was concentrated to yield **S12** that was used without further purification. To a solution of aldehyde **S12** in THF (0.6 mL) at 0 °C was added 1M TBAF in THF (0.12 mL, 0.060 mmol). The solution was maintained at 0 °C for 30 min and then SiO<sub>2</sub> (~200 mg) was added. The mixture was stirred for 30 min, loaded onto an SiO<sub>2</sub> column, and eluted with

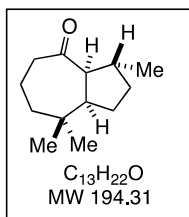
20–30% ethyl acetate/hexanes to afford the title compound **S13** (14 mg, 59%) as a clear oil:  $R_f$ : 0.25 (5% ethyl acetate/hexanes);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  5.54 (s, 1H), 4.98 (s, 1H), 4.69 (s, 1H), 4.07 (d,  $J = 10.3$  Hz, 1H), 3.69 (s, 3H), 3.03 (m, 1H) 2.66 (m, 4H), 1.82 (m, 2H), 1.54 (m, 3 H), 1.33 (m, 1H) 1.21 (m, 2H), 1.03 (s, 3H), 0.97 (s, 3H), 0.86 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  211.8, 172.6, 153.2, 117.0, 103.4, 89.3, 61.9, 55.5, 52.0, 49.3, 48.9, 39.6, 37.2, 36.6, 36.3, 35.4, 34.5, 33.5, 29.8, 25.9, 25.7, 25.2, 23.8; HRMS (ESI/TOF) calculated for  $\text{C}_{23}\text{H}_{36}\text{O}_5$  ( $\text{M}+\text{Na}$ ) $^+$  415.246, observed 415.2458.



**(1S,5R,6R,8R)-6-Acetyl-8-((1S,3aR,8aS)-1,4,4-trimethyl-8-methylenedecahydroazulen-1-yl)-2,7-dioxabicyclo[3.2.1]octan-3-one**

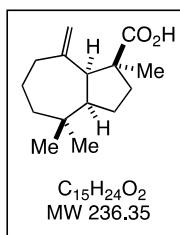
**(19):** To a solution of **S13** (3 mg, 0.007 mmol) in  $\text{CH}_2\text{Cl}_2$  (100  $\mu\text{L}$ ) at  $-78$   $^\circ\text{C}$  was added diethylaminosulfur trifluoride (2  $\mu\text{L}$ , 0.02 mmol). After 10 min, saturated aqueous  $\text{NaHCO}_3$  (1 mL) and  $\text{CH}_2\text{Cl}_2$  (1 mL) were added and the layers were separated. The aqueous layer was washed with additional  $\text{CH}_2\text{Cl}_2$  ( $2 \times 2$  mL). The organic phases were combined, dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated to yield crude **S14** as a clear oil. Crude **S14** was dissolved in EtOH (200  $\mu\text{L}$ ) and 1 N NaOH was added (21  $\mu\text{L}$ , 0.021 mmol). The mixture was stirred for 1 h at RT and 1 N HCl (4 mL) and  $\text{CH}_2\text{Cl}_2$  (2 mL) was added. The layers were separated and the aqueous layer was washed with additional  $\text{CH}_2\text{Cl}_2$  ( $5 \times 2$  mL). The organic phases were combined, dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated to yield crude **S15**, which was used without further purification. Crude **S15** was dissolved in DMF (300  $\mu\text{L}$ ) and  $\text{SnCl}_2$  (3 mg, 0.014 mmol) was added. The mixture was stirred at RT for 18 h and saturated aqueous  $\text{NaHCO}_3$  (2 mL) and  $\text{CH}_2\text{Cl}_2$  (2 mL) were added. The layers were separated and the aqueous layer was washed with additional  $\text{CH}_2\text{Cl}_2$  ( $2 \times 2$  mL). The organic phases were combined, dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated. The residue was purified by column chromatography ( $\text{SiO}_2$ , 1–2% ethyl acetate/hexanes) to give ketone **19** (2.0 mg, 79%) as a white solid:  $R_f$ : 0.14 (20% ethyl acetate/hexanes);  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 500 MHz)  $\delta$  5.58 (d,  $J = 2.4$  Hz, 1H), 4.56 (s, 1H), 4.29 (s, 1H), 3.53 (s, 1H), 2.61 (dd,  $J = 19.4, 5.6$  Hz, 1H), 2.47 (m, 1H), 2.18 (d,  $J = 8.0$  Hz, 1H), 2.13 (d,  $J = 19.4$  Hz, 1H), 2.06 (m, 1H), 1.90 (dd,  $J = 5.2, 5.0$  Hz, 1H), 1.69 (s, 3H), 1.58 (m, 1H), 1.55 (m, 2H), 1.33 (m, 4H), 1.16 (m, 4H), 0.89 (s, 3H), 0.88 (s, 3H), 0.79 (s, 3H);  $^{13}\text{C}$ -NMR ( $\text{C}_6\text{D}_6$ , 125 MHz)  $\delta$  206.6, 167.3, 153.5, 115.8, 100.9, 90.1, 61.9, 50.0, 47.8, 46.3, 37.2, 37.0, 36.7, 36.5, 36.1, 35.9, 34.3, 29.1, 26.5, 26.0, 25.95, 24.4; IR (thin film) 2931, 1750, 1458, 938  $\text{cm}^{-1}$ ; HRMS (ESI/TOF) calculated for  $\text{C}_{22}\text{H}_{32}\text{O}_4$  ( $\text{M}+\text{Na}$ ) $^+$  383.2198, observed 383.2202;  $[\alpha]_{\text{D}}^{24} -14.9^\circ$ ,  $[\alpha]_{577}^{24} -15.7^\circ$ ,  $[\alpha]_{546}^{24} -15.6^\circ$ ,  $[\alpha]_{435}^{24} -27.0^\circ$ ,  $[\alpha]_{405}^{24} -10.8^\circ$ , ( $c = 0.1$ ,  $\text{CH}_2\text{Cl}_2$ ). X-ray quality crystals

(m.p. 122–123 °C) were obtained via vapor diffusion by dissolving **19** in ethyl acetate and exposing to hexanes vapor.



**(3R,3aS,8aR)-3,8,8-Trimethyloctahydroazulen-4(5H)-one (11):** A solution of LiDBB (0.4 M in THF, 0.20 mmol, 0.50 mL) was cooled to  $-78$  °C and a solution of **8** (20 mg, 0.090 mmol) in THF (0.2 mL) was added slowly over 30 sec as the solution changed from dark green to red. Within 30 sec of the completion of addition, MeOH (0.1 mL) was added. The solution immediately

became clear. The solution was allowed to warm to RT and brine was added (2 mL). The solution was extracted with pentane ( $3 \times 1$  mL). The combined organic extracts were dried ( $\text{Na}_2\text{SO}_4$ ) and concentrated. The residue was purified by column chromatography ( $\text{SiO}_2$ , 100% hexanes) to afford the exomethylene product, (1R,3aR,8aS)-1,4,4-trimethyl-8-methylenedecahydroazulene, contaminated with 4,4'-di-*t*-butylbiphenyl.<sup>21</sup> This compound was converted to the more readily purified ketone **11**, which also exhibits a proton NMR more amenable to NOE analysis. The crude residue was dissolved in  $\text{CH}_2\text{Cl}_2$  (1 mL) and MeOH (1 mL) and cooled to  $-78$  °C.  $\text{O}_3$  was bubbled through the solution until a light blue solution was observed for 30 sec and then  $\text{O}_2$  was bubbled through to remove the  $\text{O}_3$ . Dimethyl sulfide (200  $\mu\text{L}$ ) was added to the solution. The solution was allowed to slowly warm to RT, stirred for 18 h, and then concentrated. The residue was purified by column chromatography ( $\text{SiO}_2$ , 0–10% ethyl acetate/hexanes) to afford **11** (11.0 mg, 63% over two steps) as a clear oil. The relative stereochemistry was determined by NOE as shown on page 25.  $R_f$ : 0.19 (20% ethyl acetate/hexanes);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  2.52 (dt,  $J = 3.0, 10.6$  Hz, 1H), 2.38 (m, 1H), 2.36 (m, 1H), 2.19 (m, 1H), 2.11 (m, 1H), 1.99 (m, 1H), 1.84 (m, 1H), 1.74 (m, 1H), 1.66 (m, 1H), 1.47 (m, 1H), 1.22 (m, 1H), 1.01 (d,  $J = 6.5$  Hz, 3H), 0.89 (s, 3H), 0.83 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , MHz)  $\delta$  214.6, 63.2, 51.3, 43.2, 40.2, 38.7, 36.5, 35.3, 28.9, 28.8, 28.1, 22.2, 20.2; IR (thin film) 2952, 1695, 1455  $\text{cm}^{-1}$ ; HRMS (GC/TOF) calculated for  $\text{C}_{13}\text{H}_{22}\text{ONH}_4$  ( $\text{M}+\text{NH}_4$ )<sup>+</sup> 212.2014, observed 212.2015;  $[\alpha]_{\text{D}}^{24} +22.2^\circ$ ,  $[\alpha]_{577}^{24} +16.8^\circ$ ,  $[\alpha]_{546}^{24} +23.6^\circ$ ,  $[\alpha]_{435}^{24} +55.2^\circ$ ,  $[\alpha]_{405}^{24} +85.6^\circ$ , ( $c = 0.2$ ,  $\text{CH}_2\text{Cl}_2$ ).

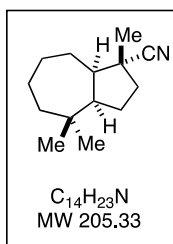


**(1S,3aR,8aS)-1,4,4-Trimethyl-8-methylenedecahydroazulene-1-carboxylic acid (12):** A solution of LiDBB (0.4 M in THF, 0.20 mmol, 0.50 mL) was cooled to  $-78$  °C and a solution of **8** (20 mg, 0.090 mmol) in THF (0.2 mL) was added slowly as the solution changed from dark green to dark red. Within 30 sec of the

<sup>21</sup> This compound was also formed from **9** by an identical procedure.



completion of addition, a balloon of dry CO<sub>2</sub> was placed on the flask and bubbled through the solution. The solution immediately became clear. The solution was allowed to warm to RT and 1 N HCl was added (2 mL). The solution was extracted with CH<sub>2</sub>Cl<sub>2</sub> (5 × 1 mL). The combined organic extracts were dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated. The residue purified by column chromatography (SiO<sub>2</sub>, 0–20% ethyl acetate/hexanes) to afford **12** (13 mg, 61%), whose relative configuration was determined by 1H NMR nOe as summarized on page 25. R<sub>f</sub>: 0.19 (20% ethyl acetate/hexanes); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) δ 4.73 (s, 1H), 4.68 (s, 1H), 2.68 (d, *J* = 7.8 Hz, 1H), 2.41 (m, 1H), 2.21 (m, 2H), 1.90 (m, 3H), 1.65 (m, 2H), 1.48 (m, 1H), 1.43 (s, 3H), 1.42 (m, 1H), 1.20 (m, 1H), 0.97 (s, 3H), 0.92 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz) δ 181.4, 152.7, 114.9, 60.4, 57.4, 51.1, 37.6, 36.1, 36.0, 34.0, 33.7, 28.6, 26.3, 26.2, 25.4; IR (thin film) 2921, 1699, 1458, 893 cm<sup>-1</sup>; HRMS (ESI/TOF) calculated for C<sub>15</sub>H<sub>24</sub>O<sub>2</sub> (M-H)<sup>-</sup> 235.1698, observed 235.1695; [α]<sub>D</sub><sup>24</sup> +3.5°, [α]<sub>577</sub><sup>24</sup> +5.5°, [α]<sub>546</sub><sup>24</sup> +3.5°, [α]<sub>435</sub><sup>24</sup> +9.5°, [α]<sub>405</sub><sup>24</sup> +6.7°, (*c* = 0.2, CH<sub>2</sub>Cl<sub>2</sub>). The identical reaction was performed with **9** (12 mg, 0.055 mmol) to afford **12** (7.5 mg, 58%).

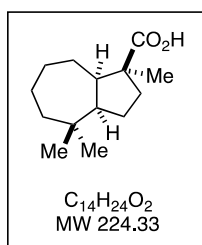


**(1S,3aR,8aR)-1,4,4-Trimethyldecahydroazulene-1-carbonitrile (13):** A

solution of **S7** (45 mg, 0.22 mmol) in EtOH (2 mL) was cooled to 0 °C and CeCl<sub>3</sub>·7H<sub>2</sub>O (9.0 mg, 0.022 mmol) and NaBH<sub>4</sub> (44 mg, 1.1 mmol) were added. The mixture was allowed to warm to RT and stirred for 18 h. A solution of 1 N HCl (3 mL) was added to the mixture and the mixture was extracted with Et<sub>2</sub>O (3 × 3 mL). The combined organic layers were dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated to yield the crude secondary alcohol as a clear oil which was used without further purification. The secondary alcohol was dissolved in THF (2 mL), cooled to 0°C, and NaH (18 mg, 0.44 mmol, 60% as a suspension in mineral oil) was added. The mixture was then stirred for 5 min and CS<sub>2</sub> (40 μL, 0.66 mmol) and MeI (27 μL, 0.44) were added sequential. The mixture was allowed to warm to RT and stirred for 18 h. A solution of saturated aqueous NH<sub>4</sub>Cl (3 mL) was added and the mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 × 5 mL). The combined organic extracts were dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated. The residue was purified by column chromatography (0–10% ethyl acetate/hexanes, SiO<sub>2</sub>) to afford the xanthate ester **S16** as a waxy solid (25 mg, 37% from **S7**): R<sub>f</sub>: 0.55 (20% ethyl acetate/hexanes); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) δ 5.87 (d, *J* = 5.8 Hz, 1H), 2.73 (m, 5H), 2.37 (d, *J* = 4.9 Hz, 1H), 2.20 (m, 1H), 1.88 (m, 3H), 1.70 (m, 3H), 1.45 (m, 1H), 1.36 (s, 3H), 1.28 (m, 1H), 1.13 (s, 3H), 0.97 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz) δ 214.6, 127.3, 82.4, 53.9, 53.8, 42.5, 37.3, 34.8, 34.2, 31.0, 29.1, 28.1, 25.7, 22.1, 19.6, 19.4; IR (thin film) 2944, 2229, 1455, 1201 cm<sup>-1</sup>; HRMS (ESI/TOF)

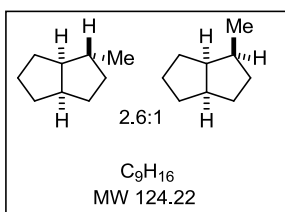
calculated for  $C_{16}H_{25}OS_2NH_4$  ( $M+Na$ )<sup>+</sup> 334.1275, observed 334.1273;  $[\alpha]_D^{24}$   $-7.7^\circ$ ,  $[\alpha]_{577}^{24}$   $-7.0^\circ$ ,  $[\alpha]_{546}^{24}$   $-7.5^\circ$ ,  $[\alpha]_{435}^{24}$   $+4.2^\circ$ ,  $[\alpha]_{405}^{24}$   $+27.2^\circ$ , ( $c = 1$ ,  $CH_2Cl_2$ ).

To a solution of **S16** (26 mg, 0.08 mmol) in toluene (1 mL) was added  $Bu_3SnH$  (36  $\mu$ L, 0.125 mmol) and AIBN (0.7 mg, 0.004 mmol) and the solution was heated to 100 °C for 18 h. The solution was cooled to rt and concentrated. The residue was purified by column chromatography (0–10% ethyl acetate/hexanes,  $SiO_2$ ) to yield **13** (13 mg, 81%) as a clear oil:  $R_f$ : 0.52 (10% ethyl acetate/hexanes);  $^1H$  NMR ( $CDCl_6$ , 500 MHz)  $\delta$  2.34 (apt t,  $J = 6.6$  Hz, 1H), 2.17 (m, 1H), 2.00 (m, 1H), 1.64 (m, 8 H), 1.22 (m, 5H), 0.89 (s, 3H), 0.88 (s, 3H);  $^{13}C$  NMR ( $CDCl_3$ , 125 MHz)  $\delta$  126.9, 52.7, 52.1, 40.0, 41.4, 37.7, 35.8, 32.2, 28.1, 26.2, 25.9, 25.5, 25.2, 20.3; IR (thin film) 2953, 2230, 1457  $cm^{-1}$ ; HRMS (ESI/TOF) calculated for  $C_{14}H_{23}NNa$  ( $M+Na$ )<sup>+</sup> 228.1728, observed 228.1724;  $[\alpha]_D^{24}$   $-9.5^\circ$ ,  $[\alpha]_{577}^{24}$   $-11.2^\circ$ ,  $[\alpha]_{546}^{24}$   $-11.7^\circ$ ,  $[\alpha]_{435}^{24}$   $-19.4^\circ$ ,  $[\alpha]_{405}^{24}$   $-20.5^\circ$ , ( $c = 0.2$ ,  $CH_2Cl_2$ ).



**(1S,3aR,8aR)-1,4,4-Trimethyldecahydroazulene-1-carbonitrile (14):**

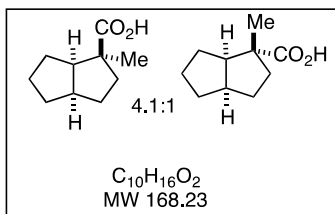
Compound **13** (15 mg, 0.070 mmol) was subjected to identical procedure used for the synthesis of **12** to yield **14** (10 mg, 75%) as a clear oil and 8.0:1 mixture of diastereomers. The indicated configuration of the major isomer was determined by NOE as shown on page 25:  $R_f$ : 0.41 (20% ethyl acetate/hexanes);  $^1H$  NMR ( $CDCl_6$ , 500 MHz, major isomer)  $\delta$  2.21 (m, 1H), 2.09 (m, 1H), 1.89 (m, 1H), 1.77 (m, 2H) 1.68 (m, 3H), 1.55 (m, 2H), 1.27 (s, 3H), 1.25 (m, 4H), 0.94 (s, 3H), 0.86 (s, 3H);  $^{13}C$  NMR ( $CDCl_3$ , 125 MHz, major isomer)  $\delta$  183.3, 54.7, 52.0, 38.7, 35.5, 34.3, 31.1, 28.1, 28.05, 27.1, 26.5, 26.1, 25.7, 24.7; IR (thin film) 2930, 1696, 1463, 1267  $cm^{-1}$ ; HRMS (ESI/TOF) calculated for  $C_{14}H_{23}O_2$  ( $M-H$ )<sup>-</sup> 223.1698, observed 223.1694;  $[\alpha]_D^{24}$   $-5.8^\circ$ ,  $[\alpha]_{577}^{24}$   $-5.8^\circ$ ,  $[\alpha]_{546}^{24}$   $-6.5^\circ$ ,  $[\alpha]_{435}^{24}$   $-9.5^\circ$ ,  $[\alpha]_{405}^{24}$   $-12.4^\circ$ , ( $c = 2.0$ ,  $CH_2Cl_2$ ).



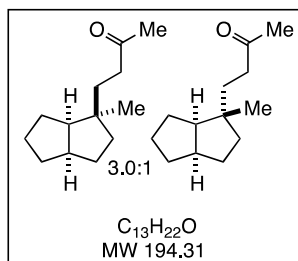
**1-Methyl-cis-octahydropentalene (16):** To a solution of LiDBB (0.4 M in THF, 2.2 mmol, 5.5 mL) at  $-78$  °C was added a solution of **15** (150 mg, 1.0 mmol). After 30 sec, MeOH (200  $\mu$ L) was added and the dark green solution became clear. The solution was allowed to warm to RT and brine was added (10 mL). The solution was extracted with pentane

( $2 \times 10$  mL). The combined organic extracts were dried ( $Na_2SO_4$ ) and carefully concentrated. The residue was purified by Kugelrohr distillation (50 °C, 10 torr.) to afford **16** (62%, 72 mg) as a clear oil containing a small amount of THF and as 2.6:1 mixture of diastereomers, whose relative configuration was determined by  $^1H$  NMR nOe as summarized on page 25:  $^1H$  NMR ( $CDCl_6$ , 500

MHz)  $\delta$  2.41 (m, 1H major isomer), 2.26 (m, 1H minor diastereomer), 1.87 (m), 1.70 (m), 1.40 (m), 1.3 (m), 1.2 (m), 0.97 (d,  $J = 6.7$  Hz, 3H major diastereomer), 0.94 (d,  $J = 6.7$  Hz, 3H minor diastereomer);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  51.8 (major), 47.8 (minor), 43.4 (major), 43.1 (minor), 42.4 (major), 37.8 (minor), 36.1 (major), 35.7 (minor), 34.1 (major), 33.7 (major), 33.1 (minor), 32.4 (major), 27.9 (minor), 27.8 (minor), 25.5 (major), 19.9 (major, C9), 15.5 (minor, C9); HRMS (GC/TOF) calculated for  $\text{C}_9\text{H}_{16}$  ( $\text{M}^+$ ) 124.1252, observed 124.1250.



**rac-1-methyl-cis-octahydropentalene (17):** A solution of LiDDB (0.4 M in THF, 2.2 mmol, 5.5 mL) was cooled to  $-78$  °C and a solution of **15** (150 mg, 1.0 mmol) in THF (0.5 mL) was added slowly. Within 30 sec of the completion of addition, a balloon of  $\text{CO}_2$  was placed on the flask and bubbled through the solution as the green solution became clear. The solution was allowed to warm to RT and 1 N HCl was added (2 mL). The solution was extracted with  $\text{CH}_2\text{Cl}_2$  ( $5 \times 5$  mL). The combined organic extracts were dried ( $\text{Na}_2\text{SO}_4$ ) and concentrated. The residue was purified by column chromatography ( $\text{SiO}_2$ , 0–20% ethyl acetate/hexanes) to afford **17** (105 mg, 63%) as a 4.1:1 mixture of diastereomers which was identical to material accessed in the accompanying communication<sup>22</sup> (although the diastereomeric ratio was different).



**rac-4-(1-methyl-cis-octahydropentalen-1-yl)butan-2-one (18):** A 1 M solution of  $\text{CuCN} \cdot 2\text{LiCl}$  was prepared according to the procedure of Knochel,<sup>23</sup> THF (0.5 mL) was added to a flask containing CuCN (45 mg, 0.5 mmol) and LiCl (42 mg, 1 mmol) and the mixture was stirred until homogenous. Separately, a solution of LiDDB (0.4 M in THF, 2.0 mmol, 5.0 mL) was added to a three-necked round bottom with a glass-stir bar and the dark-green solution was cooled to  $-78$  °C and maintained within 3 °C of that temperature by internal temperature monitoring of the reaction. The nitrile **15** (150 mg, 1.0 mmol) in THF (300  $\mu\text{L}$ ) was added to the solution slowly as a dark red solution was formed. After 30 sec., the 1.0 M  $\text{CuCN} \cdot 2\text{LiCl}$  (0.50 mL, 0.50 mmol) solution was added slowly, followed by neat TMSCl

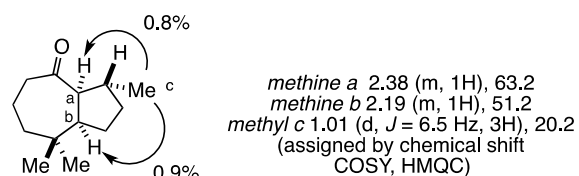
<sup>22</sup> See the following communication in this issue. This compound was prepared by hydrolysis of the corresponding tertiary nitrile and relative configuration of the nitrile was assigned by NOE analysis.

<sup>23</sup> M. Chang, P. Yeh, H. G. Chen, P. Knochel *Organic Syntheses* **1992**, 70, 195.

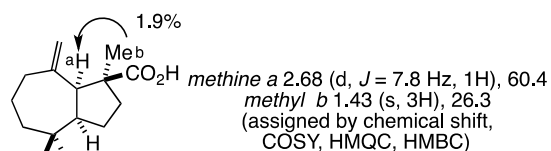
(160  $\mu$ L, 1.3 mmol). After 5 min, a solution of methyl vinyl ketone (20  $\mu$ L, 0.25 mmol) in THF (0.1 mL) was added. After 30 min, complete conversion of starting material was observed by TLC and 1N HCl was added (30 mL) and the mixture was allowed to warm to RT and stirred for 30 min. Et<sub>2</sub>O was added (50 mL) and the layers were separated. The aqueous layer was extracted with Et<sub>2</sub>O (50 mL) and the combined organic layers were dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated. The residue was purified by column chromatography (SiO<sub>2</sub>, 0–10% ethyl acetate/hexanes) to afford **18** as a clear oil (35 mg, 75%) as 3.0:1 mixture of diastereomers whose relative configuration was determined by <sup>1</sup>H NMR nOe as summarized on page 25. The minor diastereomer matched the material obtained in the following communication in this issue: R<sub>f</sub>: 0.39 (10% ethyl acetate/hexanes); <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 600 MHz)  $\delta$  2.42 (m), 2.07 (m, 2H, major), 2.00 (m, 2H, minor), 1.85 (m), 1.72 (s, 3H, major), 1.71 (s, 3H, minor), 1.60 (m), 1.49 (m, 1H, minor), 1.45 (m), 1.25 (m), 1.20 (m), 1.05 (m), 0.75 (s, 3H, minor), 0.73 (s, 3H, major); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 500 MHz, major diastereomer)  $\delta$  210.1, 54.4, 43.9, 41.7, 40.5, 36.8, 35.4, 32.3, 31.4, 29.9, 29.0, 27.7, 25.4; HRMS (GC/TOF) calculated for C<sub>13</sub>H<sub>22</sub>O<sub>4</sub> (M+NH<sub>4</sub>) 212.2014, observed 212.2009.

## Stereochemical Assignments<sup>24</sup>

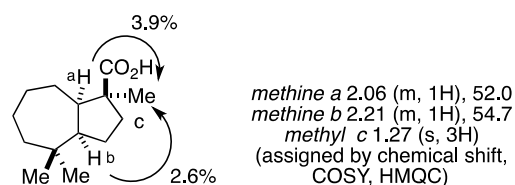
**11** assigned by 1D-NOE (key signals shown)



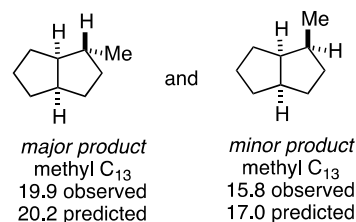
**12** assigned by 1D-NOE (key signal shown). The relative configuration was further confirmed by hydrolysis of nitrile **9** (10% KOH in ethylene glycol, 160 °C, 8 h) to provide, in unoptimized fashion, a mixture containing **9** and **12**.



**14** assigned by 1D-NOE (key signals shown)

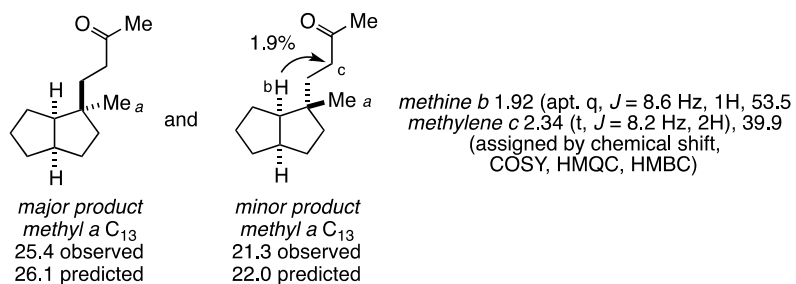


**16** assigned by the C<sub>13</sub>-shift of the tertiary methyl. The expected shielding effects were confirmed by DFT calculations at B3-LYP 6-31G\* level using Spartan<sup>25</sup> (20.2 predicted vs. 19.9 observed for the major diastereomer and 17.0 predicted vs. 15.8 observed for the minor diastereomer).



**18 (major and minor)**

assigned by 1D-nOe of the minor diastereomer (see right)<sup>26</sup> and the shift of the quaternary methyl. The expected shielding effects



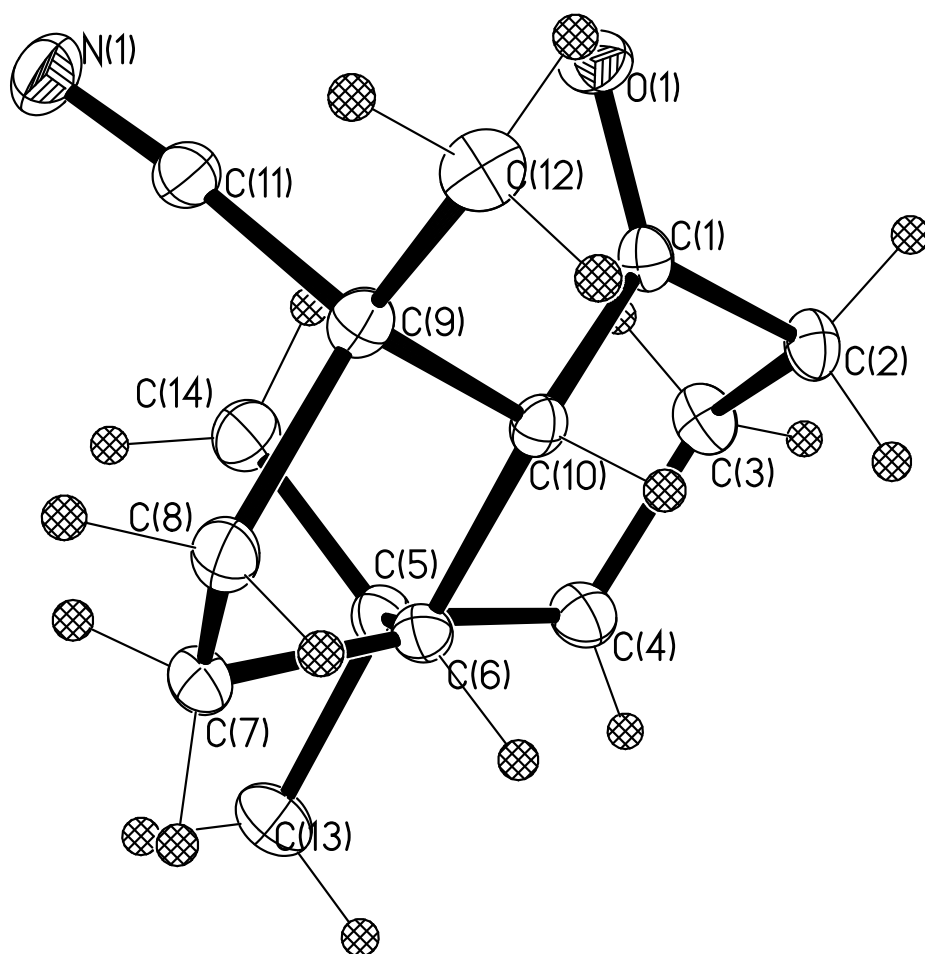
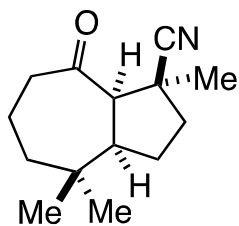
were confirmed by DFT calculations at B3-LYP 6-31G\* level using Spartan (26.1 predicted vs. 25.4 observed for the major diastereomer and 20.2 predicted vs. 21.3 observed for the minor diastereomer).

<sup>24</sup> All 1D nOe experiments were performed with a mixing time of 1 sec.

<sup>25</sup> Spartan '08 for Macintosh; Wavefunction, Inc.; Irvine, CA, 2008.

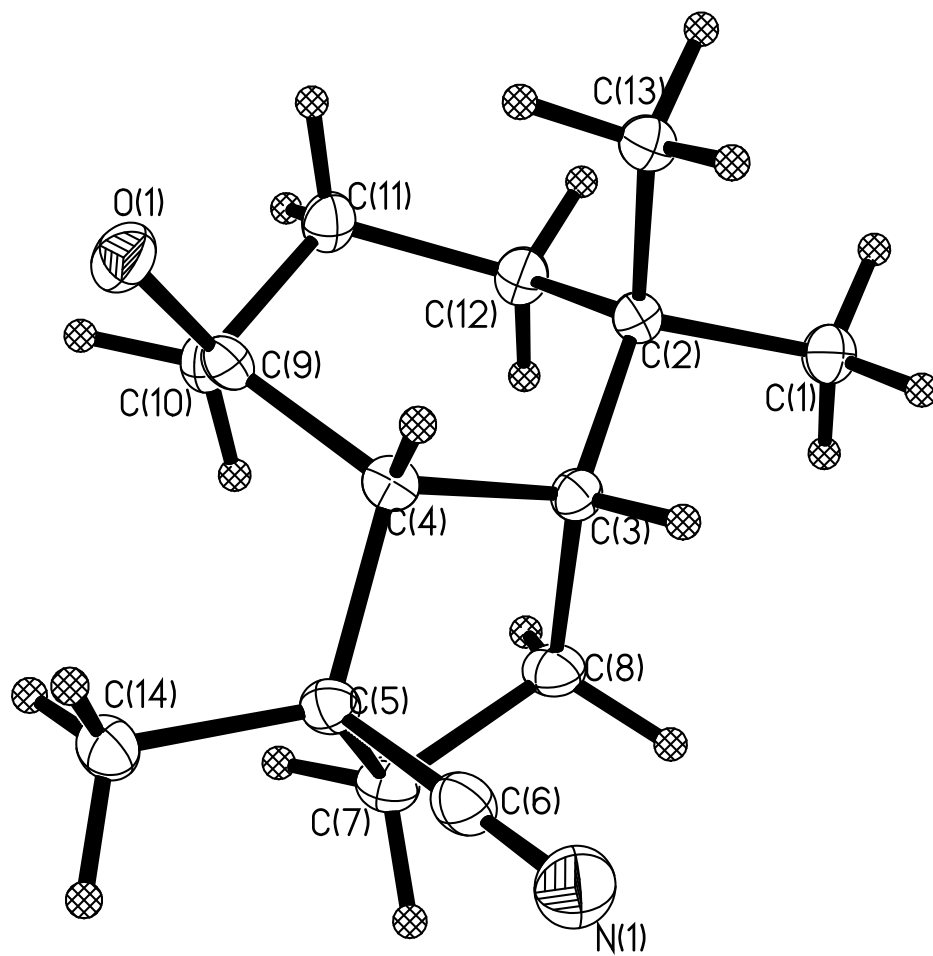
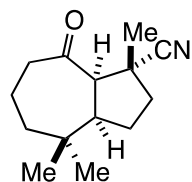
<sup>26</sup> Formed as the exclusive product in the following communication in this issue.

X-ray Structure of S6 (CCDC 885479)<sup>27</sup>



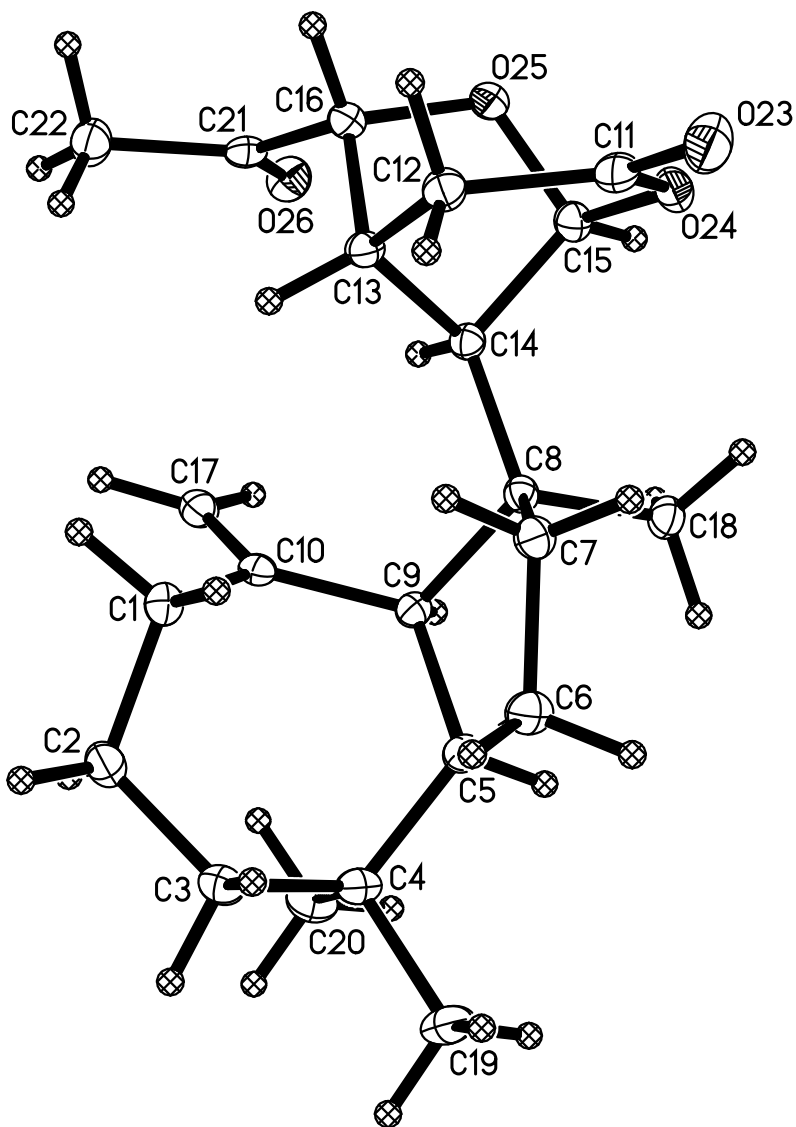
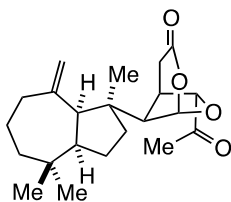
<sup>27</sup> The thermal ellipsoid plot is shown at the 50% probability level.

X-ray Structure of S7 (CCDC 885480)<sup>28</sup>



<sup>28</sup> The thermal ellipsoid plot is shown at the 50% probability level.

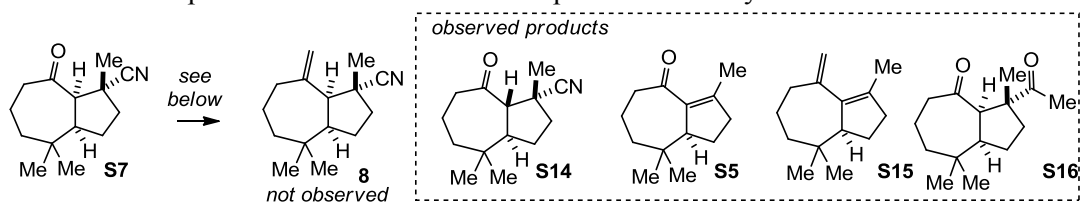
X-ray Structure of 19 (CCDC 885481)<sup>29</sup>



<sup>29</sup> The thermal ellipsoid plot is shown at the 50% probability level.



**Scheme S3:** Representative outcomes of attempted direct methylenation of **S6** and **S7**.<sup>30</sup>



Entry	Conditions	Result
1	<i>Peterson</i> 1 M TMSCH <sub>2</sub> Li, THF, THF-TMEDA, DME, or toluene	10:1 <b>S7</b> to <b>S14</b>
2	TMSCH <sub>2</sub> Li to ketone with CeCl <sub>3</sub> , THF	10:1 <b>S7</b> to <b>S14</b>
3	TMSCH <sub>2</sub> CeCl <sub>2</sub> , THF	<b>S7</b>
4	TMSCH <sub>2</sub> MgBr, THF	10:1 <b>S7</b> to <b>S14</b>
5	<i>Wittig</i> PPh <sub>3</sub> MeBr, BuLi, THF r.t	10:1 <b>S7</b> to <b>S14</b>
6	PPh <sub>3</sub> MeBr, KOtBu, toluene, 90 °C, 1 h	<b>S5</b> (40%), <b>S15</b> (21%)
7	<i>Petasis</i> Cp <sub>2</sub> TiMe <sub>2</sub> , toluene or THF	complex mixture
8	<i>Lombardo</i> TiCl <sub>4</sub> , CH <sub>2</sub> Br <sub>2</sub> , Zn (3 days) + substrate 4 h r.t.	<b>S7</b>
9	<i>Tebbe</i> Cp <sub>2</sub> TiCH <sub>2</sub> ClAlMe <sub>2</sub> , THF, -30 to 0 °C	~40% <b>S16</b>

Reaction scheme for **S6**: **S6** (6-methyl-2-cyano-1,2,3,4,5,6,7-heptahydroindole-1-one) reacts to form **S9** (6-methyl-2-cyano-1,2,3,4,5,6,7-heptahydroindole-1-one with a methyl group at the 2-position, not observed) and observed product **S17**.

Entry	Conditions	Result
1	<i>Peterson</i> 1 M TMSCH <sub>2</sub> Li, THF	10:1 <b>S6</b> to <b>S17</b>
2	TMSCH <sub>2</sub> Li to ketone with CeCl <sub>3</sub>	10:1 <b>S6</b> to <b>S17</b>
3	TMSCH <sub>2</sub> CeCl <sub>2</sub> , THF	<b>S6</b>
4	TMSCH <sub>2</sub> MgBr, THF	10:1 <b>S6</b> to <b>S17</b>
5	<i>Wittig</i> PPh <sub>3</sub> MeBr, KOtBu, toluene, 90 °C, 1 h	<b>S5</b> (60%), diene
6	<i>Lombardo</i> TiCl <sub>4</sub> , CH <sub>2</sub> Br <sub>2</sub> , Zn (3 days) + substrate 4 h r.t.	<b>S6</b>

<sup>30</sup> The conversion of nitriles to methyl ketones with the *Tebbe* reagent has been observed previously as we observed in the formation of **S16**, see: Doxsee, K. M.; Farahi, J. B. *J. Chem. Soc., Chem. Commun.*, **1990**, 1452-1453.

**Computational details:** All calculations were carried out with the B3LYP hybrid functional<sup>31</sup> and 6-31+G(d,p) basis set. Full geometry optimizations and transition structure (TS) searches were carried out with the Gaussian 09 package.<sup>32</sup> The possibility of different conformations was taken into account for all structures. Frequency analyses were carried out at the same level used in the geometry optimizations, and the nature of the stationary points was determined in each case according to the appropriate number of negative eigenvalues of the Hessian matrix. Scaled frequencies were not considered since significant errors in the calculated thermodynamic properties are not found at this theoretical level.<sup>33</sup> Where necessary, mass-weighted intrinsic reaction coordinate (IRC) calculations were carried out by using the Gonzalez and Schlegel scheme<sup>34</sup> in order to ensure that the TSs indeed connected the appropriate reactants and products. Enthalpies ( $\Delta H$ ) were used for the discussion on the relative stabilities of the considered structures. Cartesian coordinates, electronic energies, entropies, enthalpies, Gibbs free energies, lowest frequencies of the different conformations of all structures considered are available as Supporting Information.

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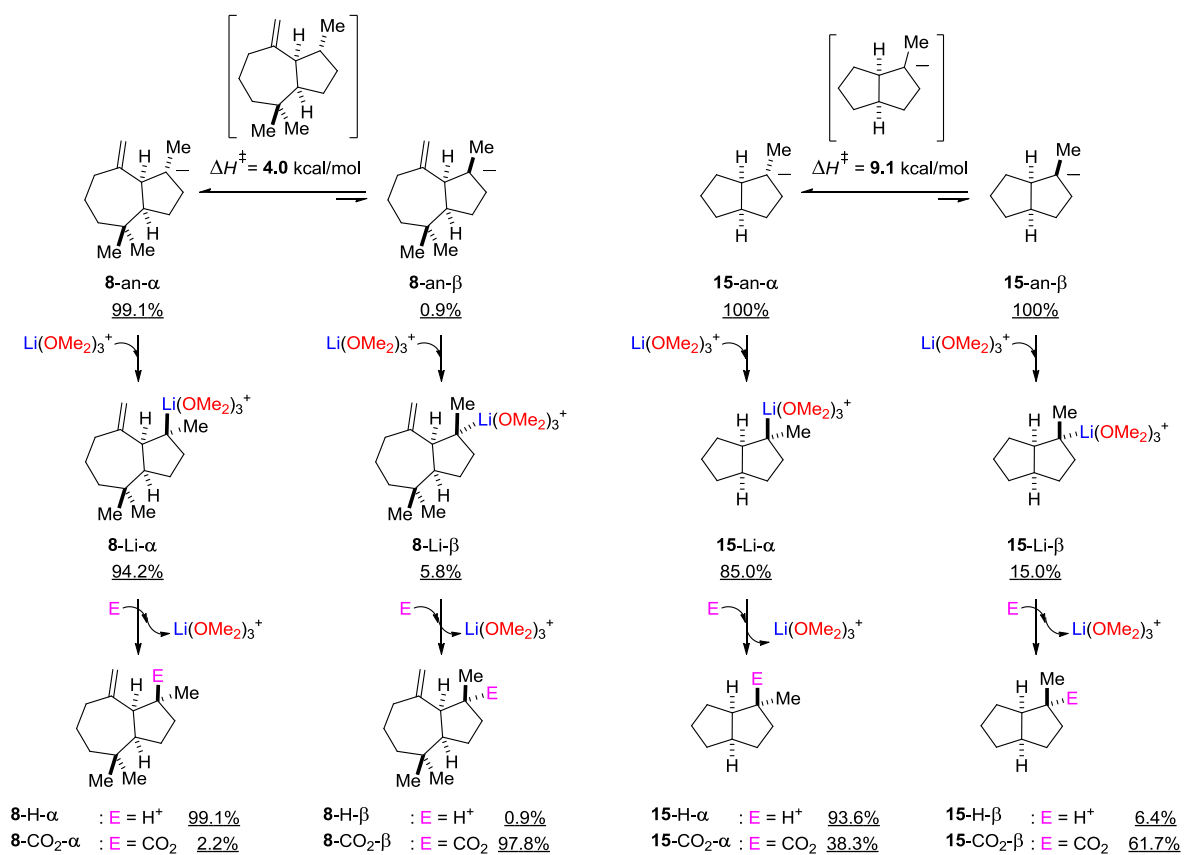
<sup>31</sup> a) C. Lee, W. Yang, R. Parr, *Phys. Rev. B* **1988**, *37*, 785. b) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648.

<sup>32</sup> Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

<sup>33</sup> a) C. W. Bauschlicher, Jr., *Chem. Phys. Lett.* **1995**, *246*, 40. b) A. P. Scott, L. Radom, *J. Phys. Chem.* **1996**, *100*, 1650. c) J. P. Merrick, D. Moran, L. Radom, *J. Phys. Chem. A* **2007**, *111*, 11683.

<sup>34</sup> a) C. Gonzalez, H. B. Schlegel, *J. Chem. Phys.* **1989**, *90*, 2154. b) C. Gonzalez, H. B. Schlegel, *J. Chem. Phys.* **1990**, *94*, 5523.

**Table S1.** B3LYP/6-31+G(d,p) absolute energies, enthalpies, free energies, entropies and relative populations (underlined) of the structures considered in this work

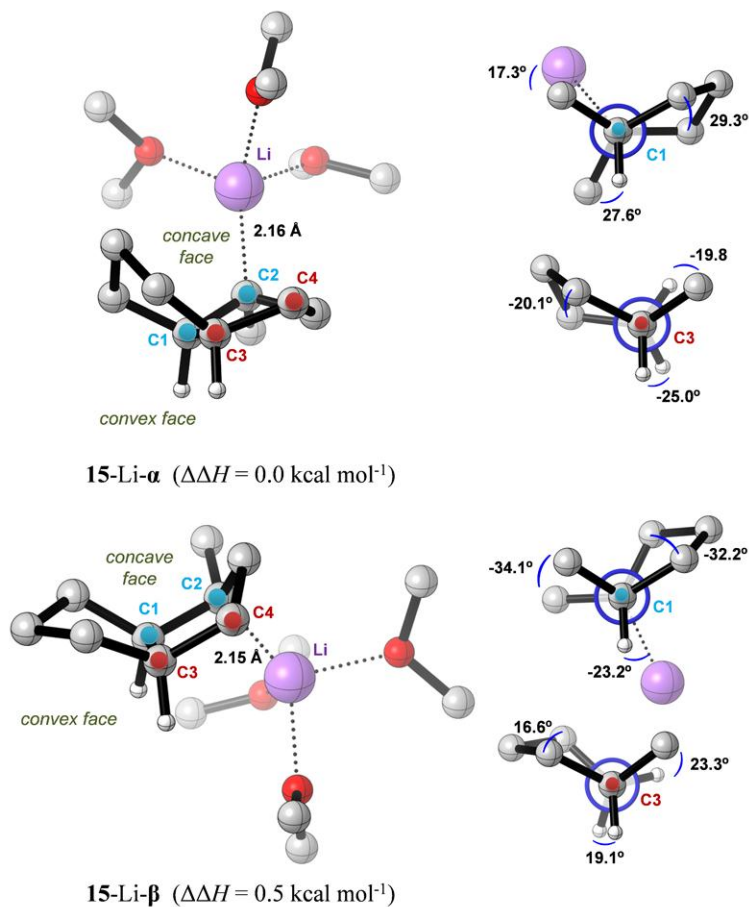


Structure	$E_{\text{elec}}$ (Hartree) <sup>[a]</sup>	$E_{\text{elec}} + \text{ZPE}$ (Hartree) <sup>[a]</sup>	$E$ (Hartree) <sup>[a]</sup>	$H$ (Hartree) <sup>[b]</sup>	$S$ (cal $\text{mol}^{-1} \text{K}^{-1}$ ) <sup>[b]</sup>	$G$ (Hartree) <sup>[b]</sup>	Lowest freq. ( $\text{cm}^{-1}$ )	$\Delta H$ ( $\text{kcal mol}^{-1}$ ) <sup>[c]</sup>
8-an- $\alpha$ _a	-547.327597	-546.994420	-546.980227	-546.979283	113.9	-547.033422	45.5	0.0
8-an- $\alpha$ _b	-547.323444	-546.990268	-546.976169	-546.975224	113.3	-547.029055	48.5	2.5
8-an- $\alpha$ _c	-547.317754	-546.984536	-546.970349	-546.969405	114.4	-547.023748	45.7	6.2
8-an- $\alpha$ _d	-547.314793	-546.982145	-546.967930	-546.966986	114.1	-547.021193	52.9	7.7
8-an- $\alpha$ _e	-547.320596	-546.987691	-546.973398	-546.972454	114.3	-547.026782	68.7	4.3
8-an- $\beta$ _a	-547.323039	-546.990181	-546.975813	-546.974868	114.2	-547.029129	61.7	2.8
8-an- $\beta$ _b	-547.311352	-546.978408	-546.964115	-546.963170	113.9	-547.017279	79.9	10.1
8-an- $\beta$ _c	-547.309457	-546.976834	-546.962484	-546.961540	113.7	-547.015575	88.3	11.1
8-an- $\beta$ _d	-547.315809	-546.982608	-546.968287	-546.967343	114.0	-547.021488	63.5	7.5
8-an- $\beta$ _e	-547.303855	-546.970272	-546.956171	-546.955227	112.6	-547.008719	73.2	15.1
8-TS	-547.319778	-546.987632	-546.973800	-546.972856	112.0	-547.026072	-175.0	4.0
8-Li- $\alpha$ _a	-	-	-	-	211.2	-	21.6	2.8
8-Li- $\alpha$ _b	1020.031272	1019.448544	1019.415115	1019.414171	-	1019.514496	-	3.3
8-Li- $\alpha$ _b	-	-	-	-	208.3	-	16.2	3.3

	1020.030149	1019.447421	1019.414375	1019.413430		1019.512398		
<b>8-Li-<math>\alpha</math>_c</b>	– 1020.035465	– 1019.452823	– 1019.419579	– 1019.418635	208.9	– 1019.517887	22.4	<b>0.0</b>
<b>8-Li-<math>\alpha</math>_d</b>	– 1020.025749	– 1019.443445	– 1019.409891	– 1019.408947	211.5	– 1019.509435	20.6	<b>6.1</b>
<b>8-Li-<math>\alpha</math>_e</b>	– 1020.025595	– 1019.443034	– 1019.409759	– 1019.408815	207.9	– 1019.507581	20.2	<b>6.2</b>
<b>8-Li-<math>\alpha</math>_f</b>	– 1020.023883	– 1019.441493	– 1019.408250	– 1019.407306	208.9	– 1019.506557	21.4	<b>7.1</b>
<b>8-Li-<math>\beta</math>_a</b>	– 1020.029573	– 1019.446980	– 1019.413547	– 1019.412603	212.8	– 1019.513729	17.0	<b>3.8</b>
<b>8-Li-<math>\beta</math>_b</b>	– 1020.025189	– 1019.442800	– 1019.409445	– 1019.408501	210.9	– 1019.508702	19.2	<b>6.4</b>
<b>8-Li-<math>\beta</math>_c</b>	– 1020.032614	– 1019.450451	– 1019.416928	– 1019.415984	213.1	– 1019.517226	15.0	<b>1.7</b>
<b>8-Li-<math>\beta</math>_d</b>	– 1020.025462	– 1019.442682	– 1019.409380	– 1019.408436	210.2	– 1019.508289	17.6	<b>6.4</b>
<b>8-Li-<math>\beta</math>_e</b>	– 1020.025501	– 1019.442428	– 1019.409287	– 1019.408343	209.2	– 1019.507731	22.7	<b>6.5</b>
<b>8-Li-<math>\beta</math>_f</b>	– 1020.023317	– 1019.440957	– 1019.407543	– 1019.406599	210.2	– 1019.506472	22.7	<b>7.6</b>
<b>8-H-<math>\alpha</math>_a</b>	–547.977048	–547.625536	–547.611173	–547.610229	115.3	–547.664996	52.7	<b>3.1</b>
<b>8-H-<math>\alpha</math>_b</b>	–547.982108	–547.630300	–547.616130	–547.615186	114.2	–547.669437	41.0	<b>0.0</b>
<b>8-H-<math>\alpha</math>_c</b>	–547.978884	–547.627143	–547.613017	–547.612073	113.6	–547.666039	48.4	<b>2.0</b>
<b>8-H-<math>\alpha</math>_d</b>	–547.974947	–547.623120	–547.608886	–547.607941	114.2	–547.662205	64.5	<b>4.5</b>
<b>8-H-<math>\alpha</math>_e</b>	–547.973668	–547.622255	–547.607924	–547.606979	114.7	–547.661469	64.8	<b>5.1</b>
<b>8-H-<math>\alpha</math>_f</b>	–547.972952	–547.621163	–547.606950	–547.606005	115.2	–547.660718	33.3	<b>5.8</b>
<b>8-H-<math>\beta</math>_a</b>	–547.974726	–547.622637	–547.608530	–547.607586	113.7	–547.661589	48.5	<b>4.8</b>
<b>8-H-<math>\beta</math>_b</b>	–547.970872	–547.618772	–547.604632	–547.603688	113.4	–547.657591	64.1	<b>7.2</b>
<b>8-H-<math>\beta</math>_c</b>	–547.977623	–547.625832	–547.611643	–547.610698	113.7	–547.664742	60.6	<b>2.8</b>
<b>8-H-<math>\beta</math>_d</b>	–547.972520	–547.620314	–547.606262	–547.605318	112.8	–547.658901	76.7	<b>6.2</b>
<b>8-H-<math>\beta</math>_e</b>	–547.970445	–547.618109	–547.604183	–547.603239	112.0	–547.656448	73.2	<b>7.5</b>
<b>8-H-<math>\beta</math>_f</b>	–547.971171	–547.619277	–547.605068	–547.604124	113.3	–547.657959	88.4	<b>6.9</b>
<b>8-CO<sub>2</sub>-<math>\alpha</math>_a</b>	–735.998701	–735.646608	–735.629730	–735.628786	128.0	–735.689599	30.2	<b>4.1</b>
<b>8-CO<sub>2</sub>-<math>\alpha</math>_b</b>	–735.997225	–735.645116	–735.628511	–735.627567	126.0	–735.687449	25.0	<b>4.9</b>
<b>8-CO<sub>2</sub>-<math>\alpha</math>_c</b>	–736.001723	–735.649229	–735.632631	–735.631687	126.5	–735.691800	31.3	<b>2.3</b>
<b>8-CO<sub>2</sub>-<math>\alpha</math>_d</b>	–735.994091	–735.641734	–735.625024	–735.624079	125.8	–735.683848	68.5	<b>7.1</b>
<b>8-CO<sub>2</sub>-<math>\alpha</math>_e</b>	–735.994558	–735.642441	–735.625781	–735.624837	125.5	–735.684475	49.7	<b>6.6</b>
<b>8-CO<sub>2</sub>-<math>\alpha</math>_f</b>	–735.990632	–735.638131	–735.621581	–735.620637	126.0	–735.680499	32.3	<b>9.2</b>
<b>8-CO<sub>2</sub>-<math>\beta</math>_a</b>	–736.001651	–735.649549	–735.632651	–735.631707	130.5	–735.693709	18.9	<b>2.3</b>
<b>8-CO<sub>2</sub>-<math>\beta</math>_b</b>	–735.999311	–735.646929	–735.630137	–735.629193	127.7	–735.689843	34.2	<b>3.8</b>
<b>8-CO<sub>2</sub>-<math>\beta</math>_c</b>	–736.005392	–735.653086	–735.636270	–735.635326	127.9	–735.696112	31.8	<b>0.0</b>
<b>8-CO<sub>2</sub>-<math>\beta</math>_d</b>	–735.997250	–735.644865	–735.628043	–735.627099	127.2	–735.687535	38.7	<b>5.2</b>
<b>8-CO<sub>2</sub>-<math>\beta</math>_e</b>	–735.996675	–735.644113	–735.627482	–735.626537	125.7	–735.686245	59.4	<b>5.5</b>
<b>8-CO<sub>2</sub>-<math>\beta</math>_f</b>	–735.997250	–735.644865	–735.628043	–735.627099	127.2	–735.687535	38.7	<b>5.2</b>

<b>15-an-<math>\alpha</math>_a</b>	-351.975135	-351.760638	-351.752155	-351.751210	89.0	-351.793502	68.6	<b>0.0</b>
<b>15-an-<math>\alpha</math>_b</b>	-351.973212	-351.758643	-351.750103	-351.749159	89.7	-351.791762	54.5	<b>1.3</b>
<b>15-an-<math>\alpha</math>_c</b>	-351.962766	-351.747919	-351.739315	-351.738371	89.6	-351.780934	65.6	<b>8.1</b>
<b>15-an-<math>\beta</math>_a</b>	-351.965533	-351.751095	-351.742591	-351.741647	89.1	-351.783996	65.2	<b>6.0</b>
<b>15-an-<math>\beta</math>_b</b>	-351.957391	-351.742444	-351.733926	-351.732981	89.2	-351.775364	58.1	<b>11.4</b>
<b>15-an-<math>\beta</math>_c</b>	-351.958435	-351.743534	-351.735094	-351.734150	88.6	-351.776232	69.6	<b>10.7</b>
<b>15-TS</b>	-351.957963	-351.745907	-351.737602	-351.736657	89.7	-351.779268	-206.4	<b>9.1</b>
<b>15-Li-<math>\alpha</math>_a</b>	-824.686582	-824.223027	-824.195402	-824.194458	186.2	-824.282908	27.4	<b>0.0</b>
<b>15-Li-<math>\alpha</math>_b</b>	-824.686630	-824.222674	-824.195227	-824.194283	184.5	-824.281932	28.5	<b>0.1</b>
<b>15-Li-<math>\alpha</math>_c</b>	-824.686938	-824.223062	-824.195457	-824.194513	187.3	-824.283522	20.9	<b>0.0</b>
<b>15-Li-<math>\beta</math>_a</b>	-824.682611	-824.218518	-824.190940	-824.189996	188.7	-824.279659	18.5	<b>2.8</b>
<b>15-Li-<math>\beta</math>_b</b>	-824.685959	-824.222233	-824.194678	-824.193734	186.5	-824.282327	20.0	<b>0.5</b>
<b>15-Li-<math>\beta</math>_c</b>	-824.683256	-824.219295	-824.191658	-824.190714	188.9	-824.280469	15.1	<b>2.4</b>
<b>15-Li-<math>\beta</math>_d</b>	-824.683249	-824.219300	-824.191649	-824.190705	188.5	-824.280271	18.8	<b>2.4</b>
<b>15-H-<math>\alpha</math>_a</b>	-352.636047	-352.403006	-352.394630	-352.393686	88.4	-352.435693	80.8	<b>0.0</b>
<b>15-H-<math>\alpha</math>_b</b>	-352.634746	-352.401887	-352.393378	-352.392434	89.9	-352.435132	46.8	<b>0.8</b>
<b>15-H-<math>\alpha</math>_c</b>	-352.633959	-352.400876	-352.392476	-352.391532	88.8	-352.433721	67.6	<b>1.4</b>
<b>15-H-<math>\alpha</math>_d</b>	-352.632067	-352.398828	-352.390439	-352.389495	89.1	-352.431822	53.1	<b>2.6</b>
<b>15-H-<math>\beta</math>_a</b>	-352.633840	-352.400727	-352.392314	-352.391369	88.7	-352.433500	76.5	<b>1.5</b>
<b>15-H-<math>\beta</math>_b</b>	-352.629813	-352.396472	-352.388140	-352.387196	88.6	-352.429296	55.0	<b>4.1</b>
<b>15-CO<sub>2</sub>-<math>\alpha</math>_a</b>	-540.656575	-540.422733	-540.411904	-540.410960	101.6	-540.459230	39.8	<b>0.7</b>
<b>15-CO<sub>2</sub>-<math>\alpha</math>_b</b>	-540.655398	-540.421774	-540.410733	-540.409789	104.0	-540.459198	24.4	<b>1.5</b>
<b>15-CO<sub>2</sub>-<math>\alpha</math>_c</b>	-540.656465	-540.422886	-540.411836	-540.410892	103.8	-540.460224	30.3	<b>0.8</b>
<b>15-CO<sub>2</sub>-<math>\beta</math>_a</b>	-540.653870	-540.419867	-540.408937	-540.407993	103.3	-540.457050	29.1	<b>2.6</b>
<b>15-CO<sub>2</sub>-<math>\beta</math>_b</b>	-540.657752	-540.424076	-540.413086	-540.412142	103.1	-540.461146	29.0	<b>0.0</b>
<b>15-CO<sub>2</sub>-<math>\beta</math>_c</b>	-540.653936	-540.419991	-540.409017	-540.408072	103.8	-540.457384	30.6	<b>2.6</b>

<sup>[a]</sup> 1 Hartree = 627.51 kcal mol<sup>-1</sup>. <sup>[b]</sup> Thermal corrections at 298.15 K. <sup>[b]</sup> Relative enthalpies derived for related structures (same shadow color)



**Figure S1.** Optimized structures of solvated organolithium intermediates derived from dehydropentalene **15** after reductive lithiation. The Newman projections of interest shown as insets are viewed from the C1→C4 and C3→C4 directions. Relative enthalpies calculated at the B3LYP/6-31+G(d,p) level are displayed. Smaller torsional strain (*i.e.* larger dihedral angles) is observed with respect to intermediates **8**-Li derived from dehydroazulene, which is translated into a small energy difference between  $\alpha$  and  $\beta$  epimers, according to experimental observations.

**Cartesian coordinates of  
the structures considered  
in this work**

Structure **8-an- $\alpha$ \_a** (B3LYP/6-31+g(d,p))

C	1.41061500	1.74189200	-1.15179700
C	2.01484600	0.33981400	-0.98322300
C	1.70463400	-0.45301200	0.31581200
C	0.23526600	-0.97401700	0.42065700
C	-0.76948200	1.49336300	0.16246100
C	-0.12898700	1.79939900	-1.17384600
C	-1.21570600	2.49168900	0.94762200
C	-0.21058800	-2.01184300	-0.63940200
H	0.22049500	-1.52374000	1.37464300
C	2.04694400	0.39242300	1.56237000
C	2.65283300	-1.67822400	0.31865800
H	1.78590800	2.14870500	-2.10360500
H	1.78730000	2.41120000	-0.36585900
H	3.11015700	0.43772200	-1.05323100
H	1.71261800	-0.27517000	-1.84147100
H	-0.52342400	1.08100800	-1.90339800
H	-0.43347600	2.80245600	-1.50265200
H	-1.17286800	3.53464600	0.63478800
H	-1.66370200	2.28424400	1.91804900
H	0.25247200	-2.99457300	-0.46554400
H	0.04200800	-1.69286400	-1.65836100
H	3.07875500	0.76904000	1.50869500
H	1.37474900	1.24582400	1.67740000
H	1.96044800	-0.21971300	2.46904900
H	2.44028100	-2.33629400	1.17024500
H	3.70107400	-1.35730100	0.39250600
H	2.54715700	-2.27163900	-0.59595000
C	-1.73467700	-2.02626100	-0.46472400
H	-2.25290300	-2.52391900	-1.29927600
H	-1.97222100	-2.65521700	0.45200700
C	-0.97790900	0.03464600	0.55096100
H	-1.25021800	0.05818500	1.64404000
C	-2.08271200	-0.57453000	-0.29938800
C	-3.47100400	-0.28811100	0.18846200
H	-3.69013800	0.78751500	0.24524300
H	-4.24087100	-0.73879500	-0.45570600
H	-3.65803200	-0.69469500	1.23065100

Structure **8-an- $\alpha$ \_b** (B3LYP/6-31+g(d,p))

C	-2.05414800	1.79449800	-0.34551200
C	-2.35187800	0.31172200	-0.61845700
C	-1.52360500	-0.78240400	0.11926100
C	-0.09334100	-0.92977900	-0.49953000
C	0.45317300	1.61905500	0.06086700
C	-0.64768200	2.28097100	-0.74205900
C	0.96165400	2.22691100	1.14368800
C	0.71308600	-2.15666800	0.01257200
H	-0.28352000	-1.11005500	-1.56884400
C	-2.28288200	-2.11147600	-0.12603800
C	-1.51101100	-0.52295900	1.64083900
H	-2.21495400	2.01463400	0.71805900
H	-2.79878800	2.38881800	-0.89793000
H	-2.26129800	0.12811600	-1.70026700
H	-3.41220700	0.14545800	-0.37119300
H	-0.60730200	3.37029200	-0.60441900
H	-0.48952100	2.08518700	-1.81336600
H	0.62685300	3.21918300	1.44830800
H	1.70952500	1.71512200	1.74419600
H	0.44482500	-3.07177200	-0.53650400
H	0.52747700	-2.33590900	1.07791300
H	-2.34797200	-2.33694500	-1.19868900
H	-1.78443400	-2.95409600	0.36245600
H	-3.30657200	-2.05181900	0.26848700
H	-1.09891400	-1.38279000	2.17868100
H	-2.53519100	-0.36081400	2.00906400
H	-0.90296200	0.34437800	1.90168400
C	2.17601200	-1.74610200	-0.18354200
H	2.87422700	-2.38169500	0.38217100
H	2.44001400	-1.90349000	-1.27758800
C	0.95714400	0.26997500	-0.44224600
H	1.17204500	0.49426900	-1.53913400
C	2.19470700	-0.29619600	0.20776000
C	3.46932900	0.40794900	-0.17387900
H	3.50953600	1.45745600	0.14655900
H	4.35590600	-0.09091200	0.24496300

H	3.61987200	0.42440100	-1.29695000
Structure <b>8-an-<math>\alpha</math>_c</b>	(B3LYP/6-31+g(d,p))		
C	-1.78887800	1.55914800	-1.08837100
C	-2.26188100	0.65850600	0.06563500
C	-1.51145000	-0.71499000	0.27066000
C	-0.18670400	-0.82806600	-0.56280900
C	0.44613700	1.61732100	0.14819900
C	-0.53775100	2.39004500	-0.70802900
C	0.85479500	2.10183200	1.33076700
C	0.59938700	-2.15934000	-0.35600900
H	-0.51348700	-0.81570300	-1.61172700
C	-2.45888900	-1.83811800	-0.22085900
C	-1.28742600	-0.90730600	1.78704400
H	-2.59805100	2.24938700	-1.36749900
H	-1.58351200	0.95719800	-1.98026300
H	-3.33185100	0.44221200	-0.06566400
H	-2.18806800	1.24326500	0.99109200
H	-0.85569200	3.29055600	-0.16413300
H	-0.03937300	2.72916000	-1.62788100
H	0.49622500	3.05995200	1.70748500
H	1.55101800	1.52964200	1.93795000
H	0.33206500	-2.90502800	-1.11989800
H	0.38515000	-2.60022600	0.62242300
H	-3.39485200	-1.83678700	0.35482600
H	-2.71534200	-1.70220500	-1.28011000
H	-2.00048400	-2.82713400	-0.11332000
H	-0.94309600	-1.91841200	2.02558700
H	-2.23195000	-0.74448000	2.32766500
H	-0.53852000	-0.20621900	2.16192600
C	2.07913900	-1.75014100	-0.41535900
C	2.73962000	-2.49470500	0.05399900
H	2.39110900	-1.71138800	-1.50741600
C	0.93063400	0.29374800	-0.42041600
C	1.19114300	0.55545000	-1.50095300
H	2.11195500	-0.38725900	0.22105500
C	3.42276000	0.32375900	0.00985100
H	3.46535200	1.31915500	0.47143200
H	4.27182100	-0.25188100	0.40713000
H	3.63981300	0.48335700	-1.09081700

Structure **8-an- $\alpha$ \_d** (B3LYP/6-31+g(d,p))

C	2.02647100	1.79300600	-0.22600500
C	2.00556500	0.36621400	-0.80683800
C	1.57231200	-0.79611300	0.12768800
C	0.01508000	-0.96567000	0.22602900
C	-0.51480600	1.62761600	-0.12004800
C	0.72548100	2.25431500	0.47683300
C	-1.20228200	2.25383300	-1.08660900
C	-0.69076200	-1.75997000	-0.89629000
H	-0.13437500	-1.59155200	1.12105700
C	2.17137700	-0.62266400	1.54313500
C	2.18791800	-2.09536700	-0.44643400
H	2.23087900	2.47508900	-1.06325000
H	2.87314800	1.90084100	0.46725300
H	3.02127800	0.15466500	-1.17606500
H	1.35116500	0.35380200	-1.68729100
H	0.66824900	3.34971600	0.42525200
H	0.76947700	1.99572500	1.54387600
H	-0.91080500	3.24361300	-1.44172100
H	-2.07515400	1.75570000	-1.50625100
H	-0.33173200	-2.79542600	-0.96617200
H	-0.56422900	-1.28138000	-1.87716200
H	2.01793900	-1.53716400	2.12957000
H	1.70410800	0.19568700	2.09653600
H	3.25293400	-0.43279900	1.49608500
H	1.84084200	-2.97693400	0.10621400
H	3.28390900	-2.06155400	-0.37464600
H	1.92470700	-2.23635300	-1.50001700
C	-2.15212300	-1.66819900	-0.43445800
H	-2.86668900	-2.00294300	-1.20382200
H	-2.27482700	-2.40916800	0.42034500
C	-0.95365100	0.26738100	0.45954300
H	-0.94811600	0.45145500	1.57165400
C	-2.30587600	-0.23033400	-0.02876100
C	-3.46169200	0.07494700	0.87592300
H	-3.36904200	-0.41629800	1.89718900
H	-3.58222000	1.14971700	1.07481900
H	-4.41951400	-0.27840500	0.46430100
Structure <b>8-an-<math>\alpha</math>_e</b>	(B3LYP/6-31+g(d,p))		
C	-0.53421500	0.89396800	1.83415400
C	-1.83837300	0.39075000	1.19639600

C	-1.77317400	-0.17030400	-0.25953500
C	-0.41509200	-0.85084000	-0.61898200
C	0.85754300	1.47552400	-0.28656500
C	0.27429100	1.93269500	1.05092100
C	1.38464200	2.39728400	-1.11289000
C	-0.07715800	-2.13281000	0.19220600
H	-0.54430300	-1.17120200	-1.66351200
C	-2.09394900	0.95034000	-1.27797300
C	-2.90444000	-1.21816700	-0.40342900
H	0.14171300	0.04857800	2.00507500
H	-0.78477300	1.32024700	2.81840600
H	-2.59814200	1.18879600	1.21408300
H	-2.22798600	-0.39726900	1.85719100
H	1.11557400	2.23144400	1.69082400
H	-0.32323300	2.84317300	0.88755500
H	1.38991400	3.45858400	-0.86256500
H	1.84508100	2.10894600	-2.05483600
H	-0.55912300	-3.02161200	-0.24167500
H	-0.41613000	-2.04908700	1.23244500
H	-3.10617800	1.34282300	-1.10580300
H	-1.39012800	1.78187100	-1.22273100
H	-2.05526300	0.55919800	-2.30284900
H	-2.94974600	-1.61015100	-1.42786800
H	-3.87945600	-0.76552100	-0.17411500
H	-2.76063300	-2.06513800	0.27490500
C	1.45530100	-2.19911300	0.14873000
H	1.87061500	-2.88212200	0.90554400
H	1.75967600	-2.63712900	-0.85503600
C	0.93540500	-0.00473400	-0.61776000
H	1.30405400	-0.04397800	-1.68451600
C	1.88261100	-0.76494200	0.30009300
C	3.33547600	-0.51401100	0.01395600
H	3.62002100	0.54183700	0.12487900
H	3.99445900	-1.09670200	0.67458800
H	3.62076800	-0.79942300	-1.04591900

Structure 8-an-β<sub>a</sub> (B3LYP/6-31+g(d,p))

C	-2.00286100	0.53421900	0.96064200
C	-1.79683100	-0.27655700	-0.34831200
C	-0.40432100	-0.97829500	-0.47613700
C	0.95639000	1.26149400	-0.16264400
C	0.40378100	1.49498100	1.22433200
C	1.63962400	2.26352500	-0.76939400
C	0.00098300	-1.91052700	0.71666800
H	-0.50232200	-1.62748900	-1.35636700
C	-2.03296700	0.62924000	-1.57552000
C	-2.88725700	-1.37579600	-0.35922400
H	-3.05338600	0.86741600	0.97769900
H	-1.89812000	-0.15158100	1.81173200
H	0.62427500	0.64681100	1.88587300
H	0.90483200	2.36945800	1.66850800
H	1.84901400	3.20370400	-0.26031500
H	2.04316900	2.14921300	-1.77363100
H	-0.22262600	-2.95513800	0.46709100
H	-0.56204900	-1.68690500	1.63304400
H	-3.02794700	1.09506700	-1.53084800
H	-1.28461100	1.42317900	-1.64361200
H	-1.97965000	0.04211000	-2.50131600
H	-2.81589200	-1.98722100	-1.26752500
H	-3.89294100	-0.93357100	-0.32920600
H	-2.79084000	-2.04644600	0.50239400
C	1.52278000	-1.70722400	0.93477100
H	1.67867300	-1.12512100	1.89593900
H	2.04184200	-2.66195700	1.12030600
C	0.85965100	-0.11934100	-0.79935500
H	0.91306900	0.04553400	-1.89049100
C	1.98816200	-1.02709100	-0.31877900
C	-1.11591400	1.76016000	1.22230800
H	-1.40442900	2.16807500	2.20411800
H	-1.32992100	2.54854300	0.48805400
C	3.41008500	-0.56169600	-0.39211500
H	4.10069100	-1.38129400	-0.14037100
H	3.68411300	-0.21531300	-1.39991900
H	3.67722000	0.29037400	0.29539500

Structure 8-an-β<sub>b</sub> (B3LYP/6-31+g(d,p))

C	-2.14766000	0.60154500	-0.81566200
C	-1.65573900	-0.68549600	-0.08368600
C	-0.14676000	-0.99637600	-0.39738700
C	0.62904200	1.37061200	0.28610200
C	-0.33859200	2.42327800	-0.21792300

C	1.27926100	1.54287200	1.45293200
C	0.61241900	-1.87028600	0.63771300
H	-0.13965700	-1.55083000	-1.34514900
C	-2.49434700	-1.86295700	-0.63970500
C	-1.97363500	-0.57772500	1.42515000
H	-1.78559500	0.57336500	-1.85341400
H	-3.24592000	0.53943800	-0.87699300
H	-0.24628400	3.34924900	0.36951100
H	-0.07369100	2.67956100	-1.25516400
H	1.12478900	2.43565400	2.06077000
H	1.98928100	0.81195700	1.82312100
H	0.31941900	-2.92845300	0.57249900
H	0.37506000	-1.54318500	1.65586500
H	-2.42579400	-1.91215100	-1.73384200
H	-2.13663000	-2.81979800	-0.24117800
H	-3.55529800	-1.75989800	-0.37069400
H	-1.31107100	0.12432400	1.93675000
H	-1.87010300	-1.55150000	1.91613500
H	-3.01151300	-0.24496000	1.57340800
C	2.12703000	-1.63575100	0.36435500
H	2.63111300	-1.36301100	1.33797200
H	2.63611700	-2.56865100	0.05913600
C	0.84385800	0.17838000	-0.66432100
H	0.62513100	0.59089300	-1.66461600
C	2.17887500	-0.54837600	-0.68898800
C	-1.81656900	1.97291100	-0.18994800
H	-2.16665200	1.98215300	0.85025600
H	-2.41576400	2.73354600	-0.71351700
C	3.44300600	0.25138100	-0.76099400
H	3.72670100	0.80118900	0.19003100
H	4.31177800	-0.38573600	-0.99084100
H	3.40345000	1.02277300	-1.54590500

Structure 8-an-β<sub>c</sub> (B3LYP/6-31+g(d,p))

C	1.96861500	0.48766000	-0.83341500
C	1.67006700	-0.68268600	0.14474700
C	0.14854900	-1.01280800	0.30575700
C	-0.67346100	1.40670900	-0.10412700
C	0.46339600	2.30444100	0.34209200
C	-1.45330500	1.77196900	-1.13680200
C	-0.55458100	-1.67713200	-0.90829100
H	0.08758700	-1.73457100	1.13148800
C	2.28406300	-0.39372600	1.53322100
C	2.38559600	-1.93713200	-0.41199100
H	3.00796300	0.38329500	-1.18494200
H	1.33578100	0.36104700	-1.71899700
H	0.23809400	3.35887500	0.12313400
H	0.56309100	2.23087300	1.43319900
H	-1.30332500	2.72448300	-1.64841100
H	-2.26005700	1.14323200	-1.49270500
H	-0.23657200	-2.71947400	-1.04396700
H	-0.29551900	-1.14618300	-1.83475100
H	1.78554700	0.43737100	2.03928500
H	2.18993600	-1.27420200	2.18095900
H	3.35286900	-0.15026900	1.45068500
H	2.09628100	-2.13857900	-1.44887500
H	2.13964200	-2.82649800	0.18169700
H	3.47637200	-1.80434700	-0.38791000
C	-2.08103800	-1.54650900	-0.62696800
H	-2.58963000	-1.14131000	-1.54945500
H	-2.54799500	-2.54056100	-0.48827400
C	-0.87319300	0.10401100	0.70514600
H	-0.68488800	0.40562500	1.75305400
C	-2.18126700	-0.65435400	0.59333300
C	1.81913900	1.93692100	-0.32513700
H	1.96574200	2.58923600	-1.19728000
C	2.64012200	2.17225500	0.36661300
C	-3.48236200	0.04726300	0.82809700
H	-3.84473000	0.72714500	-0.00600400
H	-4.30714200	-0.66799000	0.98058400
H	-3.45047100	0.68278600	1.72690200

Structure 8-an-β<sub>d</sub> (B3LYP/6-31+g(d,p))

C	1.83727500	1.19254000	-0.20561900
C	1.82911200	-0.24375500	0.39168400
C	0.42958600	-0.94619400	0.39656200
C	-0.96486000	1.25705100	0.15999600
C	-0.52891200	1.43776600	-1.27786700
C	-1.61312700	2.26803300	0.79001000
C	-0.00137500	-1.68867400	-0.90907400
H	0.49631500	-1.72547000	1.16686400



C	2.31008600	-0.11542500	1.85669300	H	2.65602300	-1.16821700	-1.43131800
C	2.85948100	-1.11984500	-0.35681300	C	-1.55657100	-1.69408700	-0.91232700
H	1.47536300	1.88665400	0.56237900	H	-1.92017800	-1.16187000	-1.84445500
H	2.88809300	1.46636500	-0.39540900	H	-1.96314900	-2.71446400	-1.02296800
H	-0.96892100	0.64774600	-0.89751500	C	-0.81921400	-0.11505100	0.81100400
H	-0.94977000	2.37971300	-1.65610100	H	-0.81866900	0.05035300	1.90297400
H	-1.85221700	3.20067500	0.28033400	C	-1.95303000	-1.04432100	0.38555200
H	-1.96288800	2.16597800	1.81563900	C	1.02265900	1.46208700	-1.48084900
H	0.41388000	-2.70471400	-0.92664300	H	1.31475400	0.76422600	-2.27640400
H	0.38156500	-1.19231300	-1.80770100	H	1.31237700	2.45923600	-1.84152900
H	3.26450600	0.42716400	1.91285800	C	-3.37766000	-0.61054300	0.54003200
H	1.57614200	0.42823800	2.46097200	H	-3.70417400	0.22312400	-0.14662000
H	2.45653300	-1.10354400	2.31164000	H	-4.06511200	-1.44745300	0.34150900
H	2.85443000	-2.14799200	0.02676500	H	-3.59940000	-0.25388900	1.55676800
H	3.87378500	-0.71703500	-0.22594400				
Structure 8-an- $\beta_e$ (B3LYP/6-31+g(d,p))				C	2.01650300	-2.72117800	1.02211300
C	-2.41093500	-0.28187600	-0.18256400	H	0.85353300	-0.11009000	-0.81417300
C	-1.15013900	-1.09639700	0.22172500	H	0.90740600	0.06076500	-1.90527900
C	0.04747300	-0.80725500	-0.74696400	C	1.98749500	-0.99329300	-0.30719200
C	0.08846900	1.85158000	-0.26784600	C	-1.07519400	1.73038900	1.28153600
C	-1.33940400	2.01061800	-0.75986900	H	-1.34280100	2.10536500	2.28262100
C	0.66885500	2.87617200	0.38142500	H	-1.30513500	2.54134200	0.57742300
C	1.22133800	-1.82656900	-0.64334900	C	3.42073000	-0.54499400	-0.35814100
H	-0.38926100	-0.90317200	-1.75750200	H	3.93039500	-0.68806300	0.61792000
C	-1.56403000	-2.58530800	0.08607500	H	4.05094500	-1.07083100	-1.10066800
C	-0.80782200	-0.83108500	1.70066700	H	3.51643500	0.53417100	-0.59180500
H	-2.61536400	-0.48026800	-1.24630100				
H	-3.26821200	-0.69469700	0.37220800	Structure 8-Li- $\alpha_a$ (B3LYP/6-31+g(d,p))			
H	-1.60050000	3.07741800	-0.73322500	C	-3.46885800	-1.87555500	-0.93136000
H	-1.39849300	1.69875800	-1.81477800	C	-4.25316500	-0.55827900	-0.88213700
H	0.12264600	3.80253300	0.56604300	C	-3.94974000	0.45899800	0.24941600
H	1.70450800	2.82562400	0.69382600	C	-2.50140500	1.04820300	0.22627700
H	1.10215800	-2.66174900	-1.35383600	C	-1.30306100	-1.29480800	0.30407800
H	1.25253700	-2.26776500	0.36140600	C	-1.93354900	-1.73492800	-1.00476400
H	-0.74907900	-3.25935200	0.36425600	C	-0.82459600	-2.23910300	1.13508100
H	-2.42453600	-2.80948300	0.73481600	C	-2.05791000	1.73498300	-1.09967800
H	-1.85104000	-2.81993700	-0.94681400	C	-2.53914000	1.84181200	0.98381500
H	-0.45782000	0.19063100	0.86263400	H	-4.22812000	-0.17582900	1.62893600
H	-0.01419600	-1.49841000	2.05044700	C	-4.94434500	1.63150500	0.06553400
H	-1.69162000	-0.99986100	2.33335400	H	-3.81306200	-2.44671100	-1.78673200
C	2.52624900	-0.99353100	-0.85229400	H	-3.70978500	-2.48634200	-0.03418900
H	3.40496500	-1.52010700	-0.45000800	H	-5.32266700	-0.80736300	-0.82318500
H	2.69426600	-0.88565400	-1.94228700	H	-4.12311900	-0.05538700	-1.84924600
C	0.84848500	0.60890100	-0.68766700	H	-1.68310800	-1.04110800	-1.81590800
H	0.97905100	0.80095200	-1.77355400	H	-1.52615300	-2.71516800	-1.28481600
C	2.26457900	0.34495200	-0.17997300	H	-0.82452000	-3.29468000	0.86832200
C	-2.40474300	1.23526100	0.03541000	H	-0.43417400	-1.98475700	2.11764400
H	-2.28906000	1.46620100	1.10271400	H	-2.26694000	2.81006700	-1.05842900
H	-3.39667900	1.61556800	-0.25427400	H	-2.60636700	1.35713800	-1.97078200
C	2.51768100	0.26057800	1.32361700	H	-5.26175800	-0.54052000	1.68789800
H	2.24037200	1.17827100	1.85830200	H	-3.56069900	-1.01490300	1.84102400
H	2.201594300	-0.56786300	1.89760300	H	-4.09149700	0.56532000	2.42596400
H	3.59307300	0.11610700	1.50461000	H	-4.79338900	2.39837900	0.83476500
				H	-5.98179700	1.28148900	0.14205200
Structure 8-TS (B3LYP/6-31+g(d,p))				H	-4.82490200	2.11105800	-0.91206100
C	-1.96703900	0.51204900	0.99939600	C	-0.52428000	1.46334900	-1.22962900
C	-1.79510900	-0.25845000	-0.33968900	H	-0.36225200	0.72420400	-2.03018400
C	-0.41347400	-0.97312100	-0.51358700	H	0.00956400	2.36925700	-1.55383300
C	0.94954000	1.26087900	-0.16899100	C	-1.26602600	0.17878300	0.68509200
C	0.44415700	1.46518800	1.23892900	H	-1.22413700	0.19269200	1.78279900
C	1.59686700	2.27797800	-0.79880600	C	-0.00910900	0.95002800	0.13940900
C	-0.01381300	-1.95701300	0.63631900	C	0.21417400	2.18252900	1.05304500
H	-0.53171800	-1.58472200	-1.41856900	H	0.40391200	1.88841800	2.09640700
C	-2.04486700	0.68629400	-1.53401200	H	1.08879700	2.76714700	0.73083500
C	-2.89797400	-1.34540800	-0.36387800	H	-0.62490000	2.91046900	1.09778900
H	-3.01680300	0.84384100	1.05201600	Li	1.93017700	0.05854900	0.04116900
H	-1.84235500	-0.20023600	1.82580200	O	2.81359700	-0.85001100	1.69427500
H	0.67996000	0.60270500	1.87767800	O	3.46974600	1.49190100	-0.31265800
H	0.95636500	2.33127400	1.68746900	O	2.58613700	-1.22552300	-1.46999700
H	1.82934600	3.21347500	-0.29012200	O	1.61519800	-2.10362200	-2.04028800
H	1.93141200	2.18445500	-1.83019400	H	2.05526600	-3.09350700	-2.22627000
H	-0.22713600	-2.98987500	0.33381200	H	0.80152900	-2.18651900	-1.32095000
H	-0.58874100	-1.78312200	1.55614200	H	1.23167000	-1.69469100	-2.98441900
H	-3.03081200	1.16588300	-1.45147800	C	3.72361100	-1.04908400	-2.30652900
H	-1.28515300	1.46962300	-1.59693900	H	3.43103500	-0.63111400	-3.28023100
H	-2.02431300	0.12538000	-2.47733800	H	4.39121200	-0.35330800	-1.79799800
H	-2.84586500	-1.93357400	-1.28882900	H	4.23610300	-2.00751300	-2.47203000
H	-3.89789400	-0.89286800	-0.30907200	C	3.25961700	-2.20256800	1.64297100
H	-2.79837900	-2.03951000	0.47853000	H	2.44717700	-2.88944800	1.91496300
C	1.50083500	-1.75653900	0.88592500	H	3.56867600	-2.39671200	0.61563100
H	1.64420600	-1.23799300	1.88696700	H	4.10785100	-2.35560900	2.32491200

C	2.34876400	-0.47914300	2.99115700	C	-2.71606600	1.32068800	1.66776400
H	3.15954200	-0.56497500	3.72837600	C	-3.30150200	-0.08511600	1.47864100
H	2.00913300	0.55489300	2.93125300	C	-3.63642900	-0.56441300	0.04048700
H	1.50875200	-1.11421300	3.29884700	C	-2.39085300	-0.84099900	-0.86078100
C	4.38506000	1.92396900	0.68802600	C	-1.44453500	1.62725700	-0.52661400
H	4.50322600	1.09633400	1.38821000	C	-1.35717800	1.56366600	0.98262400
H	5.35877300	2.17476700	0.24302900	C	-1.49406100	2.82197000	-1.14468700
H	3.99678400	2.80467200	1.21802000	C	-1.43473000	-1.96842100	-0.41390200
C	3.22668000	2.49016600	-1.30116100	H	-2.82955800	-1.20756400	-1.80053100
H	4.15275300	2.72865300	-1.84361400	C	-4.56997100	0.44520500	-0.66320700
H	2.48355000	2.08896100	-1.99109600	C	-4.42514300	-1.88854300	0.19347500
H	2.82906600	3.40465800	-0.84308900	H	-2.59344600	1.48769600	2.74787100

Structure **8-Li- $\alpha$ \_b** (B3LYP/6-31+g(d,p))

C	4.13261800	-1.37697700	0.72285700	H	-2.62087000	-0.81570500	1.93791100
C	4.29418100	0.13102600	0.49034100	H	-0.66229400	0.76355500	1.26412300
C	3.02271400	1.02651200	0.44329400	H	-0.94176000	2.50617900	1.36373900
C	2.24531700	0.83765000	-0.90144000	H	-1.43295000	3.75791000	-0.59130600
C	1.88391900	-1.77331300	-0.45111900	H	-1.60789000	2.89710300	-2.22365400
C	3.35219400	-2.14304900	-0.36036600	H	-1.89781800	-2.96033400	-0.47538400
C	0.96260200	-2.58312000	0.09526600	H	-1.10776100	-1.82134800	0.62363200
C	1.13567900	1.89155900	-1.16492900	H	-5.45851700	0.64556800	-0.05043800
H	3.01223200	1.00258600	-1.67095400	H	-4.07599600	1.39786200	-0.86667300
C	3.53427400	2.48790400	0.49492500	H	-4.91383700	0.03931000	-1.62240800
C	2.15359700	0.78371700	1.69163600	H	-4.63414300	-2.33907300	-0.78402300
H	3.66143000	-1.55906700	1.69739100	H	-5.38624000	-1.70917500	0.69093400
H	5.13986500	-1.81140400	0.78890900	H	-3.87532500	-2.62408500	0.79042300
H	4.85200000	0.28669900	-0.44512400	C	-0.25212900	-1.79779600	-1.37425700
H	4.94077800	0.51574300	1.29231800	H	0.62046500	-2.40027500	-1.06825500
H	3.44439500	-3.21721800	-0.15723000	H	-0.55294600	-2.20359700	-2.36926400
H	3.83091300	-1.96364300	-1.33411300	C	-1.43841800	0.33480300	-1.32116100
H	1.24242100	-3.50592200	0.60016400	H	-1.77679000	0.62014700	-2.33508900
H	-0.09372000	-2.34662700	0.02194800	C	0.63764700	0.14805900	-2.73331600
H	1.54576900	2.82443500	-1.57064700	H	0.74467700	1.23899300	-2.81285100
H	0.61441100	2.14353300	-0.23171800	H	1.64044000	-0.27537100	-2.89090500
H	4.17148900	2.71511000	-0.36873300	H	0.03556300	-0.16757800	-3.61826200
H	2.71098400	3.20859100	0.50130200	C	0.00379300	-0.27999100	-1.40641600
H	4.12874800	2.65557000	1.40146900	Li	1.65451300	-0.05340000	-0.03780900
H	1.32268900	1.49552000	1.74116300	O	2.86761600	1.58995600	-0.20812500
H	2.75217500	0.91105100	2.60372500	O	3.28020900	-1.47861800	-0.31160300
H	1.73116800	-0.22161600	1.69866000	O	1.64952200	-0.25963300	2.09665600
C	0.17088700	1.18763300	-2.12077400	C	2.31151700	2.80563900	-0.71976000
H	-0.78427100	1.72175600	-2.23022000	H	1.23553000	2.65484700	-0.81395200
H	0.62681300	1.18488100	-3.14058100	H	2.51964400	3.63795400	-0.03279500
C	1.53725800	-0.54561000	-1.27835200	H	2.73751600	3.03539100	-1.70509400
H	2.00703900	-0.80504200	-2.26002600	C	4.28419800	1.63927100	-0.08425100
C	-0.47860400	-1.16644000	-2.65059100	H	4.58803300	2.42865900	0.61843300
H	-0.46120300	-2.22548000	-2.36036500	H	4.60871800	0.66618800	0.28639000
H	-1.51168400	-0.92742900	-2.94896800	H	4.75269400	1.83616600	-1.05868400
H	0.13172000	-1.10099300	-3.58255000	C	3.75809100	-1.71856900	-1.63492800
C	0.04894200	-0.23309300	-1.55407500	H	3.66682800	-0.78378500	-2.18799000
Li	-1.54811300	-0.02952000	-0.08104200	H	4.81114700	-2.03204500	-1.60963400
O	-2.83718000	1.63199300	-0.43793100	H	3.15902500	-2.49095900	-2.13374800
O	-3.16914000	-1.44485300	-0.11502800	C	3.42154500	-2.62559900	0.52093700
O	-1.61044900	0.11825500	2.05582200	H	4.47044100	-2.95253700	0.55210900
C	-3.72744400	1.50972600	-1.54838600	H	3.10359900	-2.33643400	1.52230000
H	-3.97233100	0.45200200	-1.64676400	H	2.79855000	-3.45397500	0.15660000
H	-4.64288100	2.09167800	-1.37220200	C	2.00025300	0.84921100	2.92172700
H	-3.24593500	1.85944500	-2.47025600	H	2.56820600	1.54152300	2.30088600
C	-2.41939300	2.98121700	-0.23361400	H	1.10025600	1.35228200	3.29940700
H	-3.27817600	3.61363000	0.03261400	H	2.61336500	0.51898700	3.77188300
H	-1.69579500	2.98070100	0.58259500	C	0.86517300	-1.22250900	2.79786600
H	-1.93779900	3.38135000	-1.13371500	H	0.63372600	-2.02876000	2.10118300
C	-2.35573300	1.02021000	2.86361200	H	1.42344800	-1.62220600	3.65627700
H	-2.94520300	1.64872700	2.19578700	H	-0.07285000	-0.77775100	3.15400800
H	-3.03141600	0.47417800	3.53789100				
H	-1.68602200	1.64839700	3.46751400	Structure <b>8-Li-<math>\alpha</math>_d</b> (B3LYP/6-31+g(d,p))			
C	-0.87497200	-0.82067700	2.84211000	C	-3.80862900	-2.12623000	-0.27875300
H	-1.56172200	-1.44833100	3.42784000	C	-4.21151900	-0.73373900	-0.79767800
H	-0.29675900	-1.43926800	2.15587000	C	-3.97572600	0.49736800	0.11834300
H	-0.19051400	-0.29993800	3.52377200	C	-2.50037800	1.01340600	0.10685800
C	-4.27397800	-1.30574900	0.76979100	C	-1.37326500	-1.26336500	-0.26160200
H	-4.31924100	-0.25966500	1.07308700	C	-2.36527500	-2.27702700	0.27708600
H	-5.21147700	-1.58136700	0.26616100	C	-0.64733100	-1.54742200	-1.35399600
H	-4.14918200	-1.94025200	1.65853000	C	-1.99640100	1.66493500	-1.19704800
C	-3.04944700	-2.77368200	-0.62441700	H	-2.48147200	1.79942300	0.87533600
H	-3.96057900	-3.05862500	-1.16847500	C	-4.41047400	0.19076900	1.56911400
H	-2.19933400	-2.78319700	-1.30389200	C	-4.89273500	1.63339400	-0.39725900
H	-2.88096200	-3.48775700	0.19345000	H	-3.93250800	-2.82335200	-1.11744800
				H	-4.51833800	-2.45518600	0.49101800
				H	-5.28442500	-0.78227600	-1.03265500

Structure **8-Li- $\alpha$ \_c** (B3LYP/6-31+g(d,p))

H	-3.70645200	-0.55333500	-1.75399200	H	0.52006700	-2.02387500	-1.70501800
H	-2.01301000	-3.29228200	0.05642300	H	-0.65523200	-1.43171100	-2.88057500
H	-2.38994800	-2.19202600	1.37086600	C	-1.58761600	0.62162300	-1.19227700
H	-0.74962000	-2.50202900	-1.86842200	H	-1.92512000	1.03800400	-2.16220500
H	0.05167000	-0.82784900	-1.76706600	C	0.53418700	0.90414000	-2.49604900
H	-2.48839200	2.62225100	-1.40016100	H	0.51482300	1.98270400	-2.29168700
H	-2.20304300	1.01448600	-2.05660700	H	1.59048700	0.64847600	-2.67664900
H	-4.36046100	1.09887100	2.18201300	H	0.01614400	0.76835800	-3.47537600
H	-3.77715400	-0.56104100	2.04822100	C	-0.12217500	0.09461200	-1.37020000
H	-5.44516100	-0.17371400	1.59922500	Li	1.58100300	0.02558500	-0.06841200
H	-4.70215700	2.57095300	0.13913800	O	2.62259800	1.77906600	0.29333100
H	-5.94868900	1.37268700	-0.25114600	O	1.80193500	-0.83274900	1.80906400
H	-4.74111300	1.82110200	-1.46506100	O	3.23030100	-1.28697000	-0.84229600
C	-0.45920100	1.82406200	-0.99080600	C	3.36837700	-1.67181100	-2.21077700
H	0.05497800	1.56271900	-1.93108500	H	3.32833300	-2.76523400	-2.30864200
H	-0.21579900	2.88320000	-0.80919300	H	2.54015900	-1.22995100	-2.76146600
C	-1.29559600	0.06500300	0.48331600	H	4.32197200	-1.30815500	-2.61874300
H	-1.37196300	-0.18234400	1.55509500	C	4.25684100	-1.84715400	-0.03313000
C	0.16223100	1.86526200	1.45412000	H	4.07339400	-1.52445900	0.99213300
H	-0.70134200	2.52429800	1.70207200	H	4.23533400	-2.94550400	-0.07865700
H	0.37955800	1.30160700	2.37476700	H	5.24817100	-1.50190300	-0.36164000
H	1.01117200	2.54944000	1.31042600	C	4.03876000	1.90395900	0.33217400
C	-0.03116300	0.94022700	0.23001300	H	4.45067600	0.92183700	0.56555200
Li	1.92772800	0.09597700	0.03951000	H	4.42790300	2.23835500	-0.63935600
O	2.98363100	-1.05430200	-1.42611100	H	4.34553400	2.62231600	1.10565900
O	2.57626200	-1.13809100	1.56383400	C	1.97659100	3.02700600	0.01614400
O	3.37009100	1.66650300	-0.01033600	H	2.16975000	3.74168100	0.82809300
C	4.09434000	2.02563600	1.16186700	H	2.34331400	3.44424100	-0.93029200
H	4.25368900	1.11297500	1.73708600	H	0.90834300	2.83037000	-0.07102900
H	5.06470100	2.46956100	0.89772500	C	1.89120300	-0.08703200	3.02066700
H	3.52277600	2.73921500	1.76985700	H	2.21614500	0.91850200	2.75111600
C	3.07275200	2.79791700	-0.82887900	H	0.91505200	-0.03593700	3.51891500
H	4.00044500	3.26078100	-1.19458600	H	2.62204300	-0.54471800	3.70248200
H	2.47532200	2.44545000	-1.67029700	C	1.35633600	-2.17251200	2.01492100
H	2.48955200	3.54019400	-0.27085200	H	1.29120700	-2.64516300	1.03399200
C	2.62426800	-2.41322200	-1.66424700	H	2.06838200	-2.72283700	2.64598600
H	3.51476500	-3.05732700	-1.62753400	H	0.36776400	-2.18512300	2.48972900
H	1.91765100	-2.70223100	-0.88659000				
H	2.14048000	-2.52327800	-2.64359100	Structure 8-Li- $\alpha$ _f (B3LYP/6-31+g(d,p))			
C	3.86481600	-0.54531900	-2.42058900	C	-4.23972300	1.49030700	-0.47430000
H	4.77493200	-1.15926300	-2.48361900	C	-4.52527000	0.14953900	0.21854100
H	3.37722500	-0.52975700	-3.40535600	C	-3.36114100	-0.89315900	0.32433200
H	4.13372300	0.46794200	-2.12308600	C	-2.34093300	-0.72442900	-0.84753000
C	1.64038300	-1.53020700	2.56925500	C	-1.69689800	1.69156000	0.03818800
H	2.00628500	-1.24981500	3.56654300	C	-3.08527200	2.32620100	0.09509700
H	0.70901800	-1.00888600	2.35232400	C	-0.72999300	2.17554400	0.83276900
H	1.47424400	-2.61555100	2.53575100	C	-1.29213400	-1.85083900	-0.98356600
C	3.83542800	-1.78236800	1.70025900	H	-2.95834700	-0.79096600	-1.75508100
H	4.30792800	-1.52250300	2.65862900	C	-4.01126000	-2.29463800	0.21126100
H	3.72509300	-2.87481200	1.64695700	C	-2.71160900	-0.81874400	1.72391300
H	4.46363700	-1.44357900	0.87500400	H	-5.15506700	2.09573300	-0.42545000
				H	-4.06139900	1.31362500	-1.54114200
Structure 8-Li- $\alpha$ _e (B3LYP/6-31+g(d,p))				H	-5.35536400	-0.31548700	-0.33060800
C	-1.69830500	0.15918500	1.79957400	H	-4.91143500	0.34015100	1.23039900
C	-3.04337500	-0.55226300	1.59623300	H	-3.31146800	2.61546500	1.13054500
C	-3.60766300	-0.64510600	0.14447100	H	-3.04745100	3.26534500	-0.47674500
C	-2.50878900	-0.65462700	-0.96129500	H	-0.93170900	2.97244600	1.54748600
C	-1.70367100	1.79052500	-0.22921000	H	0.28214700	1.79456200	0.76445600
C	-1.57243400	1.59338600	1.28051000	H	-1.72599700	-2.77459000	-1.38457000
C	-1.86793600	3.04176800	-0.69657400	H	-0.84428800	-2.08981200	-0.00976600
C	-1.53129700	-1.85453500	-0.95265500	H	-4.83399900	-2.39235400	0.93089900
H	-3.07827900	-0.75147900	-1.89631000	H	-4.42313400	-2.46153100	-0.79148100
C	-4.60673900	0.50759000	-0.11679500	H	-3.29396800	-3.09566100	0.41853100
C	-4.42065700	-1.95864800	0.04597000	H	-1.92666700	-1.57459200	1.82890400
H	-0.90480700	-0.42683100	1.32906800	H	-3.46590500	-1.02292500	2.49457800
H	-1.48886100	0.16878000	2.87952700	H	-2.26736900	0.15594700	1.92879300
H	-3.80708800	-0.08097100	2.23172000	C	-0.23040100	-1.23560600	-1.89832400
H	-2.92366300	-1.57041200	1.99187800	H	0.67708000	-1.86017700	-1.93564800
H	-0.58596900	1.96538700	1.59350400	H	-0.62798800	-1.22863500	-2.94268100
H	-2.30348300	2.24001900	1.78504300	C	-1.47874400	0.61578100	-1.01660000
H	-1.92455300	3.90143200	-0.02973000	H	-1.90169100	1.08656400	-1.93425600
H	-1.96401600	3.24165600	-1.76054100	C	0.53129100	1.11765000	-2.42044700
H	-1.99469100	-2.76349200	-1.35475700	H	0.55083300	2.16468400	-2.08783300
H	-1.19524900	-2.09070700	0.06500500	H	1.55702000	0.86689700	-2.73597600
H	-5.44907800	0.44505700	0.58377000	C	-0.08231700	1.10339200	-3.35371100
H	-4.15168000	1.49398000	-0.01321500	C	-0.02261500	0.18138500	-1.33883400
H	-5.01389400	0.43999100	-1.13317300	Li	1.68042900	-0.05801500	-0.05234100
H	-4.88814300	-2.06076600	-0.94097100	O	1.80231300	-1.22660100	1.65009500
H	-5.22134200	-1.97140600	0.79640900	O	2.81459800	1.62506900	0.67266300
H	-3.79362300	-2.84018500	0.21497000	O	3.43985100	-0.89190200	-0.98478900
C	-0.35628900	-1.36374100	-1.80671400	C	2.91222000	2.76966200	-0.17635500

H	2.68757900	2.44096800	-1.19020300	H	-4.82428800	-2.36639400	-0.15643300
H	2.18559500	3.53659100	0.12040900	H	-1.27321500	-1.94966200	2.10480100
H	3.92702600	3.18922200	-0.13331200	C	-1.79584200	-2.90543000	2.24992200
C	3.10750600	1.93524900	2.02974000	H	-0.60513300	-2.01549000	1.24605000
H	2.37073900	2.63955600	2.44017800	H	-0.69172300	-1.71289400	3.00541500
H	3.07262500	1.00102700	2.59156100	C	-3.22872000	-1.82195900	-2.23045100
H	4.11061700	2.37612600	2.11867400	H	-3.97118300	-1.64498300	-3.02091600
C	0.97856600	-0.94088900	2.78149900	H	-2.23779200	-1.52970100	-2.57502700
H	1.54763300	-1.07190600	3.71284500	H	-3.22542800	-2.88940700	-1.97086000
H	0.63900300	0.09112100	2.68857700				
H	0.10162600	-1.59741300	2.79756600				
C	4.70273500	-0.76467700	-0.34035600	Structure <b>8-Li-<math>\beta</math>_b</b> (B3LYP/6-31+g(d,p))			
H	5.30119400	0.03049800	-0.80595400	C	-3.35357400	0.67854400	1.40949200
H	4.51303000	-0.50765900	0.70156400	C	-2.95344000	1.28001700	0.02692900
H	5.26222200	-1.70960600	-0.39426500	C	-1.58433100	0.70687500	-0.48947300
C	3.57314500	-1.24847200	-2.36072600	C	-2.30570100	-1.73620000	-0.20884600
H	2.56974700	-1.32201700	-2.77695400	C	-3.08807200	-1.92451600	1.07668800
H	4.14118900	-0.48227600	-2.90575100	C	-2.65633200	-2.40564600	-1.31939800
H	4.08725900	-2.21485700	-2.45825700	C	-1.34715300	0.74177700	-2.02101300
C	2.14392900	-2.60883000	1.56465800	H	-0.81178000	1.33979400	-0.02809900
H	2.74434100	-2.73520600	0.66358700	C	-2.76313500	2.80207700	0.24041300
H	2.72190700	-2.91989900	2.44617700	C	-4.12002000	1.10721400	-0.97187300
H	1.23937300	-3.22639800	1.48943900	H	-2.47620000	0.70046000	2.07273600
				H	-4.08304900	1.36689000	1.86039500
				H	-3.71558200	-2.82285800	1.01537600
Structure <b>8-Li-<math>\beta</math>_a</b> (B3LYP/6-31+g(d,p))				H	-2.37956900	-2.09152500	1.90219700
C	4.47989000	0.09123200	-0.43890300	H	-3.49223000	-3.10352700	-1.31541300
C	3.61174800	-0.86152700	0.42656000	H	-2.13065400	-2.28393000	-2.25905600
C	2.13245800	-0.99852300	-0.05872300	H	-1.15874300	1.76062900	-2.38791900
C	1.67845300	1.58916000	0.12961300	H	-2.24171300	0.39268300	-2.54444400
C	2.74229300	1.97518900	-0.87896900	H	-2.04237800	3.00140500	1.04370500
C	1.26084000	2.50705900	1.02178900	H	-2.39143600	3.28451000	-0.67126200
C	1.90385400	-1.46045200	-1.50890100	H	-3.70944300	3.28695200	0.51102100
H	1.72720100	-1.81289200	0.56550800	H	-4.24094800	0.07249200	-1.29949900
C	3.64146200	-0.43210300	1.90966900	H	-3.96744900	1.72468600	-1.86304500
C	4.27961100	-2.25746600	0.34402300	H	-5.06138700	1.43082400	-0.50915200
H	5.52384900	-0.03369700	-0.11642200	C	-0.17277100	-0.24056700	-2.29636800
H	4.44766300	-0.26162000	-1.47818300	H	-0.47824100	-0.95875300	-3.08645600
H	2.54339800	1.51284300	-1.85105200	H	0.69166900	0.29065700	-2.73647200
H	2.70876000	3.06114800	-1.03381400	C	-1.14878800	-0.73929600	-0.10108800
H	1.62333200	3.53323100	1.00433100	H	-0.89311700	-0.73437400	0.97186300
H	0.55591300	2.24969200	1.80883100	C	0.14772900	-0.91940400	-0.94133100
H	2.30642300	-2.46196400	-1.70770100	C	-3.99222800	-0.72488900	1.43973700
H	2.37335700	-0.77246500	-2.22281400	H	-4.86481000	-0.73239100	0.77579800
H	4.67533300	-0.37090700	2.27326700	H	-4.38681300	-0.89221000	2.45180900
H	3.16742100	0.53803500	2.07330200	C	0.60505100	-2.37105000	-1.10959300
H	3.11745900	-1.16966300	2.53099400	H	-0.07423000	-3.01835400	-1.70389500
H	3.69481700	-3.00718100	0.89087900	H	1.58138700	-2.43378400	-1.61421400
H	5.28375700	-2.23162600	0.78549800	H	0.72541900	-2.88215600	-0.14126400
H	4.38135900	-2.60139300	-0.69052700	Li	1.82201500	-0.04267800	0.05348800
C	0.37340700	-1.37966800	-1.63488200	O	1.98410300	-0.36514700	2.09618900
H	0.05374800	-1.40719600	-2.68783000	O	2.31104500	1.97929900	0.05158200
H	-0.05192800	-2.28865100	-1.16805900	O	3.70538300	-0.65412600	-0.60734900
C	1.10317900	0.18691400	0.14104100	C	1.33894600	0.57832400	2.95229000
H	0.69589000	0.06777900	1.15668600	H	0.26334000	0.37030200	3.01735000
C	4.16474400	1.59313200	-0.42125400	H	1.77766700	0.54569100	3.95906200
H	4.88495900	2.09093200	-1.08548700	H	1.48825600	1.56527100	2.51333200
H	4.33717300	2.00621600	0.58058900	C	1.79645200	-1.70969900	2.54045500
C	-0.19161400	1.03267300	-2.00426900	H	2.24029000	-1.84973900	3.53577500
H	-1.09773300	0.87640000	-2.61104500	H	0.72973400	-1.96169300	2.57512000
H	-0.28083500	2.03639500	-1.56877600	C	2.29098700	-2.36369400	1.82128900
H	0.63810900	1.09104100	-2.74421800	H	3.86455200	-0.80002700	-2.01793000
C	-0.06612500	-0.06749500	-0.92719800	H	3.87735900	-1.86015000	-2.30117300
Li	-2.00926500	-0.06531000	-0.03945600	H	3.00920500	-0.31744700	-2.49230100
O	-2.20723400	-0.90701100	1.82183200	H	4.79748200	-0.32290100	-2.34975600
O	-3.52416700	-1.02544600	-1.08315300	C	4.72810500	-1.30837700	0.13221700
O	-3.07169000	1.69543700	0.26420600	H	4.53569100	-1.11701600	1.18931000
C	-2.49647000	2.65148100	1.15588400	H	4.71484700	-2.39143600	-0.05400700
H	-3.25870500	3.36930800	1.48965000	H	5.71840200	-0.91308100	-0.13570900
H	-2.11047500	2.10149200	2.01525700	C	1.76266500	2.84991900	-0.93868200
H	-1.66772200	3.18353800	0.67434500	H	2.42973500	2.91454100	-1.80940400
C	-3.61441700	2.31250500	-0.90361800	H	0.80553100	2.42836100	-1.24243300
H	-2.83551400	2.85631500	-1.45222200	H	1.61252700	3.85610800	-0.52455200
H	-4.00890200	1.51397600	-1.53265400	C	3.58875600	2.40771200	0.50860500
H	-4.42189900	3.00549600	-0.62946300	H	3.52805000	3.41685800	0.93949900
C	-3.13228800	-0.68712100	2.87708800	H	3.91338000	1.70264900	1.27533000
H	-3.79121700	0.12619000	2.56720300	H	4.31826100	2.41035100	-0.31266500
H	-3.73003400	-1.58941300	3.07100500				
H	-2.61097600	-0.40185900	3.80175200	Structure <b>8-Li-<math>\beta</math>_c</b> (B3LYP/6-31+g(d,p))			
C	-4.79140200	-1.32769500	-0.51452900	C	-4.21088500	0.69436300	-0.45359100
H	-4.94099200	-0.64760000	0.32534100	C	-2.99473000	1.30030500	0.30025000
H	-5.59521700	-1.17956200	-1.24967200	C	-1.60047400	0.78087400	-0.18083400

C	-2.19977900	-1.74309900	0.24297600	H	-2.54133000	0.39492000	-2.25360300
C	-3.33588000	-1.74054700	-0.75939800	H	-3.54231900	2.21487700	2.27675200
C	-2.14778300	-2.72462800	1.16261100	H	-2.22090200	1.04414900	2.40856000
C	-1.31173700	0.93620300	-1.70842300	H	-1.91233200	2.66120300	1.74340400
H	-0.88083800	1.42993800	0.33697400	H	-2.63700600	3.24678200	-0.63030000
C	-3.14180700	1.07778100	1.82100900	H	-4.26637300	3.03751800	0.03117400
C	-3.04164000	2.82743300	0.04725400	H	-3.80604700	2.21590900	-1.46584400
H	-5.10683700	1.23054200	-0.10800700	C	-0.52045600	-0.44273700	-2.13817000
H	-4.11814200	0.94094000	-1.51918000	H	-1.00256800	-1.25111000	-2.73026500
H	-2.98242400	-1.44813100	-1.75443400	H	0.26246800	-0.04876400	-2.81014100
H	-3.73103700	-2.76037700	-0.85284600	C	-1.12830800	-0.64807800	0.23582800
H	-2.85905200	-3.54799300	1.16578600	H	-0.71844500	-0.53351700	1.25189400
H	-1.38447500	-2.73970100	1.93788900	C	0.03184900	-0.94340300	-0.78526400
H	-0.75928700	1.86563500	-1.89663500	C	-4.36226800	-0.72854900	-0.60433400
H	-2.23095000	1.01382500	-2.29868500	H	-4.47956500	-0.22013400	-1.56845200
H	-4.08914600	1.49654600	2.18421900	H	-5.32762700	-1.21087900	-0.40656800
H	-3.11450200	0.01925600	2.09085700	C	0.42505100	-2.42327200	-0.86905400
H	-2.32973300	1.58047100	2.36228800	H	-0.36647600	-3.08735800	-1.28002100
H	-2.22205900	3.33778100	0.56879600	H	1.30079500	-2.57567700	-1.51783700
H	-3.98350900	3.25585700	0.41150200	H	0.68785300	-2.84742900	0.11042100
H	-2.95910600	3.06463300	-1.01917200	Li	1.82958300	-0.05202100	-0.03385400
C	-0.48586600	-0.30371600	-2.12191700	O	3.57802900	-0.63663500	-0.98252900
H	-1.13620700	-1.00987500	-2.68654900	O	2.19391800	1.98908700	-0.02196600
H	0.30643800	-0.03150300	-2.83754200	O	2.35552200	-0.43850400	1.92822700
C	-1.12928100	-0.66031800	0.20390800	C	4.90661700	-0.61252100	-0.47961300
H	-0.73466000	-0.62398200	1.23146100	H	5.50430000	0.16020900	-0.98438800
C	0.04741100	-0.90714400	-0.81292600	H	4.84627000	-0.38609700	0.58637100
C	-4.49019600	-0.81007900	-0.33051600	H	5.39667100	-1.58654800	-0.61921900
H	-5.36726100	-1.03310700	-0.95410400	C	3.51771400	-0.93086500	-2.37772800
H	-4.77543900	-1.06285500	0.69851800	H	2.46675000	-0.90532000	-2.66480100
C	0.41726800	-2.38271000	-1.00211700	H	4.08130800	-0.18331300	-2.95365700
H	1.30093300	-2.49966800	-1.65038300	H	3.92942100	-1.92856400	-2.58026200
H	0.65993400	-2.88593900	-0.05528500	C	2.58700800	-1.80382300	2.27916600
H	-0.37832400	-3.00086700	-1.47259800	C	3.08958500	-2.27513400	1.43363900
Li	1.85319300	-0.04053000	-0.03405500	H	3.22263700	-1.86738400	3.17313300
O	3.43716200	0.18637400	-1.35408900	H	1.63895700	-2.32244000	2.46601600
O	2.73339800	-1.13292400	1.51458600	C	1.65384400	0.27024500	2.95099000
O	2.09322600	1.84334600	0.82375800	H	2.25685900	0.31699700	3.86829300
C	2.39505100	2.14807200	2.18104300	H	1.46935300	1.27827600	2.57742900
H	2.80330600	1.24152800	2.62903800	H	0.69373700	-0.21289900	3.16922500
H	3.14015100	2.95414100	2.24167200	C	3.29917300	2.64562900	0.58493800
H	1.49078700	2.45743800	2.72288400	H	3.67305300	1.99119600	1.37406500
C	1.60585400	2.97142400	0.09972800	H	4.09908400	2.82860600	-0.14674300
H	2.36976400	3.76054600	0.05710500	H	2.99093500	3.60635200	1.02065800
H	1.36853600	2.63004000	-0.90842700	C	1.62817900	2.74343500	-1.09458300
H	0.69687100	3.37206100	0.56610000	H	1.23348400	3.70017800	-0.72709800
C	1.86230100	-1.60126700	2.54553700	H	2.38326000	2.93859100	-1.86898700
H	2.43116900	-1.80514700	3.46328100	H	0.81785400	2.14659200	-1.51187500
H	1.12759500	-0.81741900	2.73433800				
H	1.33722100	-2.50970000	2.22794200	Structure <b>8-Li-<math>\beta_e</math></b> (B3LYP/6-31+g(d,p))			
C	3.72343100	-2.10044700	1.17015700	C	-4.53650200	-0.63142900	0.48104000
H	4.32646100	-1.67221200	0.36893800	C	-3.83425800	0.63585600	-0.08266600
H	4.36213300	-2.32290400	2.03614800	C	-2.46398500	0.88894000	0.63619100
H	3.25396500	-3.02726500	0.81618000	C	-1.42489400	-1.48771300	-0.04135900
C	4.60919700	0.96235200	-1.13542300	C	-2.51502900	-2.24357000	0.69873200
H	4.54705500	1.36140900	-0.12251700	C	-0.66196600	-2.15969600	-0.92181000
H	5.51310000	0.34470400	-1.23776500	C	-1.87501100	2.31259500	0.42515100
H	4.66611400	1.79372000	-1.85204700	H	-2.70947400	0.79396200	1.70524400
C	3.37983200	-0.36916600	-2.66826500	C	-4.78442100	1.81378800	0.25149400
H	4.22827200	-1.04651500	-2.83828600	C	-3.72354900	0.53375100	-1.61671500
H	2.44377500	-0.92066600	-2.74200500	H	-4.60606700	-0.52426300	1.57430400
H	3.39782100	0.42791300	-3.42369900	H	-5.57230200	-0.62840400	0.11251400
				H	-2.29991700	-3.31806400	0.64110200
				H	-2.49243200	-1.97286000	1.76548700
				H	-0.82993200	-3.21846100	-1.11362500
Structure <b>8-Li-<math>\beta_d</math></b> (B3LYP/6-31+g(d,p))				H	0.13425600	-1.67587400	-1.47247300
C	-4.13005300	0.29530000	0.51725300	H	-2.22174900	3.01853100	1.19088000
C	-2.96236800	1.31494100	0.36246300	H	-2.19360500	2.72003800	-0.54071900
C	-1.65011100	0.73256000	-0.26056000	H	-4.41381200	2.76327100	-0.14453000
C	-2.18513200	-1.74034700	0.35021000	H	-5.77826100	1.63947800	-0.18005900
C	-3.26751500	-1.84363100	-0.70647100	H	-4.90684700	1.92782100	1.33583800
C	-2.14160500	-2.64076800	1.34881500	H	-3.02036800	-0.24092500	-1.93079300
C	-1.57386300	0.65152200	-1.81414400	H	-3.38894900	1.47882400	-2.05546900
H	-0.86401700	1.44163900	0.03605800	H	-4.70462900	0.30033000	-2.05091500
C	-2.63841200	1.83904100	1.78098100	H	-0.33555900	2.13234000	0.41298300
C	-3.44434000	2.51935900	-0.47826300	C	0.15704800	2.98955100	-0.06905800
H	-3.98212000	-0.26527500	1.444727000	H	0.01802000	2.10980800	1.46073900
H	-5.05383900	0.87431400	0.65902800	C	-1.17782900	-0.05082100	0.37148400
H	-2.80832300	-1.82067500	-1.69940300	H	-0.81463200	-0.18859200	1.40877400
H	-3.74860200	-2.82455300	-0.61751700	C	-3.93882100	-2.00675200	0.16487200
H	-2.84586300	-3.46768400	1.40988600	H	-3.94773300	-2.18857900	-0.91726300
H	-1.38787600	-2.58527100	2.13212200				
H	-1.31153500	1.62796400	-2.24146600				

H	-4.59969400	-2.76558600	0.60659900	C	1.48563300	-0.98454700	2.89592600
C	-0.24496100	1.03420400	-1.82127200	H	0.69362500	-0.25164900	2.73921200
H	-0.19707700	0.11604300	-2.41909400	H	1.08281400	-1.98623100	2.70460700
H	-1.18600900	1.52830300	-2.12652500	H	1.85179700	-0.92329900	3.93014800
H	0.55944500	1.68950100	-2.19266200	C	4.74598700	0.57572300	-0.85852000
C	-0.05474900	0.79081500	-0.30268700	H	4.56108100	1.17369100	0.03429100
Li	1.95619800	0.11754100	0.01308900	H	5.62169600	-0.07101200	-0.70383800
O	2.46339200	-0.93309200	1.73799700	H	4.94741800	1.24421800	-1.70740400
O	2.95016500	-1.11265500	-1.39156800	C	3.68876700	-1.00880100	-2.26845300
O	3.50045100	1.55392900	0.08481400	H	4.51038700	-1.73068300	-2.16333600
C	1.49817500	-1.82430400	2.30127300	H	2.74548700	-1.53898100	-2.38845700
H	1.99071000	-2.73272400	2.67631900	H	3.87126200	-0.37966900	-3.15020400
H	0.96138100	-1.33903700	3.12676800	C	1.89478800	2.66185600	1.55169000
H	0.79398300	-2.08044200	1.50860300	C	2.21922500	1.98905700	2.34677100
C	4.76500300	1.46595000	-0.56192400	H	2.50480500	3.57574100	1.57353600
H	4.81523900	2.15601200	-1.41603800	H	0.84014000	2.93030800	1.69980800
H	5.57877900	1.70868900	0.13688400	C	1.73107100	2.76150400	-0.81516100
H	4.87226200	0.43978900	-0.91438300	H	0.68271900	3.08021700	-0.76703900
C	3.22656300	2.86538800	0.57668800	H	2.38004900	3.64628300	-0.87497900
H	3.98411900	3.16535900	1.31480800	H	1.87402200	2.13756800	-1.69842900
H	3.21752300	3.59309000	-0.24572800				
H	2.24164500	2.83833200	1.04100800				
C	2.77762800	-0.84269100	-2.78170900	Structure 8-H- $\alpha_a$ (B3LYP/6-31+g(d,p))			
H	1.95684500	-1.44103700	-3.19705900	C	1.85851200	1.56586600	-0.80906800
H	2.52947800	0.21451400	-2.87932900	C	2.20729700	0.07321200	-0.73344800
H	3.70216100	-1.06329400	-3.33390500	C	1.52394000	-0.80202200	0.35148000
C	3.23954500	-2.48364600	-1.13224500	C	-0.02473700	-0.93545700	0.20009300
H	3.35676900	-2.58462700	-0.05293000	C	-0.48822700	1.67529700	0.18531300
H	2.41724600	-3.12636600	-1.47299800	C	0.36803500	1.89280100	-1.04522500
H	4.16804700	-2.78483800	-1.63777800	C	-0.84587300	2.72469200	0.94239700
C	3.43072000	-0.50491300	2.68956000	C	-0.54812600	-1.44901000	-1.17757200
H	4.10496000	0.18124200	2.17636800	H	-0.29379200	-1.70693000	0.93402200
H	2.94860800	0.01643800	3.52844200	C	1.85756200	-0.26689400	1.76103400
H	3.99772100	-1.36159200	3.08095200	C	2.13236100	-2.21977300	0.22791000
				H	2.43825100	1.99783700	-1.63570300
				H	2.19034900	2.08463000	0.09867800
Structure 8-Li- $\beta_f$ (B3LYP/6-31+g(d,p))				H	3.29205600	-0.00944800	-0.57807300
C	-4.14758100	0.52699500	-0.27696100	H	2.02138000	-0.37632900	-1.71760300
C	-2.85602400	1.33698600	0.02183100	H	0.00039600	1.30100700	-1.89307700
C	-1.53633100	0.61497500	-0.40403200	H	0.28767900	2.94473500	-1.34210600
C	-2.40378400	-1.77316000	-0.04974500	H	-0.58229100	3.74294200	0.66733300
C	-3.47114400	-1.66422900	1.02335600	H	-1.41559000	2.60083700	1.86040000
C	-2.58059300	-2.63258300	-1.06611500	H	-0.63313500	-2.54054800	-1.16942600
C	-1.26393100	0.47908100	-1.92426400	H	0.13811100	-1.20641400	-1.99400500
H	-0.72771700	1.24064100	0.00211700	H	2.94314500	-0.23315200	1.91347000
C	-2.78492400	1.69964800	1.52215800	H	1.46519300	0.73950600	1.92975700
C	-2.95862400	2.66744000	-0.76253500	H	1.43573100	-0.92223600	2.53282200
H	-4.98900600	1.23385400	-0.31245300	H	1.70135100	-2.90073200	0.97137200
H	-4.06512000	0.10844100	-1.28642200	H	3.21601500	-2.19173900	0.39062300
H	-3.96428600	-2.63315200	1.16885300	H	1.95770100	-2.65102200	-0.76395500
H	-2.99362300	-1.41629400	1.97973800	C	-1.92690200	-0.77588200	-1.40658500
H	-3.45548300	-3.28051800	-1.10294900	H	-1.85250700	-0.01508400	-2.19178700
H	-1.87978100	-2.72058800	-1.88588500	H	-2.68978700	-1.48953700	-1.73761300
H	-1.01304700	1.44322100	-2.38262900	C	-0.93772900	0.27417000	0.58311800
H	-2.16172700	0.11609700	-2.43835300	H	-1.06483500	0.29241500	1.67162100
H	-2.63992900	0.82071000	2.15645300	C	-2.31040900	-0.10927800	-0.06518900
H	-1.94984200	2.38631400	1.71161300	C	-3.13259300	-1.04682500	0.83493000
H	-3.70401000	2.20157500	1.84963100	H	-3.35798600	-0.57458200	1.79802800
H	-3.13814100	2.49632900	-1.82881600	H	-4.08552000	-1.30072700	0.35653200
H	-2.03754800	3.25670400	-0.66805300	H	-2.60755800	-1.98727200	1.03892600
H	-3.78508700	3.27883300	-0.37970200	H	-2.90302100	0.79645400	-0.23535700
C	-0.11428600	-0.56475600	-2.05033100				
H	-0.40551900	-1.35139100	-2.77818400	Structure 8-H- $\alpha_b$ (B3LYP/6-31+g(d,p))			
H	0.77847500	-0.09557500	-2.50459000	C	1.56206800	1.69096800	-1.10221900
C	-1.20846100	-0.82158400	0.11560100	C	2.10530300	0.26798200	-0.91815400
H	-1.04360800	-0.77327700	1.20563800	C	1.69869000	-0.52886200	0.35158100
C	0.12840300	-1.10357500	-0.61579500	C	0.20227900	-0.97272800	0.38489500
C	-4.55530000	-0.59877500	0.69492600	C	-0.67576200	1.53948800	0.12090900
H	-5.41531100	-1.10597400	0.23960200	C	0.02734900	1.80921100	-1.19356100
H	-4.92646600	-0.16339400	1.63174300	C	-1.08674900	2.55893700	0.89179300
C	0.60085600	-2.55982900	-0.57112100	C	-0.27407000	-1.90916700	-0.75099700
H	0.05185200	-3.27172700	-1.22357800	H	0.12419000	-1.57389600	1.30310100
H	1.66032400	-2.67172700	-0.85882500	C	2.02754200	0.27357500	1.62970800
H	0.52367500	-2.97420600	0.44579400	C	2.57332100	-1.80686900	0.37072400
Li	1.85827200	-0.08708000	0.10373400	H	1.99017300	2.09206400	-2.03066900
O	3.57784700	-0.20216800	-1.09503500	H	1.91926400	2.34289100	-0.29555400
O	2.07417900	1.96851900	0.32066300	H	3.20239000	0.33040700	-0.92194800
O	2.53912500	-0.67903400	1.97938200	H	1.84343500	-0.32588500	-1.80435200
C	3.61924700	-1.60394700	2.07854900	H	-0.33457900	1.12230400	-1.97086800
H	3.28014700	-2.62380200	1.85440400	H	-0.22529900	2.82146200	-1.52954000
H	4.37048100	-1.30508700	1.34687800	H	-0.96141700	3.59382500	0.58248300
H	4.05712000	-1.57939500	3.08598900	H	-1.55819200	2.39203600	1.85703500

H	0.18406000	-2.90153700	-0.69733100	H	-0.42866200	-0.45645100	-2.06908000
H	-0.03357900	-1.49298600	-1.73773800	H	1.50556300	-1.92010400	2.05684000
H	3.08210300	0.57541700	1.63506100	H	1.59933300	-0.15777100	2.12367900
H	1.41938900	1.17564600	1.72587800	H	3.00021800	-1.09640700	1.59287300
H	1.85613600	-0.34143600	2.52163000	H	1.30366100	-3.16857400	-0.15684100
H	2.29588700	-2.46571000	1.20218200	H	2.91737200	-2.49394700	-0.43419800
H	3.63049700	-1.54450700	0.49299400	H	1.66133500	-2.30752800	-1.66382200
H	2.48070100	-2.37880900	-0.55834000	C	-2.31816000	-0.82741700	-1.03764600
C	-1.79399800	-1.94540600	-0.56190700	H	-2.80059000	-0.35752600	-1.90154700
H	-2.33286600	-2.35396800	-1.42446900	H	-2.87155700	-1.75293200	-0.83772800
H	-2.04784500	-2.56983000	0.30686200	C	-0.86143900	0.38611300	0.56288600
C	-0.94681300	0.10441900	0.53073500	H	-0.74288000	0.45813100	1.65211700
H	-1.23838000	0.13373400	1.58718200	C	-2.35194200	0.09479300	0.22233300
C	-2.16137200	-0.47723400	-0.28273200	C	-3.09289800	-0.55722700	1.40037900
C	-3.51142300	-0.27227200	0.40550300	H	-2.60929100	-1.49042700	1.71444200
H	-3.70693200	0.79055600	0.58592100	H	-3.12899600	0.11187900	2.26798200
H	-4.33186500	-0.66317900	-0.20773900	H	-4.12528000	-0.80049200	1.12336300
H	-3.53965400	-0.79083800	1.37220000	H	-2.86794100	1.03331700	-0.00189300
H	-2.19580000	0.03998700	-1.25165500				

Structure **8-H- $\alpha$ \_c** (B3LYP/6-31+g(d,p))

C	-2.07151800	1.80332400	-0.32869300
C	-2.38474100	0.32735800	-0.61117400
C	-1.55880800	-0.77480600	0.11471800
C	-0.13523900	-0.92433700	-0.51926800
C	0.44877900	1.62551400	0.05368700
C	-0.66623200	2.28120300	-0.73647800
C	0.98436700	2.26115500	1.10652600
C	0.66664200	-2.15310000	-0.00162300
H	-0.33142800	-1.10033800	-1.58558800
C	-2.31773200	-2.10295600	-0.13227700
C	-1.53387300	-0.52285100	1.63774000
H	-2.22282600	2.02208300	0.73550300
H	-2.80904900	2.40935800	-0.87187200
H	-2.31135700	0.14947600	-1.69480500
H	-3.44059900	0.16663400	-0.35395700
H	-0.61527900	3.36754900	-0.59887100
H	-0.52135300	2.09104900	-1.81003400
H	0.63784700	3.25103100	1.39360400
H	1.76914400	1.83266600	1.72049500
H	0.38499200	-3.07598000	-0.51774400
H	0.47622400	-2.31211000	1.06652500
H	-2.38283600	-2.33137100	-1.20332200
H	-1.83343200	-2.94922200	0.36367800
H	-3.34031900	-2.03596300	0.25637100
H	-1.11681000	-1.37999700	2.17663700
H	-2.55520900	-0.37654300	2.01051600
H	-0.94907200	0.35844900	1.90732100
C	2.14110500	-1.79159300	-0.19692100
H	2.81969000	-2.41041300	0.40137600
H	2.43171200	-1.91470100	-1.25053600
C	0.91707100	0.27675300	-0.46203200
H	1.17661800	0.46994200	-1.51564000
C	2.20039500	-0.30547300	0.18305300
C	3.49735100	0.38794000	-0.24467900
H	3.50217000	1.44958100	0.10941600
H	4.36720500	-0.08128000	0.22973500
H	3.63241700	0.31384300	-1.33134600
H	2.10614700	-0.24252700	1.27706200

Structure **8-H- $\alpha$ \_d** (B3LYP/6-31+g(d,p))

C	2.26663600	1.53788900	-0.01098100
C	2.11659300	0.16483100	-0.69369100
C	1.42104600	-0.98679800	0.08275200
C	-0.13658000	-0.90388300	0.04602100
C	-0.30880500	1.68238700	-0.01829300
C	0.98564900	2.16535900	0.60569400
C	-0.88260300	2.37905700	-1.01081900
C	-0.82978700	-1.14083600	-1.31290800
H	-0.47904300	-1.71092700	0.71247800
C	1.90636500	-1.03514000	1.54823600
C	1.84609000	-2.31685700	-0.58474500
H	2.65622900	2.22430600	-0.77275500
H	3.03894100	1.48384700	0.76597000
H	3.12991600	-0.17049900	-0.95345400
H	1.59786100	0.30035100	-1.65004300
H	1.05100500	3.25521200	0.51499200
H	0.95623900	1.95044500	1.68097000
H	-0.44084200	3.30632000	-1.36768900
H	-1.79641900	2.06440400	-1.50415500
H	-0.68714900	-2.15824000	-1.68781800

Structure **8-H- $\alpha$ \_e** (B3LYP/6-31+g(d,p))

C	-0.68460100	0.91387400	1.83492200
C	-1.93274500	0.35616500	1.13108500
C	-1.78237600	-0.23912800	-0.30537100
C	-0.38414700	-0.86779000	-0.59242900
C	0.77676700	1.52564900	-0.24446400
C	0.15232700	1.95532600	1.08180200
C	1.26494300	2.46108900	-1.07413300
C	-0.00640500	-2.08975900	0.28804300
H	-0.46356300	-1.24385900	-1.62160900
C	-2.10709900	0.83744600	-1.36885900
C	-2.85465100	-1.34446100	-0.46391700
H	-0.03694000	0.08280100	2.13051700
H	-1.01268700	1.37079900	2.77785800
H	-2.70285400	1.13872700	1.08878500
H	-2.34312700	-0.41833900	1.79219400
H	0.96189700	2.27431100	1.75360500
H	-0.45273200	2.85399700	0.90516600
H	1.20758600	3.52135300	-0.83700200
H	1.73391100	2.19903300	-2.01877700
H	-0.48461400	-3.01061700	-0.06043700
H	-0.32643900	-1.94076800	1.32649600
H	-3.14501400	1.17353500	-1.25828600
H	-1.46143500	1.71374000	-1.29898700
H	-1.99868600	0.42747200	-2.38060900
H	-2.84023300	-1.76899000	-1.47509400
H	-3.85518400	-0.92936800	-0.29328600
H	-2.71180400	-2.16202100	0.24959900
C	1.52383200	-2.16177400	0.21921600
H	1.96526500	-2.77064000	1.01671300
H	1.83836000	-2.60326600	-0.73767100
C	0.91133800	0.05650500	-0.59610100
H	1.29779800	0.03572800	-1.62235000
C	1.97268700	-0.69204200	0.27720500
C	3.41505800	-0.44875900	-0.16936200
H	3.66596400	0.61729200	-0.14667400
H	4.12376000	-0.97452400	0.48103500
H	3.57193600	-0.80857100	-1.19434400
H	1.87926500	-0.35186500	1.31734300

Structure **8-H- $\alpha$ \_f** (B3LYP/6-31+g(d,p))

C	-1.74808600	1.58289000	-1.13923000
C	-2.32982000	0.64997600	-0.06406400
C	-1.56156700	-0.69428500	0.25081200
C	-0.22608800	-0.83211600	-0.55855600
C	0.44596600	1.61316900	0.18814600
C	-0.54526900	2.40982100	-0.63606900
C	0.89985900	2.08847200	1.35646400
C	0.54883900	-2.16102400	-0.30031300
H	-0.53403700	-0.84542400	-1.61016200
C	-2.47759300	-1.86655500	-0.18028600
C	-1.35743600	-0.79511100	1.77978000
H	-2.53007100	2.28021700	-1.46450700
H	-1.47286600	1.01375600	-2.03446400
H	-3.35542700	0.39190200	-0.35426400
H	-2.42552800	1.23061700	0.86240100
H	-0.91001700	3.25104800	-0.03473700
H	-0.02450700	2.84663100	-1.50135600
H	0.54953300	3.04003300	1.74819000
H	1.62805300	1.55895400	1.96229000
H	0.24667300	-2.95215100	-0.99379100
H	0.35297600	-2.53497200	0.70962800

H	-3.43705200	-1.81560300	0.34744100	H	3.85210900	-0.82246200	-0.23433400
H	-2.68706900	-1.83081100	-1.25666500	H	2.63423800	-1.19770200	-1.45936000
H	-2.03089000	-2.84097200	0.04315300	C	-1.58689200	-1.70357200	-0.91527600
H	-0.94817800	-1.76436300	2.08206600	H	-2.03036400	-1.15794500	-1.75720000
H	-2.32308700	-0.68499900	2.28772600	H	-1.96588700	-2.72955400	-0.97994300
H	-0.69527900	-0.00982900	2.15191000	C	-0.81455100	-0.07772700	0.77767600
C	2.03759600	-1.80906300	-0.42121500	H	-0.80743500	0.06766400	1.86417800
H	2.68884600	-2.52712300	0.09014900	C	-1.99819900	-1.04098700	0.42161800
H	2.34618900	-1.78560700	-1.47637500	C	1.09809700	1.48273400	-1.45366700
C	0.88592800	0.30076500	-0.43016400	H	1.36714300	0.78471800	-2.25452100
H	1.15843600	0.55074500	-1.46929600	H	1.42848600	2.46920400	-1.79969200
C	2.13269800	-0.39271200	0.16713000	C	-3.40426700	-0.44190400	0.42123900
C	3.45913600	0.31181600	-0.13033500	H	-3.51234300	0.33602900	-0.34164000
H	3.48534600	1.32545900	0.28103100	H	-4.14934700	-1.22005100	-0.21751900
H	4.30299400	-0.24523200	0.29314600	H	-3.65039600	0.01013100	1.38870000
H	3.62126400	0.38632200	-1.21326900	H	-1.97139900	-1.81976100	1.19757800
H	2.00872700	-0.47485000	1.25715100				

Structure **8-H-β\_a** (B3LYP/6-31+g(d,p))

C	1.93539300	0.46110400	-1.07918700
C	1.77392100	-0.37478100	0.21880700
C	0.34584700	-0.97232200	0.41998100
C	-0.84222300	1.39157600	0.30568700
C	-0.35993000	1.68835500	-1.10003100
C	-1.24893900	2.39784300	1.09575000
C	-0.22486200	-1.84458600	-0.71667300
H	0.45687700	-1.65555900	1.27674900
C	2.17160000	0.45428300	1.45939700
C	2.77279500	-1.55346400	0.11138400
H	3.00637800	0.67905200	-1.19418300
H	1.67296300	-0.17384000	-1.93602500
H	-0.71439800	0.92713000	-1.80536300
H	-0.79262200	2.64158000	-1.42536100
H	-1.29292000	3.42319300	0.73609500
H	-1.55214700	2.23006500	2.12648900
H	0.36935500	-2.74494300	-0.90283000
H	-0.27247300	-1.28985900	-1.66123900
H	3.19454500	0.83584000	1.35503000
H	1.51019000	1.30806900	1.62187000
H	2.14198900	-0.16804500	2.36225900
H	2.69023100	-2.22452200	0.97461400
H	3.80302300	-1.18058500	0.07800200
H	2.60853100	-2.14701300	-0.79392400
C	-1.63774500	-2.17146400	-0.22015500
H	-2.30414200	-2.51135800	-1.02095800
H	-1.58369200	-2.98331100	0.51611300
C	-0.84831900	-0.03564700	0.83272000
H	-0.83707800	0.05800300	1.92327500
C	-2.15370800	-0.86819400	0.45228300
C	1.17641700	1.78900900	-1.20312000
H	1.42568500	2.22323700	-2.18059300
H	1.53211400	2.50476200	-0.45180900
C	-3.19338300	-0.14725100	-0.41948300
H	-4.07745500	-0.78436600	-0.53638900
H	-3.51522100	0.79818900	0.02589800
H	-2.81265900	0.07024100	-1.42370300
H	-2.65826800	-1.12271800	1.39181100

Structure **8-H-β\_b** (B3LYP/6-31+g(d,p))

C	1.88861400	1.15988700	-0.17679700
C	1.82850900	-0.29082700	0.38416100
C	0.40907300	-0.94207900	0.34723500
C	-0.92590600	1.30730600	0.15002300
C	-0.45743700	1.52619000	-1.27564200
C	-1.43056200	2.32732900	0.86093900
C	-0.03758500	-1.64265100	-0.97201900
H	0.45033200	-1.74727300	1.09579500
C	2.29473300	-0.22220200	1.85720800
C	2.82825200	-1.18549300	-0.38226800
H	1.55680400	1.85199500	0.60579500
H	2.94641600	1.39638000	-0.35446400
H	-0.92236600	0.78604600	-1.93491700
H	-0.82731700	2.50034700	-1.61205100
H	-1.54433400	3.31988200	0.43215000
H	-1.74941100	2.20318400	1.89304600
H	0.40686700	-2.63990200	-1.04639100
H	0.29452200	-1.09655700	-1.85817500
H	3.26874300	0.27572200	1.93375700
H	1.58622700	0.34073900	2.47474200
H	2.39822900	-1.22532700	2.28792400
H	2.78921400	-2.22153000	-0.02506800

Structure **8-H-β\_c** (B3LYP/6-31+g(d,p))

C	2.06948900	0.51859000	-0.92065800
C	1.80108300	-0.33993300	0.34468700
C	0.37608900	-0.97434300	0.40664700
C	-0.91558800	1.31456000	0.13064300
C	-0.29494400	1.57999700	-1.22650500
C	-1.48526000	2.32474100	0.80675200
C	-0.05423300	-1.83187000	-0.82781400
H	0.42877500	-1.67245900	1.25455500
C	2.05356100	0.49089800	1.62133900
C	2.82981700	-1.49585400	0.32266000
H	3.12658000	0.81738100	-0.88973500
H	1.97715600	-0.12320300	-1.80646800
H	-0.51649700	0.77041200	-1.93237700
H	-0.74453700	2.48847800	-1.64377000
H	-1.57092500	3.32081600	0.37915400
H	-1.88566500	2.19017300	1.80858600
H	0.23832100	-2.87707500	-0.68353600
H	0.43604800	-1.50355200	-1.74865900
H	3.07871500	0.88067800	1.62995100
H	1.37218200	1.34126100	1.70783400
H	1.92874700	-0.12938300	2.51741800
H	2.71134100	-2.14635800	1.19723600
H	3.85346400	-1.10382800	0.33523300
H	2.72418100	-2.11571100	-0.57440700
C	-1.59114000	-1.68880600	-0.94322400
C	-1.86110000	-1.05370500	-1.79656500
H	-2.09348400	-2.64981500	-1.10082300
C	-0.85296800	-0.07266100	0.75478100
H	-0.88795100	0.07974500	1.83947300
C	-2.04366500	-1.01532900	0.36631600
C	1.23437300	1.78613100	-1.15245000
H	1.56671800	2.22900800	-2.10085300
H	1.44616500	2.53265100	-0.37713100
C	-3.43774800	-0.39226800	0.30927900
H	-4.18839500	-1.16100600	0.09089100
H	-3.70964400	0.07823100	1.26078800
H	-3.50521200	0.37612400	-0.46754600
H	-2.05818100	-1.79197300	1.14602700

Structure **8-H-β\_d** (B3LYP/6-31+g(d,p))

C	-2.15476900	0.60874500	-0.83245400
C	-1.68590200	-0.67796300	-0.08629300
C	-0.17080800	-0.98740000	-0.35447800
C	0.63976200	1.37727100	0.28766500
C	-0.33215300	2.42047300	-0.22606900
C	1.23827500	1.52222000	1.47918200
C	0.57939400	-1.81297400	0.72283100
H	-0.15063500	-1.58403000	-1.27872200
C	-2.50404600	-1.85960900	-0.66057200
C	-2.03234700	-0.56880900	1.41540800
H	-1.79686200	0.57130000	-1.87150200
H	-3.25036500	0.55726700	-0.89722700
H	-0.24034500	3.34049000	0.36290400
H	-0.05502700	2.67772500	-1.25878000
H	1.04895300	2.39763700	2.09592000
H	1.92590100	0.78871700	1.88593500
H	0.26856800	-2.86328400	0.72140200
H	0.36091400	-1.41957700	1.71919900
H	-2.41135200	-1.91272800	-1.75216900
H	-2.16170000	-2.81576900	-0.24826900
H	-3.56839000	-1.75508100	-0.41871200
H	-1.39916100	0.14689700	1.94483900
H	-1.93011300	-1.53833500	1.91368600



H	-3.07548900	-0.25157200	1.53631300	H	-2.58081500	-1.04769700	-1.52184600
C	2.09044200	-1.63529200	0.41465100	H	-2.50200300	-2.50355100	-0.54766000
H	2.63710200	-1.31977500	1.31137800	C	-0.83050900	0.11559200	0.69933400
H	2.55906800	-2.56812200	0.08144700	H	-0.65000400	0.37852900	1.75010000
C	0.80791100	0.19358100	-0.65108200	C	-2.17106300	-0.66630500	0.60680600
H	0.60283000	0.57390300	-1.65920400	C	1.82445500	1.94828300	-0.28582600
C	2.17309900	-0.55248900	-0.69532800	H	1.98173000	2.61458900	-1.14285000
C	-1.81270200	1.97648500	-0.20801700	H	2.62281200	2.18477400	0.42798700
H	-2.17083100	1.99497800	0.82771100	C	-3.48083700	0.10767300	0.78077300
H	-2.39393900	2.74215900	-0.73859700	H	-3.66219700	0.82648500	-0.02139100
C	3.44754800	0.29489800	-0.69250500	H	-4.32786900	-0.58845000	0.80298700
H	3.57034000	0.85787500	0.23656600	H	-3.48592300	0.66217400	1.72661300
H	4.32868700	-0.34587200	-0.81629600	H	-2.12437000	-1.37137300	1.44927400
H	3.44523500	1.01597000	-1.51845900				
H	2.15439700	-1.08559200	-1.65700000				
Structure <b>8-H-<math>\beta_e</math></b> (B3LYP/6-31+g(d,p))				Structure <b>8-CO<sub>2</sub>-<math>\alpha_a</math></b> (B3LYP/6-31+g(d,p))			
C	-2.42290200	-0.26004000	-0.20882000	C	1.90511000	1.95769600	-0.83770800
C	-1.18043700	-1.08958000	0.22020000	C	2.64581000	0.61308300	-0.81946700
C	0.03738300	-0.80617000	-0.72567800	C	2.30054700	-0.42004900	0.28773900
C	0.07656400	1.85097500	-0.25377200	C	0.84539800	-0.99146500	0.22232800
C	-1.34101000	2.03521100	-0.76010000	C	-0.27699100	1.39083300	0.34659300
C	0.66971700	2.85413800	0.41217500	C	0.36841700	1.86999600	-0.93724600
C	1.19952800	-1.84320000	-0.60697200	C	-0.75853400	2.28644300	1.22149500
H	-0.38394900	-0.90588100	-1.73493300	C	0.43266900	-1.65192500	-1.13271400
C	-1.58862900	-2.57328300	0.04006400	H	0.85586300	-1.79991900	0.96577500
C	-0.87747000	-0.84997200	1.71210800	C	2.56251900	0.18078000	1.68540000
H	-2.60978700	-0.45271900	-1.27596800	C	3.27797900	-1.60706700	0.09988500
H	-3.29086200	-0.67028100	0.32536200	C	2.28125600	2.52661700	-1.70114300
H	-1.58752300	3.10212900	-0.71966000	H	2.16524000	2.54569100	0.05250300
H	-1.39225400	1.74325100	-1.82024300	H	3.72421700	0.82164500	-0.74359400
H	0.13655700	3.78178800	0.60498900	H	2.50887400	0.13156500	-1.79662600
H	1.69166700	2.80774600	0.76825600	H	0.08548900	1.22559800	-1.77674100
H	1.08338800	-2.67145400	-1.31295600	H	-0.02438700	2.86594300	-1.17142600
H	1.21199100	-2.28973600	0.39283900	H	-0.76616500	3.35060800	0.99399200
H	-0.79931400	-3.26168900	0.35496200	H	-1.23116500	1.97798600	2.14927300
H	-2.47848900	-2.79812800	0.63922800	H	0.60060300	-2.73536700	-1.08482200
H	-1.82902700	-2.79399800	-1.00724000	H	1.03971900	-1.29193600	-1.97164100
H	-0.52957700	0.16718400	1.90835200	H	3.60083200	0.52973600	1.76862800
H	-0.11596400	-1.54322400	2.08358300	H	1.90111500	1.02315500	1.90010200
H	-1.78188600	-1.01622100	2.31016400	H	2.40139600	-0.57593900	2.46370900
C	2.50745400	-1.06147800	-0.82853400	H	3.10218400	-2.38384600	0.85439200
H	3.38022300	-1.57266900	-0.40656500	H	4.31963800	-1.27404900	0.19801600
H	2.69531600	-0.92673000	-1.90175100	H	3.16611100	-2.06880300	-0.88742700
C	0.79716500	0.59055000	-0.69628300	C	-1.06183900	-1.31784000	-1.34749600
H	0.96768100	0.78840000	-1.76807900	H	-1.20237600	-0.51546000	-2.07601800
C	2.23298600	0.30433200	-0.16743900	H	-1.63059000	-2.17914900	-1.72008100
C	-2.41450600	1.25528100	0.01909800	C	-0.36578600	-0.09436300	0.65897500
H	-2.31578600	1.48212900	1.08801500	H	-0.48310800	-0.16419200	1.74564700
H	-3.39797400	1.63940200	-0.28294500	C	-1.61237900	-0.82675000	0.00670200
C	2.44921200	0.21871400	1.35545800	C	-2.00989600	-2.02627200	0.89206200
H	2.11548800	1.11150400	1.88781300	C	-2.37605700	-1.67160000	1.85850700
H	1.92854500	-0.63329700	1.79841000	H	-2.82790800	-2.58244300	0.41815300
H	3.51844600	0.08867600	1.56000700	H	-1.17747700	-2.72765300	1.04893900
H	2.91275800	1.07094700	-0.56067200	C	-2.85388800	0.14888500	-0.13279000
				O	-3.00660200	0.69828600	-1.25620900
				O	-3.54691300	0.28920300	0.90987500
Structure <b>8-H-<math>\beta_f</math></b> (B3LYP/6-31+g(d,p))				Structure <b>8-CO<sub>2</sub>-<math>\alpha_b</math></b> (B3LYP/6-31+g(d,p))			
C	2.00321500	0.51028600	-0.81161200	C	-2.63082800	1.74628800	0.08233900
C	1.69492900	-0.67794800	0.14042200	C	-2.95401700	0.26585800	-0.15808900
C	0.17446100	-1.00422300	0.26171600	C	-1.88752000	-0.80759900	0.20511300
C	-0.68035800	1.40338900	-0.10153100	C	-0.69458800	-0.77817300	-0.81301100
C	0.45411600	2.29713700	0.36273400	C	-0.07774600	1.73967900	-0.18792700
C	-1.40770800	1.75502600	-1.17226800	C	-1.40719900	2.29494900	-0.67401100
C	-0.52463400	-1.61583200	-0.98075400	C	0.65596700	2.44982800	0.68235800
H	0.11151200	-1.76335300	1.05693500	C	0.20923000	-2.04252100	-0.77681200
C	2.28073200	-0.41538600	1.54566100	H	-1.19181900	-0.76076400	-1.79547000
C	2.40966500	-1.92712500	-0.42804700	C	-2.60543500	-2.17179700	0.04125900
H	3.05046900	0.41934100	-1.13093000	C	-1.45452000	-0.67157000	1.67828100
H	1.40533200	0.39063800	-1.72245900	H	-2.48780400	1.92859700	1.15466900
H	0.21575800	3.34286600	0.13922600	H	-3.51457000	2.33207000	-0.21372800
H	0.53786500	2.22850900	1.45374500	H	-3.22139400	0.13370200	-1.21895400
H	-1.21880400	2.69582200	-1.68457600	H	-3.86654900	0.03416100	0.41197900
H	-2.19696900	1.13857500	-1.58466600	H	-1.39604200	3.38693500	-0.56224700
H	-0.20602300	-2.64689000	-1.15858400	H	-1.53158700	2.08882200	-1.74885900
H	-0.27472700	-1.04448900	-1.88150700	H	0.29486500	3.42095400	1.02308700
H	1.79317000	0.41951400	2.05659200	H	1.60020200	2.09251100	1.08283900
H	2.16963000	-1.30212500	2.18104200	H	-0.17738400	-2.83817300	-1.42748100
H	3.35117600	-0.18623900	1.48245600	H	0.28240800	-2.42109200	0.24368700
H	2.14579000	-2.10576400	-1.47454500	H	-2.92321300	-2.33452400	-0.99775900
H	2.15262500	-2.82751700	0.14299900				
H	3.49730000	-1.80009200	-0.37825700				
C	-2.04737400	-1.51628000	-0.68737100				

H	-1.95896800	-3.00469900	0.33054000	H	0.55491300	-2.43414500	-1.59445400
H	-3.50076000	-2.20977100	0.67515000	H	0.44830500	-0.74796000	-2.09599900
H	-0.70000300	-1.41539600	1.94435900	H	2.56128500	-1.44888800	2.10900000
H	-2.32845500	-0.79302000	2.33504100	H	2.14858800	0.26690100	2.12789500
H	-1.00151300	0.29876000	1.88788100	H	3.77526700	-0.24414700	1.64584800
C	1.60799200	-1.57402700	-1.19058400	H	2.76134400	-2.75249900	-0.06091600
H	2.38948300	-2.26470400	-0.85631900	H	4.12877500	-1.65910700	-0.34894500
H	1.67687600	-1.49490200	-2.28856600	H	2.88361700	-1.86864500	-1.59094400
C	0.34484500	0.42800300	-0.82720500	C	-1.37494600	-1.45702500	-1.11287000
H	0.38646400	0.69607000	-1.89871900	H	-1.90093000	-0.97405400	-1.93947500
C	1.77965500	-0.16580400	-0.56954900	H	-1.76031800	-2.48332600	-1.05792200
C	2.83828600	0.63950000	-1.34195900	C	-0.33903800	0.06045000	0.52221400
H	2.93848100	1.65178500	-0.94590700	H	-0.27156300	0.22073200	1.60499800
H	3.82075200	0.16389700	-1.25087800	C	-1.67864000	-0.69010200	0.20815800
H	2.57759000	0.69584000	-2.41052500	C	-1.98692800	-1.68961700	1.34955900
C	2.22123800	-0.30274700	0.96084800	H	-1.18530300	-2.42560000	1.50418600
O	1.70001100	-1.24552800	1.61382900	H	-2.16292100	-1.14470500	2.28134000
O	3.07008600	0.53473900	1.36865500	H	-2.90053000	-2.24753900	1.10973900
Structure <b>8-CO<sub>2</sub>-α<sub>c</sub></b> (B3LYP/6-31+g(d,p))				C	-2.94408800	0.26593500	0.15317900
C	1.61787200	1.83111700	-1.13548300	O	-3.14276600	0.92806000	1.20494100
C	2.18572100	0.40680200	-1.19600400	O	-3.63165800	0.24129500	-0.90336500
C	2.20915500	-0.43116600	0.11223400	Structure <b>8-CO<sub>2</sub>-α<sub>e</sub></b> (B3LYP/6-31+g(d,p))			
C	0.81600700	-0.98316300	0.55500400	C	-0.74328900	0.84314700	1.80857400
C	-0.23389900	1.48398200	0.59515000	C	-2.08760800	0.23484700	1.38058800
C	0.11548200	1.92580500	-0.81157900	C	-2.23415700	-0.29941600	-0.08018300
C	-0.43850300	2.40409800	1.55374700	C	-0.90715300	-0.81237600	-0.72401900
C	0.17198000	-2.03520500	-0.37288400	C	0.16176200	1.62648400	-0.50606400
H	1.03678400	-1.51274700	1.49626400	C	-0.16024800	1.96673800	0.94360400
C	2.84212600	0.37451600	1.26943500	C	0.32027100	2.62685400	-1.39013300
C	3.13745200	-1.64282800	-0.15317400	C	-0.26203500	-2.05655100	-0.06961800
H	1.77670100	2.29058800	-2.12190300	H	-1.21563000	-1.12964900	-1.73262200
H	2.19133500	2.43742300	-0.42055400	C	-2.87294800	0.78566500	-0.98218600
H	3.22501100	0.47591400	-1.55325100	C	-3.24171800	-1.47509600	-0.04346100
H	1.63647700	-0.15532600	-1.96168800	H	0.00336200	0.05244700	1.90826900
H	-0.44067900	1.33240000	-1.54387400	H	-0.87110400	1.24137800	2.82546200
H	-0.20307500	2.96762200	-0.93555300	H	-2.89588400	0.96375400	1.54908300
H	-0.41361900	3.46918200	1.33251800	H	-2.29074500	-0.59236000	2.07470800
H	-0.67797600	2.12205400	2.57680300	H	0.78484300	2.26840900	1.40900100
H	0.70643100	-2.99336800	-0.34467000	H	-0.83012000	2.83990000	0.95429500
H	0.12408400	-1.68155900	-1.40632200	H	0.23485900	3.66996200	-1.08984100
H	3.81957900	0.77923100	0.97275000	H	0.57543300	2.43692200	-2.43006700
H	2.21275700	1.20834600	1.58867700	H	-0.81389100	-2.97615900	-0.30216400
H	3.00267500	-0.27534900	2.13985100	H	-0.20646900	-1.95917200	1.01878700
H	3.13416500	-2.33788800	0.69624300	H	-3.87216400	1.04684000	-0.60853500
H	4.17104100	-1.30600100	-0.30708200	H	-2.27681100	1.69794500	-1.02847300
H	2.83195700	-2.20065400	-1.04442500	H	-2.98818000	0.41477000	-2.00958000
C	-1.26128200	-2.14319100	0.14926100	H	-3.42826100	-1.87096900	-1.05062400
H	-1.92773900	-2.63966200	-0.56238400	H	-4.20342400	-1.13895100	0.36658600
H	-1.27328600	-2.71634200	1.09170100	H	-2.88230600	-2.29767700	0.58236700
C	-0.36472100	0.00770300	0.93350400	C	1.16339200	-2.06640800	-0.62687400
H	-0.43445500	-0.01778500	2.02822500	H	1.83156600	-2.71422600	-0.05416500
C	-1.70845800	-0.68722800	0.41682100	H	1.14813100	-2.40868800	-1.67569200
C	-2.78205700	-0.61055800	1.51092900	C	0.30695100	0.18913600	-0.97675900
H	-3.06128600	0.42936700	1.69772200	H	0.37964000	0.27478200	-2.06845000
H	-3.69198200	-1.13505900	1.19570200	C	1.62781400	-0.59700600	-0.56234300
H	-2.42499300	-1.07039600	2.44543900	C	2.74599200	-0.30368400	-1.57604800
C	-2.27935600	-0.02915800	-0.91656400	H	3.02970200	0.75092700	-1.52924800
O	-1.81250800	-0.47464200	-2.00450300	H	3.63965700	-0.89669800	-1.34386800
O	-3.12312100	0.88724800	-0.76081900	H	2.42846900	-0.55284800	-2.60029100
Structure <b>8-CO<sub>2</sub>-α<sub>d</sub></b> (B3LYP/6-31+g(d,p))				C	2.20408900	-0.23478700	0.87910200
C	2.37017900	2.03083900	-0.03714800	O	2.09267100	-1.11471300	1.77570300
C	2.62770600	0.65821600	-0.68680000	O	2.73140700	0.90397500	0.97304400
C	2.25636700	-0.62121300	0.11090700	Structure <b>8-CO<sub>2</sub>-α<sub>f</sub></b> (B3LYP/6-31+g(d,p))			
C	0.73622400	-0.98077300	0.05655200	C	-2.81007000	1.29619900	-0.49936400
C	-0.13817400	1.42548100	-0.13171600	C	-2.66437900	0.24637000	0.61310100
C	0.93826900	2.28103300	0.51244600	C	-1.68727700	-0.95713100	0.33818600
C	-0.79963200	1.88307000	-1.20391200	C	-0.68833700	-0.66376300	-0.83348500
C	0.16611800	-1.45133600	-1.30262200	C	-0.31132200	1.78739700	0.02042600
H	0.63741900	-1.83171000	0.74501500	C	-1.63499500	2.31662700	-0.51690400
C	2.70850100	-0.49744300	1.58297800	C	0.28058000	2.39505900	1.05919900
C	3.05138400	-1.79500600	-0.51130400	C	0.29223200	-1.82549800	-1.17544100
H	2.58761500	2.78477800	-0.80575100	H	-1.33115300	-0.51735100	-1.71103700
H	3.10012700	2.20350000	0.76569300	C	-2.54492800	-2.17010700	-0.09951100
H	3.70169200	0.61079700	-0.92283100	C	-0.99345700	-1.30283400	1.67097700
H	2.10546100	0.62346200	-1.64972700	H	-3.74699400	1.85097000	-0.35139700
H	0.69135600	3.34067400	0.37656700	H	-2.91030800	0.80494500	-1.47439900
H	0.92603400	2.10422100	1.59495200	H	-3.65421100	-0.17029700	0.84709100
H	-0.59211500	2.88261000	-1.58504000	H	-2.33635700	0.76713900	1.52010100
H	-1.60253000	1.33474400	-1.68356700	H	-1.91718100	3.18700800	0.08839200

H	-1.49548100	2.68523000	-1.54509100	H	-0.96126100	2.19826100	-1.87701400
H	-0.19793800	3.25895200	1.52234200	H	-1.00616200	3.22775900	1.51052900
H	1.22404200	2.03562300	1.46528600	H	0.32353200	2.08070200	2.08798600
H	-0.08988300	-2.45134600	-1.99267100	H	0.34138700	-2.09732900	1.92212300
H	0.46165100	-2.46166900	-0.30567300	H	-0.32520200	-0.53067700	2.37417400
H	-3.26265200	-2.43766300	0.68674500	H	-1.60172400	-2.88427500	-1.18733300
H	-3.11504200	-1.94715000	-1.01210100	H	-1.58965600	-3.20149700	0.55346600
H	-1.92452900	-3.05032800	-0.29804400	H	-3.12116600	-2.83942100	-0.26696800
H	-0.34292900	-2.17704600	1.59749400	H	-2.45517600	0.28585600	1.66065100
H	-1.75641600	-1.50301700	2.43703000	H	-2.43765800	-1.41970200	2.12020000
H	-0.37009900	-0.47693000	2.02142500	H	-3.73258800	-0.80428900	1.08575500
C	1.63190100	-1.15832300	-1.52539600	C	1.70545000	-0.38330200	1.58115400
H	2.47560500	-1.83633200	-1.37373300	H	1.81724600	0.34428900	2.39829700
H	1.63322500	-0.82743300	-2.57762900	H	2.51714400	-1.10986500	1.66971400
C	0.25033100	0.60711800	-0.75193900	C	0.34118900	0.48403200	-0.27666100
H	0.24839400	0.97829100	-1.79403300	H	0.38147000	0.47321400	-1.36920900
C	1.72667700	0.08015500	-0.60299100	C	1.81525400	0.30738600	0.19654200
C	2.72948100	1.10875900	-1.15229100	C	-2.68531400	1.19364800	-1.04027800
H	2.78787400	1.98386300	-0.50183200	H	-3.34554600	1.34583900	-0.17709500
H	3.73463600	0.67211200	-1.20227400	H	-3.26285200	1.51551100	-1.91909400
H	2.44761400	1.43042500	-2.16696600	C	2.66426300	1.58936700	0.22515800
C	2.22113100	-0.36107100	0.85623000	H	2.28345800	2.33588800	0.93127800
O	2.60921100	0.57083700	1.61245900	H	3.69022600	1.33382400	0.51404200
O	2.22238000	-1.59480500	1.10206500	H	2.70125300	2.04798400	-0.76991900
Structure <b>8-CO<sub>2</sub>-β<sub>a</sub></b> (B3LYP/6-31+g(d,p))				C	2.56891900	-0.65518700	-0.85477900
C	2.85824100	0.02900400	-0.64633600	O	2.21188600	-0.54368300	-2.05853000
C	2.08112600	-0.88350400	0.33993300	O	3.47596500	-1.38024400	-0.37337700
C	0.54862700	-0.97016600	0.05575400	Structure <b>8-CO<sub>2</sub>-β<sub>c</sub></b> (B3LYP/6-31+g(d,p))			
C	0.18304300	1.63200500	0.25202000	C	2.79993500	-0.22127700	-0.62537200
C	1.12731600	1.96170200	-0.88931400	C	1.87134100	-1.06375600	0.29039900
C	-0.13870400	2.59577400	1.13244100	C	0.34502400	-0.88762700	0.01266700
C	0.10994600	-1.38357500	-1.36399300	C	0.35767800	1.73032500	0.30179500
H	0.19277800	-1.77840700	0.71338800	C	1.33497100	1.92484600	-0.84163700
C	2.31545300	-0.43472900	1.79899600	C	0.17940600	2.73196900	1.18154200
C	2.68298600	-2.30293300	0.19261600	C	-0.12443600	-1.14879700	-1.45553200
H	3.93247000	-0.12033900	-0.45754700	H	-0.13526100	-1.66051000	0.62504600
H	2.68270900	-0.33837500	-1.66665600	C	2.16559600	-0.76186300	1.77546000
H	0.78743200	1.49350000	-1.82105600	C	2.23022900	-2.54813100	0.03437400
H	1.11084000	3.04613600	-1.05928200	H	3.83676000	-0.51483300	-0.40001100
H	0.21437000	3.61909300	1.01043300	H	2.62983100	-0.52471500	-1.66686200
H	-0.78711500	2.39053700	1.98012900	H	0.93859700	1.50084500	-1.77235900
H	0.45556900	-2.38632500	-1.64794100	H	1.46634100	3.00090500	-1.01507100
H	0.49531800	-0.68623400	-2.11973300	H	0.66629100	3.69782400	1.05377500
H	3.38945100	-0.41229600	2.03038500	H	-0.47259900	2.61879600	2.04371600
H	1.90199500	0.55638400	1.99823500	H	-0.41407400	-2.19788600	-1.57721200
H	1.83634200	-1.13498800	2.49367300	H	0.67015100	-0.95795400	-2.18697300
H	2.16001300	-3.01914500	0.83728300	H	3.22172900	-0.95560100	2.00936600
H	3.74322600	-2.30574500	0.47788300	H	1.94425100	0.27604600	2.03684900
H	2.61541900	-2.66863800	-0.83787200	H	1.55311000	-1.40015700	2.42280500
C	-1.41801900	-1.29207700	-1.27906400	H	1.62100100	-3.20969300	0.66102300
H	-1.89888400	-1.21105300	-2.26034900	H	3.28636600	-2.74128400	0.26570700
H	-1.81707700	-2.19904500	-0.81078700	H	2.05973400	-2.82946400	-1.01098800
C	-0.38545100	0.23429400	0.41742900	C	-1.33582800	-0.21665600	-1.69059600
H	-0.68361500	0.13987100	1.46463200	H	-1.05355300	0.62656300	-2.33998500
C	-1.73211100	-0.05085300	-0.37969300	H	-2.18061900	-0.73500000	-2.15055100
C	2.58640900	1.53998700	-0.61786800	C	-0.37969400	0.41605700	0.47698500
H	3.22932800	2.00647500	-1.37918200	H	-0.64037100	0.32282600	1.53440300
H	2.89830400	1.96275500	0.34599600	C	-1.74280000	0.30091000	-0.29802800
C	-2.21990300	1.11406600	-1.26222200	C	2.72189000	1.31054600	-0.55260300
H	-3.17846800	0.82404900	-1.70017900	H	3.43892000	1.71224900	-1.28405200
H	-2.37327800	2.02830900	-0.68005300	H	3.05831000	1.66333600	0.43102500
H	-1.51454600	1.34577400	-2.07345500	C	-2.56611800	1.59386400	-0.37873100
C	-2.92305100	-0.43463300	0.61170900	H	-3.50274200	1.38982200	-0.91028100
O	-2.68243900	-0.43262400	1.84829800	H	-2.81874000	1.96243100	0.62145800
O	-3.99856500	-0.72718400	0.02515300	C	-2.03248100	2.39259000	-0.91063900
Structure <b>8-CO<sub>2</sub>-β<sub>b</sub></b> (B3LYP/6-31+g(d,p))				H	-2.67770200	-0.76715100	0.45644600
C	-2.39835400	-0.31408700	-1.19284400	O	-2.60621600	-0.76886200	1.71363500
C	-1.83573400	-1.08289100	0.04229500	O	-3.42102000	-1.45572400	-0.28903500
C	-0.29265900	-0.85700700	0.21183400	Structure <b>8-CO<sub>2</sub>-β<sub>d</sub></b> (B3LYP/6-31+g(d,p))			
C	-0.45984400	1.70565600	0.13937400	C	-2.73853300	0.00323600	0.45826900
C	-1.47070100	2.14011000	-0.90519100	C	-1.77181800	-1.13902100	0.04202700
C	-0.37254000	2.36555800	1.30640100	C	-0.26318000	-0.80375400	0.26058900
C	0.29925200	-1.03985000	1.63176100	C	-0.46483200	1.72898900	-0.09739500
H	0.18685700	-1.60474500	-0.43171000	C	-1.66267900	1.91215600	-1.01427000
C	-2.05146600	-2.59121600	-0.23152800	C	-0.27084900	2.61065600	0.89715000
C	-2.65797900	-0.72602100	1.30157500	C	0.24907700	-0.72242500	1.72134800
H	-1.72664300	-0.47980700	-2.04565900	H	0.28043700	-1.63008200	-0.21405600
H	-3.35359400	-0.79071800	-1.46090400	C	-2.00087200	-1.53274900	-1.43440700
H	-1.84456600	3.14742200	-0.67693700	C	-2.12228300	-2.37484800	0.90551100

H	-3.73165200	-0.43924700	0.62954100	H	0.28043700	-1.63008200	-0.21405600
H	-2.41252300	0.39335100	1.42995900	H	-2.00087200	-1.53274900	-1.43440700
H	-1.88813500	2.98014100	-1.12737700	C	-2.12228300	-2.37484800	0.90551100
H	-1.40299300	1.54209800	-2.01243700	H	-3.73165200	-0.43924700	0.62954100
H	-0.93084200	3.46981900	1.01333100	H	-2.41252300	0.39335100	1.42995900
H	0.52892800	2.51634800	1.62110700	H	-1.88813500	2.98014100	-1.12737700
H	0.30127000	-1.71347100	2.18516100	H	-1.40299300	1.54209800	-2.01243700
H	-0.42903400	-0.11494600	2.33582300	H	-0.93084200	3.46981900	1.01333100
H	-1.70442800	-0.74073000	-2.12688600	H	0.52892800	2.51634800	1.62110700
H	-1.40773000	-2.41798000	-1.68934500	H	0.30127000	-1.71347100	2.18516100
H	-3.05840300	-1.76805100	-1.61751500	H	-0.42903400	-0.11494600	2.33582300
H	-2.10135200	-2.13953000	1.97519100	H	-1.70442800	-0.74073000	-2.12688600
H	-1.41366200	-3.19232700	0.72774000	H	-1.40773000	-2.41798000	-1.68934500
H	-3.12897900	-2.74032600	0.66276600	H	-3.05840300	-1.76805100	-1.61751500
C	1.64964500	-0.05415700	1.62225500	H	-2.10135200	-2.13953000	1.97519100
H	1.71801800	0.80623100	2.30272700	H	-1.41366200	-3.19232700	0.72774000
H	2.45789400	-0.74633800	1.87201200	H	-3.12897900	-2.74032600	0.66276600
C	0.35562000	0.47967200	-0.38935300	C	1.64964500	-0.05415700	1.62225500
H	0.40455600	0.35346800	-1.47541600	H	1.71801800	0.80623100	2.30272700
C	1.81604600	0.37800000	0.14137000	H	2.45789400	-0.74633800	1.87201200
C	-2.94307000	1.18687400	-0.50790700	C	0.35562000	0.47967200	-0.38935300
H	-3.57057900	1.91717700	0.02107800	H	0.40455600	0.35346800	-1.47541600
H	-3.53122900	0.85728600	-1.37451800	C	1.81604600	0.37800000	0.14137000
C	2.69812100	1.62502900	-0.04715700	C	-2.94307000	1.18687400	-0.50790700
H	2.34176800	2.50052700	0.50561100	H	-3.57057900	1.91717700	0.02107800
H	3.71495700	1.39783900	0.29441900	H	-3.53122900	0.85728600	-1.37451800
H	2.75518900	1.89112800	-1.10867500	C	2.69812100	1.62502900	-0.04715700
C	2.57358400	-0.76603100	-0.70239100	H	2.34176800	2.50052700	0.50561100
O	2.29850900	-0.80503300	-1.93178200	H	3.71495700	1.39783900	0.29441900
O	3.39957500	-1.46648600	-0.06372700	H	2.75518900	1.89112800	-1.10867500
				C	2.57358400	-0.76603100	-0.70239100
				O	2.29850900	-0.80503300	-1.93178200
				O	3.39957500	-1.46648600	-0.06372700
Structure <b>8-CO<sub>2</sub>-<math>\beta_e</math></b> (B3LYP/6-31+g(d,p))				Structure <b>15-an-<math>\alpha_a</math></b> (B3LYP/6-31+g(d,p))			
C	-2.96203900	0.59962400	-0.42935700	C	-0.91268500	-1.58024600	0.18262900
C	-2.16405500	-0.62547100	0.09653600	C	-1.92016000	-0.822268300	-0.70272300
C	-0.81009900	-0.79550100	-0.67915400	C	-2.10168900	0.52138900	0.03449400
C	0.11254800	1.64080000	-0.02336000	C	-0.70400900	0.85682900	0.61634000
C	-1.05946800	2.34433300	-0.68624800	C	0.10533400	-0.49339100	0.61851300
C	0.92731000	2.35063600	0.77383100	C	0.15986100	1.85009800	-0.20503400
C	-0.13700900	-2.18861700	-0.48084200	C	1.55787900	1.20594200	-0.20241800
H	-1.10532200	-0.72578600	-1.73668400	C	1.26375900	-0.26473600	-0.32038500
C	-3.05536100	-1.85629200	-0.20864300	H	0.45220900	-0.72128500	1.67062100
C	-1.99411400	-0.52439300	1.62554300	H	-0.80887100	1.23912300	1.64097700
H	-3.05348700	0.50042200	-1.52206300	C	2.43944700	-1.17265500	-0.09680300
H	-3.98613400	0.52317700	-0.03308400	H	-0.42053700	-2.40488000	-0.34707100
H	-0.90630900	3.42734300	-0.60185300	H	-1.43504600	-2.00194600	1.05953300
H	-1.05950700	2.11241000	-1.76291500	H	-2.86763900	-1.36120600	-0.85187300
H	0.73114600	3.40722000	0.95258900	H	-1.46327400	-0.64801500	-1.68304500
H	1.83206000	1.94090700	1.20776800	H	-2.83011300	0.39042800	0.84957800
H	-0.46802800	-2.91367800	-1.23536500	H	-2.49013800	1.31744600	-0.61652300
H	-0.41237800	-2.60849900	0.49410200	H	0.14334000	2.86406200	0.22672600
H	-2.60893800	-2.78653600	0.15407300	H	-0.21207900	1.91758400	-1.23600800
H	-4.03588000	-1.74851200	0.27315500	H	2.06558300	1.47263100	0.77922700
H	-3.22306700	-1.96386600	-1.28809500	H	2.21394700	1.60835400	-0.98949600
H	-1.31910500	0.28502600	1.91189000	H	3.26785800	-0.97390200	-0.79275600
H	-1.59089700	-1.45226500	2.04307900	H	2.18523200	-2.23708200	-0.20426300
H	-2.96767100	-0.34542100	2.10251600	H	2.87309500	-1.06460700	0.94669500
C	1.37803300	-1.93996700	-0.52460400	Structure <b>15-an-<math>\alpha_b</math></b> (B3LYP/6-31+g(d,p))			
H	1.94996500	-2.73991900	-0.03725000	C	-1.02661900	-1.51258500	-0.00951300
H	1.73255300	-1.85275900	-1.55742100	C	-2.35593200	-0.72026700	-0.06348700
C	0.39595500	0.22078300	-0.47679400	C	-1.92109100	0.72463900	-0.37661900
H	0.78090300	0.37288200	-1.49799500	C	-0.63670800	0.91360100	0.45752600
C	1.58125900	-0.57161000	0.16831300	C	0.04854700	-0.49730500	0.48248900
C	-2.44459000	2.00580500	-0.11019400	C	0.43783700	1.89237500	-0.08407400
H	-2.42772100	2.16711000	0.97561200	C	1.74479100	1.07123400	-0.02689900
H	-3.17287100	2.72506900	-0.51386300	C	1.29505600	-0.32948600	-0.34758600
C	1.52781000	-0.76613900	1.69566500	H	0.30097000	-0.75448400	1.55694400
H	1.47079100	0.17615100	2.24294300	H	-0.92706800	1.20421000	1.47834100
H	0.67601400	-1.38290700	2.00529400	C	2.33180500	-1.39761600	-0.14559000
C	2.45127300	-1.25768300	2.01397800	H	-1.10750600	-2.39732800	0.63880800
C	2.96910500	0.06228200	-0.28936800	H	-0.74710500	-1.85129000	-1.01497700
O	3.09938800	0.20858900	-1.53490600	H	-3.07309000	-1.12328700	-0.79324200
O	3.79072400	0.34171900	0.622261000	H	-2.85024600	-0.74741700	0.91931700
Structure <b>8-CO<sub>2</sub>-<math>\beta_f</math></b> (B3LYP/6-31+g(d,p))				H	-2.70332400	1.46442900	-0.14876300
C	-2.73853300	0.00323600	0.45826900	H	-1.67813900	0.81356000	-1.44336100
C	-1.77181800	-1.13902100	0.04202700	H	0.48701500	2.82324100	0.50293100
C	-0.26318000	-0.80375400	0.26058900	H	0.21706100	2.16412100	-1.12470300
C	-0.46483200	1.72898900	-0.09739500	H	2.17477900	1.16126000	1.02159500
C	-1.66267900	1.91215600	-1.01427000				
C	-0.27084900	2.61065600	0.89715000				
C	0.24907700	-0.72242500	1.72134800				

H	2.52230100	1.46787600	-0.69764100	H	0.90331500	1.03972300	1.80050600
H	3.23814100	-1.22903700	-0.74583600	Structure 15-an- $\beta$ _c (B3LYP/6-31+g(d,p))			
H	1.96407800	-2.40209000	-0.40092000	C	1.29689500	1.12324500	0.68236900
H	2.67601200	-1.46130300	0.93403200	C	1.85379000	0.54240100	-0.63043400
Structure 15-an- $\alpha$ _c (B3LYP/6-31+g(d,p))				C	1.70755700	-0.98174300	-0.44095400
C	1.17622100	-1.35143800	0.46794300	C	0.39542300	-1.17381100	0.36148000
C	2.41466700	-0.56501500	0.00749500	C	0.06333600	0.25325900	1.01387300
C	1.87559400	0.87527500	-0.09826500	C	-0.86554400	-1.52289600	-0.45702900
C	0.46380800	0.71941100	-0.71310900	C	-1.97898600	-0.63842000	0.18091600
C	-0.03282600	-0.75905700	-0.31974500	C	-1.30299000	0.69480400	0.47324100
C	-0.61959900	1.65526000	-0.13760500	H	0.01096000	0.10584200	2.10972700
C	-1.31037000	0.79332600	0.97287900	H	0.54509000	-1.93908500	1.14130200
C	-1.35380800	-0.64138100	0.43997400	C	-1.33470900	1.63015300	-0.72298500
H	-0.16292900	-1.35748400	-1.23724700	H	1.05063100	2.18894100	0.60802600
H	0.53858000	0.82273100	-1.80462800	H	2.05971300	1.02381900	1.47307900
C	-2.56186000	-0.86955700	-0.46238300	H	2.89121100	0.84548800	-0.83648700
H	1.26511100	-2.43561200	0.32486900	H	1.24115600	0.87901400	-1.47682600
H	1.00174900	-1.18916400	1.53990800	H	2.56316300	-1.35635300	0.14214900
H	3.27712600	-0.65537800	0.68428300	H	1.71242200	-1.52639700	-1.39672300
H	2.74285900	-0.91159300	-0.98495800	H	-1.07753900	-2.60733400	-0.45474600
H	2.53239800	1.54396100	-0.67249200	H	-0.72787900	-1.22341700	-1.50715200
H	1.79308300	1.29977000	0.91360200	H	-2.32898200	-1.14600300	1.10265400
H	-1.35252800	1.90364200	-0.91718700	H	-2.86013300	-0.54217700	-0.47289000
H	-0.20130300	2.60905400	0.22774800	H	-2.37075100	1.91508000	-0.95271300
H	-2.30747100	1.18299500	1.23385400	H	-0.91542500	1.24880900	-1.70981600
H	-0.70387100	0.87928000	1.89277100	H	-0.80227800	2.57182000	-0.53245400
H	-3.50450300	-0.77949500	0.09670000	Structure 15-TS (B3LYP/6-31+g(d,p))			
H	-2.55626400	-1.88209600	-0.88988800	C	-0.97293100	-1.56236000	-0.03428700
H	-2.67299800	-0.17155000	-1.35043800	C	-2.27600000	-0.76587200	-0.26235100
Structure 15-an- $\beta$ _a (B3LYP/6-31+g(d,p))				C	-1.79910700	0.68794600	-0.43180600
C	-0.66101200	-1.49248400	-0.19400800	C	-0.68734300	0.83809600	0.62626400
C	-2.11883000	-1.01620700	-0.21907800	C	0.05298800	-0.54730000	0.64381200
C	-1.96531700	0.51189600	-0.31325600	C	0.39618000	1.88161500	0.29009300
C	-0.77208100	0.85458100	0.61606700	C	1.41306800	1.10693500	-0.58430700
C	0.08291200	-0.46587900	0.73818200	C	1.34132900	-0.27574200	-0.04517500
C	0.19667600	1.92421100	0.04607900	H	0.18323600	-0.92193200	1.69850200
C	1.32947900	1.09331900	-0.58952700	H	-1.16047800	1.04320800	1.60008600
C	1.50701100	-0.04875900	0.37547200	C	2.46445100	-1.24397900	-0.08011700
H	0.00803700	-0.87045600	1.76493000	H	-1.13878000	-2.45623800	0.58738500
H	-1.15900600	1.16153000	1.59755000	H	-0.55251500	-1.89609200	-0.99088600
C	2.43723600	-1.13953400	-0.08197400	H	-2.87617000	-1.12467200	-1.11152000
H	-0.24527800	-1.44888800	-1.21084200	H	-2.91682000	-0.83216800	0.63030300
H	-0.55017200	-2.52770000	0.15508200	H	-2.61019800	1.42014200	-0.31372400
H	-2.61911700	-1.28736700	0.72438200	H	-1.37238000	0.83295200	-1.43578000
H	-2.72151600	-1.43820700	-1.03969300	H	0.88864200	2.21219200	1.21493700
H	-2.88245800	1.06110200	-0.05573900	H	-0.02679600	2.77410000	-0.20600900
H	-1.71131300	0.77814400	-1.34949700	H	2.43277300	1.54653900	-0.52333900
H	0.60956400	2.53310600	0.85913000	H	1.12226400	1.27292700	-1.67100400
H	-0.31018500	2.59900500	-0.66446300	H	2.50158600	-1.98992700	-0.91783800
H	2.24188400	1.68586800	-0.75667300	H	2.48454000	-1.87251900	0.84042000
H	0.99610700	0.78216400	-1.63536100	H	3.44528500	-0.72455600	-0.13429400
H	2.52193400	-1.95655600	0.65252600	Structure 15-Li- $\alpha$ _a (B3LYP/6-31+g(d,p))			
H	3.45758500	-0.76208600	-0.24833800	C	-2.28903400	1.16624300	-1.22745800
H	2.14749200	-1.63652600	-1.06073900	C	-2.50881600	1.71633400	0.19270200
Structure 15-an- $\beta$ _b (B3LYP/6-31+g(d,p))				C	-3.59061300	0.78171800	0.77150100
C	-1.36424700	1.15752400	-0.49715600	C	-3.27499500	-0.61652800	0.17930200
C	-2.35769200	0.13986700	0.10957100	C	-2.33684000	-0.37300100	-1.06025800
C	-1.45105400	-0.91185800	0.77251100	C	-2.49480800	-1.59122600	1.09466900
C	-0.31791600	-1.11060700	-0.25228000	C	-1.46495800	-2.23876200	0.15595100
C	-0.10233400	0.34257800	-0.89316900	C	-0.99696000	-1.08696500	-0.75161000
C	1.07515600	-1.52912800	0.26381300	H	-2.80666300	-0.81818100	-1.96281800
C	2.04655300	-0.48204300	-0.39528100	H	-4.20654200	-1.10076200	-0.13629300
H	-0.10176500	0.19940300	-1.98911700	C	-0.40609600	-1.64230900	-2.05460700
H	-0.66615500	-1.82365000	-1.02136300	H	-1.34571300	1.50055400	-1.67519000
H	-1.80007500	1.69944100	-1.34696600	H	-3.10372100	1.51432200	-1.88066400
H	-1.11055700	1.90910000	0.25869600	H	-1.57956300	1.61391200	0.76746500
H	-3.07701400	0.59680800	0.80627100	H	-2.79794800	2.77482400	0.21729900
H	-2.94425600	-0.34013000	-0.68940100	H	-3.61632100	0.78122600	1.86916900
H	-1.98819900	-1.83744400	1.02791700	H	-4.57778700	1.12414000	0.43309200
H	-1.03723800	-0.50384000	1.70645000	H	-3.15345100	-2.31686000	1.58975100
H	1.32007500	-2.57637900	0.01827300	H	-1.97954600	-1.03566200	1.89014300
H	1.12146300	-1.43751400	1.35890100	H	-1.97926200	-3.03961700	-0.42807300
H	2.28941500	-0.85268000	-1.41020600	H	-0.66211200	-2.75008900	0.71001100
H	3.00333200	-0.41036300	0.14567700	H	0.52062000	-2.21662200	-1.89830200
C	1.27996800	0.83386600	-0.44464200	H	-0.16797900	-0.85212700	-2.78317900
C	1.33600600	1.56358900	0.89138700	H	-1.10908800	-2.33284000	-2.57882300
H	2.38265100	1.77246400	1.15411200	C	2.58217600	0.85946300	2.32405700
H	0.83837000	2.54233400	0.86243500	H	3.20644600	0.77834600	1.43480800

H	2.67810000	1.86315500	2.76222800	Structure 15-Li- $\alpha_c$	(B3LYP/6-31+g(d,p))		
H	2.90784700	0.11629000	3.06509100	C	-2.09783000	-1.35199000	0.39596100
C	0.32286100	0.67558300	3.01313400	C	-3.58900700	-1.70201200	0.28313600
H	0.57683300	-0.07585600	3.77322500	C	-4.17460000	-0.44363400	-0.38258800
H	0.33791100	1.67306600	3.47389400	C	-3.41081300	0.74376700	0.25839000
H	-0.66923900	0.46856600	2.61439400	C	-2.05211700	0.13659600	0.83340200
C	1.27705000	2.95587000	-0.48705300	C	-2.97388000	1.85163200	-0.72683500
H	1.23019300	2.82991800	0.59461600	C	-1.47677600	1.53768800	-1.01402000
H	2.10667600	3.62738100	-0.74879600	C	-0.87001000	0.99194300	0.30482700
H	0.33303100	3.38814600	-0.84316200	H	-2.08359500	0.16088600	1.93447800
C	1.52434300	1.70404700	-2.47791200	H	-4.01773200	1.16355500	1.06938600
H	1.62892100	0.67916400	-2.83428200	C	-0.66992000	2.18108500	1.27695700
H	0.59575100	2.12641200	-2.88204800	H	-1.62608200	-1.45271000	-0.59163800
H	2.37716200	2.30721100	-2.82009500	H	-1.54910200	-2.01157700	1.08128500
C	3.45726900	-1.25224500	-1.15634100	H	-4.02101700	-1.83499400	1.28519600
H	3.55000300	-0.23089000	-1.52834000	H	-3.78720900	-2.62260100	-0.28119700
H	4.43801500	-1.59811600	-0.80020400	H	-5.26279200	-0.36353500	-0.27185100
H	3.11621000	-1.91089400	-1.96654100	H	-3.96825900	-0.47980800	-1.46226200
C	2.37057200	-2.50367400	0.53466600	H	-3.06580400	2.83920000	-0.25994500
H	1.99912300	-3.24851000	-0.18007400	H	-3.59567300	1.87185400	-1.63281400
H	3.33185700	-2.83903800	0.94862900	H	-0.93851500	2.41613900	-1.40196300
H	1.64274700	-2.38860900	1.33830500	H	-1.43811400	0.77953400	-1.81444800
O	1.23845800	0.61304800	1.92034400	H	-0.23252900	1.85790300	2.23494000
O	1.48364000	1.66228300	-1.05215800	H	-1.59367700	2.73604900	1.54813100
O	2.51654700	-1.22834600	-0.08880100	H	0.01433800	2.93399200	0.85819800
Li	0.74714600	-0.03837300	-0.02492300	O	2.70971200	1.15908000	-0.60754600
				O	1.92017700	-0.74979200	1.67960200
				O	1.29219200	-1.48343700	-1.41006700
Structure 15-Li- $\alpha_b$	(B3LYP/6-31+g(d,p))			C	2.85523600	2.46053200	-0.04111900
C	-2.37297100	1.10399100	-1.02941800	H	3.91659900	2.68499800	0.13586200
C	-3.65070700	1.35219900	-0.20362500	H	2.42848500	3.22439800	-0.70430100
C	-3.56990200	0.27857700	0.90004000	H	2.31129700	2.46668900	0.90329800
C	-3.01339200	-0.96713200	0.17627800	C	3.37830400	1.03225400	-1.85725900
C	-2.21694700	-0.44088500	-1.07707800	C	2.96216000	1.73046900	-2.59721200
C	-2.02754000	-1.88256700	0.92923000	H	4.45328100	1.23305800	-1.74434400
C	-1.06270600	-2.34273500	-0.17762400	H	3.23113100	0.00624700	-2.19576700
C	-0.80164100	-1.07397100	-1.02141400	C	0.60952000	-1.35220700	-2.65656000
H	-2.75248200	-0.78920800	-1.98524600	H	-0.40129100	-1.77363700	-2.59298600
H	-3.85857800	-1.57735100	-0.16711600	H	0.53429200	-0.28665300	-2.87657500
C	-0.35662900	-1.46448200	-2.43760600	H	1.16751400	-1.86102900	-3.45534400
H	-1.50921200	1.54067300	-0.50780700	C	1.39303200	-2.84075300	-0.98769900
H	-2.41849100	1.56523800	-2.02451200	H	0.39628700	-3.28421700	-0.86420400
H	-4.53980300	1.17760400	-0.82507900	H	1.96623700	-3.43054800	-1.71666600
H	-3.72879100	2.37425800	0.19018300	H	1.90871200	-2.84007100	-0.02684700
H	-2.86662100	0.60902200	1.67775700	C	3.30943300	-0.92207000	1.92684600
H	-4.53214400	0.10085300	1.39577800	C	3.83005000	-0.72512000	0.98878700
H	-2.52392200	-2.71162000	1.45057200	H	3.66072200	-0.21475700	2.69134800
H	-1.47693000	-1.30381800	1.68497600	H	3.52410900	-1.94568600	2.26647300
H	-1.56635200	-3.14308600	-0.77088800	C	1.11848900	-0.92793500	2.84817500
H	-0.15953000	-2.81782500	0.24159300	H	1.20515600	-1.95798900	3.22140100
H	-0.27984600	-0.59914900	-3.11350000	H	1.42928300	-0.22997500	3.63713500
H	-1.07195000	-2.16506600	-2.93098800	H	0.08958600	-0.71675100	2.55823500
H	0.62310900	-1.96423000	-2.46687800	Li	1.02704900	0.05016600	0.00353900
C	1.35230800	-0.48877000	2.91276700				
H	2.03600500	-1.16288000	2.39665900	Structure 15-Li- $\beta_a$	(B3LYP/6-31+g(d,p))		
H	1.86102300	-0.02399300	3.76895700	C	2.63164000	1.62935700	0.21905500
H	0.48079900	-1.05219100	3.27050800	C	3.99970300	1.26372200	-0.38760000
C	0.04397600	1.44761000	2.52446500	C	4.42507400	0.01788600	0.41193300
H	-0.84603600	0.94255700	2.91896300	C	3.11546600	-0.77176900	0.64928100
H	0.52516800	2.01903800	3.33087000	C	1.92603500	0.27569400	0.50902500
H	-0.25729500	2.12259100	1.72234700	C	2.78948900	-1.87582800	-0.37510000
C	2.83094000	-2.33849400	-0.62118800	C	1.25079500	-1.79183300	-0.52166100
H	1.84164600	-2.79278500	-0.64225600	C	0.89781600	-0.28114500	-0.54029900
H	3.22466300	-2.27322700	-1.64421300	H	1.43500300	0.35582100	1.49194800
H	3.51069900	-2.94856100	-0.00990200	H	3.12318900	-1.21497000	1.65539600
C	3.92330800	-0.34233700	0.03253700	C	1.14045300	0.24155000	-1.97516600
H	4.65107300	-0.91430000	0.62567500	H	2.79651400	2.17652600	1.15944500
H	4.34188200	-0.16177100	-0.96738400	H	2.05053700	2.29022500	-0.43368900
H	3.72923100	0.61242900	0.52172700	H	4.73023800	2.08020500	-0.32610200
C	2.06415800	2.94408100	-0.12727000	H	3.88419900	1.00989100	-1.44792800
H	1.38800000	3.81063500	-0.10874700	H	4.85345400	0.33391400	1.37342600
H	2.27901100	2.63061400	0.89559200	H	5.19349500	-0.57606800	-0.09926700
H	2.99896500	3.23641500	-0.62698100	H	3.15765000	-2.86270000	-0.06076800
C	1.11684700	2.13933000	-2.14554200	H	3.26333100	-1.64994200	-1.33984700
H	0.41535100	2.98260500	-2.19086600	H	0.80168600	-2.31641900	0.34388000
H	2.01950300	2.38418800	-2.72254600	H	0.89081300	-2.32510500	-1.41513100
H	0.63973600	1.25028700	-2.55554100	H	0.98712400	1.32629500	-2.06472500
O	1.45779000	1.84290900	-0.78990600	H	2.14233800	0.04426600	-2.41500800
O	2.68533600	-1.03690800	-0.05226400	H	0.42598100	-0.21948300	-2.67379000
O	0.95687500	0.50425800	1.96708800	O	-2.06590900	1.79192200	-0.46483000
Li	0.82025500	-0.01348700	-0.06143500	O	-2.55517700	-1.27172000	-0.88091600

O	-1.67522900	-0.17902000	1.97194200	Structure 15-Li- $\beta_c$	(B3LYP/6-31+g(d,p))		
C	-3.28875100	1.98876600	-1.16395200	C	2.64741700	1.63356600	-0.04868700
H	-3.10032100	2.23935600	-2.21740800	C	4.17109800	1.49595100	0.16633600
H	-3.84383000	1.05121400	-1.10661500	C	4.44402100	0.00990600	-0.12540800
H	-3.87510800	2.79827200	-0.70602500	C	3.26007200	-0.71657500	0.54207400
C	-1.21519400	2.93813900	-0.48935600	C	2.03245500	0.29035700	0.43671300
H	-0.98054000	3.22344500	-1.52301800	C	2.76409700	-2.04050400	-0.07143200
H	-1.69482200	3.78418300	0.02253400	C	1.21439100	-1.88470300	-0.07356300
H	-0.29319300	2.66026500	0.02199800	C	0.90998700	-0.40011700	-0.40257300
C	-3.02631000	-2.39574500	-0.14242700	H	1.66657700	0.44827500	1.46389500
H	-3.98020900	-2.75561100	-0.55273400	H	3.51055900	-0.87557900	1.60191900
H	-2.29297300	-3.21319400	-0.16596500	C	1.11952800	-0.20267600	-1.92344300
H	-3.16874600	-2.06406300	0.88666900	H	2.23752900	2.50458000	0.47956200
C	-2.30349900	-1.58924800	-2.25000300	H	2.45399700	1.78830000	-1.11621700
H	-1.53083800	-2.36326400	-2.33272000	H	4.42705400	1.71833400	1.21224500
H	-3.22574300	-1.93242700	-2.73931000	H	4.75849800	2.17833200	-0.46158000
H	-1.94565200	-0.67986600	-2.73393800	H	5.42409400	-0.32399400	0.23823200
C	-2.51968300	0.71633100	2.68524300	H	4.42409200	-0.16176800	-1.21086300
H	-3.19822600	0.16578900	3.35248100	H	3.10971100	-2.92302300	0.48366500
H	-1.92432600	1.41985500	3.28383100	H	3.13037000	-2.14903300	-1.10070400
H	-3.09722000	1.27146200	1.94535000	H	0.85029500	-2.15924800	0.93418400
C	-0.82117200	-0.93561100	2.83008300	H	0.73208600	-2.58790700	-0.77082200
H	-0.18685500	-0.27009700	3.42942100	H	0.87403900	0.81419500	-2.26266600
H	-1.41564200	-1.57269800	3.50018700	H	0.45555400	-0.87480600	-2.48701800
H	-0.18743500	-1.55196600	2.19248900	H	2.14189400	-0.40420300	-2.31020500
Li	-1.14484100	0.00861200	-0.02299000	O	-2.56277400	-1.32172900	-0.77386000
				O	-1.81758400	-0.05073100	1.96184200
				O	-1.97088200	1.72809200	-0.71431100
Structure 15-Li- $\beta_b$	(B3LYP/6-31+g(d,p))			O	-1.06608100	2.82168900	-0.87365100
C	3.35176800	-0.44352900	-0.67047400	H	-1.37916700	3.67382600	-0.25420700
C	4.19035000	0.75591300	-1.13381600	H	-0.08580800	2.46520700	-0.55679500
C	3.73564300	1.86668800	-0.17206300	H	-1.02210000	3.13498900	-1.92528600
C	2.20989300	1.64472500	0.00641400	C	-3.29172300	2.02851200	-1.14161900
C	1.92987400	0.14969000	-0.41387300	C	-3.72025100	2.85000100	-0.54941700
C	1.70303900	1.77101300	1.46689900	H	-3.30414000	2.31469600	-2.20296200
C	1.57060800	0.31655300	1.94977100	H	-3.88950600	1.12561600	-1.00319200
C	1.04945000	-0.44882100	0.72268300	C	-2.50955000	-1.53216400	-2.18407600
H	1.41557500	0.13607500	-1.39258200	C	-3.46463300	-1.93601800	-2.54826400
H	1.67516500	2.34190000	-0.65176600	H	-2.31661700	-0.56467700	-2.64961300
C	1.25148000	-1.95948900	0.90665900	H	-1.69758700	-2.22208500	-2.44511800
H	3.34056200	-1.26966100	-1.39214300	C	-2.74921800	-2.53935100	-0.05289600
H	3.77657200	-0.83868700	0.26171700	H	-3.69806100	-3.01396100	-0.33911200
H	3.93025700	1.02138500	-2.16921100	H	-1.92039900	-3.23305700	-0.24451800
H	5.27336300	0.57889200	-1.10582100	H	-2.76812300	-2.28138500	1.00637200
H	3.97963600	2.87643500	-0.52481600	C	-2.97228500	0.63521900	2.42752600
H	4.24512900	1.73446700	0.79251200	H	-3.43524600	0.09579300	3.26589200
H	0.71791100	2.25682800	1.49805200	H	-2.71955900	1.65375000	2.75407700
H	2.37593100	2.38040000	2.08553900	H	-3.67845800	0.68583000	1.59737000
H	0.93226700	0.23647100	2.84316900	C	-0.82884900	-0.22364900	2.97805100
H	2.57534700	-0.04153900	2.27959400	H	-0.49109500	0.74895900	3.36001000
H	1.02493600	-2.53472700	-0.00437500	H	-1.23407700	-0.81909800	3.80790700
H	0.60340400	-2.37031100	1.69847800	H	0.01200500	-0.74253200	2.51943000
H	2.28476900	-2.25112700	1.19979900	Li	-1.14859400	-0.00871700	0.00144200
C	-2.78232000	1.05399800	-2.14206200				
H	-3.67841500	1.66516900	-1.96057500	Structure 15-Li- $\beta_d$	(B3LYP/6-31+g(d,p))		
H	-2.34453800	1.34831400	-3.10640200	C	2.46449400	1.55454600	-0.05921400
H	-3.05359400	-0.00191100	-2.17024900	C	3.98929000	1.52502200	0.18497300
C	-1.40669300	2.56742100	-0.94497500	C	4.37328900	0.06405900	-0.10938300
H	-0.93418300	2.92372600	-1.86998500	C	3.23142700	-0.75032200	0.53001400
H	-2.25648800	3.21976000	-0.69906100	C	1.93805500	0.16836300	0.40672200
H	-0.67715100	2.58626700	-0.13589200	C	2.84048800	-2.10007600	-0.10254500
C	-3.74595000	0.16307400	1.55495100	C	1.28345100	-2.05460200	-0.13000800
H	-4.48708700	-0.49593100	2.02906800	C	0.88034900	-0.59345300	-0.45558300
H	-3.73910300	1.12792200	2.08127500	H	1.54587400	0.29303600	1.43107300
H	-4.01670900	0.32399600	0.51067100	H	3.47205500	-0.89960600	1.59351600
C	-1.98309800	-0.69218300	2.89569800	C	1.09925200	-0.37248100	-1.97171600
H	-1.92070700	0.23985800	3.47263600	H	1.98229500	2.39135000	0.46367700
H	-2.65326300	-1.39483400	3.41034100	H	2.27975300	1.70041300	-1.12941400
H	-0.98684900	-1.12142000	2.79840500	H	4.20877600	1.75821800	1.23681500
C	-2.14401400	-3.03160900	-0.59505000	H	4.53846900	2.25160500	-0.42784000
H	-2.71701400	-2.74819800	0.28863400	H	5.36744700	-0.20112700	0.27192800
H	-2.79664000	-3.54861900	-1.31248600	H	4.38703100	-0.10058100	-1.19596600
H	-1.32523200	-3.70028200	-0.29998900	H	3.23805700	-2.96081400	0.45185500
C	-0.84010700	-2.06263900	-2.32446500	H	3.23247800	-2.17263600	-1.12541100
H	0.00865300	-2.71700800	-2.09188400	H	0.92141500	-2.36082000	0.86726000
H	-1.44765000	-2.51944700	-3.11845800	H	0.86815800	-2.78652900	-0.84076000
H	-0.46051400	-1.09617800	-2.65954700	H	0.47118900	-1.06723800	-2.54894200
O	-2.45561500	-0.43313500	1.57208200	H	2.13407200	-0.52529700	-2.34740400
O	-1.63326800	-1.82696900	-1.16190900	H	0.81357200	0.63563400	-2.30470200
O	-1.83898600	1.21526500	-1.08934000	O	-1.88418000	-0.45438400	1.87594000
Li	-1.00064900	-0.28848300	0.11061800	O	-2.61914700	-0.76856700	-1.20469400

O	-1.67382700	1.97847600	-0.10869300
C	-1.49623900	2.77741200	1.05955700
H	-0.44187000	3.05778700	1.18184300
H	-2.10941900	3.68744000	1.00045400
H	-1.81116500	2.17220300	1.91029000
C	-1.25314200	2.65374400	-1.29454300
H	-1.85434100	3.55995000	-1.45308800
H	-0.19163600	2.92180400	-1.23232300
H	-1.39779900	1.96570600	-2.12860100
C	-1.00405300	-1.06506300	2.82067700
H	0.01317400	-0.84623800	2.49766300
H	-1.17787300	-0.65627500	3.82589400
H	-1.15273600	-2.15284300	2.84115900
C	-3.25471600	-0.69865400	2.16388200
H	-3.47623900	-1.77472700	2.13619800
H	-3.52170400	-0.30485700	3.15491100
H	-3.84468000	-0.18997200	1.40021300
C	-2.36882700	-2.03193000	-1.82034400
H	-2.27597200	-1.91915600	-2.90867700
H	-1.42686100	-2.39997100	-1.41283100
H	-3.18137900	-2.73738800	-1.59650000
C	-3.80501800	-0.14319900	-1.67539900
H	-4.68907700	-0.75724800	-1.45102800
H	-3.88479000	0.81886400	-1.16605700
H	-3.75670600	0.02128700	-2.76127300
Li	-1.12364300	-0.02212000	-0.00592900

Structure 15-H- $\alpha$ _c (B3LYP/6-31+g(d,p))			
C	1.17836100	-1.36503600	0.41763400
C	2.42355900	-0.55948900	0.01206400
C	1.88416300	0.87797300	-0.06454200
C	0.48415600	0.73911500	-0.71360100
C	0.01464300	-0.73010900	-0.38635700
C	-0.60430200	1.66894000	-0.12771000
C	-1.27601900	0.82685800	0.97354600
C	-1.32800500	-0.60366900	0.38630900
H	-0.13580500	-1.30168400	-1.31010500
H	0.57664600	0.88425800	-1.79588300
H	-2.55198300	-0.81931600	-0.51783900
H	1.27678600	-2.44090100	0.23512900
H	1.00093800	-1.23828800	1.49482400
H	3.25940800	-0.67275600	0.71173400
H	2.77821000	-0.88282900	-0.97617000
H	2.53773600	1.56061600	-0.61883600
H	1.78654700	1.28284000	0.95263600
H	-1.33882300	1.93088900	-0.89847800
H	-0.19110800	2.61165300	0.24957900
H	-2.26424300	1.20335600	1.26246100
H	-0.65462000	0.83464800	1.87871000
H	-1.37180700	-1.34820500	1.19215600
H	-3.48507900	-0.69167600	0.04327500
H	-2.55234500	-1.83031500	-0.94158300
H	-2.56988900	-0.11320800	-1.35647300

Structure 15-H- $\alpha$ _a (B3LYP/6-31+g(d,p))			
C	-0.89951000	-1.59343100	0.08007400
C	-1.95926300	-0.79068800	-0.69868300
C	-2.15117900	0.46994100	0.16523700
C	-0.72896300	0.81944600	0.66512400
C	0.08657400	-0.52536500	0.61099100
C	0.05798500	1.81102000	-0.22926000
C	1.49767900	1.27737500	-0.22363300
C	1.30934800	-0.24898600	-0.30680900
H	0.45397600	-0.79967400	1.60785000
H	-0.76460300	1.21054000	1.68818000
C	2.55206400	-1.07150100	0.04044800
H	-0.40333200	-2.35762400	-0.52998600
H	-1.38099600	-2.11480300	0.91764800
H	-2.88837500	-1.34764200	-0.86150300
H	-1.57139300	-0.51478300	-1.68834900
H	-2.80308800	0.23214500	1.01593600
H	-2.62060300	1.29855300	-0.37789300
H	-0.02501600	2.84668600	0.11823500
H	-0.33674600	1.78518300	-1.25464700
H	1.99549200	1.53713000	0.72216100
H	2.11505900	1.67705700	-1.03683900
H	1.01802800	-0.48747200	-1.34212800
H	3.38361200	-0.84825700	-0.63818700
H	2.35198900	-2.14757900	-0.02429800
H	2.88759100	-0.85632600	1.06287300

Structure 15-H- $\alpha$ _d (B3LYP/6-31+g(d,p))			
C	1.14184900	-1.53894000	-0.12042700
C	1.99562000	-0.56524900	0.70885500
C	1.94174300	0.74356400	-0.10795500
C	0.56075600	0.75505400	-0.83576900
C	-0.03948200	-0.68017400	-0.61999300
C	-0.48068600	1.72094000	-0.23460000
C	-1.09668500	0.93695000	0.93569800
C	-1.20577300	-0.51867000	0.41342700
H	-0.44183200	-1.08953000	-1.55387800
H	0.71090900	0.97077500	-1.89910900
C	-2.57754500	-0.80133700	-0.21962900
H	0.81767500	-2.42287000	0.44115800
H	1.72658700	-1.89738200	-0.97853700
H	3.01826600	-0.92305100	0.87158400
H	1.54569500	-0.42082100	1.69934500
H	2.74855400	0.74297200	-0.85088700
H	2.08819100	1.63382200	0.51449800
H	-1.25304200	1.94355300	-0.98225900
H	-0.04563200	2.68036100	0.06846900
H	-2.06398900	1.33922700	1.25916500
H	-0.42799700	0.97970000	1.80434000
H	-1.06758900	-1.22644100	-1.24110100
H	-3.38292200	-0.69888700	0.51695400
H	-2.62375900	-1.81785400	-0.62751600
H	-2.78788800	-0.10640000	-1.04207200

Structure 15-H- $\beta$ _a (B3LYP/6-31+g(d,p))			
C	-1.01136900	-1.49742100	-0.17794100
C	-2.37070500	-0.78905700	-0.00422600
C	-2.02971000	0.69571100	-0.22725100
C	-0.67479500	0.88329700	0.48989400
C	0.02231100	-0.52615800	0.44493300
C	0.33566300	1.87769400	-0.13458100
C	1.69524100	1.15958200	-0.04026700
C	1.35174600	-0.31701100	-0.32038600
H	0.26084700	-0.84934700	1.46725800
H	-0.86344600	1.16123700	1.53423700
C	2.45771600	-1.31259100	0.03597100
H	-0.80318000	-1.62857200	-1.24875000
H	-0.99185800	-2.49409900	0.27588000
H	-2.74399200	-0.93755600	1.01821300
H	-3.14115300	-1.16361000	-0.68790100
H	-2.80749100	1.37599000	0.13745700
H	-1.91243800	0.88622500	-1.30326200
H	0.33421200	2.85548900	0.35916000
H	0.08600000	2.05252300	-1.18982900
H	2.10558700	1.25432000	0.97581700
H	2.44617400	1.56186300	-0.73087600
H	1.14058500	-0.40832800	-1.39767500
H	2.15368100	-2.34349600	-0.17996100
H	2.70500700	-1.25479500	1.10363100
H	3.37487300	-1.11211900	-0.53026500

Structure 15-H- $\beta$ _b (B3LYP/6-31+g(d,p))			
C	-0.66328500	-1.49029500	-0.17601300
C	-2.13114700	-1.03452300	-0.19904600
C	-2.00501500	0.49300300	-0.31783400
C	-0.80751100	0.86432400	0.59442500
C	0.04285400	-0.45507000	0.73501000
C	0.15721900	1.92810200	0.00851300
C	1.29518200	1.11461900	-0.63384900
C	1.49378100	-0.05615000	0.34856900
H	0.01777300	-0.82586400	1.76697500
H	-1.18514800	1.18767900	1.57085400
C	2.40006000	-1.18387300	-0.15273800
H	-0.26223800	-1.44455100	-1.19719800
H	-0.53189300	-2.52004000	0.17354900
H	-2.62464000	-1.30223300	0.74524600
H	-2.71221100	-1.48599100	-1.01119800
H	-2.92147500	1.02898100	-0.04743100
H	-1.77584900	0.75588700	-1.36001400
H	0.56835500	2.55183300	0.81242200
H	-0.34371300	2.60262200	-0.69544100
H	2.20928500	1.69924700	-0.78911100
H	0.98809000	0.73042200	-1.61713400
H	1.95930600	0.36450300	1.25319100
H	2.49363200	-1.98357800	0.59153100
H	3.40841800	-0.80781400	-0.36132000
H	2.01948500	-1.63192300	-1.07715100



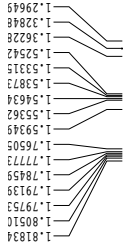
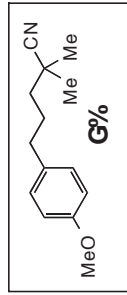
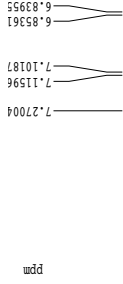


H	0.83938200	-2.50658700	-1.11126800
H	-1.40304800	-1.12383400	-1.82633700
H	0.17776600	-0.36808300	-2.15896900
H	-1.37536200	2.48425100	-0.30089200
H	-2.15662400	1.53637200	-1.57751000
H	-0.46071900	2.03916700	-1.75973700
C	-2.03553600	-0.05563600	0.56873000
O	-3.01523800	-0.54419800	-0.05493000
O	-1.92602600	0.16742200	1.80350500

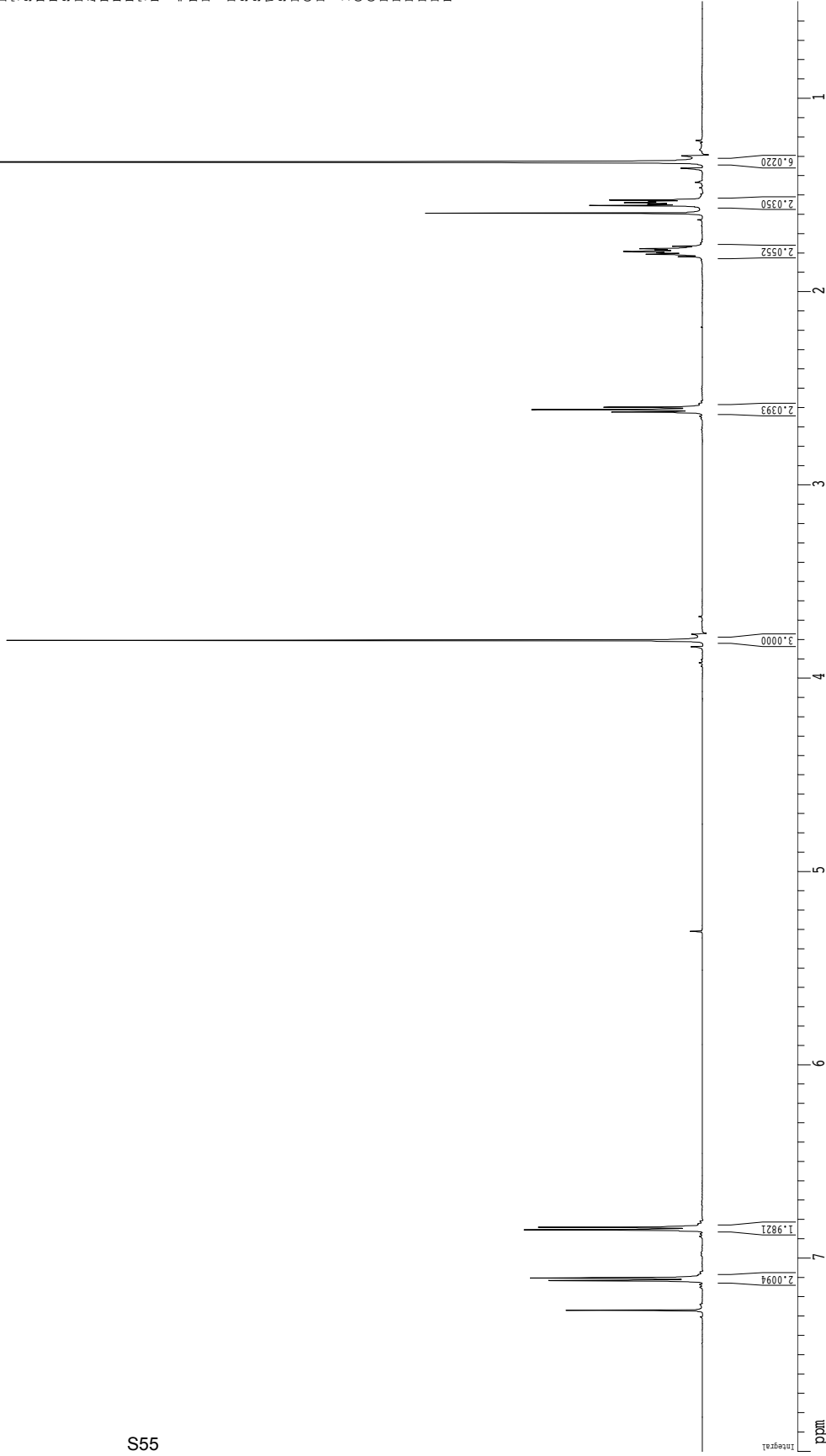
Structure **15-CO<sub>2</sub>-β<sub>c</sub>** (B3LYP/6-31+g(d,p))

C	1.18476500	-1.60222500	0.15921500
C	2.66400600	-1.31929300	-0.17393300
C	2.78373200	0.20483400	0.02182700
C	1.46877700	0.75864300	-0.56922100
C	0.41382100	-0.40510400	-0.44801500
C	0.81993200	1.98331700	0.10811000
C	-0.68896300	1.69458000	0.00430900
C	-0.84275200	0.17316900	0.29003200
H	0.06614600	-0.66926700	-1.45051400
H	1.62766700	0.98521500	-1.63264400
C	-0.84647300	-0.07554000	1.80698400
H	0.83644700	-2.56515200	-0.23162600
H	1.06786800	-1.63934800	1.24848500
H	2.87057300	-1.57447800	-1.22353500
H	3.36803500	-1.89259100	0.44475300
H	3.68424800	0.63053600	-0.44049900
H	2.83496400	0.43078400	1.09720500
H	1.10789400	2.93423000	-0.36129900
H	1.12833600	2.04112500	1.16193200
H	-1.03692400	1.88132300	-1.01839900
H	-1.29559000	2.30697500	0.68456400
H	-0.97895300	-1.13639400	2.03609900
H	-1.69704000	0.44402400	2.25784100
H	0.07669900	0.27610400	2.29213200
C	-2.18237400	-0.36728900	-0.37488200
O	-2.23867300	-0.24749800	-1.63022600
O	-3.04972600	-0.84295700	0.40384500

1H spectrum

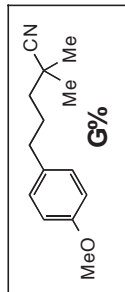


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 PULPROG zgpg30  
 TD 98074  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 9611.385 Hz  
 FIDRES 0.098042 Hz  
 AQ 5.098979 sec  
 RG 181  
 DW 52.000 usec  
 DE 1.500 usec  
 TE 292.8 K  
 D1 0.10000000 sec  
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 P1 8.00 usec  
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 SF 600.1300291 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00  
 ID NMR plot parameters  
 CX 272.0 cm  
 CY 20.00 cm  
 FIP 8.000 ppm  
 F1 4801.04 Hz  
 F2 0.500 ppm  
 FZ 300.07 Hz  
 PRMCH 0.2895 ppm/cm  
 HZCN 197.41119 Hz/cm



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

wdd



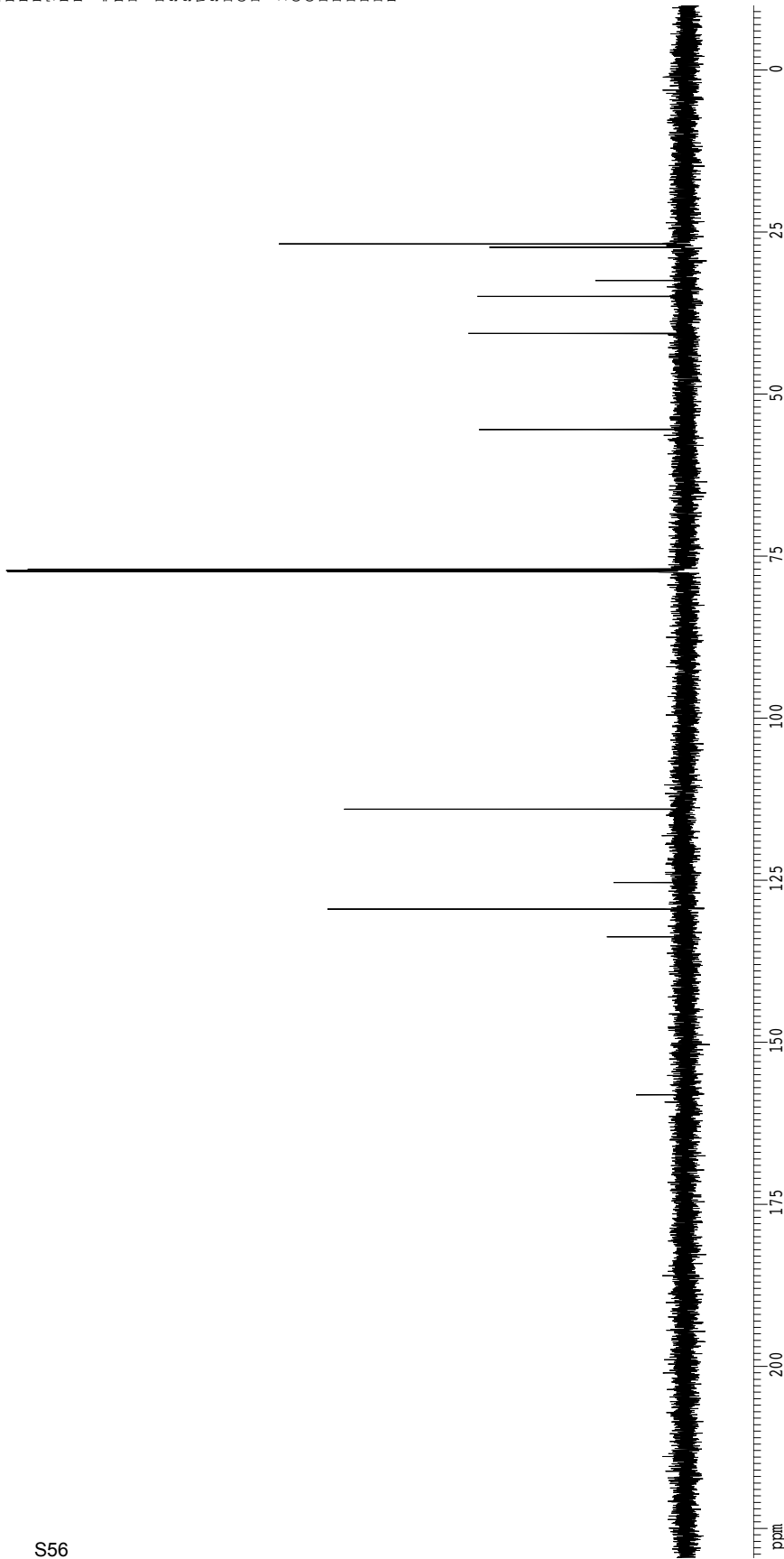
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 SOLVENT CDCl3  
 NS 361  
 DS 4  
 SWH 36231.883 Hz  
 FIDRES 0.352855 Hz  
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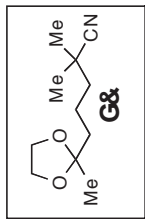
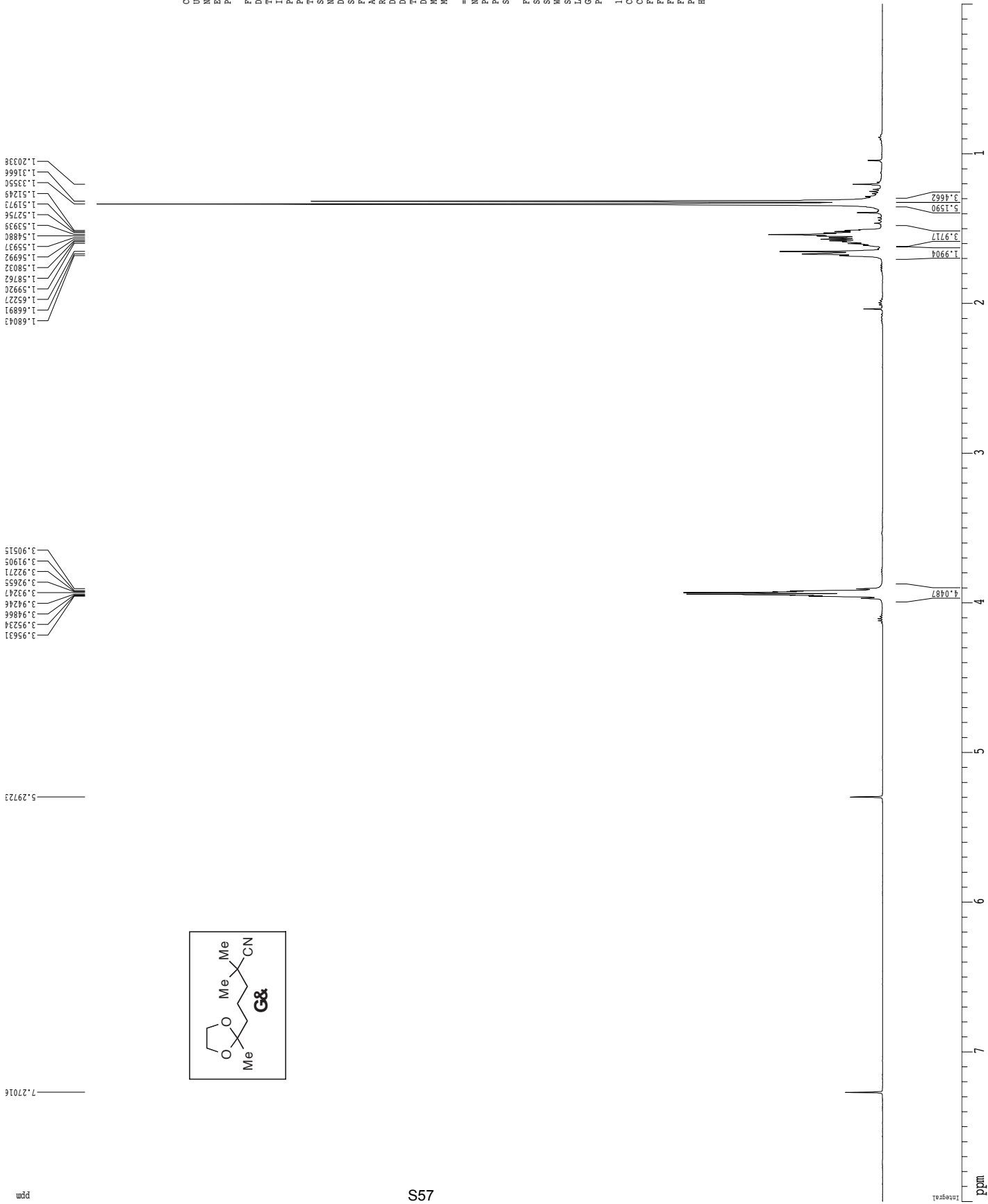
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 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 22.80 cm  
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 F1 34635.16 Hz  
 F2P -10.507 ppm  
 F2 -1585.47 Hz  
 PPMCN 10.52747 ppm/cm  
 HZCN 1586.62439 Hz/cm



<sup>1</sup>H spectrum



Current Data Parameters  
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 NAME: NUP-03-34  
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F2 - Acquisition Parameters  
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 Time: 17:23  
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 ACRESF: 0.00000000 sec  
 ACPRR: 0.01500000 sec

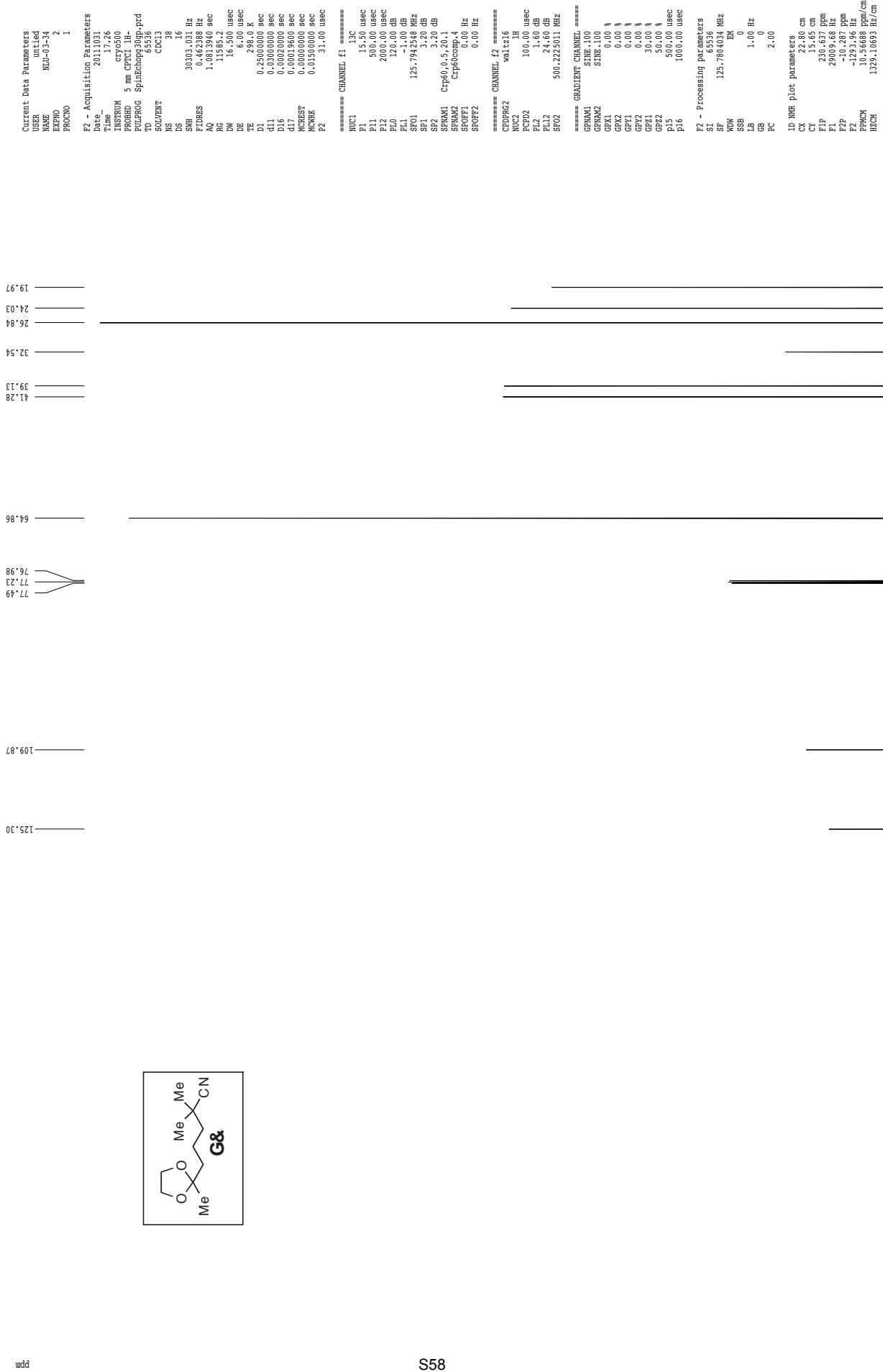
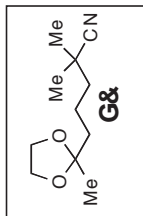
==== CHANNEL f1 =====  
 NUC1: <sup>1</sup>H  
 P1: 7.50 usec  
 PL1: 1.60 dB  
 SFO1: 500.2235015 MHz

F2 - Processing parameters  
 SI: 65536  
 SF: 500.2200271 MHz  
 WDW: EM  
 SSB: 0  
 LB: 0.20 Hz  
 GB: 0  
 PC: 4.00

ID NMR plot parameters  
 CX: 22.80 cm  
 CY: 15.00 cm  
 F1P: 8.000 ppm  
 F1: 4001.76 Hz  
 F2P: 0.000 ppm  
 F2: 0.00 Hz  
 PPMCM: 0.35088 ppm/cm  
 HZCM: 175.51581 Hz/cm

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

wdd



```

Current Data Parameters
USER          untitled
NAME          NUI-0.3-34
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20111031
Time          17:26
INSTRUM       cryo500
PROBHD        5 mm CPYCI 1H-
PULPROG       SpinEchoq3.0pp.prd
TD            65536
SOLVENT       CDCl3
NS            6
DS            6
SWH           30303.033 Hz
SF           125.7604338 MHz
AQ           1.0813940 sec
RG           11585.2
DW           16.500 usec
DE           6.00 usec
TE           298.2 K
RG           11585.2
AQ           1.0813940 sec
D11          0.0300000 sec
D16          0.0002000 sec
d17          0.00019600 sec
MCPRST       0.0000000 sec
MCNRRK       0.01500000 sec
P2           31.00 usec

===== CHANNEL f1 =====
NUC1          13C
PC           15.50 usec
PL1          500.00 usec
PL2          2000.00 usec
PL0          120.00 dB
PL1          -1.00 dB
SFO1         125.7942548 MHz
SF1          3.20 dB
SFO2          Cp60.0.5.20.1
SFO3          Cp60cm0.0
SFOF1         0.00 Hz
SFOF2         0.00 Hz

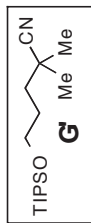
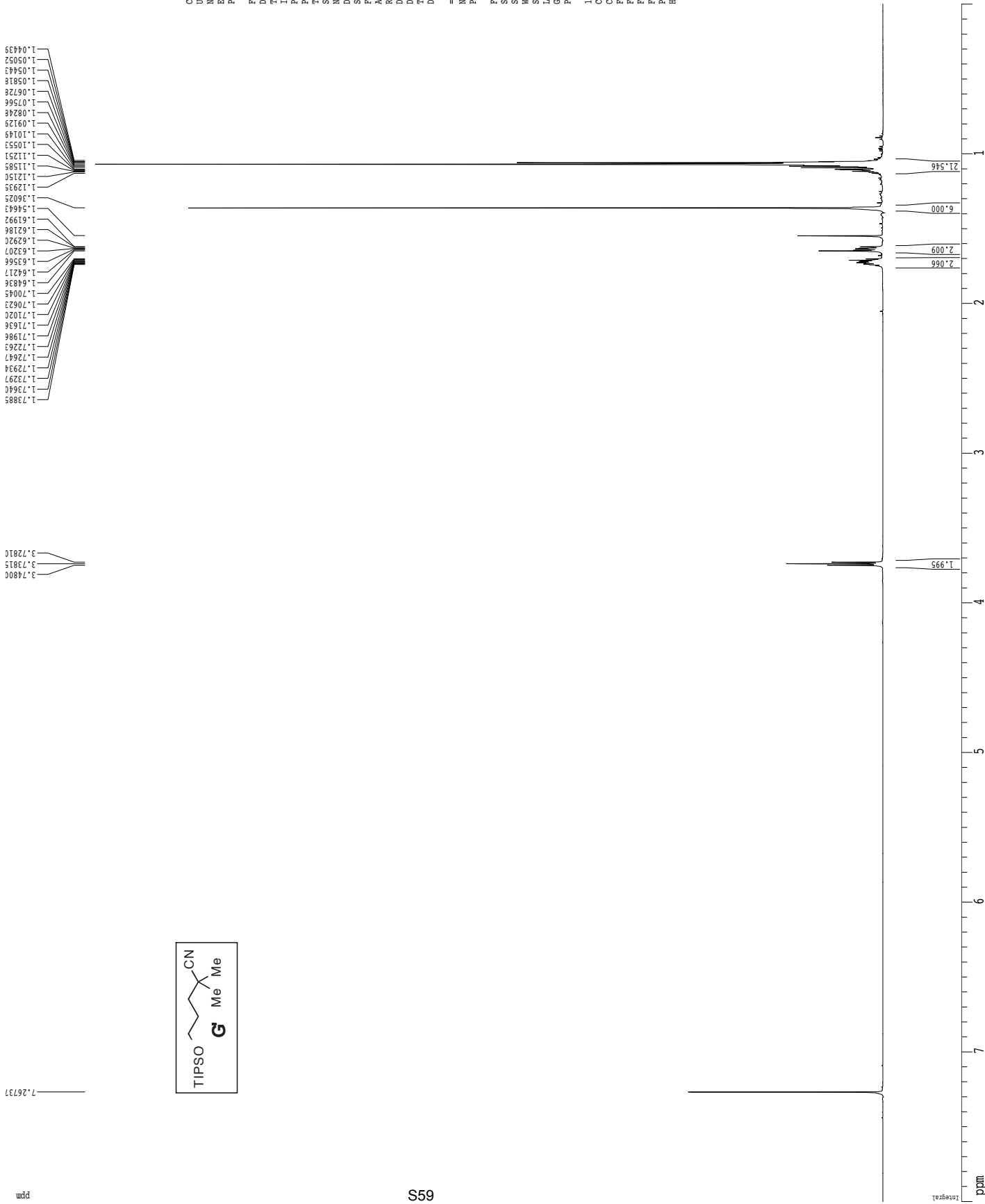
===== CHANNEL f2 =====
COPPRG2      waltz16
NUC2          1H
PCP02        100.00 usec
PLP02        2.00 dB
PL1          2.00 dB
SFO2         500.2225013 MHz

===== GRADIENT CHANNEL =====
GENAM1       SINE.100
GENAM2       SINE.100
GEX1         0.00 %
GEX2         0.00 %
GEX3         0.00 %
GEX4         0.00 %
GEX5         0.00 %
GEX6         0.00 %
GEX7         30.00 %
GEX8         50.00 %
GEX9         50.00 usec
p16          1000.00 usec

F2 - Processing parameters
SI           65536
SF           125.7604338 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           2.00

ID NMR plot parameters
CX           22.80 cm
CY           11.40 cm
EI           230.637 ppm
F1           29009.68 Hz
F2           -10.287 ppm
PRCM         10.56688 ppm/cm
HCN          1329.10693 Hz/cm
    
```

1H spectrum



Current data Parameters  
USER untitled  
NAME NMR-03-04-01  
PROCNO 1  
PRCNO 1

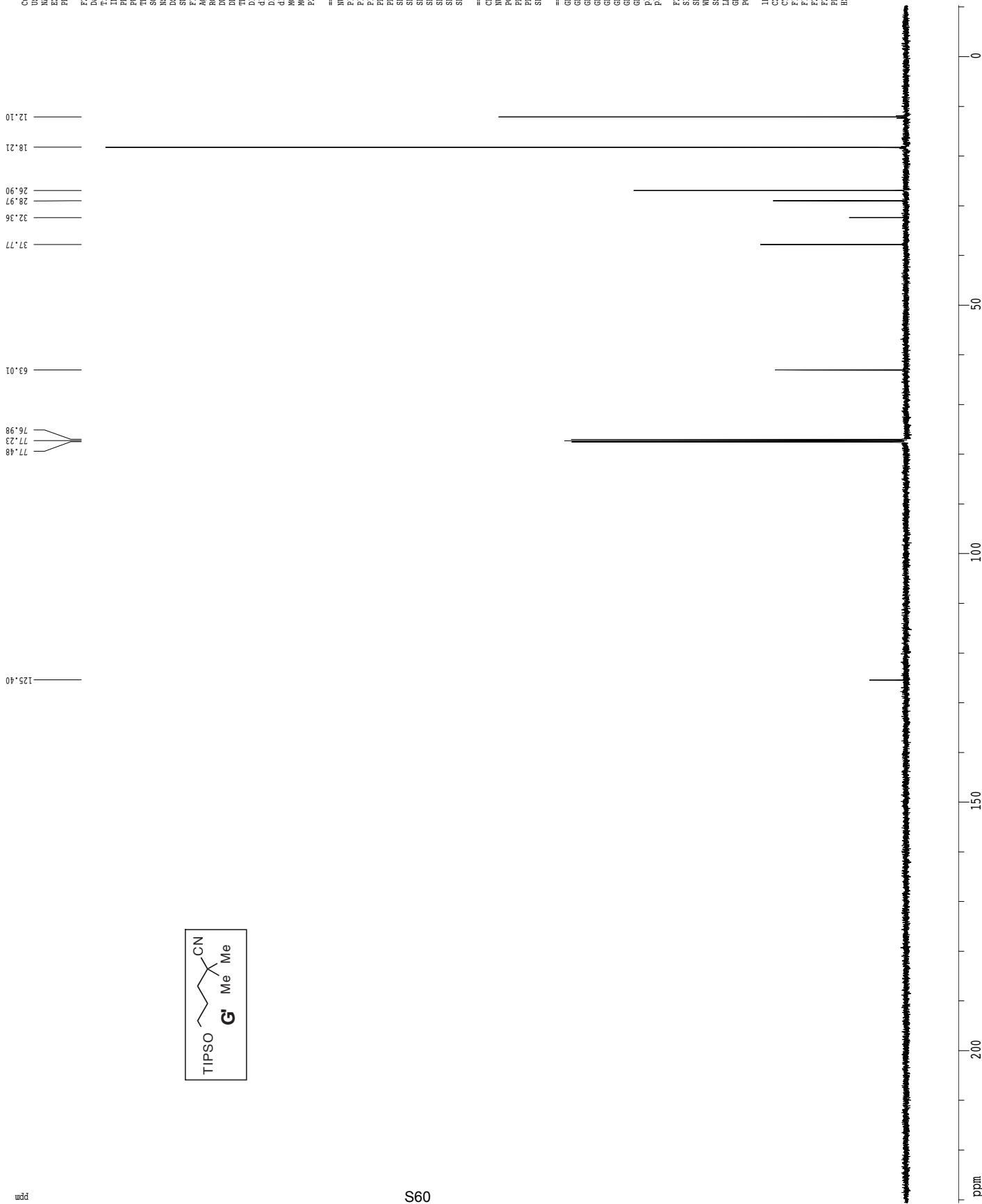
F2 - Acquisition Parameters  
Date 20111208  
Time 15:15  
INSTRUM av600  
PROBHD 5 mm TBI H/13  
PULPROG zg30  
TD 98074  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 9611.385 Hz  
FIDRES 0.090042 Hz  
AQ 5.098979 sec  
RG 256  
RW 52.000 usec  
DE 4.000 usec  
TE 298.1 K  
D1 0.1000000 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 8.00 usec

F2 - Processing parameters  
SI 65536  
SF 600.1300286 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ID NMR plot parameters  
CX 22.00 cm  
CY 15.00 cm  
FIP 8.000 ppm  
F1 4801.04 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PRMCM 0.35088 ppm/cm  
HZCM 210.57195 Hz/cm

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



Current Data Parameters  
 USER untitled  
 NAME NUI-0.3-84  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120413  
 Time\_ 17.19  
 INSTRUM cryo500  
 PROBDHD 5 mm CPYCI 1H-  
 PULPROG Spinecho30pp.prd  
 TD 65536  
 SOLVENT CCL13  
 NS 142  
 DS 4  
 SWH 30303.033 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 7298.2  
 DW 16.500 usec  
 DE 6.00 usec  
 TE 289.8 K  
 T1 0.3550000 sec  
 T1RHO 0.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.00019600 sec  
 ACQRESF 0.0000000 sec  
 MCNRRK 0.01500000 sec  
 P2 31.00 usec

==== CHANNEL f1 =====  
 NUCL1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SF01 125.7942548 MHz  
 SF1 3.20 dB  
 SF2 3.20 dB  
 SFO1 C1p60.5, Z0.1  
 SFO2 C1p60.5, Z0.1  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

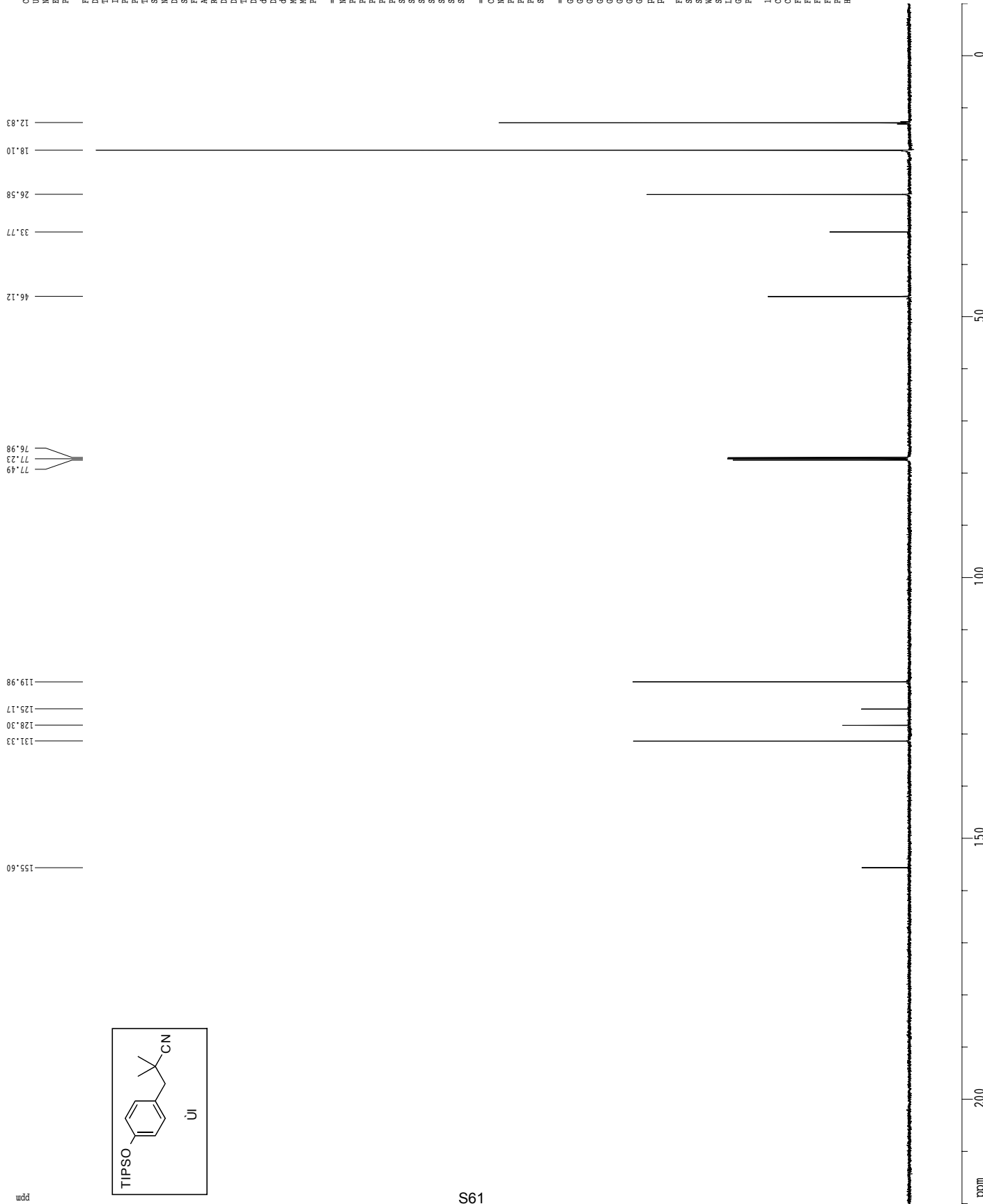
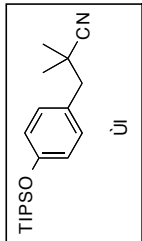
==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUCZ2 1H  
 PCPDZ 100.00 usec  
 PLZ2 2.00 dB  
 PL1 2.00 dB  
 SF02 500.2225013 MHz

==== GRADIENT CHANNEL =====  
 GENAM1 SINE.100  
 GENAM2 SINE.100  
 GX1 0.00 %  
 GX2 0.00 %  
 GY1 0.00 %  
 GY2 0.00 %  
 GZ1 30.00 %  
 GZ2 50.00 %  
 p15 500.00 usec  
 p16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.760493 MHz  
 NRG 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.50 cm  
 F1P 230.637 ppm  
 F1 29009.668 Hz  
 F2P -10.287 ppm  
 F2 -1293.96 Hz  
 PPMCM 10.56688 ppm/cm  
 HZCM 1329.10693 Hz/cm





Current Data Parameters  
 USER: NCG  
 NAME: NBC-II-053a  
 EXPNO: 2  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_: 20110503  
 Time: 16.03  
 CPU: 16.03  
 PULPROG: zgpg30  
 PRGRM: 5 mm CPDPR 1H  
 PULPROG: SpineEcho30ppm.prd  
 TD: 65536  
 SOLVENT: CDCl3  
 NS: 106  
 DS: 16  
 SWH: 30303.031 Hz  
 FIDRES: 0.462388 Hz  
 AQ: 1.96793 sec  
 RG: 36.69  
 DW: 16.500 usec  
 DE: 6.00 usec  
 TE: 298.0 K  
 D1: 1.50000000 sec  
 D11: 0.03000000 sec  
 D16: 0.00200000 sec  
 T1: 0.00350000 sec  
 T1RHO: 0.00000000 sec  
 WALTZ16: 0.00000000 sec  
 MCKR: 0.01800000 sec  
 P2: 31.00 usec

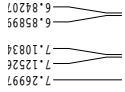
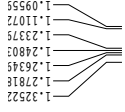
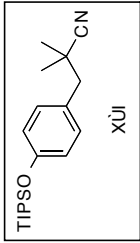
===== CHANNEL F1 =====  
 NUC1: 13C  
 P1: 15.50 usec  
 F1: 500.00 usec  
 F2: 200.00 usec  
 F3: 100.00 usec  
 F4: 1.00 dB  
 F5: 1.00 dB  
 SF01: 125.7942548 MHz  
 SF1: 3.20 dB  
 SF2: 3.20 dB  
 SFO1: Cnp60.0.5.20.1  
 SFO2: Cnp60comp.4  
 SFO3: 0.00 Hz  
 SFO4: 0.00 Hz  
 SFO5: 0.00 Hz

===== CHANNEL F2 =====  
 CDPDPR2: waltz16  
 NUC2: 1H  
 P2PD2: 100.00 usec  
 PL2: 1.60 dB  
 PL12: 24.60 dB  
 SF02: 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GPM1: SINE 100  
 SINE 100  
 GPM2: SINE 100  
 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: 100.00 usec

F2 - Processing parameters  
 SI: 65536  
 SF: 125.7804011 MHz  
 WDW: EM  
 SSB: 0  
 GB: 1.00 Hz  
 PC: 2.00

1D NMR plot parameters  
 CX: 22.80 cm  
 CY: 15.65 cm  
 FIP: 220.000 ppm  
 F1: 2767.89 Hz  
 F2: 100.000 ppm  
 F3: -1257.89 Hz  
 FPMCM: 10.06872 ppm/cm  
 HCM: 1268.83746 Hz/cm



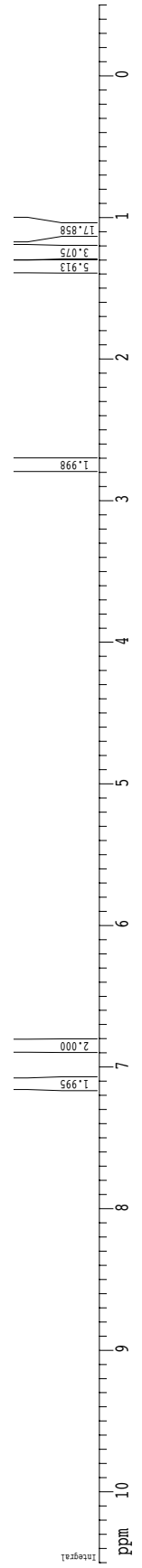
Current Data Parameters  
USER genuing  
NAME NEG-II-053a  
PROCNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20110503  
Time 15.57  
INSTRUM cryo500  
PROBHD 5 mm CPCL1.HH-  
PULPROG zg30  
TD 81728  
SOLVENT CDCl3  
NS 8  
DS 2  
FREQ 801.282 Hz  
P1 0.109026 Hz  
PC 5.0198774 sec  
RG 3.2  
DW 62.400 usec  
DE 6.00 usec  
TE 298.0 K  
D1 0.10000000 sec  
MCREST 0.00000000 sec  
MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.20 usec  
PL1 0.00 dB  
SFO1 500.2235015 MHz

F2 - Processing Parameters  
SI 65536  
SF 500.220271 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 4.00

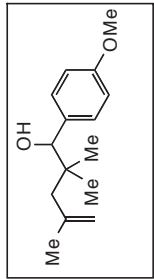
ID NMR plot parameters  
CX 22.80 cm  
CY 10.00 cm  
FLP 10.500 ppm  
F1 5252.31 Hz  
F2P -0.500 ppm  
F2 -250.11 Hz  
PRMCM 0.48246 ppm/cm  
HZCM 241.33423 Hz/cm



<sup>1</sup>H spectrum

ppm

7.27571  
7.26974  
7.25046  
7.23316  
6.87697  
6.87115  
6.85380

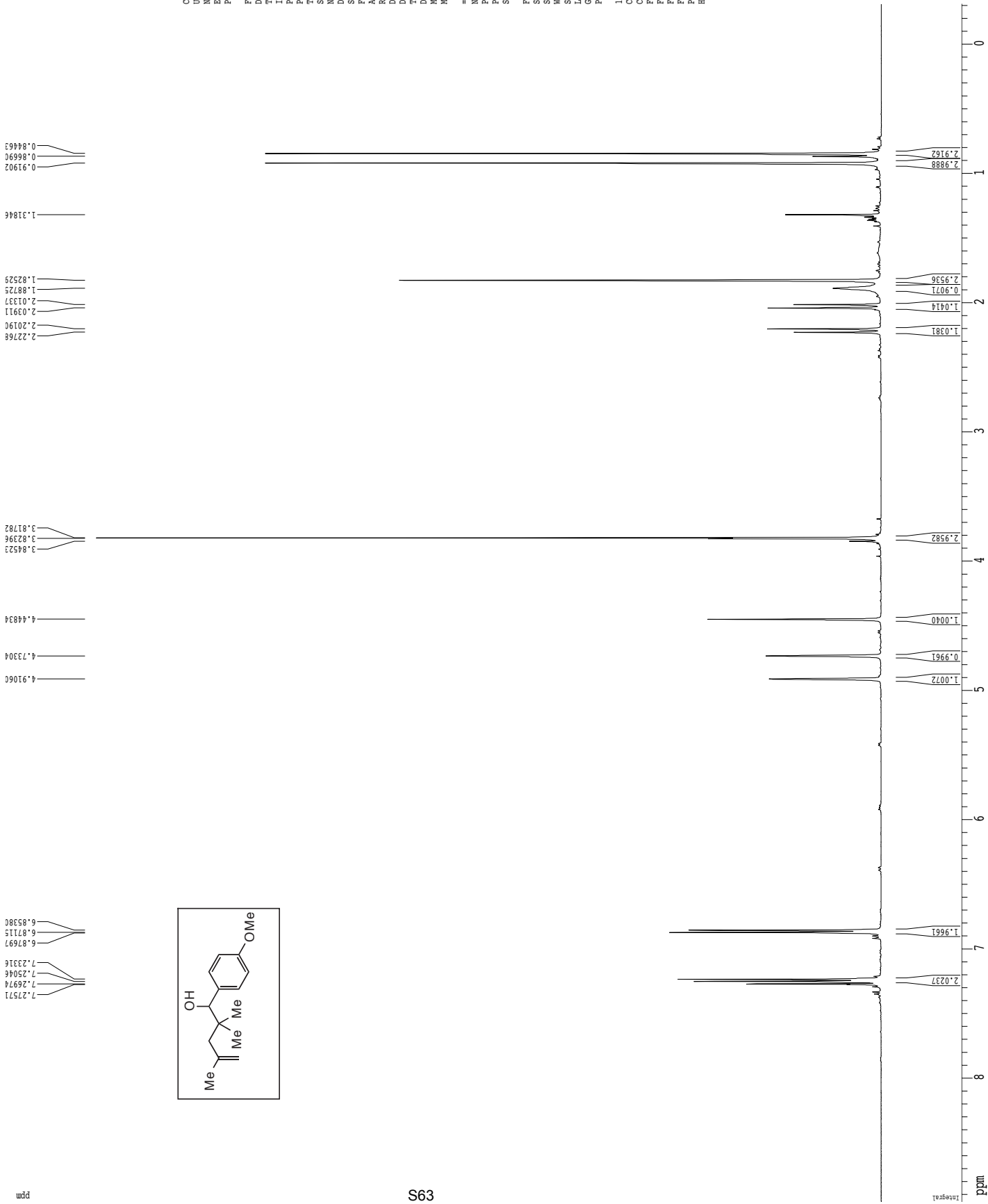


4.91060  
4.73304  
4.4834  
3.84523  
3.82396  
3.81782

2.22768  
2.20190  
2.03911  
2.01337  
1.88725  
1.82529

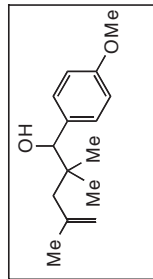
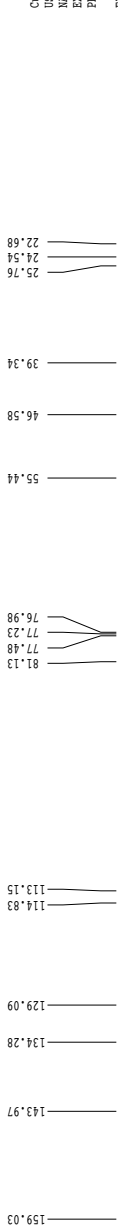
0.91902  
0.86690  
0.84463

Current Data Parameters  
 USER untied  
 NAME NUP-03-70  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120414  
 Time 14.55  
 INSTRUM cryo500  
 PROBD 5 mm CPCLP 1H-  
 PULPROG zgpg30  
 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 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 ACRESF 0.00000000 sec  
 ACPRR 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 500.2200268 MHz  
 WDW EN  
 SSB 0  
 LB 0.20 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 8.955 ppm  
 F1 4479.51 Hz  
 F2P -0.309 ppm  
 F2 -154.62 Hz  
 PPMCH 0.40652 ppm/cm  
 HZCH 201.25117 Hz/cm



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

ppm



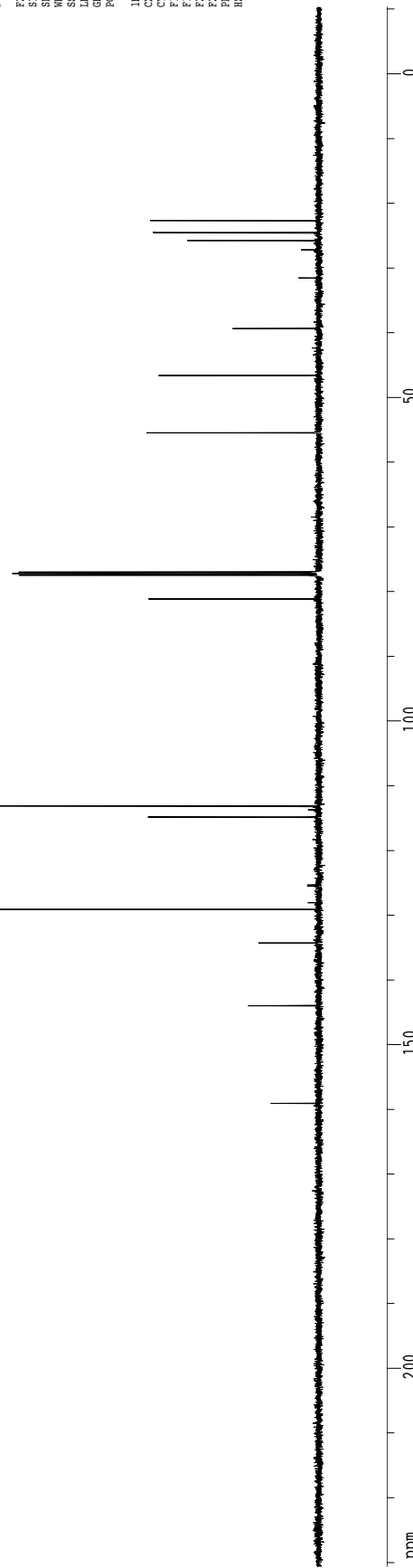
Current Data Parameters  
 USER untitled  
 NAME NLU-03-70  
 EXPNO 2  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120418  
 Time 14:57  
 INSTRUM cryo500  
 PROBH0 5 mm CPYCI 1H-  
 PULPROG Spinechoeg30pp.prd  
 TD 6536  
 SOLVENT CDCl3  
 NS 2  
 DS 2  
 SWH 30303.033 Hz  
 SF01 125.7942548 MHz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 5160.6  
 DW 16.500 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 0.2560000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.00019000 sec  
 ACRESF 0.0000000 sec  
 MCNRRK 0.0150000 sec  
 P2 31.00 usec

==== CHANNEL f1 =====  
 NUCL1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SF01 125.7942548 MHz  
 SE2 3.20 dB  
 GENAM1 Cnp60.5.20.1  
 SFOF01 Cnp60cm60  
 SFOF02 0.00 Hz  
 SFOF03 0.00 Hz

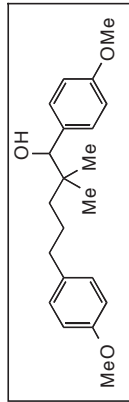
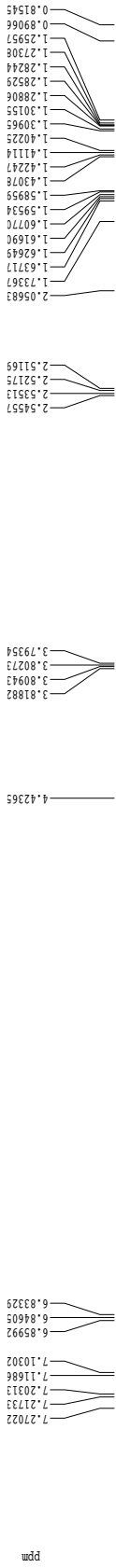
==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUCL2 1H  
 PCPDZ 100.00 usec  
 PL0 0.00 dB  
 PL1 2.00 dB  
 SF02 500.2225013 MHz

==== GRADIENT CHANNEL =====  
 GENAM1 SINE.100  
 GENAM2 SINE.100  
 GX1 0.00 %  
 GX2 0.00 %  
 GX3 0.00 %  
 GX4 0.00 %  
 GX5 30.00 %  
 GX6 50.00 %  
 p15 500.00 usec  
 p16 1000.00 usec

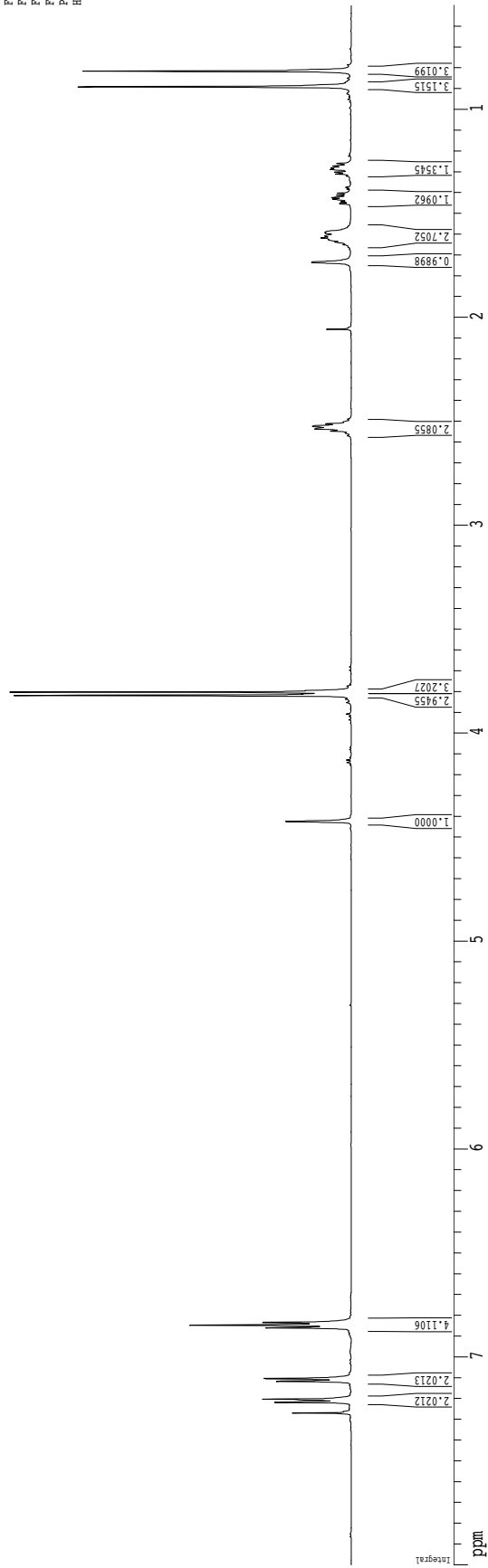
F2 - Processing parameters  
 SI 6536  
 SF 125.7942548 MHz  
 NS 2  
 DS 2  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00  
 ID NMR plot parameters  
 CX 2.80 cm  
 F1 230.637 ppm  
 F1 29009.68 Hz  
 F2P -10.287 ppm  
 F2 -1293.96 Hz  
 PPMCM 10.56688 ppm/cm  
 HCM 1329.10693 Hz/cm



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

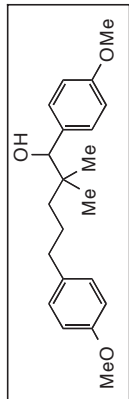
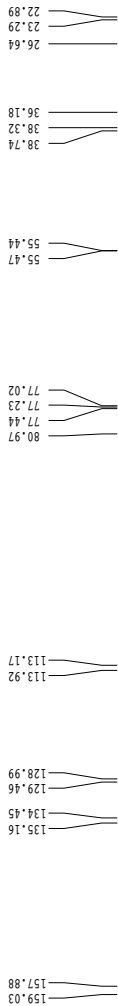


Current Data Parameters  
 USR# Untitled  
 NMR# NUL-02-239-11  
 PROCNO 1  
 PRACNO 1  
 F2 - Acquisition Parameters  
 Date 2011005  
 Time 11:17  
 INSTRUM av600  
 PROBED 5 mm TBI H/13  
 PULPROG zgpg30  
 TD 98074  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 9611.385 Hz  
 FIDRES 0.098042 Hz  
 AQ 5.098979 sec  
 RG 801.6  
 DW 52.000 usec  
 DE 4.000 usec  
 TE 298.0 K  
 D1 0.1000000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.00 usec  
 F2 - Processing parameters  
 SI 65536  
 SF 600.1300283 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00  
 ID NMR plot parameters  
 CX 22.00 cm  
 CY 5.00 cm  
 FID 8.000 ppm  
 F1 4801.04 Hz  
 F2 0.500 ppm  
 FZ 300.07 Hz  
 PRMCH 0.32895 ppm/cm  
 HZCN 197.41119 Hz/cm



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

wdd



```

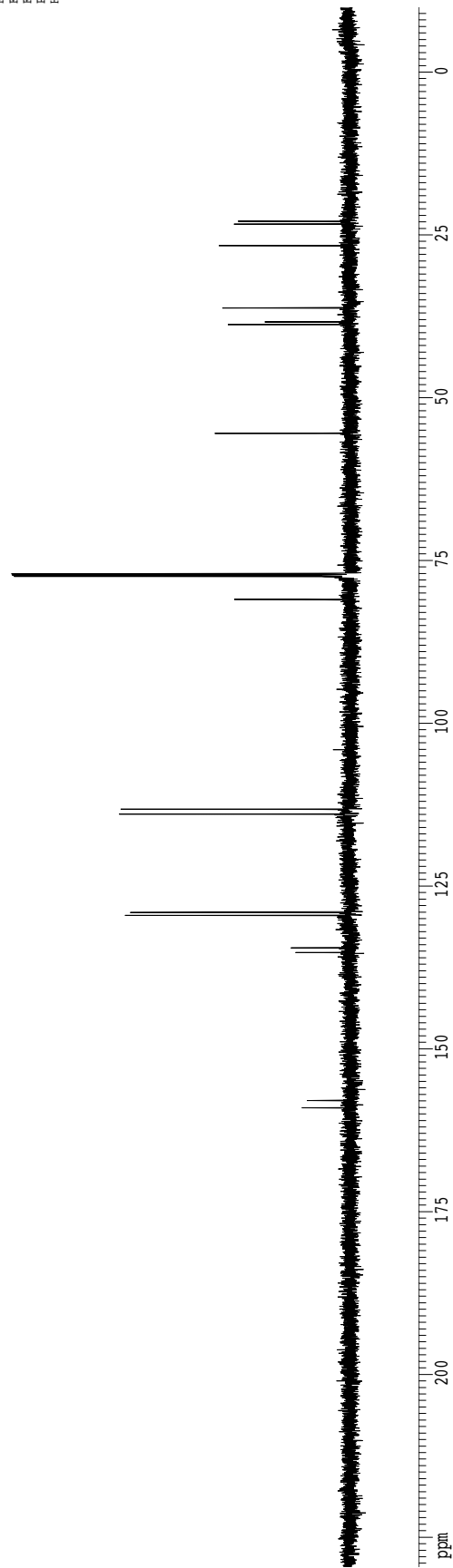
Current Data Parameters
=====
USRR      Jutilied
NAME      NUP-02-299-CL3
PRNO      1
PROCNO    1

F2 - Acquisition Parameters
=====
Date_     20111005
Time_     11.20
INSTRUM   av600
PROBHD    5 mm TBI H1/13
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         289
DS         4
SWH        36231.883 Hz
FIDRES     0.352855 Hz
AQ         0.9044468 sec
RG         2050
RW         13.800 usec
DE         4.000 usec
TE         298.0 K
D1         0.40000001 sec
D11        0.03000000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         15.00 usec

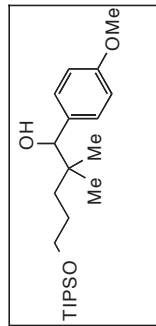
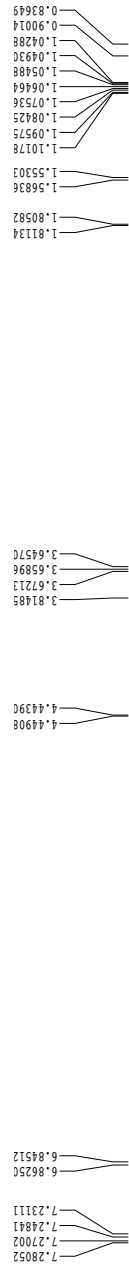
F2 - Processing parameters
=====
SI          65536
SF          150.9027836 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.00

ID NMR plot parameters
=====
CY          22.80 cm
CX          5.00 cm
F1P         229.520 ppm
F1          34635.16 Hz
F2P         -10.507 ppm
F2          -1585.47 Hz
PRMCH       10.52747 ppm/cm
HZCM        1586.62439 Hz/cm
    
```



<sup>1</sup>H spectrum

ppm



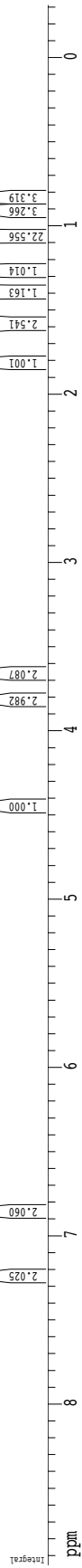
Current Data Parameters  
 USER untied  
 NAME NUP-03-87  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120414  
 Time 15.04  
 INSTRUM cryo500  
 PROBD 5 mm CPCL1 IH-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 ACRESF 0.00000000 sec  
 ACPRK 0.01500000 sec

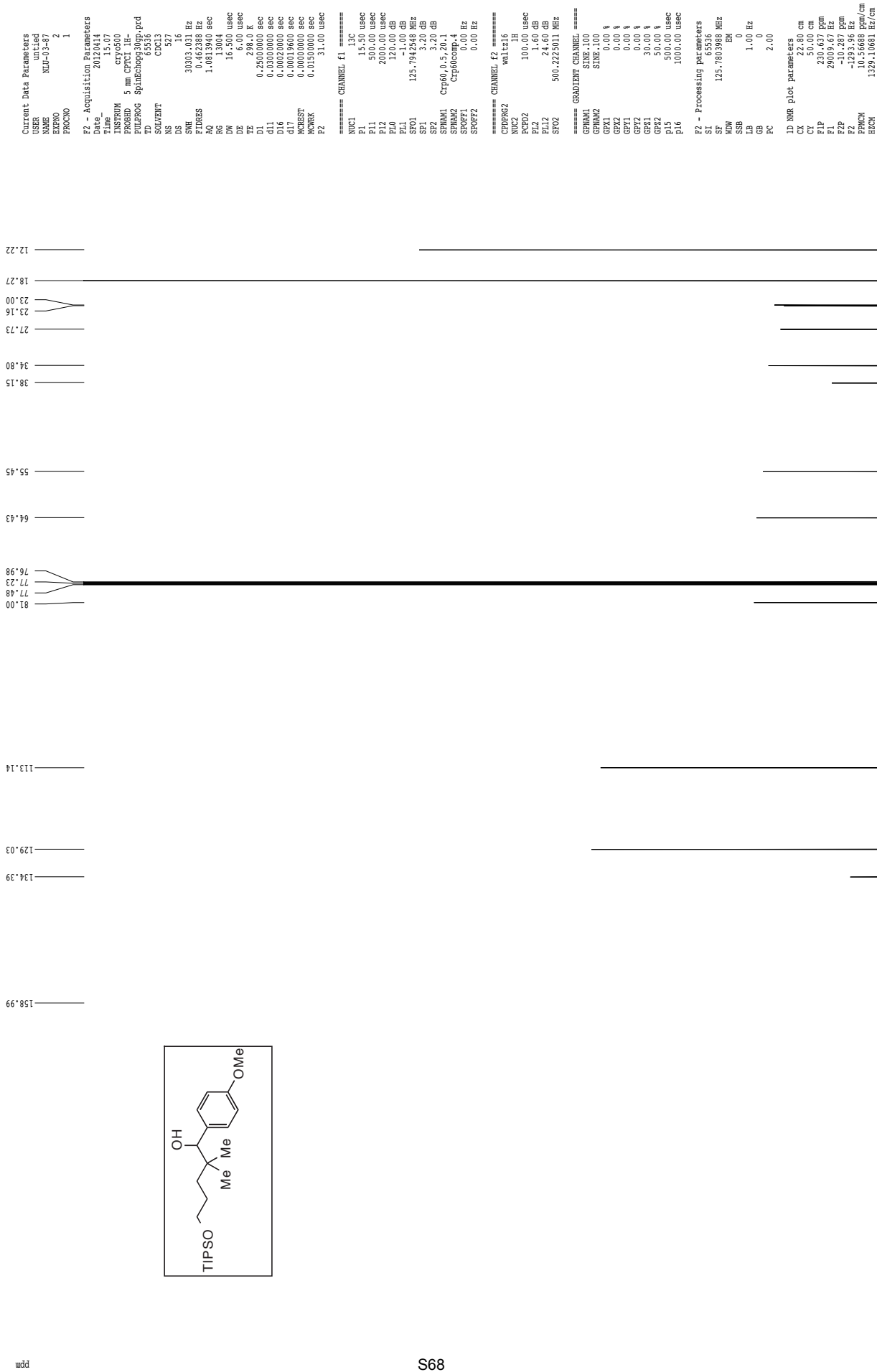
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2200271 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 F1P 8.955 ppm  
 F1 4479.51 Hz  
 F2P -0.309 ppm  
 F2 -154.62 Hz  
 PPMCM 0.40652 ppm/cm  
 HZCM 201.25117 Hz/cm

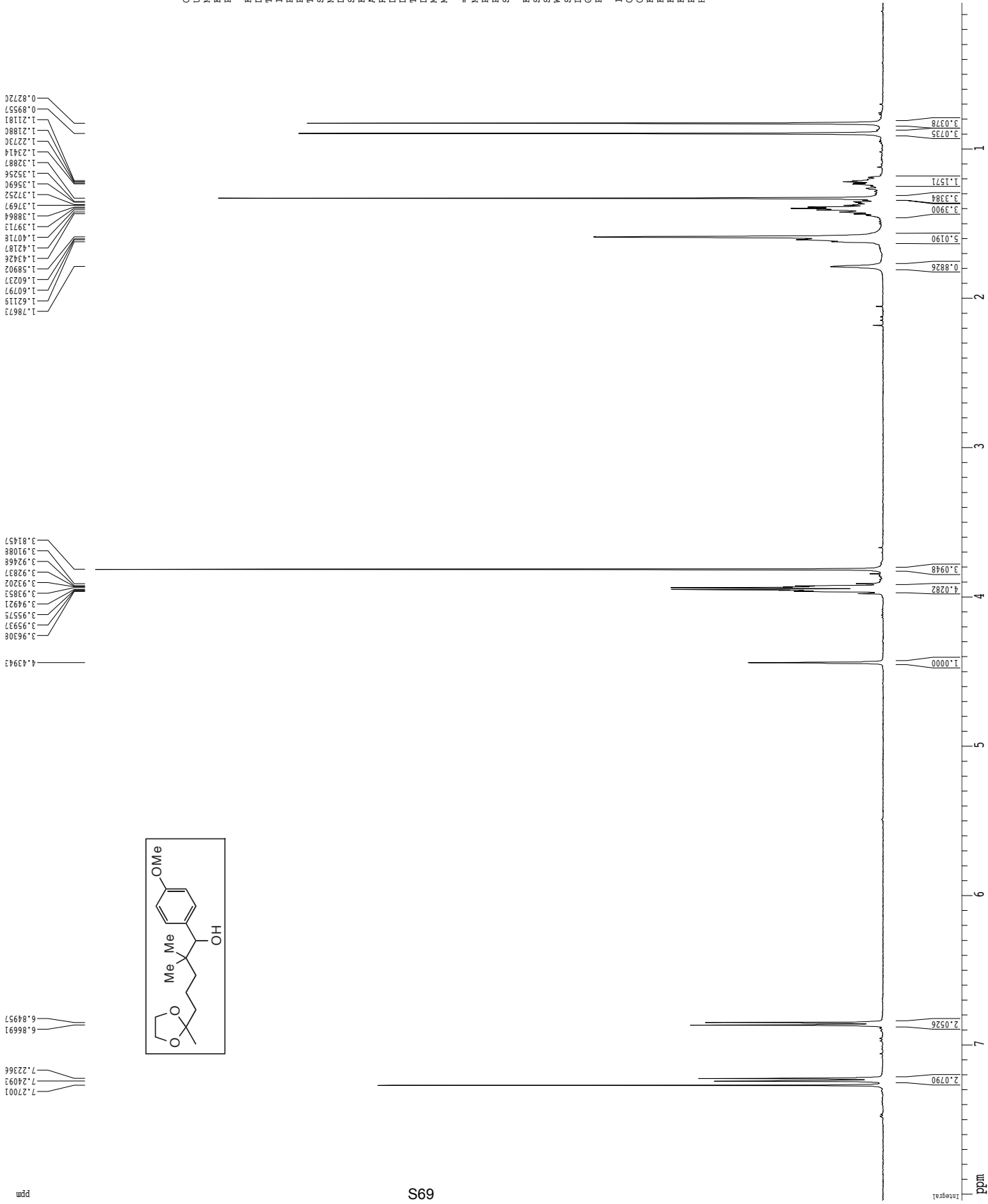


Z-restored spin-echo <sup>13</sup>C spectrum with <sup>1</sup>H decoupling





1H spectrum



Current Data Parameters  
USER untitled  
NAME NUP-03-17  
EXPNO 1  
PROCNO 1

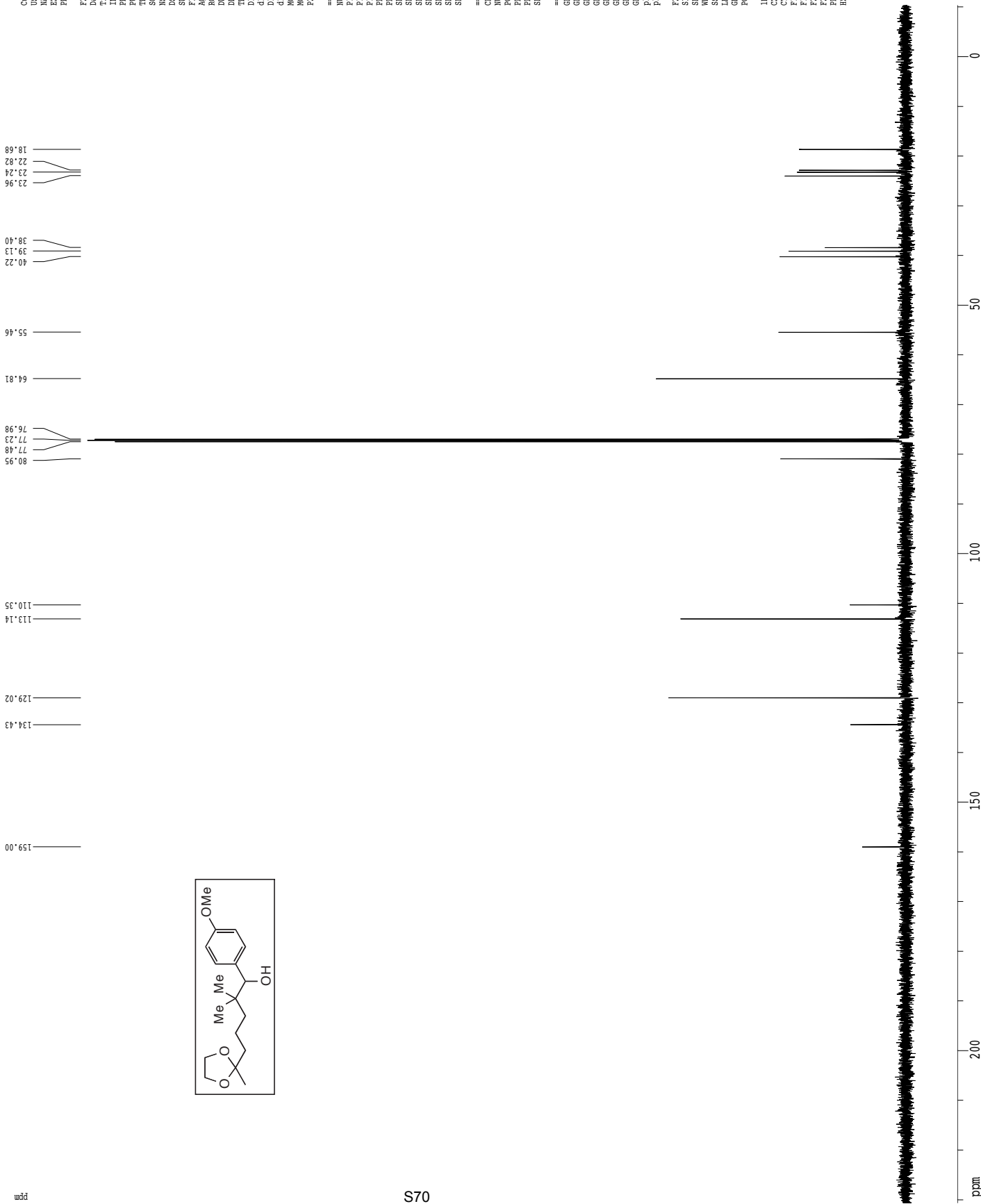
F2 - Acquisition Parameters  
Date\_ 20120414  
Time 14.42  
INSTRUM cryo500  
PROBHD 5 mm CP/CI 1H-  
PULPROG zgpg30  
AQ 8.925  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.098043 Hz  
AQ 5.0998774 sec  
RG 5.7  
DW 62.400 usec  
DE 6.00 usec  
TE 298.0 K  
D1 0.10000000 sec  
ACRESF 0.00000000 sec  
ACPRK 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 500.2200271 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 4.00

ID NMR plot parameters  
CX 22.80 cm  
CY 15.00 cm  
FIP 8.040 ppm  
F1 4021.85 Hz  
F2P 0.022 ppm  
F2 10.84 Hz  
PPMCM 0.35169 ppm/cm  
HECM 175.92148 Hz/cm

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

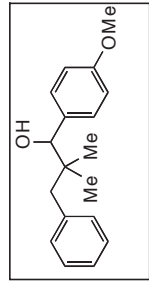
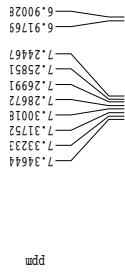


```

Current Data Parameters
USER          untitled
NAME          NUI-0.3-37
EXPNO         2
PROCNO        1
F2 - Acquisition Parameters
Date_         20120416
Time          14.45
INSTRUM       cryo500
PROBHD        5 mm CPYCI 1H-
PULPROG       SpinEcho30pp.prd
TD            65536
SOLVENT       CDCl3
NS            202
DS            4
SF            30303.033 Hz
SH            0.462388 Hz
AQ            1.0813940 sec
RG            2896.3
DW            16.500 usec
DE            6.00 usec
TE            298.0 K
T1            0.256000 sec
T1rho         0.030000 sec
d11           0.0002000 sec
d12           0.0002000 sec
d13           0.0002000 sec
d14           0.0002000 sec
d15           0.0002000 sec
d16           0.0002000 sec
d17           0.0002000 sec
d18           0.0002000 sec
d19           0.0002000 sec
d20           0.0002000 sec
MCREST       0.0000000 sec
MCNRRK       0.0150000 sec
P2            31.00 usec

===== CHANNEL f1 =====
NUC1          13C
PC            15.50 usec
PL1           500.00 usec
PL2           2000.00 usec
PL0           120.00 dB
PL1           -1.00 dB
SFO1         125.7942548 MHz
SF1           3.20 dB
SFO2          C1p60.0.5.20.1
SFO3          C1p60.0.5.20.1
SFO4          C1p60.0.5.20.1
SFO5          C1p60.0.5.20.1
SFO6          C1p60.0.5.20.1
SFO7          C1p60.0.5.20.1
SFO8          C1p60.0.5.20.1
SFO9          C1p60.0.5.20.1
SFO10         C1p60.0.5.20.1
SFO11         C1p60.0.5.20.1
SFO12         C1p60.0.5.20.1
SFO13         C1p60.0.5.20.1
SFO14         C1p60.0.5.20.1
SFO15         C1p60.0.5.20.1
SFO16         C1p60.0.5.20.1
SFO17         C1p60.0.5.20.1
SFO18         C1p60.0.5.20.1
SFO19         C1p60.0.5.20.1
SFO20         C1p60.0.5.20.1
SFO21         C1p60.0.5.20.1
SFO22         C1p60.0.5.20.1
SFO23         C1p60.0.5.20.1
SFO24         C1p60.0.5.20.1
SFO25         C1p60.0.5.20.1
SFO26         C1p60.0.5.20.1
SFO27         C1p60.0.5.20.1
SFO28         C1p60.0.5.20.1
SFO29         C1p60.0.5.20.1
SFO30         C1p60.0.5.20.1
SFO31         C1p60.0.5.20.1
SFO32         C1p60.0.5.20.1
SFO33         C1p60.0.5.20.1
SFO34         C1p60.0.5.20.1
SFO35         C1p60.0.5.20.1
SFO36         C1p60.0.5.20.1
SFO37         C1p60.0.5.20.1
SFO38         C1p60.0.5.20.1
SFO39         C1p60.0.5.20.1
SFO40         C1p60.0.5.20.1
SFO41         C1p60.0.5.20.1
SFO42         C1p60.0.5.20.1
SFO43         C1p60.0.5.20.1
SFO44         C1p60.0.5.20.1
SFO45         C1p60.0.5.20.1
SFO46         C1p60.0.5.20.1
SFO47         C1p60.0.5.20.1
SFO48         C1p60.0.5.20.1
SFO49         C1p60.0.5.20.1
SFO50         C1p60.0.5.20.1
SFO51         C1p60.0.5.20.1
SFO52         C1p60.0.5.20.1
SFO53         C1p60.0.5.20.1
SFO54         C1p60.0.5.20.1
SFO55         C1p60.0.5.20.1
SFO56         C1p60.0.5.20.1
SFO57         C1p60.0.5.20.1
SFO58         C1p60.0.5.20.1
SFO59         C1p60.0.5.20.1
SFO60         C1p60.0.5.20.1
SFO61         C1p60.0.5.20.1
SFO62         C1p60.0.5.20.1
SFO63         C1p60.0.5.20.1
SFO64         C1p60.0.5.20.1
SFO65         C1p60.0.5.20.1
SFO66         C1p60.0.5.20.1
SFO67         C1p60.0.5.20.1
SFO68         C1p60.0.5.20.1
SFO69         C1p60.0.5.20.1
SFO70         C1p60.0.5.20.1
SFO71         C1p60.0.5.20.1
SFO72         C1p60.0.5.20.1
SFO73         C1p60.0.5.20.1
SFO74         C1p60.0.5.20.1
SFO75         C1p60.0.5.20.1
SFO76         C1p60.0.5.20.1
SFO77         C1p60.0.5.20.1
SFO78         C1p60.0.5.20.1
SFO79         C1p60.0.5.20.1
SFO80         C1p60.0.5.20.1
SFO81         C1p60.0.5.20.1
SFO82         C1p60.0.5.20.1
SFO83         C1p60.0.5.20.1
SFO84         C1p60.0.5.20.1
SFO85         C1p60.0.5.20.1
SFO86         C1p60.0.5.20.1
SFO87         C1p60.0.5.20.1
SFO88         C1p60.0.5.20.1
SFO89         C1p60.0.5.20.1
SFO90         C1p60.0.5.20.1
SFO91         C1p60.0.5.20.1
SFO92         C1p60.0.5.20.1
SFO93         C1p60.0.5.20.1
SFO94         C1p60.0.5.20.1
SFO95         C1p60.0.5.20.1
SFO96         C1p60.0.5.20.1
SFO97         C1p60.0.5.20.1
SFO98         C1p60.0.5.20.1
SFO99         C1p60.0.5.20.1
SFO100        C1p60.0.5.20.1
===== CHANNEL f2 =====
C1P1RG2       waltz16
NUC2          1H
PC2           100.00 usec
PL2           2.00 dB
PL0           2.00 dB
SFO1         500.2225013 MHz
===== GRADIENT CHANNEL =====
GENAM1        SINE.100
GENAM2        SINE.100
GEX1          0.00 %
GEX2          0.00 %
GEX3          0.00 %
GEX4          0.00 %
GEX5          0.00 %
GEX6          0.00 %
GEX7          0.00 %
GEX8          0.00 %
GEX9          0.00 %
GEX10         0.00 %
GEX11         0.00 %
GEX12         0.00 %
GEX13         0.00 %
GEX14         0.00 %
GEX15         0.00 %
GEX16         0.00 %
GEX17         0.00 %
GEX18         0.00 %
GEX19         0.00 %
GEX20         0.00 %
GEX21         0.00 %
GEX22         0.00 %
GEX23         0.00 %
GEX24         0.00 %
GEX25         0.00 %
GEX26         0.00 %
GEX27         0.00 %
GEX28         0.00 %
GEX29         0.00 %
GEX30         0.00 %
GEX31         0.00 %
GEX32         0.00 %
GEX33         0.00 %
GEX34         0.00 %
GEX35         0.00 %
GEX36         0.00 %
GEX37         0.00 %
GEX38         0.00 %
GEX39         0.00 %
GEX40         0.00 %
GEX41         0.00 %
GEX42         0.00 %
GEX43         0.00 %
GEX44         0.00 %
GEX45         0.00 %
GEX46         0.00 %
GEX47         0.00 %
GEX48         0.00 %
GEX49         0.00 %
GEX50         0.00 %
GEX51         0.00 %
GEX52         0.00 %
GEX53         0.00 %
GEX54         0.00 %
GEX55         0.00 %
GEX56         0.00 %
GEX57         0.00 %
GEX58         0.00 %
GEX59         0.00 %
GEX60         0.00 %
GEX61         0.00 %
GEX62         0.00 %
GEX63         0.00 %
GEX64         0.00 %
GEX65         0.00 %
GEX66         0.00 %
GEX67         0.00 %
GEX68         0.00 %
GEX69         0.00 %
GEX70         0.00 %
GEX71         0.00 %
GEX72         0.00 %
GEX73         0.00 %
GEX74         0.00 %
GEX75         0.00 %
GEX76         0.00 %
GEX77         0.00 %
GEX78         0.00 %
GEX79         0.00 %
GEX80         0.00 %
GEX81         0.00 %
GEX82         0.00 %
GEX83         0.00 %
GEX84         0.00 %
GEX85         0.00 %
GEX86         0.00 %
GEX87         0.00 %
GEX88         0.00 %
GEX89         0.00 %
GEX90         0.00 %
GEX91         0.00 %
GEX92         0.00 %
GEX93         0.00 %
GEX94         0.00 %
GEX95         0.00 %
GEX96         0.00 %
GEX97         0.00 %
GEX98         0.00 %
GEX99         0.00 %
GEX100        0.00 %
===== Processing parameters =====
SI            65536
SF            125.7942548 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            2.00
ID NMR plot parameters
CX            22.80 cm
SI            15.50 usec
F1P           230.637 ppm
F1           29009.67 Hz
F2P          -10.287 ppm
F2           -1293.96 Hz
PRMCM        10.56688 ppm/cm
HCM          1329.10681 Hz/cm
    
```

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



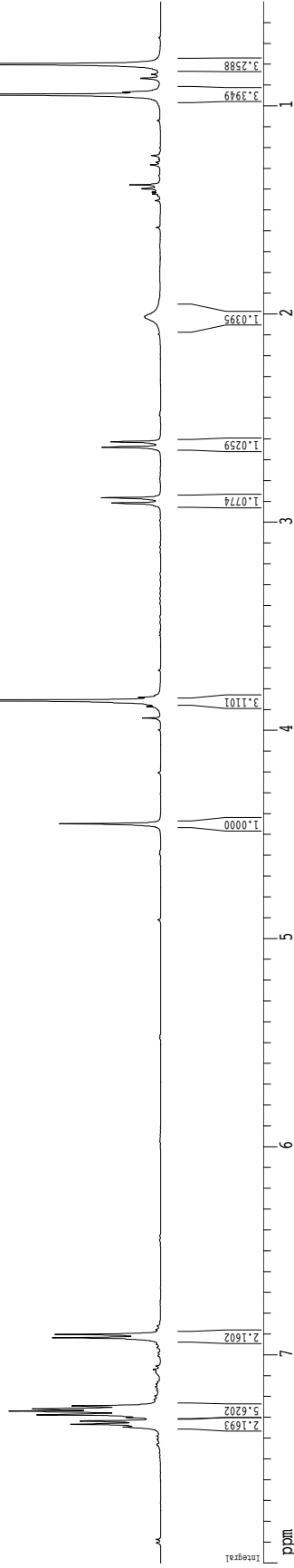
Current Data Parameters  
 USER untitled  
 NAME MUJ-03-190  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120428  
 Time 15.40  
 INSTRUM cryo500  
 PROBDI 5 mm CPCL1 IH-  
 PULPROG zgpg30  
 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 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 ACRESF 0.00000000 sec  
 ACPRR 0.01500000 sec

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

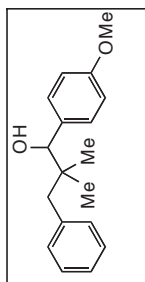
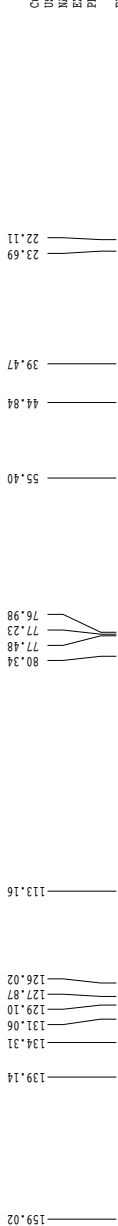
F2 - Processing parameters  
 SI 65536  
 SF 500.2200117 MHz  
 WDW EM  
 SSB 0  
 LB 0.20 Hz  
 GB 0  
 PC 4.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 5.00 cm  
 FIP 8.000 ppm  
 F1 4001.76 Hz  
 F2P 0.500 ppm  
 F2 250.11 Hz  
 PPMCH 0.32895 ppm/cm  
 HZCM 164.54605 Hz/cm



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

wdd



Current Data Parameters  
 USER untitled  
 NAME NLIJ-03-190  
 EXPNO 2  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120428  
 Time 15:44  
 INSTRUM cryo500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG Spinechoeg30pp.prd  
 TD 65536  
 SOLVENT CDCl3  
 NS 6  
 DS 6  
 SWH 30303.033 Hz  
 SFH 0.462388 Hz  
 FIDRES 1.0813940 sec  
 AQ 5160.6  
 RG 16.500 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 0.2550000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.00019600 sec  
 ACRESF 0.0000000 sec  
 MCNRRK 0.0150000 sec  
 P2 31.00 usec

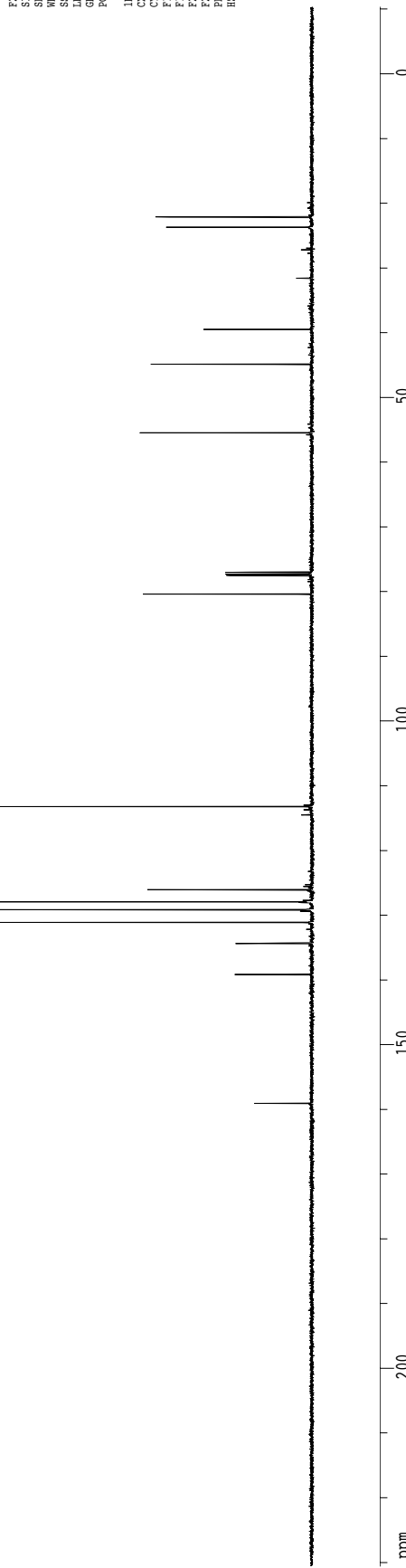
==== CHANNEL f1 =====  
 NUCL1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SF01 125.7942548 MHz  
 SF1 3.20 dB  
 SF2 3.20 dB  
 GENAM1 Cnp60.0.5.20.1  
 GENAM2 Cnp60cm0.0  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUCL2 1H  
 PCPDZ 100.00 usec  
 PL0 0.00 dB  
 PL1 2.00 dB  
 SF02 500.2225013 MHz

==== GRADIENT CHANNEL =====  
 GENAM1 SINE.100  
 GENAM2 SINE.100  
 GX1 0.00 %  
 GX2 0.00 %  
 GY1 0.00 %  
 GY2 0.00 %  
 GZ1 30.00 %  
 GZ2 50.00 %  
 p15 500.00 usec  
 p16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.760490 MHz  
 NS 6  
 DS 6  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 24.80 cm  
 F1 230.637 ppm  
 F2 29009.68 Hz  
 F3 -10.287 ppm  
 F4 -1293.96 Hz  
 PPMCM 10.56688 ppm/cm  
 HCM 1329.10693 Hz/cm



1H spectrum



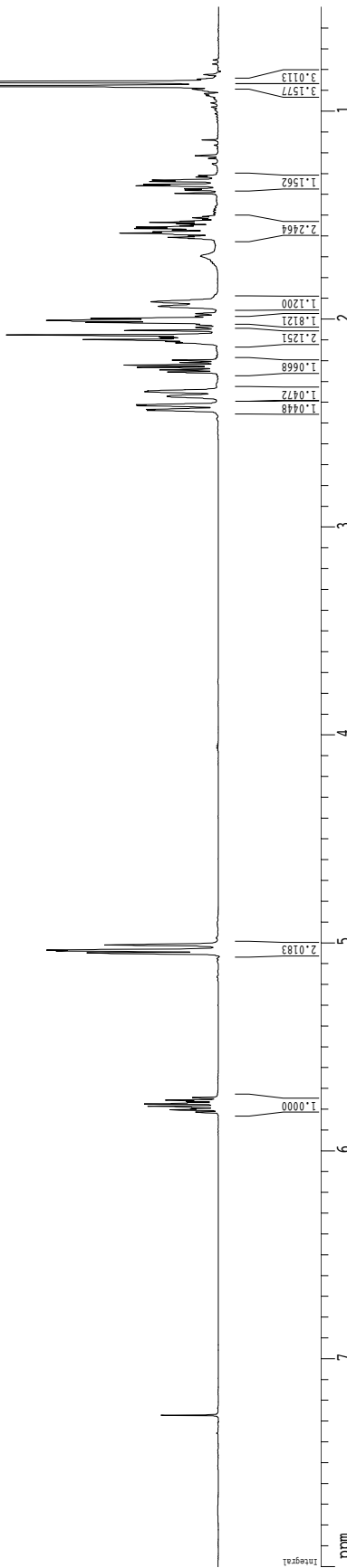
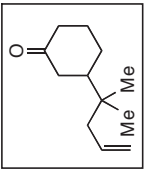
Current Data Parameters  
 USER untitled  
 NAME NUL-02-27-01  
 F2PNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110825  
 Time\_ 22.13  
 INSTRUM av600  
 PROBED 5 mm TBI H/13  
 PULPROG zgpg30  
 TD 98074  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 9611.385 Hz  
 FIDRES 0.1090042 Hz  
 AQ 5.098979 sec  
 RG 45.2  
 DW 52.000 usec  
 DE 1.00 usec  
 TE 298.1 K  
 D1 0.10000000 sec

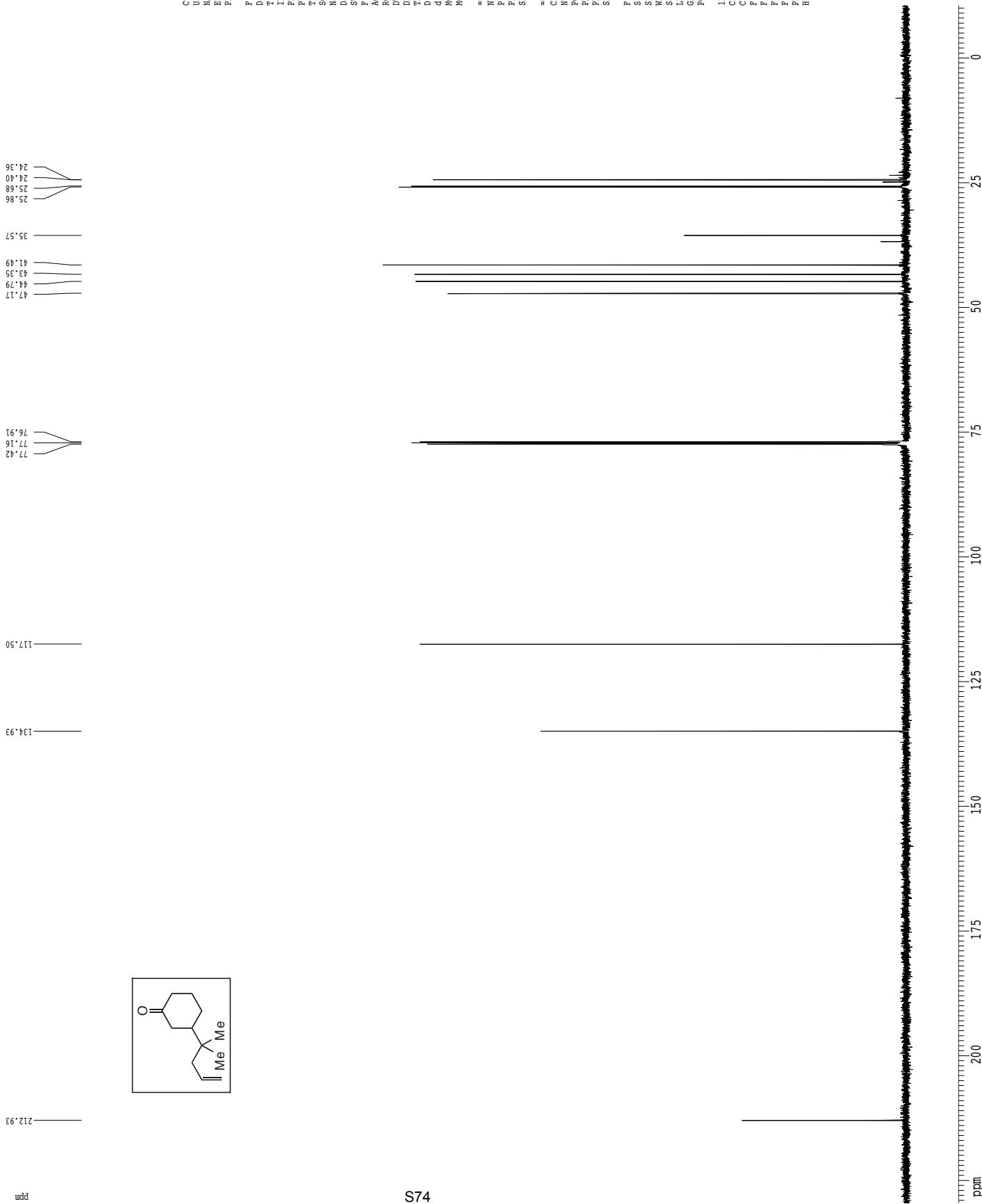
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 600.1300281 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 32.00 cm  
 CY 15.00 cm  
 FID 8.000 ppm  
 F1 4801.04 Hz  
 F2 0.500 ppm  
 FZ 300.07 Hz  
 PRCM 0.2895 ppm/cm  
 HZCN 197.41119 Hz/cm



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



Current Data Parameters  
 USER untitled  
 NAME NMR-02-277-C13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110825  
 Time\_ 22.54  
 INSTRUM qm500  
 PROBED 5 mm broadband  
 PULPROG zgpgc30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 30301.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 46341  
 DW 16.300 usec  
 DE 2.200 usec  
 TE 298.0 K  
 D1 0.25000000 sec  
 d11 0.03000000 sec  
 MCREST 0.00000000 sec  
 MCORE 0.01500000 sec

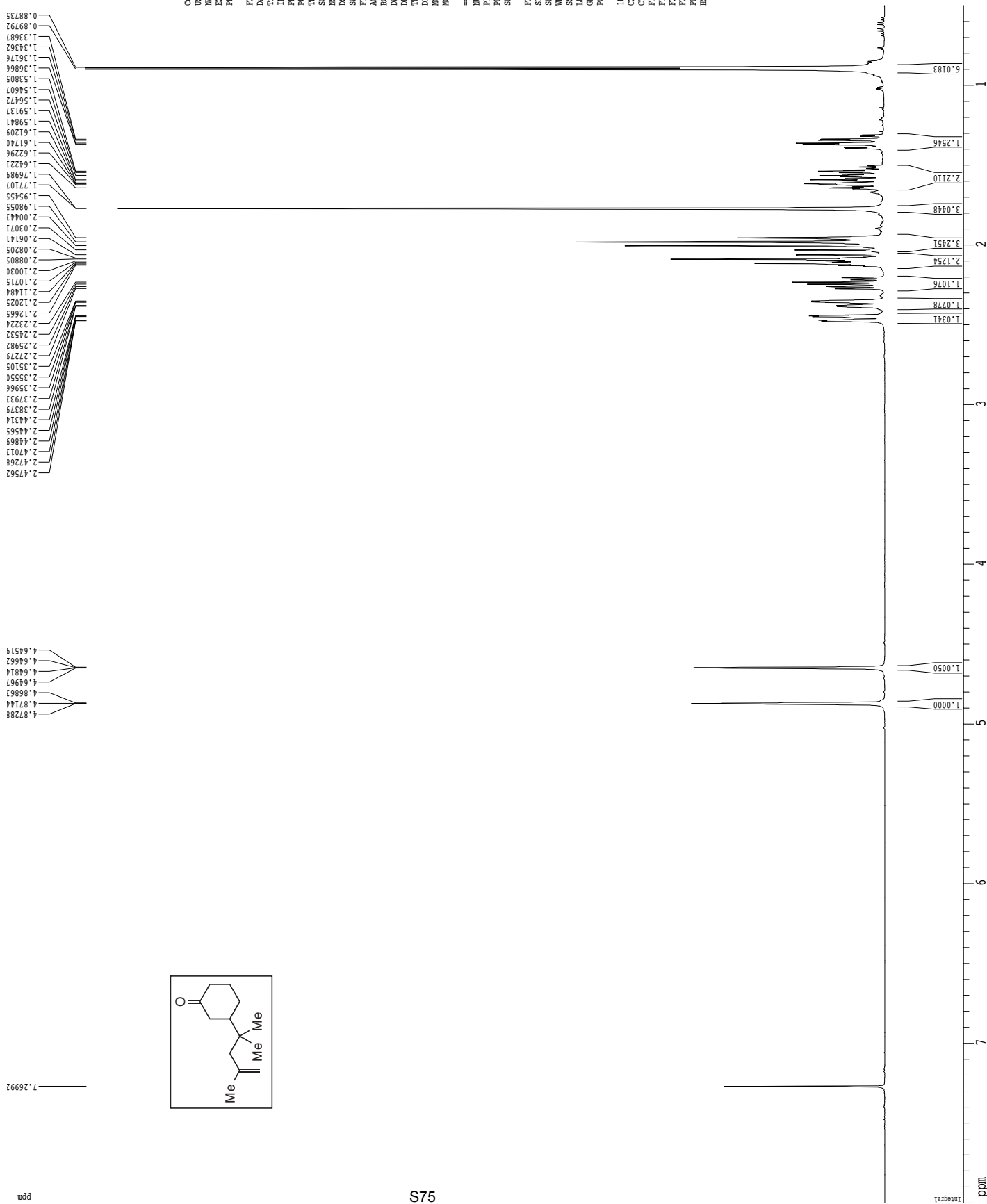
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 7.70 usec  
 PL1 0.00 dB  
 SFO1 125.6157052 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 13.00 dB  
 PL12 13.00 dB  
 SFO2 499.5124975 MHz

F2 - Processing parameters  
 SI 65536  
 SF 125.6038777 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 225.520 ppm  
 F1 28828.10 Hz  
 F2 -110.362 ppm  
 F3 0.00000000 Hz  
 FWHM 110.52747 Hz/cm  
 HCON 1322.26978 Hz/cm

<sup>1</sup>H spectrum



Current Data Parameters  
 USER untied  
 NAME NUP-03-82  
 EXPNO 1  
 PROCNO 1

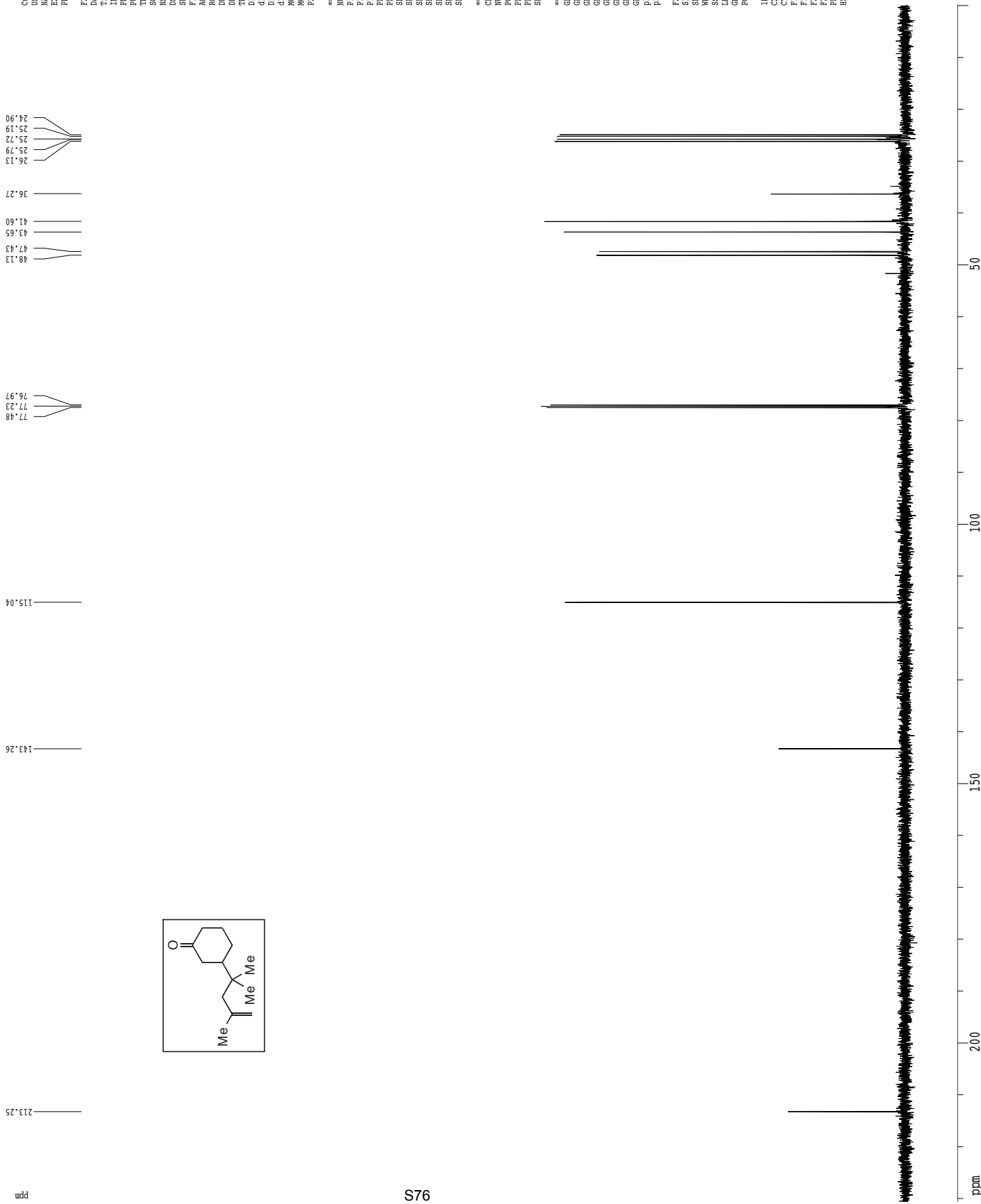
F2 - Acquisition Parameters  
 Date\_ 20120413  
 Time 17.25  
 INSTRUM cryo500  
 PROBD 5 mm CPCL1 IH-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 289.8 K  
 D1 0.10000000 sec  
 ACRESF 0.00000000 sec  
 ACPRK 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 500.2200272 MHz  
 WDW EN  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 20.00 cm  
 F1P 8.000 ppm  
 F1 4001.76 Hz  
 F2P 0.500 ppm  
 F2 250.11 Hz  
 PPMCM 0.32895 ppm/cm  
 HZCM 164.54607 Hz/cm

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



```

Current Data Parameters
USER      untitled
NAME      NLU-0.3-82
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20120413
Time      17:27
INSTRUM   cryo500
PROBHD    5 mm CPYCI 1H-
PULPROG   Spinechoeg30pp.prd
TD         65536
SOLVENT    CDCl3
NS         0
DS         0
SWH        30303.033 Hz
FIDRES     0.462388 Hz
AQ         1.0813940 sec
RG         3251
DE         16.500 usec
TE         289.8 K
AQ         0.2550000 sec
d11        0.0300000 sec
d16        0.0002000 sec
d17        0.00019000 sec
MCRESTF    0.0000000 sec
MCNRRK     0.01500000 sec
P2         31.00 usec

===== CHANNEL f1 =====
NUC1       13C
PC         15.50 usec
P1         500.00 usec
P11        2000.00 usec
P12        120.00 dB
P13        -1.00 dB
SFO1       125.7942548 MHz
SF1        3.20 dB
SFO2        Cp60.5, 20.1
SFO3        Cp60.5, 20.1
SFO4        0.00 Hz
SFO5        0.00 Hz
SFO6        0.00 Hz
SFO7        0.00 Hz
SFO8        0.00 Hz

===== CHANNEL f2 =====
CPCPRG2    waltz16
NUC2       1H
PC2        100.00 usec
P2         2.00 dB
P21        2.00 dB
SFO2       500.2225013 MHz

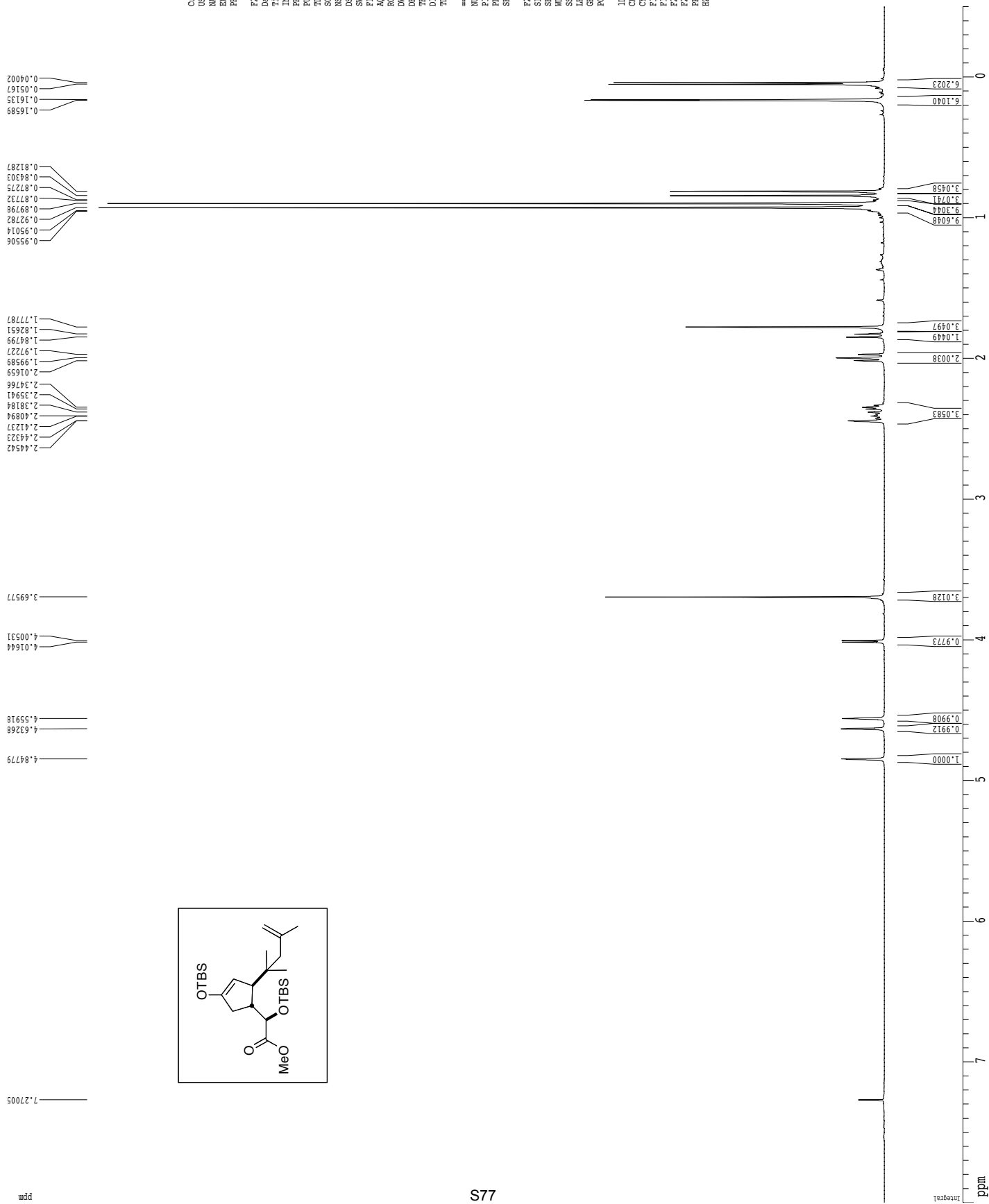
===== GRADIENT CHANNEL =====
GENAM1     SINE.100
GENAM2     SINE.100
GX1        0.00 %
GX2        0.00 %
GX3        0.00 %
GX4        0.00 %
GX5        30.00 %
GX6        50.00 %
GX7        100.00 usec
p15        500.00 usec
p16        1000.00 usec

F2 - Processing parameters
SI         65536
SF         125.7604893 MHz
WDW        0
SSB        0
LB         1.00 Hz
GB         0
PC         2.00

ID NMR plot parameters
CX         2.80 cm
CY         7.50 cm
F1P        230.577 ppm
F1         29002.04 Hz
F2P        0.000 ppm
F2         0.00 Hz
PRCM       10.11302 ppm/cm
HCM        1272.01941 Hz/cm
    
```



<sup>1</sup>H spectrum



```

Current Data Parameters
USER          untied
NAME          02-14-F1
EXPNO         1
PROCNO        1

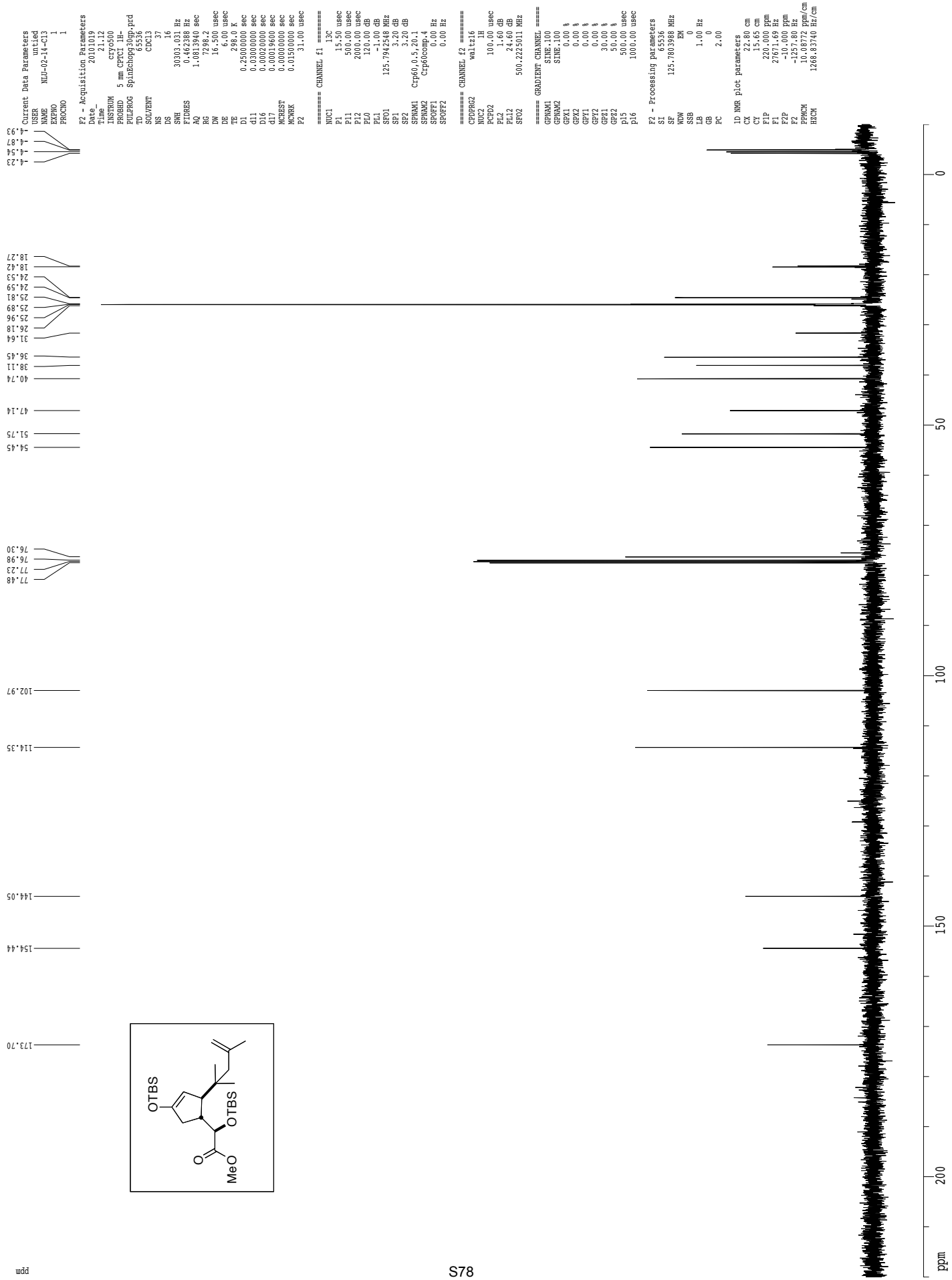
F2 - Acquisition Parameters
Date_         20101213
Time          17.42
INSTRUM       av600
PROBHD        5 mm TBI 1H/13
PULPROG       zg30
AQ             8.074
RG             256
SI             2
SF             9615.385 Hz
WDW            EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00

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

F2 - Processing Parameters
SI             65536
SF            600.1300286 MHz
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
F1P           8.000 ppm
F2P           4801.04 Hz
P2P           -0.500 ppm
P3P           0.37281 ppm/cm
RGCH          223.73288 Hz/cm
    
```

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

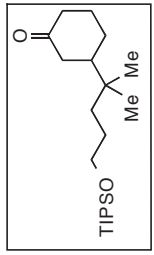


1H spectrum

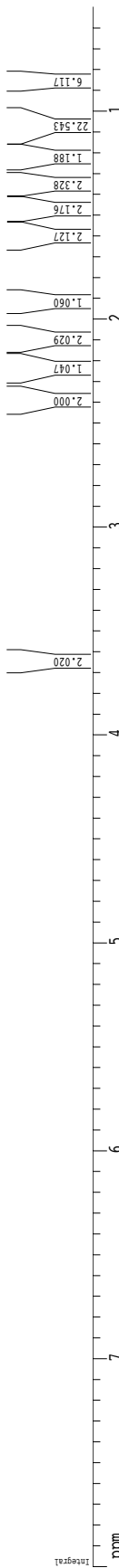
7.27003  
7.26867

3.65893  
3.64434

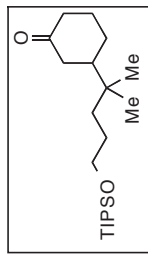
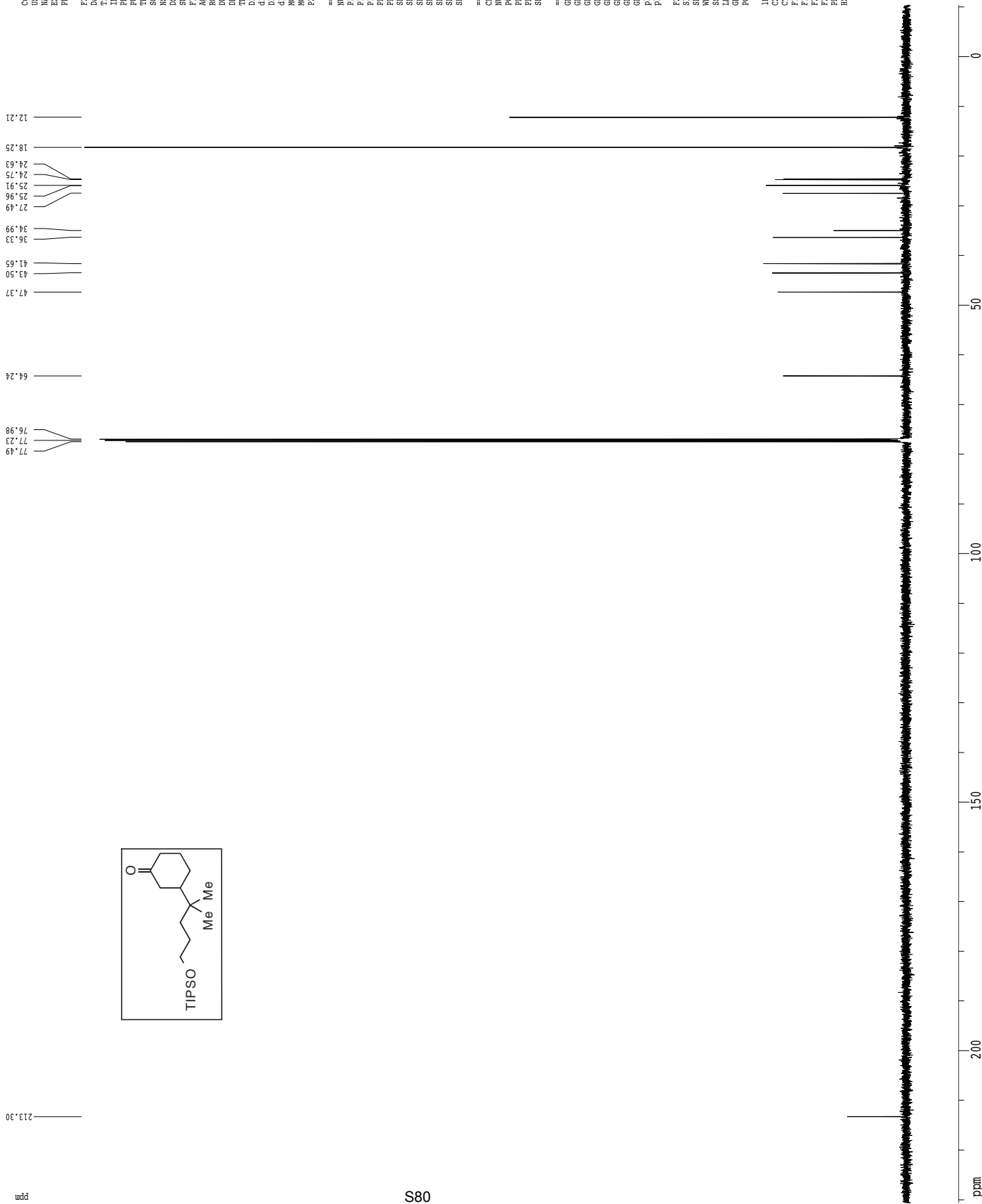
1.46039  
1.32419  
1.10343  
1.08679  
1.07707  
1.06731  
1.05734  
1.04586  
0.87377  
0.85889



Current Data Parameters  
 USER untied  
 NAME NUP-03-97  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120414  
 Time 16.24  
 INSTRUM cryo500  
 PROBD 5 mm CPCLP1H-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 8  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 ACRESF 0.00000000 sec  
 ACPRK 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  
 WDW EN  
 SSB 0  
 LB 0.20 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 8.000 ppm  
 F1 4001.76 Hz  
 F2P 0.500 ppm  
 F2 250.11 Hz  
 FPMCH 0.32895 ppm/cm  
 HZCM 164.54607 Hz/cm



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



```

Current Data Parameters
USER          untitled
NAME          NUI-03-97
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20120416
Time          16:27
INSTRUM       cryo500
PROBHD        5 mm CPVC 1H-
PULPROG       Spinechoeg30pp.prd
TD            65536
SOLVENT       CDCl3
NS            442
DS            4
SWH           30303.033 Hz
SF           125.760358 MHz
AQ           1.0813940 sec
RG           7298.2
DN           16.500 usec
DE           6.000 usec
TE           298.0 K
FIDRES       0.356000 sec
AQRES        0.030000 sec
D1           0.0002000 sec
D16          0.0002000 sec
d17          0.00019600 sec
MCREST       0.0000000 sec
MCNRRK       0.01500000 sec
P2           31.00 usec

===== CHANNEL f1 =====
NUC1          13C
PC           15.50 usec
PL1          500.00 usec
PL2          2000.00 usec
PL0          120.00 dB
PL1          -1.00 dB
SFO1         125.7942548 MHz
SF1          3.20 dB
SFO2         C1p60.0, 5.20, 1
SFO3         C1p60.0, 5.20, 1
SFO4         C1p60.0, 5.20, 1
SFO5         C1p60.0, 5.20, 1
SFO6         C1p60.0, 5.20, 1
SFO7         C1p60.0, 5.20, 1
SFO8         C1p60.0, 5.20, 1
SFO9         C1p60.0, 5.20, 1
SFO10        C1p60.0, 5.20, 1
SFO11        C1p60.0, 5.20, 1
SFO12        C1p60.0, 5.20, 1
SFO13        C1p60.0, 5.20, 1
SFO14        C1p60.0, 5.20, 1
SFO15        C1p60.0, 5.20, 1
SFO16        C1p60.0, 5.20, 1
SFO17        C1p60.0, 5.20, 1
SFO18        C1p60.0, 5.20, 1
SFO19        C1p60.0, 5.20, 1
SFO20        C1p60.0, 5.20, 1
SFO21        C1p60.0, 5.20, 1
SFO22        C1p60.0, 5.20, 1
SFO23        C1p60.0, 5.20, 1
SFO24        C1p60.0, 5.20, 1
SFO25        C1p60.0, 5.20, 1
SFO26        C1p60.0, 5.20, 1
SFO27        C1p60.0, 5.20, 1
SFO28        C1p60.0, 5.20, 1
SFO29        C1p60.0, 5.20, 1
SFO30        C1p60.0, 5.20, 1
SFO31        C1p60.0, 5.20, 1
SFO32        C1p60.0, 5.20, 1
SFO33        C1p60.0, 5.20, 1
SFO34        C1p60.0, 5.20, 1
SFO35        C1p60.0, 5.20, 1
SFO36        C1p60.0, 5.20, 1
SFO37        C1p60.0, 5.20, 1
SFO38        C1p60.0, 5.20, 1
SFO39        C1p60.0, 5.20, 1
SFO40        C1p60.0, 5.20, 1
SFO41        C1p60.0, 5.20, 1
SFO42        C1p60.0, 5.20, 1
SFO43        C1p60.0, 5.20, 1
SFO44        C1p60.0, 5.20, 1
SFO45        C1p60.0, 5.20, 1
SFO46        C1p60.0, 5.20, 1
SFO47        C1p60.0, 5.20, 1
SFO48        C1p60.0, 5.20, 1
SFO49        C1p60.0, 5.20, 1
SFO50        C1p60.0, 5.20, 1
SFO51        C1p60.0, 5.20, 1
SFO52        C1p60.0, 5.20, 1
SFO53        C1p60.0, 5.20, 1
SFO54        C1p60.0, 5.20, 1
SFO55        C1p60.0, 5.20, 1
SFO56        C1p60.0, 5.20, 1
SFO57        C1p60.0, 5.20, 1
SFO58        C1p60.0, 5.20, 1
SFO59        C1p60.0, 5.20, 1
SFO60        C1p60.0, 5.20, 1
SFO61        C1p60.0, 5.20, 1
SFO62        C1p60.0, 5.20, 1
SFO63        C1p60.0, 5.20, 1
SFO64        C1p60.0, 5.20, 1
SFO65        C1p60.0, 5.20, 1
SFO66        C1p60.0, 5.20, 1
SFO67        C1p60.0, 5.20, 1
SFO68        C1p60.0, 5.20, 1
SFO69        C1p60.0, 5.20, 1
SFO70        C1p60.0, 5.20, 1
SFO71        C1p60.0, 5.20, 1
SFO72        C1p60.0, 5.20, 1
SFO73        C1p60.0, 5.20, 1
SFO74        C1p60.0, 5.20, 1
SFO75        C1p60.0, 5.20, 1
SFO76        C1p60.0, 5.20, 1
SFO77        C1p60.0, 5.20, 1
SFO78        C1p60.0, 5.20, 1
SFO79        C1p60.0, 5.20, 1
SFO80        C1p60.0, 5.20, 1
SFO81        C1p60.0, 5.20, 1
SFO82        C1p60.0, 5.20, 1
SFO83        C1p60.0, 5.20, 1
SFO84        C1p60.0, 5.20, 1
SFO85        C1p60.0, 5.20, 1
SFO86        C1p60.0, 5.20, 1
SFO87        C1p60.0, 5.20, 1
SFO88        C1p60.0, 5.20, 1
SFO89        C1p60.0, 5.20, 1
SFO90        C1p60.0, 5.20, 1
SFO91        C1p60.0, 5.20, 1
SFO92        C1p60.0, 5.20, 1
SFO93        C1p60.0, 5.20, 1
SFO94        C1p60.0, 5.20, 1
SFO95        C1p60.0, 5.20, 1
SFO96        C1p60.0, 5.20, 1
SFO97        C1p60.0, 5.20, 1
SFO98        C1p60.0, 5.20, 1
SFO99        C1p60.0, 5.20, 1
SFO100       C1p60.0, 5.20, 1

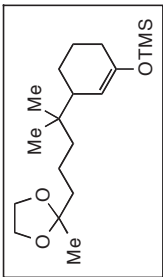
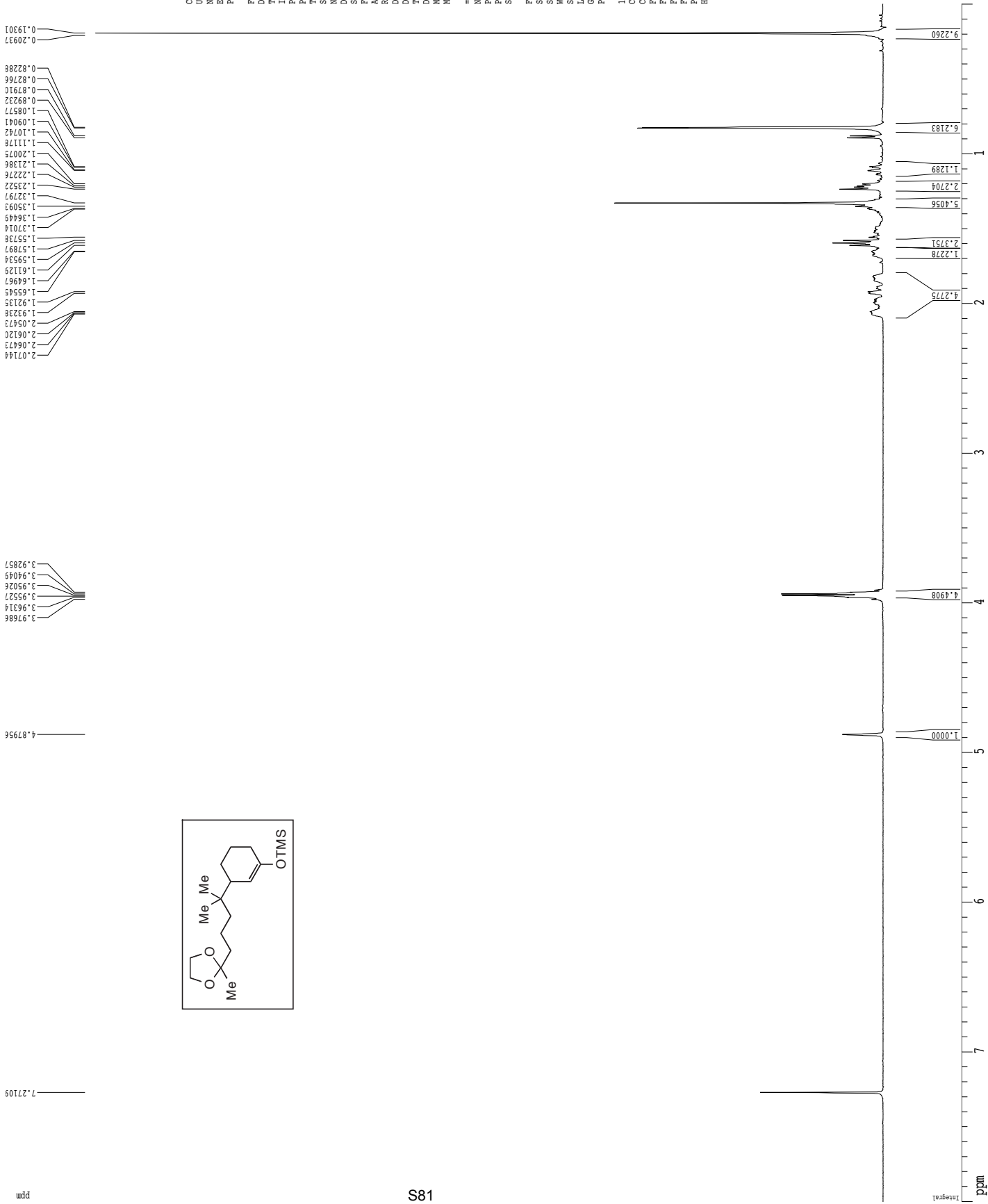
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PC2          100.00 usec
PL2          2.00 dB
PL0          120.00 dB
SFO2         500.2225013 MHz

===== GRADIENT CHANNEL =====
GENAM1       SINE.100
GENAM2       SINE.100
GX1          0.00 %
GX2          0.00 %
GY1          0.00 %
GY2          0.00 %
GZ1          30.00 %
GZ2          50.00 %
p15          500.00 usec
p16          1000.00 usec

F2 - Processing parameters
SI           65536
SF           125.760358 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           2.00

ID NMR plot parameters
CX           22.80 cm
CY           1.50 cm
F1P          230.637 ppm
F1           290095.63 Hz
F2P          -10.287 ppm
F2           -1293.96 Hz
P1PCMK      10.56688 ppm/cm
P2PCMK      1329.10681 Hz/cm
    
```

<sup>1</sup>H spectrum



Current Data Parameters  
 NMR Unit Used  
 NUC-03-41-H-1  
 EXNO 1  
 PROCNO 1

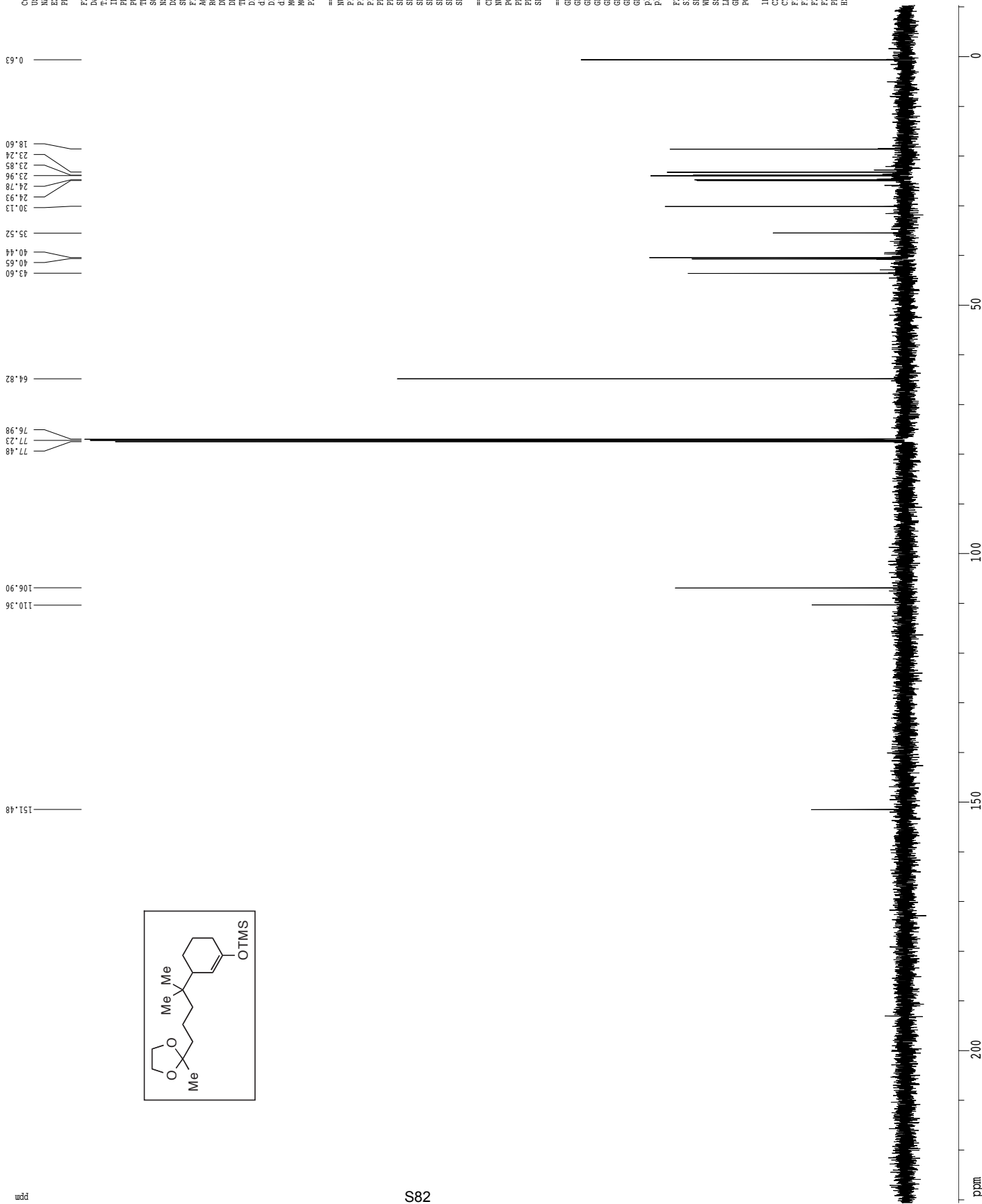
F2 - Acquisition Parameters  
 Date\_ 20111109  
 Time\_ 15.29  
 INSTRUM gn500  
 PROBED 5 mm broadband  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 9  
 DS 4  
 SF 8012.820 Hz  
 EQ 0.098043 Hz  
 FIDRES 5.0998774 sec  
 RG 812.7  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUCL1 1H  
 P1 12.00 usec  
 PL1 0.00 dB  
 PR1 -5.00 dB  
 SFO1 499.5134966 MHz

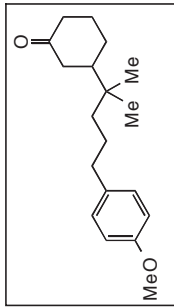
F2 - Processing parameters  
 SI 65536  
 SF 499.5100217 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CD 25.80 cm  
 CX 15.00 cm  
 CY 8.00 cm  
 EI 3996.08 Hz  
 F2 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 0.35088 ppm/cm  
 HZCM 175.26668 Hz/cm

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



1H spectrum



Current Data Parameters  
USER untitled  
NAME NUL-02-208-F1  
PROCNO 1  
PRCNO 1

F2 - Acquisition Parameters  
Date\_ 20111003  
Time\_ 16.45  
INSTRUM av600  
PROBHD 5 mm TBI H/13  
PULPROG zgpg30  
TD 98074  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 9613.385 Hz  
FIDRES 0.098042 Hz  
AQ 5.098979 sec  
RG 221.6  
DW 52.000 usec  
DE 4.000 usec  
TE 298.2 K  
D1 0.10000000 sec

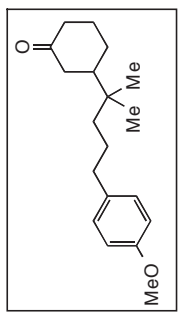
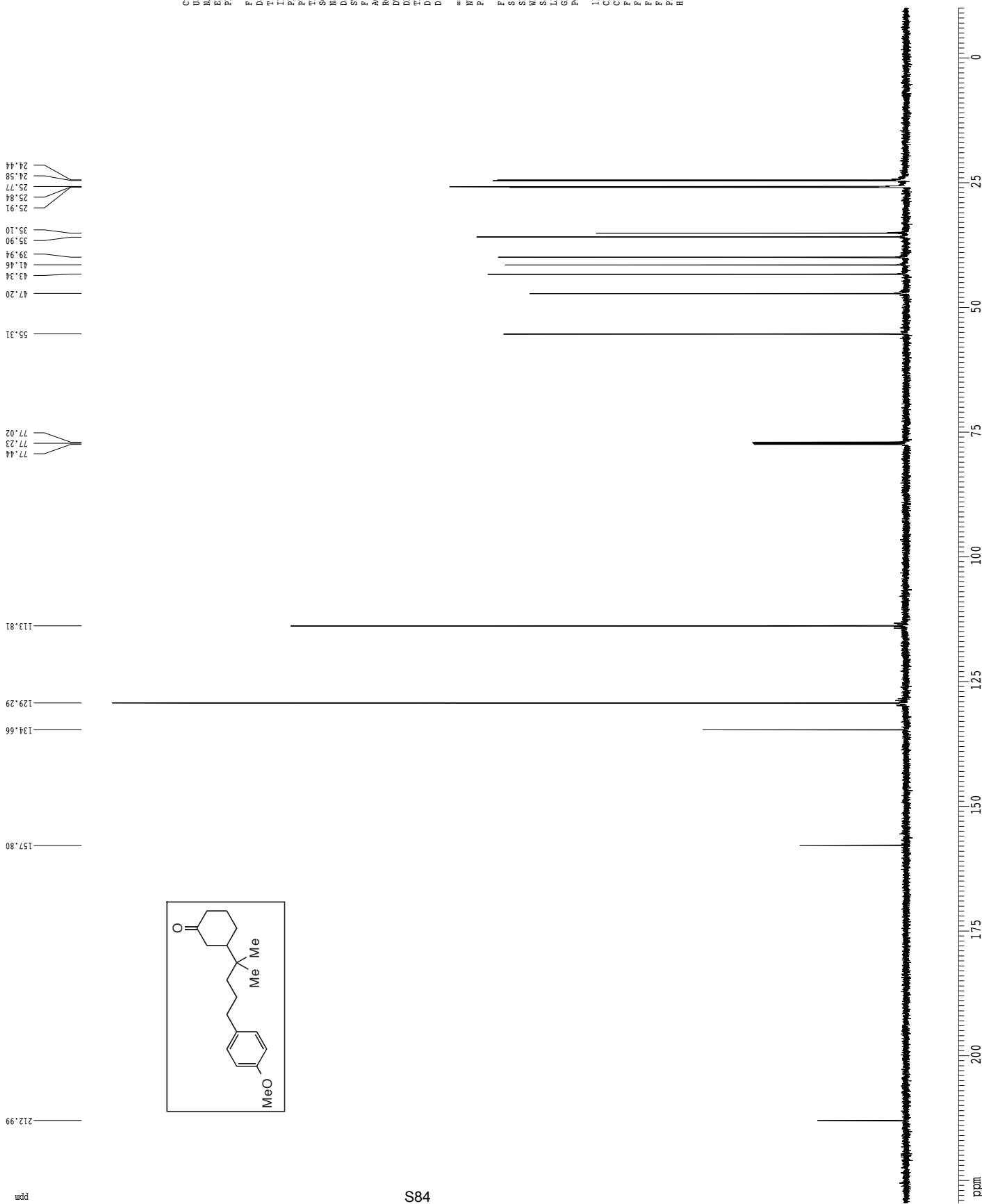
==== CHANNEL f1 =====  
NUC1 1H  
P1 8.00 usec

F2 - Processing parameters  
SI 65536  
SF 600.1300286 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
F2 298.200 MHz  
CX 15.00 cm  
FLP 8.000 ppm  
F1 4801.04 Hz  
FZP 0.500 ppm  
F2 300.07 Hz  
PRMCH 0.2895 ppm/cm  
HZCN 197.41119 Hz/cm



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



Current Data Parameters  
 USER Utilized  
 NAME NUP-02-246-CL3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20111003  
 Time\_ 16.52  
 INSTRUM av600  
 PROBEID 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 234  
 DS 4  
 SWH 36231.883 Hz  
 FIDRES 0.352855 Hz  
 AQ 0.904468 sec  
 RG 2050  
 DW 13.800 usec  
 DE 4.000 usec  
 TE 298.1 K  
 D1 0.4000001 sec  
 D11 0.0300000 sec

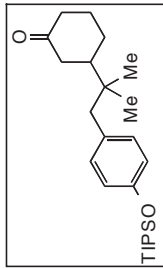
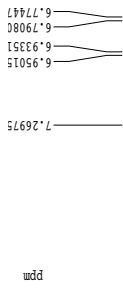
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 150.9028019 MHz  
 WDW BH  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CY 212.80 cm  
 CX 15.85 cm  
 F1P 228.520 ppm  
 F1 34635.16 Hz  
 F2P -10.507 ppm  
 F2 -1585.47 Hz  
 PPMCH 10.52747 ppm/cm  
 HZCM 1588.62451 Hz/cm



<sup>1</sup>H spectrum



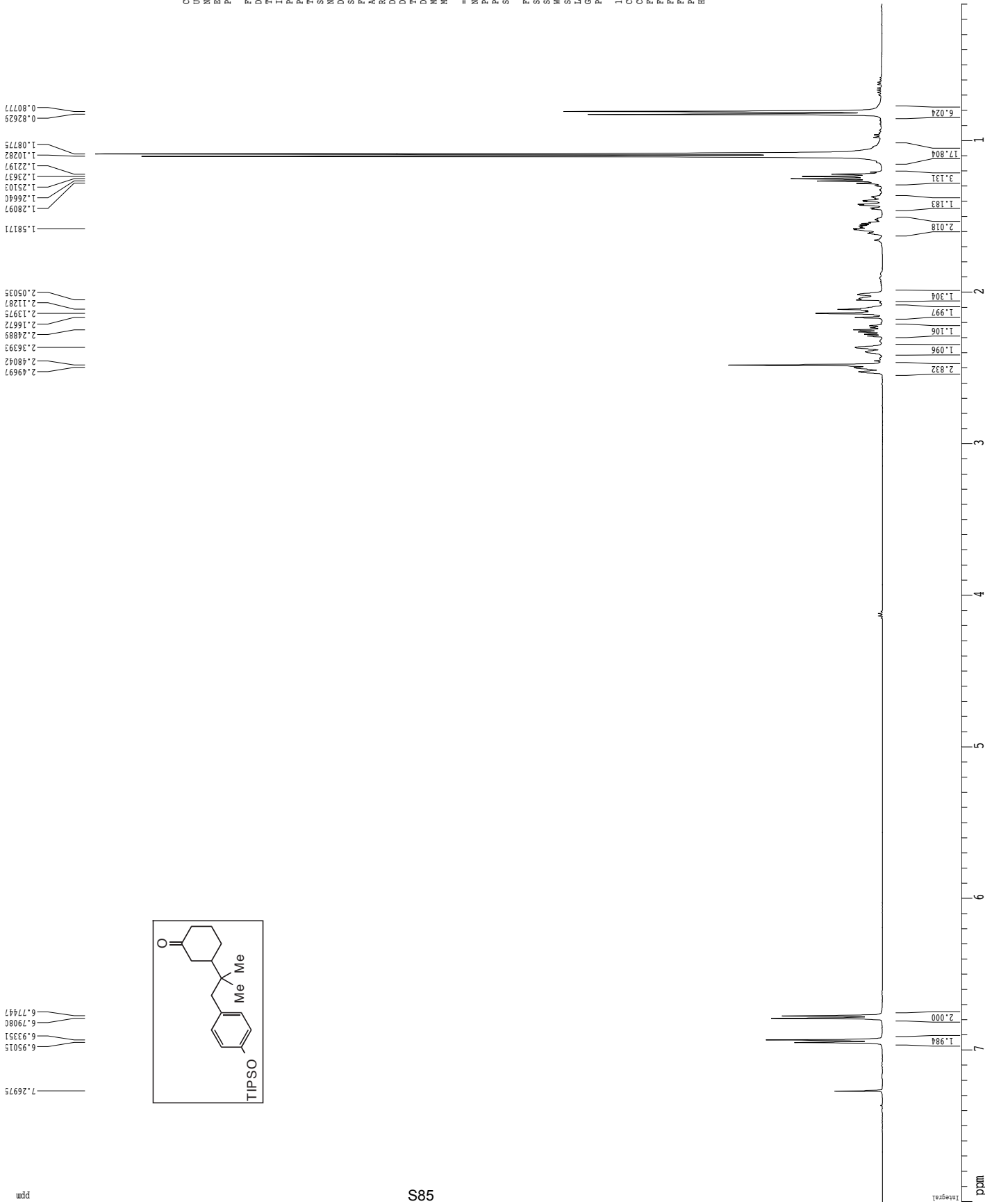
Current Data Parameters  
 USER untitled  
 NAME MUJ-43-210  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120522  
 Time 16.31  
 INSTRUM cryo500  
 PROBDI 5 mm CPCLP1H-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.1000000 sec  
 ACRESF 0.0000000 sec  
 ACPRR 0.0150000 sec

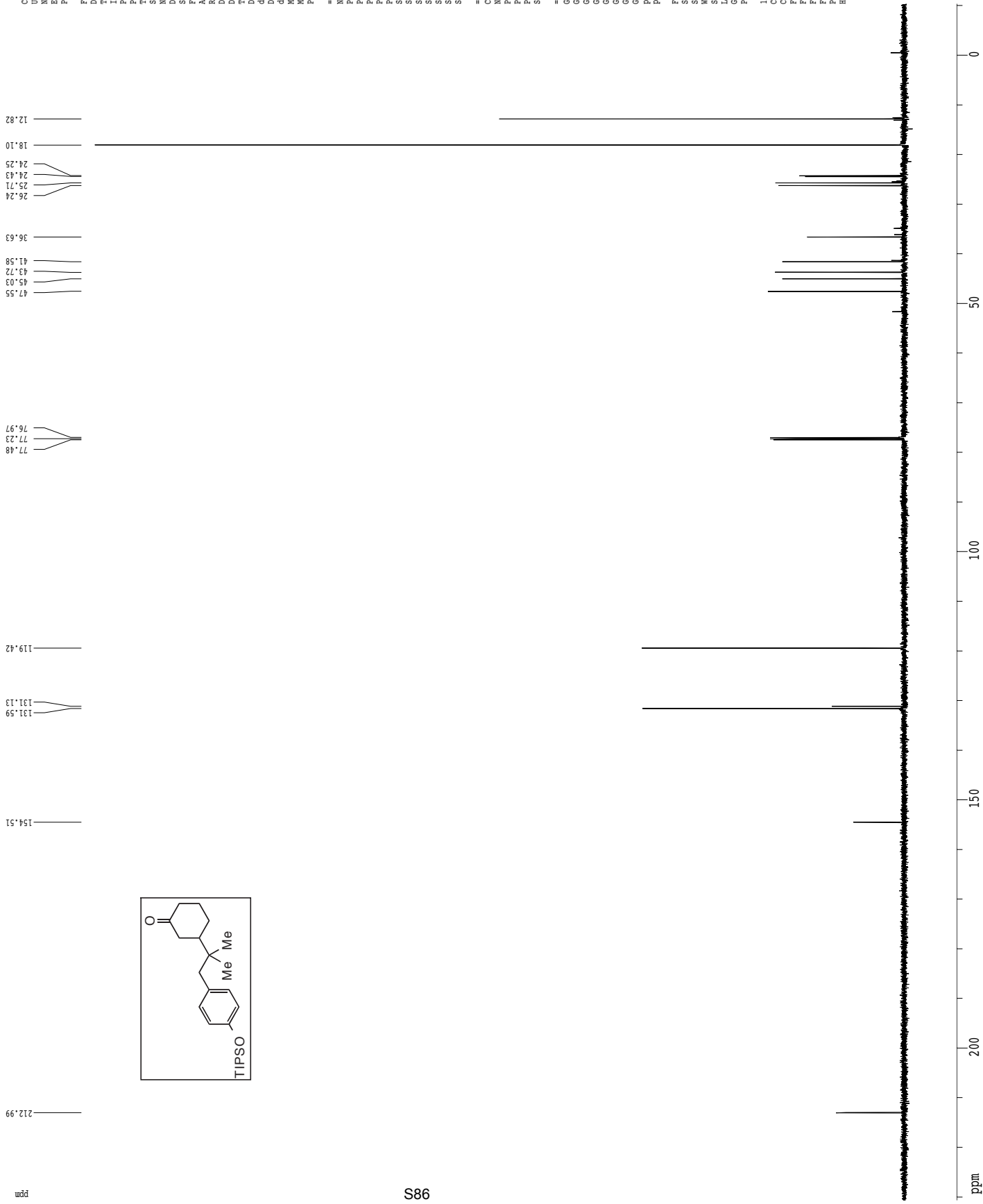
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2200288 MHz  
 WDW EM  
 SSB 0  
 LB 0.20 Hz  
 GB 0  
 PC 4.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 8.000 ppm  
 F1 4001.76 Hz  
 F2P 0.100 ppm  
 F2 50.02 Hz  
 PPMCM 0.34649 ppm/cm  
 HZCM 173.32185 Hz/cm



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



Current Data Parameters  
 USER untitled  
 NAME NLIJ-03-210  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120522  
 Time\_ 16:33  
 INSTRUM cryo500  
 PROBH0 5 mm CPYCI 1H-  
 PULPROG Spinechoeg30pp.prd  
 TD 65536  
 SOLVENT CDCl3  
 NS 6  
 DS 6  
 SWH 30303.033 Hz  
 SF01 125.7942548 MHz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 14596.5  
 DW 16.500 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 0.2550000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.0001900 sec  
 MCPRST 0.0000000 sec  
 MCKRRK 0.0150000 sec  
 P2 31.00 usec

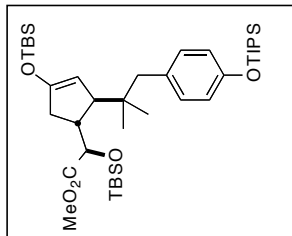
==== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 -1.00 dB  
 SF01 125.7942548 MHz  
 SF1 3.20 dB  
 SF2 3.20 dB  
 SFO1 C1p60.0\_5\_20.1  
 SFO2 C1p60cm60  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPDZ 100.00 usec  
 PL2 2.00 dB  
 PL3 2.00 dB  
 SF02 500.2225013 MHz

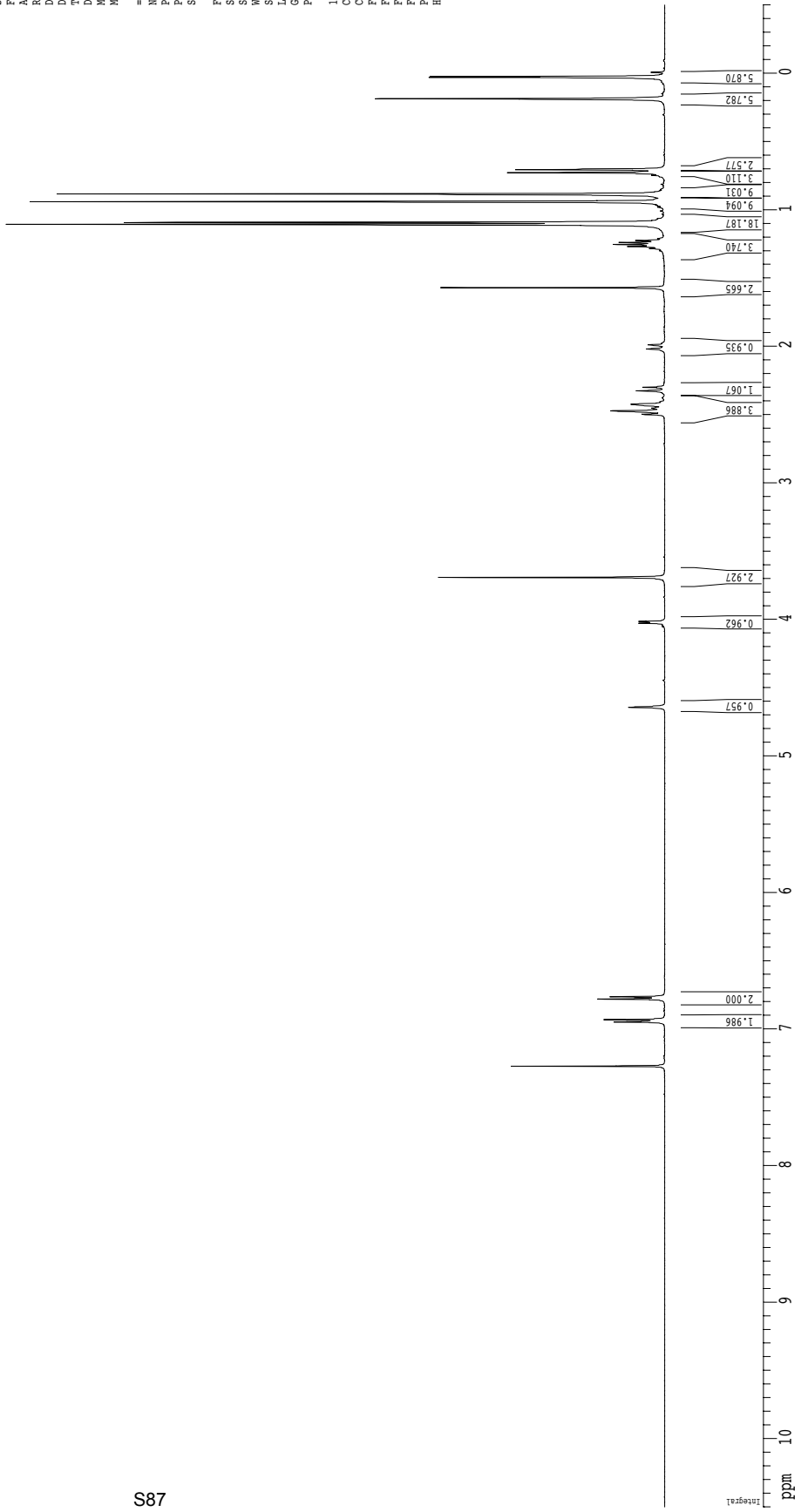
==== GRADIENT CHANNEL =====  
 GENAM1 SINE.100  
 GENAM2 SINE.100  
 GRX1 0.00 %  
 GRX2 0.00 %  
 GRX3 0.00 %  
 GRX4 0.00 %  
 GRX5 30.00 %  
 GRX6 50.00 %  
 p15 500.00 usec  
 p16 1000.00 usec

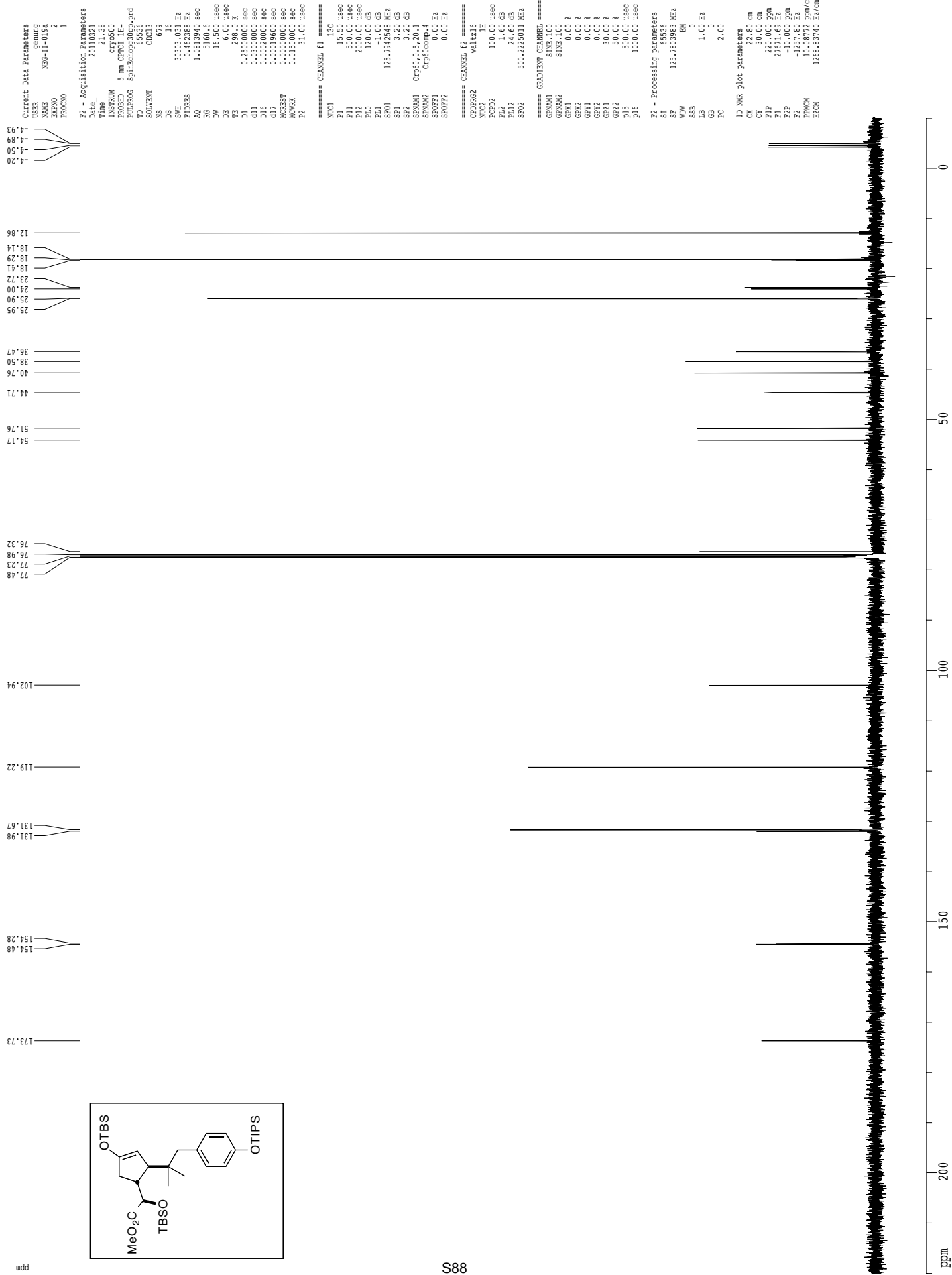
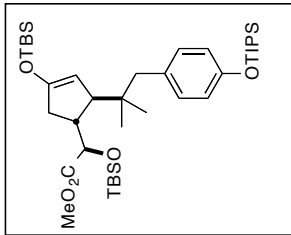
F2 - Processing parameters  
 SI 65536  
 SF 125.760480 MHz  
 NWDW 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 F1 230.637 ppm  
 F1 29009.68 Hz  
 F2P -10.287 ppm  
 F2 -1293.96 Hz  
 PPMCM 10.56688 ppm/cm  
 HCM 1329.10693 Hz/cm



Current Data Parameters  
 USER genny  
 SAMPLE NEG-II-019a  
 EXPTNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date 20110321  
 Time 21.29  
 INSTRUM cry500  
 PROHDH 5 mm CPCL1.H  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 FHS 8012.822 Hz  
 AQRES 0.109626 Hz  
 RG 5.0398774 sec  
 RC 7.1  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 0.00 dB  
 SFO1 500.2235015 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 500.220258 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 10.50 cm  
 FL1 10.500 mm  
 F1 5252.31 Hz  
 F2P -0.500 ppm  
 F2 -250.11 Hz  
 PPMCM 0.48246 ppm/cm  
 HZCM 241.33423 Hz/cm





Current Data Parameters  
 USER NEG-II-019a  
 NAME NEG-II-019a  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 2011021  
 Time 21:36  
 CPU 10  
 PROBHD 5 mm CPYCI 1H  
 PULPROG zgpg30p3upprpd  
 TD 65536  
 SOLVENT CDCl3  
 NS 679  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.90668 sec  
 RG 51.608  
 DW 16.500 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.25000000 sec  
 D11 0.03000000 sec  
 D16 0.00200000 sec  
 DELTA 0.00350000 sec  
 ACQRES 1.90668 sec  
 WDESS 0.462388 Hz  
 WDCEN 0.01800000 sec  
 P2 31.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 F1 500.00 usec  
 P2 200.00 usec  
 F2 125.760 MHz  
 PL1 1.00 dB  
 PL2 1.00 dB  
 SF01 125.7642548 MHz  
 SF1 3.20 dB  
 SF2 3.20 dB  
 SPAN1 Cpp60 0.5, 20.1  
 SPAN2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

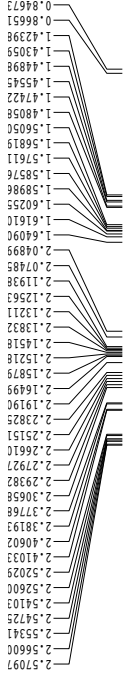
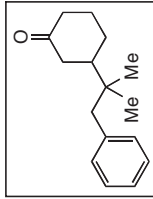
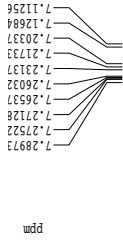
===== CHANNEL F2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P1 100.00 usec  
 F1 500.00 MHz  
 PL2 1.60 dB  
 PL3 24.60 dB  
 SF02 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GPM1 SINE 100  
 GPM2 SINE 100  
 GAX1 0.00 %  
 GAX2 0.00 %  
 GAX3 0.00 %  
 GAZ1 0.00 %  
 GAZ2 0.00 %  
 GAZ3 0.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

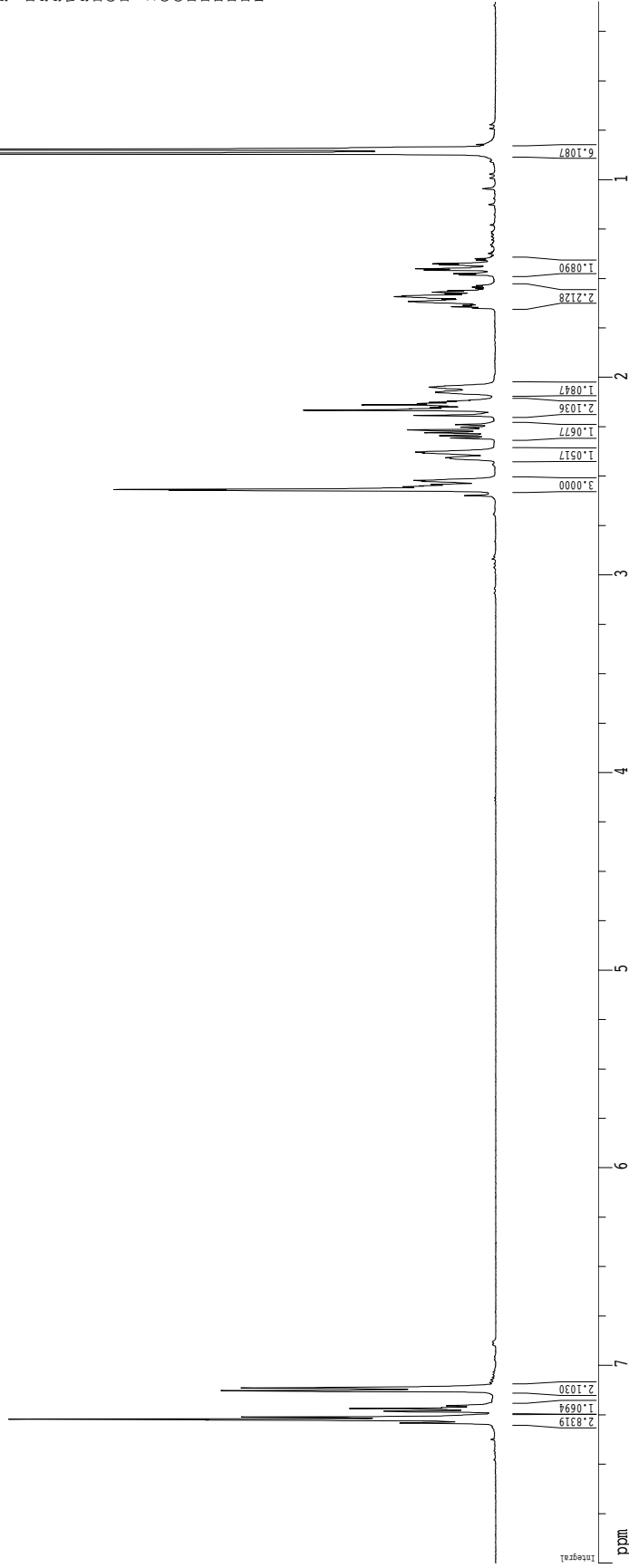
F2 - Processing parameters  
 SI 65536  
 SF 125.7803983 MHz  
 WDW EM  
 SSB 0  
 GB 1.00 Hz  
 PC 2.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 30.00 cm  
 FIP 220.000 ppm  
 FZ 2767.68 Hz  
 F2 500.000 MHz  
 F2 -1257.80 Hz  
 PPMCK 10.08772 ppm/cm  
 HZCK 1268.83746 Hz/cm

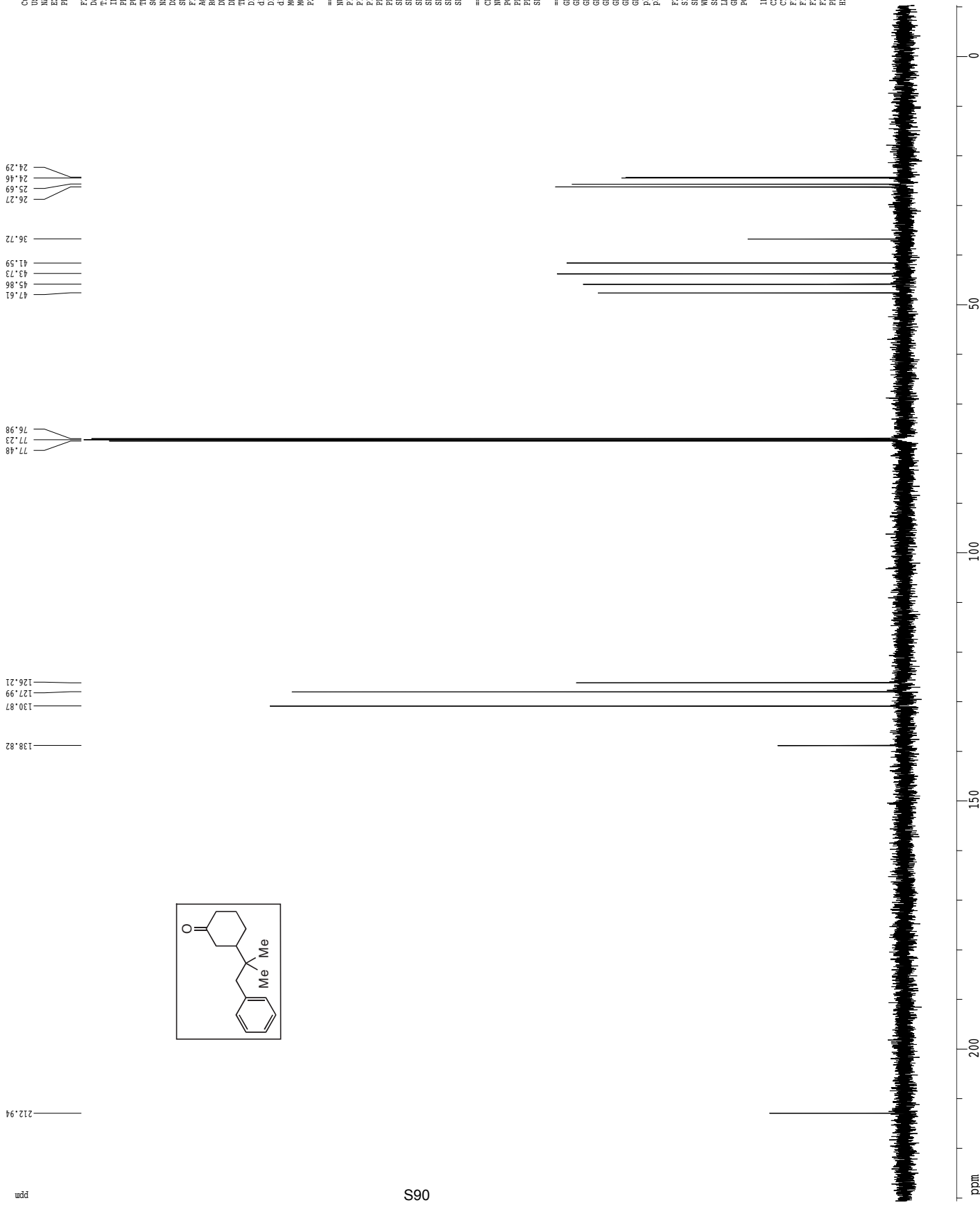
<sup>1</sup>H spectrum



Current Data Parameters  
 USER untitled  
 NAME NUJ-403-208  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120522  
 Time 16.22  
 INSTRUM cryo500  
 PROBD 5 mm CPCLP1 IH-  
 PULPROG zgpg30  
 SOLVENT CCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 8  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 ACRESF 0.00000000 sec  
 ACPRK 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 500.2200265 MHz  
 WDW EN  
 SSB 0  
 LB 0.20 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 8.000 ppm  
 F1 4001.76 Hz  
 F2P 0.100 ppm  
 F2 50.02 Hz  
 PPMCM 0.34649 ppm/cm  
 HZCM 173.32185 Hz/cm



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



```

Current Data Parameters
NAME      untitled
EXPNO     2
PROCNO    1
F2 - Acquisition Parameters
Date_     20120522
Time      16:25
INSTRUM   cryo500
PROBHD    5 mm CPYCI 1H-
PULPROG   Spinecho30pp.prd
TD        65536
SOLVENT   CDCl3
NS         7
DS         7
SF         30303.033 Hz
SH         0.462388 Hz
AQ         1.0813940 sec
RG         7298.2
DW         16.500 usec
DE         6.00 usec
TE         298.0 K
F1         101.626000 sec
D11        0.0300000 sec
D16        0.0002000 sec
d17        0.00019600 sec
MCREST    0.0000000 sec
MCNRRK    0.01500000 sec
P2         31.00 usec

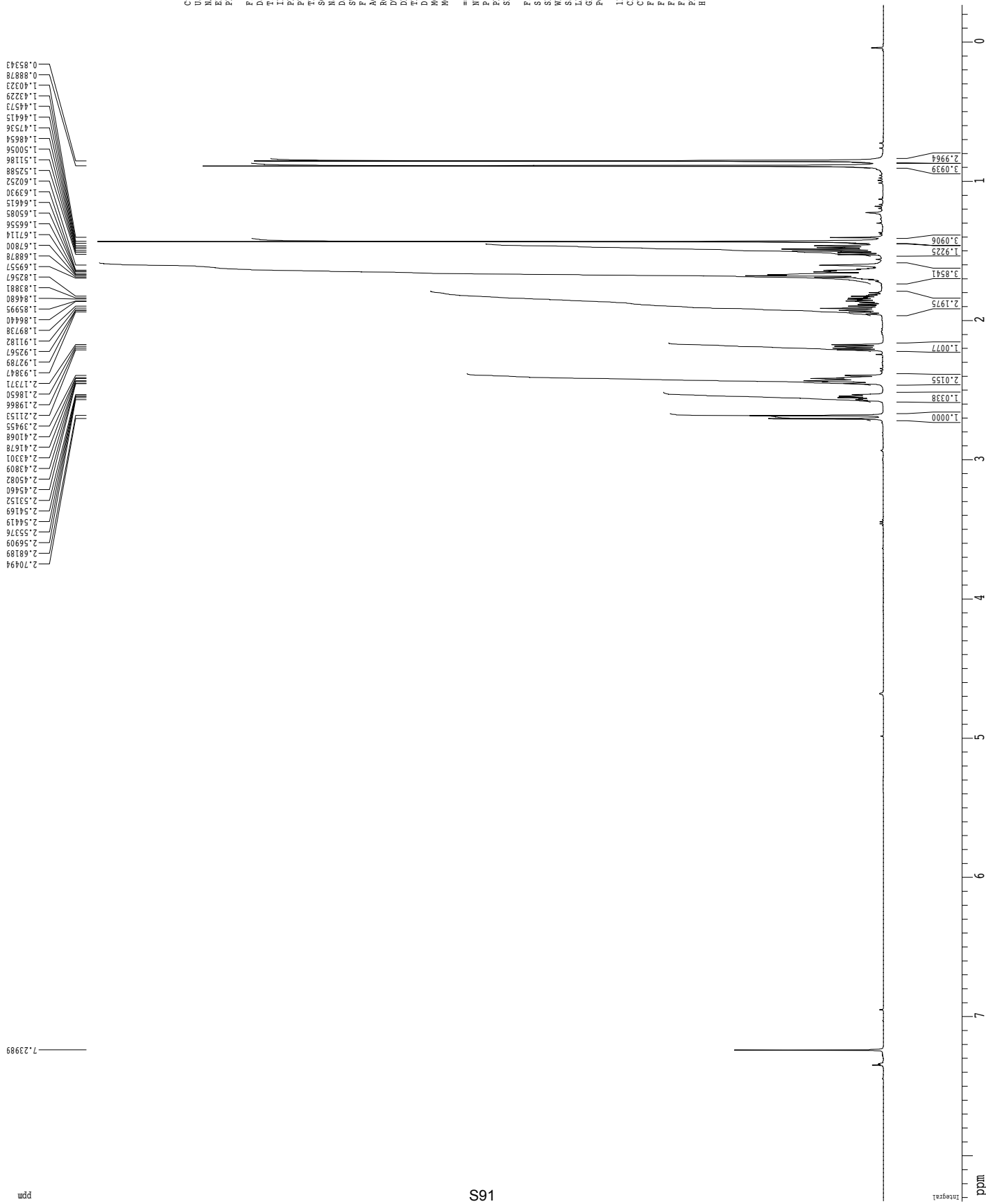
===== CHANNEL f1 =====
NUC1       13
PC         15.50 usec
P1         500.00 usec
P12        2000.00 usec
PL0        120.00 dB
PL1        -1.00 dB
SFO1       125.7942548 MHz
SFO2        3.20 dB
SFO3
SFO4
SFO5
SFO6
SFO7
SFO8
SFO9
SFO10
SFO11
SFO12
SFO13
SFO14
SFO15
SFO16
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PC2         100.00 usec
P12         2.00 dB
PL0         2.00 dB
PL1         2.00 dB
SFO1        500.2225013 MHz

===== GRADIENT CHANNEL =====
GENAM1     SINE.100
GENAM2     SINE.100
GCX1        0.00 %
GCX2        0.00 %
GCY1        0.00 %
GCY2        0.00 %
GZ1         30.00 %
GZ2         50.00 %
p15         500.00 usec
p16         1000.00 usec

F2 - Processing parameters
SI         65536
SF          125.7942548 MHz
WDW         0
SSB         0
LB          1.00 Hz
GB          0
PC          2.00

ID NMR plot parameters
CX         22.80 cm
CY         1.50 cm
EI         230.637 ppm
F1         290009.68 Hz
F2         -10.287 ppm
PRCM       10.56688 ppm/cm
HCM        1329.10693 Hz/cm
    
```

1H spectrum



7.23989  
 2.70494  
 2.68189  
 2.55376  
 2.54419  
 2.53152  
 2.45460  
 2.45082  
 2.43809  
 2.43301  
 2.41678  
 2.41068  
 2.39455  
 2.21153  
 2.19866  
 2.18650  
 2.17371  
 2.17371  
 1.93847  
 1.92789  
 1.92567  
 1.91182  
 1.89738  
 1.86440  
 1.85995  
 1.84680  
 1.83881  
 1.82561  
 1.69597  
 1.68878  
 1.67800  
 1.67114  
 1.66556  
 1.65985  
 1.64615  
 1.63930  
 1.60252  
 1.52588  
 1.51186  
 1.50056  
 1.48654  
 1.47536  
 1.46415  
 1.44573  
 1.43229  
 1.43229  
 1.40323  
 0.88878  
 0.85343

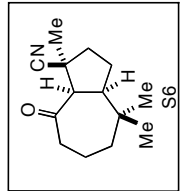
Current Data Parameters  
 USER schner  
 NAME ms02-299a-3-ic13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20100602  
 Time 8.35  
 INSTRUM crys500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 17  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.096043 Hz  
 AQ 5.0998774 sec  
 RG 63  
 DR 6.00 usec  
 DE 288.0 K  
 TE 0.1000000 sec  
 D1 0.0000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

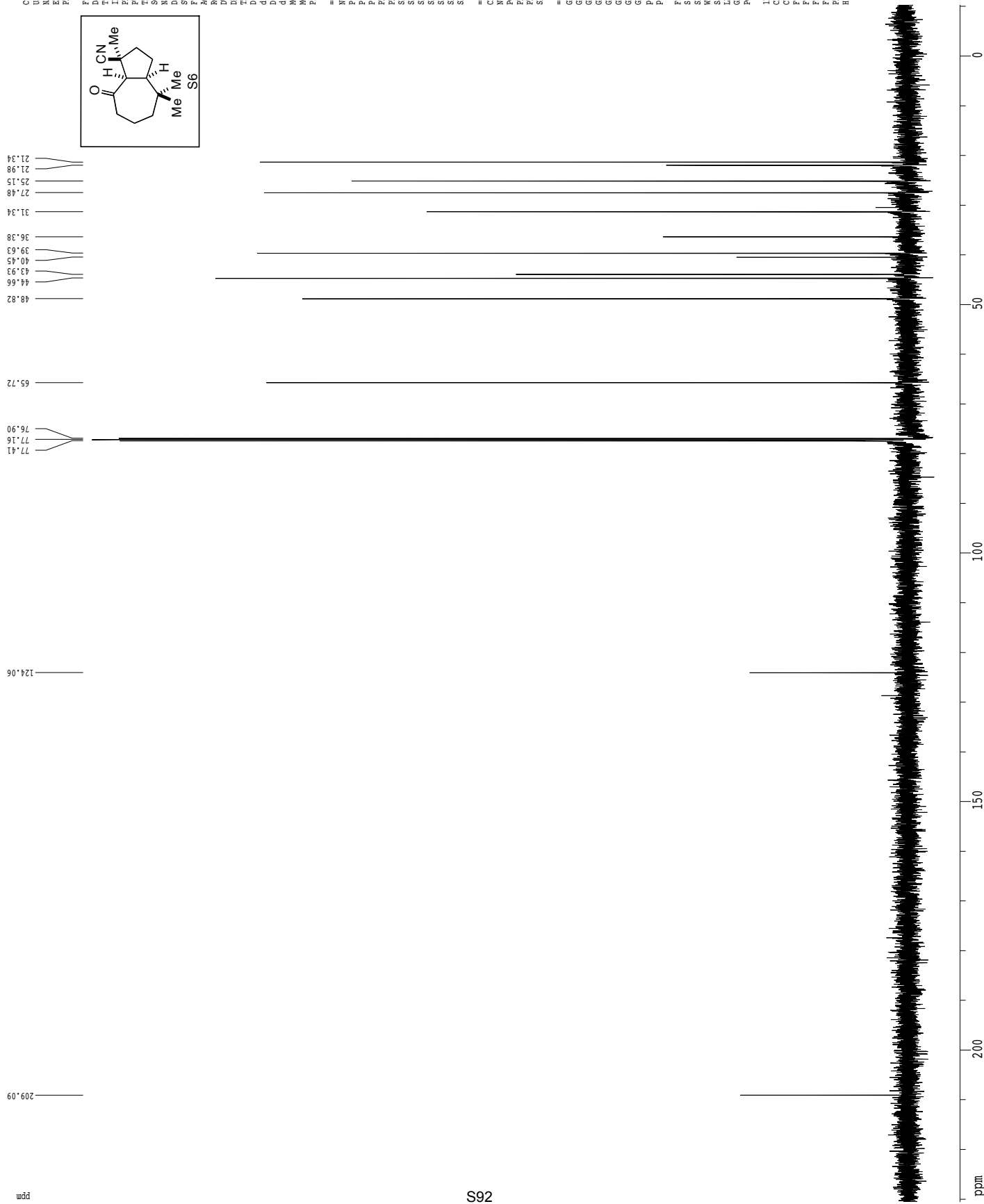
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.225015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220423 MHz  
 GSSS  
 MDW 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 8.326 ppm  
 F2 4104.83 Hz  
 F3 10.51 ppm  
 F4 -132.59 ppm  
 PPMCM 0.37680 ppm/cm  
 HZCM 188.48347 Hz/cm



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



Current Data Parameters  
 USER Scuser  
 MS02-2398-1-1313  
 EXNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20100602  
 Time 8:39  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 109  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 728.7  
 DR 6.00 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.25000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01000000 sec  
 F2 31.00 usec

===== CHANNEL F1 =====  
 NUC1 <sup>13</sup>C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 20.00 dB  
 PL2 20.00 dB  
 SFO1 125.764568 MHz  
 SFO2 500.132500 MHz  
 SP1 31.20 dB  
 SP2 31.20 dB  
 SPNAM1 Cyp60.0.5.20.1  
 SPNAM2 Cyp60comp.4  
 SPOFF1 0.00 Hz  
 SPOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPREG wd1616  
 NUC2 <sup>1</sup>H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

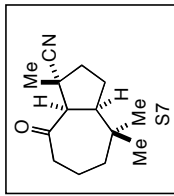
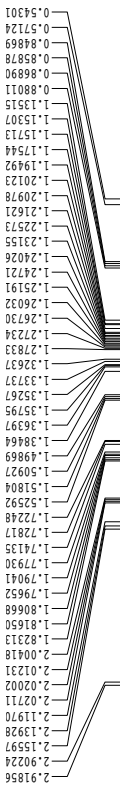
===== GRADIENT CHANNEL =====  
 GSPAM1 100.00 usec  
 GSPAM2 100.00 usec  
 GFL1 0.00 %  
 GFL2 0.00 %  
 GFL3 0.00 %  
 GFL4 0.00 %  
 GFL5 0.00 %  
 GFL6 0.00 %  
 GFL7 0.00 %  
 GFL8 0.00 %  
 GFL9 0.00 %  
 GFL10 0.00 %  
 GFL11 0.00 %  
 GFL12 0.00 %  
 GFL13 0.00 %  
 GFL14 0.00 %  
 GFL15 0.00 %  
 GFL16 0.00 %  
 GFL17 0.00 %  
 GFL18 0.00 %  
 GFL19 0.00 %  
 GFL20 0.00 %  
 GFL21 0.00 %  
 GFL22 0.00 %  
 GFL23 0.00 %  
 GFL24 0.00 %  
 GFL25 0.00 %  
 GFL26 0.00 %  
 GFL27 0.00 %  
 GFL28 0.00 %  
 GFL29 0.00 %  
 GFL30 0.00 %  
 GFL31 0.00 %  
 GFL32 0.00 %  
 GFL33 0.00 %  
 GFL34 0.00 %  
 GFL35 0.00 %  
 GFL36 0.00 %  
 GFL37 0.00 %  
 GFL38 0.00 %  
 GFL39 0.00 %  
 GFL40 0.00 %  
 GFL41 0.00 %  
 GFL42 0.00 %  
 GFL43 0.00 %  
 GFL44 0.00 %  
 GFL45 0.00 %  
 GFL46 0.00 %  
 GFL47 0.00 %  
 GFL48 0.00 %  
 GFL49 0.00 %  
 GFL50 0.00 %  
 GFL51 0.00 %  
 GFL52 0.00 %  
 GFL53 0.00 %  
 GFL54 0.00 %  
 GFL55 0.00 %  
 GFL56 0.00 %  
 GFL57 0.00 %  
 GFL58 0.00 %  
 GFL59 0.00 %  
 GFL60 0.00 %  
 GFL61 0.00 %  
 GFL62 0.00 %  
 GFL63 0.00 %  
 GFL64 0.00 %  
 GFL65 0.00 %  
 GFL66 0.00 %  
 GFL67 0.00 %  
 GFL68 0.00 %  
 GFL69 0.00 %  
 GFL70 0.00 %  
 GFL71 0.00 %  
 GFL72 0.00 %  
 GFL73 0.00 %  
 GFL74 0.00 %  
 GFL75 0.00 %  
 GFL76 0.00 %  
 GFL77 0.00 %  
 GFL78 0.00 %  
 GFL79 0.00 %  
 GFL80 0.00 %  
 GFL81 0.00 %  
 GFL82 0.00 %  
 GFL83 0.00 %  
 GFL84 0.00 %  
 GFL85 0.00 %  
 GFL86 0.00 %  
 GFL87 0.00 %  
 GFL88 0.00 %  
 GFL89 0.00 %  
 GFL90 0.00 %  
 GFL91 0.00 %  
 GFL92 0.00 %  
 GFL93 0.00 %  
 GFL94 0.00 %  
 GFL95 0.00 %  
 GFL96 0.00 %  
 GFL97 0.00 %  
 GFL98 0.00 %  
 GFL99 0.00 %  
 GFL100 0.00 %

F2 - Processing parameters  
 SI 65536  
 SF 125.7804103 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

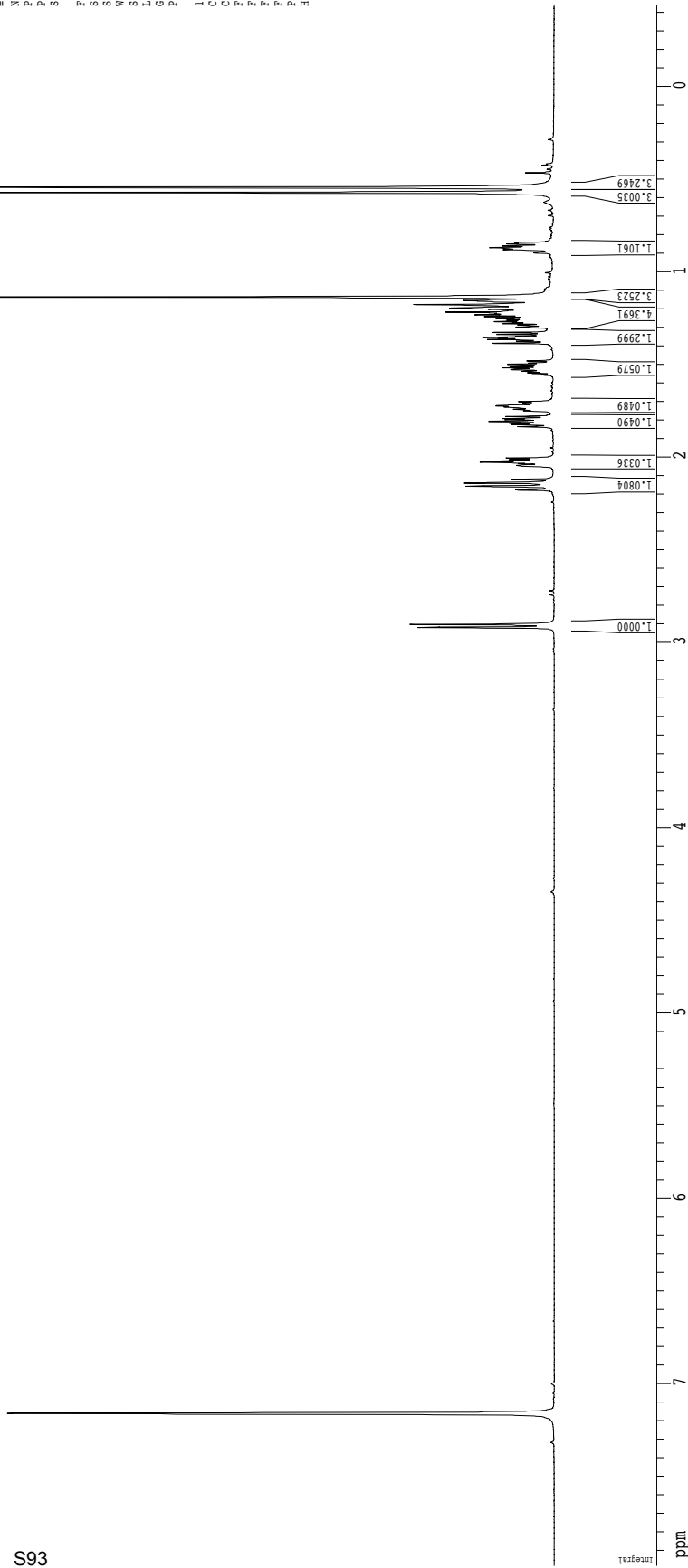
ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.65 cm  
 FIP 230.637 ppm  
 F1 29005.68 Hz  
 F2 -10.287 ppm  
 F2 1293.96 Hz  
 F2 13.568 ppm/cm  
 HECKN 1329.1093 Hz/cm



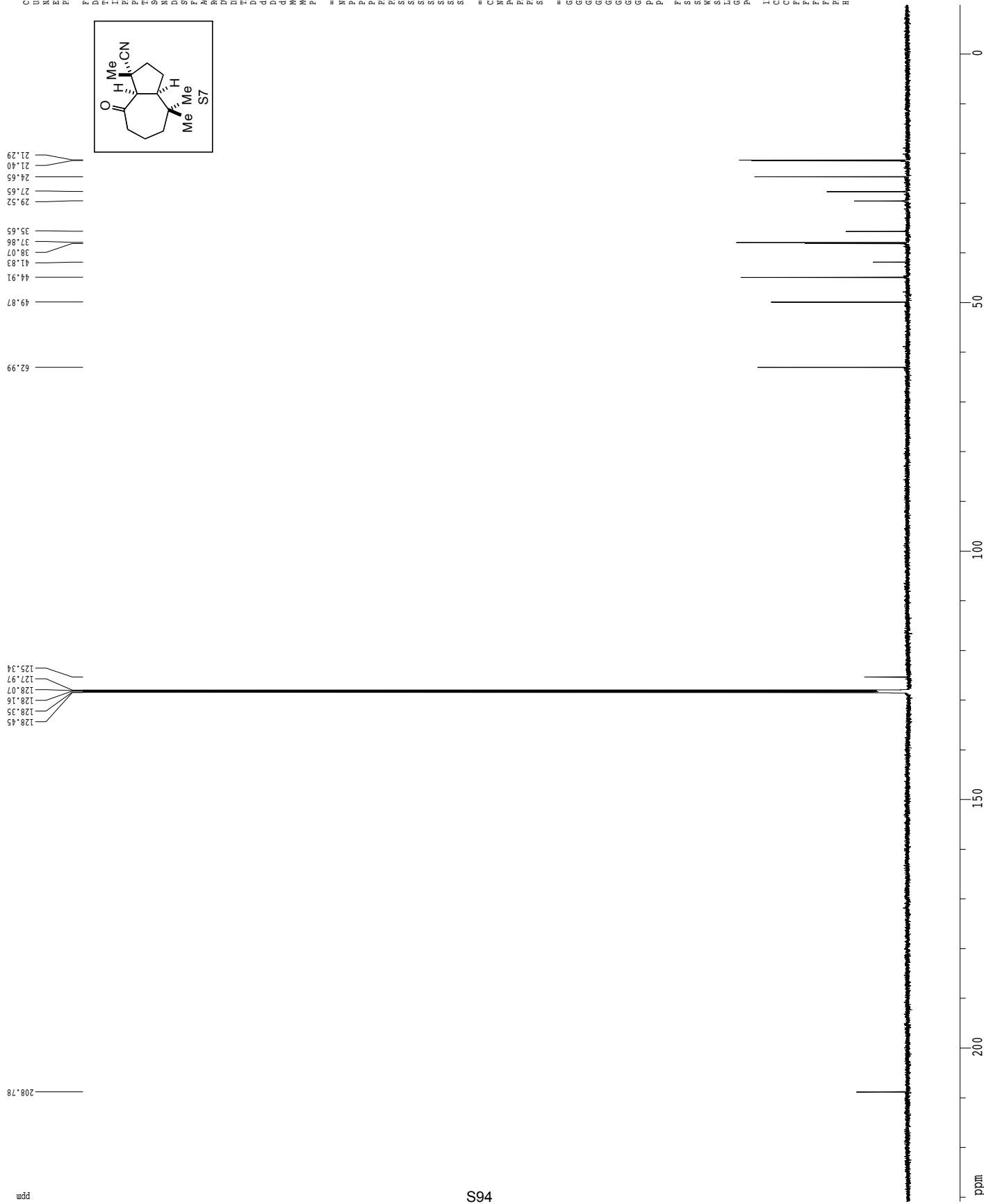
1H spectrum



Current Data Parameters  
 USER schmer  
 NAME ms003-21-3-Ibenzd  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20100623  
 Time\_ 18.00  
 INSTRUM crys500  
 PROBRD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 11  
 DS 2  
 SWH 8012.822 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 8  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 MCRESF 0.00000000 sec  
 MCNRF 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 500.2200514 MHz  
 WDW EN  
 EN  
 GB 0  
 CB 0.30 Hz  
 SC 4.00  
 PC 4.00  
 1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 7.981 ppm  
 F1 3992.25 Hz  
 F2 -0.435 ppm  
 F3 13.47 Hz  
 FREQ0 0.1601 Hz/cm  
 FREQ1 184.6367 Hz/cm



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



Current Data Parameters  
 USER Scms  
 EXPNO ms003-21-5-11gen2d  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20100623  
 Time 18.16  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 99  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 5120.6  
 DR 6.00 usec  
 DE 6.00 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 3.00 usec

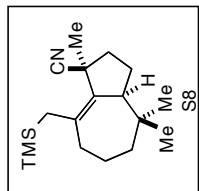
===== CHANNEL F1 =====  
 NUC1 <sup>13</sup>C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.784568 dB  
 PL2 120.00 dB  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO1 Ccp60.0.5.20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 P2 100.00 usec  
 P21 1.60 dB  
 P22 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPRMR SFR 1.0  
 GSRMZ SFR 1.0  
 GEX1 0.00 %  
 GEX2 0.00 %  
 GFL1 0.00 %  
 GFL2 0.00 %  
 GZ1 30.00 %  
 GZ2 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803760 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 25.00 cm  
 FIP 231.032 ppm  
 F1 29055.27 Hz  
 F2 -9.888 ppm  
 FZ 1241.77 Hz  
 HPCOM 1.668 ppm/cm  
 HPCON 1329.00957 Hz/cm



Current Data Parameters  
 USER schner  
 NAME mjs1-81b-3c13  
 EXPNO 1  
 PROCNO 1

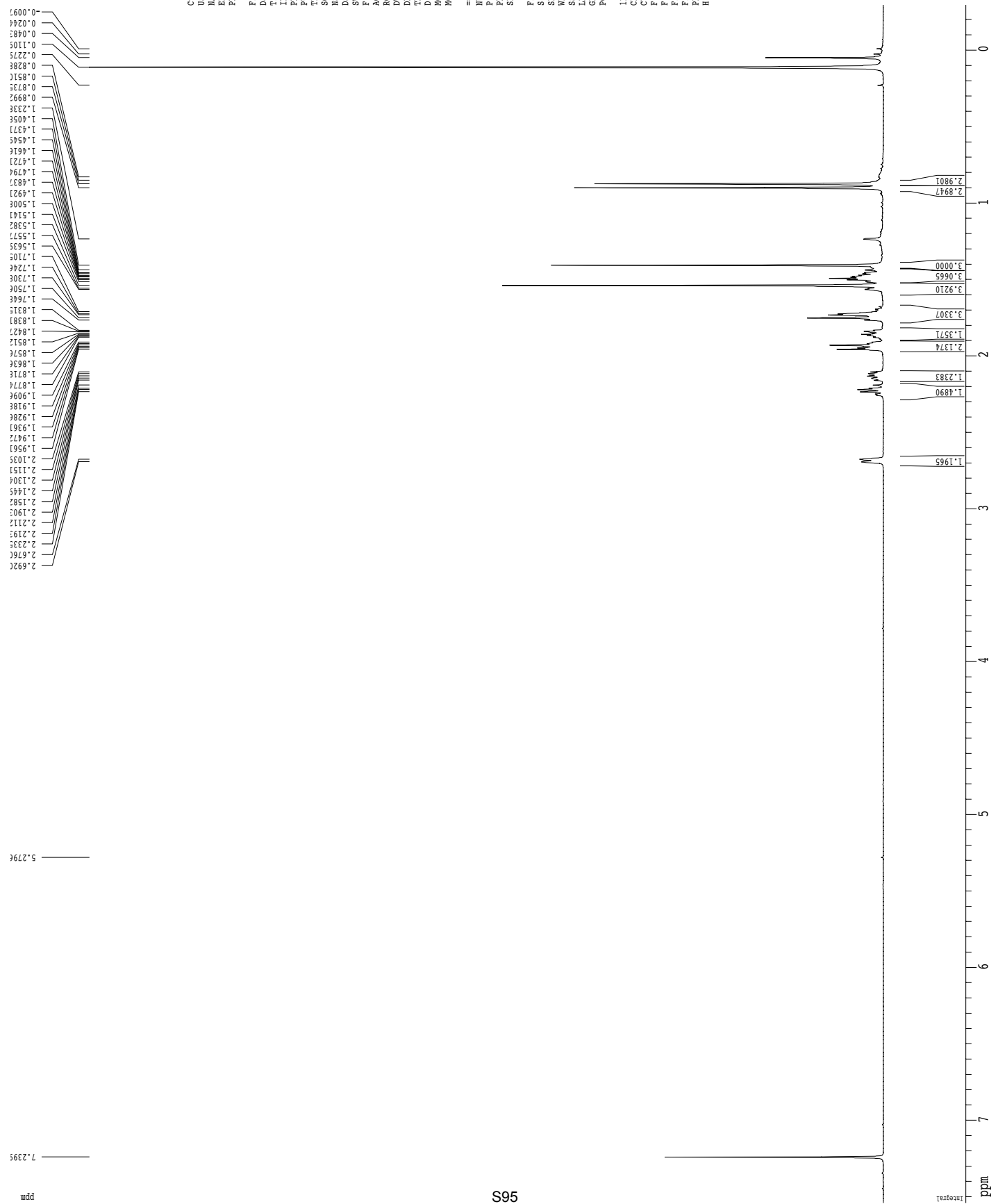
F2 - Acquisition Parameters  
 Date\_ 20110511  
 Time 14.18  
 INSTRUM cryo300  
 PULPROG zgpg30  
 FIDRES 5 mm CPIC1  
 TD 81728  
 SOLVENT C6D6  
 NS 8  
 DS 2

SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 4.5  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 MCRST 0.10000000 sec  
 MCRBK 0.01500000 sec

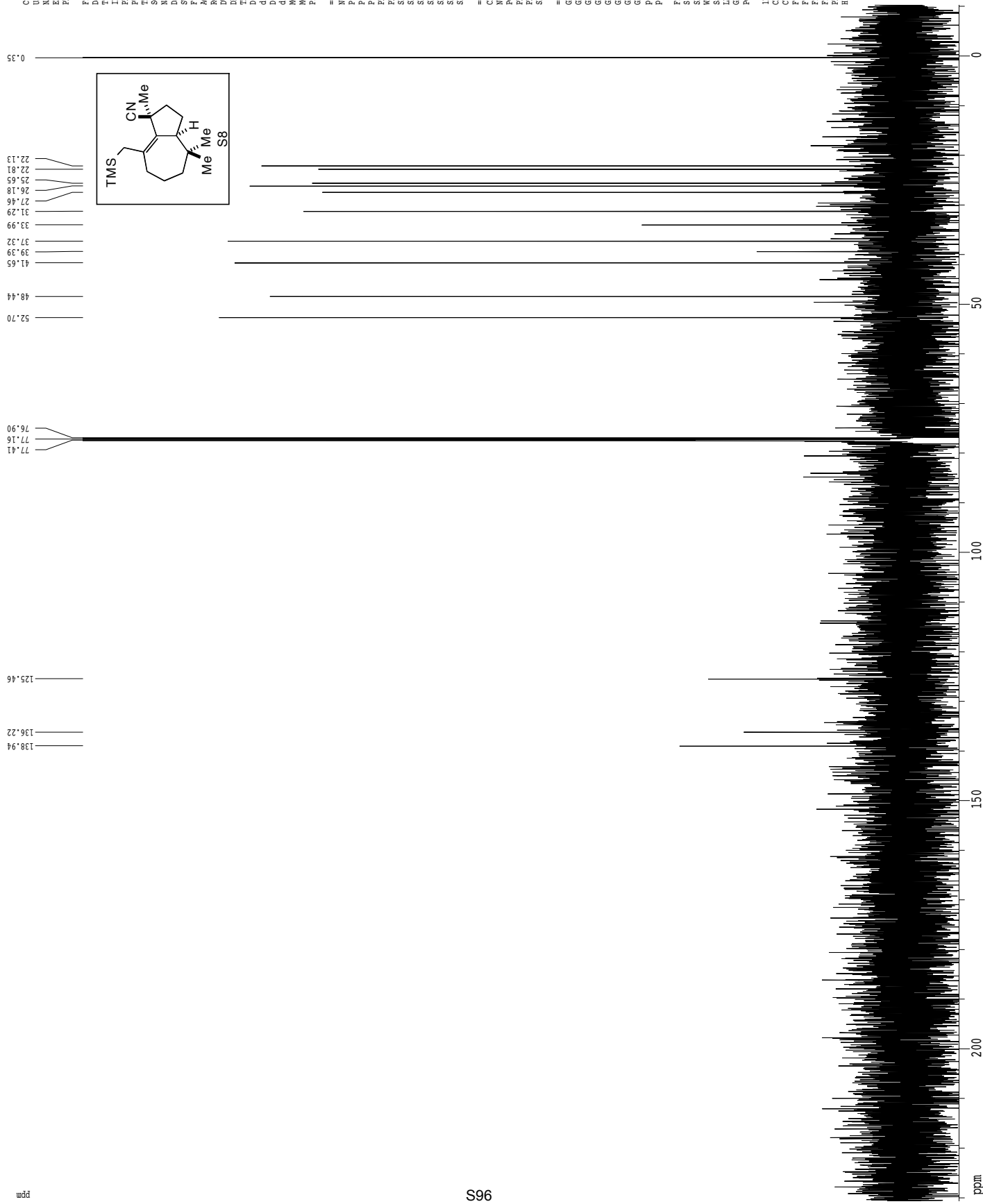
==== CHANNEL f1 =====  
 NUCL 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2199874 MHz  
 EQ  
 F2 0.30 Hz  
 GB 0  
 PC 0.25

1D NMR plot parameters  
 CX 22.80 cm  
 CY 20.00 cm  
 F1P 7.539 ppm  
 F1 3771.05 Hz  
 F2P -0.294 ppm  
 F2 -147.05 Hz  
 PRCH 0.38354 ppm/cm  
 HZCX 171.84618 Hz/cm



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



Current Data Parameters  
 USER SCHEUC  
 EXPNO mjs-81b-3C12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110511  
 Time 14.19  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 162  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 728.7  
 DR 6.00 usec  
 DE 6.00 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 31.00 usec

===== CHANNEL F1 =====  
 NUC1 <sup>13</sup>C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 PL2 125.794568 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 wd1616  
 NUC2 <sup>1</sup>H  
 P2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GBRM1 0  
 GBRM2 10  
 GBRM3 10  
 GBX1 0.00 %  
 GBX2 0.00 %  
 GBX3 0.00 %  
 GBY1 0.00 %  
 GBY2 0.00 %  
 GBY3 0.00 %  
 GZ1 50.00 %  
 GZ2 50.00 %  
 GZ3 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803946 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.50

ID NMR plot parameters  
 CX 22.80 cm  
 CY 75.00 cm  
 FIP 230.637 ppm  
 F1 29005.67 Hz  
 F2 -10.287 ppm  
 F3 -1295.96 Hz  
 F4 -1295.96 Hz  
 HCON 1329.1688 Hz/cm  
 HCON 1329.1688 Hz/cm

<sup>1</sup>H spectrum

ppm

7.26117

0.11927

0.76438

0.87718

1.36248

1.43032

1.56119

1.58249

1.80219

1.83135

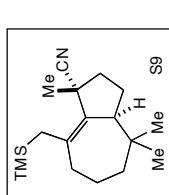
1.98702

1.99718

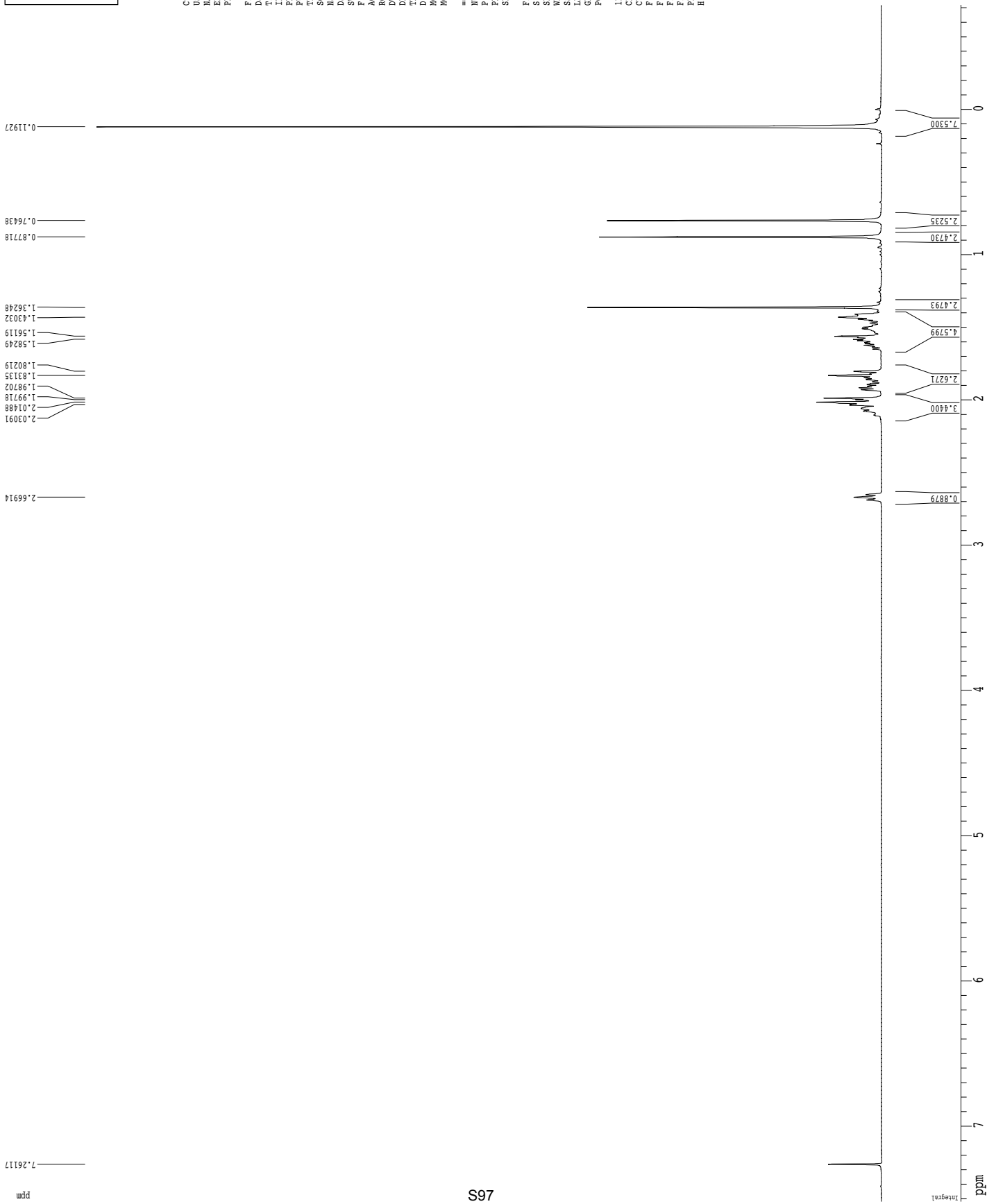
2.01488

2.03091

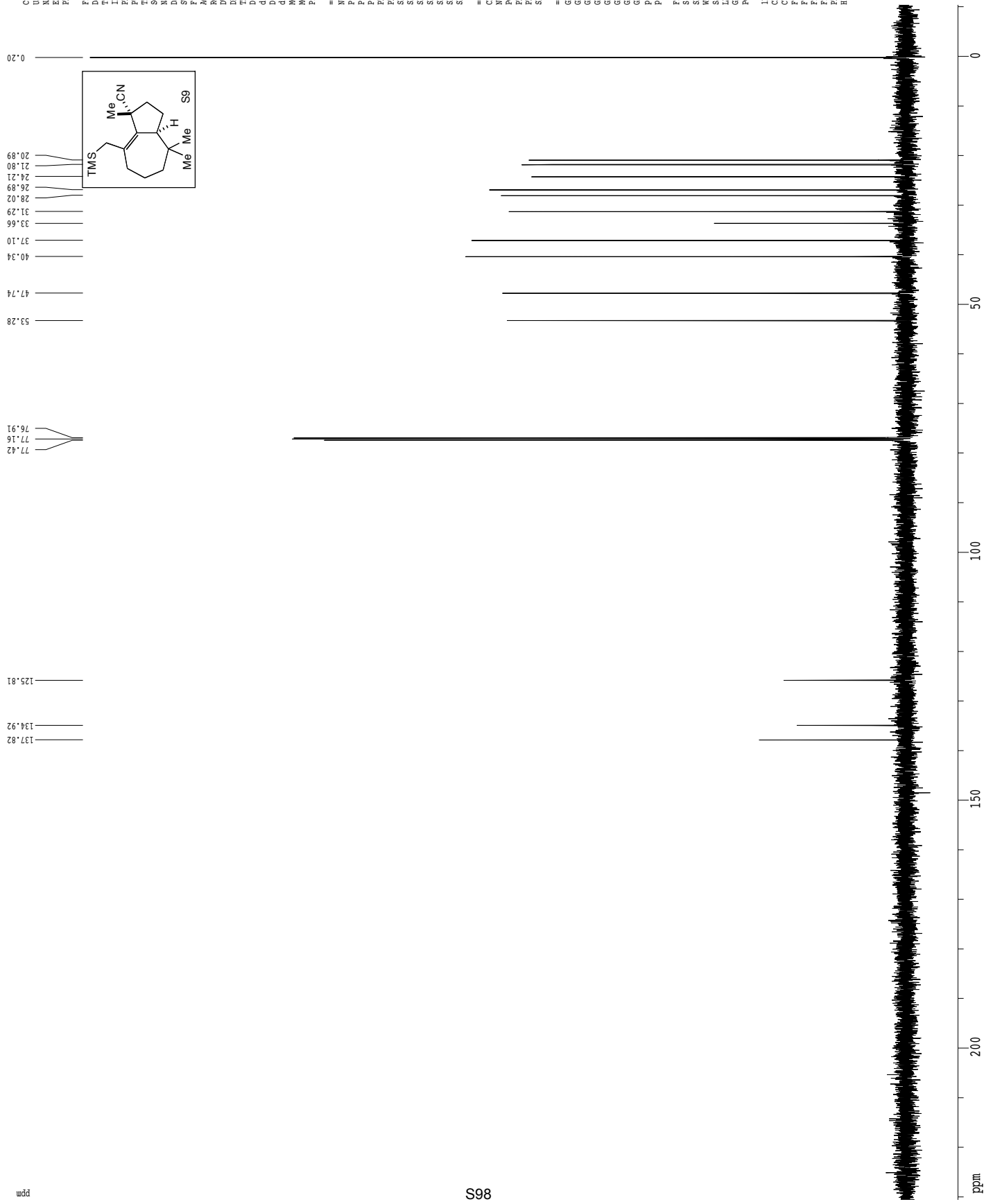
2.66914



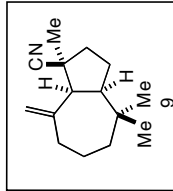
Current Data Parameters  
 USER schner  
 NAME ms003-81a-3-ic13  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20100913  
 Time 8.38  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0996774 sec  
 RG 711  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 500.220313 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 7.517 ppm  
 F2 3700.39 Hz  
 F3 46.25 Hz  
 F4 -358.35 Hz  
 PPM0 0.36113 ppm/cm  
 HZCM 180.64648 Hz/cm



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



1H spectrum



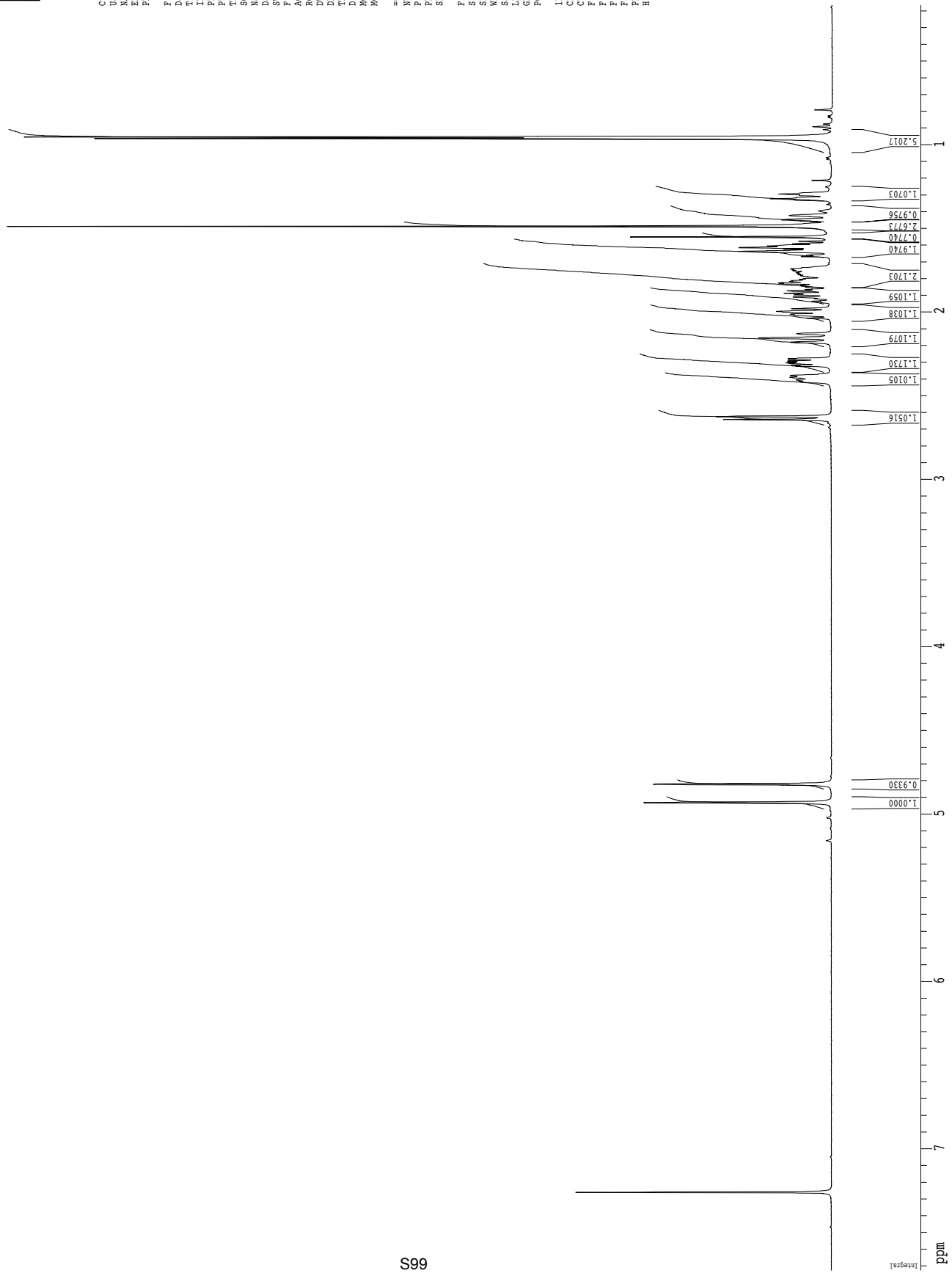
Current Data Parameters  
 USER schner  
 NAME ms003-302-3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110318  
 Time 8.57  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 10  
 DS 2  
 SWH 801.2820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0999398 sec  
 RG 71  
 DE 62.40 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

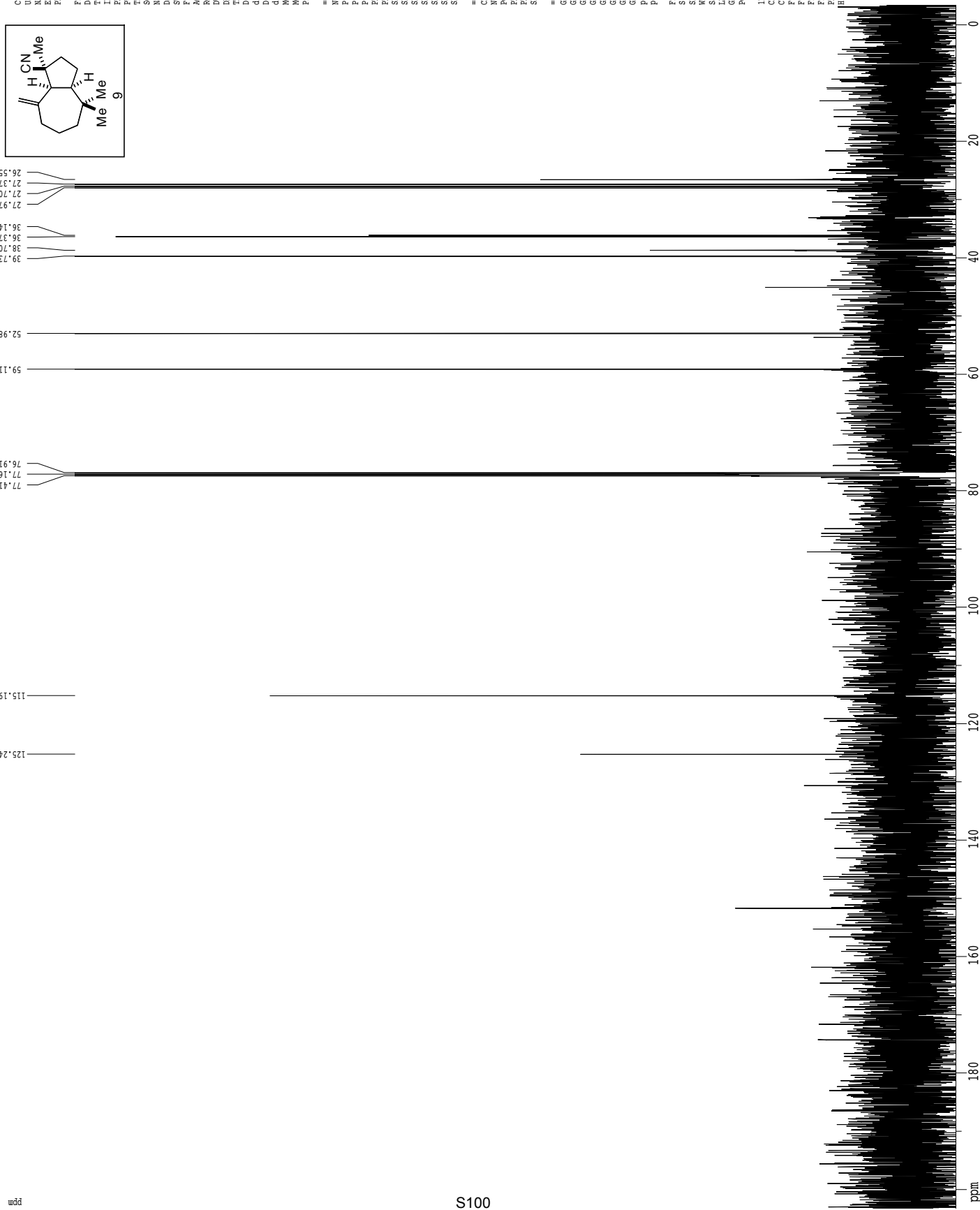
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.2200312 MHz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 7.725 ppm  
 FZ 3964.08 Hz  
 PZ 81.00 ppm  
 PRGM 0.33143 ppm/cm  
 HZCN 165.78963 Hz/cm



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



Current Data Parameters  
 USER: scmic  
 MS03-502-2  
 EXNO: 1  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_: 20110318  
 Time: 8:59  
 INSTRUM: cryo500  
 PROBHD: 5 mm CPXI 1H  
 PULPROG: zgpg30  
 TD: 65536  
 SOLVENT: CDCl3  
 NS: 215  
 DS: 16  
 SWH: 30303.031 Hz  
 FIDRES: 0.462388 Hz  
 AQ: 1.0813940 sec  
 RG: 406  
 NG: 16  
 DR: 6.00 usec  
 DE: 6.00 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: 3.00 usec

===== CHANNEL F1 =====  
 NUC1: 13C  
 P1: 15.50 usec  
 P11: 500.00 usec  
 P12: 2000.00 usec  
 PL0: 120.00 dB  
 PL1: 75.00 dB  
 SP1: 125.794568 MHz  
 SP2: 5.20 dB  
 SFO1: 125.761568 MHz  
 SFO2: 3.20 dB  
 SPNAM1: Ccp60.0.5.20.1  
 SPNAM2: Ccp60comp.4  
 SFOFF1: 0.00 Hz  
 SFOFF2: 0.00 Hz

===== CHANNEL F2 =====  
 CDPREG2: wd t615  
 NUC2: 1H  
 PCPD2: 100.00 usec  
 PL2: 1.60 dB  
 PL12: 24.60 dB  
 SFO2: 500.2225011 MHz

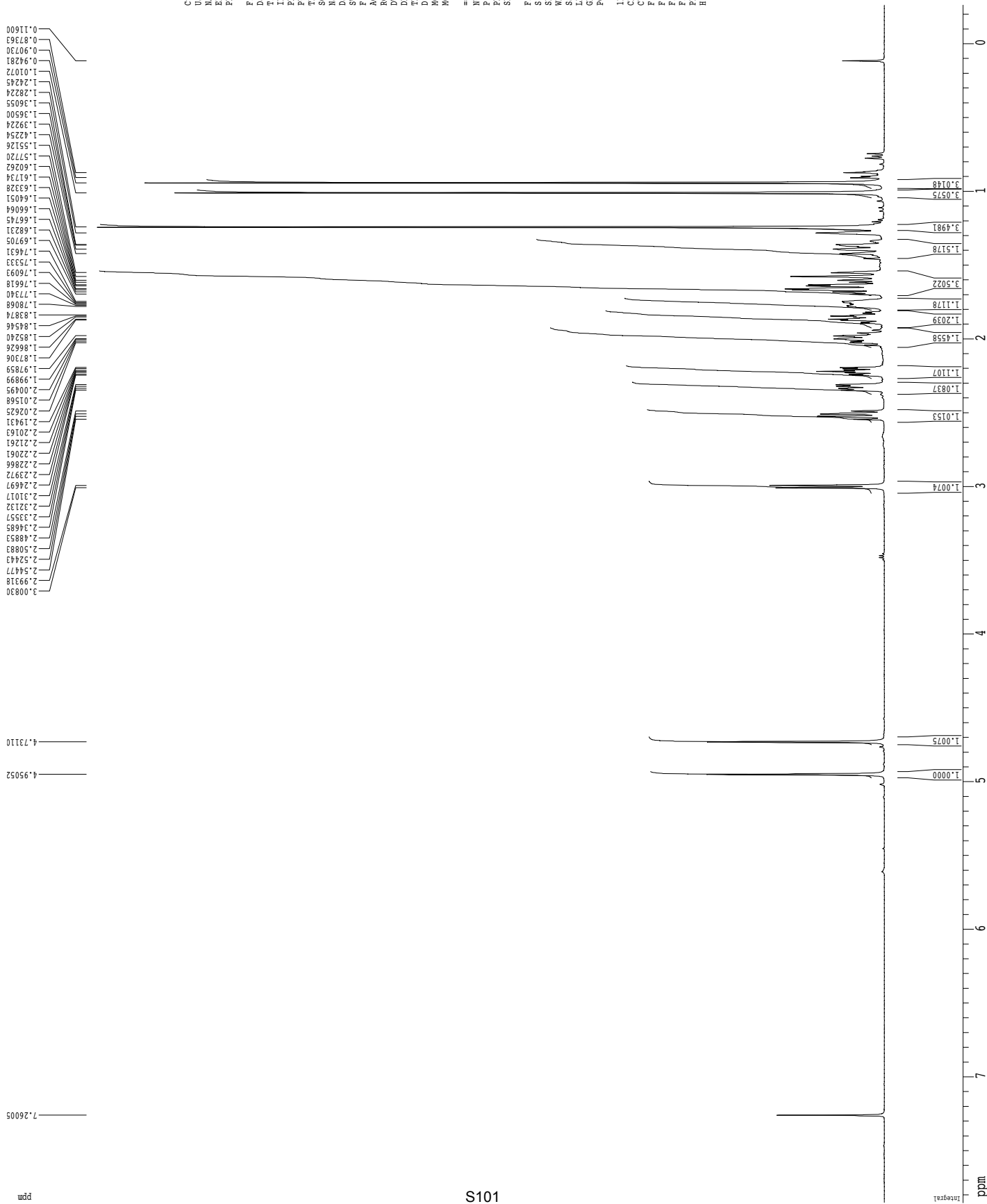
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 GSPAM4: 0.00 %  
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 GSPAM6: 0.00 %  
 GSPAM7: 0.00 %  
 GSPAM8: 0.00 %  
 GSPAM9: 0.00 %  
 GSPAM10: 0.00 %  
 GSPAM11: 0.00 %  
 GSPAM12: 0.00 %  
 GSPAM13: 0.00 %  
 GSPAM14: 0.00 %  
 GSPAM15: 0.00 %  
 GSPAM16: 0.00 %  
 GSPAM17: 0.00 %  
 GSPAM18: 0.00 %  
 GSPAM19: 0.00 %  
 GSPAM20: 0.00 %  
 GSPAM21: 0.00 %  
 GSPAM22: 0.00 %  
 GSPAM23: 0.00 %  
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 GSPAM26: 0.00 %  
 GSPAM27: 0.00 %  
 GSPAM28: 0.00 %  
 GSPAM29: 0.00 %  
 GSPAM30: 0.00 %  
 GSPAM31: 0.00 %  
 GSPAM32: 0.00 %  
 GSPAM33: 0.00 %  
 GSPAM34: 0.00 %  
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 GSPAM36: 0.00 %  
 GSPAM37: 0.00 %  
 GSPAM38: 0.00 %  
 GSPAM39: 0.00 %  
 GSPAM40: 0.00 %  
 GSPAM41: 0.00 %  
 GSPAM42: 0.00 %  
 GSPAM43: 0.00 %  
 GSPAM44: 0.00 %  
 GSPAM45: 0.00 %  
 GSPAM46: 0.00 %  
 GSPAM47: 0.00 %  
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 GSPAM49: 0.00 %  
 GSPAM50: 0.00 %  
 GSPAM51: 0.00 %  
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 GSPAM54: 0.00 %  
 GSPAM55: 0.00 %  
 GSPAM56: 0.00 %  
 GSPAM57: 0.00 %  
 GSPAM58: 0.00 %  
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 GSPAM60: 0.00 %  
 GSPAM61: 0.00 %  
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 GSPAM67: 0.00 %  
 GSPAM68: 0.00 %  
 GSPAM69: 0.00 %  
 GSPAM70: 0.00 %  
 GSPAM71: 0.00 %  
 GSPAM72: 0.00 %  
 GSPAM73: 0.00 %  
 GSPAM74: 0.00 %  
 GSPAM75: 0.00 %  
 GSPAM76: 0.00 %  
 GSPAM77: 0.00 %  
 GSPAM78: 0.00 %  
 GSPAM79: 0.00 %  
 GSPAM80: 0.00 %  
 GSPAM81: 0.00 %  
 GSPAM82: 0.00 %  
 GSPAM83: 0.00 %  
 GSPAM84: 0.00 %  
 GSPAM85: 0.00 %  
 GSPAM86: 0.00 %  
 GSPAM87: 0.00 %  
 GSPAM88: 0.00 %  
 GSPAM89: 0.00 %  
 GSPAM90: 0.00 %  
 GSPAM91: 0.00 %  
 GSPAM92: 0.00 %  
 GSPAM93: 0.00 %  
 GSPAM94: 0.00 %  
 GSPAM95: 0.00 %  
 GSPAM96: 0.00 %  
 GSPAM97: 0.00 %  
 GSPAM98: 0.00 %  
 GSPAM99: 0.00 %  
 GSPAM100: 0.00 %

F2 - Processing parameters  
 SI: 65536  
 SF: 125.7804076 MHz  
 WDW: EM  
 SSB: 0  
 LB: 1.00 Hz  
 GB: 0  
 PC: 2.00

ID NMR plot parameters  
 CX: 22.80 cm  
 CY: 100.00 cm  
 FIP: 283.222 ppm  
 F1: 2556.144 Hz  
 F2: -3.417 ppm  
 F3: 0.42382 Hz  
 FWHM: 1139.9727 Hz/cm  
 HZCM: 1139.9727 Hz/cm



<sup>1</sup>H spectrum

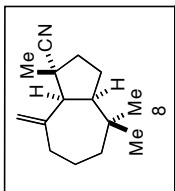


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0.90730  
0.94281  
1.01072  
1.24245  
1.28224  
1.36055  
1.36500  
1.39224  
1.42254  
1.55126  
1.57720  
1.60262  
1.61794  
1.63328  
1.64951  
1.66064  
1.66745  
1.68231  
1.69705  
1.74631  
1.75333  
1.76993  
1.76618  
1.77340  
1.78068  
1.83874  
1.84546  
1.85240  
1.86826  
1.87306  
1.87306  
1.97859  
1.99899  
2.00495  
2.01568  
2.02625  
2.19131  
2.20163  
2.21261  
2.22061  
2.22866  
2.23972  
2.24697  
2.31017  
2.32132  
2.33557  
2.34685  
2.48853  
2.50883  
2.52443  
2.54477  
2.99318  
3.00830

4.73110  
4.95052

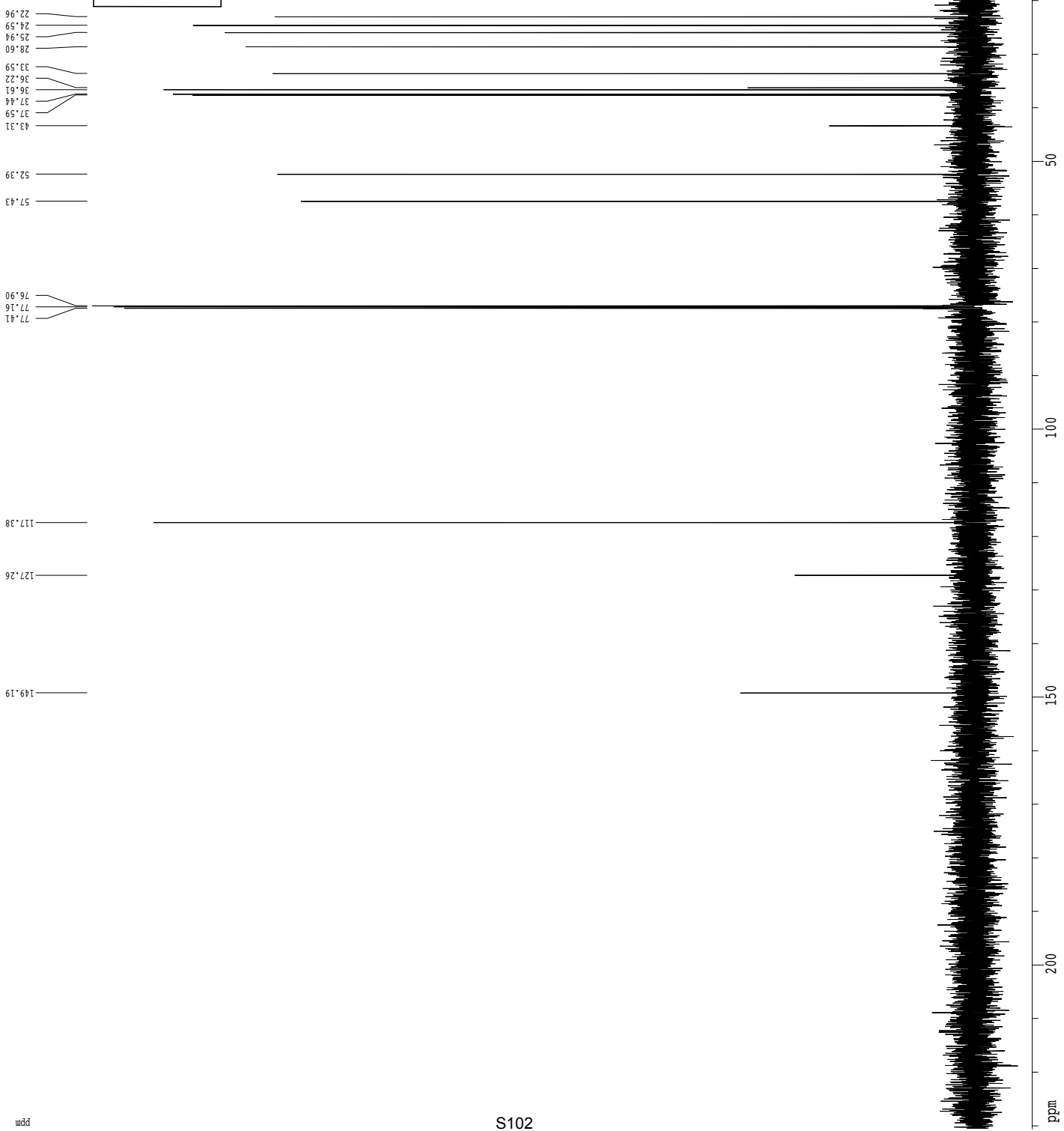
7.26095

ppm



Current Data Parameters  
 USER schner  
 NAME ms003-133-3-2c13  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20101013  
 Time 14.28  
 INSTRUM cryo500  
 PROBHD 5 mm CPCL1 H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 13  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 0  
 DW 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 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 500.220322 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 7.852 ppm  
 FZ 3927.79 Hz  
 GZ 0.60 ppm  
 PZ -130.44  
 PRMCM 0.35583 ppm/cm  
 HZCM 177.99275 Hz/cm

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



Current Data Parameters  
 USER Scuser  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20101013  
 Time 14:30  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 40  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0812940 sec  
 RG 676  
 NG 16  
 DR 6.00 usec  
 DE 6.00 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  
 ASWAK 0.01500000 sec  
 F2 3.00 usec

===== CHANNEL F1 =====  
 NUC1 <sup>13</sup>C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 P10 120.00 dB  
 P11 120.00 dB  
 P12 125.794548 MHz  
 SFO1 125.761488 MHz  
 SFO2 500.2225011 MHz  
 SP1 3.20 dB  
 SP2 3.20 dB  
 SPNAM1 Ccp60.0.5.20.1  
 SPNAM2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPRES2 wd t615  
 NUC2 <sup>1</sup>H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GRAM1 0  
 GRAM2 0  
 GRAM3 0  
 GR1 0.00 %  
 GR2 0.00 %  
 GR3 0.00 %  
 GR4 0.00 %  
 GR5 0.00 %  
 GR6 0.00 %  
 GR7 0.00 %  
 GR8 0.00 %  
 GR9 0.00 %  
 GR10 0.00 %  
 GR11 0.00 %  
 GR12 0.00 %  
 GR13 0.00 %  
 GR14 0.00 %  
 GR15 0.00 %  
 GR16 0.00 %  
 GR17 0.00 %  
 GR18 0.00 %  
 GR19 0.00 %  
 GR20 0.00 %  
 GR21 0.00 %  
 GR22 0.00 %  
 GR23 0.00 %  
 GR24 0.00 %  
 GR25 0.00 %  
 GR26 0.00 %  
 GR27 0.00 %  
 GR28 0.00 %  
 GR29 0.00 %  
 GR30 0.00 %  
 GR31 0.00 %  
 GR32 0.00 %  
 GR33 0.00 %  
 GR34 0.00 %  
 GR35 0.00 %  
 GR36 0.00 %  
 GR37 0.00 %  
 GR38 0.00 %  
 GR39 0.00 %  
 GR40 0.00 %  
 GR41 0.00 %  
 GR42 0.00 %  
 GR43 0.00 %  
 GR44 0.00 %  
 GR45 0.00 %  
 GR46 0.00 %  
 GR47 0.00 %  
 GR48 0.00 %  
 GR49 0.00 %  
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 GR60 0.00 %  
 GR61 0.00 %  
 GR62 0.00 %  
 GR63 0.00 %  
 GR64 0.00 %  
 GR65 0.00 %  
 GR66 0.00 %  
 GR67 0.00 %  
 GR68 0.00 %  
 GR69 0.00 %  
 GR70 0.00 %  
 GR71 0.00 %  
 GR72 0.00 %  
 GR73 0.00 %  
 GR74 0.00 %  
 GR75 0.00 %  
 GR76 0.00 %  
 GR77 0.00 %  
 GR78 0.00 %  
 GR79 0.00 %  
 GR80 0.00 %  
 GR81 0.00 %  
 GR82 0.00 %  
 GR83 0.00 %  
 GR84 0.00 %  
 GR85 0.00 %  
 GR86 0.00 %  
 GR87 0.00 %  
 GR88 0.00 %  
 GR89 0.00 %  
 GR90 0.00 %  
 GR91 0.00 %  
 GR92 0.00 %  
 GR93 0.00 %  
 GR94 0.00 %  
 GR95 0.00 %  
 GR96 0.00 %  
 GR97 0.00 %  
 GR98 0.00 %  
 GR99 0.00 %  
 GR100 0.00 %

F2 - Processing parameters  
 SI 65536  
 SF 125.7800094 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 230.637 ppm  
 F1 29005.68 Hz  
 F2 -10.287 ppm  
 F3 -1293.96 Hz  
 F4 -15.068 ppm/cm  
 F5 1329.1093 Hz/cm  
 HECK

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



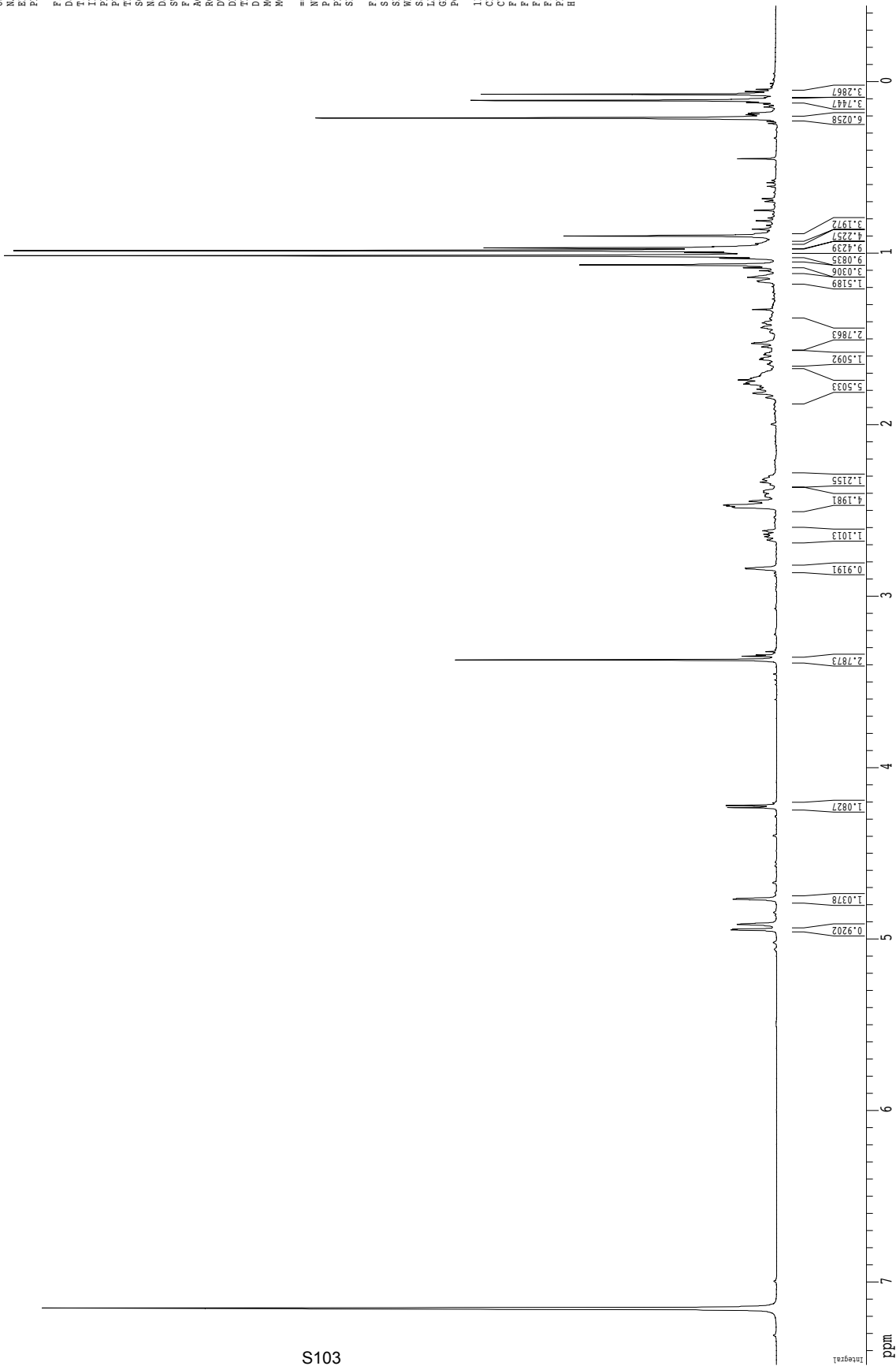
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 USER schner  
 NAME ms03-711-32d  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110221  
 Time 10.25  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 13  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 62.400 usec  
 DR 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

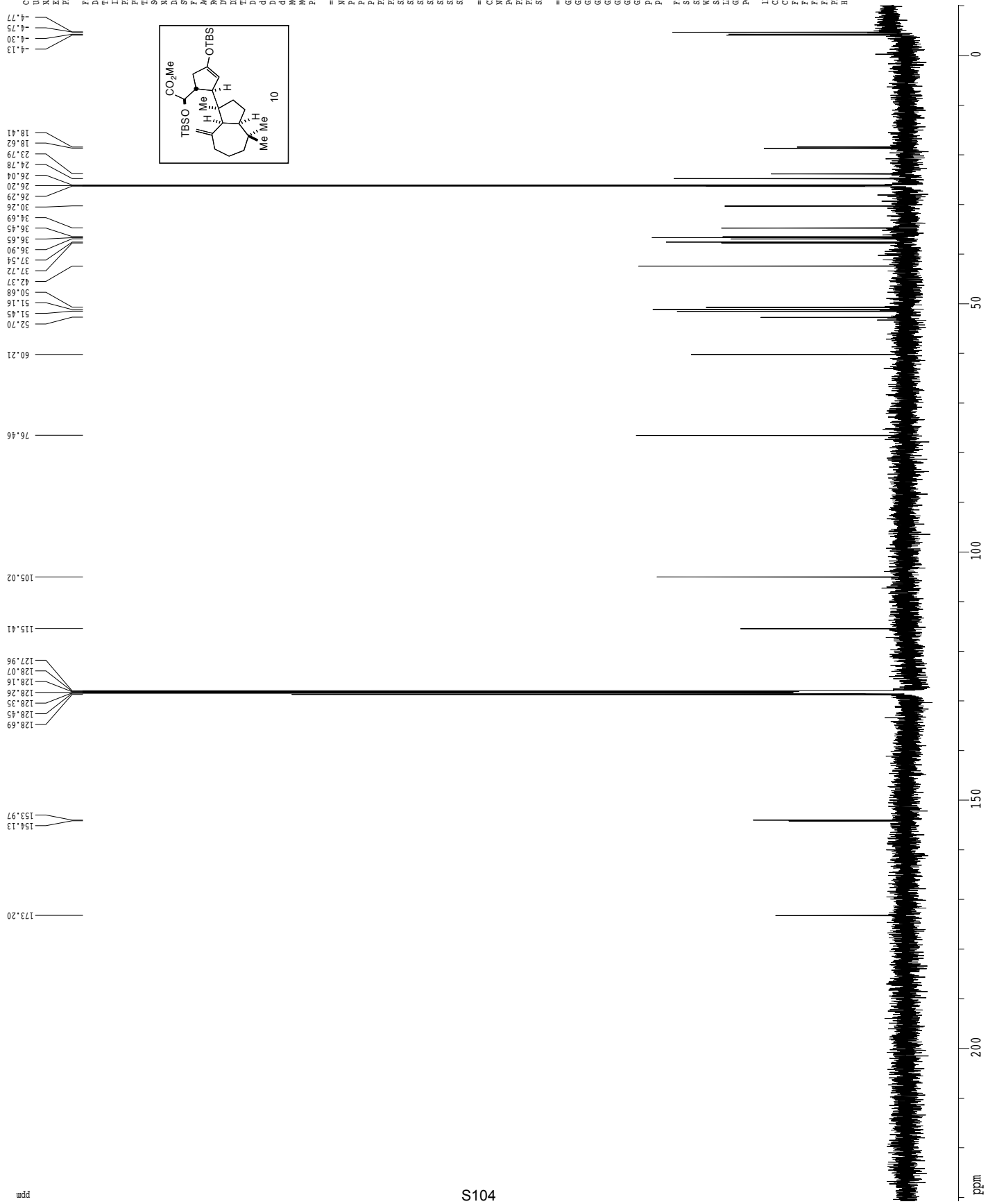
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.2205688 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

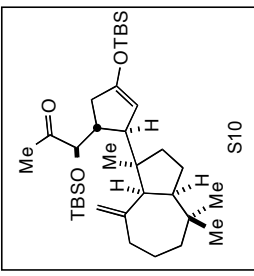
1D NMR plot parameters  
 CX 22.80 cm  
 CY 13.00 cm  
 FIP 7.460 ppm  
 F2 3741.68 Hz  
 F3 -220.88 ppm  
 PPM0 0.34744 ppm/cm  
 HZCM 173.78643 Hz/cm



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



1H spectrum



Current Data Parameters  
 USER schner  
 NAME ms003-266-3-2  
 EXPNO 1  
 PROCNO 1

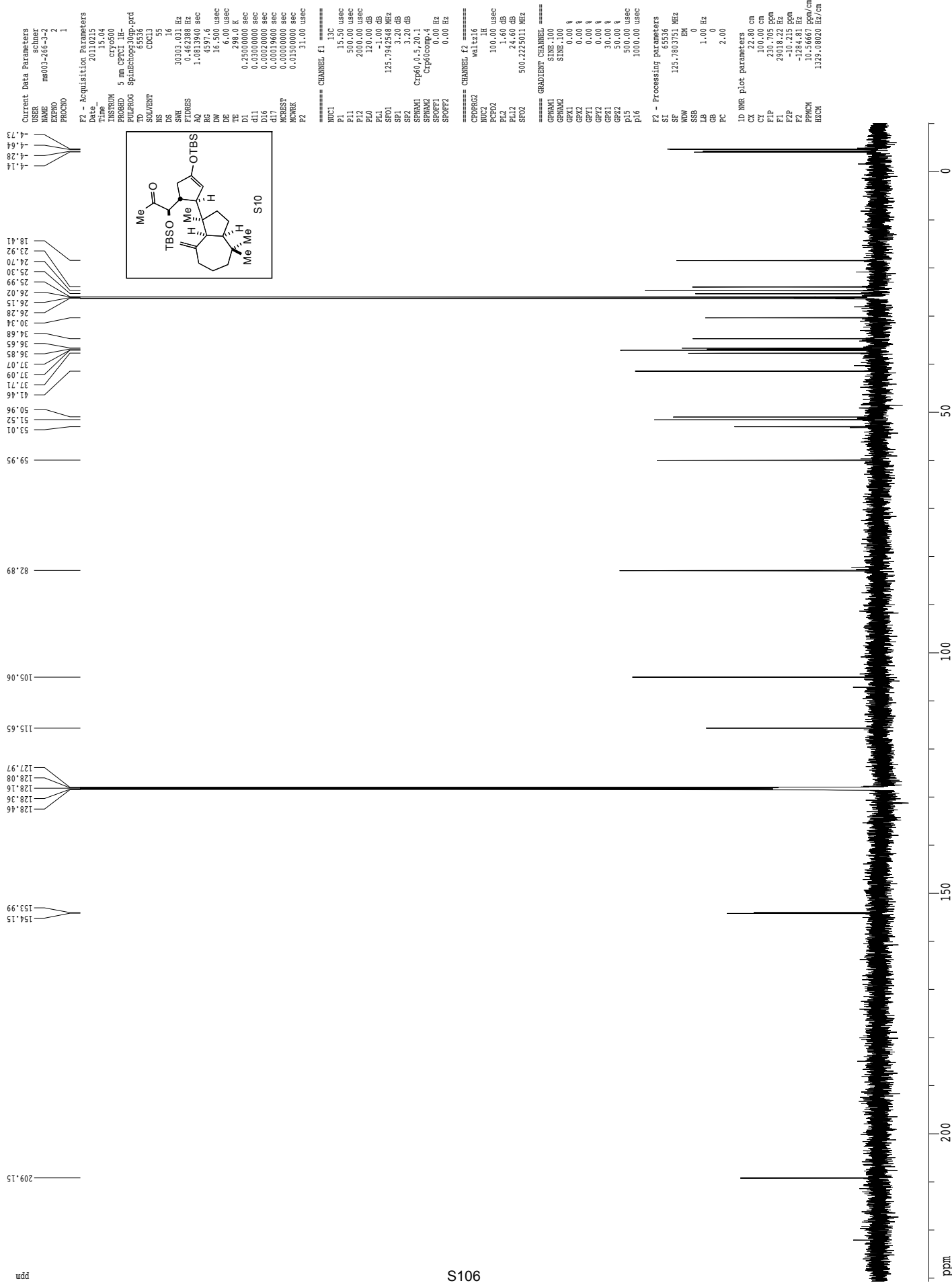
F2 - Acquisition Parameters  
 Date\_ 20110215  
 Time 15.62  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 11  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0990774 sec  
 RG 415  
 DE 62.600 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

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

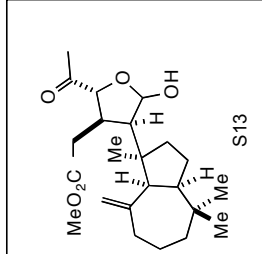
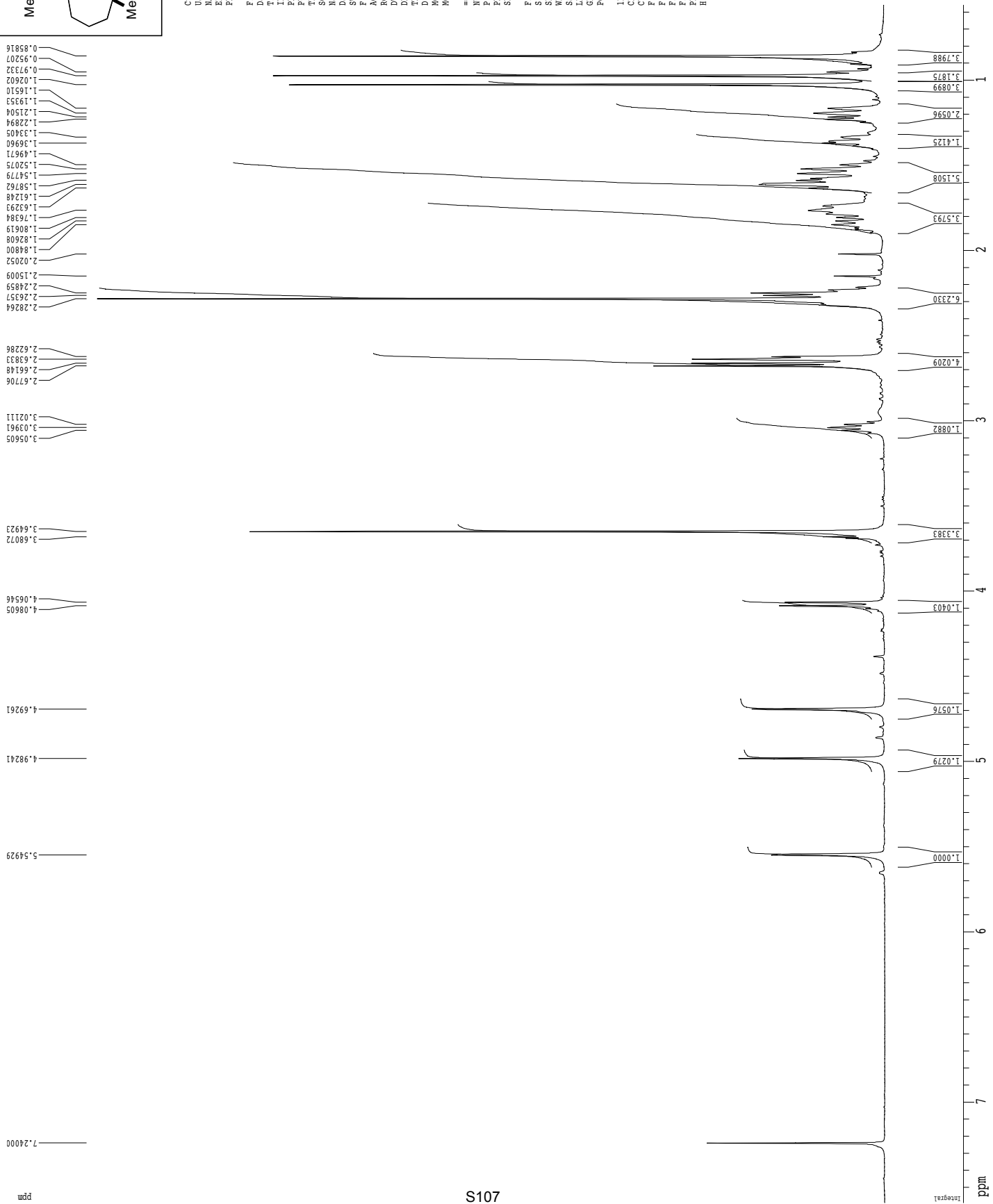
F2 - Processing parameters  
 SI 65536  
 SF 500.2201608 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 7.970 ppm  
 F1 3986.88 Hz  
 F2 -28.62 ppm  
 F3 0.00000000 ppm  
 PRGM 0.37470 ppm/cm  
 HZCM 187.43440 Hz/cm

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



1H spectrum



Current Data Parameters  
 USER schner  
 NAME ms003-175-3  
 EXPNO 1  
 PROCNO 1

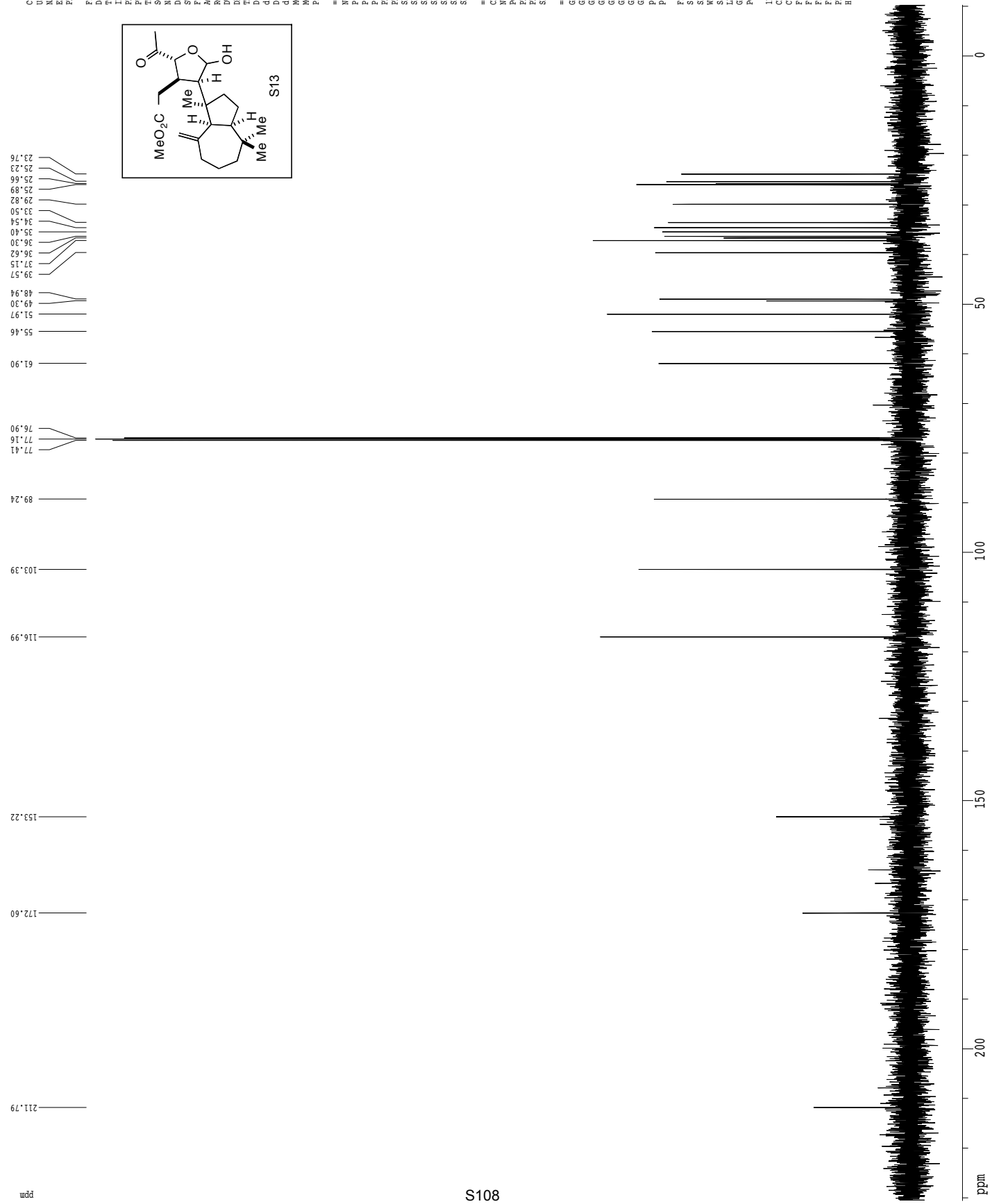
F2 - Acquisition Parameters  
 Date\_ 20101109  
 Time\_ 10.31  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 6  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099874 sec  
 RG 0  
 DE 62.40 usec  
 TE 298.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

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

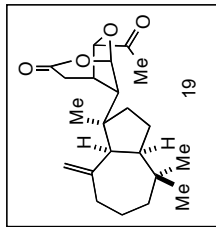
F2 - Processing parameters  
 SI 32768  
 SF 500.2204221 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 7.590 ppm  
 FZ 3796.88 Hz  
 PZ 0.00 ppm  
 PR 280.00 ppm  
 PRCM 0.30834 ppm/cm  
 HZCM 154.23898 Hz/cm

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







Current Data Parameters  
 USER schner  
 NAME ms603-233-3c13  
 EXPNO 1  
 PROCNO 1

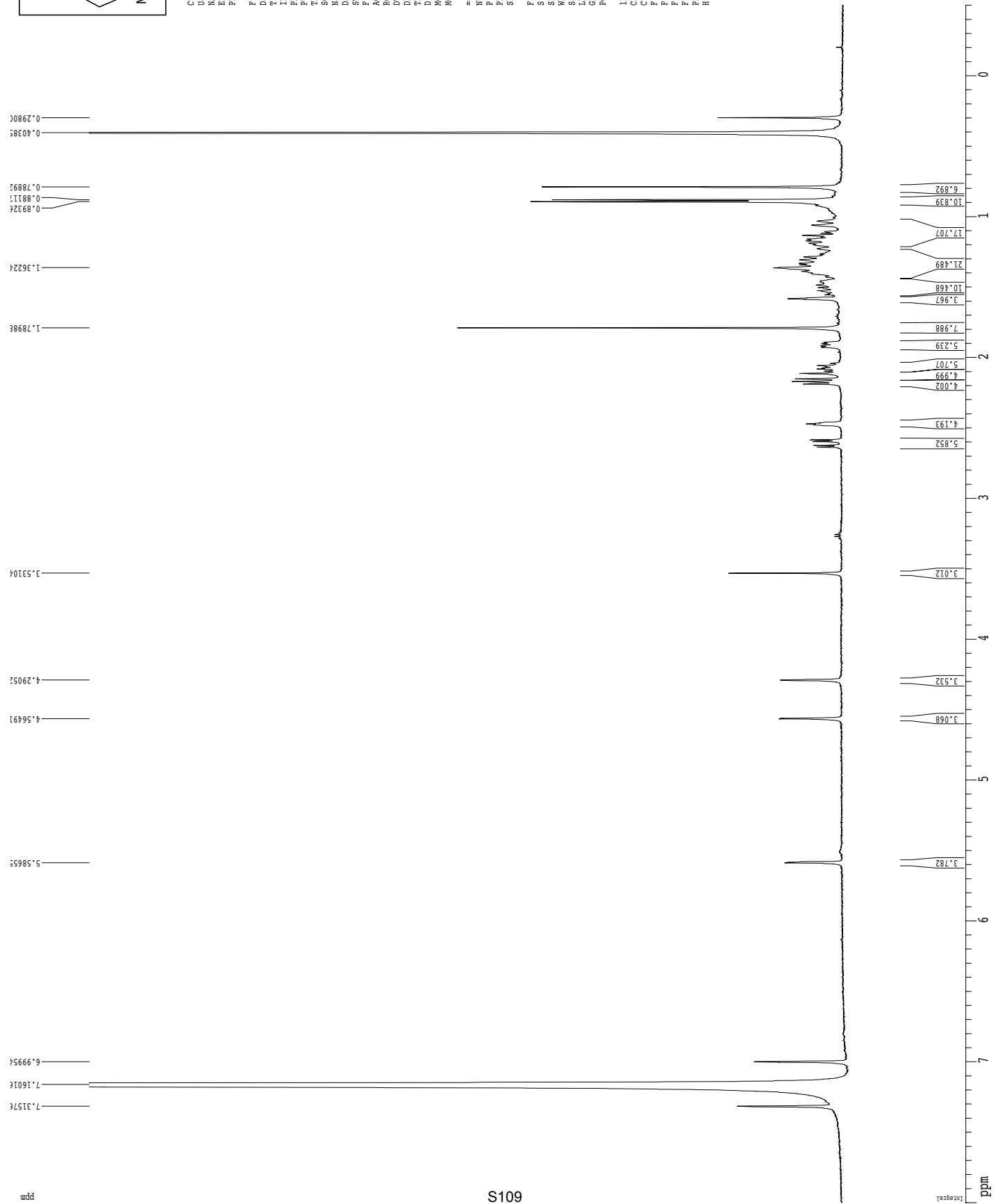
F2 - Acquisition Parameters  
 Date\_ 20101222  
 Time 21:34  
 INSTRUM cryo500  
 PULPROG zgpg30  
 FIDRES 5 mm CPFG1.620  
 TD 81728  
 SOLVENT 6006  
 NS 33  
 DS 2

SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 MCFRESF 0.1000000 sec  
 MCFRES 0.0000000 sec  
 MCFREK 0.01500000 sec

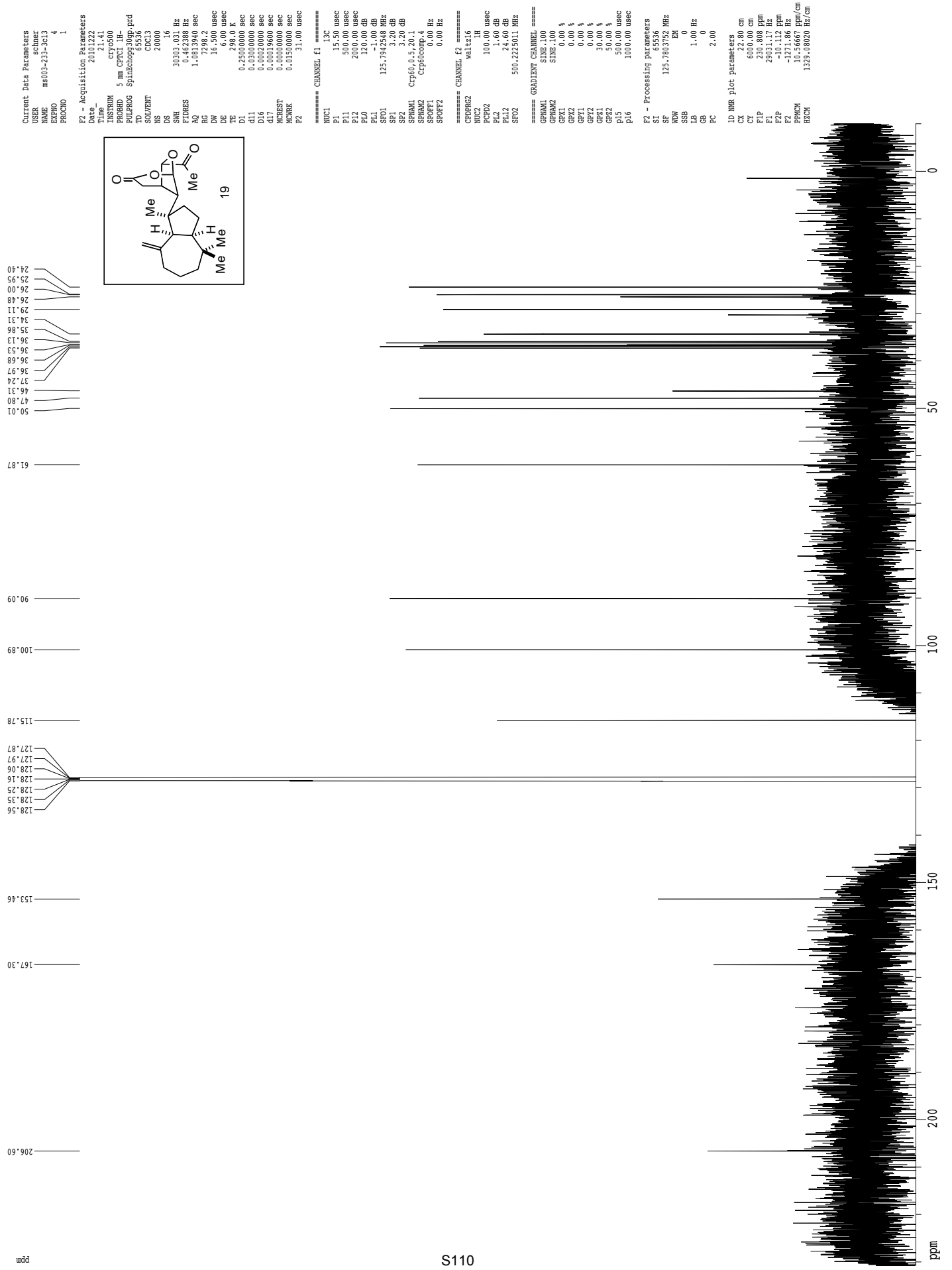
==== CHANNEL f1 =====  
 NUCL 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2200009 MHz  
 WDW EM  
 SS 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 300.00 cm  
 FIP 8.000 ppm  
 F1 4001.76 Hz  
 F2 -0.500 ppm  
 F2 -250.11 Hz  
 PRCH 0.37261 ppm/cm  
 HZCX 186.46553 Hz/cm



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



Current Data Parameters  
USER SCHEM  
NAME ms003-233-0112  
EXPER 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20101222  
Time 21.41  
INSTRUM cryo500  
PROBHD 5 mm CPXI 1H  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 20000  
DS 16  
SWH 30303.031 Hz  
FIDRES 0.462388 Hz  
AQ 1.0815940 sec  
RG 1298.7  
DE 6.00 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  
ACWRR 0.01500000 sec  
F2 31.00 usec

===== CHANNEL F1 =====  
NUC1 13C  
P1 15.50 usec  
PL1 500.00 usec  
PL2 2000.00 usec  
PL0 120.00 dB  
PL1 125.7947568 dB  
SP1 5.20 dB  
SP2 31.20 dB  
SFO1 Ccp60.05.20.1  
SFO2 Ccp60comp.4  
SFOFF1 0.00 Hz  
SFOFF2 0.00 Hz

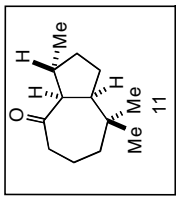
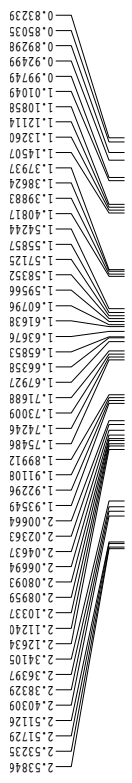
===== CHANNEL F2 =====  
CPDPRG2 wd1616  
NUC2 1H  
PCPD2 100.00 usec  
PL2 1.60 dB  
PL12 24.60 dB  
SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
GGRM1 0.00 %  
GGRM2 0.00 %  
GGRM3 0.00 %  
GGRM4 0.00 %  
GGRM5 30.00 %  
GGRM6 50.00 %  
P15 500.00 usec  
P16 1000.00 usec

F2 - Processing parameters  
SI 65536  
SF 125.7803752 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 2.00

ID NMR plot parameters  
CX 22.80 cm  
CY 600.00 cm  
FIP 230.808 ppm  
F1 2903.17 Hz  
F2 -10.112 ppm  
FZ -1271.86 Hz  
H1 1.660 ppm/cm  
H2CN 1329.0020 Hz/cm

1H spectrum



Current Data Parameters  
 USER schner  
 NAME ms003-260-32d  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110209  
 Time 10.45  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 8  
 DS 2

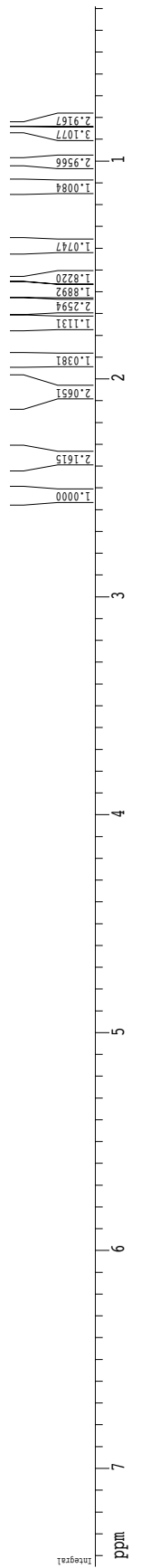
SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 65  
 RT 62.40 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

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

F2 - Processing parameters  
 SI 65536  
 SF 500.2204236 MHz  
 DS 4  
 MVM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

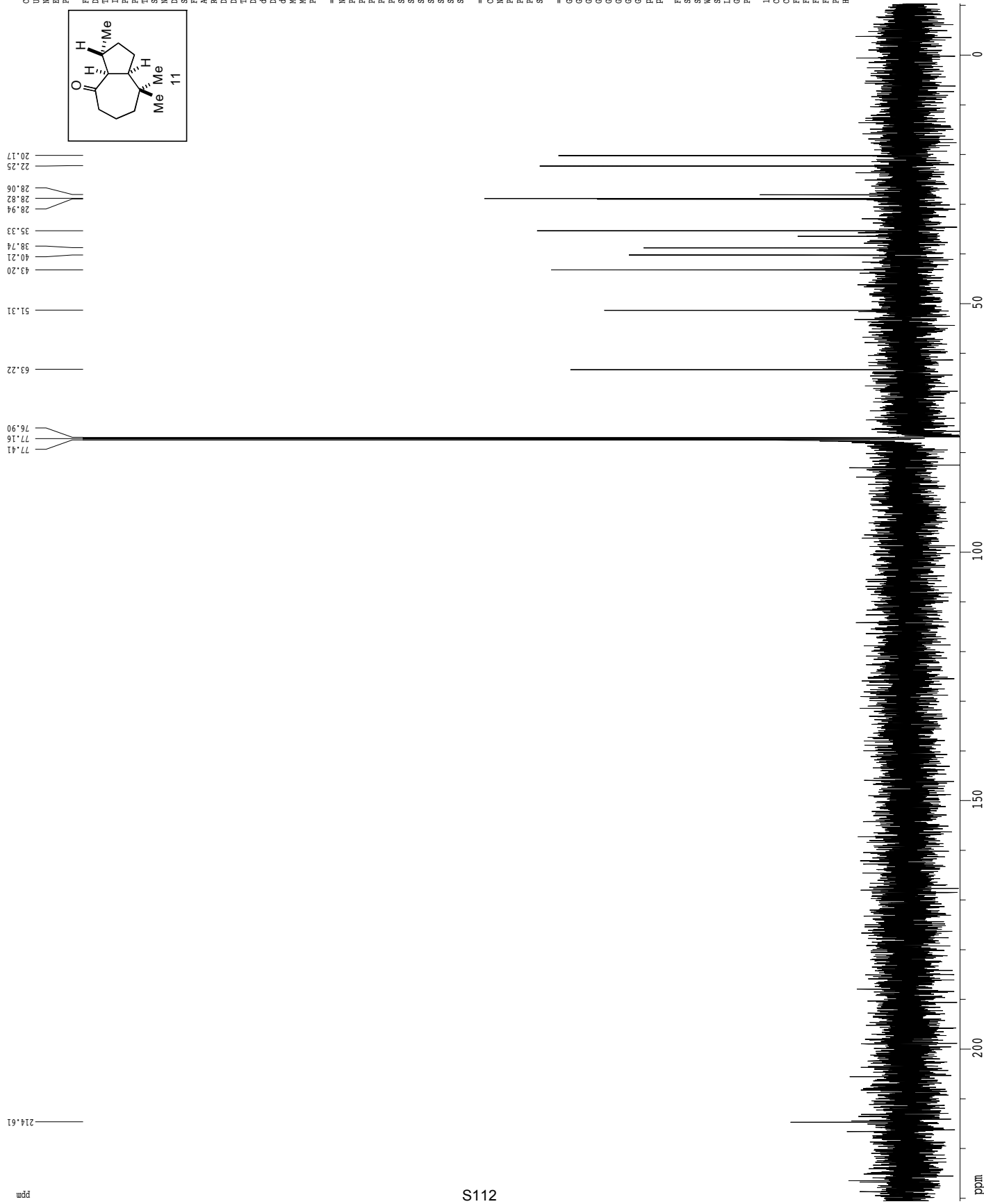
1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 7.469 ppm  
 F2 3726.07 Hz  
 F2 146.21 ppm  
 PPMCM 0.31388 ppm/cm  
 HZCM 157.01131 Hz/cm

S111

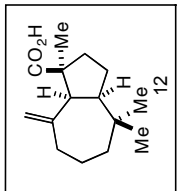
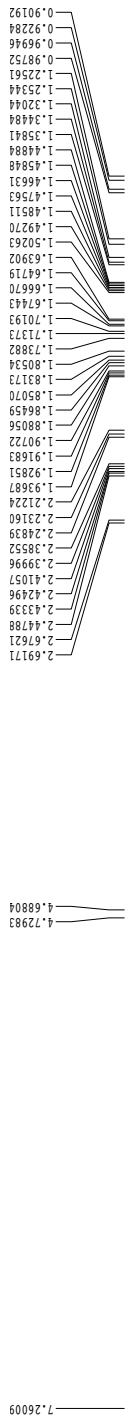


Integral

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



1H spectrum



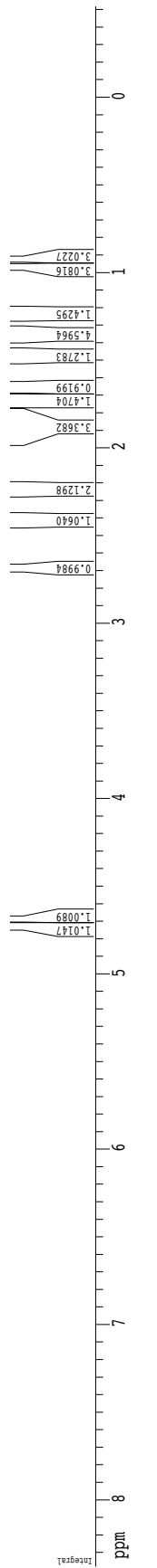
Current Data Parameters  
 USER schner  
 NAME ms003-45-32d  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20100825  
 Time 16.20  
 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 5.0996774 sec  
 RG 71  
 DR 62.40 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

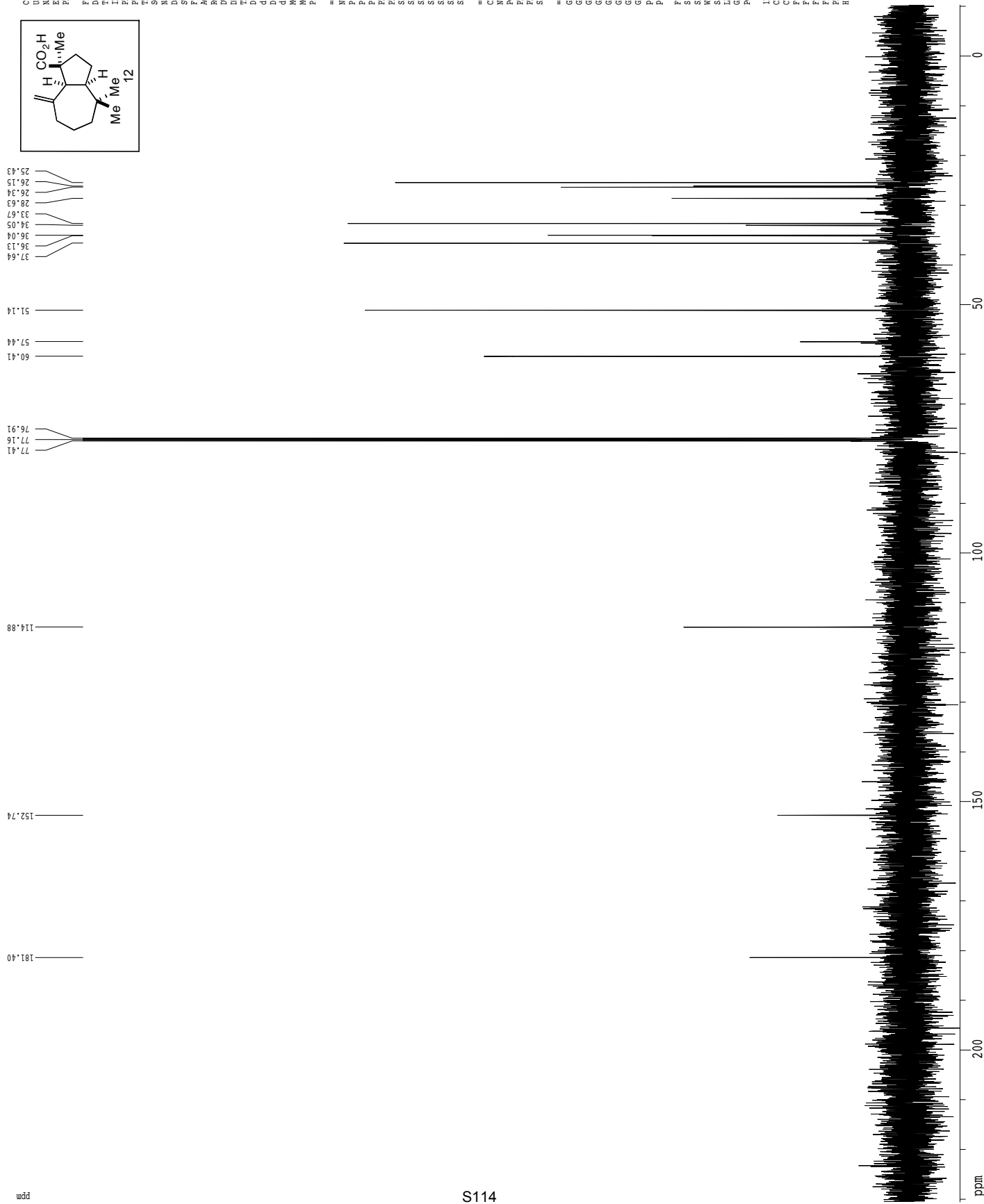
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2203116 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

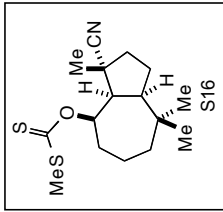
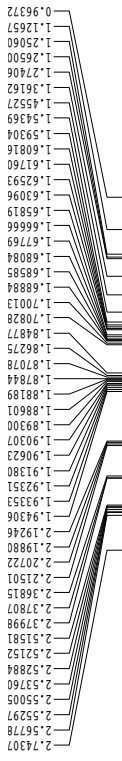
1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 8.379 ppm  
 F2 4191.52 Hz  
 F3 -25.73 ppm  
 PPM0 0.38008 ppm/cm  
 HZCM 198.12761 Hz/cm



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



1H spectrum



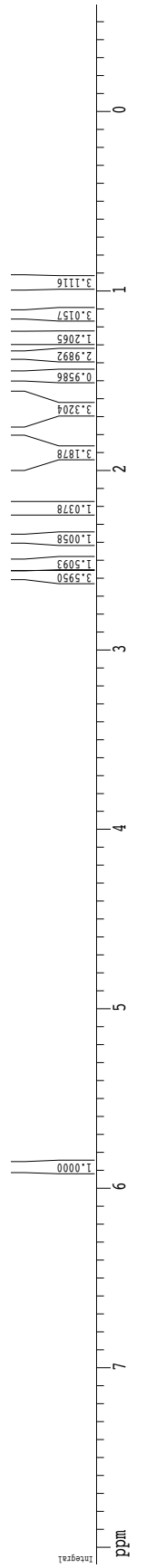
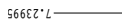
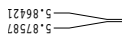
Current Data Parameters  
 USER: schmer  
 NAME: mjs4-12-3  
 EXPNO: 1  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_: 20110321  
 Time: 14.23  
 INSTRUM: av600  
 PROBHD: 5 mm TBI 1H/13  
 PULPROG: zg30  
 AQ: 0.7938  
 SOLVENT: CDCl3  
 NS: 7  
 DS: 2  
 SWH: 9615.385 Hz  
 FIDRES: 0.098178 Hz  
 AQ: 5.0928259 sec  
 RG: 203  
 DW: 52.000 usec  
 DE: 6.00 usec  
 TE: 298.0 K  
 D1: 0.10000000 sec

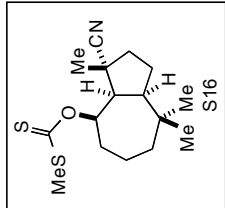
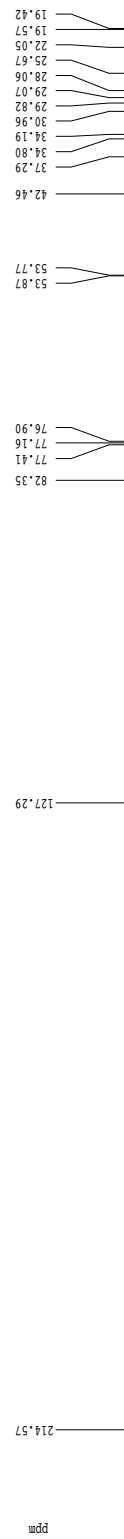
==== CHANNEL f1 =====  
 NUC1: 1H  
 P1: 8.00 usec

F2 - Processing parameters  
 SI: 6536  
 SF: 600.1300460 MHz  
 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  
 F1P: 8.095 ppm  
 F1: 4858.15 Hz  
 F2P: -0.593 ppm  
 F2: -356.16 Hz  
 PPMCH: 0.38108 ppm/cm  
 HZCM: 228.69795 Hz/cm



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



Current Data Parameters  
 USER schmer  
 NAME mjs4-12b-2  
 EXPNO 2  
 PROCNO 1

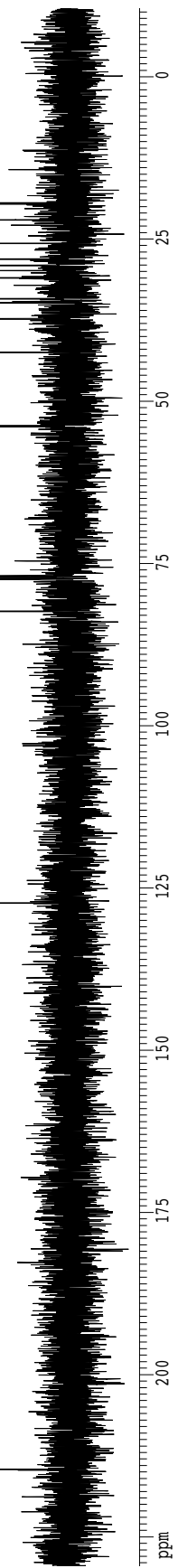
F2 - Acquisition Parameters  
 Date\_ 20110322  
 Time 10.28  
 INSTRUM gfb500  
 PROBD 5 mm broadband  
 PULPROG zgpg30  
 TD 6536  
 SOLVENT CDCl3  
 NS 69  
 DS 4  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 2580.3  
 DW 16.500 usec  
 DE 4.50 usec  
 TE 298.0 K  
 d1 0.25000000 sec  
 d11 0.03000000 sec  
 MCRST 0.00000000 sec  
 MCRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 PC 1.70 usec  
 PL1 0.00 dB  
 SF01 125.6157092 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PL2 -3.00 dB  
 PL12 13.20 dB  
 SF02 499.5124975 MHz

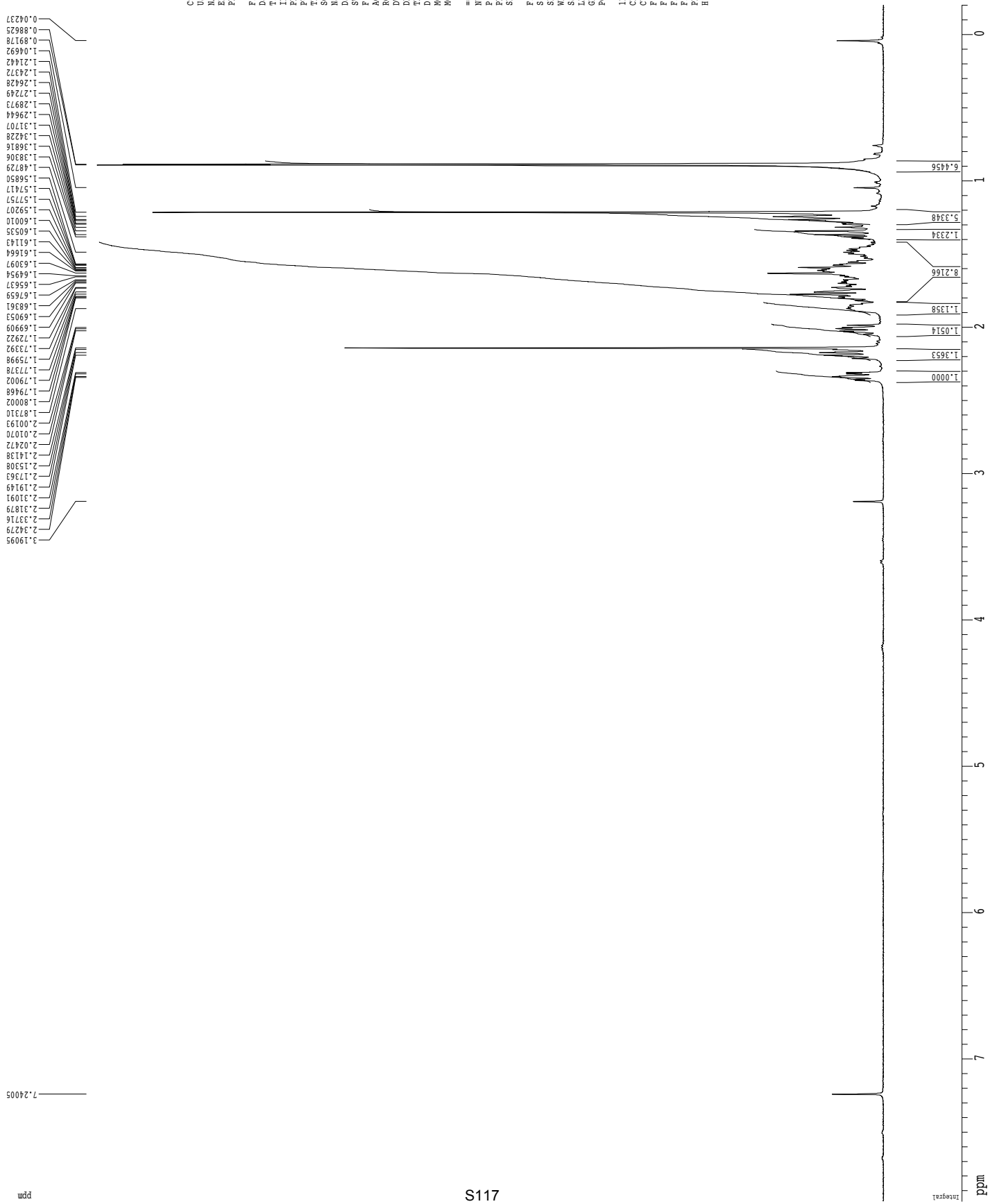
F2 - Processing parameters  
 SI 65536  
 SF 125.6018786 MHz  
 MDW EN  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 2.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.65 cm  
 E1P 299.520 ppm  
 F1 28828.10 Hz  
 F2P -10.507 ppm  
 F2 -1319.65 Hz  
 PPMCM 10.52747 ppm/cm  
 HZCM 1322.26978 Hz/cm

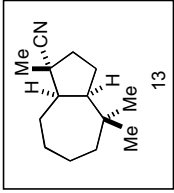




1H spectrum



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



```

Current Data Parameters
USER          schmer
NAME          njs4-13-3c13
EXPNO        2
PROCNO       1

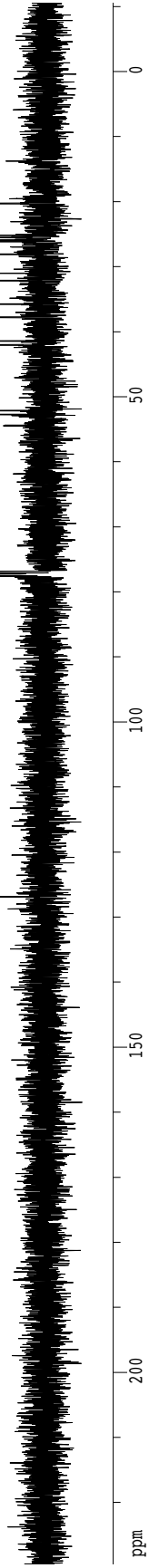
F2 - Acquisition Parameters
Date_        20110323
Time         9.37
INSTRUM      gfb500
PROBHD       5 mm broadband
PULPROG      zgpg30
AQ           6536
RG           131
DS           4
SWH          30303.031 Hz
FIDRES       0.462388 Hz
AQ           1.0813940 sec
RG           46341
DW           16.500 usec
DE           4.50 usec
TE           298.0 K
d1           0.25000000 sec
d11          0.03000000 sec
MCRETST     0.00000000 sec
MCPRK       0.01500000 sec

===== CHANNEL f1 =====
NUC1         13C
P1           7.70 usec
PL1          0.00 dB
SFO1         125.6157032 MHz

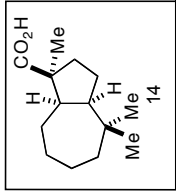
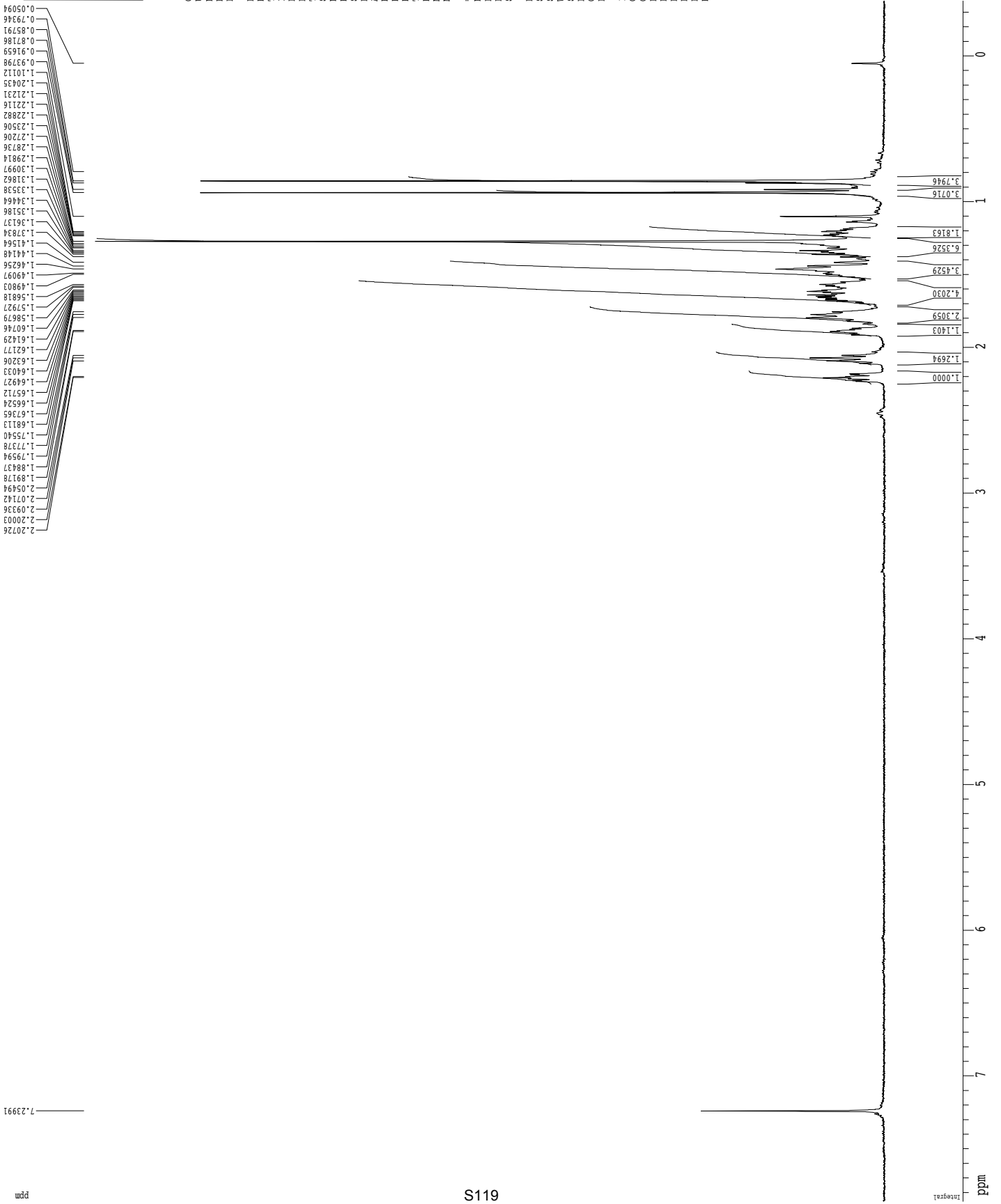
===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2       80.00 usec
PL2         -3.00 dB
PL12        13.20 dB
SFO2        499.5124975 MHz

F2 - Processing parameters
SI           65536
SF           125.6018807 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           2.00

ID NMR plot parameters
CY           22.80 cm
CX           15.65 cm
E1P         299.520 ppm
F1          28828.10 Hz
F2P         -10.507 ppm
F2          -1319.65 Hz
PPHMCN     10.52747 ppm/cm
HZCN       1322.26990 Hz/cm
    
```



1H spectrum



Current Data Parameters  
USER schner  
NAME m184-15-3c4c13  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20110323  
Time 19:05  
INSTRUM spect  
PROBHD 5 mm broadband  
PULPROG zgpg30  
TD 81728  
FIDRES 0.098043 Hz  
AQ 5.0998774 sec  
RG 812.7  
DW 62.400 usec  
DE 6.00 usec  
TE 298.0 K  
MCHRESF 0.1000000 sec  
MCNRFK 0.01500000 sec  
===== CHANNEL f1 =====  
NUC1 1H  
P1 12.20 usec  
PL1 -5.00 dB  
SFO1 499.3134966 MHz

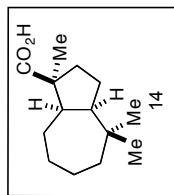
F2 - Processing parameters  
SI 65536  
SF 499.3100370 MHz  
WDW EM  
SSB 0  
GB 0.30 Hz  
GC 1.00  
PC 1.00

1D NMR plot parameters  
CX 22.80 cm  
CY 15.00 cm  
F1P 7.860 ppm  
F1 3926.00 Hz  
F2P -0.376 ppm  
F2 -188.04 Hz  
PRCH 0.36124 ppm/cm  
HZCX 180.44028 Hz/cm

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



ppm



Current Data Parameters  
 USER schmer  
 NAME mjs4-15-3cdc13  
 EXPNO 2  
 PROCNO 1

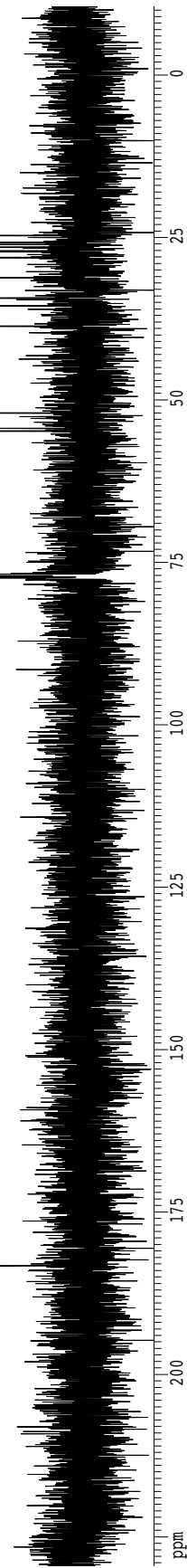
F2 - Acquisition Parameters  
 Date\_ 20110323  
 Time 19.06  
 INSTRUM gwb00  
 PROBD 5 mm broadband  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 166  
 DS 4  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 91.95.2  
 DW 16.500 usec  
 DE 4.50 usec  
 TE 298.0 K  
 D1 0.25000000 sec  
 d11 0.03000000 sec  
 MCRST 0.00000000 sec  
 MCRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 7.70 usec  
 PL1 0.00 dB  
 SF01 125.6157092 MHz

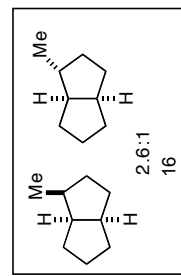
==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PL2 -3.00 dB  
 PL12 13.20 dB  
 SF02 499.5124975 MHz

F2 - Processing parameters  
 SI 65536  
 SF 125.6018774 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.50

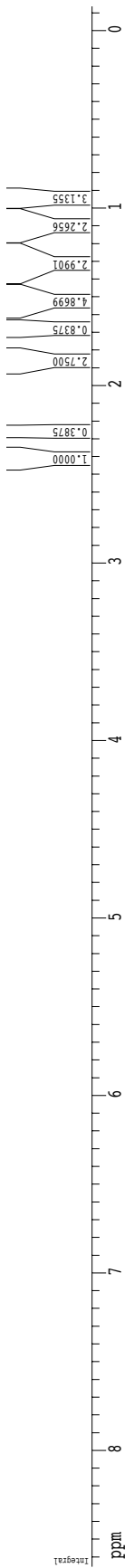
1D NMR plot parameters  
 CX 22.80 cm  
 CY 40.00 cm  
 E1P 29.520 ppm  
 F1 28828.10 Hz  
 F2P -10.507 ppm  
 F2 -1319.65 Hz  
 PPMCM 10.52747 ppm/cm  
 HZCM 1322.26978 Hz/cm



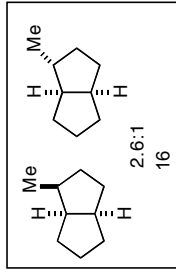
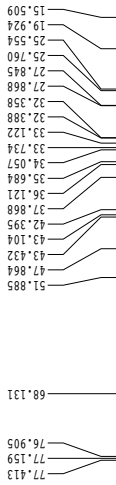
0.93751  
0.91513  
0.92963  
0.97561  
1.03636  
1.04501  
1.04943  
1.05734  
1.06376  
1.12741  
1.12827  
1.12900  
1.13052  
1.13156  
1.13615  
1.14614  
1.14696  
1.17263  
1.17921  
1.18766  
1.19563  
1.19563  
1.51156  
1.51444  
1.53008  
1.53021  
1.58243  
1.58243  
1.58442  
1.58442  
1.68105  
1.68105  
1.68135  
1.68172  
1.68172  
1.68204  
1.68916  
1.68916  
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1.69603  
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1.69561  
1.69561  
1.69777  
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1.68156  
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1.68851  
1.64388  
1.64388  
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1.64075  
1.64756  
1.64756  
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1.64144  
1.63905  
1.63905  
1.64574  
1.64574  
1.64305  
1.64305  
1.73352  
1.73352  
1.74616  
1.74616  
1.75991  
1.75991  
1.72606  
1.72606



Current Data Parameters  
 USER schner  
 NAME m1st-239-3c13  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120426  
 Time 9:33  
 NSBROW cryo300  
 PULPROG zgpg30  
 PRGNAME 5 mm CPAC1  
 FIDRES 0.098043 Hz  
 TO 81728  
 SOLVENT CDCl3  
 NS 5  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 5  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 MCFREQ 0.100000000 sec  
 MCHNK 0.015000000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 500.2200321 MHz  
 WDW EM  
 SS 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 8.653 ppm  
 F1 4328.33 Hz  
 F2P -0.133 ppm  
 F2 -66.72 Hz  
 PRCH 0.38536 ppm/cm  
 HZCX 192.76561 Hz/cm



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



```

Current Data Parameters
USER          SCuser
EXPNO         m34-239-3C12
PROCNO        1
PROCNO        1

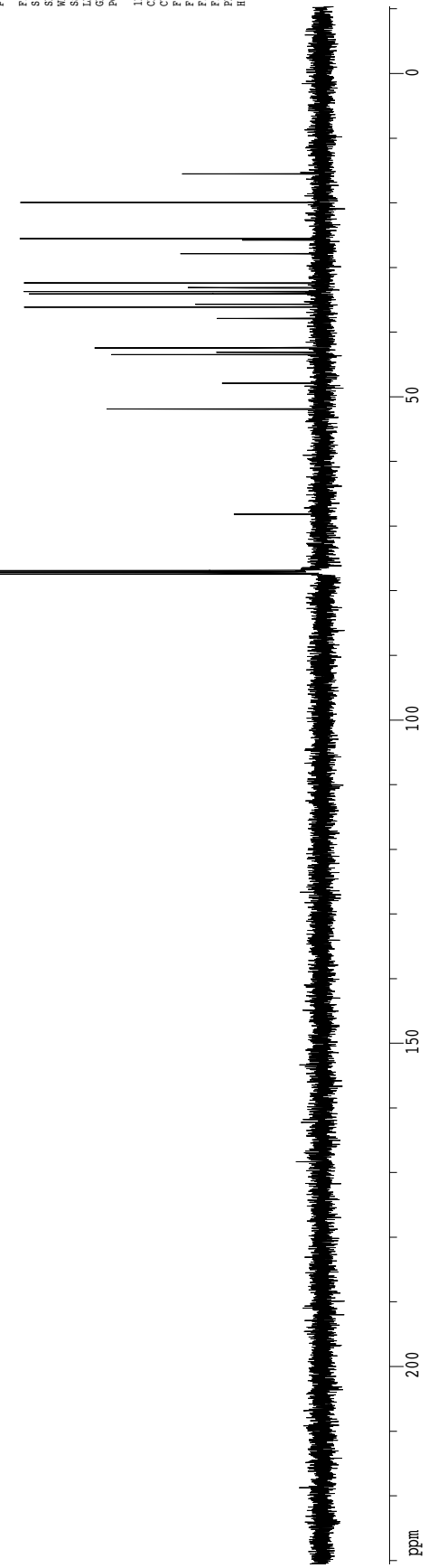
F2 - Acquisition Parameters
Date_         20120426
Time          9.36
INSTRUM       cryo500
PROBHD        5 mm CPXI 1H
PULPROG       zgpg30
SOLVENT       CDCl3
NS            121
DS            16
SWH           30303.031 Hz
AQ            0.462388 Hz
RG            10221.5
DR            6.00 usec
TE            298.2 K
D1            0.25000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00015600 sec
ACQRESF       0.00000000 sec
AQRESF        0.01500000 sec
F2            3.00 usec

===== CHANNEL f1 =====
NUC1          13C
P1            15.50 usec
PL1           500.00 usec
P12           2000.00 usec
PL2           120.00 dB
P13           125.784568 MHz
SFO1          500.136299 MHz
SFO2          500.136299 MHz
SFO3          500.136299 MHz
SFO4          500.136299 MHz
SFO5          500.136299 MHz
SFO6          500.136299 MHz
SFO7          500.136299 MHz
SFO8          500.136299 MHz
SFO9          500.136299 MHz
SFO10         500.136299 MHz
SFO11         500.136299 MHz
SFO12         500.136299 MHz
SFO13         500.136299 MHz
SFO14         500.136299 MHz
SFO15         500.136299 MHz
SFO16         500.136299 MHz
SFO17         500.136299 MHz
SFO18         500.136299 MHz
SFO19         500.136299 MHz
SFO20         500.136299 MHz
===== CHANNEL f2 =====
CPDPRG2       wdcp16
NUC2          1H
PCPD2         100.00 usec
PL2           1.60 dB
PL12          24.60 dB
SFO2         500.2225011 MHz

===== GRADIENT CHANNEL =====
GMR1          10.00 usec
GMR2          10.00 usec
GMR3          10.00 usec
GMR4          10.00 usec
GMR5          10.00 usec
GMR6          10.00 usec
GMR7          10.00 usec
GMR8          10.00 usec
GMR9          10.00 usec
GMR10         10.00 usec
GMR11         10.00 usec
GMR12         10.00 usec
GMR13         10.00 usec
GMR14         10.00 usec
GMR15         10.00 usec
GMR16         10.00 usec
GMR17         10.00 usec
GMR18         10.00 usec
GMR19         10.00 usec
GMR20         10.00 usec

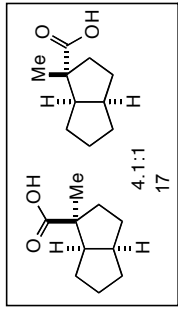
F2 - Processing parameters
SI            65536
SF            125.7804076 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            2.00

ID NMR plot parameters
CX            22.80 cm
CY            15.65 cm
FIP           230.551 ppm
F1            28994.80 Hz
F2            -10.395 ppm
F3            -130.423 Hz
F4            10.668 ppm/cm
HEXCN        1329.00032 Hz/cm
    
```



1H spectrum

7.22412  
 2.71330  
 2.69897  
 2.53504  
 2.52090  
 2.50658  
 2.49519  
 2.44800  
 2.22968  
 2.04926  
 2.03587  
 1.87291  
 1.86612  
 1.86054  
 1.85666  
 1.85252  
 1.84543  
 1.83978  
 1.83581  
 1.77631  
 1.76521  
 1.60660  
 1.59991  
 1.59642  
 1.58668  
 1.44676  
 1.43453  
 1.42511  
 1.34957  
 1.33442  
 1.33011  
 1.32705  
 1.20655  
 1.20144  
 1.28265  
 1.27904  
 1.27307  
 1.26371  
 1.22778  
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 1.11910  
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 1.09987  
 0.93864



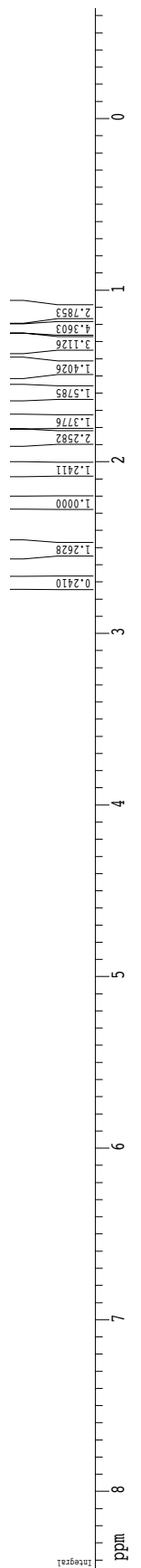
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 NAME m184-127a-3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
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 PROBHD 5 mm TBI 1H/13  
 PULPROG zg30  
 AQ 9.7938  
 SOLVENT CDCl3  
 NS 14  
 DS 2  
 SWH 9615.385 Hz  
 FIDRES 0.098178 Hz  
 AQ 5.0928259 sec  
 RG 1030  
 DW 52.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec

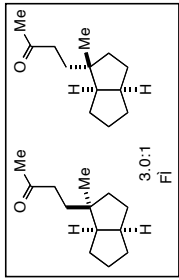
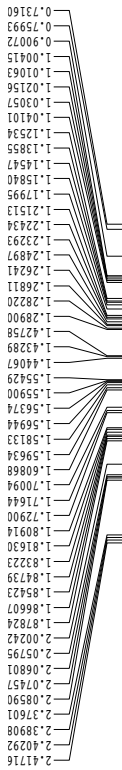
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.00 usec

F2 - Processing parameters  
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 WWDW 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 8.446 ppm  
 F1 5068.46 Hz  
 F2 -0.642 ppm  
 FZ -385.04 Hz  
 PPMXN 0.39856 ppm/cm  
 HZCN 239.18869 Hz/cm



1H spectrum



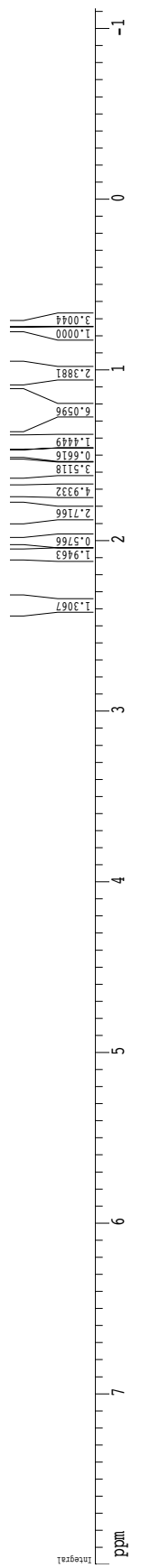
Current Data Parameters  
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 EXPNO 1  
 PROCNO 1

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 Time 13.43  
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 TD 65536  
 SFO 400.136099  
 SOLVENT CDCl3  
 NS 10  
 DS 2  
 SWH 9615.385 Hz  
 SF 0.098178 Hz  
 FTRES 5.0928259 sec  
 RG 456  
 DW 52.000 usec  
 DE 6.00 usec  
 TE 298.1 K  
 D1 0.10000000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 400.136099 MHz  
 DS 2  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 8.000 ppm  
 F1 4801.04 Hz  
 F2 -1.116 ppm  
 FZ -669.80 Hz  
 PPMCH 0.39983 ppm/cm  
 HZCM 239.94931 Hz/cm





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

