

Palladium- and Nickel-Catalyzed C–C Bond Insertion Reactions with
Alkylidenesilacyclopropanes

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Supporting Information

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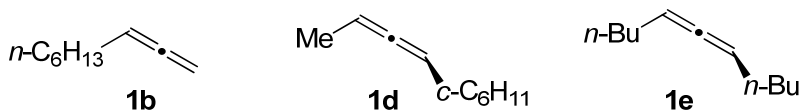
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Experimental Section

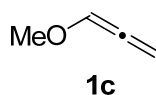
General Procedures. ^1H NMR and ^{13}C NMR spectra were recorded at ambient temperature using Bruker DRX 400 (400 and 100 MHz, respectively) or DRX 500 (500 and 125 MHz, respectively) spectrometers, as indicated. The data are reported as follows: chemical shift in ppm from internal tetramethylsilane on the δ scale, multiplicity (appar = apparent, br = broad, s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, m = multiplet), coupling constants (Hz), and integration. Due to difficulties with purification for certain products, only distinctive peaks are listed in tabulated ^1H NMR spectral data as indicated, and the structures were assigned using a combination of COSY, HMQC, HMBC, and nOe experiments. ^{29}Si NMR spectra were recorded at ambient temperature using a Bruker DRX 500 (99.3 MHz) spectrometer relative to an external tetramethylsilane standard on the δ scale. NMR yields were determined relative to a known concentration of internal standard (PhSiMe_3). Infrared (IR) spectra were obtained using a Mattson Galaxy FT-IR 5000 spectrometer. Gas chromatography–mass spectrometry (GC-MS) was performed with a Thermo-Finnigan Trace Mass Spectrometer Plus quadrupole system with a fused silica capillary column ($30\text{ m} \times 0.32\text{ mm} \times 0.25\text{ }\mu\text{m}$) wall-coated with DB-5 (J & W Scientific) using electron ionization (70 eV). High resolution mass spectra (HRMS) were acquired on a Waters LCT Premier quadrupole time-of-flight spectrometer or a Waters GCT Premier orthogonal acceleration time-of-flight spectrometer and were obtained by peak matching. Microanalyses were performed by Atlantic Microlab Inc., Norcross, GA. Melting points were obtained using a Büchi 510 melting point apparatus and were reported uncorrected. Analytical thin layer chromatography was performed on EMD Chemicals Inc. silica gel 60 F₂₅₄ plates. Liquid chromatography was performed using forced flow (flash chromatography) of the indicated solvent system on Sorbent Technologies silica gel (SiO_2) 60 (230–400 mesh). Metal catalysts and silacyclopropanes were stored and manipulated in an Innovative Technologies nitrogen-atmosphere dry box. All reactions were performed under an

atmosphere of nitrogen in glassware that had been flame-dried under vacuum. Solvents were distilled and degassed before use. DMSO was distilled over CaH₂ and dried sequentially over 4Å molecular sieves according to the procedure outlined by Burfield et al.¹ Unless otherwise noted, all reagents and substrates were commercially available.

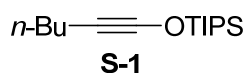
I. Syntheses of Starting Materials



The syntheses of **1b**, **1d**, and **1e** were previously published by our laboratory.²

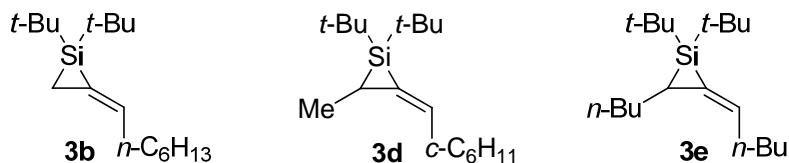


Allene 1c. A procedure reported by Trofimov³ was used to prepare allene **1c**. To a solution of anhydrous KOH (2.8 g, 50 mmol) in DMSO (14 mL) was added methyl propargyl ether (8.5 mL, 100 mmol). The resulting orange-brown solution was stirred at 22 °C for 18 h. The reaction mixture was distilled at ambient pressure into a receiving flask cooled to -78 °C. The fraction collected with bp 51–53 °C afforded allene ether **1c** as a colorless liquid (3.3 g, 47%). The spectral data are consistent with the data reported:⁴ ¹H NMR (400 MHz, C₆D₆) δ 6.73 (t, *J* = 5.9, 1H), 5.25 (d, *J* = 5.9, 2H), 3.18 (s, 3H); ¹³C NMR (125 MHz, C₆D₆) δ 201.3, 123.0, 90.5, 55.2.



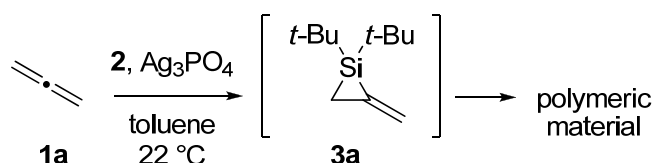
Alkyne S-1. A procedure reported by Kozmin⁵ was used to prepare alkyne **S-3**. A solution of LiOO*t*-Bu was prepared by adding THF (36 mL) and LiHMDS (12 mL, 1.0 M in THF, 12 mmol) to an anhydrous solution of HOO*t*-Bu⁶ (3.3 mL, 3.625 M in toluene, 12 mmol). The prepared solution was added to a cooled (-78 °C) solution of 1-hexyne (1.3 mL, 11 mmol) and LiHMDS (13 mL, 1.0 M in THF, 13 mmol) in THF (36 mL). The reaction mixture was warmed to 0 °C. After 2 h, the reaction mixture was cooled to -78 °C and *i*-Pr₃SiOTf (2.6 mL, 11.9 mmol) was added dropwise. The reaction mixture was warmed to 0 °C. After 30 min, the reaction mixture was warmed to 22 °C, diluted with hexanes (100 mL), and the layers were separated. The organic layer was washed with saturated NaHCO₃ (50 mL) and brine (40 mL), dried with Na₂SO₄, and concentrated *in vacuo*. Kugelrohr distillation under vacuum (0.3 mm Hg) from 110 – 135 °C yielded alkyne **S-3** as a colorless oil (2.0 g, 68%). The spectral data are consistent with the data reported:⁵ ¹H NMR (400 MHz, CDCl₃) δ 2.08 (t, *J* = 6.2, 2H), 1.53–1.37 (m, 4H), 1.30–1.18 (m, 3H), 1.14–0.96 (m, 18H), 0.90 (t, *J* = 6.9, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 86.7, 32.1, 30.5, 21.9, 17.4, 16.9, 13.7, 11.9; HRMS (APCI) *m/z* calcd for C₁₆H₃₅O₂ (M + H + CH₃OH)⁺ 287.2406, found 287.2401.

II. Syntheses of Alkylidenesilacyclopropanes

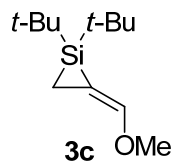


The syntheses of **3b**, **3d**, and **3e** were previously published by our laboratory.²

Alkylidenesilacyclopropane 3d. Previously, we were unable to obtain high resolution mass spectral data for compound **3d** and could only report the low resolution data.² We have since been able to obtain the desired data: HRMS (GCMS) m/z calcd for $\text{C}_{18}\text{H}_{35}\text{Si}$ ($\text{M} + \text{H}$)⁺ 279.2508, found 279.2503.

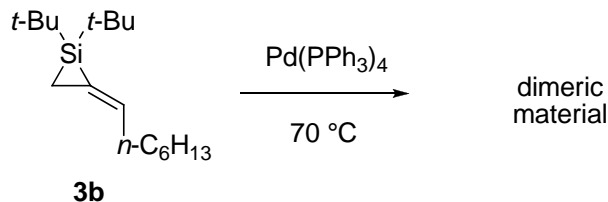


Alkylidenesilacyclopropane 3a. A procedure reported by Woerpel² was adapted to observe alkylidenesilacyclopropane **3a**. A solution of Ag_3PO_4 (0.068 g, 0.16 mmol) in toluene (20 mL) was saturated with allene (**1a**) by bubbling the gas through the solution for 5 min. To the reaction mixture was added a solution of silacyclopropane **2**^{7,8} (0.674 g, 3.00 mmol) in toluene (10 mL). The reaction mixture was saturated a second time with allene (**1a**) for 3 min and then stirred for 4 h at 22 °C. Alkylidenesilacyclopropane **3a** was observed in the reaction mixture (~50%) by ¹H NMR spectroscopic analysis: ¹H NMR (400 MHz, C_6D_6) δ 6.24 (s, 1H), 6.08 (s, 1H), 1.43 (s, 2H), 1.27 (s, 18H). The reaction mixture was filtered through Celite and concentrated *in vacuo* to afford an insoluble white film containing no trace of alkylidenesilacyclopropane **3a** by ¹H NMR spectroscopic analysis.

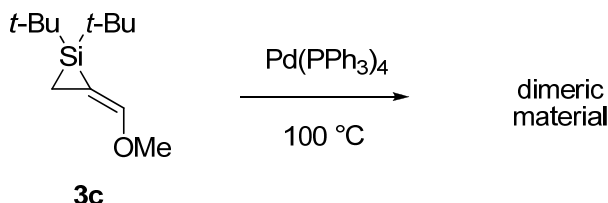


Alkylidenesilacyclopropane 3c. A procedure reported by Woerpel² was used to prepare alkylidenesilacyclopropane **3c**. To a solution of allene **1c** (1.06 g, 15.1 mmol) and silacyclopropane **2**^{7,8} (3.88 g, 17.3 mmol) in toluene (30 mL) was added Ag_3PO_4 (0.60 g, 1.4 mmol). The reaction mixture was stirred at 22 °C for 40 h. The reaction mixture was filtered through Celite and concentrated *in vacuo*. Kugelrohr distillation under vacuum (0.3 mm Hg) at 75 °C yielded alkylidenesilacyclopropane **3c** as a colorless oil (2.0 g, 61%): ¹H NMR (400 MHz, C_6D_6) δ 6.59 (t, $J = 2.5$, 1H), 3.49 (s, 3H), 1.39 (d, $J = 2.4$, 2H), 1.11 (s, 18H); ¹³C NMR (125 MHz, C_6D_6) δ 147.7, 99.1, 57.4, 29.0, 18.4, 4.4; ²⁹Si NMR (99.3 MHz, C_6D_6) δ -52.0; IR (neat) 2962, 1686, 1654, 1471, 1364, 1204 cm^{-1} ; HRMS (GCMS) m/z calcd for $\text{C}_{12}\text{H}_{25}\text{OSi}$ ($\text{M} + \text{H}$)⁺ 213.1675, found 213.1665.

III. Dimerization of Alkylidenesilacyclopropanes

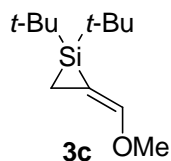


Dimeric 3b. To a solution of silacyclopropane **3b** (0.206 g, 0.773 mmol) in toluene (10 mL) was added Pd(PPh₃)₄ (0.060 g, 0.05 mmol). The reaction mixture was heated to 70 °C. After 24 h, the reaction mixture was cooled to 22 °C, filtered through SiO₂ with hexanes, and concentrated *in vacuo*. The resulting oil was purified by flash chromatography (hexanes) to afford dimeric material as a colorless oil (0.055 g, 13%): ¹H NMR (400 MHz, C₆D₆, distinctive peaks) δ 6.00 (t, *J* = 6.6, 2H), 2.37–2.27 (m, 4H), 1.96 (s, 4H); ¹³C NMR (125 MHz, C₆D₆, distinctive peaks) δ 140.5, 134.7; IR (neat) 2929, 2856, 1470, 1389, 1363 cm⁻¹; HRMS (GCMS) *m/z* calcd for C₃₄H₆₉Si₂ (M + H)⁺ 533.4938, found 533.4929.



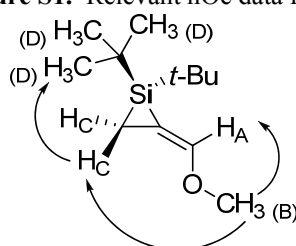
Dimeric 3c. To a solution of silacyclopropane **3c** (0.550 mL, 0.154 mmol, 0.281 M solution of **3c** and 0.0465 M solution of PhSiMe₃ in *tol-d*₈) was added Pd(PPh₃)₄ (0.007 g, 0.006 mmol). The reaction mixture was heated to 100 °C. After 10 min, the reaction mixture was cooled to 22 °C and the reaction mixture was observed to give dimeric material in quantitative yield by ¹H NMR spectroscopic analysis (relative to the PhSiMe₃ internal standard) using a single scan. The reaction mixture was filtered through Davisil with hexanes, and concentrated *in vacuo* to afford dimeric material as a colorless oil: ¹H NMR (500 MHz, C₆D₆) δ 6.15 (t, *J* = 1.5, 1H), 6.13 (t, *J* = 1.5, 1H), 3.261 (s, 3H), 3.257 (s, 3H), 2.15 (d, *J* = 1.2, 2H), 2.06 (d, *J* = 1.2, 2H), 1.26 (s, 9H), 1.20 (s, 18H), 1.15 (s, 9H); ¹³C NMR (125 MHz, C₆D₆) δ 151.3, 150.2, 107.3, 106.7, 58.4, 58.4, 30.6, 29.6, 29.6, 28.2, 21.1, 10.0, 9.5; HRMS (ESI) *m/z* calcd for C₂₄H₅₀O₂Si₂ (M + H)⁺ 425.3271, found 425.3264.

IV. Regiochemistry and Stereochemistry of Products



Alkylidenesilacyclopropane 3c. Analysis of nOe data was consistent with an assignment of (*E*) to the exocyclic alkene (Fig S1). The observed nOe between H^B and H^C suggests a proximal relationship and is consistent with the stereochemical assignment. No nOe was observed from H^A to H^D, which is consistent with observations by Lippmaa et al. that suggest a large difference in relaxation processes between *tert*-butyl and *sp*²-hybridized protons.⁹ These differences can result in significantly different nOe's, depending on the proton irradiated.^{10,11}

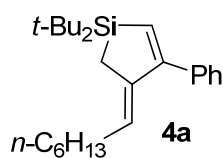
Figure S1. Relevant nOe data for **3c**



(*E*)-3c

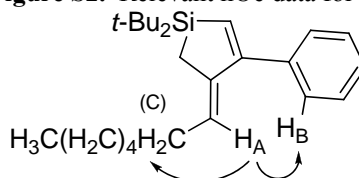
H^B irradiated: H^A (5.5%), H^C (0.9%)

H^C irradiated: H^D (0.4%)



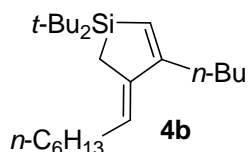
Silacyclopentene 4a. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkene (Fig S2). The observed nOe between H^A and H^B suggests a proximal relationship and supports the stereo- and regiochemical assignments.

Figure S2. Relevant nOe data for **4a**



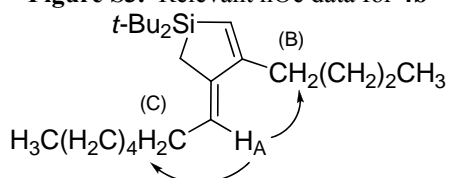
(*Z*)-4a

H^A irradiated: H^B (2.7%), H^C (2.2%)



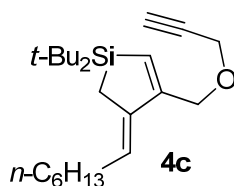
Silacyclopentene 4b. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkene (Fig S3). The observed nOe between H^A and H^B suggests a proximal relationship and supports the stereo- and regiochemical assignments.

Figure S3. Relevant nOe data for **4b**



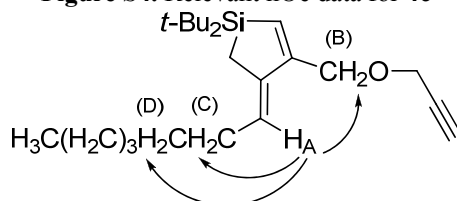
(Z)-4b

H^A irradiated: H^B (6.2%), H^C (2.3%)



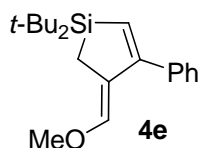
Silacyclopentene 4c. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkene (Fig S4). The observed nOe between H^A and H^B suggests a proximal relationship and supports the stereo- and regiochemical assignments.

Figure S4. Relevant nOe data for **4c**



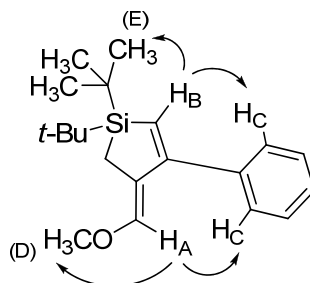
(Z)-4c

H^A irradiated: H^B (6.4%), H^C (2.4%), H^D (1.6%)



Silacyclopentene 4e. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkene (Fig S5). The observed nOe between H^A and H^C suggests a proximal relationship and supports the stereo- and regiochemical assignments. In addition, an observed nOe between H^B and H^E further supports the regiochemical assignment of the endocyclic alkene.

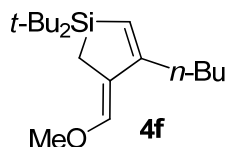
Figure S5. Relevant nOe data for **4e**



(*Z*)-4e

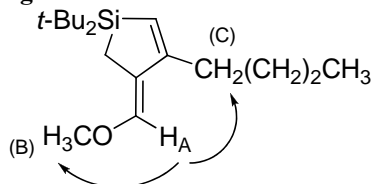
H^A irradiated: H^C (2.2%), H^D (2.4%)

H^B irradiated: H^C (1.0%), H^E (2.0%)



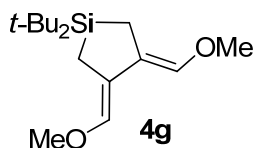
Silacyclopentene 4f. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkene (Fig S6). The observed nOe between H^A and H^C suggests a proximal relationship and supports the stereo- and regiochemical assignments.

Figure S6. Relevant nOe data for **4f**



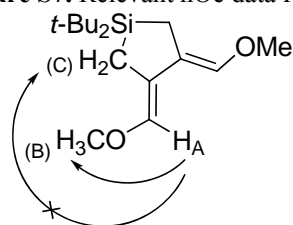
(*Z*)-4f

H^A irradiated: H^B (2.5%), H^C (3.6%)



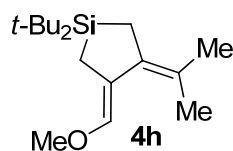
Silacyclopentane 4g. By ^1H NMR spectroscopy, **4g** was observed to have an internal plane of symmetry. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkenes (Fig S7). Due to symmetry, no nOe was observed to the proximal vinyl proton. Both the observed nOe between H^{A} and H^{B} and the absence of an nOe between H^{A} and H^{C} support the stereo- and regiochemical assignments.

Figure S7. Relevant nOe data for **4g**



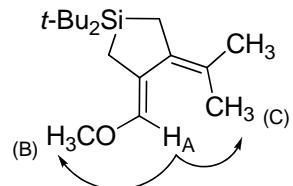
(Z)-4g

H^{A} irradiated: H^{B} (2.1%), H^{C} (0%)



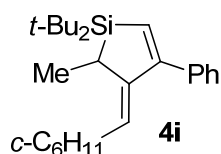
Silacyclopentane 4h. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkene (Fig S8). The observed nOe between H^{A} and H^{C} suggests a proximal relationship and supports both the stereo- and regiochemical assignments.

Figure S8. Relevant nOe data for **4h**



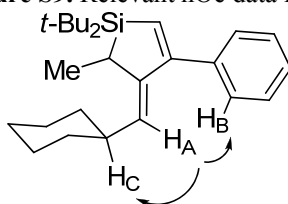
(Z)-4h

H^{A} irradiated: H^{B} (1.8%), H^{C} (1.2%)

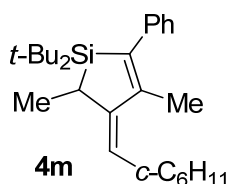


Silacyclopentene 4i. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkene (Fig S9). The observed nOe between H^A and H^B suggests a proximal relationship and supports both the stereo- and regiochemical assignments.

Figure S9. Relevant nOe data for **4i**

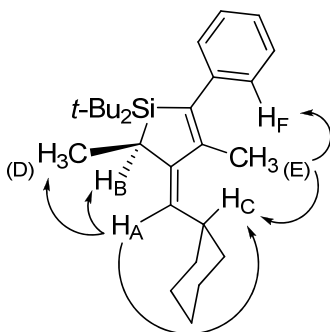


(Z)-4i
H^A irradiated: H^B (3.6%), H^C (2.3%)

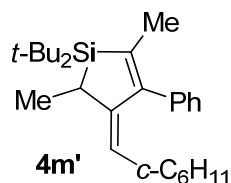


Silacyclopentene 4m. Analysis of nOe data was consistent with the assignment of (*E*) to the exocyclic alkene (Fig S10). The observed nOe between H^A and H^{B/D} suggests a proximal relationship and supports the stereochemical assignment. The observed nOe between H^E and H^C suggests a proximal relationship and supports the regiochemical assignment.

Figure S10. Relevant nOe data for **4m**

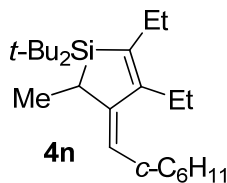
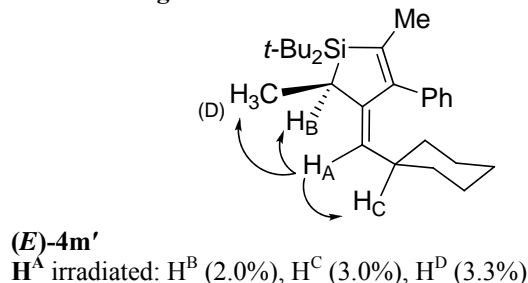


(E)-4m
H^A irradiated: H^B (2.7%), H^C (2.2%), H^D (3.6%)
H^E irradiated: H^C (8.2%), H^F (1.7%)



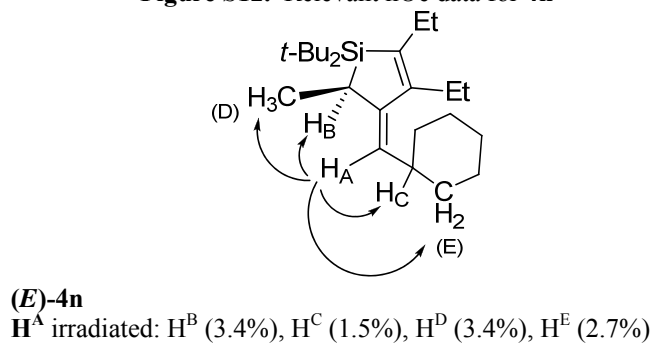
Silacyclopentene 4m'. Analysis of nOe data was consistent with the assignment of (*E*) to the exocyclic alkene (Fig S11). The observed nOe between H^A and H^{B/D} suggests a proximal relationship and supports the stereochemical assignment.

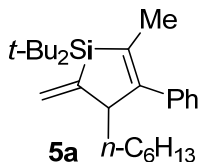
Figure S11. Relevant nOe data for **4m'**



Silacyclopentene 4n. Analysis of nOe data was consistent with the assignment of (*E*) to the exocyclic alkene (Fig S12). The observed nOe between H^A and H^{B/D} suggests a proximal relationship and supports the stereochemical assignment.

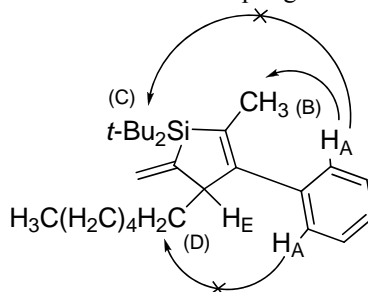
Figure S12. Relevant nOe data for **4n**





Silacyclopentane 5a. Analysis of coupling constant data was consistent with the proximal *t*-Bu₂Si–Me relationship (Fig S13). When H^A was irradiated, no nOe was observed with either H^C or H^D. Coupling constant data for H^B (d, *J* = 2.2) supports the regiochemical assignment. If H^B and H^E were on geminal carbons then no coupling constant would be observed, so the presence of a *J*-value (2.2 Hz) between H^B and H^E suggests a *transoid* homoallylic relationship.¹²

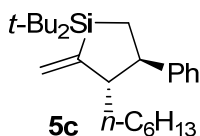
Figure S13. Relevant nOe and coupling constant data for **5a**



5a

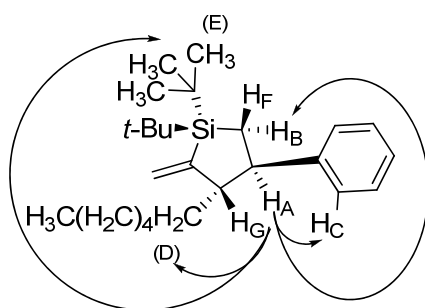
H^A irradiated: H^B (0.8%), H^C (0%), H^D (0%)

H^B: d, *J* = 2.2 Hz (*transoid*^B–*transoid*^E)



Silacyclopentane 5c. Analysis of nOe data was consistent with a *trans* *n*-hexyl–Ph stereochemical relationship (Fig. S14). The observed nOe between H^A and H^{B/D} suggests a proximal relationship and supports the assigned stereochemistry. Coupling constant data for H^A (td, $J = 12.6, 6.4$) and H^G (dtd, $J = 12.5, 4.7, 1.6$) further supports this assignment. The large H^A and H^G J -values (12.6 and 12.5 Hz) suggest *trans* H^A–H^F and H^A–H^G relationships. The smaller H^A J -value (6.4 Hz) suggests a *cis* H^A–H^B relationship. For silacyclopentanes, a *trans* relationship would be characterized by J -values on the order of ~ 5 –10 Hz, while a *cis* relationship would exhibit coupling constants from ~ 1 –4 Hz.¹³⁻¹⁵

Figure S14. Relevant nOe and coupling constant data for **5c**

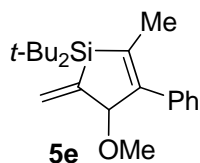


***trans*-5c**

H^A irradiated: H^B (7.9%), H^C (8.8%), H^D (1.4%), H^E (0.9%)

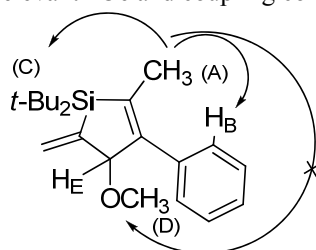
H^A: td, $J = 12.6, 6.4$ Hz (*trans*^A–*trans*^F, *trans*^A–*trans*^G, *cis*^A–*cis*^B)

H^G: dtd, $J = 12.5, 4.7, 1.6$ Hz (*trans*^G–*trans*^A)



Silacyclopentene 5e. Analysis of nOe data was consistent with a proximal *t*-Bu₂Si–Me regiochemical assignment (Fig S15). Both the observed nOe between H^A and H^C and the absence of an nOe between H^A and H^D suggests a proximal *t*-Bu₂Si–Me relationship and supports the regiochemical assignment. Coupling constant data for H^A (d, *J* = 1.9) further supports the regiochemical assignment. If H^A and H^E were on geminal carbons then no coupling constant would be observed, so the presence of a *J*-value (1.9 Hz) between H^A and H^E suggests a *transoid* homoallylic relationship.¹²

Figure S15. Relevant nOe and coupling constant data for **5e**



5e

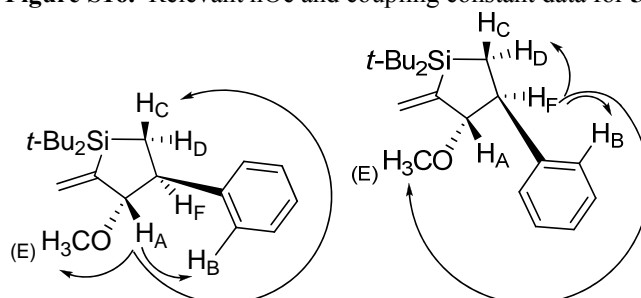
H^A irradiated: H^B (2.6%), H^C (0.3%), H^D (0%)

H^A: d, *J* = 1.9 Hz (*transoid*^A–*transoid*^E)



Silacyclopentane 5g. Analysis of nOe data was consistent with a *trans* Ph–OMe stereochemical relationship (Fig. S16). The observed nOe between H^A and H^{B/C} and between H^F and H^{D/E} suggests a proximal relationship and supports the stereochemical assignment. Coupling constant data for H^A (dt, $J = 11.4, 2.7$) and H^F (ddd, $J = 12.7, 11.5, 7.0$) further supports this assignment. The large H^A J -value (11.4 Hz) suggests a *trans* H^A–H^F relationship, while the large H^F J -values (12.7 and 11.5 Hz) suggest a *trans* H^F–H^{A/C} relationship. The small H^F J -value (7.0 Hz) suggests a *cis* H^F–H^D relationship. For silacyclopentanes, a *trans* H^F–H^{A/C} relationship would be characterized by J -values on the order of ~ 5 –10 Hz, while a *cis* relationship would exhibit coupling constants from ~ 1 –4 Hz.^{13–15}

Figure S16. Relevant nOe and coupling constant data for **5g**



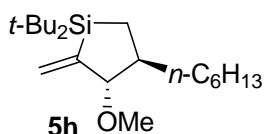
***trans*-5g**

H^A irradiated: H^B (2.1%), H^C (8.7%), H^E (1.2%)

H^F irradiated: H^B (3.8%), H^D (6.3%), H^E (0.3%)

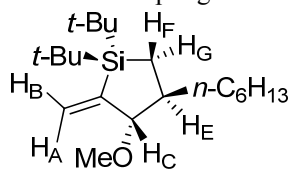
H^A: dt, $J = 11.4, 2.7$ Hz (*trans*^A–*trans*^F)

H^F: ddd, $J = 12.5, 11.5, 7.0$ Hz (*trans*^F–*trans*^A, *trans*^F–*trans*^C, *cis*^F–*cis*^D)



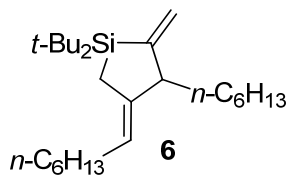
Silacyclopentane 5h. Analysis of coupling constant data was consistent with a *trans* *n*-hexyl–OMe stereochemical relationship (Fig. S17). The large J -values (11.2 Hz) suggest a *trans* H^C–H^E relationship. For silacyclopentanes, a *trans* H^C–H^E relationship would be characterized by J -values on the order of ~ 5 –10 Hz, while a *cis* relationship would exhibit coupling constants from ~ 1 –4 Hz.^{13–15}

Figure S17. Relevant coupling constant data for **5h**



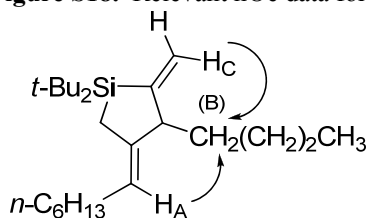
***trans*-5h**

H^C: dt, $J = 11.2, 2.7$ Hz (*trans*^C–*trans*^E, alkyl^C–vinyl^A, alkyl^C–vinyl^B)



Silacyclopentane 6. Analysis of nOe data was consistent with the assignment of (*Z*) to the exocyclic alkene (Fig S18). The observed nOe between H^A and H^B suggests a proximal relationship and supports the stereochemical assignment. The observed nOe between H^C and H^B suggests a proximal relationship and supports the regiochemical assignment.

Figure S18. Relevant nOe data for **6**



(Z)-6

H^A irradiated: H^B (4.3%)

H^C irradiated: H^B (1.6%)

V. X-Ray Crystallographic Data (Silacycloheptadiene 13a)

X-ray Data Collection, Structure Solution and Refinement for Silacycloheptadiene 13a.

A colorless crystal of approximate dimensions 0.13 x 0.30 x 0.38 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2¹ program package was used to determine the unit-cell parameters and for data collection (25 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT² and SADABS³ to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL⁴ program. The diffraction symmetry was $2/m$ and the systematic absences were consistent with the monoclinic space group $P2_1/c$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors⁵ for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model.

At convergence, $wR2 = 0.1105$ and $Goof = 1.025$ for 323 variables refined against 6639 data (0.78\AA), $R1 = 0.0441$ for those 5760 data with $I > 2.0\sigma(I)$.

References.

1. APEX2 Version 2.2-0, Bruker AXS, Inc.; Madison, WI 2007.
2. SAINT Version 7.46a, Bruker AXS, Inc.; Madison, WI 2007.
3. Sheldrick, G. M. SADABS, Version 2008/1, Bruker AXS, Inc.; Madison, WI 2008.
4. Sheldrick, G. M. SHELXTL, Version 2008/3, Bruker AXS, Inc.; Madison, WI 2008.
5. International Tables for X-Ray Crystallography 1992, Vol. C., Dordrecht: Kluwer Academic Publishers.

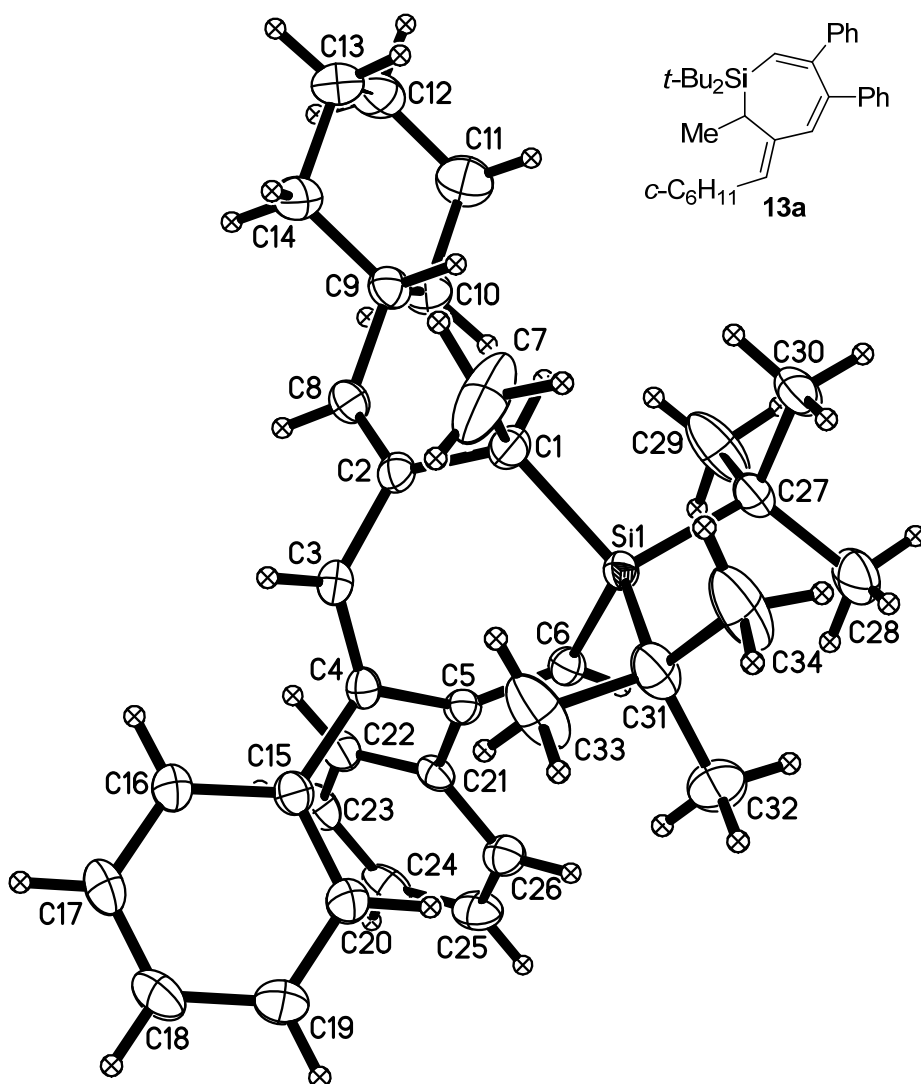
Definitions:

$$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$$

$$R1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$$

$Goof = S = [\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.

Table 1. Crystal data and structure refinement for **13a**.

Identification code	kaw142 (Kay Buchner)	
Empirical formula	C ₃₄ H ₄₆ Si	
Formula weight	482.80	
Temperature	148(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 13.6833(8) Å	α = 90°.
	b = 10.0323(6) Å	β = 99.5161(7)°.

	$c = 22.2163(13) \text{ \AA}$	$\gamma = 90^\circ$.
Volume	$3007.8(3) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.066 Mg/m^3	
Absorption coefficient	0.097 mm^{-1}	
F(000)	1056	
Crystal color	colorless	
Crystal size	$0.38 \times 0.30 \times 0.13 \text{ mm}^3$	
theta range for data collection	$1.51 \text{ to } 27.10^\circ$	
Index ranges	$-17 \leq h \leq 17, -12 \leq k \leq 12, -28 \leq l \leq 28$	
Reflections collected	33135	
Independent reflections	6639 [R(int) = 0.0253]	
Completeness to theta = 27.10°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9875 and 0.9641	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6639 / 0 / 323	
Goodness-of-fit on F^2	1.025	
Final R indices [$I > 2\sigma(I) = 5760$ data]	R1 = 0.0411, wR2 = 0.1049	
R indices (all data, 0.78 \AA)	R1 = 0.0484, wR2 = 0.1105	
Largest diff. peak and hole	0.338 and $-0.266 \text{ e.\AA}^{-3}$	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **13a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	2686(1)	5609(1)	2465(1)	19(1)
C(1)	2037(1)	6720(1)	2973(1)	29(1)
C(2)	1769(1)	8082(1)	2698(1)	22(1)
C(3)	1152(1)	8097(1)	2080(1)	23(1)
C(4)	1468(1)	7890(1)	1548(1)	20(1)
C(5)	2525(1)	7598(1)	1506(1)	20(1)
C(6)	3067(1)	6677(1)	1850(1)	21(1)
C(7)	1156(2)	6121(2)	3224(1)	76(1)
C(8)	1996(1)	9229(1)	2988(1)	26(1)
C(9)	2540(1)	9446(1)	3627(1)	27(1)
C(10)	3552(1)	10088(2)	3633(1)	34(1)
C(11)	4093(1)	10317(2)	4285(1)	43(1)
C(12)	3471(1)	11146(2)	4653(1)	46(1)
C(13)	2465(1)	10517(2)	4648(1)	45(1)
C(14)	1925(1)	10302(2)	3996(1)	40(1)
C(15)	763(1)	7935(1)	961(1)	23(1)
C(16)	0(1)	8868(2)	864(1)	32(1)

C(17)	-671(1)	8885(2)	324(1)	41(1)
C(18)	-587(1)	7978(2)	-128(1)	42(1)
C(19)	170(1)	7051(2)	-46(1)	38(1)
C(20)	845(1)	7035(1)	494(1)	29(1)
C(21)	2944(1)	8416(1)	1047(1)	21(1)
C(22)	2765(1)	9784(1)	1010(1)	25(1)
C(23)	3161(1)	10563(1)	593(1)	30(1)
C(24)	3722(1)	9982(2)	201(1)	32(1)
C(25)	3894(1)	8623(2)	228(1)	32(1)
C(26)	3513(1)	7842(1)	652(1)	27(1)
C(27)	3891(1)	5080(1)	2977(1)	28(1)
C(28)	4501(1)	4091(2)	2667(1)	54(1)
C(29)	4512(1)	6337(2)	3152(1)	56(1)
C(30)	3695(1)	4433(2)	3571(1)	36(1)
C(31)	1932(1)	4138(1)	2073(1)	36(1)
C(32)	2435(2)	3631(2)	1549(1)	61(1)
C(33)	876(1)	4555(2)	1790(1)	51(1)
C(34)	1837(2)	2976(2)	2514(1)	59(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for **13a**.

Si(1)-C(6)	1.8758(12)	C(19)-C(20)	1.3876(19)
Si(1)-C(1)	1.9080(13)	C(21)-C(26)	1.3922(17)
Si(1)-C(27)	1.9164(13)	C(21)-C(22)	1.3935(18)
Si(1)-C(31)	1.9241(14)	C(22)-C(23)	1.3873(18)
C(1)-C(2)	1.5169(17)	C(23)-C(24)	1.381(2)
C(1)-C(7)	1.532(2)	C(24)-C(25)	1.383(2)
C(2)-C(8)	1.3299(18)	C(25)-C(26)	1.3895(19)
C(2)-C(3)	1.4884(17)	C(27)-C(28)	1.532(2)
C(3)-C(4)	1.3390(17)	C(27)-C(29)	1.534(2)
C(4)-C(15)	1.4895(16)	C(27)-C(30)	1.5344(19)
C(4)-C(5)	1.4941(16)	C(31)-C(32)	1.534(3)
C(5)-C(6)	1.3416(17)	C(31)-C(33)	1.537(2)
C(5)-C(21)	1.4947(16)	C(31)-C(34)	1.541(2)
C(8)-C(9)	1.5055(18)		
C(9)-C(10)	1.5257(19)	C(6)-Si(1)-C(1)	108.05(6)
C(9)-C(14)	1.5309(19)	C(6)-Si(1)-C(27)	106.00(6)
C(10)-C(11)	1.531(2)	C(1)-Si(1)-C(27)	104.43(6)
C(11)-C(12)	1.523(2)	C(6)-Si(1)-C(31)	107.57(6)
C(12)-C(13)	1.512(3)	C(1)-Si(1)-C(31)	116.62(7)
C(13)-C(14)	1.529(2)	C(27)-Si(1)-C(31)	113.59(6)
C(15)-C(16)	1.3923(18)	C(2)-C(1)-C(7)	110.30(12)
C(15)-C(20)	1.3938(18)	C(2)-C(1)-Si(1)	113.16(8)
C(16)-C(17)	1.385(2)	C(7)-C(1)-Si(1)	117.22(11)
C(17)-C(18)	1.375(2)	C(8)-C(2)-C(3)	119.33(11)
C(18)-C(19)	1.382(2)	C(8)-C(2)-C(1)	124.23(11)

C(3)-C(2)-C(1)	116.30(11)	C(17)-C(18)-C(19)	120.01(13)
C(4)-C(3)-C(2)	126.62(11)	C(18)-C(19)-C(20)	119.96(14)
C(3)-C(4)-C(15)	120.79(11)	C(19)-C(20)-C(15)	120.82(13)
C(3)-C(4)-C(5)	122.88(11)	C(26)-C(21)-C(22)	118.69(12)
C(15)-C(4)-C(5)	116.33(10)	C(26)-C(21)-C(5)	121.39(11)
C(6)-C(5)-C(4)	123.27(11)	C(22)-C(21)-C(5)	119.92(11)
C(6)-C(5)-C(21)	121.92(11)	C(23)-C(22)-C(21)	120.72(12)
C(4)-C(5)-C(21)	114.80(10)	C(24)-C(23)-C(22)	120.08(13)
C(5)-C(6)-Si(1)	127.91(9)	C(23)-C(24)-C(25)	119.81(12)
C(2)-C(8)-C(9)	128.41(12)	C(24)-C(25)-C(26)	120.32(13)
C(8)-C(9)-C(10)	112.04(11)	C(25)-C(26)-C(21)	120.37(13)
C(8)-C(9)-C(14)	110.83(11)	C(28)-C(27)-C(29)	109.08(15)
C(10)-C(9)-C(14)	109.70(12)	C(28)-C(27)-C(30)	107.38(12)
C(9)-C(10)-C(11)	111.55(12)	C(29)-C(27)-C(30)	107.31(12)
C(12)-C(11)-C(10)	111.37(14)	C(28)-C(27)-Si(1)	113.04(10)
C(13)-C(12)-C(11)	110.93(13)	C(29)-C(27)-Si(1)	108.00(10)
C(12)-C(13)-C(14)	111.32(14)	C(30)-C(27)-Si(1)	111.87(10)
C(13)-C(14)-C(9)	111.32(13)	C(32)-C(31)-C(33)	106.75(14)
C(16)-C(15)-C(20)	118.08(12)	C(32)-C(31)-C(34)	109.05(15)
C(16)-C(15)-C(4)	121.06(12)	C(33)-C(31)-C(34)	107.08(14)
C(20)-C(15)-C(4)	120.86(11)	C(32)-C(31)-Si(1)	108.84(12)
C(17)-C(16)-C(15)	121.04(13)	C(33)-C(31)-Si(1)	112.03(10)
C(18)-C(17)-C(16)	120.07(14)	C(34)-C(31)-Si(1)	112.88(11)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **13a**. The anisotropic displacement factor exponent takes the form: $-\frac{1}{2}\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	22(1)	16(1)	20(1)	1(1)	2(1)	1(1)
C(1)	42(1)	24(1)	25(1)	5(1)	14(1)	8(1)
C(2)	23(1)	24(1)	22(1)	3(1)	9(1)	4(1)
C(3)	21(1)	20(1)	27(1)	2(1)	5(1)	3(1)
C(4)	19(1)	16(1)	24(1)	1(1)	2(1)	1(1)
C(5)	19(1)	21(1)	18(1)	-2(1)	3(1)	0(1)
C(6)	19(1)	24(1)	21(1)	0(1)	4(1)	2(1)
C(7)	101(2)	37(1)	113(2)	29(1)	88(2)	22(1)
C(8)	30(1)	23(1)	25(1)	6(1)	4(1)	2(1)
C(9)	33(1)	21(1)	25(1)	3(1)	3(1)	0(1)
C(10)	34(1)	35(1)	32(1)	-2(1)	6(1)	-4(1)
C(11)	40(1)	47(1)	40(1)	-5(1)	0(1)	-9(1)
C(12)	68(1)	33(1)	32(1)	-7(1)	-4(1)	-1(1)
C(13)	56(1)	53(1)	27(1)	-4(1)	7(1)	14(1)
C(14)	39(1)	52(1)	28(1)	-1(1)	7(1)	7(1)
C(15)	19(1)	24(1)	26(1)	1(1)	3(1)	0(1)

C(16)	27(1)	34(1)	31(1)	-3(1)	0(1)	8(1)
C(17)	30(1)	48(1)	41(1)	0(1)	-7(1)	14(1)
C(18)	33(1)	51(1)	34(1)	-2(1)	-12(1)	2(1)
C(19)	39(1)	41(1)	31(1)	-10(1)	-4(1)	0(1)
C(20)	28(1)	30(1)	29(1)	-4(1)	1(1)	4(1)
C(21)	17(1)	27(1)	18(1)	2(1)	0(1)	0(1)
C(22)	23(1)	28(1)	25(1)	4(1)	3(1)	2(1)
C(23)	28(1)	29(1)	31(1)	9(1)	-1(1)	-2(1)
C(24)	28(1)	44(1)	22(1)	11(1)	2(1)	-8(1)
C(25)	29(1)	46(1)	24(1)	-2(1)	9(1)	-4(1)
C(26)	25(1)	30(1)	26(1)	-1(1)	5(1)	0(1)
C(27)	28(1)	32(1)	24(1)	5(1)	-1(1)	5(1)
C(28)	42(1)	80(1)	39(1)	10(1)	5(1)	35(1)
C(29)	42(1)	57(1)	57(1)	26(1)	-24(1)	-20(1)
C(30)	47(1)	32(1)	27(1)	9(1)	-2(1)	5(1)
C(31)	44(1)	20(1)	39(1)	2(1)	-12(1)	-5(1)
C(32)	90(2)	39(1)	44(1)	-19(1)	-16(1)	14(1)
C(33)	47(1)	35(1)	60(1)	16(1)	-23(1)	-17(1)
C(34)	63(1)	28(1)	73(1)	21(1)	-29(1)	-18(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **13a**.

	x	y	z	U(eq)
H(1A)	2548	6898	3342	35
H(3A)	465	8271	2061	27
H(6A)	3723	6551	1773	26
H(7A)	985	6696	3548	113
H(7B)	1333	5232	3390	113
H(7C)	586	6051	2894	113
H(8A)	1787	10013	2763	31
H(9A)	2646	8557	3831	32
H(10A)	3465	10953	3415	41
H(10B)	3959	9506	3413	41
H(11A)	4246	9446	4488	52
H(11B)	4728	10781	4271	52
H(12A)	3819	11221	5080	55
H(12B)	3385	12055	4479	55
H(13A)	2061	11100	4869	54
H(13B)	2548	9649	4863	54
H(14A)	1789	11176	3793	47
H(14B)	1282	9859	4007	47
H(16A)	-60	9503	1173	38
H(17A)	-1191	9524	267	50

H(18A)	-1050	7988	-498	50
H(19A)	229	6425	-359	46
H(20A)	1370	6403	546	35
H(22A)	2368	10187	1272	30
H(23A)	3047	11497	578	36
H(24A)	3988	10514	-86	38
H(25A)	4275	8222	-44	39
H(26A)	3642	6912	671	32
H(28A)	5137	3930	2931	81
H(28B)	4617	4460	2276	81
H(28C)	4137	3249	2594	81
H(29A)	5112	6098	3437	83
H(29B)	4123	6978	3347	83
H(29C)	4698	6736	2785	83
H(30A)	4327	4219	3829	54
H(30B)	3310	3614	3476	54
H(30C)	3322	5053	3788	54
H(32A)	2061	2873	1351	91
H(32B)	3113	3349	1711	91
H(32C)	2452	4347	1251	91
H(33B)	533	3797	1570	77
H(33C)	906	5294	1505	77
H(33D)	514	4839	2113	77
H(34D)	1396	2294	2302	89
H(34A)	1562	3308	2865	89
H(34B)	2492	2588	2654	89

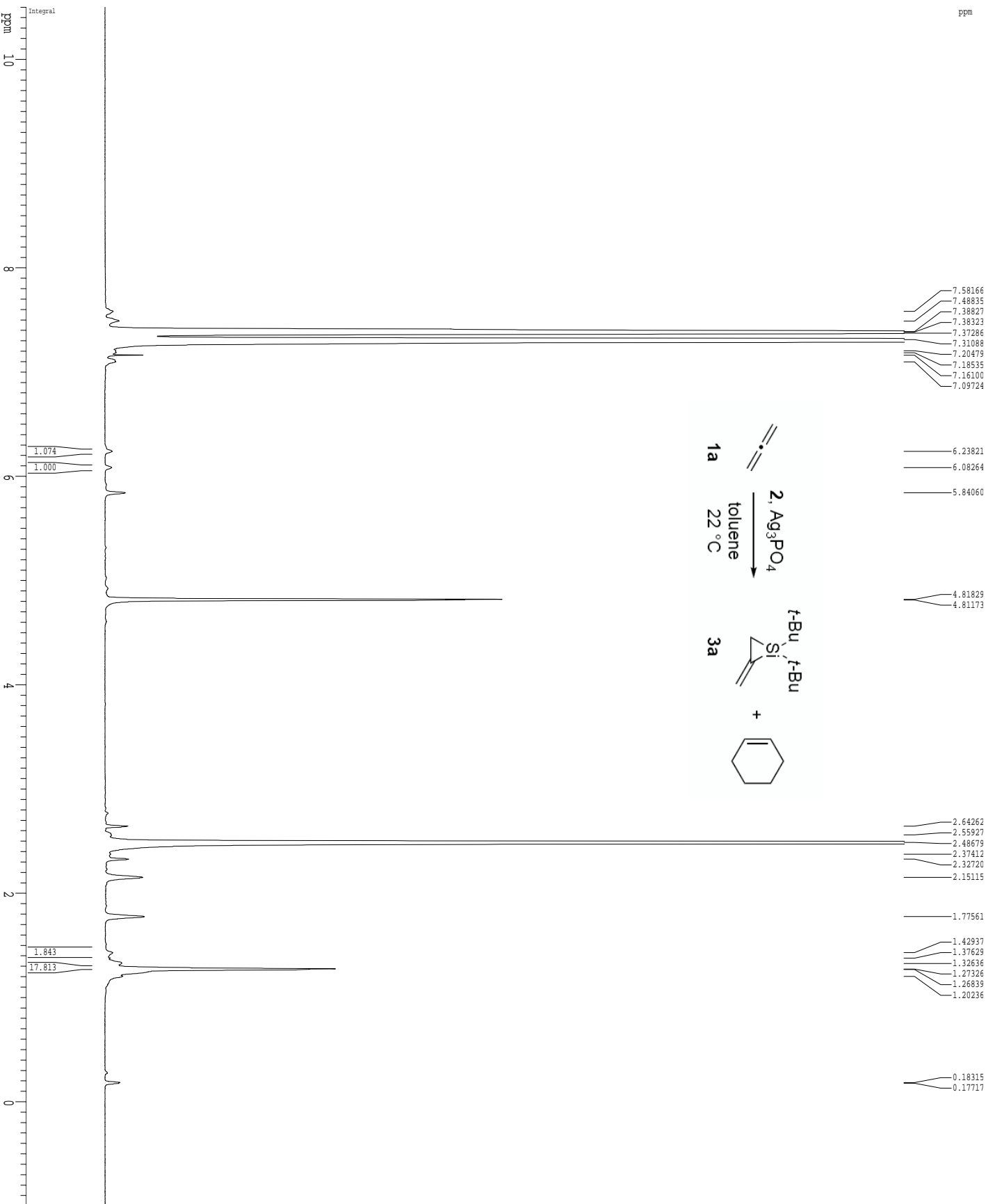
Table 6. Torsion angles [°] for **13a**.

C(6)-Si(1)-C(1)-C(2)	13.03(12)
C(27)-Si(1)-C(1)-C(2)	125.56(10)
C(31)-Si(1)-C(1)-C(2)	-108.19(11)
C(6)-Si(1)-C(1)-C(7)	143.15(14)
C(27)-Si(1)-C(1)-C(7)	-104.32(15)
C(31)-Si(1)-C(1)-C(7)	21.93(16)
C(7)-C(1)-C(2)-C(8)	97.63(18)
Si(1)-C(1)-C(2)-C(8)	-128.84(12)
C(7)-C(1)-C(2)-C(3)	-78.02(17)
Si(1)-C(1)-C(2)-C(3)	55.51(14)
C(8)-C(2)-C(3)-C(4)	105.41(15)
C(1)-C(2)-C(3)-C(4)	-78.72(16)
C(2)-C(3)-C(4)-C(15)	179.98(11)
C(2)-C(3)-C(4)-C(5)	0.3(2)
C(3)-C(4)-C(5)-C(6)	48.48(18)
C(15)-C(4)-C(5)-C(6)	-131.18(13)
C(3)-C(4)-C(5)-C(21)	-131.41(12)
C(15)-C(4)-C(5)-C(21)	48.93(14)
C(4)-C(5)-C(6)-Si(1)	-2.40(18)
C(21)-C(5)-C(6)-Si(1)	177.49(9)
C(1)-Si(1)-C(6)-C(5)	-45.84(13)
C(27)-Si(1)-C(6)-C(5)	-157.31(12)
C(31)-Si(1)-C(6)-C(5)	80.85(13)
C(3)-C(2)-C(8)-C(9)	175.16(12)
C(1)-C(2)-C(8)-C(9)	-0.4(2)
C(2)-C(8)-C(9)-C(10)	112.24(15)
C(2)-C(8)-C(9)-C(14)	-124.87(15)
C(8)-C(9)-C(10)-C(11)	179.42(12)
C(14)-C(9)-C(10)-C(11)	55.89(16)
C(9)-C(10)-C(11)-C(12)	-55.80(18)
C(10)-C(11)-C(12)-C(13)	55.08(18)
C(11)-C(12)-C(13)-C(14)	-55.66(19)
C(12)-C(13)-C(14)-C(9)	56.92(19)
C(8)-C(9)-C(14)-C(13)	179.39(13)
C(10)-C(9)-C(14)-C(13)	-56.37(17)
C(3)-C(4)-C(15)-C(16)	38.67(18)
C(5)-C(4)-C(15)-C(16)	-141.67(13)
C(3)-C(4)-C(15)-C(20)	-140.87(13)
C(5)-C(4)-C(15)-C(20)	38.80(17)
C(20)-C(15)-C(16)-C(17)	1.4(2)
C(4)-C(15)-C(16)-C(17)	-178.17(13)
C(15)-C(16)-C(17)-C(18)	-0.5(2)
C(16)-C(17)-C(18)-C(19)	-0.3(3)
C(17)-C(18)-C(19)-C(20)	0.1(3)

C(18)-C(19)-C(20)-C(15)	0.8(2)
C(16)-C(15)-C(20)-C(19)	-1.5(2)
C(4)-C(15)-C(20)-C(19)	178.02(13)
C(6)-C(5)-C(21)-C(26)	44.71(17)
C(4)-C(5)-C(21)-C(26)	-135.39(12)
C(6)-C(5)-C(21)-C(22)	-135.30(13)
C(4)-C(5)-C(21)-C(22)	44.59(15)
C(26)-C(21)-C(22)-C(23)	-1.08(18)
C(5)-C(21)-C(22)-C(23)	178.94(11)
C(21)-C(22)-C(23)-C(24)	1.4(2)
C(22)-C(23)-C(24)-C(25)	-0.5(2)
C(23)-C(24)-C(25)-C(26)	-0.6(2)
C(24)-C(25)-C(26)-C(21)	0.9(2)
C(22)-C(21)-C(26)-C(25)	-0.03(18)
C(5)-C(21)-C(26)-C(25)	179.95(11)
C(6)-Si(1)-C(27)-C(28)	-70.01(13)
C(1)-Si(1)-C(27)-C(28)	176.00(12)
C(31)-Si(1)-C(27)-C(28)	47.89(14)
C(6)-Si(1)-C(27)-C(29)	50.76(12)
C(1)-Si(1)-C(27)-C(29)	-63.23(12)
C(31)-Si(1)-C(27)-C(29)	168.66(12)
C(6)-Si(1)-C(27)-C(30)	168.64(10)
C(1)-Si(1)-C(27)-C(30)	54.64(11)
C(31)-Si(1)-C(27)-C(30)	-73.47(12)
C(6)-Si(1)-C(31)-C(32)	41.68(12)
C(1)-Si(1)-C(31)-C(32)	163.17(10)
C(27)-Si(1)-C(31)-C(32)	-75.30(12)
C(6)-Si(1)-C(31)-C(33)	-76.13(13)
C(1)-Si(1)-C(31)-C(33)	45.35(14)
C(27)-Si(1)-C(31)-C(33)	166.89(12)
C(6)-Si(1)-C(31)-C(34)	162.90(13)
C(1)-Si(1)-C(31)-C(34)	-75.62(14)
C(27)-Si(1)-C(31)-C(34)	45.92(15)

VI. Reference and Notes

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1H spectrum in CDCl₃

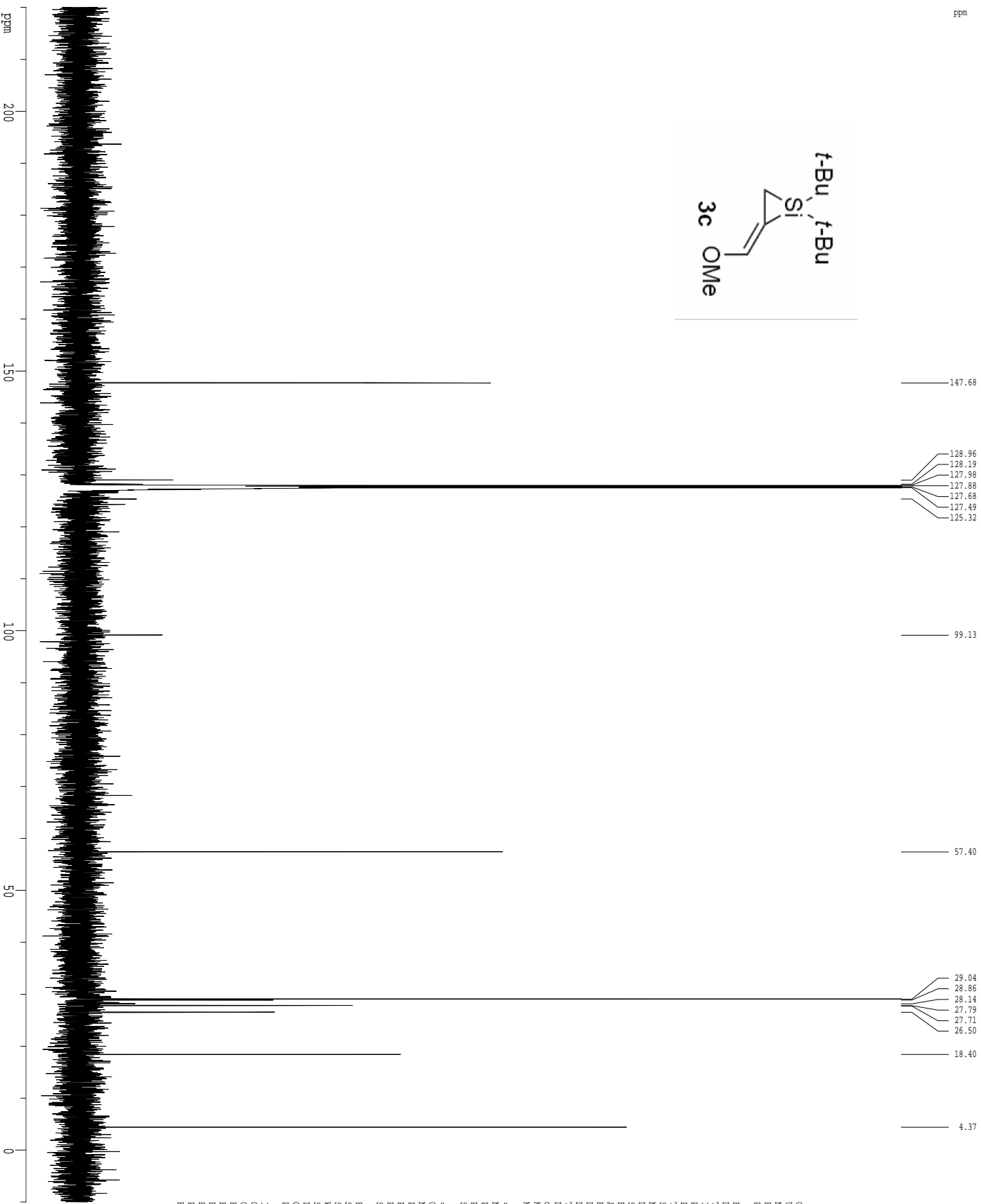
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 PROCNO 1

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 PULPROG zgpg30
 TD 65536
 SFO1 400.126009 MHz
 CDCL3
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 DS 2
 SWH 6410.256 Hz
 FIDRES 0.097913 Hz
 AQ 5.118579 sec
 RG 32
 DW 78.000 usec
 DE 4.50 usec
 TE 298.1 K
 D1 0.1000000 sec
 DELT 0.0000000 sec
 ACQRES 0.0000000 sec
 KCMAX 0.01500000 sec

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 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.126009 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300615 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

JD NMR plot parameters
 CX 22.80 cm
 CY 75.00 cm
 FIP 10.500 ppm
 F1 4201.37 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.50439 ppm/cm
 HZCM 201.81999 Hz/cm

^{13}C spectrum with ^1H decoupling in CDCl_3 

```

Current Data Parameters
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NAME          RB-I-45
EXPNO        11
PROCNO       1

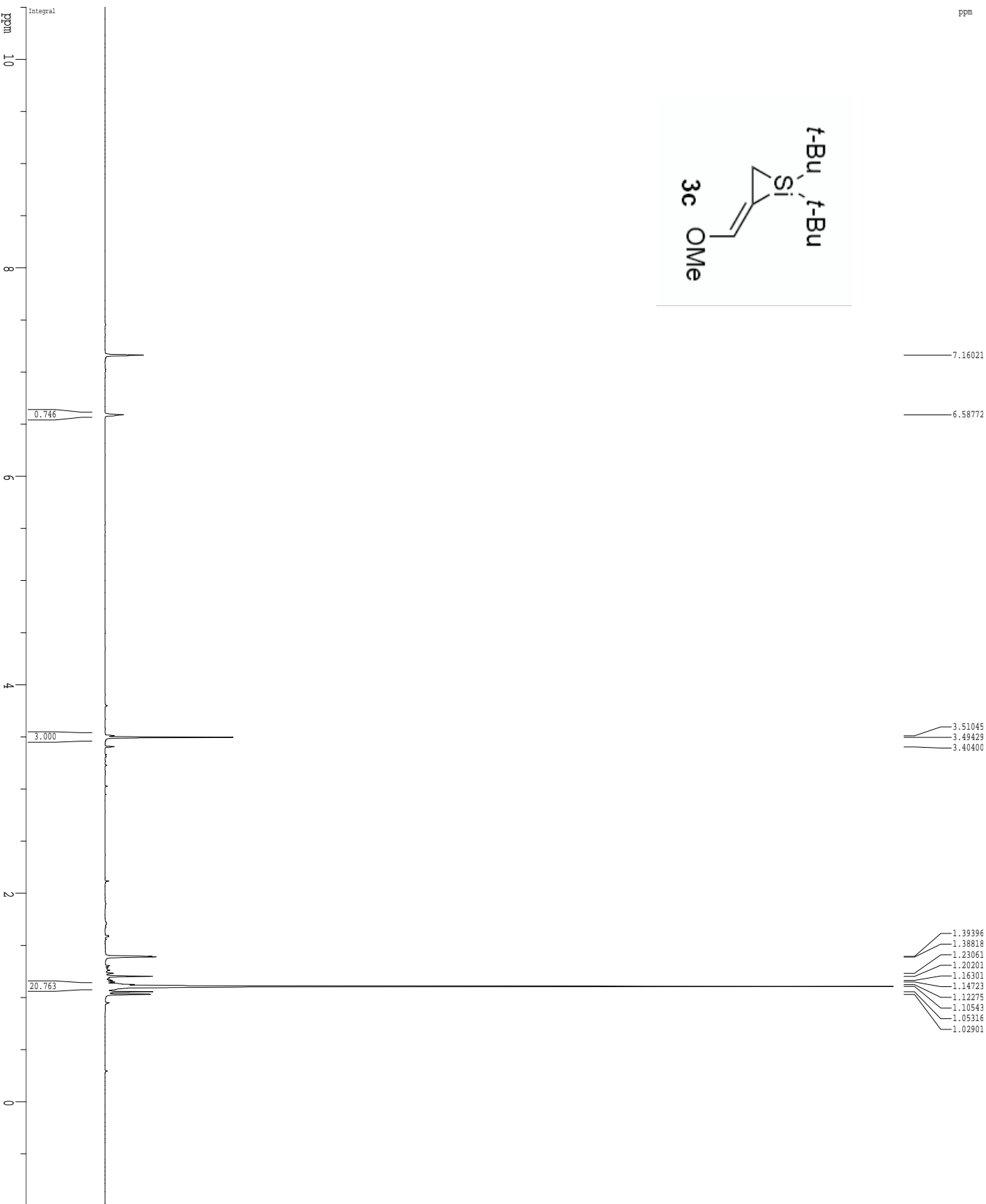
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Time          9.38
INSTRUM      sm500
PROBHD       5 mm broadband
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS            88
DS            4
SWH           30303.011 Hz
FIDRES       0.423388 Hz
AQ           1.083248 sec
RG            5792.6
DW           16.500 usec
DE           4.50 usec
TE           298.0 K
D1           0.25000000 sec
d11          0.03000000 sec
NUC1         13C
NUC2         13C
MCKEY        0.01500000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            7.08 usec
PL1           0.00 dB
SFO1         125.6949209 MHz

===== CHANNEL f2 =====
NUC2          13C
P2            80.00 usec
PL2           -3.00 dB
SFO2         499.8274991 MHz

F2 - Processing parameters
=====
SI            65536
SF           125.6810960 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.50

JD NMR plot parameters
=====
CX            62.80 cm
CY            1.00 cm
PL1           220.00 ppm
PL2           2766.84 ppm
F2P           -10.000 ppm
F2            -126.81 Hz
PCKM         10.08772 ppm/cm
HZCM         1267.83569 Hz/cm
  
```

¹H spectrum in CDCl₃

Current Data Parameters
 USER huchne
 NAME RB-1-45
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070821
 Time 16:15

INSTRUM dx400
 PROBRD 5 mm QNP H/P
 PULPROG zgpg30
 TD 65536
 DO 256
 CQ 8
 NS 2
 DS 2

SWH 6410.256 Hz
 FIDRES 0.0977813 Hz
 AQ 5.1118579 sec
 RG 143.7

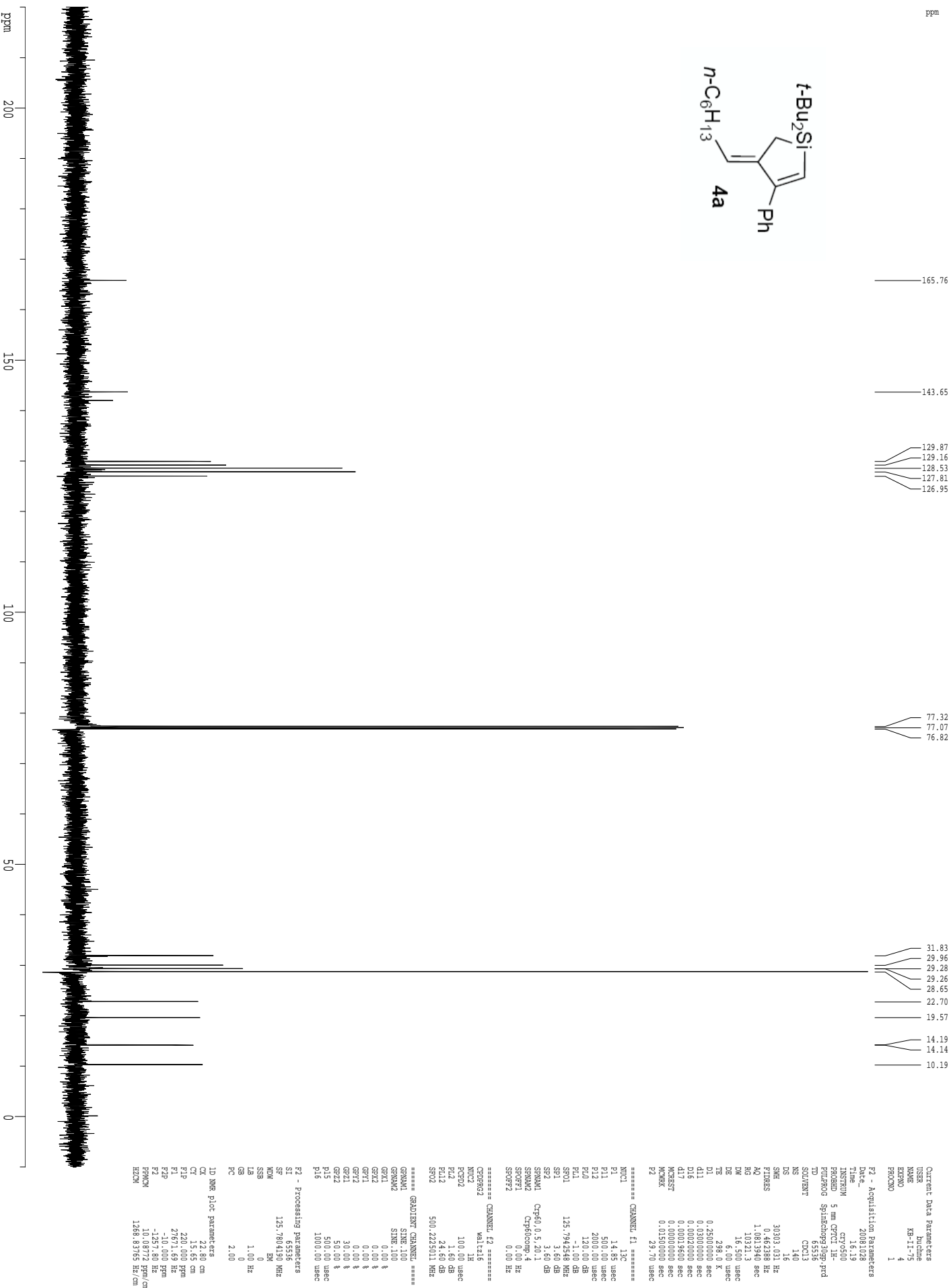
DW 78.000 usec
 DE 4.50 usec
 TE 298.1 K

DI 0.1000000 sec
 SFO1 400.1228009 MHz

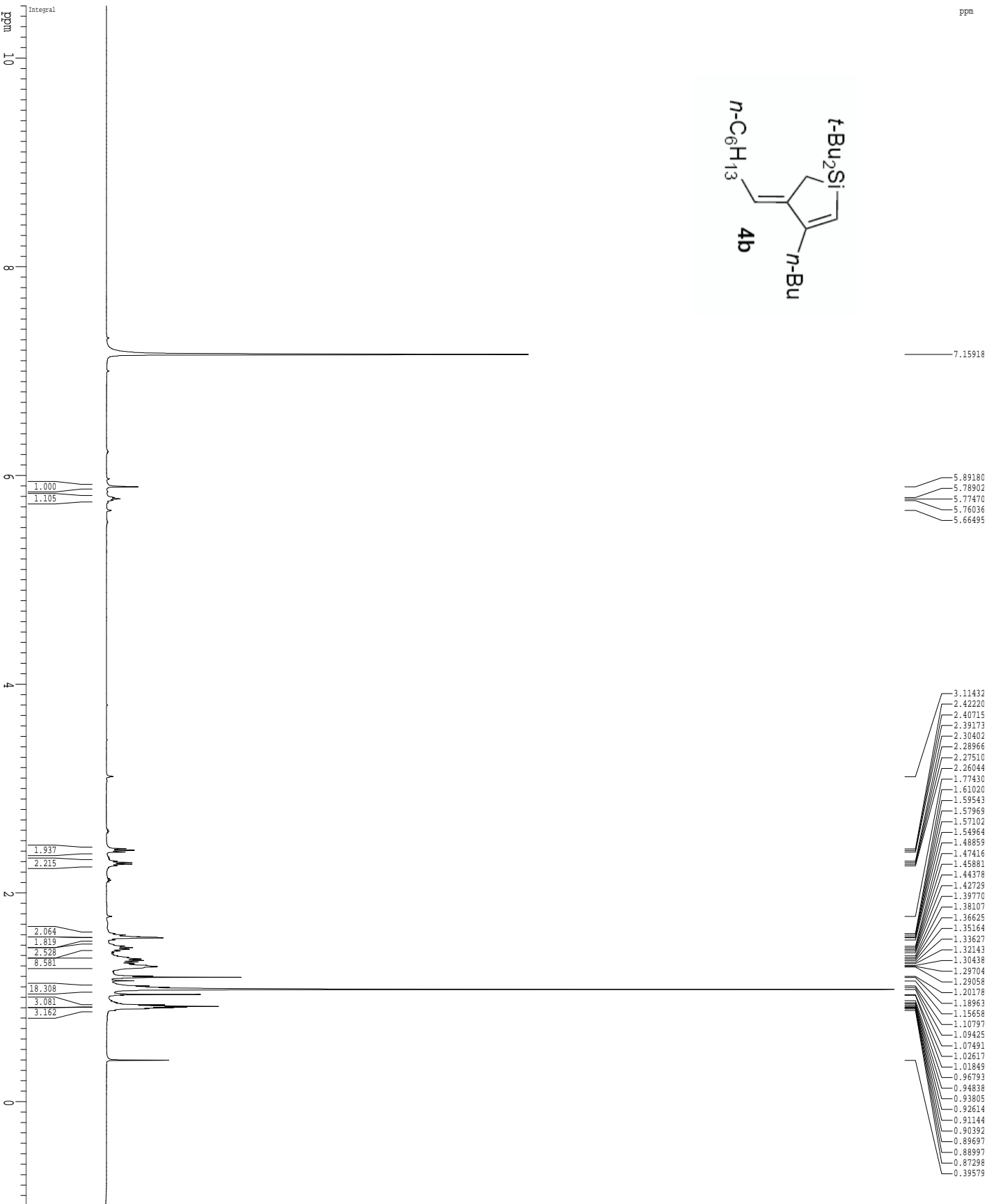
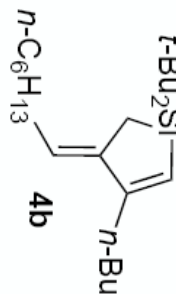
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 PL 0.00 dB
 SFO1 400.1228009 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1229966 MHz
 WDW EM
 SSB 0
 GB 0
 LB 0.30 Hz
 GB 0
 PC 0.50

JD NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 4201.37 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.50449 ppm/cm
 HZCM 201.81996 Hz/cm

Z-restored spin-echo ^{13}C spectrum with ^1H decoupling in CDCl_3 

¹H spectrum in CDCl₃



```

Current Data Parameters
USER             buchne
NAME             KB-II-37
EXPNO            2
PROCNO           1

F2 - Acquisition Parameters
Date_            20090624
Time             17.04
INSTRUM          cryo500
PROBHD           5 mm CPXI 1H-
PULPROG          zgpg30
TD               65536
AQ               8.128
RG               655
WDW               EM
SSB               0
GB               0
PC               1.00

F2 - Processing parameters
SI               65536
SF               500.220000 MHz
WDW              EM
SSB              0
GB               0
PC               1.00

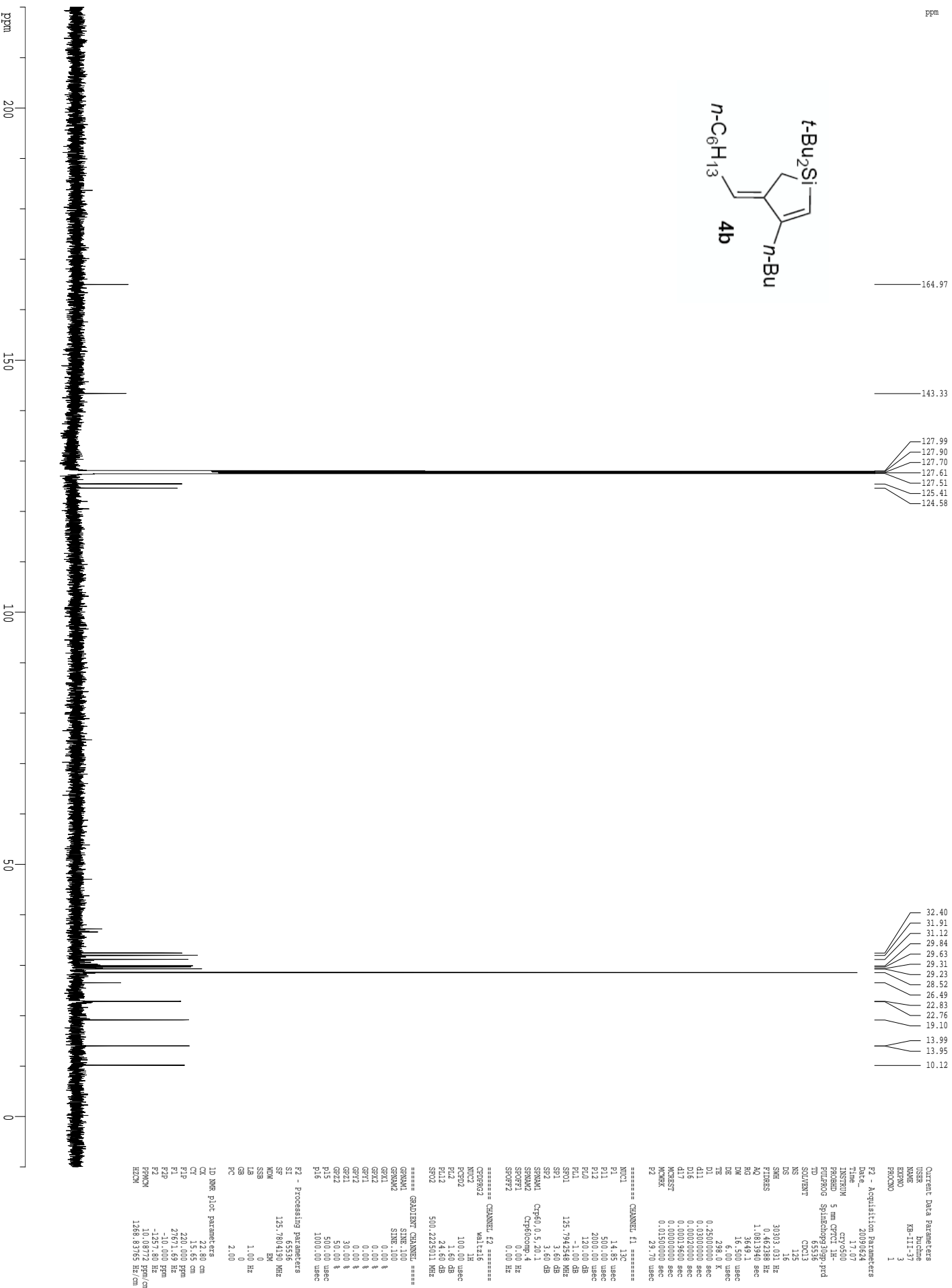
JD NMR plot parameters
CY               22.80 cm
CX               15.00 cm
F1P              10.500 ppm
F1                5252.31 Hz
F2P              -1.000 ppm
F2                -500.22 Hz
PNUCM            0.50459 ppm/cm
HZCM             252.30396 Hz/cm

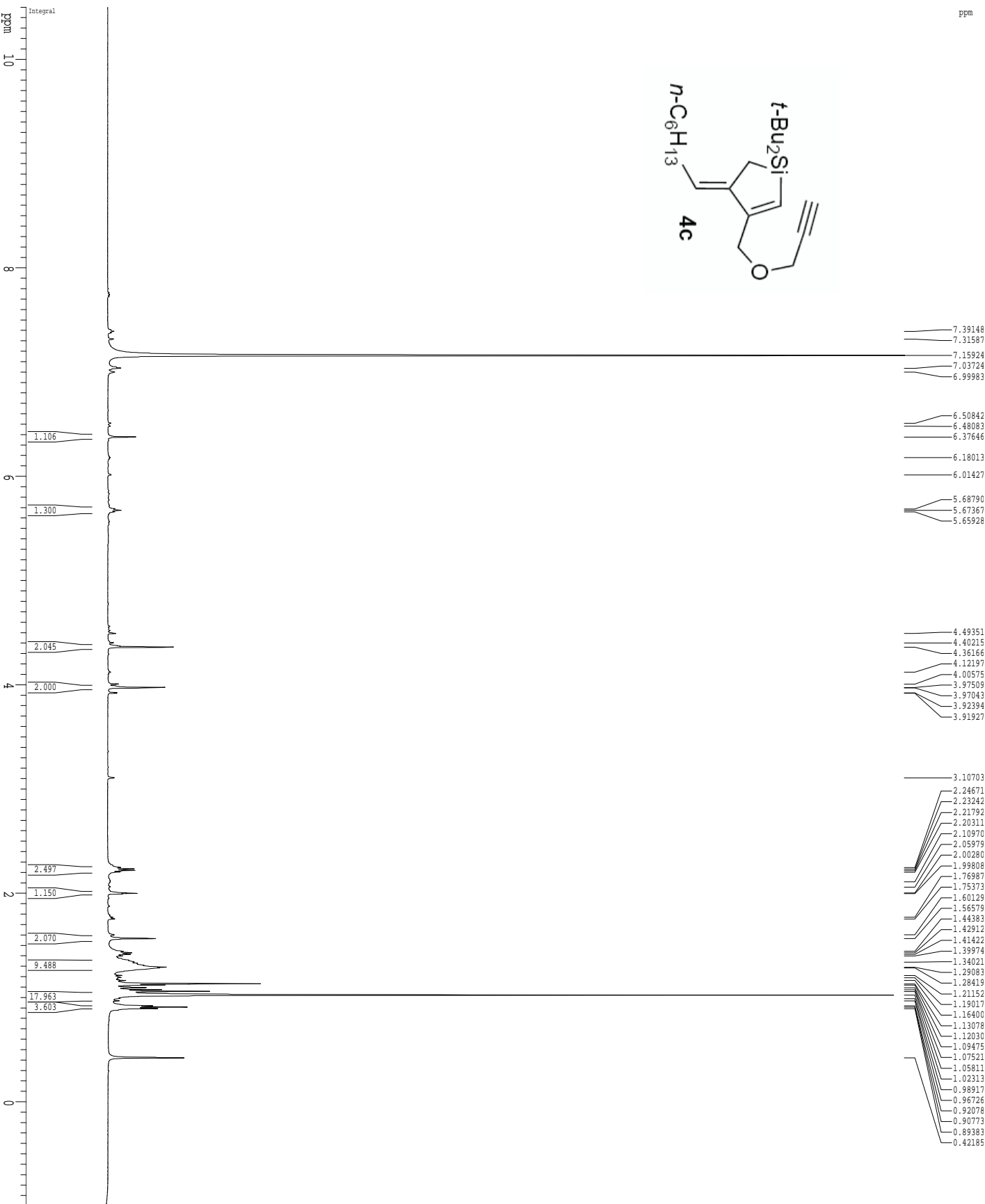
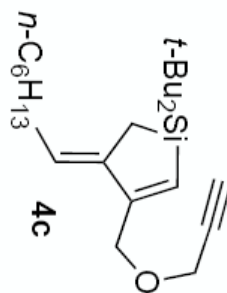
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NUC1              1H
P1                7.50 usec
PL1              1.60 dB
SFO1             500.2235015 MHz

F2 - Acquisition Parameters
Date_            20090624
Time             17.04
INSTRUM          cryo500
PROBHD           5 mm CPXI 1H-
PULPROG          zgpg30
TD               65536
AQ               8.128
RG               655
WDW              EM
SSB              0
GB               0
PC               1.00

F2 - Processing parameters
SI               65536
SF               500.220000 MHz
WDW              EM
SSB              0
GB               0
PC               1.00

JD NMR plot parameters
CY               22.80 cm
CX               15.00 cm
F1P              10.500 ppm
F1                5252.31 Hz
F2P              -1.000 ppm
F2                -500.22 Hz
PNUCM            0.50459 ppm/cm
HZCM             252.30396 Hz/cm
    
```

Z-restored spin-echo ^{13}C spectrum with ^1H decoupling in C_6D_6 

1H spectrum in CDCl₃

```

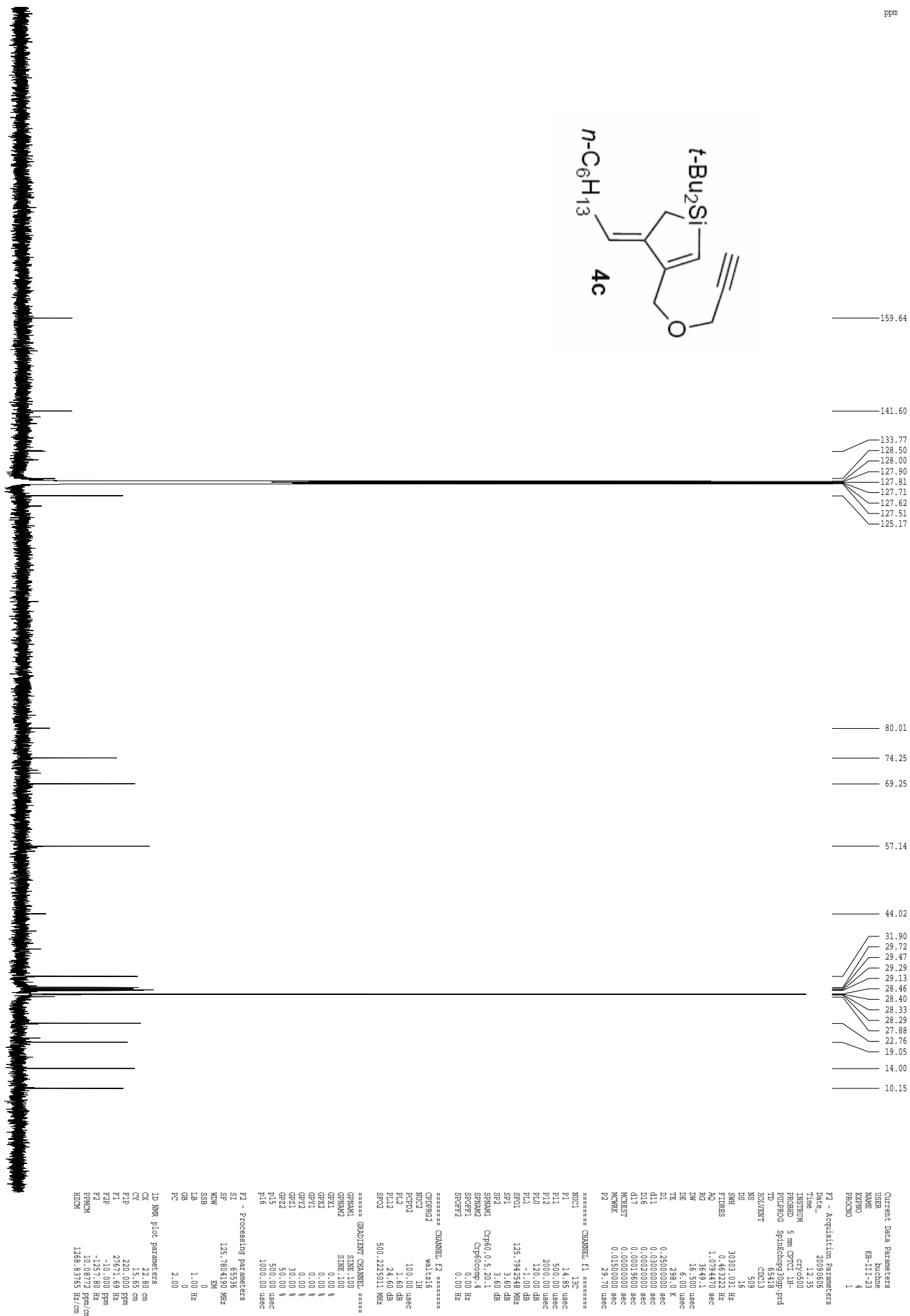
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PROCNO           1

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PROBHD           5 mm CRY1 H-
PULPROG          zgpg30
TD               65536
AQ               8.178
RG               655
DELTA            0.000000 sec
DE               6.00 usec
TE              298.0 K
D1               0.1000000 sec
MRESST          0.0000000 sec
KCMAX            0.0150000 sec

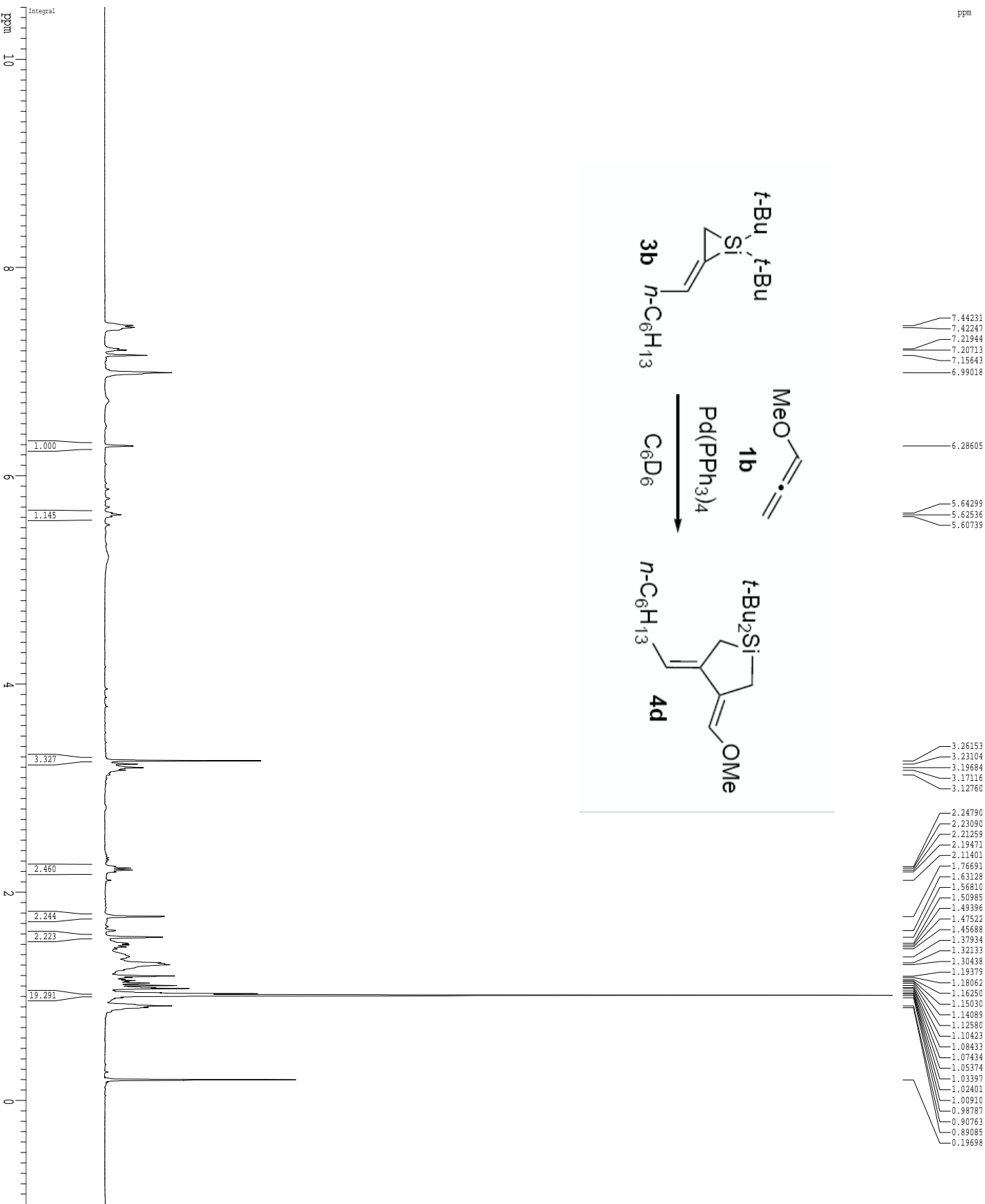
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P1                7.50 usec
PL1               1.60 dB
SFO1              500.2235015 MHz

P2 - Processing parameters
SI                65536
SF                500.2200000 MHz
WDW               EM
SSB               0
GB                0
PC                1.00

JD NMR plot parameters
CY                22.80 cm
CV                15.00 cm
F1P              10.500 ppm
F1                5252.31 Hz
F2P              -1.000 ppm
F2                -500.22 Hz
PFGM              0.50459 ppm/cm
HZCM              252.30396 Hz/cm
  
```

Z-restored spin-echo ^{13}C spectrum with ^1H decoupling in C_6D_6 

1H spectrum in C6D6 (reaction mixture)



Current Data Parameters
 USER buchoe
 NAME KB-11-47
 EXPRNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081018
 Time 12.03

INSTRUM dx400
 PROBRD 5 mm QNP H/P/P
 EPROBHD zsg30
 TD 65536
 TD0LENGTH 65536
 CQ1.1
 NS 1
 DS 0

SWH 6410.266 Hz
 FIDRES 0.0977813 Hz
 AQ 5.1118979 sec
 RG 50.8

DW 78.000 usec
 DE 4.50 usec
 TE 298.1 K

DI 0.1000000 sec
 SFO1 400.1280009 MHz
 KICKOFF 0.0150000 sec
 KCMAX 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.1280009 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1289987 MHz
 WDW EM
 SSB 0
 GB 0.30 Hz
 PC 1.00

JD NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 4201.37 Hz
 F2P -1.000 ppm
 F2 -400.113 Hz
 PPMXN 0.50459 ppm/cm
 HZCM 2011.81996 Hz/cm

1H spectrum in CDCl3



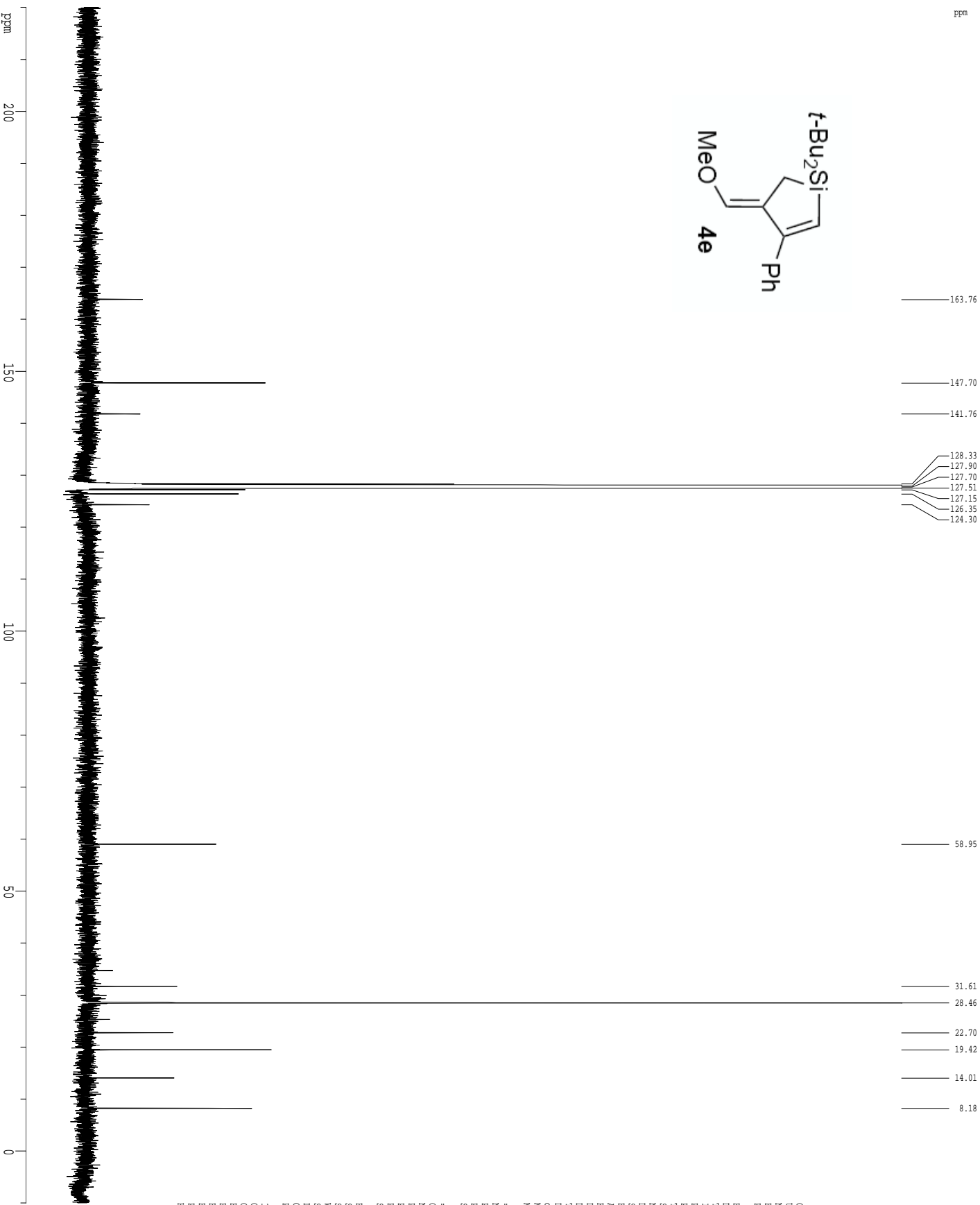
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 EXPRNO 3
 PROCNO 1

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 Time 10.12
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 PULPROG zgpg30
 TD 65536
 SFO1 400.126000
 D0 JMOD
 CQ1 8
 NS 2
 DS 2
 SWH 6410.256 Hz
 FIDRES 0.097913 Hz
 AQ 5.118579 sec
 RG 256
 DW 78.000 usec
 DE 4.50 usec
 TE 298.1 K
 D1 0.1000000 sec
 ACQST 0.0000000 sec
 KCXKX 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.126000 MHz

F2 - Processing parameters
 SI 65536
 SF 400.126000 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 10.500 ppm
 F1 4201.37 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMX 0.50459 ppm/cm
 HZCM 201.81996 Hz/cm

¹³C spectrum with ¹H decoupling in C6D6

Current Data Parameters
 USER huchne
 NAME KP-1-162
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080225

Time 11.18
 INSTRUM cryo500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65418
 SOLVENT CDCl3
 NS 267
 DS 4
 SFO 300.011 MHz
 FIDRES 0.0000000 Hz
 AQ 1.0794478 sec
 RQ 2864.3
 DW 16.500 usec
 DE 6.100 usec
 TE 298.0 K

TI 0.25000000 sec
 D1 0.03000000 sec
 d11 0.00000000 sec
 NUCREST 0.01500000 sec
 MCKEY 0.01500000 sec

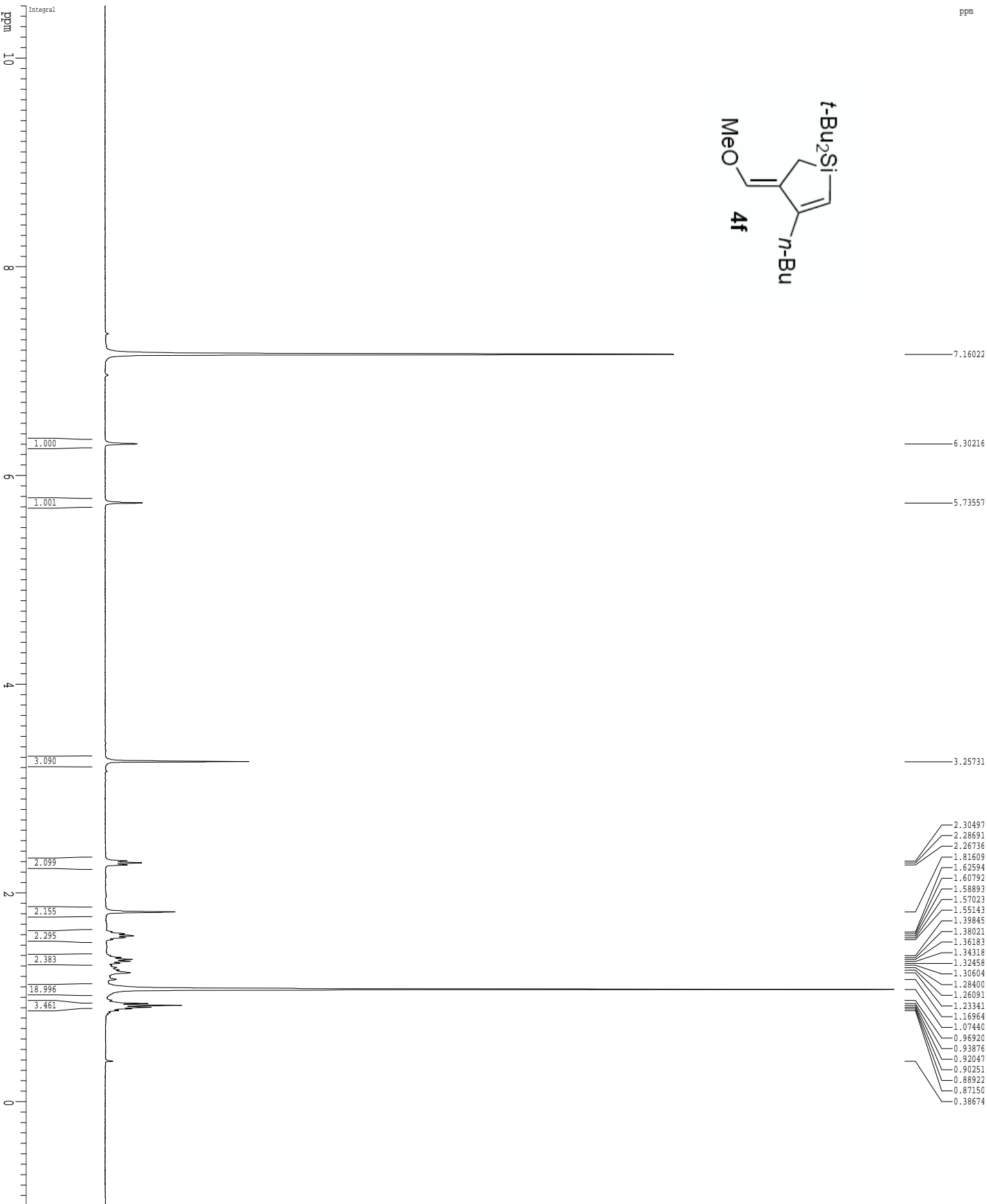
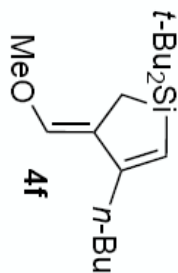
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 SFO1 125.7942948 MHz

===== CHANNEL f2 =====
 NUC2 ¹³C
 P2 100.00 usec
 PL2 1.60 dB
 SFO2 500.225011 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7804190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

JD NMR plot parameters
 CX 2.80 cm
 CY 2.80 cm
 F1D 20.00 cm
 F1 2671.69 ppm
 F2P -10.000 ppm
 F2 -125.80 Hz
 PCKM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm

¹H spectrum in C6D6



- 2.30497
- 2.28691
- 2.26736
- 1.81609
- 1.62594
- 1.60792
- 1.58893
- 1.57023
- 1.55143
- 1.39845
- 1.38021
- 1.36183
- 1.34318
- 1.32458
- 1.30604
- 1.28400
- 1.26091
- 1.23341
- 1.16964
- 1.07440
- 0.96920
- 0.93876
- 0.92047
- 0.90251
- 0.88922
- 0.87150
- 0.38674

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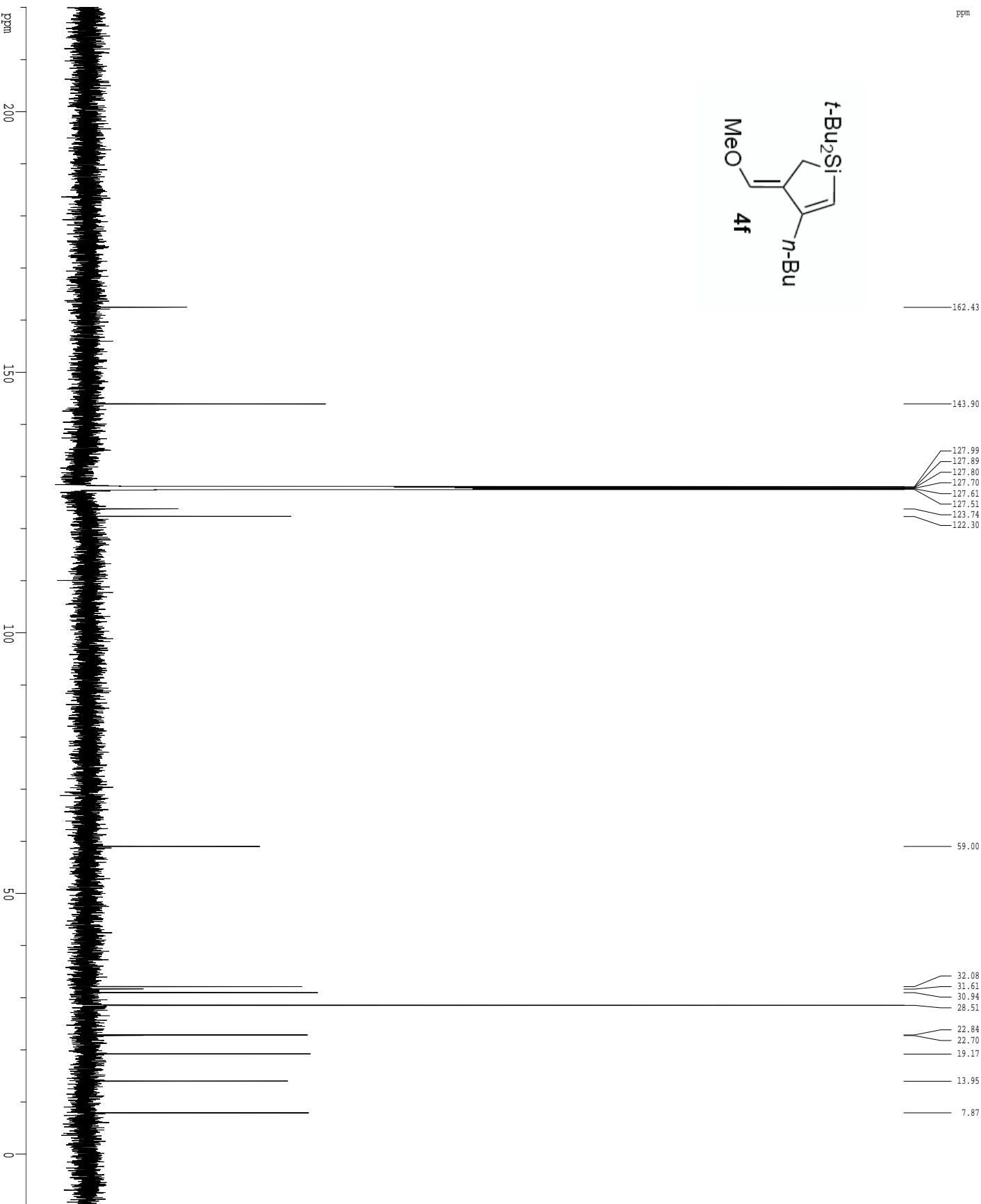
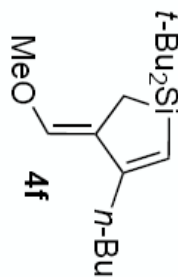
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PROCNO           1

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RG               382
DE               78.000 usec
TE               297.9 K
D1               0.1000000 sec
SFO1             400.128009 MHz
===== CHANNEL f1 =====
NUC1              1H
P1                12.00 usec
PL1              -0.00 dB
SFO1             400.128009 MHz

P2 - Processing parameters
SI               65536
SF               400.1289972 MHz
WDW              EM
SSB              0
GB               0
PC               1.00

JD NMR plot parameters
CY               22.80 cm
CX               15.00 cm
F1P             10.500 ppm
F1               4201.37 Hz
F2P             -1.000 ppm
F2              -400.13 Hz
PNUCM           0.50449 ppm/cm
HZCM            2011.81996 Hz/cm
    
```

¹³C spectrum with ¹H decoupling in C6D6



Current Data Parameters
 USER biochem
 NAME KP-1-161
 EXPNO 7
 PROCNO 1

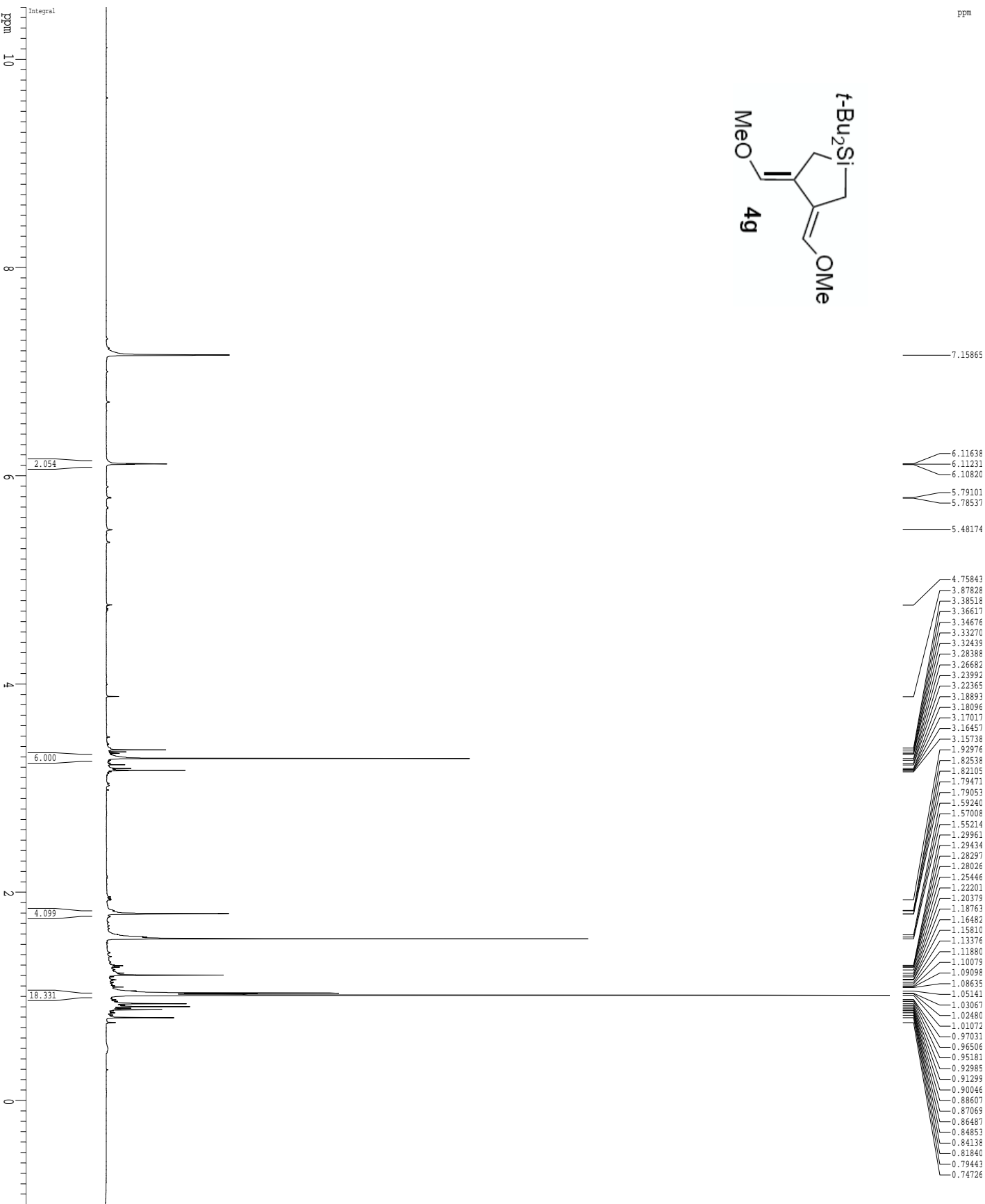
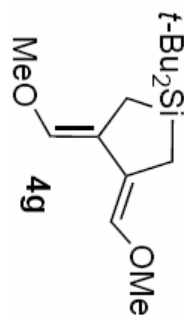
F2 - Acquisition Parameters
 Date_ 20080221
 Time 11.27
 INSTRUM cryo500
 PROBHD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65418
 SOLVENT CDCl3
 NS 158
 DS 4
 SWH 3033.031 Hz
 FWHSS 0.162472 Hz
 AQ 1.079272 sec
 RG 3251
 DW 16.500 usec
 DE 6.100 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 NUCREST 0.00000000 sec
 NUCNCK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 14.75 usec
 PL1 -1.00 dB
 SFO1 125.7942948 MHz

===== CHANNEL f2 =====
 NUC2 ¹³C
 P2 100.00 usec
 PL2 1.60 dB
 SFO2 500.225011 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7804190 MHz
 WDM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

ID NMR plot parameters
 CX 2.80 cm
 CY 2.80 cm
 FID 20.00 cm
 F1 2671.69 ppm
 F2 -10.000 ppm
 F2 -1257.80 Hz
 PNMCM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm

1H spectrum in CDCl₃

Current Data Parameters
 USER buchoe
 NAME KB-1-175
 EXPNO 6
 PROCNO 1

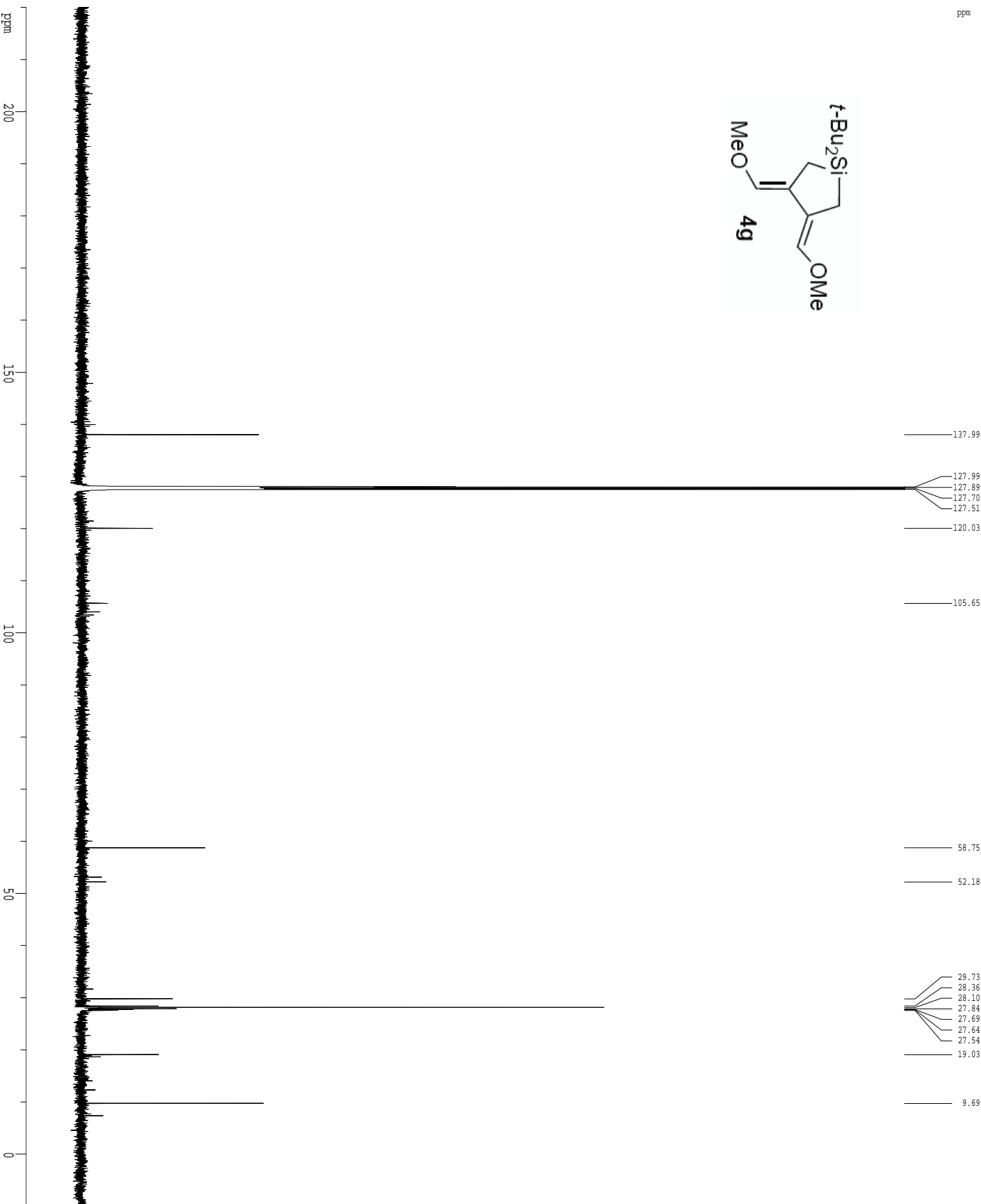
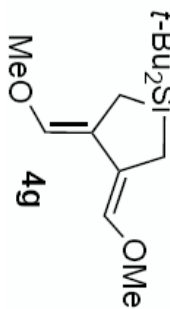
P2 - Acquisition Parameters
 Date_ 20080320
 Time 16:00
 INSTRUM cryo500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65536
 SFO1 500.136261
 F2 500.136261
 F1 125.0681305
 DDF 2
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098083 Hz
 AQ 5.0998774 sec
 RG 4.5
 DE 62.400 usec
 DW 6.00 usec
 TE 298.0 K
 D1 0.1000000 sec
 MRESST 0.0000000 sec
 KCMAX 0.0150000 sec

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

P2 - Processing parameters
 SI 65536
 SF 500.2200000 MHz
 WDW EM
 SSB 0
 GB 0.30 Hz
 LB 0
 GC 0
 FC 1.00

ID NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -500.22 Hz
 PPMCM 0.50459 ppm/cm
 HZCM 252.30396 Hz/cm

¹³C spectrum with ¹H decoupling in C6D6



Current Data Parameters
 USER huchne
 NAME KP-1-175
 EXPNO 8
 PROCNO 1

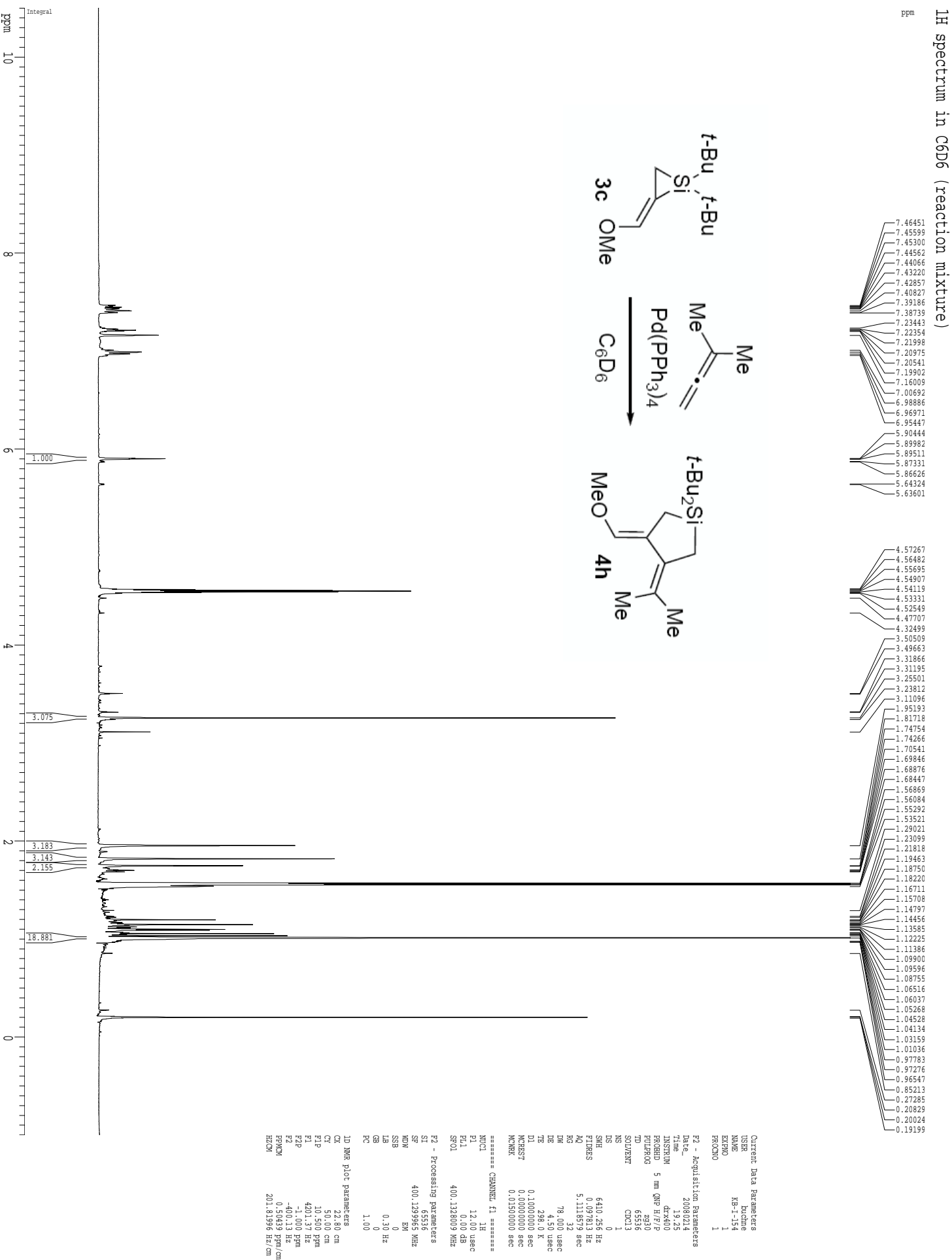
F2 - Acquisition Parameters
 Date_ 20080320
 Time 16.05
 INSTRUM cryo500
 PROBHD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65418
 SOLVENT CDCl3
 NS 229
 DS 4
 SFO 300.001 MHz
 FIDRES 0.162472 Hz
 AQ 1.078472 sec
 RQ 3251
 DW 16.500 usec
 DE 6.100 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 NUCREST 0.00000000 sec
 MCNCRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 14.75 usec
 PL1 -1.00 dB
 SFO1 125.7942948 MHz

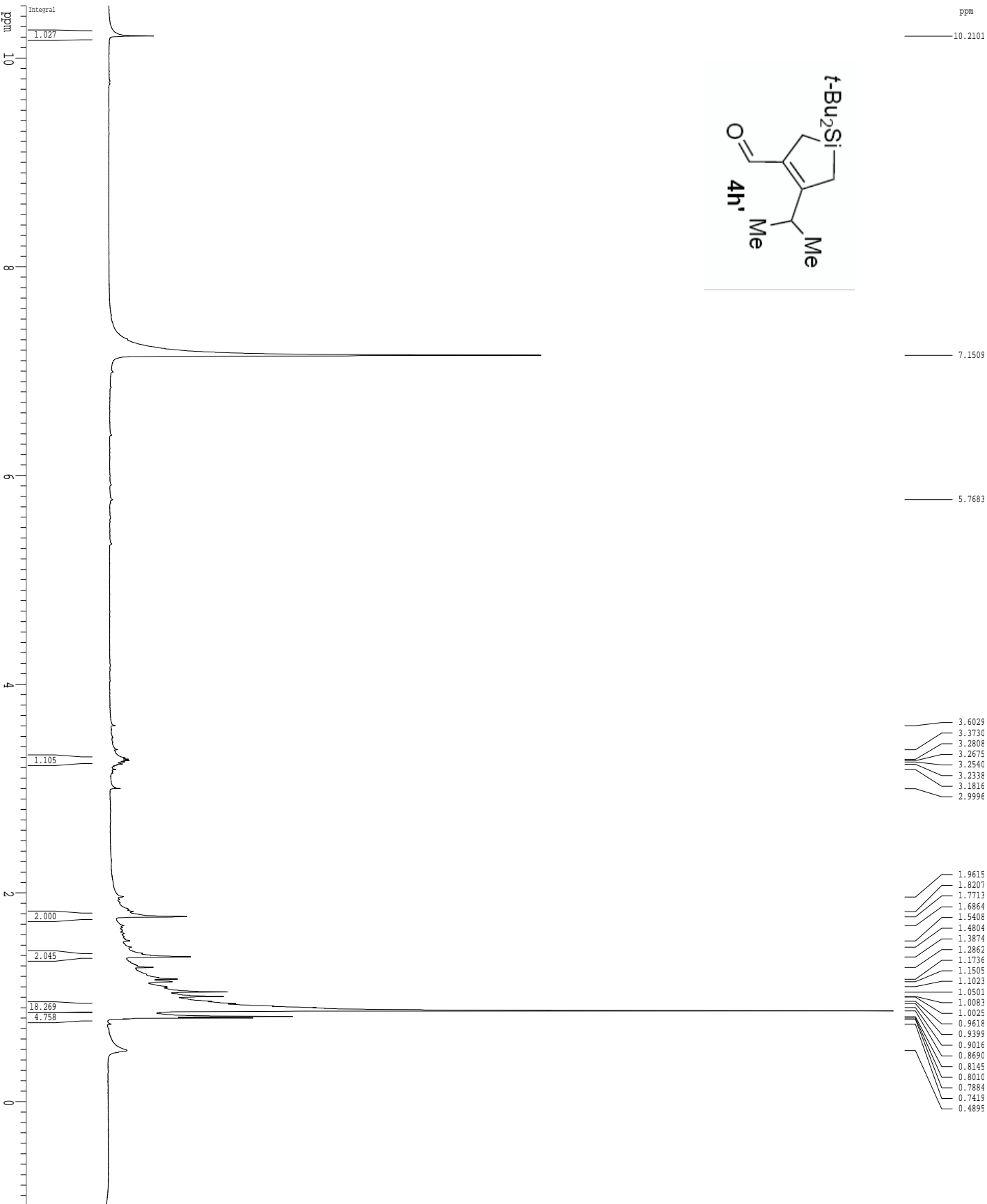
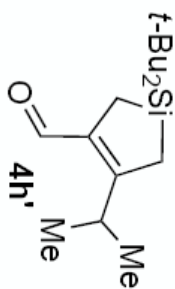
===== CHANNEL f2 =====
 NUC2 ¹³C
 P2 100.00 usec
 PL2 1.60 dB
 SFO2 500.225011 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7804190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

JD NMR plot parameters
 CX 2.80 cm
 CY 2.80 cm
 FID 220.00 cm
 F1 2767.69 ppm
 F2 -10.000 ppm
 F2 -1257.80 Hz
 PRCM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm



¹H spectrum in C6D6



ppm

10.2101
7.1509
5.7683
3.6029
3.3730
3.2808
3.2675
3.2540
3.2338
3.1816
2.9996
1.9615
1.8207
1.7713
1.6864
1.5408
1.4804
1.3874
1.2862
1.1736
1.1505
1.1023
1.0501
1.0083
1.0025
0.9618
0.9399
0.9016
0.8690
0.8145
0.8010
0.7884
0.7419
0.4895

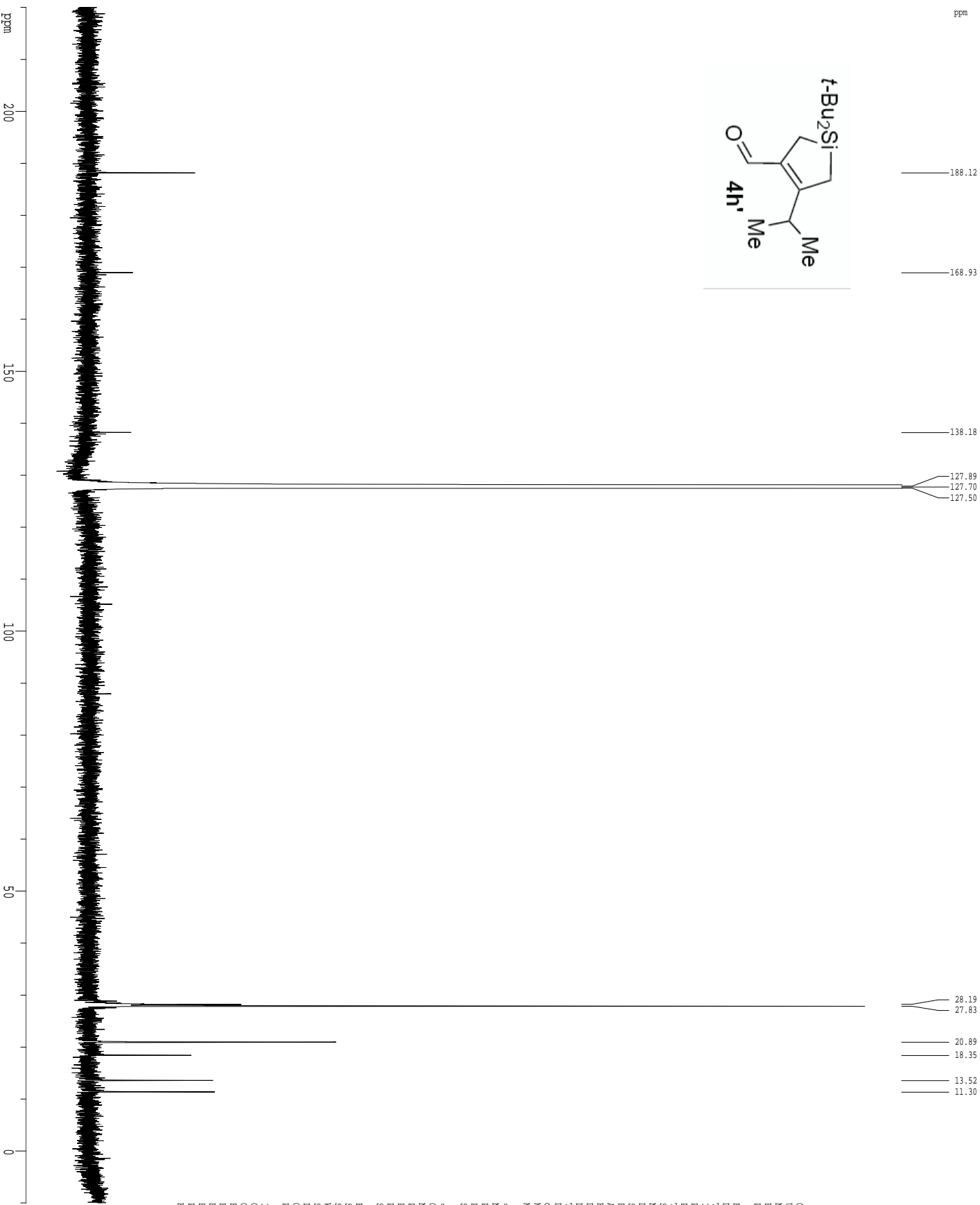
```

Current Data Parameters
=====
USER          buchne
NAME          KB-1-42
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
=====
Date_         20080915
Time          10.15
INSTRUM      cryo500
PROBHD       5 mm CPXI 1H-
PULPROG      zgpg30
TD            65536
AQ            8.178
RG            655.36
DE            0.000000 sec
TE            298.0 K
D1            0.1000000 sec
SFO1          500.2235015 MHz
===== CHANNEL f1 =====
NUC1          1H
P1            7.38 usec
PL1           1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameters
=====
SI            65536
SF            500.2200000 MHz
WDW           EM
SSB           0
GB            0
PC            1.00

JD NMR plot parameters
=====
CY            22.80 cm
CX            15.00 cm
F1P          10.500 ppm
F1           5252.31 Hz
F2P          -1.000 ppm
F2           -500.22 Hz
PFGMCM       0.50459 ppm/cm
HZCM         252.30396 Hz/cm
    
```

¹³C spectrum with ¹H decoupling in C6D6

Current Data Parameters
 USER
 NAME KP-11-42
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20080915
 Time 10.17
 INSTRUM cryo500
 PROBHD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65418
 SOLVENT CDCl3
 NS 398
 DS 4
 SFO 300.001 MHz
 FWHSS 0.162472 Hz
 AQ 1.073231 sec
 RQ 3251
 DW 16.500 usec
 DE 6.100 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 NUCREST 0.00000000 sec
 MCKMRK 0.01500000 sec

===== CHANNEL f1 =====

NUC1 ¹³C
 P1 14.75 usec
 PL1 -1.00 dB
 SFO1 125.7942948 MHz

===== CHANNEL f2 =====

NUC2 ¹³C
 P2 100.00 usec
 PL2 1.60 dB
 SFO2 500.225011 MHz

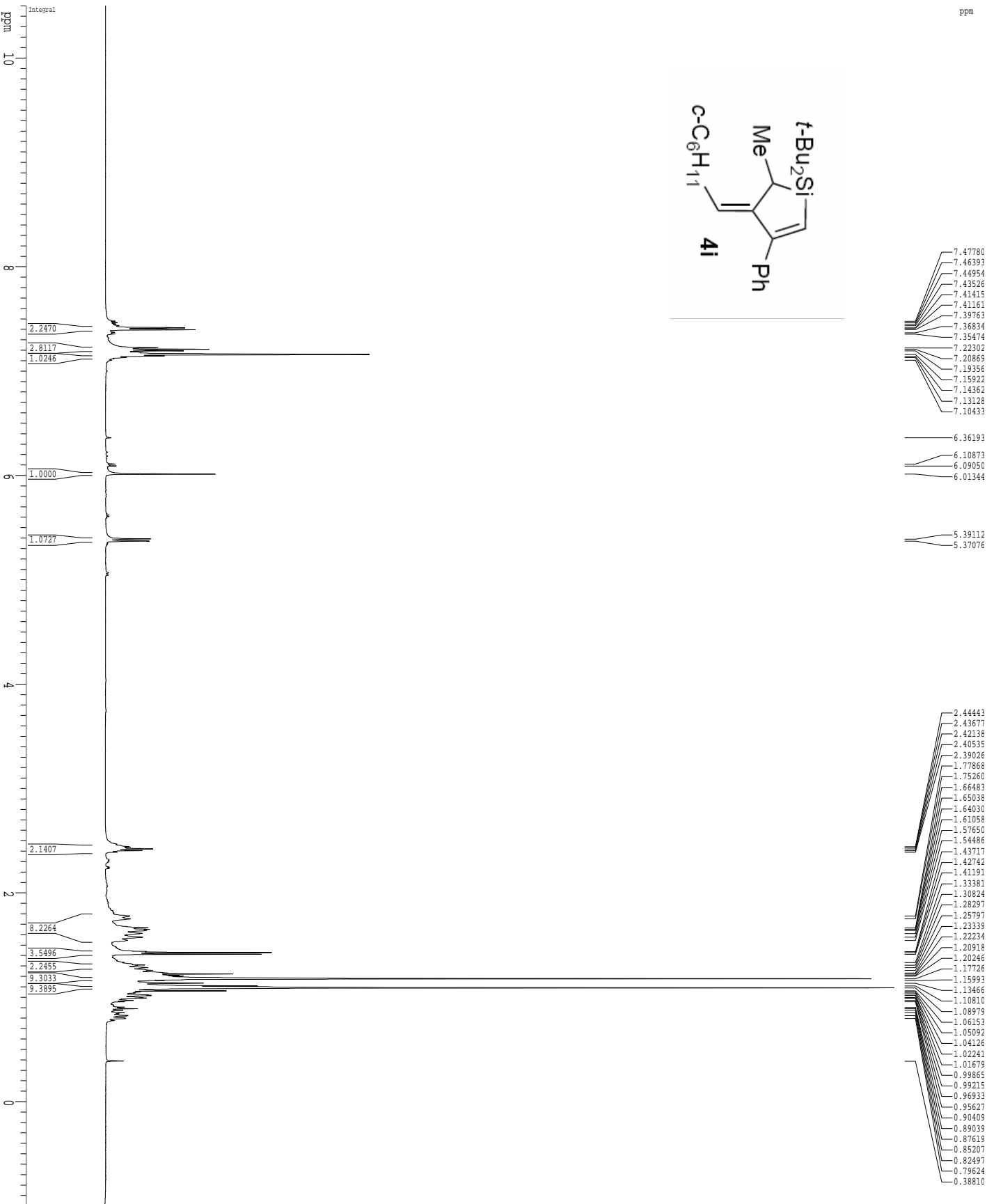
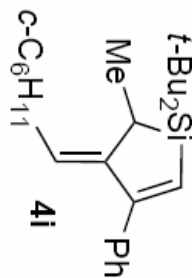
F2 - Processing parameters

SI 65536
 SF 125.7804190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

JD NMR plot parameters

CX 42.80 cm
 CY 42.80 cm
 P1D 220.00 cm
 F1 2767.69 ppm
 F2 -10.000 ppm
 F2 -1257.80 Hz
 PCKM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm

¹H spectrum in C6D6



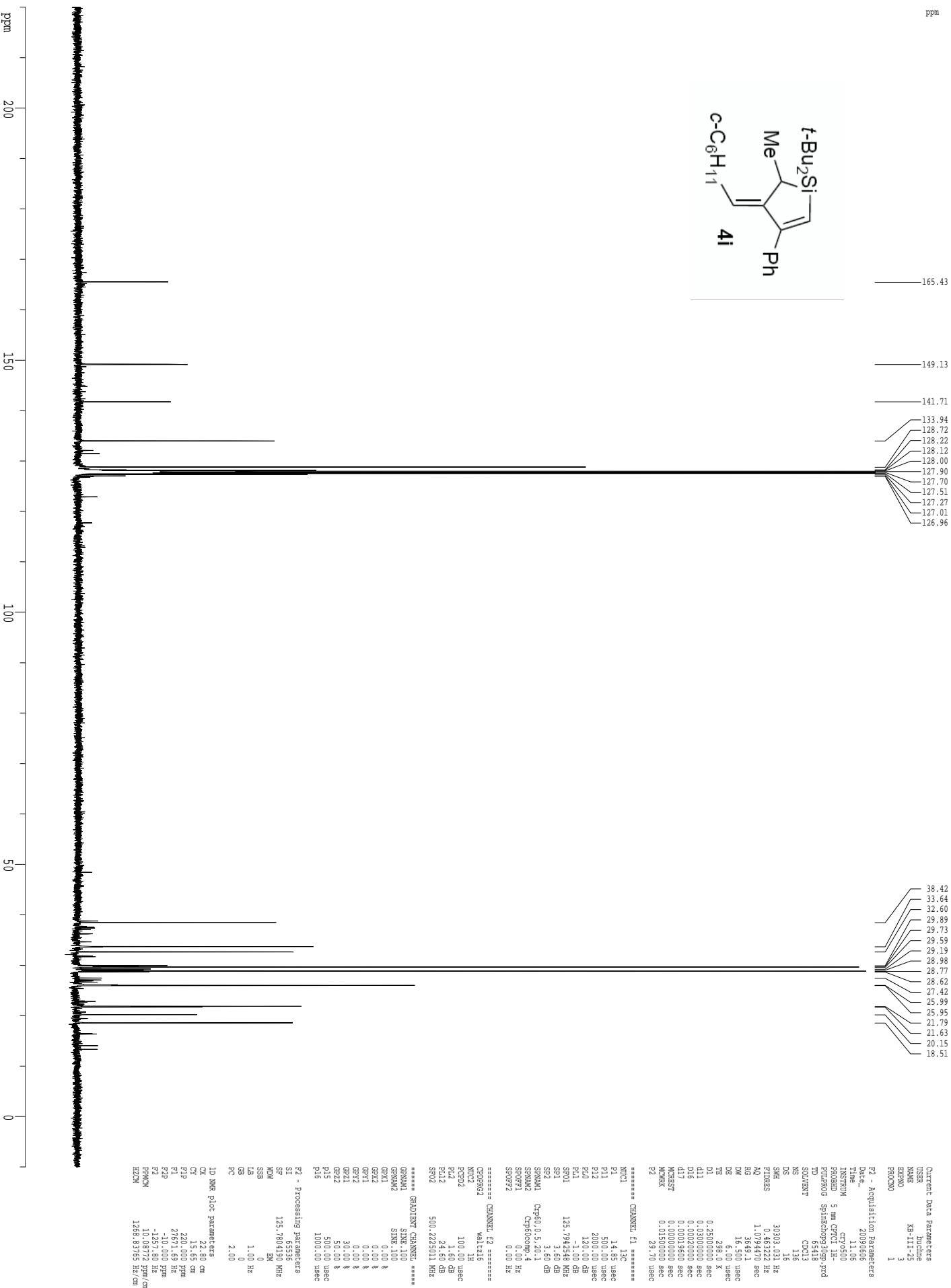
Current Data Parameters
 USER huchne
 NAME KB-II-25
 EXPRNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090606
 Time 11.03
 INSTRUM cryo500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 4920
 SFO1 500.130762 MHz
 FIDRES 0.1000000 Hz
 AQ 5.0998774 sec
 RG 5
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 KRESST 0.0000000 sec
 KCXKX 0.01500000 sec

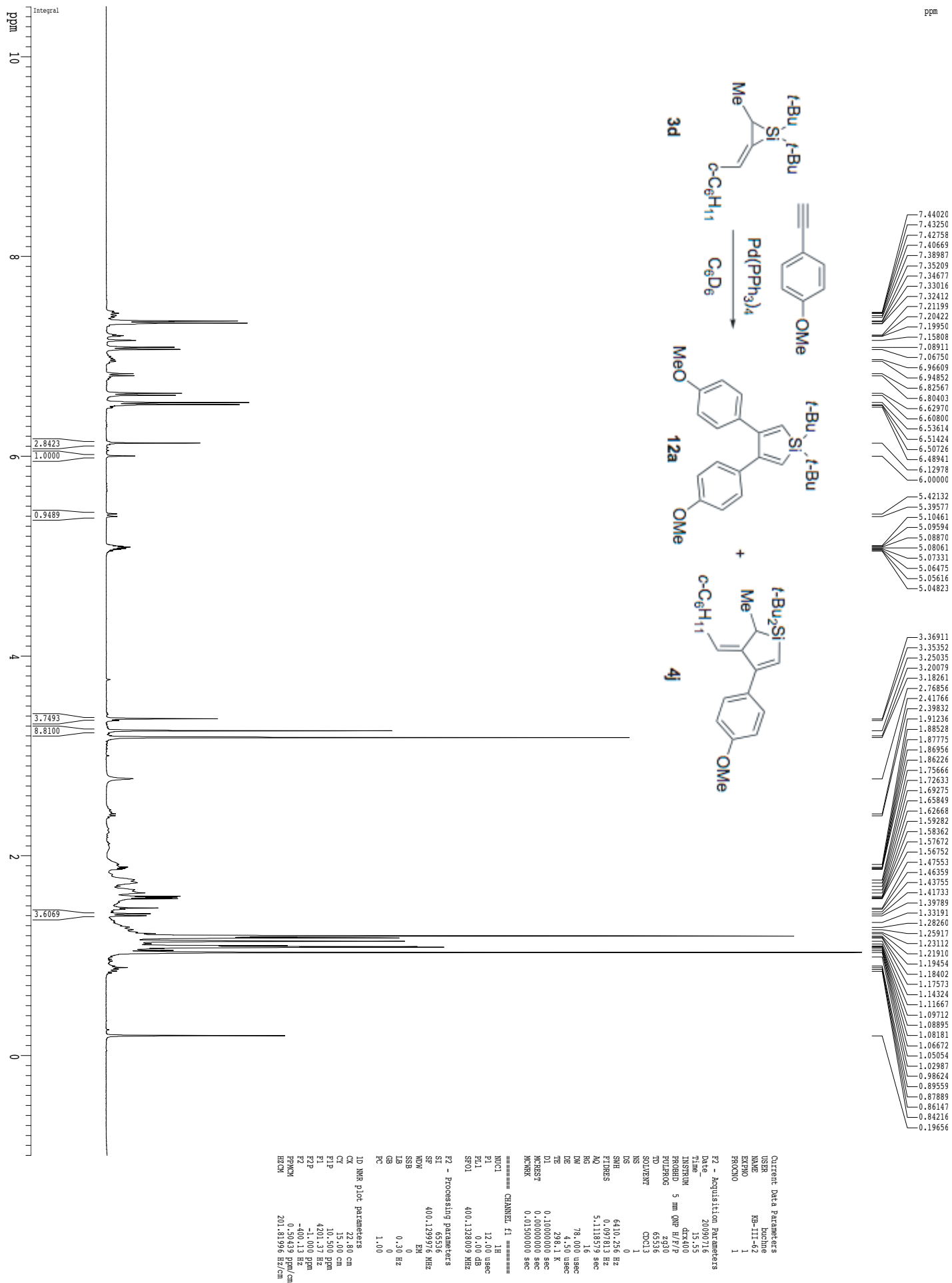
***** CHANNEL f1 *****
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2235015 MHz

F2 - Processing parameters
 SI 65536
 SF 500.2200000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

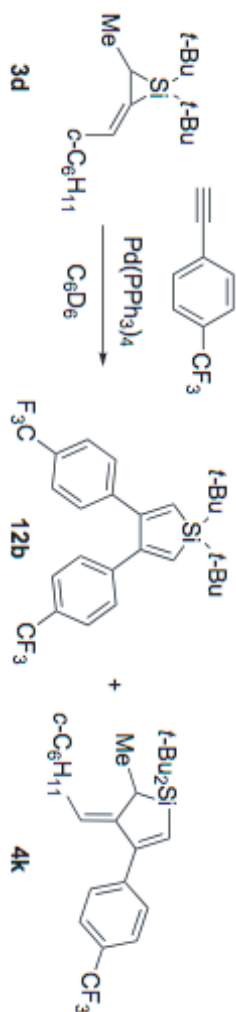
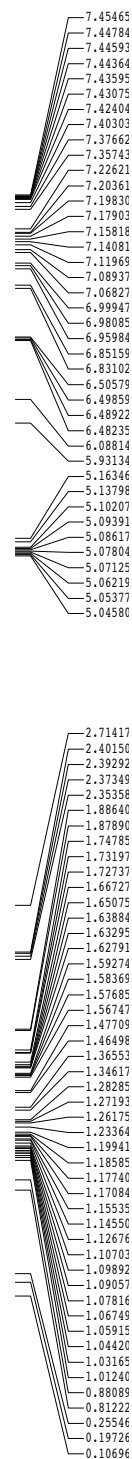
ID NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -500.22 Hz
 PPMX 0.50459 ppm/cm
 HZCM 252.30396 Hz/cm

Z-restored spin-echo ^{13}C spectrum with ^1H decoupling in C_6D_6 

1H spectrum in C6D6 (reaction mixture)

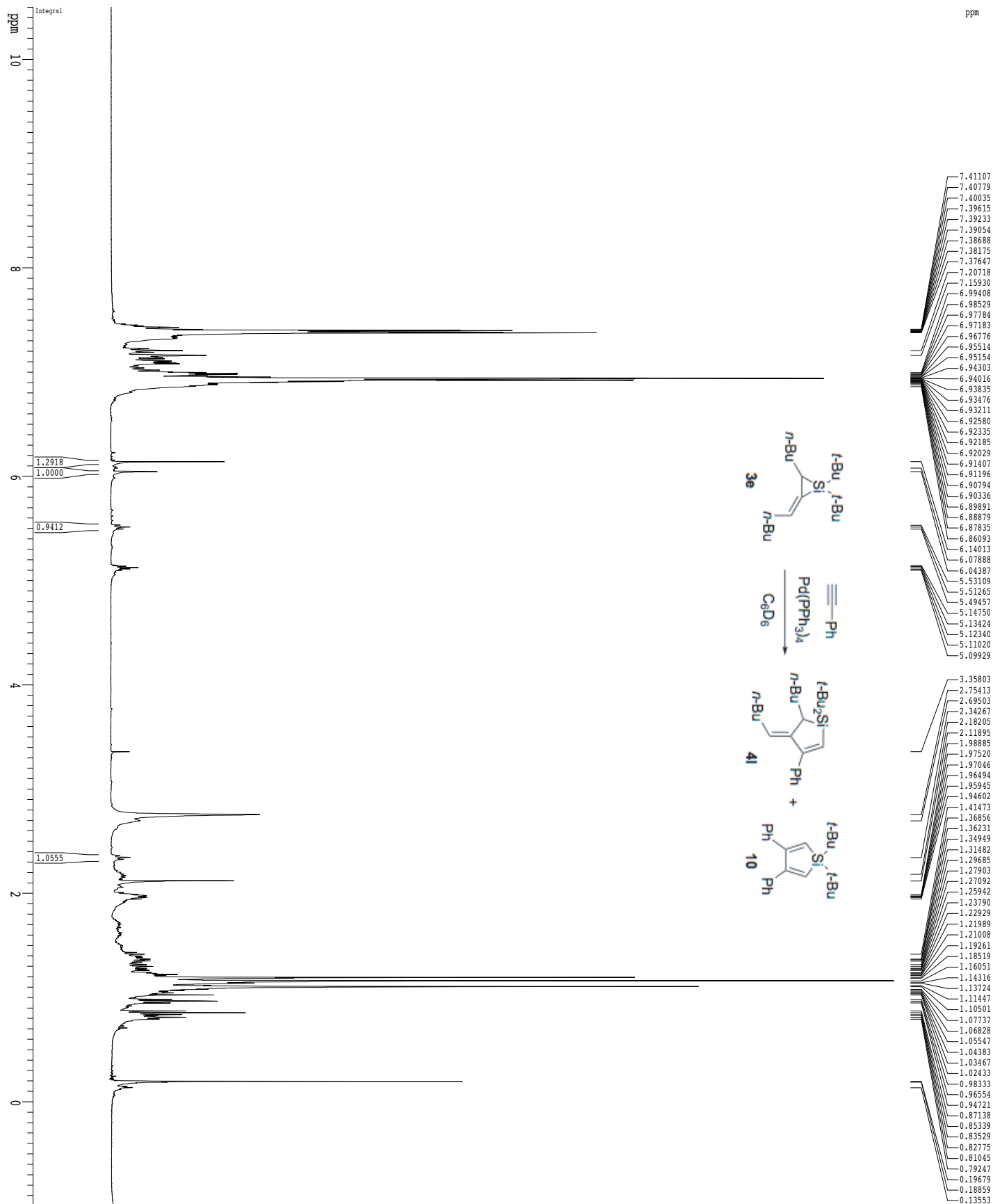


1H spectrum in C6D6 (reaction mixture)



```

Current Data Parameters
USER          Buchhe
NAME          KB-III-63
EXPNO        2
PROCNO       1
===== CHANNEL f1 =====
NUC1          1H
P1            12.00 usec
P2            0.00 dB
SFO1         400.132809 MHz
=====
F2 - Acquisition Parameters
Date_        20090716
Time        12:34
INSTRUM     spect
PROBHD     5 mm QNP 1H/1
PULPROG    zgpg30
TD          65536
SOLVENT    CDCl3
NS          1
DS          0
SWH         6410.235 Hz
FIDRES     0.097813 Hz
AQ         5.118579 sec
RG          16
WDW         78.000 usec
SSB         0
LB          3.00 Hz
GB          0
PC          1.00
=====
F2 - Processing parameters
SI          65536
SF          400.129983 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         10.500 ppm
F2P         4201.37 Hz
E2P         -1.000 ppm
F2PCMH     400.13 Hz
PFKCMH     0.50449 ppm/cm
MICH       20.101390 Hz/cm
  
```


¹H spectrum in C6D6 (reaction mixture)

Current Data Parameters
 USER pudine
 NAME RP-1-169
 EXPTNO 1
 PROCNO 1

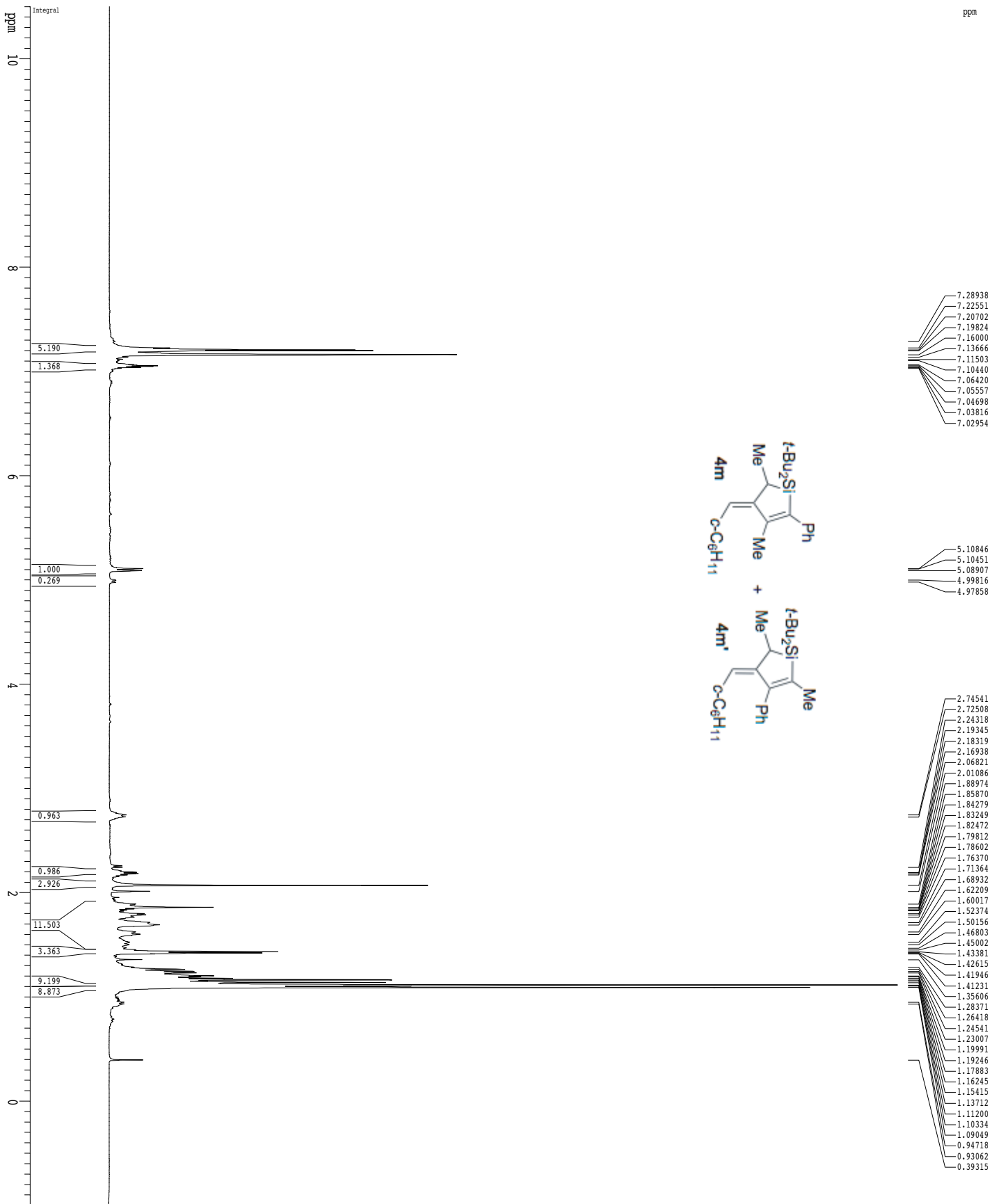
Acquisition Parameters
 Date_ 20080311
 Time 13.35
 INSTRUM dtx400
 PROBD 5 mm QNP H/F/P
 PULPROG zg30
 TD 65536
 SOLVENT CMC13
 NS 1
 DS 0
 SM 640.226 Hz
 FIDRES 0.197813 Hz
 AQ 5.118017 sec
 IN 78.000 usec
 DE 4.50 usec
 TE 298.1 K
 D1 0.1000000 sec
 ACQRES 0.0000000 sec
 MCRES 0.0150000 sec

===== CHANNEL f1 =====
 NUCL1 ¹H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.132809 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1299972 MHz
 MDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.80 cm
 CT 1.00
 C1P 13.00 cm
 F1 4201.37 Hz
 F2P -1.000 DM
 -400.13 Hz
 PPMCM 0.50439 ppm/cm
 HZCM 201.81995 Hz/cm

¹H spectrum in C6D6 (regioisomeric mixture)



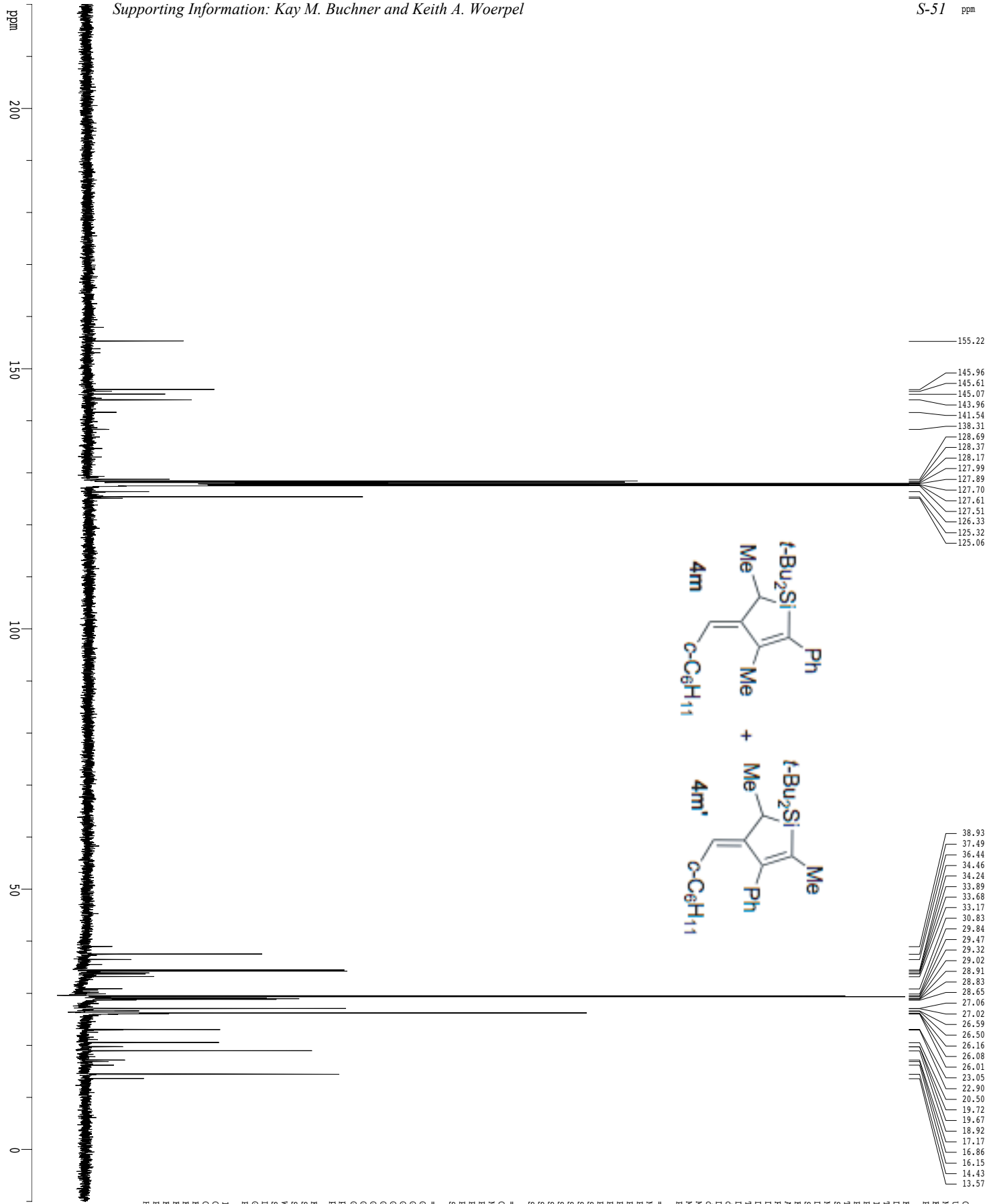
Current Data Parameters
 USER buchner
 NAME RB-11-102
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090501
 Time 12.11
 INSTRUM cryo600
 PROBHD 5 mm CPCL1 1H-
 PULPROG zgpg30
 TD 65536
 SFO 500.136250
 SOLVENT CDCl3
 DS 2
 SFR 8012.820 Hz
 FIDRES 0.086043 Hz
 AQ 5.098774 sec
 RG 3.6
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.1000000 sec
 ACQRES 0.0000000 sec
 MCNKR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL 1.60 dB
 SFO1 500.225015 MHz

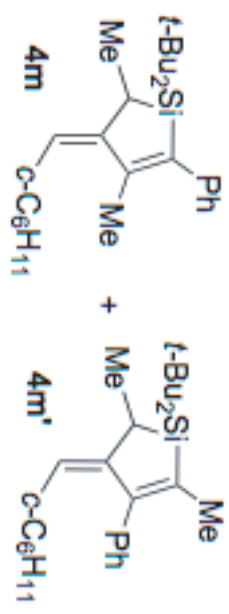
F2 - Processing parameters
 SI 65536
 SF 500.2200003 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters:
 CX 222.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -5104.22 Hz
 PPMCH 0.50439 ppm/cm
 HZCH 252.30396 Hz/cm



- 155.22
- 145.96
- 145.61
- 145.07
- 143.96
- 141.54
- 138.31
- 128.69
- 128.37
- 128.17
- 127.99
- 127.89
- 127.70
- 127.61
- 127.51
- 126.33
- 125.32
- 125.06

- 38.93
- 37.49
- 36.44
- 34.46
- 34.24
- 33.89
- 33.68
- 33.17
- 30.83
- 29.84
- 29.47
- 29.32
- 29.02
- 28.91
- 28.83
- 28.65
- 27.06
- 27.02
- 26.59
- 26.50
- 26.16
- 26.08
- 26.01
- 23.05
- 22.90
- 20.50
- 19.72
- 19.67
- 18.92
- 17.17
- 16.86
- 16.15
- 14.43
- 13.57



```

Current Data Parameters
=====
USER          buchne
NAME          kb-11-182
EXPNO         10
PROCNO        1

F2 - Acquisition Parameters
=====
Date_         20001215
Time          12.15
INSTRUM      crys00
PROBHD       5 mm CPXI 1H-
PULPROG      zgpg30
TD            65418
SOLVENT      CDCl3
NS           156
DS           16
SMH          3030.1031 Hz
FIDRES       0.46322 Hz
AQ           1.079470 sec
RG           36.500 usec
DE           6.00 usec
TE           298.0 K
D1           0.25000000 sec
d11          0.03000000 sec
d16          0.00020000 sec
d17          0.00019600 sec
ACQRES      0.00000000 sec
WCWRES      0.01500000 sec
PC           29.70 usec

===== CHANNEL f1 =====
NUC1          13C
P1            14.65 usec
P2            500.00 usec
PCPD2        2000.00 usec
PZ1          120.00 dB
PZ2          -1.00 dB
SF01         125.7942548 MHz
SR1          3.60 dB
SR2          3.60 dB
SFOHM1       Cp(60, 0.5, 20, 1
SFOHM2       Cp(60, 0.5, 20, 4
SFOFT1       0.00 Hz
SFOFT2       0.00 Hz

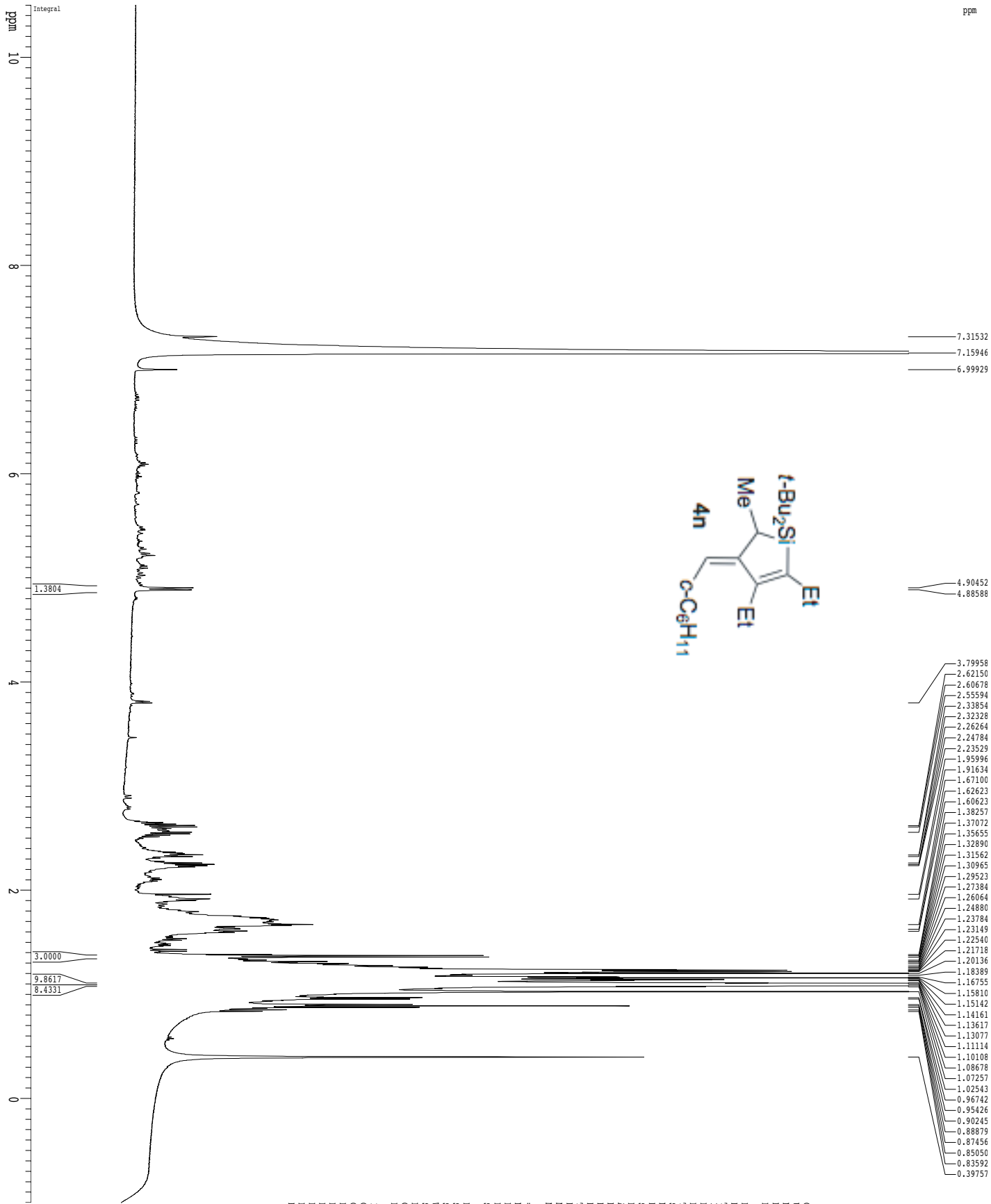
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PZ1          1.60 dB
PZ2          24.60 dB
SF02         500.2225011 MHz

===== CHANNEL CHANNELS =====
GPRM1       SINE:100
GPRM2       SINE:100
GPRF1       0.00 %
GPRF2       0.00 %
GPR1        0.00 %
GPR2        0.00 %
GPR3        0.00 %
GPR4        0.00 %
GPR5        30.00 %
GPR6        50.00 %
GPR7        500.00 usec
GPR8        1000.00 usec

F2 - Processing parameters
=====
SI           65358
SR           125.7804390 MHz
WDW          EM
SSB          0
GB           0
PC           2.00

ID NMR plot parameters
=====
CX           22.80 cm
CY           15.65 cm
F1P          220.000 ppm
F2P          27871.69 Hz
ZNP          -101.000 ppm
SFO1         125.7942548 MHz
SFO2         500.2225011 MHz
HSCN         1268.83765 Hz/cm
    
```

¹H spectrum in C6D6



Current Data Parameters
 USER: jmoehle
 NAME: RB-11-207
 EXPNO: 2
 PROCNO: 1

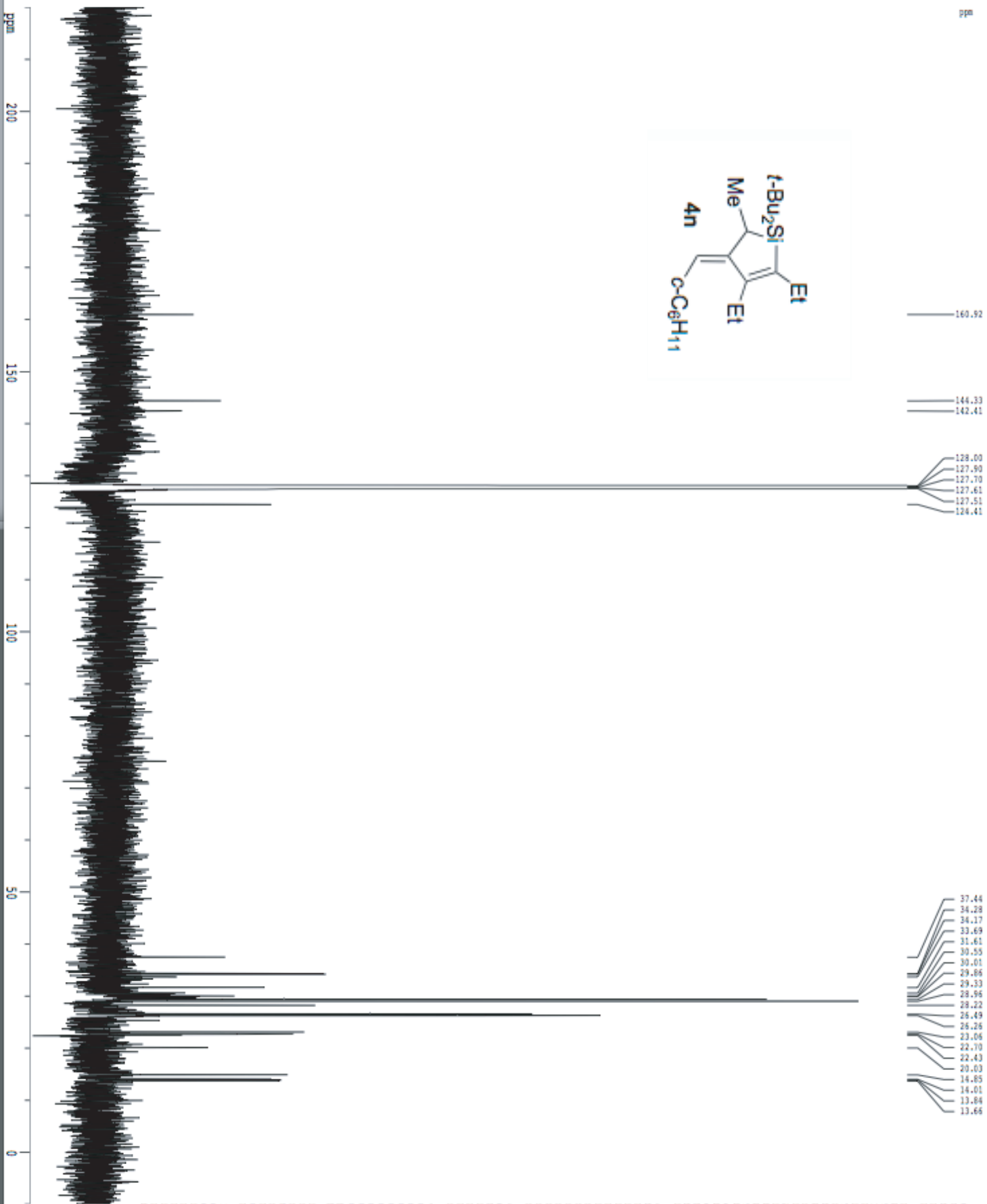
F2 - Acquisition Parameters
 Date_: 20090522
 Time: 15.17
 INSTRUM: cryo500
 PROBHD: 5 mm CPYCI 1H-
 PULPROG: zgpg30
 TD: 65536
 SFO1: 500.136261 MHz
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.098043 Hz
 AQ: 0.0998774 sec
 RG: 5
 DW: 62.400 usec
 DE: 6.00 usec
 TE: 298.4 K
 D1: 0.10000000 sec
 ACQRES: 0.00000000 sec
 MCWRR: 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: 500.2200000 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 22.80 cm
 CY: 50.00 cm
 P1P: 10.500 ppm
 F1: 5252.31 Hz
 F2P: -1.000 ppm
 P2: -500.22 Hz
 PPKCM: 0.50439 ppm/cm
 HZCM: 252.30396 Hz/cm

Z-restored spin-echo ¹³C spectrum with ¹H decoupling in C6D6



160.92
144.33
142.41
128.00
127.90
127.70
127.61
127.51
124.41

37.44
34.28
34.17
33.69
31.61
30.55
30.01
29.33
28.96
28.22
26.49
26.26
23.98
22.70
22.43
20.03
16.85
14.01
13.84
13.59

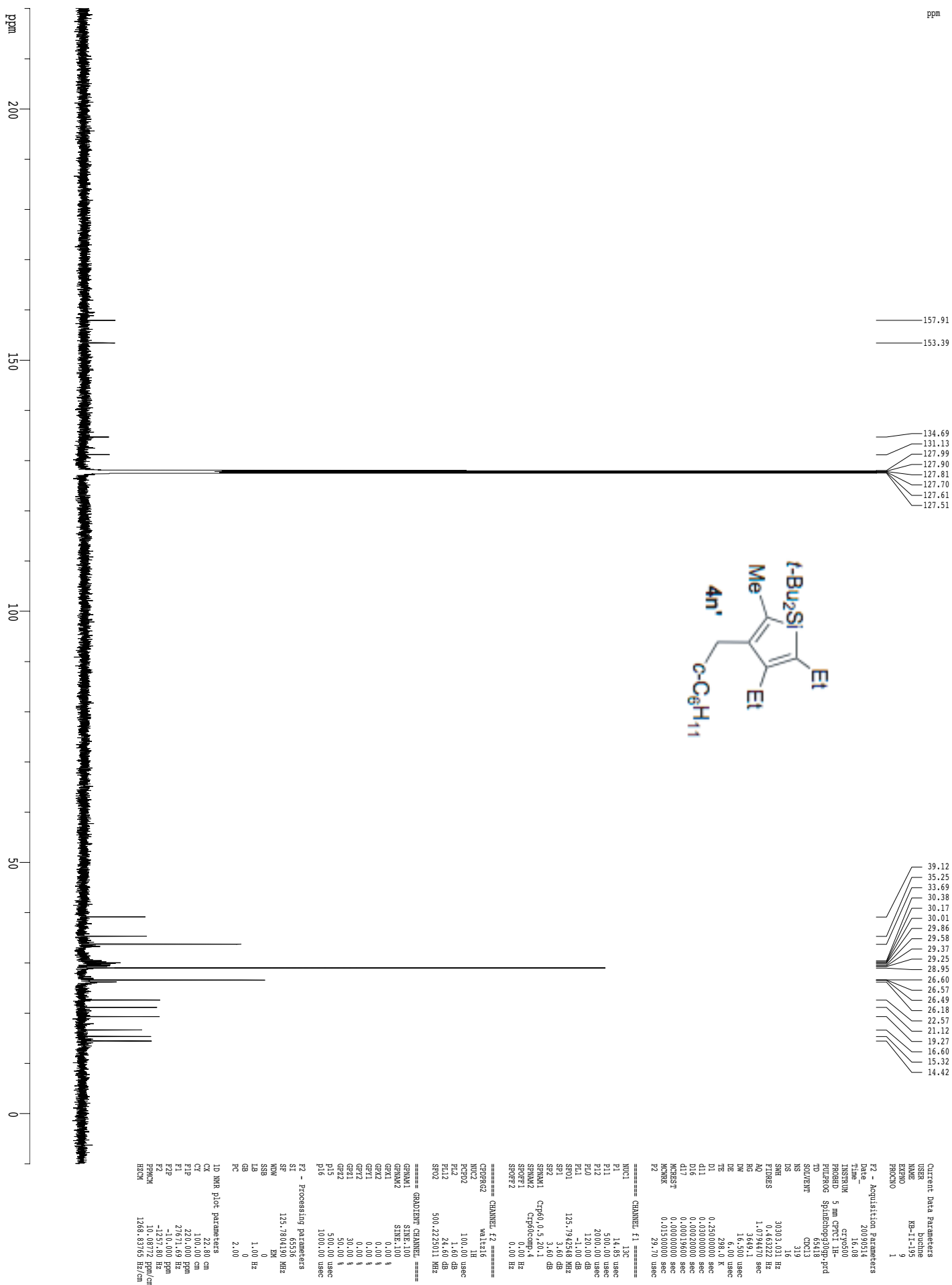
Current Data Parameters
DATE_ 2009032
TIME 15.12
INSTRUM spect
PROBHD 5 mm CPY130
PULPROG zgpg30
TD 65536
SOLVENT C6D13
NS 1024
DS 16
SWH 20303.031 MHz
F2RES 0.463232 Hz
AQ 1.0194479 sec
RG 3190.4
SQ 18.500 sec
WDW EM
SSB 0
GB 0
PC 0.2500000 sec
DT 0.0100000 sec
FIDRES 0.0002000 sec
AQRES 0.0001860 sec
RGRES 0.0000000 sec
MCKRES 0.0100000 sec
MCKM 0.0100000 sec
SFO 29.70 sec

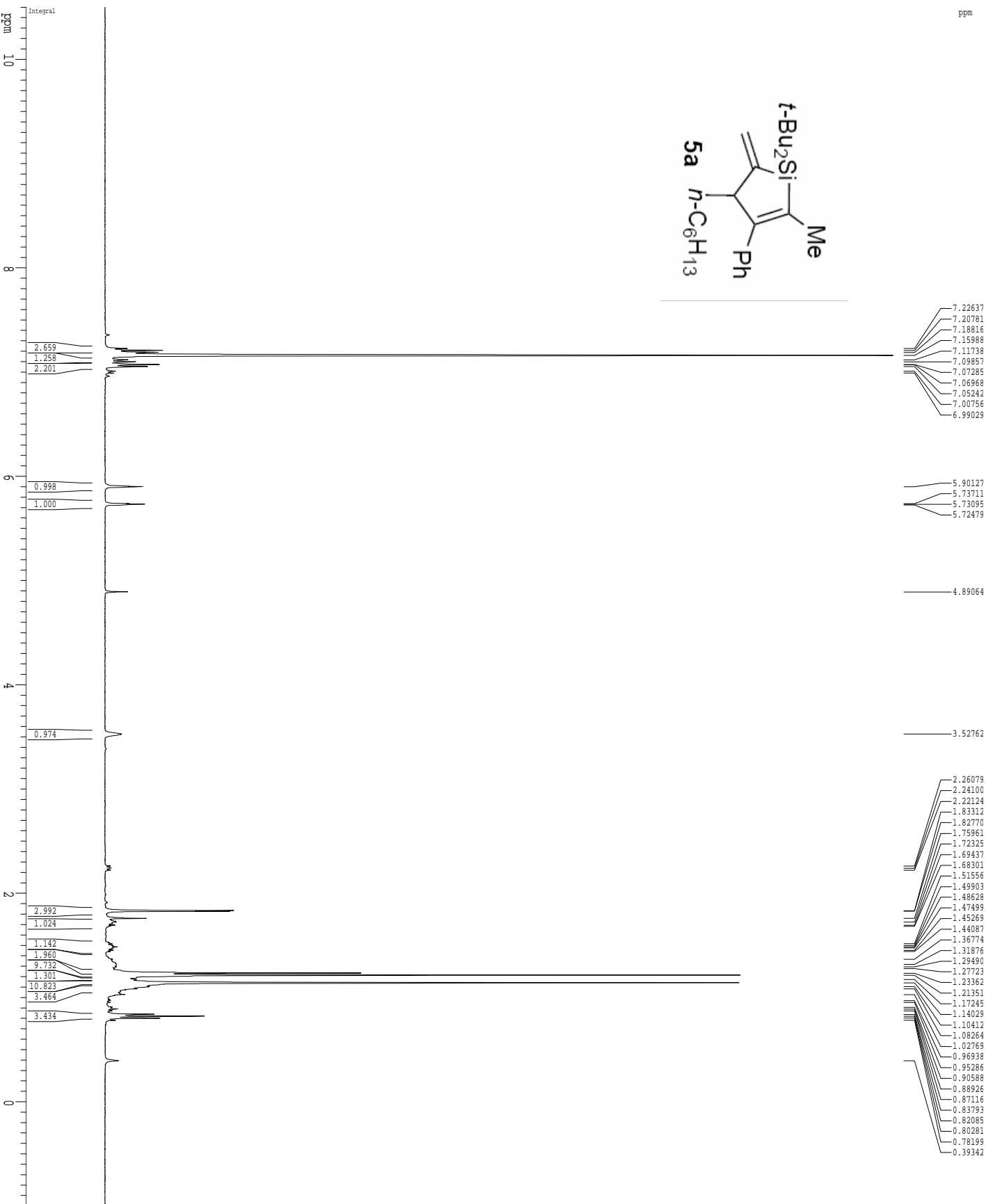
===== CHANNEL f1 =====
NUC1 13C
P1 14.12 sec
PL1 0.00 dB
PL2 0.00 dB
PL3 2000.00 dB
PL4 0.00 dB
PL5 0.00 dB
PL6 -1.00 dB
PL7 0.00 dB
PL8 126.794248 MHz
PL9 0.00 dB
PL10 0.00 dB
PL11 0.00 dB
PL12 0.00 dB
PL13 0.00 dB
PL14 0.00 dB
PL15 0.00 dB
PL16 0.00 dB
PL17 0.00 dB
PL18 0.00 dB
PL19 0.00 dB
PL20 0.00 dB
PL21 0.00 dB
PL22 0.00 dB
PL23 0.00 dB
PL24 0.00 dB
PL25 0.00 dB
PL26 0.00 dB
PL27 0.00 dB
PL28 0.00 dB
PL29 0.00 dB
PL30 0.00 dB
PL31 0.00 dB
PL32 0.00 dB
PL33 0.00 dB
PL34 0.00 dB
PL35 0.00 dB
PL36 0.00 dB
PL37 0.00 dB
PL38 0.00 dB
PL39 0.00 dB
PL40 0.00 dB
PL41 0.00 dB
PL42 0.00 dB
PL43 0.00 dB
PL44 0.00 dB
PL45 0.00 dB
PL46 0.00 dB
PL47 0.00 dB
PL48 0.00 dB
PL49 0.00 dB
PL50 0.00 dB
PL51 0.00 dB
PL52 0.00 dB
PL53 0.00 dB
PL54 0.00 dB
PL55 0.00 dB
PL56 0.00 dB
PL57 0.00 dB
PL58 0.00 dB
PL59 0.00 dB
PL60 0.00 dB
PL61 0.00 dB
PL62 0.00 dB
PL63 0.00 dB
PL64 0.00 dB
PL65 0.00 dB
PL66 0.00 dB
PL67 0.00 dB
PL68 0.00 dB
PL69 0.00 dB
PL70 0.00 dB
PL71 0.00 dB
PL72 0.00 dB
PL73 0.00 dB
PL74 0.00 dB
PL75 0.00 dB
PL76 0.00 dB
PL77 0.00 dB
PL78 0.00 dB
PL79 0.00 dB
PL80 0.00 dB
PL81 0.00 dB
PL82 0.00 dB
PL83 0.00 dB
PL84 0.00 dB
PL85 0.00 dB
PL86 0.00 dB
PL87 0.00 dB
PL88 0.00 dB
PL89 0.00 dB
PL90 0.00 dB
PL91 0.00 dB
PL92 0.00 dB
PL93 0.00 dB
PL94 0.00 dB
PL95 0.00 dB
PL96 0.00 dB
PL97 0.00 dB
PL98 0.00 dB
PL99 0.00 dB
PL100 0.00 dB

===== CHANNEL f2 =====
NUC2 13C
P1 14.12 sec
PL1 0.00 dB
PL2 0.00 dB
PL3 2000.00 dB
PL4 0.00 dB
PL5 0.00 dB
PL6 -1.00 dB
PL7 0.00 dB
PL8 126.794248 MHz
PL9 0.00 dB
PL10 0.00 dB
PL11 0.00 dB
PL12 0.00 dB
PL13 0.00 dB
PL14 0.00 dB
PL15 0.00 dB
PL16 0.00 dB
PL17 0.00 dB
PL18 0.00 dB
PL19 0.00 dB
PL20 0.00 dB
PL21 0.00 dB
PL22 0.00 dB
PL23 0.00 dB
PL24 0.00 dB
PL25 0.00 dB
PL26 0.00 dB
PL27 0.00 dB
PL28 0.00 dB
PL29 0.00 dB
PL30 0.00 dB
PL31 0.00 dB
PL32 0.00 dB
PL33 0.00 dB
PL34 0.00 dB
PL35 0.00 dB
PL36 0.00 dB
PL37 0.00 dB
PL38 0.00 dB
PL39 0.00 dB
PL40 0.00 dB
PL41 0.00 dB
PL42 0.00 dB
PL43 0.00 dB
PL44 0.00 dB
PL45 0.00 dB
PL46 0.00 dB
PL47 0.00 dB
PL48 0.00 dB
PL49 0.00 dB
PL50 0.00 dB
PL51 0.00 dB
PL52 0.00 dB
PL53 0.00 dB
PL54 0.00 dB
PL55 0.00 dB
PL56 0.00 dB
PL57 0.00 dB
PL58 0.00 dB
PL59 0.00 dB
PL60 0.00 dB
PL61 0.00 dB
PL62 0.00 dB
PL63 0.00 dB
PL64 0.00 dB
PL65 0.00 dB
PL66 0.00 dB
PL67 0.00 dB
PL68 0.00 dB
PL69 0.00 dB
PL70 0.00 dB
PL71 0.00 dB
PL72 0.00 dB
PL73 0.00 dB
PL74 0.00 dB
PL75 0.00 dB
PL76 0.00 dB
PL77 0.00 dB
PL78 0.00 dB
PL79 0.00 dB
PL80 0.00 dB
PL81 0.00 dB
PL82 0.00 dB
PL83 0.00 dB
PL84 0.00 dB
PL85 0.00 dB
PL86 0.00 dB
PL87 0.00 dB
PL88 0.00 dB
PL89 0.00 dB
PL90 0.00 dB
PL91 0.00 dB
PL92 0.00 dB
PL93 0.00 dB
PL94 0.00 dB
PL95 0.00 dB
PL96 0.00 dB
PL97 0.00 dB
PL98 0.00 dB
PL99 0.00 dB
PL100 0.00 dB

===== CHANNEL f3 =====
NUC3 13C
P1 14.12 sec
PL1 0.00 dB
PL2 0.00 dB
PL3 2000.00 dB
PL4 0.00 dB
PL5 0.00 dB
PL6 -1.00 dB
PL7 0.00 dB
PL8 126.794248 MHz
PL9 0.00 dB
PL10 0.00 dB
PL11 0.00 dB
PL12 0.00 dB
PL13 0.00 dB
PL14 0.00 dB
PL15 0.00 dB
PL16 0.00 dB
PL17 0.00 dB
PL18 0.00 dB
PL19 0.00 dB
PL20 0.00 dB
PL21 0.00 dB
PL22 0.00 dB
PL23 0.00 dB
PL24 0.00 dB
PL25 0.00 dB
PL26 0.00 dB
PL27 0.00 dB
PL28 0.00 dB
PL29 0.00 dB
PL30 0.00 dB
PL31 0.00 dB
PL32 0.00 dB
PL33 0.00 dB
PL34 0.00 dB
PL35 0.00 dB
PL36 0.00 dB
PL37 0.00 dB
PL38 0.00 dB
PL39 0.00 dB
PL40 0.00 dB
PL41 0.00 dB
PL42 0.00 dB
PL43 0.00 dB
PL44 0.00 dB
PL45 0.00 dB
PL46 0.00 dB
PL47 0.00 dB
PL48 0.00 dB
PL49 0.00 dB
PL50 0.00 dB
PL51 0.00 dB
PL52 0.00 dB
PL53 0.00 dB
PL54 0.00 dB
PL55 0.00 dB
PL56 0.00 dB
PL57 0.00 dB
PL58 0.00 dB
PL59 0.00 dB
PL60 0.00 dB
PL61 0.00 dB
PL62 0.00 dB
PL63 0.00 dB
PL64 0.00 dB
PL65 0.00 dB
PL66 0.00 dB
PL67 0.00 dB
PL68 0.00 dB
PL69 0.00 dB
PL70 0.00 dB
PL71 0.00 dB
PL72 0.00 dB
PL73 0.00 dB
PL74 0.00 dB
PL75 0.00 dB
PL76 0.00 dB
PL77 0.00 dB
PL78 0.00 dB
PL79 0.00 dB
PL80 0.00 dB
PL81 0.00 dB
PL82 0.00 dB
PL83 0.00 dB
PL84 0.00 dB
PL85 0.00 dB
PL86 0.00 dB
PL87 0.00 dB
PL88 0.00 dB
PL89 0.00 dB
PL90 0.00 dB
PL91 0.00 dB
PL92 0.00 dB
PL93 0.00 dB
PL94 0.00 dB
PL95 0.00 dB
PL96 0.00 dB
PL97 0.00 dB
PL98 0.00 dB
PL99 0.00 dB
PL100 0.00 dB

===== CHANNEL f4 =====
NUC4 13C
P1 14.12 sec
PL1 0.00 dB
PL2 0.00 dB
PL3 2000.00 dB
PL4 0.00 dB
PL5 0.00 dB
PL6 -1.00 dB
PL7 0.00 dB
PL8 126.794248 MHz
PL9 0.00 dB
PL10 0.00 dB
PL11 0.00 dB
PL12 0.00 dB
PL13 0.00 dB
PL14 0.00 dB
PL15 0.00 dB
PL16 0.00 dB
PL17 0.00 dB
PL18 0.00 dB
PL19 0.00 dB
PL20 0.00 dB
PL21 0.00 dB
PL22 0.00 dB
PL23 0.00 dB
PL24 0.00 dB
PL25 0.00 dB
PL26 0.00 dB
PL27 0.00 dB
PL28 0.00 dB
PL29 0.00 dB
PL30 0.00 dB
PL31 0.00 dB
PL32 0.00 dB
PL33 0.00 dB
PL34 0.00 dB
PL35 0.00 dB
PL36 0.00 dB
PL37 0.00 dB
PL38 0.00 dB
PL39 0.00 dB
PL40 0.00 dB
PL41 0.00 dB
PL42 0.00 dB
PL43 0.00 dB
PL44 0.00 dB
PL45 0.00 dB
PL46 0.00 dB
PL47 0.00 dB
PL48 0.00 dB
PL49 0.00 dB
PL50 0.00 dB
PL51 0.00 dB
PL52 0.00 dB
PL53 0.00 dB
PL54 0.00 dB
PL55 0.00 dB
PL56 0.00 dB
PL57 0.00 dB
PL58 0.00 dB
PL59 0.00 dB
PL60 0.00 dB
PL61 0.00 dB
PL62 0.00 dB
PL63 0.00 dB
PL64 0.00 dB
PL65 0.00 dB
PL66 0.00 dB
PL67 0.00 dB
PL68 0.00 dB
PL69 0.00 dB
PL70 0.00 dB
PL71 0.00 dB
PL72 0.00 dB
PL73 0.00 dB
PL74 0.00 dB
PL75 0.00 dB
PL76 0.00 dB
PL77 0.00 dB
PL78 0.00 dB
PL79 0.00 dB
PL80 0.00 dB
PL81 0.00 dB
PL82 0.00 dB
PL83 0.00 dB
PL84 0.00 dB
PL85 0.00 dB
PL86 0.00 dB
PL87 0.00 dB
PL88 0.00 dB
PL89 0.00 dB
PL90 0.00 dB
PL91 0.00 dB
PL92 0.00 dB
PL93 0.00 dB
PL94 0.00 dB
PL95 0.00 dB
PL96 0.00 dB
PL97 0.00 dB
PL98 0.00 dB
PL99 0.00 dB
PL100 0.00 dB

Z-restored spin-echo ^{13}C spectrum with ^1H decoupling in C_6D_6 (after pumping)

1H spectrum in CDCl₃

Current Data Parameters
 USER hachne
 NAME KB-II-42
 EXPRNO 2
 PROCNO 1

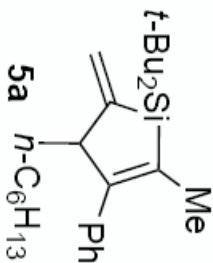
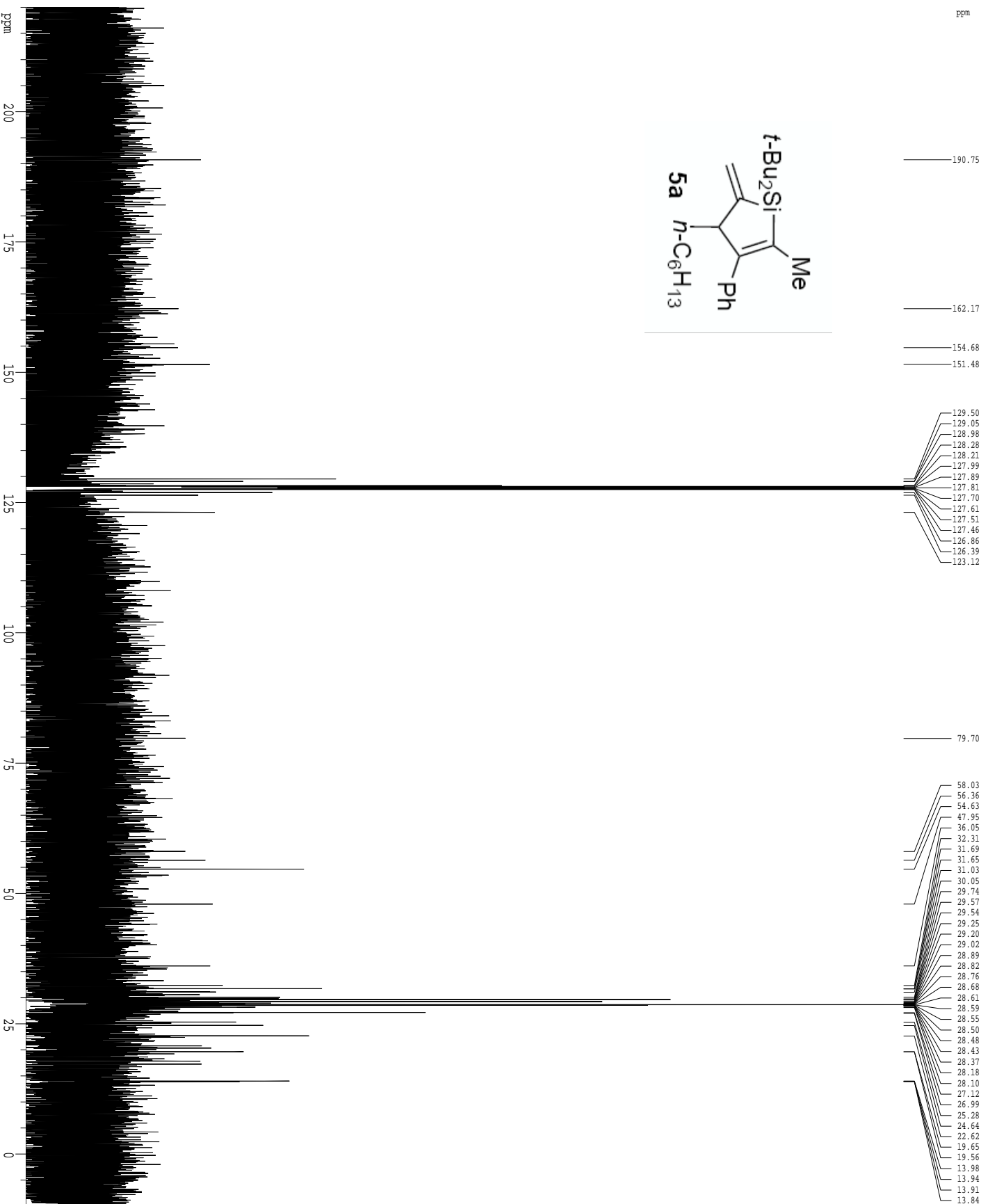
F2 - Acquisition Parameters
 Date_ 20090630
 Time 12.13
 INSTRUM dx400
 PROBRD 5 mm QNP H/P/P
 PULPROG zgpg30
 TD 65536
 SFO1 400.126131
 D0 DULPRXT
 NS 8
 DS 2
 SWH 6410.26 Hz
 FIDRES 0.097813 Hz
 AQ 5.111879 sec
 RG 228.1
 DW 78.000 usec
 DE 4.50 usec
 TE 297.9 K
 D1 0.1000000 sec
 DELT 0.0000000 sec
 ACQRES 0.0150000 sec
 KCMAX

***** CHANNEL f1 *****
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.126131 MHz

F2 - Processing parameters
 SI 65536
 SF 400.126131 MHz
 WDW EM
 SSB 0
 GB 0.30 Hz
 PC 1.00

JD NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 4201.37 Hz
 F2P -1.000 ppm
 F2 -40.13 Hz
 PPMX 0.50459 ppm/cm
 HZCM 201.81996 Hz/cm

Z-restored spin-echo ¹³C spectrum with ¹H decoupling in C6D6



ppm

190.75

162.17

154.68

151.48

129.50

129.05

128.98

128.28

128.21

127.99

127.89

127.81

127.70

127.61

127.51

127.46

126.86

126.39

123.12

79.70

58.03

56.36

54.63

47.95

36.05

32.31

31.69

31.65

31.03

30.05

29.74

29.57

29.54

29.25

29.20

29.02

28.89

28.82

28.76

28.68

28.61

28.59

28.55

28.50

28.48

28.43

28.37

28.18

28.10

27.12

26.99

25.28

24.64

22.62

19.56

19.27

18.91

18.84

```

Current Data Parameters
Date_ 20090818
Time 14.26
INSTRUM cryo500
PROBHD 5 mm CPXI 1H-
PULPROG Spinhirg30pp.prd
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30303.031 Hz
F2 100.626131 MHz
AQ 0.462388 sec
RG 3649.1
DE 16.500 usec
TE 298.15 K
D1 0.250000 sec
d11 0.0002000 sec
d16 0.0002000 sec
d17 0.00019600 sec
WCRES7 0.00000000 sec
WCRES8 0.01500000 sec
P2 29.70 usec

===== CHANNEL f1 =====
NUC1 13C
P1 14.00 usec
PL1 500.00 usec
P2 2000.00 usec
PL2 120.00 dB
PL1 -1.00 dB
SFO1 125.794548 MHz
SFO2 500.2225011 MHz
SE1 3.60 dB
SE2 3.60 dB
SFO1M1 Cp60 0.5, 50.1
SFO1M2 Cp60 0.5, 50.1
SFO1M3 Cp60 0.5, 50.1
SFO1M4 Cp60 0.5, 50.1
SFO1M5 Cp60 0.5, 50.1
SFO1M6 Cp60 0.5, 50.1
SFO1M7 Cp60 0.5, 50.1
SFO1M8 Cp60 0.5, 50.1
SFO1M9 Cp60 0.5, 50.1
SFO1M10 Cp60 0.5, 50.1
SFO1M11 Cp60 0.5, 50.1
SFO1M12 Cp60 0.5, 50.1
SFO1M13 Cp60 0.5, 50.1
SFO1M14 Cp60 0.5, 50.1
SFO1M15 Cp60 0.5, 50.1
SFO1M16 Cp60 0.5, 50.1
SFO1M17 Cp60 0.5, 50.1
SFO1M18 Cp60 0.5, 50.1
SFO1M19 Cp60 0.5, 50.1
SFO1M20 Cp60 0.5, 50.1
SFO1M21 Cp60 0.5, 50.1
SFO1M22 Cp60 0.5, 50.1
SFO1M23 Cp60 0.5, 50.1
SFO1M24 Cp60 0.5, 50.1
SFO1M25 Cp60 0.5, 50.1
SFO1M26 Cp60 0.5, 50.1
SFO1M27 Cp60 0.5, 50.1
SFO1M28 Cp60 0.5, 50.1
SFO1M29 Cp60 0.5, 50.1
SFO1M30 Cp60 0.5, 50.1
SFO1M31 Cp60 0.5, 50.1
SFO1M32 Cp60 0.5, 50.1
SFO1M33 Cp60 0.5, 50.1
SFO1M34 Cp60 0.5, 50.1
SFO1M35 Cp60 0.5, 50.1
SFO1M36 Cp60 0.5, 50.1
SFO1M37 Cp60 0.5, 50.1
SFO1M38 Cp60 0.5, 50.1
SFO1M39 Cp60 0.5, 50.1
SFO1M40 Cp60 0.5, 50.1
SFO1M41 Cp60 0.5, 50.1
SFO1M42 Cp60 0.5, 50.1
SFO1M43 Cp60 0.5, 50.1
SFO1M44 Cp60 0.5, 50.1
SFO1M45 Cp60 0.5, 50.1
SFO1M46 Cp60 0.5, 50.1
SFO1M47 Cp60 0.5, 50.1
SFO1M48 Cp60 0.5, 50.1
SFO1M49 Cp60 0.5, 50.1
SFO1M50 Cp60 0.5, 50.1
SFO1M51 Cp60 0.5, 50.1
SFO1M52 Cp60 0.5, 50.1
SFO1M53 Cp60 0.5, 50.1
SFO1M54 Cp60 0.5, 50.1
SFO1M55 Cp60 0.5, 50.1
SFO1M56 Cp60 0.5, 50.1
SFO1M57 Cp60 0.5, 50.1
SFO1M58 Cp60 0.5, 50.1
SFO1M59 Cp60 0.5, 50.1
SFO1M60 Cp60 0.5, 50.1
SFO1M61 Cp60 0.5, 50.1
SFO1M62 Cp60 0.5, 50.1
SFO1M63 Cp60 0.5, 50.1
SFO1M64 Cp60 0.5, 50.1
SFO1M65 Cp60 0.5, 50.1
SFO1M66 Cp60 0.5, 50.1
SFO1M67 Cp60 0.5, 50.1
SFO1M68 Cp60 0.5, 50.1
SFO1M69 Cp60 0.5, 50.1
SFO1M70 Cp60 0.5, 50.1
SFO1M71 Cp60 0.5, 50.1
SFO1M72 Cp60 0.5, 50.1
SFO1M73 Cp60 0.5, 50.1
SFO1M74 Cp60 0.5, 50.1
SFO1M75 Cp60 0.5, 50.1
SFO1M76 Cp60 0.5, 50.1
SFO1M77 Cp60 0.5, 50.1
SFO1M78 Cp60 0.5, 50.1
SFO1M79 Cp60 0.5, 50.1
SFO1M80 Cp60 0.5, 50.1
SFO1M81 Cp60 0.5, 50.1
SFO1M82 Cp60 0.5, 50.1
SFO1M83 Cp60 0.5, 50.1
SFO1M84 Cp60 0.5, 50.1
SFO1M85 Cp60 0.5, 50.1
SFO1M86 Cp60 0.5, 50.1
SFO1M87 Cp60 0.5, 50.1
SFO1M88 Cp60 0.5, 50.1
SFO1M89 Cp60 0.5, 50.1
SFO1M90 Cp60 0.5, 50.1
SFO1M91 Cp60 0.5, 50.1
SFO1M92 Cp60 0.5, 50.1
SFO1M93 Cp60 0.5, 50.1
SFO1M94 Cp60 0.5, 50.1
SFO1M95 Cp60 0.5, 50.1
SFO1M96 Cp60 0.5, 50.1
SFO1M97 Cp60 0.5, 50.1
SFO1M98 Cp60 0.5, 50.1
SFO1M99 Cp60 0.5, 50.1
SFO1M100 Cp60 0.5, 50.1
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 usec
PL2 2.00 dB
PL1 2.00 dB
SFO2 500.2225011 MHz

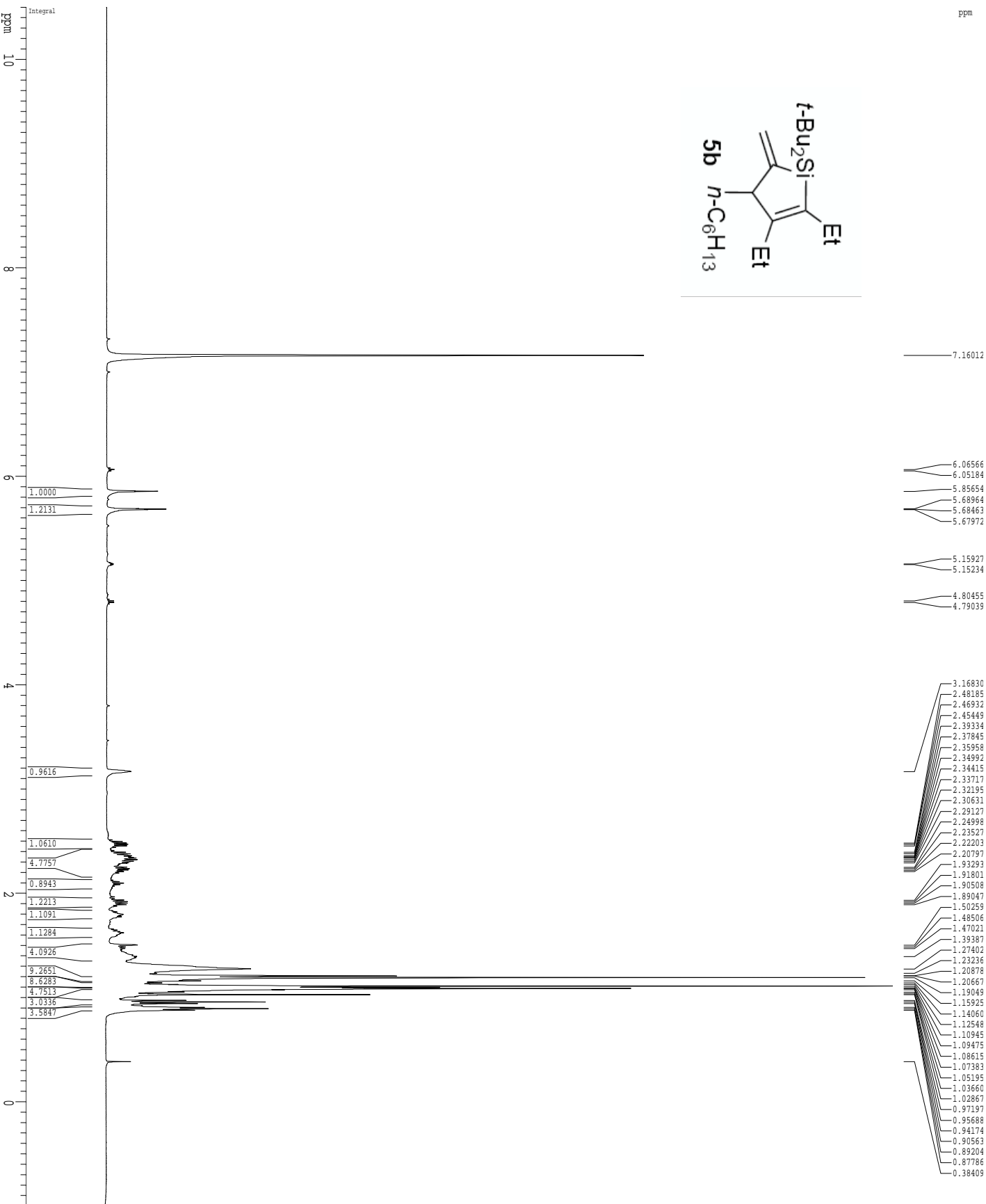
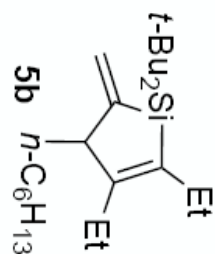
===== GRADIENT CHANNEL =====
GRNMA1 SINE:100
GRNMA2 SINE:100
GRX1 0.00 %
GRX2 0.00 %
GRY1 0.00 %
GRY2 0.00 %
GRZ1 0.00 %
GRZ2 30.00 %
GRZ3 50.00 %
p15 500.00 usec
p16 1000.00 usec

F2 - Processing parameters
SI 65336
SF 125.794548 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

ID NMR plot parameters
CX 22.80 cm
CY 10.00 cm
TZ 230.00 cm
FT 2701.68 Hz
F1 -10.000 ppm
F2 -1257.80 Hz
PRGCM HZCM
HZCM 1268.8365 Hz/cm
    
```

1H spectrum in CDCl₃

ppm



Current Data Parameters
 USER buchoe
 NAME KB-111-22
 EXPRNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090609
 Time 17.55

INSTRUM cryo500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 4930
 SFO1 500.136410 MHz
 F2 500.136410 MHz
 CQX1 8
 NS 2
 DS 2

SWH 8012.820 Hz
 FIDRES 0.098083 Hz
 AQ 5.0998774 sec
 RG 5.7

DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K

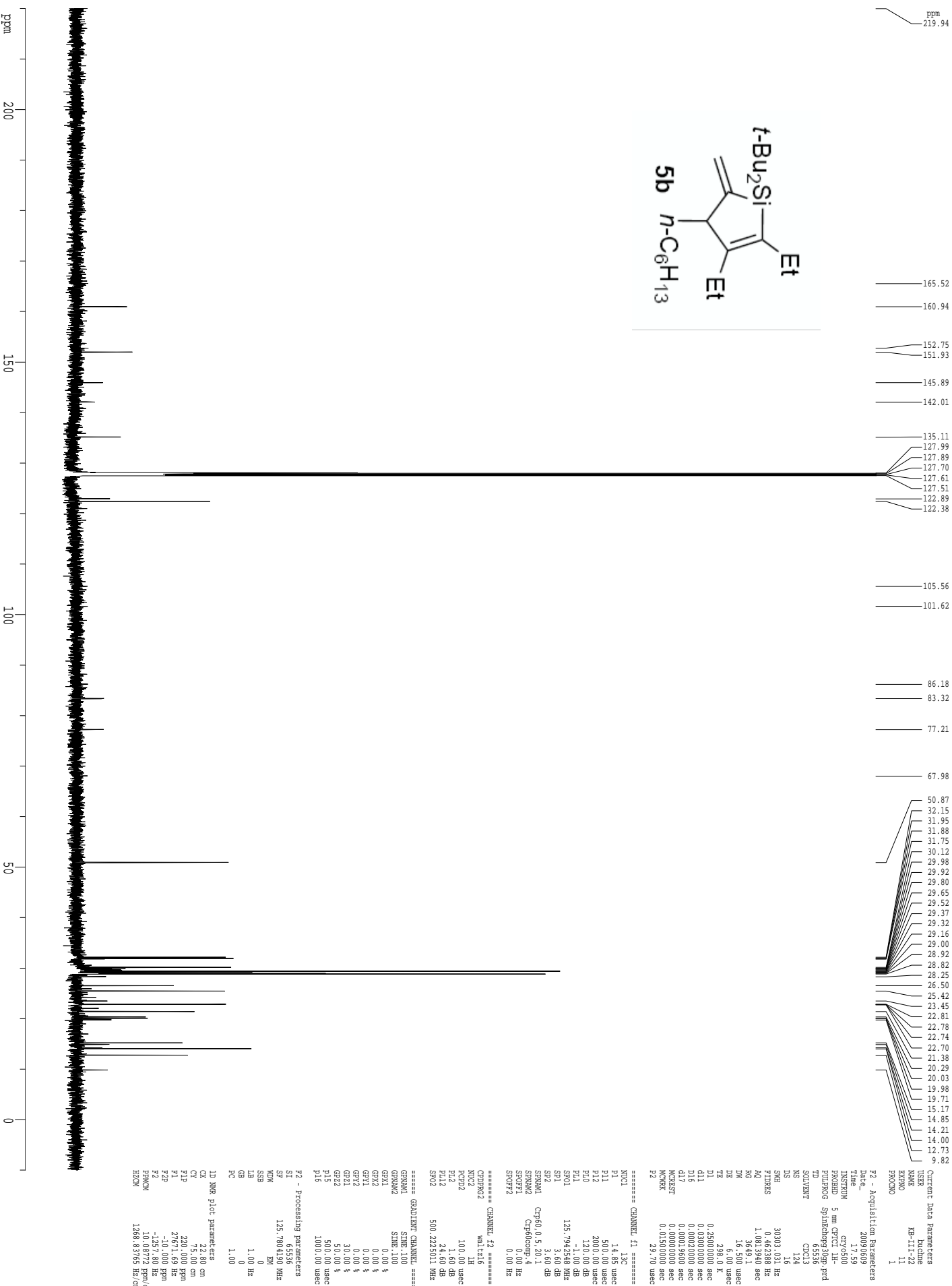
DI 0.1000000 sec
 ACQST 0.0000000 sec
 KCXST 0.0150000 sec

KCMXK 0.0150000 sec

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

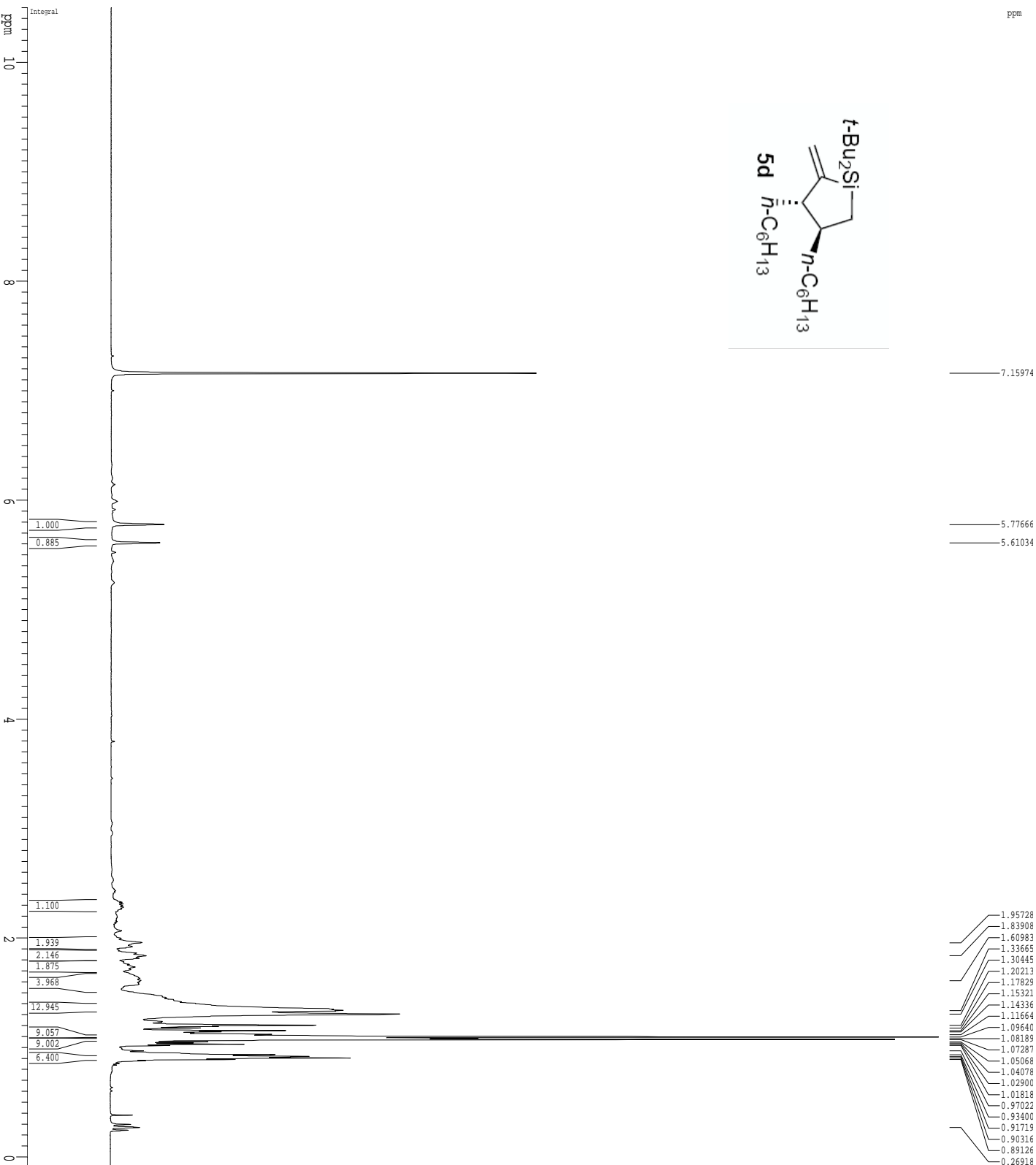
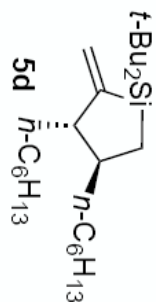
F2 - Processing parameters
 SI 65536
 SF 500.220000 MHz
 WDW EM
 SSB 0
 GB 0
 LB 0.30 Hz
 PC 1.00

JD NMR plot parameters
 CY 22.80 cm
 CV 15.00 cm
 F1P 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -500.22 Hz
 PPM/CM 0.50459 ppm/cm
 HZ/CM 252.30396 Hz/cm

Z-restored spin-echo ^{13}C spectrum with ^1H decoupling (in C_6D_6 after vacuum for 4h)

1H spectrum in CDCl₃

ppm



Current Data Parameters
 USER hachne
 NAME KB-II-40
 EXPMO 2
 PROCNO 1

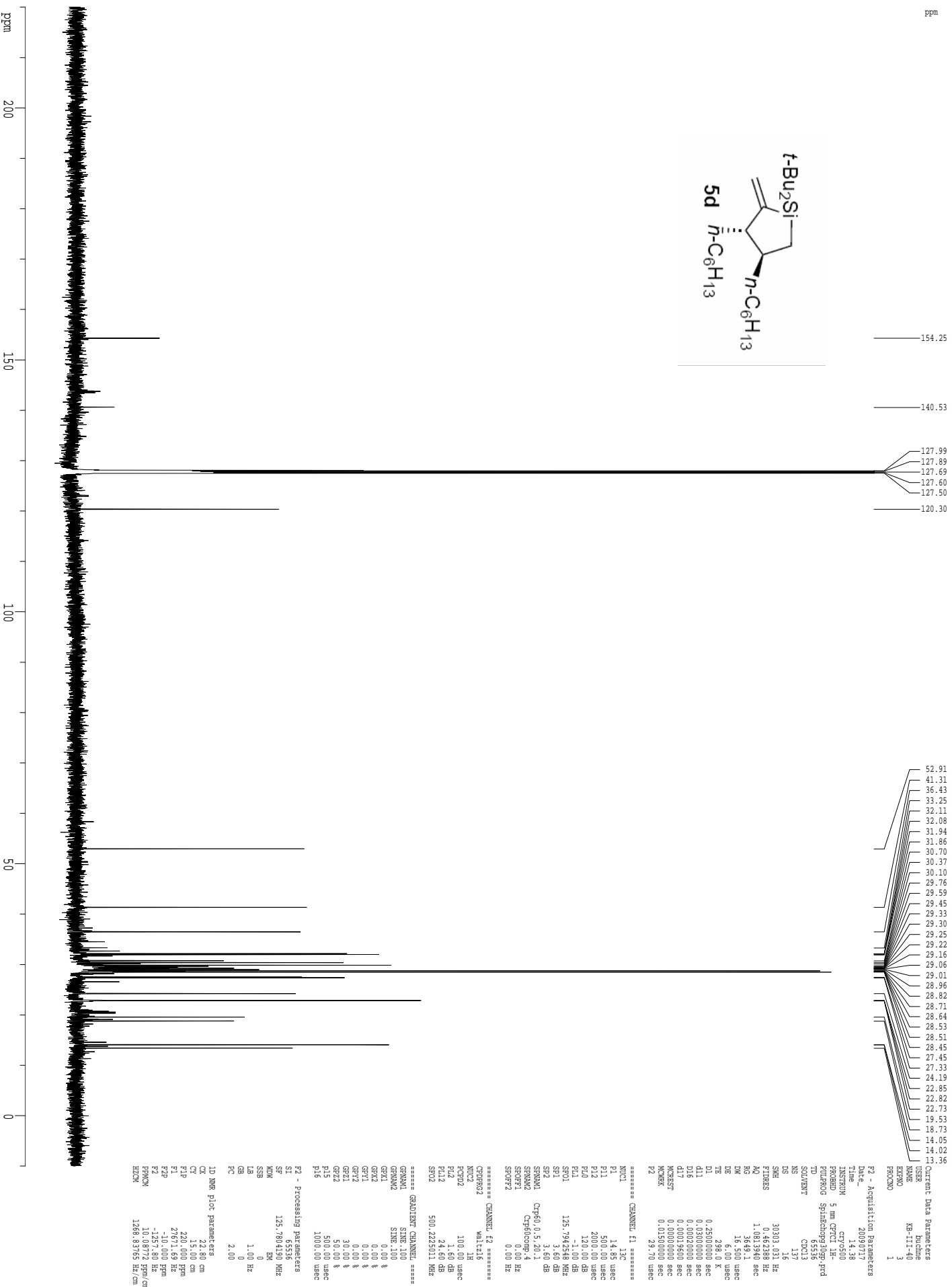
F2 - Acquisition Parameters
 Date_ 20090717
 Time 14.34

INSTRM cryo500
 PROBD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 4920
 SFO1 500.136261
 F2 500.136261
 D0 11.23
 D1 1.23
 D2 0.000000
 D3 0.000000
 D4 0.000000
 D5 0.000000
 D6 0.000000
 D7 0.000000
 D8 0.000000
 D9 0.000000
 D10 0.000000
 D11 0.000000
 D12 0.000000
 D13 0.000000
 D14 0.000000
 D15 0.000000
 D16 0.000000
 D17 0.000000
 D18 0.000000
 D19 0.000000
 D20 0.000000
 D21 0.000000
 D22 0.000000
 D23 0.000000
 D24 0.000000
 D25 0.000000
 D26 0.000000
 D27 0.000000
 D28 0.000000
 D29 0.000000
 D30 0.000000
 D31 0.000000
 D32 0.000000
 D33 0.000000
 D34 0.000000
 D35 0.000000
 D36 0.000000
 D37 0.000000
 D38 0.000000
 D39 0.000000
 D40 0.000000
 D41 0.000000
 D42 0.000000
 D43 0.000000
 D44 0.000000
 D45 0.000000
 D46 0.000000
 D47 0.000000
 D48 0.000000
 D49 0.000000
 D50 0.000000
 D51 0.000000
 D52 0.000000
 D53 0.000000
 D54 0.000000
 D55 0.000000
 D56 0.000000
 D57 0.000000
 D58 0.000000
 D59 0.000000
 D60 0.000000
 D61 0.000000
 D62 0.000000
 D63 0.000000
 D64 0.000000
 D65 0.000000
 D66 0.000000
 D67 0.000000
 D68 0.000000
 D69 0.000000
 D70 0.000000
 D71 0.000000
 D72 0.000000
 D73 0.000000
 D74 0.000000
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 D80 0.000000
 D81 0.000000
 D82 0.000000
 D83 0.000000
 D84 0.000000
 D85 0.000000
 D86 0.000000
 D87 0.000000
 D88 0.000000
 D89 0.000000
 D90 0.000000
 D91 0.000000
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 D95 0.000000
 D96 0.000000
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 D98 0.000000
 D99 0.000000
 D100 0.000000

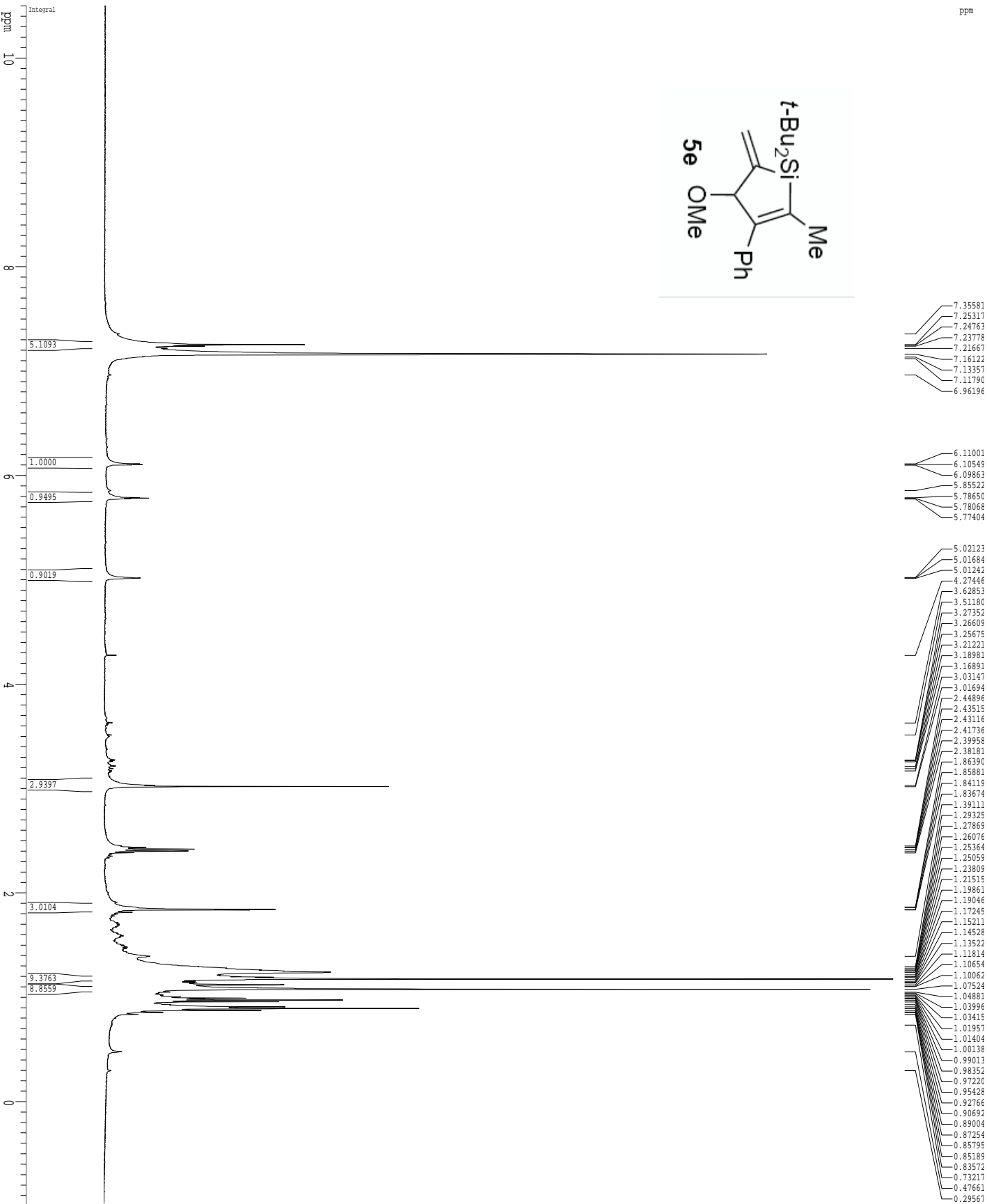
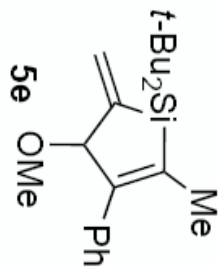
===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2235015 MHz

F2 - Processing parameters
 SI 65536
 SF 500.220000 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 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -500.22 Hz
 PPM/CM 0.50459 ppm/cm
 HZ/CM 252.30396 Hz/cm

Z-restored spin-echo ^{13}C spectrum with ^1H decoupling in C_6D_6 

¹H spectrum in CDCl₃



- 7.35581
- 7.25317
- 7.24763
- 7.23778
- 7.21667
- 7.16122
- 7.13357
- 7.11790
- 6.96196
- 6.11001
- 6.10549
- 6.09863
- 5.85522
- 5.78650
- 5.78068
- 5.77404
- 5.02123
- 5.01684
- 5.01242
- 4.27446
- 3.62853
- 3.51180
- 3.27352
- 3.26609
- 3.25675
- 3.23221
- 3.18961
- 3.16891
- 3.03147
- 3.01694
- 2.44896
- 2.43515
- 2.43116
- 2.41736
- 2.39958
- 2.38181
- 1.86390
- 1.85881
- 1.84119
- 1.83674
- 1.39111
- 1.29325
- 1.27869
- 1.26076
- 1.25364
- 1.25059
- 1.23809
- 1.23515
- 1.19861
- 1.19046
- 1.17245
- 1.15211
- 1.14528
- 1.13522
- 1.11814
- 1.10654
- 1.10062
- 1.07524
- 1.04881
- 1.03996
- 1.03415
- 1.01957
- 1.01404
- 1.00138
- 0.99013
- 0.98352
- 0.97220
- 0.95428
- 0.92766
- 0.90692
- 0.89004
- 0.87825
- 0.85795
- 0.85189
- 0.83572
- 0.73217
- 0.47661
- 0.29567

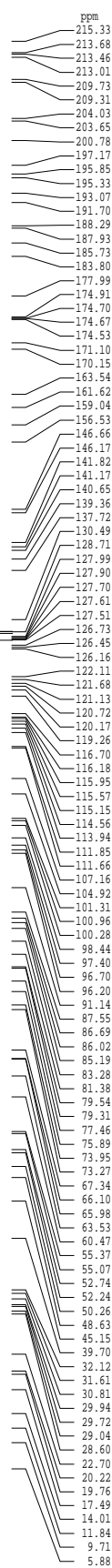
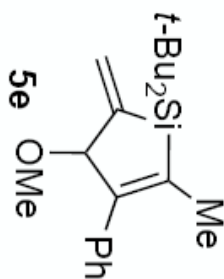
Current Data Parameters
 USER buche
 NAME KB-1-80
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080522
 Time 18.25
 INSTRUM dx400
 PROBRD 5 mm QNP H/P/P
 F2P1 420.13
 F2P2 100.625
 TD 65536
 SFO1 400.126009 MHz
 CQ1 2
 NS 2
 DS 2
 SWH 6410.26 Hz
 FIDRES 0.097813 Hz
 AQ 5.111879 sec
 RG 228.1
 DW 78.000 usec
 DE 4.50 usec
 TE 298.0 K
 D1 0.1000000 sec
 DELTA 0.0000000 sec
 ACQRESPT 0.0150000 sec
 KCMAX 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.126009 MHz

F2 - Processing parameters
 SI 65536
 SF 400.126009 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 10.500 ppm
 F1 4201.37 Hz
 F2P -1.000 ppm
 F2 -40.13 Hz
 PPM/CM 0.50439 ppm/cm
 HZ/CM 201.81996 Hz/cm

¹³C spectrum with ¹H decoupling

Current Data Parameters
 USER buchner
 NAME KP-1-180
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080523
 Time 11.38
 INSTRUM cryo500
 PROBRD 5 mm CPTCI 1H-
 PULPROG zgpg30
 TD 65418
 SOLVENT CDCl3
 NS 540
 DS 4
 SM 30303.001 Hz
 SFO 125.762222 Hz
 FIDRES 0.162472 Hz
 AQ 1.073231 sec
 RQ 3251
 DW 16.500 usec
 DE 6.100 usec
 TE 298.0 K

TD 0.25000000 sec
 D1 0.03000000 sec
 d11 0.03000000 sec
 NUC1 13C
 NUC2 13C
 NUC3 13C
 P1 14.75 usec
 P11 -1.00 dB
 P12 125.7942948 MHz
 SFO1 125.7942948 MHz

===== CHANNEL f1 =====
 NUC1 13C
 P1 14.75 usec
 P11 -1.00 dB
 P12 125.7942948 MHz
 SFO1 125.7942948 MHz

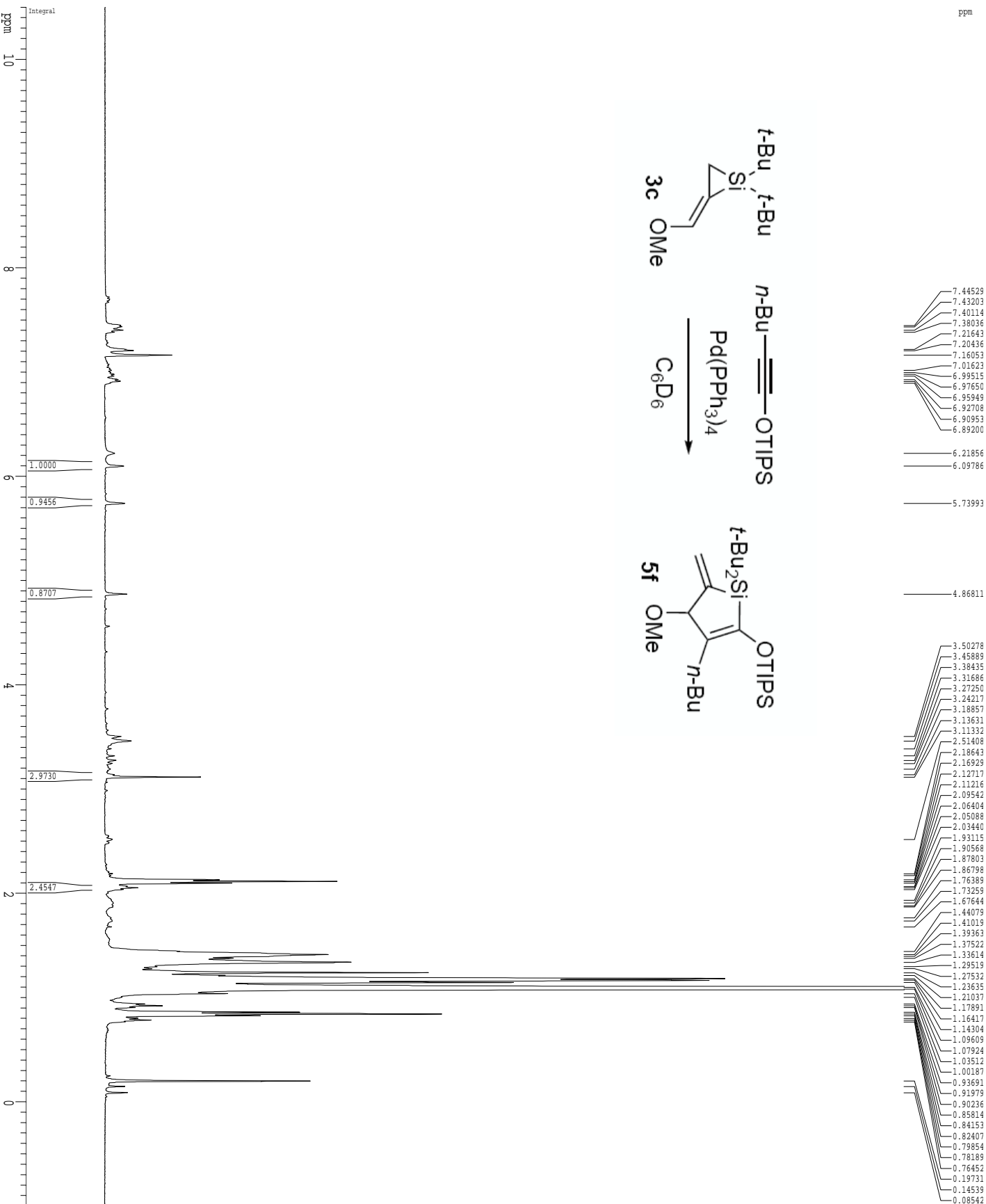
===== CHANNEL f2 =====
 NUC2 13C
 P2 100.00 usec
 P21 1.60 dB
 P22 24.80 dB
 SFO2 500.225011 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7804190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

JD NMR plot parameters
 CX 42.80 cm
 CY 42.80 cm
 F1P 13.00 cm
 F1D 220.00 cm
 F1 2671.69 ppm
 F2P -10.000 ppm
 F2 -1257.80 Hz
 PPMCM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm

ppm

1H spectrum in C6D6



Current Data Parameters
 USER buchoe
 NAME KB-1-16
 EXPNO 2
 PROCNO 1

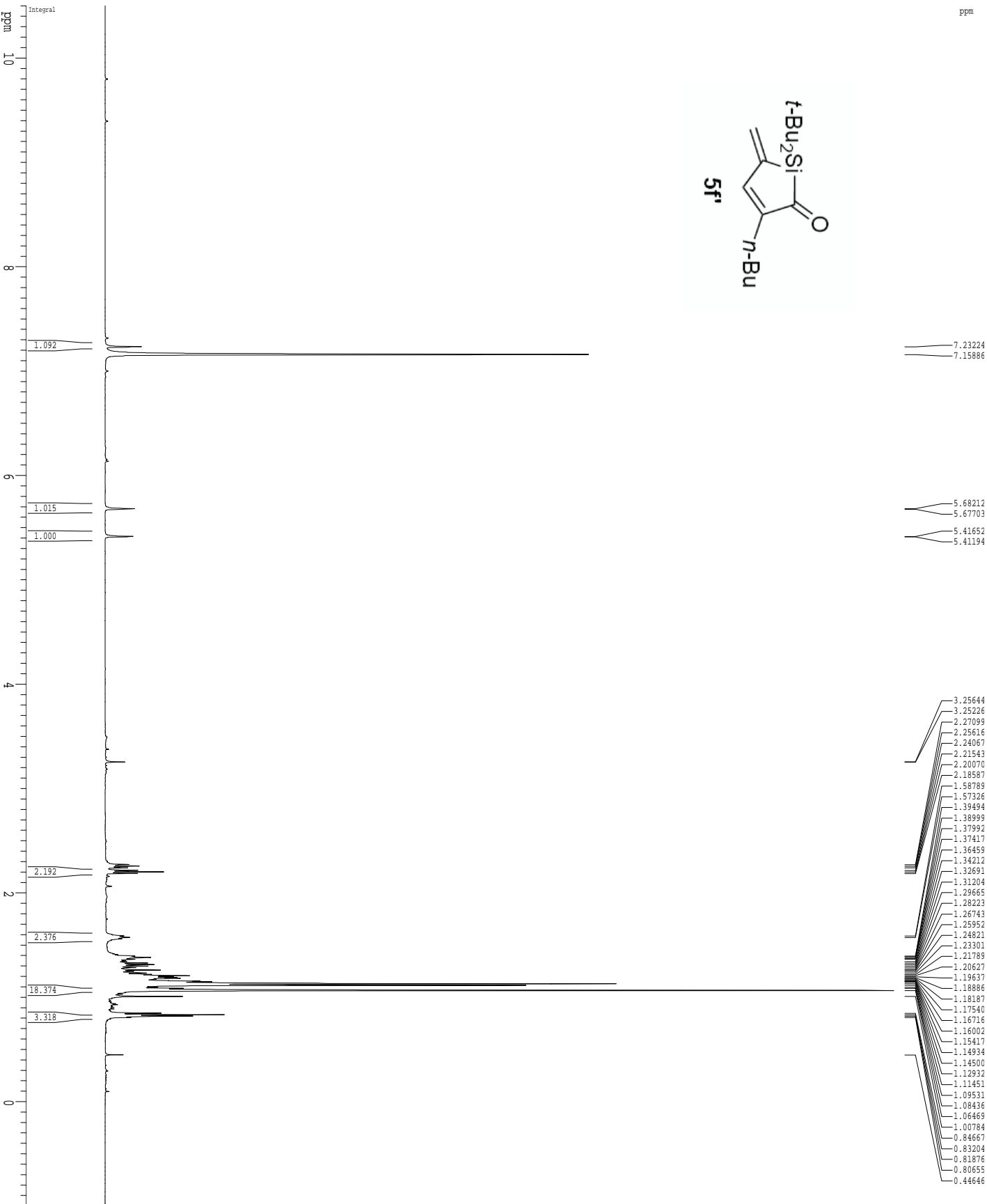
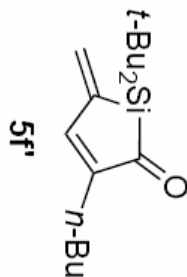
P2 - Acquisition Parameters
 Date_ 20080216
 Time 9:32
 INSTRUM dx400
 PROBRD 5 mm QNP H/P/P
 F1 420.137 Hz
 F2 -1.000 ppm
 TD 65536
 SFO1 400.128009 MHz
 D0 0.000000 sec
 D1 0.100000 sec
 DE 4.50 usec
 TE 297.9 K
 DI 0.100000 sec
 ACQ 5.118579 sec
 RG 18
 DW 78.000 usec
 DR 0.000000 sec
 KEYSF 0.000000 sec
 KCMAX 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.128009 MHz

P2 - Processing parameters
 SI 65536
 SF 400.128009 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ID NMR parameters
 CX 22.80 cm
 CY 50.00 cm
 FIP 10.500 ppm
 F1 4201.37 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCKM 0.50459 ppm/cm
 HZCM 2011.81996 Hz/cm

¹H spectrum in CDCl₃

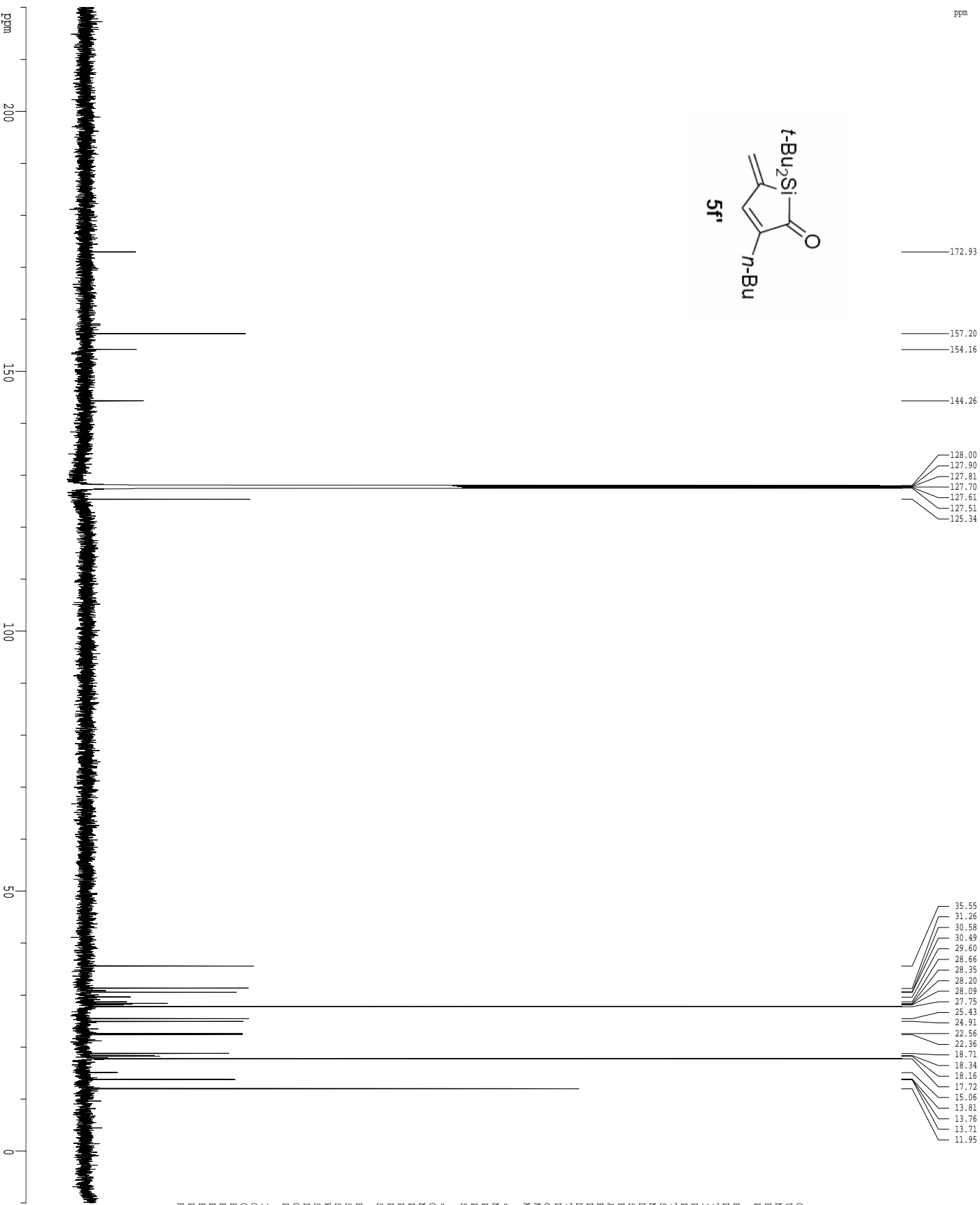
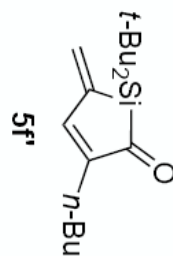


Current Data Parameters
 USER buchoe
 NAME KB-1-45
 EXPRNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080919
 Time 17:06
 INSTRUM crys500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 4920
 SFO 500.136261
 TO 1728
 T1 2.00
 T2 0.10
 T3 0.10
 T4 0.10
 T5 0.10
 T6 0.10
 T7 0.10
 T8 0.10
 T9 0.10
 T10 0.10
 T11 0.10
 T12 0.10
 T13 0.10
 T14 0.10
 T15 0.10
 T16 0.10
 T17 0.10
 T18 0.10
 T19 0.10
 T20 0.10
 T21 0.10
 T22 0.10
 T23 0.10
 T24 0.10
 T25 0.10
 T26 0.10
 T27 0.10
 T28 0.10
 T29 0.10
 T30 0.10
 T31 0.10
 T32 0.10
 T33 0.10
 T34 0.10
 T35 0.10
 T36 0.10
 T37 0.10
 T38 0.10
 T39 0.10
 T40 0.10
 T41 0.10
 T42 0.10
 T43 0.10
 T44 0.10
 T45 0.10
 T46 0.10
 T47 0.10
 T48 0.10
 T49 0.10
 T50 0.10
 T51 0.10
 T52 0.10
 T53 0.10
 T54 0.10
 T55 0.10
 T56 0.10
 T57 0.10
 T58 0.10
 T59 0.10
 T60 0.10
 T61 0.10
 T62 0.10
 T63 0.10
 T64 0.10
 T65 0.10
 T66 0.10
 T67 0.10
 T68 0.10
 T69 0.10
 T70 0.10
 T71 0.10
 T72 0.10
 T73 0.10
 T74 0.10
 T75 0.10
 T76 0.10
 T77 0.10
 T78 0.10
 T79 0.10
 T80 0.10
 T81 0.10
 T82 0.10
 T83 0.10
 T84 0.10
 T85 0.10
 T86 0.10
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 T89 0.10
 T90 0.10
 T91 0.10
 T92 0.10
 T93 0.10
 T94 0.10
 T95 0.10
 T96 0.10
 T97 0.10
 T98 0.10
 T99 0.10
 T100 0.10

F2 - Processing parameters
 SI 65536
 SF 500.220000 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 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -500.22 Hz
 PPM/CM 0.50459 ppm/cm
 HZ/CM 252.30396 Hz/cm

¹³C spectrum with ¹H decoupling in C6D6

Current Data Parameters
 USER Name
 NAME KP-11-45
 EXPNO 2
 PROCNO 1

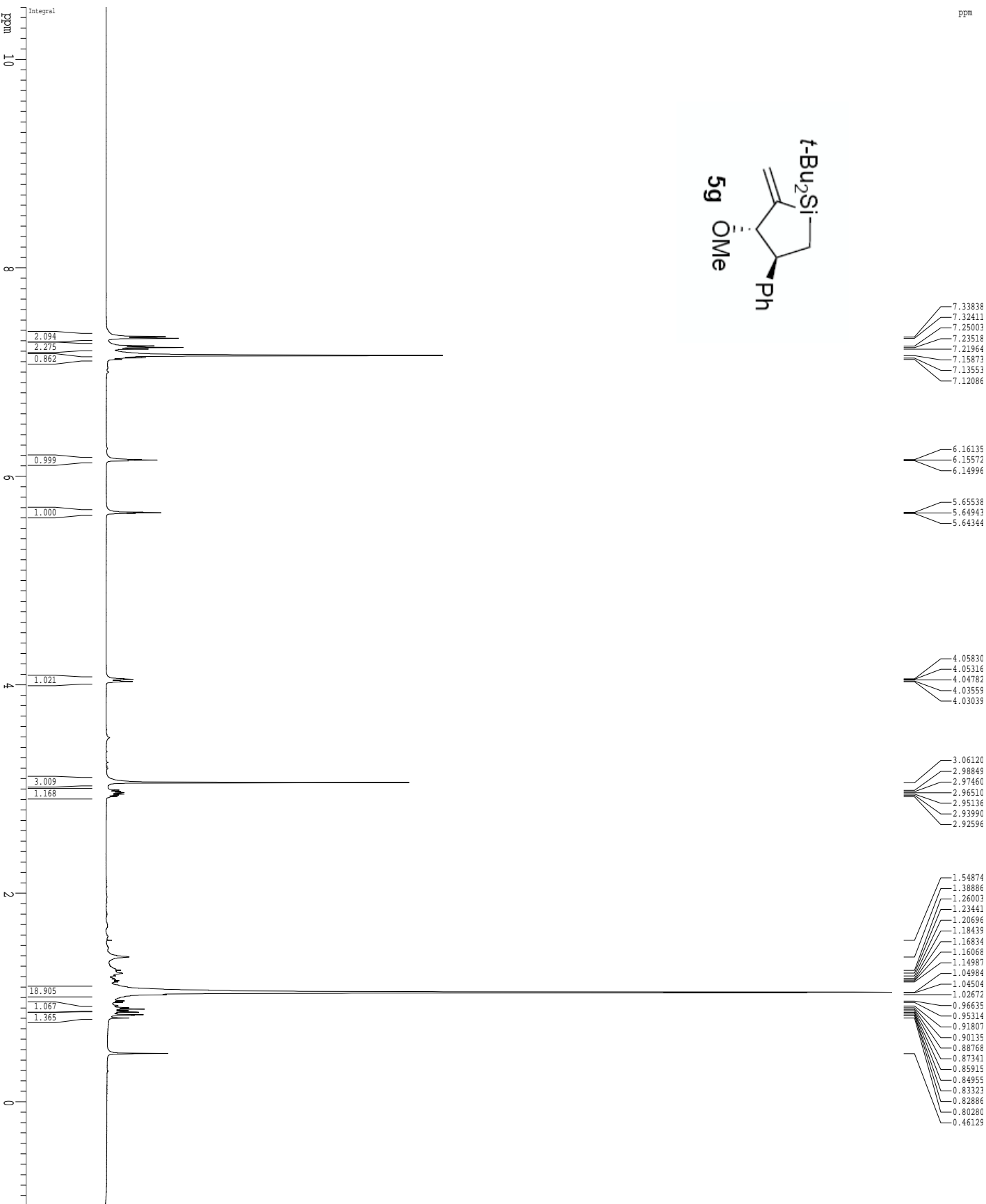
F2 - Acquisition Parameters
 Date_ 20080919
 Time 17.09
 INSTRUM cryo500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65418
 SOLVENT CDCl3
 NS 223
 DS 4
 SFO 303.031 MHz
 FIDRES 0.162472 Hz
 AQ 1.078472 sec
 RQ 3251
 DW 16.500 usec
 DE 6.100 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 NUCBR1 0.00000000 sec
 NUCBR2 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 14.75 usec
 PL1 -1.00 dB
 SFO1 125.7942949 MHz

===== CHANNEL f2 =====
 NUC2 ¹³C
 P2 100.00 usec
 PL2 1.60 dB
 SFO2 500.225011 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7894190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

JD NMR plot parameters
 CX 2.80 cm
 CY 2.80 cm
 F1D 202.00 cm
 F1 2767.69 ppm
 F2P -10.000 ppm
 F2 -1257.80 Hz
 PPMCM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm

1H spectrum in CDCl₃

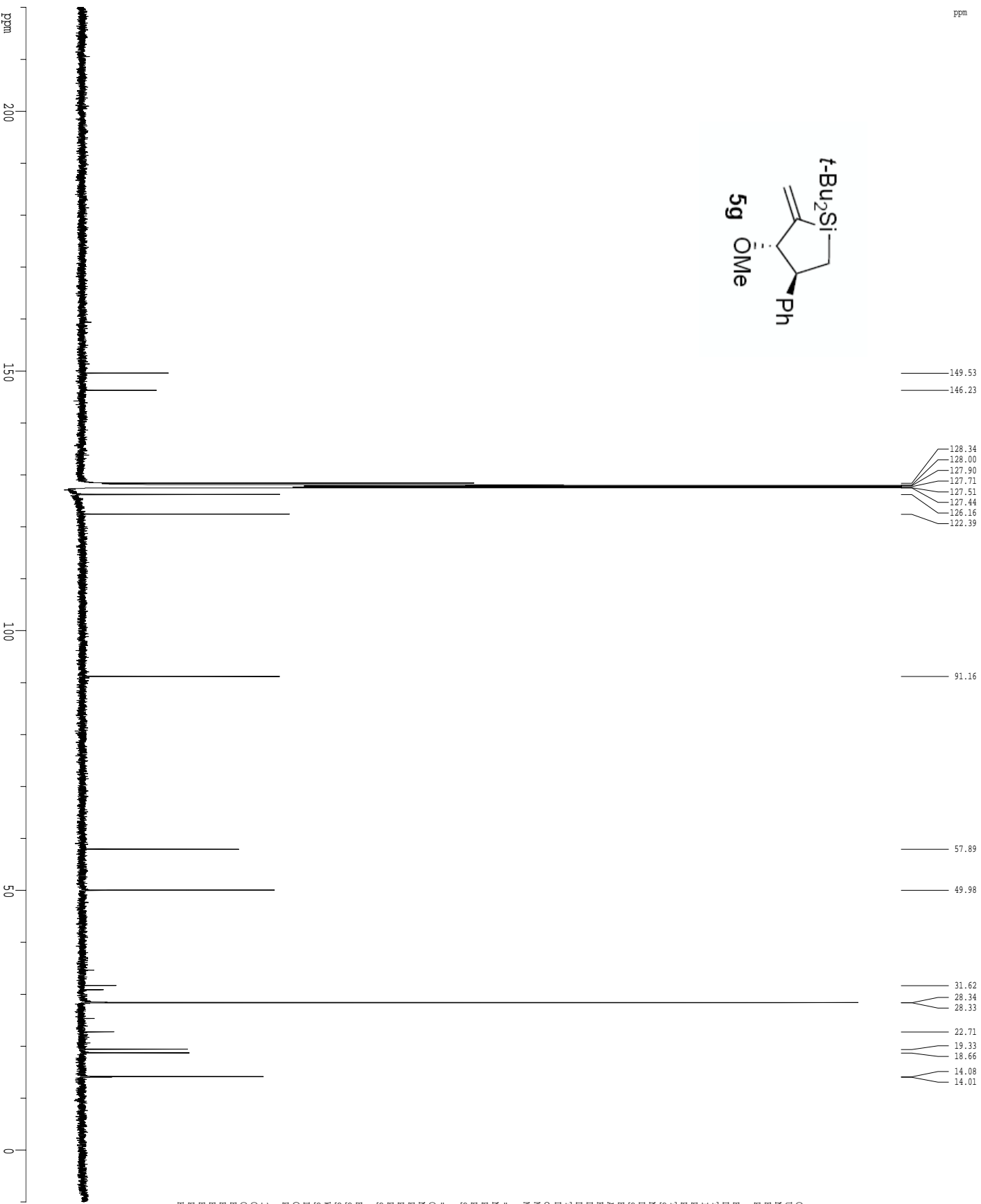
Current Data Parameters
 USER buchu
 NAME KB-1-43
 EXPRNO 2
 PROCNO 1

P2 - Acquisition Parameters
 Date_ 20080915
 Time 16:06
 INSTRM cryo500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 4920
 SFO 500.136261
 F2 500.136261
 D0 8128
 CQX1 8
 NS 2
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098083 Hz
 AQ 5.0998774 sec
 RG 4
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.1000000 sec
 MRESST 0.0000000 sec
 KCMAX 0.0150000 sec

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

P2 - Processing parameters
 SI 65536
 SF 500.220000 MHz
 WDW EM
 SSB 0
 GB 0.30 Hz
 LB 0
 PC 1.00

ID NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -500.22 Hz
 PPMCM 0.50459 ppm/cm
 HZCM 252.30396 Hz/cm

¹³C spectrum with ¹H decoupling in C6D6

Current Data Parameters
 USER kbr
 NAME KP-11-43
 EXPNO 3
 PROCNO 1

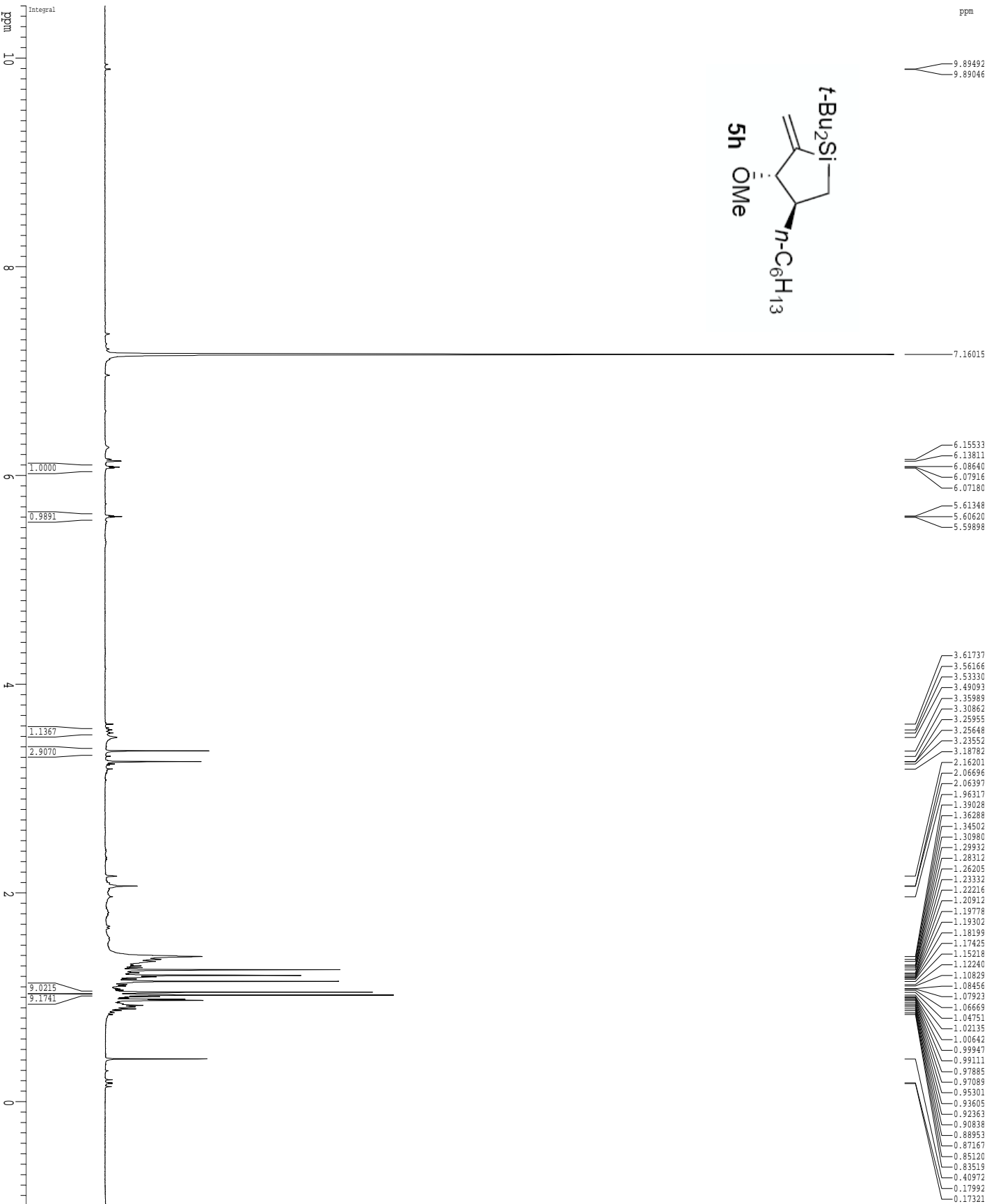
F2 - Acquisition Parameters
 Date_ 20080915
 Time 16.10
 INSTRUM cryo500
 PROBHD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65418
 SOLVENT CDCl3
 NS 231
 DS 4
 SWH 3030.031 Hz
 FIDRES 0.162472 Hz
 AQ 1.078272 sec
 RG 3251
 DW 16.500 usec
 DE 6.100 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 NUCERST 0.00000000 sec
 MCNCRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 14.75 usec
 PL1 -1.00 dB
 SFO1 125.7942948 MHz

===== CHANNEL f2 =====
 NUC2 ¹³C
 P2 100.00 usec
 PL2 1.60 dB
 SFO2 500.225011 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7804190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

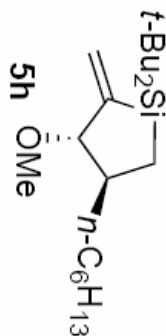
JD NMR plot parameters
 CX 42.80 cm
 CY 4.00 cm
 P1D 13.00 cm
 P1B 220.00 ppm
 F1 2767.69 Hz
 F2P -10.000 ppm
 F2 -1257.80 Hz
 PPMCM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm

1H spectrum in CDCl₃

ppm

9.89492
9.89046

7.16015

6.15533
6.13811
6.08640
6.07916
6.07180
5.61348
5.60620
5.598983.61737
3.56166
3.53330
3.49093
3.35989
3.30862
3.25955
3.25648
3.23552
3.18782
2.16201
2.06696
2.06397
1.96317
1.39028
1.36288
1.34502
1.30980
1.29932
1.28312
1.26205
1.23332
1.22216
1.20912
1.18778
1.18302
1.18199
1.17425
1.15218
1.12240
1.10829
1.08456
1.07923
1.06669
1.04751
1.02135
1.00642
0.99947
0.99111
0.97885
0.97089
0.95301
0.93605
0.92363
0.90838
0.88953
0.87167
0.85120
0.83519
0.40972
0.17992
0.17321

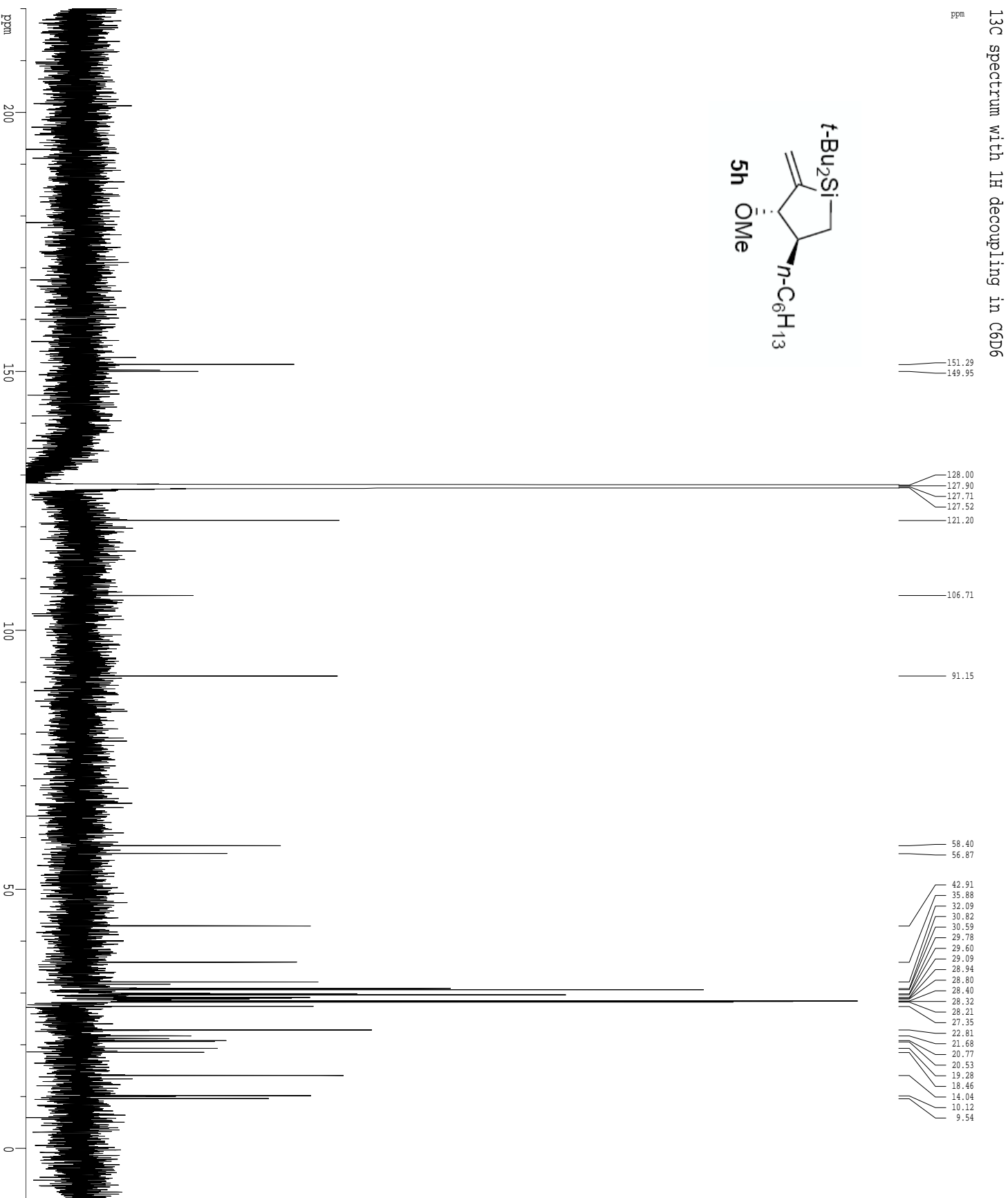
Current Data Parameters
 USER buchoe
 NAME KB-1-52
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081003
 Time 18.25
 INSTRUM dx400
 PROBRD 5 mm QNP H/P/P
 EPROBHD zgpg30
 PULPROG zgpg30
 TD 65536
 SFO1 400.126000 MHz
 NS 8
 DS 2
 SWH 6410.256 Hz
 FIDRES 0.097813 Hz
 AQ 5.111879 sec
 RG 256
 DE 78.000 usec
 DW 4.50 usec
 TE 298.0 K
 D1 0.1000000 sec
 KICKST 0.0000000 sec
 KICKAX 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.126000 MHz

F2 - Processing parameters
 SI 65536
 SF 400.126000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

JD NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 4201.37 Hz
 F2P -1.000 ppm
 F2 -40.13 Hz
 PPMCM 0.50439 ppm/cm
 HZCM 201.81996 Hz/cm



Current Data Parameters
 USER Name
 NAME KP-11-42
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081014
 Time 14.05
 INSTRUM cryo500
 PROBHD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65418
 SOLVENT CDCl3
 NS 364
 DS 4
 SWH 3033.031 Hz
 FIDRES 0.162472 Hz
 AQ 1.079277 sec
 RG 3251
 DW 16.500 usec
 DE 6.100 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 NUC1 13C
 NUC2 1H
 MCKEY 0.01500000 sec

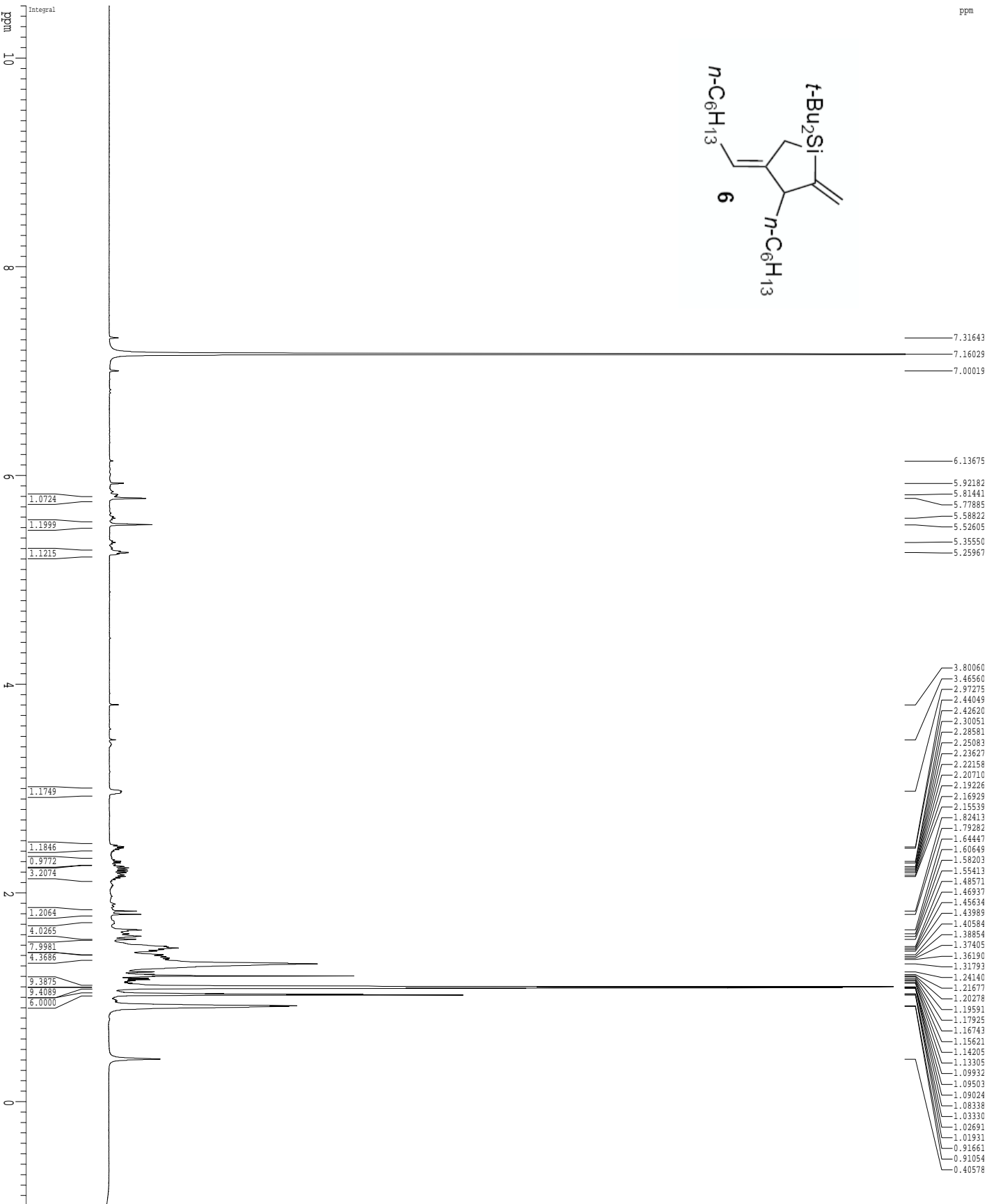
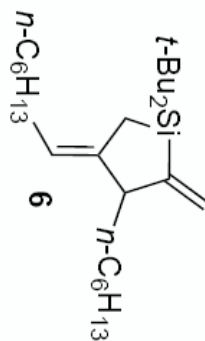
===== CHANNEL f1 =====
 NUC1 13C
 P1 14.85 usec
 PL1 -1.00 dB
 SFO1 125.7942949 MHz

===== CHANNEL f2 =====
 NUC2 1H
 P2 100.00 usec
 PL2 1.60 dB
 SFO2 500.225011 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7894190 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

JD NMR plot parameters
 CX 42.80 cm
 CY 4.00 cm
 F1D 13.00 cm
 F1D 228.000 ppm
 F1 2767.69 Hz
 F2P -10.000 ppm
 F2 -1257.80 Hz
 PCKM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm

¹H spectrum in CDCl₃



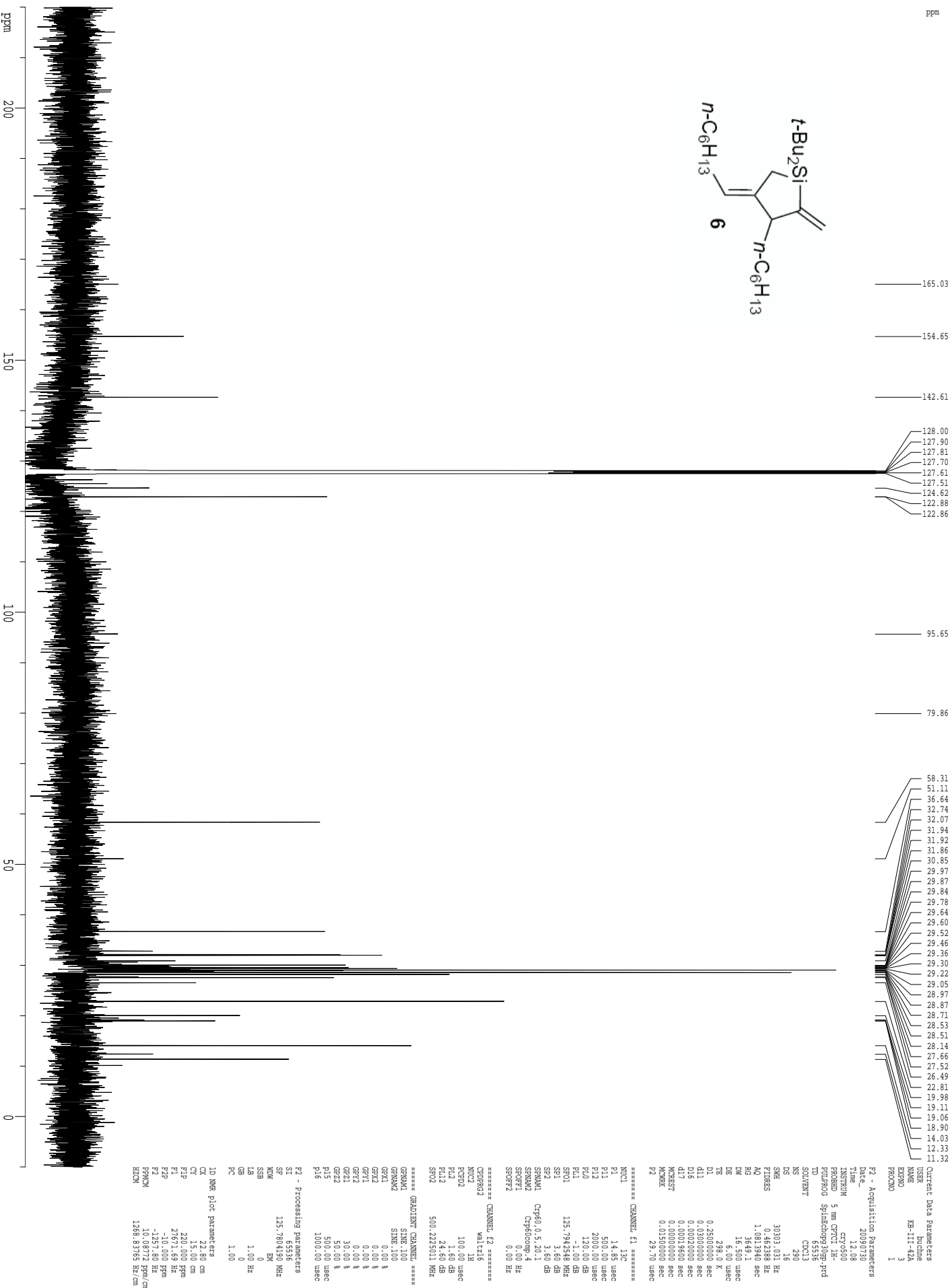
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Current Data Parameters
=====
USER             buchu
NAME             KB-III-42A
EXPNO            2
PROCNO           1

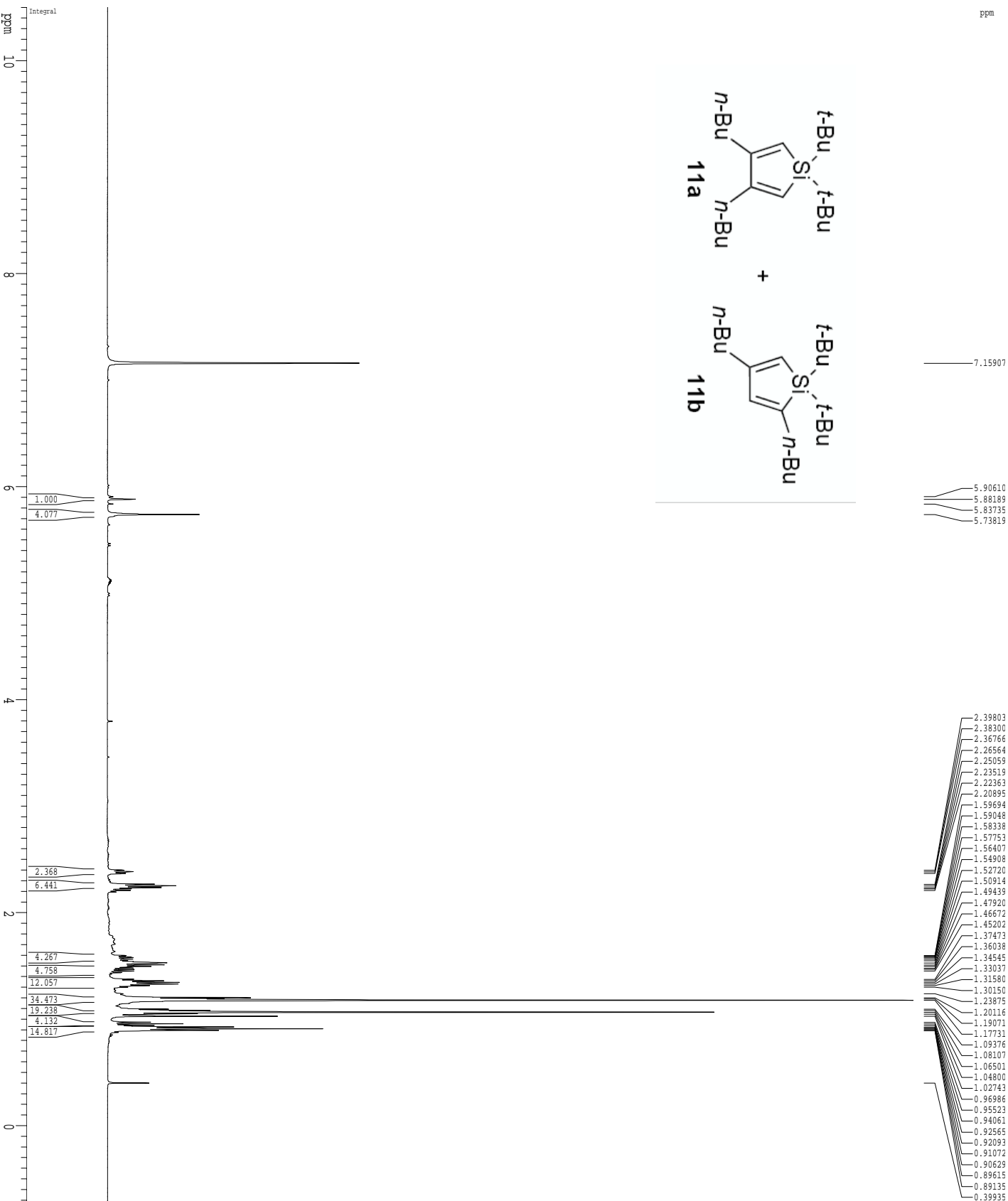
F2 - Acquisition Parameters
=====
Date_            20090730
Time             12.06
INSTRUM         cryo500
PROBHD          5 mm CPXI 1H-
PULPROG         zgpg30
TD              65536
AQ              8.173
RG              655
WDW              EM
SSB              0
GB              0
PC              1.00

F2 - Processing parameters
=====
SI              65536
SF              500.219997 MHz
WDW             EM
SSB             0
SGB             0
PC             1.00

JD NMR plot parameters
=====
CY              22.80 cm
CV              15.00 cm
F1P            10.500 ppm
F1              5252.31 Hz
F2P            -1.000 ppm
F2              -500.422 Hz
PNUCM          0.50459 ppm/cm
HZCM           252.30396 Hz/cm
    
```

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

1H spectrum in CDCl3 (regioisomeric mixture)



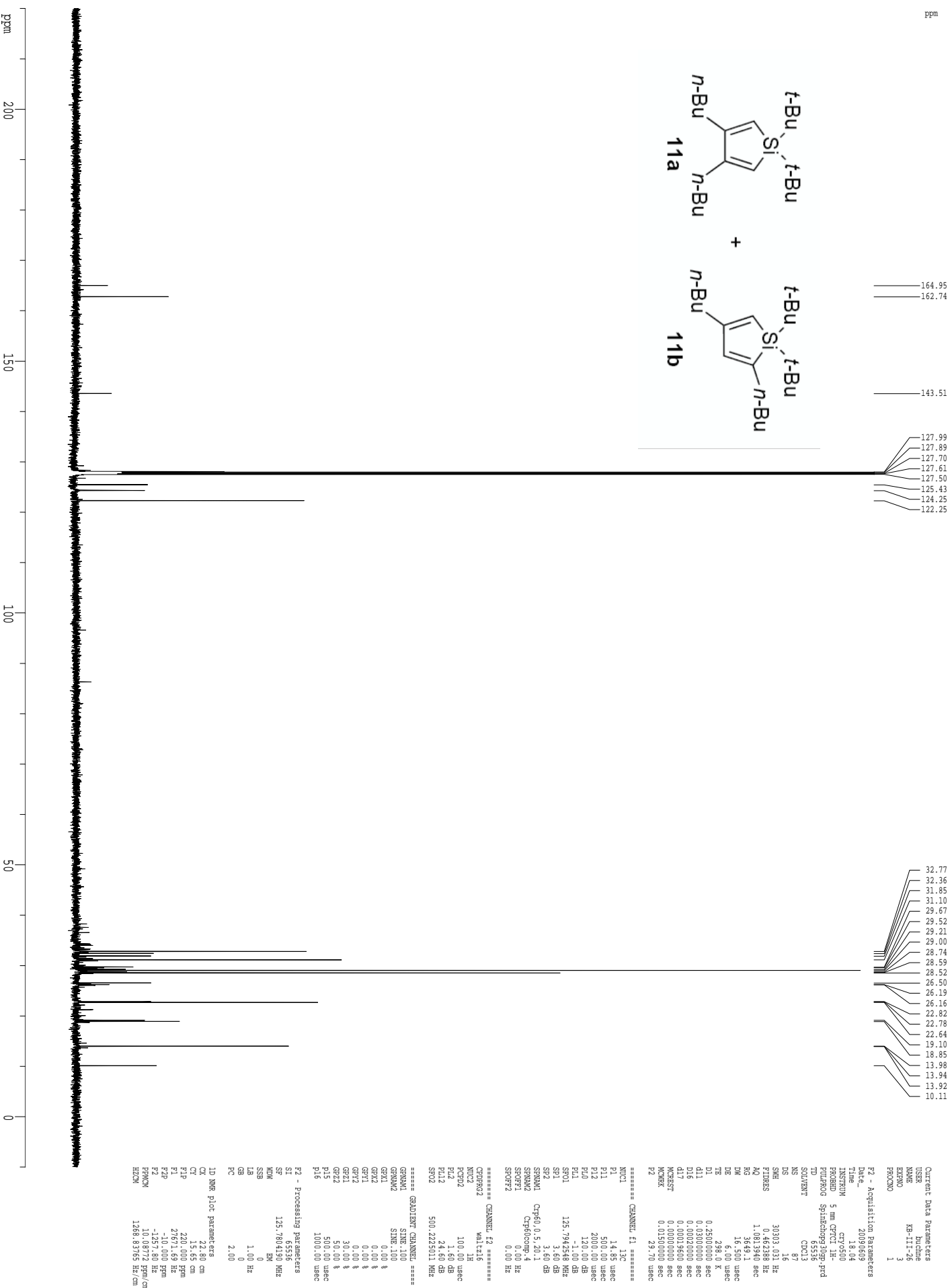
Current Data Parameters
 USER huchne
 NAME KB-II-26
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090609
 Time 18:07
 INSTRUM crys500
 PROBD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65536
 SFO1 500.130761 MHz
 FIDRES 0.098083 Hz
 AQ 5.0998774 sec
 RG 10.1
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.1000000 sec
 DELTA 0.0000000 sec
 ACQRESPT 0.0150000 sec
 KCMAX 0.0150000 sec

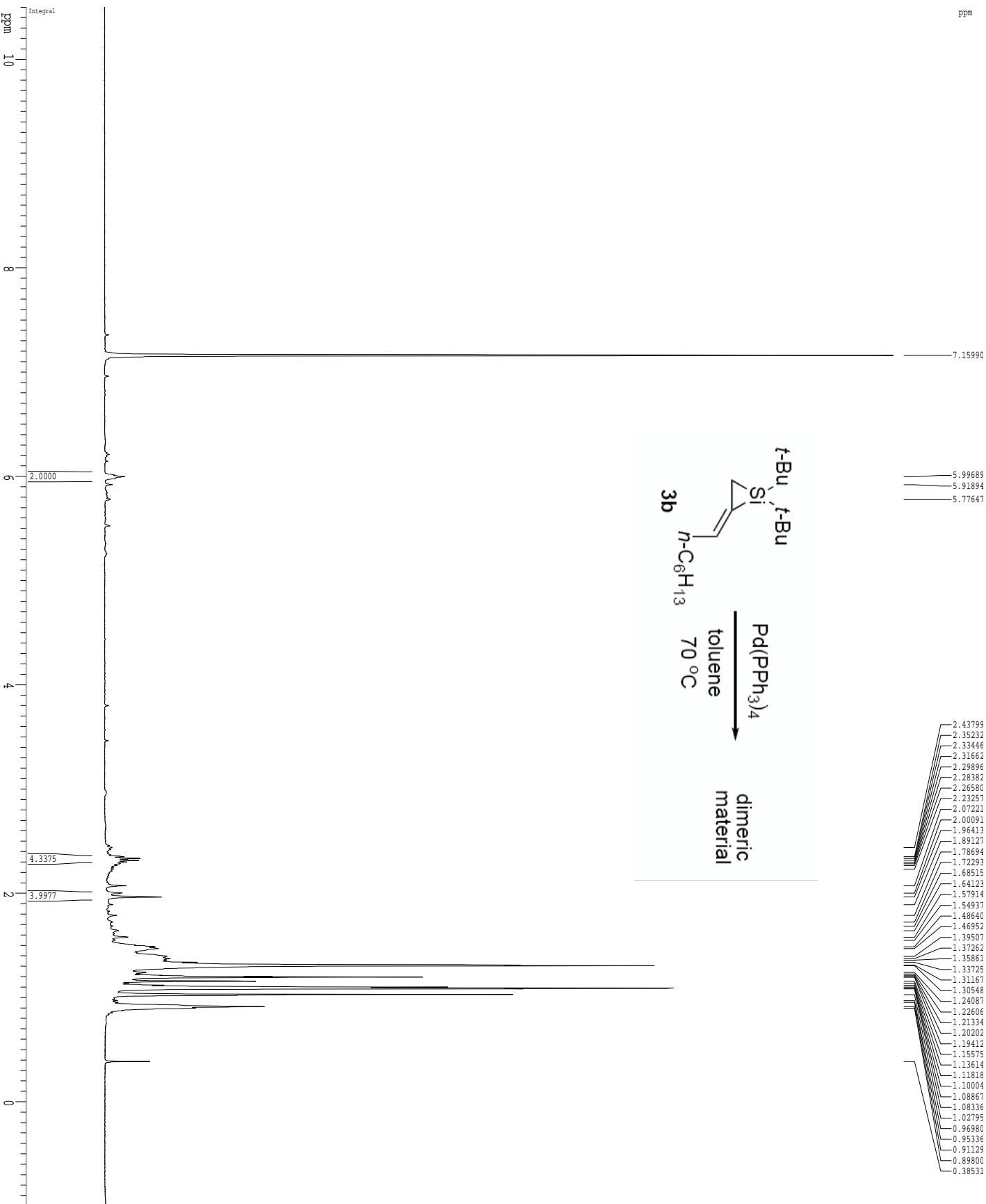
***** CHANNEL f1 *****
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2235015 MHz

F2 - Processing parameters
 SI 65536
 SF 500.2200000 MHz
 WDW EM
 SSB 0
 GB 0.30 Hz
 PC 1.00

ID NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -500.22 Hz
 PPM/CM 0.50459 ppm/cm
 HZ/CM 252.30396 Hz/cm

Z-restored spin-echo ¹³C spectrum with ¹H decoupling in C6D6 (regioisomeric mixture)

1H spectrum in C6D6



Current Data Parameters

USER	huchne
NAME	KB-II-50
EXPMO	1
PROCNO	1

P2 - Acquisition Parameters

Date_	20090717
Time	14.03
INSTRM	dx400
PROBHD	5 mm QNP H/P/P
PULPROG	zgpg30
TD	65536
TD0	1
TD1	65536
TD2	65536
TD3	65536
TD4	65536
TD5	65536
TD6	65536
TD7	65536
TD8	65536
TD9	65536
TD10	65536
TD11	65536
TD12	65536
TD13	65536
TD14	65536
TD15	65536
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TD86	65536
TD87	65536
TD88	65536
TD89	65536
TD90	65536
TD91	65536
TD92	65536
TD93	65536
TD94	65536
TD95	65536
TD96	65536
TD97	65536
TD98	65536
TD99	65536
TD100	65536

P2 - Processing parameters

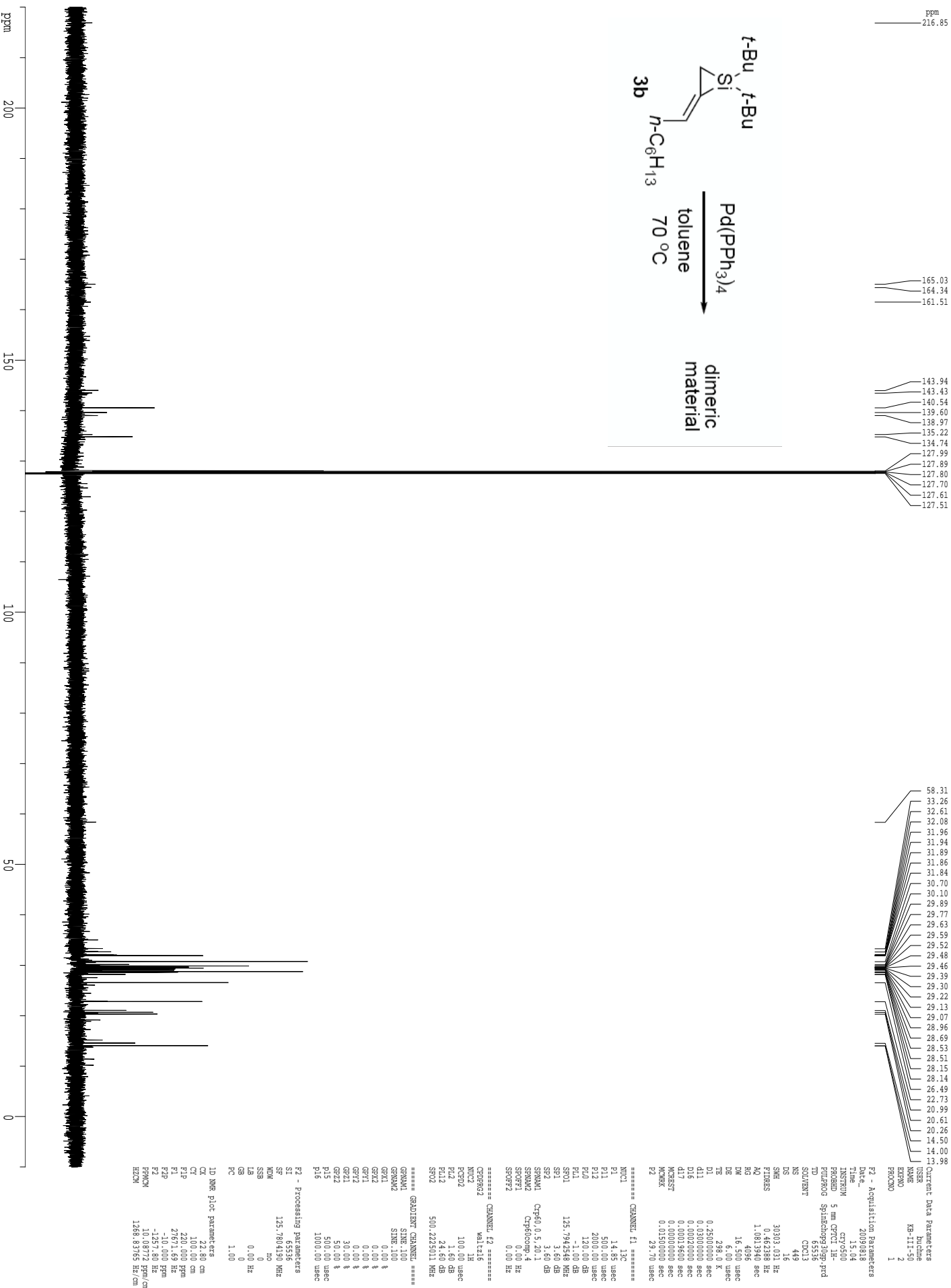
SI	65536
SF	400.129970 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

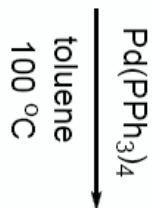
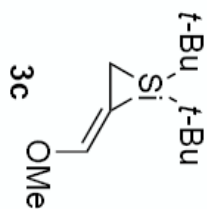
JD NMR plot parameters

CX	22.80 cm
CY	15.00 cm
F1P	10.500 ppm
F1	4201.37 Hz
F2P	-1.000 ppm
F2	-40.13 Hz
PRGCM	0.50449 ppm/cm
HZCM	201.81996 Hz/cm

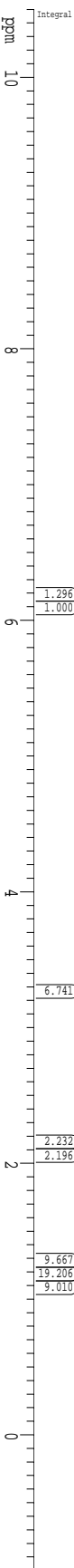
***** CHANNEL f1 *****

NUC1	1H
PL	12.00 usec
PL1	0.00 dB
SFO1	400.128009 MHz

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

1H spectrum in CDCl₃dimeric
material7.46755
7.45249
7.22569
7.21390
7.160066.31910
6.29745
6.15002
6.13290
5.93502

4.00831

3.26108
3.25699
3.23262
3.17687
3.087622.15311
2.05749
2.02854
1.99245
1.96461
1.94369
1.91496
1.88776
1.38288
1.33012
1.30132
1.27852
1.25817
1.25024
1.20395
1.17059
1.16034
1.14699
1.11395
1.10759
1.08373
1.07796
1.02840
0.96915
0.95595
0.90399
0.89045
0.87619
0.85232
0.83758
0.40360
0.28982
0.20290

Current Data Parameters
 USER buchoe
 NAME KB-1-51
 EXPRNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081004
 Time 12:53
 INSTRUM cryo500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 TD 65536
 TO DULTEXT
 NS 2
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098083 Hz
 AQ 5.0998774 sec
 RG 5.7
 DE 62.400 usec
 DW 6.00 usec
 TE 298.0 K
 D1 0.1000000 sec
 WALTZ16 0.0000000 sec
 MCKEST 0.0150000 sec
 KCMAX

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

F2 - Processing parameters
 SI 65536
 SF 500.2199985 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 10.500 ppm
 F1 5252.31 Hz
 F2P -1.000 ppm
 F2 -500.22 Hz
 PPMX 0.50459 ppm/cm
 HZCM 252.30396 Hz/cm

¹³C spectrum with ¹H decoupling in C6D6