Uncatalyzed Carboboration of Seven-Membered-Ring *trans*-Alkenes: Formation of Air-Stable Trialkylboranes

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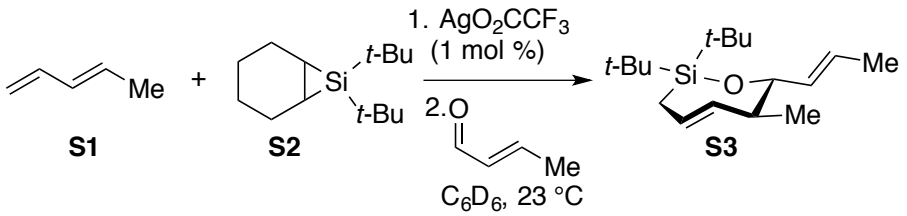
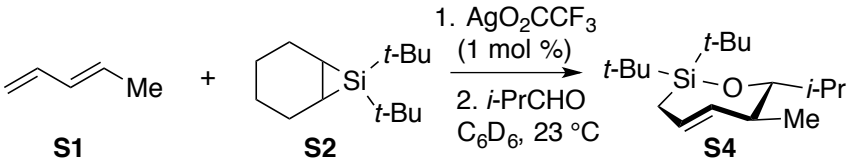
I. General Experimental

All ^{1}H, ^{13}C, ^{11}B, ^{19}F, and ^{29}Si NMR spectra were recorded at ambient temperature using Bruker AVIII-400 (400, 100, 128 and 376 MHz, respectively), AV-500 (500 and 125 MHz, respectively) and AVIII-600 with TCI cryoprobe (600 and 150 MHz, respectively) spectrometers. The data were reported as follows: chemical shifts are reported in ppm from internal tetramethylsilane or from residual solvent peaks (^{1}H NMR: $CDCl_3$ δ 7.26; C_6D_6 δ 7.16; CD_3OD δ 3.31 and ^{13}C NMR: $CDCl_3$ δ 77.2; C_6D_6 δ 128.4) on the δ scale, multiplicity (s = singlet, b = broad, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet), coupling constants (Hz), and integration. ^{29}Si NMR spectra (AV-500 99 MHz) were referenced against external tetramethylsilane (δ 0). ^{19}F NMR spectra were referenced against external hexafluorobenzene (δ –164.9) unless noted otherwise. ^{11}B NMR spectra were referenced against external boron trifluoride diethyl etherate (δ 0). Multiplicity of carbon peaks was determined using HSQC or DEPT experiments. Due to difficulties in isolation and purification of certain products, diagnostic ^{1}H and ^{13}C peaks were assigned using a combination of COSY, HSQC, HMBC, and nOe experiments. Infrared (IR) spectra were recorded using a Thermo Nicolet AVATAR Fourier Transform IR spectrometer using attenuated total reflectance (ATR). High-resolution mass spectra (HRMS) were recorded using an Agilent 6224 Accurate-Mass time-of-flight spectrometer with atmospheric pressure chemical ionization (APCI) or electrospray ionization (ESI) ionization sources. Melting points were reported uncorrected. Analytical thin layer chromatography was performed on Silicycle silica gel 60 Å F_{254} plates. Liquid chromatography was performed using forced flow (flash chromatography) of the indicated solvent system on Silicycle silica gel (SiO_2) 60 (230-400 mesh). THF, DMF, and CH_2Cl_2 were dried by filtration through alumina according to the method of Grubbs.[1] All reactions were run under a nitrogen atmosphere in glassware that had been flame-dried under vacuum unless otherwise stated. Metal catalysts, silacyclopropanes, and *trans*-oxasilacycloheptenes were stored and manipulated in a nitrogen-atmosphere dry box. All solvents and reagents were degassed before use. The synthesis and characterization of compounds **1**,[2] **S2**,[3] **S5**,[4] **S8**,[5] and **S27**[6] were reported previously. Unless otherwise noted, all reagents were commercially available. *trans*-Oxasilacycloheptenes were unable to be purified due to decomposition upon exposure to air and column chromatography. *trans*-Alkenes also undergo formal [1,3]-sigmatropic rearrangements at room temperature, preventing facile isolation.[2] All *trans*-oxasilacycloheptene concentrations were calculated by ^{1}H NMR spectroscopy relative to a known amount of internal standard (mesitylene) as described below. CCDC 1539169 (**2**) and CCDC 1539170 (*ent*-**10**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

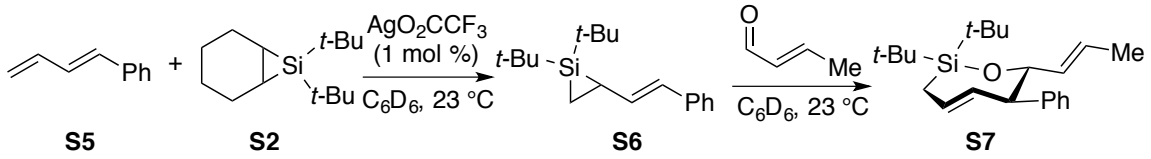
II. Synthesis of *trans*-Oxasilacycloheptenes



Representative Procedure for the One-Step Synthesis of *trans*-Alkenes (*trans*-Oxasilacycloheptene S3). The synthesis of *trans*-oxasilacycloheptene **S3** was adapted from a reported procedure.[2] To a solution of diene **S1** (0.0075 mL, 0.075 mmol), cyclohexene silacyclopropane **S2** (0.022 g, 0.098 mmol), and mesitylene (0.0020 mL, 0.014 mmol, internal standard) in C_6D_6 (0.475 mL) in an NMR tube was added $AgOCOCF_3$ (0.025 mL, 0.0030 M in C_6H_6 1 mol %). After 10 min, crotonaldehyde (0.0063 mL, 0.076 mmol) was added. *trans*-Oxasilacycloheptene **S3** was formed in 10 min in 56% yield over two steps based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the allylic ether CH peak (~δ 3.60). *trans*-Oxasilacycloheptene **S3** was unable to be purified and was used without further purification: ^{1}H NMR (500 MHz, C_6D_6, diagnostic peaks) δ 5.58 (dqd, J = 15.2, 6.4, 0.9, 1H), 5.44 (ddq, J = 15.2, 6.7, 1.5, 1H), 4.98 (ddd, J = 16.8, 10.1, 0.9, 1H), 3.62–3.59 (m, 1H), 2.35–2.26 (m, 2H), 1.85 (dd, J = 12.0, 4.5, 1H), 1.57–1.55 (m, 3H), 1.08 (s, 9H), 1.00 (s, 9H); ^{13}C NMR (125 MHz, C_6D_6, diagnostic peaks) δ 133.4, (CH), 130.7 (CH), 126.2 (CH), 81.0 (CH), 49.1 (CH), 29.1 (CH_3), 28.4 (CH_3), 18.7 (CH_2), 18.2 (CH_3); HRMS (APCI) m / z calcd for $C_{17}H_{33}OSi$ $(M + H)^+$ 281.2295, found 281.2297.

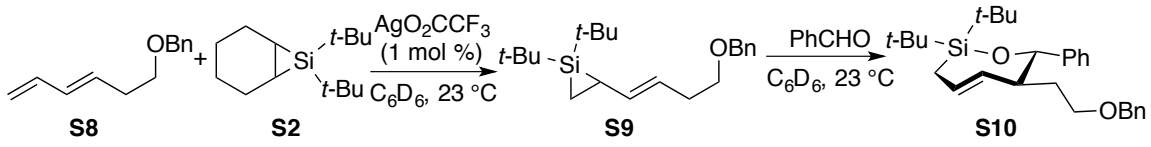


***trans*-Oxasilacycloheptene S4**. *trans*-Oxasilacycloheptene **S4** was prepared using the representative procedure for the synthesis of *trans*-alkenes using diene **S1** (0.012 mL, 0.12 mmol), cyclohexene silacyclopropane **S2** (0.034 g, 0.15 mmol), $AgOCOCF_3$ (0.036 mL, 0.010 M in C_6D_6, 0.3 mol %), and isobutyraldehyde (0.011 mL, 0.12 mmol). *trans*-Oxasilacycloheptene **S4** was formed in 10 min in 63% yield over two steps based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the ether CH peak (δ 3.15). *trans*-Oxasilacycloheptene **S4** was unable to be purified and was used without further purification: ^{1}H NMR (400 MHz, C_6D_6, diagnostic peaks) δ 4.93 (dd, J = 16.9, 9.9, 1H), 3.15 (dd, J = 9.1, 1.6, 1H), 2.52–2.42 (m, 1H), 2.29–2.22 (m, 1H), 1.82 (dd, J = 12.0, 4.4, 1H), 1.07 (s, 9H), 0.99 (s, 9H), 0.93 (d, J = 6.6, 3H), 0.88 (d, J = 6.8, 3H), 0.72 (d, J = 7.0, 3H); ^{13}C NMR (100 MHz, C_6D_6, diagnostic peaks) δ 134.8 (CH), 131.6 (CH), 84.0 (CH), 45.4 (CH), 30.7 (CH), 29.1 (CH_3), 28.5 (CH_3), 18.9 (CH_2), 16.9 (CH_3), 15.6 (CH_3), 15.1 (CH_3); HRMS (APCI) m / z calcd for $C_{17}H_{35}OSi$ $(M + H)^+$ 283.2452, found 283.2450.



***trans*-Alkene (S7).** The synthesis of *trans*-oxasilacycloheptene **S7** was adapted from a reported procedure.[2] To a solution of diene **S5** (0.010 g, 0.077 mmol), cyclohexene silacyclopropane **S2** (0.029 g, 0.13 mmol), and mesitylene (0.0020 mL, 0.014 mmol, internal standard) in C_6D_6 (0.50 mL) in an NMR tube was added $AgOCOCF_3$ (0.025 mL, 0.030 M in C_6D_6, 1 mol %). Vinylsilacyclopropane **S6** was formed in 10 min in 72% yield based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (~δ 6.71) and the area of the alkene CH peak (δ 6.43). Vinylsilacyclopropane **S6** was unable to be purified and was used without further purification: ^{1}H NMR (500 MHz, C_6D_6) δ 7.35–7.33 (m, 2H), 7.19–7.16 (m, 2H), 7.05–7.01 (m, 1H), 6.55 (dd, *J* = 15.7, 7.7, 1H), 6.43 (d, *J* = 15.7, 1H), 2.00–1.94 (m, 1H), 1.07 (s, 9H), 1.00 (s, 9H), 0.90–0.84 (m, 2H); ^{13}C NMR (125 MHz, C_6D_6, diagnostic peaks) δ 135.0 (CH), 129.2 (CH), 127.7 (CH), 126.4 (CH), 125.9 (CH), 124.9 (CH), 30.9 (CH_3), 29.9 (CH_3), 19.6 (CH), 3.6 (CH_2); ^{29}Si NMR (99 MHz, C_6D_6) δ –47.1.

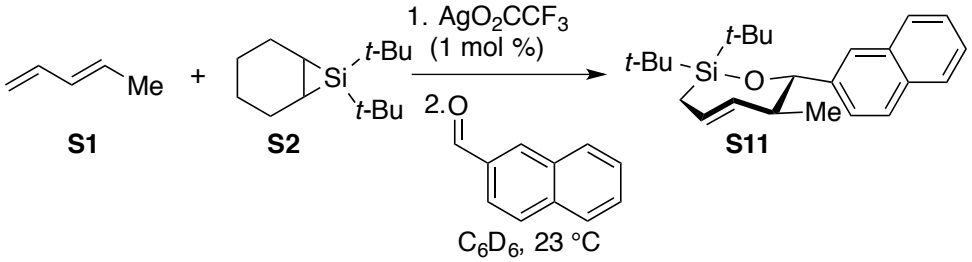
To a solution of vinylsilacyclopropane **S6** (0.015 g, 0.055 mmol) in C_6D_6 (0.525 mL) was added crotonaldehyde (0.0065 mL, 0.079 mmol). *trans*-Oxasilacycloheptene **S7** was formed in 10 min in 86% yield from vinylsilacyclopropane **S6** based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH peak (δ 4.24). *trans*-Oxasilacycloheptene **S7** was unable to be purified and was used without further purification: ^{1}H NMR (500 MHz, C_6D_6, diagnostic peaks) δ 7.22–7.17 (m, 4H), 7.10–7.06 (m, 1H), 5.99–5.92 (m, 1H), 5.59–5.48 (m, 2H), 5.41–5.36 (m, 1H), 4.24 (ddt, *J* = 9.0, 5.2, 1.2, 1H), 3.43 (t, *J* = 9.7, 1H), 2.37–2.32 (m, 1H), 1.42 (dt, *J* = 6.5, 1.4, 3H), 1.12 (s, 9H), 1.04 (s, 9H); ^{13}C NMR (125 MHz, C_6D_6, diagnostic peaks) δ 135.1 (CH), 132.1 (CH), 125.5 (CH), 79.9 (CH), 61.7 (CH), 29.1 (CH_3), 28.4 (CH_3), 19.1 (CH_2), 18.1 (CH_3); HRMS (APCI) *m* / *z* calcd for $C_{22}H_{35}OSi$ $(M + H)^+$ 343.2452, found 343.2447.



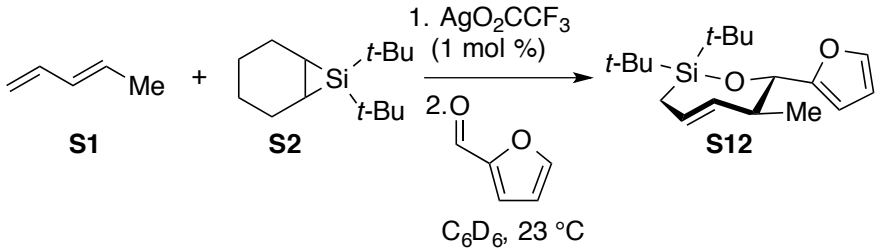
***trans*-Alkene (S10).** The synthesis of *trans*-oxasilacycloheptene **S10** was adapted from a reported procedure.[2] To a solution of diene **S8** (0.014 g, 0.074 mmol), cyclohexene silacyclopropane **S2** (0.021 g, 0.094 mmol), and mesitylene (0.0020 mL, 0.014 mmol, internal standard) in C_6D_6 (0.475 mL) in an NMR tube was added $AgOCOCF_3$ (0.025 mL, 0.030 M in C_6D_6, 1 mol %). Vinylsilacyclopropane **S9** was formed in 10 min in 82% yield based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the alkene CH peak (~δ 5.51). Vinylsilacyclopropane **S9** was unable to be purified and was used without further purification: ^{1}H NMR (500 MHz, C_6D_6, diagnostic peaks) δ 7.32–7.30 (m, 2H), 7.11–7.08 (m, 1H), 5.85–5.80 (m, 1H),

5.54–5.48 (m, 1H), 4.35 (s, 2H), 4.43–3.40 (m, 2H), 2.46–2.42 (m, 2H), 1.83–1.77 (m, 1H), 1.09 (s, 9H), 0.90 (t, J = 11.2, 1H), 0.74 (dd, J = 11.2, 9.0); ^{13}C NMR (125 MHz, C_6D_6, diagnostic peaks) δ 135.3 (CH), 128.1 (CH), 127.8 (CH), 121.5 (CH), 73.3 (CH_2), 71.5 (CH_2), 34.3 (CH_2), 31.0 (CH_3), 30.0 (CH_3), 17.9, (CH), 2.9 (CH_2); ^{29}Si NMR (99 MHz, C_6D_6) δ –48.5.

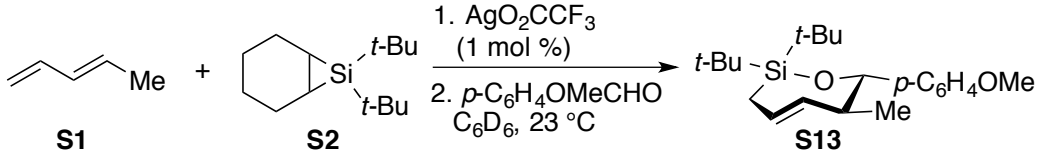
To a solution of vinylsilacyclopropane **S9** (0.021 g, 0.061 mmol) in C_6D_6 (0.50 mL) was added benzaldehyde (0.0075 mL, 0.074 mmol). *trans*-Oxasilacycloheptene **S10** was formed in 10 min in 88% yield from vinylsilacyclopropane **S9** based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of one of the ether CH_2 peaks (~δ 3.35). *trans*-Oxasilacycloheptene **S10** was unable to be purified and was used without further purification: ^{1}H NMR (500 MHz, C_6D_6, diagnostic peaks) δ 6.05–5.97 (m, 1H), 5.00 (dd, J = 16.8, 10.1, 1H), 4.25 (s, 2H and m, 1H), 3.49–3.44 (m, 1H), 3.38–3.33 (m, 1H), 2.74–2.68 (m, 1H), 2.37–2.32 (m, 1H), 1.63–1.56 (m, 1H), 1.46–1.39 (m, 1H), 1.02 (s, 9H), 0.97 (s, 9H); ^{13}C NMR (125 MHz, C_6D_6, diagnostic peaks) δ 137.6 (CH), 129.2 (CH), 81.8 (CH), 73.4 (CH_2), 70.0 (CH_2), 54.5 (CH), 31.2 (CH_2), 29.1 (CH_3), 28.3 (CH_3), 19.2 (CH_2); ^{29}Si NMR (99 MHz, C_6D_6) δ –1.7; HRMS (APCI) m / z calcd for $C_{28}H_{41}O_2Si$ $(M + H)^+$ 438.2899, found 438.2896.



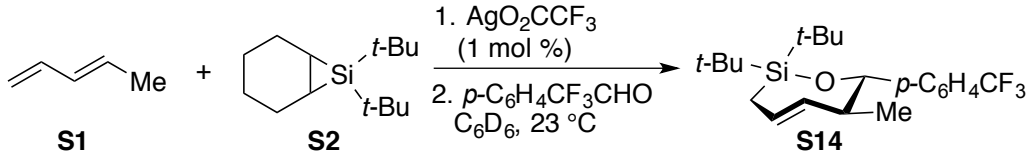
***trans*-Oxasilacycloheptene S11**. *trans*-Oxasilacycloheptene **S11** was prepared using the representative procedure for the synthesis of *trans*-alkenes using diene **S1** (0.0080 mL, 0.080 mmol), cyclohexene silacyclopropane **S2** (0.024 g, 0.11 mmol), $AgOCOCF_3$ (0.027 mL, 0.030 M in C_6D_6, 1 mol %), and 2-naphthaldehyde (0.012 g, 0.077 mmol). *trans*-Oxasilacycloheptene **S11** was formed in 10 min in 62% yield over two steps based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH peak (δ 4.30). *trans*-Oxasilacycloheptene **S11** was unable to be purified and was used without further purification: ^{1}H NMR (400 MHz, C_6D_6, diagnostic peaks) δ 7.73–7.61 (m, 4H), 7.29–7.24 (m, 2H), 7.23–7.17 (m, 1H), 6.10–6.01 (m, 1H), 5.12 (dd, J = 16.8, 9.8, 1H), 4.30 (d, J = 8.9, 1H), 2.70–2.61 (m, 1H), 2.41–2.35 (m, 1H), 1.07 (s, 9H), 1.01 (s, 9H), 0.91 (d, J = 6.6, 3H); ^{13}C NMR (100 MHz, C_6D_6, diagnostic peaks) δ 136.3 (CH), 130.7 (CH), 126.4 (CH), 83.2 (CH), 51.0 (CH), 29.1 (CH_3), 28.3 (CH_3), 19.0 (CH_2), 16.5 (CH_3); HRMS (APCI) m / z calcd for $C_{24}H_{35}OSi$ $(M + H)^+$ 367.2452, found 367.2448.



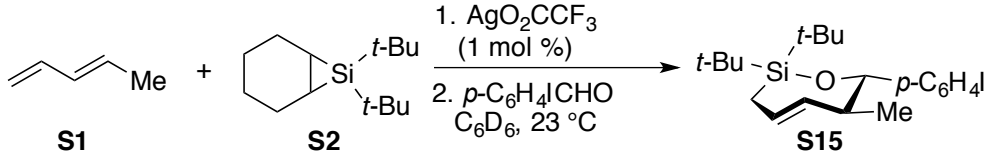
***trans*-Oxasilacycloheptene S12**. *trans*-Oxasilacycloheptene **S12** was prepared using the representative procedure for the synthesis of *trans*-alkenes using diene **S1** (0.0075 mL, 0.075 mmol), cyclohexene silacyclopropane **S2** (0.022 g, 0.098 mmol), $AgOCOCF_3$ (0.025 mL, 0.030 M in C_6D_6, 1 mol %), and furfural (0.0065 mL, 0.078 mmol). *trans*-Oxasilacycloheptene **S12** was formed in 10 min in 64% yield over two steps based on ^1H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH peak (δ 4.27). *trans*-Oxasilacycloheptene **S12** was unable to be purified and was used without further purification: ^1H NMR (400 MHz, C_6D_6, diagnostic peaks) δ 7.08 (t, J = 1.3, 1H), 6.02, (d, J = 1.3, 2H), 6.01 (dddd, J = 16.8, 13.2, 4.5, 0.8, 1H), 5.00 (ddd, J = 16.8, 10.0, 1.1, 1H) 4.27 (d, J = 9.3, 1H), 2.96–2.86 (m, 1H), 2.29 (ddd, J = 13.2, 12.0, 1.1, 1H), 1.86 (dd, J = 12.0, 4.5, 1H), 1.02 (s, 9H), 0.99 (s, 9H); ^{13}C NMR (100 MHz, C_6D_6, diagnostic peaks) δ 142.2 (CH), 136.7 (CH), 130.2 (CH), 110.6 (CH), 106.7 (CH), 75.7 (CH), 48.1 (CH), 29.0 (CH_3), 28.2 (CH_3), 19.0 (CH_2); HRMS (APCI) m / z calcd for $C_{18}H_{31}OSi$ $(M + H)^+$ 307.2088, found 307.2078.



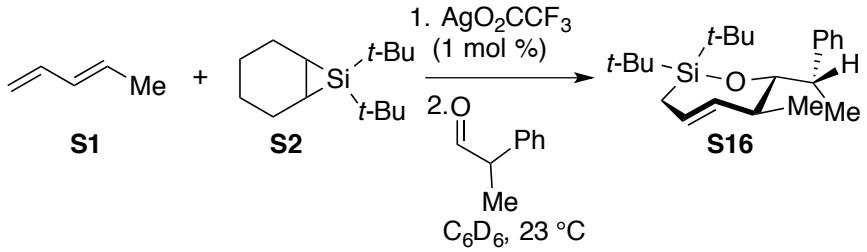
***trans*-Oxasilacycloheptene S13**. *trans*-Oxasilacycloheptene **S13** was prepared using the representative procedure for the synthesis of *trans*-alkenes using diene **S1** (0.0070 mL, 0.070 mmol), cyclohexene silacyclopropane **S2** (0.018 g, 0.080 mmol), $AgOCOCF_3$ (0.020 mL, 0.010 M in C_6D_6, 0.3 mol %), and *p*-methoxybenzaldehyde (0.0085 mL, 0.070 mmol). *trans*-Oxasilacycloheptene **S13** was formed in 10 min in 58% yield over two steps based on ^1H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the methoxy CH_3 peak (δ 3.32). *trans*-Oxasilacycloheptene **S13** was unable to be purified and was used without further purification: ^1H NMR (600 MHz, C_6D_6, diagnostic peaks) δ 7.17 (d, J = 8.7, 2H), 6.79 (d, J = 8.7, 2H), 6.04–5.98 (m, 1H), 5.10 (dd, J = 16.8, 10.0, 1H), 4.12 (d, J = 8.9, 1H), 3.32 (s, 3H), 2.60–2.54 (m, 1H), 2.37–2.33 (m, 1H), 1.06 (s, 9H), 1.00 (s, 9H), 0.92 (d, J = 6.6, 3H); ^{13}C NMR (150 MHz, C_6D_6, diagnostic peaks) δ 136.0 (CH), 131.1 (CH), 114.3 (CH), 82.7 (CH), 55.1 (CH_3), 51.2 (CH), 29.1 (CH_3), 28.3 (CH_3), 19.0 (CH_2), 16.6 (CH_3); HRMS (APCI) m / z calcd for $C_{21}H_{35}O_2Si$ $(M + H)^+$ 347.2401, found 347.2398.



***trans*-Oxasilacycloheptene S14**. *trans*-Oxasilacycloheptene **S14** was prepared using the representative procedure for the synthesis of *trans*-alkenes using diene **S1** (0.0080 mL, 0.080 mmol), cyclohexene silacyclopropane **S2** (0.024 g, 0.11 mmol), $AgOCOCF_3$ (0.027 mL, 0.030 M in C_6D_6, 1 mol %), and *p*-(trifluoromethyl)benzaldehyde (0.011 mL, 0.081 mmol). *trans*-Oxasilacycloheptene **S14** was formed in 10 min in 70% yield over two steps based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH peak (δ 4.01). *trans*-Oxasilacycloheptene **S14** was unable to be purified and was used without further purification: ^{1}H NMR (400 MHz, C_6D_6, diagnostic peaks) δ 7.35 (d, *J* = 8.1, 2H), 7.08 (d, *J* = 8.1, 2H), 5.98–5.89 (m, 1H), 4.99 (dd, *J* = 16.7, 10.0, 1H), 4.01 (d, *J* = 8.9, 1H), 2.41–2.28 (m, 2H), 1.01 (s, 9H), 0.95 (s, 9H), 0.76 (d, *J* = 6.6, 3H); ^{13}C NMR (100 MHz, C_6D_6, diagnostic peaks) δ 136.5 (CH), 130.0 (CH), 127.7 (CH), 125.7 (q, *J* = 4.0, CH), 82.3 (CH), 51.2 (CH), 29.0 (CH_3), 28.2 (CH_3), 18.9 (CH_2), 16.2 (CH_3); ^{19}F NMR (377 MHz, C_6D_6, internal reference *p*-CF_3-C_6H_4CHO δ –63.2) δ –62.0; HRMS (APCI) *m* / *z* calcd for $C_{21}H_{32}F_3OSi$ $(M + H)^+$ 385.2169, found 385.2154.

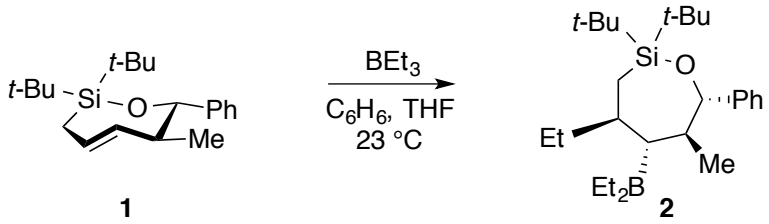


***trans*-Oxasilacycloheptene S15**. *trans*-Oxasilacycloheptene **S15** was prepared using the representative procedure for the synthesis of *trans*-alkenes using diene **S1** (0.0080 mL, 0.080 mmol), cyclohexene silacyclopropane **S2** (0.023 g, 0.10 mmol), $AgOCOCF_3$ (0.027 mL, 0.030 M in C_6D_6, 1 mol %), and *p*-iodobenzaldehyde (0.018 g, 0.078 mmol). *trans*-Oxasilacycloheptene **S15** was formed in 10 min in 57% yield over two steps based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH peak (δ 3.92). *trans*-Oxasilacycloheptene **S15** was unable to be purified and was used without further purification: ^{1}H NMR (600 MHz, C_6D_6, diagnostic peaks) δ 7.45 (d, *J* = 8.3, 2H), 6.76 (d, *J* = 8.3, 2H), 5.94–5.89 (m, 1H), 4.99 (dd, *J* = 16.8, 10.0, 1H), 3.92 (d, *J* = 8.9, 1H), 2.40–2.34 (m, 1H), 2.33–2.28 (m, 1H), 1.00 (s, 9H), 0.95 (s, 9H), 0.78 (d, *J* = 6.6, 3H); ^{13}C NMR (150 MHz, C_6D_6, diagnostic peaks) δ 137.8 (CH), 136.4 (CH), 131.0 (CH), 128.4 (CH), 82.3 (CH), 51.1 (CH), 29.0 (CH_3), 28.2 (CH_3), 18.9 (CH_2), 16.3 (CH_3); HRMS (APCI) *m* / *z* calcd for $C_{20}H_{30}IOSi$ $(M + H)^+$ 443.1262, found 443.1253.



***trans*-Oxasilacycloheptene S16**. *trans*-Oxasilacycloheptene **S16** was prepared using the representative procedure for the synthesis of *trans*-alkenes using diene **S1** (0.0080 mL, 0.080 mmol), cyclohexene silacyclopropane **S2** (0.030 g, 0.13 mmol), $AgOCOCF_3$ (0.027 mL, 0.030 M in C_6D_6 1 mol %), and 2-phenylpropionaldehyde (0.011 mL, 0.082 mmol). *trans*-Oxasilacycloheptene **S16** was formed in 10 min in 57% yield over two steps based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH peak (δ 3.39). *trans*-Oxasilacycloheptene **S16** was unable to be purified and was used without further purification: ^{1}H NMR (600 MHz, C_6D_6, diagnostic peaks) δ 7.21–7.18 (m, 2H), 7.08–7.06 (m, 2H), 6.85 (d, J = 7.7, 1H), 5.81–5.78 (m, 1H), 4.89 (dd, J = 16.8, 9.9, 1H), 3.39 (d, J = 9.2, 1H), 2.92 (q, J = 7.0, 1H), 2.57–2.51 (m, 1H), 2.24–2.19 (m, 1H), 1.81 (dd, J = 12.0, 4.2, 1H), 1.06 (s, 9H), 0.62 (s, 9H); ^{13}C NMR (150 MHz, C_6D_6, diagnostic peaks) δ 135.4 (CH), 130.8 (CH), 128.9 (CH), 128.7 (CH), 126.5 (CH), 85.0 (CH), 53.4 (CH), 45.9 (CH), 41.4 (CH), 28.6 (CH_3), 28.5 (CH_3), 19.3 (CH_2); HRMS (APCI) m / z calcd for $C_{22}H_{37}OSi$ $(M + H)^+$ 345.2608, found 345.2620.

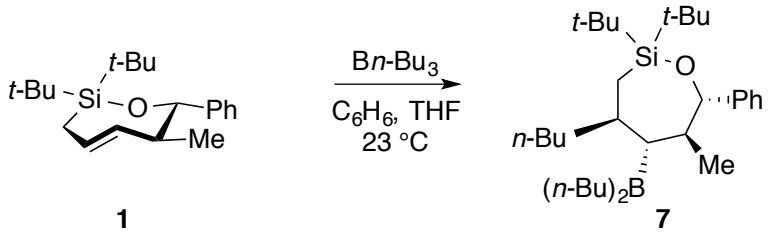
III. Synthesis of Trialkylboranes



Representative Procedure for the Synthesis of Trialkylboranes (trialkylborane 2). To a solution of *trans*-alkene **1** (0.132 g, 0.417 mmol) in C_6H_6 (4.00 mL) was added triethylborane (3.60 mL, 1.0 M in THF, 3.6 mmol). After 2 h, 1 M NaOH (5.0 mL) was added, followed by 30% H_2O_2 in H_2O (3.0 mL) (*caution the ensuing reaction was exothermic*). After 20 min, Et_2O (30 mL) and brine (15 mL) were added and the layers were separated. The aqueous layer was extracted with Et_2O (2 x 30 mL). The combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo*. Purification by flash chromatography (hexanes) afforded trialkylborane **2** as a white solid (0.159 g, 92%): mp = 66–69 °C; ^{1}H NMR (500 MHz, C_6D_6) δ 7.31 (d, J = 7.1, 2H), 7.21–7.17 (m, 2H), 7.10–7.07 (m, 1H), 4.64 (d, J = 9.5, 1H), 2.28–2.22 (m, 1H), 2.10–2.02 (m, 1H), 1.57 (t, J = 10.2, 1H), 1.23 (m, 5H and s, 9H), 1.08 (t, J = 7.6, 6H), 1.02 (s, 9H and m, 1H), 0.94–0.88 (m, 4H), 0.76 (dd, J = 15.5, 11.9, 1H), 0.17 (d, J = 7.0, 3H); ^{13}C NMR (150 MHz, C_6D_6, 25 °C) δ 145.8 (C), 128.7 (CH), 127.6 (CH), 127.5 (CH), 85.2 (CH), 52.7 (CH), 44.5 (CH), 39.5 (CH), 33.6 (CH_2), 29.5 (CH_3), 29.2 (CH_3), 22.3 (C), 21.6 (C), 20.3 (CH_3), 17.2 (CH_2), 12.5 (CH_3), 10.2 (CH_3); (Some ^{13}C shifts next to the boron atom are

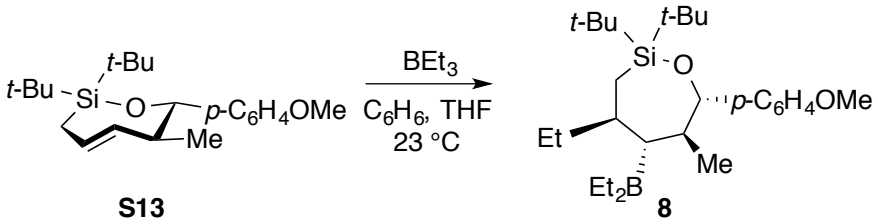
too broad to resolve at 25 °C) ^{13}C NMR (125 MHz, $CDCl_3$, –40 °C) δ 145.3 (C), 127.7 (CH), 126.8 (CH), 126.6 (CH), 83.7 (CH), 50.7 (CH), 42.6 (CH), 35.6 (CH), 36.2 (CH_2), 28.7 (CH_3), 28.5 (CH_3), 22.0 (C), 21.9 (CH_2), 21.0 (C), 19.6 (CH_3), 16.0 (CH_2), 15.7 (CH_2), 12.4 (CH_3), 9.9 (CH_3), 9.8 (CH_3); ^{11}B NMR (128 MHz, C_6D_6) δ 32.1; IR (ATR) 1081, 1054, 823, 698 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{22}H_{37}OSi$ $(M - BEt_2)^+$ 345.2608, found 345.2610.

Note: The ^{1}H, ^{13}C, and ^{11}B NMR spectra are consistent with trialkylboranes having multiple conformational isomers, despite being a single stereoisomer. Subsequent oxidation of the boron–carbon bond results in a sinlge stereoisomer with one conformational isomer on the NMR time scale. Due to the slow rotation around the carbon–boron bonds, methylene carbons next to the boron atom are too broad to resolve at 25 °C in the ^{13}C NMR spectra of most trialkylboranes. The methyl groups on the BEt_2 group are not diastereotopic at 25 °C in the ^{13}C NMR spectrum (as evidenced by the ^{13}C NMR spectrum at 25 °C), but are diastereotopic at –40 °C. Additionally, some trialkylboranes exhibit two ^{11}B NMR resonances, likely due to the impeded rotation. Variable temperature NMR studies were unable to resolve these peaks, however.



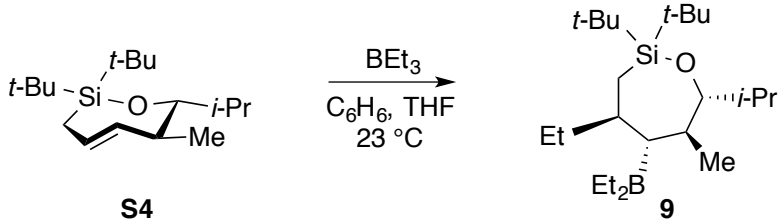
1 **7**

Trialkylborane 7. Trialkylborane **7** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **1** (0.028 g, 0.088 mmol), tributylborane (0.150 mL, 0.615 mmol) (*caution: neat tributylborane reacts violently with oxygen)*, and C_6H_6 (1.00 mL). Purification by flash chromatography (hexanes) afforded trialkylborane **7** as a colorless oil (0.032 g, 73%): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29–7.25 (m, 4H), 7.22–7.19 (m, 1H), 4.52 (d, *J* = 7.9, 1H), 2.18–2.13 (m, 1H), 1.91–1.84 (m, 1H), 1.46–1.38 (m, 6H), 1.36–1.32 (m, 4H), 1.24–1.14 (m, 6H), 1.08 (m, 1H and s, 9H), 1.03–0.97 (m, 2H), 0.95 (s, 9H), 0.92–0.88 (m, 9H), 0.77–0.68 (m, 2H), 0.07 (d, *J* = 7.0, 3H); ^{13}C NMR (125 MHz, C_6D_6) δ 145.8 (C), 128.7 (CH), 127.6 (CH), 127.5 (CH), 85.2 (CH), 53.6 (CH), 44.6 (CH), 41.3 (CH_2), 38.1 (CH), 30.5 (CH_2), 29.5 (CH_3), 29.2 (CH_3), 28.9 (CH_2), 26.9 (CH_2), 23.8 (CH_2), 22.4 (C), 21.6 (C), 20.7 (CH_3), 18.2 (CH_2), 14.7 (CH_3), 14.6 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, C_6D_6) δ 54.0, 32.8 (see note under trialkylborane **2**, p. S10); IR (ATR) 1081, 1066, 823, 698 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{24}H_{41}OSi$ $(M - B^nBu_2)^+$ 373.2921, found 373.2924.



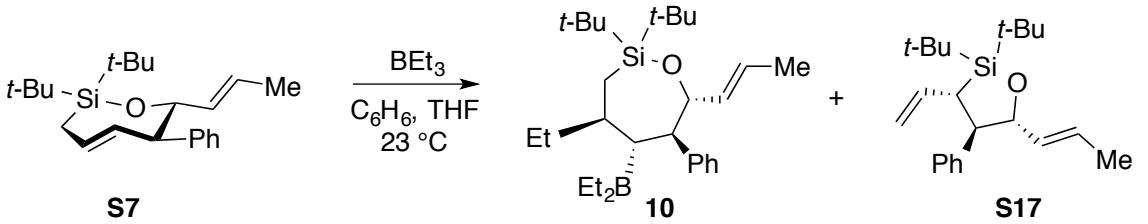
S13 **8**

Trialkylborane 8. Trialkylborane **8** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S13** (0.012 g, 0.035 mmol), triethylborane (0.450 mL, 1.0 M in THF, 0.45 mmol), and C_6H_6 (0.530 mL). Purification by flash chromatography (hexanes) afforded trialkylborane **8** as a colorless oil (0.013 g, 84%): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.17 (d, J = 8.6, 2H), 6.82 (d, J = 8.6, 2H), 4.49 (d, J = 8.0, 1H), 3.80 (s, 3H), 2.11–2.06 (m, 1H), 1.89–1.83 (m, 1H), 1.45 (t, J = 10.2, 1H), 1.23–1.18 (m, 4H), 1.08 (m, 2H and s, 9H), 1.00 (t, J = 7.6, 6H), 0.95 (s, 9H), 0.91 (t, J = 8.0, 3H), 0.87–0.82 (m, 1H), 0.66 (dd, J = 15.5, 11.9, 1H), 0.07 (d, J = 7.0, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.51 (C), 137.9 (C), 127.8 (CH), 113.2 (CH), 83.8 (CH), 55.3 (CH_3), 51.9 (CH), 43.9 (CH), 38.9 (CH), 32.9 (CH_2), 29.0 (CH_3), 28.8 (CH_3), 22.0 (C), 21.1 (C), 19.8 (CH_3), 16.6 (CH_2), 12.2 (CH_3), 9.7 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, $CDCl_3$) δ 55.4; IR (ATR) 1244, 1074, 1041, 820 cm^{-1}; HRMS (APCI) m / z calcd for $C_{27}H_{50}BO_2Si$ $(M + H)^+$ 445.3673, found 445.3664.



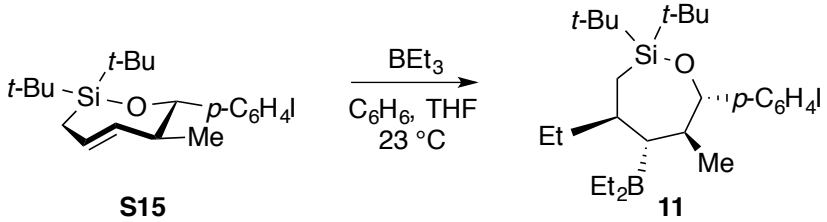
S4 **9**

Trialkylborane 9. Trialkylborane **9** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S4** (0.021 g, 0.075 mmol), triethylborane (0.480 mL, 1.0 M in THF, 0.48 mmol), and C_6H_6 (0.400 mL). Purification by flash chromatography (hexanes) afforded trialkylborane **9** as a colorless oil that could not be further purified (0.028 g, 97% unpurified yield): ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.49 (dd, J = 8.5, 1.8, 1H), 1.87–1.79 (m, 2H), 1.76–1.71 (m, 1H), 1.35 (t, J = 10.1, 1H), 1.16–1.13 (m, 4H), 1.03 (s, 9H and m, 2H), 1.01 (s, 9H and m, 8H), 0.90–0.85 (m, 4H), 0.81 (m, 1H and t, J = 6.7, 3H), 0.45 (m, 1H and d, J = 6.9, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 84.2 (CH), 50.7 (CH), 40.4 (CH), 39.1 (CH), 32.6 (CH_2), 30.8 (CH), 29.0 (CH_3), 28.6 (CH_3), 22.4 (C), 21.7 (C), 21.5 (CH_3), 18.5 (CH_3), 17.5 (CH_2), 13.9 (CH_3), 12.4 (CH_3), 9.7 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, C_6D_6) δ 54.2, 32.2 (see note under trialkylborane **2**, p. S10); IR (ATR) 1062, 820, 621 cm^{-1}; HRMS (APCI) m / z calcd for $C_{23}H_{49}BKOSi$ $(M + K)^+$ 419.3282, found 419.3277.



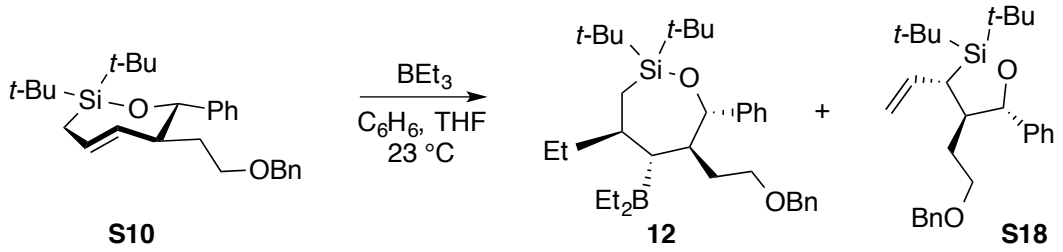
S7 **10** **S17**

Trialkylborane 10. Trialkylborane **10** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S7** (0.015 g, 0.044 mmol), triethylborane (0.450 mL, 1.0 M in THF, 0.45 mmol), and C_6H_6 (0.525 mL). ^{1}H NMR spectroscopic analysis of the unpurified reaction mixture after workup showed a mixture of trialkylborane **10** and alkene **S17** in a 77:23 (**10**:**S17**) ratio. (The spectral data are consistent with the data reported below for alkene **S17**, the result of rearrangement of the starting *trans*-alkene.) Purification by flash chromatography (hexanes–3:97 EtOAc:hexanes) afforded trialkylborane **10** as a white solid (0.010 g, 53%): mp = 75–77 °C; ^{1}H NMR (600 MHz, C_6D_6) δ 6.99–6.75 (m, 5H), 5.66–5.60 (m, 1H), 5.17 (ddd, *J* = 15.1, 5.6, 1.6, 1H), 4.70–4.68 (m, 1H), 2.91 (dd, *J* = 10.8, 8.4, 1H), 2.26–2.21 (m, 1H), 2.14 (t, *J* = 10.4, 1H), 1.35 (d, *J* = 6.6, 3H), 1.28 (s, 9H and m, 2H), 1.17 (s, 9H and m, 2H), 1.09–1.03 (m, 2H), 0.95–0.89 (m, 10H), 0.82 (dd, *J* = 15.5, 11.8, 1H); ^{13}C NMR (150 MHz, C_6D_6) δ 143.5 (C), 134.6 (CH), 131.3 (CH), 128.7 (CH), 126.8 (CH), 124.5 (CH), 81.3 (CH), 57.0 (CH), 52.5 (CH), 40.3 (CH), 33.6 (CH_2), 29.5 (CH_3), 29.3 (CH_3), 22.6 (CH_2), 22.5 (C), 21.7 (C), 18.1 (CH_3), 18.0 (CH_2), 17.8 (CH_2), 12.9 (CH_3), 10.1 (CH_3), 9.7 (CH_3); ^{11}B NMR (128 MHz, C_6D_6) δ 54.0; IR (ATR) 1600, 1474, 1070, 822 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{24}H_{39}OSi$ (M – BEt_2)$^+$ 371.2765, found 371.2764. Anal. Calcd for $C_{28}H_{49}BOSi$: C, 76.33; H, 11.21. Found: C, 76.05; H, 11.27.



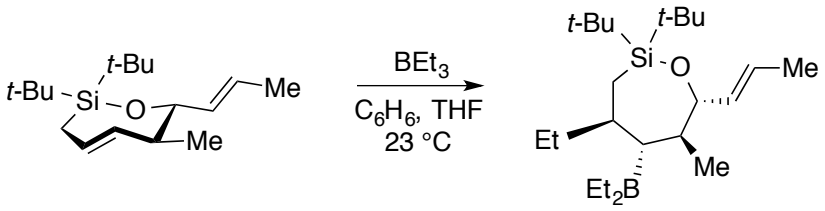
S15 **11**

Trialkylborane 11. Trialkylborane **11** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S15** (0.019 g, 0.043 mmol), triethylborane (0.450 mL, 1.0 M in THF, 0.45 mmol), and C_6H_6 (0.530 mL). Purification by flash chromatography (hexanes) afforded trialkylborane **11** as a white solid (0.018 g, 78%): mp = 91–93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.4, 2H), 7.01 (d, *J* = 8.4, 2H), 4.47 (d, *J* = 8.0, 1H), 2.12–2.05 (m, 1H), 1.92–1.80 (m, 1H), 1.45 (t, *J* = 10.2, 1H), 1.24–1.16 (m, 4H), 1.11 (dd, *J* = 15.4, 1.1, 1H), 1.07 (s, 9H), 1.00 (m, 1H and t, *J* = 7.5, 6H), 0.92 (s, 9H and t, *J* = 6.3, 3H), 0.86–0.79 (m, 1H), 0.66 (dd, *J* = 15.4, 11.9, 1H), 0.07 (d, *J* = 7.0, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2 (C), 137.1 (CH), 129.0 (CH), 92.1 (C), 83.8 (CH), 51.9 (CH), 43.7 (CH), 38.8 (CH), 32.9 (CH_2), 28.9 (CH_3), 28.7 (CH_3), 22.0 (C), 21.1 (C), 19.7 (CH_3), 16.6 (CH_2), 12.1 (CH_3), 9.6 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.3; IR (ATR) 1078, 1006, 848, 823 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{22}H_{36}IOSi$ (M – BEt_2)$^+$ 471.1575, found 471.1577.



S10 **12** **S18**

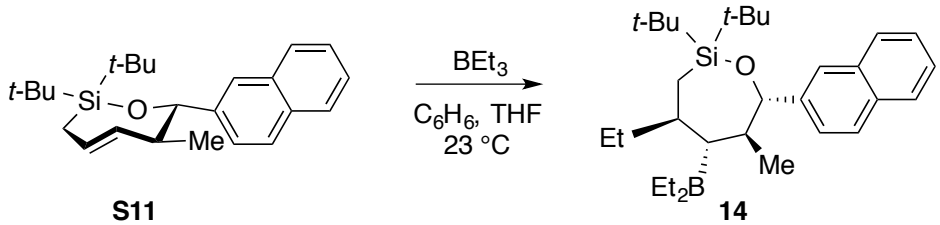
Trialkylborane 12. Trialkylborane **12** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S10** (0.048 g, 0.11 mmol), triethylborane (0.900 mL, 1.0 M in THF, 0.90 mmol), and C_6H_6 (1.00 mL). ^{1}H NMR spectroscopic analysis of the unpurified reaction mixture after workup showed a mixture of trialkylborane **12** and alkene **S18** in a 41:59 (**12**:**S18**) ratio. (The spectral data are consistent with the data reported below for alkene **S18**, the result of rearrangement of the starting *trans*-alkene.) Purification by flash chromatography (1:99 EtOAc:hexanes) afforded trialkylborane **12** as a colorless oil (0.015 g, 26%): ^{1}H NMR (500 MHz, C_6D_6) δ 7.32 (d, J = 7.2, 2H), 7.15–7.11 (m, 6H), 7.09–7.03 (m, 2H), 4.74 (d, J = 8.2, 1H), 4.07 (d, J = 12.2, 1H), 4.02 (d, J = 12.2, 1H), 2.76 (td, J = 9.2, 6.6, 1H), 2.53 (td, J = 9.2, 4.7, 1H), 2.27–2.21 (m, 1H), 2.16–2.11 (m, 1H), 1.79 (t, J = 10.4, 1H), 1.43–1.28 (m, 6H), 1.21 (s, 9H), 1.15 (m, 2H and t, J = 7.5, 6H), 0.99 (s, 9H), 0.94–0.92 (m, 4H), 0.74 (dd, J = 15.5, 11.8, 1H); ^{13}C NMR (150 MHz, C_6D_6) δ 145.4 (C), 139.7 (C), 128.8 (CH), 128.7 (CH), 128.1 (CH), 127.9 (CH), 127.85 (CH), 127.78 (CH), 83.6 (CH), 73.1 (CH_2), 68.5 (CH_2), 51.3 (CH), 47.1 (CH), 39.7 (CH), 34.5 (CH_2), 33.1 (CH_2), 29.5 (CH_3), 29.3 (CH_3), 22.2 (C), 21.5 (C), 17.2 (CH_2), 12.7 (CH_3), 10.2 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, C_6D_6) δ 54.3, 32.9 (see note under trialkylborane **2**, p. S10); IR (ATR) 1306, 1082, 823, 699 cm^{-1}; HRMS (APCI) m / z calcd for $C_{30}H_{45}O_2Si$ (M – BEt_2)$^+$ 465.3183, found 465.3181.



S3 **13**

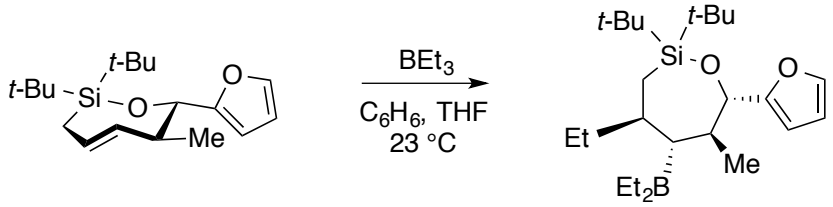
Trialkylborane 13. Trialkylborane **13** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S3** (0.022 g, 0.079 mmol), triethylborane (0.975 mL, 1.0 M in THF, 0.98 mmol), and C_6H_6 (1.00 mL). Purification by flash chromatography (hexanes) afforded trialkylborane **13** as a colorless oil (0.020 g, 67%): ^{1}H NMR (500 MHz, C_6D_6) δ 5.63–5.51 (m, 2H), 4.12–4.09 (m, 1H), 2.18–2.10 (m, 1H), 1.87–1.79 (m, 1H), 1.59 (d, J = 6.1, 3H), 1.45 (t, J = 10.3, 1H), 1.22 (m, 3H and s, 9H), 1.12 (s, 9H and m, 10H), 0.92–0.89 (m, 3H), 0.68 (dd, J = 15.4, 11.9, 1H), 0.46 (d, J = 7.0, 3H) (Some of trialkylborane **13** decomposed to alkene **S19** (vide infra) and is present in the ^{1}H NMR spectrum); ^{13}C NMR (125 MHz, C_6D_6) δ 135.1 (CH), 124.8 (CH), 83.2 (CH), 52.7 (CH), 43.2 (CH), 39.4 (CH), 33.6 (CH_2), 29.6 (CH_3), 29.3 (CH_3), 22.5 (C), 21.6 (C), 19.8 (CH_3), 18.2 (CH_3), 17.2 (CH_2), 12.5 (CH_3), 10.2 (CH_3) (see note under

trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, C_6D_6) δ 54.0, 32.0 (see note under trialkylborane **2**, p. S10); IR (ATR) 1079, 1048, 821, 643 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{19}H_{37}OSi$ (M – BEt_2)$^+$ 309.2608, found 309.2616.



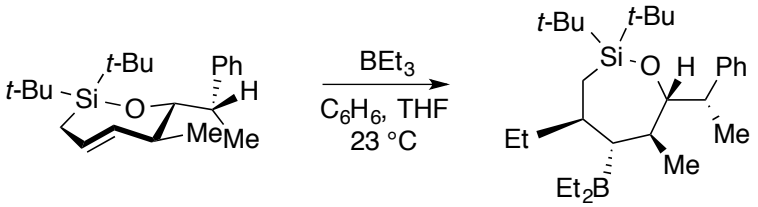
S11 **14**

Trialkylborane 14. Trialkylborane **14** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S11** (0.018 g, 0.050 mmol) and triethylborane (0.300 mL, 1.0 M in THF, 0.30 mmol). Purification by flash chromatography (hexanes) afforded trialkylborane **14** as a colorless oil (0.020 g, 87%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83–7.79 (m, 3H), 7.60 (s, 1H), 7.52 (dd, *J* = 8.4, 1.4, 1H), 7.48–7.41 (m, 2H), 4.71 (d, *J* = 8.0, 1H), 2.19–2.11 (m, 1H), 2.07–1.97 (m, 1H), 1.54 (t, *J* = 10.2, 1H), 1.26–1.17 (m, 5H), 1.11 (s, 9H), 1.02 (t, *J* = 7.6, 6H and m, 2H), 0.96 (s, 9H and m, 3H), 0.73 (dd, *J* = 15.5, 11.9, 1H), 0.09 (d, *J* = 7.0, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9 (C), 133.2 (C), 132.9 (C), 128.0 (CH), 127.83 (CH), 127.78 (CH), 125.8 (CH), 125.5 (CH), 125.40 (CH), 125.38 (CH), 84.5 (CH), 52.0 (CH), 43.5 (CH), 38.9 (CH), 33.0 (CH_2), 29.0 (CH_3), 28.7 (CH_3), 22.0 (C), 21.2 (C), 19.8 (CH_3), 16.7 (CH_2), 12.2 (CH_3), 9.7 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.5; IR (ATR) 1076, 823, 668 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{26}H_{39}OSi$ (M – BEt_2)$^+$ 395.2765, found 395.2765.



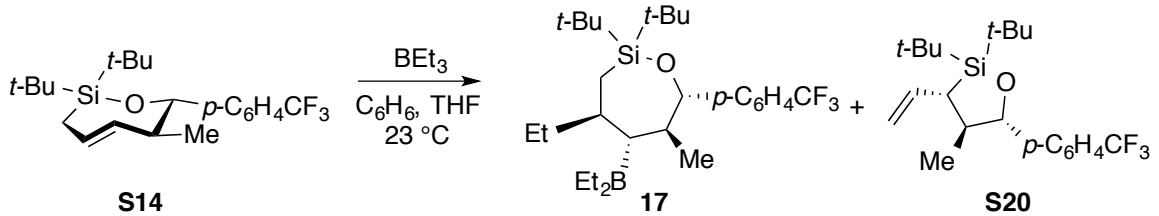
S12 **15**

Trialkylborane 15. Trialkylborane **15** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S12** (0.011 g, 0.035 mmol), triethylborane (0.45 mL, 1.0 M in THF, 0.45 mmol), and C_6H_6 (0.500 mL). Purification by flash chromatography (hexanes) afforded trialkylborane **15** as a colorless oil (0.009 g, 64%): ^{1}H NMR (400 MHz, C_6D_6) δ 7.09 (dd, *J* = 1.8, 0.7, 1H), 6.14 (dd, *J* = 3.1, 0.7, 1H), 6.09 (dd, *J* = 3.1, 1.8, 1H), 4.79 (d, *J* = 8.2, 1H), 2.37–2.27 (m, 1H), 2.25–2.17 (m, 1H), 1.52 (t, *J* = 10.4, 1H), 1.20 (s, 9H and m, 3H), 1.16–1.12 (m, 2H), 1.06 (m, 6H and s, 9H), 1.00–0.94 (m, 1H), 0.90–0.83 (m, 4H), 0.70 (dd, *J* = 15.5, 11.9, 1H), 0.32 (d, *J* = 7.0, 3H); ^{13}C NMR (100 MHz, C_6D_6) δ 158.4 (C), 141.7 (CH), 110.5 (CH), 106.3 (CH), 78.6 (CH), 52.4 (CH), 43.5 (CH), 39.3 (CH), 33.5 (CH_2), 29.4 (CH_3), 29.1 (CH_3), 22.4 (C), 21.5 (C), 19.0 (CH_3), 17.1 (CH_2), 12.4 (CH_3), 10.1 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, C_6D_6) δ 54.0; IR (ATR) 1504, 1009, 823, 729 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{20}H_{35}O_2Si$ (M – BEt_2)$^+$ 335.2401, found 335.2397.



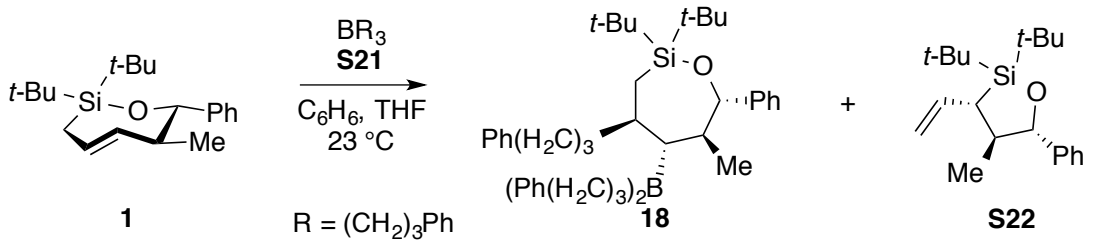
S16 **16**

Trialkylborane 16. Trialkylborane **16** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S16** (0.013 g, 0.038 mmol), triethylborane (0.400 mL, 1.0 M in THF, 0.40 mmol), and C_6H_6 (0.530 mL). Purification by flash chromatography (hexanes) afforded trialkylborane **16** as a white solid that could not be further purified (0.011 g, 65% unpurified yield): mp = 89–92 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.27–7.26 (m, 4H), 7.17–7.14 (m, 1H), 3.69 (dd, *J* = 8.5, 1.8, 1H), 3.02 (qd, *J* = 7.0, 1.8, 1H), 1.91–1.83 (m, 2H), 1.39 (t, *J* = 10.1, 1H), 1.26 (d, *J* = 7.0, 3H and m, 4H), 1.04 (m, 6H and s, 9H), 1.01–0.98 (m, 1H), 0.87–0.82 (m, 5H), 0.63 (d, *J* = 6.7, 3H), 0.46 (s, 9H), 0.35 (dd, *J* = 15.3, 12.1, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 146.4 (C), 129.1 (CH), 127.9 (CH), 125.8 (CH), 84.7 (CH), 50.6 (CH), 42.0 (CH), 40.5 (CH), 39.1 (CH), 32.5 (CH_2), 28.9 (CH_3), 27.9 (CH_3), 21.8 (C), 21.6 (C), 19.2 (CH_3), 17.7 (CH_2), 12.4 (CH_3), 10.6 (CH_3), 9.8 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, C_6D_6) δ 53.8; IR (ATR) 1105, 1091, 822, 698 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{24}H_{41}OSi$ $(M - BEt_2)^+$ 373.2921, found 373.2926.



S14 **17** **S20**

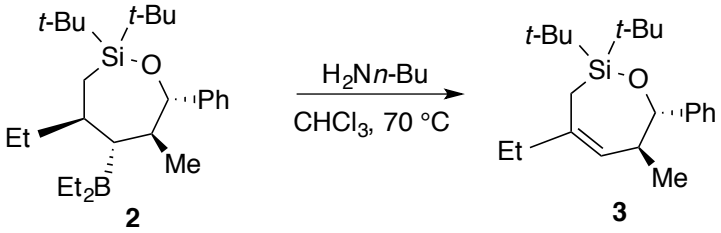
Trialkylborane 17. Trialkylborane **17** was prepared using the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **S14** (0.022 g, 0.056 mmol), triethylborane (0.450 mL, 1.0 M in THF, 0.45 mmol), and C_6H_6 (0.530 mL). ^{1}H NMR spectroscopic analysis of the unpurified reaction mixture after workup showed a mixture of trialkylborane **17** and alkene **S20** in a 70:30 (**17**:**S20**) ratio. (The spectral data are consistent with the data reported below for alkene **S20**, the result of rearrangement of the starting *trans*-alkene.) Purification by flash chromatography (hexanes) afforded trialkylborane **17** as a colorless oil (0.015 g, 56%): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0, 2H), 7.37 (d, *J* = 8.0, 2H), 4.59 (d, *J* = 8.0, 1H), 2.13–2.08 (m, 1H), 1.93–1.87 (m, 1H), 1.48 (t, *J* = 10.2, 1H), 1.26–1.16 (m, 4H), 1.14–1.11 (m, 1H), 1.08 (s, 9H), 1.01 (t, *J* = 7.6, 6H and m, 1H), 0.94 (s, 9H), 0.91 (t, *J* = 6.8, 3H), 0.87–0.81 (m, 1H), 0.68 (dd, *J* = 15.5, 11.9, 1H), 0.07 (d, *J* = 7.0, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.3 (C), 129.0 (q, *J* = 32.0, C), 127.2 (CH), 125.0 (q, *J* = 3.8, CH), 124.4 (q, *J* = 270.1, C), 83.8 (CH), 51.9 (CH), 43.7 (CH), 38.8 (CH), 32.9 (CH_2), 28.9 (CH_3), 28.7 (CH_3), 22.0 (C), 21.1 (C), 19.7 (CH_3), 16.6 (CH_2), 12.1 (CH_3), 9.6 (CH_3) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ –65.4; IR (ATR) 1324, 1126, 849, 822 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{23}H_{36}F_3OSi$ $(M - BEt_2)^+$ 413.2482, found 413.2466.



Trialkylborane 18. Trialkylborane **18** was prepared following the representative procedure for the synthesis of trialkylboranes using *trans*-alkene **1** (0.030 g, 0.094 mmol), trialkylborane **S21**[7] (0.150 g, 0.407 mmol); (*caution: neat trialkylboranes reacts violently with oxygen)*, and C_6H_6 (0.97 mL). ^{1}H NMR spectroscopic analysis of the unpurified reaction mixture after workup showed a mixture of trialkylborane **18** and alkene **S22** in a 73:37 (**18**:**S22**) ratio. The spectral data are consistent with the data reported previously for alkene **S22**,[2] the result of rearrangement of the starting *trans*-alkene. Purification by flash chromatography (1:99 EtOAc:hexanes) afforded trialkylborane **18** as a colorless oil (0.019 g, 30%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.24 (m, 8H), 7.22–7.16 (m, 10H), 7.10–7.08 (m, 2H), 4.47 (d, J = 7.9, 1H), 2.59–2.42 (m, 6H), 2.15–2.07 (m, 1H), 1.85–1.77 (m, 2H), 1.71–1.57 (m, 3H), 1.44–1.39 (m, 2H), 1.14 (t, J = 8.0, 4H), 1.07 (s, 9H and m, 2H), 0.92 (m, 1H and s, 9H), 0.72–0.65 (m, 2H), 0.01 (d, J = 7.0, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2 (C), 143.0 (C), 142.4 (C), 128.62 (CH), 128.58 (CH), 128.5 (CH), 128.4 (CH), 127.9 (CH), 126.9 (CH), 126.8 (CH), 125.9 (CH), 125.8 (CH), 84.1 (CH), 52.1 (CH), 43.8 (CH), 40.4 (CH_2), 39.5 (CH_2), 37.3 (CH), 36.4 (CH_2), 29.4 (CH_2), 29.0 (CH_3), 28.7 (CH_3), 27.9 (CH_2), 21.9 (C), 21.1 (C), 19.9 (CH_3), 17.5 (CH_2) (see note under trialkylborane **2**, p. S10); ^{11}B NMR (128 MHz, C_6D_6) δ 32.9 (see note under trialkylborane **2**, p. S10); IR (ATR) 1080, 1029, 823, 697 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{29}H_{43}OSi$ (M – $C_{16}H_{22}B$)$^+$ 435.3078, found 435.3071.

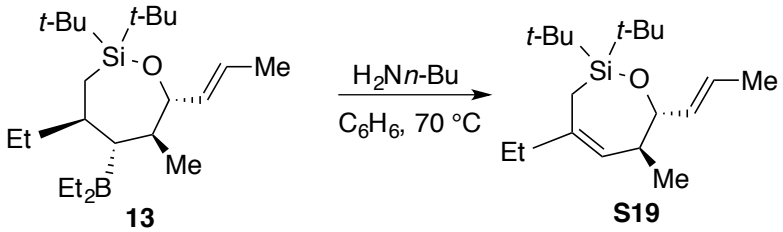
A compound similar to alkene **3**, but with a 1-phenylpropyl group, resulting from the decomposition of **18**, was also isolated (0.007 g, 17%, clear oil): ^{1}H NMR (500 MHz, $CDCl_3$, diagnostic peaks) δ 5.09–5.07 (m, 1H), 4.73 (d, J = 9.3, 1H), 2.69–2.60 (m, 8H), 1.07 (s, 9H), 1.00 (s, 9H), 0.56 (d, J = 7.2, 3H).

IV. Transformations of Trialkylboranes

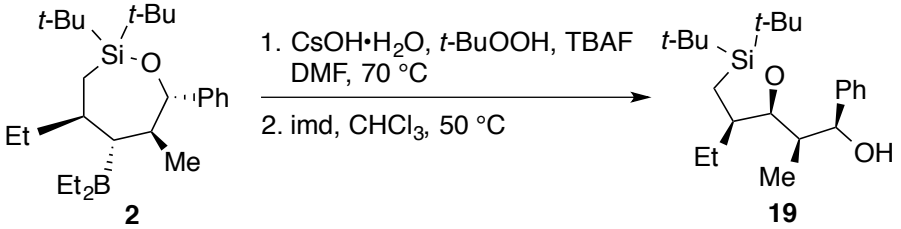


Alkene 3. A solution of trialkylborane **2** (0.034 g, 0.082 mmol) and H_2N^nBu (0.130 mL, 1.19 mmol) in $CHCl_3$ (2.0 mL) was heated to 70 °C. After 16 h, the reaction mixture was cooled and CH_2Cl_2 (5 mL) and H_2O (5 mL) were added. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (5 mL). The combined organic layers were

washed with brine (10 mL), dried with $MgSO_4$, and concentrated *in vacuo*. Purification by flash chromatography (hexanes) afforded alkene **3** as a colorless oil (0.019 g, 68%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32–7.31 (m, 4H), 7.25–7.21 (m, 1H), 5.02–5.01 (m, 1H), 4.70 (d, J = 9.2, 1H), 2.72–2.62 (m, 1H), 2.21–2.14 (m, 2H), 1.99 (d, J = 15.2, 1H), 1.53 (d, J = 15.2, 1H), 1.06 (m, 3H and s, 9H), 0.99 (s, 9H), 0.53 (d, J = 7.1, 3H); ^{13}C NMR (150 MHz, C_6D_6) δ 145.2 (C), 139.3 (C), 128.7 (CH), 128.3 (CH), 127.8 (CH), 127.6 (CH), 82.3 (CH), 43.0 (CH), 35.6 (CH_2), 29.2 (CH_3), 28.7 (CH_3), 23.1 (C), 21.5 (C), 20.3 (CH_3), 15.5 (CH_2), 13.3 (CH_3); IR (ATR) 1603, 1096, 823 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{22}H_{37}OSi$ $(M + H)^+$ 345.2608, found 345.2604. Anal. Calcd for $C_{22}H_{36}OSi$: C, 76.68; H, 10.53. Found: C, 76.53; H, 10.76.

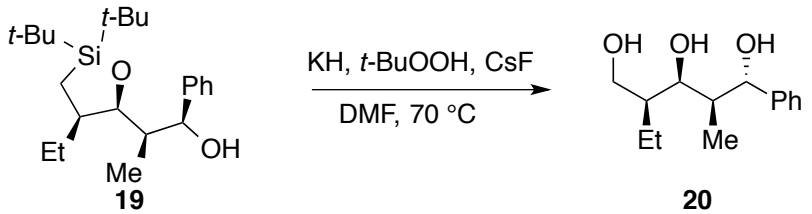


Alkene S19. A solution of trialkylborane **13** (0.014 g, 0.037 mmol) and H_2N^nBu (0.060 mL, 0.61 mmol) in C_6H_6 (1.5 mL) was heated to 70 °C. After 18 h, the reaction mixture was cooled and Et_2O (15 mL) and H_2O (15 mL) were added. The layers were separated and the aqueous layer was extracted with Et_2O (15 mL). The combined organic layers were washed with brine (2 x 15 mL), dried with $MgSO_4$, and concentrated *in vacuo*. Purification by flash chromatography (hexanes) afforded alkene **S19** as a colorless oil (0.012 g, 100%): ^{1}H NMR (600 MHz, C_6D_6) δ 5.55–5.54 (m, 2H), 5.00 (d, J = 5.7, 1H), 4.14–4.12 (m, 1H), 2.52–2.49 (m, 1H), 2.17–2.09 (m, 2H), 1.94 (d, J = 15.2, 1H), 1.56 (s, 3H), 1.35 (d, J = 15.2, 1H), 1.12 (s, 18H), 1.07–1.05 (m, 3H), 0.87 (d, J = 7.0, 3H); ^{13}C NMR (150 MHz, C_6D_6) δ 139.9 (C), 134.7 (CH), 127.5 (CH), 126.5 (CH), 80.7 (CH), 40.8 (CH), 34.9 (CH_2), 29.2 (CH_3), 28.8 (CH_3), 22.8 (C), 21.6 (C), 19.7 (CH_3), 18.0 (CH_3), 15.6 (CH_2), 13.2 (CH_3); IR (ATR) 1673, 1363, 1096, 822 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{19}H_{37}OSi$ $(M + H)^+$ 309.2608, found 309.2610. Anal. Calcd for $C_{19}H_{36}OSi$: C, 73.95; H, 11.76. Found: C, 74.25; H, 11.77.



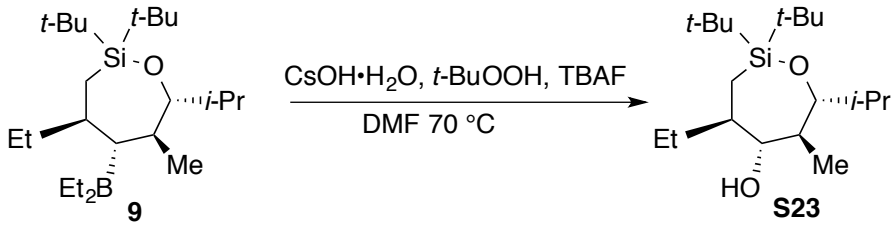
Alcohol 19. A solution of trialkylborane **2** (0.091 g, 0.22 mmol), ^{t}BuOOH (0.620 mL, 5–6 M in decane, 3 mmol), $CsOH•H_2O$ (0.517 g, 3.08 mmol), and TBAF (1.1 mL, 1.0 M in THF, 1.1 mmol) in DMF (3.4 mL) was heated to 70 °C. After 19 h, the reaction mixture was cooled and Et_2O (5 mL) and saturated aqueous $Na_2S_2O_3$ (5 mL) were added. The layers were separated and the aqueous layer was extracted with Et_2O (2 x 5 mL). The combined organic layers were washed with H_2O (10 mL) and brine (10 mL). These

layers were dried with $MgSO_4$, and concentrated *in vacuo*. To a solution of the resulting oil in $CHCl_3$ (6 mL) was added imidazole (0.114 g, 1.67 mmol) and the reaction mixture was heated to 50 °C. After 3 d, the reaction mixture was cooled and CH_2Cl_2 (10 mL) and H_2O (10 mL) were added. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (2 x 10 mL). The combined organic layers were washed with H_2O (20 mL) and brine (20 mL), dried with $MgSO_4$ and concentrated *in vacuo*. Purification by flash chromatography (3:97 EtOAc:hexanes) afforded alcohol **19** as a yellow oil (0.053 g, 66% over two steps): ^{1}H NMR (400 MHz, C_6D_6) δ 7.44–7.42 (m, 2H), 7.25–7.22 (m, 2H), 7.12–7.08 (m, 1H), 4.82 (dd, *J* = 6.5, 4.2, 1H), 4.34 (dd, *J* = 7.9, 1.9, 1H), 3.88 (d, *J* = 6.5, 1H), 2.02–1.95 (m, 1H), 1.87–1.77 (m, 1H), 1.37–1.27 (m, 1H), 1.17 (d, *J* = 6.9, 3H and m, 1H), 1.06 (s, 9H), 0.97 (s, 9H), 0.75 (t, *J* = 7.3, 3H and m, 1H), 0.36 (dd, *J* = 15.1, 7.4, 1H); ^{13}C NMR (100 MHz, C_6D_6) δ 146.3 (C), 128.7 (CH), 127.4 (CH), 126.8 (CH), 80.5 (CH), 79.2 (CH), 44.0 (CH), 42.6 (CH), 29.1 (CH_3), 28.6 (CH_3), 25.5 (CH_2), 21.7 (C), 20.3 (C), 14.6 (CH_3), 13.8 (CH_3), 11.0 (CH_2); IR (ATR) 3458, 1062, 970, 823 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{22}H_{38}NaO_2Si$ $(M + Na)^+$ 385.2533, found 385.2525. Anal. Calcd for $C_{22}H_{38}O_2Si$: C, 72.87; H, 10.55. Found: C, 72.72; H, 10.72.

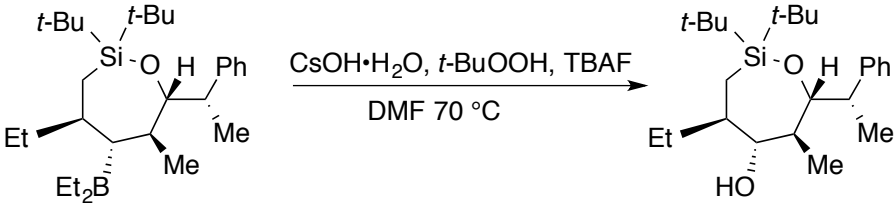


19 **20**

Triol 20. To a solution of KH (0.012 g, 0.30 mmol) in DMF (0.40 mL) was added ^{t}BuOOH (0.065 mL, 5–6 M in decane, 0.4 mmol), followed by alcohol **19** (0.008 g, 0.022 mmol) in DMF (0.20 mL). After 10 min, CsF (0.019 g, 0.13 mmol) was added and the reaction mixture was heated to 70 °C. After 17 h, the reaction mixture was cooled to 23 °C and Et_2O (5 mL) and saturated aqueous $Na_2S_2O_3$ (5 mL) were added. The layers were separated and the aqueous layer was extracted with Et_2O (2 x 5 mL). The combined organic layers were washed with H_2O (10 mL) and brine (10 mL). These layers were dried with $MgSO_4$ and concentrated *in vacuo*. Purification by flash chromatography (1:1 EtOAc:hexanes) afforded alcohol **20** as a colorless oil (0.003 g, 57%): ^{1}H NMR (600 MHz, CD_3OD) δ 7.33–7.31 (m, 4H), 7.25–7.23 (m, 1H), 4.58 (d, *J* = 7.9, 1H), 3.95 (d, *J* = 8.7, 1H), 3.56 (dd, *J* = 11.3, 4.5, 1H), 3.51 (dd, *J* = 11.3, 4.6, 1H), 2.04–1.99 (m, 1H), 1.76–1.69 (m, 1H), 1.56–1.51 (m, 1H), 1.47–1.40 (m, 1H), 0.94 (t, *J* = 7.5, 3H), 0.70 (d, *J* = 7.0, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.9 (C), 128.5 (CH), 127.6 (CH), 126.1 (CH), 78.7 (CH), 72.6 (CH), 63.2 (CH_2), 45.3 (CH), 41.5 (CH), 19.6 (CH_2), 11.9 (CH_3), 11.7 (CH_3); IR (ATR) 3338, 1017 cm^{-1}; HRMS (ESI) *m* / *z* calcd for $C_{14}H_{22}NaO_3$ $(M + Na)^+$ 261.1461, found 261.1460. Anal. Calcd for $C_{14}H_{22}O_3$: C, 70.56; H, 9.30. Found: C, 70.30; H, 9.20.

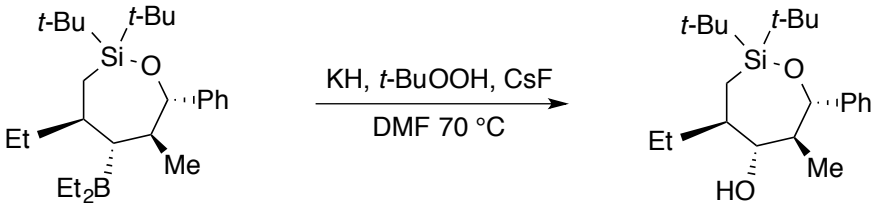


Alcohol S23. To a solution of trialkylborane **9** (0.028 g, 0.074 mmol), ^{t}BuOOH (0.210 mL, 5–6 M in decane, 1 mmol), and CsOH•H_2O (0.174 g, 1.04 mmol) in DMF (1.2 mL) was added TBAF (0.370 mL, 1.0 M in THF, 0.37 mmol). After 30 min, Et_2O (5 mL) and saturated aqueous $Na_2S_2O_3$ (2.5 mL) were added. The layers were separated and the aqueous layer was extracted with Et_2O (2 x 5 mL). The combined organic layers were washed with H_2O (10 mL) and brine (10 mL). These layers were dried with $MgSO_4$ and concentrated *in vacuo*. Purification by flash chromatography (5:95 EtOAc:hexanes) afforded alcohol **S23** as a colorless oil (0.019 g, 76% over two steps): ^{1}H NMR (600 MHz, C_6D_6) δ 3.43 (dd, *J* = 9.0, 1.8, 1H), 2.78–2.75 (m, 1H), 1.88–1.83 (m, 1H), 1.80–1.74 (m, 1H), 1.73–1.68 (m, 1H), 1.54–1.49 (m, 1H), 1.48–1.41 (m, 1H), 1.10 (s, 9H), 1.08 (d, *J* = 6.7, 3H), 1.03 (s, 9H), 0.97 (t, *J* = 7.4, 3H), 0.92–0.91 (m, 6H), 0.78 (br s, 1H and dd, *J* = 15.4, 1.5, 1H), 0.56 (dd, *J* = 15.4, 12.5, 1H); ^{13}C NMR (100 MHz, C_6D_6) δ 81.3 (CH), 80.2 (CH), 47.8 (CH), 43.5 (CH), 32.1 (CH), 29.3 (CH_3), 29.2 (CH_2), 29.0 (CH_3), 22.7 (C), 22.2 (CH_3), 21.9 (C), 15.4 (CH_3), 14.5 (CH_3), 13.2 (CH_2), 10.7 (CH_3); IR (ATR) 3351, 1139, 1062, 823 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{19}H_{41}O_2Si$ (M + H)$^+$ 329.2870, found 329.2862. Anal. Calcd for $C_{19}H_{40}O_2Si$: C, 69.45; H, 12.27. Found: C, 69.64; H, 12.34.



Alcohol S24. To a solution of trialkylborane **16** (0.011 g, 0.025 mmol), ^{t}BuOOH (0.070 mL, 5–6 M in decane, 0.4 mmol), and CsOH•H_2O (0.058 g, 0.35 mmol) in DMF (0.400 mL) was added TBAF (0.125 mL, 1.0 M in THF, 0.13 mmol). After 100 min, Et_2O (5 mL) and saturated aqueous $Na_2S_2O_3$ (2.0 mL) were added. The layers were separated and the aqueous layer was extracted with Et_2O (2 x 5 mL). The combined organic layers were washed with H_2O (10 mL) and brine (10 mL). These layers were dried with $MgSO_4$ and concentrated *in vacuo*. Purification by flash chromatography (5:95 EtOAc:hexanes) afforded alcohol **S24** as a white solid (0.008 g, 53% over two steps): mp = 126–128 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27–7.26 (m, 4H), 7.17–7.13 (m, 1H), 3.75 (dd, *J* = 9.0, 1.9, 1H), 3.16 (qd, *J* = 7.0, 1.9, 1H), 2.99 (t, *J* = 8.9, 1H), 1.91–1.85 (m, 1H), 1.78–1.65 (m, 2H), 1.54 (br s, 1H), 1.50–1.40 (m, 1H), 1.29 (d, *J* = 7.0, 3H), 1.18 (d, *J* = 6.7, 3H), 1.01 (s, 9H), 0.94 (t, *J* = 7.4, 3H), 0.73 (dd, *J* = 15.6, 1.5, 1H), 0.51 (dd, *J* = 15.6, 12.5, 1H), 0.45 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.9 (C), 129.1 (CH), 128.0 (CH), 126.0 (CH), 81.2 (CH), 79.9 (CH), 47.2 (CH), 42.6 (CH), 42.3 (CH), 28.7 (CH_3), 28.6

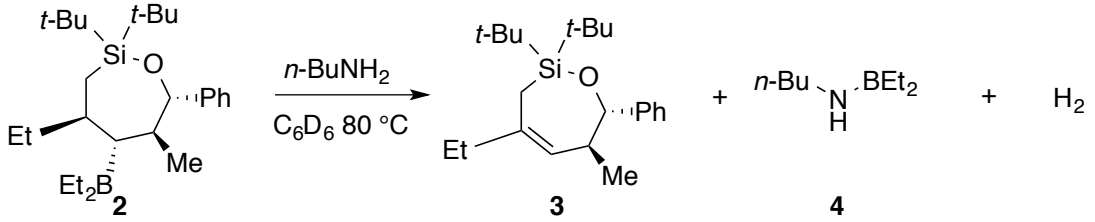
(CH_2), 27.8 (CH_3), 21.8 (C), 21.5 (C), 15.9 (CH_3), 12.6 (CH_2), 10.7 (CH_3), 9.9 (CH_3); IR (ATR) 3348, 1041, 1029, 1009, 824 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{24}H_{43}O_2Si$ $(M + H)^+$ 391.3027, found 391.3038.



2 **S25**

Alcohol S25. To a solution of KH (0.025 g, 0.55 mmol) in DMF (0.70 mL) was added ^{t}BuOOH (0.110 mL, 5–6 M in decane, 0.6 mmol), followed by trialkylborane **2** (0.016 g, 0.039 mmol) in DMF (0.40 mL) and THF (0.15 mL). After 10 min, CsF (0.037 g, 0.24 mmol) was added and the reaction mixture was heated to 70 °C. After 14 h, the reaction mixture was cooled to 23 °C, $Na_2S_2O_3$ (0.037 g) was added, and the reaction mixture was concentrated *in vacuo*. The reaction mixture was partitioned in Et_2O (10 mL) and brine (10 mL). The layers were separated and the aqueous layer was extracted with Et_2O (2 x 5 mL). The combined organic layers were dried with $MgSO_4$ and concentrated *in vacuo*. Purification by flash chromatography (5:95 EtOAc:hexanes) afforded alcohol **S25** as a white solid (0.010 g, 71%): mp = 99–100 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31–7.29 (m, 2H), 7.26–7.22 (m, 3H), 4.51 (d, *J* = 8.5, 1H), 3.05 (t, *J* = 9.2, 1H), 2.11–2.04 (m, 1H), 1.85–1.74 (m, 2H), 1.59–1.53 (m, 2H), 1.06 (s, 9H), 0.99 (t, *J* = 7.4, 3H), 0.93 (s, 9H), 0.85–0.84 (m, 2H), 0.60 (d, *J* = 6.8, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.0 (C), 128.1 (CH), 127.0 (2 CH), 81.8 (CH), 78.7 (CH), 50.3 (CH), 42.0 (CH), 28.9 (CH_3 and CH_2), 28.6 (CH_3), 21.8 (C), 21.0 (C), 17.4 (CH_3), 11.2 (CH_2), 9.6 (CH_3); IR (ATR) 3346, 1078, 1057, 909, 823 cm^{-1}; HRMS (ESI) *m* / *z* calcd for $C_{22}H_{37}O$ $(M - OH)^+$ 345.2608, found 345.2606.

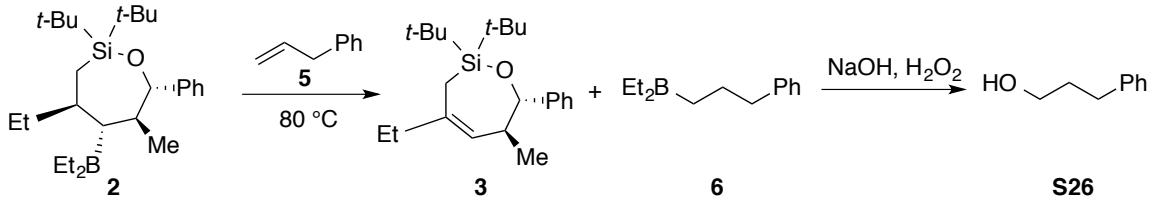
V. Control Experiments



2 **3** **4**

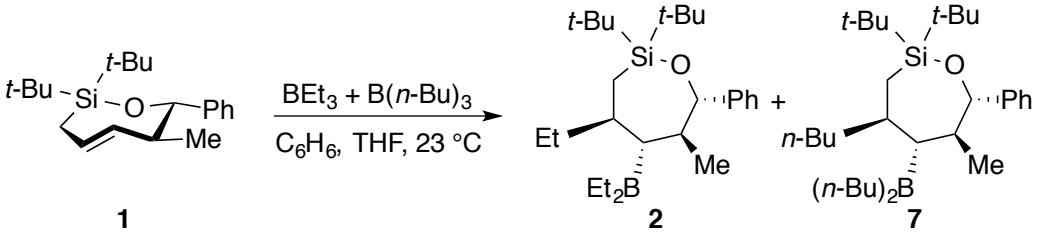
Amine 4 and Alkene 3. To a solution of trialkylborane **2** (0.018 g, 0.043 mmol) and mesitylene (0.0020 mL, 0.014 mmol, internal standard) in C_6D_6 (0.600 mL) in a NMR tube was added ^{n}BuNH$_2$ (0.050 mL, 0.50 mmol). The NMR tube was flame-sealed under vacuum. After 24 h, the reaction mixture was heated to 80 °C. After 24 h, alkene **3** was formed in 95% yield based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH peak (δ 4.70). The spectral data are consistent with the data reported above for alkene **3**. Amine **4** was formed in 85% yield based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71)

and the area of the NH peak (δ 3.77): ^{1}H NMR (600 MHz, C_6D_6, diagnostic peaks) δ 3.77 (br s, 1H), 2.84–2.80 (m, 2H); ^{13}C NMR (150 MHz, C_6D_6, diagnostic peaks) δ 42.8 (CH_2), 36.2 (CH_2), 9.7 (CH_3); ^{11}B NMR (128 MHz, C_6D_6) δ 45.9.

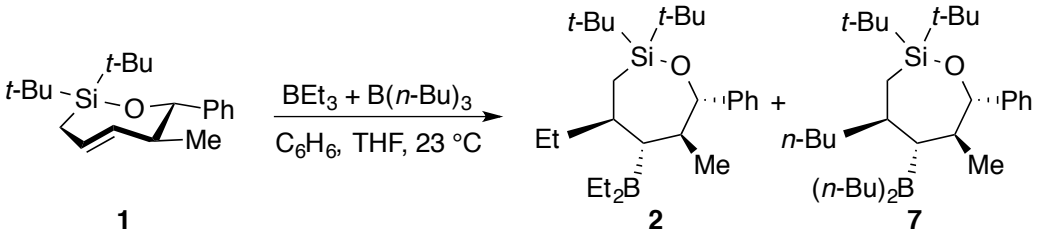


Alkene 3 and Trialkylborane 6. To a solution of trialkylborane **2** (0.013 g, 0.031 mmol) and mesitylene (0.0020 mL, 0.014 mmol, internal standard) in C_6D_6 (0.550 mL) in a NMR tube was added allylbenzene **5** (0.006 mL, 0.045 mmol). The NMR tube was flame-sealed under vacuum. After 24 h, the reaction mixture was heated to 80 °C. After 24 h, alkene **3** was formed in 96% yield based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH peak (δ 4.70). The spectral data are consistent with the data reported above for alkene **3**. Trialkylborane **6** was formed in 74% yield based on ^{1}H NMR spectroscopic analysis of the area of a peak of the standard (δ 6.71) and the area of the benzylic CH_2 peak (δ 2.51): ^{1}H NMR (600 MHz, C_6D_6, diagnostic peaks) δ 2.51 (t, J = 7.6, 2H), 1.69–1.63 (m, 2H); ^{13}C NMR (150 MHz, C_6D_6, diagnostic peaks) δ 39.8 (CH_2), 27.9 (CH_2), 27.3 (CH_2), 20.0 (CH_2), 8.7 (CH_3); ^{11}B NMR (128 MHz, C_6D_6) δ 85.9.

Alcohol S26. Oxidation of trialkylborane **6** was performed to confirm the identity of **6**. The above reaction mixture was transferred to a flask containing 1 M NaOH (1.0 mL) and 30% H_2O_2 (0.5 mL) using Et_2O (2 mL). The layers were separated and the aqueous layer was extracted with Et_2O (2 x 3 mL). The combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo*. The spectral data for alcohol **S26** matched the data previously reported.[8]

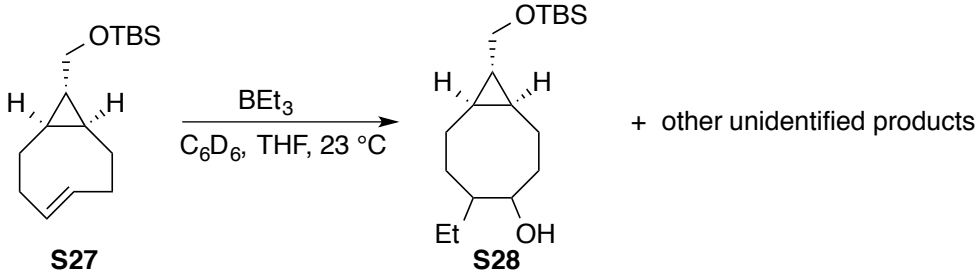


Crossover experiment with BEt_3 (5 equiv) and $B(n\text{-}Bu)_3$ (5 equiv). To a solution of *trans*-alkene **1** (0.007 g, 0.021 mmol) in C_6H_6 (0.200 mL) was added tri-*n*-butylborane (0.024 mL, 0.098 mmol), immediately followed by triethylborane (0.100 mL, 1.0 M in THF, 0.10 mmol). After 2 h, 1 M NaOH (0.80 mL) was added, followed by 30% H_2O_2 in H_2O (0.40 mL) (*caution the ensuing reaction was exothermic*). After 20 min, Et_2O (5 mL) and brine (5 mL) were added and the layers were separated. The aqueous layer was extracted with Et_2O (2 x 5 mL). The combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo*. ^{1}H NMR spectroscopic analysis of the unpurified reaction mixture showed a mixture of trialkylboranes **2** and **7** in a 83:17 (**2**:**7**) ratio. The spectral data are consistent with the data reported above for trialkylboranes **2** and **7**.



1 **2** **7**

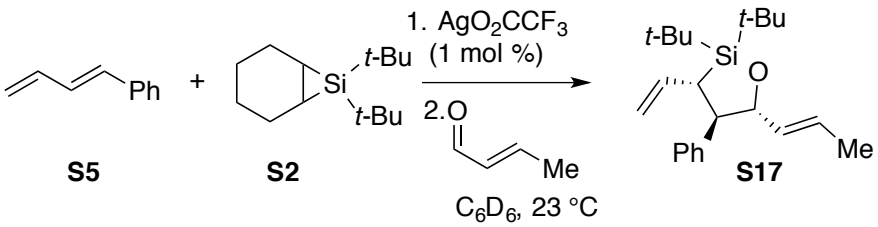
Crossover experiment with BEt_3 (5 equiv) and $B(n\text{-Bu})_3$ (20 equiv). To a solution of *trans*-alkene **1** (0.007 g, 0.021 mmol) in C_6H_6 (0.200 mL) was added tri-*n*-butylborane (0.100 mL, 0.410 mmol), immediately followed by triethylborane (0.100 mL, 1.0 M in THF, 0.10 mmol). After 2 h, 1 M NaOH (0.80 mL) was added, followed by 30% H_2O_2 in H_2O (0.40 mL) (*caution the ensuing reaction was exothermic*). After 20 min, Et_2O (5 mL) and brine (5 mL) were added and the layers were separated. The aqueous layer was extracted with Et_2O (2 x 5 mL). The combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo*. ^{1}H NMR spectroscopic analysis of the unpurified reaction mixture showed a mixture of trialkylboranes **2** and **7** in a 59:41 (**2**:**7**) ratio. The spectral data are consistent with the data reported above for trialkylboranes **2** and **7**.



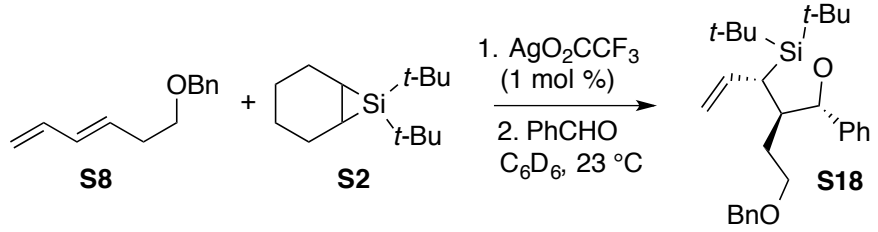
S27 **S28**

Alcohol S28. To a solution of *trans*-alkene **S27** (0.017 g, 0.062 mmol) in C_6D_6 (0.610 mL) in a J. Young NMR tube was added triethylborane (0.370 mL, 1.0 M in THF, 0.37 mmol). The reaction mixture was monitored by ^{1}H NMR spectroscopy until *trans*-alkene **S28** was consumed. After 13 d, 1 M NaOH (1.0 mL) was added, followed by 30% H_2O_2 in H_2O (0.50 mL) (*caution the ensuing reaction was exothermic*). After 20 min, Et_2O (5 mL) and brine (5 mL) were added and the layers were separated. The aqueous layer was extracted with Et_2O (2 x 10 mL). The combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo*. Purification by flash chromatography (hexanes) afforded alcohol **S28** as a clear oil that could not be purified further (0.004 g, 21% unpurified yield): ^{1}H NMR (600 MHz, C_6D_6) δ 3.46–3.44 (m, 2H), 3.24–3.21 (m, 1H), 2.01–1.96 (m, 1H), 1.85–1.80 (m, 2H), 1.75–1.68 (m, 1H), 1.62–1.56 (m, 2H), 1.52–1.42 (m, 1H), 1.32–1.19 (m, 3H), 1.01 (s, 9H), 0.88–0.79 (m, 4H), 0.57–0.52 (m, 1H), 0.48–0.43 (m, 2H), 0.39–0.34 (m, 1H), 0.08 (s, 6H); ^{13}C NMR (150 MHz, C_6D_6) δ 75.1 (CH), 67.1 (CH_2), 44.2 (CH), 40.7 (CH_2), 33.5 (CH_2), 27.4 (CH), 26.5 (CH_3), 26.3 (CH_2), 24.9 (CH_2), 24.0 (CH_2), 21.51 (CH), 21.50 (CH), 18.9 (C), 13.7 (CH_3), –4.6 (CH_3); IR (ATR) 3406, 1074, 836 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{18}H_{36}NaO_2Si$ $(M + Na)^+$ 335.2377, found 335.2374.

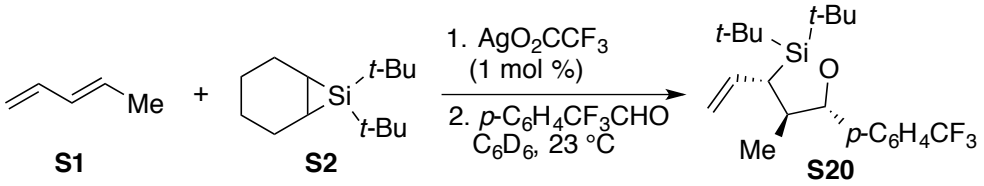
VI. Rearrangement of Seven-Membered-Ring *trans*-Alkenes



Alkene S17. The synthesis of alkene **S17** was adapted from a reported procedure.[2] To a solution of diene **S5** (0.011 g, 0.084 mmol) and cyclohexene silacyclopropane **S2** (0.021 g, 0.094 mmol) in C_6H_6 (0.50 mL) was added $AgOCOCF_3$ (0.024 mL, 0.010 M in C_6H_6, 0.3 mol %). After 10 min, crotonaldehyde (0.007 mL, 0.08 mmol) was added. After 1 d, the reaction mixture was concentrated *in vacuo*. Purification by flash chromatography (3:97 EtOAc:hexanes) afforded alkene **S17** as a colorless oil (0.015 g, 52% over three steps): ^{1}H NMR (400 MHz, C_6D_6) δ 7.18–7.11 (m, 4H), 7.07–7.02 (m, 1H), 5.89 (ddd, *J* = 17.0, 10.3, 8.3, 1H), 5.71–5.62 (m, 1H), 5.59–5.53 (m, 1H), 4.83 (dt, *J* = 17.0, 1.5, 1H), 4.78–4.74 (m, 1H), 4.47 (ddt, *J* = 10.3, 5.2, 1.0, 1H), 3.04 (dd, *J* = 12.6, 10.3, 1H), 2.73 (ddt, *J* = 12.6, 8.3, 1.0, 1H), 1.47 (dt, *J* = 6.2, 1.3, 3H), 1.20 (s, 9H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, C_6D_6) δ 142.1 (C), 138.1 (CH), 132.6 (CH), 129.0 (CH), 128.9 (CH), 127.2 (CH), 126.0 (CH), 113.4 (CH_2), 84.4 (CH), 58.4 (CH), 40.4 (CH), 28.6 (CH_3), 28.4 (CH_3), 22.4 (C), 22.2 (C), 18.0 (CH_3); IR (ATR) 1628, 1472, 837 cm^{-1}; HRMS (ESI) *m* / *z* calcd for $C_{22}H_{33}Si$ $(M - OH)^+$ 325.2346, found 325.2347.



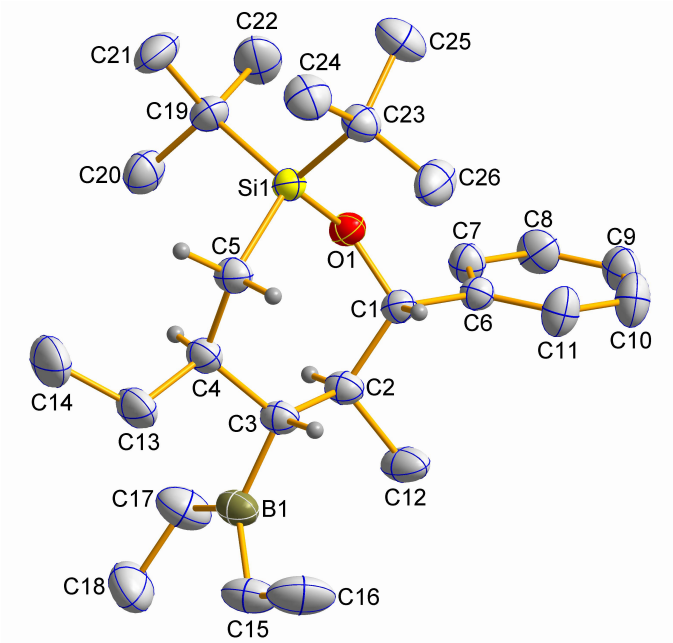
Alkene S18. The synthesis of alkene **S18** was adapted from a reported procedure.[2] To a solution of diene **S8** (0.014 g, 0.074 mmol) and cyclohexene silacyclopropane **S2** (0.021 g, 0.094 mmol) in C_6D_6 (0.50 mL) was added $AgOCOCF_3$ (0.025 mL, 0.030 M in C_6H_6, 1 mol %). After 10 min, benzaldehyde (0.0075 mL, 0.074 mmol) was added. After 1 d, the reaction mixture was concentrated *in vacuo*. Purification by flash chromatography (3:97 EtOAc:hexanes) afforded alkene **S18** as a colorless oil (0.020 g, 63% over three steps): ^{1}H NMR (600 MHz, C_6D_6) δ 7.52 (d, *J* = 7.7, 2H), 7.24 (d, *J* = 7.6, 2H), 7.21–7.18 (m, 2H), 7.14–7.07 (m, 4H), 6.00–5.94 (m, 1H), 5.00 (d, *J* = 17.1, 1H), 4.89 (d, *J* = 10.3, 1H), 4.64 (d, *J* = 9.5, 1H), 4.18 (s, 2H), 3.29–3.23 (m, 2H), 2.36–2.27 (m, 2H), 1.75–1.71 (m, 2H), 1.21 (s, 9H), 1.13 (s, 9H); ^{13}C NMR (150 MHz, C_6D_6) δ 144.2 (C), 140.1 (CH), 139.6 (C), 128.84 (CH), 128.82 (CH), 128.7 (CH), 128.1 (CH), 127.91 (CH), 127.87 (CH), 112.6 (CH_2), 85.4 (CH), 73.2 (CH_2), 68.1 (CH_2), 49.6 (CH), 38.5 (CH), 31.6 (CH_2), 28.59 (CH_3), 28.58 (CH_3), 22.5 (C), 22.2 (C); IR (ATR) 1625, 1472, 1002, 822 cm^{-1}; HRMS (APCI) *m* / *z* calcd for $C_{28}H_{41}O_2Si$ $(M + H)^+$ 437.2870, found 437.2873.



Alkene S20. The synthesis of alkene **S20** was adapted from a reported procedure.[2] To a solution of diene **S1** (0.0080 mL, 0.080 mmol) and cyclohexene silacyclopropane **S2** (0.022 g, 0.098 mmol) in C_6H_6 (0.50 mL) was added $AgOCOCF_3$ (0.022 mL, 0.010 M in C_6H_6, 0.3 mol %). After 10 min, *p*-(trifluoromethyl)benzaldehyde (0.010 mL, 0.073 mmol) was added. After 4 d, the reaction mixture was concentrated *in vacuo*. Purification by flash chromatography (3:97 EtOAc:hexanes) afforded alkene **S20** as a colorless oil (0.009 g, 29% over three steps): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.2, 2H), 7.52 (d, J = 8.2, 2H), 5.93 (ddd, J = 17.0, 10.3, 8.8, 1H), 5.02–4.95 (m, 2H), 4.37 (d, J = 10.0, 1H), 2.09–2.04 (m, 1H), 1.98–1.87 (m, 1H), 1.17 (s, 9H), 1.12 (s, 9H), 0.90 (d, J = 6.3, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 147.3 (C), 137.9 (CH), 129.9 (q, J = 32.1, C), 126.9 (CH), 125.4 (q, J = 3.6, CH), 124.4 (q, J = 270.7, C), 113.3 (CH_2), 85.8 (CH), 47.4 (CH), 40.2 (CH), 28.1 (CH_3), 28.0 (CH_3), 22.0 (C), 21.8 (C), 15.8 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ –65.6; IR (ATR) 1622, 1473, 1323, 1067, 823 cm^{-1}; HRMS (APCI) m / z calcd for $C_{21}H_{31}F_3NaOSi$ $(M + Na)^+$ 407.1988, found 407.1982. Anal. Calcd for $C_{21}H_{31}F_3OSi$: C, 65.59; H, 8.13. Found: C, 65.84; H, 8.27.

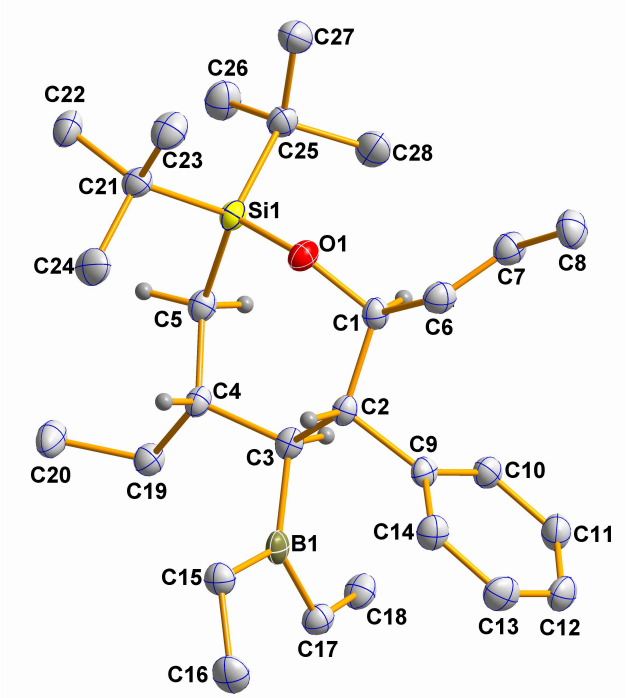
VII. X-ray Crystallographic Data

A. X-ray Data Collection, Structure Solution, and Refinement for Trialkylborane **2** (CCDC 1539169)



Single-crystal structure determination. The X-ray intensity data of the crystal were recorded on a Bruker D8 APEX-II CCD system using graphite-monochromated and 0.5 mm-MonoCap-collimated Mo-Kα radiation (λ = 0.71073 Å) with the ω scan method at 100 K. The temperature was controlled by an Oxford Cryosystems 700+ Cooler. The dataset was processed with the INTEGRATE program of the APEX2 software for reduction and cell refinement[9] Multi-scan absorption corrections were applied by using the SCALE program for the area detector. The structure was solved by intrinsic phasing methods (SHELXT)[10] and the structure model was completed and refined using the full-matrix least-square methods on F^2 (SHELXL).[11] Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms on carbons were placed in idealized positions (C-H = 0.95-1.00 Å) and included as riding with *U*iso(H) = 1.2 or 1.5 *U*eq(non-H).

B. X-ray Data Collection, Structure Solution, and Refinement for Trialkylborane *ent*-**10** (CCDC 1539170)



Single-crystal structure determination. The X-ray intensity data of the crystal were recorded on a Bruker D8 APEX-II CCD system using graphite-monochromated and 0.5 mm-MonoCap-collimated Mo-Kα radiation (λ = 0.71073 Å) with the ω scan method at 100 K. The temperature was controlled by an Oxford Cryosystems 700+ Cooler. The dataset was processed with the INTEGRATE program of the APEX2 software for reduction and cell refinement[9] Multi-scan absorption corrections were applied by using the SCALE program for the area detector. The structure was solved by intrinsic phasing methods (SHELXT)[10] and the structure model was completed and refined using the full-matrix least-square methods on F^2 (SHELXL).[11] Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms on carbons were placed in idealized positions (C-H = 0.95-1.00 Å) and included as riding with *U*iso(H) = 1.2 or 1.5 *U*eq(non-H).

VIII. Stereochemical Proofs

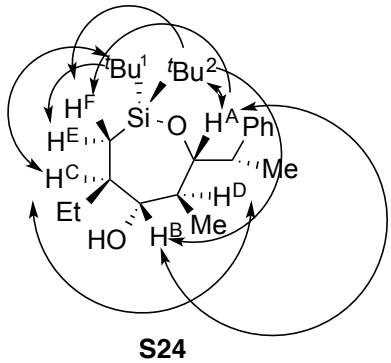
A. Assignment by analogy

The relative stereochemistry of *trans*-alkenes **S3**, **S4**, **S7**, **S10**–**S16** and alkenes **S17**, **S18**, and **S20** were assigned by analogy to previously reported structures.[2] The relative stereochemistry of trialkylboranes **7**–**18** were assigned by analogy to X-ray crystallographic structures of compounds **2** and ent-**10**. The relative stereochemistry of alcohol **20** was assigned by analogy to alcohols **S23** and **S24** (nOe data reported below).

B. General Procedure for DPFGSE–nOe Experiments

All DPFGSE-nOe data were collected on degassed C_6D_6 samples with a mixing time of 0.50 seconds. All peaks in the ^1H NMR spectra were assigned using $^1H/^1H$ COSY, $^1H/^{13}C$ HSQC, and ^1H NMR chemical shifts.

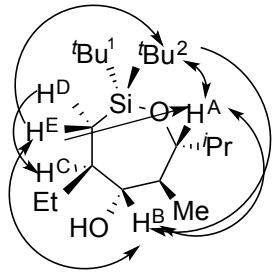
C. DPFGSE–nOe Data



S24

Relevant nOe Data for Alcohol S24 (C_6D_6)

H^A irradiated: H^B (2.1%), H^F (0.7%)
H^B irradiated: H^A (2.2%)
H^C irradiated: H^D (2.1%), ^{t}Bu^1 (3.3%)
H^D irradiated: H^C (2.4%)
^{t}Bu^1 irradiated: H^C (0.8%), H^D (0.4%), H^E (0.5%)
^{t}Bu^2 irradiated: H^A (0.9%), H^B (0.6%), H^F (0.8%)
Note: There was no nOe observed between H^A and H^C. These data indicate the relative stereochemistry shown above.



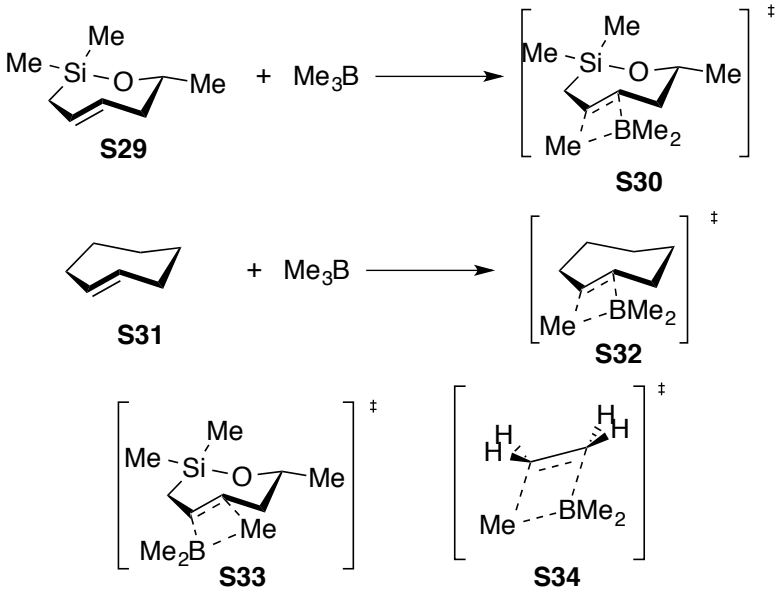
S23

Relevant nOe Data for Alcohol S23 (C_6D_6)

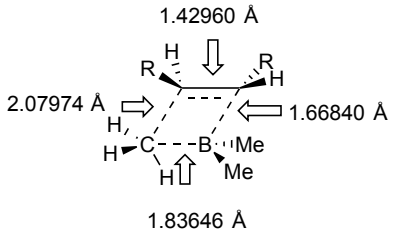
H^A irradiated: H^B (1.6%)
H^B irradiated: H^A (1.6%)
H^D irradiated: H^C (1.2%)
H^E irradiated: H^A (0.7%), H^B (2.0%), ^{t}Bu^2 (2.7%)
^{t}Bu^2 irradiated: H^A (0.7%), H^B (0.4%)
Note: There was no nOe observed between H^A and H^D. These data indicate the relative stereochemistry shown above.

IX. Computational Investigations of the Carboboration Reaction

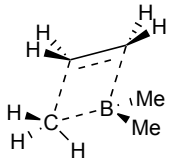
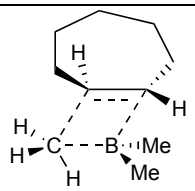
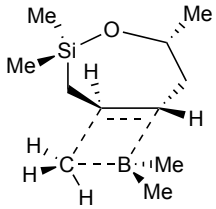
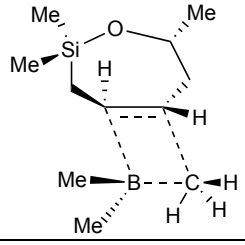
Computational studies of the carboboration reaction of *trans*-oxasilacycloheptenes were performed on model compounds. A conformational search of a model compound using the Merck Molecular Force Field (MMFF) as implemented in Spartan16[12] produced structure **S29** that resides in a conformation that resembles the X-ray crystal structure of a *trans*-oxasilacycloheptene.[13] This structure was further minimized using semi-empirical methods (PM3), then Hartree–Fock methods (HF/6-31G(d)) and then density functional methods (B3LYP/6-31G(d)). Additional optimization of **S29** was performed with Gaussian09[14] (M06-2X/6-311+G(2d,p)) using the integrated equation formalism of the polarizable continuum model (IEFPCM) with THF as the solvent; the structures from the different methods were not significantly different. The minimization protocol was repeated for trimethylborane, ethylene, and *trans*-cycloheptene **S31**. All structures were determined to be energy minima by vibrational calculations, which showed no imaginary frequencies.



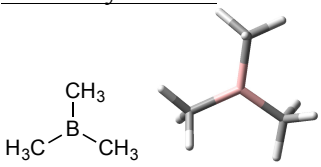
Transition structures for carboboration reactions were optimized. The transition structures were first identified at the B3LYP/6-31G(d) level without solvent (as implemented in Spartan16) by reducing the distance between the boron atom and the alkene. At approximately 2.0 Å, the energy of the system, which had slowly risen, dropped significantly. The highest energy structures were minimized at the B3LYP/6-31G(d) level to obtain transition structures. All transition structures structurally resembled those identified for hydroboration.[15] These structures were optimized further using Gaussian09 (M06-2X/6-311+G(2d,p)) with the polarizable continuum model (IEFPCM) with THF as the solvent. The transition state for the formation of **S33**, shown below, is representative. That these structures were transition states was confirmed by vibration calculations, which showed only one imaginary frequency (421 cm^{-1} in the case of **S33**). Transition states were also located for the other carboboration reactions.



Summary of Computational Data

Transition State Description and Number	Transition State Structure	ΔΔE‡ (kcal/mol)
ethylene and trimethylborane (**S34**)		21.4
trans-cycloheptene and trimethylborane (**S32**)		1.13
Major regioisomer and trimethylborane (**S30**)		3.42
Minor regioisomer and trimethylborane (**S33**)		8.60

Trimethylborane



Gaussian09: MO6-2X/6-311+G(2d,p), THF (IEPCM) (note: convergence required the "calcfc" keyword)
Energy: –144.56553199
Number of imaginary vibrations: 0

Table S1: Cartesian Coordinates for Trimethylborane

Center	Atomic	X (Å)	Y (Å)	Z (Å)

Number	Number			
1	5	-0.002519	-0.002270	-0.002306
2	6	-1.547399	-0.286728	-0.004649
3	1	-1.822489	-1.338963	-0.090029
4	1	-1.964146	0.095807	0.936065
5	1	-2.051388	0.280371	-0.793330
6	6	1.021381	-1.192839	0.008940
7	1	1.027780	-1.613025	-1.006428
8	1	2.048073	-0.913572	0.251342
9	1	0.702467	-2.010617	0.660518
10	6	0.524681	1.477920	-0.005029
11	1	1.001986	1.668609	0.964613
12	1	1.318374	1.612244	-0.746694
13	1	-0.240035	2.240378	-0.160098

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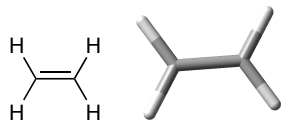
ethylene

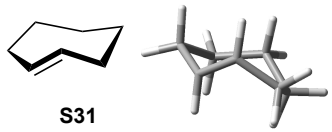


Gaussian09: MO6-2X/6-311+G(2d,p), THF (IEPCM)
Energy: –78.56741412
Number of imaginary vibrations: 0

Table S2: Cartesian Coordinates for Ethylene

Center Number	Atomic Number	X (Å)	Y (Å)	Z (Å)
1	6	0.661928	0.000000	0.000004
2	6	-0.661928	0.000000	-0.000004
3	1	1.229122	0.923425	-0.000010
4	1	1.229122	-0.923425	0.000023
5	1	-1.229122	-0.923425	0.000010
6	1	-1.229122	0.923425	-0.000023

trans-cycloheptene

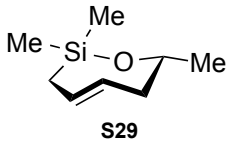


Gaussian09: MO6-2X/6-311+G(2d,p), THF (IEPCM)
Energy: –273.85136156 au
Number of imaginary vibrations: 0

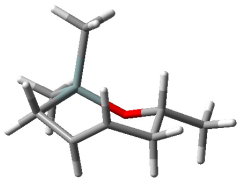
Table S3: Cartesian Coordinates for *trans*-Cycloheptene

Center Number	Atomic Number	X (Å)	Y (Å)	Z (Å)
1	1	0.366651	-1.192109	1.516442
2	6	0.569537	-1.241617	0.448757
3	6	-0.471866	-1.298059	-0.377507
4	1	-0.277247	-1.259531	-1.450226
5	6	1.802945	-0.520468	-0.018030
6	1	2.580732	-0.505908	0.745942
7	1	2.230129	-0.952674	-0.924917
8	6	-1.735290	-0.631832	0.068887
9	1	-1.912206	-0.801981	1.133790
10	1	-2.633225	-0.907269	-0.486698
11	6	1.280657	0.926316	-0.321130
12	1	1.106295	1.003942	-1.398230
13	1	2.060024	1.653479	-0.079358
14	6	-1.393533	0.870076	-0.171050
15	1	-2.189564	1.486616	0.256728
16	1	-1.402325	1.055856	-1.250149
17	6	-0.033860	1.367129	0.393683
18	1	0.023297	1.132081	1.461294
19	1	-0.064107	2.458236	0.333714

trans-oxasilacycloheptene model compound



S29

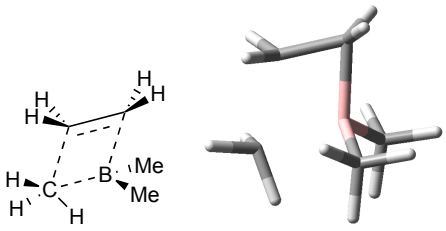


Gaussian09: MO6-2X/6-311+G(2d,p), THF (IEPCM)
Energy: –679.16022095 au
Number of imaginary vibrations: 0

Table S4: Cartesian Coordinates for **S29**

Center Number	Atomic Number	X (Å)	Y (Å)	Z (Å)
1	14	1.178548	-0.253742	0.014051
2	8	-0.346764	-0.773024	-0.452129
3	6	1.399488	1.638059	-0.297801
4	6	-2.149763	0.867118	-0.007475
5	6	-1.583284	-0.563681	0.233788
6	6	2.346153	-1.276848	-1.011076
7	6	1.386466	-0.543256	1.846331
8	1	1.712053	2.100181	0.641148
9	1	2.089605	1.903652	-1.096891
10	1	-3.031642	1.002285	0.622138
11	1	-2.450694	0.947324	-1.056037
12	1	2.209942	-2.341069	-0.810416
13	1	2.171437	-1.103567	-2.074820
14	1	3.381839	-1.011299	-0.788802
15	1	2.425878	-0.361005	2.129021
16	1	1.134861	-1.573608	2.107406
17	1	0.756704	0.123624	2.438573
18	6	-2.557574	-1.630169	-0.227600
19	1	-3.521174	-1.504520	0.269125
20	1	-2.173933	-2.625584	-0.002719
21	1	-2.708284	-1.550080	-1.305990
22	1	-1.408644	-0.672836	1.311668
23	6	-1.008217	1.783474	0.300783
24	1	-0.757378	1.923315	1.351813
25	6	-0.039435	1.864371	-0.615310
26	1	-0.319138	1.645348	-1.644733

transition state for addition of trimethylborane to ethylene



Gaussian09: MO6-2X/6-311+G(2d,p), THF (IEPCM)
Energy: –223.09893940
Number of imaginary vibrations: 1 (–511.65 cm^{-1})

Table S5: Cartesian Coordinates for Carboboration of Ethylene

Center Number	Atomic Number	X (Å)	Y (Å)	Z (Å)
1	5	0.336308	-0.143723	0.076425
2	6	1.025291	-1.023351	-1.072564
3	1	1.535102	-1.887425	-0.635602
4	1	1.772920	-0.452910	-1.634703
5	1	0.302322	-1.412776	-1.797702
6	6	1.246332	0.642781	1.136328
7	1	1.829046	-0.071271	1.726092
8	1	0.656148	1.237203	1.840695
9	1	1.952101	1.321469	0.644508
10	6	-0.363418	1.329846	-0.853206
11	1	-0.551585	2.177672	-0.200917
12	1	-1.062051	1.334177	-1.685150
13	1	0.631288	1.442634	-1.284339
14	1	-0.905080	-2.028230	0.529373
15	6	-0.862006	-0.996624	0.852514
16	6	-1.533228	-0.034966	0.033769
17	1	-0.881952	-0.837591	1.922449
18	1	-1.967036	-0.387830	-0.890681
19	1	-2.070581	0.777375	0.502805

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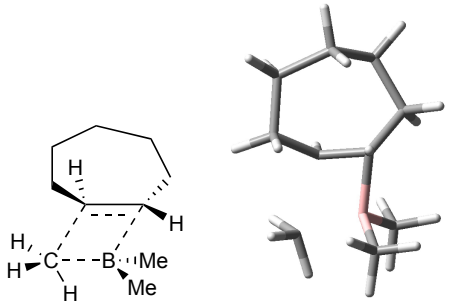
transition state for addition of trimethylborane to *trans*-cycloheptene



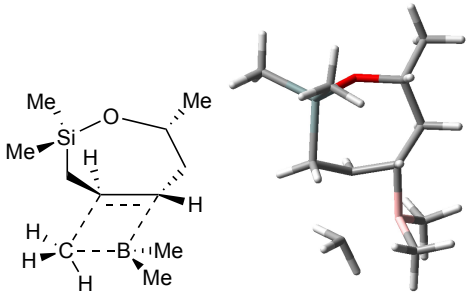
Gaussian09: MO6-2X/6-311+G(2d,p), THF (IEPCM)
Energy: –418.41508651
Number of imaginary vibrations: 1 (–383.28 cm^{-1})

Table S6: Cartesian Coordinates for Carboboration of *trans*-Cycloheptene

Center Number	Atomic Number	X (Å)	Y (Å)	Z (Å)
1	5	-1.694092	-0.168282	0.087693
2	6	-1.887529	1.436830	-0.698545
3	1	-2.966531	1.296187	-0.798786
4	1	-1.510974	1.678247	-1.691247
5	1	-1.717846	2.276579	-0.027253
6	6	-2.490839	0.075169	1.467451
7	1	-2.028277	0.849975	2.087580
8	1	-2.525653	-0.840943	2.064706
9	1	-3.523604	0.387195	1.273414
10	6	-2.288272	-1.230184	-0.963528
11	1	-2.288934	-2.243217	-0.548942
12	1	-1.729343	-1.270789	-1.904901
13	1	-3.324570	-0.982918	-1.219773
14	1	0.092038	-0.261576	1.533706
15	6	-0.086025	-0.545437	0.499878
16	6	0.010571	0.537940	-0.393863
17	1	0.110724	0.263840	-1.441158
18	6	0.691667	-1.779702	0.086169
19	1	0.701847	-2.494890	0.911066
20	1	0.226634	-2.281567	-0.764983
21	6	0.809326	1.729195	0.014574
22	1	0.606940	1.971688	1.060585
23	1	0.622622	2.614448	-0.596106
24	6	2.139446	-1.357985	-0.278073
25	1	2.196052	-1.172542	-1.355736
26	1	2.819545	-2.189861	-0.080758
27	6	2.279242	1.269039	-0.160179
28	1	2.919364	2.040835	0.273116

29	1	2.505415	1.245363	-1.231135
30	6	2.674202	-0.097690	0.443817
31	1	2.408822	-0.126989	1.505075
32	1	3.765462	-0.140712	0.406857

transition state for addition of trimethylborane to *trans*-oxasilacycloheptene, observed regioisomer



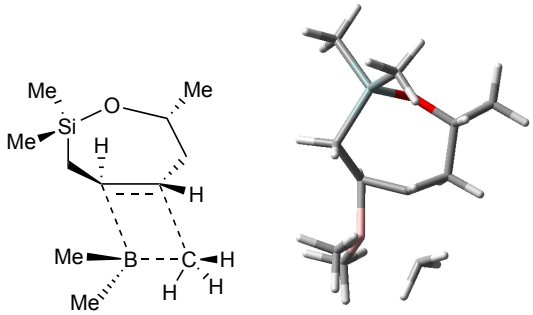
Gaussian09: MO6-2X/6-311+G(2d,p), THF (IEPCM)
Energy: –823.72030262
Number of imaginary vibrations: 1 (–421.12 cm^{-1})

Table S7: Cartesian Coordinates for Carboboration of **S30**, Observed Regioisomer

Center Number	Atomic Number	X (Å)	Y (Å)	Z (Å)
1	14	-1.825701	-0.849551	0.010507
2	8	-1.648464	0.722038	-0.503243
3	6	1.011774	0.454313	0.484493
4	6	0.777330	-0.603563	-0.448081
5	6	-0.122195	-1.732570	-0.096967
6	6	0.452472	1.803799	0.092533
7	6	-1.072971	1.798773	0.245582
8	6	-3.030120	-1.632011	-1.167270
9	6	-2.420460	-0.904335	1.776236
10	1	0.768558	0.182299	1.513002
11	1	0.708848	-0.268075	-1.477606
12	1	0.116366	-2.133513	0.891272
13	1	-0.113948	-2.542139	-0.828555
14	1	0.864284	2.604995	0.713018
15	1	0.699662	2.034884	-0.948272
16	1	-4.005817	-1.147374	-1.099463
17	1	-2.672366	-1.544091	-2.194972
18	1	-3.155436	-2.692466	-0.939418
19	1	-2.622794	-1.939957	2.059832
20	1	-3.343553	-0.332443	1.893265
21	1	-1.677252	-0.507269	2.470349
22	6	-1.702745	3.090232	-0.237934

23	1	-1.288750	3.941817	0.304608
24	1	-2.782586	3.071487	-0.088729
25	1	-1.500445	3.223952	-1.302561
26	1	-1.312690	1.656190	1.307356
27	5	2.555017	-0.045013	0.093791
28	6	3.276168	0.965689	-0.927403
29	1	2.751889	1.063588	-1.884363
30	1	4.294541	0.632104	-1.155132
31	1	3.350186	1.971226	-0.500402
32	6	2.539271	-1.653564	-0.792149
33	1	2.119043	-1.854314	-1.776168
34	1	2.341802	-2.492581	-0.129358
35	1	3.619109	-1.569027	-0.932157
36	6	3.331044	-0.471426	1.436572
37	1	4.311206	-0.909519	1.216636
38	1	2.772219	-1.202967	2.029775
39	1	3.492950	0.403661	2.074253

transition state for addition of trimethylborane to *trans*-oxasilacycloheptene, other regioisomer



Gaussian09: MO6-2X/6-311+G(2d,p), THF (IEPCM)
Energy: –823.71204962
Number of imaginary vibrations: 1 (–453.43 cm^{-1})

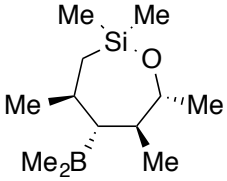
Table S8: Cartesian Coordinates for Carboboration of **S33**, Other Regioisomer

Center Number	Atomic Number	X (Å)	Y (Å)	Z (Å)
1	14	-1.782264	-0.930967	-0.018151
2	8	-1.678364	0.659479	-0.530780
3	6	0.966489	0.541095	0.398935
4	6	0.868172	-0.548122	-0.509861
5	6	-0.046558	-1.695069	-0.102322
6	6	0.389921	1.870791	0.021975
7	6	-1.138999	1.750002	0.205138
8	6	-2.977292	-1.733014	-1.197448
9	6	-2.414659	-0.973412	1.741206

10	1	0.807404	0.270630	1.440852
11	1	0.704131	-0.224701	-1.534876
12	1	0.235666	-2.091377	0.876944
13	1	0.013280	-2.520924	-0.814872
14	1	0.747330	2.687340	0.653185
15	1	0.615113	2.102879	-1.022484
16	1	-3.963948	-1.271072	-1.130395
17	1	-2.621005	-1.637415	-2.225176
18	1	-3.079236	-2.796759	-0.972109
19	1	-2.594550	-2.010320	2.035894
20	1	-3.353400	-0.423940	1.839240
21	1	-1.693195	-0.553015	2.445616
22	6	-1.838416	3.017958	-0.247538
23	1	-1.462405	3.883849	0.299368
24	1	-2.911851	2.933785	-0.077553
25	1	-1.665460	3.173607	-1.314030
26	1	-1.335958	1.595870	1.274306
27	5	2.499864	-0.447763	-0.125301
28	6	2.945243	-1.588156	0.913335
29	1	2.749123	-2.586465	0.509428
30	1	2.427788	-1.525744	1.876949
31	1	4.018571	-1.525119	1.124167
32	6	3.335923	-0.263534	-1.486508
33	1	3.262612	-1.166518	-2.100467
34	1	4.397895	-0.084893	-1.282226
35	1	2.976019	0.571509	-2.095862
36	6	2.929789	1.124481	0.718885
37	1	3.954286	0.766168	0.834399
38	1	2.594307	1.433333	1.706733
39	1	2.939099	1.977688	0.045039

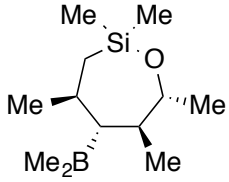
Computational Investigations of NBO Calculations

Additional calculations were performed to evaluate the bonding of the borane to explain the unusual chemical shift of the trialkylborane products. These studies were performed on a model compound, borane **S35**. A conformational search using the Merck Molecular Force Field (MMFF, with keywords "montecarlo" and "findboats" resulting in more conformers) as implemented in Spartan16[12] produced 13 low-energy conformers. One structure, the lowest energy one, was found to occupy a conformation that resembles the X-ray crystal structure of the product **2**. These structures were refined using semi-empirical methods (PM3), then Hartree–Fock methods (HF/3-31G(d)), which produced five unique conformers. These structures were optimized with Gaussian09[14] (M06-2X/6-311+G(2d,p)). The structure resembling the X-ray crystal structure was >0.9 kcal/mol lower in energy than all others. This structure was determined to be an energy minima by vibrational calculations, which showed no imaginary frequencies.

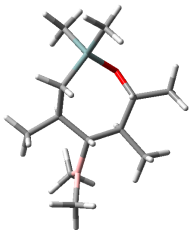


S35

borane model compound (**S35**)



S35



Gaussian09: MO6-2X/6-311+G(2d,p)
Energy: –863.087061105 au
Number of imaginary vibrations: 0

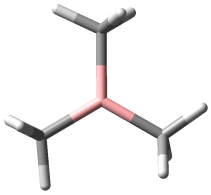
Table S9: Cartesian Coordinates for **S35**

Standard orientation:

		Coordinates (Angstroms)		
Center Number	Atomic Number	X	Y	Z
1	8	1.539515	0.835524	0.663553
2	6	-1.277836	-0.101018	-0.389199
3	6	0.874306	-1.479241	-0.814397
4	6	-0.466738	-1.382640	-0.055304
5	14	2.246062	-0.511594	0.013509

6	6	0.654069	1.622090	-0.126475
7	6	-0.796916	1.246252	0.214125
8	6	2.966234	-1.453261	1.449541
9	6	3.579040	-0.043309	-1.210886
10	1	0.731703	-1.160866	-1.852942
11	1	1.192659	-2.527218	-0.866774
12	1	3.646735	-0.818071	2.019686
13	1	3.524170	-2.327078	1.106464
14	1	2.179876	-1.793960	2.125878
15	1	4.395358	0.484381	-0.713494
16	1	3.994688	-0.932623	-1.690645
17	1	3.185545	0.604837	-1.997247
18	6	1.011201	3.076226	0.140379
19	1	2.083374	3.206108	-0.009388
20	1	0.778015	3.336127	1.175832
21	1	0.482717	3.758196	-0.525336
22	6	-1.766543	2.351269	-0.228444
23	1	-1.560861	3.298787	0.267768
24	1	-2.804595	2.093830	-0.002978
25	1	-1.702510	2.510471	-1.309533
26	6	-1.311042	-2.623932	-0.375852
27	1	-2.238922	-2.660713	0.203399
28	1	-0.757416	-3.538688	-0.156820
29	1	-1.572940	-2.636918	-1.438434
30	5	-2.780356	-0.307581	0.090179
31	6	-3.959412	-0.358538	-0.947484
32	1	-4.946641	-0.175033	-0.518210
33	1	-3.977325	-1.377267	-1.359138
34	1	-3.804234	0.304873	-1.801667
35	6	-3.095694	-0.443324	1.626854
36	1	-2.243420	-0.712890	2.253230
37	1	-3.918200	-1.136941	1.820155
38	1	-3.450752	0.536480	1.973917
39	1	-1.257290	0.010096	-1.484256
40	1	-0.270307	-1.383626	1.024279
41	1	-0.830230	1.171131	1.308203
42	1	0.817576	1.419162	-1.197541

$\underline{BMe_3}$:



Gaussian09: MO6-2X/6-311+G(2d,p)
Energy: –144.564980142 au
Number of imaginary vibrations: 0

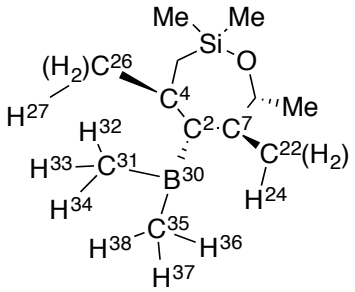
Table S10: Cartesian Coordinates for BMe_3:

		Coordinates (Angstroms)		
Center Number	Atomic Number	X	Y	Z
1	6	0.637229	1.434376	-0.004682
2	1	-0.067021	2.254342	-0.150473
3	1	1.141985	1.588737	0.957363
4	1	1.430835	1.510990	-0.754608
5	6	-1.563668	-0.166486	-0.004731
6	1	-1.950506	0.228651	0.943357
7	1	-2.027530	0.451606	-0.779655
8	1	-1.919981	-1.192097	-0.108419
9	5	-0.001405	-0.001087	-0.003723
10	6	0.925029	-1.268994	0.007897
11	1	0.556601	-2.040065	0.689418
12	1	0.874554	-1.719525	-0.992609
13	1	1.976555	-1.070583	0.223339

Computational studies of ^{11}B NMR chemical shifts were performed using the method of Wrackmeyer. Employing the same computational models used in that work (GIAO method, B3LYP/6-311+(d,p)) reproduced the chemical shift for BMe_3 from that paper,[16] but that method suggested that the product should have a chemical shift of δ 88 ppm, which is not consistent with the experimental results.

A natural bond order calculation was performed on both **S35** and BMe_3 using the computational methods employed to find minima. The results of those calculations are summarized in Tables S11 and S12.

Table 11. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis for **S35**



					E(2)	E(j)-E(i)	F(I,j)
Donor NBO (i)			Acceptor NBO (j)			a.u.	a.u.
3. BD	C2	C4	64. LP*	B30	2.61	0.71	0.040
4. BD	C2	C7	64. LP*	B30	3.45	0.71	0.046
11. BD	C4	C26	64. LP*	B30	1.48	0.74	0.031
18. BD	C7	C22	64. LP*	B30	1.24	0.74	0.028
19. BD	C7	H41	64. LP*	B30	0.62	0.61	0.018
30. BD	C22	H24	64. LP*	B30	8.01	0.64	0.066
32. BD	C26	H27	64. LP*	B30	8.52	0.64	0.068
34. BD	C26	H29	64. LP*	B30	1.08	0.64	0.024
37. BD	C31	H32	64. LP*	B30	0.86	0.62	0.021
38. BD	C31	H33	64. LP*	B30	13.61	0.61	0.084
39. BD	C31	H34	64. LP*	B30	2.68	0.62	0.038
40. BD	C35	H36	64. LP*	B30	0.56	0.62	0.017
41. BD	C35	H37	64. LP*	B30	3.31	0.62	0.042
42. BD	C35	H38	64. LP*	B30	12.92	0.61	0.082

Table 12. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis for BMe_3

					E(2)	E(j)-E(i)	F(I,j)
Donor NBO (i)			Acceptor NBO (j)		kcal/mol	a.u	a.u.
2. BD	C1	H3	17. LP*	B9	8.99	0.61	0.068
3. BD	C1	H4	17. LP*	B9	5.15	0.62	0.052
5. BD	C5	H6	17. LP*	B9	9.27	0.61	0.069
6. BD	C5	H7	17. LP*	B9	4.87	0.62	0.050
10. BD	C10	H11	17. LP*	B9	3.74	0.62	0.044
11. BD	C10	H12	17. LP*	B9	10.54	0.61	0.074

The NBO analysis suggests an explanation for the unusually high upfield chemical shift for the ^{11}B atom of borane **S35**. As the electron density of a boron atom increases, the chemical shift should move upfield, so contributions to electron density of the boron atom was evaluated by NBO analysis, and the chemical shifts were compared to BMe_3. The hyperconjugative interactions of $\sigma_{CH} \rightarrow n_B$ were of a similar magnitude between these compounds. Where BMe_3 had a third set of those interactions, borane **S35** had $\sigma_{CC} \rightarrow n_B$ interactions. Borane **S35**, however, also had large $\sigma_{CH} \rightarrow n_B$ interactions from remote C–H bonds, which are held rigidly over the boron atom. These interactions (underlined in Table 11) donate electron density at boron and thus could be responsible for the higher chemical shifts. No unusual chemical shifts were present for those remote methyl groups, but that interaction could be averaged by bond rotation, making it difficult to detect. These interactions of remote carbon–hydrogen bonds to electron-deficient atoms resemble interactions observed in alkyl-substiututed carbocations.[17]

X. References

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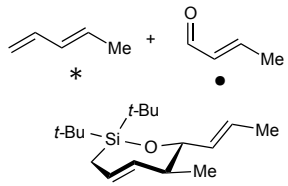
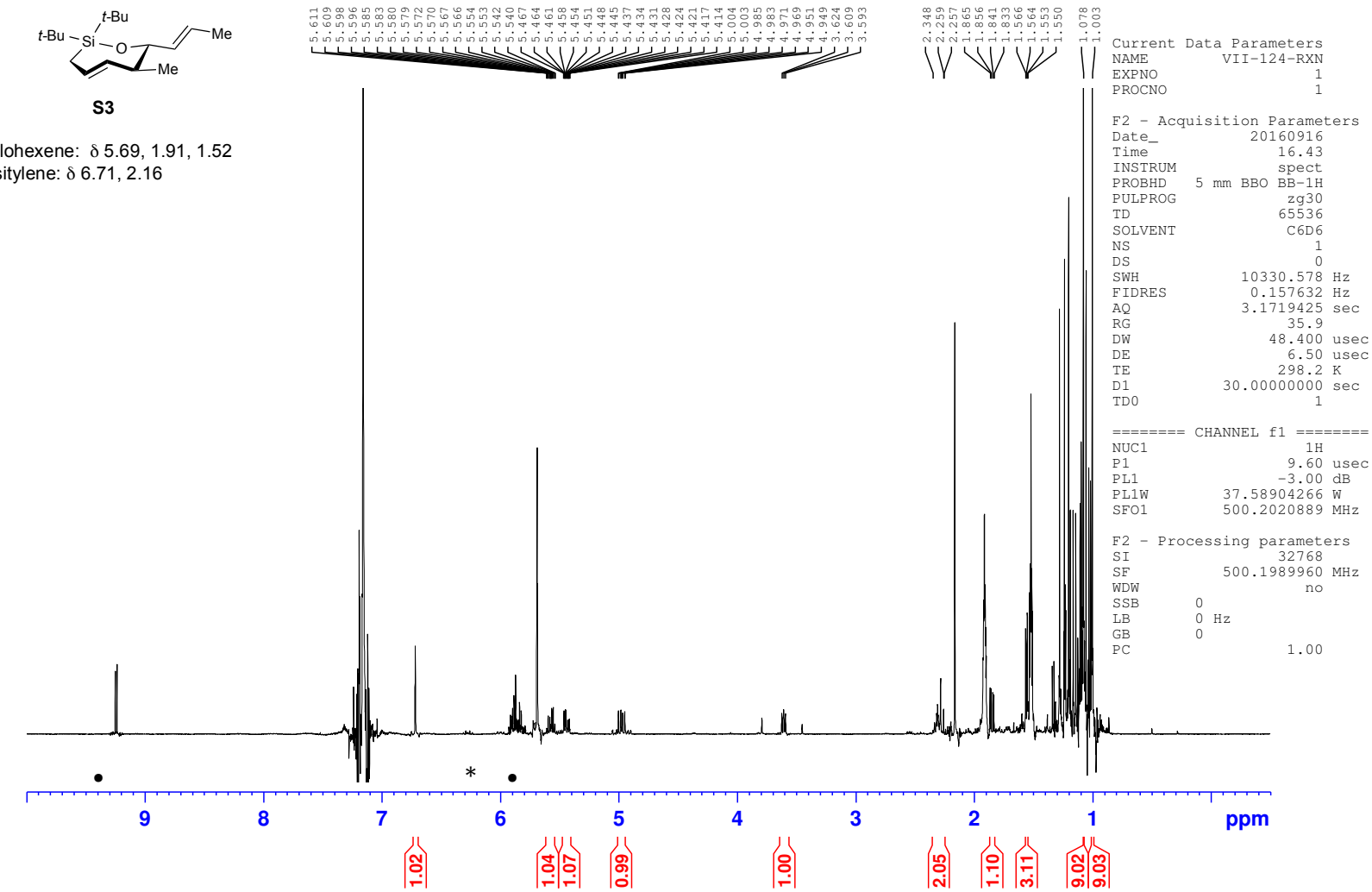
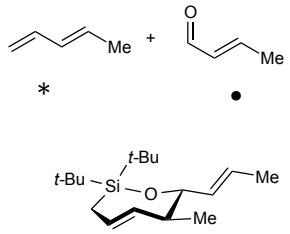
XII. ^{1}H and ^{13}C NMR Spectra (Side products, starting materials, and standards from *in situ* reactions listed above relevant spectra.)



S3

Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16





S3

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8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PROCNO                 1

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DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
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PL1                 2.30 dB
PL1W        46.00027084 W
SFO1        125.7877161 MHz

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PL12               15.31 dB
PL13               18.31 dB
PL2W        37.58904266 W
PL12W        0.55470389 W
PL13W        0.27801058 W
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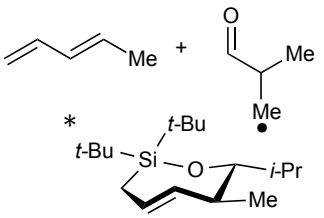
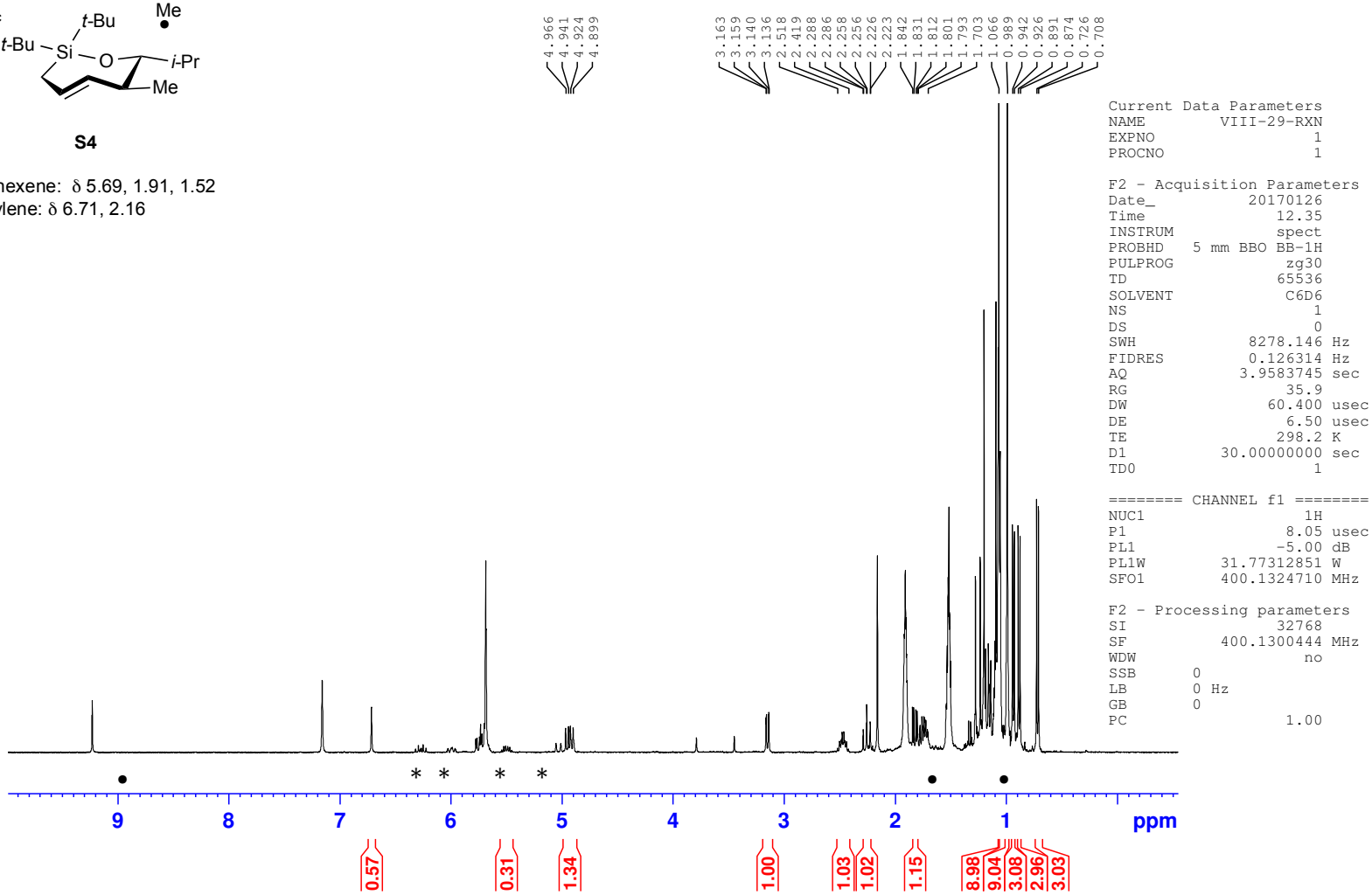
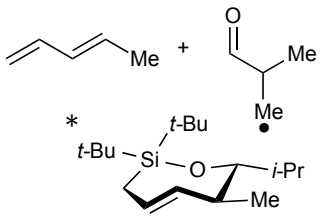


S4

Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16





S4

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8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EXPNO                  3
PROCNO                 1

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DS                     2
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DW                20.850 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

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PL1                 -2.70 dB
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SFO1        100.6228298 MHz

======== CHANNEL f2 ========
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PL12                14.95 dB
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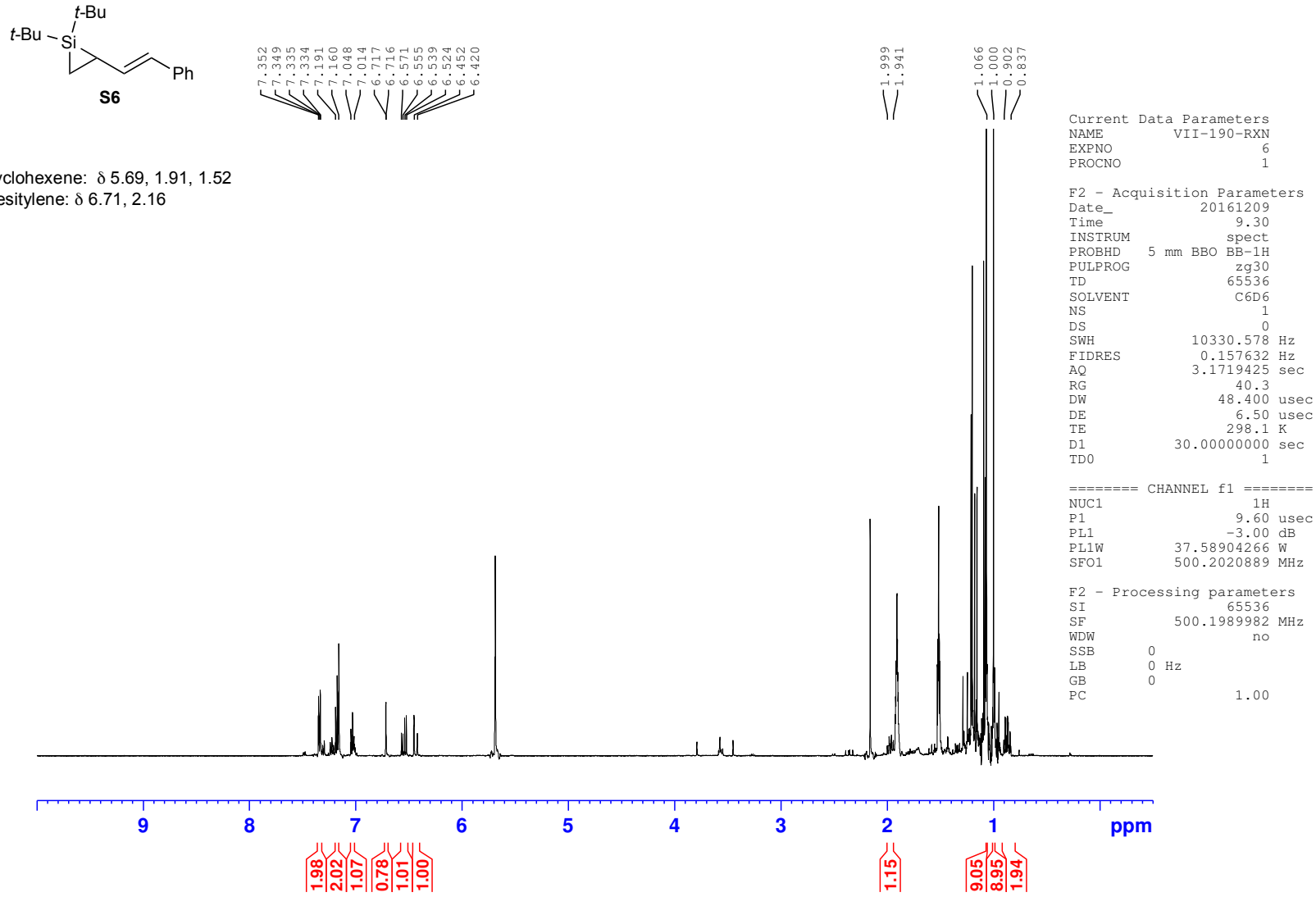
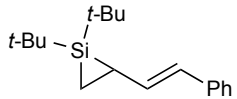
PL13W        0.20799839 W
SFO2        400.1316005 MHz

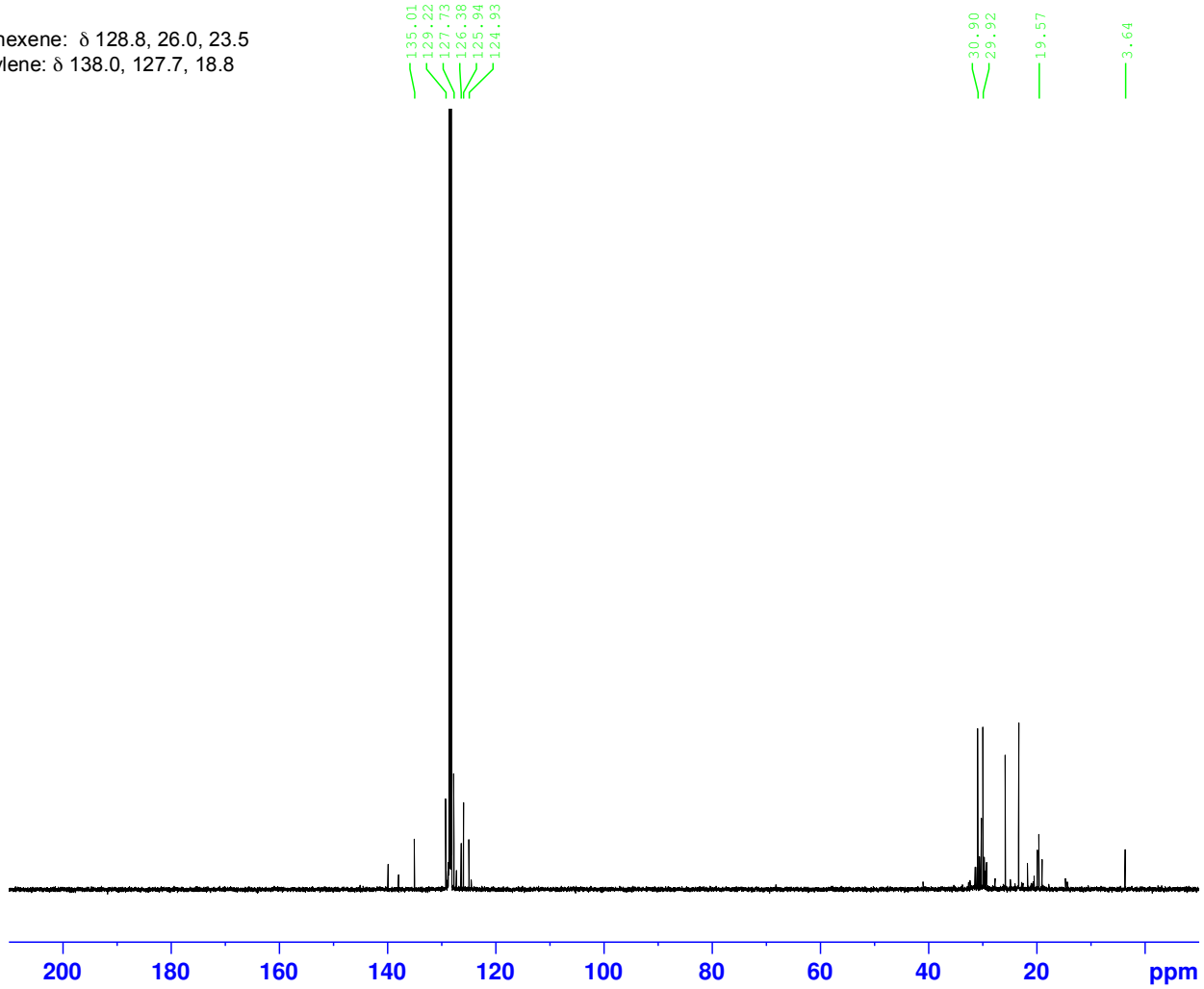
F2 - Processing parameters
SI                  32768
SF          100.6127076 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```


t-Bu
t-Bu
Si
Ph
S6
7.352
7.349
7.335
7.334
7.191
7.160
7.048
7.014
6.717
6.716
6.571
6.555
6.539
6.524
6.452
6.420
1.999
1.941
1.066
1.000
0.902
0.837
Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16
Current Data Parameters
NAME VII-190-RXN
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161209
Time 9.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 1
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 40.3
DW 48.400 usec
DE 6.50 usec
TE 298.1 K
D1 30.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 65536
SF 500.1989982 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
1.98
2.02
1.07
0.78
1.01
1.00
1.15
9.05
8.95
1.94



S6

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8



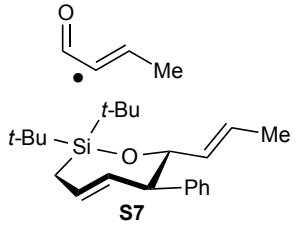

```
Current Data Parameters
NAME         VII-190-RXN
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161209
Time                9.07
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT              C6D6
NS                     74
DS                      2
SWH            30030.029 Hz
FIDRES          0.458222 Hz
AQ              1.0911744 sec
RG                 9195.2
DW                16.650 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

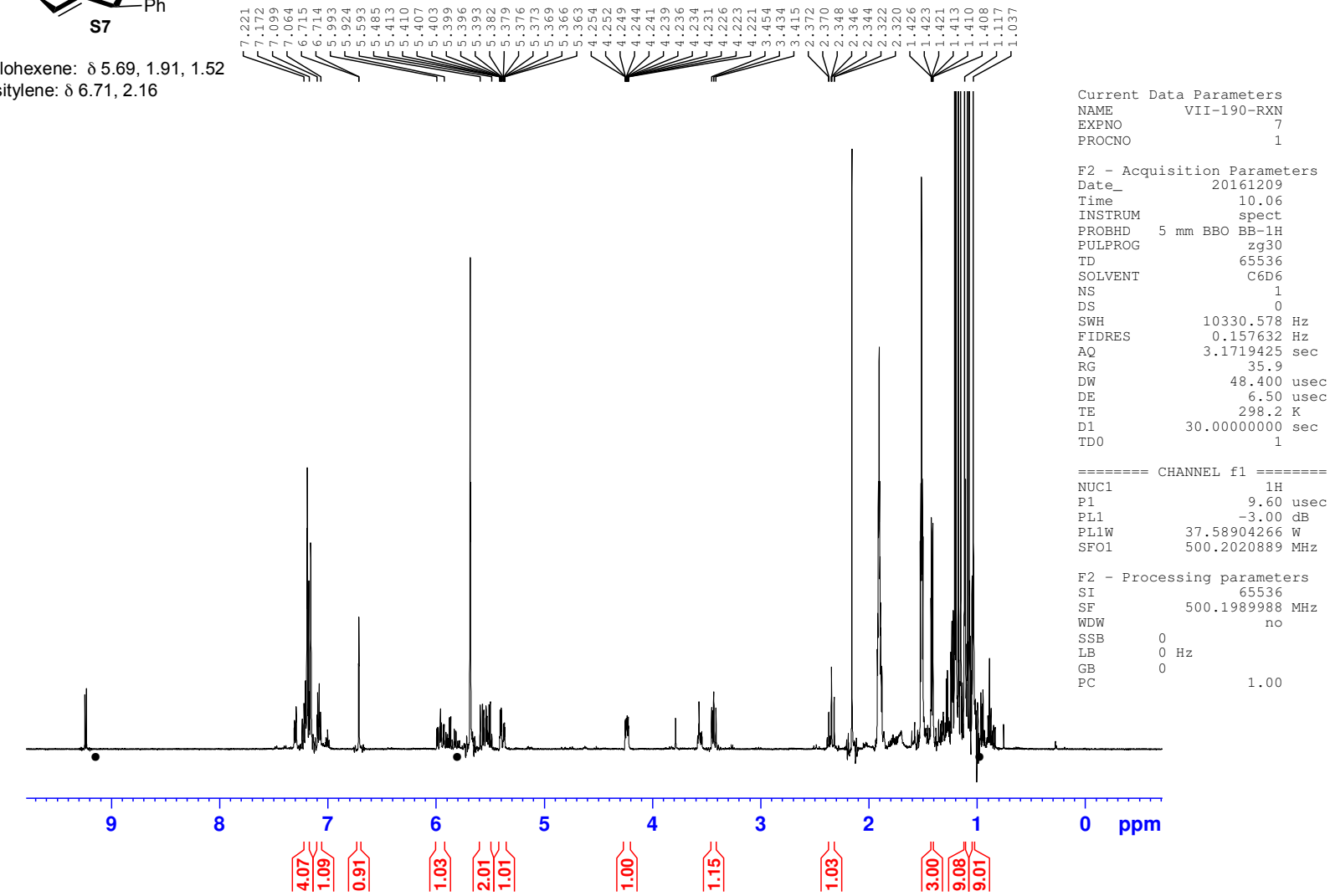
======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 2.30 dB
PL1W         46.00027084 W
SFO1         125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               15.31 dB
PL13               18.31 dB
PL2W         37.58904266 W
PL12W         0.55470389 W
PL13W         0.27801058 W
SFO2         500.2010008 MHz

F2 - Processing parameters
SI                 32768
SF           125.7750480 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16

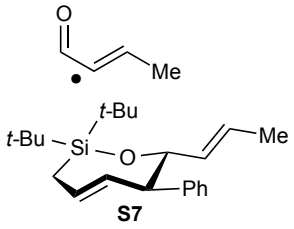



```
Current Data Parameters
NAME         VII-190-RXN
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161209
Time               10.06
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT              C6D6
NS                      1
DS                      0
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719425 sec
RG                   35.9
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1           30.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                   9.60 usec
PL1                 -3.00 dB
PL1W         37.58904266 W
SFO1         500.2020889 MHz

F2 - Processing parameters
SI                 65536
SF           500.1989988 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```



S7

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8

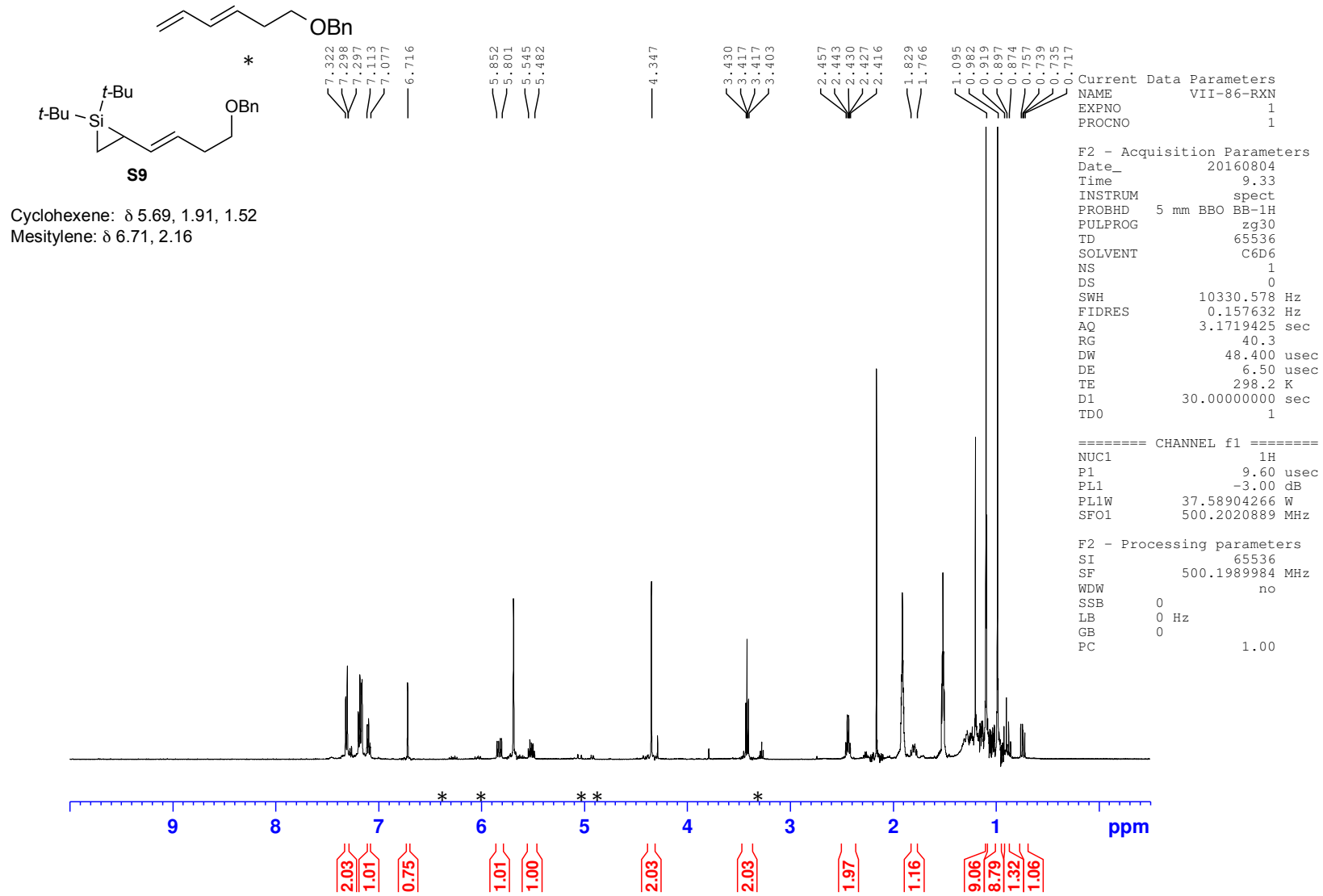

```
Current Data Parameters
NAME         VII-190-RXN
EXPNO                  8
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161209
Time               10.13
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT            C6D6
NS                   64
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0911744 sec
RG               11585.2
DW                16.650 usec
DE                 6.50 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

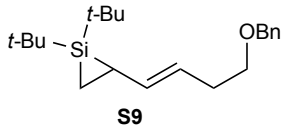
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                2.30 dB
PL1W        46.00027084 W
SFO1        125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              15.31 dB
PL13              18.31 dB
PL2W        37.58904266 W
PL12W        0.55470389 W
PL13W        0.27801058 W
SFO2        500.2010008 MHz

F2 - Processing parameters
SI                32768
SF          125.7750471 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16



S9

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8

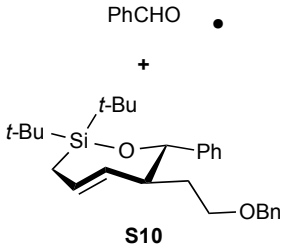

```
Current Data Parameters
NAME          VII-86-RXN
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160804
Time                9.38
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT            C6D6
NS                   45
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0911744 sec
RG               2896.3
DW               16.650 usec
DE                6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

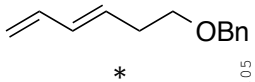
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                2.30 dB
PL1W        46.00027084 W
SFO1       125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              15.31 dB
PL13              18.31 dB
PL2W        37.58904266 W
PL12W        0.55470389 W
PL13W        0.27801058 W
SFO2       500.2010008 MHz

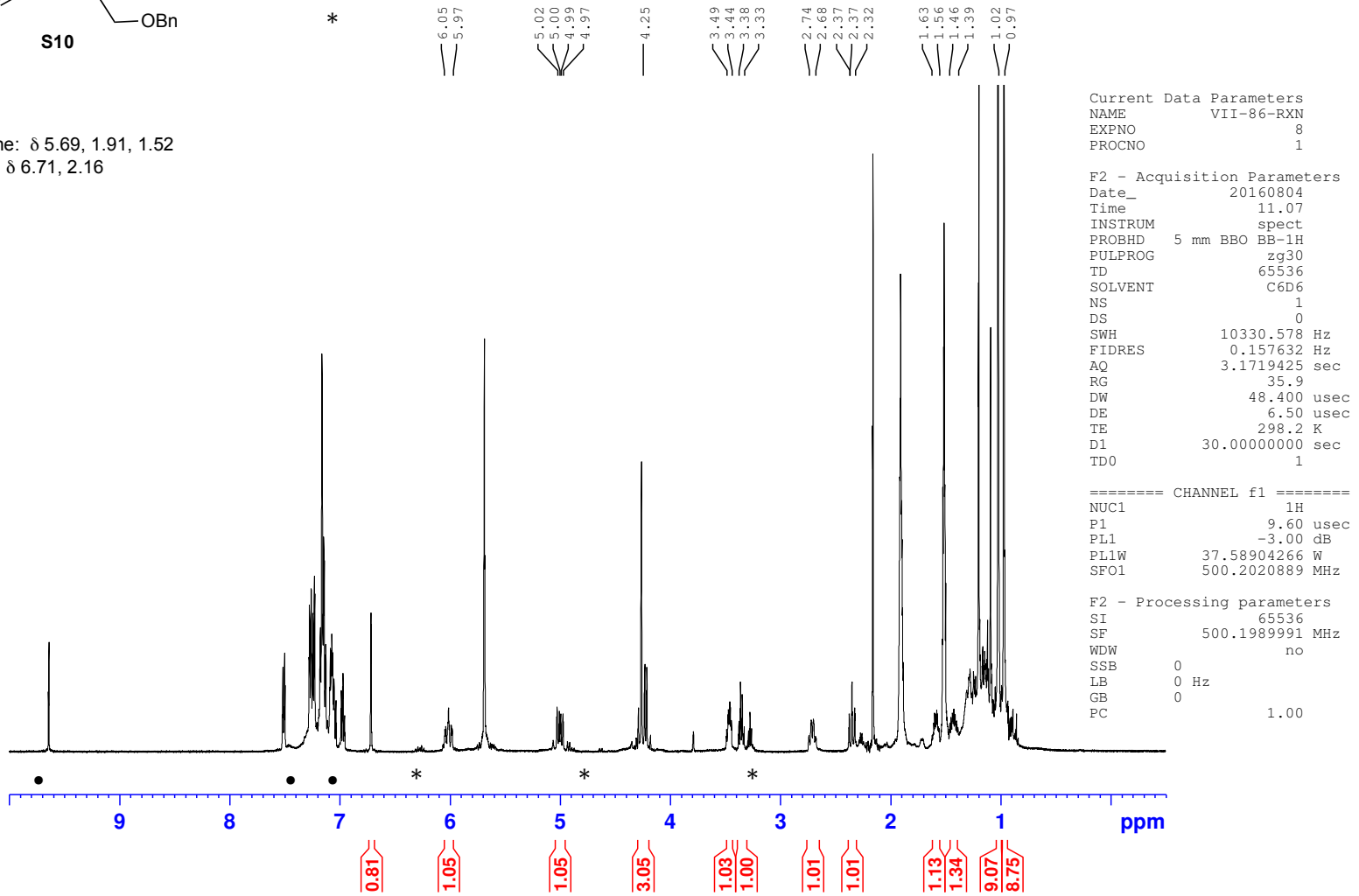
F2 - Processing parameters
SI                32768
SF          125.7750484 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```



S10



Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16




```
Current Data Parameters
NAME          VII-86-RXN
EXPNO                  8
PROCNO                 1

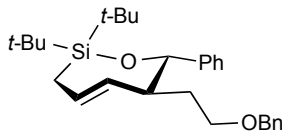
F2 - Acquisition Parameters
Date_           20160804
Time               11.07
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     1
DS                     0
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719425 sec
RG                  35.9
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.60 usec
PL1               -3.00 dB
PL1W        37.58904266 W
SFO1        500.2020889 MHz

F2 - Processing parameters
SI                 65536
SF          500.1989991 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

PhCHO •

+



S10

Cyclohexene: δ 128.8, 26.0, 23.5

Mesitylene: δ 138.0, 127.7, 18.8

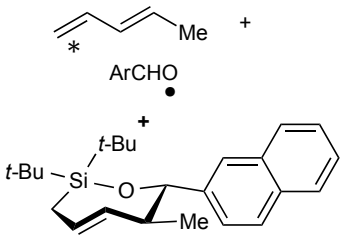

```
Current Data Parameters
NAME          VII-86-RXN
EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160804
Time               11.12
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                    70
DS                     2
SWH            30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0911744 sec
RG                9195.2
DW                16.650 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                2.30 dB
PL1W         46.00027084 W
SFO1         125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               15.31 dB
PL13               18.31 dB
PL2W         37.58904266 W
PL12W         0.55470389 W
PL13W         0.27801058 W
SFO2         500.2010008 MHz

F2 - Processing parameters
SI                 32768
SF           125.7750491 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



S11

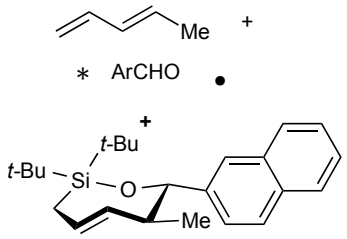
Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16


```
Current Data Parameters
NAME         VII-179-RXN
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161130
Time               16.18
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     1
DS                     0
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9583745 sec
RG                  35.9
DW                60.400 usec
DE                 6.50 usec
TE                298.2 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.05 usec
PL1               -5.00 dB
PL1W         31.77312851 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300441 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



S11

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8

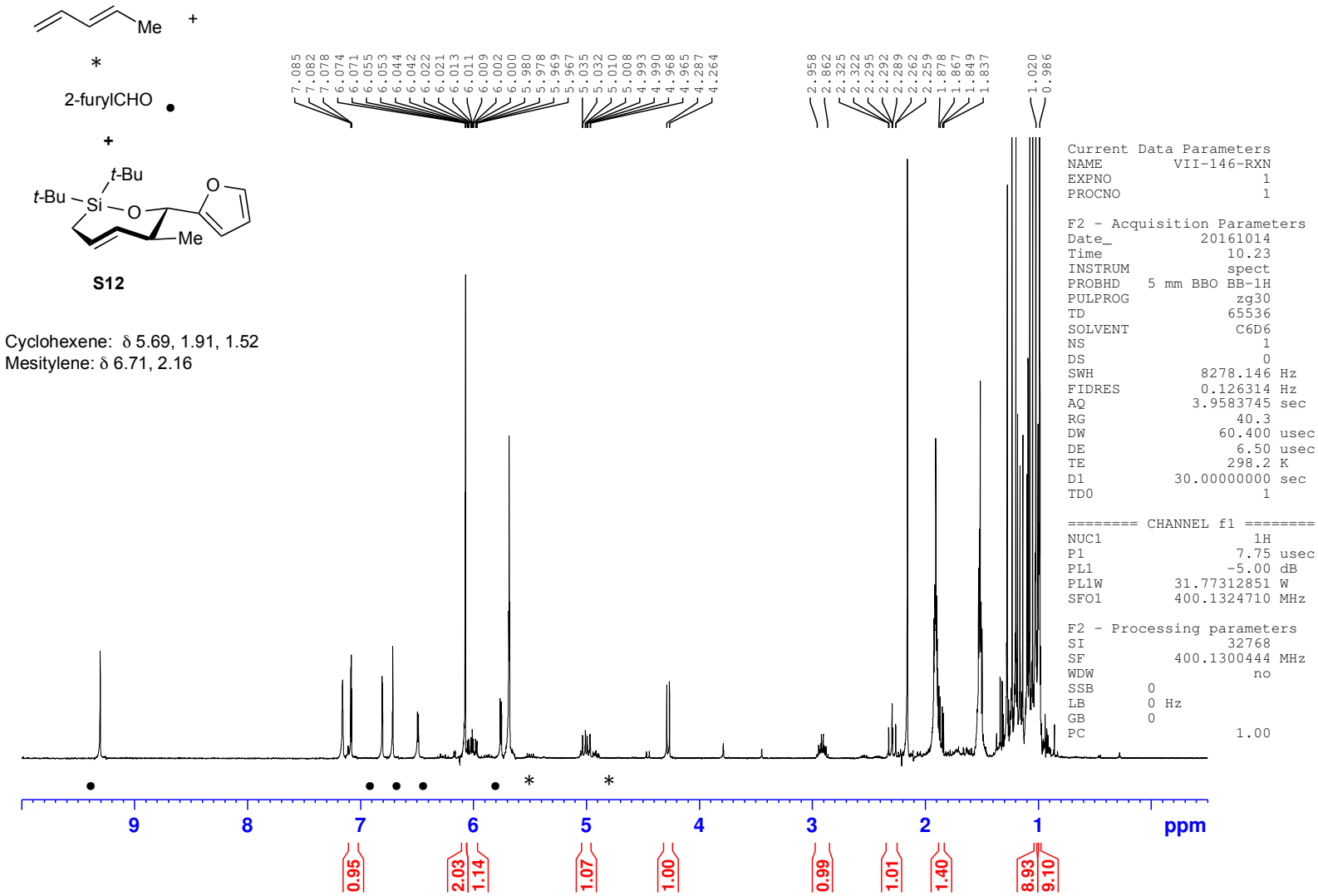

```
Current Data Parameters
NAME         VII-179-RXN
EXPNO                  2
PROCNO                 1

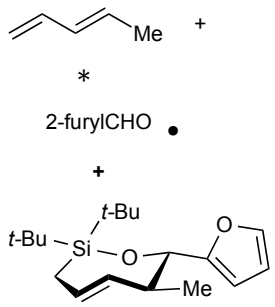
F2 - Acquisition Parameters
Date_           20161130
Time               16.22
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                    74
DS                     2
SWH            23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664256 sec
RG               14596.5
DW                20.850 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.75 usec
PL1                 -2.70 dB
PL1W         18.70940590 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2               80.00 usec
PL2                 -5.00 dB
PL12                14.95 dB
PL13                16.84 dB
PL2W         31.77312851 W
PL12W         0.32141048 W
PL13W         0.20799839 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127082 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
                    1.40
```


Me
+
*
2-furylCHO
•
+
t-Bu
t-Bu
Si
O
O
Me
S12
Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16
7.085 7.082 7.078 6.074 6.071 6.055 6.053 6.044 6.042 6.022 6.021 6.013 6.011 6.009 6.002 6.000 5.980 5.978 5.969 5.967 5.035 5.032 5.010 5.008 4.993 4.990 4.968 4.965 4.287 4.264
2.958 2.862 2.325 2.322 2.295 2.292 2.289 2.262 2.259 1.878 1.867 1.849 1.837
1.020 0.986
Current Data Parameters
NAME VII-146-RXN
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161014
Time 10.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 1
DS 0
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 40.3
DW 60.400 usec
DE 6.50 usec
TE 298.2 K
D1 30.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.75 usec
PL1 -5.00 dB
PL1W 31.77312851 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300444 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
0.95
2.03
1.14
1.07
1.00
0.99
1.01
1.40
8.93
9.10



S12

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8

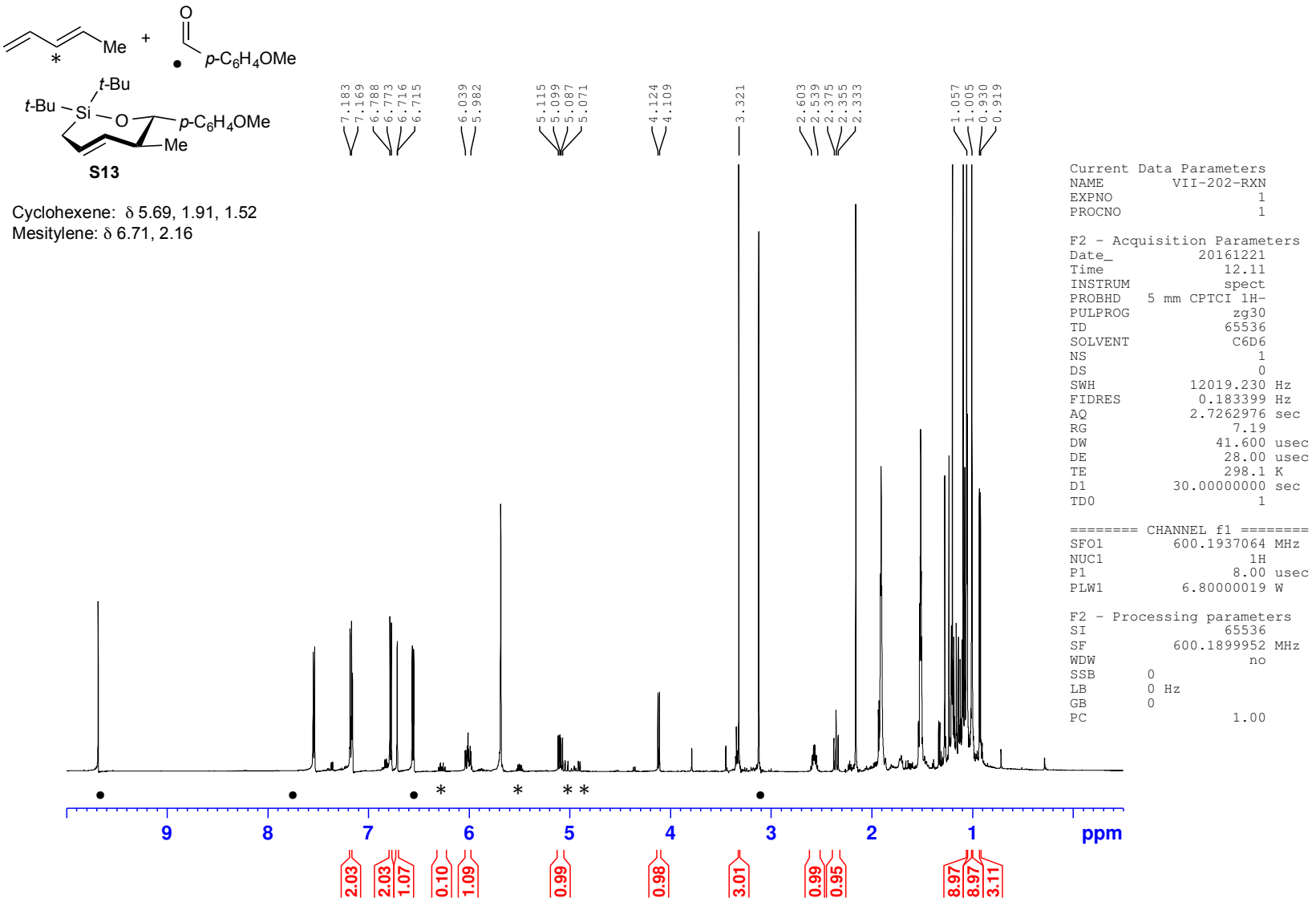

```
Current Data Parameters
NAME         VII-146-RXN
EXPNO                  2
PROCNO                 1

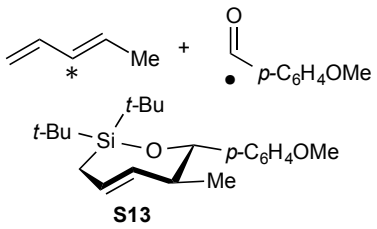
F2 - Acquisition Parameters
Date_           20161014
Time              10.29
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                  140
DS                    2
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664256 sec
RG              14596.5
DW               20.850 usec
DE                6.50 usec
TE               298.2 K
D1           2.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.75 usec
PL1                -2.70 dB
PL1W        18.70940590 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -5.00 dB
PL12               14.95 dB
PL13               16.84 dB
PL2W        31.77312851 W
PL12W        0.32141048 W
PL13W        0.20799839 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127082 MHz
WDW                  EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```


Me
+
O
p-C6H4OMe
t-Bu
t-Bu
Si
O
p-C6H4OMe
Me
S13
Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16
7.183
7.169
6.788
6.773
6.716
6.715
6.039
5.982
5.115
5.099
5.087
5.071
4.124
4.109
3.321
2.603
2.539
2.375
2.355
2.333
1.057
1.005
0.930
0.919
Current Data Parameters
NAME VII-202-RXN
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161221
Time 12.11
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 1
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 7.19
DW 41.600 usec
DE 28.00 usec
TE 298.1 K
D1 30.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1899952 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.03
2.03
1.07
0.10
1.09
0.99
0.98
3.01
0.99
0.95
8.97
8.97
3.11



S13

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8

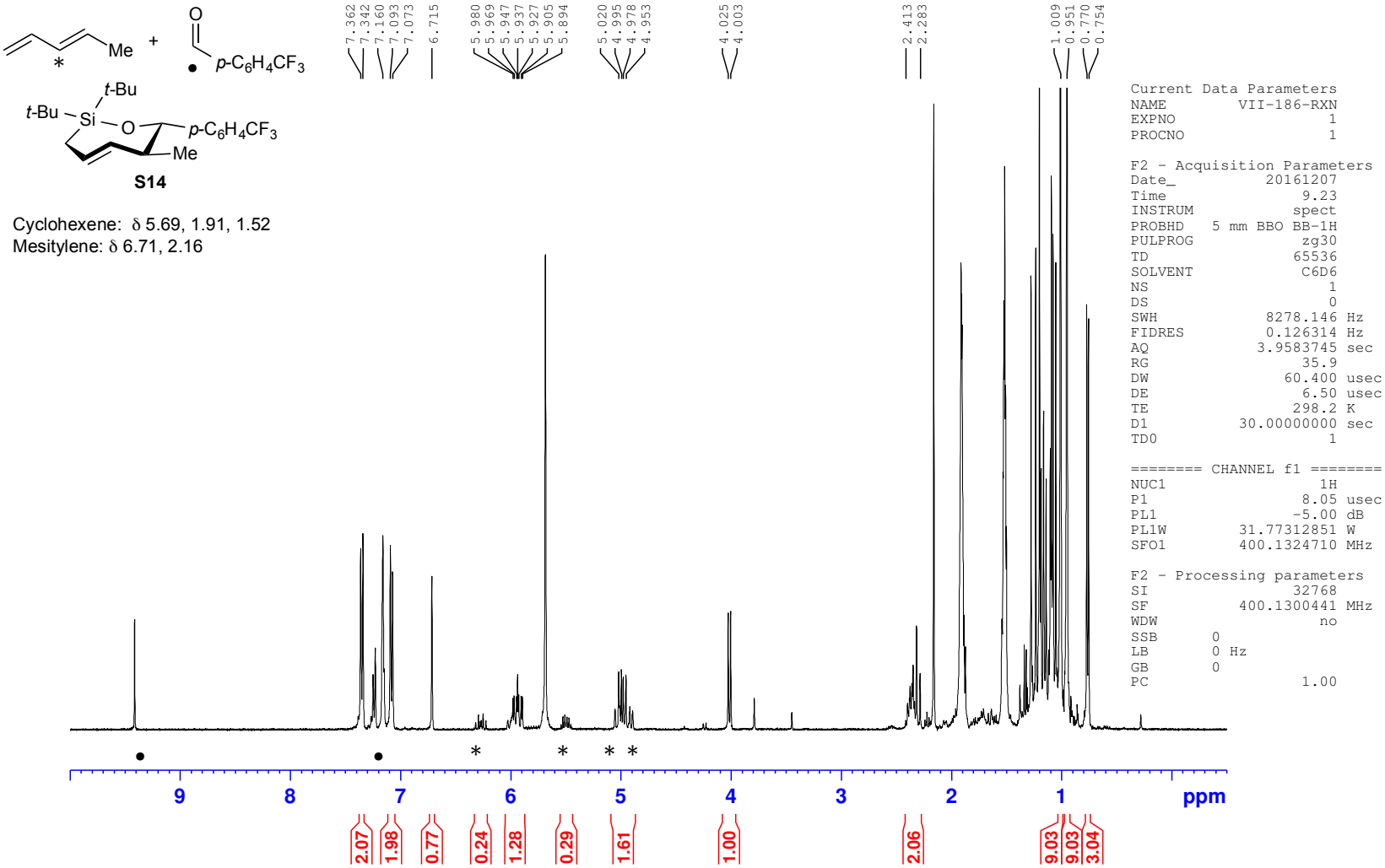

```
Current Data Parameters
NAME         VII-202-RXN
EXPNO                  2
PROCNO                 1

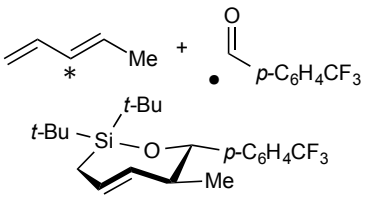
F2 - Acquisition Parameters
Date_           20161221
Time              12.13
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                    20
DS                     2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG               184.65
DW               13.867 usec
DE                18.00 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                13C
P1                11.63 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

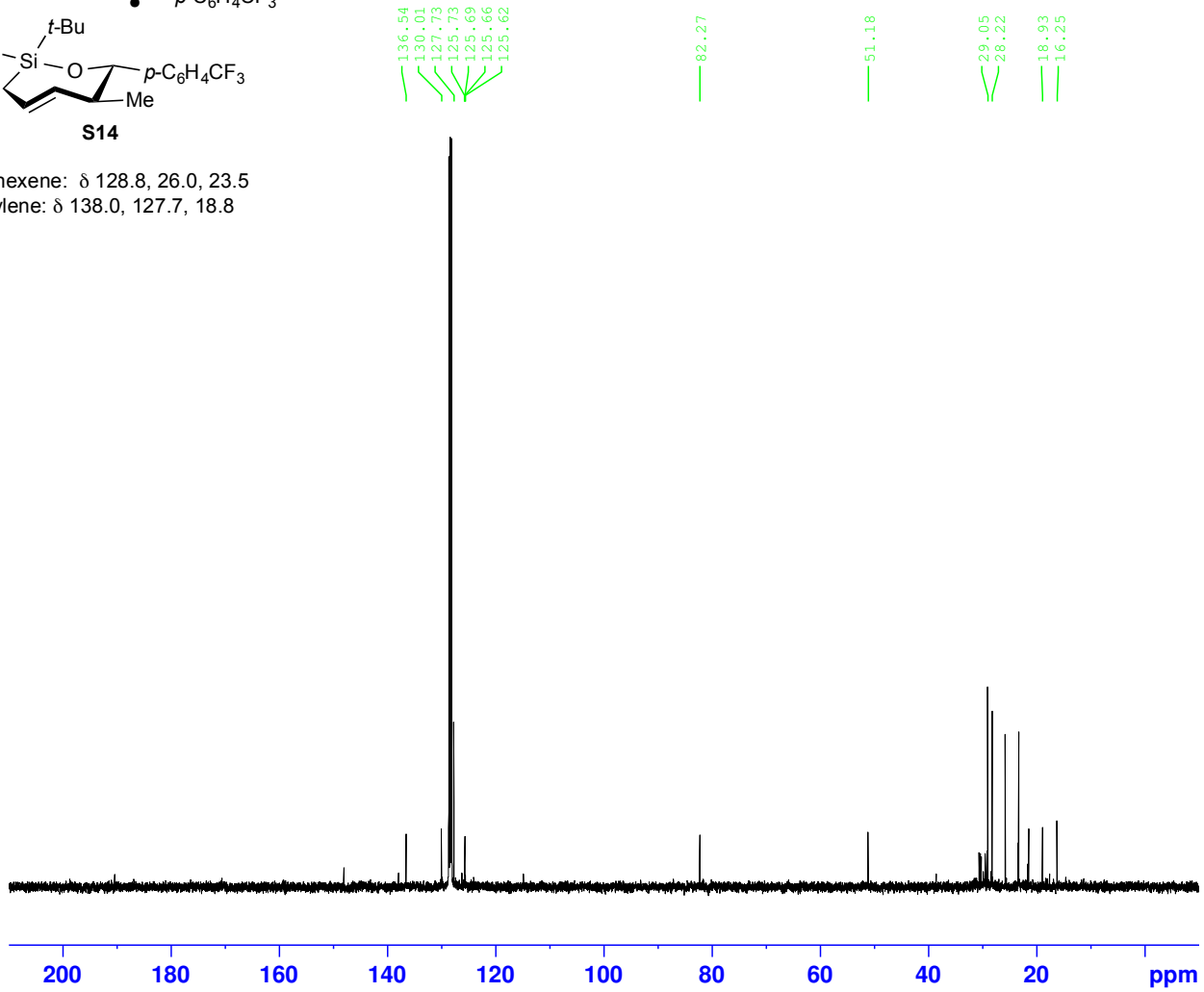
F2 - Processing parameters
SI                 32768
SF          150.9177876 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


Me
+
O
p-C6H4CF3
t-Bu
t-Bu
Si
O
p-C6H4CF3
Me
S14
Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16
7.362
7.342
7.160
7.093
7.073
6.715
5.980
5.969
5.947
5.937
5.927
5.905
5.894
5.020
4.995
4.978
4.953
4.025
4.003
2.413
2.283
1.009
0.951
0.770
0.754
Current Data Parameters
NAME VII-186-RXN
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161207
Time 9.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 1
DS 0
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 35.9
DW 60.400 usec
DE 6.50 usec
TE 298.2 K
D1 30.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.05 usec
PL1 -5.00 dB
PL1W 31.77312851 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300441 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.07
1.98
0.77
0.24
1.28
0.29
1.61
1.00
2.06
9.03
9.03
3.04



S14

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8



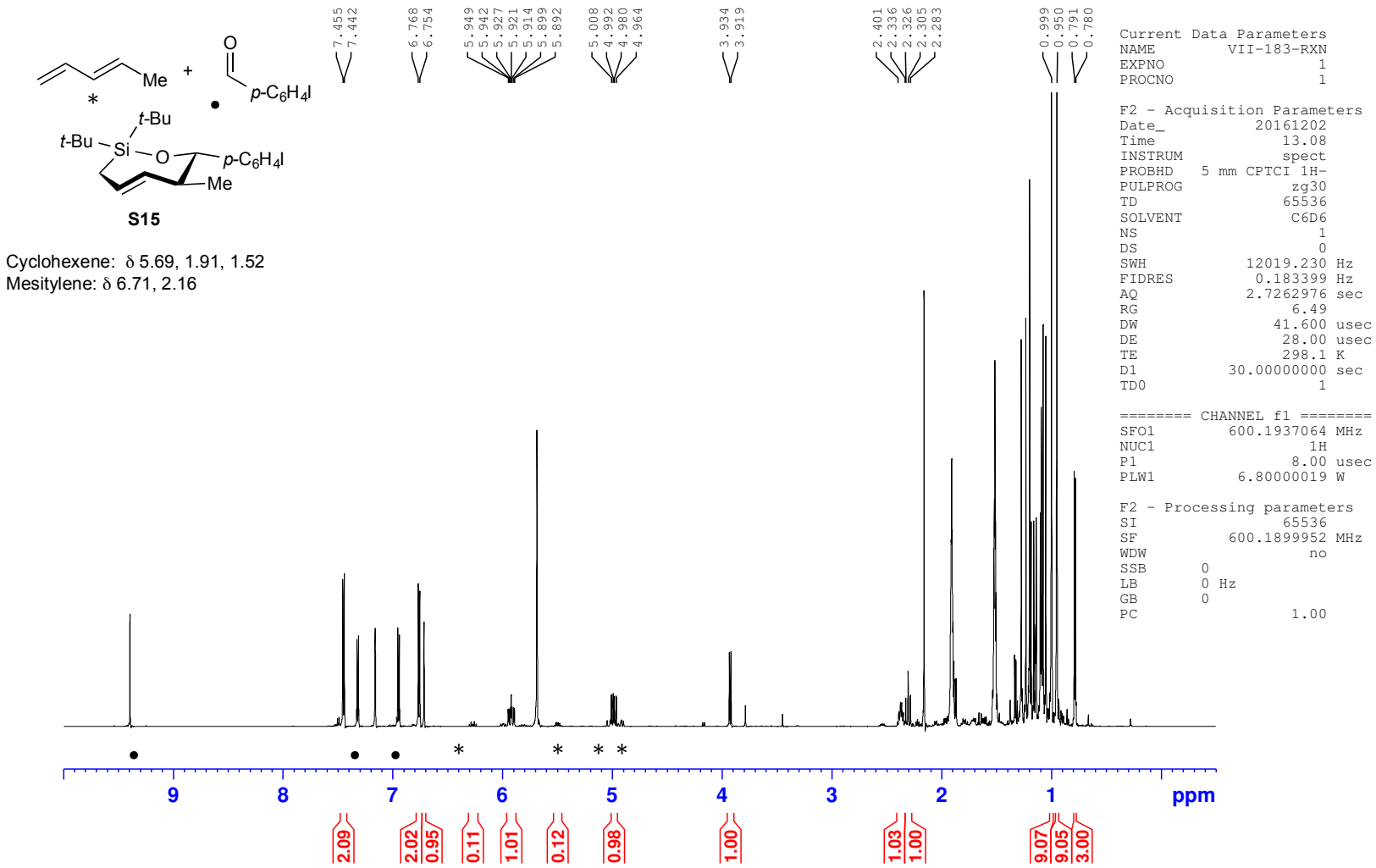

```
Current Data Parameters
NAME         VII-186-RXN
EXPNO                  2
PROCNO                 1

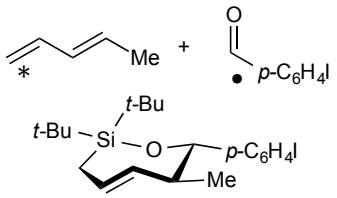
F2 - Acquisition Parameters
Date_           20161207
Time                9.25
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT              C6D6
NS                     38
DS                      2
SWH            23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664256 sec
RG                 13004
DW                20.850 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.75 usec
PL1                -2.70 dB
PL1W        18.70940590 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -5.00 dB
PL12               14.95 dB
PL13               16.84 dB
PL2W        31.77312851 W
PL12W        0.32141048 W
PL13W        0.20799839 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127065 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


Me
+
O
p-C6H4I
t-Bu
t-Bu
Si
O
p-C6H4I
Me
S15
Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16
7.455
7.442
6.768
6.754
5.949
5.942
5.927
5.921
5.914
5.899
5.892
5.008
4.992
4.980
4.964
3.934
3.919
2.401
2.336
2.326
2.305
2.283
0.999
0.950
0.791
0.780
Current Data Parameters
NAME VII-183-RXN
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161202
Time 13.08
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 1
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 6.49
DW 41.600 usec
DE 28.00 usec
TE 298.1 K
D1 30.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1899952 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.09
2.02
0.95
0.11
1.01
0.12
0.98
1.00
1.03
1.00
9.07
9.05
3.00



S15

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8

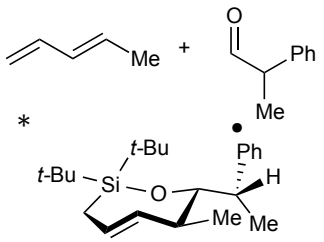

```
Current Data Parameters
NAME         VII-183-RXN
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161202
Time              13.10
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                    16
DS                     2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG               184.65
DW               13.867 usec
DE                18.00 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                  13C
P1                11.63 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                 32768
SF          150.9177885 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



S16

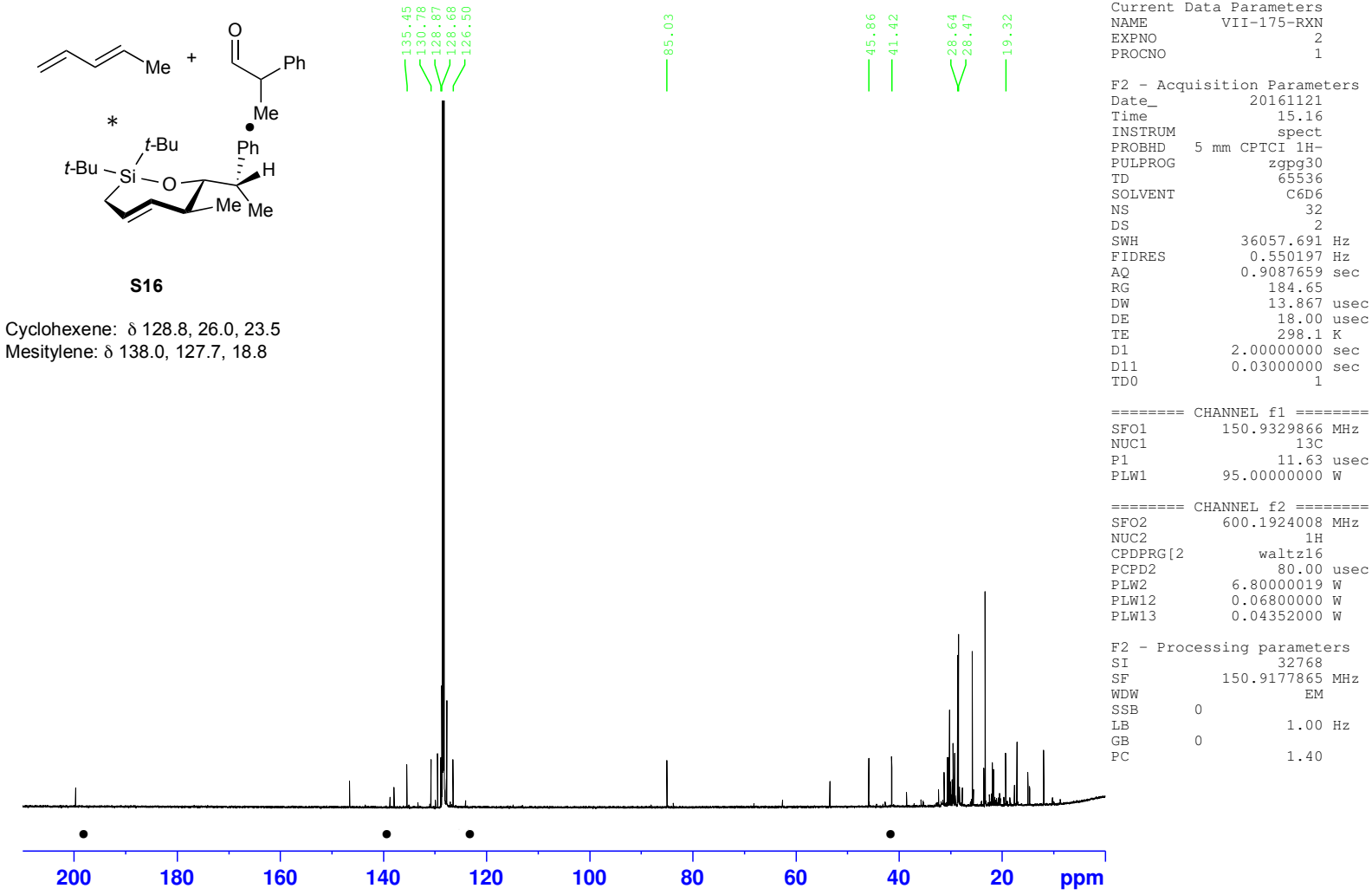
Cyclohexene: δ 5.69, 1.91, 1.52
Mesitylene: δ 6.71, 2.16


```
Current Data Parameters
NAME         VII-175-RXN
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161121
Time               15.12
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     1
DS                     0
SWH            12019.230 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                  6.49
DW                41.600 usec
DE                28.00 usec
TE                298.1 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         600.1937064 MHz
NUC1                   1H
P1                  8.00 usec
PLW1          6.80000019 W

F2 - Processing parameters
SI                 65536
SF            600.1899952 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



S16

Cyclohexene: δ 128.8, 26.0, 23.5
Mesitylene: δ 138.0, 127.7, 18.8

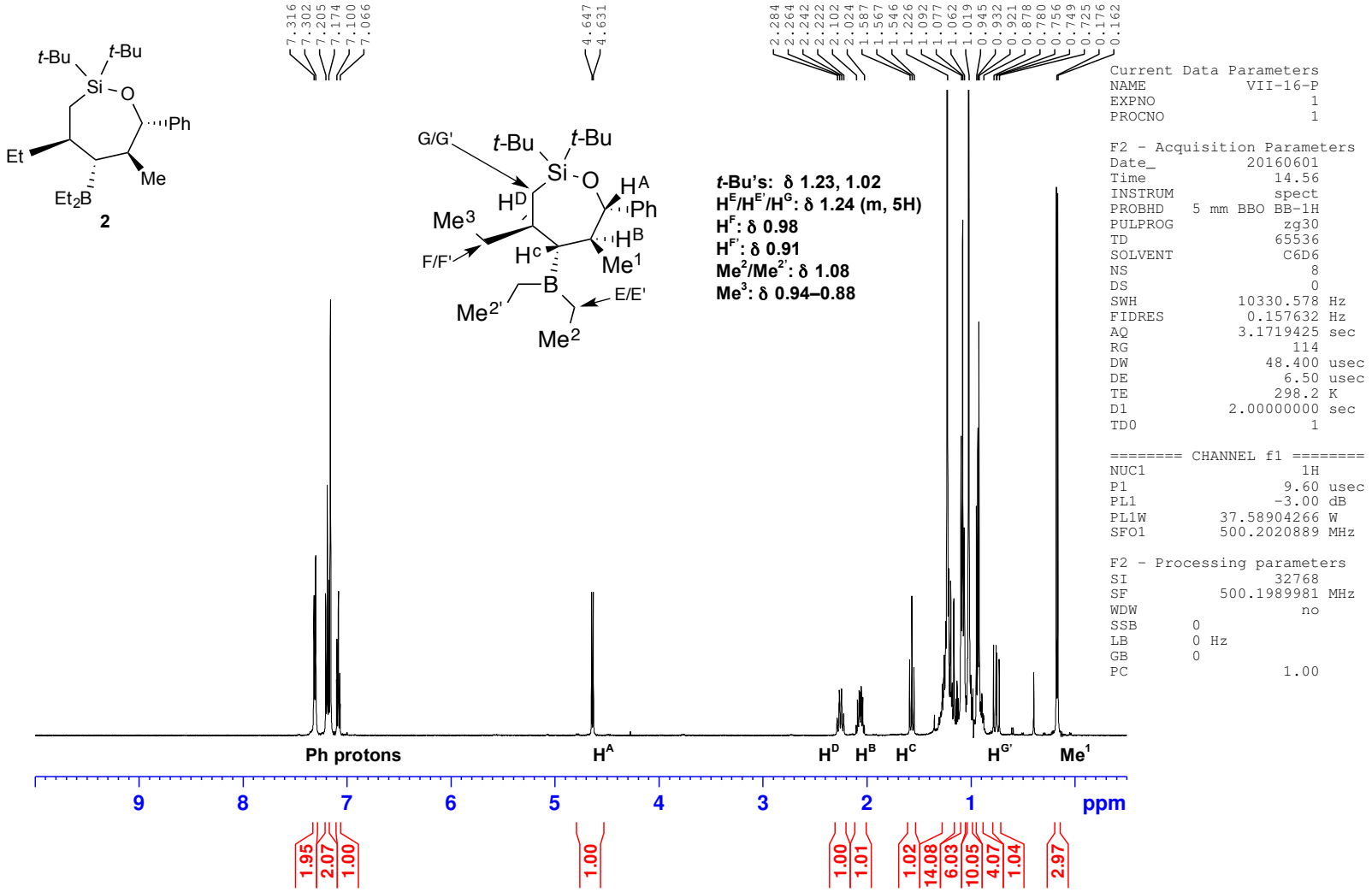
```
Current Data Parameters
NAME         VII-175-RXN
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161121
Time               15.16
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                    32
DS                     2
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                184.65
DW                13.867 usec
DE                 18.00 usec
TE                 298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

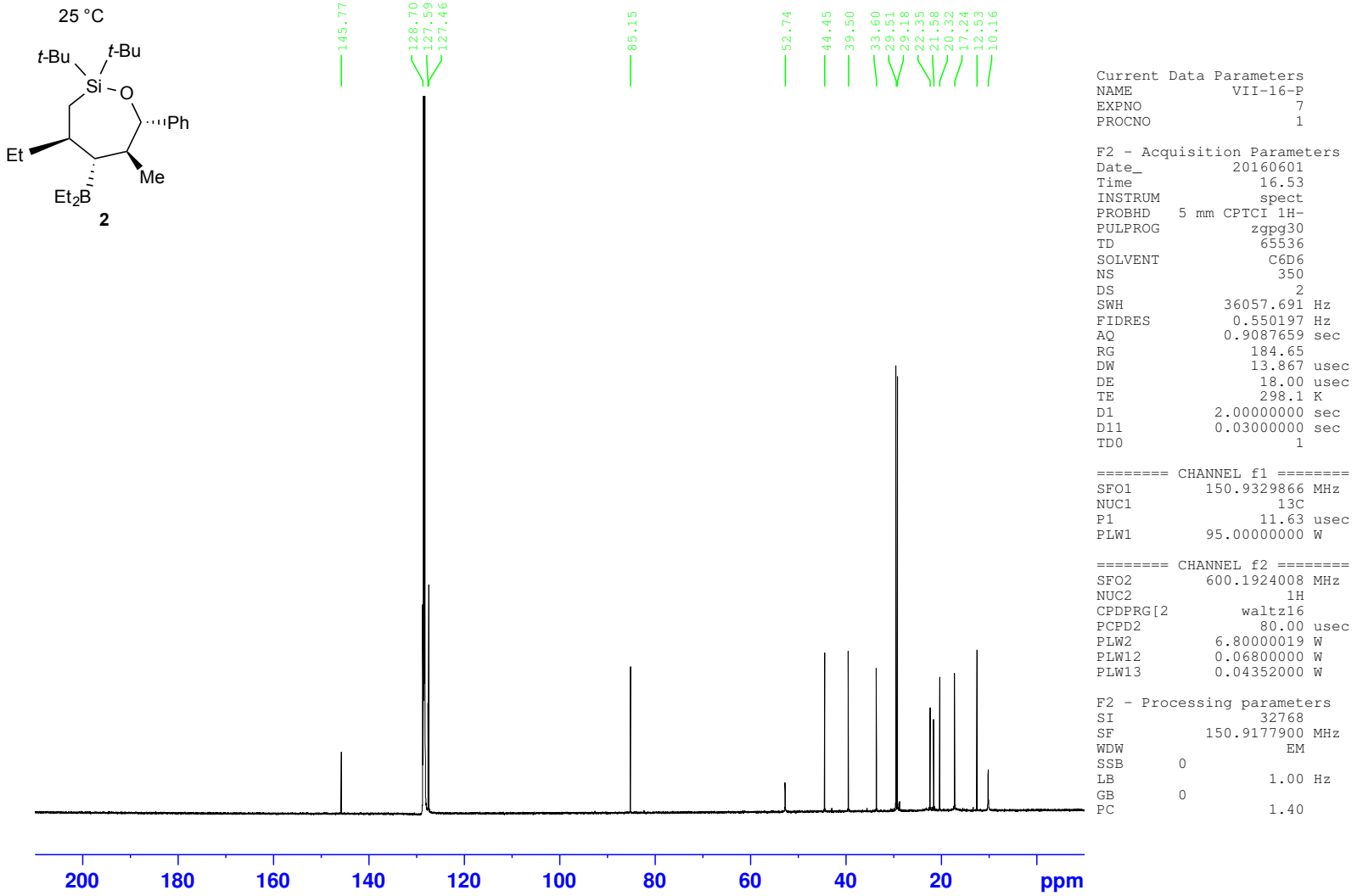
======== CHANNEL f1 ========
SFO1         150.9329866 MHz
NUC1                  13C
P1                 11.63 usec
PLW1         95.00000000 W

======== CHANNEL f2 ========
SFO2         600.1924008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                 32768
SF           150.9177865 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



1H NMR assignments by HSQC and COSY experiments



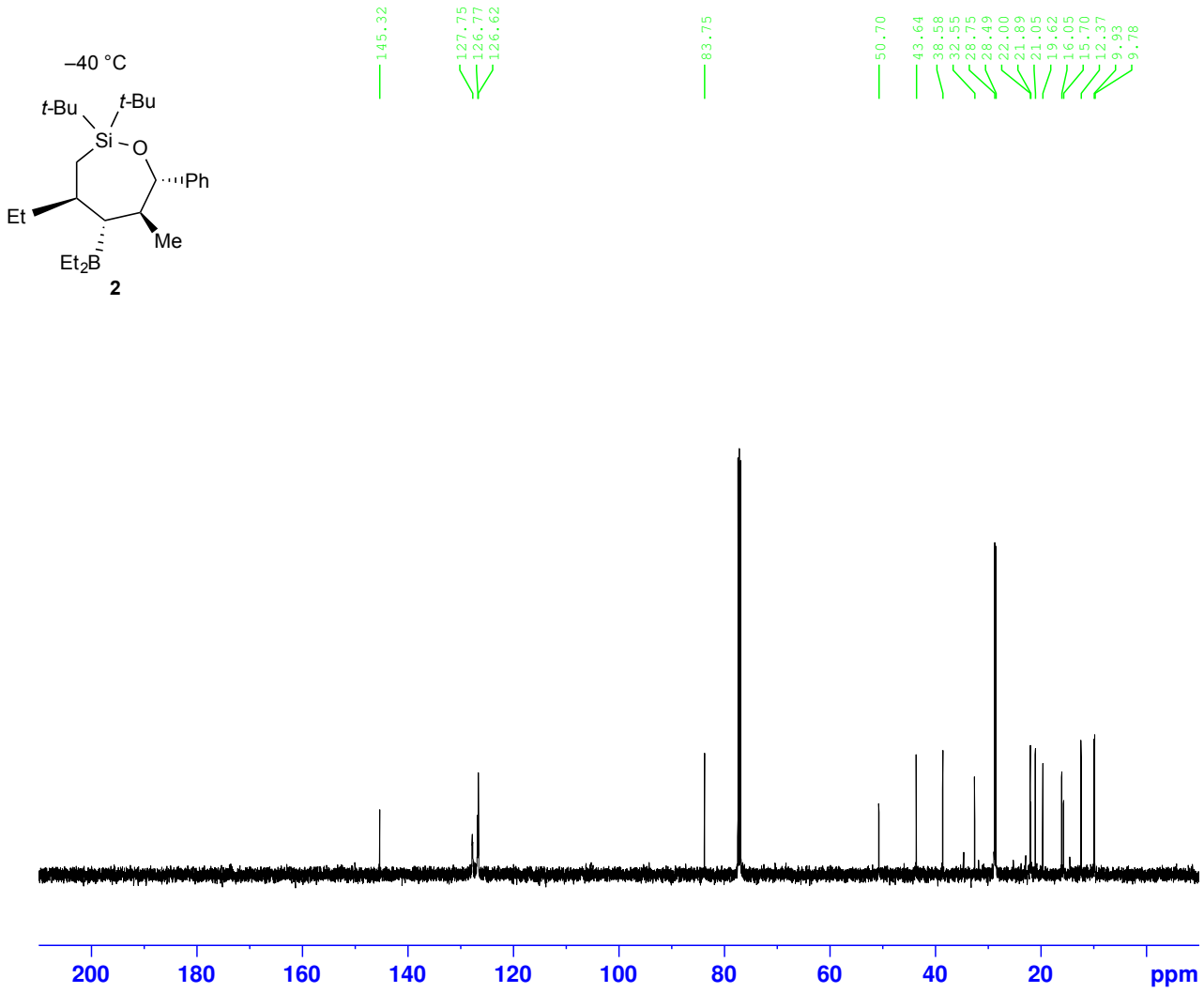

```
Current Data Parameters
NAME            VII-16-P
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160601
Time               16.53
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT              C6D6
NS                    350
DS                      2
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                184.65
DW                13.867 usec
DE                 18.00 usec
TE                 298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         150.9329866 MHz
NUC1                  13C
P1                 11.63 usec
PLW1         95.00000000 W

======== CHANNEL f2 ========
SFO2         600.1924008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                 32768
SF           150.9177900 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



2

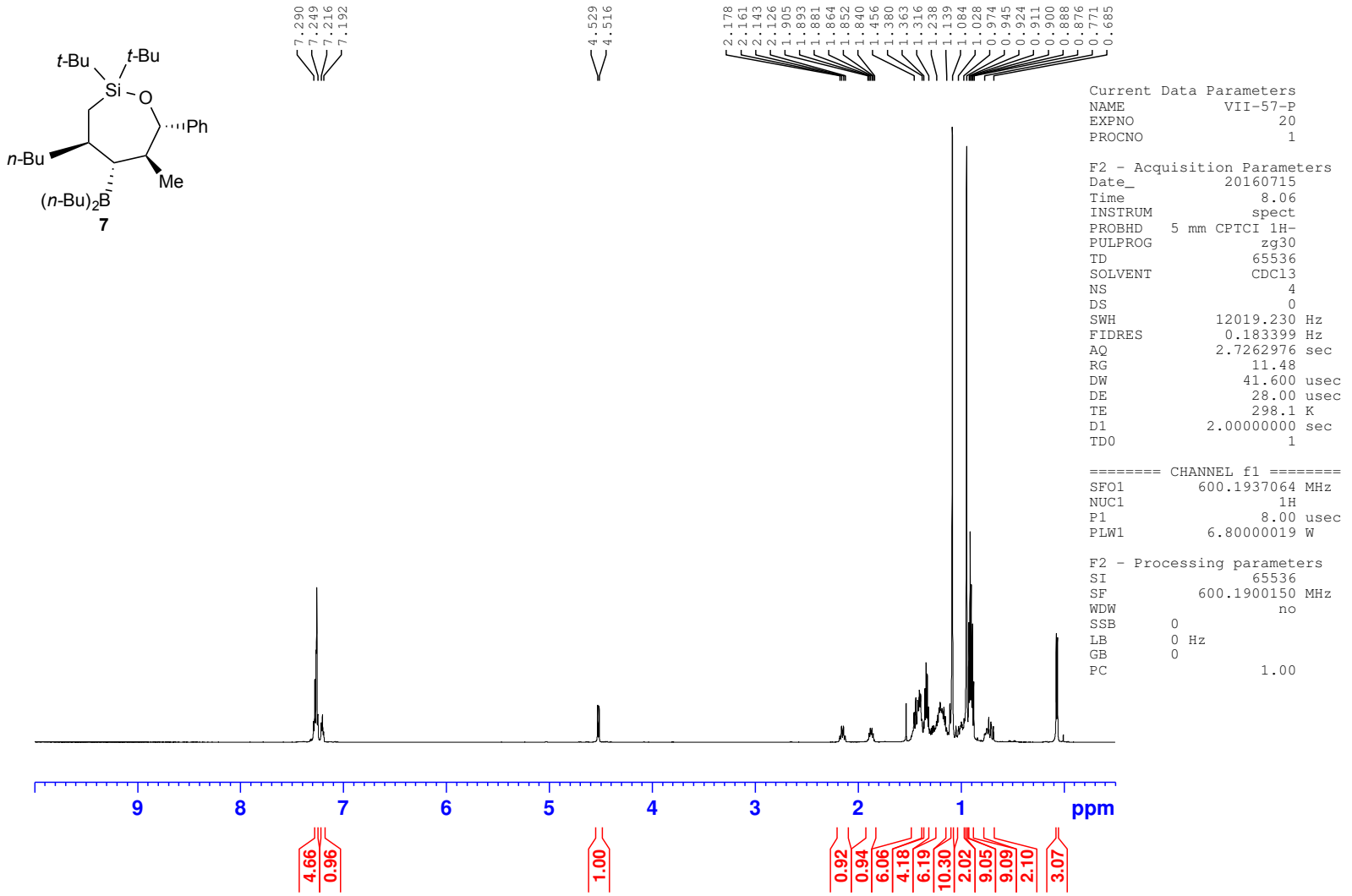
```
Current Data Parameters
NAME      VII-48-P-VTCOLD
EXPNO                   6
PROCNO                  1

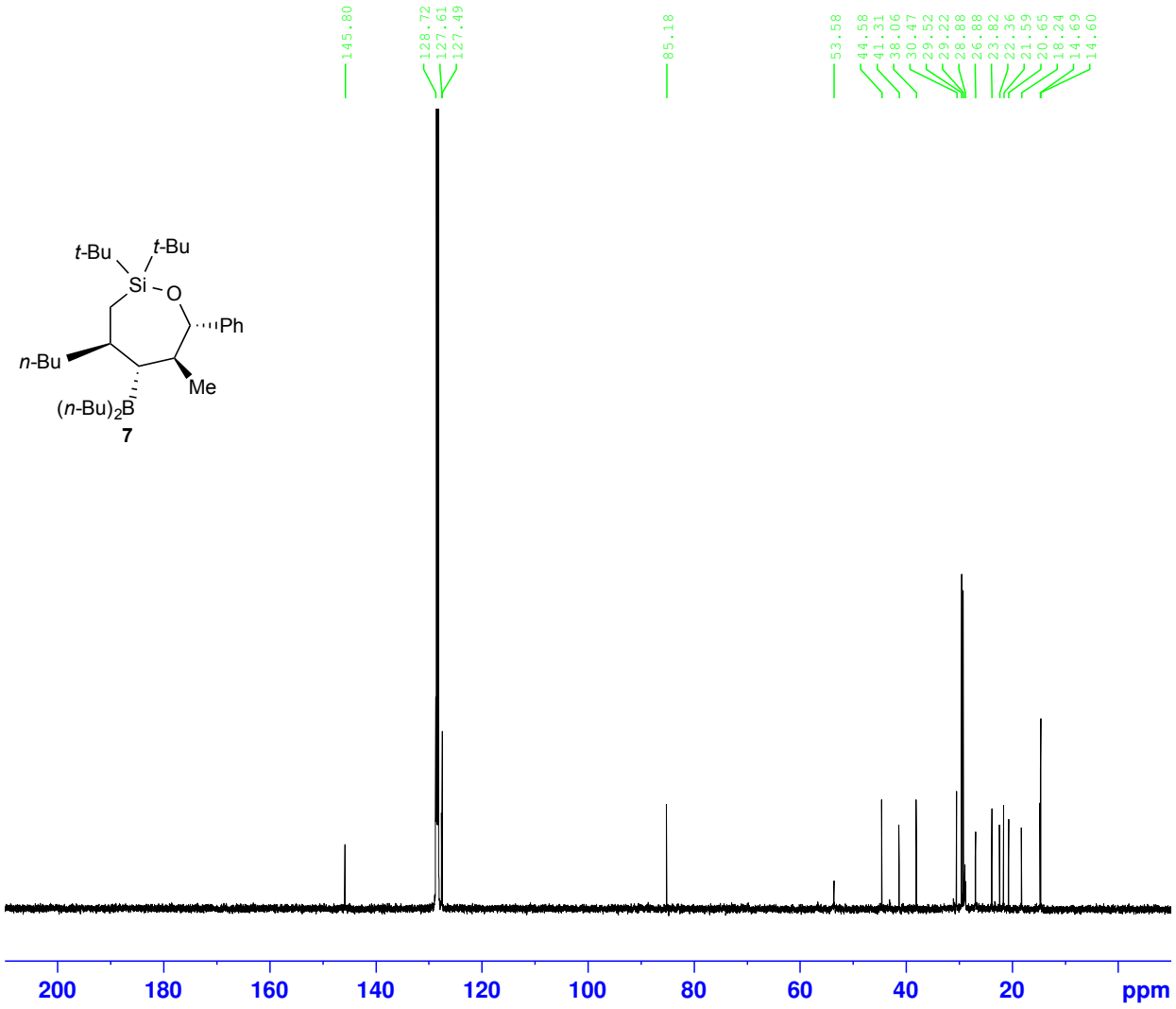
F2 - Acquisition Parameters
Date_           20160719
Time               10.28
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   39
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0911744 sec
RG               11585.2
DW                16.650 usec
DE                 6.50 usec
TE                233.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                2.30 dB
PL1W        46.00027084 W
SFO1        125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              15.31 dB
PL13              18.31 dB
PL2W        37.58904266 W
PL12W        0.55470389 W
PL13W        0.27801058 W
SFO2        500.2010008 MHz

F2 - Processing parameters
SI                32768
SF          125.7751556 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


t-Bu
t-Bu
Si
O
Ph
n-Bu
Me
(n-Bu)2B
7
7.290
7.249
7.216
7.192
4.529
4.516
2.178
2.161
2.143
2.126
1.905
1.893
1.881
1.864
1.852
1.840
1.456
1.380
1.363
1.316
1.238
1.139
1.084
1.028
0.974
0.945
0.924
0.911
0.900
0.888
0.876
0.771
0.685
Current Data Parameters
NAME VII-57-P
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160715
Time 8.06
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 11.48
DW 41.600 usec
DE 28.00 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1900150 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
4.66
0.96
1.00
0.92
0.94
6.06
4.18
6.19
10.30
2.02
9.05
9.09
2.10
3.07



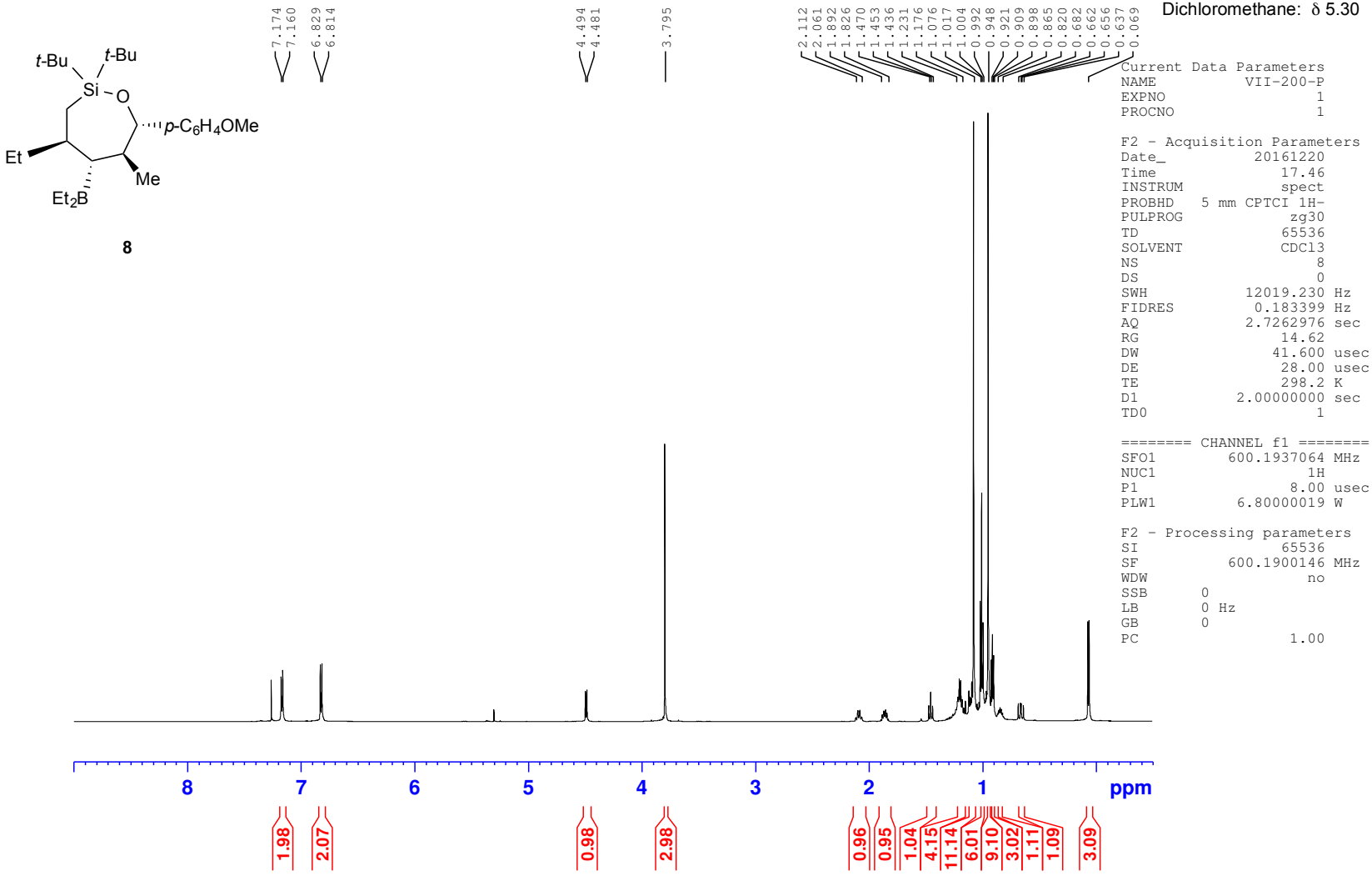

```
Current Data Parameters
NAME            VII-57-P
EXPNO                  4
PROCNO                 1

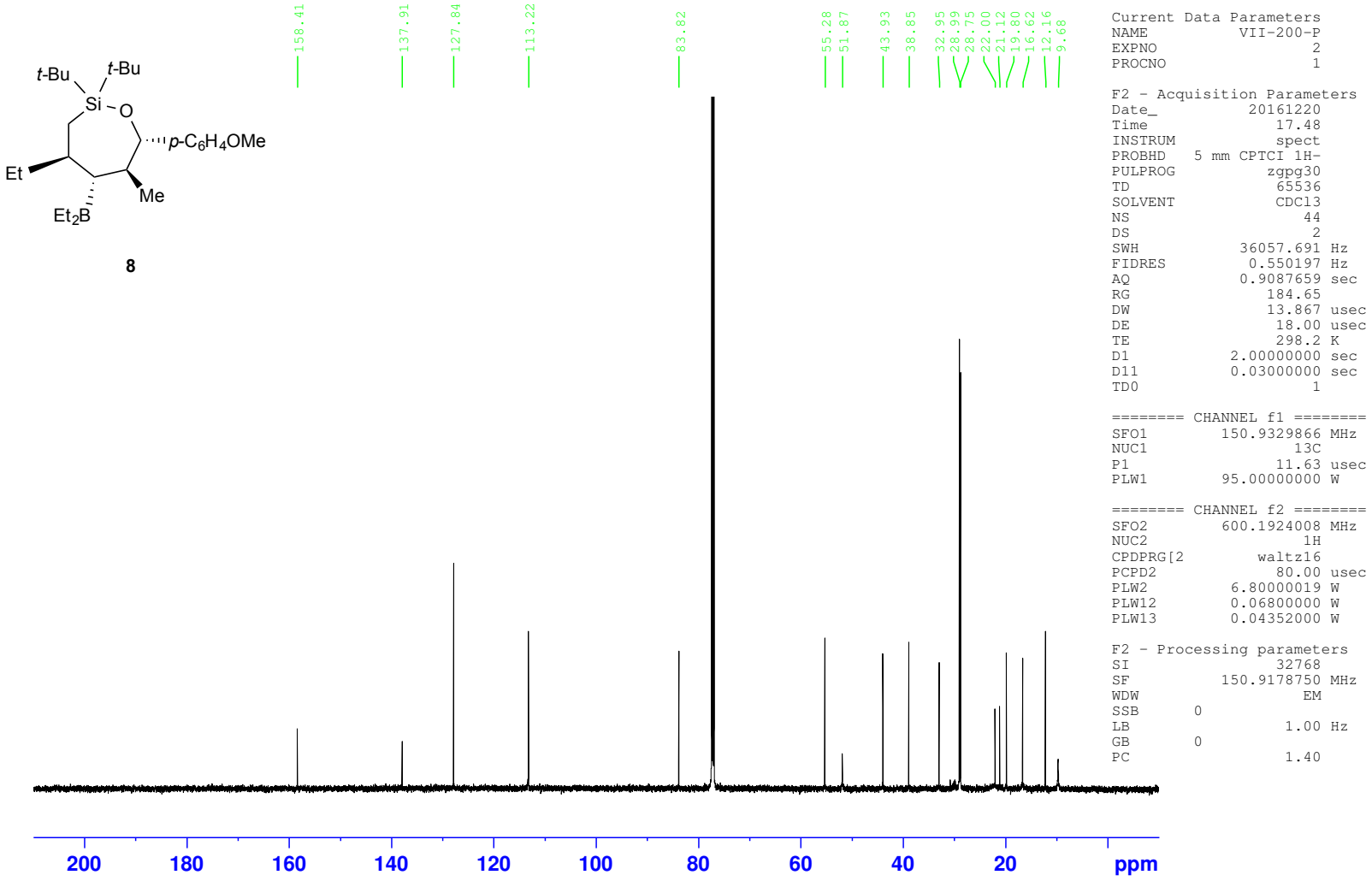
F2 - Acquisition Parameters
Date_           20160713
Time                7.28
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 65536
SOLVENT             C6D6
NS                   258
DS                     2
SWH            30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0911744 sec
RG                  8192
DW                16.650 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 2.30 dB
PL1W         46.00027084 W
SFO1         125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               15.31 dB
PL13               18.31 dB
PL2W         37.58904266 W
PL12W         0.55470389 W
PL13W         0.27801058 W
SFO2         500.2010008 MHz

F2 - Processing parameters
SI                 32768
SF           125.7750486 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


t-Bu
t-Bu
Si
O
p-C6H4OMe
Et
Me
Et2B
8
7.174
7.160
6.829
6.814
4.494
4.481
3.795
2.112
2.061
1.892
1.826
1.470
1.453
1.436
1.231
1.176
1.076
1.017
1.004
0.992
0.948
0.921
0.909
0.898
0.865
0.820
0.682
0.662
0.656
0.637
0.069
Dichloromethane: δ 5.30
Current Data Parameters
NAME VII-200-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161220
Time 17.46
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 14.62
DW 41.600 usec
DE 28.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1900146 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
ppm
1.98
2.07
0.98
2.98
0.96
0.95
1.04
4.15
11.14
6.01
9.10
3.02
1.11
1.09
3.09



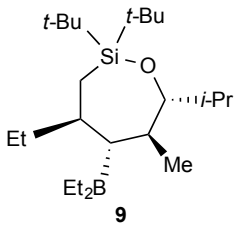

```
Current Data Parameters
NAME            VII-200-P
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161220
Time                17.48
INSTRUM             spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    44
DS                     2
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                184.65
DW                13.867 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

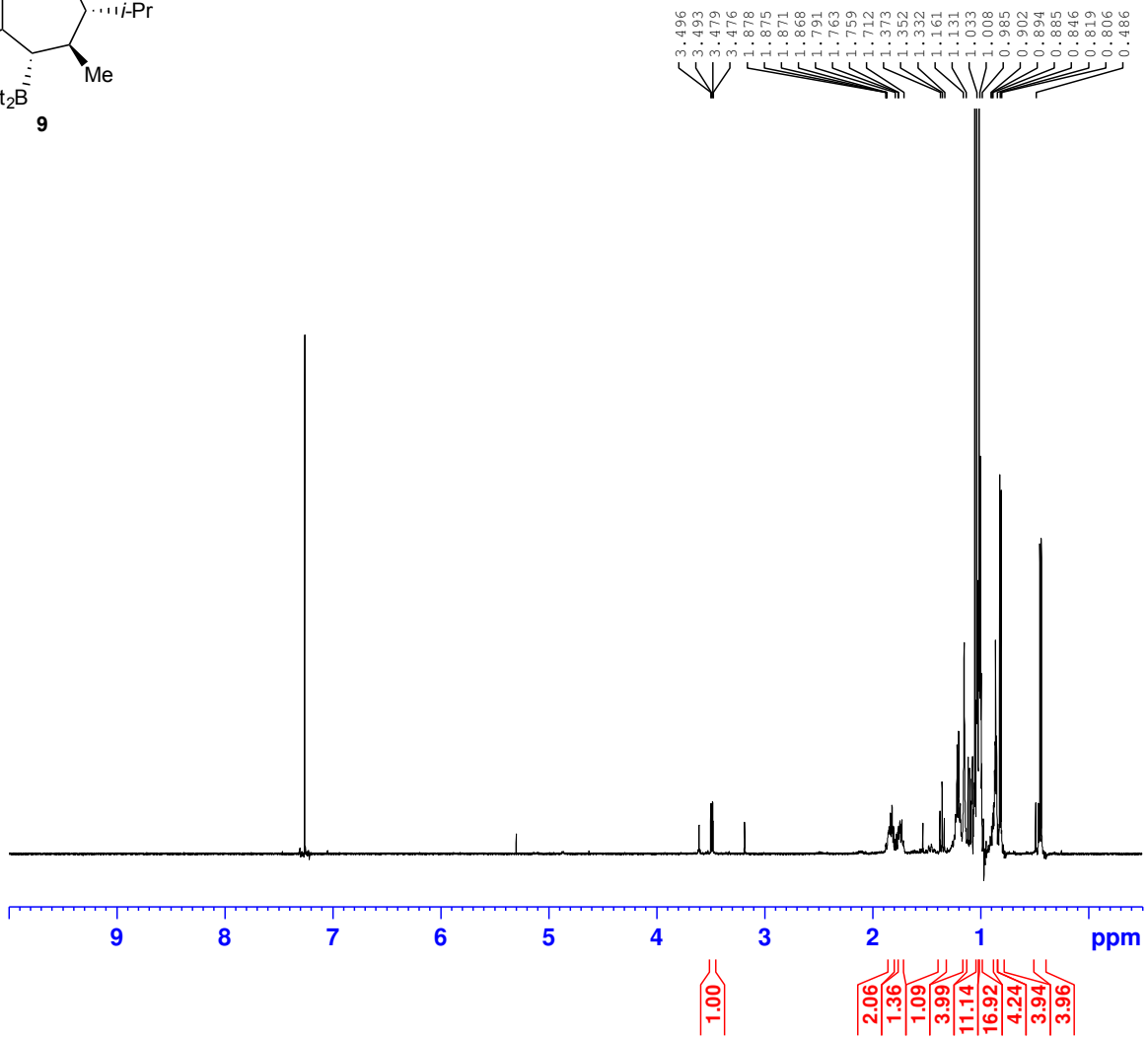
======== CHANNEL f1 ========
SFO1         150.9329866 MHz
NUC1                  13C
P1                11.63 usec
PLW1         95.00000000 W

======== CHANNEL f2 ========
SFO2         600.1924008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                 32768
SF           150.9178750 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



9

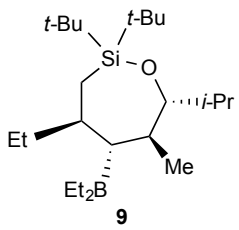



```
Current Data Parameters
NAME           VIII-23-P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170123
Time               13.17
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719425 sec
RG                   256
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.60 usec
PL1               -3.00 dB
PL1W        37.58904266 W
SFO1        500.2020889 MHz

F2 - Processing parameters
SI                 65536
SF          500.1990143 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



9


```
Current Data Parameters
NAME          VIII-23-P
EXPNO                 4
PROCNO                1

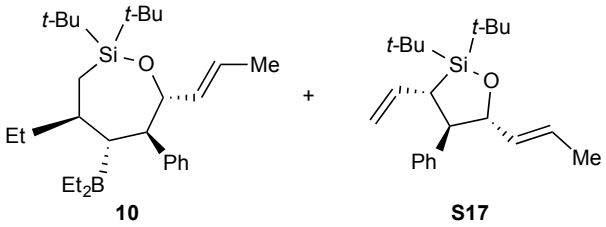
F2 - Acquisition Parameters
Date_          20170123
Time              14.06
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG               184.65
DW               13.867 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                13C
P1                11.63 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                32768
SF          150.9178746 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{1}H NMR of unpurified reaction mixture



10

+

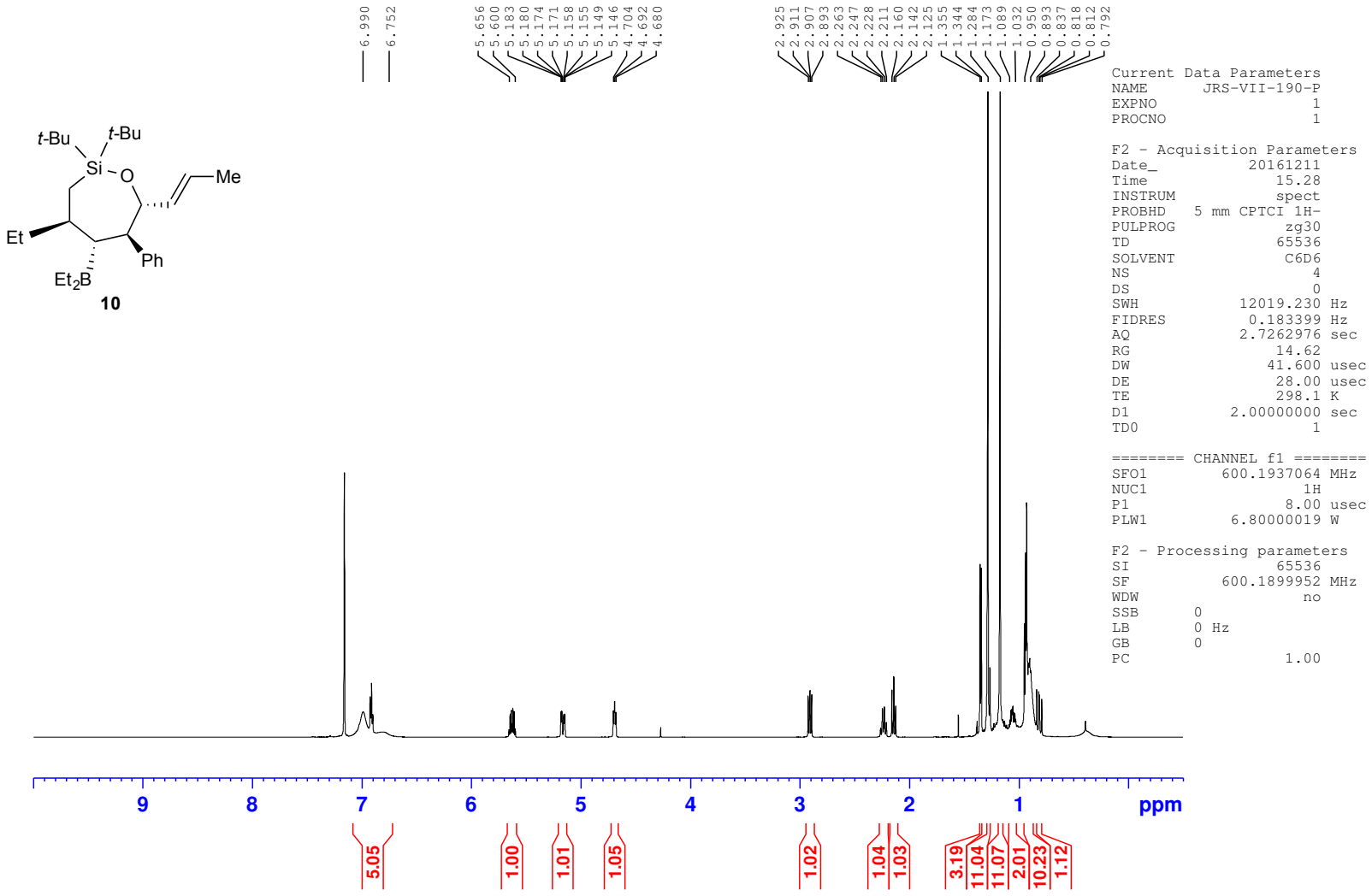
S17

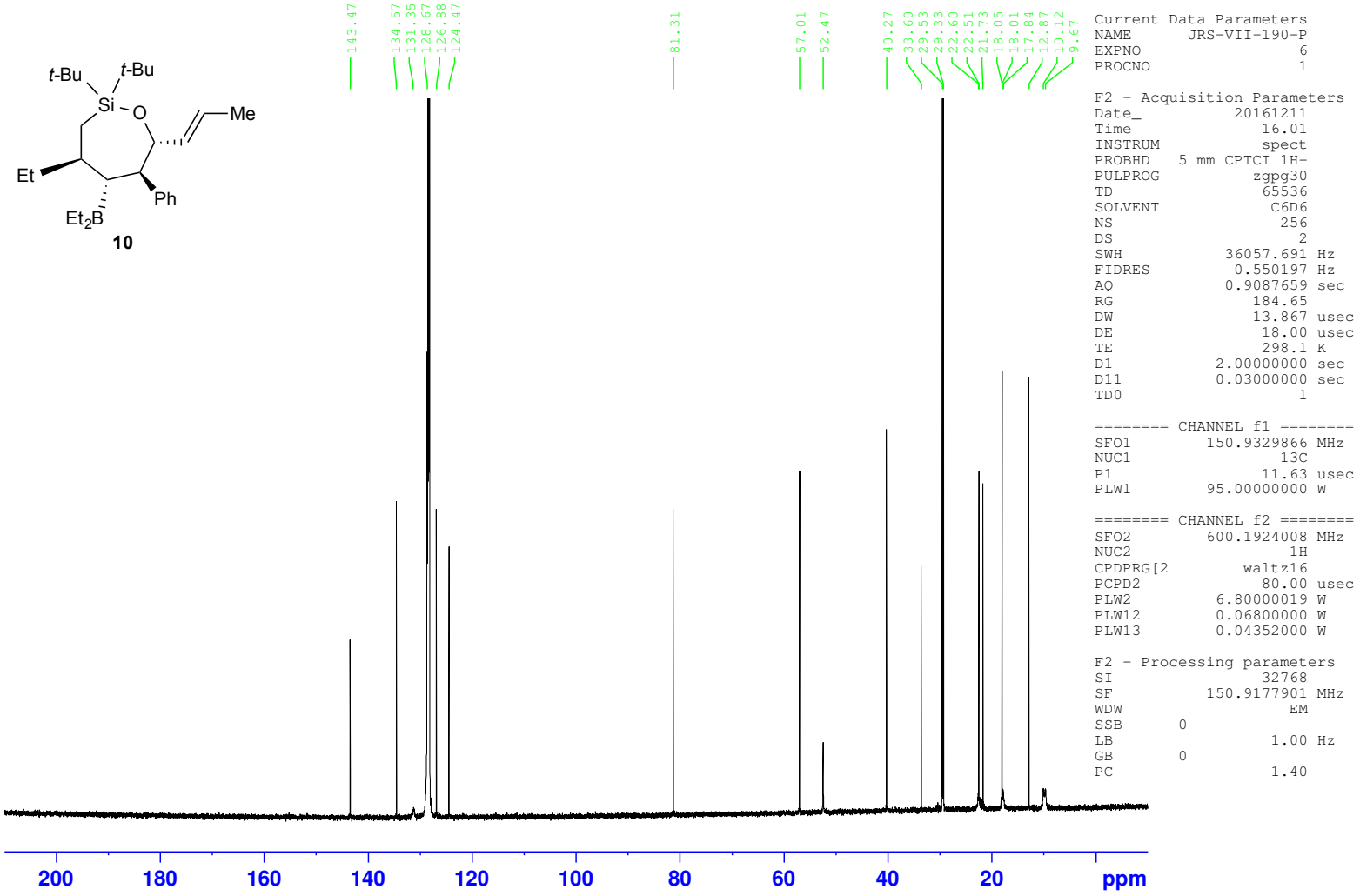

```
Current Data Parameters
NAME          VII-190-CR
EXPNO                  1
PROCNO                 1

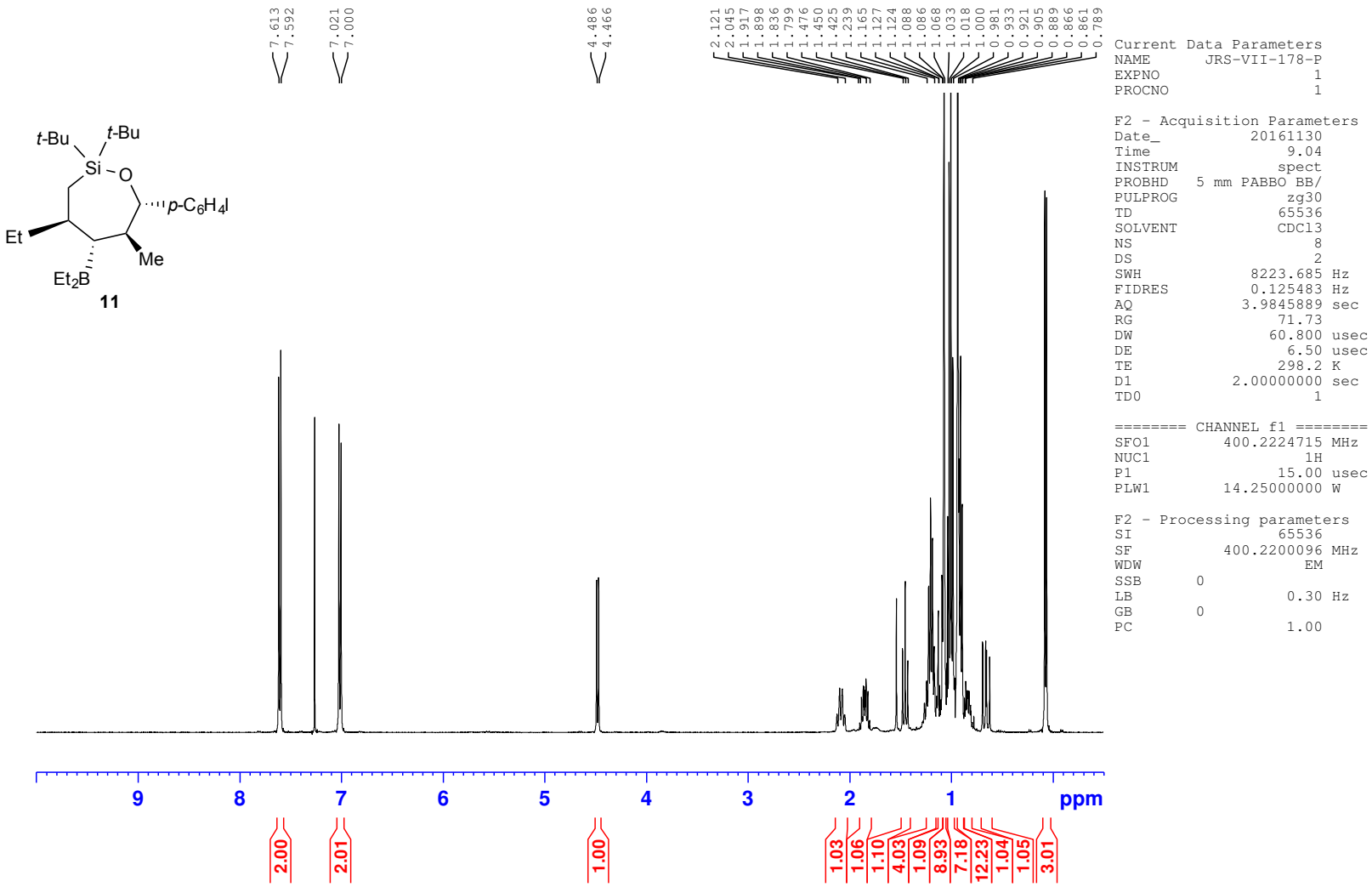
F2 - Acquisition Parameters
Date_           20161209
Time               15.52
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     1
DS                     0
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719425 sec
RG                  71.8
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.60 usec
PL1               -3.00 dB
PL1W        37.58904266 W
SFO1        500.2020889 MHz

F2 - Processing parameters
SI                 65536
SF          500.1990000 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```


6.990
6.752
5.656
5.600
5.183
5.180
5.174
5.171
5.158
5.155
5.149
5.146
4.704
4.692
4.680
2.925
2.911
2.907
2.893
2.263
2.247
2.228
2.211
2.160
2.142
2.125
1.355
1.344
1.284
1.173
1.089
1.032
0.950
0.893
0.837
0.818
0.812
0.792
t-Bu
t-Bu
Si
O
Me
Et
Ph
Et2B
10
Current Data Parameters
NAME JRS-VII-190-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161211
Time 15.28
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 4
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 14.62
DW 41.600 usec
DE 28.00 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1899952 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
5.05
1.00
1.01
1.05
1.02
1.04
1.03
3.19
11.04
11.07
2.01
10.23
1.12


t-Bu
t-Bu
Si
O
Me
Et
Ph
Et2B
10
143.47
134.57
131.35
128.67
126.88
124.47
81.31
57.01
52.47
40.27
33.60
29.53
29.33
22.60
22.51
21.73
18.05
18.01
17.84
12.87
10.12
9.67
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME JRS-VII-190-P
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161211
Time 16.01
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 256
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 184.65
DW 13.867 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 150.9329866 MHz
NUC1 13C
P1 11.63 usec
PLW1 95.00000000 W
======== CHANNEL f2 ========
SFO2 600.1924008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 6.80000019 W
PLW12 0.06800000 W
PLW13 0.04352000 W
F2 - Processing parameters
SI 32768
SF 150.9177901 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

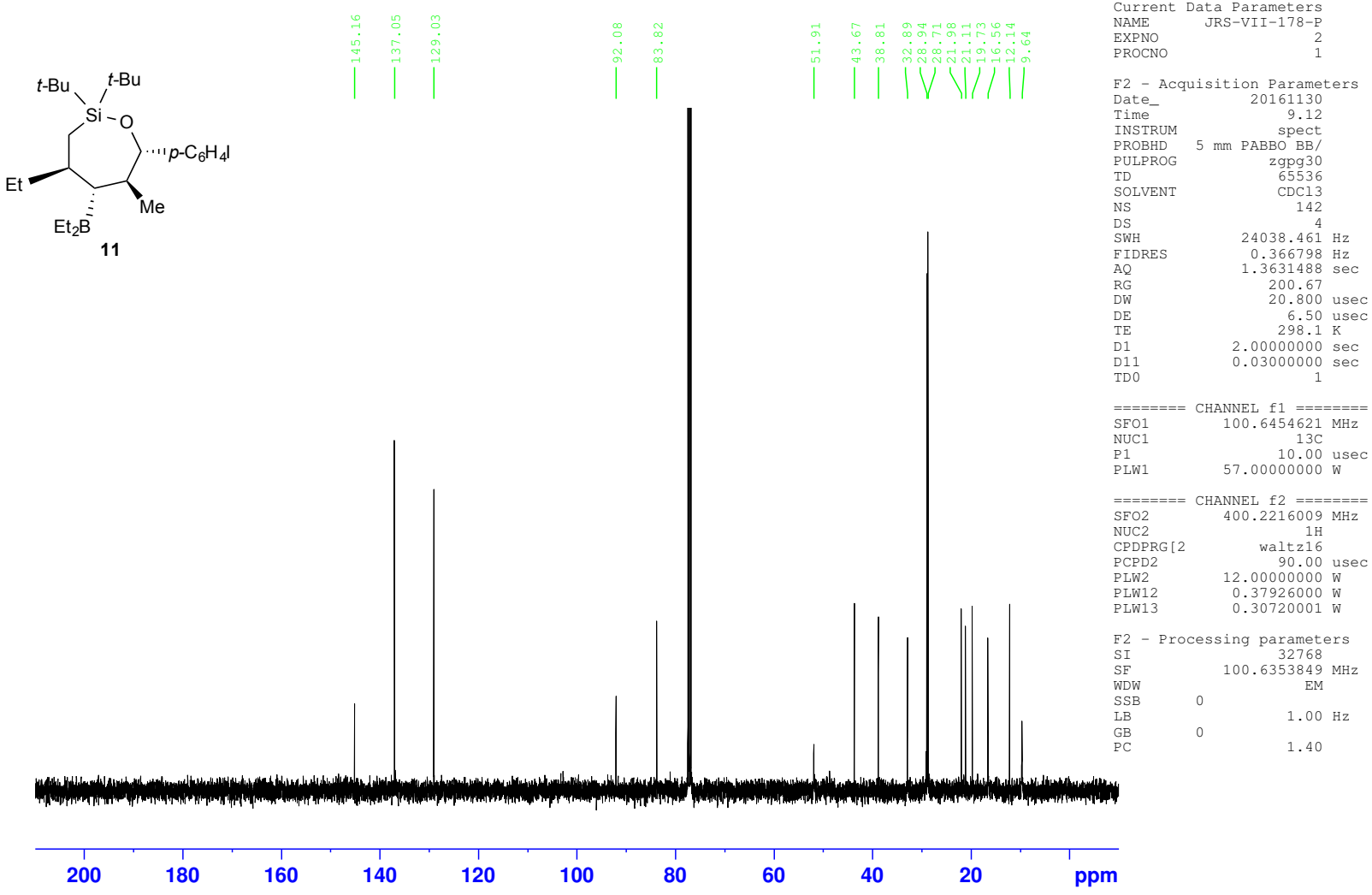



```
Current Data Parameters
NAME      JRS-VII-178-P
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20161130
Time               9.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ           3.9845889 sec
RG               71.73
DW               60.800 usec
DE                6.50 usec
TE               298.2 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.2224715 MHz
NUC1                1H
P1                15.00 usec
PLW1        14.25000000 W

F2 - Processing parameters
SI                65536
SF          400.2200096 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```




```
Current Data Parameters
NAME      JRS-VII-178-P
EXPNO                 2
PROCNO                1

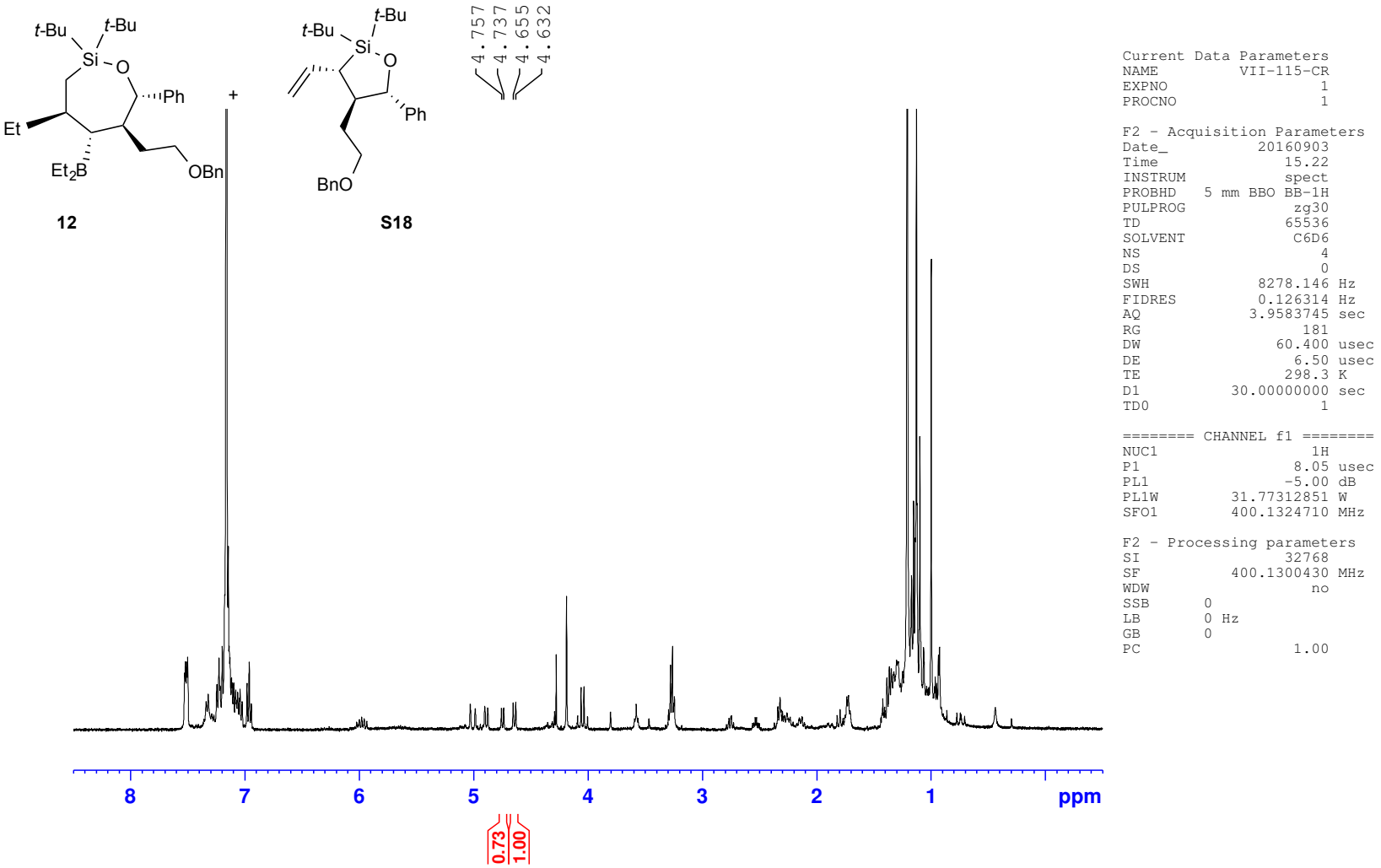
F2 - Acquisition Parameters
Date_          20161130
Time               9.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT         CDCl3
NS                142
DS                  4
SWH         24038.461 Hz
FIDRES       0.366798 Hz
AQ          1.3631488 sec
RG             200.67
DW             20.800 usec
DE              6.50 usec
TE             298.1 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1       100.6454621 MHz
NUC1              13C
P1              10.00 usec
PLW1       57.00000000 W

======== CHANNEL f2 ========
SFO2       400.2216009 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.37926000 W
PLW13       0.30720001 W

F2 - Processing parameters
SI               32768
SF         100.6353849 MHz
WDW                EM
SSB      0
LB              1.00 Hz
GB       0
PC              1.40
```

^{1}H NMR of unpurified reaction mixture

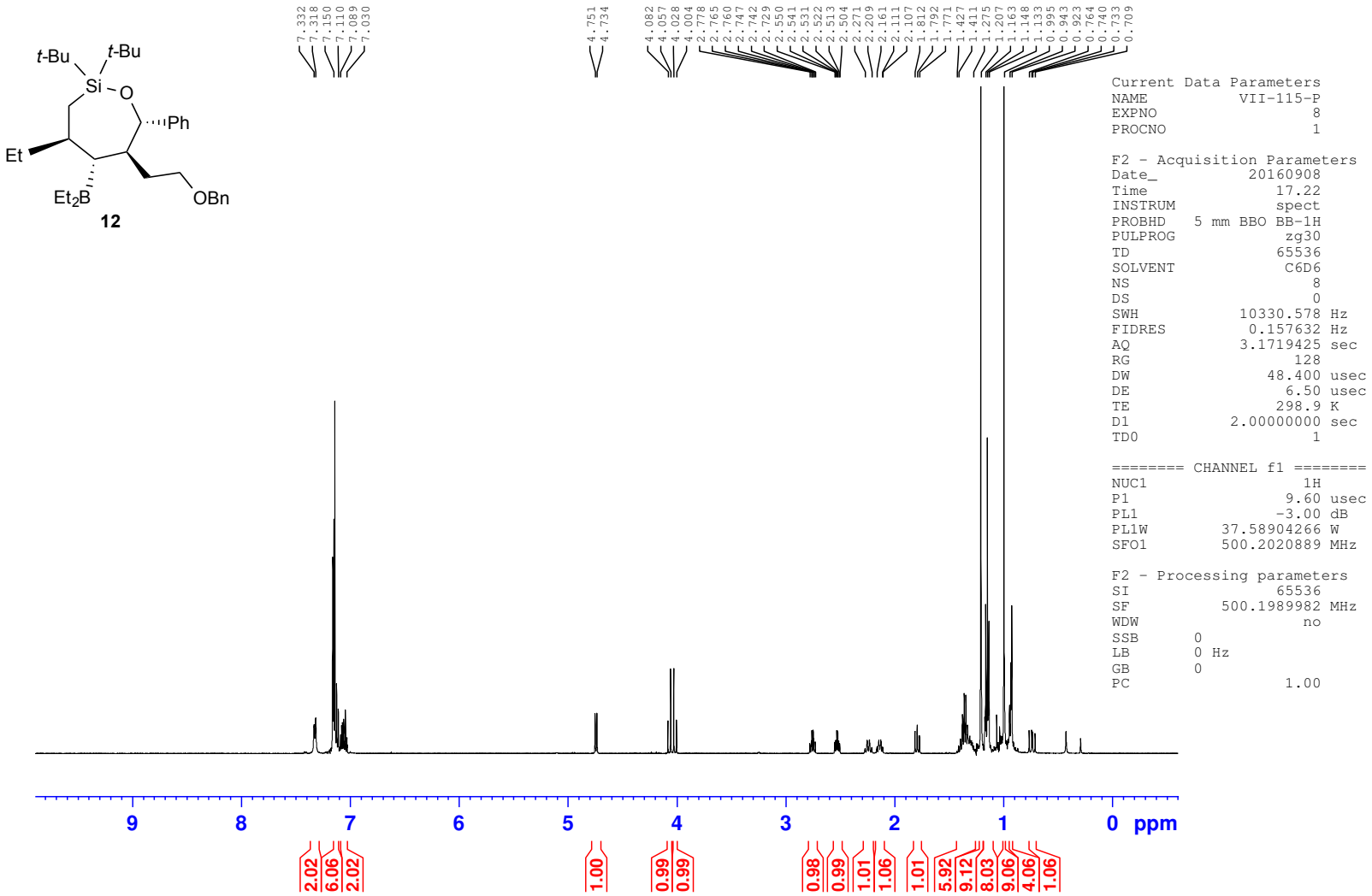


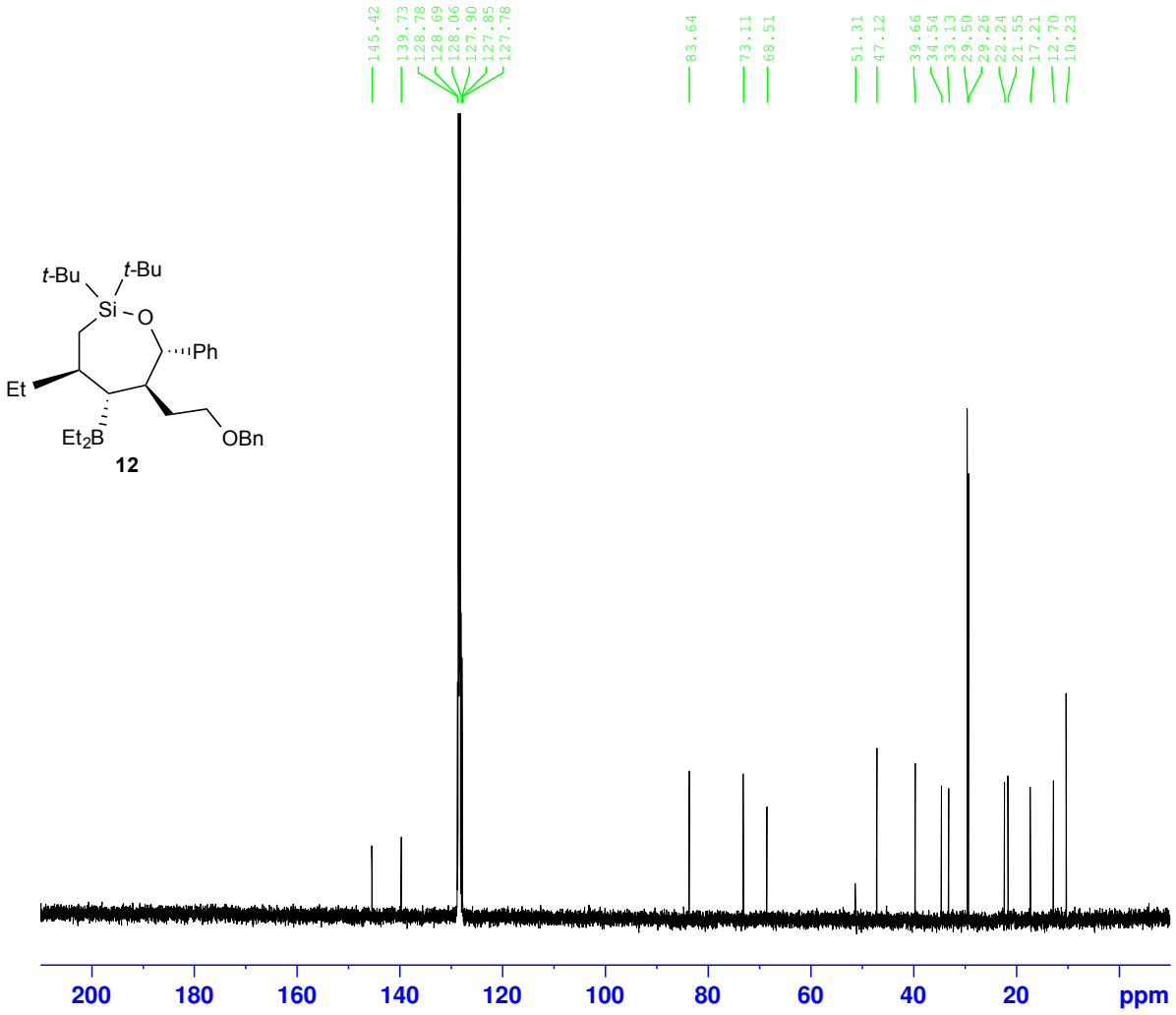

```
Current Data Parameters
NAME          VII-115-CR
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160903
Time               15.22
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     4
DS                     0
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9583745 sec
RG                   181
DW                60.400 usec
DE                 6.50 usec
TE                298.3 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.05 usec
PL1               -5.00 dB
PL1W         31.77312851 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300430 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```


t-Bu
t-Bu
Si
O
Ph
Et
Et2B
OBn
12
7.332
7.318
7.150
7.110
7.089
7.030
4.751
4.734
4.082
4.057
4.028
4.004
2.778
2.765
2.760
2.747
2.742
2.729
2.550
2.541
2.531
2.522
2.513
2.504
2.271
2.209
2.161
2.111
2.107
1.812
1.792
1.771
1.427
1.411
1.275
1.207
1.163
1.148
1.133
0.995
0.943
0.923
0.764
0.740
0.733
0.709
Current Data Parameters
NAME VII-115-P
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160908
Time 17.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 65536
SF 500.1989982 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0 ppm
2.02
6.06
2.02
1.00
0.99
0.99
0.98
0.99
1.01
1.06
1.01
5.92
9.12
8.03
9.06
4.06
1.06



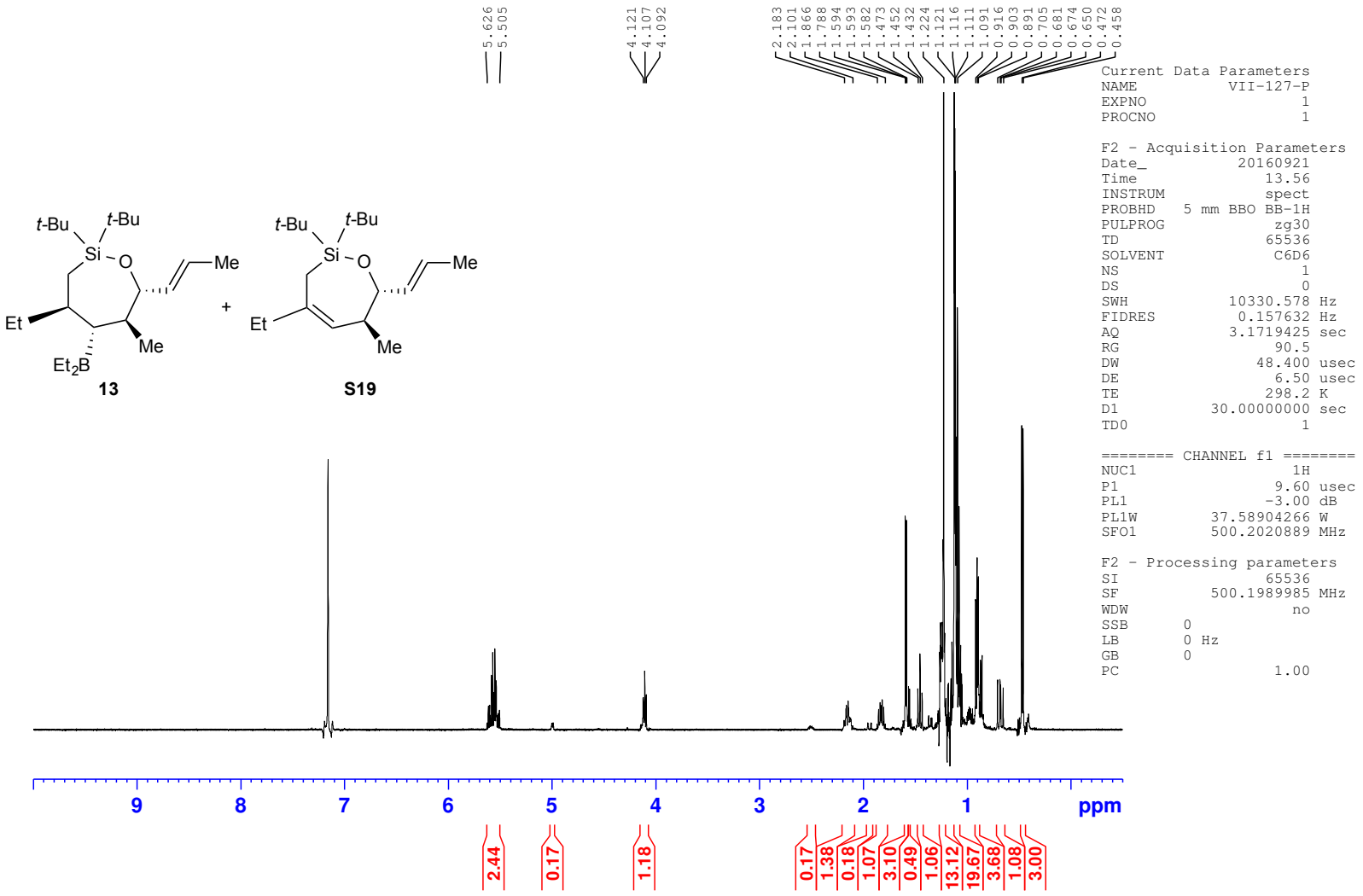

```
Current Data Parameters
NAME           VII-115-P
EXPNO                  4
PROCNO                 1

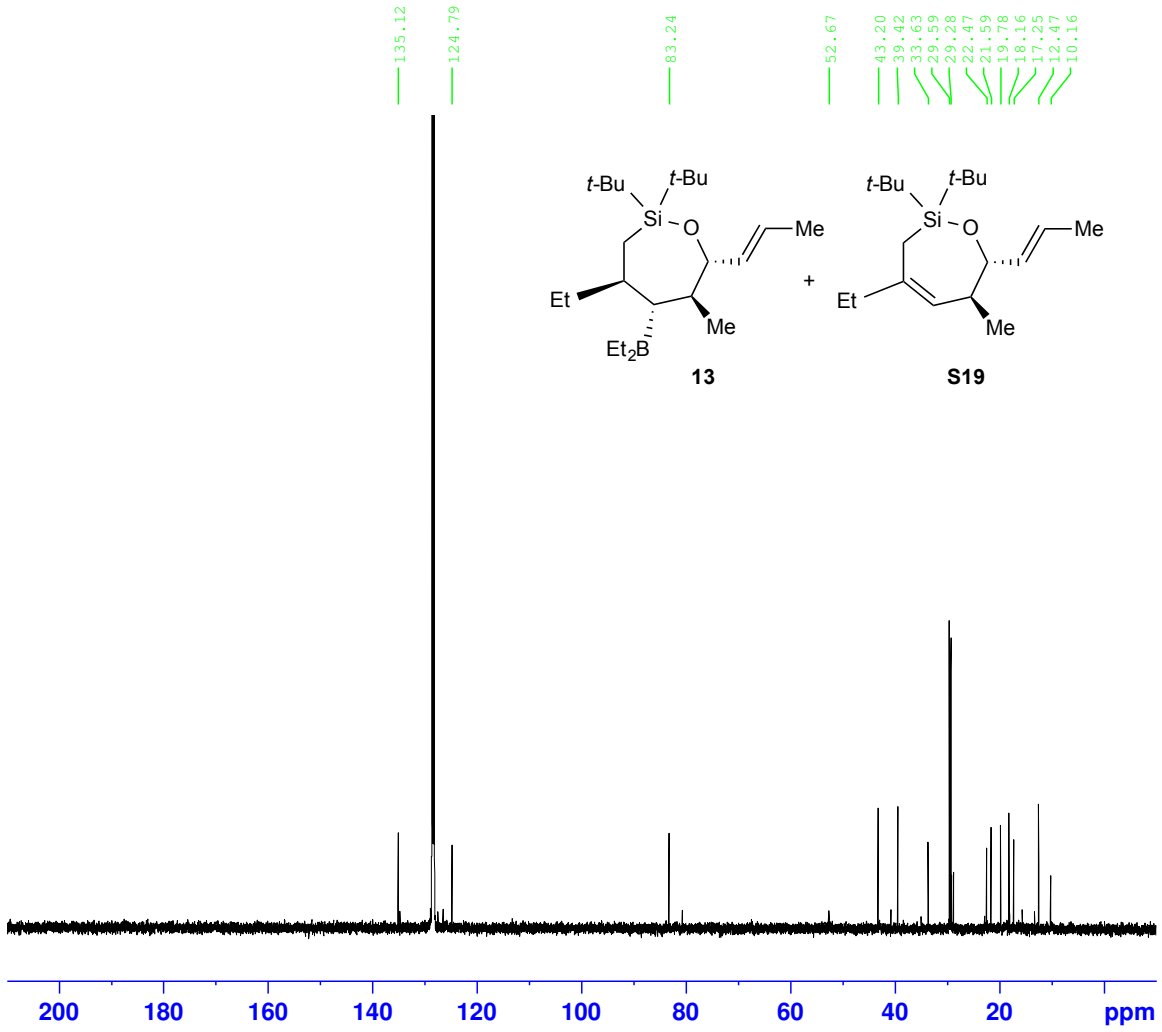
F2 - Acquisition Parameters
Date_           20160908
Time               13.11
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT             C6D6
NS                    16
DS                     2
SWH            36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9087659 sec
RG                184.65
DW                13.867 usec
DE                 18.00 usec
TE                 298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         150.9329866 MHz
NUC1                  13C
P1                 11.63 usec
PLW1         95.00000000 W

======== CHANNEL f2 ========
SFO2         600.1924008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                 32768
SF           150.9177887 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


5.626
5.505
4.121
4.107
4.092
2.183
2.101
1.866
1.788
1.594
1.593
1.582
1.473
1.452
1.432
1.224
1.121
1.116
1.111
1.091
0.916
0.903
0.891
0.705
0.681
0.674
0.650
0.472
0.458
t-Bu
t-Bu
Si
O
Me
Et
Me
Et2B
13
+
t-Bu
t-Bu
Si
O
Me
Et
Me
S19
Current Data Parameters
NAME VII-127-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160921
Time 13.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 1
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 90.5
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 30.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 65536
SF 500.1989985 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.44
0.17
1.18
0.17
1.38
0.18
1.07
3.10
0.49
1.06
13.12
19.67
3.68
1.08
3.00



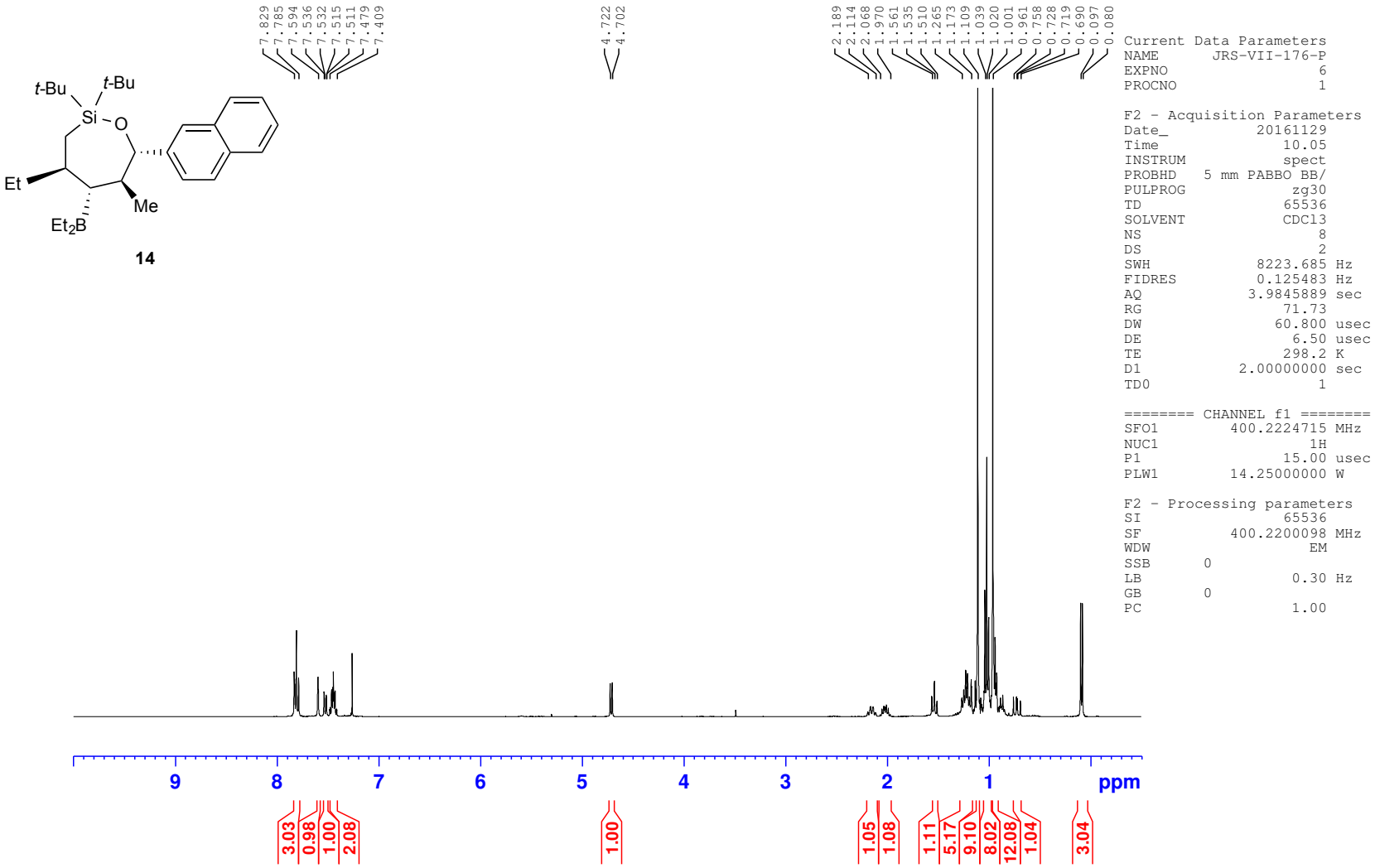

```
Current Data Parameters
NAME           VII-127-P
EXPNO                  3
PROCNO                 1

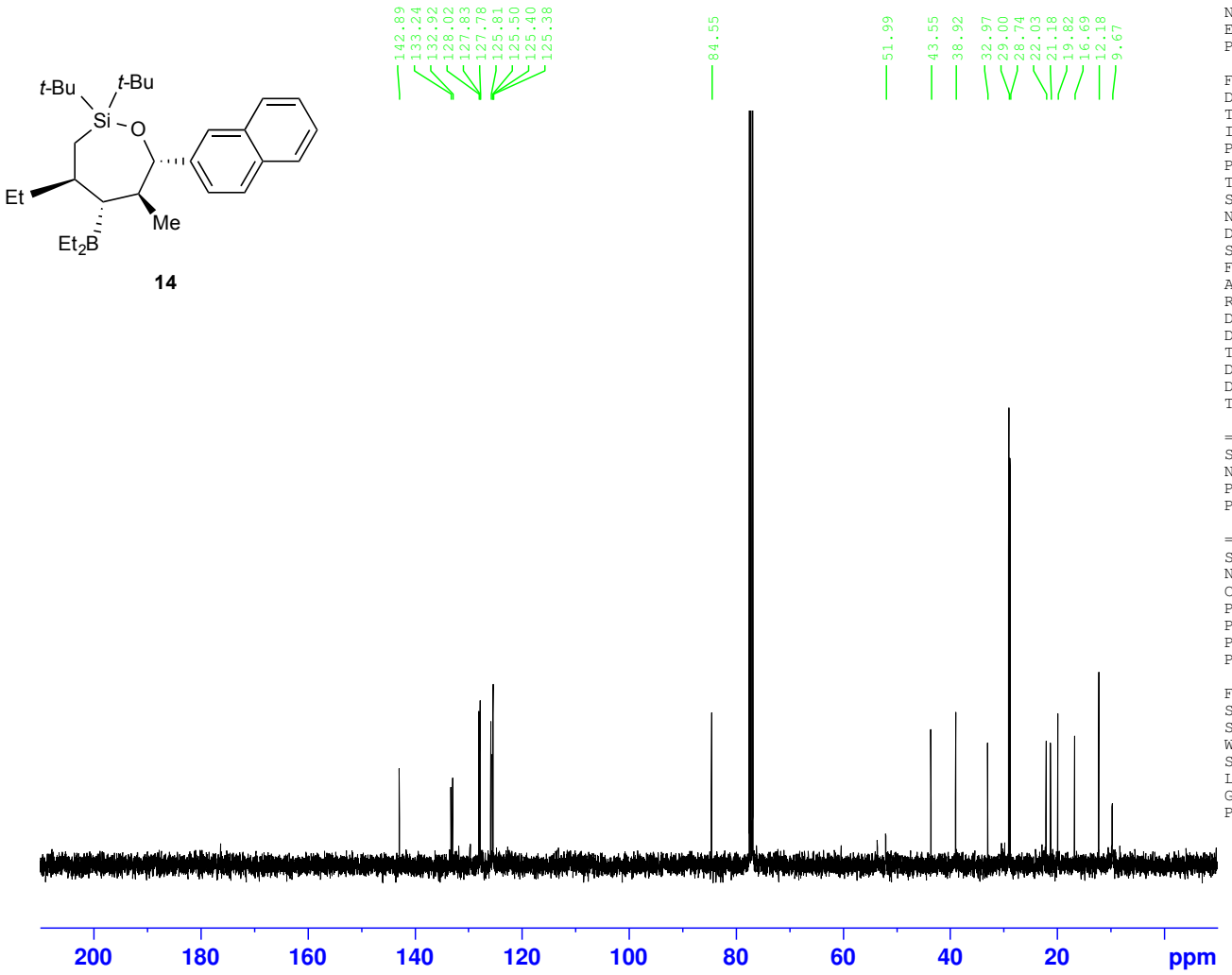
F2 - Acquisition Parameters
Date_           20160921
Time               14.03
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                   200
DS                     2
SWH            30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0911744 sec
RG                5792.6
DW                16.650 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 2.30 dB
PL1W         46.00027084 W
SFO1         125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               15.31 dB
PL13               18.31 dB
PL2W         37.58904266 W
PL12W         0.55470389 W
PL13W         0.27801058 W
SFO2         500.2010008 MHz

F2 - Processing parameters
SI                 32768
SF           125.7750500 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


7.829
7.785
7.594
7.536
7.532
7.515
7.511
7.479
7.409
4.722
4.702
2.189
2.114
2.068
1.970
1.561
1.535
1.510
1.265
1.173
1.109
1.039
1.020
1.001
0.961
0.758
0.728
0.719
0.690
0.097
0.080
t-Bu
t-Bu
Si
O
Et
Me
Et2B
14
Current Data Parameters
NAME JRS-VII-176-P
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161129
Time 10.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 71.73
DW 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.2224715 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.25000000 W
F2 - Processing parameters
SI 65536
SF 400.2200098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
3.03
0.98
1.00
2.08
1.00
1.05
1.08
1.11
5.17
9.10
8.02
12.08
1.04
3.04



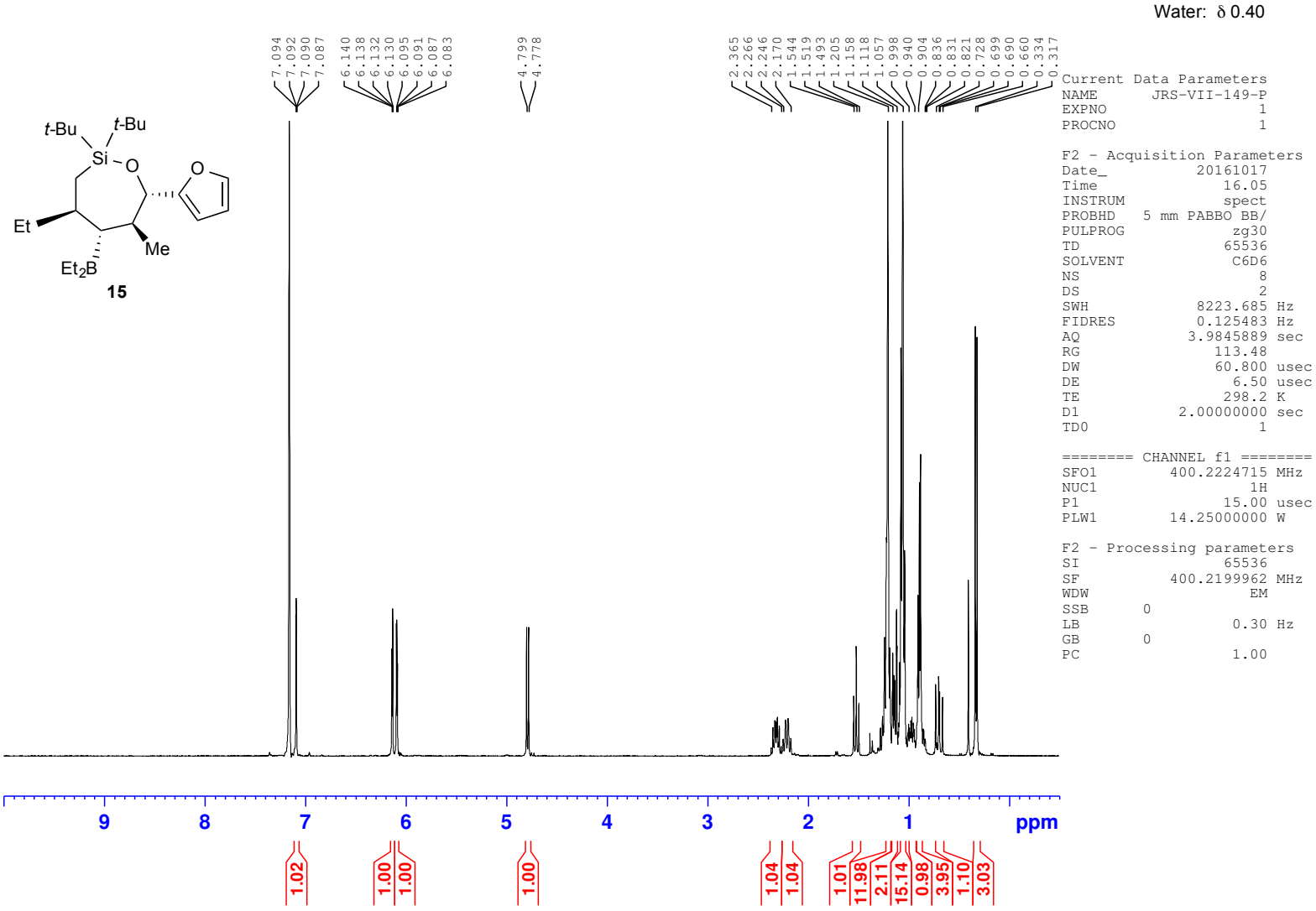

```
Current Data Parameters
NAME      JRS-VII-176-P
EXPNO                 2
PROCNO                1

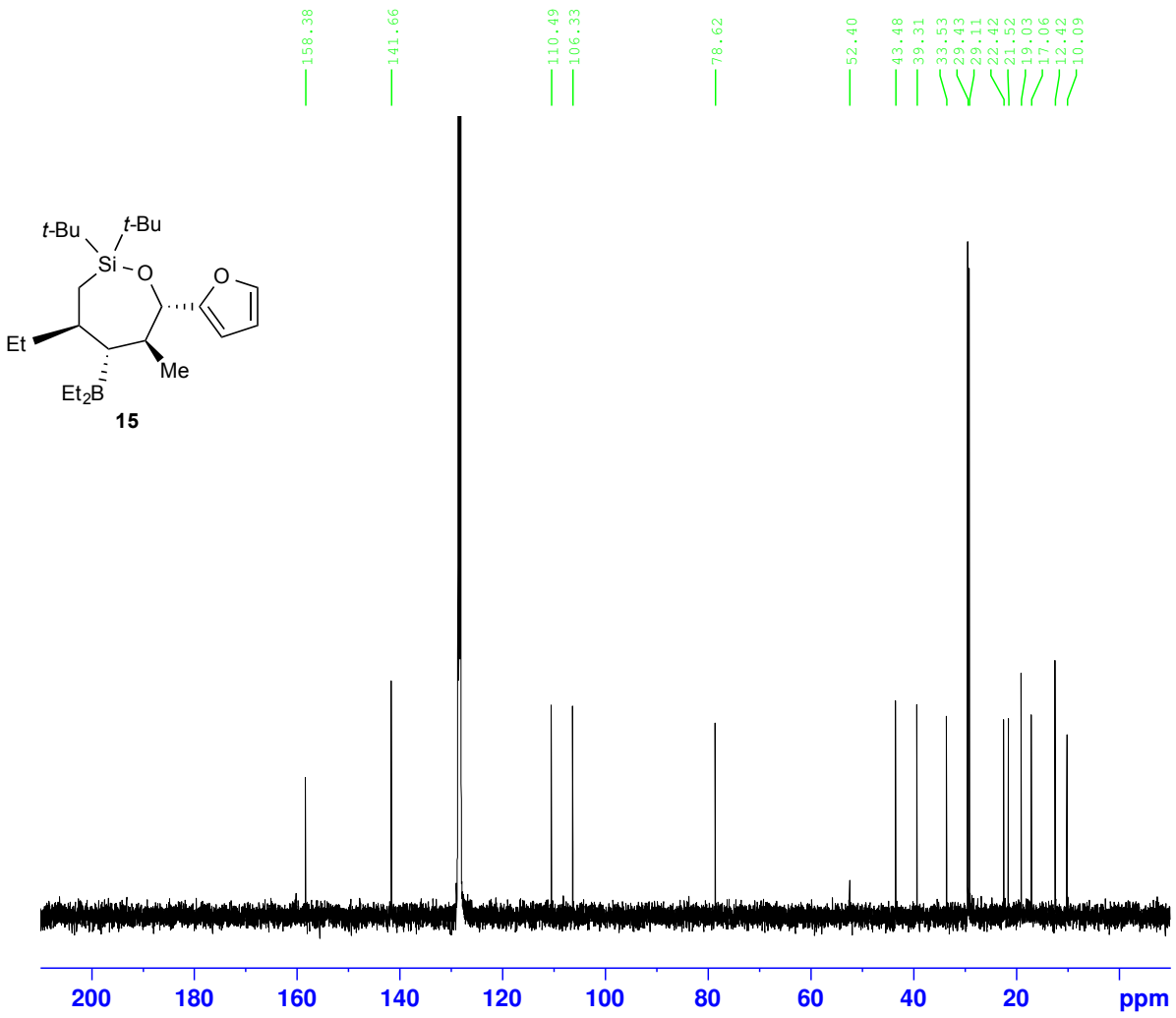
F2 - Acquisition Parameters
Date_          20161128
Time              17.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  110
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               200.67
DW               20.800 usec
DE                6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6454621 MHz
NUC1                13C
P1                10.00 usec
PLW1        57.00000000 W

======== CHANNEL f2 ========
SFO2        400.2216009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.00000000 W
PLW12        0.37926000 W
PLW13        0.30720001 W

F2 - Processing parameters
SI                32768
SF          100.6353855 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


t-Bu
t-Bu
Si
O
O
Et
Me
Et2B
15
Water: δ 0.40
7.094
7.092
7.090
7.087
6.140
6.138
6.132
6.130
6.095
6.091
6.087
6.083
4.799
4.778
2.365
2.266
2.246
2.170
1.544
1.519
1.493
1.205
1.158
1.118
1.057
0.998
0.940
0.904
0.836
0.831
0.821
0.728
0.699
0.690
0.660
0.334
0.317
Current Data Parameters
NAME JRS-VII-149-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161017
Time 16.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.48
DW 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.2224715 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.25000000 W
F2 - Processing parameters
SI 65536
SF 400.2199962 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
1.02
1.00
1.00
1.00
1.04
1.04
1.01
11.98
2.11
15.14
0.98
3.95
1.10
3.03



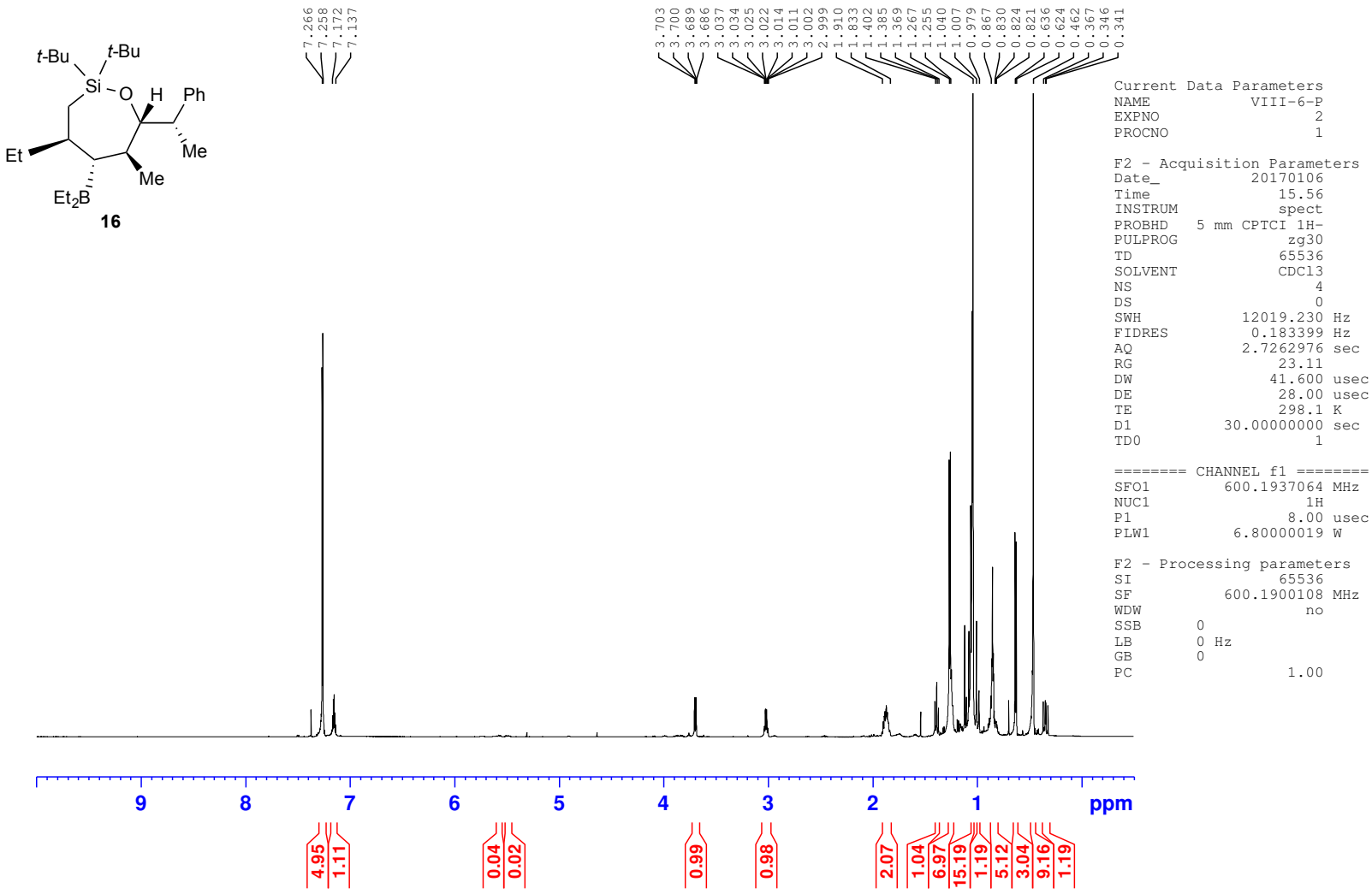

```
Current Data Parameters
NAME      JRS-VII-149-P
EXPNO                 2
PROCNO                1

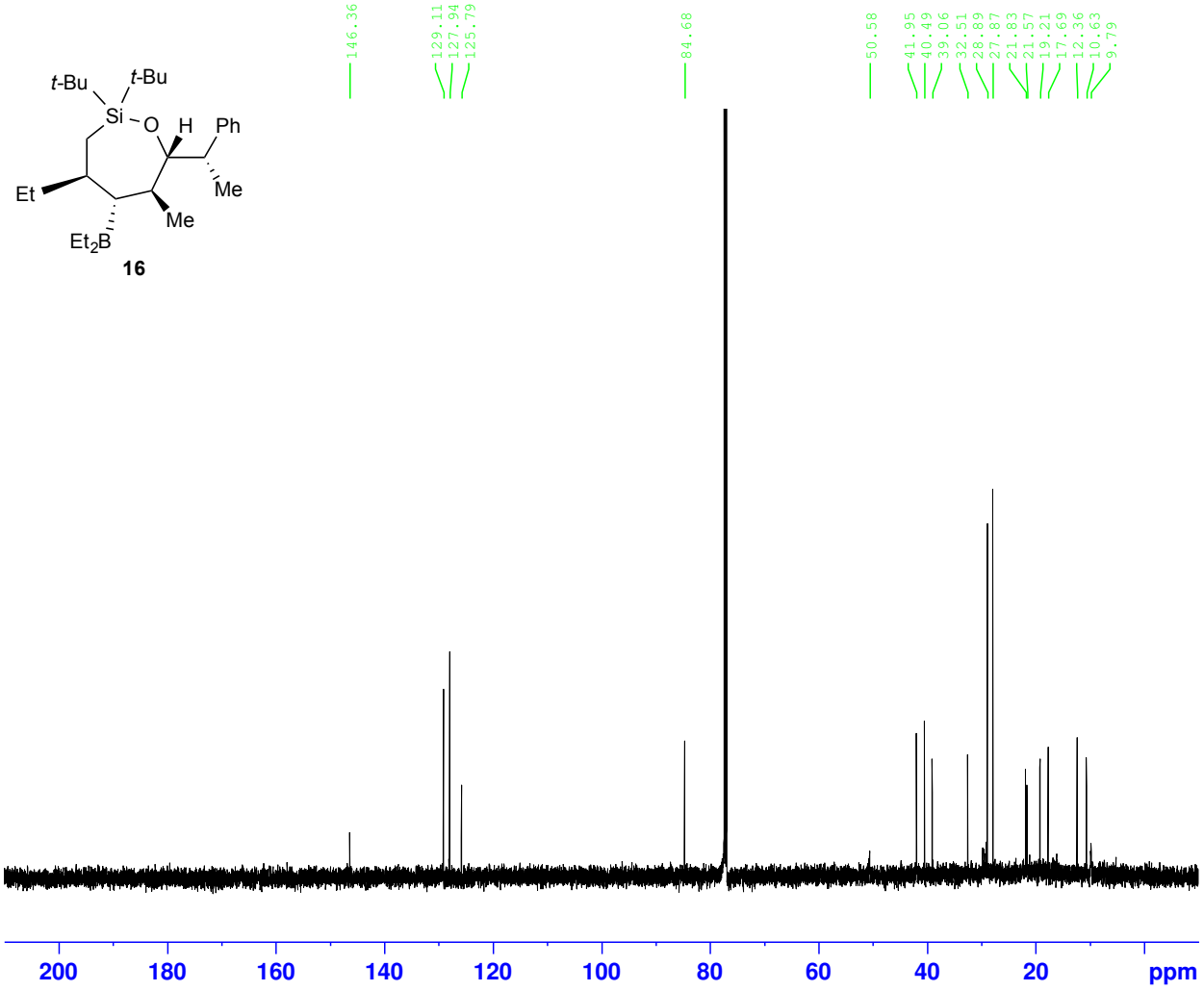
F2 - Acquisition Parameters
Date_          20161017
Time               16.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                   415
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                200.67
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6454621 MHz
NUC1                 13C
P1                10.00 usec
PLW1         57.00000000 W

======== CHANNEL f2 ========
SFO2         400.2216009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.37926000 W
PLW13         0.30720001 W

F2 - Processing parameters
SI                 32768
SF           100.6353285 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


t-Bu
t-Bu
Si
O
H
Ph
Et
Me
Me
Et2B
16
7.266
7.258
7.172
7.137
3.703
3.700
3.689
3.686
3.037
3.034
3.025
3.022
3.014
3.011
3.002
2.999
1.910
1.833
1.402
1.385
1.369
1.267
1.255
1.040
1.007
0.979
0.867
0.830
0.824
0.821
0.636
0.624
0.462
0.367
0.346
0.341
Current Data Parameters
NAME VIII-6-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170106
Time 15.56
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 23.11
DW 41.600 usec
DE 28.00 usec
TE 298.1 K
D1 30.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1900108 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
4.95
1.11
0.04
0.02
0.99
0.98
2.07
1.04
6.97
15.19
1.19
5.12
3.04
9.16
1.19



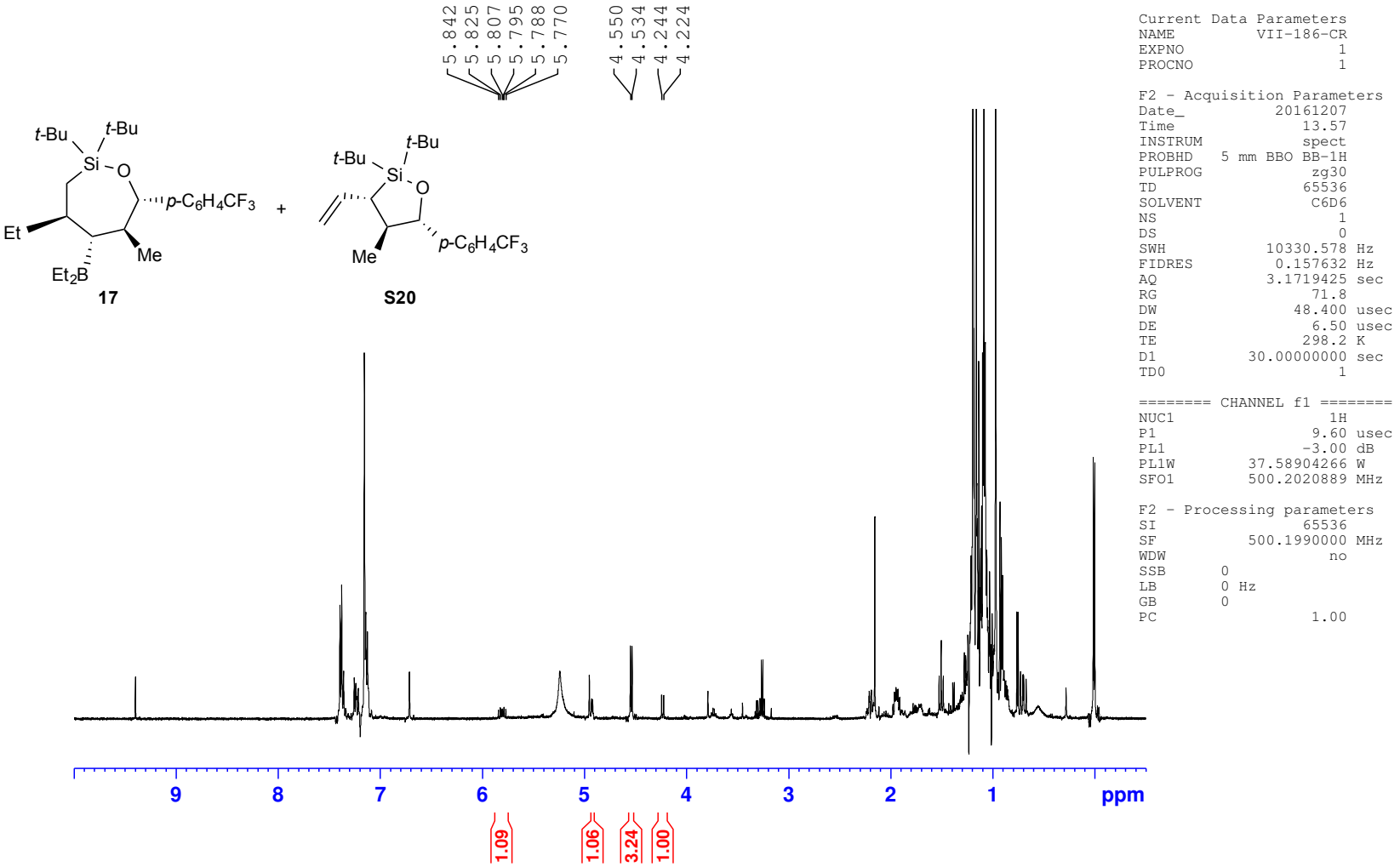

```
Current Data Parameters
NAME            VIII-6-P
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170106
Time               16.10
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG               184.65
DW               13.867 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                 13C
P1                11.63 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         6.80000019 W
PLW12        0.06800000 W
PLW13        0.04352000 W

F2 - Processing parameters
SI                32768
SF          150.9178748 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

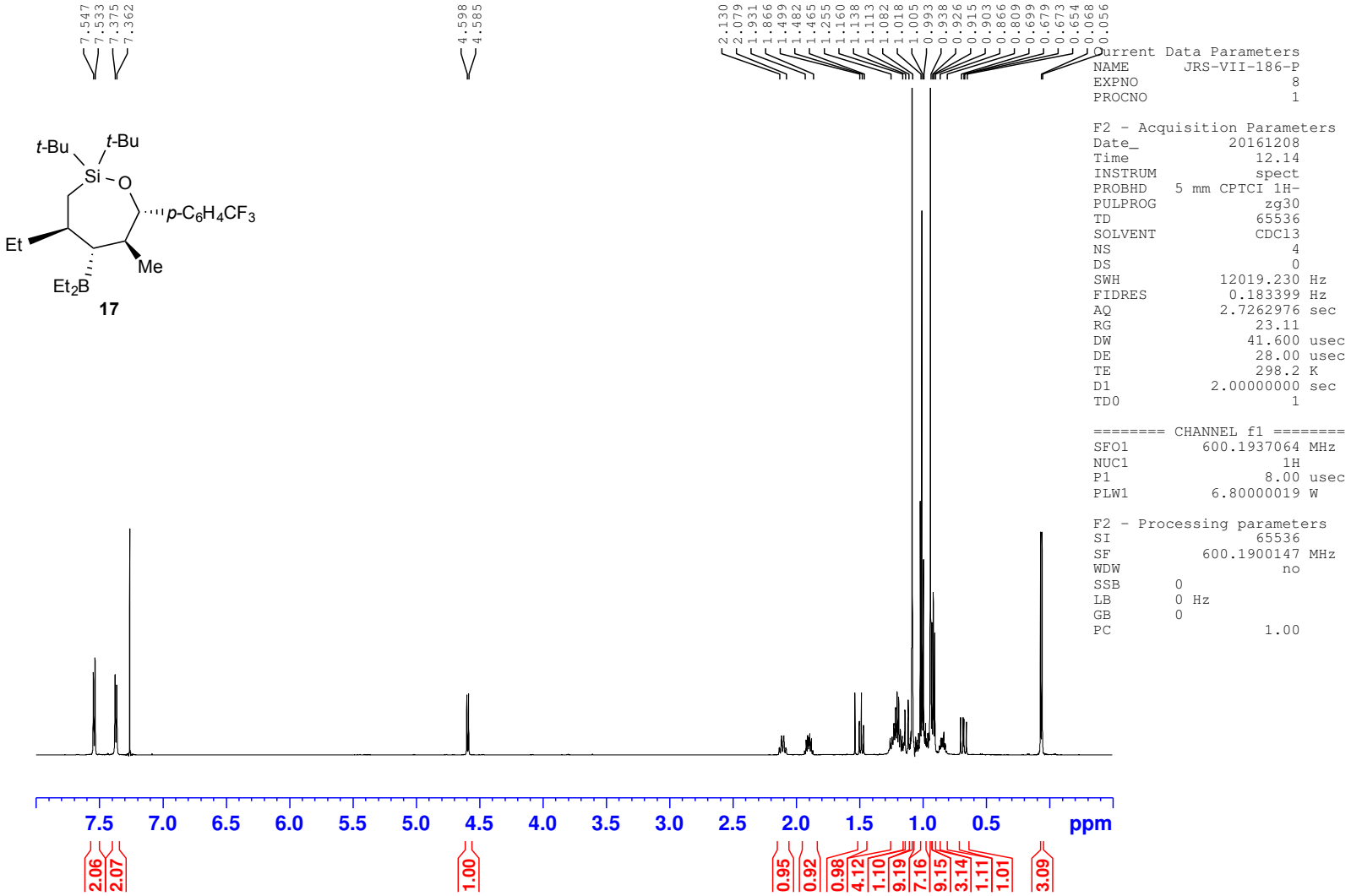


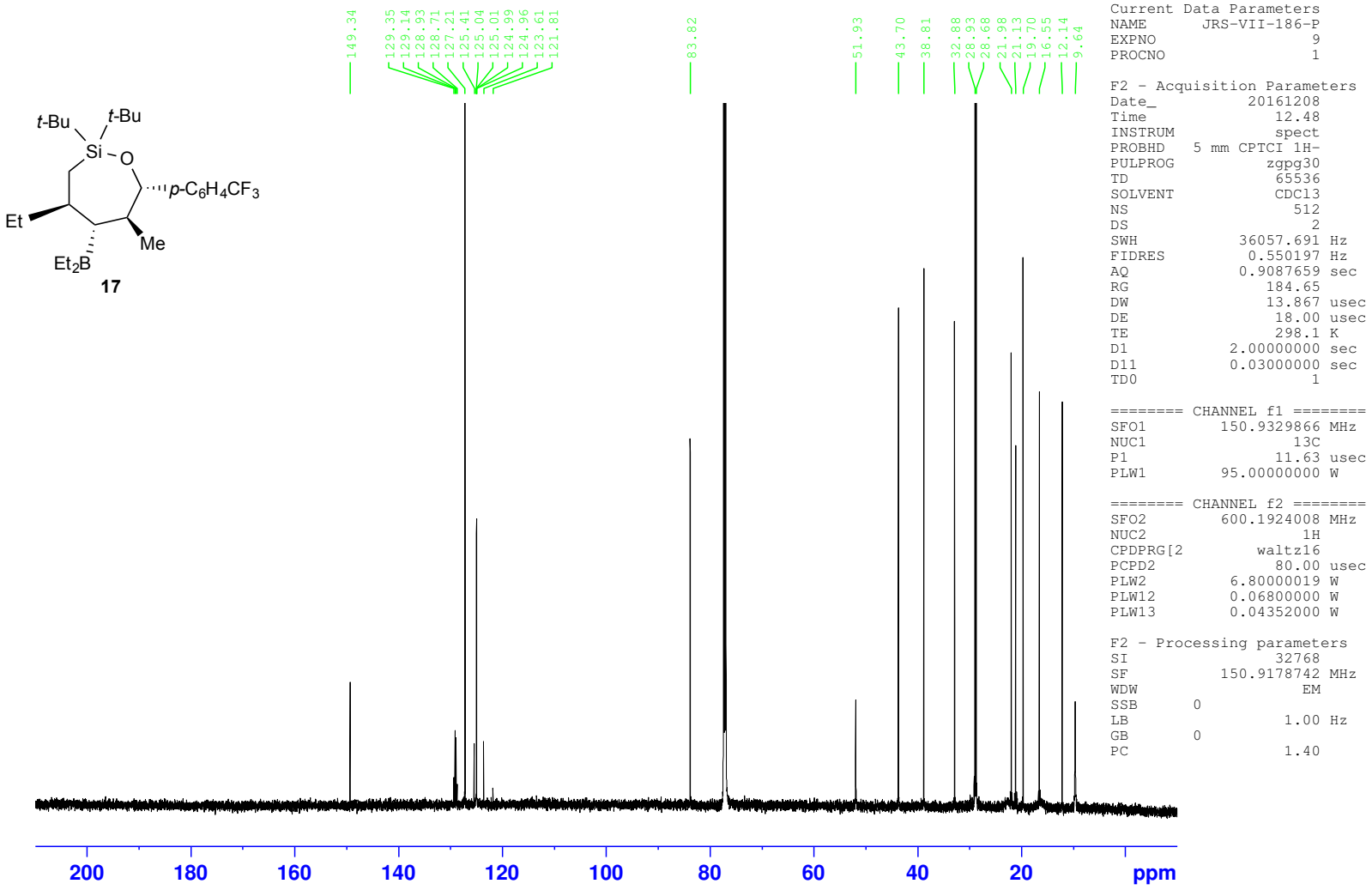

```
Current Data Parameters
NAME          VII-186-CR
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161207
Time               13.57
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     1
DS                     0
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719425 sec
RG                  71.8
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.60 usec
PL1                -3.00 dB
PL1W         37.58904266 W
SFO1         500.2020889 MHz

F2 - Processing parameters
SI                 65536
SF           500.1990000 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```


7.547
7.533
7.375
7.362
4.598
4.585
2.130
2.079
1.931
1.866
1.499
1.482
1.465
1.255
1.160
1.138
1.113
1.082
1.018
1.005
0.993
0.938
0.926
0.915
0.903
0.866
0.809
0.699
0.679
0.673
0.654
0.068
0.056
t-Bu
t-Bu
Si
O
p-C6H4CF3
Et
Me
Et2B
17
Current Data Parameters
NAME JRS-VII-186-P
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161208
Time 12.14
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 23.11
DW 41.600 usec
DE 28.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1900147 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.06
2.07
1.00
0.95
0.92
0.98
4.12
1.10
9.19
7.16
9.15
3.14
1.11
1.01
3.09



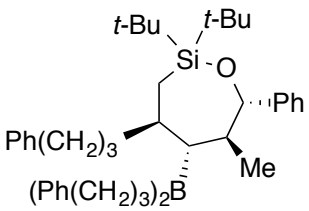

```
Current Data Parameters
NAME      JRS-VII-186-P
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20161208
Time              12.48
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG               184.65
DW               13.867 usec
DE                18.00 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

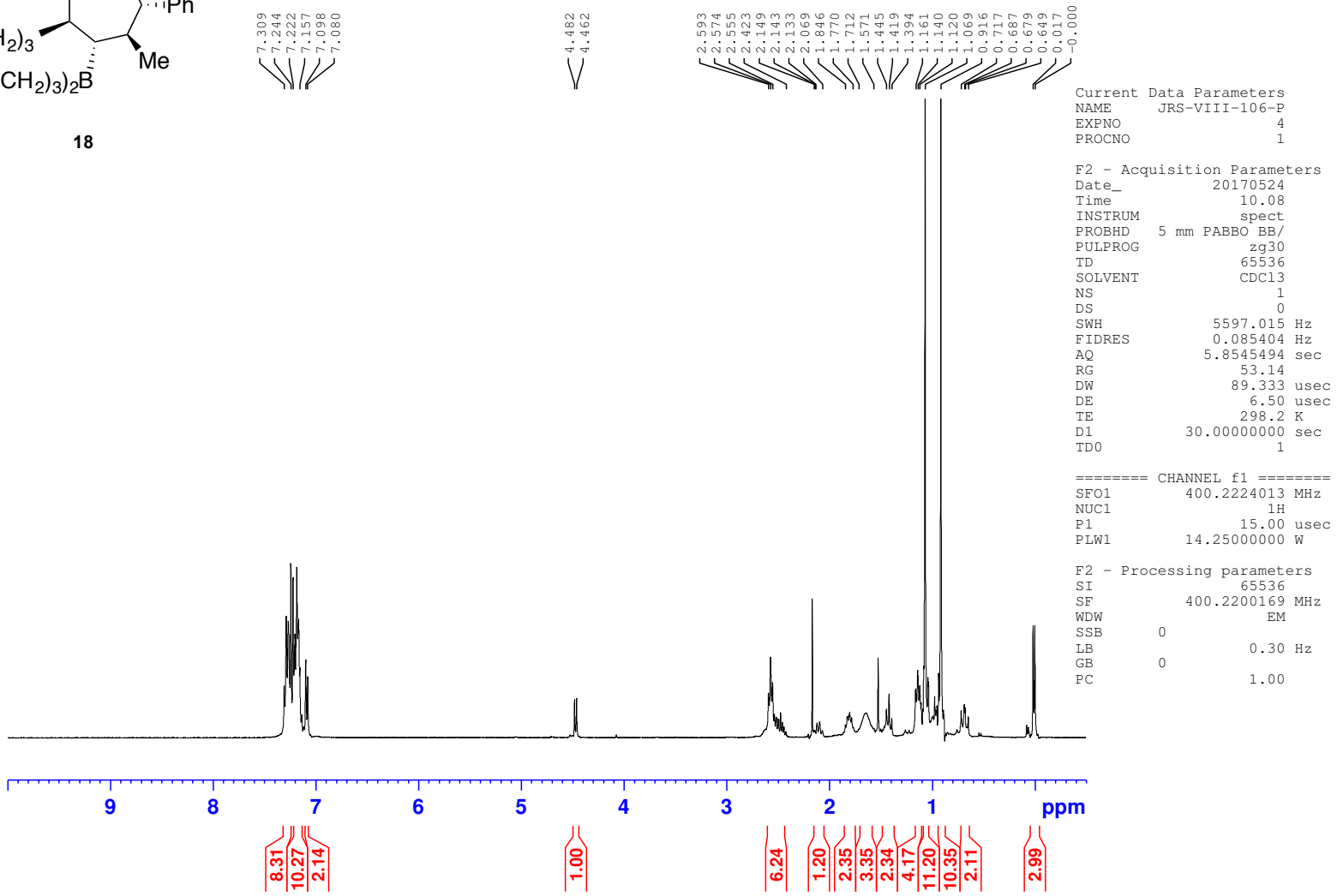
======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                13C
P1                11.63 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                 32768
SF          150.9178742 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```



18

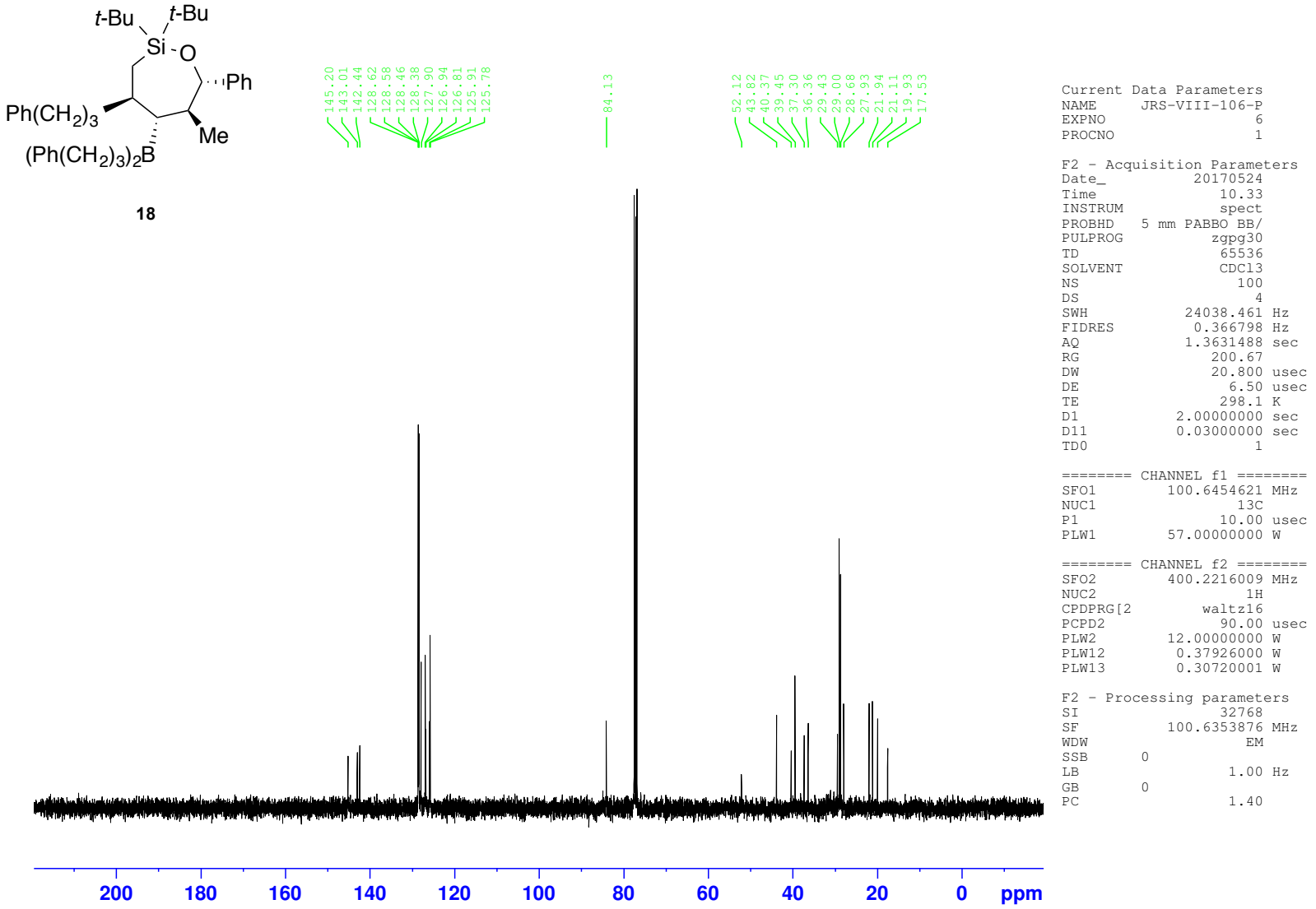



```
Current Data Parameters
NAME      JRS-VIII-106-P
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170524
Time               10.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     1
DS                     0
SWH             5597.015 Hz
FIDRES          0.085404 Hz
AQ             5.8545494 sec
RG                 53.14
DW                89.333 usec
DE                  6.50 usec
TE                 298.2 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.2224013 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         14.25000000 W

F2 - Processing parameters
SI                 65536
SF           400.2200169 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



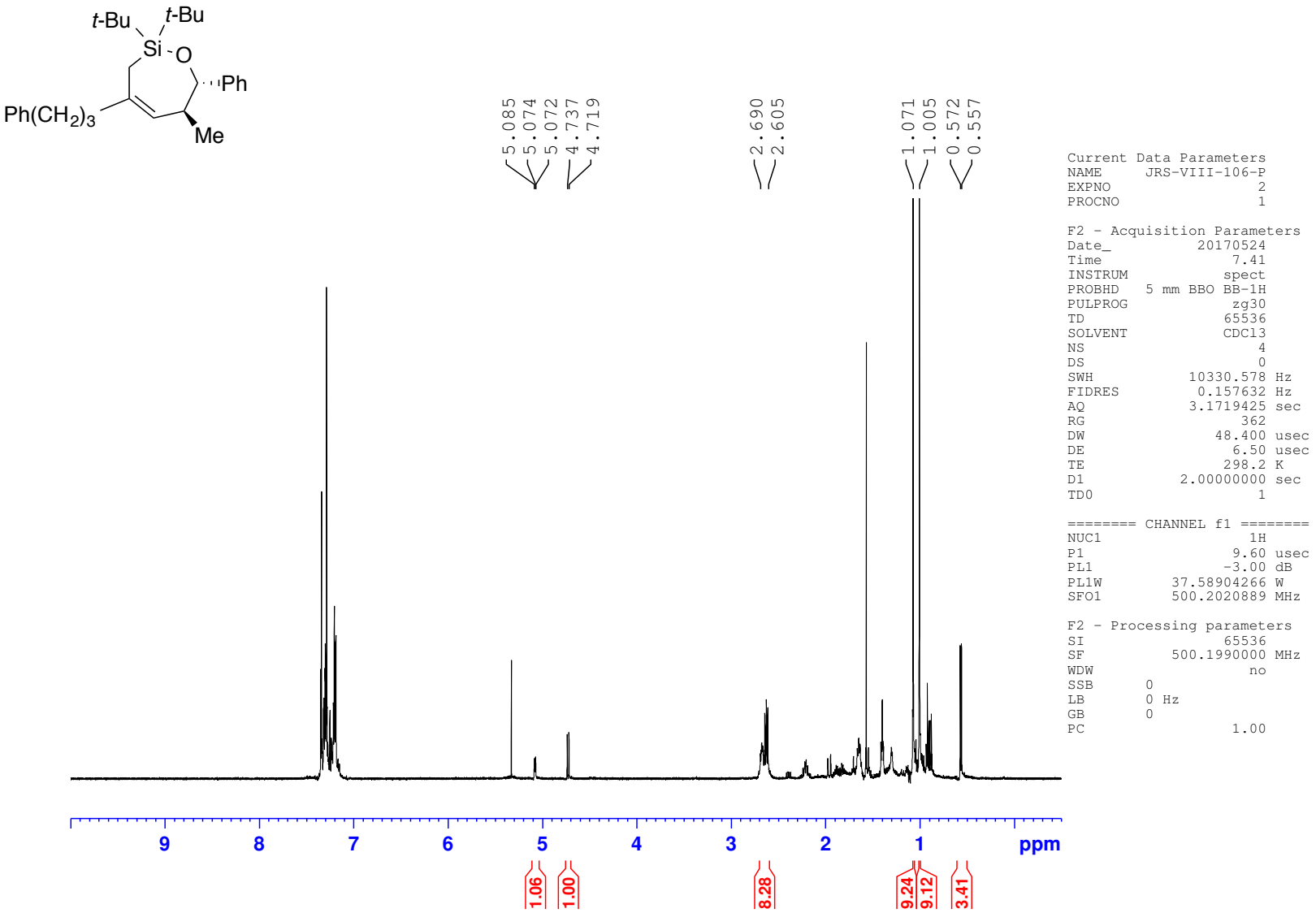

```
Current Data Parameters
NAME      JRS-VIII-106-P
EXPNO                   6
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170524
Time               10.33
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               200.67
DW               20.800 usec
DE                6.50 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6454621 MHz
NUC1                13C
P1                10.00 usec
PLW1         57.00000000 W

======== CHANNEL f2 ========
SFO2         400.2216009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.37926000 W
PLW13         0.30720001 W

F2 - Processing parameters
SI                 32768
SF           100.6353876 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

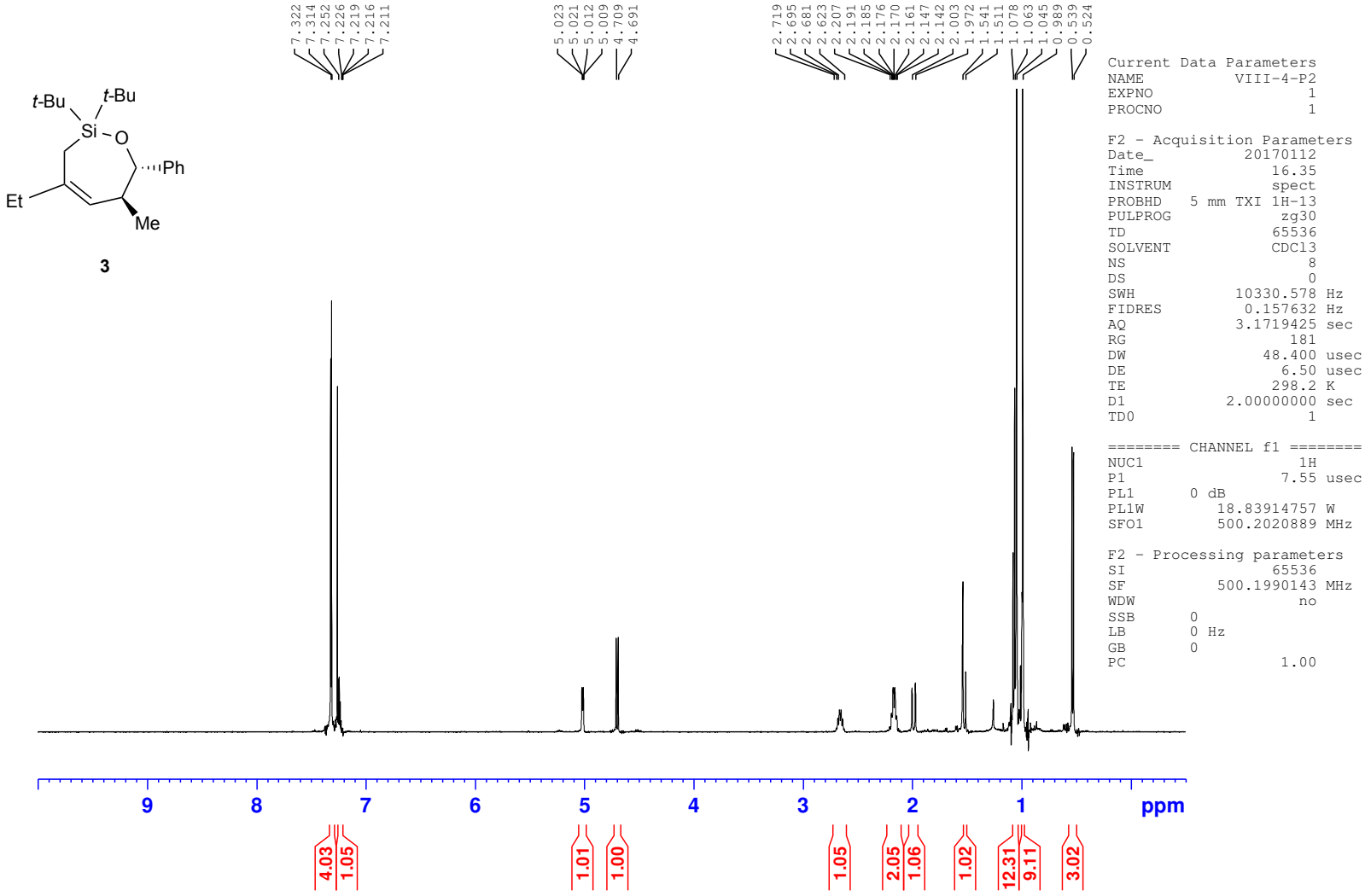


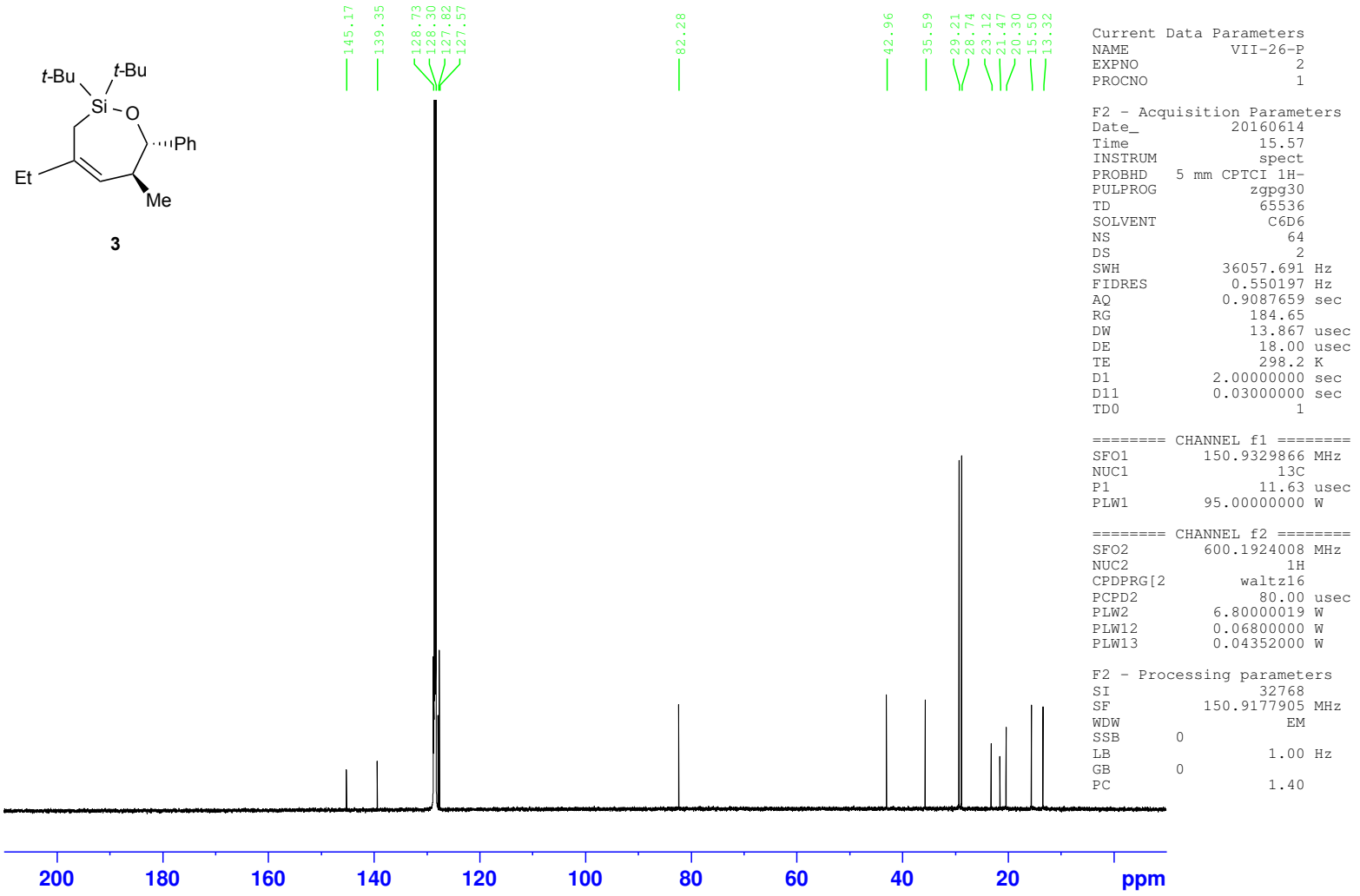

```
Current Data Parameters
NAME      JRS-VIII-106-P
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170524
Time               7.41
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    0
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719425 sec
RG                  362
DW               48.400 usec
DE                6.50 usec
TE                298.2 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.60 usec
PL1               -3.00 dB
PL1W        37.58904266 W
SFO1        500.2020889 MHz

F2 - Processing parameters
SI                65536
SF          500.1990000 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                1.00
```


t-Bu
t-Bu
Si
O
Ph
Et
Me
3
7.322
7.314
7.252
7.226
7.219
7.216
7.211
5.023
5.021
5.012
5.009
4.709
4.691
2.719
2.695
2.681
2.623
2.207
2.191
2.185
2.176
2.170
2.161
2.147
2.142
2.003
1.972
1.541
1.511
1.078
1.063
1.045
0.989
0.539
0.524
Current Data Parameters
NAME VIII-4-P2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170112
Time 16.35
INSTRUM spect
PROBHD 5 mm TXI 1H-13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.55 usec
PL1 0 dB
PL1W 18.83914757 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 65536
SF 500.1990143 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
4.03
1.05
1.01
1.00
1.05
2.05
1.06
1.02
12.31
9.11
3.02



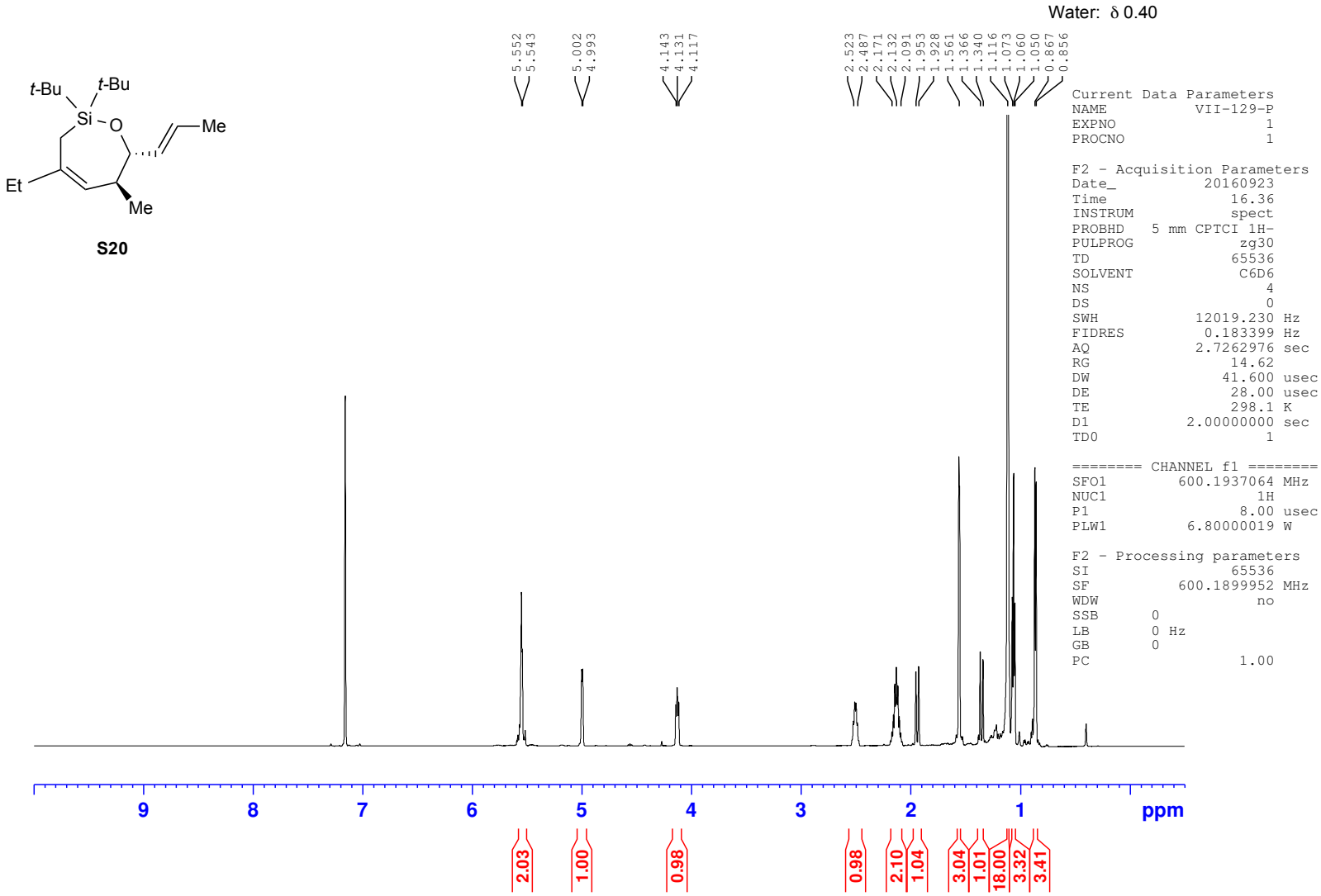

```
Current Data Parameters
NAME            VII-26-P
EXPNO                  2
PROCNO                 1

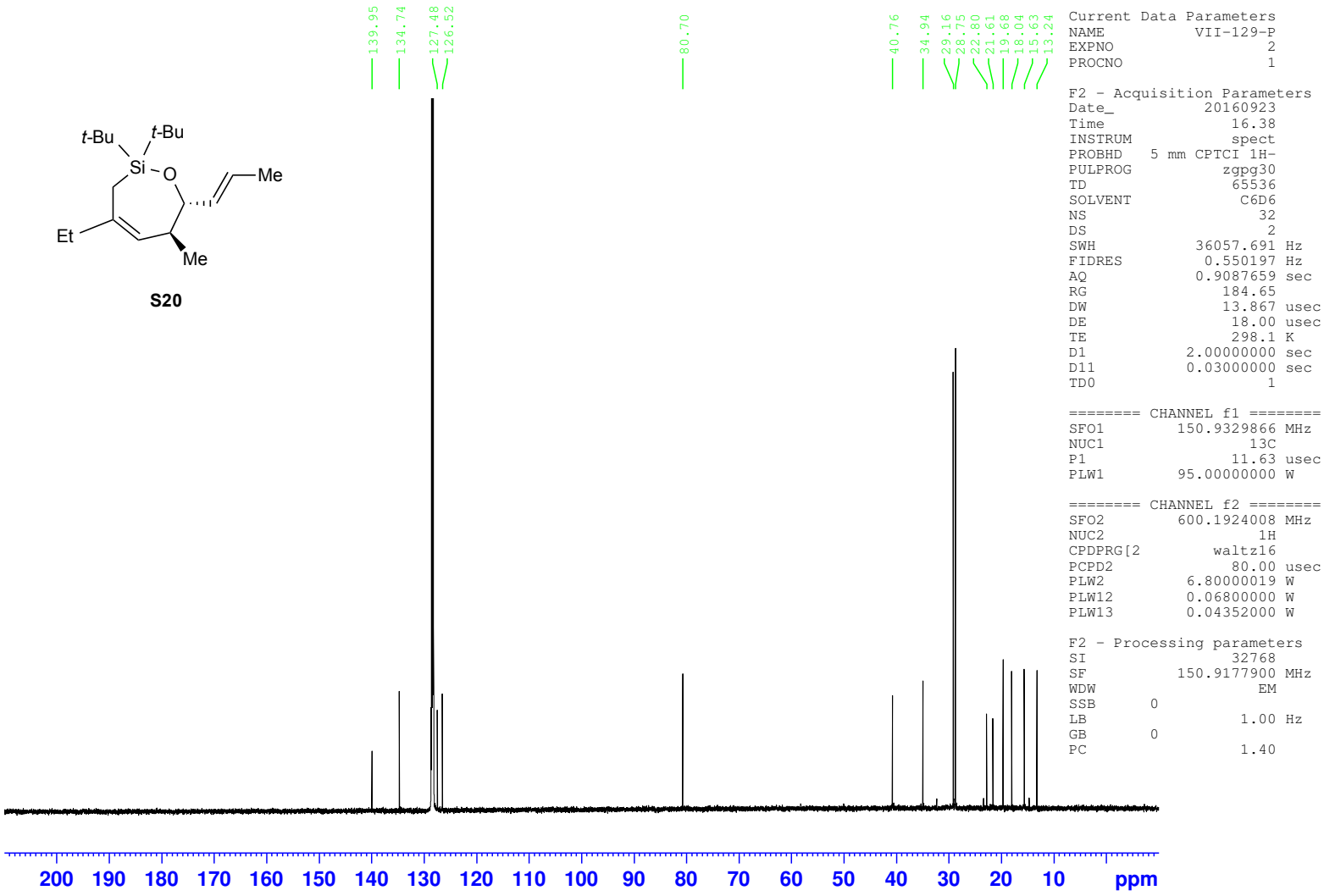
F2 - Acquisition Parameters
Date_           20160614
Time               15.57
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT              C6D6
NS                     64
DS                      2
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                184.65
DW                13.867 usec
DE                 18.00 usec
TE                 298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

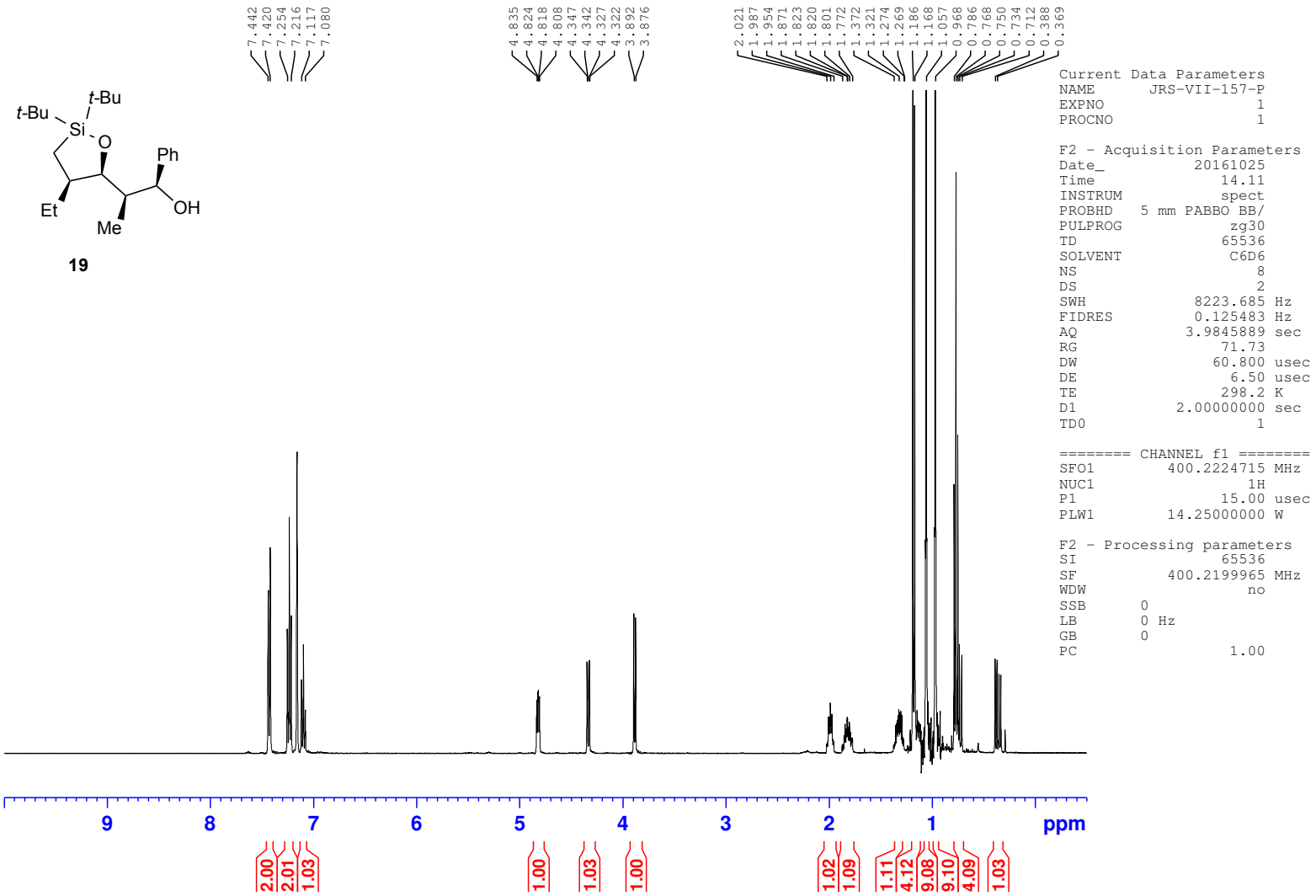
======== CHANNEL f1 ========
SFO1         150.9329866 MHz
NUC1                  13C
P1                 11.63 usec
PLW1         95.00000000 W

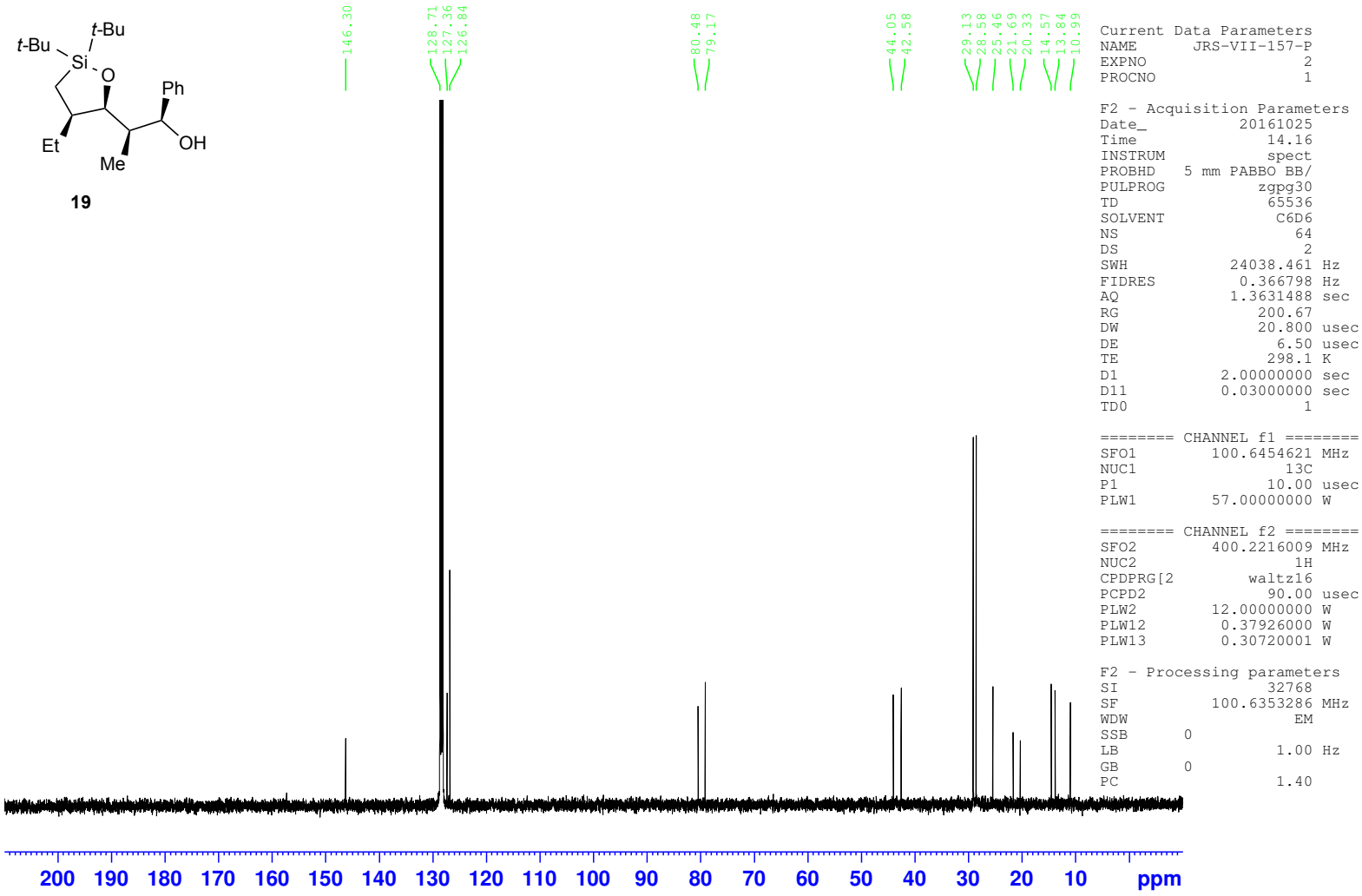
======== CHANNEL f2 ========
SFO2         600.1924008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

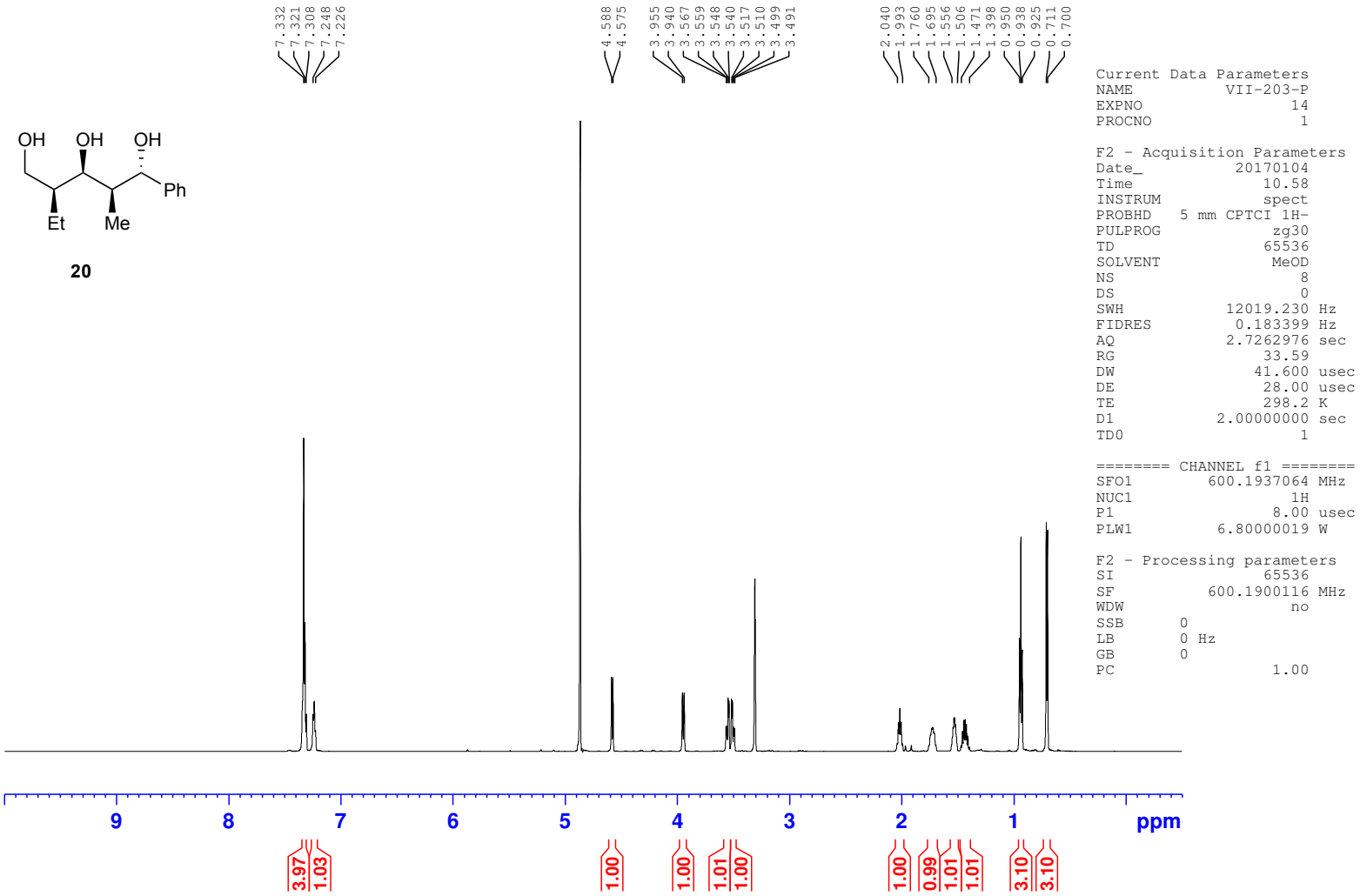
F2 - Processing parameters
SI                 32768
SF           150.9177905 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

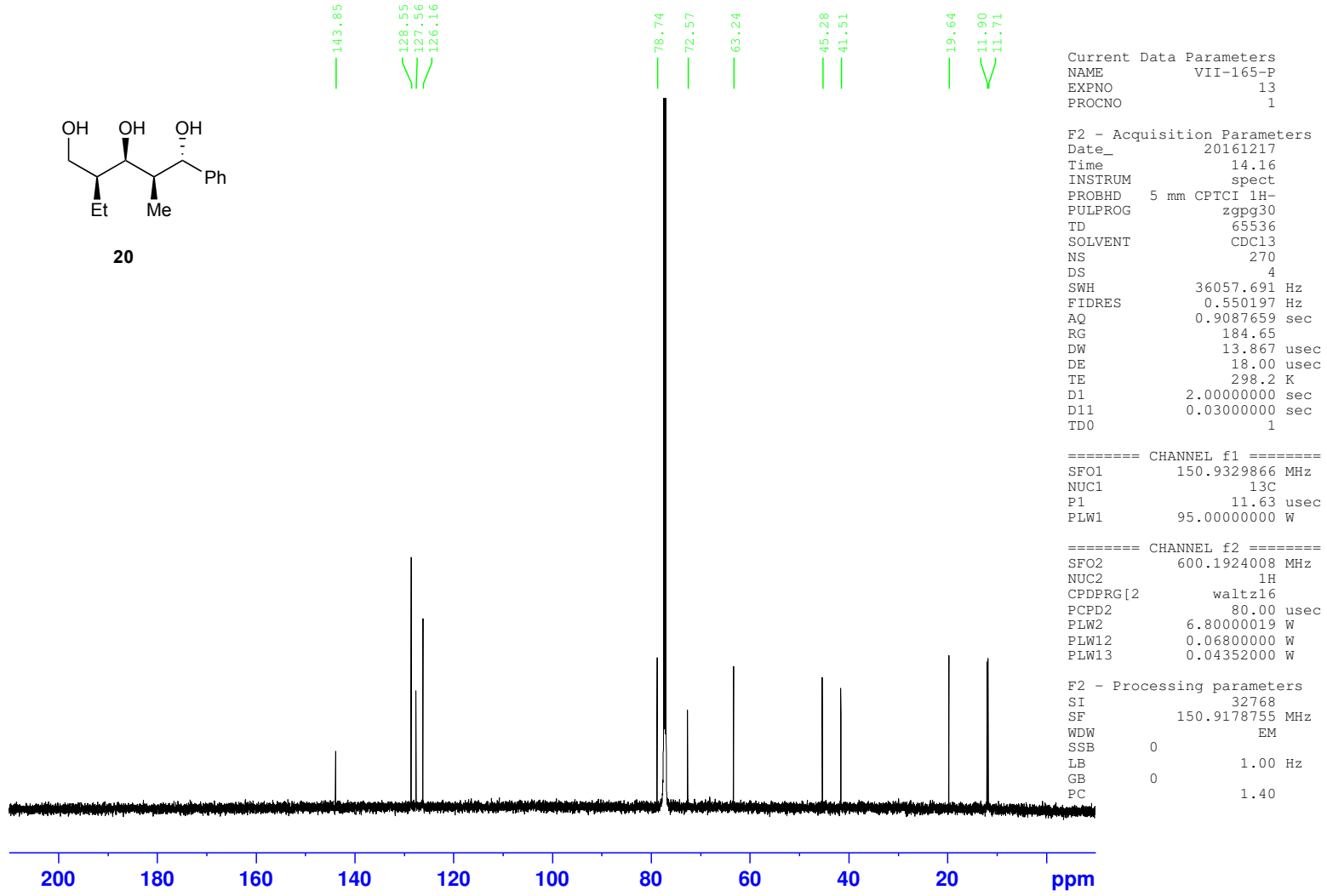

t-Bu
t-Bu
Si
O
Me
Et
Me
S20
Water: δ 0.40
5.552
5.543
5.002
4.993
4.143
4.131
4.117
2.523
2.487
2.171
2.132
2.091
1.953
1.928
1.561
1.366
1.340
1.116
1.073
1.060
1.050
0.867
0.856
Current Data Parameters
NAME VII-129-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160923
Time 16.36
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 4
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 14.62
DW 41.600 usec
DE 28.00 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1899952 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.03
1.00
0.98
0.98
2.10
1.04
3.04
1.01
18.00
3.32
3.41

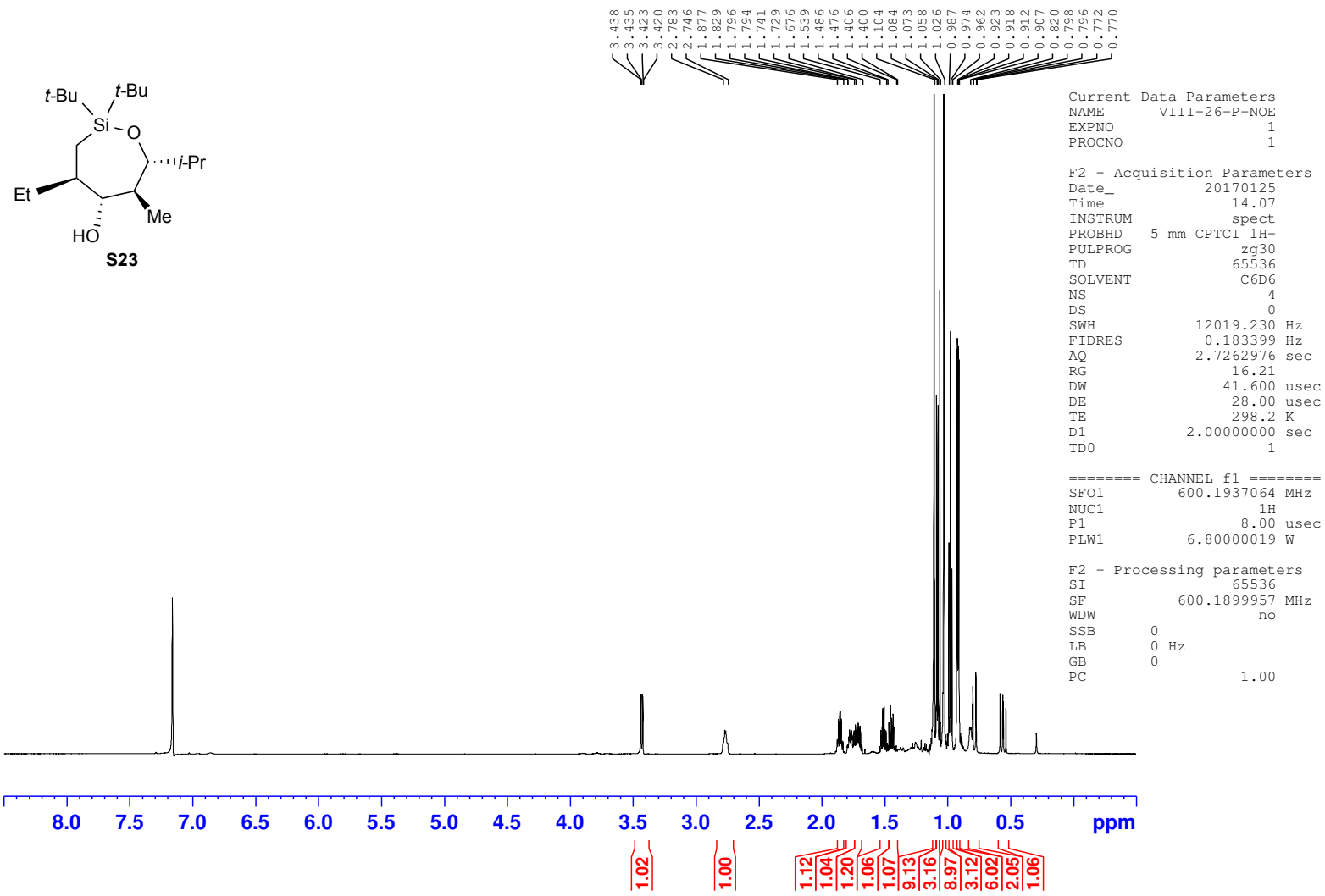

139.95
134.74
127.48
126.52
80.70
40.76
34.94
29.16
28.75
22.80
21.61
19.68
18.04
15.63
13.24
t-Bu
t-Bu
Si
O
Me
Et
Me
S20
Current Data Parameters
NAME VII-129-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160923
Time 16.38
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 32
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 184.65
DW 13.867 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 150.9329866 MHz
NUC1 13C
P1 11.63 usec
PLW1 95.00000000 W
======== CHANNEL f2 ========
SFO2 600.1924008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 6.80000019 W
PLW12 0.06800000 W
PLW13 0.04352000 W
F2 - Processing parameters
SI 32768
SF 150.9177900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

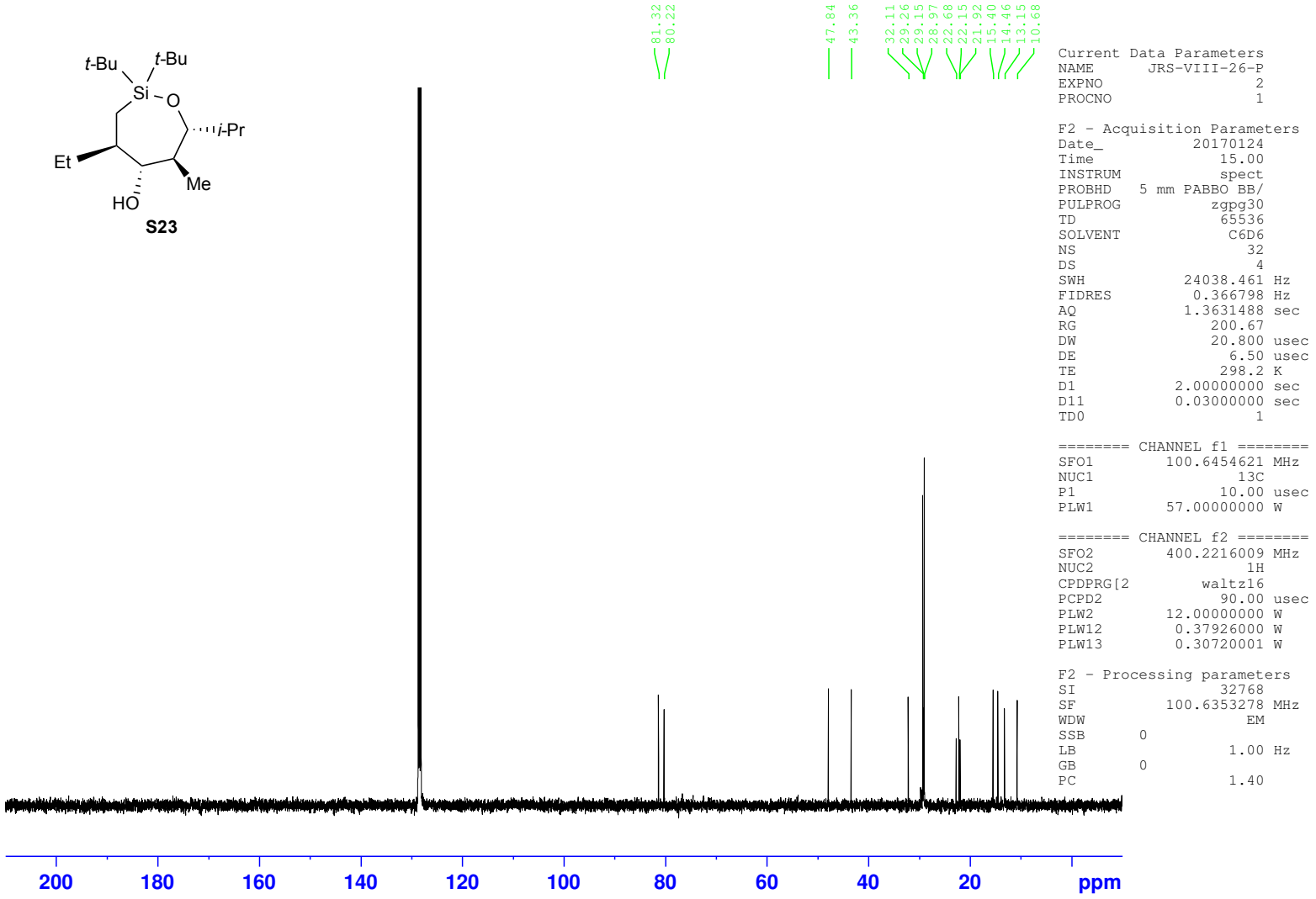

7.442
7.420
7.254
7.216
7.117
7.080
4.835
4.824
4.818
4.808
4.347
4.342
4.327
4.322
3.892
3.876
2.021
1.987
1.954
1.871
1.823
1.820
1.801
1.772
1.372
1.321
1.274
1.269
1.186
1.168
1.057
0.968
0.786
0.768
0.750
0.734
0.712
0.388
0.369
t-Bu
t-Bu
Si
O
Ph
Et
OH
Me
19
Current Data Parameters
NAME JRS-VII-157-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 14.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 71.73
DW 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.2224715 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.25000000 W
F2 - Processing parameters
SI 65536
SF 400.2199965 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.00
2.01
1.03
1.00
1.03
1.00
1.02
1.09
1.11
4.12
9.08
9.10
4.09
1.03

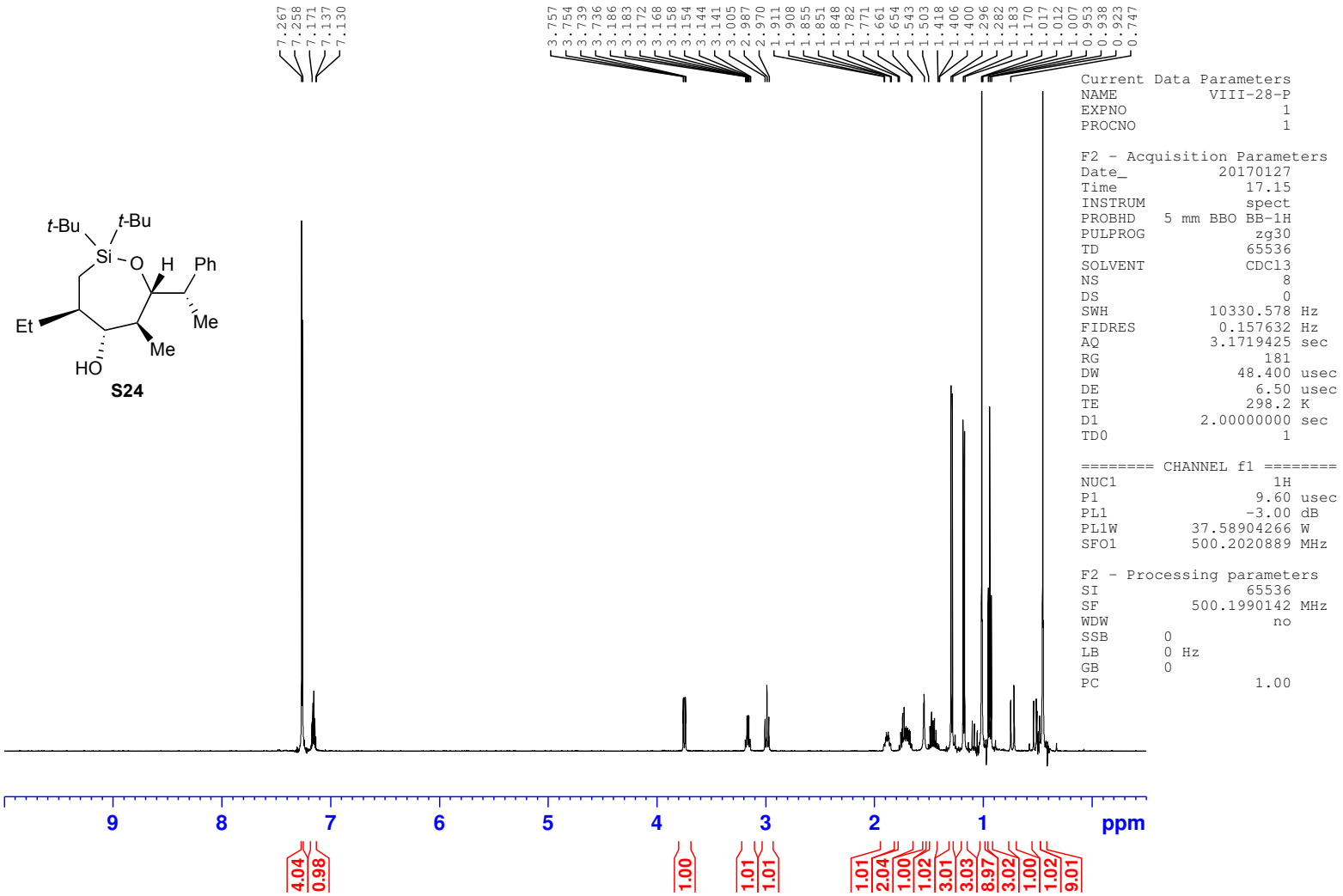

t-Bu
t-Bu
Si
O
Ph
Et
Me
OH
19
146.30
128.71
127.36
126.84
80.48
79.17
44.05
42.58
29.13
28.58
25.46
21.69
20.33
14.57
13.84
10.99
Current Data Parameters
NAME JRS-VII-157-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 14.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 64
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 200.67
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6454621 MHz
NUC1 13C
P1 10.00 usec
PLW1 57.00000000 W
======== CHANNEL f2 ========
SFO2 400.2216009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.37926000 W
PLW13 0.30720001 W
F2 - Processing parameters
SI 32768
SF 100.6353286 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

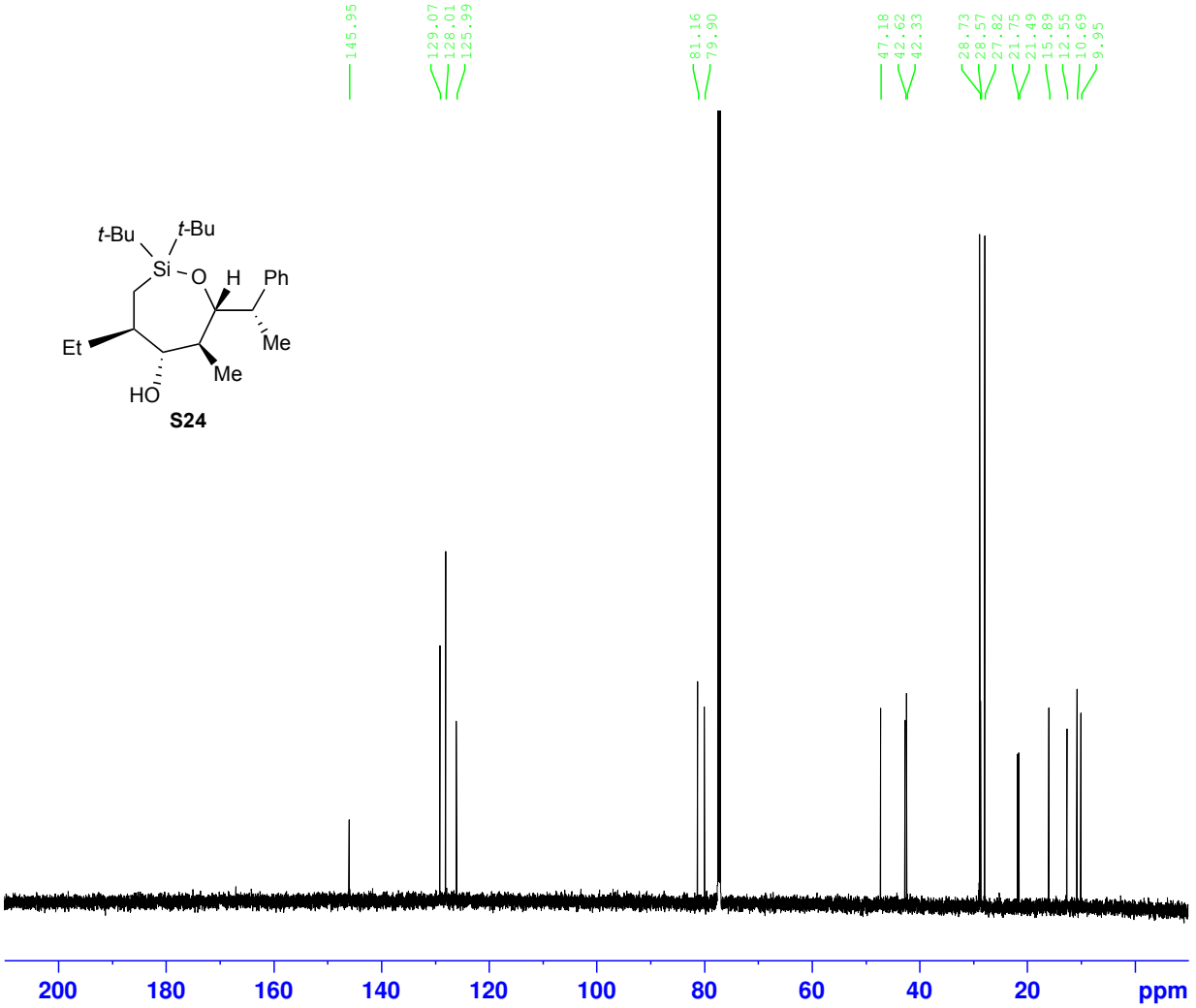

7.332
7.321
7.308
7.248
7.226
4.588
4.575
3.955
3.940
3.567
3.559
3.548
3.540
3.517
3.510
3.499
3.491
2.040
1.993
1.760
1.695
1.556
1.506
1.471
1.398
0.950
0.938
0.925
0.711
0.700
OH
OH
OH
Ph
Et
Me
20
Current Data Parameters
NAME VII-203-P
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170104
Time 10.58
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 33.59
DW 41.600 usec
DE 28.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1900116 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
3.97
1.03
1.00
1.00
1.01
1.00
1.00
0.99
1.01
1.01
3.10
3.10


143.85
128.55
127.56
126.16
78.74
72.57
63.24
45.28
41.51
19.64
11.90
11.71
OH
OH
OH
Et
Me
Ph
20
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME VII-165-P
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161217
Time 14.16
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 270
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 184.65
DW 13.867 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 150.9329866 MHz
NUC1 13C
P1 11.63 usec
PLW1 95.00000000 W
======== CHANNEL f2 ========
SFO2 600.1924008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 6.80000019 W
PLW12 0.06800000 W
PLW13 0.04352000 W
F2 - Processing parameters
SI 32768
SF 150.9178755 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


t-Bu
t-Bu
Si
O
i-Pr
Et
Me
HO
S23
3.438
3.435
3.423
3.420
2.783
2.746
1.877
1.829
1.796
1.794
1.741
1.729
1.676
1.539
1.486
1.476
1.406
1.400
1.104
1.084
1.073
1.058
1.026
0.987
0.974
0.962
0.923
0.918
0.912
0.907
0.820
0.798
0.796
0.772
0.770
Current Data Parameters
NAME VIII-26-P-NOE
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170125
Time 14.07
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 4
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 16.21
DW 41.600 usec
DE 28.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1899957 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.02
1.00
1.12
1.04
1.20
1.06
1.07
9.13
3.16
8.97
3.12
6.02
2.05
1.06


t-Bu
t-Bu
Si
O
i-Pr
Et
Me
HO
S23
81.32
80.22
47.84
43.36
32.11
29.26
29.15
28.97
22.68
22.15
21.92
15.40
14.46
13.15
10.68
Current Data Parameters
NAME JRS-VIII-26-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170124
Time 15.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 32
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 200.67
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6454621 MHz
NUC1 13C
P1 10.00 usec
PLW1 57.00000000 W
======== CHANNEL f2 ========
SFO2 400.2216009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.37926000 W
PLW13 0.30720001 W
F2 - Processing parameters
SI 32768
SF 100.6353278 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
ppm


7.267
7.258
7.171
7.137
7.130
3.757
3.754
3.739
3.736
3.186
3.183
3.172
3.168
3.158
3.154
3.144
3.141
3.005
2.987
2.970
1.911
1.908
1.855
1.851
1.848
1.782
1.771
1.661
1.654
1.543
1.503
1.418
1.406
1.400
1.296
1.282
1.183
1.170
1.017
1.012
1.007
0.953
0.938
0.923
0.747
t-Bu
t-Bu
Si
O
H
Ph
Et
Me
Me
HO
S24
Current Data Parameters
NAME VIII-28-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170127
Time 17.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 65536
SF 500.1990142 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
4.04
0.98
1.00
1.01
1.01
1.01
2.04
1.00
1.02
3.01
3.03
8.97
3.02
1.00
1.02
9.01



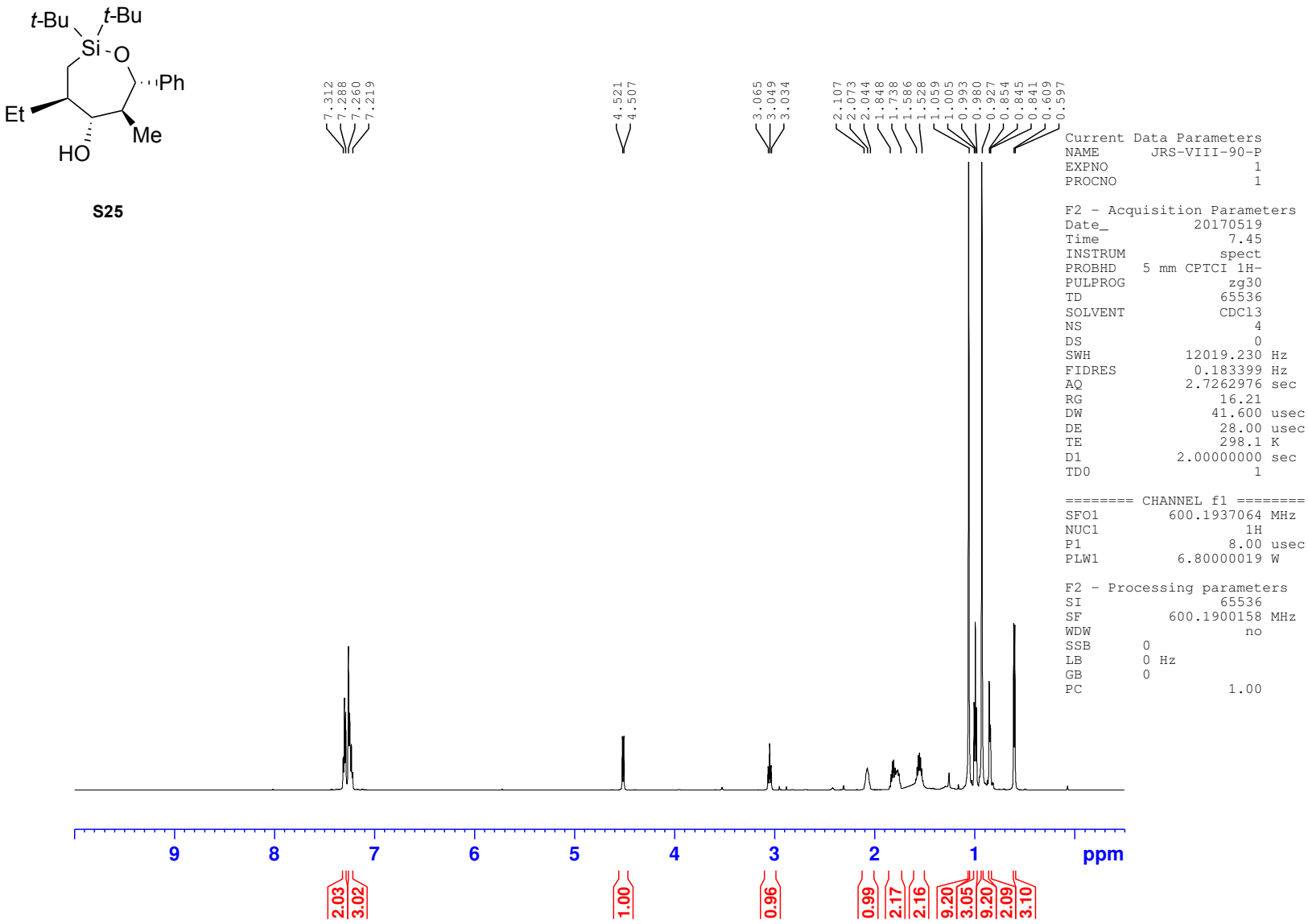

```
Current Data Parameters
NAME          VIII-22-P
EXPNO                 4
PROCNO                1

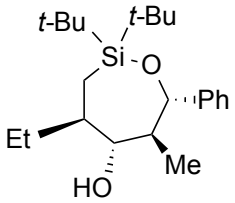
F2 - Acquisition Parameters
Date_          20170122
Time              13.59
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9087659 sec
RG                184.65
DW                13.867 usec
DE                 18.00 usec
TE                 298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                13C
P1                11.63 usec
PLW1        95.00000000 W

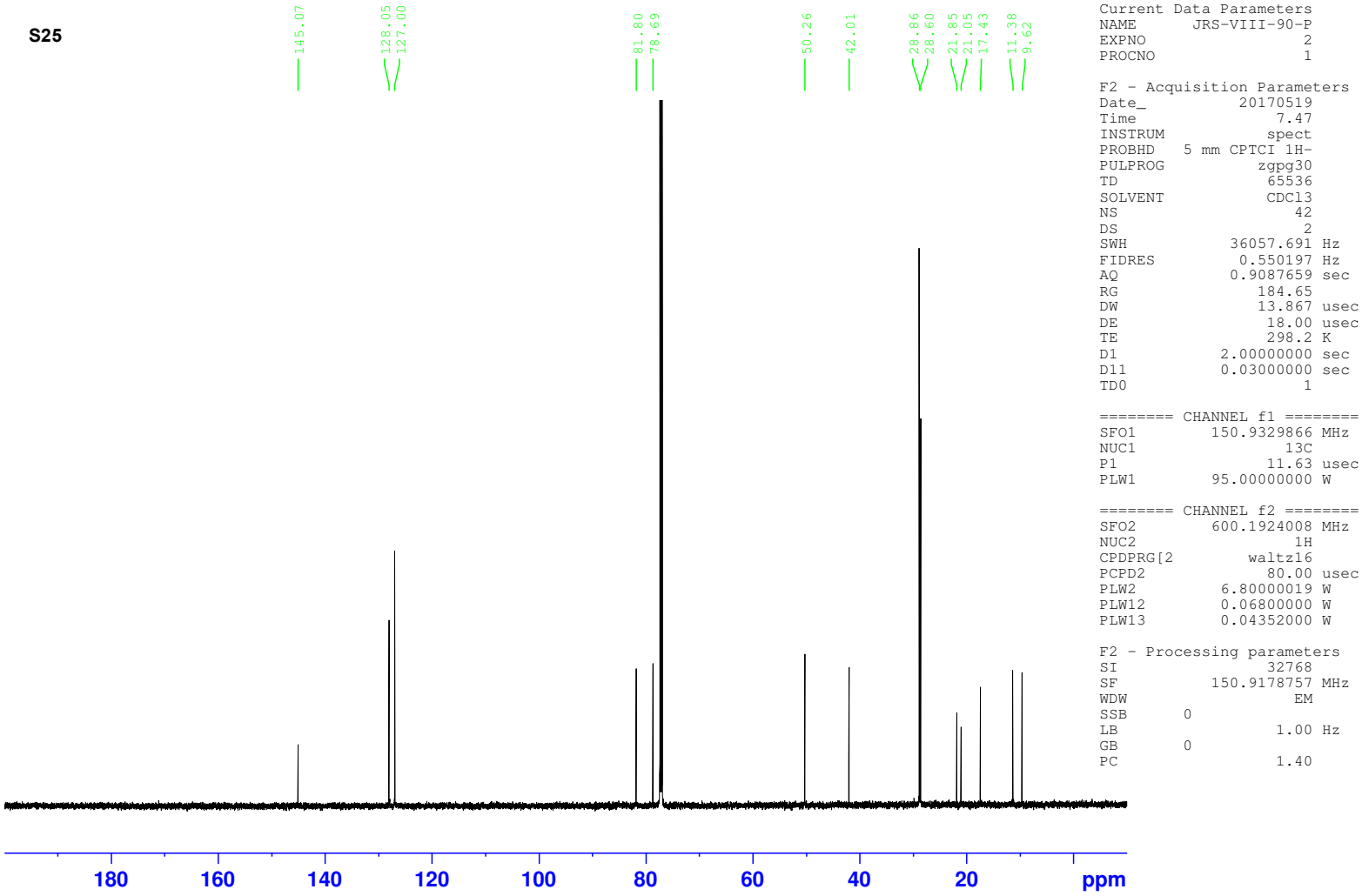
======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         6.80000019 W
PLW12        0.06800000 W
PLW13        0.04352000 W

F2 - Processing parameters
SI                32768
SF          150.9178755 MHz
WDW                EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


t-Bu
t-Bu
Si
O
Ph
Et
Me
HO
S25
7.312
7.288
7.260
7.219
4.521
4.507
3.065
3.049
3.034
2.107
2.073
2.044
1.848
1.738
1.586
1.528
1.059
1.005
0.993
0.980
0.927
0.854
0.845
0.841
0.609
0.597
Current Data Parameters
NAME JRS-VIII-90-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170519
Time 7.45
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 16.21
DW 41.600 usec
DE 28.00 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1900158 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.03
3.02
1.00
0.96
0.99
2.17
2.16
9.20
3.05
9.20
2.09
3.10



S25



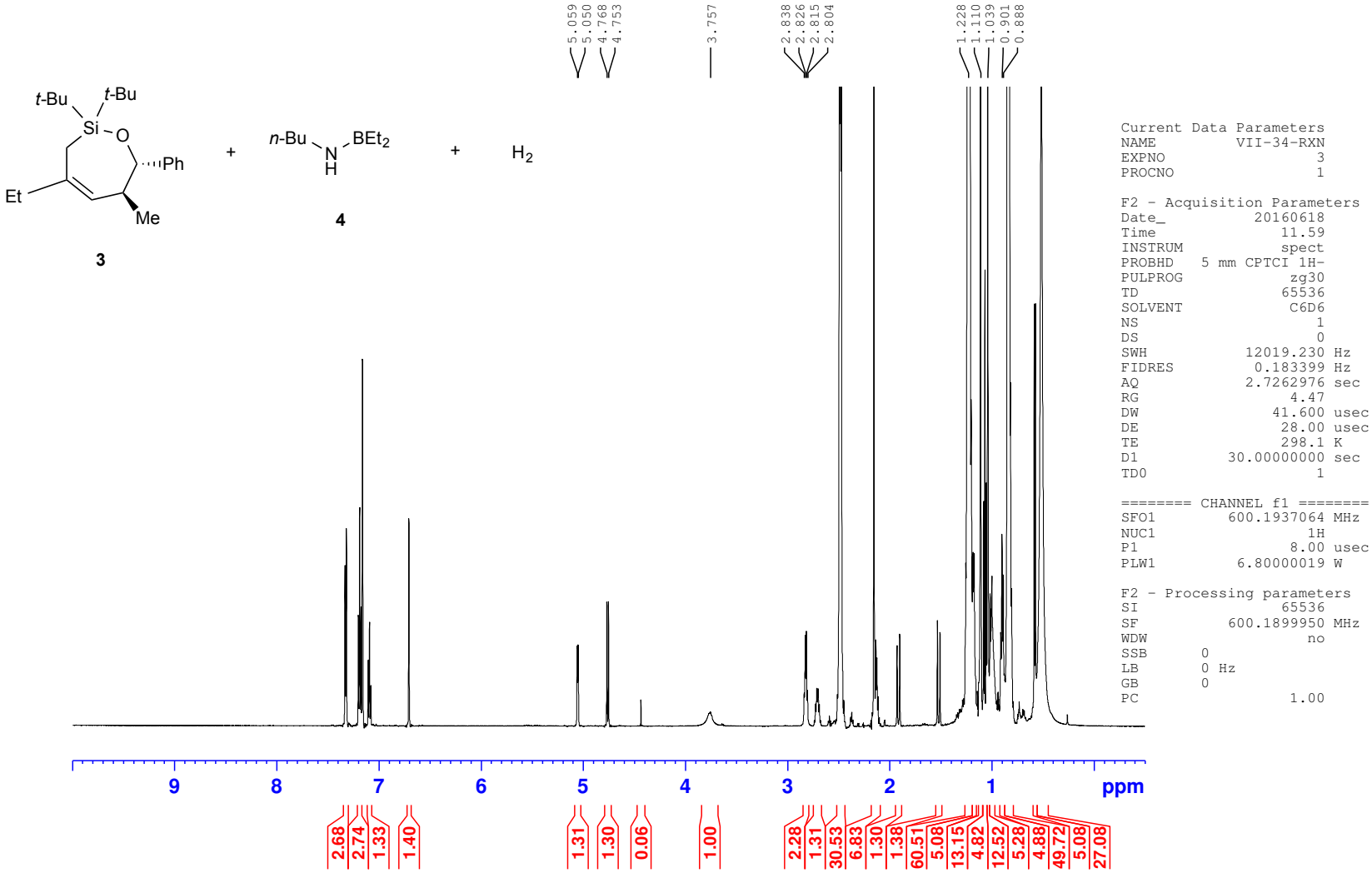

```
Current Data Parameters
NAME      JRS-VIII-90-P
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170519
Time               7.47
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   42
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG               184.65
DW               13.867 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                 13C
P1                11.63 usec
PLW1         95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                32768
SF          150.9178757 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

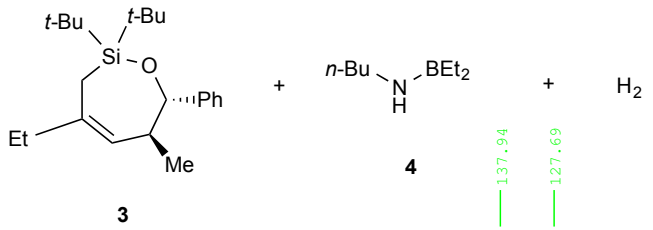



```
Current Data Parameters
NAME          VII-34-RXN
EXPNO                  3
PROCNO                 1

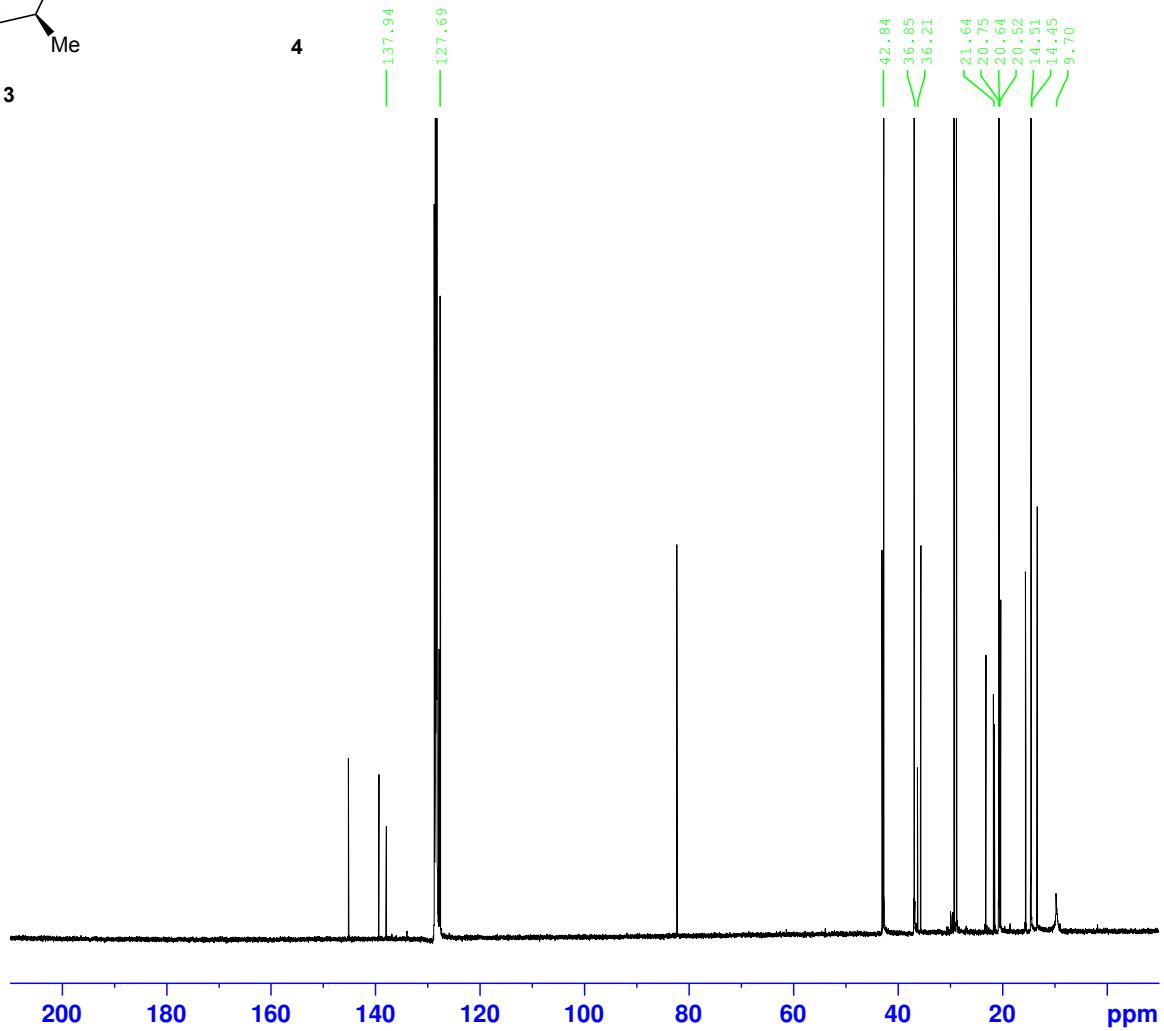
F2 - Acquisition Parameters
Date_           20160618
Time               11.59
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     1
DS                     0
SWH            12019.230 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                  4.47
DW                41.600 usec
DE                28.00 usec
TE                298.1 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         600.1937064 MHz
NUC1                   1H
P1                  8.00 usec
PLW1          6.80000019 W

F2 - Processing parameters
SI                 65536
SF           600.1899950 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



3 + **4** + H_2



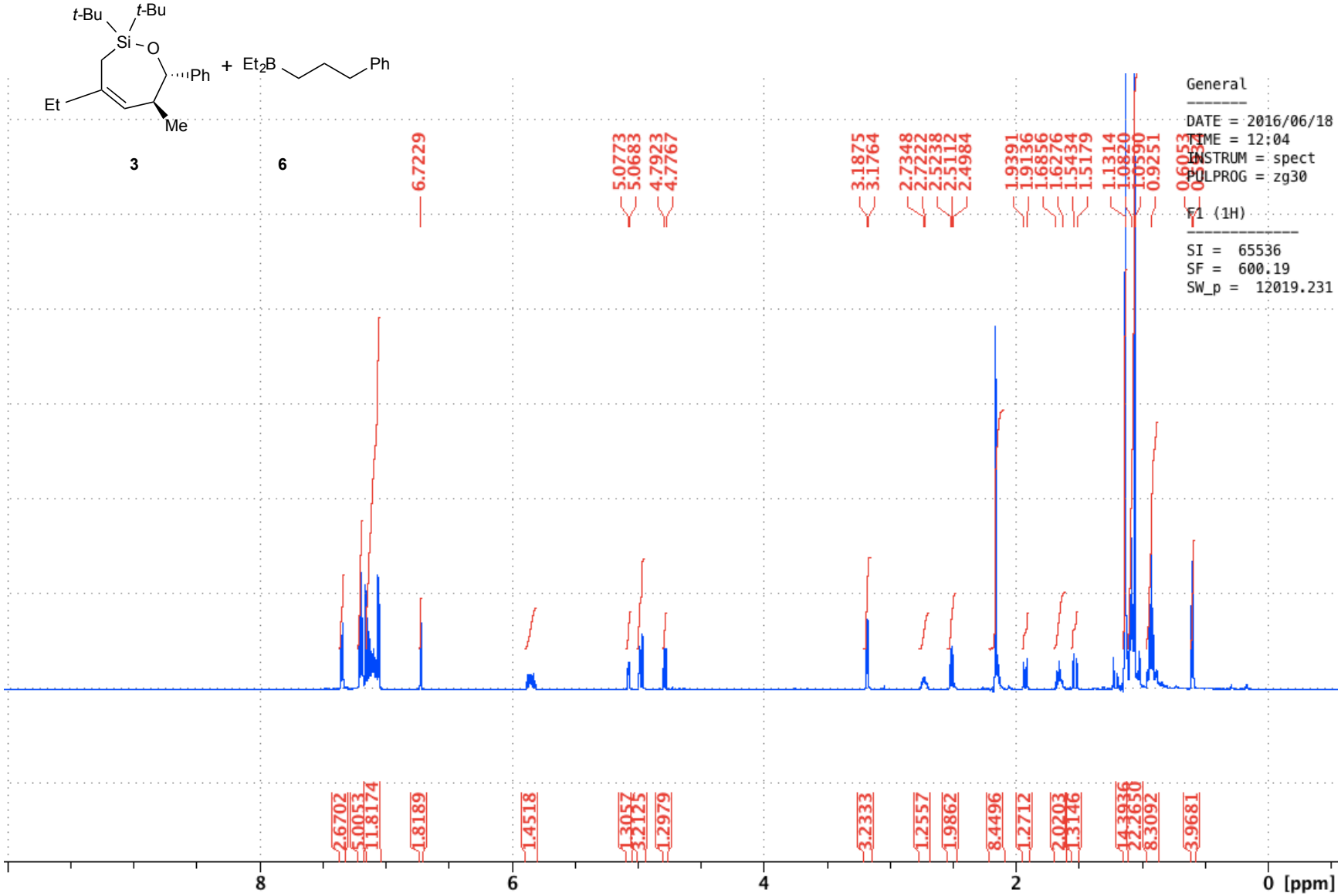

```
Current Data Parameters
NAME          VII-34-RXN
EXPNO                  5
PROCNO                 1

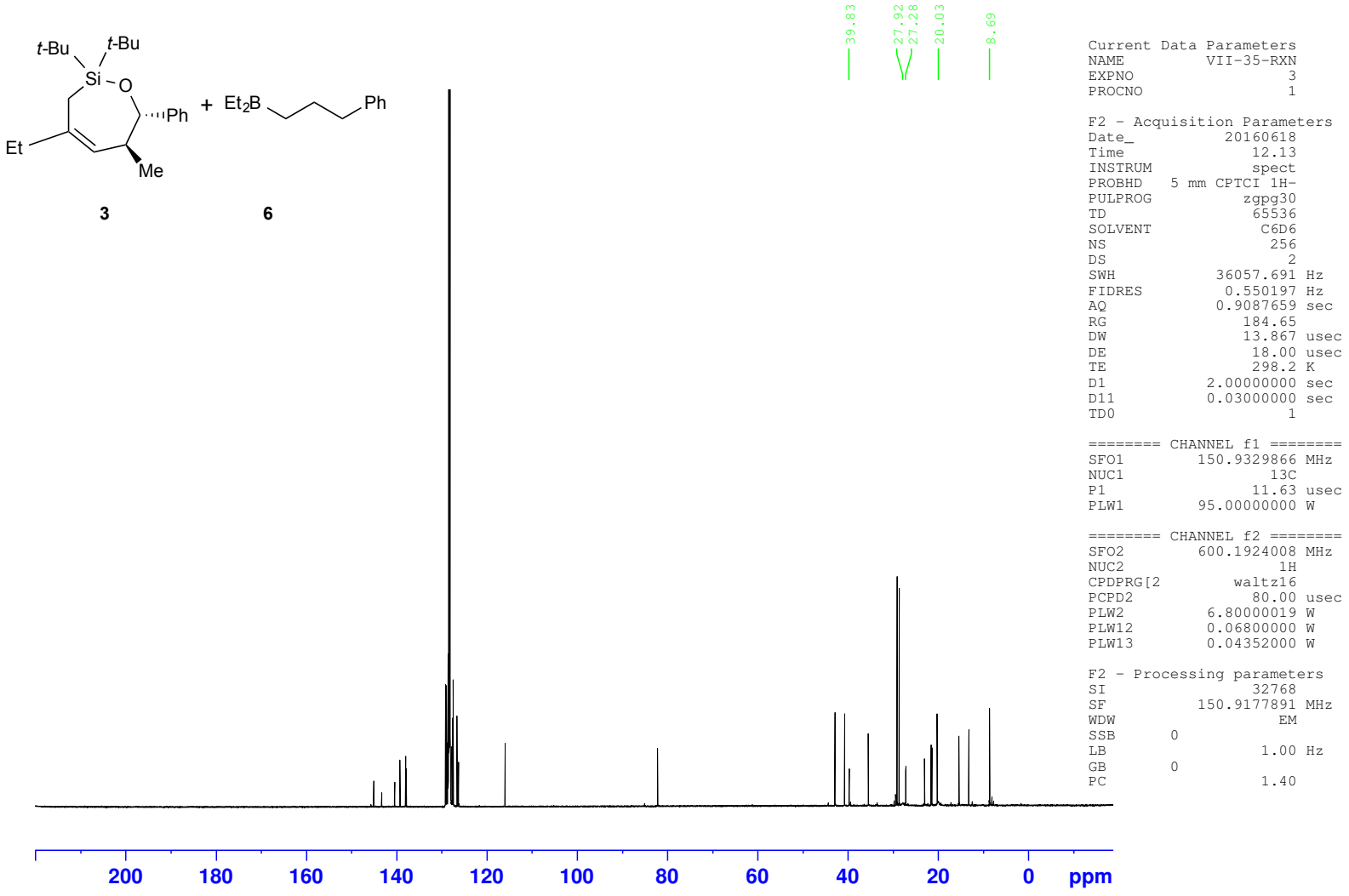
F2 - Acquisition Parameters
Date_           20160620
Time                8.26
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                   256
DS                     2
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                184.65
DW                13.867 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         150.9329866 MHz
NUC1                  13C
P1                 11.63 usec
PLW1         95.00000000 W

======== CHANNEL f2 ========
SFO2         600.1924008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          6.80000019 W
PLW12         0.06800000 W
PLW13         0.04352000 W

F2 - Processing parameters
SI                 32768
SF           150.9177848 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


t-Bu
t-Bu
Si
O
Ph
Et
Me
3
+ Et2B
Ph
6
6.7229
5.0773
5.0683
4.7923
4.7767
3.1875
3.1764
2.7348
2.7222
2.5238
2.5112
2.4984
1.9391
1.9136
1.6856
1.6276
1.5434
1.5179
1.1314
1.0820
1.0590
0.9251
0.6053
General
DATE = 2016/06/18
TIME = 12:04
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 600.19
SW_p = 12019.231
2.6702
5.0053
11.8174
1.8189
1.4518
1.3057
3.2125
1.2979
3.2333
1.2557
1.9862
8.4496
1.2712
2.0203
1.3146
14.3936
22.2650
8.3092
3.9681
8
6
4
2
0 [ppm]



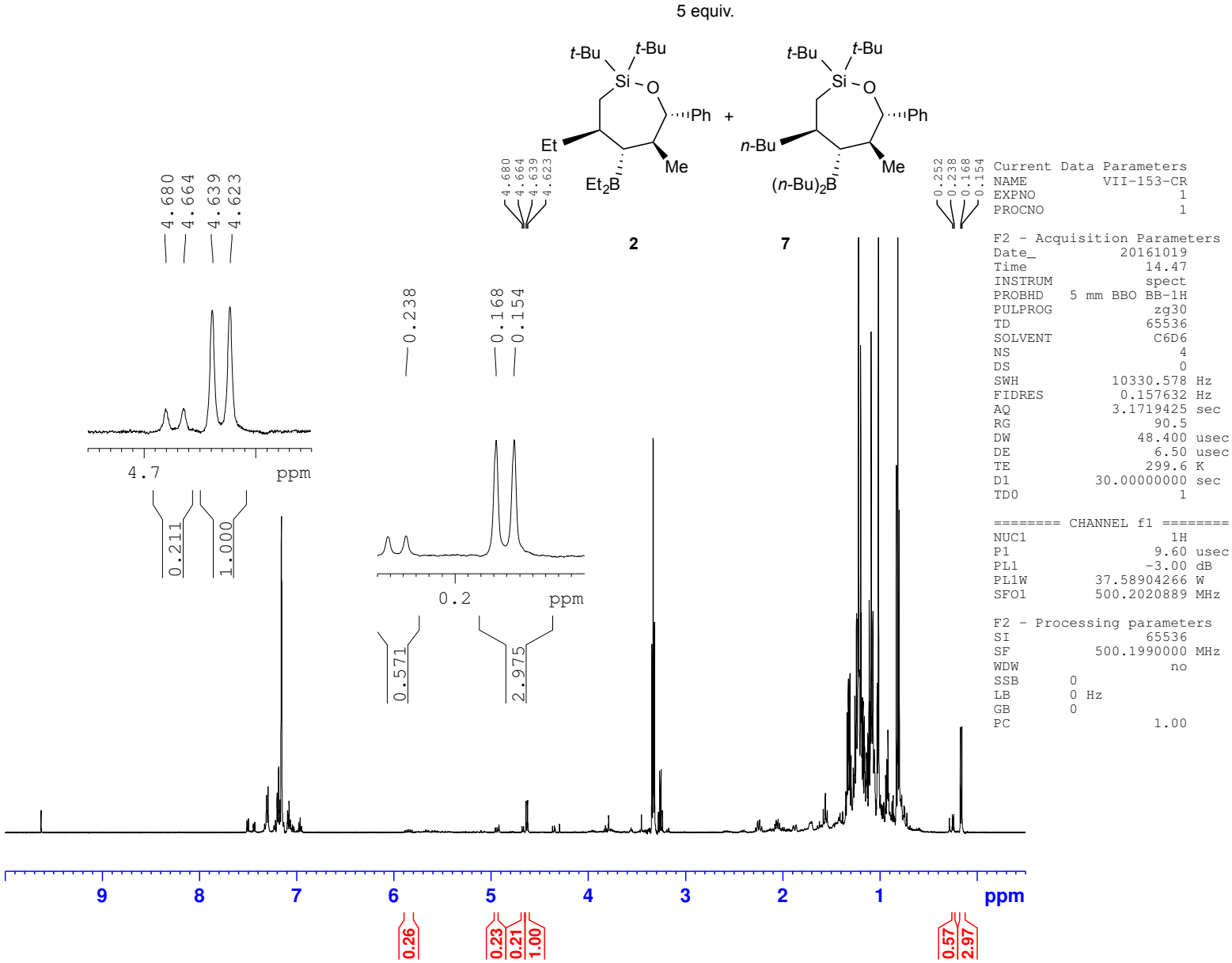

```
Current Data Parameters
NAME          VII-35-RXN
EXPNO                  3
PROCNO                 1

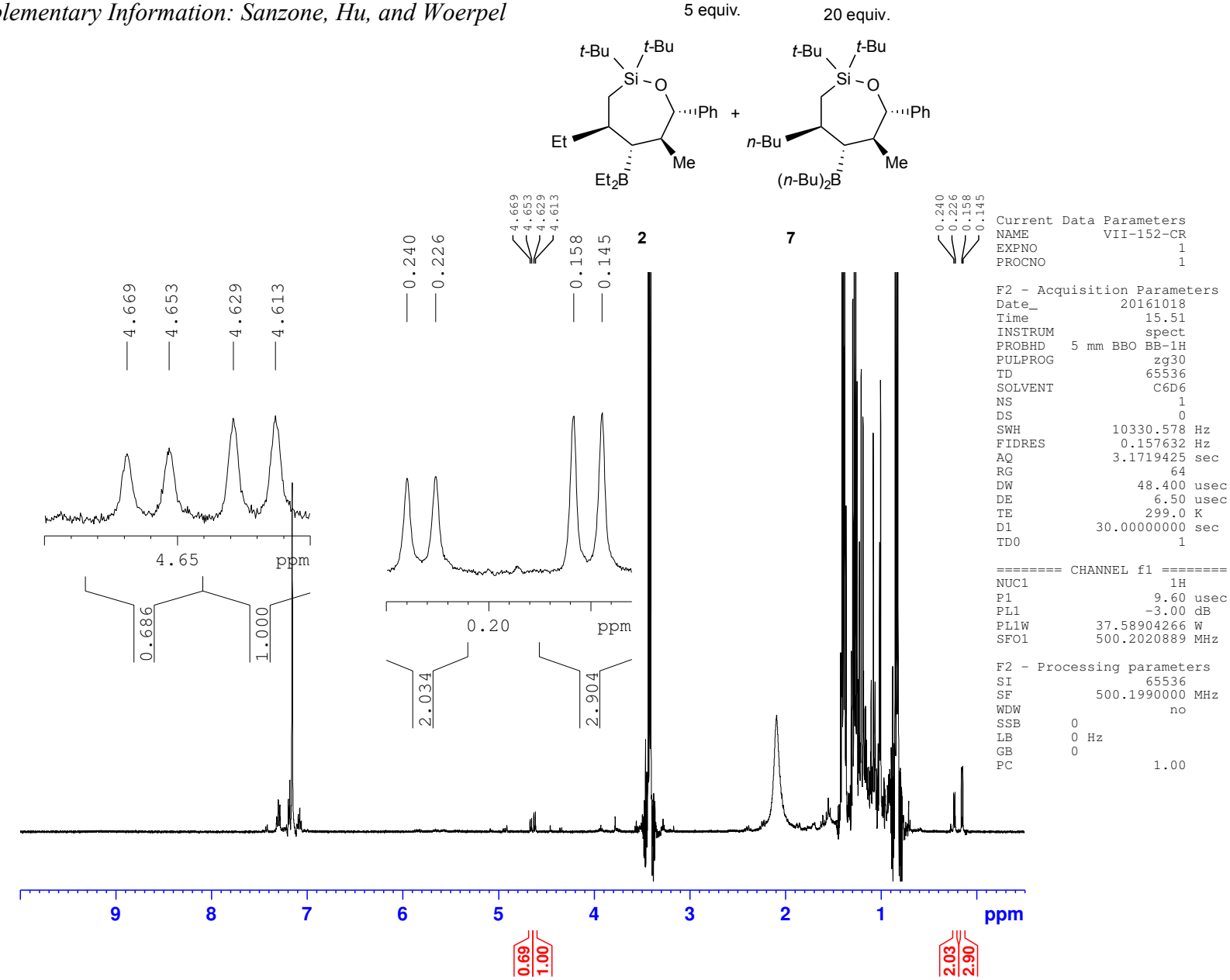
F2 - Acquisition Parameters
Date_           20160618
Time               12.13
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT            C6D6
NS                  256
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG               184.65
DW               13.867 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                13C
P1                11.63 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         6.80000019 W
PLW12        0.06800000 W
PLW13        0.04352000 W

F2 - Processing parameters
SI                 32768
SF          150.9177891 MHz
WDW                   EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```


5 equiv.
t-Bu
t-Bu
Si
O
Ph
Et
Me
Et2B
+
n-Bu
(n-Bu)2B
2
7
4.680
4.664
4.639
4.623
0.252
0.238
0.168
0.154
4.7
ppm
0.211
1.000
0.2
0.571
2.975
9
8
7
6
5
4
3
2
1
0.26
0.23
0.21
1.00
0.57
2.97
Current Data Parameters
NAME VII-153-CR
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161019
Time 14.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 4
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 90.5
DW 48.400 usec
DE 6.50 usec
TE 299.6 K
D1 30.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 65536
SF 500.1990000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

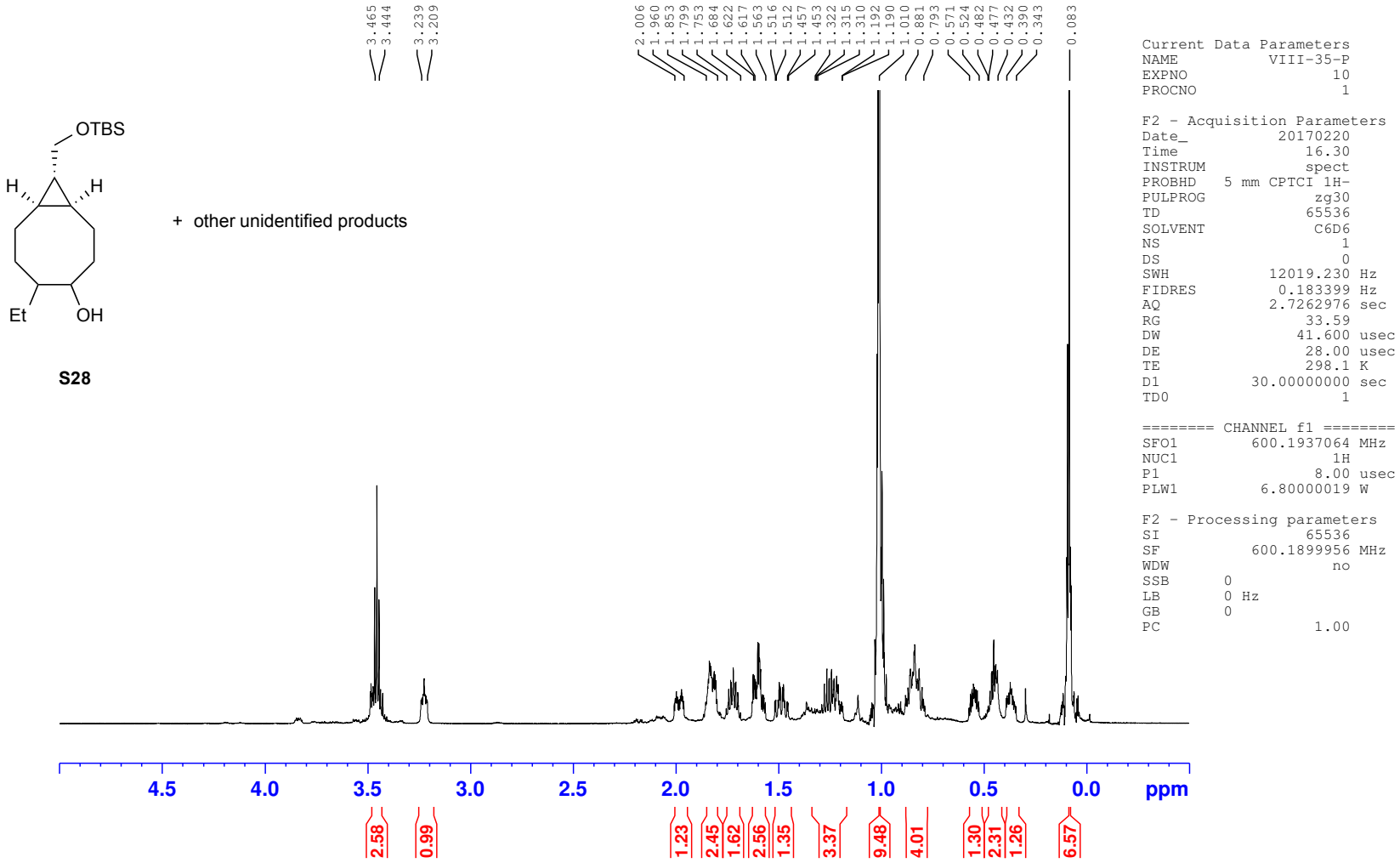



```
Current Data Parameters
NAME          VII-152-CR
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161018
Time               15.51
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     1
DS                     0
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719425 sec
RG                    64
DW                48.400 usec
DE                 6.50 usec
TE                299.0 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.60 usec
PL1               -3.00 dB
PL1W         37.58904266 W
SFO1         500.2020889 MHz

F2 - Processing parameters
SI                 65536
SF           500.1990000 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

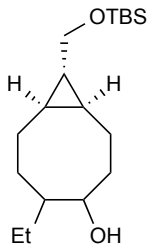



```
Current Data Parameters
NAME          VIII-35-P
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20170220
Time              16.30
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               65536
SOLVENT           C6D6
NS                   1
DS                   0
SWH          12019.230 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG                33.59
DW               41.600 usec
DE               28.00 usec
TE               298.1 K
D1           30.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        600.1937064 MHz
NUC1                1H
P1                8.00 usec
PLW1         6.80000019 W

F2 - Processing parameters
SI               65536
SF          600.1899956 MHz
WDW                 no
SSB      0
LB       0 Hz
GB       0
PC                1.00
```



S28

\+ other unidentified products

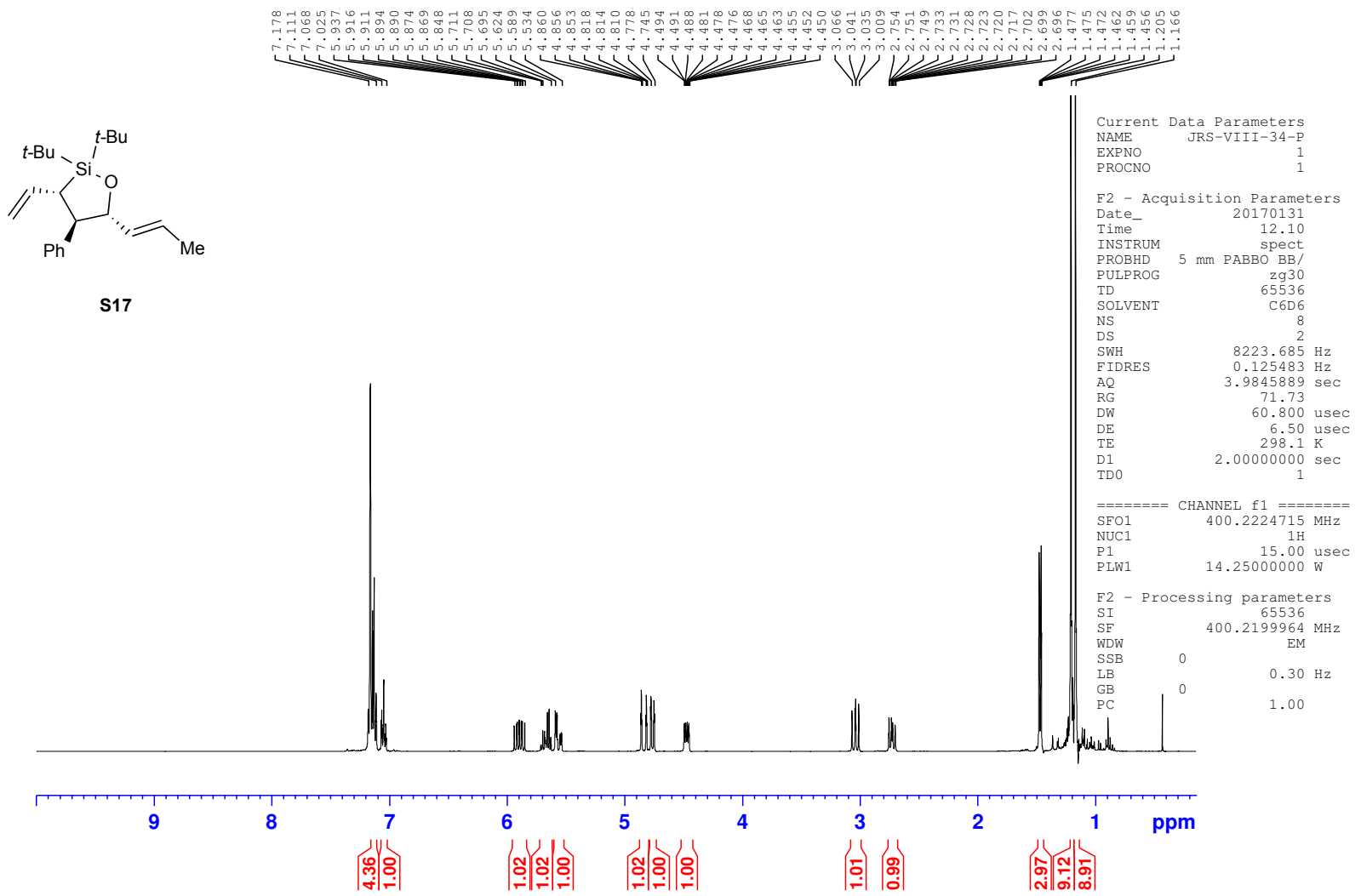

```
Current Data Parameters
NAME            VIII-35-P
EXPNO                  12
PROCNO                  1

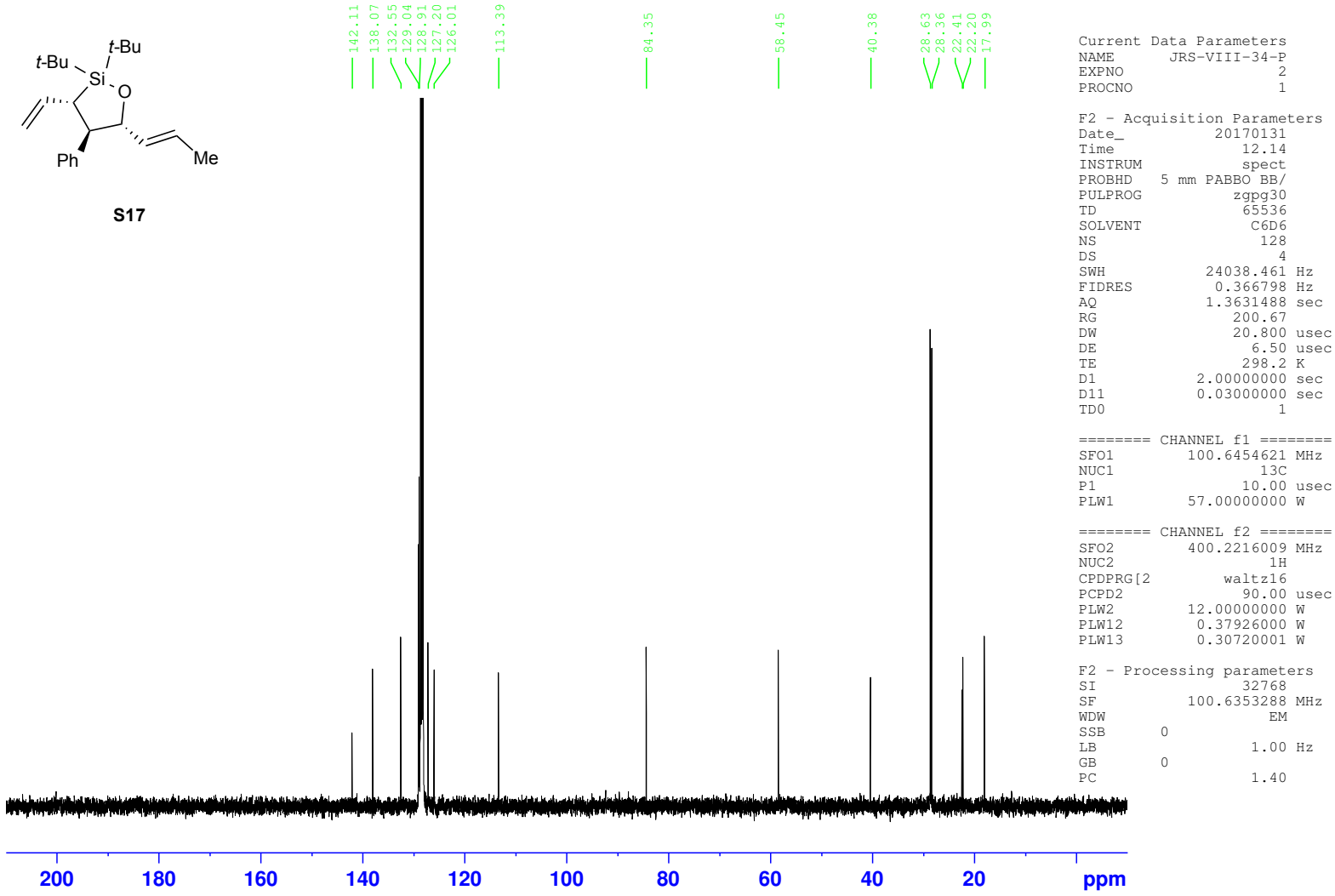
F2 - Acquisition Parameters
Date_            20170220
Time                16.37
INSTRUM             spect
PROBHD    5 mm CPTCI 1H-
PULPROG            zgpg30
TD                  65536
SOLVENT              C6D6
NS                     16
DS                      2
SWH             36057.691 Hz
FIDRES           0.550197 Hz
AQ               0.9087659 sec
RG                 184.65
DW                 13.867 usec
DE                  18.00 usec
TE                  298.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          150.9329866 MHz
NUC1                   13C
P1                  11.63 usec
PLW1          95.00000000 W

======== CHANNEL f2 ========
SFO2          600.1924008 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2           6.80000019 W
PLW12          0.06800000 W
PLW13          0.04352000 W

F2 - Processing parameters
SI                  32768
SF            150.9177911 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```


7.178
7.111
7.068
7.025
5.937
5.916
5.911
5.894
5.890
5.874
5.869
5.848
5.711
5.708
5.695
5.624
5.589
5.534
4.860
4.856
4.853
4.818
4.814
4.810
4.778
4.745
4.494
4.491
4.488
4.481
4.478
4.476
4.468
4.465
4.463
4.455
4.452
4.450
3.066
3.041
3.035
3.009
2.754
2.751
2.749
2.733
2.731
2.728
2.723
2.720
2.717
2.702
2.699
2.696
1.477
1.475
1.472
1.462
1.459
1.456
1.205
1.166
t-Bu
t-Bu
Si
O
Ph
Me
S17
Current Data Parameters
NAME JRS-VIII-34-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170131
Time 12.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 71.73
DW 60.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.2224715 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.25000000 W
F2 - Processing parameters
SI 65536
SF 400.2199964 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
4.36
1.00
1.02
1.02
1.00
1.02
1.00
1.00
1.01
0.99
2.97
9.12
8.91



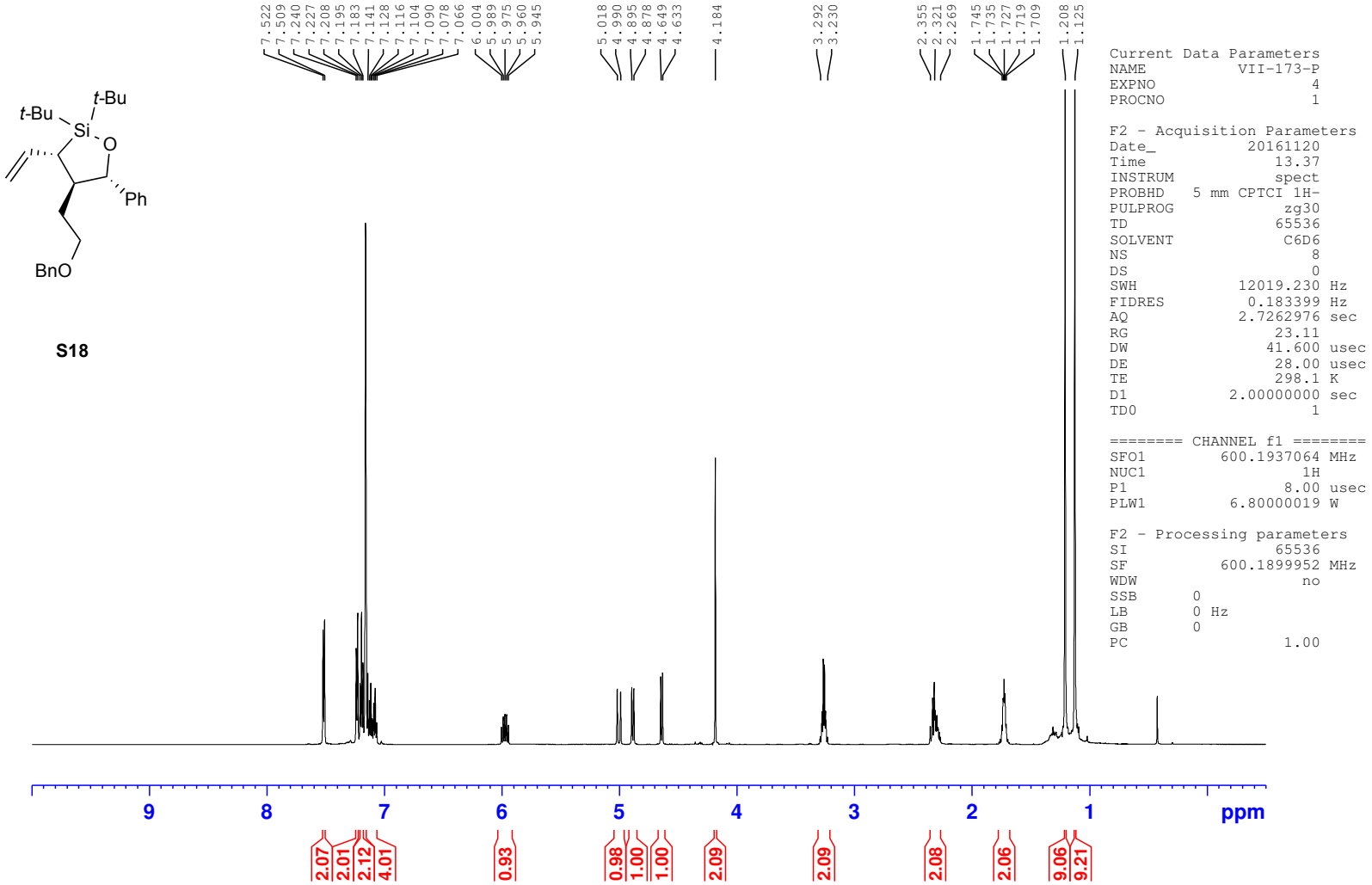

```
Current Data Parameters
NAME      JRS-VIII-34-P
EXPNO                 2
PROCNO                1

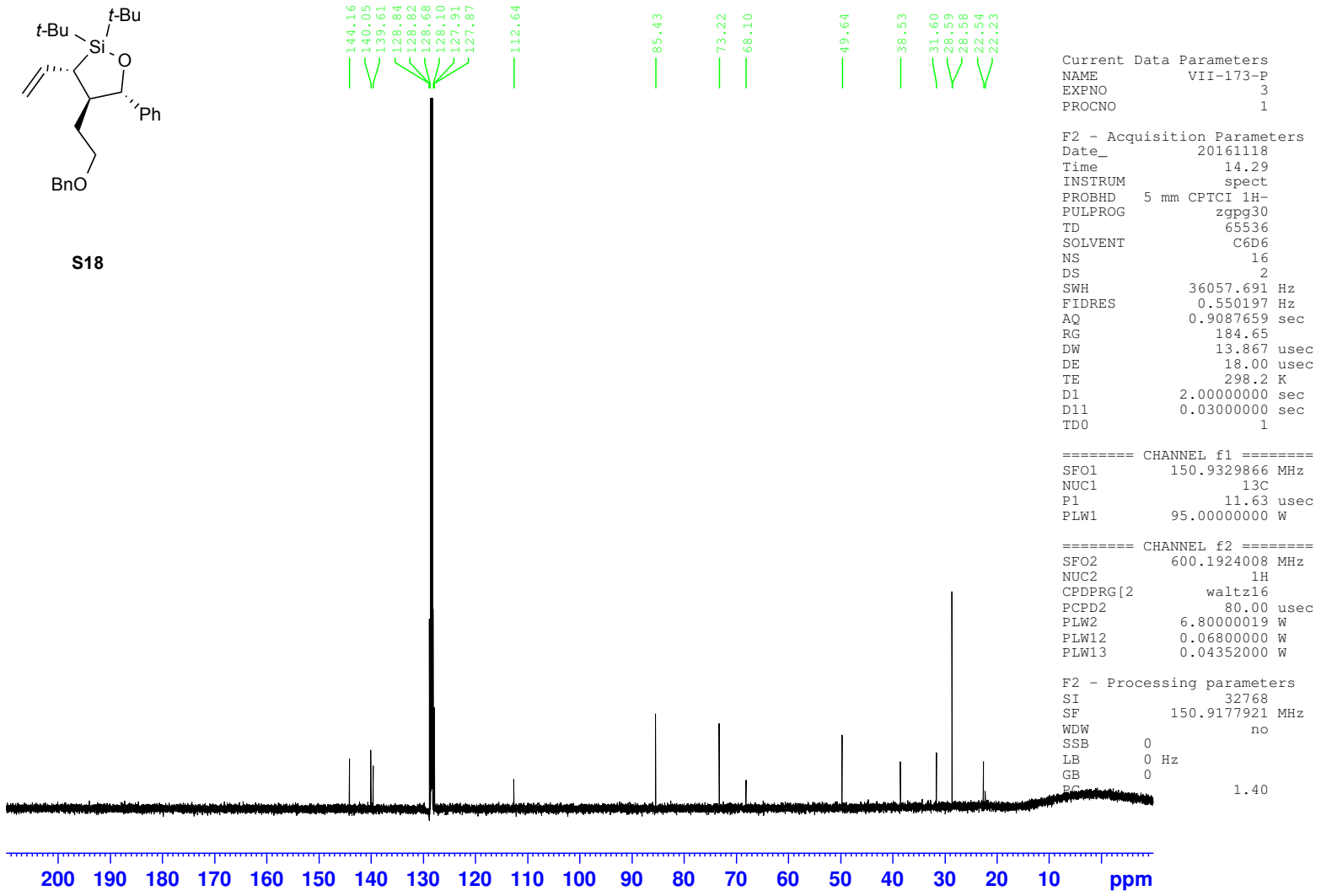
F2 - Acquisition Parameters
Date_          20170131
Time              12.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           C6D6
NS                 128
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631488 sec
RG              200.67
DW              20.800 usec
DE               6.50 usec
TE              298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6454621 MHz
NUC1               13C
P1               10.00 usec
PLW1        57.00000000 W

======== CHANNEL f2 ========
SFO2        400.2216009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        12.00000000 W
PLW12        0.37926000 W
PLW13        0.30720001 W

F2 - Processing parameters
SI                32768
SF          100.6353288 MHz
WDW                EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
```


7.522
7.509
7.240
7.227
7.208
7.195
7.183
7.141
7.128
7.116
7.104
7.090
7.078
7.066
6.004
5.989
5.975
5.960
5.945
5.018
4.990
4.895
4.878
4.649
4.633
4.184
3.292
3.230
2.355
2.321
2.269
1.745
1.735
1.727
1.719
1.709
1.208
1.125
t-Bu
t-Bu
Si
O
Ph
BnO
S18
Current Data Parameters
NAME VII-173-P
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161120
Time 13.37
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 23.11
DW 41.600 usec
DE 28.00 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.80000019 W
F2 - Processing parameters
SI 65536
SF 600.1899952 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.07
2.01
2.12
4.01
0.93
0.98
1.00
1.00
2.09
2.09
2.08
2.06
9.06
9.21



S18

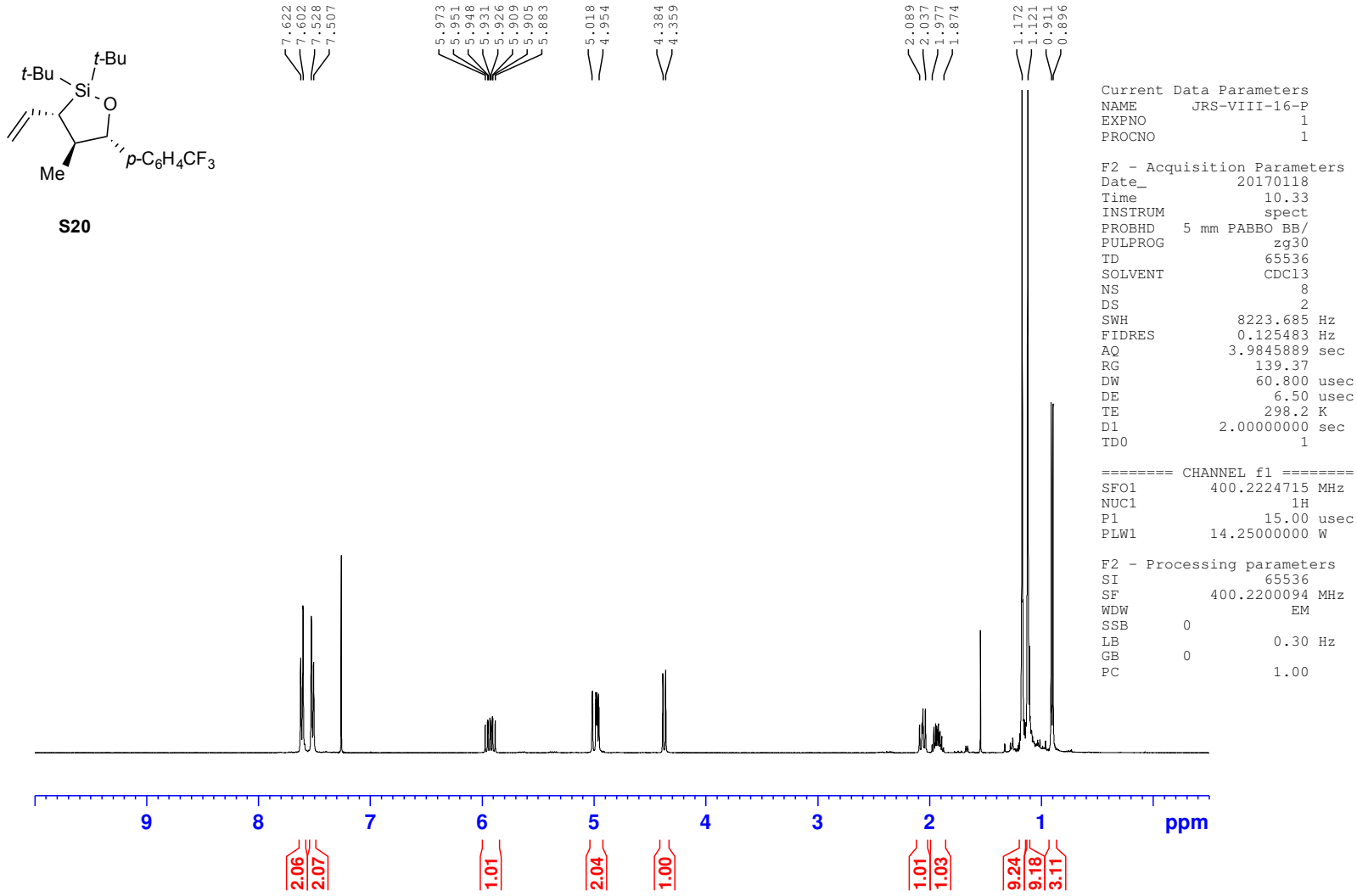
```
Current Data Parameters
NAME          VII-173-P
EXPNO                 3
PROCNO                1

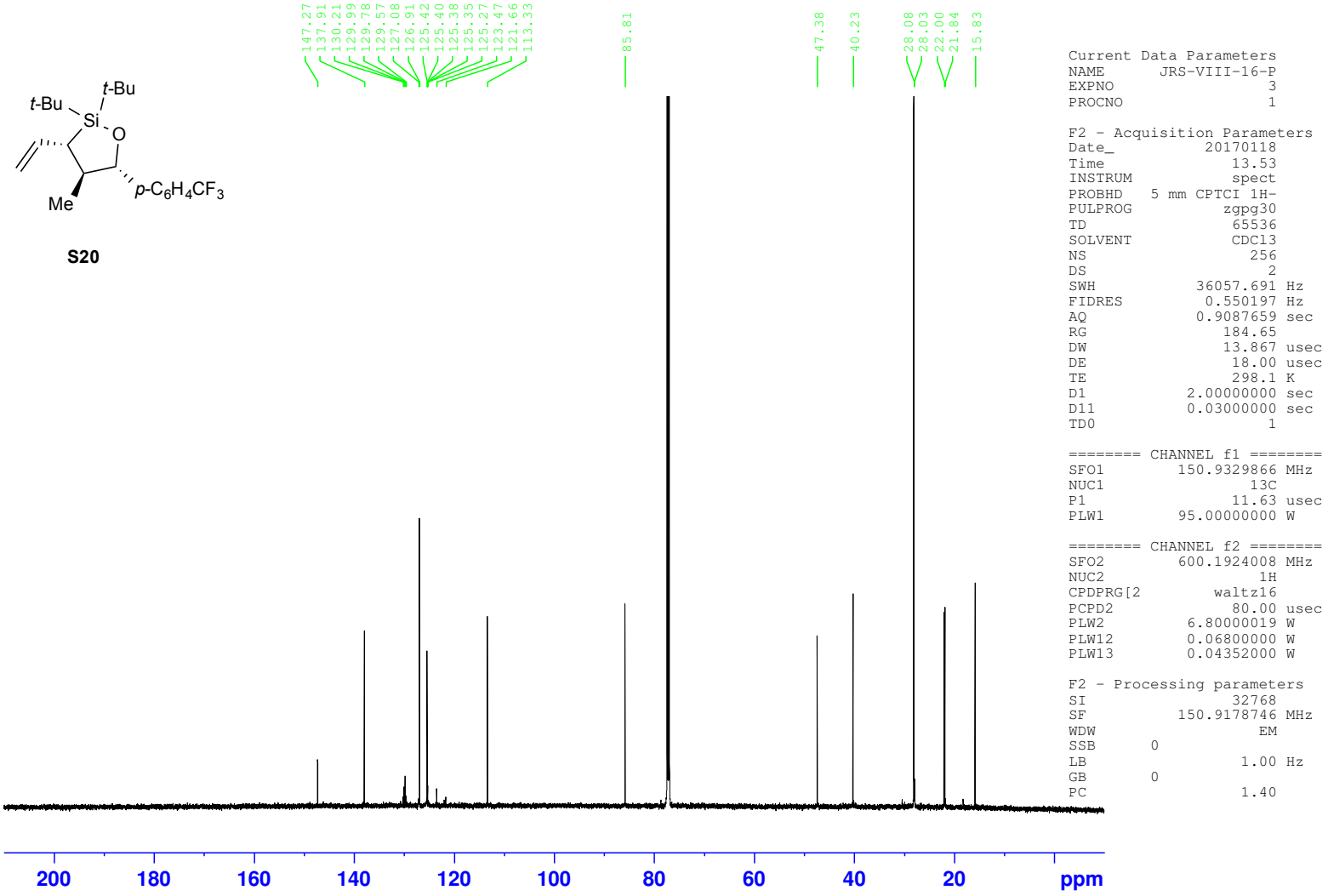
F2 - Acquisition Parameters
Date_          20161118
Time              14.29
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                   16
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG               184.65
DW               13.867 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9329866 MHz
NUC1                13C
P1                11.63 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1924008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         6.80000019 W
PLW12        0.06800000 W
PLW13        0.04352000 W

F2 - Processing parameters
SI                32768
SF          150.9177921 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                1.40
```


t-Bu
t-Bu
Si
O
Me
p-C6H4CF3
S20
7.622
7.602
7.528
7.507
5.973
5.951
5.948
5.931
5.926
5.909
5.905
5.883
5.018
4.954
4.384
4.359
2.089
2.037
1.977
1.874
1.172
1.121
0.911
0.896
Current Data Parameters
NAME JRS-VIII-16-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170118
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 139.37
DW 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.2224715 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.25000000 W
F2 - Processing parameters
SI 65536
SF 400.2200094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.06
2.07
1.01
2.04
1.00
1.01
1.03
9.24
9.18
3.11


147.27
137.91
130.21
129.99
129.78
129.57
127.08
126.91
125.42
125.40
125.38
125.35
125.27
123.47
121.66
113.33
85.81
47.38
40.23
28.08
28.03
22.00
21.84
15.83
t-Bu
t-Bu
Si
O
Me
p-C6H4CF3
S20
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME JRS-VIII-16-P
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170118
Time 13.53
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 184.65
DW 13.867 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 150.9329866 MHz
NUC1 13C
P1 11.63 usec
PLW1 95.00000000 W
======== CHANNEL f2 ========
SFO2 600.1924008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 6.80000019 W
PLW12 0.06800000 W
PLW13 0.04352000 W
F2 - Processing parameters
SI 32768
SF 150.9178746 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40