Cycloadditions of Cyclohexynes and Cyclopentyne

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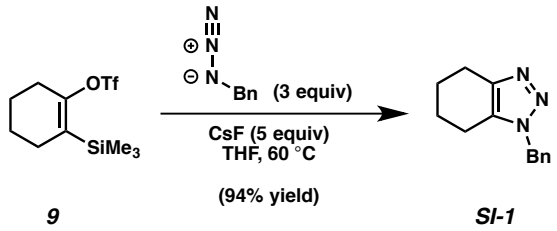
Supporting Information – Table of Contents

Materials and Methods. Unless stated otherwise, reactions were conducted in flame-dried glassware under an atmosphere of nitrogen using anhydrous solvents (freshly distilled or passed through activated alumina columns). All commercially obtained reagents were used as received unless otherwise specified. Cesium fluoride (CsF) was obtained from Strem Chemicals. *N*-phenyl-bis(trifluoromethanesulfonimide) was obtained from Oakwood Products, Inc. *N*-tert-butyl-α-phenylnitrone, 1,3-dimethyl-2-imidazolidinone, and methyl 2-acetamidoacrylate were obtained from Alfa Aesar. Methyl thiolsalicylate was obtained from Acros Organics. Ethyl diazoacetate, L-selectride (1 M in THF), and (trimethylsilyl)diazomethane (1 M in Et_2O) were obtained from Sigma Aldrich. *Caution: (trimethylsilyl)diazomethane is a flammable liquid that is very toxic when inhaled. Inhalation can cause pulmonary edema. It may be harmful if ingested or absorbed through the skin. It causes respiratory tract, skin, and eye irritation.* Trimethylsilyl chloride (TMSCl) was distilled over CaH_2 prior to use. Reaction temperatures were controlled using an IKAmag temperature modulator and, unless stated otherwise, reactions were performed at room temperature (rt, approximately 23 °C). Thin-layer chromatography (TLC) was conducted with EMD gel 60 F254 pre-coated plates (0.25 mm) and visualized using a combination of UV light and potassium permanganate staining. Silicycle Siliaflash P60 (particle size 0.040–0.063 mm) was used for flash column chromatography. ^{1}H NMR and 2D-NOESY spectra were recorded on Bruker spectrometers (at 500 MHz) and are reported relative to deuterated solvent signals. Data for ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. ^{13}C NMR spectra were recorded on Bruker spectrometers (at 125 MHz) and are reported relative to deuterated solvent signals. Data for ^{13}C NMR spectra are reported in terms of chemical shift and, when necessary, multiplicity, and coupling constant (Hz). ^{19}F NMR spectra were recorded on Bruker spectrometers (at 376 MHz) and reported in terms of chemical shift. IR spectra were obtained using on a Perkin-Elmer 100 spectrometer and are reported in terms of frequency of absorption (cm^{-1}). High-resolution mass spectra were obtained on Waters LCT Premier with ACQUITY LC and Thermo Scientific™ Exactive Mass Spectrometers with DART ID-CUBE.

Experimental Procedures.

A. Cyclohexyne Trapping Experiments.

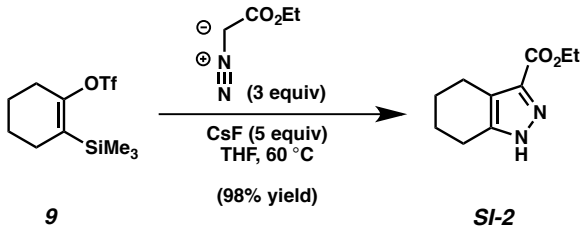


9 *SI-1*

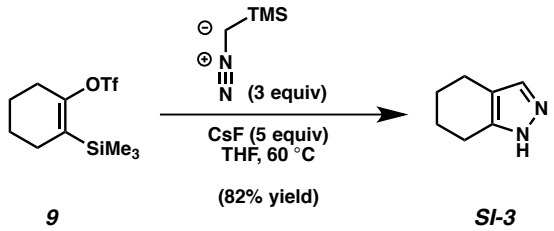
Representative Procedure (Preparation of triazole SI-1 is used as an example).

SI-1 (Table 1, entry 1). To a stirred solution of silyltriflate **9**[1] (52.0 mg, 0.172 mmol) and benzylazide (0.8 M in PhH, 640 μL, 0.512 mmol, 3.0 equiv) in THF (5.90 mL) was added CsF (0.130 g, 0.857 mmol, 5.0 equiv). The reaction vessel was purged with N_2 gas, sealed, and placed in a preheated aluminum heating block maintained at 60 °C for 24 h. After cooling to 23 °C, the reaction mixture was filtered over silica gel (EtOAc eluent, 12 mL). Evaporation under reduced pressure and further purification by preparative thin layer chromatography (3:2 EtOAc : hexanes) afforded triazole **SI-1** as a white amorphous solid (94% yield, average of two experiments). R_f 0.30 (3:2 EtOAc : hexanes); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34–7.27 (m, 3H), 7.19–7.17 (app. d, J = 7.5, 2H), 5.41 (s, 2H), 2.72 (app. t, J = 5.0, 2H), 2.40 (app. t, J = 5.2, 2H), 1.78–1.72 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.0, 135.1, 132.1, 129.0, 128.3, 127.6, 51.9, 22.6, 22.5, 22.0, 20.2; IR (film): 2934, 2855, 1586, 1497, 1456, 1440 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{13}H_{16}N_3$, 214.1339; found, 214.1332.

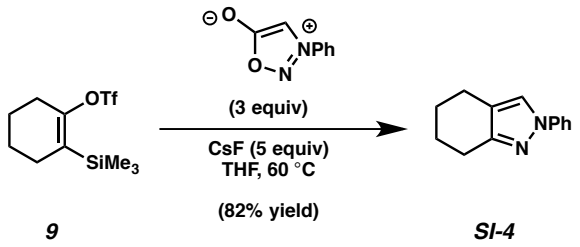
Any modifications of the conditions shown in this representative procedure are specified in the following schemes, which depict all of the results shown in Tables 1 in addition to several other examples of cyclohexyne trapping.



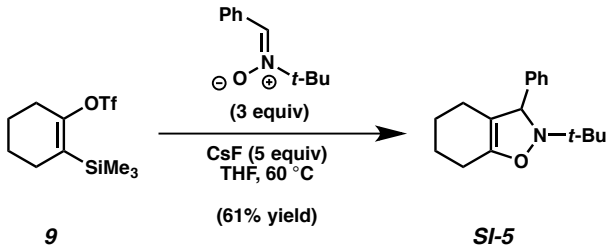
SI-2 (Table 1, entry 2). Purification by preparative thin layer chromatography (1:1 hexanes : EtOAc) afforded pyrazole **SI-2** as a faint yellow oil (98% yield, average of two experiments). R_f 0.40 (1:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 11.55 (br s, 1H), 4.34 (q, J = 7.0, 2H), 2.72 (t, J = 5.9, 2H), 2.68 (t, J = 5.9, 2H), 1.85–1.67 (m, 4H), 1.34 (t, J = 7.1, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.2, 145.3, 135.8, 119.6, 60.6, 23.0, 22.7, 22.2, 21.6, 14.4; IR (film): 2934, 2855, 1714, 1442, 1256, 1143 cm^{-1}; HRMS-ESI (*m/z*) $[M - H]^-$ calcd for $C_{10}H_{13}N_2O_2$, 193.0972; found, 193.0981.



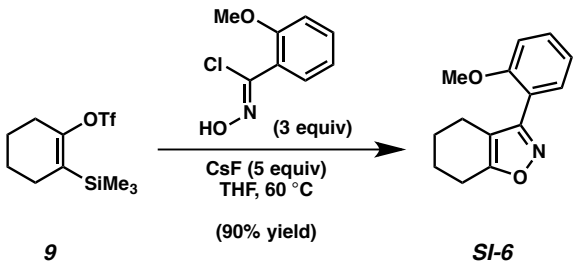
SI-3 (Table 1, entry 3). Purification by preparative thin layer chromatography (2:1 EtOAc : hexanes) afforded pyrazole **SI-3** as a colorless oil (82% yield, average of two experiments). R_f 0.20 (2:1 EtOAc : hexanes); ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.16 (br s, 1H), 7.30 (s, 1H), 2.68 (t, J = 6.1, 2H), 2.54 (t, J = 6.1, 2H), 1.86–1.78 (m, 2H), 1.78–1.70 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.5, 132.2, 115.2, 23.6, 23.3, 22.2, 20.6; IR (film): 3155, 3103, 2923, 2849, 1593, 1444 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_7H_{11}N_2$, 123.0917; found, 123.0914.



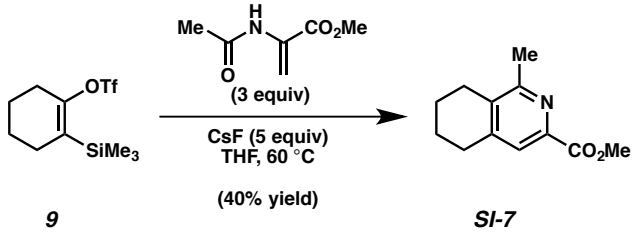
SI-4 (Table 1, entry 4). The sydnone trapping agent was synthesized using a known procedure.[2] Purification by preparative thin layer chromatography (9:1 hexanes : EtOAc) afforded pyrazole **SI-4** as a faint orange oil (82% yield, average of two experiments). R_f 0.55 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.62 (dd, J = 8.7, 1.0, 2H), 7.61 (s, 1H), 7.40 (tt, J = 7.2, 1.8, 2H), 7.20 (tt, J = 7.3, 1.0, 1H), 2.78 (t, J = 6.4, 2H), 2.62 (t, J = 6.4, 2H), 1.89–1.83 (m, 2H), 1.81–1.75 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.4, 140.6, 129.4, 125.6, 123.8, 118.7, 118.3, 23.6, 23.6, 23.5, 20.8; IR (film): 2928, 2855, 1598, 1570, 1504, 1376 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{13}H_{15}N_2$, 199.1230; found, 199.1227.



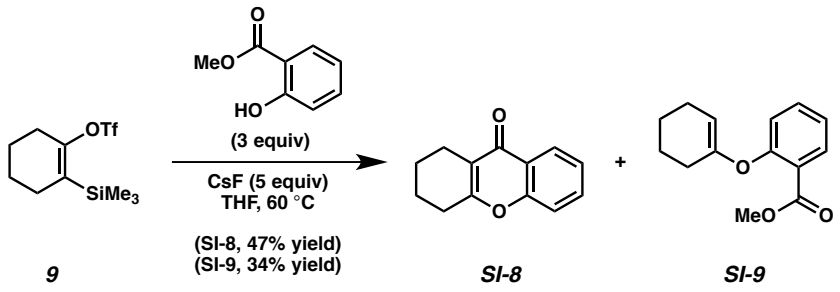
SI-5 (Table 1, entry 5). Purification by preparative thin layer chromatography (9:1 hexanes : EtOAc) afforded isoxazoline **SI-5** as a colorless oil (61% yield, average of two experiments). R_f 0.65 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.36–7.28 (m, 4H), 7.22 (app. tt, J = 6.4, 1.7, 1H), 4.88 (s, 1H), 2.21–2.07 (m, 2H), 1.86–1.78 (m, 1H), 1.70–1.58 (m, 3H), 1.58–1.52 (m, 2H), 1.11 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.0, 143.8, 128.4, 127.5, 127.1, 106.5, 70.6, 60.3, 25.2, 22.8, 22.7, 21.4, 21.2; IR (film): 2972, 2932, 1724, 1453, 1361, 1211 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{17}H_{24}NO$, 258.1852; found, 258.1851.



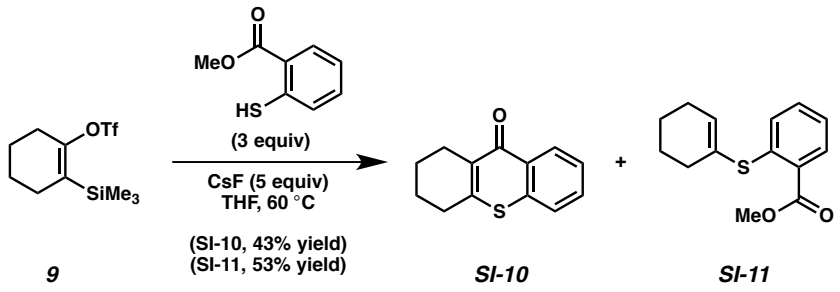
SI-6 (Table 1, entry 6). The chloro-oxime trapping agent was synthesized using a known procedure.[3] Purification by preparative thin layer chromatography (9:1 hexanes : EtOAc) afforded isoxazole **SI-6** as a faint yellow oil (90% yield, average of two experiments). R_f 0.40 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.47 (dd, *J* = 7.5, 1.7, 1H), 7.41 (ddd, *J* = 8.3, 7.4, 1.7, 1H), 7.02 (dt, *J* = 7.5, 1.0, 1H), 6.98 (d, *J* = 8.3, 1H), 3.84 (s, 3H), 2.74 (tt, *J* = 6.4, 1.5, 2H), 2.39 (tt, *J* = 6.4, 1.5, 2H), 1.94–1.86 (m, 2H), 1.77–1.70 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.8, 159.8, 157.4, 131.1, 131.0, 120.8, 118.9, 113.5, 111.1, 55.5, 22.9, 22.8, 22.3, 20.7; IR (film): 2937, 2856, 1634, 1604, 1510, 1470 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{14}H_{16}NO_2$, 230.1176; found, 230.1179.



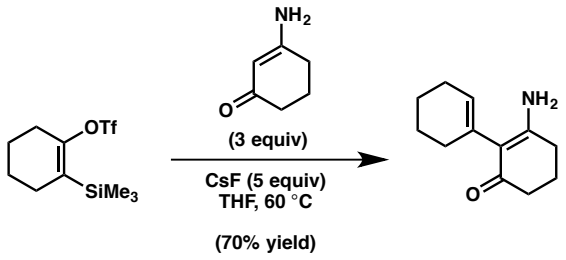
SI-7. Purification by preparative thin layer chromatography (9:1 hexanes : EtOAc) afforded tetrahydroisoquinoline **SI-7** as a colorless oil (40% yield, average of two experiments). R_f 0.10 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.71 (s, 1H), 3.96 (s, 3H), 2.78 (t, *J* = 6.4, 2H), 2.66 (t, *J* = 6.4, 2H), 2.51 (s, 3H), 1.89–1.85 (m, 2H), 1.80–1.76 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.6, 157.8, 146.9, 143.8, 135.6, 124.1, 52.8, 29.5, 26.5, 22.8, 22.6, 21.9; IR (film): 2935, 1741, 1717, 1590, 1436, 1214 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{12}H_{16}NO_2$, 206.1176; found, 206.1173.



SI-8 and SI-9. Purification by preparative thin layer chromatography (9:1 hexanes : EtOAc) afforded adducts **SI-8** (47% yield, average of two experiments) and **SI-9** (34% yield, average of two experiments) as colorless oils. **SI-8**: R_f 0.22 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.19 (dd, *J* = 8.0, 1.7, 1H), 7.59 (ddd, *J* = 8.6, 7.1, 1.7, 1H), 7.36 (dd, *J* = 8.6, 0.6, 1H), 7.33 (ddd, *J* = 8.1, 7.1, 1.1, 1H), 2.66 (tt, *J* = 6.4, 1.5, 2H), 2.57 (tt, *J* = 6.4, 1.5, 2H), 1.90–1.84 (m, 2H), 1.78–1.73 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 177.8, 163.9, 156.0, 133.0, 125.8, 124.5, 123.3, 118.5, 117.7, 28.3, 22.0, 21.8, 21.1; IR (film): 2943, 2872, 1638, 1622, 1609, 1468 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{13}H_{13}O_2$, 201.0910; found, 201.0910. **SI-9**: R_f 0.55 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (dd, *J* = 7.8, 1.7, 1H), 7.44 (ddd, *J* = 8.2, 7.3, 1.7, 1H), 7.10 (dt, *J* = 7.6, 1.1, 1H), 7.06 (dd, *J* = 8.2, 1.1, 1H), 4.84 (tt, *J* = 3.9, 1.2, 1H), 3.88 (s, 3H), 2.26–2.21 (m, 2H), 2.07–2.00 (m, 2H), 1.78–1.72 (m, 2H), 1.61–1.55 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.6, 155.6, 154.2, 133.3, 131.7, 123.0, 122.9, 120.8, 105.5, 52.2, 26.9, 23.7, 23.0, 22.4; IR (film): 2932, 2843, 1733, 1716, 1602, 1227 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{14}H_{17}O_3$, 233.1172; found, 233.1174.

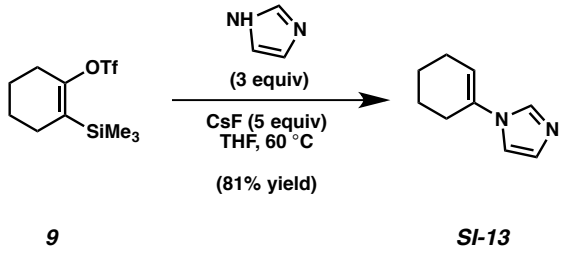


SI-10 and SI-11. Purification by preparative thin layer chromatography (9:1 hexanes : EtOAc) afforded adducts **SI-10** (43% yield, average of two experiments) and **SI-11** (53% yield, average of two experiments) as colorless oils. **SI-10**: R_f 0.25 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (dd, *J* = 8.1, 1.4, 1H), 7.54–7.44 (m, 3H), 2.73–2.65 (m, 4H), 1.88–1.80 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.1, 147.4, 137.2, 131.5, 130.9, 130.5, 129.0, 127.0, 125.7, 31.3, 24.8, 22.4, 22.2; IR (film): 3065, 2934, 2867, 1605, 1581, 1548 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{13}H_{13}OS$, 217.0682; found, 217.0682. **SI-11**: R_f 0.55 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (dd, *J* = 7.9, 1.5, 1H), 7.38 (ddd, *J* = 8.1, 7.3, 1.5, 1H) 7.24 (dd, *J* = 8.1, 0.8, 1H), 7.14 (ddd, *J* = 8.4, 7.9, 1.2, 1H), 6.39–6.37 (m, 1H), 3.91 (s, 3H), 2.27–2.23 (m, 2H), 2.18–2.15 (m, 2H), 1.75–1.70 (m, 2H), 1.68–1.63 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.0, 141.4, 139.6, 132.2, 131.4, 130.1, 127.8, 127.2, 124.3, 52.2, 30.4, 27.3, 23.8, 21.6; IR (film): 2931, 1717, 1588, 1562, 1434, 1249 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{14}H_{17}O_2S$, 249.0944; found, 249.0945.



9 ***SI-12***

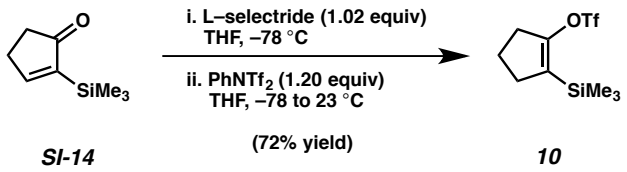
SI-12. Purification by preparative thin layer chromatography (1:1 hexanes : EtOAc) afforded adduct **SI-12** as an amorphous white solid (70% yield, average of two experiments). R_f 0.10 (1:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.53–5.50 (m, 1H), 4.80 (br s, 2H), 2.40 (t, J = 6.1, 2H), 2.31 (t, J = 6.1, 2H), 2.12–2.07 (m, 2H), 2.07–1.98 (m, 2H), 1.96–1.90 (m, 2H), 1.72–1.66 (m, 2H), 1.65–1.59 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 194.8, 159.4, 133.7, 127.9, 115.3, 37.0, 29.1, 28.3, 25.6, 23.1, 22.3, 21.5; IR (film): 3449, 3303, 3164, 2928, 1529, 1405 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{12}H_{18}ON$, 192.1383; found, 192.1376.



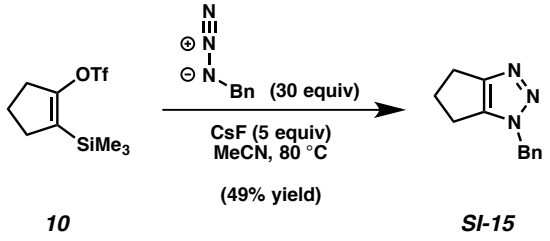
9 ***SI-13***

SI-13. Purification by preparative thin layer chromatography (1:1 hexanes : EtOAc) afforded adduct **SI-13** as a colorless oil (81% yield, average of two experiments). R_f 0.15 (1:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.64 (s, 1H), 7.06 (d, J = 9.8, 2H), 5.83–5.79 (m, 1H), 2.44–2.38 (m, 2H), 2.22–2.15 (m, 2H), 1.85–1.78 (m, 2H), 1.69–1.62 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 134.6, 133.9, 129.4, 116.7, 116.5, 27.4, 24.2, 22.5, 21.8; IR (film): 3390, 3115, 2931, 2861, 1673, 1490 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_9H_{12}N_2$, 149.1073; found, 149.1070.

B. Synthesis of Cyclopentyne Precursor and Trapping Experiments

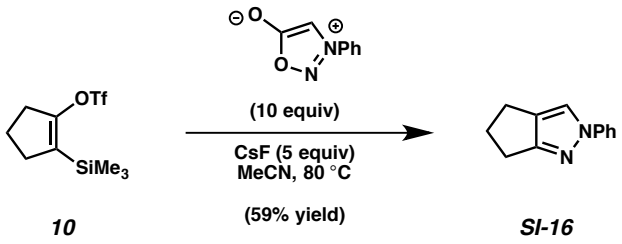


Silyl triflate 10. To a solution of known silyl enone **SI-14**[4] (0.963 g, 67.2 mmol, 1 equiv) in THF (22 mL) at –78 °C was added L-selectride (1 M in THF, 6.37 mL, 6.37 mmol, 1.02 equiv) dropwise over 5 min. The reaction was stirred for 3 h, then a solution of $NPhTf_2$ (2.68 g, 7.49 mmol, 1.2 equiv) in THF (6.2 mL) was added over 5 min. The reaction was allowed to slowly warm to room temperature and was then stirred for 15 h. The reaction was quenched with saturated aqueous ammonium chloride (20 mL). The layers were separated and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine (50 mL), dried over Na_2SO_4, and concentrated *in vacuo* to provide the crude product, which was purified by flash chromatography (hexanes) to afford silyl triflate **10** (1.30 g, 72% yield) as a colorless oil. R_f 0.52 (hexanes); ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.65–2.69 (m, 2H), 2.40–2.44 (m, 2H), 1.97–2.03 (m, 2H), 0.16 (s, 9H); ^{13}C (125 MHz, $CDCl_3$): δ 155.0, 130.5, 118.6 (q, J = 319.8), 32.6, 32.5, 22.2, –1.7; ^{19}F NMR (376 MHz, $CDCl_3$): δ -74.3, IR (film): 2959, 2902, 2857, 1638, 1418, 1315, 1288, 1250, 1204, 1142, 1122, 1068 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_9H_{16}F_3O_3SSi$, 289.0536; found, 289.0525.

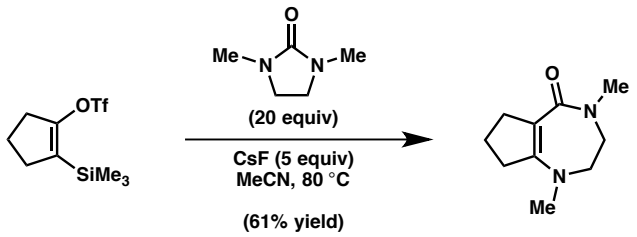


SI-15 (Table 2, entry 1). Silyl triflate **10** (65.4 mg, 0.227 mmol, 1 equiv) was added to a flame-dried vial. In a separate flame-dried vial, benzylazide (0.8 M in benzene, 8.5 mL, 6.8 mmol, 30 equiv) was added and the benzene was removed *in vacuo*. The neat benzylazide was then transferred to the vial containing **10** with MeCN (0.91 mL). CsF (0.172 g, 1.13 mmol, 5 equiv) was added and the vial was capped and heated to 80 °C in a pre-heated aluminum heating block. After heating for 6 d, the reaction

was cooled to room temperature and filtered through a small plug of silica gel (EtOAc eluent, 10 mL). The solvent was removed *in vacuo* and the crude material was purified by flash chromatography (3:1→1:1 hexanes : EtOAc) to provide triazole **SI-15** (49% yield, average of two experiments) as a white solid. R_f 0.39 (1:1 hexanes : EtOAc); Mp: 7.4–73.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33–7.37 (m, 3H), 7.24–7.26 (m, 2H), 5.41 (s, 2H), 2.72–2.74 (m, 2H), 2.51–2.57 (m, 2H), 2.38–2.41 (m, 2H); ^{13}C (125 MHz, $CDCl_3$): δ 156.8, 142.1, 134.7, 129.1, 128.7, 128.3, 53.3, 30.4, 22.7, 21.8; IR (film): 3063, 3032, 2978, 2955, 2937, 2921, 2866, 1572, 1495, 1452, 1373, 1275, 1230, 1176, 1084, 1059 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{12}H_{14}N_3$, 200.1182; found, 200.1174.



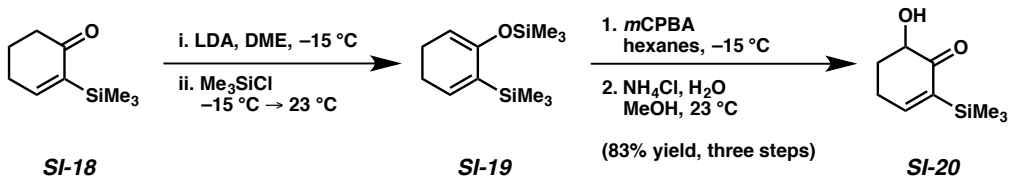
SI-16 (Table 2, entry 2). To a solution of silyl triflate **10** (50.4 mg, 0.175 mmol, 1 equiv) in MeCN (1.4 mL) in a flame-dried vial was added the sydnone (0.283 g, 1.75 mmol, 10 equiv), and CsF (0.133 g, 0.874 mmol, 5 equiv). The vial was capped and heated to 80 °C in a pre-heated aluminum block. After stirring for 17 h, the reaction was cooled to room temperature and filtered through a small plug of silica gel (EtOAc eluent, 10 mL). The solvent was removed *in vacuo* and the crude material was purified by flash chromatography (39:1→19:1 hexanes : EtOAc) to afford pyrazole **SI-16** (59% yield, average of two experiments) as a white solid. R_f 0.36 (9:1 hexanes : EtOAc); Mp: 74.9–75.6 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.61–7.63 (m, 2H), 7.53 (s, 1H), 7.38–7.42 (m, 2H), 7.19–7.26 (m, 1H), 2.79–2.82 (m, 2H), 2.70–2.73 (m, 2H), 2.42–2.47 (m, 2H); ^{13}C (125 MHz, $CDCl_3$): δ 164.0, 141.1, 129.5, 127.4, 125.6, 120.6, 118.7, 30.1, 24.7, 23.2; IR (film): 3109, 3051, 2962, 2947, 2866, 2853, 1598, 1577, 1504, 1460, 1440, 1376, 1212, 1036 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{12}H_{13}N_2$, 185.1073; found, 185.1065.



10 ***SI-17***

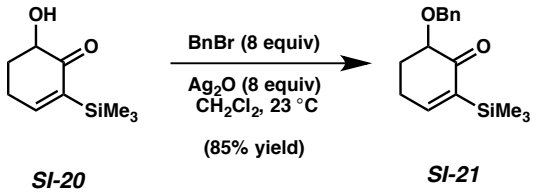
SI-17 (Table 2, entry 3). To a solution of silyl triflate **10** (44.8 mg, 0.155 mmol, 1 equiv) in MeCN (0.62 mL) in a flame-dried vial was added DMI (0.34 mL, 3.11 mmol, 20 equiv) and CsF (0.118 g, 0.777 mmol, 5 equiv). The vial was capped and heated to 80 °C in a pre-heated aluminum block. After stirring for 23 h, the reaction was cooled to room temperature and filtered through a small plug of silica gel (EtOAc eluent, 10 mL). The solvent was removed *in vacuo* and the crude product was purified by flash chromatography (EtOAc→49:1→19:1 CH_2Cl_2 : MeOH) to afford vinylogous urea **SI-17** (61% yield, average over two experiments) as a colorless oil. R_f 0.34 (9:1 CH_2Cl_2 : MeOH); ^{1}H NMR (500 MHz, $CDCl_3$): δ 3.45–3.46 (m, 2H), 3.31–3.33 (m, 2H), 2.98 (s, 3H), 2.89 (s, 3H), 2.73 (t, J = 7.3, 2H), 2.60 (t, J = 7.6, 2H), 1.75 (p, J = 7.5, 2H); ^{13}C (125 MHz, $CDCl_3$): δ 168.9, 152.1, 101.4, 55.6, 49.2, 41.1, 36.6, 36.4, 34.5, 20.6; IR (film): 2938, 2845, 1587, 1574, 1560 1490, 1431, 1404, 1305, 1204, 1090 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{10}H_{17}N_2O$, 181.1335; found, 181.1327.

C. Synthesis of 3-Benzyloxy-Cyclohexyne Precursor.



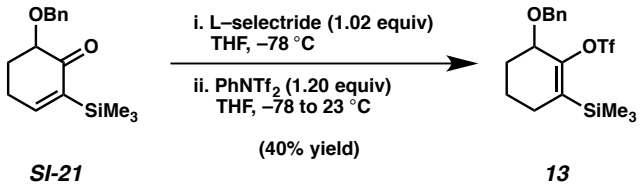
α-Hydroxy-silylenone SI-20. To a solution of *i*Pr_2NH (0.5 mL, 3.57 mmol, 1.2 equiv) in DME (7.4 mL) at –15 °C was added *n*–BuLi (2.52 M in hexanes, 1.3 mL, 3.27 mmol, 1.1 equiv). The reaction was stirred for 20 min, then known ketone **SI-18**[4] (0.500 g, 2.97 mmol, 1 equiv) in DME (3.5 mL) was added. After stirring for 30 min at –15 °C, TMSCl (0.75 mL, 5.94 mmol, 2 equiv) was added and the mixture was allowed to warm to room temperature. After stirring for 2 h, the solvent was removed *in vacuo*. The residue was suspended in pentane (15 mL), filtered and concentrated *in vacuo* to give silyl enol ether **SI-19**, which was used in the next step without further purification.

Silyl enol ether **SI-19** was dissolved in hexanes (5 mL) and added to a mixture of *m*CPBA (77%, 0.732 g, 4.24 mmol, 1.1 equiv) in hexanes (42 mL) at –15 °C. The reaction was allowed to warm to room temperature, stirred for 2 h, and then filtered and concentrated *in vacuo*. The residue was dissolved in MeOH (5 mL) and saturated aqueous ammonium chloride (5 mL) was added. After stirring for 25 min, saturated aqueous sodium bicarbonate (20 mL) was added. The layers were separated and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine (40 mL), dried over Na_2SO_4 and concentrated *in vacuo* to give a crude oil. Purification by flash chromatography (9:1 hexanes : EtOAc) provided α–hydroxy-silylenone **SI-20** (0.457 g, 83% yield) as a yellow oil. R_f 0.27 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.06–7.08 (m, 1H), 4.09 (dd, *J* =13.8, 5.7, 1H), 3.82 (bs, 1H), 2.47 (m, 2H), 2.28–2.33 (m, 1H), 1.72–1.81 (m, 1H), 0.09 (s, 9H); ^{13}C (125 MHz, $CDCl_3$): δ 203.2, 159.1, 139.1, 72.5, 31.3, 27.5, –1.5; IR (film): 3483, 2954, 2899, 2870, 2824, 1664, 1591, 1457, 1423, 1332, 1246, 1167, 1144, 1113, 1076 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_9H_{17}O_2Si$, 185.0992; found, 185.0989.



SI-20 ***SI-21***

Benzyloxy-silylenone SI-21. α–Hydroxy-silylenone **SI-20** (1.00 g, 5.43 mmol, 1 equiv) was dissolved in CH_2Cl_2 (22 mL) and BnBr (5.2 mL, 43.41 mmol, 8 equiv) and Ag_2O (10.06 g, 43.41 mmol, 8 equiv) were added. After stirring for 14 h at room temperature, the reaction was filtered through celite (CH_2Cl_2 eluent, 30 mL) and concentrated *in vacuo*. The crude product was purified by flash chromatography (benzene→99:1→49:1 benzene : EtOAc) to give benzyloxy-silylenone **SI-21** (1.269 g, 85% yield) as a white solid. Mp: 56.5–59.5 °C; R_f 0.60 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38 (app. dd, *J* = 7.3, 1.4, 2H), 7.34 (app dt, *J* = 7.3, 1.8, 2H), 7.28 (app. tt, *J* = 6.5, 2.1, 1H), 7.06 (ddd, *J* = 3.9, 3.0, 0.6, 1H), 4.87 (d, *J* = 11.9, 1H), 4.60 (d, *J* = 11.9, 1H), 3.89 (dd, *J* = 11.0, 4.6, 1H), 2.57 (dq, *J* = 19.4, 4.4, 1H), 2.46–2.36 (m, 1H), 2.21 (dq, *J* = 13.2, 4.4, 1H), 2.14–2.03 (m, 1H), 0.17 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 201.5, 157.3, 140.8, 138.4, 128.4, 127.9, 127.7, 78.7, 72.1, 29.6, 26.9, -1.3; IR (film): 3031, 2953, 1749, 1673, 1593, 1338 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{16}H_{23}O_2Si$, 275.1462; found, 275.1453.

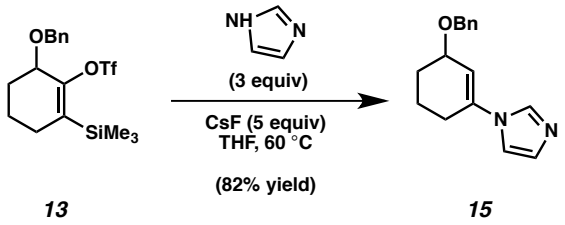


SI-21 ***13***

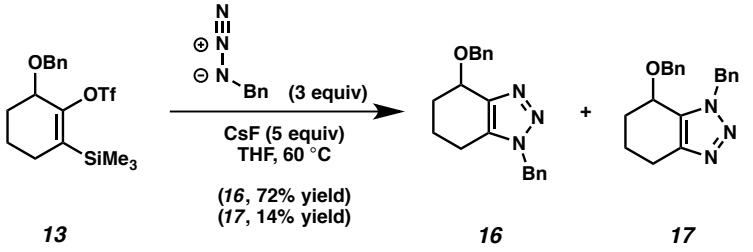
Benzyloxy-silyltriflate 13. To a solution of benzyloxy-silylenone **SI-21** (0.148 mg, 0.541 mmol, 1 equiv) in THF (2.2 mL) at –78 °C was added L-selectride (1 M in THF, 552 μL, 0.552 mmol, 1.02 equiv) dropwise over 5 min. The reaction was stirred for 3 h at –78 °C, then a solution of $NPhTf_2$ (233 mg, 0.649 mmol, 1.20 equiv) in THF (0.5 mL) was added dropwise over 5 min. The reaction was allowed to slowly warm to 23 °C and was stirred for an additional 15 h. The reaction was then quenched with saturated NH_4Cl (4 mL). The layers were separated and the aqueous layer was extracted with EtOAc (3 × 4 mL). The combined organic layers were washed with brine (5 mL), dried over Na_2SO_4 and concentrated *in vacuo*. Further purification by column chromatography with basic Brockman Grade I 58

Å Al_2O_3 (Activity 1) as the stationary (hexanes) afforded benzyloxy-silyltriflate **13** (88.6 mg, 40% yield) as a colorless oil. R_f 0.80 (9:1 hexanes : EtOAc); ^{1}H NMR (500 MHz, C_6D_6): δ 7.34 (d, J = 7.6, 2H), 7.19–7.12 (m, 2H), 7.08 (t, J = 7.6, 1H), 4.32 (dd, J = 46.3, 10.9, 2H), 4.16 (app. t, J = 4.2, 1H), 1.91 (dt, J = 17.9, 4.2, 1H), 1.77–1.61 (m, 2H), 1.53–1.41 (m, 1H), 1.30 (app. tt, J = 12.3, 3.3, 1H), 1.16–1.04 (m, 1H), 0.15 (s, 9H); ^{13}C (125 MHz, CD_2Cl_2): δ 152.9, 138.7, 134.1, 128.6, 128.3, 128.0, 118.8 (q, J = 332.0), 73.4, 70.9, 29.3, 28.2, 17.9, -1.3 ; IR (film): 3210, 3035, 2950, 2868, 1643, 1401 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{17}H_{24}O_4SSiF_3$, 409.1111; found, 409.1094.

D. 3-Benzyloxy-Cyclohexyne Trapping Experiments.



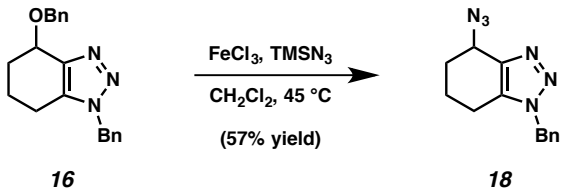
Imidazoyl-cyclohexene 15 (Figure 3). To a solution of silyl triflate **13** (51.6 mg, 0.126 mmol, 1 equiv) in THF (5.1 mL) in a flame-dried vial was added imidazole (25.8 mg, 0.379 mmol, 3 equiv) and CsF (95.9 mg, 0.632 mmol, 5 equiv). The vial was capped and heated to 60 °C in a pre-heated aluminum block. After stirring for 17.5 h, the reaction was cooled to room temperature and filtered through a small plug of silica gel (EtOAc eluent, 10 mL). The solvent was removed *in vacuo* and the crude product was purified by flash chromatography (3:1 EtOAc : hexanes) to afford imidazoyl-cyclohexene **15** as a colorless oil (82% yield, average of two experiments). R_f 0.50 (EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.70 (s, 1H), 7.36–7.27 (m, 5H), 7.12 (s, 1H), 7.07 (s, 1H), 5.92 (m, 1H), 4.65 (d, J = 11.8, 1H), 4.57 (d, J = 11.8, 1H), 4.18–4.15 (m, 1H), 2.53–2.48 (m, 1H), 2.44–2.38 (m, 1H), 2.06–2.01 (m, 1H), 1.88–1.74 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.6, 136.9, 134.6, 129.8, 128.6, 127.8, 127.8, 116.5, 115.7, 71.7, 70.7, 27.7, 27.3, 18.6; IR (film): 3396, 3117, 2942, 2866, 1669, 1491, 1454, 1392, 1292, 1246, 1073 cm^{-1}; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{16}H_{19}N_2O$, 255.1492; found, 255.1483.



Triazoles 16 and 17 (Figure 3). Silyl triflate **13** (50.7 mg, 0.124 mmol, 1 equiv) was added to a flame-dried vial. In a separate flame-dried vial benzylazide (0.8 M in benzene, 0.47 mL, 0.37 mmol, 3 equiv) was added and the benzene was removed *in vacuo*. The neat benzylazide was then transferred to the vial containing **13** with THF (5.0 mL). CsF (0.094 g, 0.62 mmol, 5 equiv) was added and the vial was capped and heated to 60 °C in a pre-heated aluminum heating block. After 21 h, the reaction was cooled

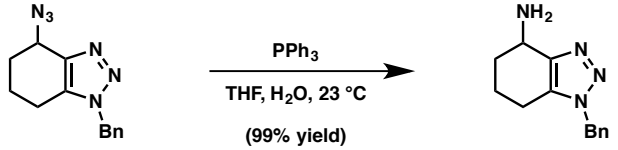
to room temperature and filtered through a small plug of silica gel (EtOAc eluent, 10 mL). The solvent was removed *in vacuo* and the crude product was purified by flash chromatography (5:3:2 hexanes : EtOAc : benzene) to provide triazole **16** (72% yield, average over two experiments) as a colorless oil and triazole **17** (14% yield, average over two experiments) as a colorless oil. Triazole **16**: R_f 0.47 (5:3:2 hexanes : EtOAc : benzene); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.19–7.42 (m, 10H), 5.49 (d, *J* = 15.4, 1H), 5.40 (d, *J* = 15.4, 1H), 4.88 (d, *J* = 12.0, 1H), 4.80 (d, *J* = 12.0, 1H), 4.70 (t, *J* = 3.6, 1H), 2.55 (ddd, *J* = 16.5, 5.8, 3.0, 1H), 2.29 (ddd, *J* = 16.5, 10.5, 6.0, 1H), 2.11–2.16 (m, 1H), 1.99–2.08 (m, 1H), 1.77–1.83 (m, 1H), 1.65–1.71 (m, 1H); ^{13}C (125 MHz, $CDCl_3$): δ 144.2, 138.8, 134.7, 133.9, 129.1, 128.4, 128.4, 127.9, 127.7, 127.5, 10.7, 67.9, 52.0, 29.4, 20.2, 18.1; IR (film): 3063, 3031, 2946, 2866, 1605, 1586, 1497, 1455, 1436, 1314, 1237, 1208, 1116, 1089, 1070, 1047, 1028 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{20}H_{22}N_3O$, 320.1757; found, 320.1744. Triazole **17**: R_f 0.35 (5:3:2 hexanes : EtOAc : benzene); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.39–7.27 (m, 8H), 7.04–7.03 (m, 2H), 5.64 (d, *J* = 15.1, 1H), 5.31 (d, 15.1, 1H), 4.65 (d, *J* = 11.3, 1H), 4.40 (t, *J* = 4.7, 1H), 4.39 (d, *J* = 11.3, 1H), 2.84 (dt, *J* = 16.0, 5.5, 1H), 2.69 (ddd, *J* = 16.0, 8.3, 5.6, 1H), 2.09–2.03 (m, 1H), 2.01–1.93 (m, 1H), 1.88–1.82 (m, 1H), 1.80–1.74 (m, 1H); ^{13}C (125 MHz, $CDCl_3$): δ 145.8, 137.8 135.3, 131.6, 128.9, 128.8, 128.2, 128.2, 128.1, 127.6, 70.4, 67.9, 52.4, 27.9, 22.1, 19.5; IR (film): 3064, 3031, 2943, 2861, 1587, 1497, 1455, 1358, 1311, 1198, 1159, 1072 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{20}H_{22}N_3O$, 320.1757; found, 320.1745.

E. Derivatization of Triazole 16.



16 *18*

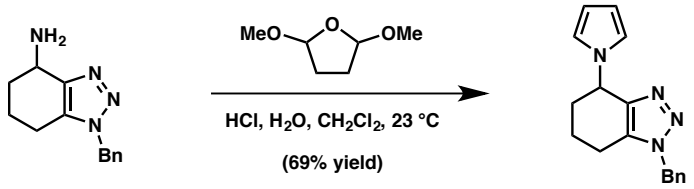
Azide 18 (Scheme 1). Triazole **16** (24.6 mg, 0.077 mmol, 1 equiv) in CH_2Cl_2 (0.39 mL) was added to a vial containing $FeCl_3$ (18.7 mg, 0.116 mmol, 1.5 equiv). $TMSN_3$ (61 μL, 0.462 mmol, 6 equiv) was then added and the vial was capped and heated to 45 °C. After stirring for 18 h, the vial was cooled to room temperature and water (1 mL) was added. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 1 mL). The combined organic layers were washed with brine (3 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The crude product was purified by preparative thin layer chromatography (5:3:2 hexanes : EtOAc : PhH) to provide azide **18** (11.2 mg, 57% yield) as a white solid. R_f 0.40 (5:3:2 hexanes : EtOAc : PhH); Mp: 53.4–55.1 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.37–7.31 (m, 3H), 7.21–7.19 (m, 2H), 5.52 (d, J = 15.4, 1H), 5.43 (d, J = 15.4, 1H), 4.83 (t, J = 4.1, 1H), 2.56–2.51 (m, 1H), 2.35–2.29 (m, 1H), 1.98–1.80 (m, 4H); ^{13}C (125 MHz, $CDCl_3$): δ 142.1, 134.5, 133.9, 129.2, 128.7, 127.7, 53.0, 52.3, 29.2, 20.0, 18.6; IR (film): 3064, 3033, 2949, 2866, 2096, 1587, 1497, 1456, 1436, 1240, 1091, 1071 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{13}H_{15}N_6$, 255.1353; found, 255.1347.



18 *SI-22*

Amine SI-22 (Scheme 1). Water (21 μL, 1.18 mmol, 10 equiv) was added to a mixture of azide **18** (30 mg, 0.118 mmol, 1 equiv) and PPh_3 (93 mg, 0.354 mmol, 3 equiv) in THF (1.2 mL) at room temperature. After stirring for 18 h, the reaction was concentrated *in vacuo*. The crude material was purified by flash chromatography (EtOAc→9:1 CH_2Cl_2 : MeOH) to afford amine **SI-22** (26.5 mg, 99% yield) as a colorless oil. R_f 0.21 (9:1 CH_2Cl_2 : MeOH); Mp: 89.6–91.6 °C; ^{1}H NMR (500 MHz, $CDCl_3$):

δ 7.35–7.30 (m, 3H), 7.19–7.18 (m, 2H), 2.43 (s, 2H), 4.19 (t, *J* = 5.6, 1H), 2.50 (bs, 2H), 2.46–2.35 (m, 2H), 2.06–1.95 (m, 2H), 1.76–1.69 (m, 1H), 1.60–1.54 (m, 1H); ^{13}C (125 MHz, $CDCl_3$): δ 147.3, 134.8, 132.4, 129.1, 128.5, 127.7, 52.1, 44.6, 32.1, 20.2, 19.9; IR (film): 3361, 3063, 3032, c2932, 2860, 1586, 1497, 1456, 1303, 1242, 1204, 1098, 1074 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{13}H_{17}N_4$, 229.1448; found, 229.1449.



SI-22 ***19***

Triazolopyrrole 19 (Scheme 1). To a vial containing HCl (0.1 M in H_2O, 0.22 mL) was added 2,5-dimethoxytetrahydrofuran (28.4 μL, 0.219 mmol, 4 equiv) and the mixture was heated to 100 °C. After 30 min, the vial was cooled to room temperature and the mixture was added to a solution of amine **SI-22** (11.8 mg, 0.055 mmol, 1 equiv) in CH_2Cl_2 (0.55 mL). The reaction was stirred at room temperature for 15 h, then aqueous sodium hydroxide (1 M in H_2O, 1 mL) was added. The solution was extracted with CH_2Cl_2 (3 × 1 mL). The combined organic layers were washed with brine (2 mL), dried over Na_2SO_4, filtered and concentrated *in vacuo*. The crude product was purified by flash chromatography (3:2 hexanes : EtOAc) to provide triazolopyrrole **19** (10.5 mg, 69% yield) as a white solid. R_f 0.46 (1:1 hexanes : EtOAc); Mp: 168.4–170.6 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.37–7.34 (m, 3H), 7.23–7.21 (m, 2H), 6.61 (t, *J* = 2.2, 2H), 6.14 (t, *J* = 2.2, 2H), 5.53 (d, *J* = 15.3, 1H), 5.47 (d, *J* = 15.3, 1H), 5.41 (t, *J* = 4.8, 1H), 2.57 (dt, *J* = 16.5, 5.2, 1H), 2.40 (dt, *J* = 16.5, 7.5, 1H), 2.18–2.13 (m, 1H), 2.10–2.03 (m, 1H), 1.85–1.80 (m, 2H); ^{13}C (125 MHz, $CDCl_3$): δ 142.3, 134.6, 134.3, 129.2, 128.7, 127.7, 119.8, 108.2, 52.3, 51.3, 31.8, 20.0, 19.0; IR (film): 3096, 3064, 3033, 2930, 2864, 1587, 1488, 1455, 1434, 1277, 1247, 1089, 1072 cm $^{-1}$; HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{17}H_{19}N_4$, 279.1604; found, 279.1599.

Computational Methods. All calculations were carried out with the meta-hybrid M06-2X[5] functional and 6-311+G(2d,p) basis set. Full geometry optimizations and transition structure (TS) searches were carried out with the Gaussian 09 package.[6] Thermal and entropic corrections to energy were calculated from vibrational frequencies. The nature of the stationary points was determined in each case according to the appropriate number of negative eigenvalues of the Hessian matrix from the frequency calculations. Scaled frequencies were not considered. Mass-weighted intrinsic reaction coordinate (IRC) calculations were carried out using the Gonzalez and Schlegel scheme[7] in order to ensure that the TSs indeed connected the appropriate reactants and products. Bulk solvent effects were considered implicitly during optimization through the IEF-PCM polarizable continuum model[8] as implemented in Gaussian 09. The parameters for tetrahydrofuran were used to calculate solvation free energies (ΔG_{solv}). The possibility of different conformations was taken into account for all structures. Gibbs free energies (ΔG) were used for the discussion on the relative stabilities of the considered structures. Cartesian coordinates, electronic energies, entropies, enthalpies, Gibbs free energies, and lowest frequencies of the different conformations of all structures are provided.

F. Bent´s Rule and Alkyne Distortion Determine Regioselectivity of Nucleophilic Addition. Henry Bent stated in 1961 that *"atomic s character concentrates in orbitals directed toward electropositive substituents"*. The rationale for this rule is that bonds between elements of different electronegativities are polarized in a way that the electron density will be shifted towards the more electronegative element. Due to the inherent higher stability of *s* orbitals, the hybrid orbitals from the more electronegative atoms will increase their *s* character in order to stabilize the withdrawn electron density. To compensate for this shift in electron density, the less electronegative atoms will direct hybrid orbitals with an increased *p* character toward the more electronegative atoms to which they are bound, without a significant energy penalty. As a result, the hybrid orbitals that constitute these polarized bonds deviate from ideal sp^n (n = 1, 2 or 3) hybridizations, which translates into distorted geometries.

In restrained alkynes bearing an electron-withdrawing substituent, such as 3-methoxycyclohexyne, the C2–C3 is polarized as revealed by the increment in the atomic charge (Δq) at C2 with respect to cyclohexyne (Figure SI-1a); following Bent´s rule, the σ-bonding orbitals (*sp*) at C2 possess more *p* character, which translates into a more compressed internal angle (124º) with respect to cyclohexyne (132º). In turn, the *sp* σ-bonding orbitals of C1 rehybridize to increase their *s* character, which causes the internal angle to be more linear (138º) with respect to cyclohexyne (132º). This change in geometry is associated with a very slight polarization of the C1–C2 bond and an increase of the *p* character of the reacting orbital and a slightly greater contribution of C1 to the LUMO, but, more importantly, involves a pre-distortion of the reactant towards the geometry that is required to achieve the transition state for nucleophilic addition. For the *distal* attack, only minimal geometric and electronic changes are required to reach the saddle point in the potential energy surface, resulting in a generally early transition state and low activation barrier (Figures SI-1b and 4 in the manuscript). Conversely, attack at the *proximal* position, besides minor electrostatic and steric repulsions, requires a complete redistribution of the electron density and modification of the geometry (*i.e.* distortion) to reallocate the developing negative charge in the C1; this reaction pathway is thus associated to a normally late transition state and a high activation barrier (Figures SI-1b and 4 in the manuscript). Another benefit for regioselectivity is the stabilization of the negative charge of the developing anion at C2, whose non-bonding orbital has an increased *s* character, upon nucleophilic attack at C1.

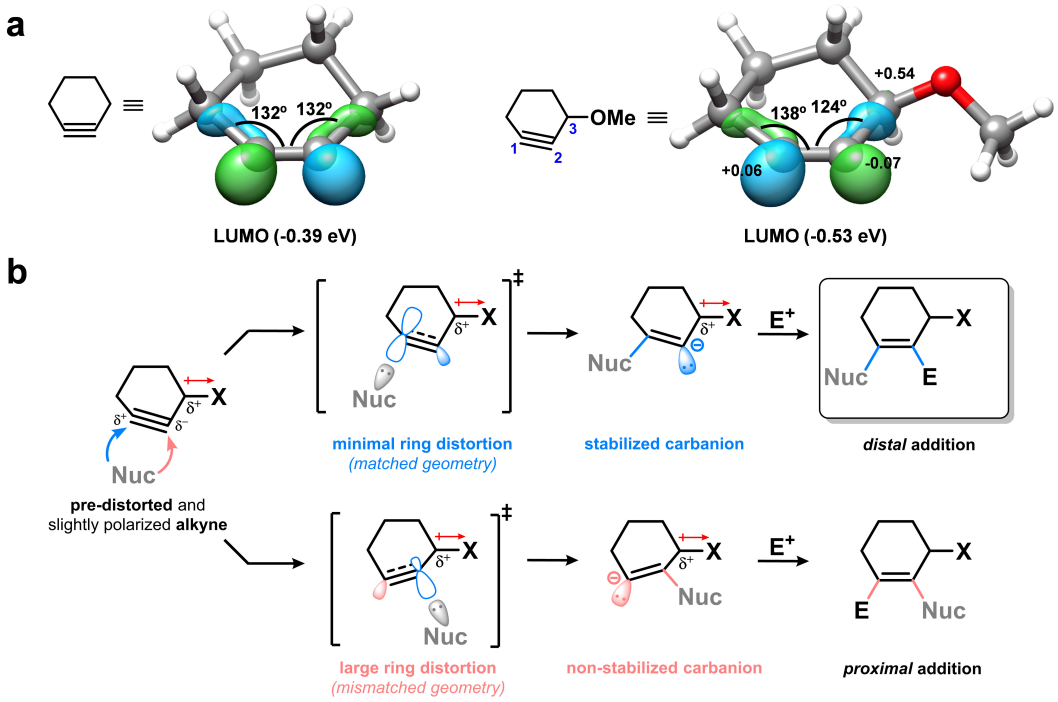
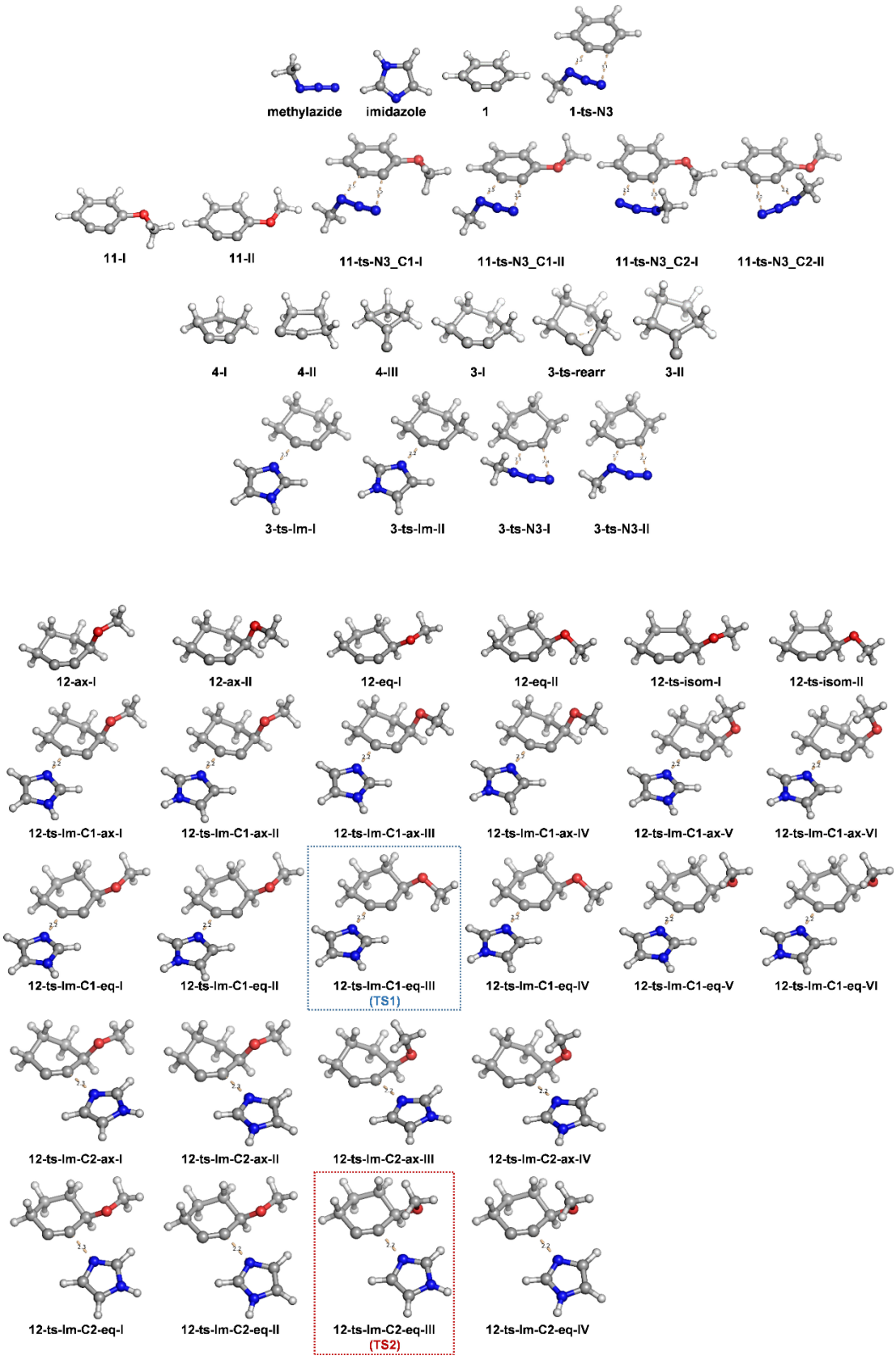


Figure SI-1. a) Structures and isosurface representation of the LUMO of cyclohexyne and 3-methoxycyclohexyne calculated at the PCM(THF)/M06-2X/6-311+G(2d,p) level. Incremental atomic charges (NPA) with respect to cyclohexane are shown. b) Distortion-accelerated regioselective nucleophilic addition at the *distal* position (C1) of strained cycloalkynes.


methylazide
imidazole
1
1-ts-N3
11-I
11-II
11-ts-N3_C1-I
11-ts-N3_C1-II
11-ts-N3_C2-I
11-ts-N3_C2-II
4-I
4-II
4-III
3-I
3-ts-rearr
3-II
3-ts-Im-I
3-ts-Im-II
3-ts-N3-I
3-ts-N3-II
12-ax-I
12-ax-II
12-eq-I
12-eq-II
12-ts-isom-I
12-ts-isom-II
12-ts-Im-C1-ax-I
12-ts-Im-C1-ax-II
12-ts-Im-C1-ax-III
12-ts-Im-C1-ax-IV
12-ts-Im-C1-ax-V
12-ts-Im-C1-ax-VI
12-ts-Im-C1-eq-I
12-ts-Im-C1-eq-II
12-ts-Im-C1-eq-III
(TS1)
12-ts-Im-C1-eq-IV
12-ts-Im-C1-eq-V
12-ts-Im-C1-eq-VI
12-ts-Im-C2-ax-I
12-ts-Im-C2-ax-II
12-ts-Im-C2-ax-III
12-ts-Im-C2-ax-IV
12-ts-Im-C2-eq-I
12-ts-Im-C2-eq-II
12-ts-Im-C2-eq-III
(TS2)
12-ts-Im-C2-eq-IV

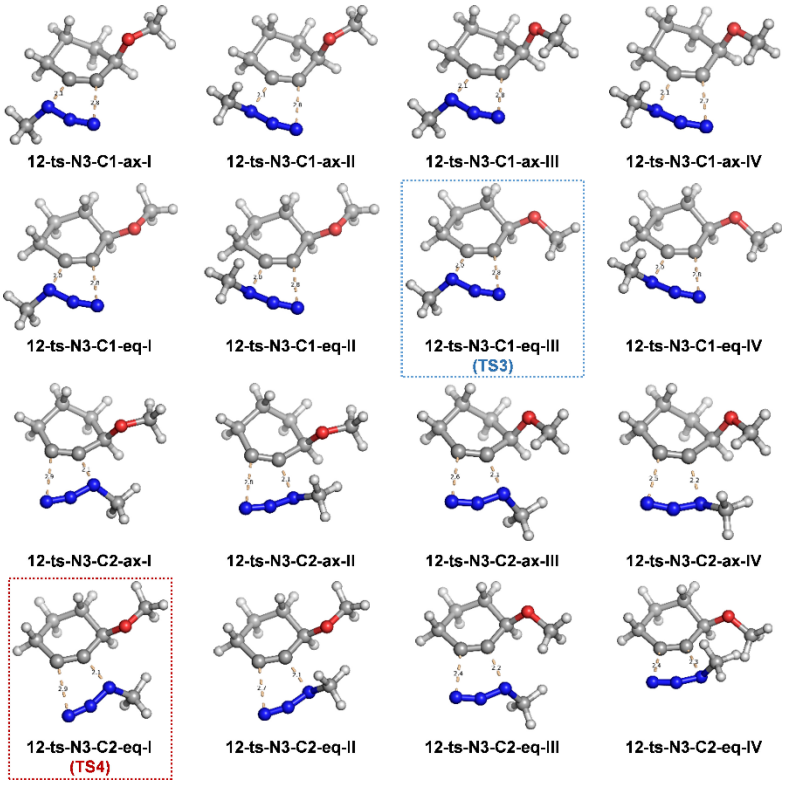


Figure SI-2. **Geometries calculated at the PCM(THF)/M06-2X/6-311+G(2d,p) level.** The minimum energy transition states for 3-methoxycyclohexyne are labeled as TS1-TS4 as shown in Figure 4 of the manuscript.

G. Table SI-1. **Energies, enthalpies, free energies, and entropies of the structures calculated at the PCM(THF)/M06-2X/6-311+G(2d,p) level.**

Structure	E_0	E_0+ZPE	H	S	G	Lowest freq.
	(Hartree)[a]	(Hartree)[a]	(Hartree)[a]	(cal mol^{-1} K^{-1})[b]	(Hartree)[a]	(cm^{-1})
methylazide	–204.069524	–204.018649	–204.013286	67.2	–204.045233	105.8
imidazole	–226.202555	–226.130419	–226.125799	64.9	–226.156640	573.7
1	–230.878167	–230.802434	–230.797046	68.9	–230.829767	393.9
1-ts-N3	–434.950394	–434.822419	–434.811989	97.9	–434.858514	–116.3
11-I	–345.400552	–345.291894	–345.283997	82.2	–345.323071	88.1
11-II	–345.397789	–345.288702	–345.280992	81.1	–345.319529	100.3
11-ts-N3_C1-I	–549.475642	–549.315051	–549.301834	113.2	–549.355610	–22.2
11-ts-N3_C1-II	–549.472332	–549.311289	–549.298277	112.0	–549.351475	–65.0
11-ts-N3_C2-I	–549.468182	–549.306996	–549.294232	109.0	–549.346033	–258.2
11-ts-N3_C2-II	–549.468606	–549.307182	–549.294315	110.1	–549.346617	–127.0
4-II	–193.938760	–193.847196	–193.840924	74.8	–193.876483	18.2
4-I	–193.931905	–193.839749	–193.833657	71.2	–193.867484	166.4
4-III	–193.934091	–193.843322	–193.837020	73.5	–193.871964	64.2
3-I	–233.294602	–233.172350	–233.165836	73.6	–233.200822	220.2
3-ts-rearr	–233.266845	–233.145944	–233.139629	73.5	–233.174555	–279.9
3-II	–233.274581	–233.153708	–233.146671	79.2	–233.184308	22.6
3-ts-N3-I	–437.358527	–437.183951	–437.172698	99.9	–437.220178	–254.5
3-ts-N3-II	–437.358352	–437.183755	–437.172485	100.1	–437.220035	–262.7
3-ts-Im-I	–459.490404	–459.294913	–459.284066	100.3	–459.331718	–149.5
3-ts-Im-II	–459.489721	–459.294291	–459.283418	100.6	–459.331231	–149.6
12-ax-I	–347.804816	–347.649578	–347.640560	87.4	–347.682085	76.6
12-ax-II	–347.808374	–347.652964	–347.644036	86.6	–347.685177	91.2
12-eq-I	–347.805789	–347.650487	–347.641527	87.0	–347.682843	77.7
12-eq-II	–347.809663	–347.654307	–347.645385	86.5	–347.686470	101.3
12-ts-isom-I	–347.794583	–347.639455	–347.630927	85.7	–347.671634	–195.1
12-ts-isom-II	–347.797951	–347.642836	–347.634293	85.8	–347.675050	–189.8
12-ts-N3-C1-ax-I	–551.869777	–551.662152	–551.648313	113.7	–551.702345	–232.6
12-ts-N3-C1-ax-II	–551.869730	–551.662041	–551.648227	113.4	–551.702127	–238.6
12-ts-N3-C1-ax-III	–551.873313	–551.665602	–551.651815	113.3	–551.705641	–248.6
12-ts-N3-C1-ax-IV	–551.873040	–551.665315	–551.651532	113.3	–551.705373	–255.8
12-ts-N3-C1-eq-I	–551.872162	–551.664584	–551.650777	113.5	–551.704692	–215.3
12-ts-N3-C1-eq-II	–551.872052	–551.664345	–551.650636	112.5	–551.704111	–215.3
12-ts-N3-C1-eq-III	–551.875995	–551.668317	–551.654566	112.9	–551.708230	–228.1
12-ts-N3-C1-eq-IV	–551.875920	–551.668118	–551.654438	112.5	–551.707867	–231.7
12-ts-N3-C2-ax-I	–551.870525	–551.662842	–551.649073	112.8	–551.702648	–199.5

12-ts-N3-C2-ax-II	–551.871266	–551.663722	–551.649931	112.9	–551.703574	–212.5
12-ts-N3-C2-ax-III	–551.871594	–551.663903	–551.650166	112.8	–551.703737	–290.4
12-ts-N3-C2-ax-IV	–551.870128	–551.662248	–551.648653	111.6	–551.701666	–315.8
12-ts-N3-C2-eq-I	–551.871229	–551.663389	–551.649739	111.3	–551.702638	–211.7
12-ts-N3-C2-eq-II	–551.870799	–551.663099	–551.649324	112.9	–551.702944	–254.1
12-ts-N3-C2-eq-III	–551.870263	–551.662308	–551.648696	111.8	–551.701819	–340.1
12-ts-N3-C2-eq-IV	–551.869761	–551.661668	–551.648058	112.1	–551.701326	–351.3
12-ts-Im-C1-ax-I	–574.002341	–573.773880	–573.760421	114.7	–573.814916	–136.3
12-ts-Im-C1-ax-II	–574.001586	–573.773181	–573.759691	115.1	–573.814384	–137.7
12-ts-Im-C1-ax-III	–574.005826	–573.777163	–573.763818	113.3	–573.817653	–140.7
12-ts-Im-C1-ax-IV	–574.005155	–573.776492	–573.763141	113.4	–573.817012	–139.9
12-ts-Im-C1-ax-V	–574.002596	–573.773656	–573.760443	112.6	–573.813920	–144.4
12-ts-Im-C1-ax-VI	–574.001827	–573.772935	–573.759692	113.0	–573.813401	–144.6
12-ts-Im-C1-eq-I	–574.005167	–573.776671	–573.763283	113.7	–573.817317	–130.2
12-ts-Im-C1-eq-II	–574.004410	–573.775909	–573.762522	113.8	–573.816572	–128.6
12-ts-Im-C1-eq-III	–574.009116	–573.780513	–573.767187	112.9	–573.820843	–134.7
12-ts-Im-C1-eq-IV	–574.008479	–573.779863	–573.766533	113.1	–573.820249	–131.7
12-ts-Im-C1-eq-V	–574.006685	–573.778075	–573.764687	113.9	–573.818796	–135.3
12-ts-Im-C1-eq-VI	–574.006004	–573.777504	–573.764062	114.8	–573.818605	–133.5
12-ts-Im-C2-ax-I	–574.002396	–573.774125	–573.760587	114.9	–573.815185	–122.8
12-ts-Im-C2-ax-II	–574.002866	–573.774556	–573.761054	114.4	–573.815409	–121.7
12-ts-Im-C2-ax-III	–574.003910	–573.775438	–573.762030	113.8	–573.816099	–122.4
12-ts-Im-C2-ax-IV	–574.003894	–573.775305	–573.761943	113.2	–573.815751	–119.8
12-ts-Im-C2-eq-I	–574.002460	–573.774222	–573.760689	114.7	–573.815201	–116.9
12-ts-Im-C2-eq-II	–574.002531	–573.774280	–573.760734	115.1	–573.815434	–119.5
12-ts-Im-C2-eq-III	–574.004123	–573.775543	–573.762113	113.8	–573.816198	–129.3
12-ts-Im-C2-eq-IV	–574.004223	–573.775521	–573.762168	112.7	–573.815730	–129.0

[a] 1 Hartree = 627.5 kcal mol^{-1}. [b] Thermal corrections at 298.15 K.

H. Cartesian coordinates of the structures calculated at the PCM(THF)/M06-2X/6-311+G(2d,p) level.

Structure **methylazide**

N	-0.39258	-0.64808	-0.00047
N	0.71041	-0.11252	-0.00030
N	1.75818	0.28788	0.00067
C	-1.52609	0.29808	-0.00003
H	-2.42886	-0.30374	-0.00062
H	-1.51189	0.92553	0.89233
H	-1.51150	0.92671	-0.89157

Structure **imidazole**

N	0.13485	-1.22075	0.00009
C	-0.98467	-0.53818	0.00002
C	1.13640	-0.27758	-0.00009
H	-1.98091	-0.94986	0.00003
C	0.60478	0.97963	0.00010
H	2.17723	-0.55555	-0.00014
H	-1.45425	1.52086	-0.00013
H	1.05236	1.95753	0.00016
N	-0.75351	0.79650	-0.00007

Structure **1**

C	-0.70045	1.05163	0.00000
C	-1.45847	-0.12952	0.00000
C	-0.61946	-1.22723	0.00000
C	0.61700	-1.22753	0.00000
C	1.45847	-0.13200	0.00000
C	0.70239	1.05047	0.00000
H	-1.22239	2.00135	0.00000
H	-2.53898	-0.13017	0.00000
H	2.53896	-0.13472	0.00000
H	1.22597	1.99929	0.00000

Structure **1**-ts-N3

C	-2.40041	-1.04392	0.11052
C	-1.03721	-1.29213	0.32094
C	-0.34009	-0.12003	0.18435
C	-0.66799	1.06444	-0.06977
C	-2.02268	1.34412	-0.28376
C	-2.87684	0.24176	-0.18448
H	-3.09925	-1.86873	0.18242
H	-0.64298	-2.27069	0.55687
H	-2.41481	2.32890	-0.50821
H	-3.94113	0.38093	-0.33587
N	2.33194	1.80157	0.15446
N	2.22766	0.69335	0.25179
N	1.91273	-0.48468	0.44338
C	2.36758	-1.42312	-0.60361
H	3.45340	-1.51271	-0.59186
H	1.92756	-2.38495	-0.35970
H	2.02678	-1.10301	-1.58904

Structure **11-I**

C	-1.90640	0.81795	0.00011
C	-2.32940	-0.52721	-0.00035
C	-1.19975	-1.29829	-0.00018
C	0.02134	-1.08018	-0.00019
C	0.47393	0.23653	-0.00059
C	-0.56207	1.18996	-0.00014
H	-2.66393	1.59331	0.00050
H	-3.36300	-0.83385	-0.00023
H	-0.29088	2.23848	0.00015
O	1.75139	0.65042	-0.00028
C	2.72833	-0.38322	-0.00020
H	3.69590	0.10978	0.00018
H	2.62274	-1.00411	0.89112
H	2.62324	-1.00369	-0.89187

Structure **11-II**

C	-1.98900	0.78248	0.00003
C	-2.34683	-0.57312	-0.00011
C	-1.17964	-1.29985	0.00040
C	0.01997	-1.00337	0.00023
C	0.42723	0.32815	-0.00065
C	-0.65761	1.22580	-0.00034
H	-2.77972	1.52426	0.00035
H	-3.36510	-0.92799	0.00017
H	-0.47600	2.29196	-0.00020
O	1.72716	0.66945	-0.00040
C	2.03567	2.05698	-0.00069
H	3.11943	2.12222	-0.00033
H	1.63730	2.54088	-0.89441
H	1.63667	2.54140	0.89247

Structure **11-ts-N3_C1-I**

C	1.03114	2.38353	0.01151
C	-0.35718	2.22820	0.19146
C	-0.60998	0.88758	0.22227
C	0.04500	-0.17424	0.13610
C	1.42126	-0.02791	-0.03947
C	1.89551	1.29472	-0.10113
H	1.43818	3.38681	-0.03732
H	-1.05136	3.04825	0.28891
H	2.95743	1.45804	-0.23720
N	-2.66196	-1.81229	0.37137
N	-2.91830	-0.72540	0.30680
O	2.31285	-1.03399	-0.15280
C	1.77234	-2.34549	-0.07403
H	1.05078	-2.50998	-0.87626
H	2.61111	-3.02782	-0.17890
H	1.28046	-2.49868	0.88811
N	-3.08105	0.49444	0.33507
C	-3.62084	1.06458	-0.91726
H	-3.61378	2.14237	-0.78902
H	-2.99570	0.79492	-1.76981
H	-4.64450	0.72882	-1.08433

Structure **11-ts-N3_C1-II**

C	0.90423	2.44654	0.11028
C	-0.47621	2.24238	0.22764
C	-0.68913	0.88847	0.21946
C	0.01316	-0.13959	0.13942
C	1.39255	0.04712	0.02329
C	1.81859	1.38735	0.01022
H	1.28144	3.46268	0.09960
H	-1.20170	3.03646	0.31345
H	2.86909	1.62851	-0.07533
N	-2.66610	-1.85558	0.32617

N	-2.93323	-0.77229	0.25447
O	2.21575	-1.02010	-0.06621
C	3.60706	-0.76491	-0.17855
H	3.97549	-0.22477	0.69615
H	4.08773	-1.73714	-0.23605
H	3.82638	-0.19334	-1.08294
N	-3.10149	0.44803	0.27667
C	-3.64873	1.00881	-0.97662
H	-3.65711	2.08674	-0.84936
H	-3.01950	0.74658	-1.82843
H	-4.66751	0.65862	-1.14324

Structure **11-ts-N3_C2-I**

C	1.87690	1.08069	-0.00013
C	1.32053	-0.20799	-0.04865
C	-0.06668	-0.26671	-0.02230
C	-0.71604	0.81641	0.03276
C	-0.33110	2.13202	0.09107
C	1.06995	2.21650	0.06698
H	2.95562	1.17940	-0.01410
H	1.53941	3.19293	0.09792
N	-2.84819	0.33877	-0.05316
N	-2.67593	-0.78279	-0.12179
H	-0.97674	2.99660	0.13784
O	2.16295	-1.26491	-0.11077
C	1.54262	-2.54114	-0.09103
H	0.84679	-2.64515	-0.92598
H	2.34236	-3.27177	-0.17514
H	1.00213	-2.68499	0.84736
N	-2.05555	-1.81960	-0.29617
C	-2.13441	-2.82651	0.77707
H	-1.95456	-2.37414	1.75220
H	-3.10879	-3.31389	0.75987
H	-1.36635	-3.56174	0.55942

Structure **11-ts-N3_C2-II**

C	1.88388	1.16139	0.10013
C	1.15119	-0.02623	-0.04951
C	-0.20193	0.23810	-0.10562
C	-0.80881	1.33073	-0.05271
C	-0.14309	2.54961	0.09570
C	1.24269	2.41013	0.16897
H	2.96346	1.12580	0.16175
H	1.86022	3.29477	0.28059
N	-3.35090	-0.28476	-0.38249
N	-2.50874	-1.01753	-0.31418
H	-0.61781	3.52034	0.14707
O	1.65150	-1.27484	-0.13061
C	3.06504	-1.40439	-0.06759
H	3.44618	-1.02815	0.88382
H	3.27372	-2.46677	-0.15186
H	3.53897	-0.86943	-0.89280
N	-1.43411	-1.62534	-0.32521
C	-1.20474	-2.50788	0.83859
H	-1.35716	-1.96637	1.77306
H	-1.86498	-3.37321	0.79329
H	-0.17106	-2.82874	0.76524

Structure **4-II**

C	0.41699	-0.09200	-0.18207
C	0.03747	1.07079	-0.45054
C	1.61400	1.23873	0.21859
C	1.28665	-1.17254	0.29289
C	2.34723	-0.10150	0.64967
H	1.58976	-1.86698	-0.48632
H	0.88639	-1.71404	1.14610
H	3.26526	-0.23255	0.08476
H	2.57514	-0.08827	1.71127
H	2.15288	1.75040	-0.56997
H	1.44327	1.88926	1.06813

Structure **4-I**

C	-0.12490	-0.46442	-0.25326
C	1.08555	-0.46360	-0.19531
C	1.72971	0.88005	0.07010
C	0.47498	1.79388	-0.21646
C	-0.79761	0.87533	-0.04843
H	2.06244	0.93422	1.10670
H	2.57369	1.12116	-0.57225
H	0.44453	2.69602	0.39750
H	0.52317	2.11161	-1.25903
H	-1.22554	0.92720	0.95277
H	-1.57883	1.11386	-0.76658

Structure **4-III**

C	0.54061	-0.10712	-0.12892
C	0.63918	-1.32442	-0.52699
C	1.54899	1.02859	0.12625
C	0.42561	2.02878	-0.23542
C	-0.61739	0.90407	-0.03499
H	1.80815	1.05975	1.18382
H	2.44645	1.01205	-0.48472
H	0.32806	2.90862	0.39541
H	0.48618	2.32823	-1.27979
H	-1.03148	0.89637	0.97252
H	-1.40717	0.79041	-0.77143

Structure **3-I**

C	1.29419	-0.05998	-0.80867
C	2.72869	-0.20708	-1.14298
C	3.20266	1.28607	-1.14312
C	2.61327	2.14900	-0.01384
C	1.05020	2.25222	-0.01478
C	0.66439	0.86286	-0.34946
H	4.29291	1.30385	-1.07422
H	3.24406	-0.79092	-0.37842
H	2.92770	-0.67183	-2.10797
H	2.92190	1.73493	0.94966
H	3.02742	3.15774	-0.08188
H	0.68947	2.60688	0.95006
H	0.69478	2.94499	-0.77947
H	2.93022	1.72492	-2.10657

Structure **3-ts-rearr**

C	1.30547	0.25929	-0.64916
C	2.67678	-0.04367	-1.07879
C	3.33183	1.35082	-1.16852
C	2.70821	2.13511	-0.02366
C	1.17647	2.05317	-0.11365
C	0.14194	0.56968	-0.32051
H	4.41713	1.28835	-1.10438
H	3.17994	-0.66347	-0.33495
H	2.68057	-0.57047	-2.03236
H	3.03445	1.71399	0.93016
H	2.98755	3.19054	-0.03612
H	0.73590	2.34647	0.83221

H	0.79515	2.67101	-0.92078
H	3.07004	1.81090	-2.12344

Structure **3-II**

C	1.20585	0.53912	-0.38174
C	2.55640	0.04789	-0.92843
C	3.30302	1.36195	-1.20406
C	2.82102	2.28966	-0.09236
C	1.30716	2.03331	-0.03613
C	0.15609	-0.19238	-0.24148
H	4.38305	1.21735	-1.21219
H	3.06216	-0.51901	-0.14524
H	2.44896	-0.59064	-1.80213
H	3.28003	2.00189	0.85630
H	3.04515	3.34028	-0.27495
H	0.85454	2.27327	0.92316
H	0.79557	2.60446	-0.81236
H	3.00358	1.76004	-2.17635

Structure **3-ts-N3-I**

C	-2.29338	-1.03150	-0.35073
C	-2.68540	0.18136	0.50444
C	-1.89476	1.46141	0.14006
C	-0.45046	1.07638	-0.03601
C	-0.12496	-0.10961	-0.16744
C	-0.79192	-1.42130	-0.20795
H	-2.26413	1.88829	-0.79658
H	-2.50130	-0.05345	1.55763
H	-3.75742	0.36794	0.39986
H	-2.48637	-0.80319	-1.40271
H	-2.91020	-1.89212	-0.08482
H	-0.62109	-1.98566	0.71302
H	-0.47740	-2.04698	-1.04529
N	2.19980	1.89298	-0.10611
N	2.27750	0.77711	-0.18964
N	1.91123	-0.39623	-0.37567
C	2.43780	-1.39527	0.56901
H	2.22948	-1.10882	1.60099
H	1.92618	-2.32505	0.33683
H	3.50808	-1.53391	0.42451
H	-2.03686	2.22709	0.90458

Structure **3-ts-N3-II**

C	2.25464	-1.11921	0.21685
C	2.76069	0.25811	-0.23239
C	1.90091	1.42695	0.30839
C	0.45871	1.04449	0.12225
C	0.12730	-0.12968	-0.07573
C	0.80019	-1.42690	-0.25160
H	2.09459	1.58689	1.37265
H	2.75464	0.29956	-1.32605
H	3.79798	0.38543	0.08818
H	2.27653	-1.16643	1.30936
H	2.91870	-1.90152	-0.15592
H	0.77652	-1.74377	-1.29733
H	0.37863	-2.23459	0.34945
N	-2.12929	1.92210	-0.01117
N	-2.25215	0.81800	-0.17303
N	-1.91430	-0.35354	-0.41492
C	-2.54029	-1.39198	0.41988
H	-3.60719	-1.45983	0.21267
H	-2.06732	-2.32877	0.14035
H	-2.37370	-1.19725	1.48042
H	2.16204	2.35785	-0.19763

Structure **3-ts-Im-I**

C	-3.34567	-0.11599	0.39843
C	-2.76449	1.14594	-0.25309
C	-1.23626	1.31376	0.01012
C	-0.76644	-0.06588	-0.08225
C	-1.16710	-1.23590	-0.12827
C	-2.67815	-1.41233	-0.11013
H	-0.79085	1.97720	-0.73284
H	-2.91841	1.09117	-1.33441
H	-3.28691	2.03415	0.10700
H	-3.20349	-0.05211	1.48207
H	-4.42368	-0.15557	0.21893
H	-3.01158	-1.63823	-1.12732
H	-2.98419	-2.26049	0.50559
N	1.39680	0.16289	-0.01595
C	2.37621	1.12558	0.02583
C	2.00654	-0.99399	-0.01413
C	3.60034	0.52333	0.05296
H	2.14375	2.17751	0.03388
H	1.50549	-1.94964	-0.04262
H	4.60029	0.91862	0.08700
H	4.03310	-1.56192	0.03637
N	3.34470	-0.82523	0.02687
H	-1.04456	1.73719	0.99963

Structure **3-ts-Im-II**

C	-2.75278	-1.15914	0.25061
C	-3.34955	0.09707	-0.39784
C	-2.69930	1.40035	0.11584
C	-1.18722	1.24184	0.13500
C	-0.76870	0.07867	0.08607
C	-1.22224	-1.30652	-0.01151
H	-3.01552	2.24662	-0.49737
H	-3.20499	0.03855	-1.48149
H	-4.42825	0.12195	-0.21978
H	-2.90846	-1.10928	1.33193
H	-3.26353	-2.05297	-0.11242
H	-1.02510	-1.72434	-1.00244
H	-0.77060	-1.96786	0.72985
N	1.39525	-0.11716	0.01607
C	2.05753	1.07889	0.00384
C	2.30975	-1.05768	-0.01481
C	3.40201	0.85284	-0.03480
H	1.50760	2.00676	0.02588
H	2.13282	-2.12100	-0.01542
H	4.24769	1.51709	-0.05438
H	4.41620	-1.02164	-0.07224
N	3.54572	-0.51278	-0.04643
H	-3.03686	1.61861	1.13335

Structure **12-ax-I**

C	1.28779	1.13871	-0.32359
C	0.14193	0.93487	0.67895
C	-0.65691	-0.40386	0.50726
C	0.43301	-1.36646	0.21188
C	1.58584	-1.18015	-0.09602
C	2.40076	0.03849	-0.26854
H	-1.19410	-0.62747	1.43468
H	0.53460	0.95483	1.69935
H	-0.56646	1.76214	0.58829
H	0.87645	1.15158	-1.33541

H	1.75101	2.11155	-0.14449
H	3.06464	0.17758	0.58660
H	3.00755	0.05713	-1.17258
O	-1.56963	-0.36172	-0.56679
C	-2.81062	0.21808	-0.21192
H	-2.69299	1.25132	0.12691
H	-3.43309	0.20795	-1.10373
H	-3.29819	-0.36279	0.57704

Structure **12-ax-II**

C	1.57527	0.82924	-0.54894
C	0.52126	1.20478	0.50373
C	-0.67449	0.21764	0.62101
C	-0.00438	-1.12469	0.50525
C	1.12295	-1.36490	0.14136
C	2.26980	-0.55304	-0.30119
H	-1.18184	0.35141	1.58221
H	0.99143	1.26732	1.48847
H	0.10672	2.18845	0.27203
H	1.10127	0.79832	-1.53216
H	2.34430	1.60417	-0.57804
H	3.02421	-0.49189	0.48515
H	2.75597	-0.90735	-1.20898
O	-1.57653	0.46297	-0.42480
C	-2.71644	-0.36931	-0.36482
H	-3.24205	-0.24080	0.58707
H	-3.37190	-0.08131	-1.18339
H	-2.43159	-1.42056	-0.47563

Structure **12-eq-I**

C	1.54680	1.12735	0.22617
C	0.07606	0.97378	-0.19008
C	-0.62872	-0.31326	0.35451
C	0.40466	-1.35547	0.12891
C	1.59753	-1.19834	0.00606
C	2.48455	-0.04775	-0.22699
H	-0.82313	-0.21085	1.43005
H	-0.00643	0.93828	-1.28037
H	-0.47571	1.85096	0.15694
H	1.60523	1.20115	1.31496
H	1.94132	2.05966	-0.18353
H	2.74358	0.03365	-1.28358
H	3.40582	-0.04871	0.35330
O	-1.83726	-0.58924	-0.31044
C	-2.86445	0.33163	0.00206
H	-2.67147	1.31558	-0.43326
H	-3.78646	-0.06559	-0.41646
H	-2.97686	0.43570	1.08660

Structure **12-eq-II**

C	1.87255	0.85117	0.27142
C	0.44643	1.18371	-0.18819
C	-0.63750	0.19049	0.30213
C	-0.01274	-1.16058	0.05106
C	1.17977	-1.35152	-0.04279
C	2.39907	-0.55042	-0.20492
H	-0.80553	0.29586	1.38142
H	0.39713	1.19488	-1.28032
H	0.17472	2.18133	0.16480
H	1.91417	0.87194	1.36315
H	2.55799	1.61768	-0.09536
H	2.71218	-0.52321	-1.24953
H	3.24592	-0.86801	0.40123
O	-1.82355	0.46028	-0.38705
C	-2.90143	-0.33488	0.06114
H	-3.09822	-0.16198	1.12419
H	-3.77637	-0.05407	-0.52042
H	-2.68293	-1.39658	-0.09291

Structure **12-ts-isom-I**

C	-3.78046	0.52446	1.07270
C	-2.30719	0.77919	0.62735
C	-1.67735	0.03028	-0.62365
C	-2.59998	-1.08278	-0.89773
C	-3.77099	-1.16283	-0.61420
C	-4.71523	-0.45537	0.24147
H	-1.66742	0.70848	-1.48496
H	-2.16666	1.84908	0.46537
H	-1.65775	0.49954	1.45821
H	-3.74789	0.12062	2.08317
H	-4.30133	1.47976	1.13659
H	-5.43916	0.09921	-0.35537
H	-5.27139	-1.09790	0.92234
O	-0.35712	-0.38734	-0.36709
C	0.55473	0.69258	-0.31998
H	0.35291	1.35523	0.52653
H	1.54939	0.26739	-0.20743
H	0.51299	1.27540	-1.24642

Structure **12-ts-isom-II**

C	-3.77622	0.48291	1.09329
C	-2.30319	0.75709	0.66432
C	-1.68393	0.07566	-0.60801
C	-2.57771	-1.07543	-0.94173
C	-3.75046	-1.13022	-0.65092
C	-4.70816	-0.44073	0.20024
H	-1.70726	0.76791	-1.45769
H	-2.15419	1.83115	0.54621
H	-1.65365	0.44152	1.48054
H	-3.74712	0.01601	2.07623
H	-4.29532	1.43363	1.21478
H	-5.40122	0.15110	-0.39768
H	-5.29680	-1.09471	0.84169
O	-0.34841	-0.23112	-0.31156
C	0.35415	-0.71028	-1.43882
H	-0.10440	-1.63146	-1.81304
H	0.36051	0.03500	-2.24096
H	1.37502	-0.91283	-1.12341

Structure **12-ts-N3-C1-ax-I**

C	-1.09479	1.99490	-0.33829
C	-1.82060	1.14282	0.70841
C	-1.57933	-0.37883	0.53713
C	-0.11857	-0.58884	0.23634
C	0.59436	0.37308	-0.07543
C	0.45005	1.82080	-0.28642
H	-1.87065	-0.89275	1.46073
H	-1.48181	1.42614	1.71001
H	-2.89376	1.34492	0.66643
H	-1.43891	1.70426	-1.33366
H	-1.34097	3.04883	-0.19788
H	0.88058	2.38782	0.54383
H	0.91130	2.17412	-1.20997
O	-2.34038	-0.91361	-0.53602
N	2.04540	-2.34909	0.06885
N	2.49187	-1.34617	-0.15466

N	2.55423	-0.14079	-0.45270
C	3.51366	0.66611	0.32091
H	3.33628	0.56727	1.39279
H	3.35267	1.69615	0.01586
H	4.53621	0.38066	0.07932
C	-3.66894	-1.22325	-0.17224
H	-4.21605	-0.34009	0.17162
H	-4.16209	-1.61717	-1.05883
H	-3.68967	-1.98122	0.61775

Structure **12-ts-N3-C1-ax-II**

C	1.15714	1.97651	0.17752
C	1.95218	1.02559	-0.72324
C	1.61148	-0.46716	-0.48638
C	0.11215	-0.58261	-0.40159
C	-0.57834	0.42289	-0.19595
C	-0.38108	1.87036	-0.03441
H	2.01432	-1.06406	-1.31291
H	1.74740	1.25440	-1.77372
H	3.02257	1.18119	-0.56632
H	1.37633	1.73974	1.22130
H	1.47014	3.00710	0.00140
H	-0.70000	2.40784	-0.93128
H	-0.90889	2.29998	0.81829
O	2.16728	-0.94719	0.72910
N	-2.09942	-2.22525	-0.50050
N	-2.54470	-1.21505	-0.30537
N	-2.61118	0.02335	-0.21668
C	-3.33314	0.54768	0.95530
H	-4.38697	0.27823	0.90719
H	-3.24372	1.62865	0.90630
H	-2.89173	0.18193	1.88355
C	3.51957	-1.33427	0.60458
H	4.15780	-0.49969	0.29888
H	3.84524	-1.68427	1.58225
H	3.62687	-2.14601	-0.12236

Structure **12-ts-N3-C1-ax-III**

C	-1.19406	2.09867	-0.43881
C	-1.92852	1.33705	0.66999
C	-1.70747	-0.18805	0.62779
C	-0.24393	-0.45326	0.32381
C	0.47885	0.47850	-0.05210
C	0.34767	1.90851	-0.37061
H	-1.98479	-0.62254	1.59614
H	-1.58538	1.69658	1.64469
H	-3.00211	1.52886	0.60919
H	-1.54236	1.74059	-1.41027
H	-1.42730	3.16299	-0.37581
H	0.78580	2.53126	0.41451
H	0.81427	2.18531	-1.31734
O	-2.55813	-0.72613	-0.36489
N	1.85106	-2.24673	0.23517
N	2.33462	-1.28056	-0.06508
N	2.41681	-0.09839	-0.44255
C	3.41673	0.73405	0.24719
H	3.28166	0.69679	1.32904
H	3.25698	1.74841	-0.10741
H	4.42503	0.42070	-0.01861
C	-2.51424	-2.13553	-0.42261
H	-2.76648	-2.57239	0.55018
H	-3.24929	-2.45175	-1.16026
H	-1.52107	-2.48441	-0.71834

Structure **12-ts-N3-C1-ax-IV**

C	1.33012	2.03442	0.36958
C	2.13614	1.15197	-0.58949
C	1.75782	-0.34030	-0.52073
C	0.24340	-0.43611	-0.47430
C	-0.42814	0.56925	-0.21330
C	-0.19955	1.98994	0.08832
H	2.15500	-0.85922	-1.40166
H	1.97588	1.48955	-1.61757
H	3.20344	1.24488	-0.37605
H	1.50154	1.69481	1.39345
H	1.67512	3.06773	0.30320
H	-0.46871	2.61722	-0.76552
H	-0.75217	2.35310	0.95612
O	2.35812	-0.89302	0.63326
N	-1.95283	-2.01880	-0.70305
N	-2.41396	-1.02730	-0.44969
N	-2.47158	0.20418	-0.28712
C	-3.21358	0.66950	0.89616
H	-4.26877	0.41479	0.81125
H	-3.11329	1.75065	0.90976
H	-2.79642	0.24833	1.81218
C	2.16143	-2.28660	0.73958
H	2.54004	-2.80159	-0.15039
H	2.71408	-2.62577	1.61358
H	1.10067	-2.52426	0.85904

Structure **12-ts-N3-C1-eq-I**

C	-0.87916	2.21424	0.15223
C	-1.88758	1.14633	-0.28798
C	-1.60026	-0.22968	0.35771
C	-0.14762	-0.52822	0.15893
C	0.64578	0.41269	0.00076
C	0.59243	1.86716	-0.21756
H	-1.80078	-0.16819	1.43739
H	-1.85401	1.01739	-1.37438
H	-2.89316	1.48298	-0.02487
H	-0.93998	2.33079	1.23787
H	-1.13867	3.17760	-0.28990
H	0.80869	2.10787	-1.26136
H	1.27975	2.43948	0.40743
O	-2.41025	-1.26002	-0.18492
N	1.93226	-2.41414	-0.13415
N	2.41790	-1.41189	-0.23979
N	2.55398	-0.18619	-0.39786
C	3.57373	0.46011	0.44748
H	4.56625	0.08731	0.20027
H	3.52758	1.52040	0.21829
H	3.36204	0.30092	1.50570
C	-3.77953	-1.11993	0.12718
H	-4.24545	-0.30194	-0.42946
H	-4.26922	-2.05288	-0.14608
H	-3.92088	-0.94366	1.19985

Structure **12-ts-N3-C1-eq-II**

C	0.92259	2.19955	-0.28585
C	1.85083	1.13322	0.30938
C	1.62728	-0.25877	-0.32677
C	0.15458	-0.53015	-0.33923
C	-0.63511	0.42438	-0.28048
C	-0.58741	1.88172	-0.08286
H	1.98427	-0.23875	-1.36702

H	1.67684	1.03854	1.38612
H	2.88685	1.45032	0.16771
H	1.11345	2.27609	-1.35987
H	1.14403	3.17419	0.15220
H	-0.90778	2.15357	0.92655
H	-1.19837	2.44259	-0.79216
O	2.32380	-1.28453	0.36175
N	-1.98261	-2.37637	-0.33495
N	-2.45678	-1.36792	-0.23535
N	-2.59835	-0.13260	-0.26244
C	-3.36557	0.45298	0.85117
H	-2.91184	0.20542	1.81200
H	-3.34220	1.52806	0.69937
H	-4.39940	0.11319	0.82285
C	3.72726	-1.17637	0.25702
H	4.12005	-0.34740	0.85250
H	4.15049	-2.10721	0.63012
H	4.03267	-1.03851	-0.78666

Structure **12-ts-N3-C1-eq-III**

C	-0.85550	2.41518	0.18907
C	-1.92110	1.43272	-0.30809
C	-1.74448	0.02929	0.29217
C	-0.30279	-0.37910	0.10866
C	0.55019	0.51637	-0.00306
C	0.59577	1.97913	-0.16652
H	-1.95289	0.05901	1.37138
H	-1.86777	1.33856	-1.39660
H	-2.91665	1.80622	-0.05729
H	-0.93101	2.50107	1.27651
H	-1.03994	3.40719	-0.22619
H	0.84863	2.24218	-1.19668
H	1.30892	2.47907	0.49094
O	-2.68675	-0.82333	-0.32391
N	1.61214	-2.37065	-0.20985
N	2.19101	-1.41489	-0.28269
N	2.41666	-0.19787	-0.40389
C	3.47672	0.35196	0.45865
H	4.44265	-0.07689	0.19740
H	3.50042	1.41979	0.26318
H	3.25590	0.17386	1.51199
C	-2.71849	-2.10724	0.25877
H	-2.99485	-2.04776	1.31777
H	-3.46714	-2.68891	-0.27555
H	-1.74323	-2.59523	0.17489

Structure **12-ts-N3-C1-eq-IV**

C	0.88889	2.39502	-0.28753
C	1.86183	1.42205	0.38735
C	1.76863	0.00560	-0.19952
C	0.31250	-0.39723	-0.25453
C	-0.53934	0.50663	-0.26286
C	-0.59968	1.97177	-0.12851
H	2.15203	0.00756	-1.23019
H	1.64363	1.35541	1.45740
H	2.88627	1.78675	0.28152
H	1.11858	2.44645	-1.35530
H	1.02024	3.39825	0.12079
H	-0.97969	2.26053	0.85525
H	-1.22201	2.45555	-0.88331
O	2.58726	-0.83777	0.58318
N	-1.66668	-2.36616	-0.23452
N	-2.22926	-1.39904	-0.19617
N	-2.45194	-0.17818	-0.28578
C	-3.31147	0.40224	0.76052
H	-2.89016	0.23226	1.75254
H	-3.35464	1.46815	0.55715
H	-4.31689	-0.01083	0.70114
C	2.71277	-2.13220	0.03701
H	3.16678	-2.09192	-0.95970
H	3.35641	-2.70499	0.70183
H	1.73569	-2.61739	-0.03925

Structure **12-ts-N3-C2-ax-I**

C	-2.18705	1.62786	-0.15436
C	-2.10982	0.35920	0.70135
C	-0.87909	-0.54451	0.37969
C	0.16903	0.44037	0.08580
C	0.27458	1.66554	-0.05838
C	-0.95073	2.53683	0.02213
H	-0.65150	-1.15477	1.26332
H	-2.04899	0.63467	1.75826
H	-3.01398	-0.23968	0.57482
H	-2.26430	1.34255	-1.20732
H	-3.09582	2.17946	0.09924
H	-0.96759	3.02601	1.00060
H	-0.94792	3.33441	-0.72221
O	-1.07743	-1.40213	-0.72786
N	1.89145	-0.63138	-0.23767
N	2.70673	0.30119	-0.28201
N	3.13627	1.32834	-0.40018
C	2.14593	-1.69959	0.74003
H	1.32737	-2.40526	0.62691
H	2.15939	-1.30672	1.75789
H	3.08372	-2.20676	0.51926
C	-1.79521	-2.57393	-0.39785
H	-2.80412	-2.34835	-0.04106
H	-1.86737	-3.17172	-1.30378
H	-1.26892	-3.14841	0.37245

Structure **12-ts-N3-C2-ax-II**

C	2.14722	-1.60659	-0.43728
C	2.16978	-0.46676	0.58783
C	0.94106	0.48247	0.47479
C	-0.15968	-0.45112	0.20398
C	-0.29715	-1.64659	-0.08652
C	0.91105	-2.52142	-0.28509
H	0.80866	1.03167	1.41495
H	2.18066	-0.87989	1.60063
H	3.07656	0.13024	0.46967
H	2.14248	-1.17509	-1.44216
H	3.06187	-2.19729	-0.34340
H	1.01482	-3.16958	0.59016
H	0.81217	-3.18247	-1.14729
O	1.06886	1.41166	-0.59066
N	-1.92101	0.58569	0.44911
N	-2.71360	-0.29827	0.08907
N	-3.12009	-1.31058	-0.16545
C	-2.01585	1.87826	-0.25351
H	-1.21658	2.49516	0.14463
H	-2.97596	2.34946	-0.04819
H	-1.87148	1.75094	-1.32651
C	1.80946	2.56049	-0.23245
H	2.82632	2.30854	0.08220
H	1.86098	3.19760	-1.11286
H	1.31458	3.10524	0.57932

Structure **12-ts-N3-C2-ax-III**

C	2.59935	-1.02387	-0.01668
C	2.17059	0.08957	0.94746
C	0.89472	0.84510	0.49462
C	0.02255	-0.25443	0.00958
C	0.20652	-1.44123	-0.27044
C	1.52894	-2.13255	-0.17589
H	0.46317	1.39087	1.34326
H	1.97529	-0.33306	1.93674
H	2.96664	0.82950	1.05132
H	2.79517	-0.58325	-0.99759
H	3.53581	-1.46423	0.33401
H	1.51984	-2.79529	0.69394
H	1.74652	-2.75826	-1.04227
O	1.26689	1.76843	-0.50660
N	-2.04787	0.24670	-0.11097
N	-2.44255	-0.91260	-0.32174
N	-2.33867	-1.99698	-0.60556
C	-2.55029	0.88748	1.11482
H	-2.02957	1.83760	1.19401
H	-2.33757	0.27689	1.99399
H	-3.62001	1.07746	1.03900
C	0.18850	2.55733	-0.96408
H	-0.27487	3.10175	-0.13292
H	0.59276	3.27427	-1.67569
H	-0.56987	1.94205	-1.45510

Structure **12-ts-N3-C2-ax-IV**

C	2.55592	-1.00697	0.01045
C	2.10380	0.10624	0.96633
C	0.88541	0.91211	0.44823
C	-0.00586	-0.14433	-0.10433
C	0.18399	-1.33345	-0.35052
C	1.46473	-2.08322	-0.23963
H	0.41498	1.46720	1.26878
H	1.83244	-0.32374	1.93410
H	2.91948	0.81304	1.13186
H	2.82570	-0.55684	-0.94811
H	3.45367	-1.48401	0.41032
H	1.40209	-2.78542	0.59581
H	1.69883	-2.67005	-1.12841
O	1.35364	1.82377	-0.52278
N	-2.20697	0.15050	0.05249
N	-2.45485	-1.00843	-0.30997
N	-2.16891	-2.07890	-0.53812
C	-2.90838	1.22833	-0.65889
H	-2.49206	2.16018	-0.28833
H	-3.97392	1.20474	-0.43224
H	-2.75650	1.16108	-1.73744
C	0.32680	2.60713	-1.08564
H	-0.22330	3.14853	-0.30725
H	0.79463	3.32337	-1.75789
H	-0.37300	1.98352	-1.65128

Structure **12-ts-N3-C2-eq-I**

C	2.01138	-1.83124	0.54945
C	2.19646	-0.41128	-0.00046
C	0.94834	0.49756	0.19863
C	-0.16101	-0.41780	-0.10968
C	-0.32749	-1.64055	-0.19226
C	0.83544	-2.58968	-0.11153
H	0.89730	0.83831	1.24354
H	2.38589	-0.44882	-1.07778
H	3.06042	0.05679	0.47586
H	1.82641	-1.77375	1.62664
H	2.93930	-2.39329	0.41608
H	1.10194	-2.90463	-1.12421
H	0.60444	-3.49836	0.44622
O	0.95073	1.62801	-0.64687
N	-1.86154	0.72475	-0.22675
N	-2.70186	-0.18819	-0.24726
N	-3.15307	-1.20570	-0.37308
C	-1.96931	1.69206	0.87838
H	-1.10266	2.34014	0.78260
H	-2.87615	2.28639	0.77884
H	-1.95355	1.18655	1.84521
C	1.93434	2.57968	-0.29231
H	1.75901	3.46350	-0.90185
H	1.85082	2.84967	0.76668
H	2.94430	2.20875	-0.48571

Structure **12-ts-N3-C2-eq-II**

C	-2.03843	-1.91954	-0.24259
C	-2.20462	-0.43777	0.11684
C	-1.01657	0.45653	-0.34493
C	0.15509	-0.37606	-0.03095
C	0.34092	-1.57991	0.17208
C	-0.77240	-2.55930	0.38126
H	-1.07850	0.64052	-1.42651
H	-2.27962	-0.32284	1.20295
H	-3.12946	-0.05848	-0.32316
H	-1.97504	-2.01722	-1.33060
H	-2.92691	-2.47082	0.07543
H	-0.91130	-2.72030	1.45362
H	-0.57737	-3.53654	-0.06226
O	-0.98516	1.70139	0.32459
N	1.92505	0.67240	-0.42093
N	2.69967	-0.27541	-0.20881
N	3.01663	-1.34119	-0.04658
C	2.15611	1.87720	0.40060
H	1.32960	2.54519	0.18694
H	2.15687	1.62834	1.46269
H	3.09854	2.34722	0.12271
C	-2.06053	2.54770	-0.03099
H	-1.84873	3.52881	0.38923
H	-2.14538	2.63340	-1.11979
H	-3.00982	2.18603	0.37277

Structure **12-ts-N3-C2-eq-III**

C	2.50603	-1.16165	0.62091
C	2.41471	0.29296	0.14712
C	1.00358	0.92799	0.25827
C	0.08864	-0.17324	-0.15900
C	0.29879	-1.37754	-0.28871
C	1.57800	-2.12129	-0.17561
H	0.78617	1.22069	1.29480
H	2.69431	0.35299	-0.90865
H	3.11368	0.91697	0.70804
H	2.23270	-1.21704	1.67857
H	3.54050	-1.50286	0.53755
H	1.98401	-2.31664	-1.17109
H	1.48582	-3.08207	0.33178
O	1.01503	2.07878	-0.55350
N	-2.13322	0.08861	-0.18113
N	-2.32225	-1.12916	-0.32917

N	-1.98576	-2.18616	-0.55195
C	-2.63142	0.64641	1.08799
H	-2.22124	1.64939	1.16108
H	-3.71910	0.70912	1.07930
H	-2.29675	0.04985	1.93820
C	-0.16166	2.85148	-0.45010
H	-0.01708	3.74100	-1.05978
H	-1.02787	2.29587	-0.82023
H	-0.33867	3.15509	0.58805

Structure **12-ts-N3-C2-eq-IV**

C	2.28670	-1.11245	0.30302
C	2.01456	0.24957	-0.35152
C	0.75177	0.94851	0.20356
C	-0.27564	-0.13040	0.18526
C	-0.10176	-1.34606	0.22666
C	1.13890	-2.14764	0.10687
H	0.93026	1.26050	1.24062
H	1.87498	0.13112	-1.42987
H	2.86858	0.91304	-0.19757
H	2.43290	-0.96349	1.37677
H	3.21706	-1.52585	-0.09227
H	1.18889	-2.60620	-0.88354
H	1.21889	-2.95094	0.83963
O	0.47105	2.08689	-0.57636
N	-2.51810	0.15019	-0.19081
N	-2.64970	-1.07892	-0.26832
N	-2.28668	-2.14616	-0.14313
C	-2.77338	0.87353	-1.45109
H	-2.42432	1.88980	-1.30012
H	-2.22770	0.41950	-2.27928
H	-3.84084	0.89158	-1.66927
C	-0.36324	2.99930	0.10981
H	-0.65991	3.77115	-0.59799
H	-1.25482	2.49754	0.50040
H	0.17300	3.46019	0.94547

Structure **12-ts-Im-C1-ax-I**

C	-1.78990	1.88068	-0.27700
C	-2.52048	0.96701	0.71301
C	-2.17345	-0.52856	0.52383
C	-0.66802	-0.67933	0.37374
C	-0.05906	0.35698	0.08762
C	-0.23907	1.78357	-0.15049
H	-2.53711	-1.09214	1.39128
H	-2.25546	1.24678	1.73750
H	-3.60015	1.10759	0.61482
H	-2.06873	1.59309	-1.29306
H	-2.09581	2.91778	-0.13038
H	0.13410	2.37517	0.68957
H	0.24693	2.13842	-1.05989
N	2.12733	0.12655	-0.03276
C	3.28323	0.82446	-0.28829
C	2.48123	-1.10962	0.20703
C	4.35102	-0.02011	-0.19705
H	3.27648	1.87676	-0.51911
H	1.79473	-1.90912	0.44102
H	5.40806	0.13396	-0.32443
H	4.33758	-2.10065	0.25982
N	3.82081	-1.24638	0.11900
O	-2.78744	-1.06025	-0.64311
C	-4.12685	-1.45338	-0.43376
H	-4.75701	-0.61417	-0.12346
H	-4.50087	-1.84049	-1.37982
H	-4.18844	-2.23989	0.32585

Structure **12-ts-Im-C1-ax-II**

C	-1.77406	1.88207	-0.25845
C	-2.51774	0.96977	0.72306
C	-2.18847	-0.52859	0.52286
C	-0.68551	-0.69524	0.37244
C	-0.06113	0.33397	0.09613
C	-0.22489	1.76502	-0.12968
H	-2.55946	-1.09428	1.38582
H	-2.25147	1.23851	1.75020
H	-3.59544	1.12415	0.62364
H	-2.05423	1.60576	-1.27729
H	-2.06780	2.92167	-0.10445
H	0.15275	2.34519	0.71644
H	0.26620	2.12310	-1.03529
N	2.12021	0.07738	-0.02098
C	2.52989	-1.20259	0.23303
C	3.20025	0.77548	-0.28221
C	3.88741	-1.27557	0.12257
H	1.81049	-1.96948	0.47437
H	3.23908	1.82466	-0.52661
H	4.58090	-2.08879	0.24306
H	5.24951	0.28978	-0.36414
N	4.29872	-0.00744	-0.20612
O	-2.80883	-1.04340	-0.64839
C	-4.15157	-1.42578	-0.44085
H	-4.77257	-0.58418	-0.11860
H	-4.53160	-1.79739	-1.39073
H	-4.21928	-2.22097	0.30911

Structure **12-ts-Im-C1-ax-III**

C	-1.89106	1.95840	-0.39523
C	-2.64184	1.12855	0.65135
C	-2.30558	-0.37162	0.59631
C	-0.78998	-0.57026	0.45154
C	-0.17467	0.44966	0.11517
C	-0.34664	1.85760	-0.22744
H	-2.65725	-0.85372	1.51730
H	-2.38780	1.49086	1.65198
H	-3.72044	1.24803	0.52394
H	-2.15359	1.59758	-1.39199
H	-2.19139	3.00559	-0.33241
H	0.01428	2.50733	0.57447
H	0.16247	2.14155	-1.14915
N	1.98534	0.20192	-0.01405
C	3.13184	0.89309	-0.32362
C	2.35233	-1.01311	0.30180
C	4.20808	0.06551	-0.18776
H	3.11260	1.92845	-0.62077
H	1.67487	-1.80116	0.59362
H	5.26256	0.22060	-0.33370
H	4.21840	-1.98147	0.40129
N	3.69216	-1.14274	0.21066
O	-3.01228	-0.93161	-0.49327
C	-2.88239	-2.33327	-0.57711
H	-3.19063	-2.80953	0.36063
H	-3.53326	-2.67096	-1.38161
H	-1.84972	-2.61896	-0.79354

Structure **12-ts-Im-C1-ax-IV**

C	1.87468	-1.95918	-0.40187

C	2.63934	-1.14007	0.64311
C	2.31864	0.36392	0.59359
C	0.80560	0.57762	0.45317
C	0.17565	-0.43315	0.11829
C	0.33225	-1.84287	-0.22613
H	2.67797	0.83937	1.51508
H	2.38631	-1.50221	1.64407
H	3.71595	-1.27088	0.51004
H	2.13563	-1.59772	-1.39883
H	2.16481	-3.00956	-0.34387
H	-0.03027	-2.48995	0.57732
H	-0.18325	-2.12200	-1.14594
N	-1.97959	-0.15543	-0.00907
C	-2.39453	1.10498	0.32111
C	-3.05645	-0.84393	-0.30656
C	-3.75276	1.17649	0.21932
H	-1.67737	1.85895	0.60590
H	-3.08989	-1.87746	-0.61097
H	-4.45024	1.97732	0.38945
H	-5.10837	-0.36595	-0.35154
N	-4.15841	-0.07270	-0.18128
O	3.02810	0.91991	-0.49646
C	2.91141	2.32316	-0.57572
H	3.23142	2.79373	0.36094
H	3.55956	2.65647	-1.38423
H	1.88003	2.61966	-0.78339

Structure **12-ts-Im-C1-ax-V**

C	1.94654	1.73558	0.41788
C	2.71576	0.90809	-0.62198
C	2.22909	-0.55730	-0.83355
C	0.72998	-0.66233	-0.58899
C	0.15929	0.37813	-0.24009
C	0.41278	1.75956	0.15439
H	2.42920	-0.82009	-1.87316
H	2.62706	1.41167	-1.58954
H	3.78060	0.88947	-0.37458
H	2.10514	1.32759	1.41746
H	2.32458	2.75975	0.41998
H	0.14992	2.45849	-0.64404
H	-0.12486	2.05605	1.05553
N	-1.99789	0.19399	-0.02322
C	-3.11138	0.91016	0.34503
C	-2.41134	-1.00364	-0.34822
C	-4.21500	0.11531	0.23611
H	-3.05161	1.93828	0.66125
H	-1.76824	-1.80363	-0.68225
H	-5.25809	0.29638	0.42709
H	-4.30619	-1.91784	-0.39302
N	-3.74949	-1.09810	-0.20606
O	2.98538	-1.51308	-0.10784
C	2.91608	-1.38360	1.29486
H	1.87737	-1.34016	1.63614
H	3.39805	-2.26235	1.72012
H	3.44630	-0.49080	1.64128

Structure **12-ts-Im-C1-ax-VI**

C	1.92800	1.73771	0.42933
C	2.71118	0.92753	-0.61358
C	2.24280	-0.54223	-0.83743
C	0.74555	-0.66697	-0.59629
C	0.15811	0.36235	-0.24332
C	0.39519	1.74476	0.15994
H	2.44780	-0.79422	-1.87877
H	2.61994	1.43709	-1.57779
H	3.77522	0.92018	-0.36216
H	2.08762	1.32378	1.42636
H	2.29363	2.76634	0.44093
H	0.12799	2.44548	-0.63561
H	-0.14797	2.03100	1.06128
N	-1.99252	0.14412	-0.02983
C	-2.45145	-1.10201	-0.35579
C	-3.04007	0.85810	0.31002
C	-3.80664	-1.13899	-0.20733
H	-1.76432	-1.87129	-0.67188
H	-3.03653	1.88959	0.62293
H	-4.53018	-1.92004	-0.35952
H	-5.10096	0.43304	0.42184
N	-4.16533	0.11674	0.21690
O	3.01034	-1.49392	-0.11796
C	2.93406	-1.37817	1.28554
H	1.89357	-1.35263	1.62313
H	3.42684	-2.25381	1.70477
H	3.45029	-0.48106	1.64200

Structure **12-ts-Im-C1-eq-I**

C	-1.66146	2.12322	0.16473
C	-2.52562	0.96500	-0.35306
C	-2.19348	-0.37258	0.34831
C	-0.70145	-0.56955	0.31754
C	-0.02486	0.45768	0.21215
C	-0.13018	1.89146	-0.03283
H	-2.51254	-0.31559	1.39928
H	-2.36596	0.82532	-1.42693
H	-3.57795	1.22007	-0.20559
H	-1.84996	2.25457	1.23363
H	-1.94685	3.05248	-0.33091
H	0.18491	2.13993	-1.04895
H	0.44595	2.50309	0.66238
N	2.16164	0.11042	0.03112
C	3.35965	0.76216	-0.13798
C	2.43849	-1.16584	0.10782
C	4.37312	-0.15120	-0.16271
H	3.41888	1.83384	-0.23114
H	1.70536	-1.94663	0.24199
H	5.43797	-0.04749	-0.27499
H	4.23017	-2.26828	0.02187
N	3.76746	-1.37286	-0.00469
O	-2.85846	-1.47346	-0.25378
C	-4.26006	-1.43826	-0.09272
H	-4.72634	-0.67301	-0.71969
H	-4.64319	-2.41359	-0.38773
H	-4.52986	-1.25079	0.95317

Structure **12-ts-Im-C1-eq-II**

C	-1.64797	2.12193	0.17139
C	-2.52516	0.97450	-0.34852
C	-2.20411	-0.36935	0.34652
C	-0.71469	-0.57989	0.30928
C	-0.02695	0.43971	0.20803
C	-0.11965	1.87558	-0.03157
H	-2.51837	-0.31292	1.39898
H	-2.37016	0.83759	-1.42342
H	-3.57447	1.23946	-0.19678
H	-1.83199	2.25060	1.24141
H	-1.92567	3.05610	-0.31945

H	0.19408	2.12487	-1.04798
H	0.46388	2.47989	0.66411
N	2.15511	0.06763	0.02435
C	2.47364	-1.26045	0.10241
C	3.28489	0.71778	-0.12651
C	3.82505	-1.41199	-0.00457
H	1.70078	-2.00226	0.22970
H	3.39946	1.78544	-0.22176
H	4.45968	-2.28023	0.00835
H	5.29845	0.10756	-0.25430
N	4.32693	-0.14226	-0.14995
O	-2.88313	-1.46072	-0.25699
C	-4.28330	-1.41282	-0.08783
H	-4.67756	-2.38269	-0.38619
H	-4.54543	-1.22875	0.96063
H	-4.74568	-0.63951	-0.70780

Structure **12-ts-Im-C1-eq-III**

C	-1.73054	2.26829	0.19846
C	-2.61174	1.16615	-0.40186
C	-2.33874	-0.20503	0.23212
C	-0.84039	-0.47572	0.22307
C	-0.14294	0.54535	0.18364
C	-0.20553	1.99450	0.01919
H	-2.66547	-0.19913	1.28191
H	-2.42408	1.08004	-1.47619
H	-3.66634	1.42048	-0.27099
H	-1.94015	2.34872	1.26836
H	-1.97515	3.23072	-0.25319
H	0.13881	2.28971	-0.97486
H	0.37665	2.54599	0.75847
N	2.02286	0.16924	0.03445
C	3.22787	0.82003	-0.07818
C	2.28956	-1.11125	0.05519
C	4.23567	-0.09861	-0.12596
H	3.29536	1.89451	-0.11828
H	1.54831	-1.89151	0.13665
H	5.30325	0.00258	-0.21120
H	4.07600	-2.22086	-0.04638
N	3.61916	-1.32204	-0.03971
O	-3.11115	-1.15745	-0.46986
C	-3.07481	-2.43460	0.12425
H	-3.46427	-2.40015	1.14831
H	-3.70148	-3.09142	-0.47613
H	-2.05211	-2.82151	0.14916

Structure **12-ts-Im-C1-eq-IV**

C	-1.71377	2.27223	0.20431
C	-2.60753	1.18107	-0.39755
C	-2.34765	-0.19492	0.23205
C	-0.85269	-0.47969	0.21919
C	-0.14348	0.53267	0.18298
C	-0.19185	1.98297	0.02177
H	-2.67203	-0.18852	1.28259
H	-2.42283	1.09605	-1.47248
H	-3.65913	1.44621	-0.26393
H	-1.92062	2.35165	1.27484
H	-1.94918	3.23853	-0.24404
H	0.15306	2.27726	-0.97243
H	0.39640	2.52769	0.76145
N	2.01724	0.12708	0.03257
C	2.31876	-1.20678	0.05986
C	3.15622	0.76949	-0.07662
C	3.66965	-1.37005	-0.03538
H	1.53510	-1.94305	0.14592
H	3.28405	1.83872	-0.12646
H	4.29404	-2.24567	-0.04972
H	5.16381	0.14050	-0.20304
N	4.18812	-0.10162	-0.12169
O	-3.13160	-1.13707	-0.47095
C	-3.10287	-2.41764	0.11648
H	-3.73791	-3.06609	-0.48422
H	-2.08330	-2.81294	0.13430
H	-3.48704	-2.38523	1.14261

Structure **12-ts-Im-C1-eq-V**

C	1.83787	2.15126	-0.03908
C	2.69350	0.91357	0.26232
C	2.30669	-0.27803	-0.63916
C	0.80457	-0.48769	-0.54562
C	0.16248	0.52754	-0.25166
C	0.31341	1.91011	0.19208
H	2.53977	-0.02265	-1.67587
H	2.55841	0.63166	1.31018
H	3.75130	1.14636	0.11495
H	1.98400	2.43905	-1.08360
H	2.16154	2.99079	0.57794
H	0.04777	2.01383	1.24690
H	-0.28157	2.62300	-0.37994
N	-2.00795	0.20330	-0.02306
C	-3.17642	0.85145	0.29785
C	-2.33088	-1.03286	-0.30419
C	-4.21953	-0.02344	0.20567
H	-3.19521	1.89306	0.57242
H	-1.62968	-1.79911	-0.59807
H	-5.27607	0.09032	0.37309
H	-4.15630	-2.08101	-0.34099
N	-3.66178	-1.21747	-0.17846
O	3.09661	-1.42782	-0.38882
C	2.85904	-2.05122	0.85448
H	1.78877	-2.22559	1.00083
H	3.37978	-3.00710	0.83549
H	3.24377	-1.45844	1.68928

Structure **12-ts-Im-C1-eq-VI**

C	1.82011	2.15519	-0.02873
C	2.68986	0.92675	0.27001
C	2.32105	-0.26545	-0.63869
C	0.82190	-0.49266	-0.55168
C	0.16482	0.51178	-0.25618
C	0.29782	1.89402	0.19526
H	2.55511	-0.00198	-1.67318
H	2.55486	0.63814	1.31605
H	3.74517	1.17339	0.12730
H	1.96667	2.44966	-1.07134
H	2.13101	2.99580	0.59344
H	0.02766	1.98934	1.24978
H	-0.30282	2.60343	-0.37549
N	-2.00183	0.15627	-0.03077
C	-2.36820	-1.13272	-0.30582
C	-3.10265	0.80684	0.26386
C	-3.71975	-1.25996	-0.17239
H	-1.62655	-1.86623	-0.58110
H	-3.17658	1.84873	0.53046
H	-4.38434	-2.09602	-0.29930
H	-5.13072	0.24270	0.36924

N	-4.17222	-0.01562	0.19093
O	3.12488	-1.40600	-0.39027
C	2.88080	-2.04630	0.84318
H	3.42514	-2.98894	0.82490
H	3.23625	-1.45212	1.68994
H	1.81279	-2.24785	0.96884

Structure **12-ts-Im-C2-ax-I**

C	3.17177	-0.78446	-0.40877
C	2.67269	0.28218	0.57483
C	1.14670	0.60293	0.43593
C	0.61180	-0.71509	0.12601
C	0.95769	-1.86617	-0.13590
C	2.44383	-2.13703	-0.24505
H	0.76815	0.99943	1.38507
H	2.84562	-0.05532	1.60071
H	3.22881	1.21219	0.43933
H	3.01388	-0.42545	-1.42973
H	4.24860	-0.92011	-0.27742
H	2.76756	-2.64232	0.66962
H	2.68670	-2.80766	-1.07070
N	-1.59865	-0.23935	0.14947
C	-2.43982	-1.31849	0.11338
C	-2.35176	0.82664	0.02679
C	-3.72773	-0.89040	-0.02873
H	-2.05556	-2.32389	0.18232
H	-2.00684	1.84768	0.00193
H	-4.66305	-1.41700	-0.09753
H	-4.42980	1.11440	-0.19324
N	-3.65452	0.47946	-0.08121
O	0.86074	1.52634	-0.59746
C	1.03082	2.86938	-0.19503
H	2.06127	3.07862	0.10731
H	0.78178	3.49530	-1.04948
H	0.36374	3.11349	0.63917

Structure **12-ts-Im-C2-ax-II**

C	3.14596	-0.86725	-0.33522
C	2.66055	0.23277	0.61776
C	1.16299	0.63153	0.40048
C	0.57234	-0.66405	0.09565
C	0.86762	-1.83549	-0.14200
C	2.34285	-2.17872	-0.19313
H	0.76191	1.07299	1.32001
H	2.76649	-0.10366	1.65308
H	3.27073	1.13098	0.50165
H	3.05072	-0.50946	-1.36442
H	4.20766	-1.05721	-0.15667
H	2.60534	-2.69398	0.73555
H	2.58216	-2.86669	-1.00546
N	-1.61636	-0.13382	0.08849
C	-2.48023	0.93020	0.17996
C	-2.35613	-1.20060	-0.07013
C	-3.76561	0.48369	0.07367
H	-2.12797	1.94016	0.30944
H	-1.97579	-2.20483	-0.17896
H	-4.71300	0.99301	0.09280
H	-4.43485	-1.52029	-0.19667
N	-3.66734	-0.87614	-0.08538
O	0.98215	1.53903	-0.66887
C	1.19419	2.88269	-0.28944
H	2.21251	3.04829	0.07529
H	1.03382	3.49567	-1.17388
H	0.48679	3.18291	0.49099

Structure **12-ts-Im-C2-ax-III**

C	3.19660	0.39427	0.35306
C	2.65683	-0.55275	-0.73061
C	1.09192	-0.70013	-0.80463
C	0.65675	0.59702	-0.28839
C	1.08905	1.67325	0.12593
C	2.58742	1.81149	0.28294
H	0.80715	-0.83743	-1.84834
H	2.98426	-0.19047	-1.70863
H	3.06819	-1.55702	-0.60345
H	2.98407	-0.01761	1.34257
H	4.28460	0.45149	0.25911
H	2.97275	2.35595	-0.58409
H	2.86949	2.39241	1.16250
N	-1.55438	0.26046	-0.24715
C	-2.30736	1.35902	0.06698
C	-2.37909	-0.75759	-0.30716
C	-3.61615	0.99422	0.19312
H	-1.84824	2.32766	0.18739
H	-2.10560	-1.77774	-0.52167
H	-4.50473	1.55339	0.42699
H	-4.46097	-0.94898	-0.02959
N	-3.64479	-0.35704	-0.04900
O	0.56944	-1.84097	-0.15726
C	0.73219	-1.86277	1.24655
H	0.32015	-0.95902	1.70373
H	0.19013	-2.73351	1.61114
H	1.78604	-1.96093	1.52373

Structure **12-ts-Im-C2-ax-IV**

C	3.18944	0.44877	0.33846
C	2.66499	-0.52158	-0.73193
C	1.10399	-0.71550	-0.78630
C	0.63866	0.57335	-0.27592
C	1.04184	1.66566	0.12756
C	2.53829	1.84678	0.26574
H	0.81149	-0.86892	-1.82564
H	2.97068	-0.15765	-1.71636
H	3.10616	-1.51269	-0.60188
H	3.00116	0.03798	1.33330
H	4.27408	0.53743	0.23092
H	2.89745	2.39579	-0.60962
H	2.81356	2.44212	1.13779
N	-1.56188	0.18874	-0.22152
C	-2.46763	-0.83769	-0.33387
C	-2.24658	1.26071	0.08335
C	-3.72382	-0.36168	-0.09120
H	-2.15444	-1.84042	-0.57176
H	-1.82262	2.23915	0.24993
H	-4.68852	-0.83767	-0.07865
H	-4.29678	1.63163	0.39637
N	-3.56397	0.97633	0.17259
O	0.62312	-1.86466	-0.12423
C	0.78856	-1.86503	1.27897
H	0.34130	-0.97378	1.72751
H	0.28181	-2.75256	1.65340
H	1.84584	-1.91821	1.55577

Structure **12-ts-Im-C2-eq-I**

C	3.18638	-0.99813	0.40203
C	2.68726	0.39788	0.00453

C	1.16146	0.62036	0.26190
C	0.62063	-0.67649	-0.13086
C	0.97874	-1.83780	-0.31547
C	2.45969	-2.14137	-0.34524
H	0.97622	0.81790	1.32663
H	2.84556	0.55987	-1.06627
H	3.25412	1.15861	0.54548
H	3.03510	-1.13613	1.47710
H	4.26327	-1.05912	0.22278
H	2.78649	-2.18825	-1.38757
H	2.70398	-3.10621	0.10189
N	-1.58678	-0.24343	0.04122
C	-2.37985	0.79979	-0.00147
C	-2.39362	-1.34743	0.09480
H	-2.06508	1.82867	-0.06076
C	-3.70181	-0.95882	0.08853
H	-1.97249	-2.34004	0.12529
H	-4.47719	1.02388	-0.00160
H	-4.62284	-1.51351	0.11959
N	-3.67567	0.41270	0.02812
O	0.63354	1.68578	-0.49750
C	1.09054	2.94947	-0.06140
H	2.15277	3.09348	-0.27752
H	0.51661	3.70147	-0.59939
H	0.92670	3.07335	1.01500

Structure **12-ts-Im-C2-eq-II**

C	3.13232	-1.06544	0.45401
C	2.69976	0.34636	0.03603
C	1.17629	0.63163	0.24457
C	0.59678	-0.64913	-0.14559
C	0.91233	-1.82587	-0.31568
C	2.38257	-2.18230	-0.30918
H	0.96633	0.85339	1.29991
H	2.89603	0.49563	-1.03031
H	3.27927	1.08814	0.58960
H	2.94560	-1.19209	1.52487
H	4.21058	-1.16953	0.30537
H	2.73268	-2.24299	-1.34321
H	2.58031	-3.15469	0.14464
N	-1.59392	-0.16317	0.00787
C	-2.46004	0.89829	0.10271
C	-2.32982	-1.24390	-0.02182
H	-2.10509	1.91473	0.13583
H	-1.94763	-2.25034	-0.09954
H	-4.69341	0.93768	0.19636
H	-4.40780	-1.58695	0.04224
N	-3.64212	-0.93111	0.05085
C	-3.74407	0.43571	0.13162
O	0.71606	1.70304	-0.54807
C	1.19296	2.95693	-0.10613
H	0.67323	3.71912	-0.68321
H	0.97788	3.10265	0.95845
H	2.26943	3.06236	-0.26829

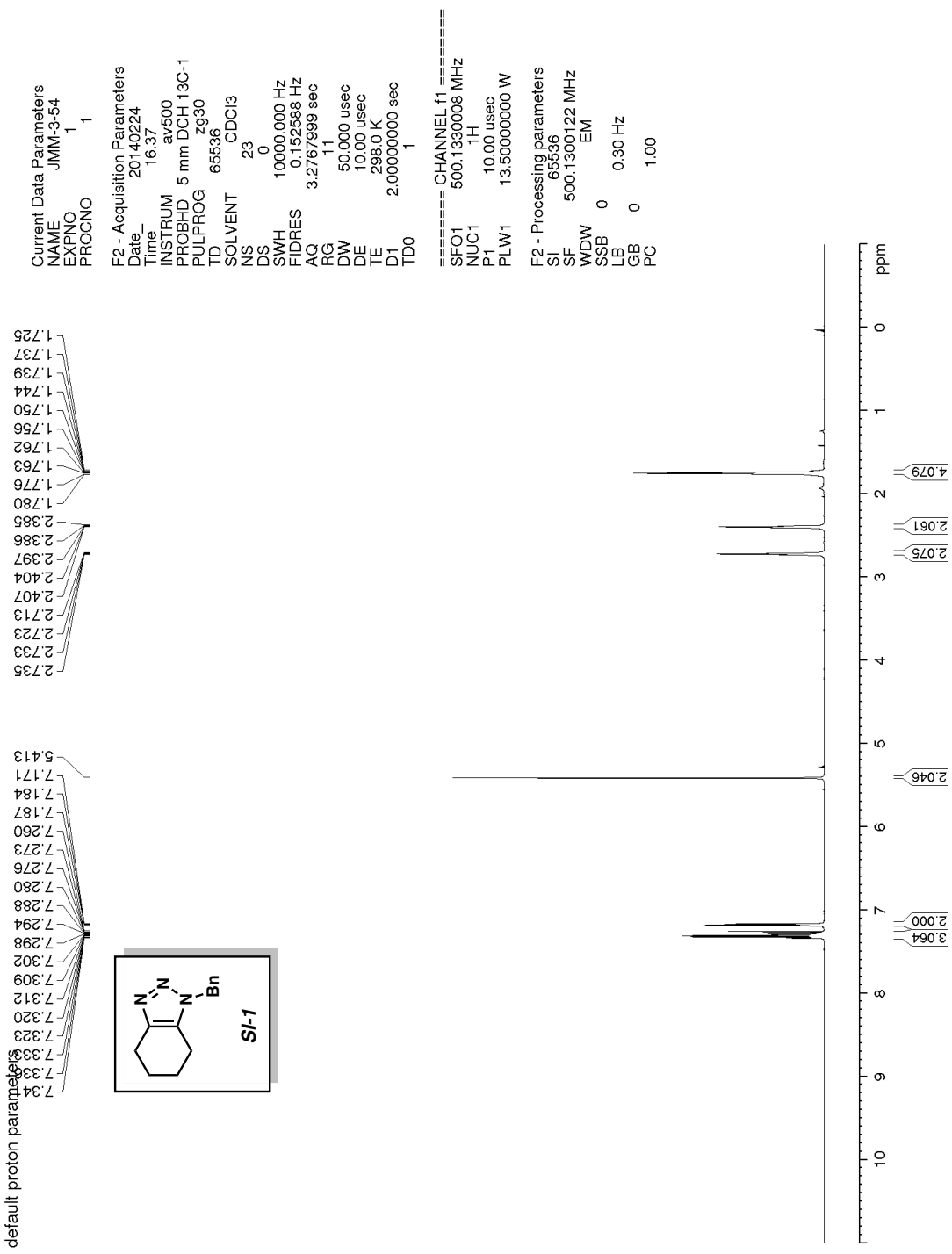
Structure **12-ts-Im-C2-eq-III**

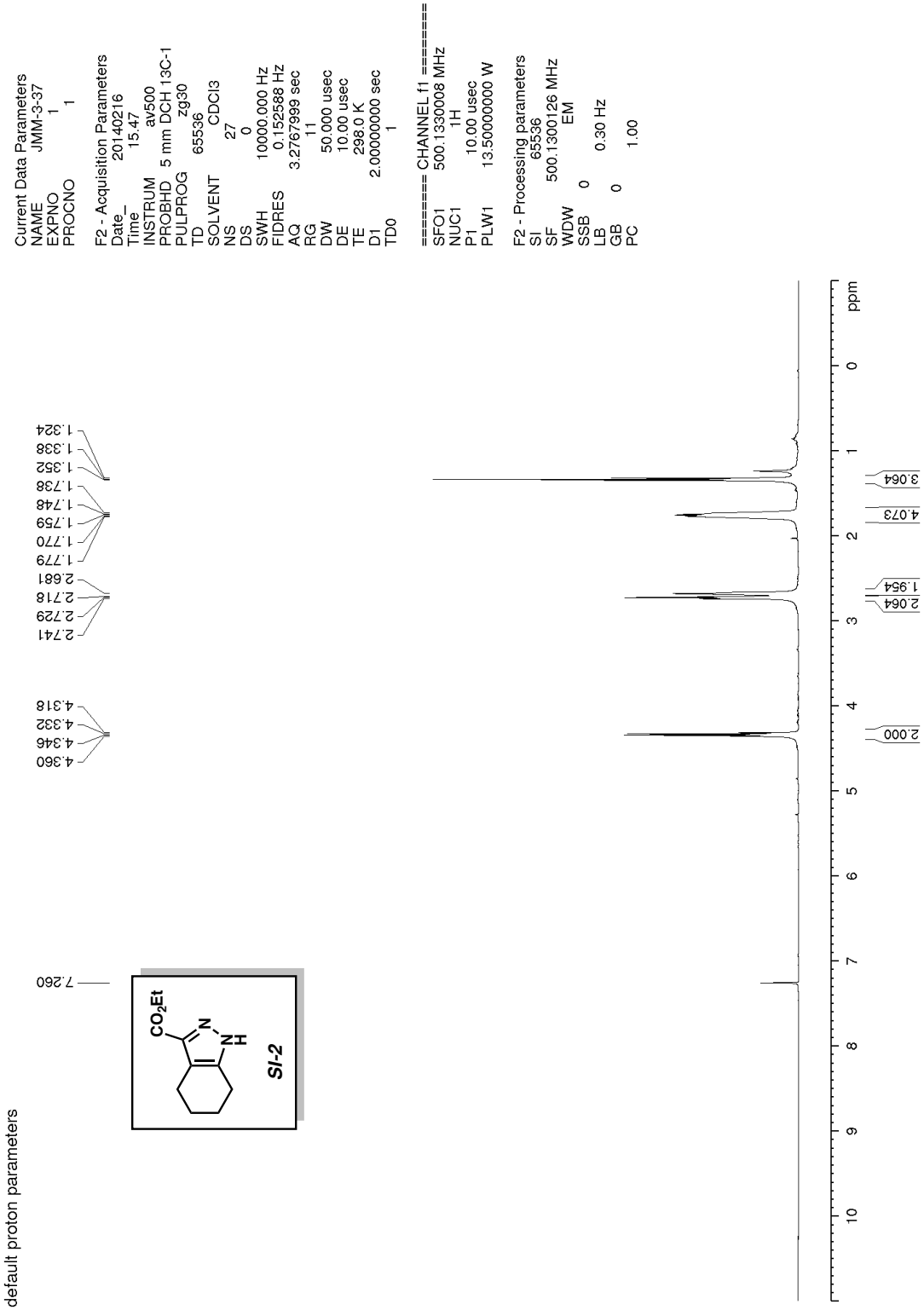
C	-3.29217	-0.68166	-0.49296
C	-2.66893	0.71240	-0.33847
C	-1.13483	0.73871	-0.62165
C	-0.70447	-0.50877	0.02019
C	-1.16946	-1.57902	0.41542
C	-2.67545	-1.72633	0.46618
H	-0.95528	0.69552	-1.69842
H	-2.83104	1.06286	0.68390
H	-3.14853	1.42494	-1.01253
H	-3.14528	-1.02588	-1.52146
H	-4.37142	-0.61546	-0.33051
H	-3.00930	-1.54889	1.49243
H	-3.00867	-2.73110	0.20134
N	1.49556	-0.29148	-0.14240
C	2.36391	0.65776	-0.39960
C	2.21565	-1.41222	0.16877
H	2.12514	1.67278	-0.67279
C	3.54890	-1.13154	0.09406
H	1.71855	-2.33430	0.42643
H	4.47106	0.72164	-0.41168
H	4.42580	-1.73160	0.26091
N	3.62575	0.19035	-0.26913
O	-0.50758	1.93362	-0.20749
C	-0.36928	2.09629	1.19173
H	0.14672	1.24053	1.63401
H	0.22681	2.99514	1.33987
H	-1.33432	2.23080	1.68645

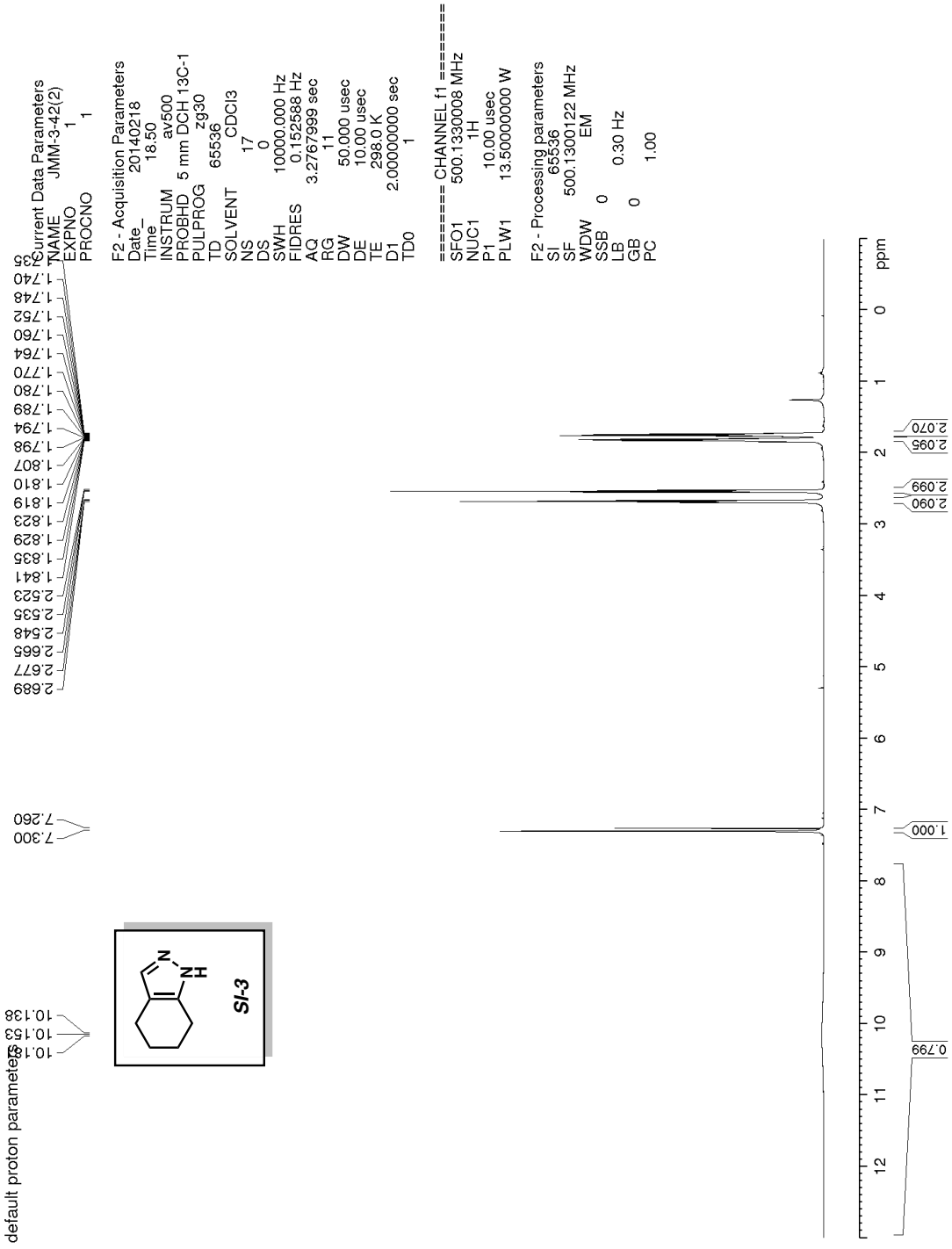
Structure **12-ts-Im-C2-eq-IV**

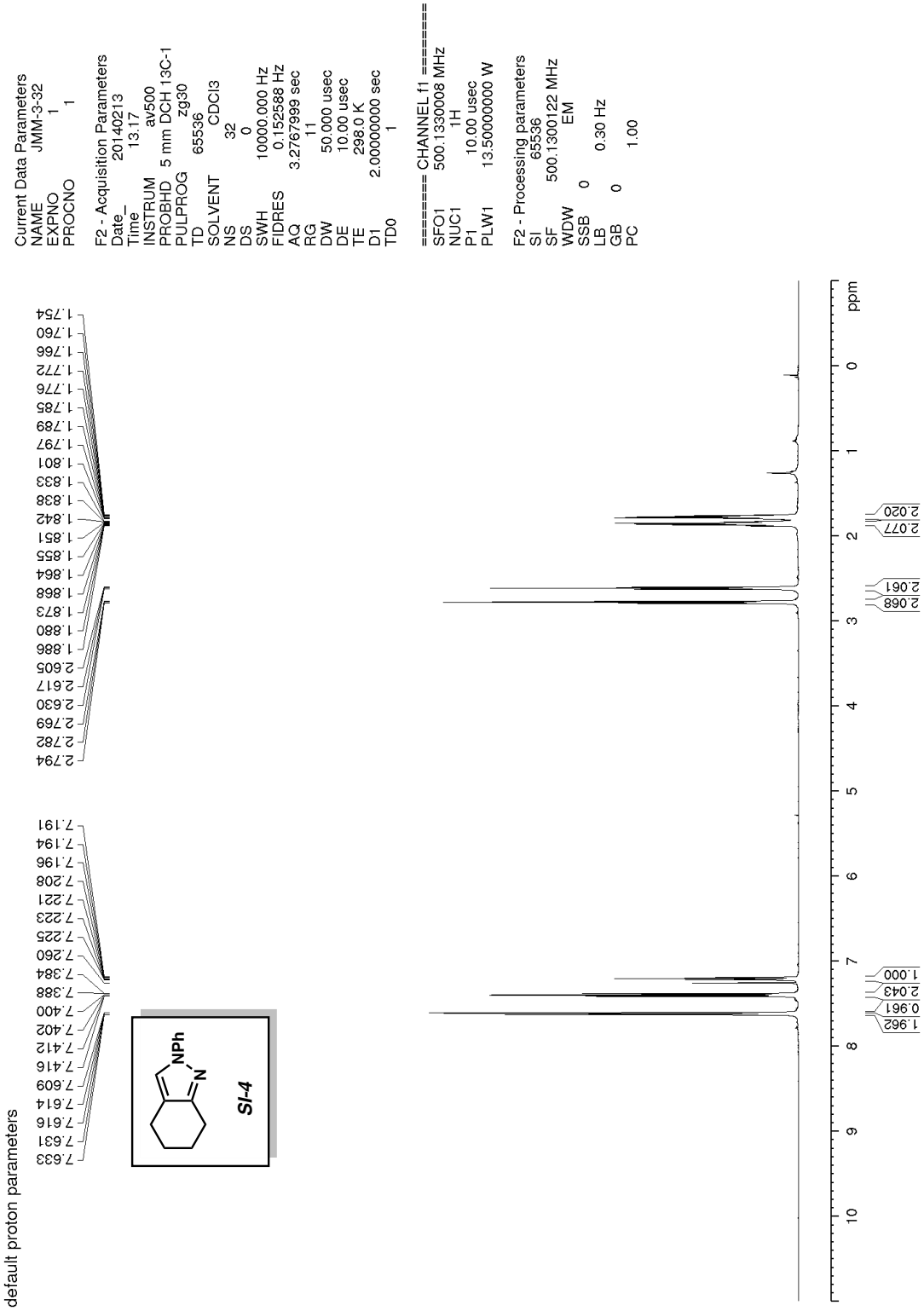
C	-3.26343	-0.74977	-0.49249
C	-2.68745	0.66557	-0.35219
C	-1.15244	0.74103	-0.62301
C	-0.68568	-0.48814	0.02763
C	-1.11434	-1.57102	0.43317
C	-2.61673	-1.76159	0.48120
H	-0.96217	0.70001	-1.69805
H	-2.86944	1.02621	0.66333
H	-3.18379	1.35280	-1.04015
H	-3.10068	-1.10102	-1.51622
H	-4.34501	-0.71759	-0.33526
H	-2.95845	-1.58096	1.50435
H	-2.91824	-2.77964	0.22926
N	1.50048	-0.22197	-0.13977
C	2.43893	0.74296	-0.41532
C	2.15831	-1.31317	0.15559
H	2.15228	1.74593	-0.68446
H	1.70406	-2.25395	0.42657
H	4.67095	0.62705	-0.40644
H	4.20830	-1.78386	0.26390
N	3.48958	-1.10050	0.08211
C	3.68770	0.20869	-0.28159
O	-0.57440	1.95917	-0.20649
C	-0.40753	2.10725	1.19088
H	0.08481	3.06622	1.34188
H	-1.36359	2.11637	1.72058
H	0.21880	1.30791	1.59427

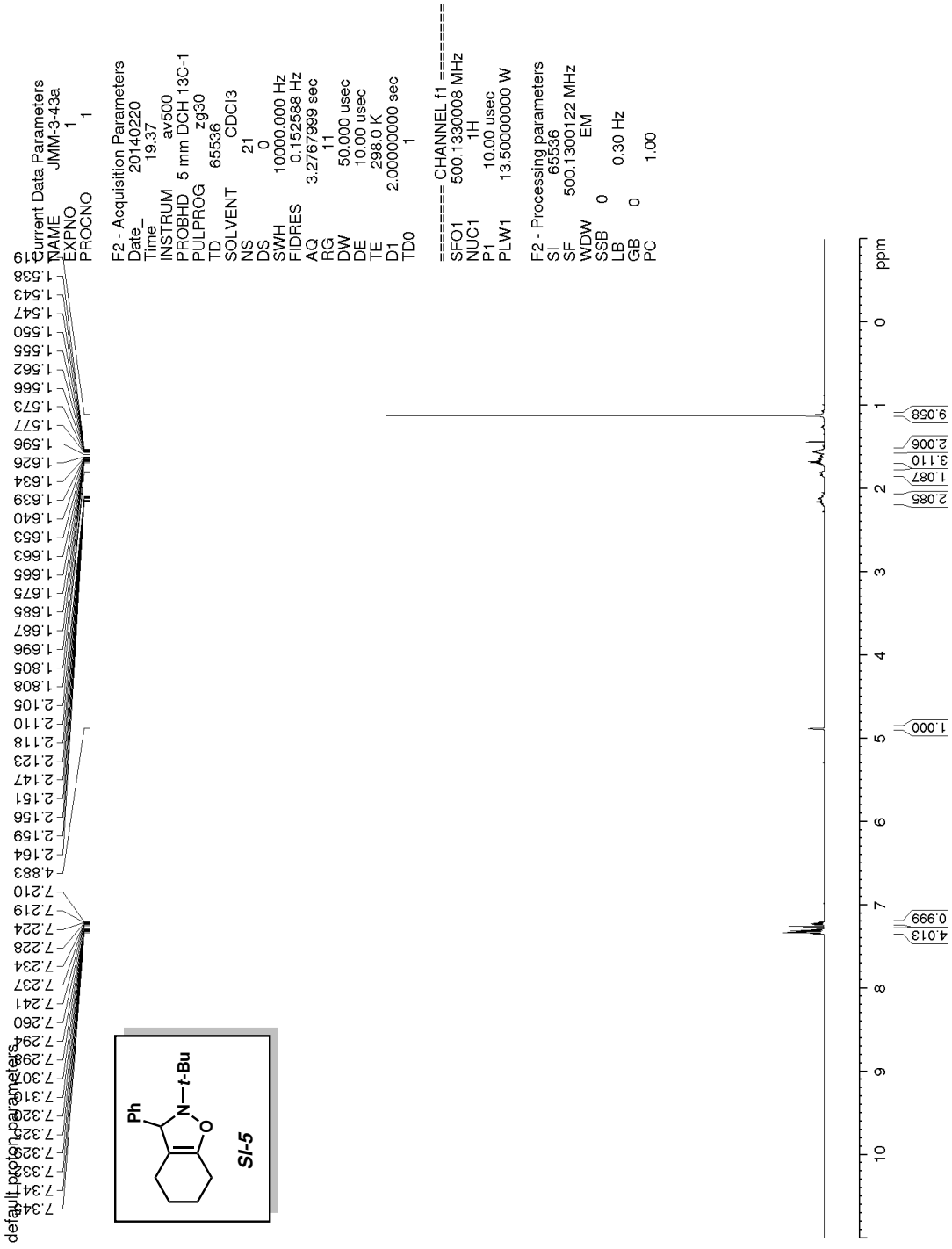
^{1}H NMR Spectra:

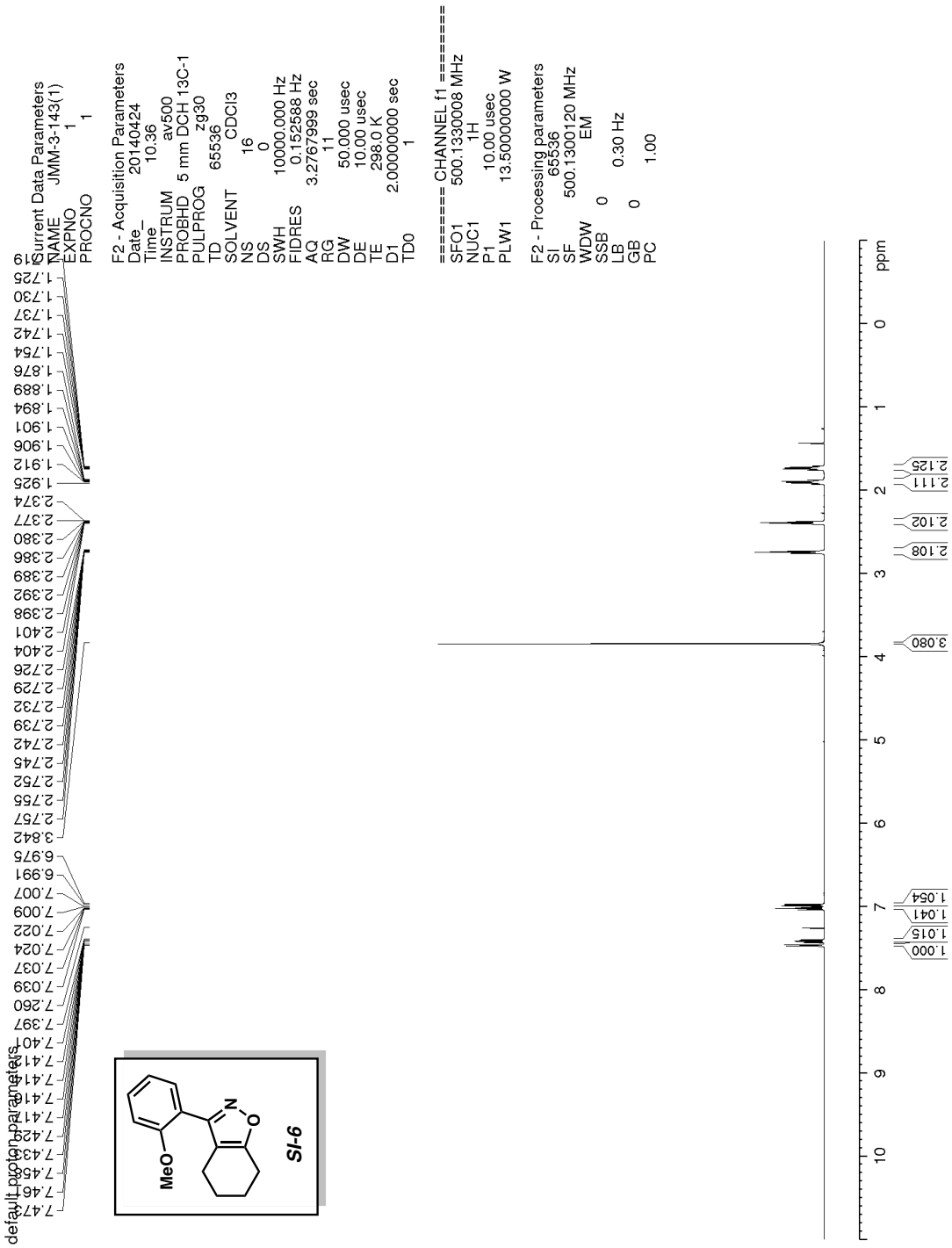

Current Data Parameters
NAME JMM-3-54
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140224
Time 16.37
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 23
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
default proton parameters
SI-1
Bn
ppm
4.079
2.061
2.075
2.046
3.064
2.000

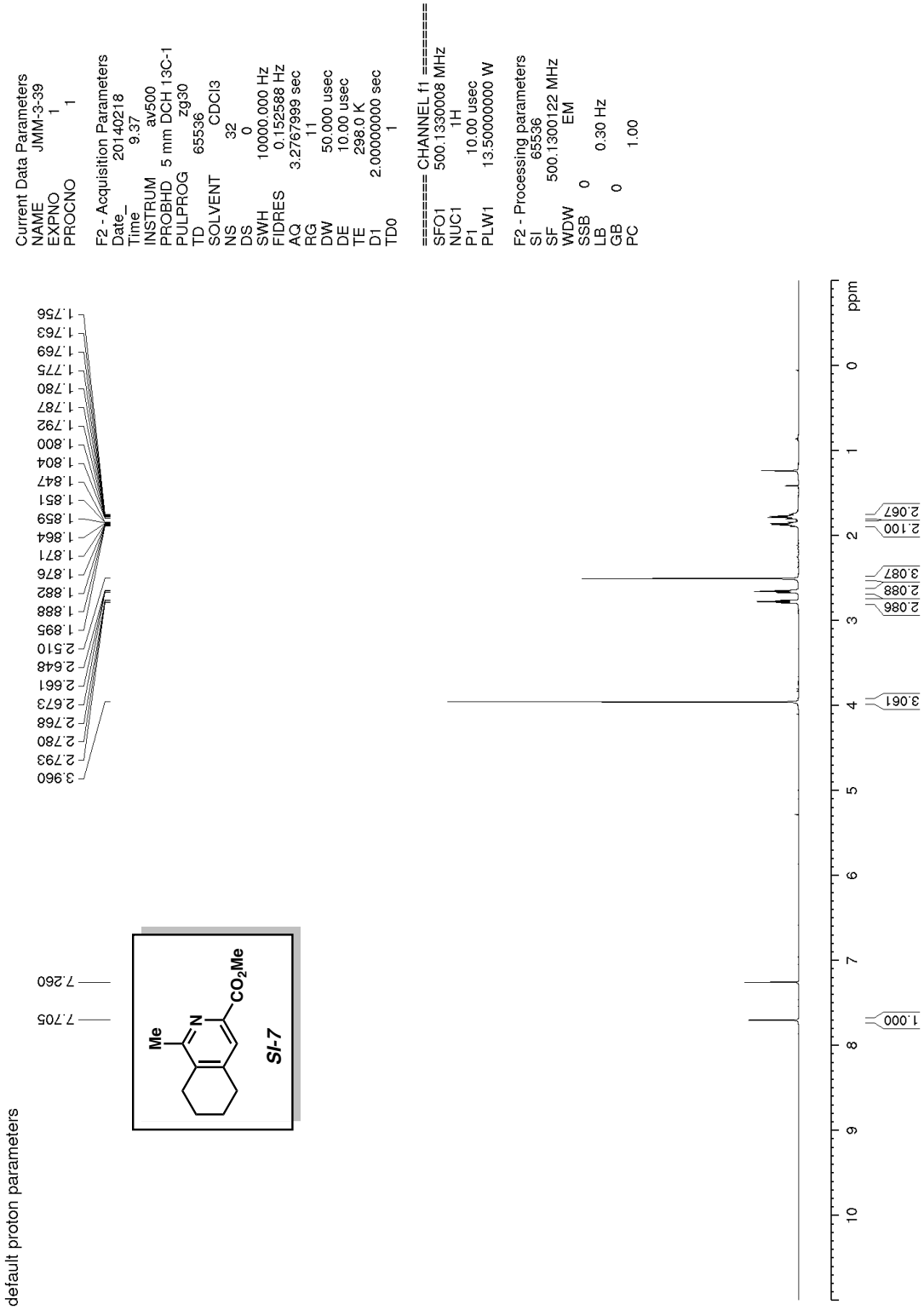

default proton parameters
7.260
4.360
4.346
4.332
4.318
2.741
2.729
2.718
2.681
1.779
1.770
1.759
1.748
1.738
1.352
1.338
1.324
CO2Et
N
N
H
SI-2
Current Data Parameters
NAME JMM-3-37
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140216
Time 15.47
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 27
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3.064
4.073
1.954
2.064
2.000
ppm

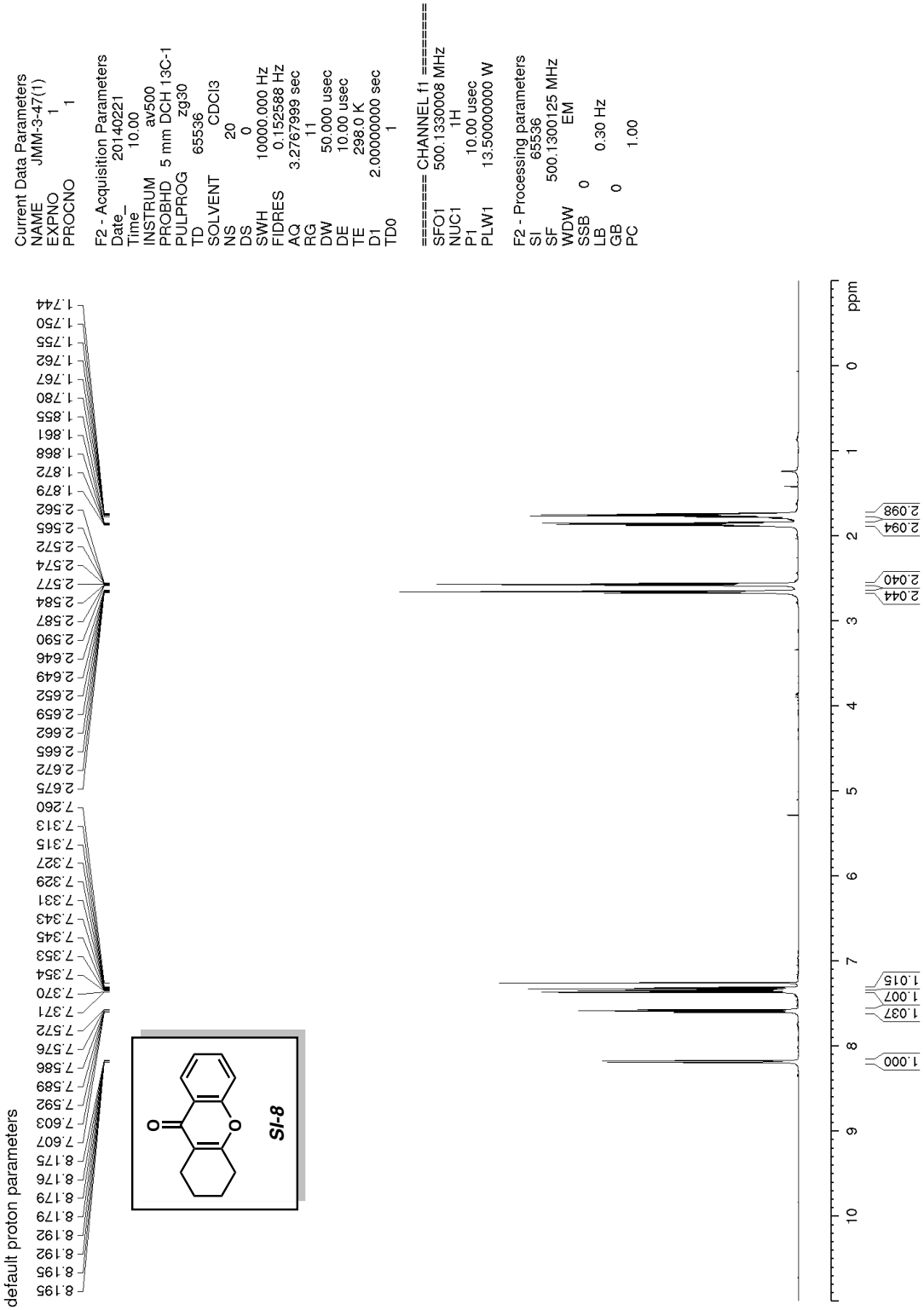

default proton parameters
SI-3
ppm

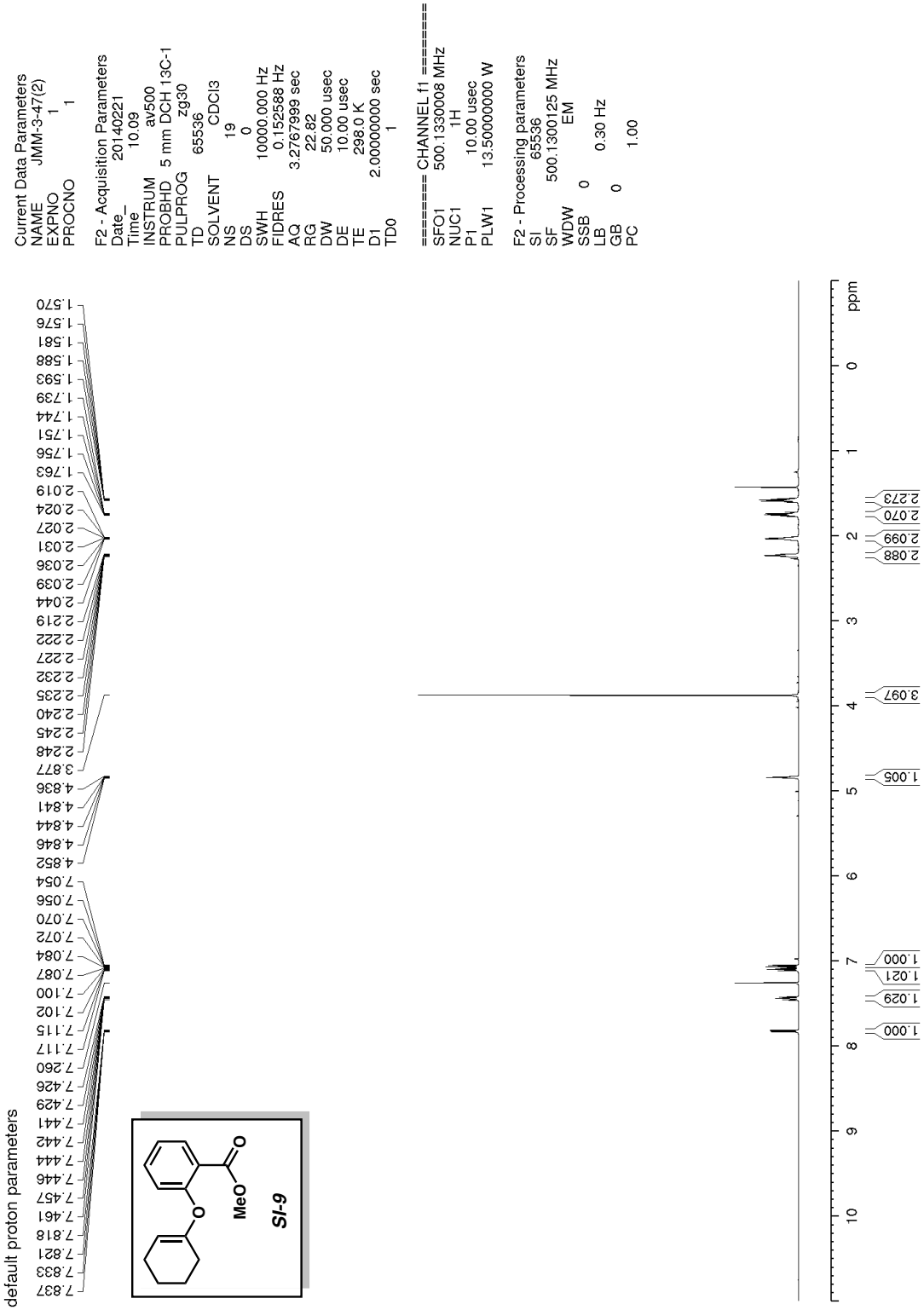

default proton parameters
7.633
7.631
7.616
7.614
7.609
7.416
7.412
7.402
7.400
7.388
7.384
7.260
7.225
7.223
7.221
7.208
7.196
7.194
7.191
2.794
2.782
2.769
2.630
2.617
2.605
1.886
1.880
1.873
1.868
1.864
1.855
1.851
1.842
1.838
1.833
1.801
1.797
1.789
1.785
1.776
1.772
1.766
1.760
1.754
NPh
N
SI-4
Current Data Parameters
NAME JMM-3-32
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140213
Time 13.17
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.962
0.961
2.043
1.000
2.068
2.061
2.077
2.020
10
9
8
7
6
5
4
3
2
1
0
ppm

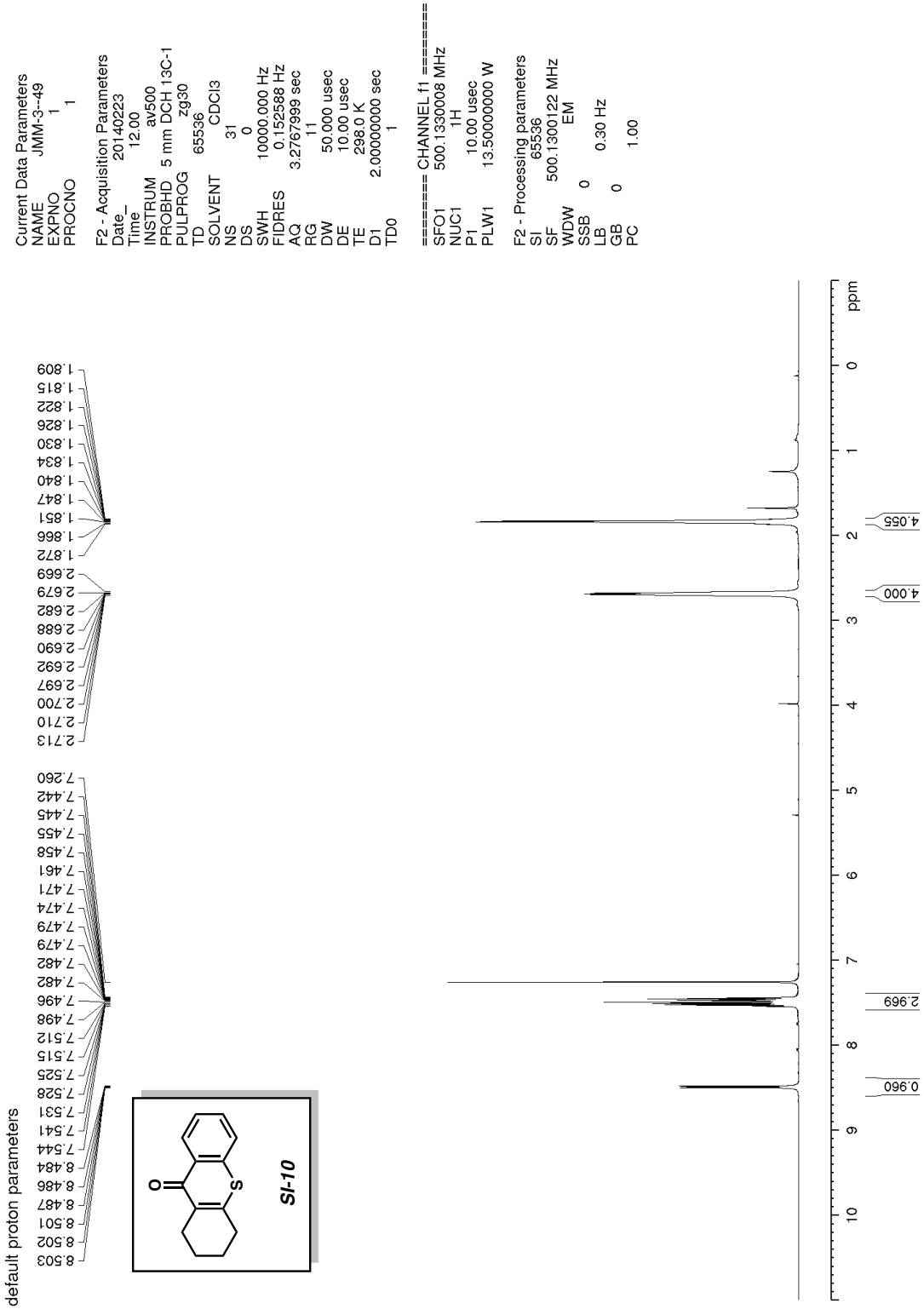

Current Data Parameters
NAME JMM-3-43a
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140220
Time 19.37
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 21
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
default proton parameters
Ph
N—t-Bu
O
SI-5
9.058
2.006
3.110
1.087
2.085
1.000
4.013
0.999
ppm

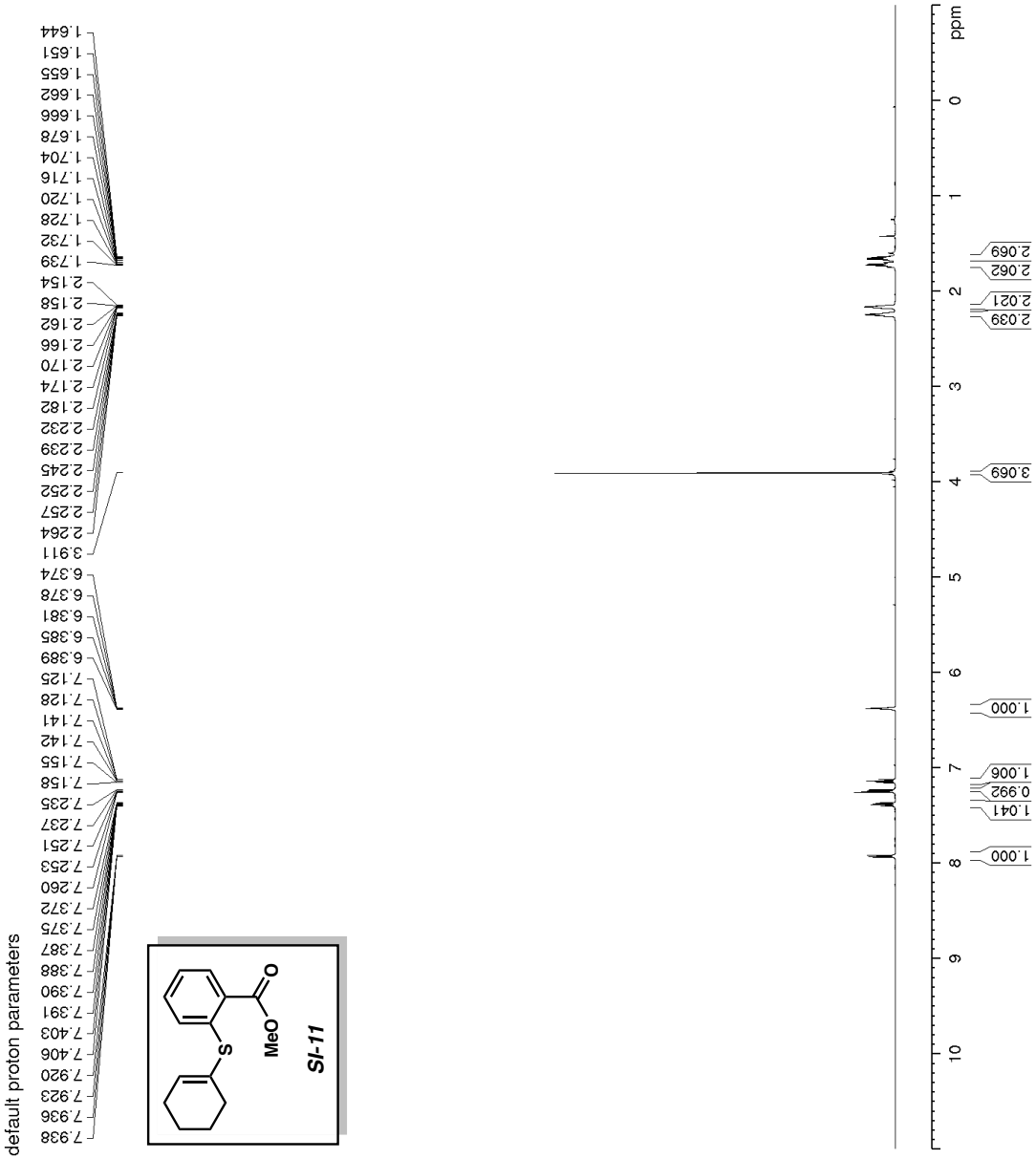

$Current Data Parameters
NAME JMM-3-143(1)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140424
Time 10.36
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
default proton parameters
MeO
SI-6
1.000
1.015
1.041
1.054
3.080
2.108
2.102
2.111
2.125
ppm

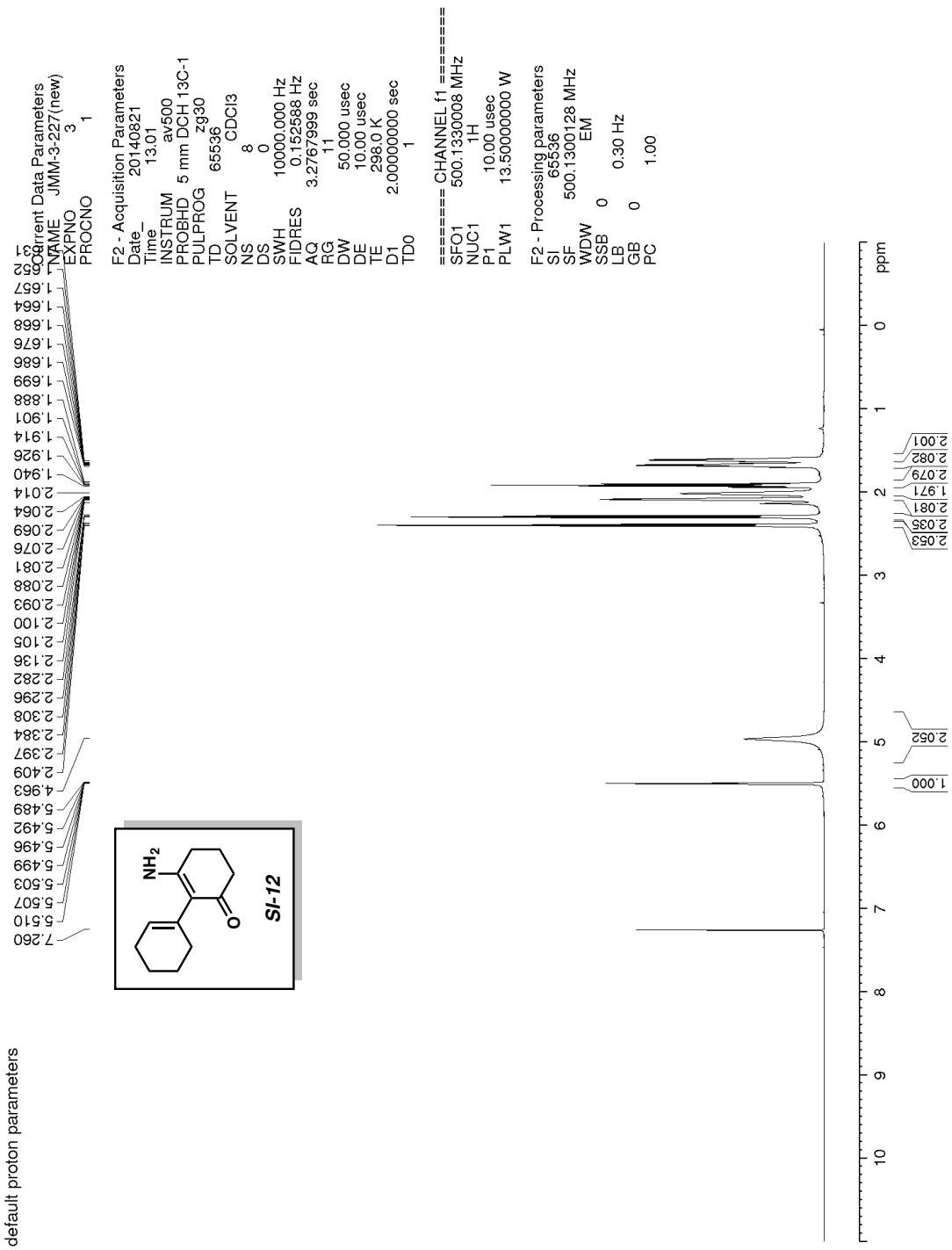

default proton parameters
Current Data Parameters
NAME JMM-3-39
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140218
Time 9.37
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.705
7.260
Me
N
CO2Me
SI-7
3.960
2.793
2.780
2.768
2.673
2.661
2.510
2.648
1.895
1.888
1.882
1.876
1.871
1.864
1.859
1.851
1.847
1.804
1.800
1.792
1.787
1.780
1.775
1.769
1.763
1.756
3.061
2.086
2.088
3.087
2.067
2.100
1.000
ppm

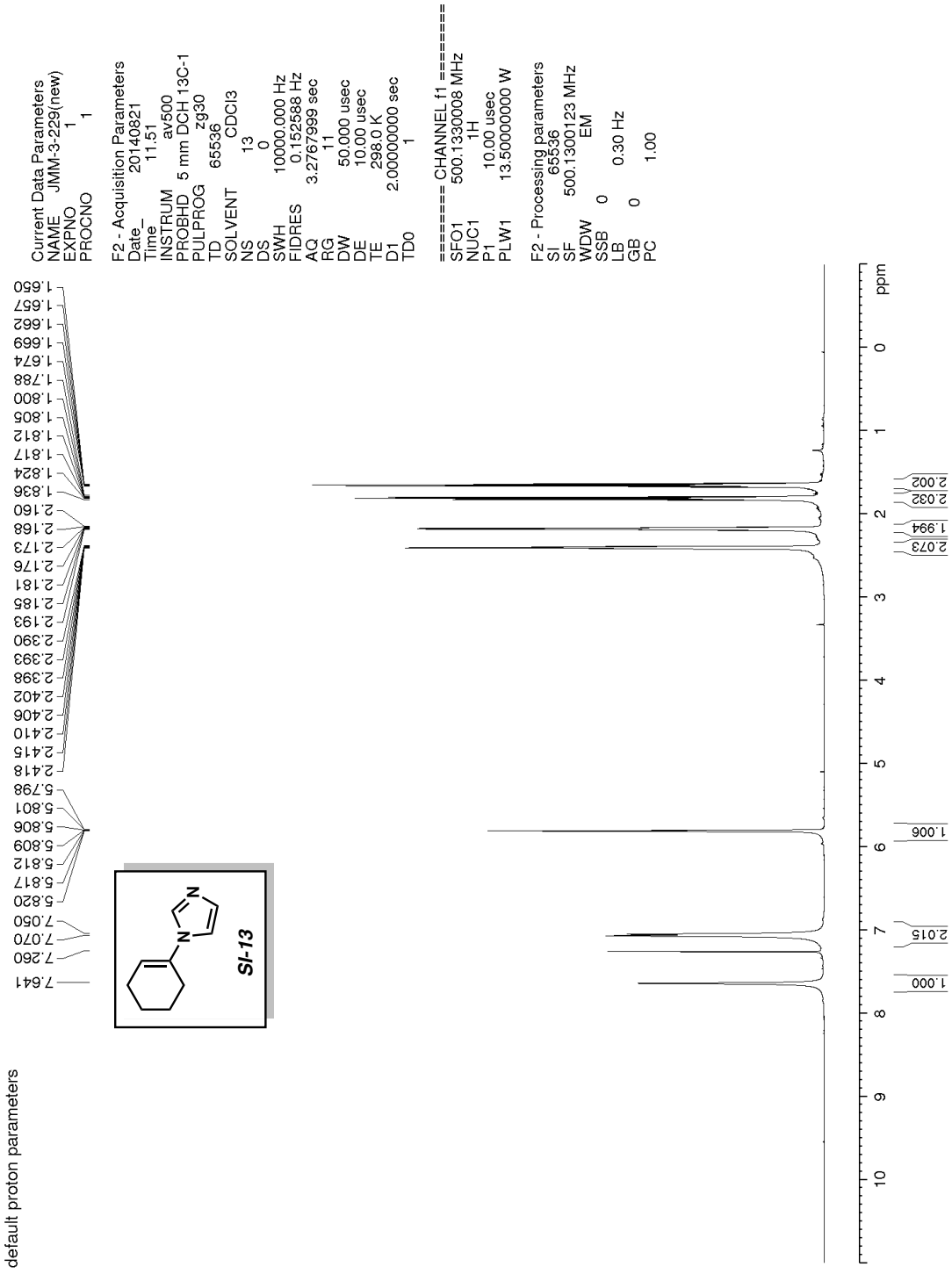

Current Data Parameters
NAME JMM-3-47(1)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140221
Time 10.00
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 20
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
default proton parameters
SI-8
2.098
2.094
2.044
2.040
1.037
1.007
1.015
1.000
ppm

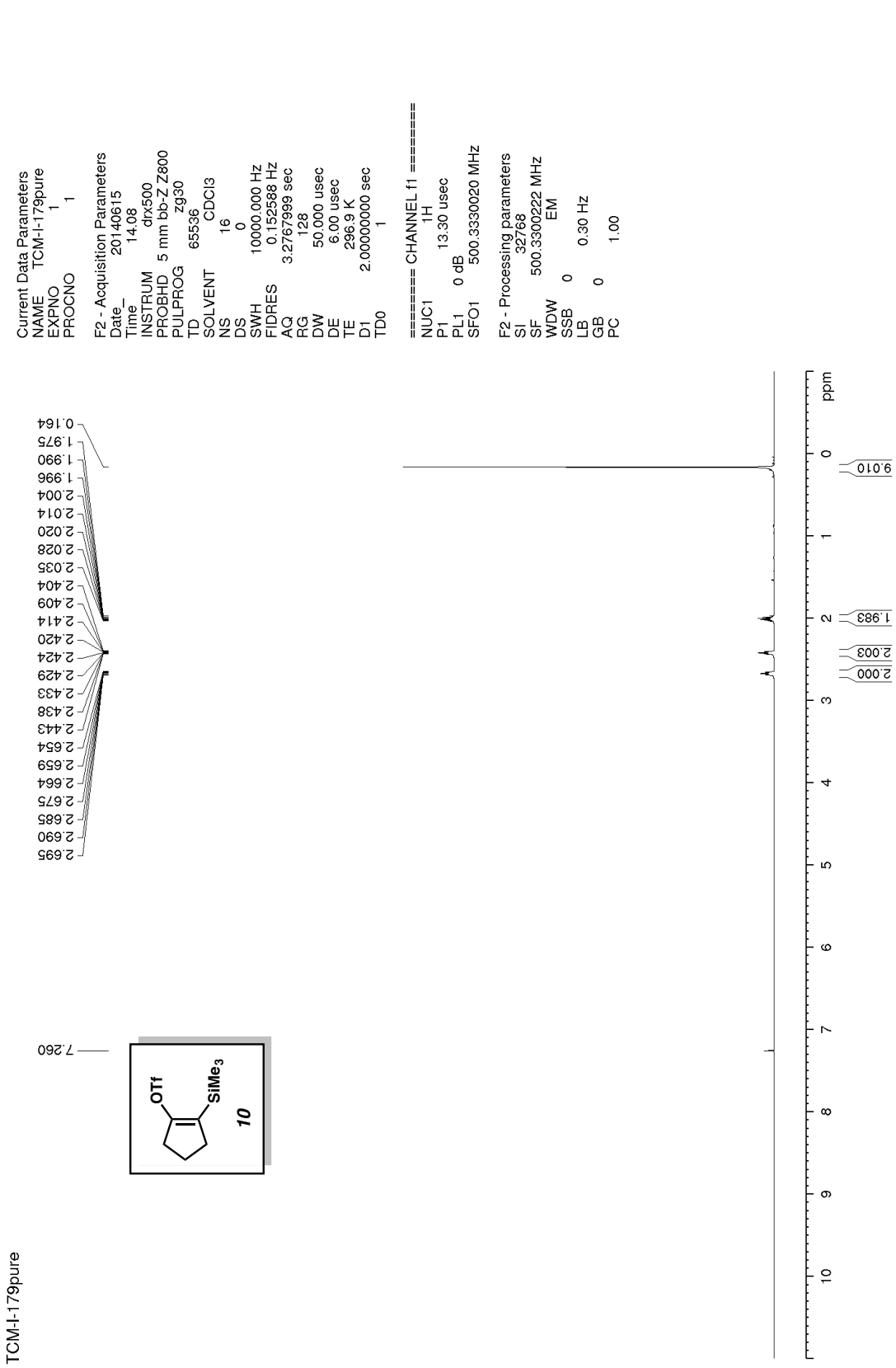

Current Data Parameters
NAME JMM-3-47(2)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140221
Time 10.09
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 19
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 22.82
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
default proton parameters
7.837
7.833
7.821
7.818
7.461
7.457
7.446
7.444
7.442
7.441
7.429
7.426
7.260
7.117
7.115
7.102
7.100
7.087
7.084
7.072
7.070
7.056
7.054
4.852
4.846
4.844
4.841
4.836
3.877
2.248
2.245
2.240
2.235
2.232
2.227
2.222
2.219
2.044
2.039
2.036
2.031
2.027
2.024
2.019
1.763
1.756
1.751
1.744
1.739
1.593
1.588
1.581
1.576
1.570
MeO
O
O
SI-9
1.000
1.029
1.021
1.000
1.005
3.097
2.088
2.099
2.070
2.273
ppm

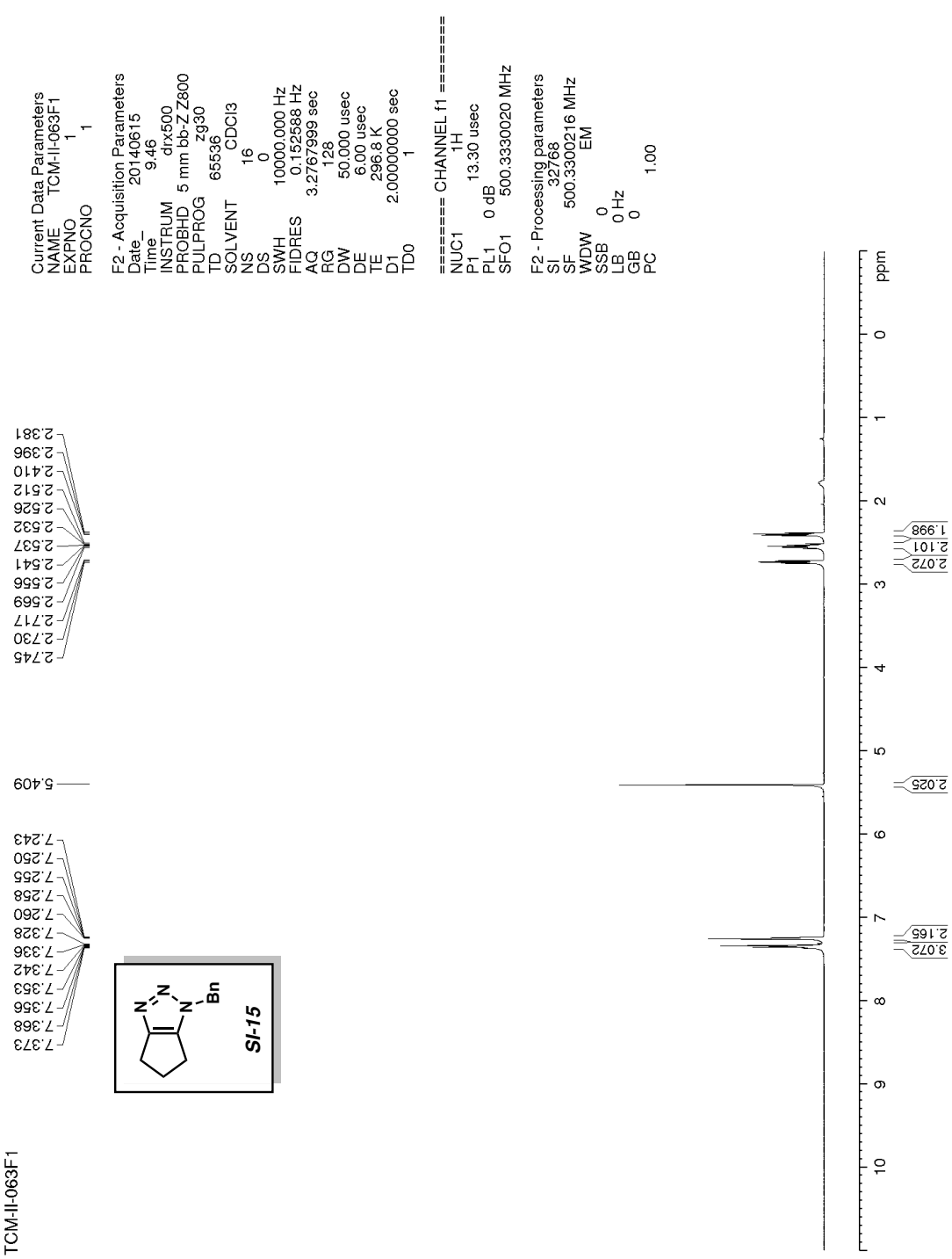

Current Data Parameters
NAME JMM-3--49
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140223
Time 12.00
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 31
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
default proton parameters
8.503
8.502
8.501
8.487
8.486
8.484
7.544
7.541
7.531
7.528
7.525
7.515
7.512
7.498
7.496
7.482
7.482
7.479
7.479
7.474
7.471
7.461
7.458
7.455
7.445
7.442
7.260
2.713
2.710
2.700
2.697
2.692
2.690
2.688
2.682
2.679
2.669
1.872
1.866
1.851
1.847
1.840
1.834
1.830
1.826
1.822
1.815
1.809
SI-10
4.055
4.000
2.969
0.960
ppm

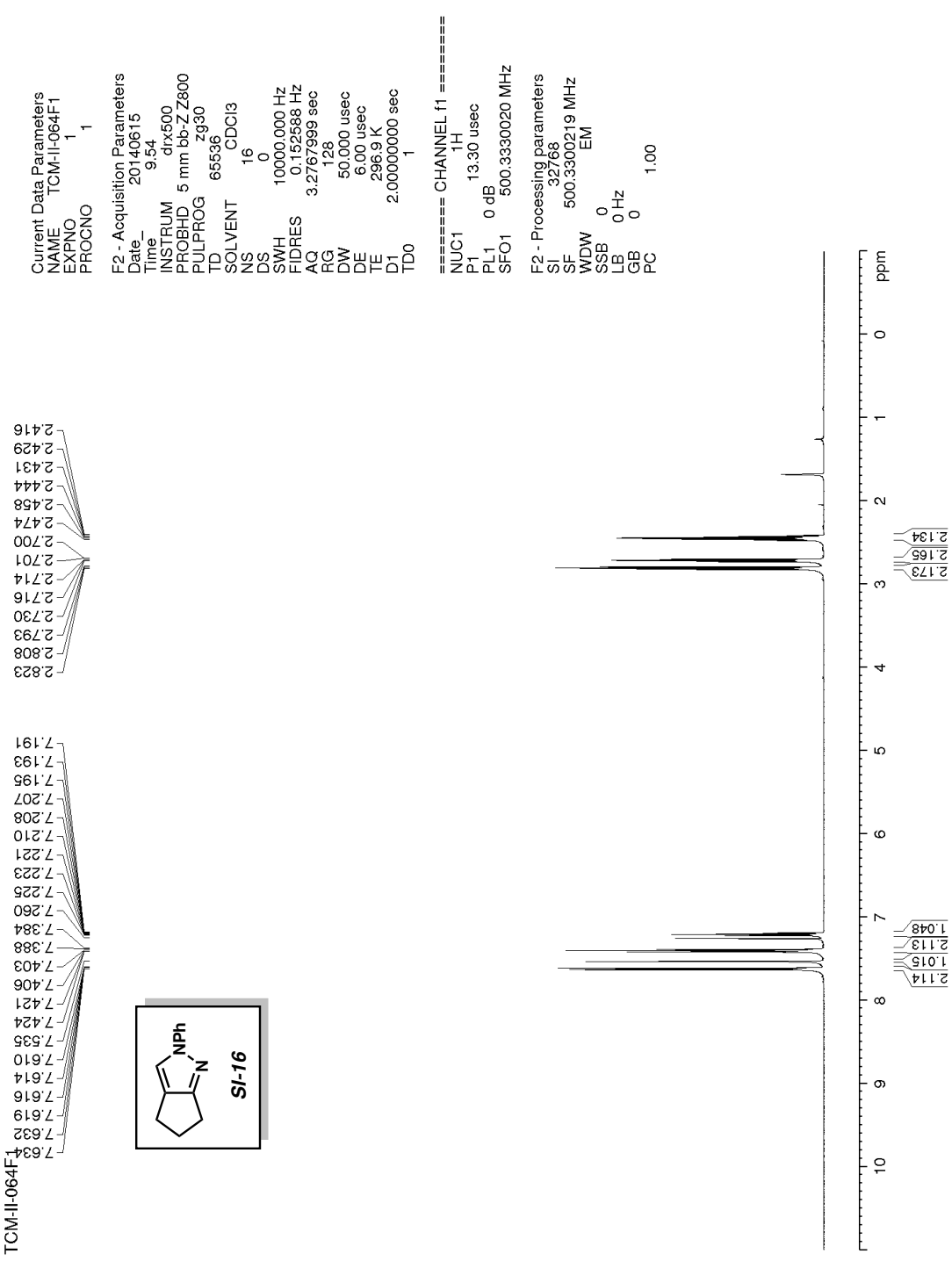

default proton parameters
Current Data Parameters
NAME JMM-3-49-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140222
Time 19.03
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 20
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
O
S
SI-11
7.938
7.936
7.923
7.920
7.406
7.403
7.391
7.390
7.388
7.387
7.375
7.372
7.260
7.253
7.251
7.237
7.235
7.158
7.155
7.142
7.141
7.128
7.125
6.389
6.385
6.381
6.378
6.374
3.911
2.264
2.257
2.252
2.245
2.239
2.232
2.182
2.174
2.170
2.166
2.162
2.158
2.154
1.739
1.732
1.728
1.720
1.716
1.704
1.678
1.666
1.662
1.655
1.651
1.644
3.069
2.069
2.062
2.039
2.021
1.000
1.041
0.992
1.006
1.000
ppm

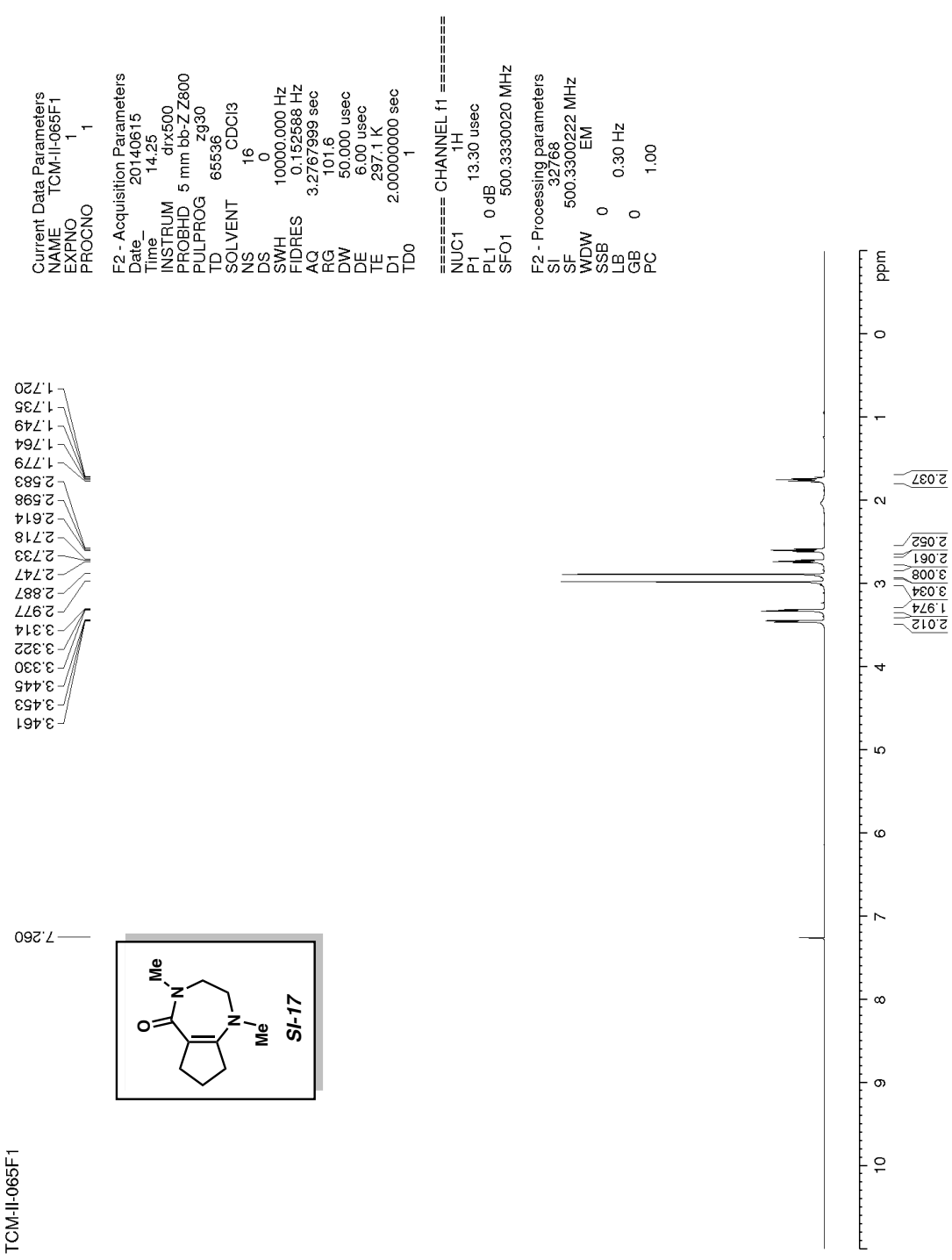

default proton parameters
Current Data Parameters
NAME JMM-3-227(new)
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140821
Time 13.01
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
SI-12
ppm

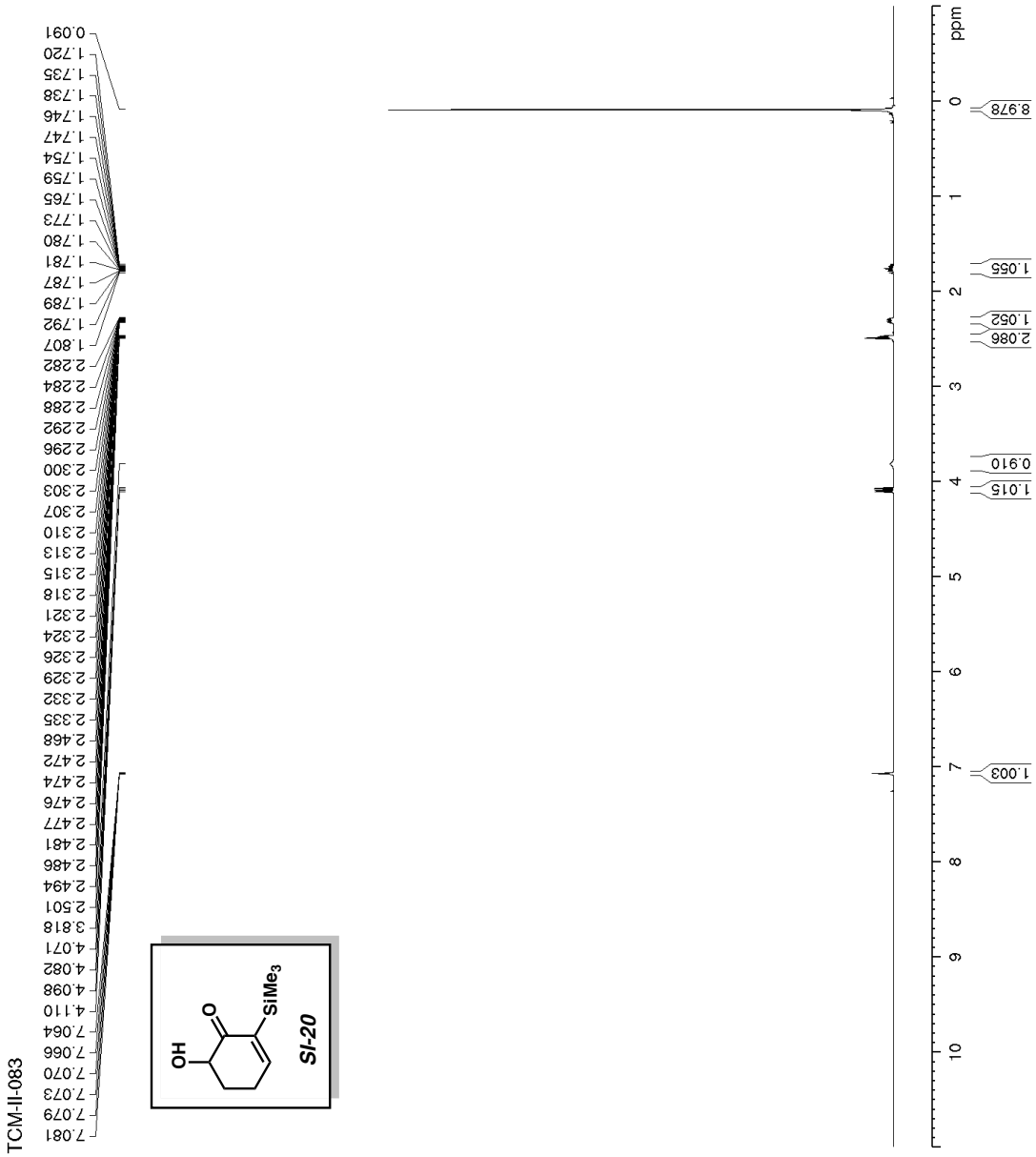

default proton parameters
Current Data Parameters
NAME JMM-3-229(new)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140821
Time 11.51
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 13
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
SI-13
7.641
7.260
7.070
7.050
5.820
5.817
5.812
5.809
5.806
5.801
5.798
2.418
2.415
2.410
2.406
2.402
2.398
2.393
2.390
2.193
2.185
2.181
2.176
2.173
2.168
2.160
1.836
1.824
1.817
1.812
1.805
1.800
1.788
1.674
1.669
1.662
1.657
1.650
2.002
2.032
1.994
2.073
1.006
2.015
1.000
ppm

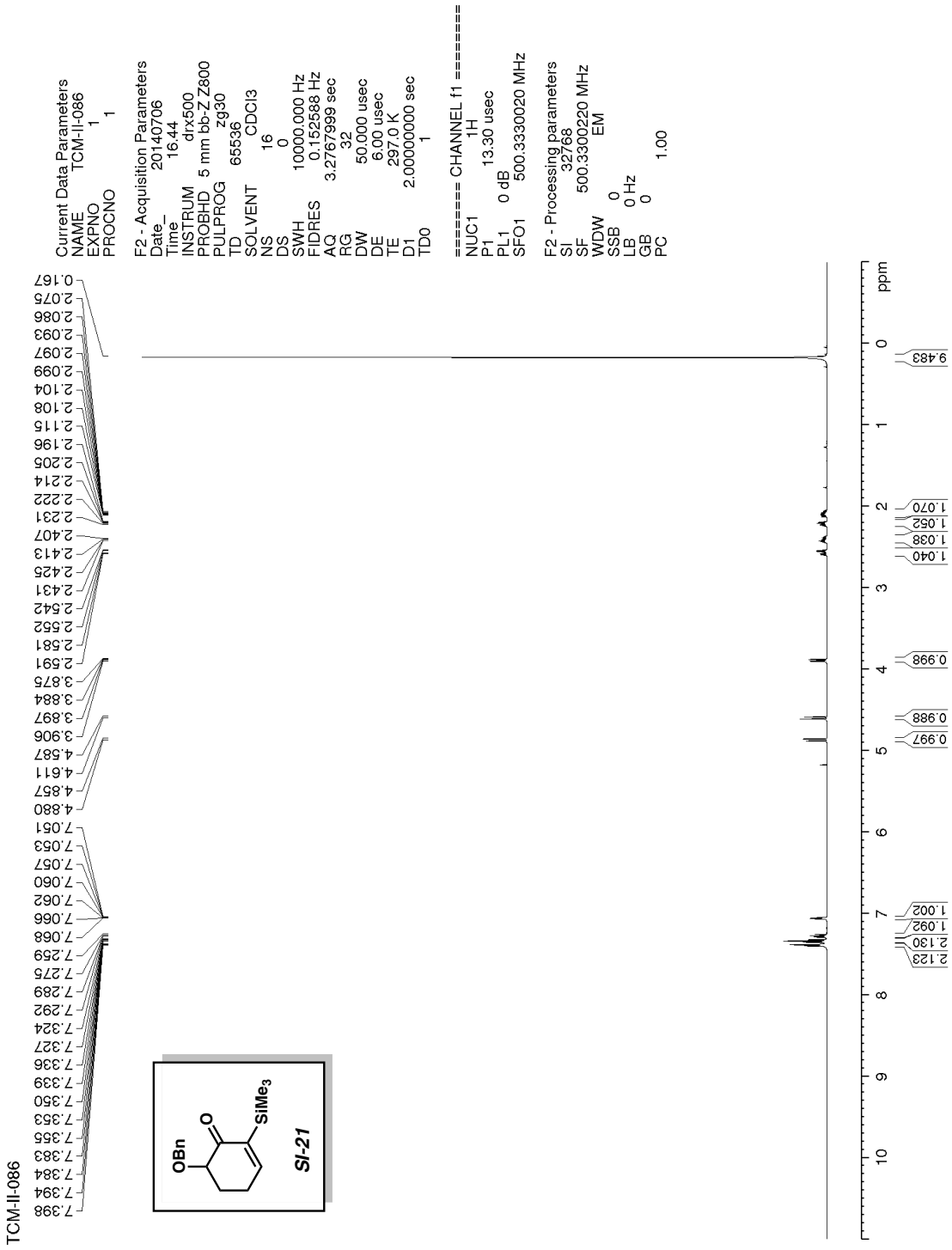

TCM-I-179pure
Current Data Parameters
NAME TCM-I-179pure
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140615
Time 14.08
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300222 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.260
2.695
2.690
2.685
2.675
2.664
2.659
2.654
2.443
2.438
2.433
2.429
2.424
2.420
2.414
2.409
2.404
2.035
2.028
2.020
2.014
2.004
1.996
1.990
1.975
0.164
OTf
SiMe3
10
9.010
1.983
2.003
2.000
ppm

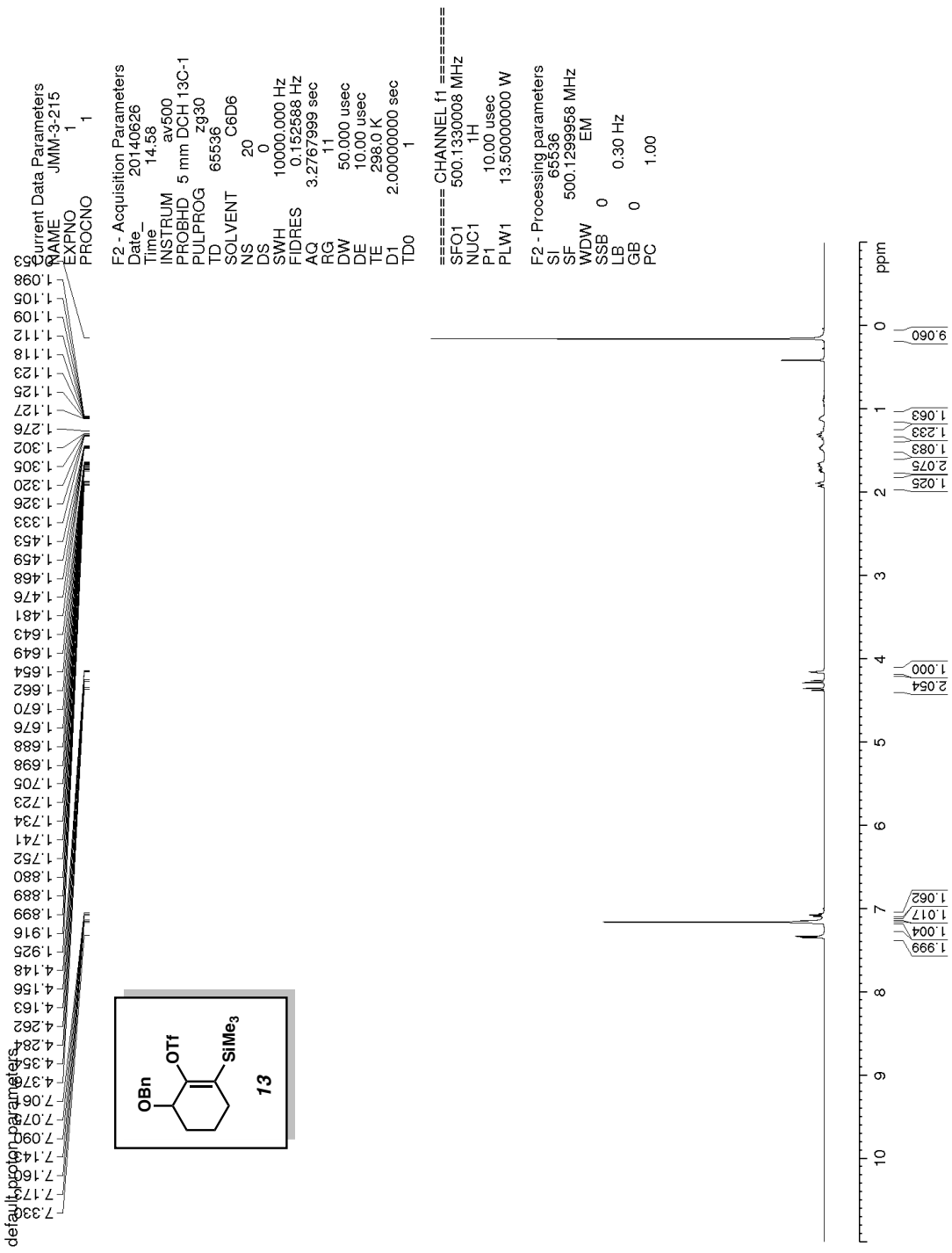

TCM-II-063F1
Current Data Parameters
NAME TCM-II-063F1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140615
Time 9.46
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 296.8 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300216 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
SI-15
Bn
7.373
7.368
7.356
7.353
7.342
7.336
7.328
7.260
7.258
7.255
7.250
7.243
5.409
2.745
2.730
2.717
2.569
2.556
2.541
2.537
2.532
2.526
2.512
2.410
2.396
2.381
3.072
2.165
2.072
2.101
1.998
2.025
ppm

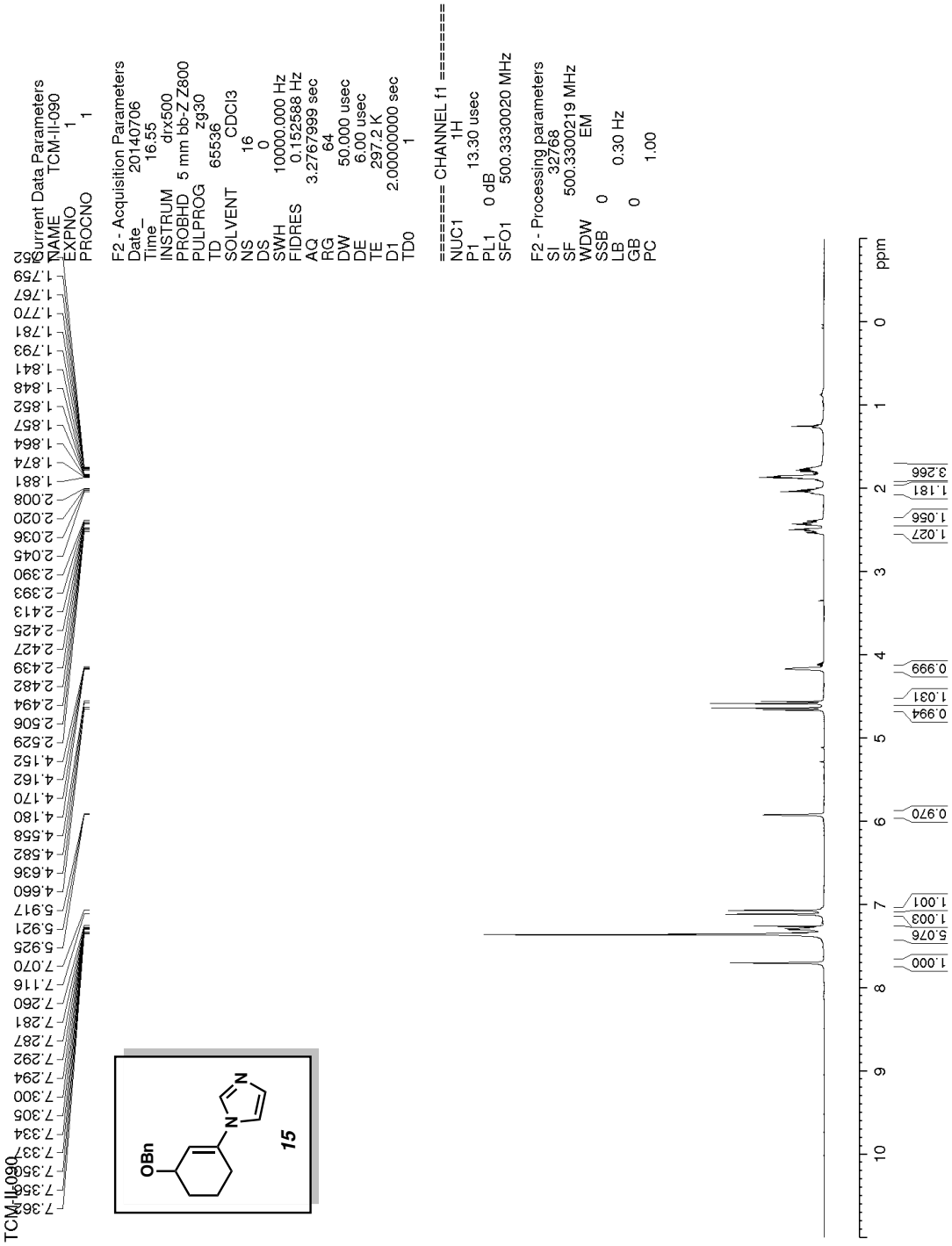

Current Data Parameters
NAME TCM-II-064F1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140615
Time 9.54
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300219 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
TCM-II-064F1
NPh
N
SI-16
7.634
7.632
7.619
7.616
7.614
7.610
7.535
7.424
7.421
7.406
7.403
7.388
7.384
7.260
7.225
7.223
7.221
7.210
7.208
7.207
7.195
7.193
7.191
2.823
2.808
2.793
2.730
2.716
2.714
2.701
2.700
2.474
2.458
2.444
2.431
2.429
2.416
2.114
1.015
2.113
1.048
2.173
2.165
2.134
ppm

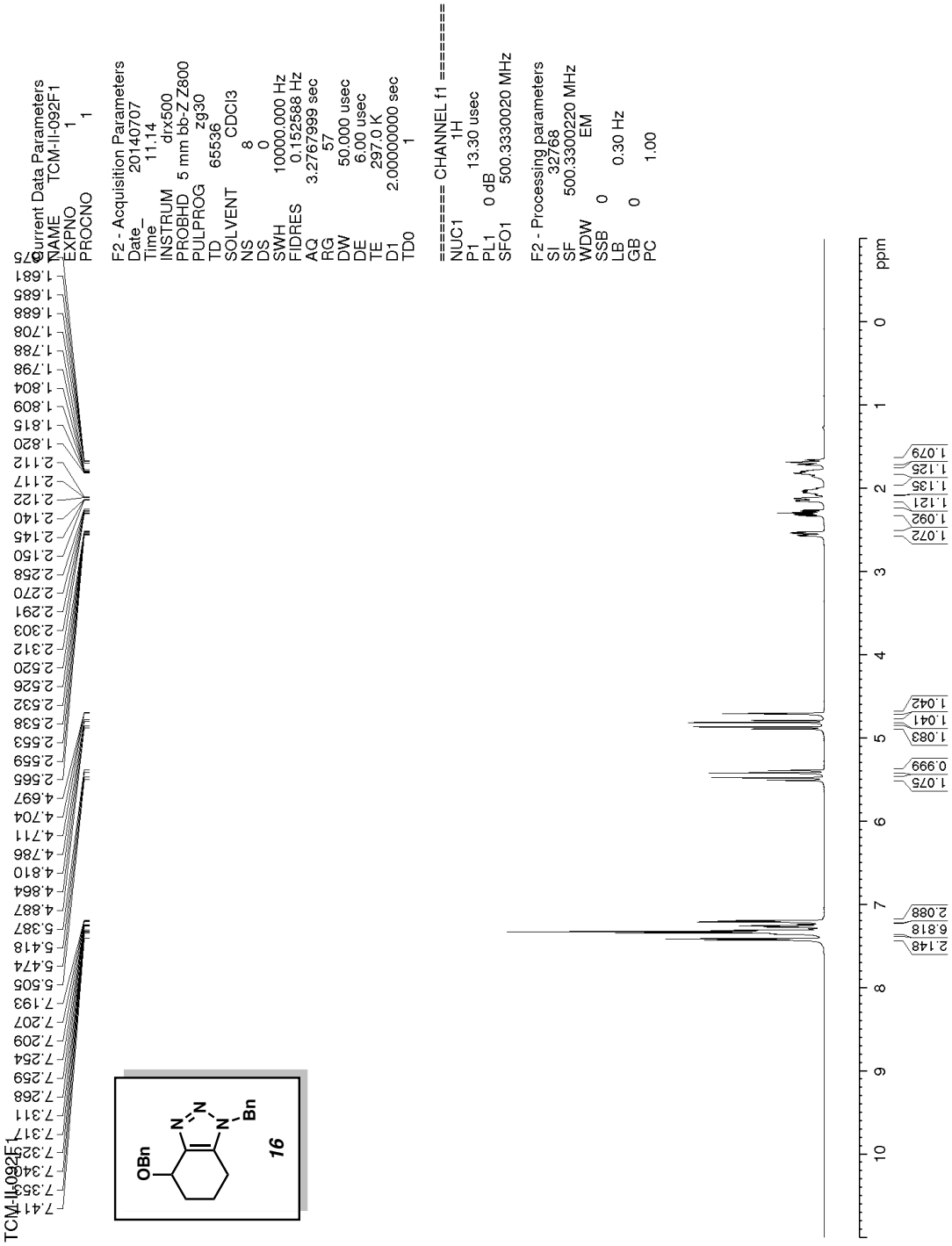

TCM-II-065F1
7.260
Me
N
O
N
Me
SI-17
3.461
3.453
3.445
3.330
3.322
3.314
2.977
2.887
2.747
2.733
2.718
2.614
2.598
2.583
1.779
1.764
1.749
1.735
1.720
2.012
1.974
3.034
3.008
2.061
2.052
2.037
ppm
Current Data Parameters
NAME TCM-II-065F1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140615
Time 14.25
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 101.6
DW 50.000 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300222 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

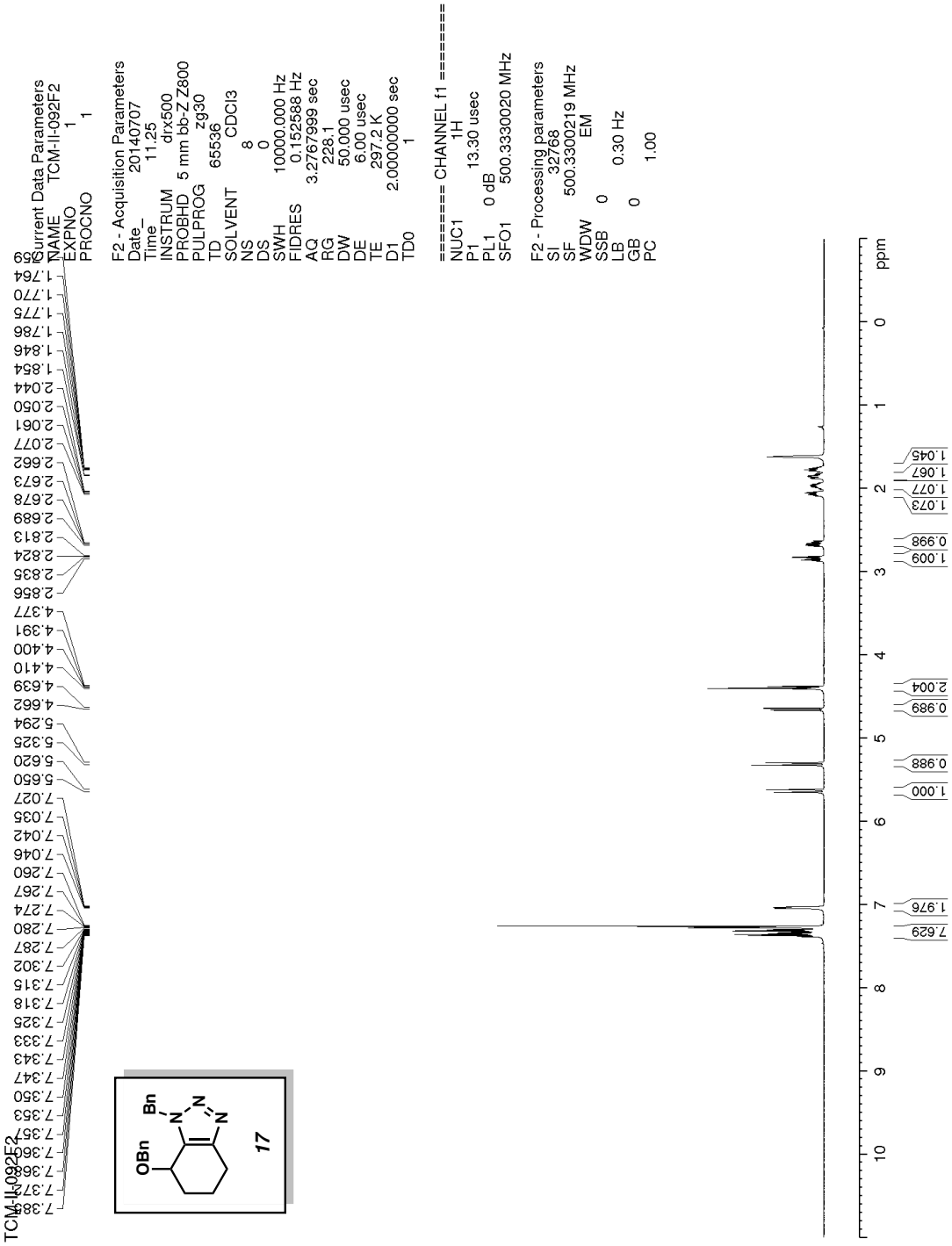

Current Data Parameters
NAME TCM-II-083
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140626
Time 17.18
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 22.6
DW 50.000 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300216 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
TCM-II-083
7.081
7.079
7.073
7.070
7.066
7.064
4.110
4.098
4.082
4.071
3.818
2.501
2.494
2.486
2.481
2.477
2.476
2.474
2.472
2.468
2.335
2.332
2.329
2.326
2.324
2.321
2.318
2.315
2.313
2.310
2.307
2.303
2.300
2.296
2.292
2.288
2.284
2.282
1.807
1.792
1.789
1.787
1.781
1.780
1.773
1.765
1.759
1.754
1.747
1.746
1.738
1.735
1.720
0.091
OH
O
SiMe3
SI-20
ppm
8.978
1.055
2.086
1.052
0.910
1.015
1.003

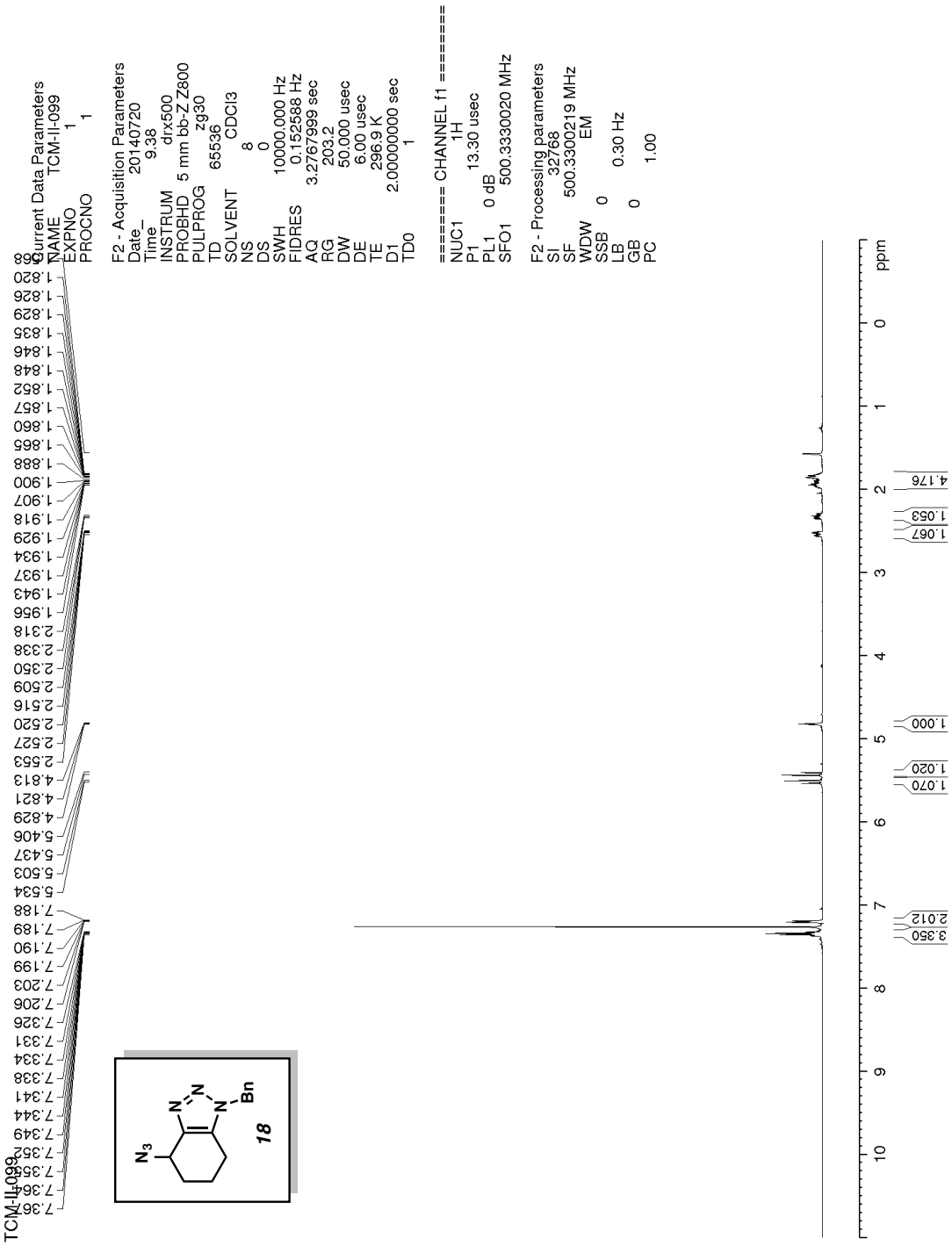

TCM-II-086
Current Data Parameters
NAME TCM-II-086
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140706
Time 16.44
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 32
DW 50.000 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
OBn
SiMe3
SI-21
ppm

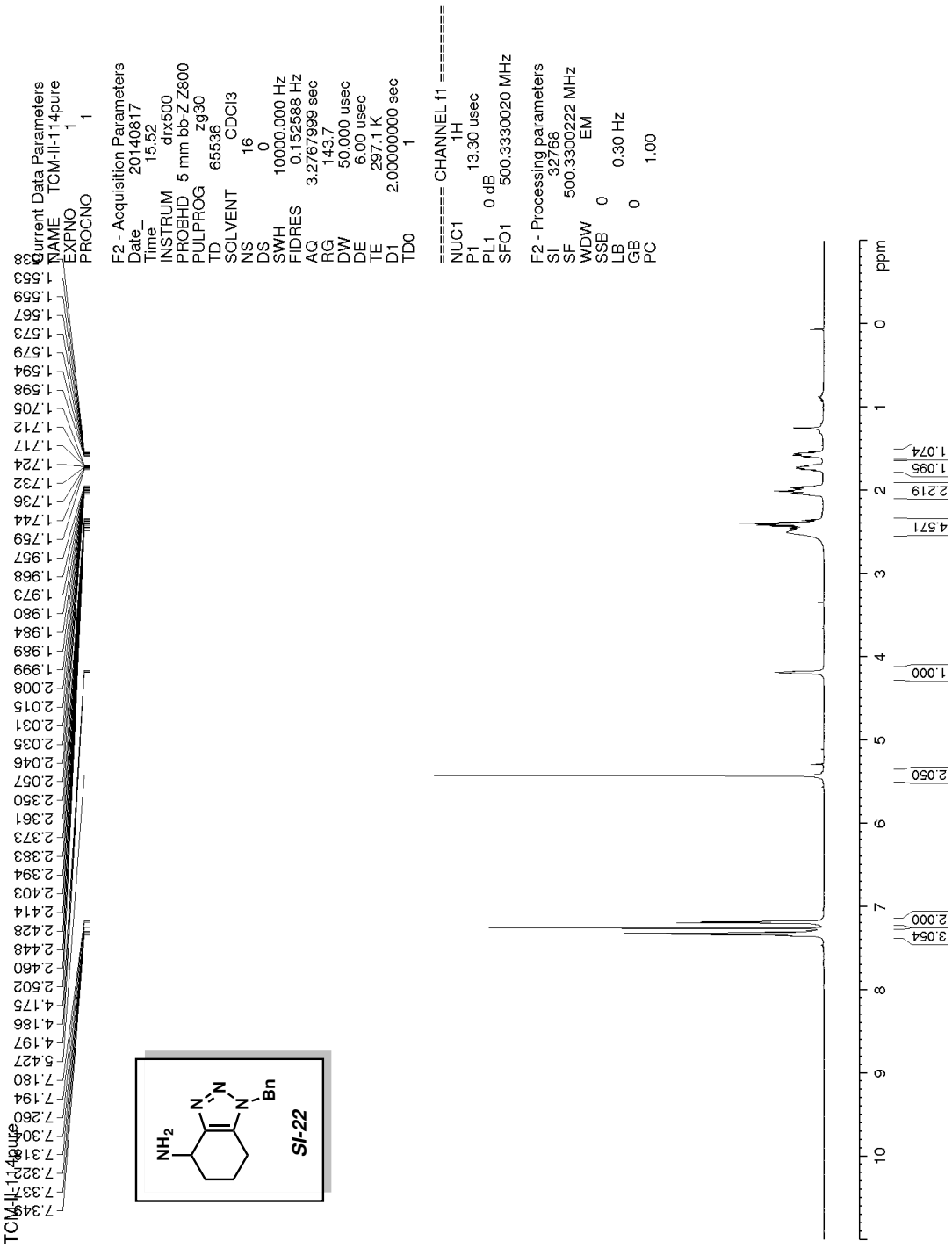

default proton parameters
$Current Data Parameters
NAME JMM-3-215
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140626
Time 14.58
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 20
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1299958 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OBn
OTf
SiMe3
13
ppm
9.060
2.054
1.000
1.999
1.004
1.017
1.062
1.025
2.075
1.083
1.233
1.063

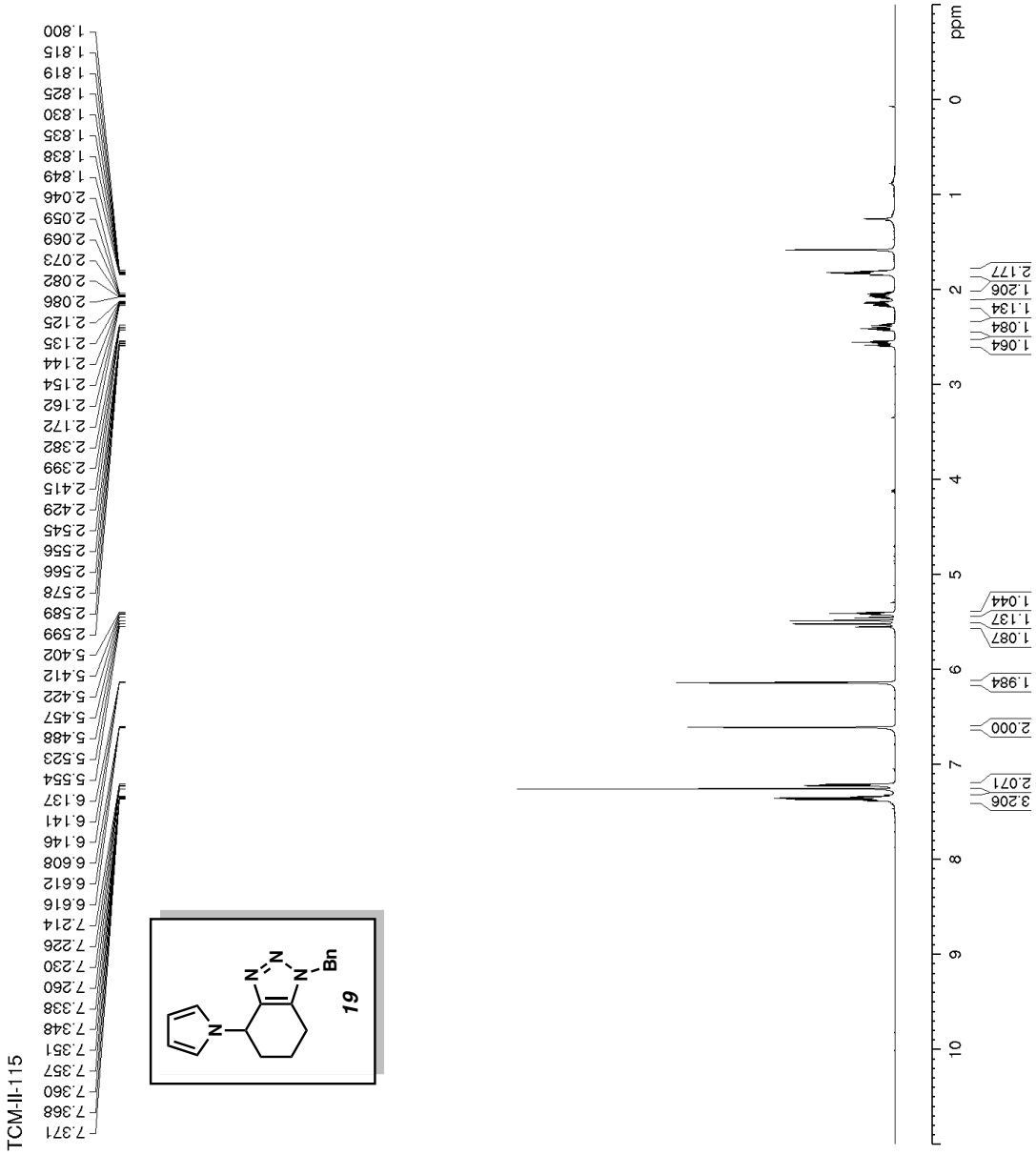

$Current Data Parameters
NAME TCM-II-090
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140706
Time 16.55
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 64
DW 50.000 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300219 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TCM-II-090
OBn
15
1.000
5.076
1.003
1.001
0.970
0.994
1.031
0.999
1.027
1.056
1.181
3.266
ppm


$Current Data Parameters
NAME TCM-II-092F1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140707
Time 11.14
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 57
DW 50.000 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OBn
Bn
16
TCM-II-092F1
ppm

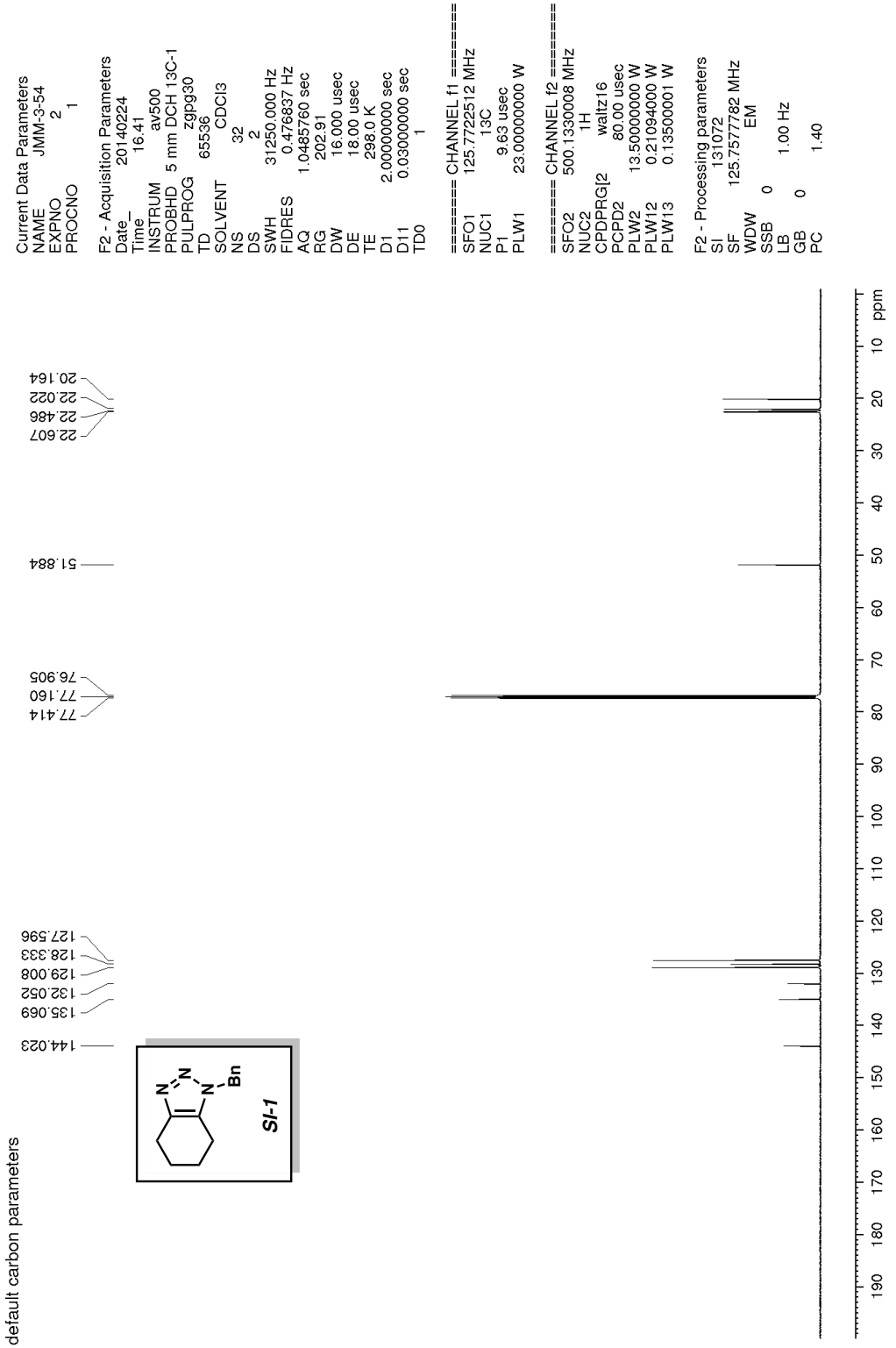

TCM-II-092F2
$Current Data Parameters
NAME TCM-II-092F2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140707
Time 11.25
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 228.1
DW 50.000 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300219 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OBn
Bn
N
N
N
17
7.629
1.976
1.000
0.988
0.989
2.004
1.009
0.998
1.073
1.077
1.067
1.045
ppm

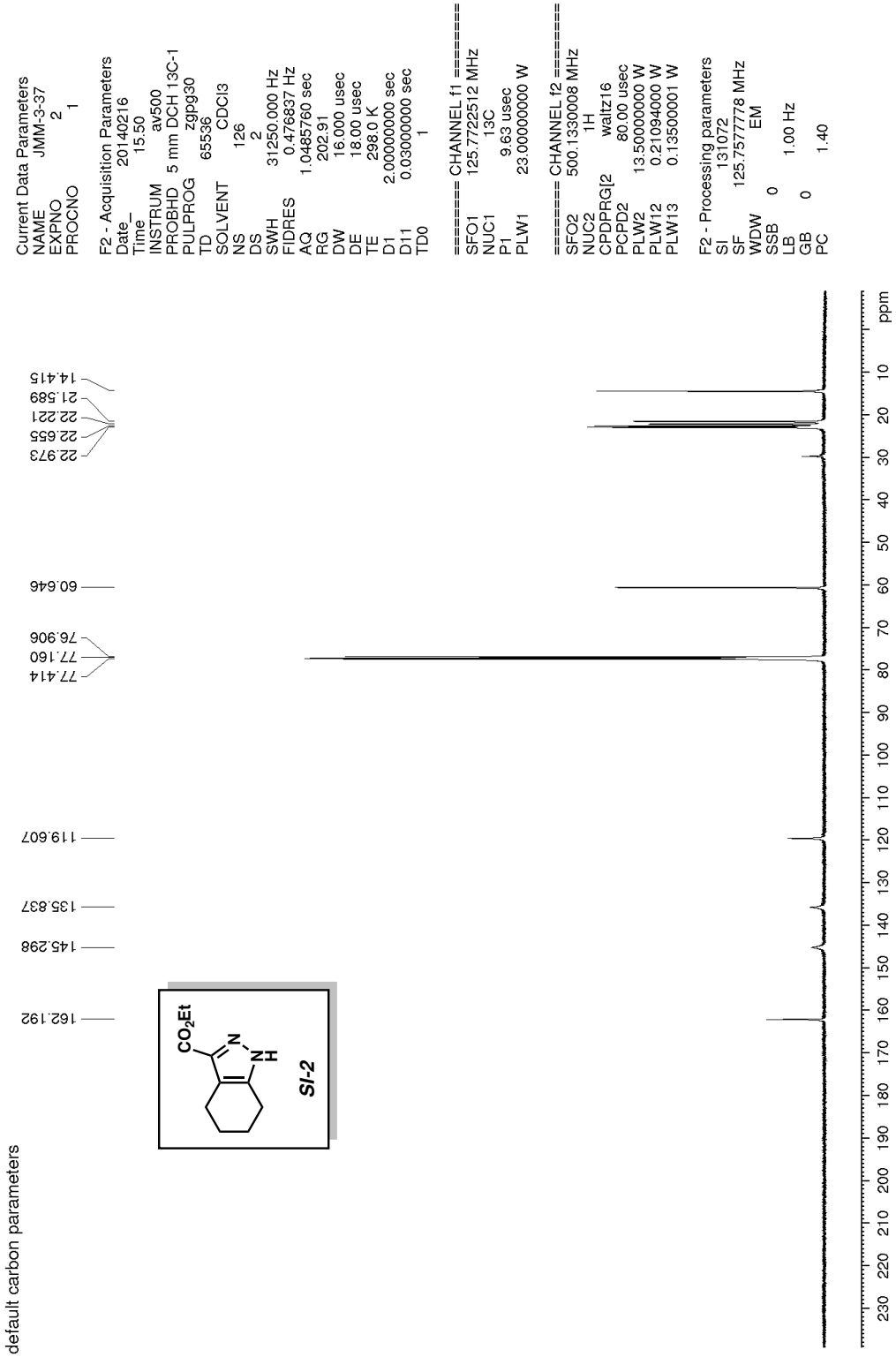

TCM-II-099
7.368
7.355
7.352
7.349
7.344
7.341
7.338
7.334
7.331
7.326
7.206
7.203
7.199
7.190
7.189
7.188
5.534
5.503
5.437
5.406
4.829
4.821
4.813
2.553
2.527
2.520
2.516
2.509
2.350
2.338
2.318
1.956
1.943
1.937
1.934
1.929
1.918
1.907
1.900
1.888
1.865
1.860
1.857
1.852
1.848
1.846
1.835
1.829
1.826
1.820
1.788
Current Data Parameters
NAME TCM-II-099
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140720
Time 9.38
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 203.2
DW 50.000 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300219 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N3
N
N
N
Bn
18
4.176
1.067
1.053
1.000
1.070
1.020
3.350
2.012
ppm

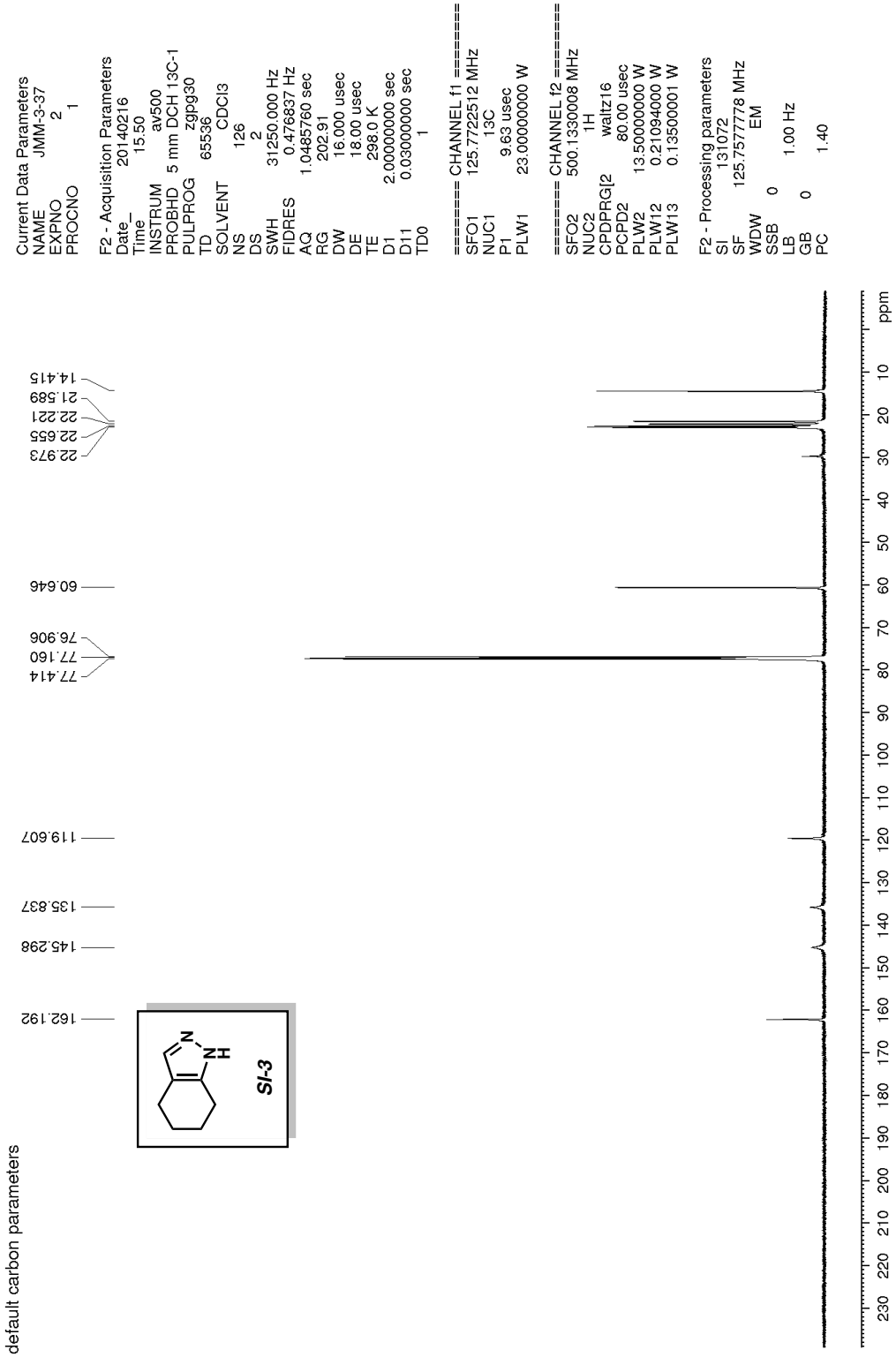

TCM-II-114pure
7.349
7.337
7.322
7.318
7.260
7.194
7.180
5.427
4.197
4.186
4.175
2.502
2.460
2.448
2.428
2.414
2.403
2.394
2.383
2.373
2.361
2.350
2.057
2.046
2.035
2.031
2.015
2.008
1.999
1.989
1.984
1.980
1.973
1.968
1.957
1.759
1.744
1.736
1.732
1.724
1.717
1.712
1.705
1.598
1.594
1.579
1.573
1.567
1.559
1.553
1.538
Current Data Parameters
NAME TCM-II-114pure
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140817
Time 15.52
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 143.7
DW 50.000 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300222 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NH2
N
N
N
Bn
SI-22
10
9
8
7
6
5
4
3
2
1
0
ppm
3.054
2.000
2.050
1.000
4.571
2.219
1.095
1.074

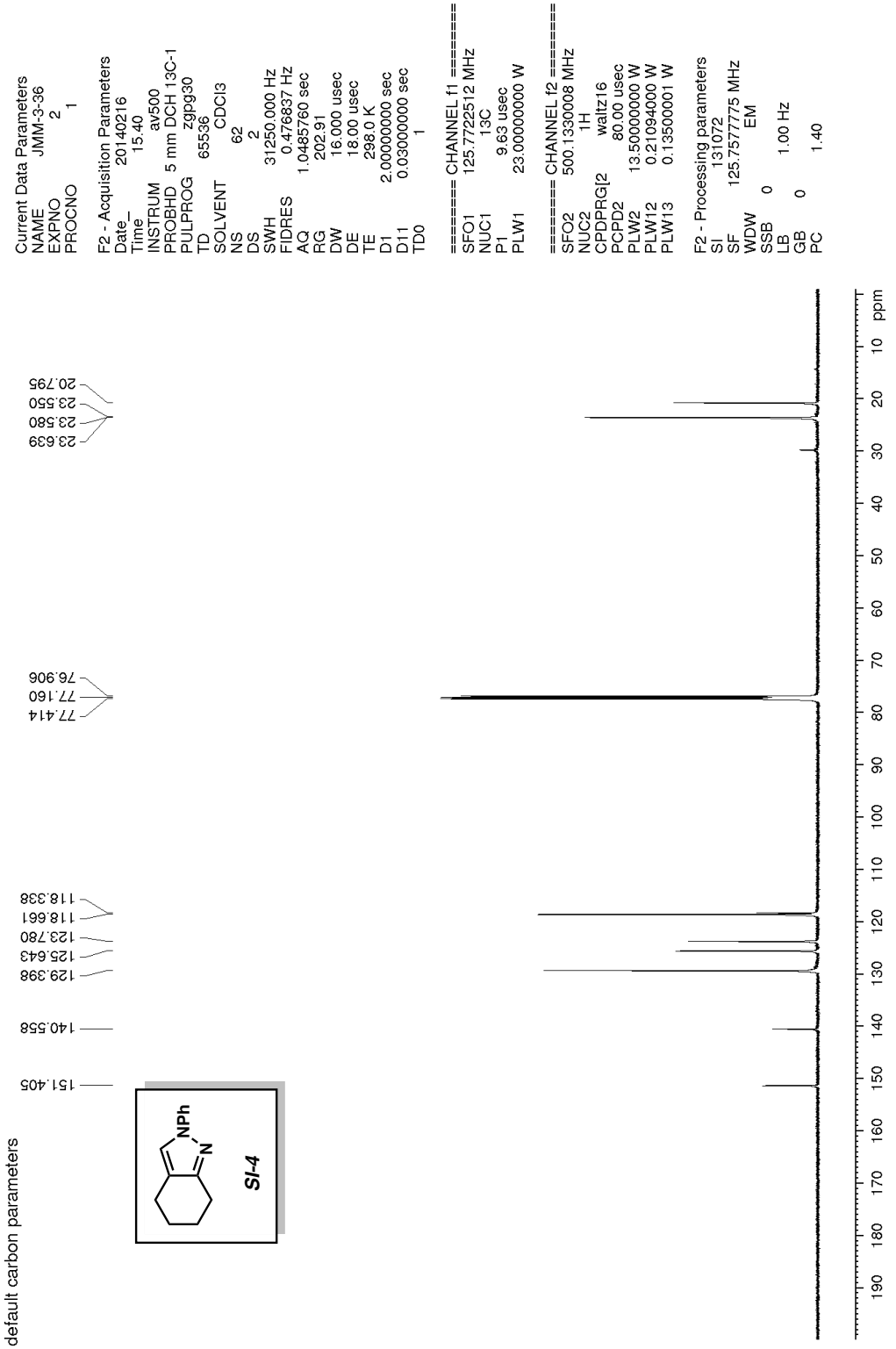

TCM-II-115
Current Data Parameters
NAME TCM-II-115
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140808
Time 16.06
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 161.3
DW 50.000 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300219 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Bn
19
ppm

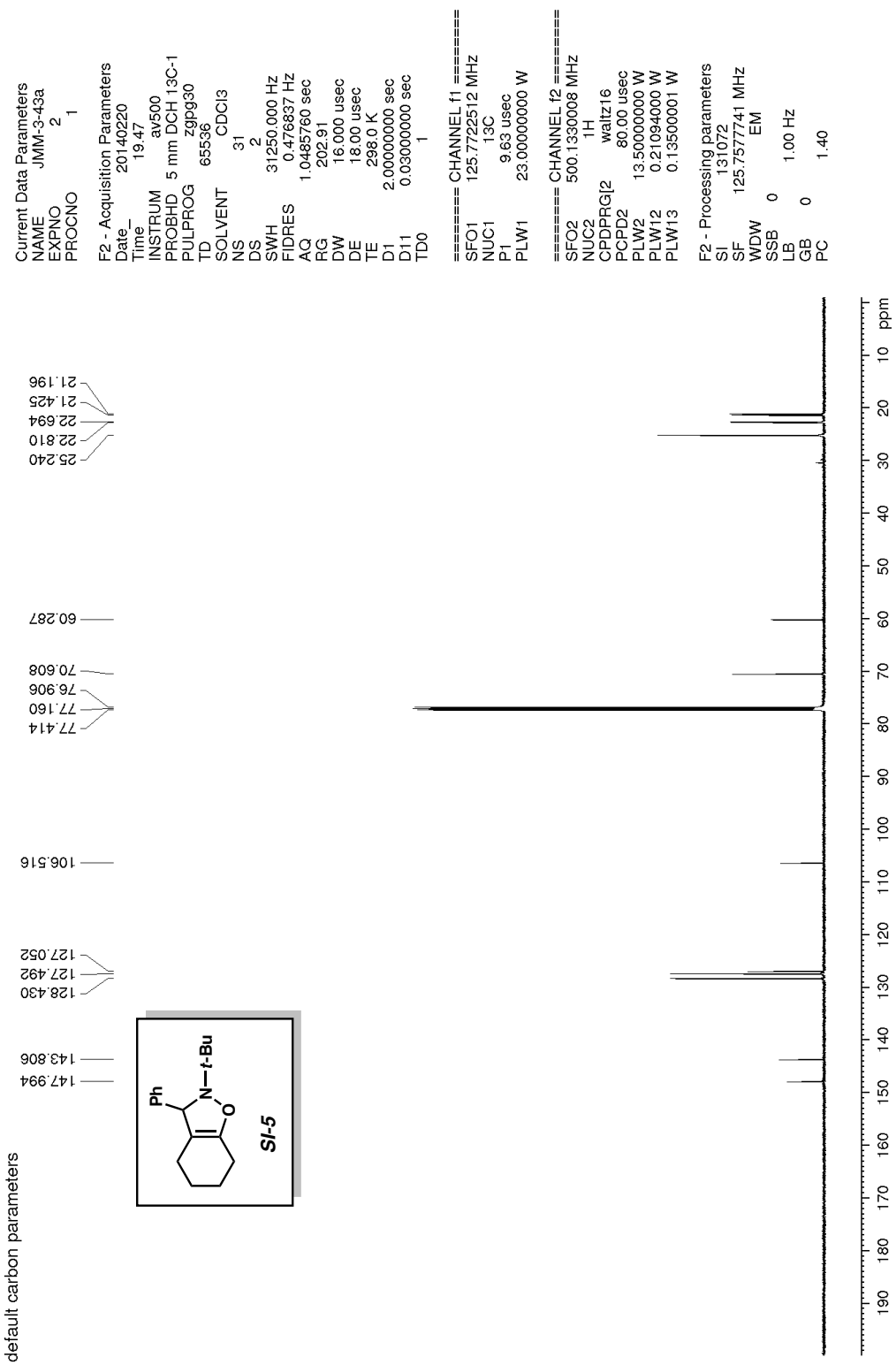
^{13}C NMR Spectra:

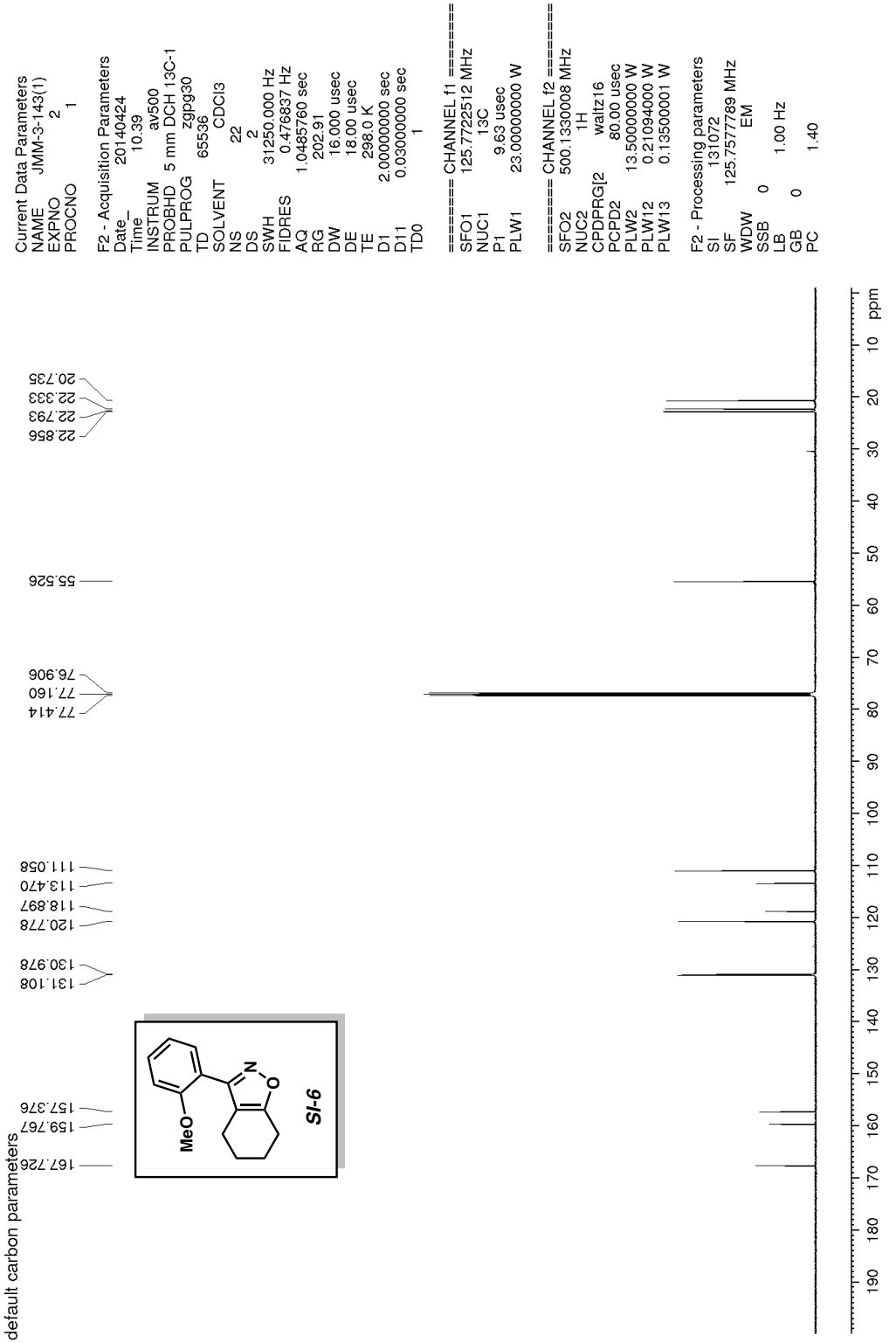

default carbon parameters
Current Data Parameters
NAME JMM-3-54
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140224
Time 16.41
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577782 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
144.023
135.069
132.052
129.008
128.333
127.596
77.414
77.160
76.905
51.884
22.607
22.486
22.022
20.164
N
N
N
Bn
SI-1
ppm

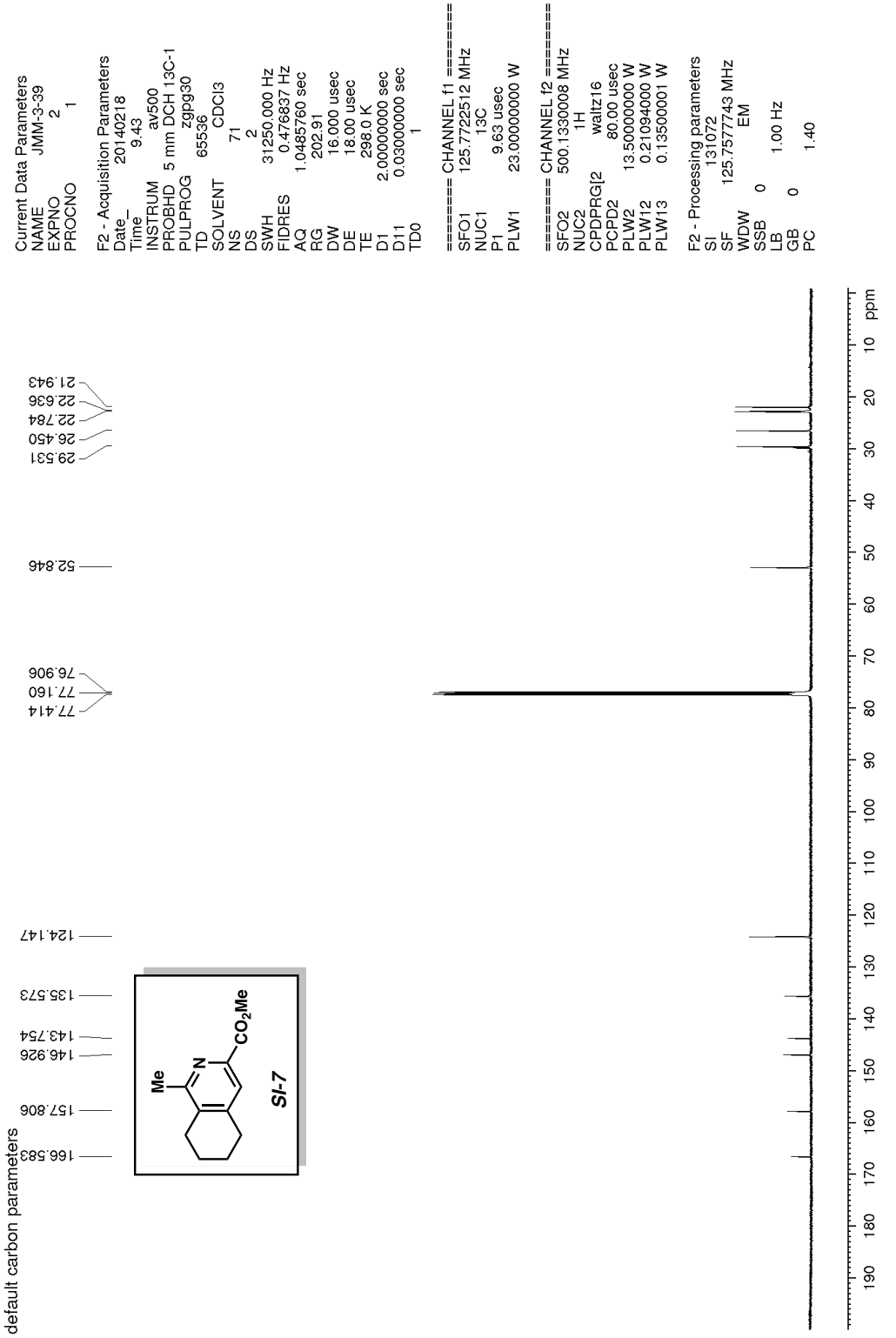

default carbon parameters
Current Data Parameters
NAME JMM-3-37
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140216
Time 15.50
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 126
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577778 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
CO2Et
N
N
H
SI-2
162.192
145.298
135.837
119.607
77.414
77.160
76.906
60.646
22.973
22.655
22.221
21.589
14.415
ppm

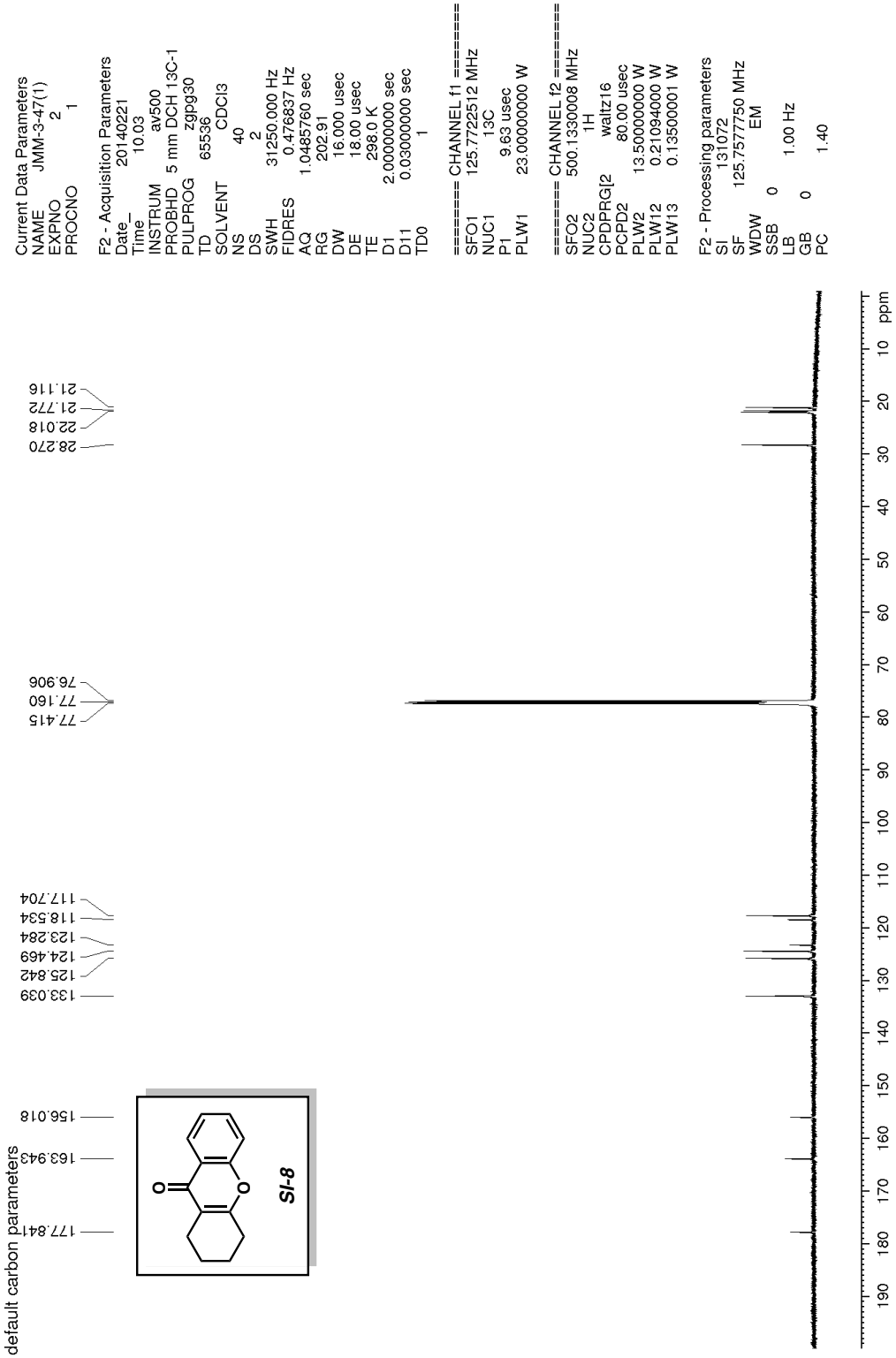

default carbon parameters
Current Data Parameters
NAME JMM-3-37
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140216
Time 15.50
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 126
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577778 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
14.415
21.589
22.221
22.655
22.973
60.646
76.906
77.160
77.414
119.607
135.837
145.298
162.192
SI-3
ppm

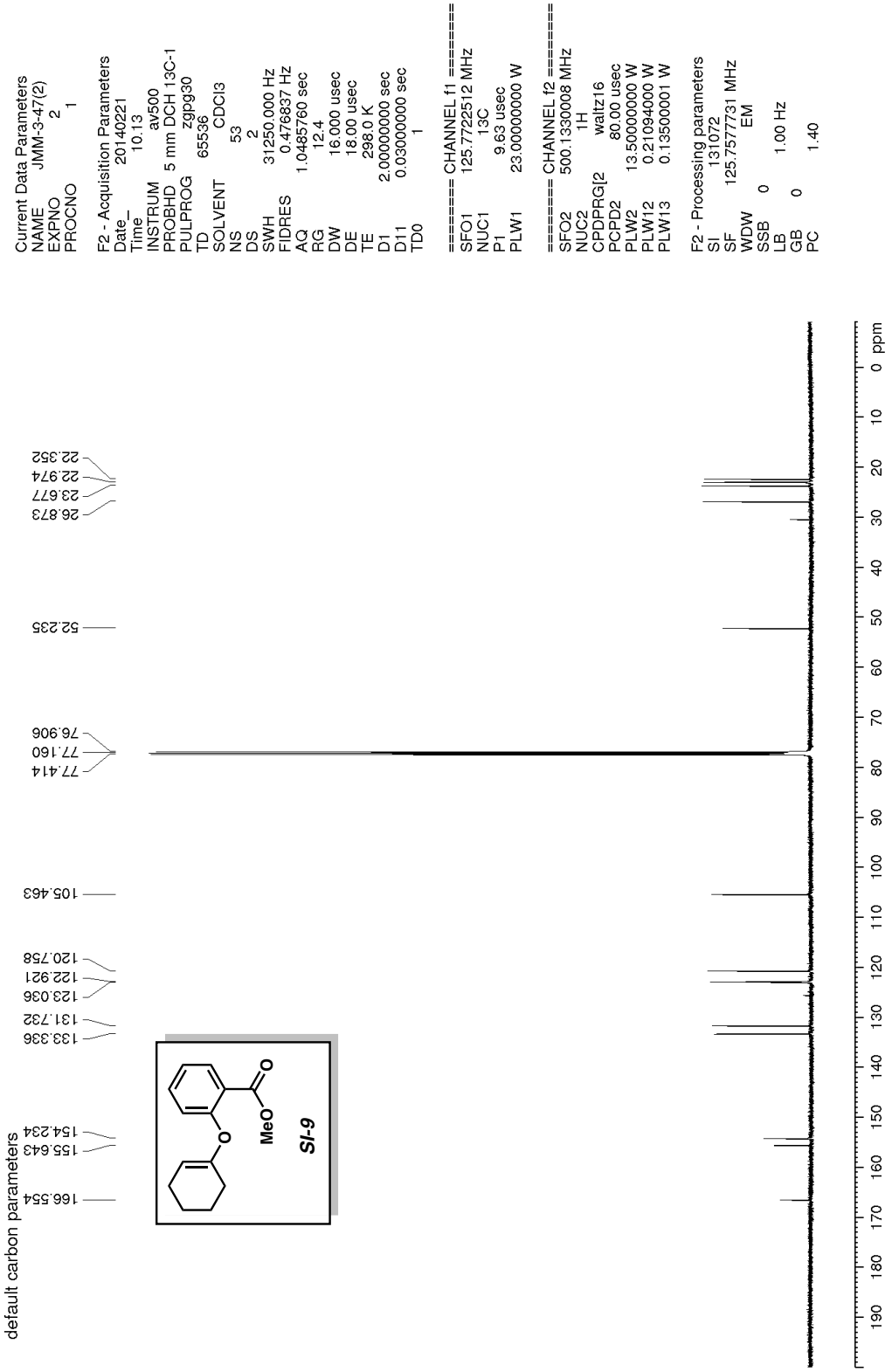

default carbon parameters
Current Data Parameters
NAME JMM-3-36
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140216
Time 15.40
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 62
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577775 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
151.405
140.558
129.398
125.643
123.780
118.661
118.338
77.414
77.160
76.906
23.639
23.580
23.550
20.795
NPh
N
SI-4
ppm

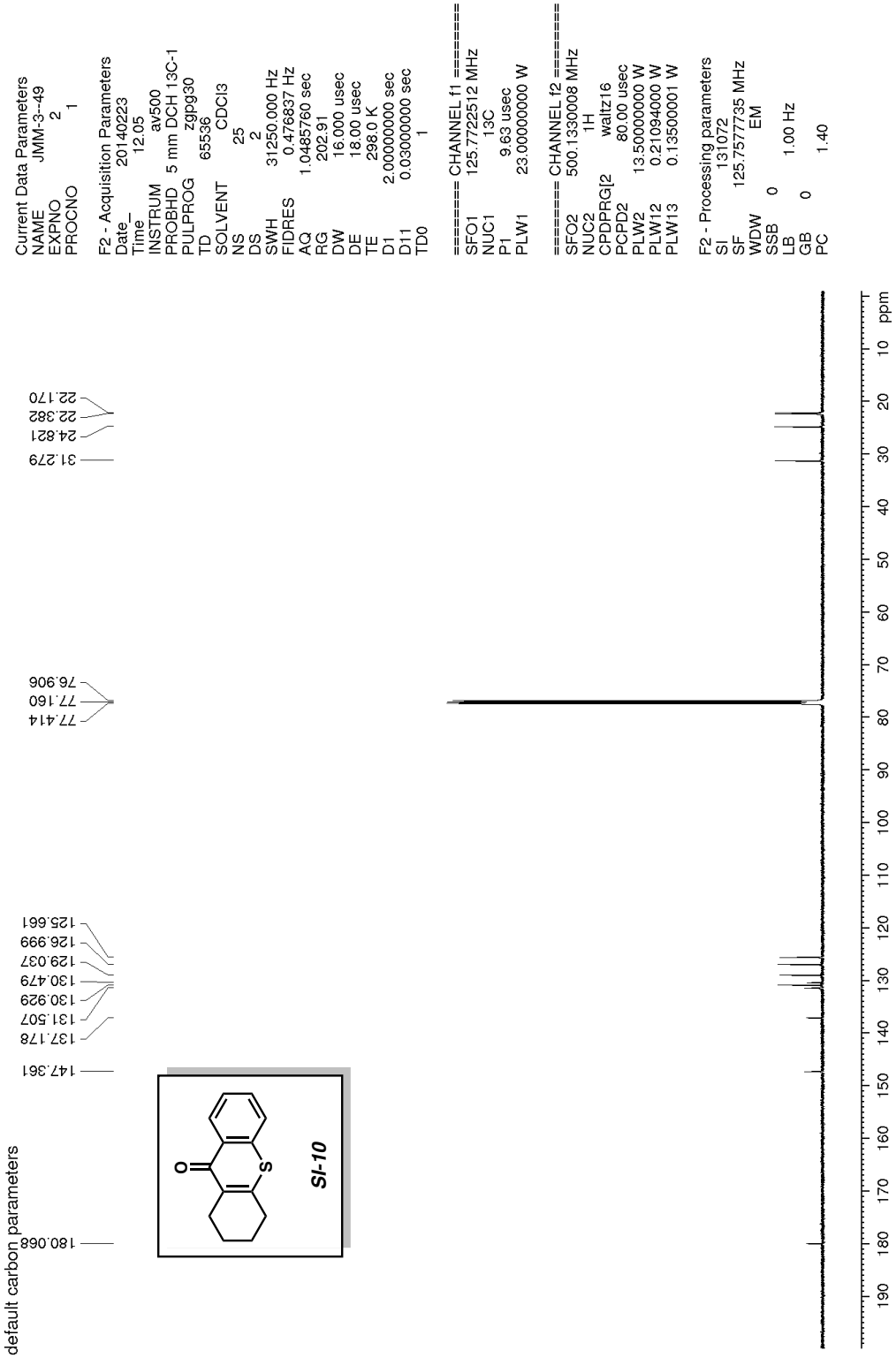

default carbon parameters
Current Data Parameters
NAME JMM-3-43a
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140220
Time 19.47
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 31
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577741 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
N—t-Bu
O
SI-5
147.994
143.806
128.430
127.492
127.052
106.516
77.414
77.160
76.906
70.608
60.287
25.240
22.810
22.694
21.425
21.196
ppm

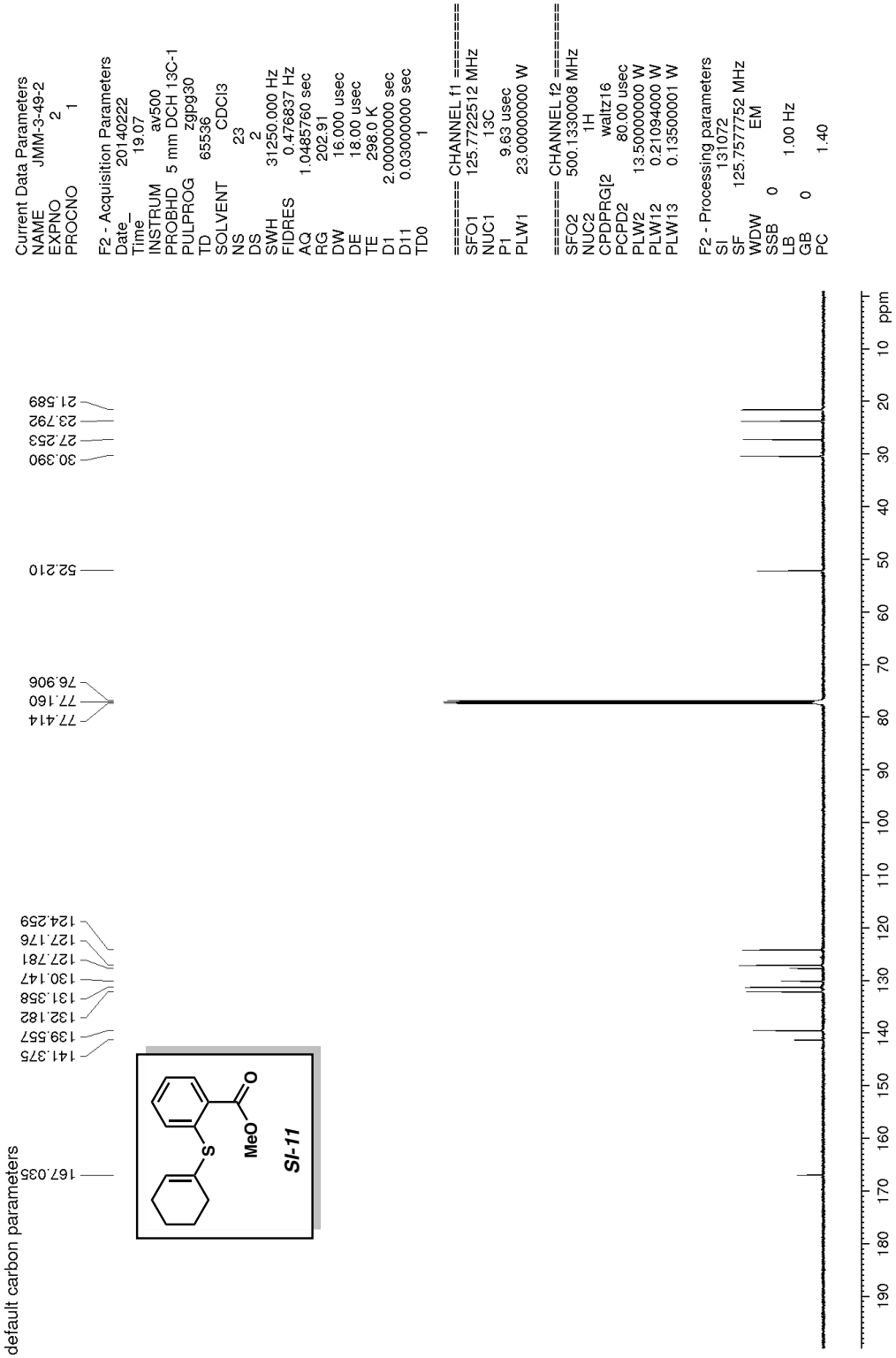

Current Data Parameters
NAME JMM-3-143(1)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140424
Time 10.39
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 22
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577789 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
default carbon parameters
MeO
SI-6
167.726
159.767
157.376
131.108
130.978
120.778
118.897
113.470
111.058
77.414
77.160
76.906
55.526
22.856
22.793
22.333
20.735
ppm

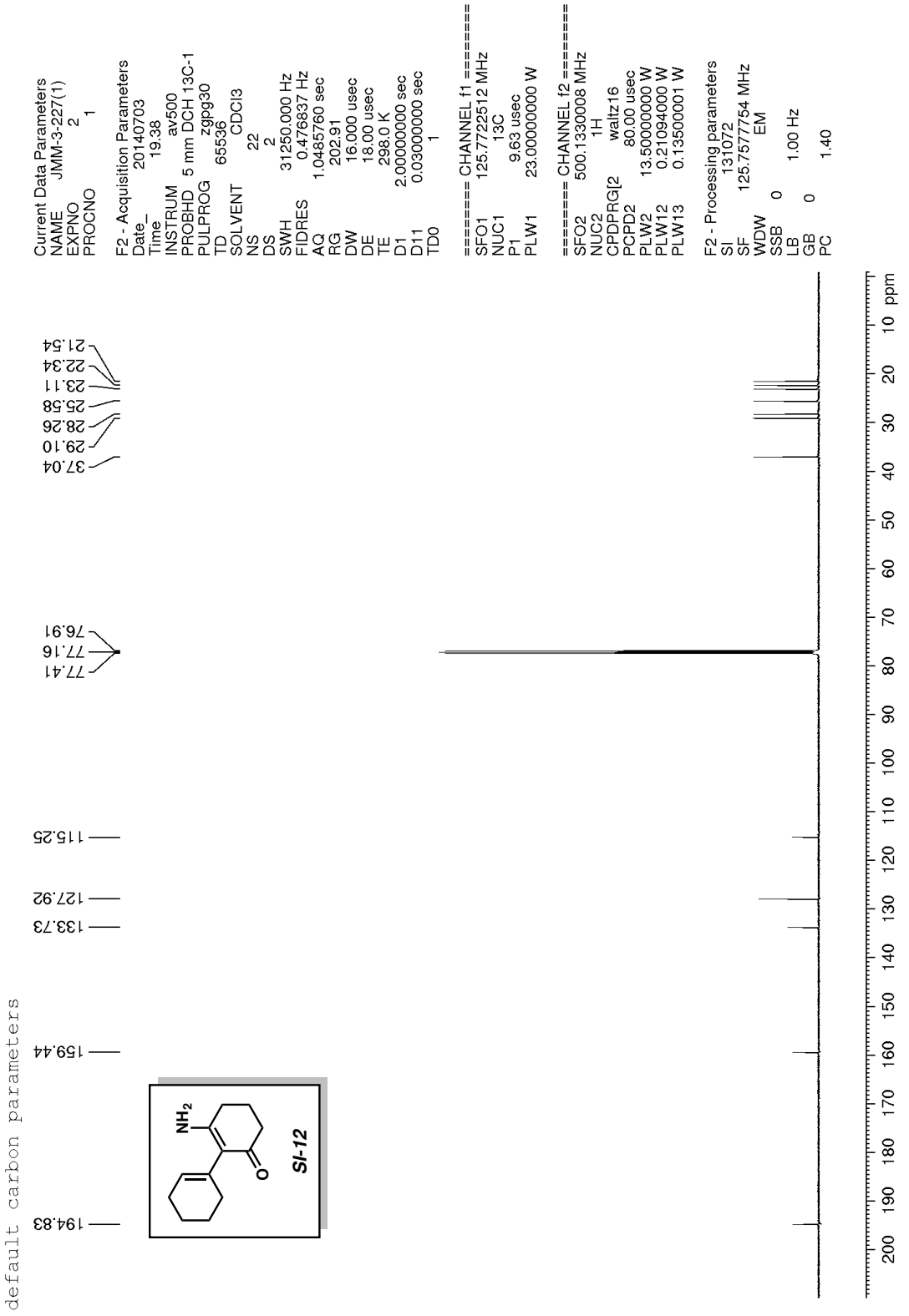

default carbon parameters
166.583
157.806
146.926
143.754
135.573
124.147
77.414
77.160
76.906
52.846
29.531
26.450
22.784
22.636
21.943
Me
N
CO2Me
SI-7
Current Data Parameters
NAME JMM-3-39
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140218
Time 9.43
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 71
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577743 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

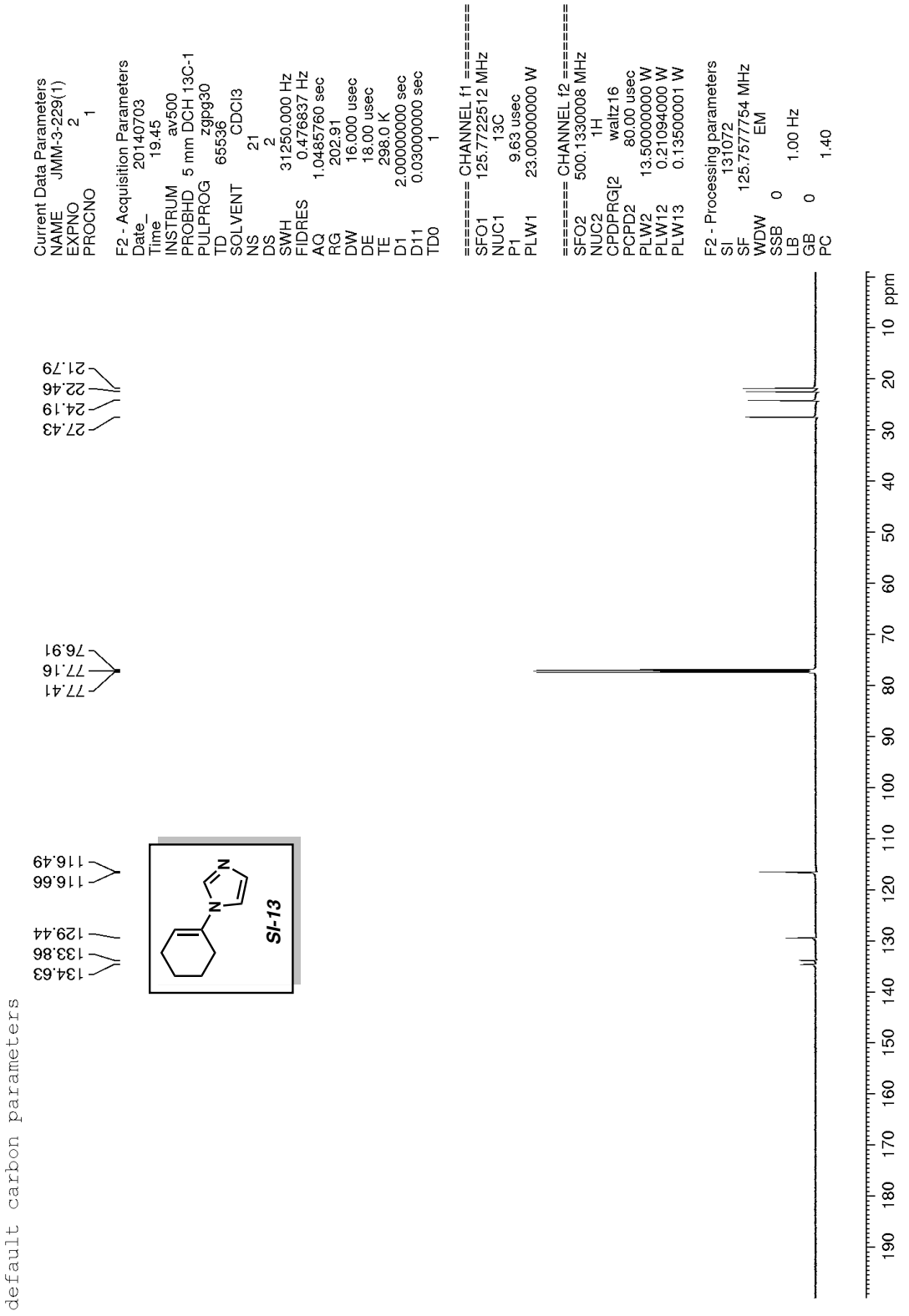

Current Data Parameters
NAME JMM-3-47(1)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140221
Time 10.03
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 40
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577750 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
default carbon parameters
177.841
163.943
156.018
133.039
125.842
124.469
123.284
118.534
117.704
77.415
77.160
76.906
28.270
22.018
21.772
21.116
SI-8
ppm

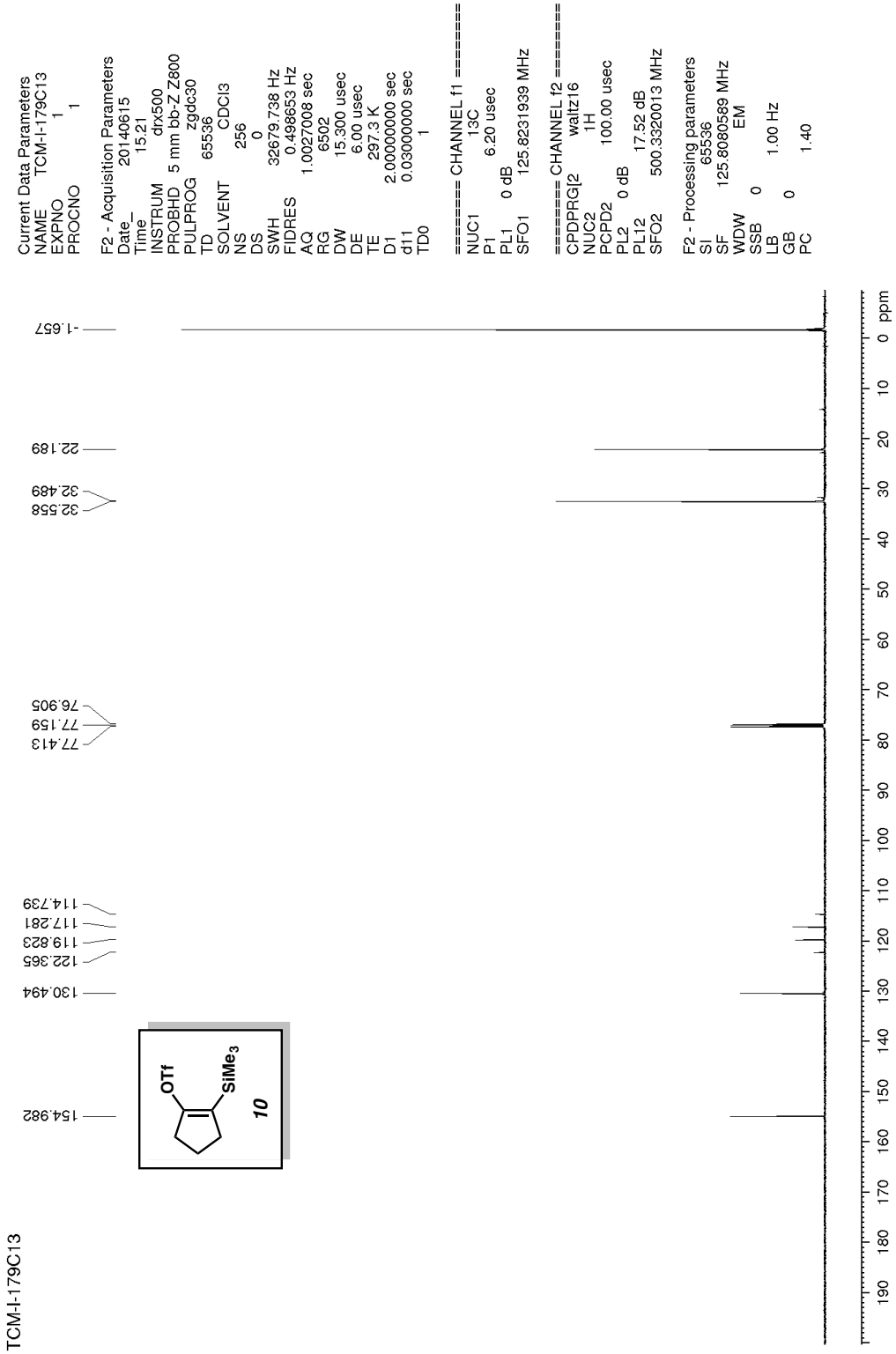

Current Data Parameters
NAME JMM-3-47(2)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140221
Time 10.13
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 53
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 12.4
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577731 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
default carbon parameters
166.554
155.643
154.234
133.336
131.732
123.036
122.921
120.758
105.463
77.414
77.160
76.906
52.235
26.873
23.677
22.974
22.352
MeO
O
O
SI-9
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

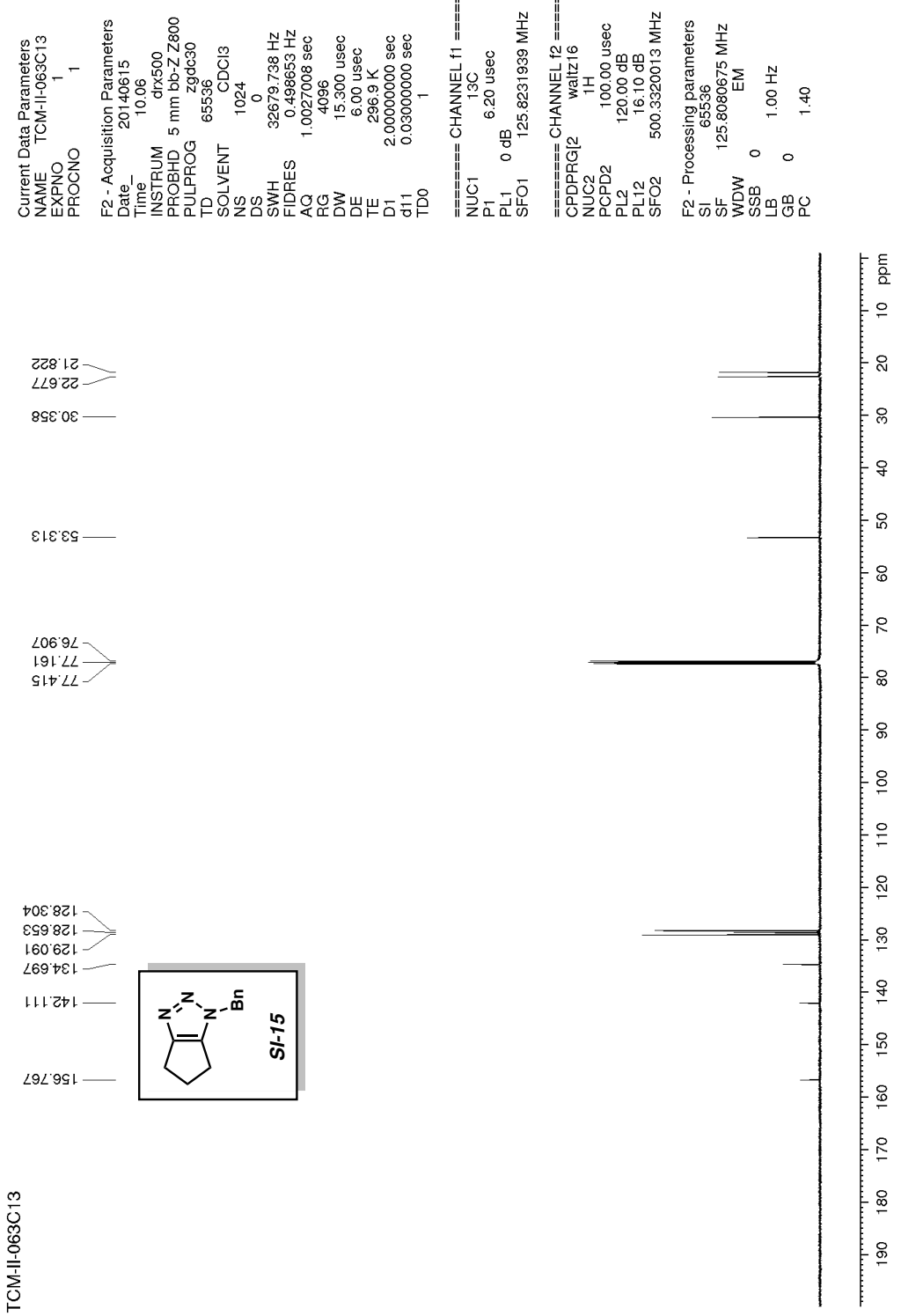

default carbon parameters
180.068
147.361
137.178
131.507
130.929
130.479
129.037
126.999
125.661
77.414
77.160
76.906
31.279
24.821
22.382
22.170
SI-10
O
S
Current Data Parameters
NAME JMM-3--49
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140223
Time 12.05
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 25
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577735 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

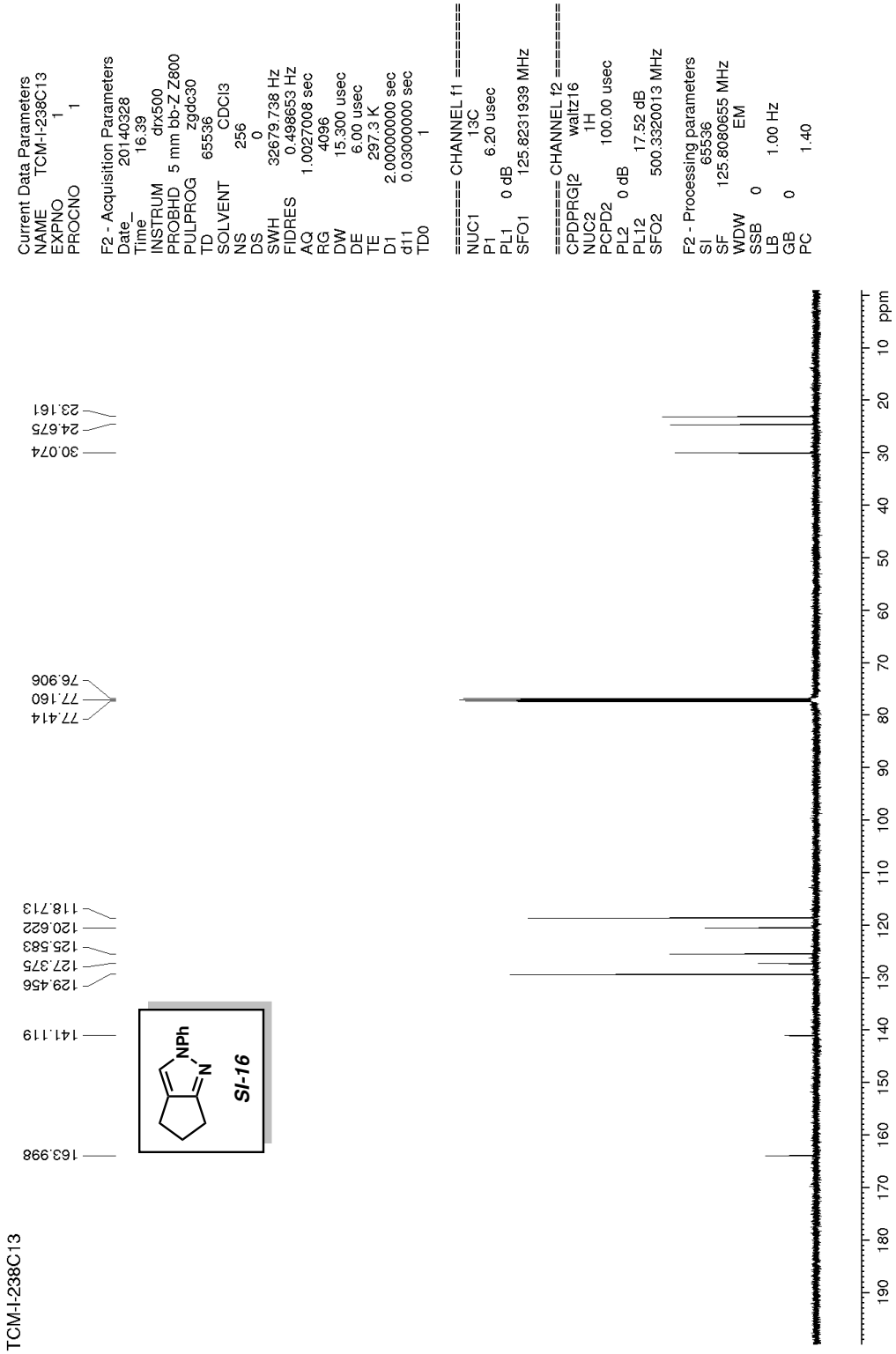

default carbon parameters
167.035
141.375
139.557
132.182
131.358
130.147
127.781
127.176
124.259
77.414
77.160
76.906
52.210
30.390
27.253
23.792
21.589
MeO
S
O
SI-11
Current Data Parameters
NAME JMM-3-49-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140222
Time 19.07
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 23
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577752 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

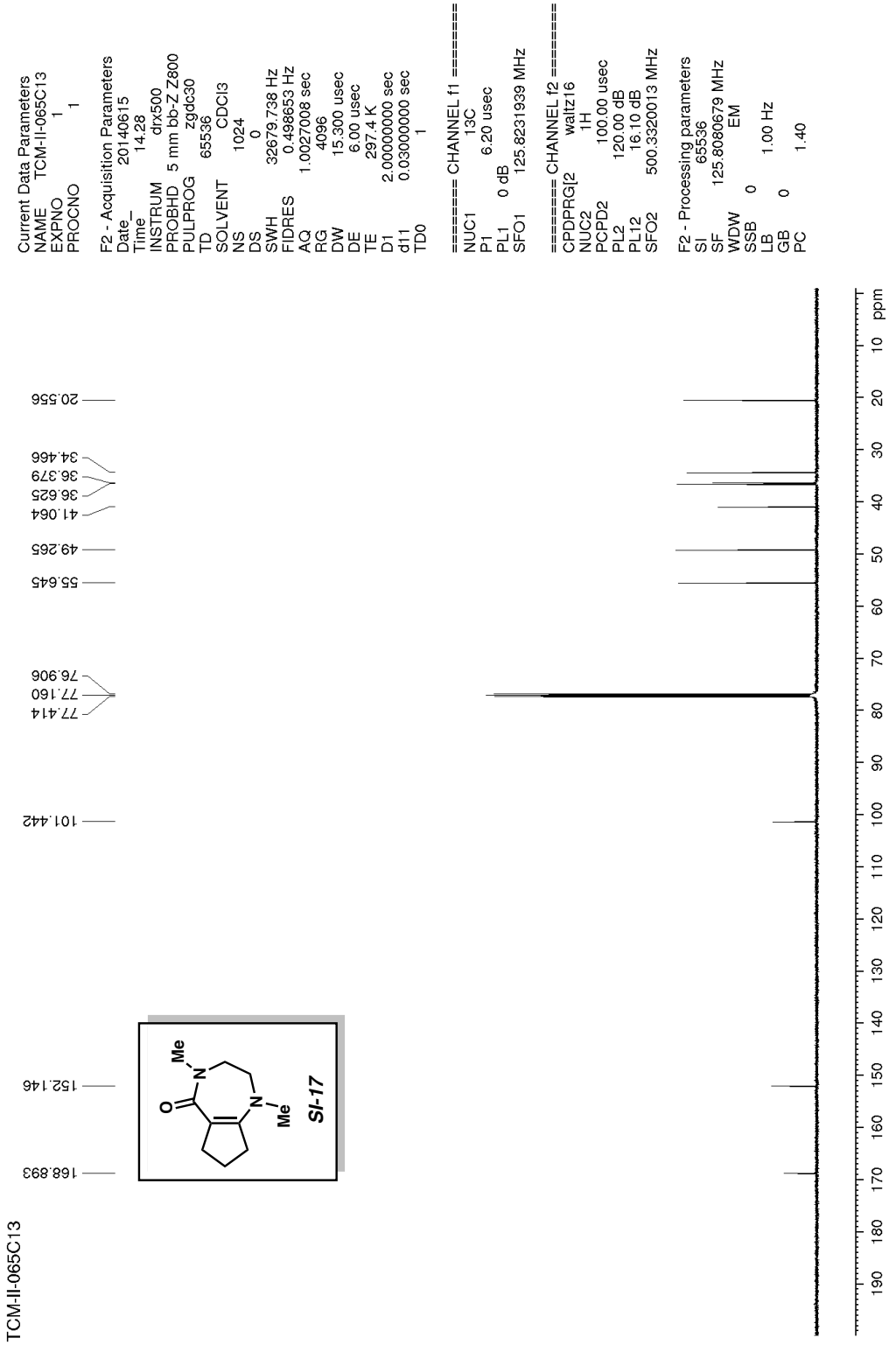

default carbon parameters
194.83
159.44
133.73
127.92
115.25
77.41
77.16
76.91
37.04
29.10
28.26
25.58
23.11
22.34
21.54
NH2
O
SI-12
Current Data Parameters
NAME JMM-3-227(1)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140703
Time 19.38
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 22
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577754 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

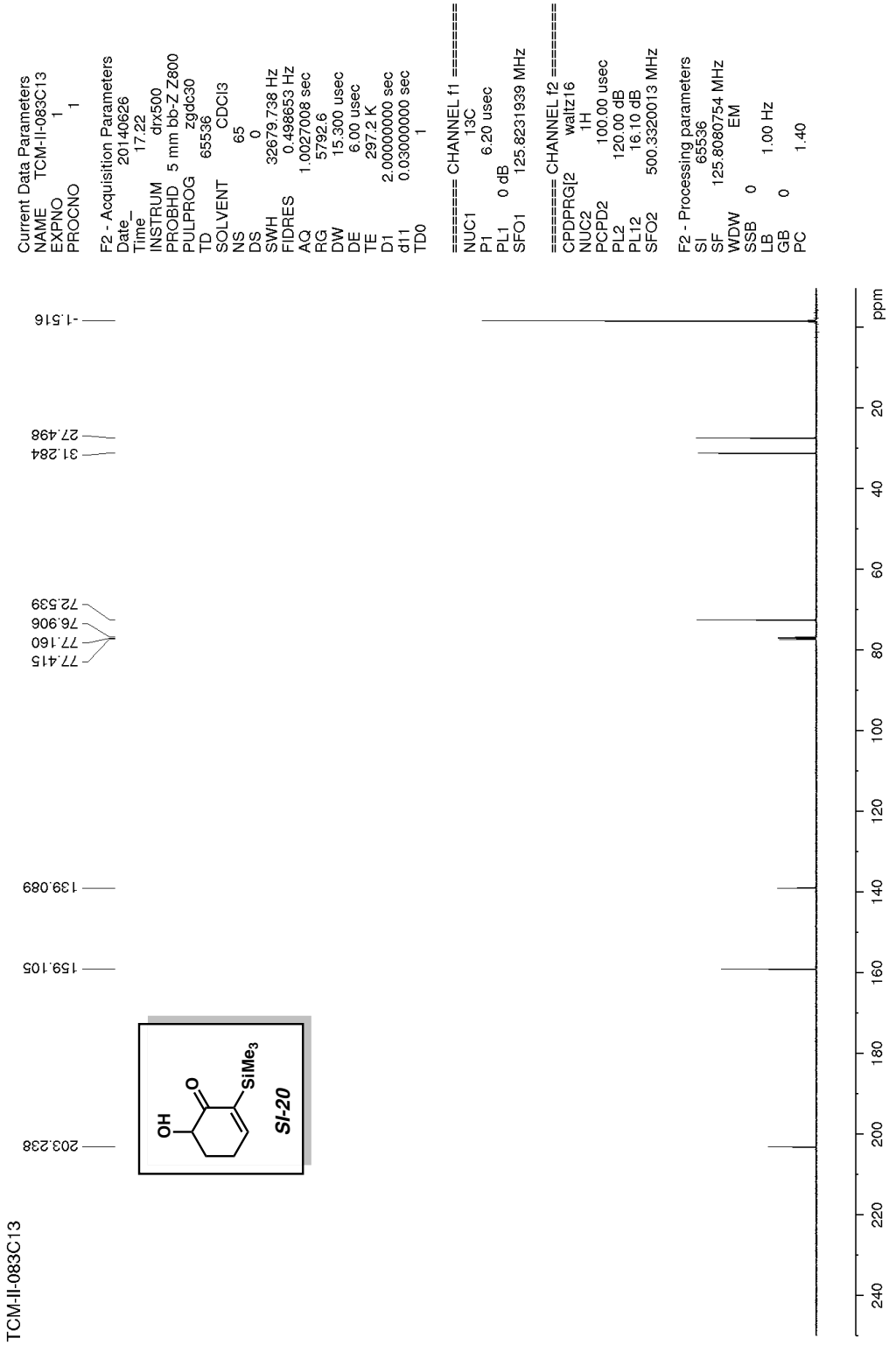

default carbon parameters
Current Data Parameters
NAME JMM-3-229(1)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140703
Time 19.45
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 21
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577754 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
134.63
133.86
129.44
116.66
116.49
77.41
77.16
76.91
27.43
24.19
22.46
21.79
SI-13
N
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

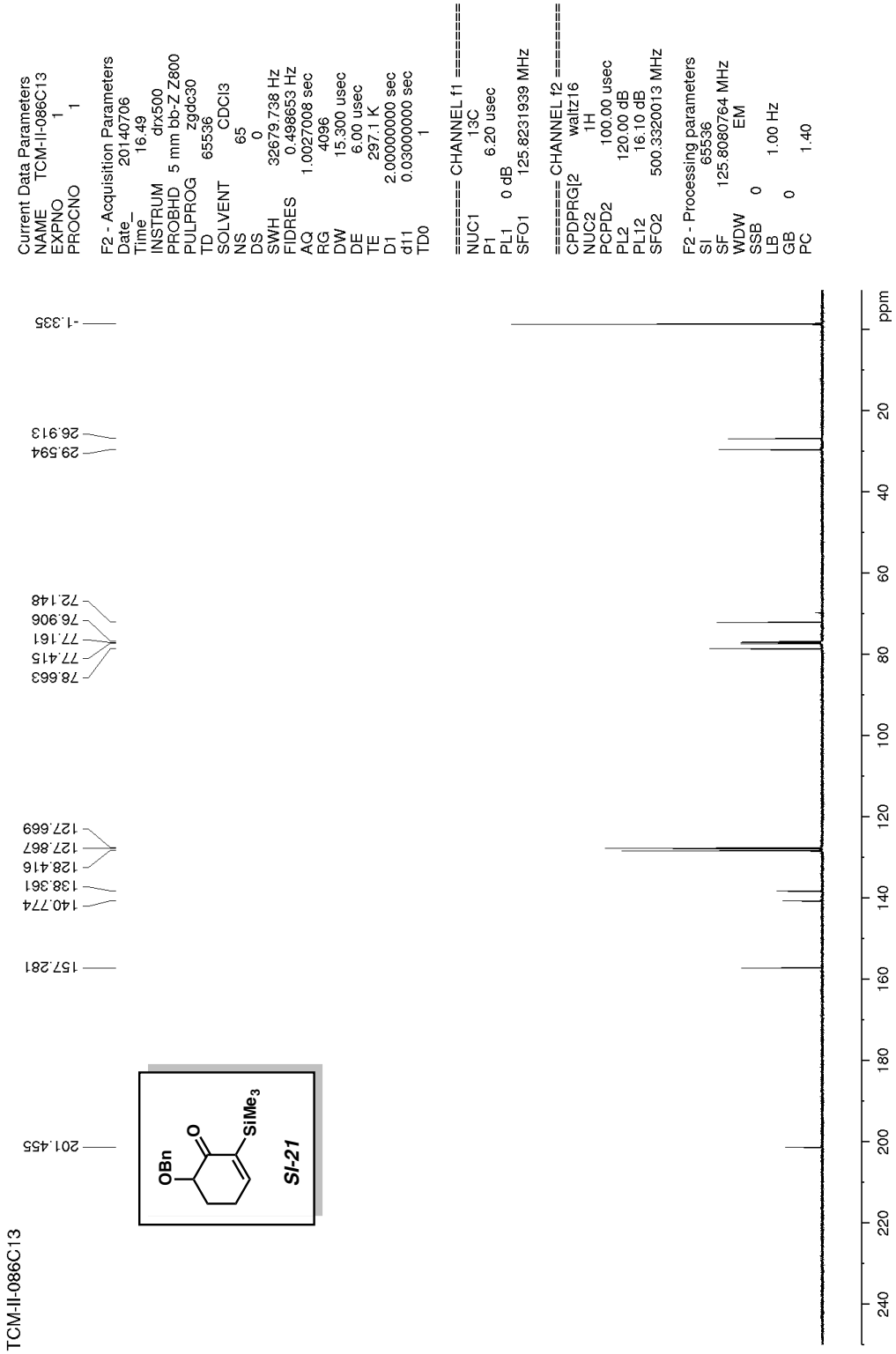

TCM-I-179C13
Current Data Parameters
NAME TCM-I-179C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140615
Time 15.21
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 6502
DW 15.300 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0 dB
PL12 17.52 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OTf
SiMe3
10
154.982
130.494
122.365
119.823
117.281
114.739
77.413
77.159
76.905
32.558
32.489
22.189
-1.657
ppm

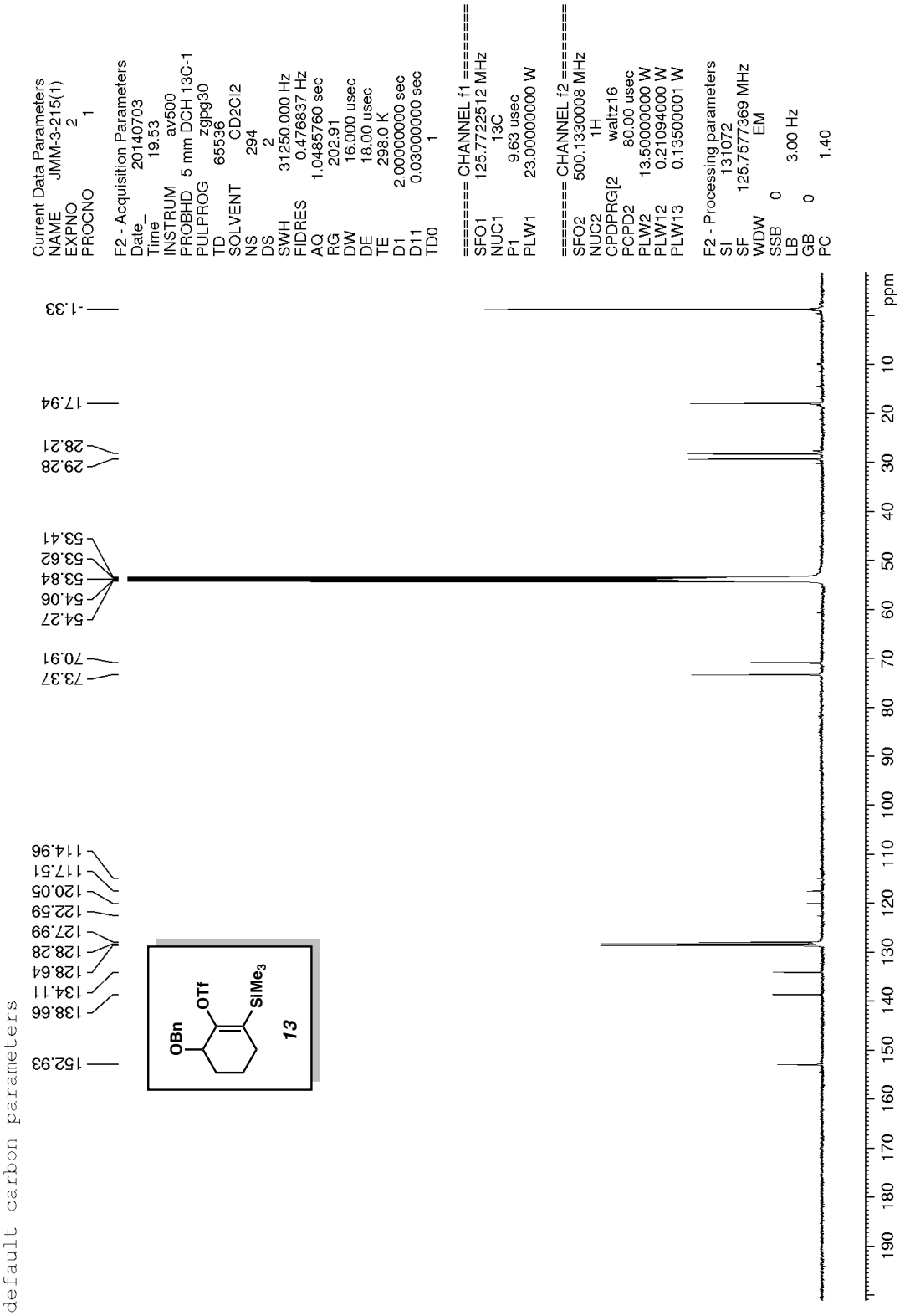

TCM-II-063C13
Current Data Parameters
NAME TCM-II-063C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140615
Time 10.06
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1024
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080675 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
156.767
142.111
134.697
129.091
128.653
128.304
77.415
77.161
76.907
53.313
30.358
22.677
21.822
N
N
N
Bn
SI-15
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

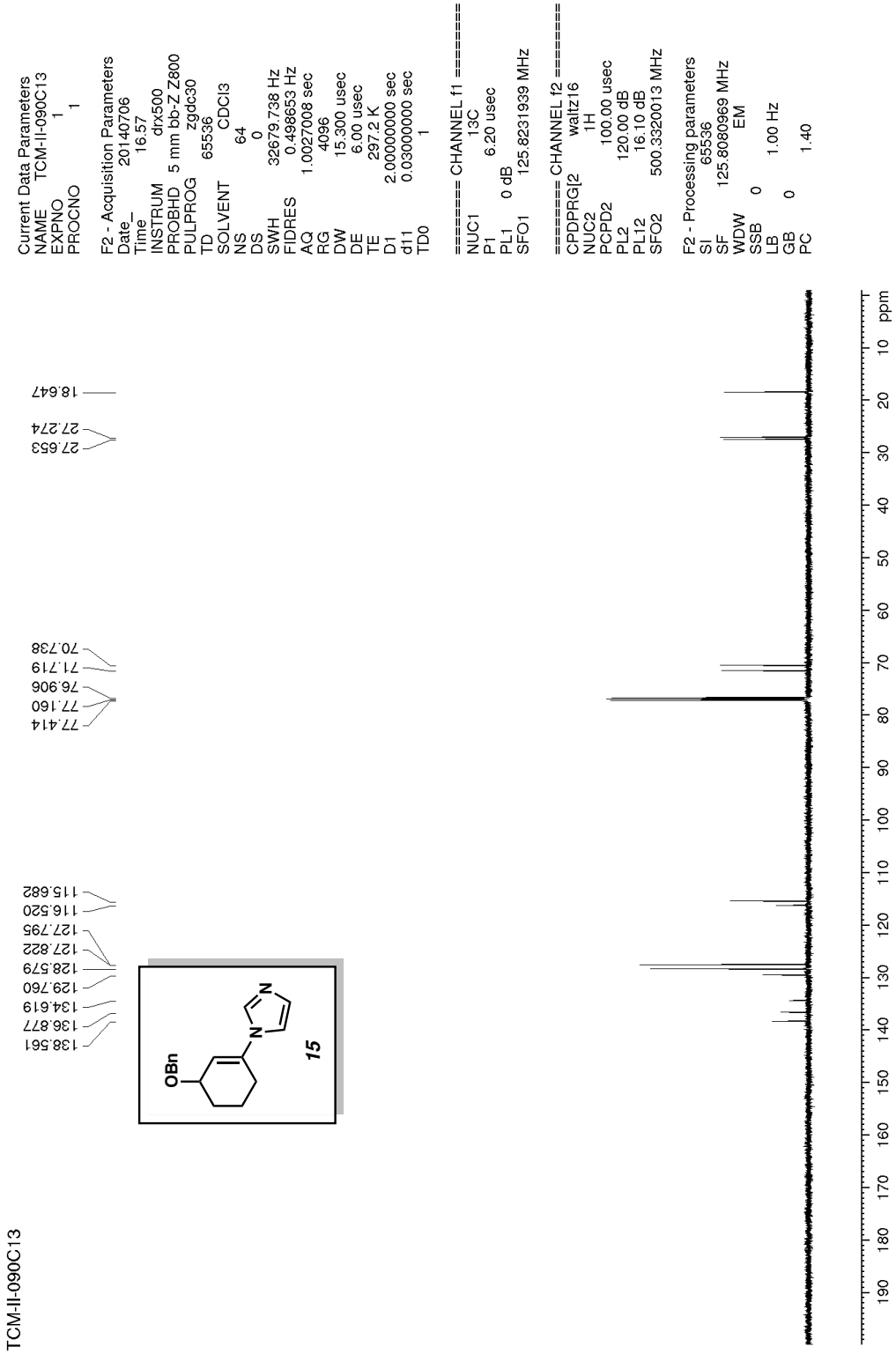

TCM-I-238C13
Current Data Parameters
NAME TCM-I-238C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140328
Time 16.39
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0 dB
PL12 17.52 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080655 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
NPh
N
SI-16
163.998
141.119
129.456
127.375
125.583
120.622
118.713
77.414
77.160
76.906
30.074
24.675
23.161
ppm

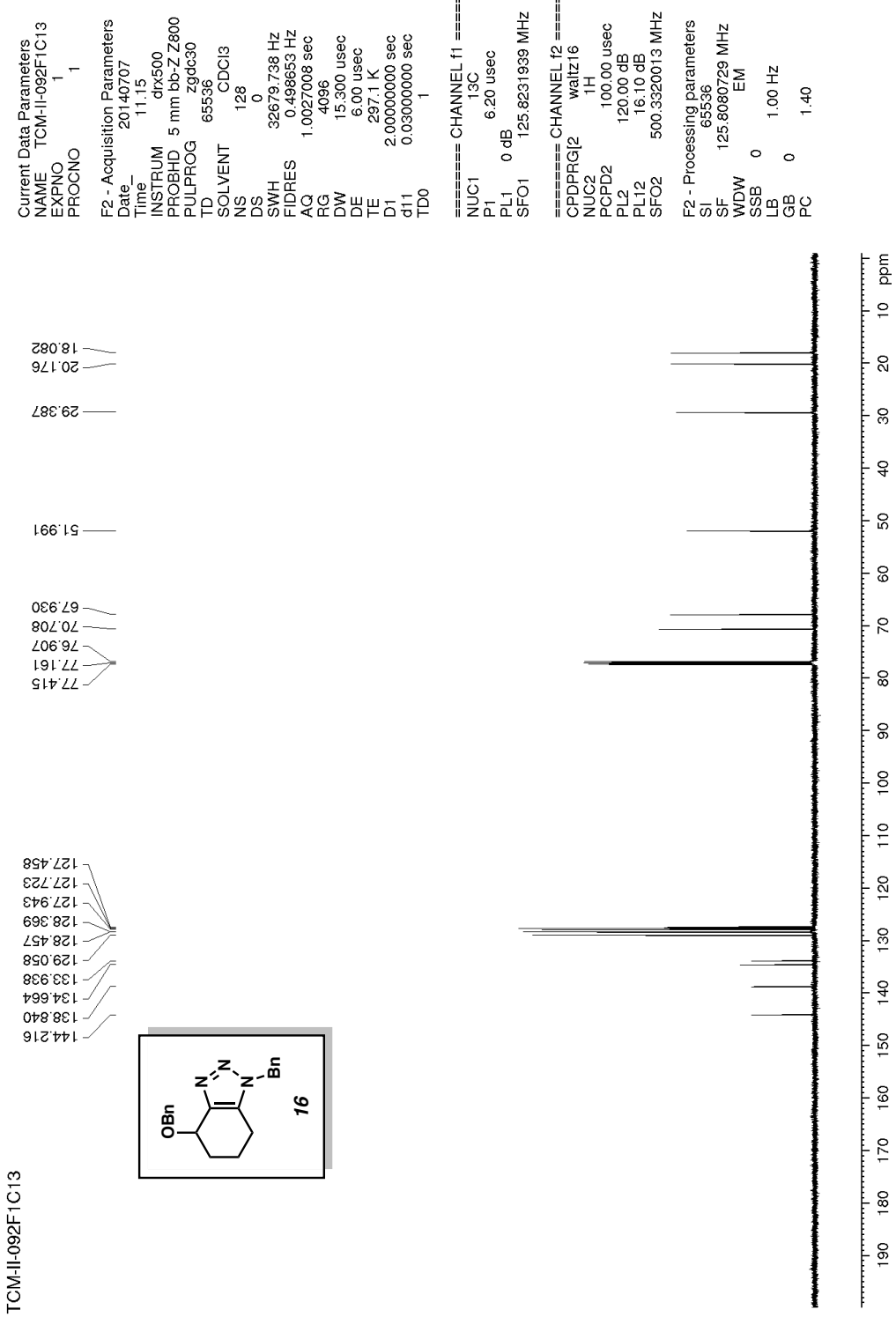

TCM-II-065C13
Current Data Parameters
NAME TCM-II-065C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140615
Time 14.28
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1024
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080679 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
168.893
152.146
101.442
77.414
77.160
76.906
55.645
49.265
41.064
36.625
36.379
34.466
20.556
Me
N
O
N
Me
SI-17
ppm

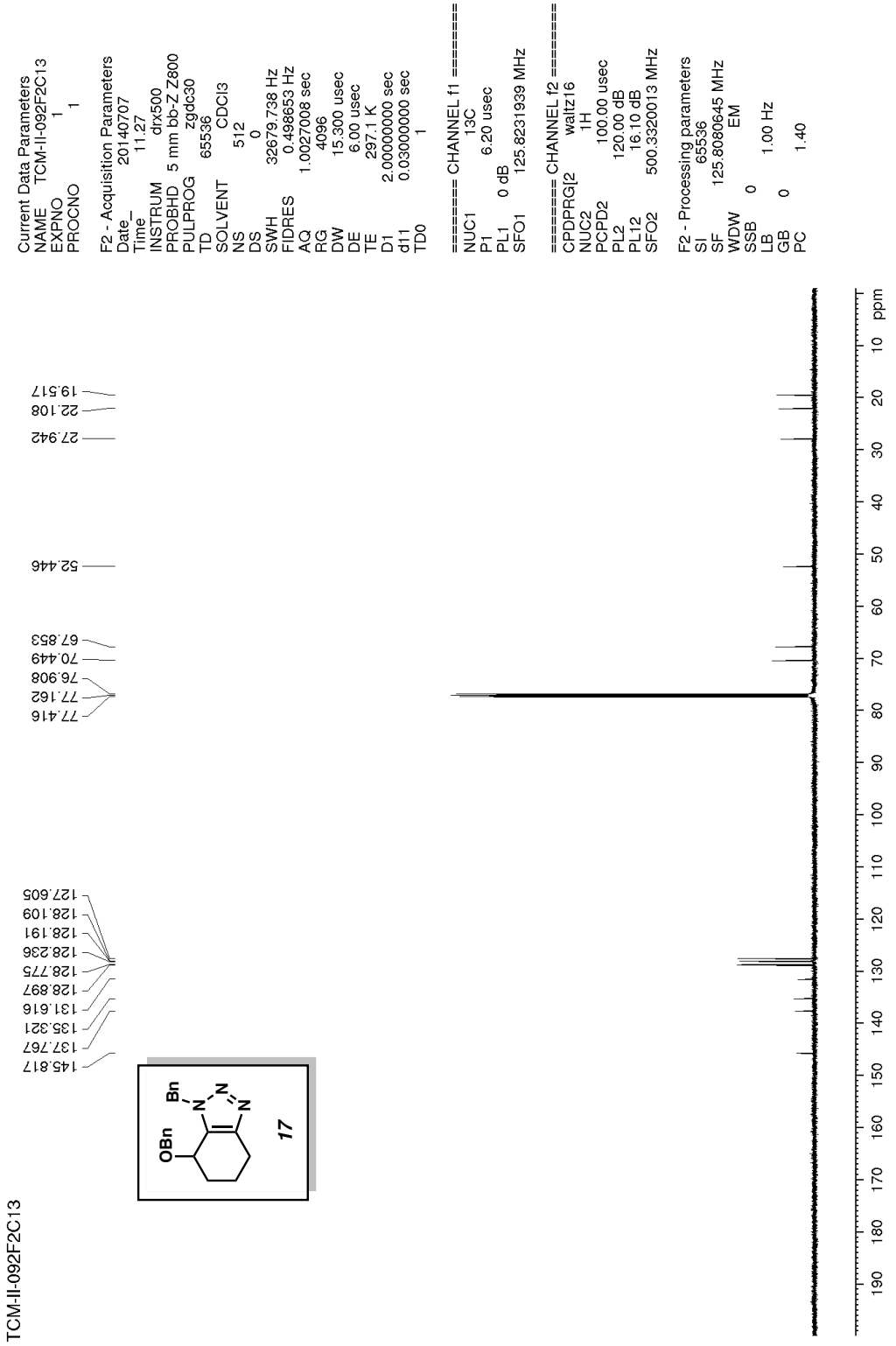

TCM-II-083C13
Current Data Parameters
NAME TCM-II-083C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140626
Time 17.22
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 65
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.00027008 sec
RG 5792.6
DW 15.300 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080754 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
-1.516
27.498
31.284
72.539
76.906
77.160
77.415
139.089
159.105
203.238
OH
O
SiMe3
SI-20
ppm
240
220
200
180
160
140
120
100
80
60
40
20

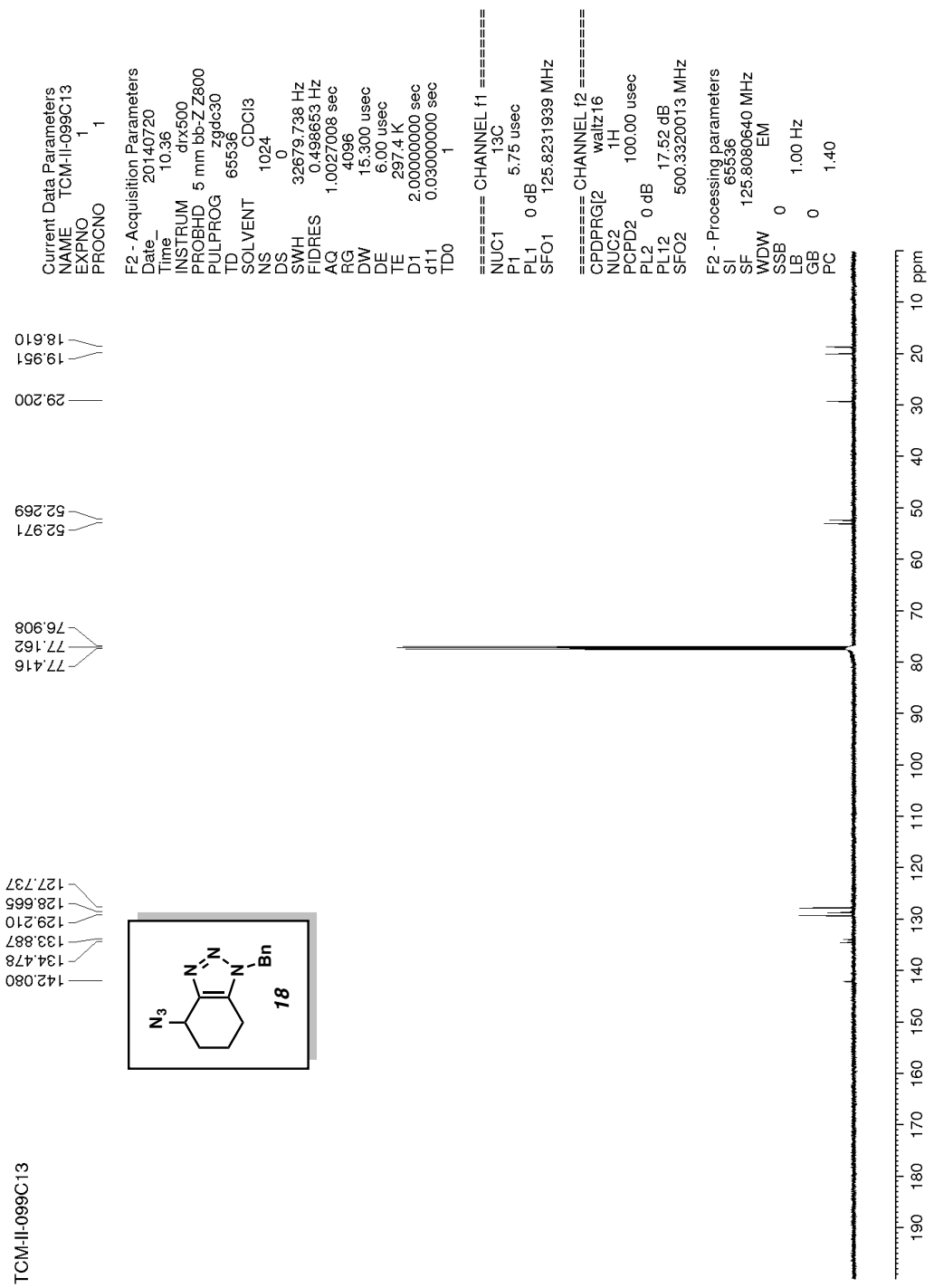

TCM-II-086C13
Current Data Parameters
NAME TCM-II-086C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140706
Time 16.49
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 65
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080764 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
-1.335
26.913
29.594
72.148
76.906
77.161
77.415
78.663
127.669
127.867
128.416
138.361
140.774
157.281
201.455
OBn
O
SiMe3
SI-21
ppm
240
220
200
180
160
140
120
100
80
60
40
20

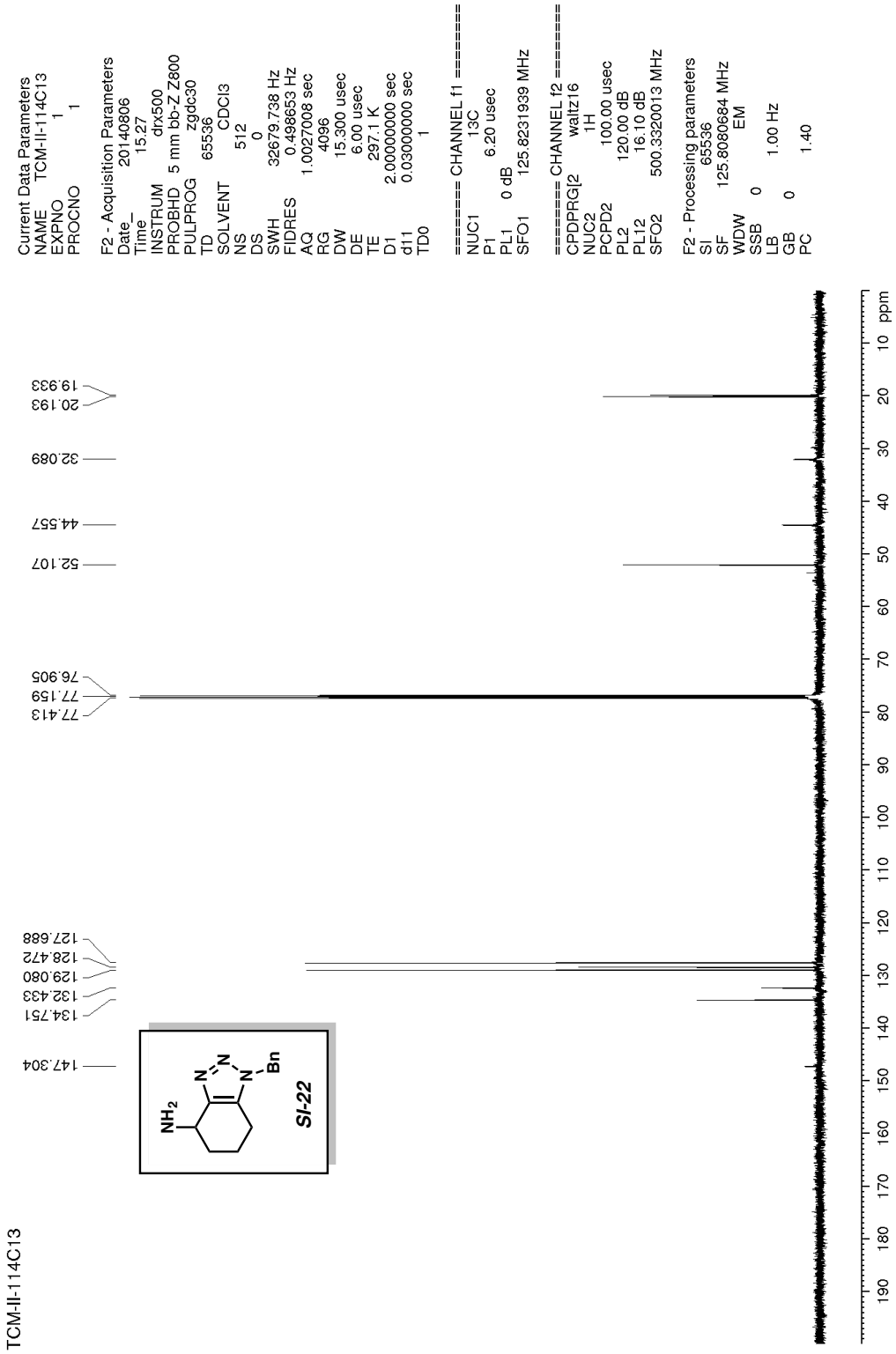

default carbon parameters
Current Data Parameters
NAME JMM-3-215(1)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140703
Time 19.53
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 294
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7722512 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
======== CHANNEL f2 ========
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
F2 - Processing parameters
SI 131072
SF 125.7577369 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
-1.33
17.94
28.21
29.28
53.41
53.62
53.84
54.06
54.27
70.91
73.37
114.96
117.51
120.05
122.59
127.99
128.28
128.64
134.11
138.66
152.93
OBn
OTf
SiMe3
13
ppm

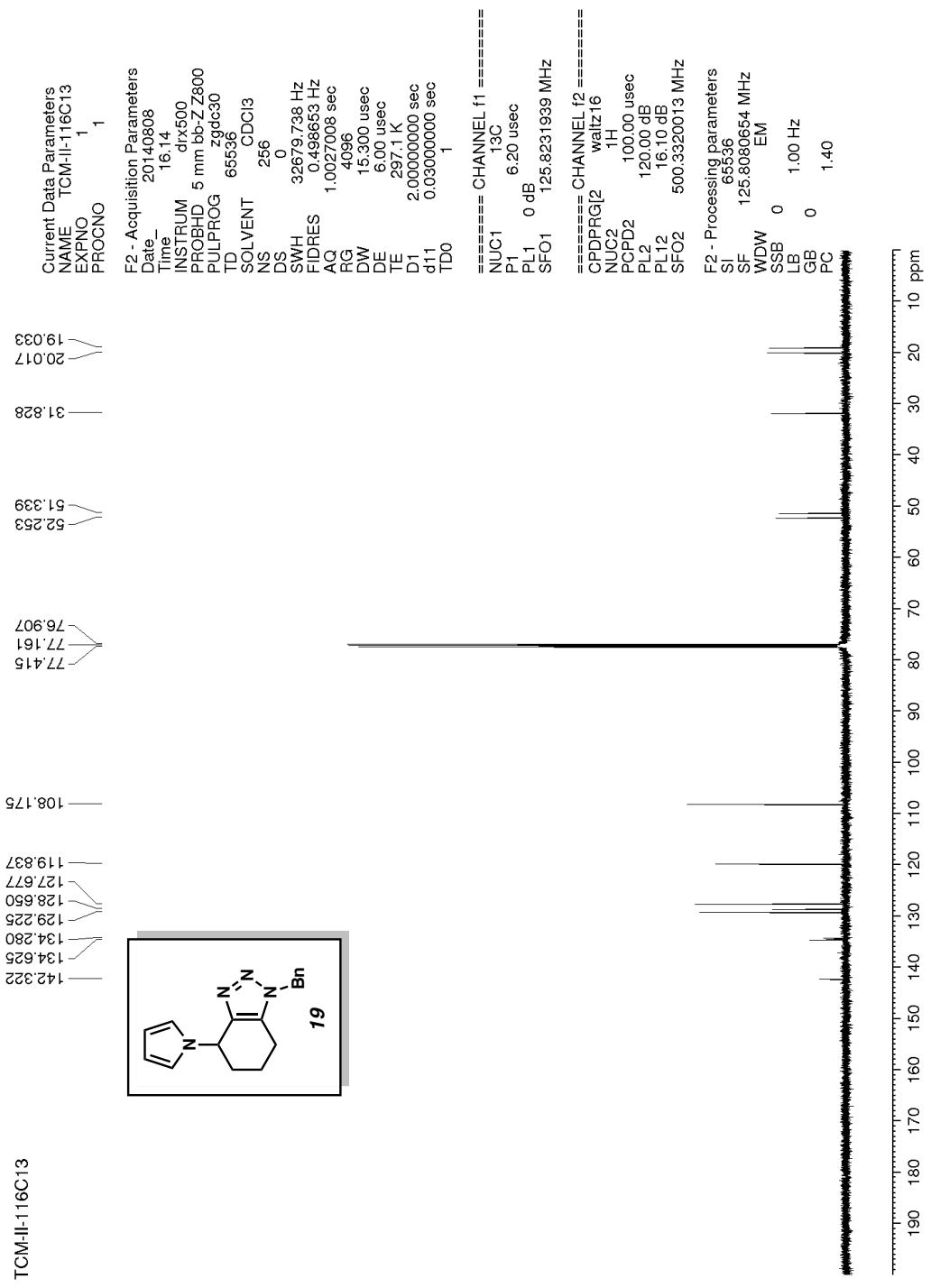

TCM-II-090C13
Current Data Parameters
NAME TCM-II-090C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140706
Time 16.57
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OBn
15
138.561
136.877
134.619
129.760
128.579
127.822
127.795
116.520
115.682
77.414
77.160
76.906
71.719
70.738
27.653
27.274
18.647
ppm


TCM-II-092F1C13
Current Data Parameters
NAME TCM-II-092F1C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140707
Time 11.15
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OBn
N
N
N
Bn
16
144.216
138.840
134.664
133.938
129.058
128.457
128.369
127.943
127.723
127.458
77.415
77.161
76.907
70.708
67.930
51.991
29.387
20.176
18.082
ppm


TCM-II-092F2C13
Current Data Parameters
NAME TCM-II-092F2C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140707
Time 11.27
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080645 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
19.517
22.108
27.942
52.446
67.853
70.449
76.908
77.162
77.416
127.605
128.109
128.191
128.236
128.775
128.897
131.616
135.321
137.767
145.817
OBn
Bn
N
N
N
17
ppm


TCM-II-099C13
Current Data Parameters
NAME TCM-II-099C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140720
Time 10.36
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1024
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 5.75 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0 dB
PL12 17.52 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080640 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
142.080
134.478
133.887
129.210
128.665
127.737
77.416
77.162
76.908
52.971
52.269
29.200
19.951
18.610
N3
Bn
18
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


TCM-II-114C13
Current Data Parameters
NAME TCM-II-114C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140806
Time 15.27
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080684 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
147.304
134.751
132.433
129.080
128.472
127.688
77.413
77.159
76.905
52.107
44.557
32.089
20.193
19.933
NH2
N
N
N
Bn
SI-22
ppm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Current Data Parameters
NAME TCM-II-116C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140808
Time 16.14
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.20 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz
F2 - Processing parameters
SI 65536
SF 125.8080654 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
19.033
20.017
31.828
51.339
52.253
76.907
77.161
77.415
108.175
119.837
127.677
128.650
129.225
134.280
134.625
142.322
N
N
N
Bn
19
ppm

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