Understanding and Interrupting the Fischer Azaindolization Reaction

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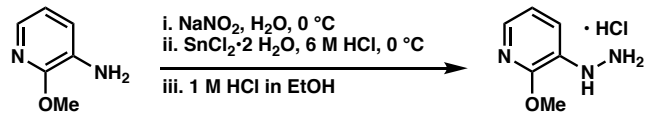
Supporting Information – Table of Contents

Part I: Experimental Section

Materials and Methods. Unless stated otherwise, reactions were conducted in flame-dried glassware under an atmosphere of air and commercially obtained reagents were used as received. Non-commercially available substrates were synthesized following protocols specified in Section A of the Experimental Procedures. Di-*tert*-buyl hydrazodiformate (**SI-4**), amine **SI-2**, boronate ester **SI-9,** $Pd_2(dba)_3$, $Cu(OAc)_2$, and dppf were obtained from Sigma-Aldrich and used as received. Di-*tert*-butyl azodicarboxylate (**SI-7**), bromopyridines **SI-3**, **SI-12**, amine **SI-1**, and boronate ester **SI-14** were obtained from Combi-Blocks and used as received. Amines **SI-11** and **SI-13** were obtained from Oakwood and used as received. Boronic acid **SI-6** was obtained from Frontier Scientific and used as received. Solid supported thiol-resin MetSThiol® was obtained from SiliCycle (Product # R51030B). Reaction temperatures were controlled using an IKAmag temperature modulator, and unless stated otherwise, reactions were performed at elevated temperatures (approximately 120 °C). Thin-layer chromatography (TLC) was conducted with EMD gel 60 F254 pre-coated plates (0.25 mm for analytical chromatography and 0.50 mm for preparative chromatography) and visualized using a combination of UV, anisaldehyde, iodine, and potassium permanganate staining techniques. Silicycle Siliaflash P60 (particle size 0.040–0.063 mm) was used for flash column chromatography. ^{1}H NMR spectra were recorded on Bruker spectrometers (at 300, 400 and 500 MHz) and are reported relative to residual solvent signals. Data for ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (at 100 and 125 MHz). IR spectra were recorded on a Perkin-Elmer UATR Two FT-IR spectrometer and are reported in terms of frequency absorption (cm^{-1}). DART-MS spectra were collected on a Thermo Exactive Plus MSD (Thermo Scientific) equipped with an ID-CUBE ion source and a Vapur Interface (IonSense Inc.). Both the source and MSD were controlled by Excalibur software v. 3.0. The analyte was spotted onto OpenSpot sampling cards (IonSense Inc.) using volatile solvents (e.g. chloroform, dichloromethane). Ionization was accomplished using UHP He (Airgas Inc.) plasma with no additional ionization agents. The mass calibration was carried out using Pierce LTQ Velos ESI (+) and (–) Ion calibration solutions (Thermo Fisher Scientific). Optical rotations were measured with a Rudolf Autopol III Automatic Polarimeter.

A. Syntheses of Hydrazine Substrates

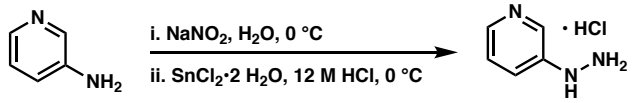
Representative Procedure A for the synthesis of hydrazine substrates from Tables 1 and 2. (37 is used as an example).



SI-1 **(90% yield)** ***37***

Hydrazine 37. To a solution of aniline **SI-1** (200.0 mg, 1.60 mmol, 1.0 equiv) in 6 M HCl (3.0 mL, 0.5 M) at 0 °C was added dropwise a solution of $NaNO_2$ (107.0 mg, 1.55 mmol, 1.0 equiv) in deionized H_2O (4.0 mL, 0.4 M) over 1 min under an air atmosphere. After stirring at 0 °C for 30 min, a solution of $SnCl_2$•2 H_2O (878.0 mg, 3.90 mmol, 2.5 equiv) in 6 M HCl (3.0 mL, 1.3 M) was added dropwise over 1 min. The reaction was allowed to stir at 0 °C for 1 h, then quenched with a solution of 40% w/w KOH in deionized H_2O until a pH of 12 had been reached (ca. 10 mL). The solution was transferred to a separatory funnel and extracted with EtOAc (4 x 20 mL). The organic layers were combined, dried over $MgSO_4$, and the volatiles were removed under reduced pressure. The resulting crude residue was taken up in EtOAc (6.0 mL) and cooled to 0 °C. Next, 1 M HCl in EtOH (8.0 mL, 0.2 M) was added dropwise over 1 min. The resulting precipitate was collected by filtration through a vacuum filter. The solid residue was washed with CH_2Cl_2 (5 mL) and dried under reduced pressure to yield hydrazine **37** as a solid (252.8 mg, 90% yield). Hydrazine **37**: mp: 151–152 ºC; R_f 0.57 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.40 (br. s, 3H), 8.09 (br. s, 2H), 7.72 (dd, J = 5.1, 1.5, 1H), 7.40 (dd, J = 7.7, 1.5, 1H), 6.94 (dd, J = 7.7, 5.1, 1H) 3.90 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 152.3, 138.0, 129.4, 120.8, 117.0, 53.4; IR (film): 3347, 3091, 2589, 1565, 788 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_6H_{10}N_3O^+$, 140.08184; found 140.08159.

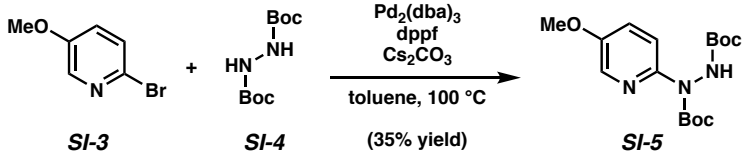
Representative Procedure B for the synthesis of hydrazine substrates from Table 2. (41 is used as an example).



SI-2 **(67% yield)** ***41***

Hydrazine 41. To a solution of aniline **SI-2** (1.0 g, 10.60 mmol, 1.0 equiv) in 12 M HCl (10.0 mL, 1.1 M) at 0 °C was added dropwise a solution of $NaNO_2$ (768.0 mg, 11.10 mmol, 1.0 equiv) in deionized H_2O (10.0 mL, 1.1 M) over 1 min under an air atmosphere. After stirring at 0 °C for 30 min, a solution of $SnCl_2$•2 H_2O (6.0 g, 26.50 mmol, 2.5 equiv) in 12 M HCl (10.0 mL, 2.6 M) was added dropwise over 1 min. The reaction was allowed to stir at 0 °C for 30 min. The precipitate was then removed by vacuum filtration. The filtrate was left to evaporate over 48 h allowing crystals to form. The resulting solid was transferred to a filter paper, washed with Et_2O (10 mL), and dried under reduced pressure to yield hydrazine **41** as a solid (1.03 g, 67% yield). Hydrazine **41**: mp: 181–183 ºC; R_f 0.08 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.45 (br. s, 3H), 9.54 (br. s, 1H), 8.45–8.43 (m, 2H), 8.04–8.02 (m, 1H), 7.96–7.93 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 144.9, 133.8, 129.3, 127.3, 126.8; IR (film): 3500, 3060, 2656, 1548, 787 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_5H_8N_3^+$, 110.07127; found 110.07105.

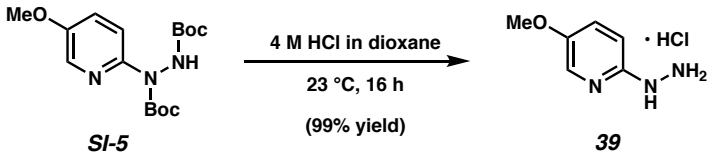
Representative Procedure C for the synthesis of hydrazine substrates from Table 2. (39 is used as an example).



SI-3 ***SI-4*** **(35% yield)** ***SI-5***

Boc-Hydrazine SI-5. A 1-dram vial charged with a magnetic stir bar and Cs_2CO_3 (876.7 mg, 2.69 mmol, 1.25 equiv) was flame-dried under reduced pressure, and allowed to cool under a N_2 atmosphere. Bromide **SI-3** (505.9 mg, 2.69 mmol, 1.25 equiv) and di-*tert*-butyl hydrazodiformate (**SI-4**) (500.0 mg, 2.15 mmol, 1.0 equiv) were added and the vial was flushed with N_2 for 5 min. The vial was taken into a glovebox and charged with $Pd_2(dba)_3$ (98.5 mg, 0.11 mmol, 0.05 equiv), dppf (179.1 mg, 0.32 mmol, 0.15 equiv), and toluene (3.6 mL, 0.75 M). The

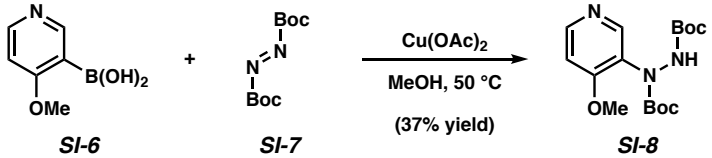
vial was then capped with a Teflon-lined screw cap and taken out of the glovebox where it was placed in a pre-heated aluminum block and allowed to stir at 100 °C for 24 h. After cooling to room temperature, the reaction mixture was diluted with CH_2Cl_2 (15 mL) and filtered through a plug of celite (30 mL of CH_2Cl_2 as eluent). The organics were transferred to a separatory funnel and washed sequentially with deionized water (2 x 15 mL), saturated aqueous NaCl (15 mL), and dried over Na_2SO_4. The volatiles were removed under reduced pressure. The resulting crude residue was purified by flash chromatography (1:1 Hexanes:EtOAc) to yield Boc-hydrazine **SI-5** (253.9 mg, 35% yield) as a light brown solid.



SI-5 *39*

Hydrazine 39. A 20 mL scintillation vial equipped with a magnetic stir bar was charged with Boc-hydrazine **SI-5** (269.5 mg, 0.79 mmol, 1.0 equiv) and 4 M HCl in dioxane (5.3 mL, 0.15 M). After stirring at 23 °C for 16 h, the volatiles were removed under reduced pressure. The resulting crude solid was transferred to a filter paper, washed with EtOAc (5 mL), and dried under reduced pressure to yield hydrazine **39** (141.1 mg, 99% yield) as a yellow solid. Hydrazine **39**: mp: 198–200 ºC; R_f 0.09 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.70 (br. s, 3H), 9.03 (br. s, 1H), 7.88 (d, J = 2.8, 1H), 7.44 (dd, J = 9.1, 2.8, 1H), 6.88 (app. dd, J = 9.1, 2.8, 1H), 3.78 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 150.8, 150.3, 130.3, 126.6, 110.6, 56.0; IR (film): 3308, 2940, 2646, 1620, 1584 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_6H_{10}N_3O^+$, 140.08184; found 140.08163.

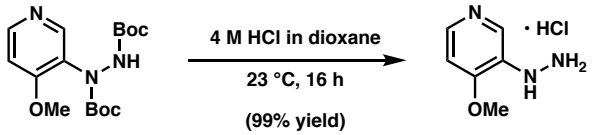
Representative Procedure D for the synthesis of hydrazine substrates from Table 2. (33 is used as an example).



SI-6 *SI-7* *SI-8*

Boc-Hydrazine SI-8. A 20 mL scintillation vial was charged with a magnetic stir bar, flame-dried under reduced pressure, and allowed to cool under a N_2 atmosphere. Boronic acid **SI-6** (300.0 mg, 1.76 mmol, 1.0 equiv), di-*tert*-butyl azodicarboxylate (**SI-7**) (444.6 mg, 1.93 mmol, 1.1 equiv), $Cu(OAc)_2$ (31.9 mg, 0.17 mmol, 0.10 equiv), and MeOH (7.0 mL, 0.25 M) were

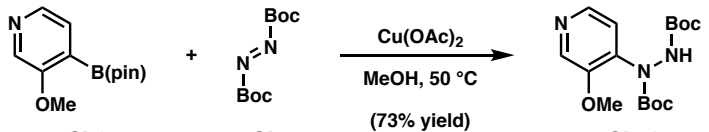
added under an atmosphere of air. The vial was capped with a Teflon-lined screw cap, placed in a pre-heated aluminum block, and allowed to stir at 50 °C for 3 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The reaction mixture was then transferred to a separatory funnel with deionized water (5 mL) and CH_2Cl_2 (5 mL). The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (3 x 5 mL). The organic layers were combined, washed with saturated aqueous NaCl (15 mL), and then dried over Na_2SO_4. The volatiles were removed under reduced pressure. The resulting crude residue was purified by flash chromatography (1:10 Hexanes:EtOAc, 2% Et_3N) to yield Boc-hydrazine **SI-8** (221.7 mg, 37% yield) as a white solid.



SI-8 ***33***

Hydrazine 33. A 20 mL scintillation vial equipped with a magnetic stir bar was charged with Boc-hydrazine **SI-8** (221.7 mg, 0.65 mmol, 1.0 equiv) and 4 M HCl in dioxane (4.4 mL, 0.15 M). After stirring at 23 °C for 16 h, the volatiles were removed under reduced pressure. The resulting crude residue was transferred to a filter paper, washed with EtOAc (5 mL), and dried under reduced pressure to yield hydrazine **33** (140.4 mg, 99% yield) as a light brown solid. Hydrazine **33**: mp: 178–180 ºC; R_f 0.07 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.81 (br. s, 1H), 8.52 (dd, J = 6.5, 0.7, 1H), 8.42 (d, J = 0.7, 1H), 7.59 (d, J = 6.5, 1H), 4.12 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 158.9, 136.7, 134.2, 124.1, 108.3, 58.1; IR (film): 3382, 3206, 2851, 2051, 1505 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_6H_{10}N_3O^+$, 140.08184; found 140.08165.

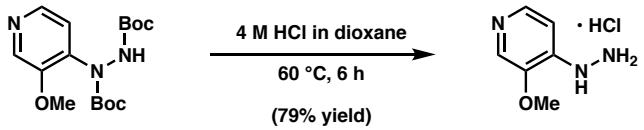
Representative Procedure E for the synthesis of hydrazine substrates from Table 2. (35 is used as an example).



SI-9 ***SI-7*** ***SI-10***

Boc-Hydrazine SI-10. A 20 mL scintillation vial was charged with a magnetic stir bar, flame-dried under reduced pressure, and allowed to cool under a N_2 atmosphere. Boronate ester **SI-9** (300.0 mg, 1.28 mmol, 1.0 equiv), di-*tert*-butyl azodicarboxylate (**SI-7**) (326.0 mg, 1.40 mmol,

1.1 equiv), $Cu(OAc)_2$ (23.2 mg, 0.13 mmol, 0.10 equiv), and MeOH (5.1 mL, 0.25 M) were added under an atmosphere of air. The vial was capped with a Teflon-lined screw cap, placed in a pre-heated aluminum block, and then allowed to stir at 50 °C for 3 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The reaction mixture was then transferred to a separatory funnel with deionized water (5 mL) and CH_2Cl_2 (5 mL). The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (3 x 5 mL). The organic layers were combined, washed with saturated aqueous NaCl (15 mL), and then dried over Na_2SO_4. The volatiles were removed under reduced pressure. The resulting crude residue was purified by flash chromatography (1:10 Hexanes: EtOAc, 2% Et_3N) to yield Boc-hydrazine **SI-10** (316.3 mg, 73% yield) as a colorless foam.

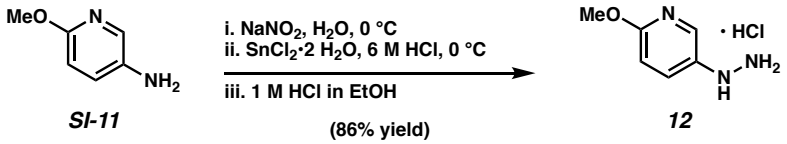


SI-10 ***35***

Hydrazine 35. A 20 mL scintillation vial equipped with a magnetic stir bar was charged with Boc-hydrazine **SI-10** (131.8 mg, 0.39 mmol, 1.0 equiv) and 4 M HCl in dioxane (2.6 mL, 0.15 M). The vial was then capped with a Teflon-lined screw cap and was placed in a pre-heated aluminum block at 60 °C for 6 h. Once at room temperature, the volatiles were removed under reduced pressure. The resulting crude residue was transferred to a filter paper, washed with EtOAc (5 mL), and dried under reduced pressure to yield hydrazine **35** (53.7 mg, 79% yield) as a yellow solid. Hydrazine **35**: mp: 225–228 ºC; R_f 0.00 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.70 (br. s, 1H), 8.19 (d, J = 6.6, 1H), 8.08 (s, 1H), 7.21 (d, J = 6.6, 1H), 3.94 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 149.1, 141.9, 135.7, 120.0, 104.0, 57.2; IR (film): 3366, 3215, 2834, 1631, 1536 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_6H_{10}N_3O^+$, 140.08184; found 140.08159.

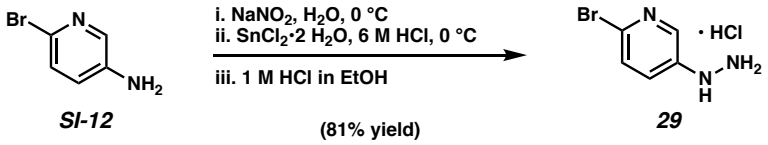
Note: Supporting information for the syntheses of some substrates (i.e., lactols, hemiaminals, ketones) used in Tables 1 and 2 and Figure 4 have previously been reported: **14**[1], **16**[1], **18**[1], **20**[1], **22**[1], **24**[1], **26**[2], and **46**[3]. Syntheses for the remaining substrates shown in Tables 1 and 2 and Figure 4 are as follows:

Any modification of the conditions shown in the representative procedures above are specified in the following schemes.



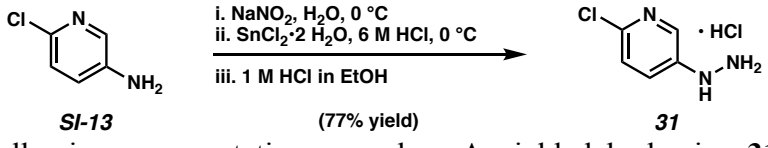
SI-11 ***12***

Hydrazine 12. Following representative procedure A yielded hydrazine **12** (2.42 g, 86% yield) as a light brown solid. Hydrazine **12**: mp: 175–178 ºC; R_f 0.27 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.45 (br. s, 4H), 7.99 (d, J = 2.8, 1H), 7.65 (dd, J = 9.1, 2.8, 1H), 6.90 (d, J = 9.1, 1H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 158.8, 136.7, 132.4, 130.3, 110.7, 54.0; IR (film): 3368, 3201, 2564, 1627, 1562 cm^{-1}; HRMS-APCI (*m/z*) [M + H]$^+$ calcd for $C_6H_{10}N_3O^+$, 140.08184; found 140.08154.



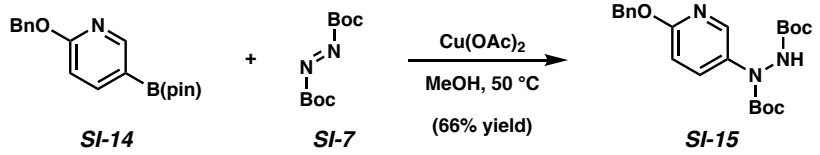
SI-12 ***29***

Hydrazine 29. Following representative procedure A yielded hydrazine **29** (280.7 mg, 81% yield) as an orange solid. Hydrazine **29**: mp: 211–213 ºC; R_f 0.37 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.43 (br. s, 3H), 8.69 (br. s, 1H), 8.08 (d, J = 3.0, 1H), 7.56 (d, J = 8.5, 1H), 7.35 (dd, J = 8.5, 3.0, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): 142.1, 136.9, 131.9, 127.7, 125.4; IR (film): 3070, 2883, 2645, 1927, 1619 cm^{-1}; HRMS-APCI (*m/z*) [M + H]$^+$ calcd for $C_5H_7N_3Br^+$, 187.98179; found 187.98140.



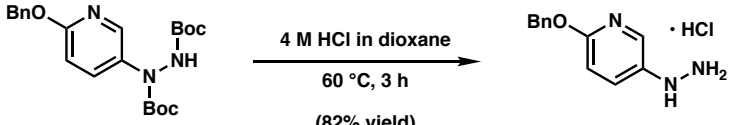
SI-13 ***31***

Hydrazine 31. Following representative procedure A yielded hydrazine **31** (215.3 mg, 77% yield) as a light brown solid. Hydrazine **31**: mp: 208–209 ºC; R_f 0.37 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.45 (br. s, 3H), 8.72 (br. s, 1H), 8.10–8.09 (m, 1H), 7.47–7.43 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): 141.9, 141.6, 136.1, 125.5, 124.0; IR (film): 3378, 3197, 2662, 1617, 1470 cm^{-1}; HRMS-APCI (*m/z*) [M + H]$^+$ calcd for $C_5H_7N_3Cl^+$, 144.03230; found 144.03195.



SI-14 *SI-7* *SI-15*

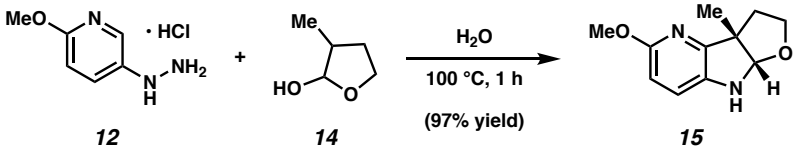
Boc-Hydrazine SI-15. Following representative procedure E. Purification by flash chromatography (5:1 Hexanes:EtOAc) yielded Boc-hydrazine **SI-15** (560.0 mg, 66% yield) as a light yellow solid.



SI-15 *43*

Hydrazine 43. Following representative procedure E yielded hydrazine **43** (280.1 mg, 82% yield) as a yellow solid. Hydrazine **43**: mp: 125–128 ºC; R_f 0.33 (EtOAc); ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.11 (br. s, 3H), 9.90 (br. s, 1H), 7.89 (d, J = 2.5, 1H), 7.47 (app. dt, J = 8.8, 2.5, 1H), 7.38 (d, J = 7.3, 2H), 7.33 (t, J = 7.3, 2H), 7.27 (t, J = 7.3, 1H), 6.84 (d, J = 8.8, 1H), 5.26 (s, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): 158.8, 137.4, 136.5, 133.8, 129.2, 128.4, 127.8, 127.7, 110.8, 67.0; IR (film): 3389, 2894, 2646, 1946, 1556 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{12}H_{14}N_3O^+$, 216.11314; found 216.11281.

B. Scope of Methodology

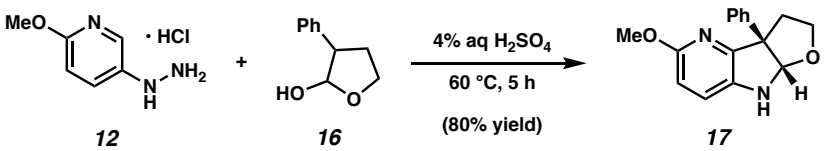


12 *14* *15*

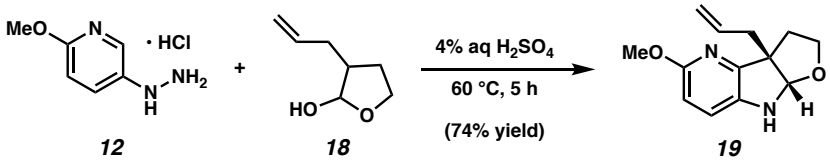
Representative Procedure (azaindoline 15 is used as an example). Azaindoline 15. A scintillation vial containing a magnetic stir bar was charged with lactol **14** (23.6 mg, 0.231 mmol, 1.0 equiv) and deionized H_2O (4.6 mL, 0.05 M). Hydrazine **12** (60.9 mg, 0.347 mmol, 1.5 equiv) was added and the vial was capped with a Teflon-lined screw cap. The reaction mixture was then placed in a pre-heated aluminum block and allowed to stir at 100 °C for 1 h. After cooling to room temperature, the reaction mixture was transferred to a separatory funnel with deionized H_2O (3 mL) and EtOAc (3 mL). The reaction mixture was then basified to a pH of 12 by the addition of 40% w/w KOH in deionized H_2O (ca. 4 mL). The layers were separated and the aqueous layer was extracted with EtOAc (3 x 5 mL). The combined organic layers were washed with saturated aqueous NaCl (5 mL), and then dried over Na_2SO_4. The volatiles were

removed under reduced pressure, and the crude residue was purified by preparative thin-layer chromatography (2:1 Hexanes:EtOAc) to yield azaindoline **15** (97% yield, average of two experiments) as a yellow oil. Azaindoline **15**: R_f 0.55 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.88 (d, *J* = 8.4, 1H), 6.43 (d, *J* = 8.4, 1H), 5.27 (s, 1H), 3.96 (ddd, *J* = 8.9, 7.6, 1.7, 1H), 3.87 (s, 3H), 3.53 (ddd, *J* = 10.9, 8.9, 5.3, 1H), 2.40 (ddd, *J* = 12.1, 5.3, 1.7, 1H), 2.03 (ddd, *J* = 12.1, 10.9, 7.6, 1H), 1.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.7, 151.2, 136.8, 119.7, 107.4, 99.1, 67.6, 54.3, 53.8, 39.6, 22.6; IR (film): 3347, 2961, 2867, 1603, 1471 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{11}H_{15}N_2O_2^+$, 207.11280; found 207.11237.

Any modifications of the conditions shown in the representative procedure above are specified in the following schemes, which depict all of the results shown in Tables 1 and 2.

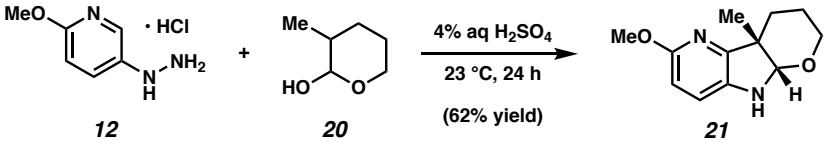


Azaindoline 17. Purification by preparative thin-layer chromatography (2:1 Hexanes:EtOAc) yielded azaindoline **17** (80% yield, average of two experiments) as an amorphous solid. Azaindoline **17**: R_f 0.63 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.42 (d, *J* = 7.8, 2H), 7.32 (t, *J* = 7.8, 2H), 7.26–7.21 (m, 1H), 6.94 (d, *J* = 8.6, 1H), 6.47 (d, *J* = 8.6, 1H), 5.69 (s, 1H), 4.39 (s, 1H), 4.18–4.15 (m, 1H), 3.85 (s, 3H), 3.67–3.62 (m, 1H), 2.85–2.82 (m, 1H), 2.65–2.59 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.8, 149.1, 142.6, 137.6, 128.6, 126.9, 126.5, 120.5, 108.4, 99.7, 68.6, 62.4, 53.8, 39.7; IR (film): 3341, 2866, 2973, 1602, 1470 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{16}H_{17}N_2O_2^+$, 269.12845; found 269.12688.



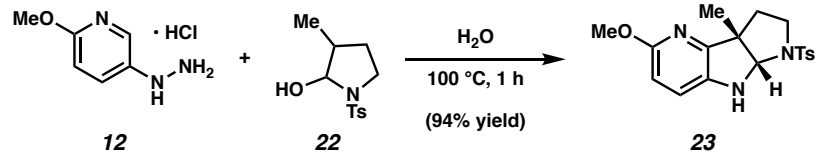
Azaindoline 19. Purification by preparative thin-layer chromatography (3:2 Hexanes:EtOAc) yielded azaindoline **19** (74% yield, average of two experiments) as a red oil. Azaindoline **19**: R_f 0.62 (1:1 Hexanes:EtOAc); ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.88–6.86 (m, 1H), 6.45–6.42 (m,

1H), 5.75–5.65 (m, 1H), 5.39 (s, 1H), 5.10–5.06 (m, 1H), 5.03–4.99 (m, 1H), 3.98–3.93 (m, 1H), 3.87 (s, 3H), 3.53 (ddd, *J* = 11.2, 8.8, 5.3, 1H), 2.75–2.69 (m, 1H), 2.52–2.47 (m, 1H), 2.34–2.29 (m, 1H), 2.09 (app. ddd, *J* = 11.2, 11.2, 7.4, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.8, 149.9, 137.7, 134.4, 119.9, 118.0, 107.8, 96.8, 67.3, 58.1, 53.9, 40.9, 37.9; IR (film): 3343, 2973, 2947, 1603, 1471 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{13}H_{17}N_2O_2^+$, 233.12845; found 233.12790.



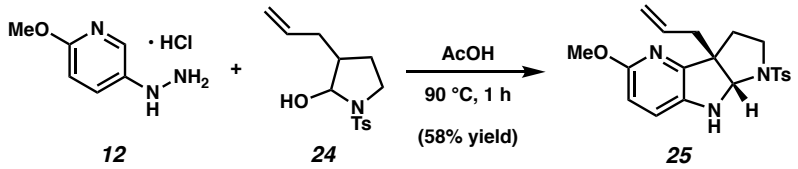
12 ***20*** ***21***

Azaindoline 21. Purification by preparative thin-layer chromatography (3:2 Hexanes:EtOAc) yielded azaindoline **21** (62% yield, average of two experiments) as an amorphous solid. Azaindoline **21**: R_f 0.59 (1:1 Hexanes:EtOAc); ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.93 (d, *J* = 8.1, 1H), 6.41 (d, *J* = 8.1, 1H), 4.74 (s, 1H), 4.04 (br. s, 1H), 3.87 (s, 3H), 3.75 (dddd, *J* = 11.2, 4.0, 4.0, 1.6, 1H), 3.40 (ddd, *J* = 11.2, 10.0, 3.0, 1H), 2.45 (dddd, *J* = 13.3, 4.0, 4.0, 1.6, 1H), 1.62 (ddd, *J* = 13.6, 11.8, 4.7, 1H), 1.55–1.47 (m, 1H), 1.47–1.36 (m, 1H), 1.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.7, 152.9, 136.4, 120.4, 106.2, 94.9, 63.0, 53.9, 44.2, 29.2, 24.7, 22.2; IR (film): 3319, 2950, 2851, 1603, 1464 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{12}H_{17}N_2O_2^+$, 221.12845; found 221.12779.



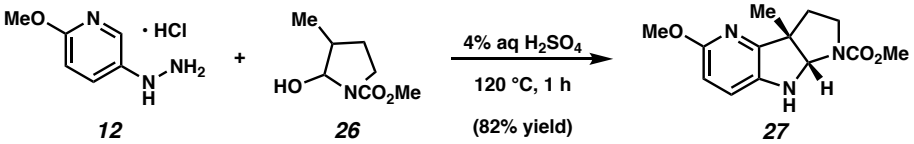
12 ***22*** ***23***

Azaindoline 23. Purification by preparative thin-layer chromatography (2:1 Hexanes:EtOAc) yielded azaindoline **23** (94% yield, average of two experiments) as a colorless oil. Azaindoline **23**: R_f 0.77 (1:1 Hexanes:EtOAc); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.3, 2H), 7.32 (d, *J* = 8.3, 2H), 6.90 (d, *J* = 8.4, 1H), 6.44 (d, *J* = 8.4, 1H), 4.98 (s, 1H), 3.84 (s, 3H), 3.39 (ddd, *J* = 10.5, 8.2, 2.3, 1H), 3.10 (ddd, *J* = 10.5, 10.5, 6.4, 1H), 2.44 (s, 3H), 2.41 (ddd, *J* = 12.5, 6.4, 2.3, 1H), 1.70 (ddd, *J* = 12.5, 10.5, 8.2, 1H), 1.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.9, 150.2, 143.8, 136.3, 136.0, 129.9, 127.2, 120.9, 107.9, 84.1, 54.6, 53.9, 47.7, 36.1, 22.4, 21.7; IR (film): 3375, 2963, 2867, 1597, 1470 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{18}H_{22}N_3O_3S^+$, 360.13764; found 360.13632.



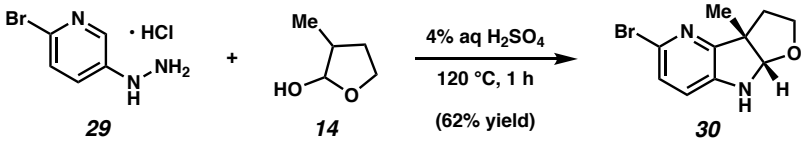
12 ***24*** ***25***

Azaindoline 25. Purification by preparative thin-layer chromatography (2:1 Hexanes:EtOAc) yielded azaindoline **25** (58% yield, average of two experiments) as a colorless oil. Azaindoline **25**: R_f 0.70 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.74 (d, *J* = 7.8, 2H), 7.32 (d, *J* = 7.8, 2H), 6.89 (d, *J* = 8.4, 1H), 6.45 (d, *J* = 8.4, 1H), 5.54 (dddd, *J* = 17.4, 10.0, 7.4, 7.4, 1H), 5.11 (s, 1H), 4.98–4.93 (m, 2H), 4.52 (br. s, 1H), 3.84 (s, 3H), 3.38 (ddd, *J* = 10.3, 8.3, 2.3, 1H), 3.10 (ddd, *J* = 10.3, 10.3, 6.2, 1H), 2.44 (s, 3H), 2.41–2.38 (m, 1H), 2.32–2.27 (m, 2H), 1.78 (ddd, *J* = 12.2, 10.2, 8.3, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.8, 149.0, 143.8, 137.0, 136.0, 133.5, 129.9, 127.3, 120.8, 118.5, 108.2, 81.6, 58.2, 53.9, 47.5, 40.5, 34.2, 21.7; IR (film): 3376, 3072, 2950, 1598, 1471 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{20}H_{24}N_3O_3S^+$, 386.15329; found 386.15111.



12 ***26*** ***27***

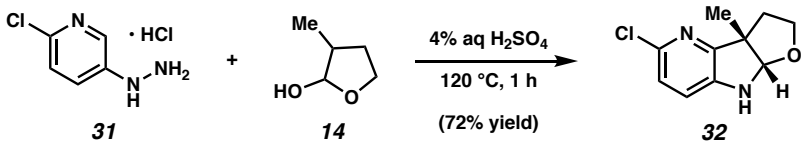
Azaindoline 27. Purification by preparative thin-layer chromatography (1:1 Hexanes:EtOAc) yielded azaindoline **27** (82% yield, average of two experiments) as an amorphous solid. Azaindoline **27**: R_f 0.46 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$, 58 °C): δ 6.85 (d, *J* = 8.3, 1H), 6.43 (d, *J* = 8.3, 1H), 5.10 (br. s, 1H), 3.88 (s, 3H), 3.72–3.64 (m, 4H), 3.09–3.04 (m, 1H), 2.53–2.49 (m, 1H), 2.02–1.95 (m, 1H), 1.42 (s, 3H); ^{13}C NMR (125 MHz, C_6D_6, **Major rotational isomer**): 160.0, 155.4, 150.2, 137.0, 120.7, 109.0, 82.1, 53.4, 53.2, 51.9, 45.9, 35.4, 22.2; ^{13}C NMR (125 MHz, C_6D_6, **Minor rotational isomer**, 11 of 13 peaks seen): 160.2, 154.4, 150.3, 136.6, 120.6, 109.1, 81.4, 54.6, 52.1, 46.4, 22.7; IR (film): 3360, 2956, 2869, 1696, 1605 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{13}H_{18}N_3O_3^+$, 264.13427; found 264.13304.



29 ***14*** ***30***

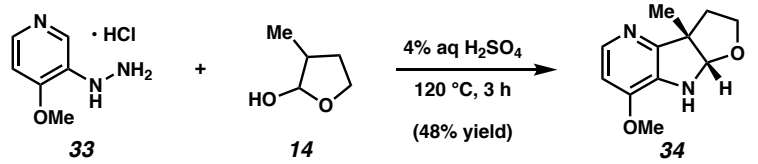
Azaindoline 30. Purification by preparative thin-layer chromatography (1:1 Hexanes:EtOAc) yielded azaindoline **30** (62% yield, average of two experiments) as a light brown solid. Azaindoline **30**: mp: 170–171 ºC; R_f 0.50 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ

7.08 (d, *J* = 8.3, 1H), 6.89 (d, *J* = 8.3, 1H), 5.29 (s, 1H), 4.64 (br. s, 1H), 3.98 (ddd, *J* = 8.9, 7.6, 1.6, 1H), 3.52 (dddd, *J* = 11.3, 8.9, 5.3, 1H), 2.43 (ddd, *J* = 12.3, 5.3, 1.6, 1H), 2.05 (ddd, *J* = 12.3, 11.3, 7.6, 1H), 1.50 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 156.1, 142.2, 129.8, 126.2, 116.7, 98.5, 67.7, 54.2, 39.9, 22.8; IR (film): 3328, 2963, 2866, 1595, 1426 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{10}H_{12}N_2OBr^+$, 255.01275; found 255.01276.



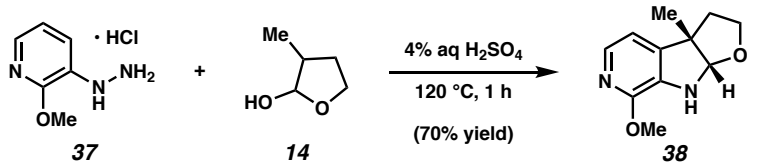
31 ***14*** ***32***

Azaindoline 32. Purification by preparative thin-layer chromatography (1:1 Hexanes:EtOAc) yielded azaindoline **32** (72% yield, average of two experiments) as a brown solid. Azaindoline **32**: mp: 143–145 ºC; R_f 0.50 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.95 (d, *J* = 8.3, 1H), 6.77 (d, *J* = 8.3, 1H), 5.31 (s, 1H), 4.62 (br. s, 1H), 3.99 (ddd, *J* = 8.9, 7.6, 1.6, 1H), 3.53 (ddd, *J* = 11.3, 8.9, 5.3, 1H), 2.43 (ddd, *J* = 12.3, 5.3, 1.6, 1H), 2.06 (ddd, *J* = 12.3, 11.3, 7.6, 1H), 1.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 155.3, 141.8, 140.5, 122.5, 116.7, 98.6, 67.7, 54.2, 39.9, 22.8; IR (film): 3319, 2965, 2867, 1596, 1430 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{10}H_{12}N_2OCl^+$, 211.06327; found 211.06329.



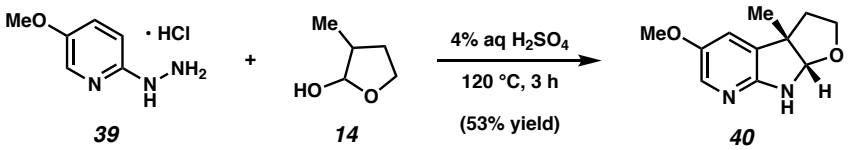
33 ***14*** ***34***

Azaindoline 34. Purification by preparative thin-layer chromatography (EtOAc) yielded azaindoline **34** (48% yield, average of two experiments) as an amorphous solid. Azaindoline **34**: R_f 0.26 (EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.94 (d, *J* = 5.3, 1H), 6.61 (d, *J* = 5.3, 1H), 5.33 (s, 1H), 4.51 (br. s, 1 H), 3.99 (ddd, *J* = 8.8, 7.6, 1.5, 1H), 3.88 (s, 3H), 3.54 (ddd, *J* = 11.2, 8.8, 5.5, 1H), 2.45 (ddd, *J* = 12.2, 5.5, 1.5, 1H), 2.08 (ddd, *J* = 12.2, 11.2, 7.6, 1H), 1.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 154.2, 149.8, 141.9, 132.3, 105.7, 98.8, 67.9, 55.5, 54.9, 39.8, 22.8; IR (film): 3308, 2926, 2867, 1614, 1498 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{11}H_{15}N_2O_2^+$, 207.11280; found 207.11210.



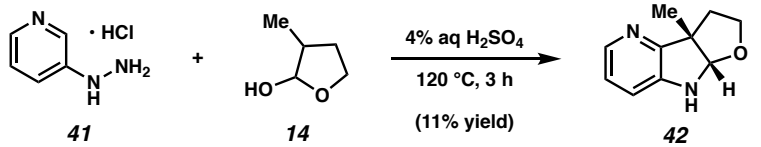
37 ***14*** ***38***

Azaindoline 38. Purification by preparative thin-layer chromatography (2:1 Hexanes:EtOAc) yielded azaindoline **38** (70% yield, average of two experiments) as a colorless solid. Azaindoline **38**: mp: 143–145 ºC; R_f 0.51 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.64 (d, *J* = 5.1, 1H), 6.70 (d, *J* = 5.1, 1H), 5.34 (s, 1H), 4.48 (br. s, 1H), 3.99–3.95 (m, 4H), 3.54 (ddd, *J* = 11.2, 8.7, 5.1, 1H), 2.16 (ddd, *J* = 12.3, 5.1, 1.6, 1H), 2.07 (ddd, *J* = 12.3, 11.2, 7.3, 1H), 1.47 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 150.0, 142.3, 137.1, 132.9, 112.3, 99.9, 67.6, 55.1, 53.2, 40.8, 23.9; IR (film): 3328, 2956, 2867, 1611, 1471 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{11}H_{15}N_2O_2^+$, 207.11280; found 207.11261.



39 ***14*** ***40***

Azaindoline 40. Purification by preparative thin-layer chromatography (1:1 Hexanes:EtOAc) yielded azaindoline **40** (53% yield, average of two experiments) as a yellow solid. Azaindoline **40**: mp: 87–90 ºC; R_f 0.13 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.56 (d, *J* = 2.7, 1H), 6.95 (d, *J* = 2.7, 1H), 5.31 (s, 1H), 5.11 (br. s, 1H), 3.97 (ddd, *J* = 8.8, 7.0, 1.6, 1H), 3.78 (s, 3H), 3.58 (ddd, *J* = 10.9, 8.8, 5.4, 1H), 2.13–2.03 (m, 2H), 1.47 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 156.7, 150.5, 130.9, 128.8, 120.6, 98.0, 67.2, 56.8, 52.6, 41.5, 24.7; IR (film): 3206, 2956, 2866, 1627, 1480 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{11}H_{15}N_2O_2^+$, 207.11280; found 207.11214.

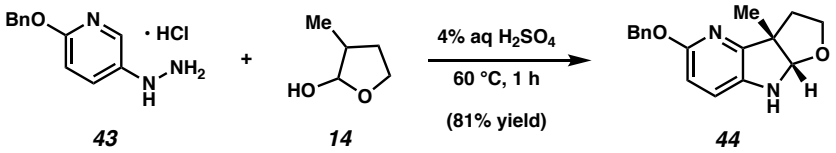


41 ***14*** ***42***

Azaindoline 42. Purification by preparative thin-layer chromatography (98:2 EtOAc:Et_3N) yielded azaindoline **42** (11% yield, average of two experiments) as an amorphous solid. Azaindoline **42**: R_f 0.44 (EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.95 (dd, *J* = 5.1, 1.4, 1H), 6.93 (dd, *J* = 7.9, 5.1, 1H), 6.79 (dd, *J* = 7.9, 1.4, 1H), 5.31 (s, 1H), 4.59 (br. s, 1H), 3.99 (ddd, *J* = 8.9, 7.6, 1.6, 1H), 3.53 (ddd, *J* = 11.2, 8.9, 5.3, 1H), 2.43 (ddd, *J* = 12.2, 5.3, 1.6, 1H), 2.09 (ddd, *J* = 12.2, 11.2, 7.6, 1H), 1.52 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 155.0, 142.7, 140.1,

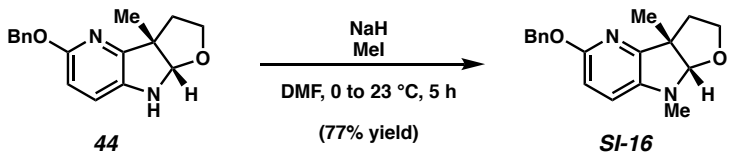
122.5, 113.9, 98.3, 67.7, 54.0, 40.1, 22.9; IR (film): 3330, 2961, 2867, 1602, 1436 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{10}H_{13}N_2O^+$, 177.10224; found 177.10093.

C. Synthesis of an Aza-Analogue of Phensvenine



43 *14* *44*

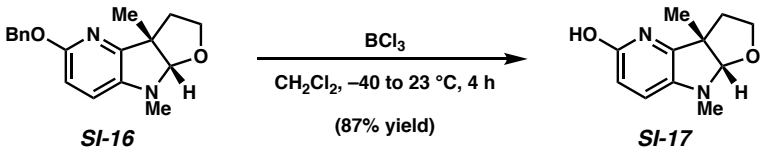
Azaindoline 44. A round-bottom flask containing a magnetic stir bar was charged with lactol **14** (37.2 mg, 0.364 mmol, 1.0 equiv) and 4% aqueous H_2SO_4 (7.3 mL, 0.05 M). Hydrazine **43** (274.3 mg, 1.092 mmol, 3.0 equiv) was added and the flask equipped with an air condenser. The reaction mixture was then placed in a pre-heated oil bath and allowed to stir at 60 °C for 1 h. After cooling to room temperature, the reaction mixture was transferred to a separatory funnel with deionized H_2O (5 mL) and EtOAc (5 mL). The reaction mixture was then basified to a pH of 9 with saturated aqueous $NaHCO_3$ (ca. 10 mL). The layers were separated and the aqueous layer was extracted with EtOAc (3 x 10 mL). The combined organic layers were washed with saturated aqueous NaCl (10 mL), and then dried over Na_2SO_4. The volatiles were removed under reduced pressure, and the crude residue was purified by flash chromatography (2:1 Hexanes:EtOAc) to yield azaindoline **44** (83.2 mg, 81% yield) as a yellow oil. Azaindoline **44**: R_f 0.54 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.2, 2H), 7.35 (t, *J* = 7.2, 2H), 7.30–7.28 (m, 1H), 6.87 (d, *J* = 8.5, 1H), 6.48 (d, *J* = 8.5, 1H), 5.31 (s, 1H), 5.30 (s, 1H), 5.27 (s, 1H), 4.25 (br. s, 1H), 3.97 (ddd, *J* = 9.1, 7.7, 1.7, 1H), 3.53 (ddd, *J* = 11.1, 9.1, 5.1. 1H), 2.39 (ddd, *J* = 12.1, 5.1, 1.7, 1H), 2.04 (ddd, *J* = 12.1, 11.1 7.7, 1H), 1.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.1, 151.0, 138.1, 137.1, 128.5, 128.3, 127.8, 119.9, 108.6, 99.2, 68.1, 67.7, 54.5, 39.7, 22.8; IR (film): 3348, 2963, 2930, 1603, 1447 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{17}H_{19}N_2O_2^+$, 283.14410; found 283.14342.



44 *SI-16*

Azaindoline SI-16. A 1-dram vial was charged with a magnetic stir bar, flame-dried under reduced pressure, and allowed to cool under a N_2 atmosphere. Azaindoline **44** (83.0 mg, 0.294 mmol, 1.0 equiv) was added and the vial was flushed with N_2 for 5 min. DMF (294 μL, 1.0 M)

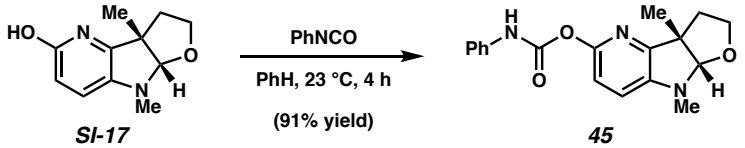
was added and the reaction mixture cooled to 0 °C under an N_2 atmosphere. NaH (60% dispersion in mineral oil, 26.0 mg, 0.647 mmol, 2.2 equiv) was added in one portion and the reaction was left to stir for 30 min at 0 °C. MeI (44 μL, 0.706 mmol, 2.4 equiv) was then added dropwise over 1 min. After 30 min stirring at 0 °C, the reaction mixture was warmed to 23 °C and allowed to stir for 4 h. The reaction mixture was then transferred to a separatory funnel with deionized H_2O (3 mL) and CH_2Cl_2 (3 mL). The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (3 x 5 mL). The combined organic layers were washed sequentially with deionized H_2O (3 x 3 mL) and saturated aqueous NaCl (10 mL), and then dried over Na_2SO_4. The volatiles were removed under reduced pressure, and the crude residue was purified by flash chromatography (3:1 Hexanes:EtOAc) to yield azaindoline **SI-16** (61.0 mg, 77% yield) as a colorless oil. Azaindoline **SI-16**: R_f 0.46 (3:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.5, 2H), 7.35 (t, *J* = 7.5, 2H), 7.30–7.27 (m, 1H), 6.64 (d, *J* = 8.3, 1H), 6.50 (d, *J* = 8.3, 1H), 5.32–5.27 (m, 2H), 5.04 (s, 1H), 3.96 (ddd, *J* = 9.0, 7.6, 1.6, 1H), 3.43 (ddd, *J* = 11.2, 9.0, 5.6, 1H), 2.88 (s, 3H), 2.36 (ddd, *J* = 12.2, 5.6, 1.6, 1H), 2.02 (ddd, *J* = 12.2, 11.2, 7.6, 1H), 1.47 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 157.9, 151.5, 139.7, 138.2, 128.4, 128.3, 127.7, 115.8, 108.0, 104.3, 68.2, 67.7, 53.4, 39.7, 32.0, 22.7; IR (film): 2930, 2864, 1595, 1457, 1421 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{18}H_{21}N_2O_2^+$, 297.15975; found 297.15959.



SI-16 *SI-17*

Hydroxyazaindoline SI-17. A 1-dram vial was charged with a magnetic stir bar, flame-dried under reduced pressure, and allowed to cool under a N_2 atmosphere. Azaindoline **SI-16** (3.3 mg, 0.011 mmol, 1.0 equiv) was added and the vial was flushed with N_2 for 5 min. CH_2Cl_2 (222 μL, 0.05 M) was added and the reaction mixture cooled to –40 °C. BCl_3 (1 M in CH_2Cl_2, 78.0 μL, 0.078 mmol, 7.0 equiv) was added dropwise over 1 min and the reaction mixture was stirred at –40 °C. After 5 min, the reaction mixture was warmed to 23 °C and allowed to stir for 4 h. The reaction mixture was then transferred to separatory funnel containing ice-cold deionized H_2O (5 mL). The reaction mixture was basified to a pH of 9 with saturated aqueous $NaHCO_3$ (5 mL) and then extracted with EtOAc (5 x 3 mL). The combined organic layers were washed with saturated aqueous NaCl (10 mL), and subsequently dried over Na_2SO_4. The volatiles were removed under reduced pressure, and the crude residue was purified by preparative thin-layer chromatography

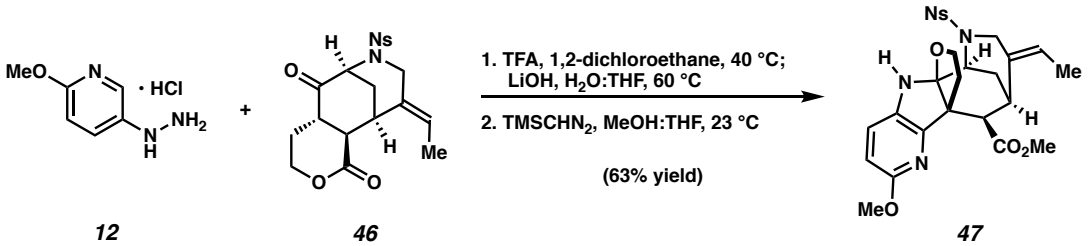
(EtOAc) to yield hydroxyazaindoline **SI-17** (1.9 mg, 87% yield) as a brown solid. Hydroxyazaindoline **SI-17**: mp: 169–170 ºC; R_f 0.36 (EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.77 (d, *J* = 8.5, 1H), 6.49 (d, *J* = 8.5, 1H), 5.01 (s, 1H), 3.97 (ddd, *J* = 8.8, 7.4, 1.6, 1H), 3.47 (ddd, *J* = 11.2, 8.8, 5.2, 1H), 2.88 (s, 3H), 2.44 (ddd, *J* = 12.2, 5.2, 1.6, 1H), 2.08 (ddd, *J* = 12.2, 11.2, 7.4, 1H), 1.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.2, 148.9, 138.5, 118.9, 109.2, 104.5, 67.9, 53.2, 39.5, 32.3, 22.7; IR (film): 2964, 2926, 2669, 1614, 1488 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{11}H_{15}N_2O_2^+$, 207.11280; found 207.11227.



SI-17 ***45***

Aza-phensvenine 45. A 1-dram vial was charged with a magnetic stir bar, flame-dried under reduced pressure, and allowed to cool under a N_2 atmosphere. Hydroxyazaindoline **SI-17** (5.0 mg, 0.024 mmol, 1.0 equiv) was added and the vial was flushed with N_2 for 5 min. The vial was then charged with a stock solution of PhNCO (1.7 uL, 0.022 mmol, 1.5 equiv) in PhH (200 µL, 0.075 M), and the reaction mixture was allowed to stir at 23 °C under an N_2 atmosphere. After 4 h, the volatiles were removed under reduced pressure to yield aza-phensvenine **45** (7.2 mg, 91% yield) as an amorphous solid. Aza-phensvenine **45**: R_f 0.40 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, C_6D_6): δ 7.27 (d, *J* = 8.0, 2H), 7.05–7.02 (m, 2H), 6.83–6.80 (m, 1H), 6.77 (d, *J* = 8.1, 1H), 6.61 (br. s, 1H), 6.13 (d, *J* = 8.1, 1H), 4.86 (s, 1H), 3.65 (ddd, *J* = 8.9, 7.6, 1.6, 1H), 3.25 (ddd, *J* = 11.2, 8.9, 5.4, 1H), 2.52 (s, 3H), 2.26 (ddd, *J* = 12.2, 5.4, 1.6, 1H), 1.67 (ddd, *J* = 12.2, 11.2, 7.6, 1H), 1.32 (s, 3H); ^{13}C NMR (125 MHz, C_6D_6): 154.0, 152.0, 150.6, 143.5, 138.4, 129.1, 123.7, 119.0, 114.9, 113.0, 103.9, 67.4, 53.2, 40.2, 30.8, 22.7; IR (film): 3281, 2926, 1746, 1646, 1597 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{18}H_{20}N_3O_3^+$, 326.14992; found 326.14895.

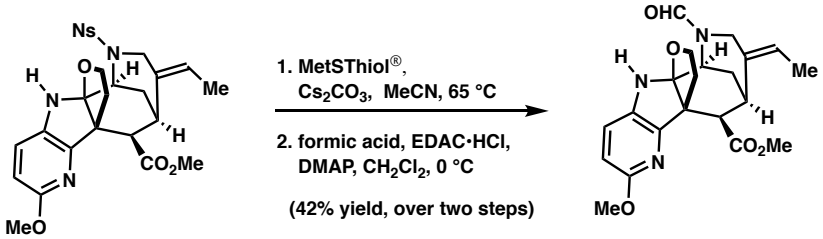
D. Synthesis of an Aza-Analogue of Aspidophylline A



12 ***46*** ***47***

Aza-furoindoline 47. A 1-dram vial was charged with a magnetic stir bar, flame-dried under reduced pressure, and allowed to cool under a N_2 atmosphere. Ketolactone **46** (10.0 mg, 0.0238 mmol, 1.0 equiv) was added and suspended in 1,2-dichloroethane (1.0 mL, 0.020 M). Hydrazine **12** (35.0 mg, 0.119 mmol, 5.0 equiv) and TFA (10.0 μL, 0.119 mmol, 5.0 equiv) were added to the reaction vial. The mixture was degassed via the freeze-pump-thaw method using a –78 °C dry ice/acetone bath. After warming to 23 °C, the reaction vessel was placed into a pre-heated 80 °C aluminum heating block and allowed to stir for 12 h. After cooling to room temperature, the reaction mixture was filtered over Na_2SO_4, washed with CH_2Cl_2 (10 mL), and concentrated under reduced pressure. The resultant residue was suspended in 1:1 THF/H_2O (1.0 mL, 0.02 M) in a 1-dram vial. LiOH (5.0 mg, 0.230 mmol, 10.0 equiv) was added and the reaction vessel was placed into a pre-heated 60 °C aluminum heating block. Upon stirring for 2 h at 60 °C, the reaction was cooled to 23°C. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (4 x 2 mL). The organic layers were combined, dried over Na_2SO_4, and concentrated under reduced pressure. The resultant residue was suspended in 1:1 THF/MeOH (1.0 mL, 0.02 M) in a 1-dram vial. $TMSCHN_2$ (77.0 μL, 0.046 mmol, 2.0 equiv) was added and the resultant solution stirred at room temperature. Upon stirring for 1.5 h, the reaction was diluted with 2 mL of H_2O and the layers were separated. The aqueous layer was extracted with EtOAc (4 x 2 mL). The organic layers were combined, dried over Na_2SO_4, and then concentrated under reduced pressure. The crude residue was purified by flash chromatography (9:1 Hexanes:EtOAc → 7:3 Hexanes:EtOAc) to afford aza-furoindoline **47** (8.0 mg, 63% yield) as a yellow oil. Aza-furoindoline **47:** R_f 0.50 (1:1 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07–8.03 (m, 1H), 7.69–7.61 (m, 3H), 6.88 (d, *J* = 8.5, 1H), 6.44 (d, *J* = 8.2, 1H), 5.53 (q, *J* = 7.0, 1H), 4.38 (br. s, 1H), 4.04 (d, *J* = 15.0, 1H), 3.93 (d, *J* = 15.0, 1H), 3.78 (br. s, 4H), 3.67 (s, 3H), 3.35–3.28 (m, 1H), 3.21 (q, *J* = 3.8, 1H), 3.08–3.00 (m, 1H), 2.90 (d, *J* = 4.8, 1H), 2.47 (dd, *J* = 13.6, 5.6, 1H), 2.06 (dt, *J* = 13.5, 3.7, 1H), 1.96 (dt, *J* = 13.3, 2.6, 1H), 1.52 (dd, *J* = 6.9, 1.8, 3H); ^{13}C

NMR (125 MHz, $CDCl_3$): 171.8, 159.8, 151.2, 148.1, 134.4, 134.0, 133.1, 131.5, 131.1, 129.5, 125.0, 124.4, 120.4, 108.9, 100.8, 68.5, 54.4, 54.2, 53.4, 52.0, 51.7, 48.5, 34.4, 31.2, 30.1, 12.7; IR (film): 3360, 2950, 2872, 1742, 1163 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{26}H_{29}N_4O_8S^+$, 557.17006; found 557.16905; $[\alpha]^{25.9}_D$ –165.33° (c = 0.1, CH_2Cl_2).



47 ***48***

(–)-10-Methoxy-9-aza-aspidophylline A (48). To a 1-dram vial, a suspension of aza-furoindoline **47** (10.0 mg, 0.017 mmol, 1.0 equiv) and Cs_2CO_3 (18.0 mg, 0.0539 mmol, 3.0 equiv) in MeCN (1.0 mL, 0.02 M) was added MetSThiol® (58.0 mg, 0.0718 mmol, 4.0 equiv). The reaction vessel was placed in an aluminum block and heated to 65 °C. After stirring for 12 h, the reaction was cooled to 23 °C and filtered through a plug of celite (100 mg) and washed with 10 mL of MeCN. The filtrate was concentrated under reduced pressure to afford the corresponding secondary amine, which was used subsequently without further purification.

In a 20 mL scintillation vial, HCOOH (9.6 μL, 0.255 mmol, 15.0 equiv) was added to a solution of DMAP (44 mg, 0.358 mmol, 20.0 equiv) and EDAC•HCl (34 mg, 0.179 mmol, 10.0 equiv) in CH_2Cl_2 (3.8 mL, 0.005 M) at 0 °C. This mixture was stirred at 0 °C for 15 min, at which point a 400 μL aliquot of this stock solution was added to the crude denosylated product in a 1-dram vial equipped with a magnetic stir bar. The reaction mixture was cooled to 0 °C and stirred for 1.5 h. The reaction mixture was then quenched with saturated aqueous $NaHCO_3$ (2 mL). The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (4 x 2 mL). The organic layers were combined, dried over Na_2SO_4, and concentrated under reduced pressure. The crude mixture was purified via flash chromatography (1:1 Hexanes:EtOAc → 1:9 Hexanes:EtOAc) to afford (–)-10-methoxy-9-aza-aspidophylline A (**48**) as a colorless oil (3.0 mg, 42% yield). (–)-10-methoxy-9-aza-aspidophylline A (**48**) was observed as a 5:1 mixture of rotational isomers in $CDCl_3$. (–)-10-methoxy-9-aza-aspidophylline A (**48**) **(Major rotational isomer)**: R_f 0.27 (1:9 Hexanes:EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.12 (s, 1H), 6.95 (d, *J* = 8.5, 1H), 6.49 (d, *J* = 8.5, 1H), 5.62 (q, *J* = 6.8, 1H), 4.38 (d, *J* = 18.0, 1H), 4.01–3.96 (m, 2H),

3.85 (t, J = 3.0, 1H), 3.80 (s, 3H), 3.70 (d, J = 3.2, 1H), 3.69 (s, 3H), 3.55–3.47 (m, 1H), 3.31 (q, J = 4.1, 1H), 2.95–2.86 (m, 1H), 2.82 (d, J = 4.8, 1H), 2.67 (dd, J = 13.6, 5.6, 1H), 2.10 (dt, J = 13.3, 2.7, 1H), 2.00 (dt, J = 13.5, 3.8, 1H), 1.54 (br. s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 171.6, 164.3, 160.1, 151.6, 134.1, 129.1, 124.3, 121.4, 109.7, 101.2, 69.2, 54.3, 54.2, 53.5, 52.0, 51.8, 44.6, 33.2, 30.8, 30.4, 12.9; IR (film): 3318, 2927, 2862, 1744, 1421 cm^{-1}; HRMS-APCI (*m/z*) $[M + H]^+$ calcd for $C_{21}H_{26}N_3O_5^+$, 400.18670; found 400.18560; $[\alpha]^{28.5}_D$ –4.00° (c = 0.1, CH_2Cl_2).

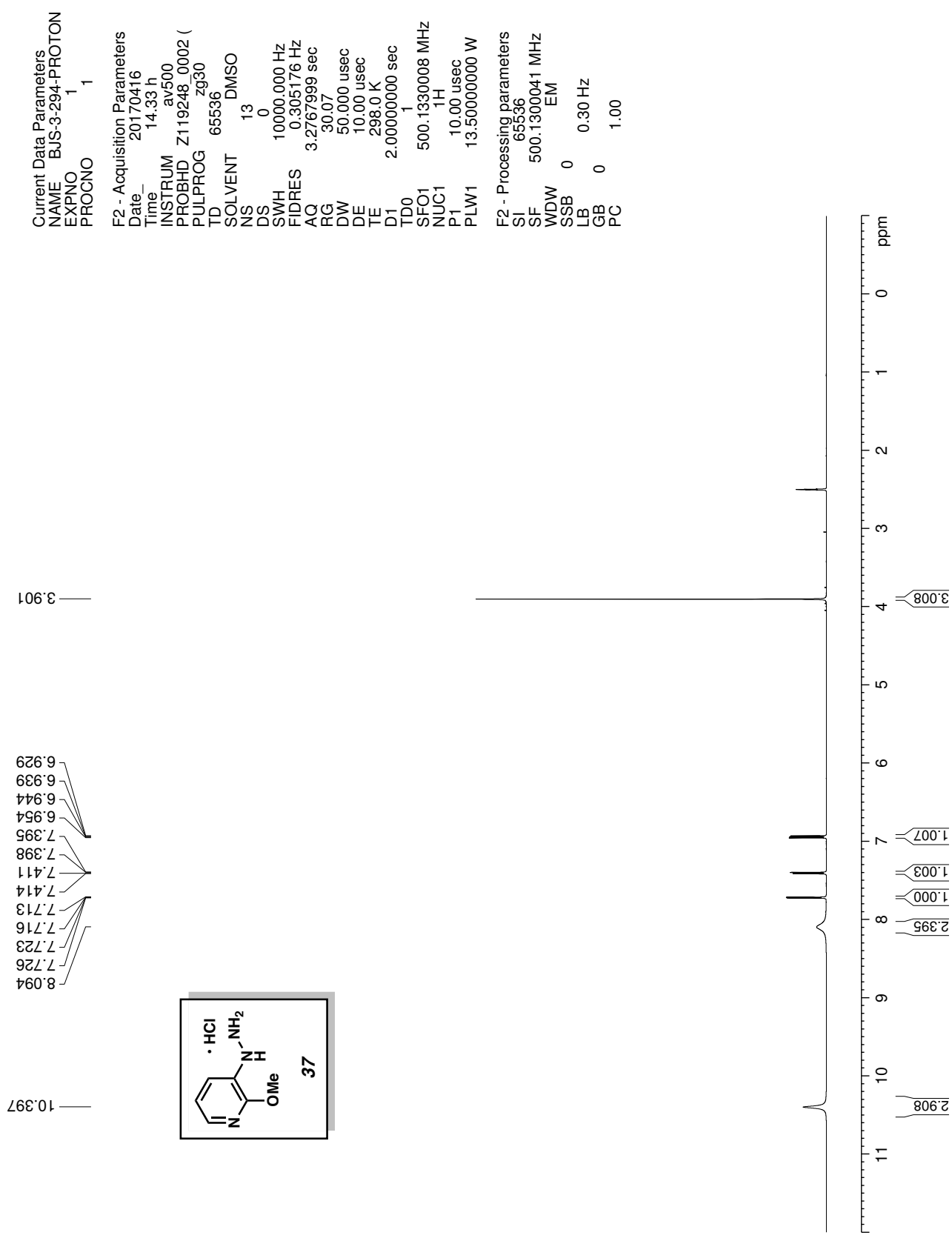
References

[1] Boal, B. W.; Schammel, A. W.; Garg, N. K. *Org. Lett.* **2009**, *11*, 3458–3461.

[2] Schammel, A. W.; Boal, B. W.; Zu, L.; Mesganaw, T.; Garg, N. K. *Tetrahedron* **2010**, *66*, 4687–4695.

[3] Moreno, J.; Picazo, E.; Morrill, L. A.; Smith, J. M.; Garg, N. K. *J. Am. Chem. Soc.* **2016**, *138*, 1162–1165.

^{1}H NMR Spectra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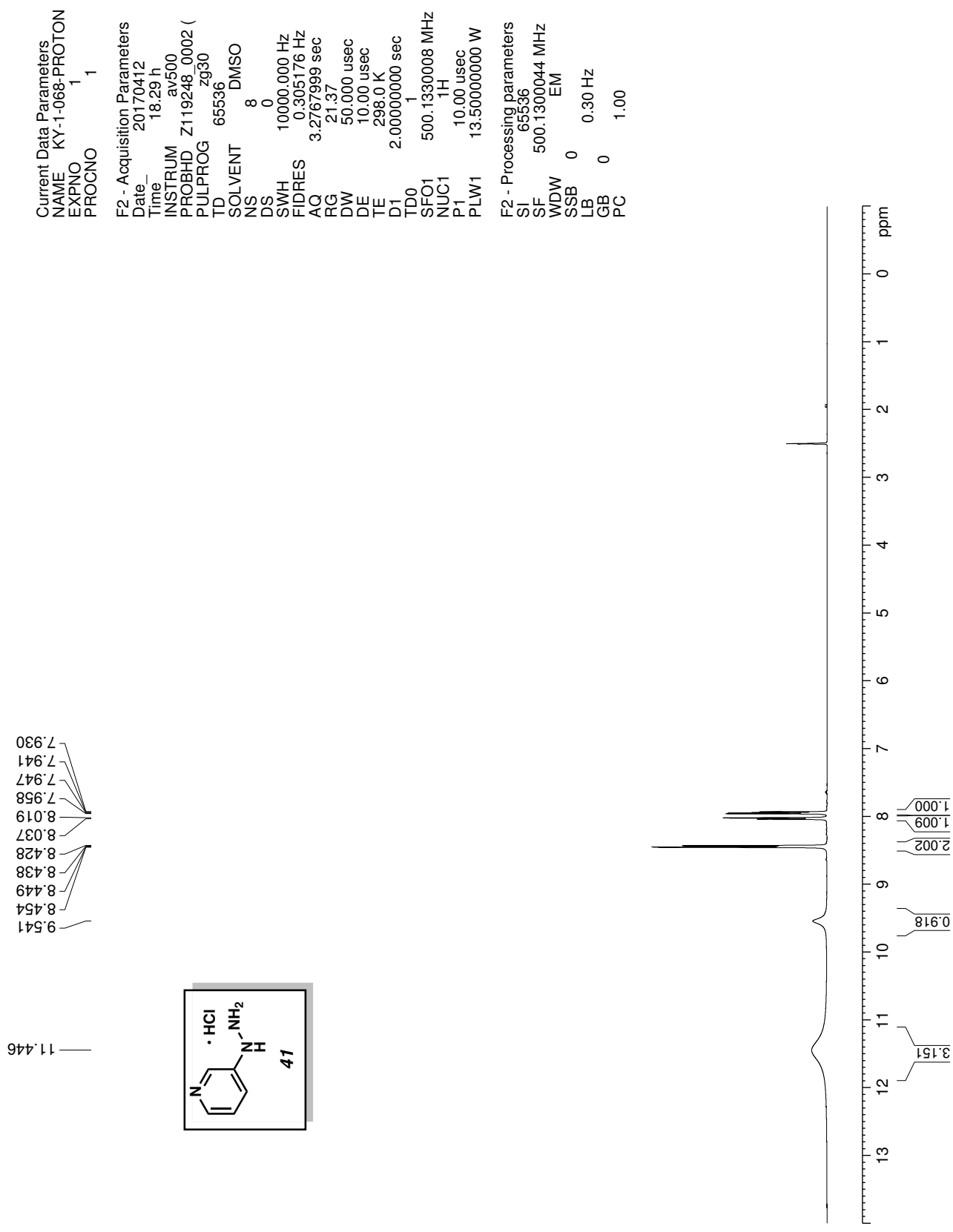
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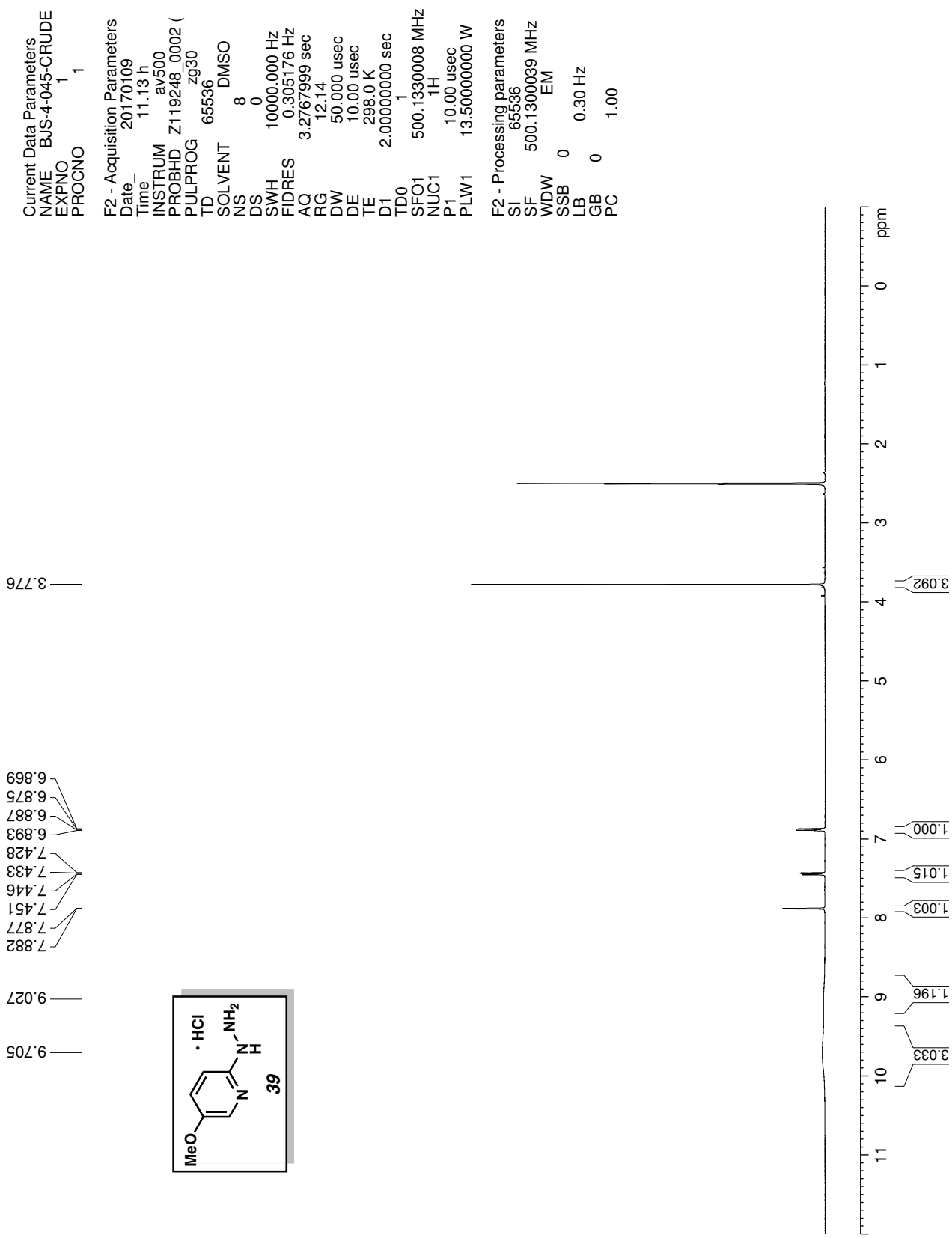
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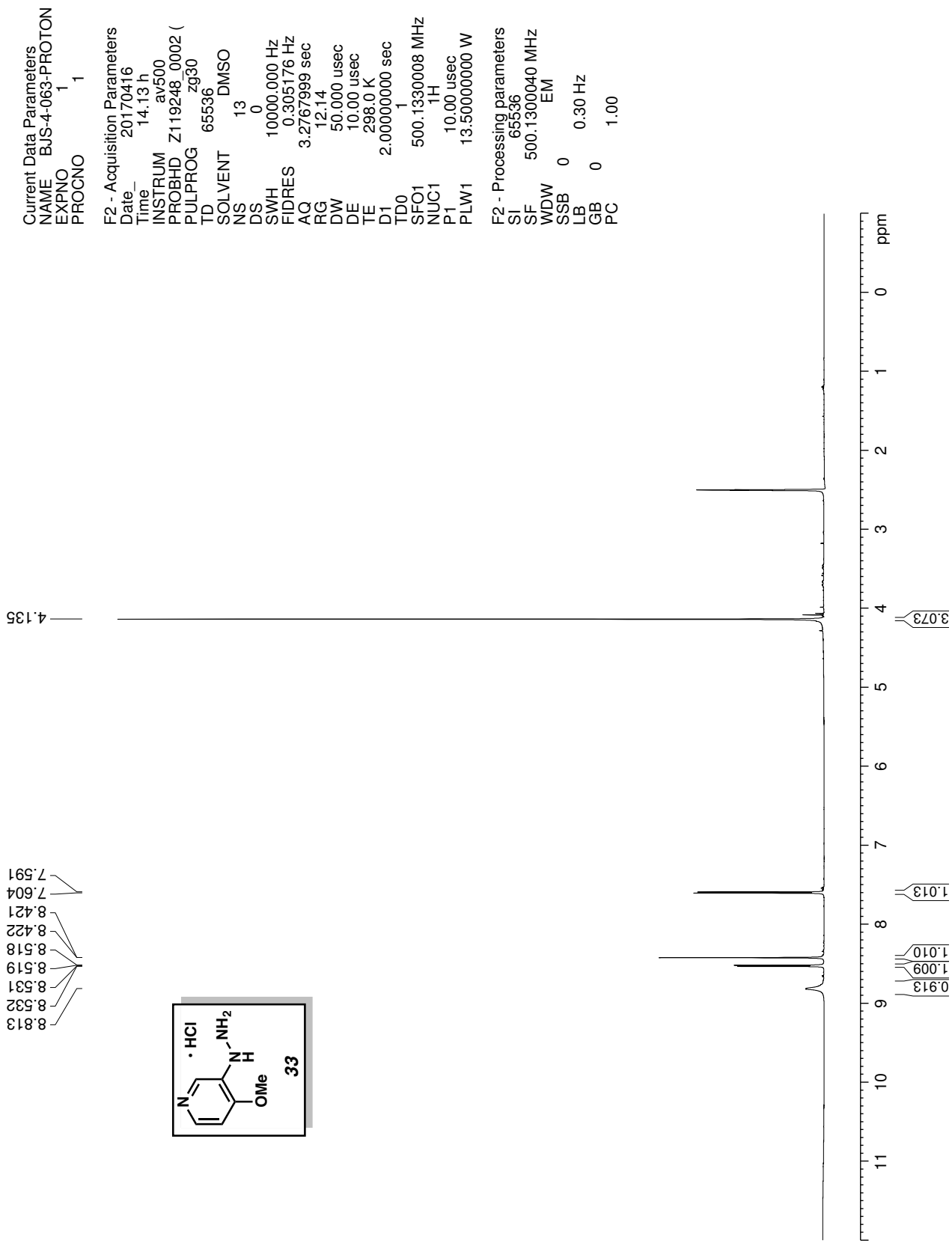
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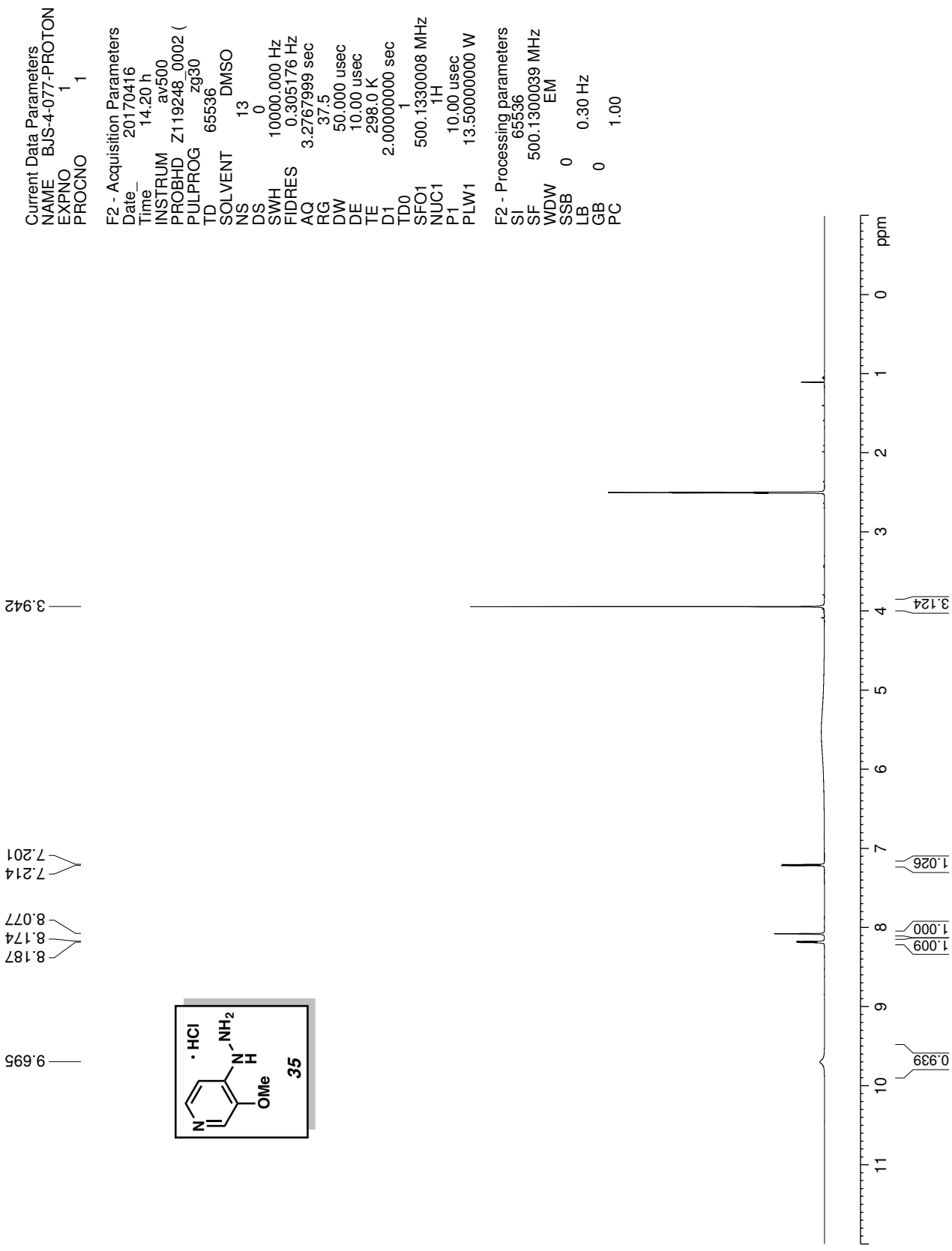
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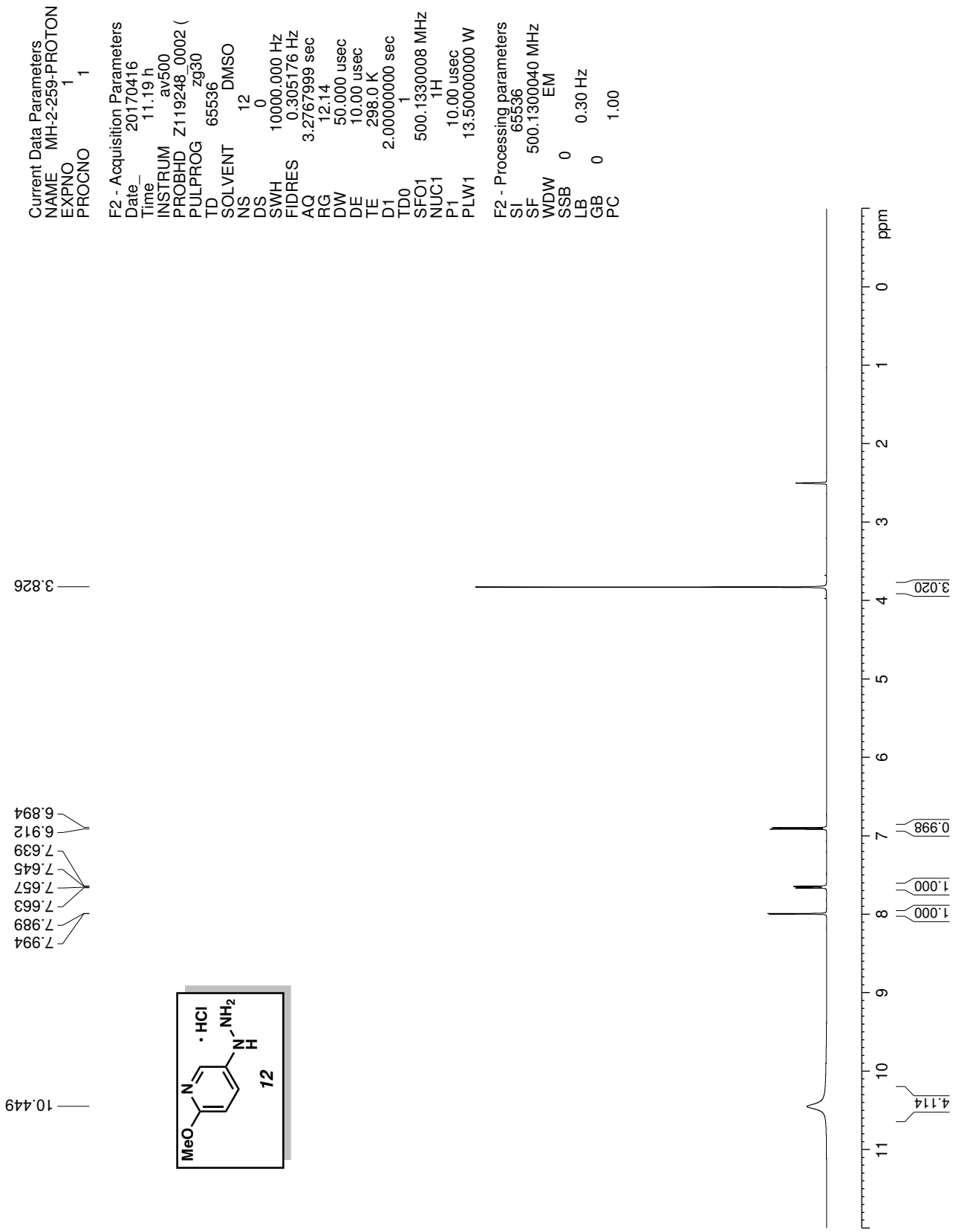
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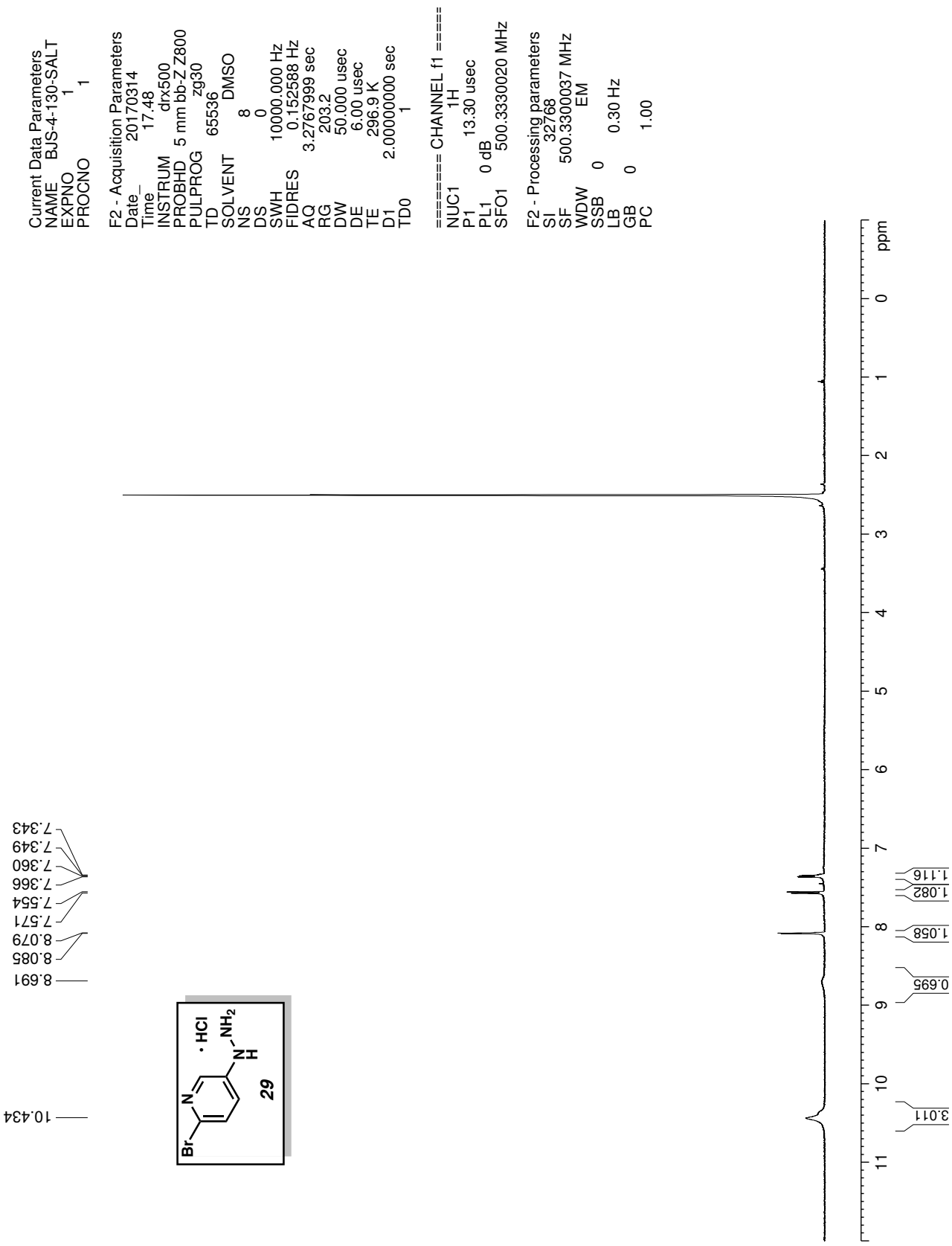
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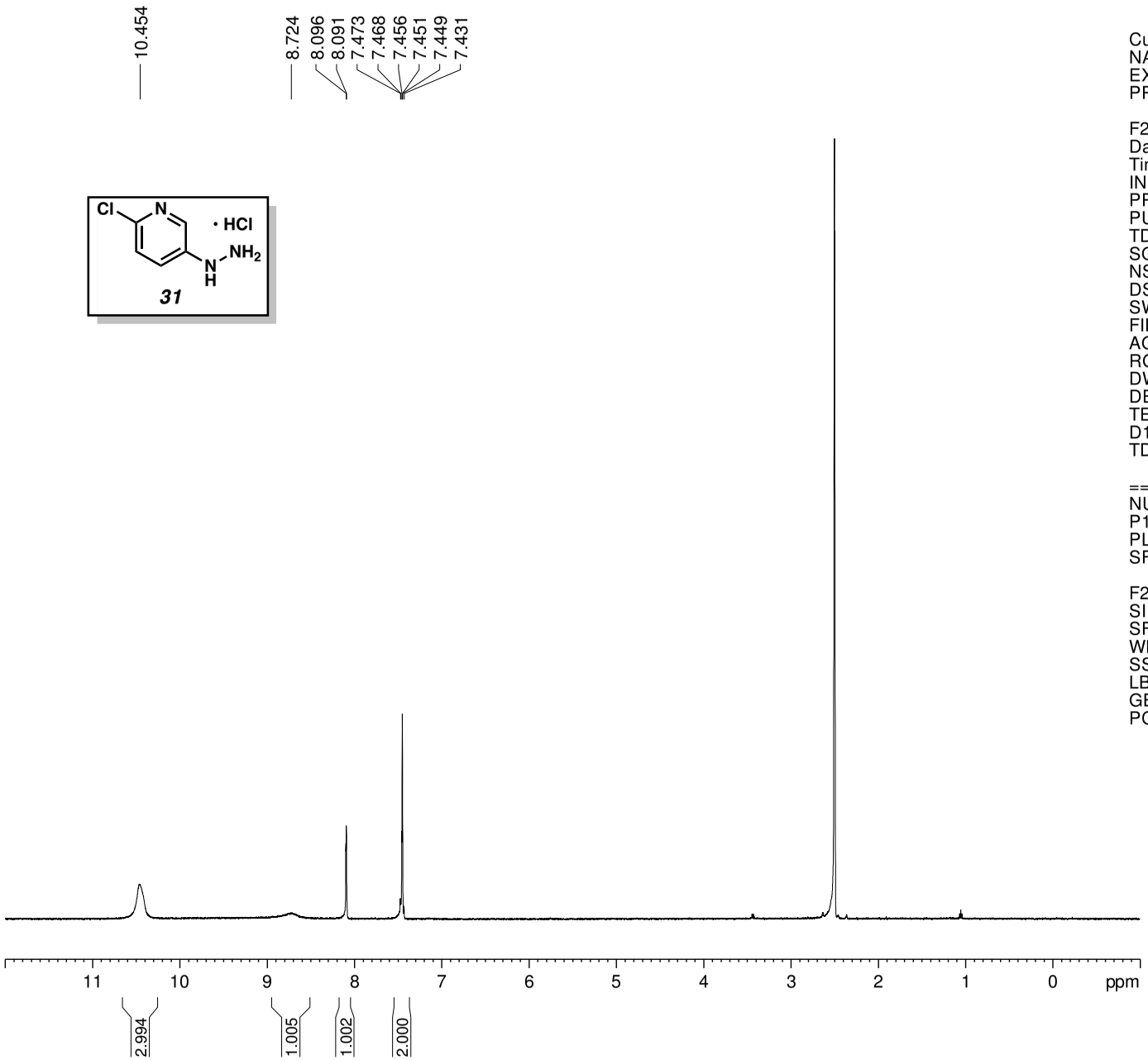
DW 50.000 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300037 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10.434
8.691
8.085
8.079
7.571
7.554
7.366
7.360
7.349
7.343
29
3.011
0.695
1.058
1.082
1.116
ppm

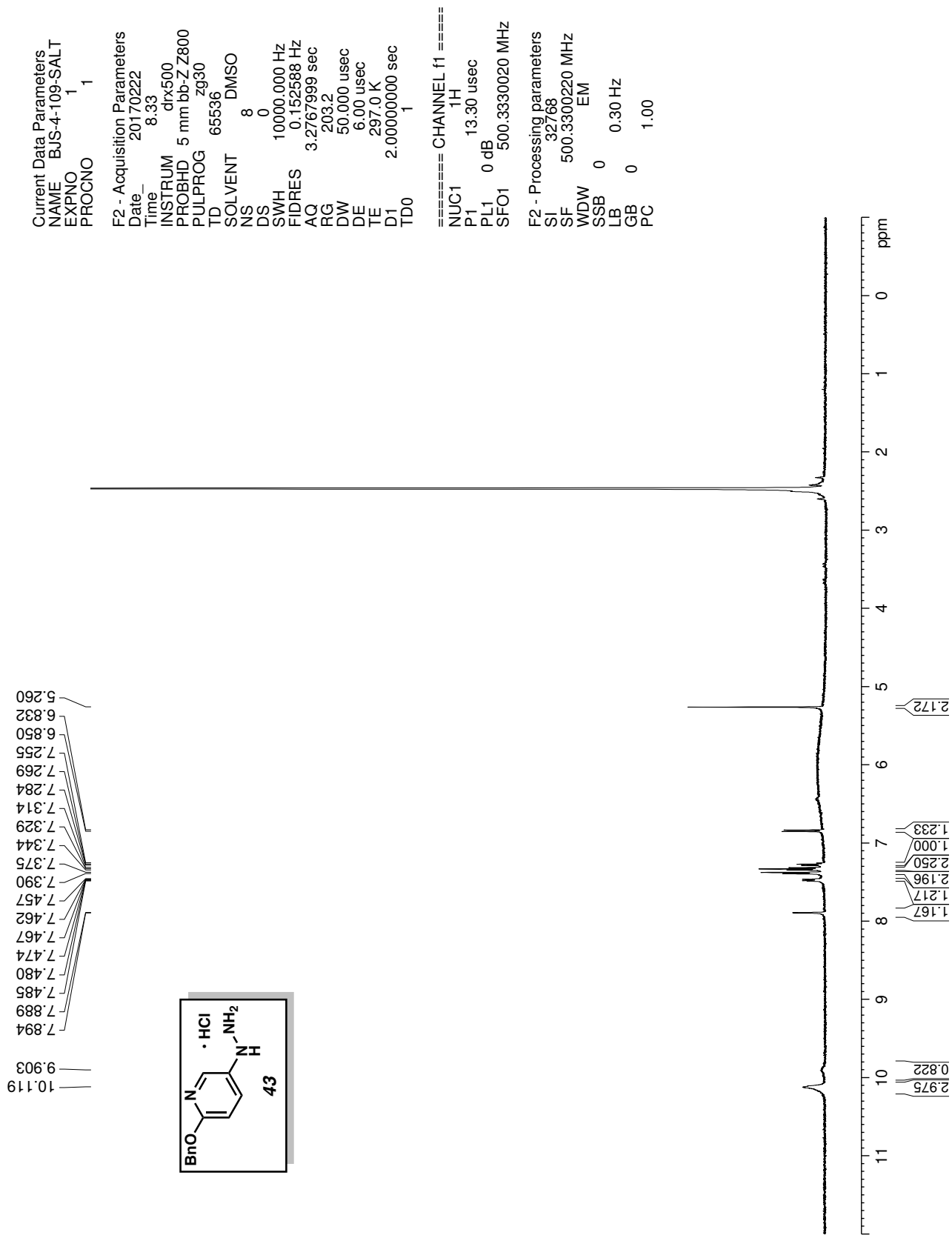


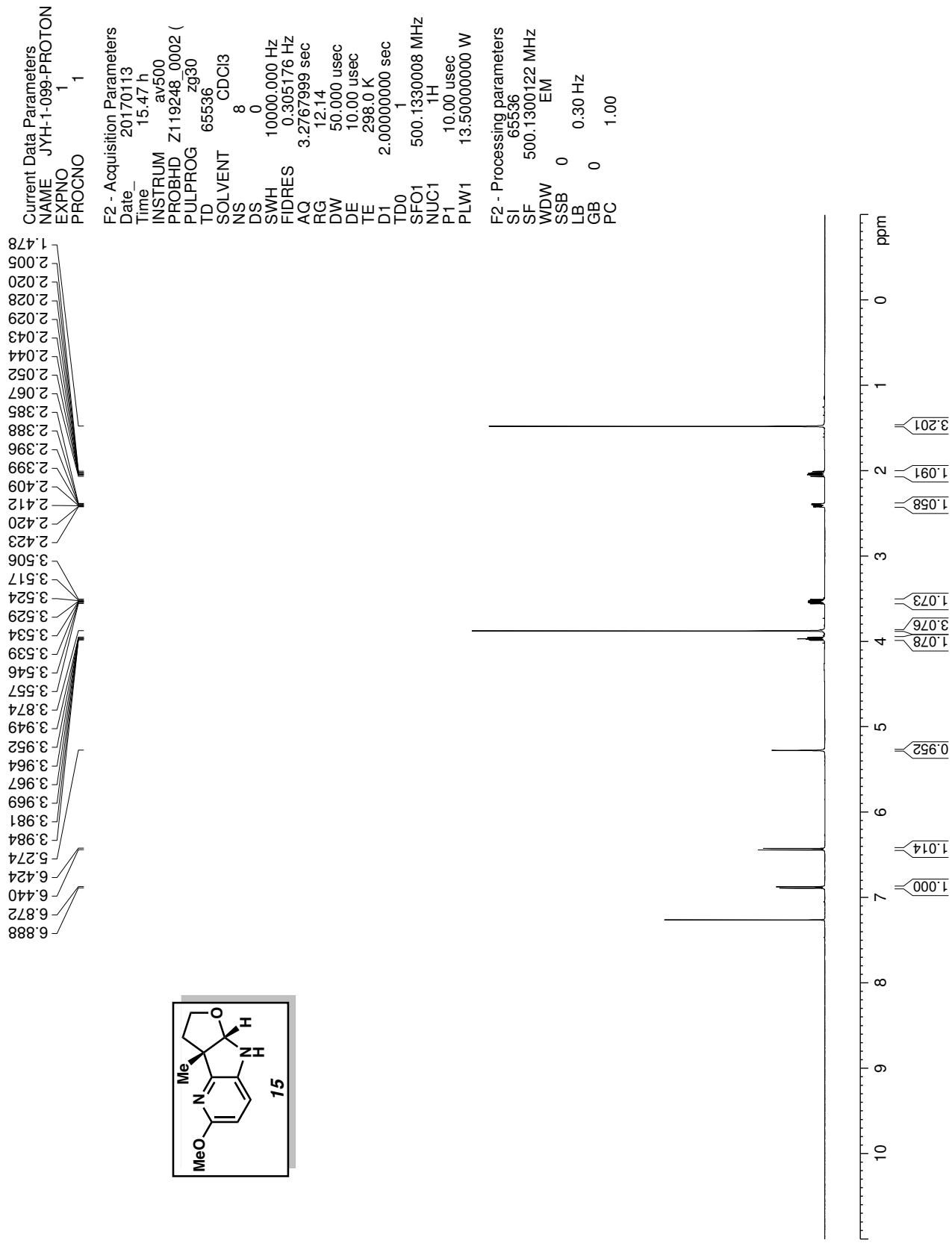
Current Data Parameters
NAME BJS-3-285-CRUDE
EXPNO 1
PROCNO 1

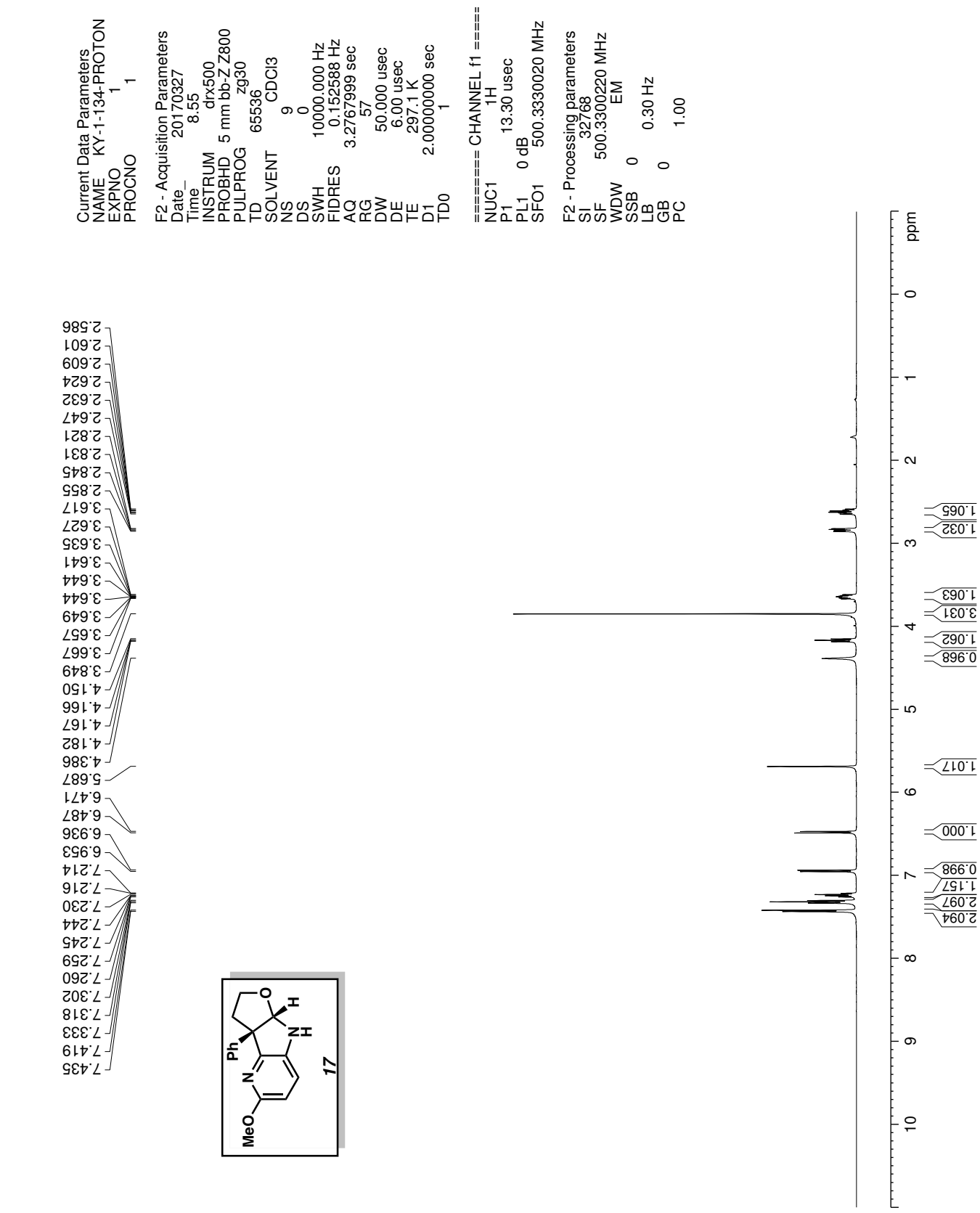
F2 - Acquisition Parameters
Date_ 20161109
Time 13.37
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
TD0 1

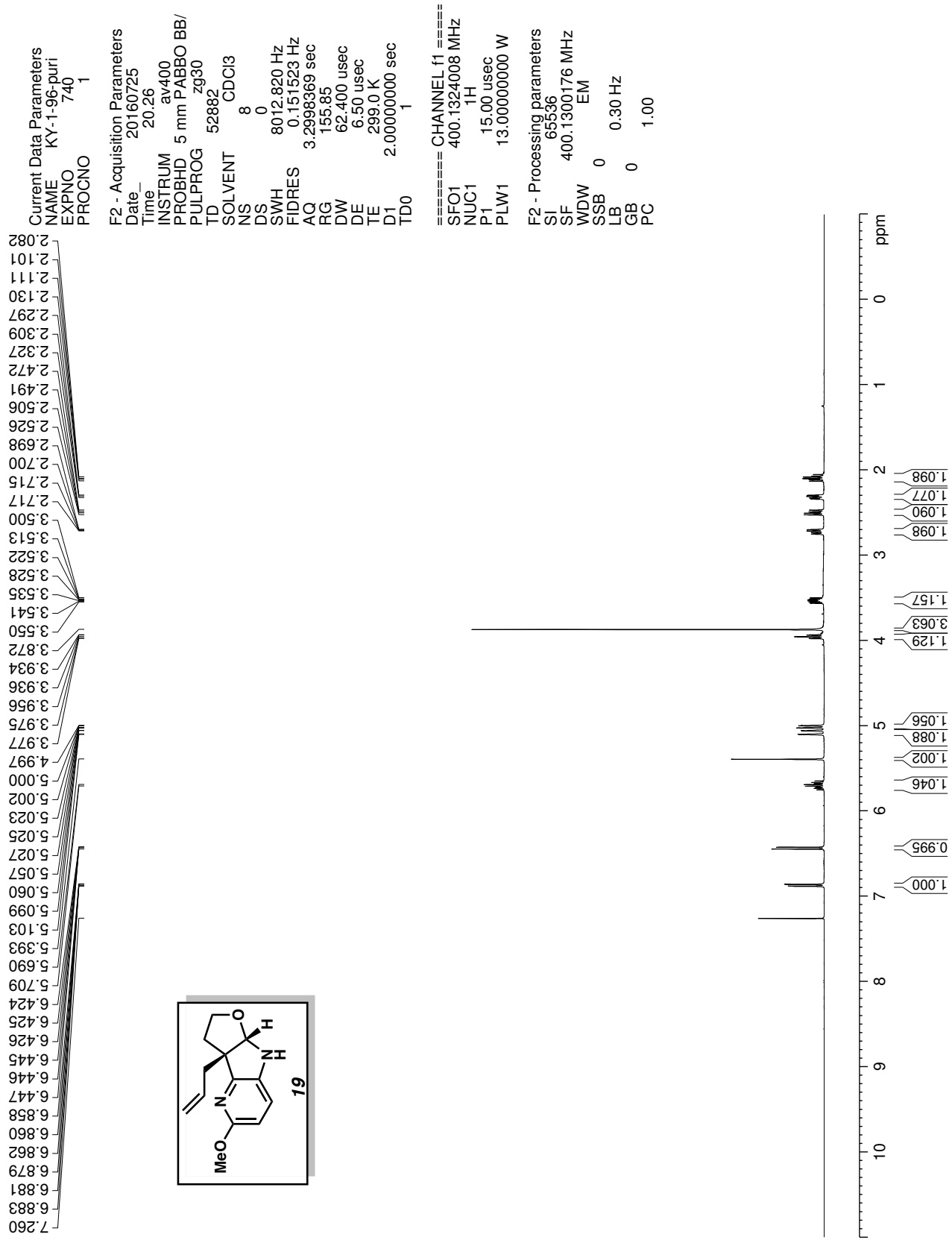
======== CHANNEL f1 =====
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz

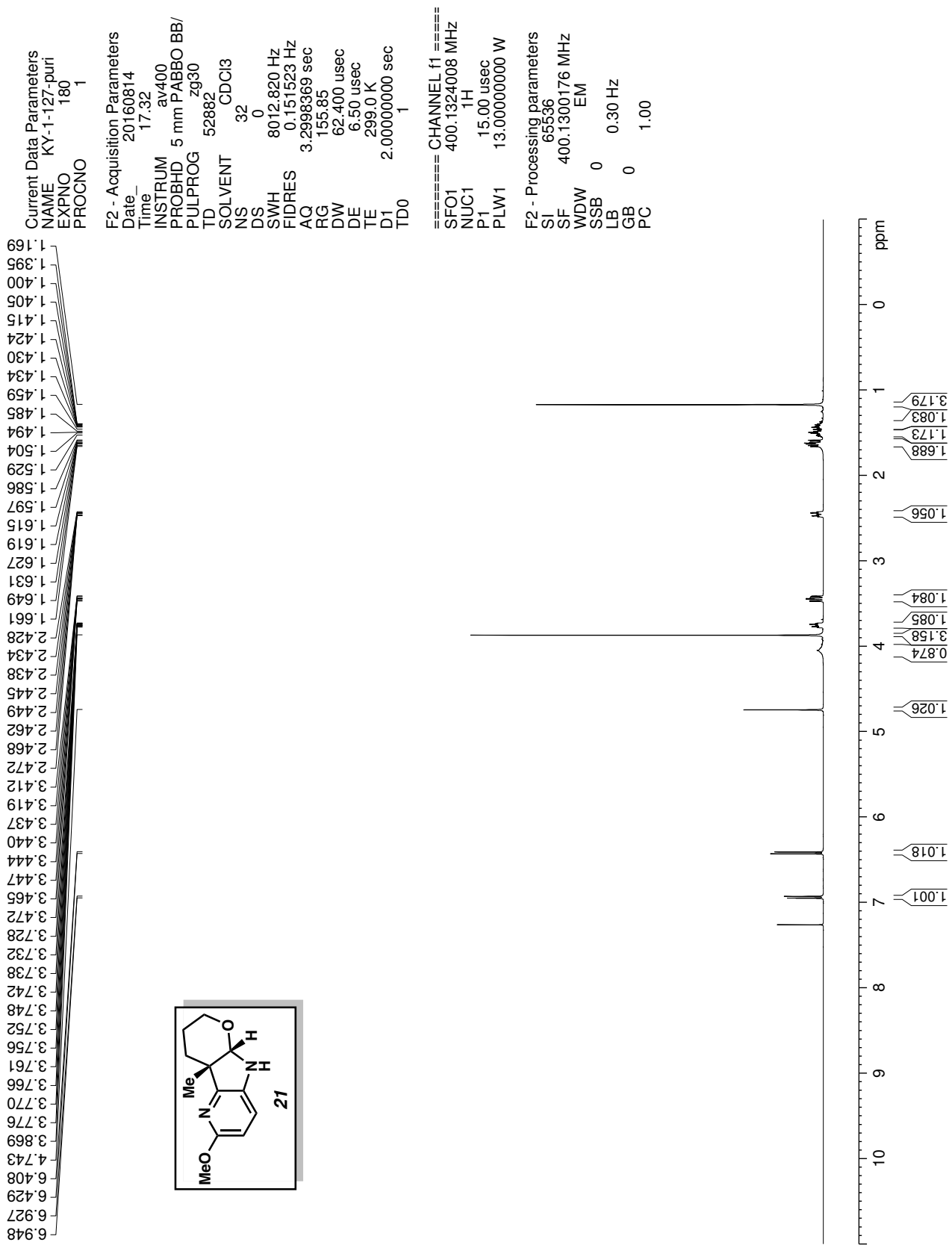
F2 - Processing parameters
SI 32768
SF 500.3300046 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

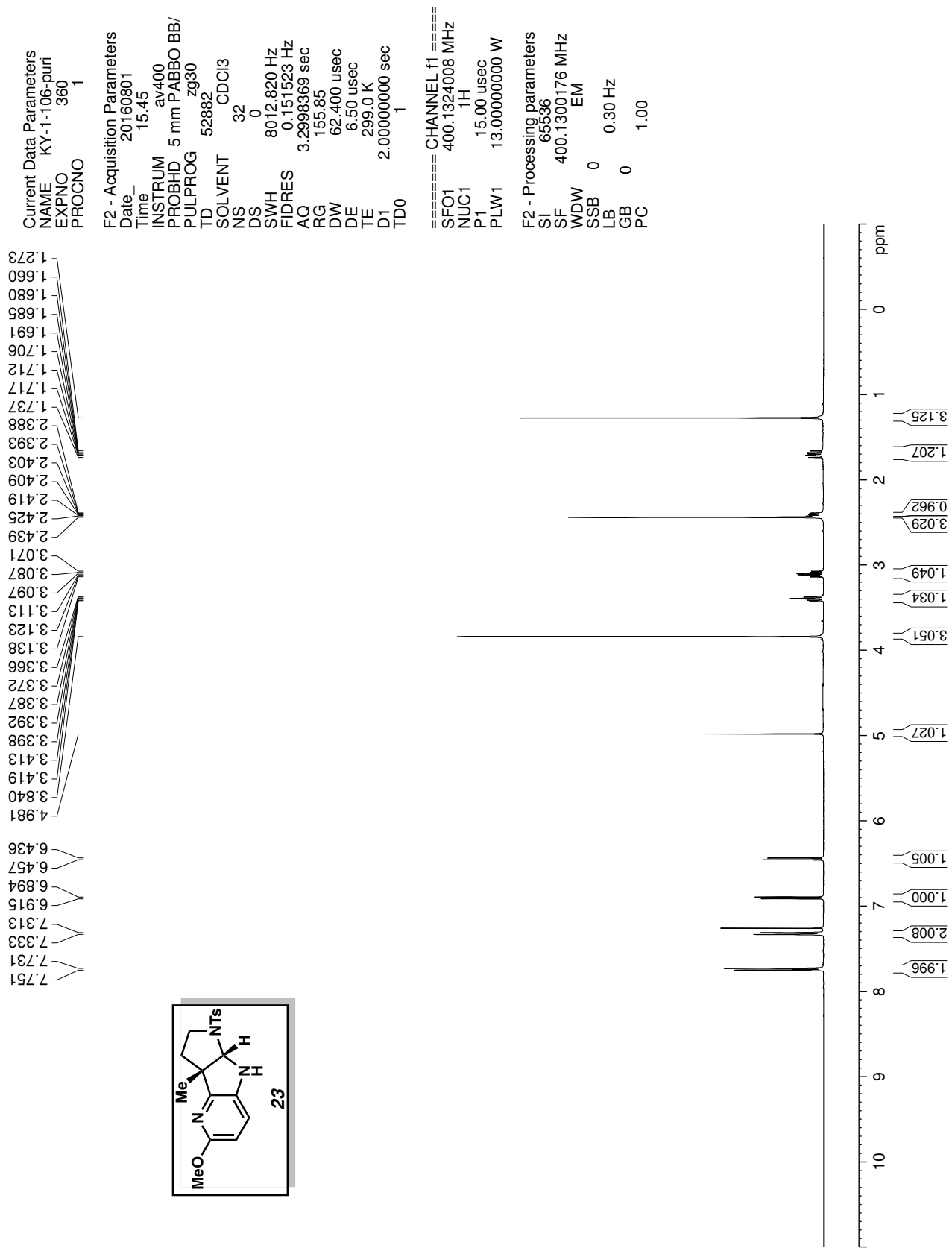

Current Data Parameters
NAME BJS-4-109-SALT
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170222
Time_ 8.33
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 203.2
DW 50.000 usec
DE 6.00 usec
TE 297.0 K
D1 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
10.119
9.903
7.894
7.889
7.485
7.480
7.474
7.467
7.462
7.457
7.390
7.375
7.344
7.329
7.314
7.284
7.269
7.255
6.850
6.832
5.260
BnO
HCl
NH2
43
2.975
0.822
1.167
1.217
2.196
2.250
1.000
1.233
2.172
ppm

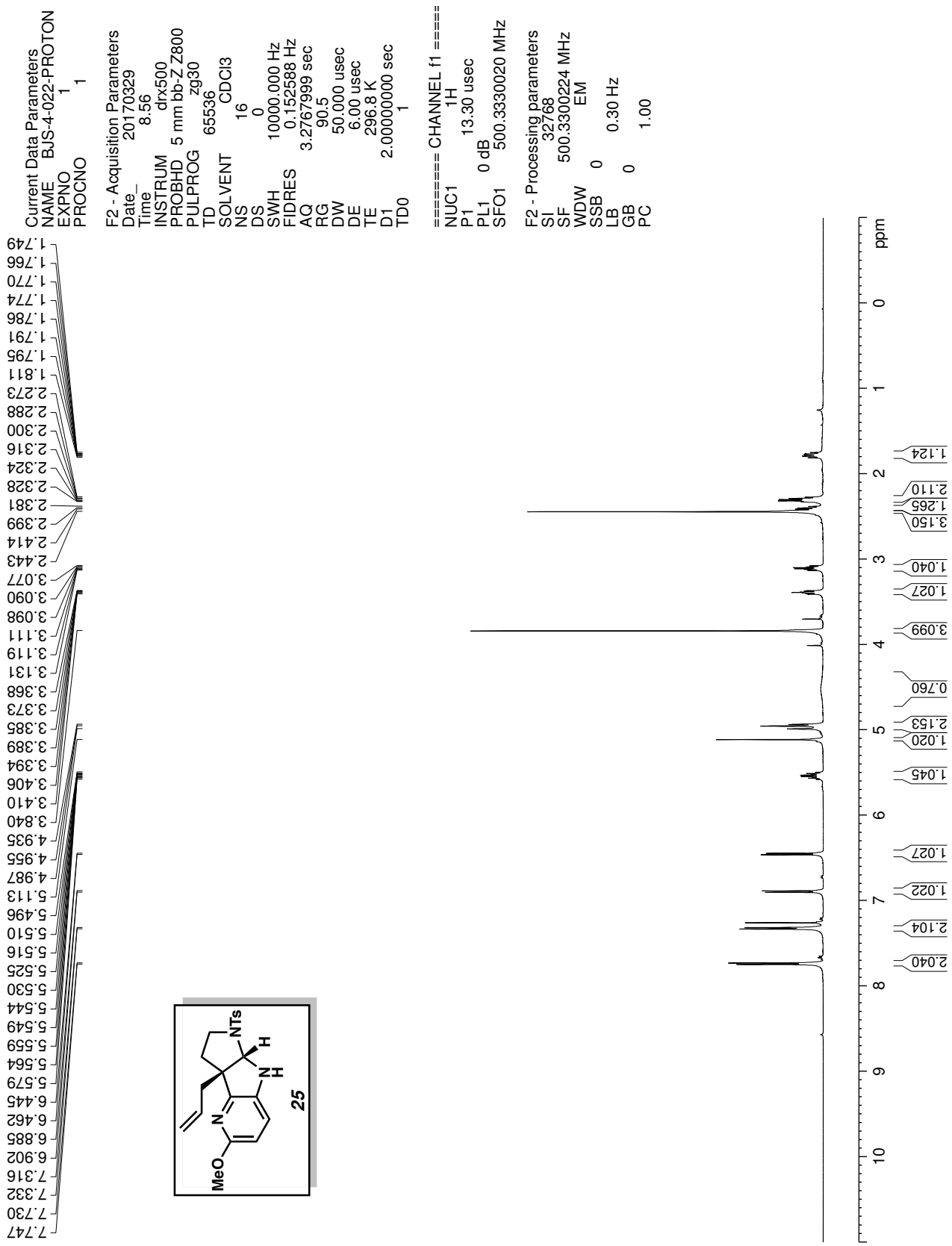

Current Data Parameters
NAME JYH-1-099-PROTON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170113
Time_ 15.47 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 12.14
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
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
1.478
2.005
2.020
2.028
2.029
2.043
2.044
2.052
2.067
2.385
2.388
2.396
2.399
2.409
2.412
2.420
2.423
3.506
3.517
3.524
3.529
3.534
3.539
3.546
3.557
3.874
3.949
3.952
3.964
3.967
3.969
3.981
3.984
5.274
6.424
6.440
6.872
6.888
Me
MeO
N
N
H
O
H
15
ppm
0
1
2
3
4
5
6
7
8
9
10
3.201
1.091
1.058
1.073
3.076
1.078
0.952
1.014
1.000

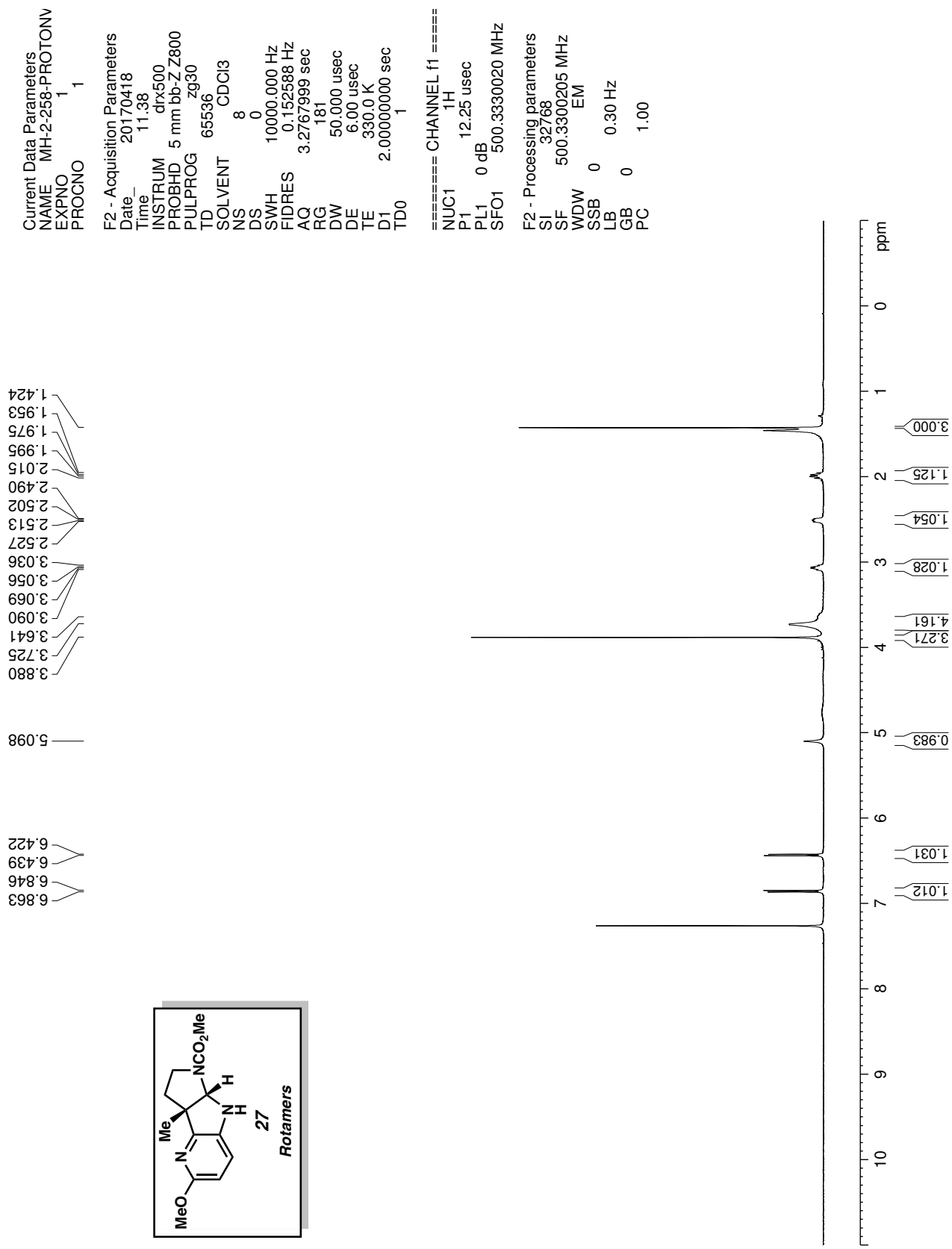

Current Data Parameters
NAME KY-1-134-PROTON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170327
Time_ 8.55
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 57
DW 50.000 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 =====
NUC1 1H
P1 13.30 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.435
7.419
7.333
7.318
7.302
7.260
7.259
7.245
7.244
7.230
7.216
7.214
6.953
6.936
6.487
6.471
5.687
4.386
4.182
4.167
4.166
4.150
3.849
3.667
3.657
3.649
3.644
3.644
3.641
3.635
3.627
3.617
2.855
2.845
2.831
2.821
2.647
2.632
2.624
2.609
2.601
2.586
MeO
Ph
17
2.094
2.097
1.157
0.998
1.000
1.017
0.968
1.062
3.031
1.063
1.032
1.065
ppm

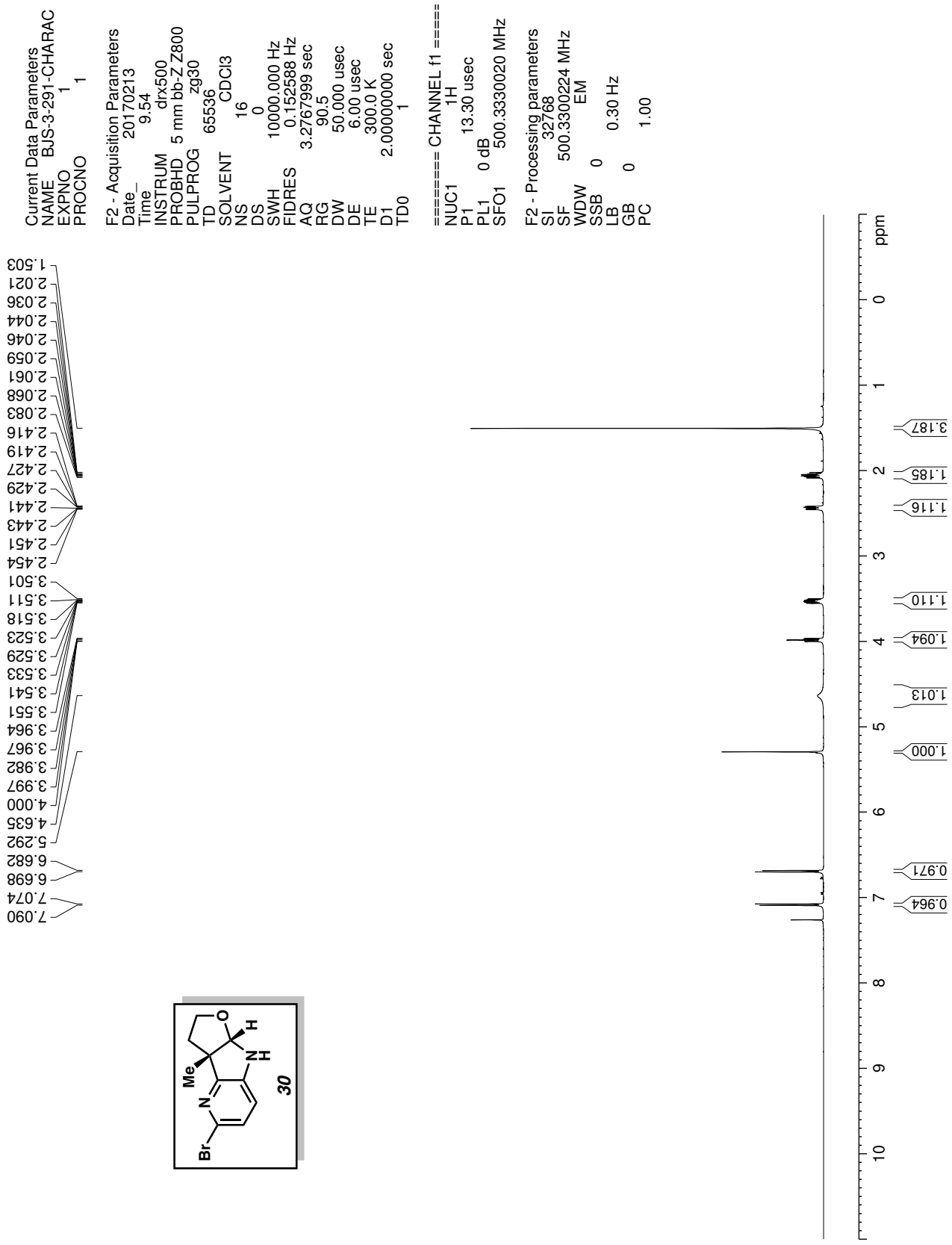

Current Data Parameters
NAME KY-1-96-puri
EXPNO 740
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160725
Time_ 20.26
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 155.85
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300176 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
19
ppm
1.098
1.077
1.090
1.098
1.157
3.063
1.129
1.056
1.088
1.002
1.046
0.995
1.000

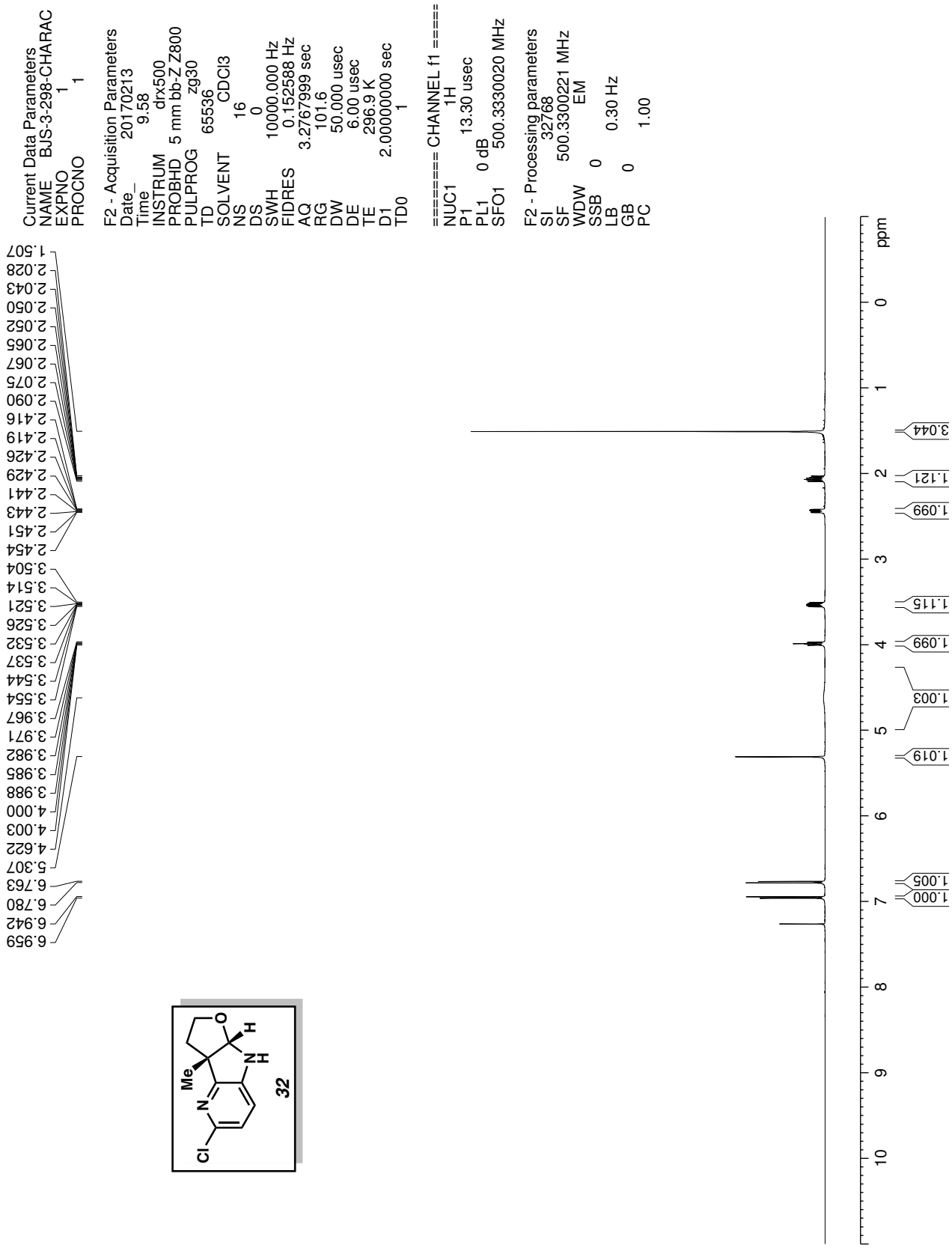

Current Data Parameters
NAME KY-1-127-puri
EXPNO 180 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160814
Time_ 17.32
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CDCl3
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 155.85
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300176 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
MeO
N
NH
O
21
ppm
3.179
1.083
1.173
1.688
1.056
1.084
1.085
3.158
0.874
1.026
1.018
1.001

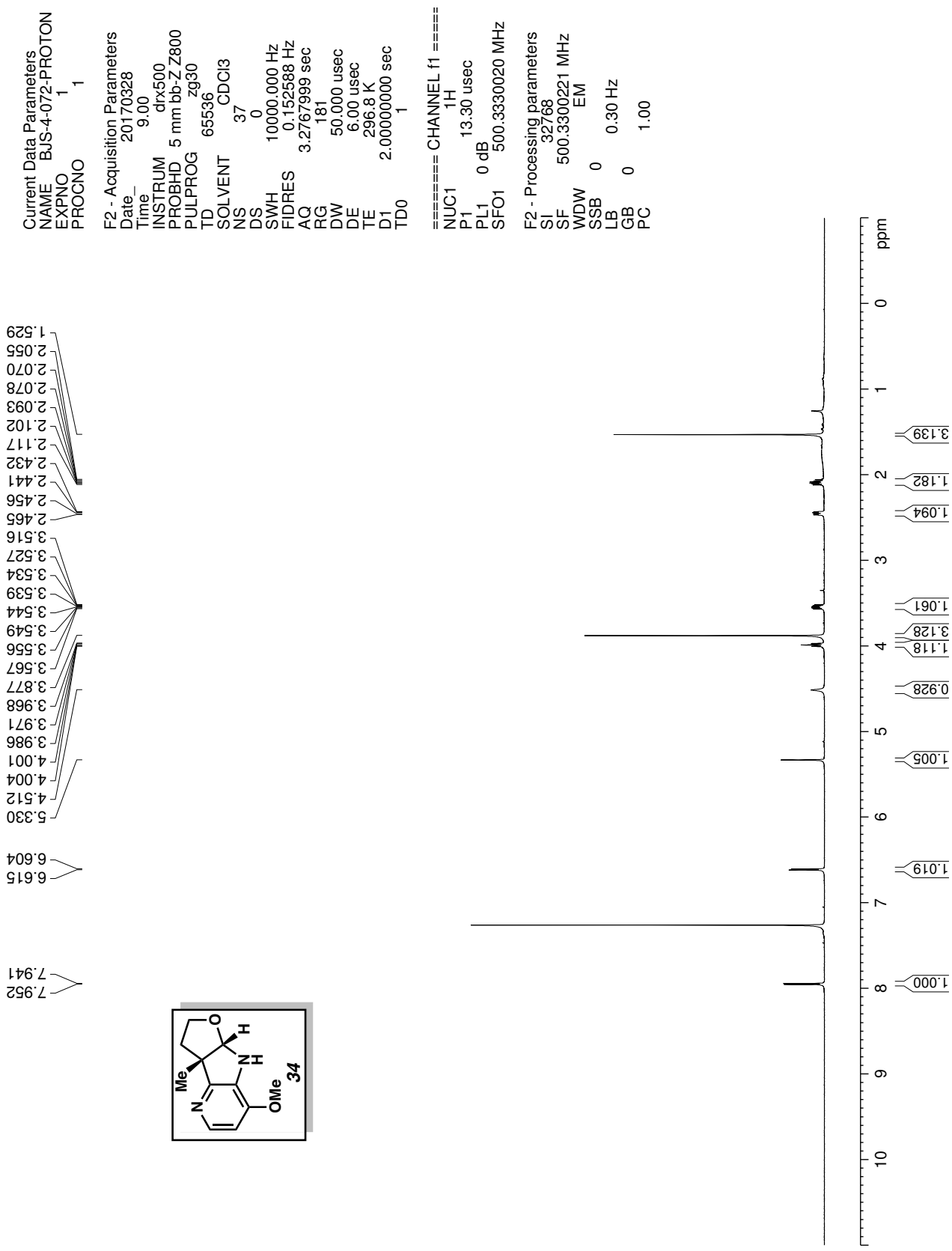

Current Data Parameters
NAME KY-1-106-puri
EXPNO 360
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160801
Time 15.45
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CDCl3
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 155.85
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300176 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.751
7.731
7.333
7.313
6.915
6.894
6.457
6.436
4.981
3.840
3.419
3.413
3.398
3.392
3.387
3.372
3.366
3.138
3.123
3.113
3.097
3.087
3.071
2.439
2.425
2.419
2.409
2.403
2.393
2.388
1.737
1.717
1.712
1.706
1.691
1.685
1.680
1.660
1.273
Me
NTs
H
N
H
N
MeO
23
ppm
0
1
2
3
4
5
6
7
8
9
10
3.125
1.207
3.029
0.962
1.049
1.034
3.051
1.027
1.005
1.000
2.008
1.996

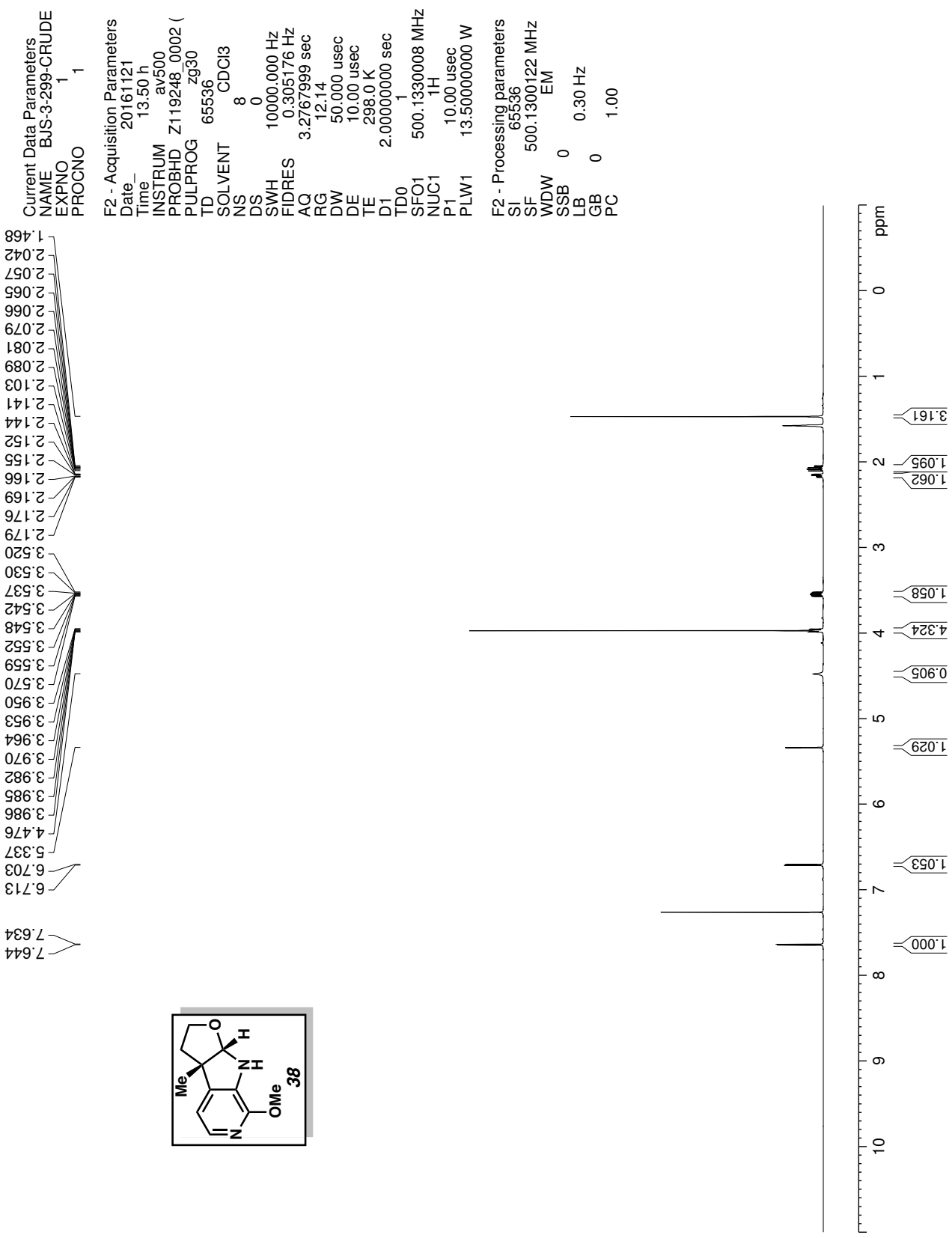

Current Data Parameters
NAME BJS-4-022-PROTON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170329
Time_ 8.56
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 6.00 usec
TE 296.8 K
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 500.3300224 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
NTs
H
N
H
25
ppm

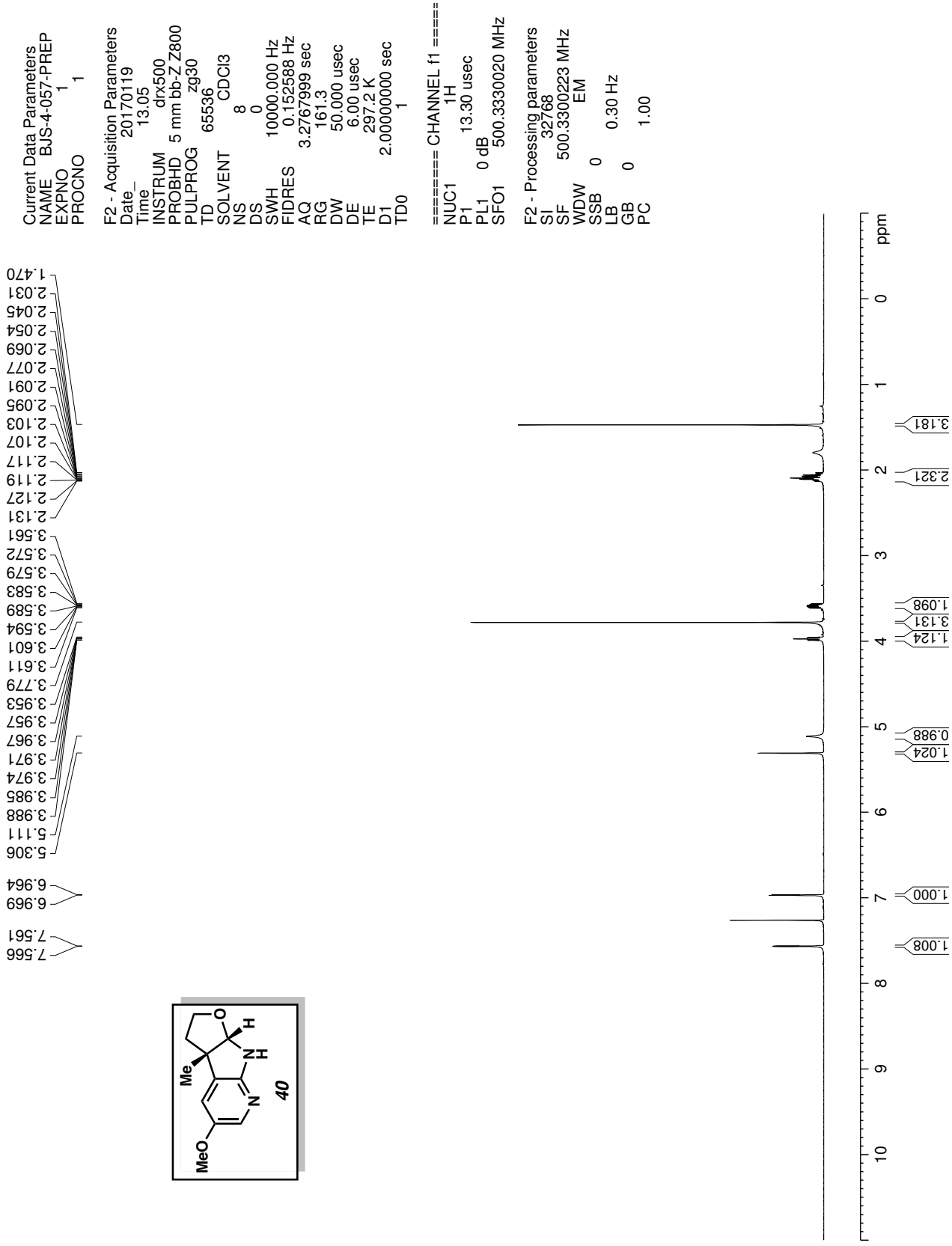

Current Data Parameters
NAME MH-2-258-PROTONv
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170418
Time_ 11.38
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 6.00 usec
TE 330.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 =====
NUC1 1H
P1 12.25 usec
PL1 0 dB
SFO1 500.3330020 MHz
F2 - Processing parameters
SI 32768
SF 500.3300205 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.424
1.953
1.975
1.995
2.015
2.490
2.502
2.513
2.527
3.036
3.056
3.069
3.090
3.641
3.725
3.880
5.098
6.422
6.439
6.846
6.863
3.000
1.125
1.054
1.028
4.161
3.271
0.983
1.031
1.012
ppm
MeO
N
Me
NCO2Me
H
N
H
27
Rotamers

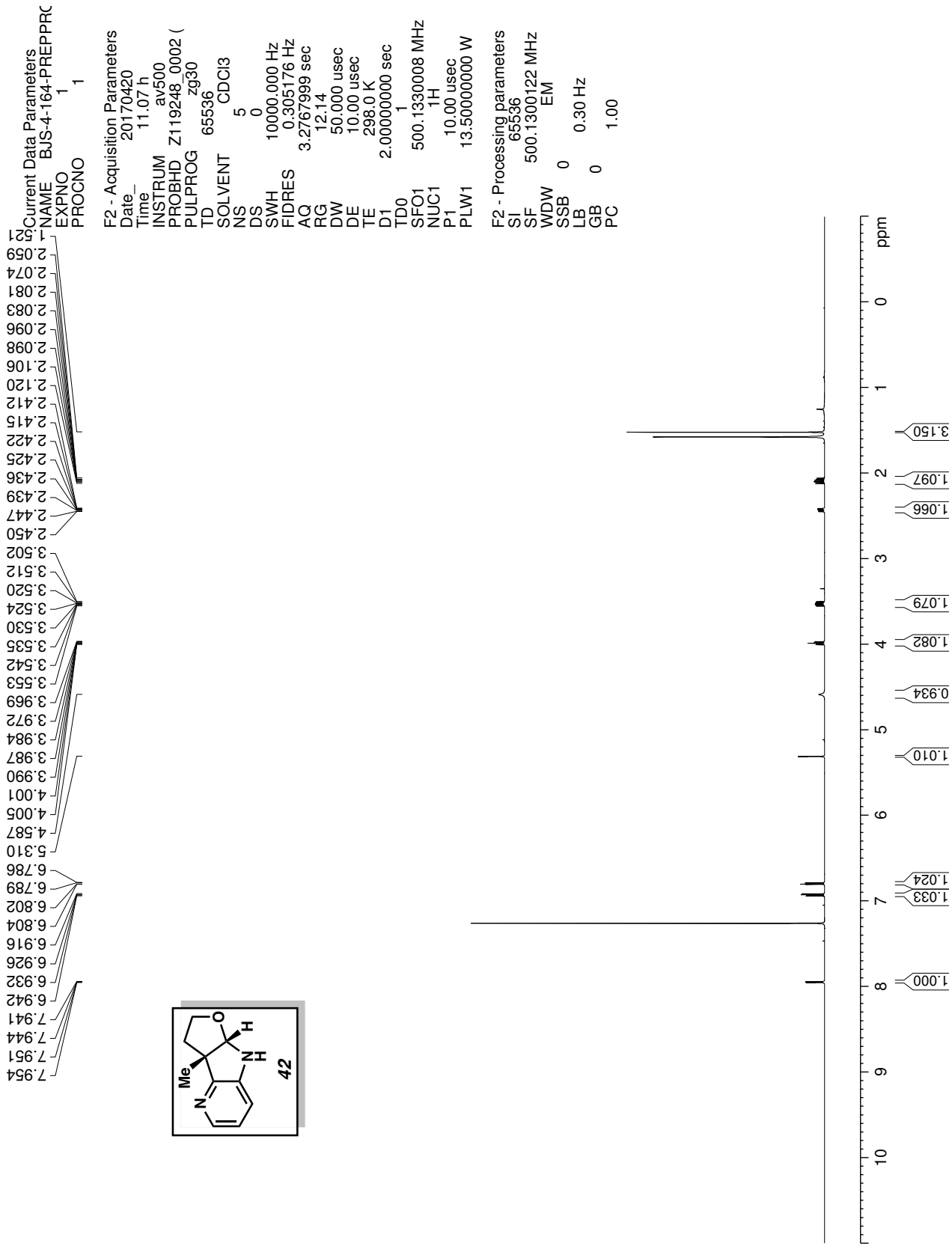

Current Data Parameters
NAME BJS-3-291-CHARAC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170213
Time_ 9.54
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 6.00 usec
TE 300.0 K
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 500.3300224 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.503
2.021
2.036
2.044
2.046
2.059
2.061
2.068
2.083
2.416
2.419
2.427
2.429
2.441
2.443
2.451
2.454
3.501
3.511
3.518
3.523
3.529
3.533
3.541
3.551
3.964
3.967
3.982
3.997
4.000
4.635
5.292
6.682
6.698
7.074
7.090
Me
N
Br
H
N
O
H
30
ppm
0
1
2
3
4
5
6
7
8
9
10
3.187
1.185
1.116
1.110
1.094
1.013
1.000
0.971
0.964

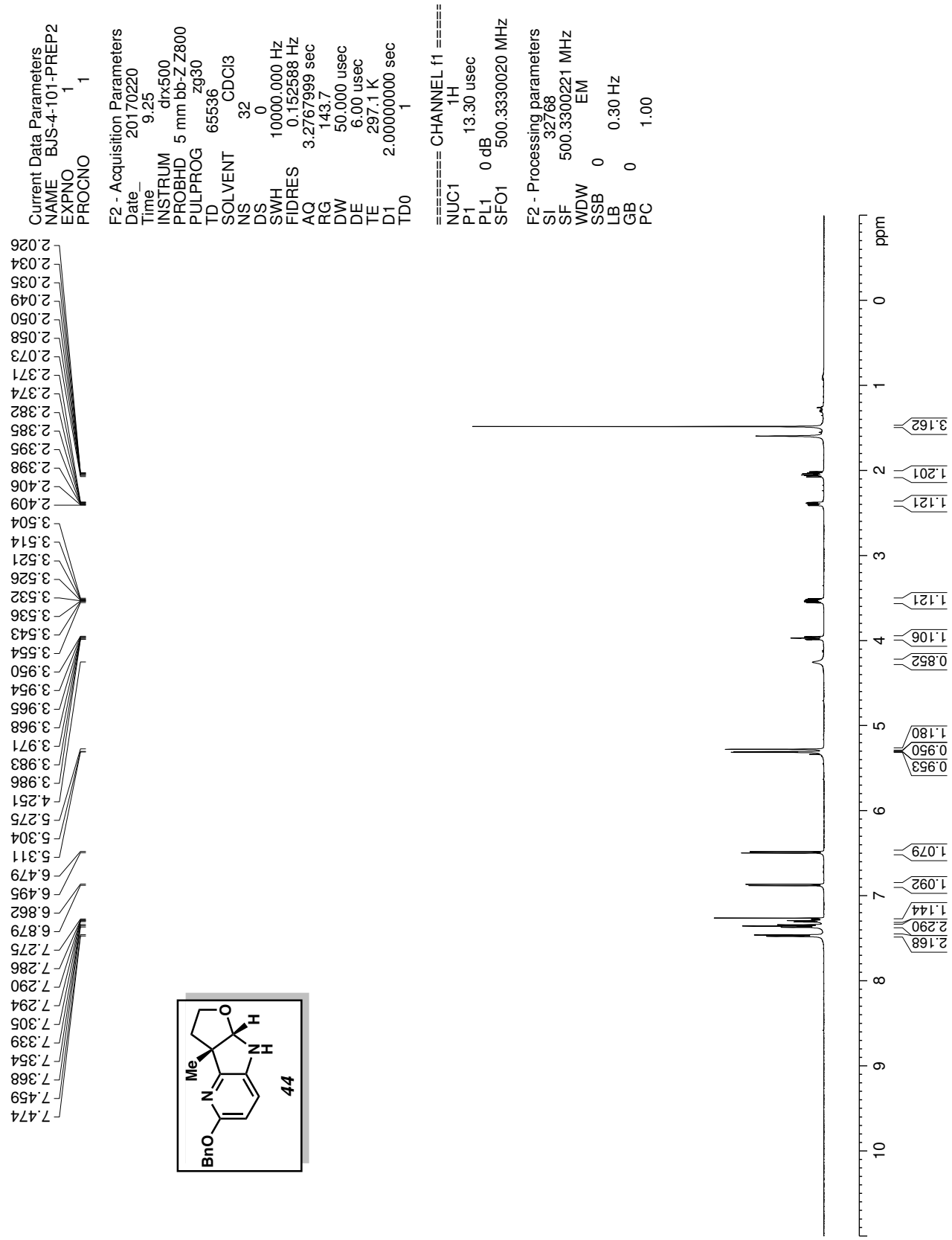

Current Data Parameters
NAME BJS-3-298-CHARAC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170213
Time_ 9.58
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 101.6
DW 50.000 usec
DE 6.00 usec
TE 296.9 K
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 500.3300221 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.507
2.028
2.043
2.050
2.052
2.065
2.067
2.075
2.090
2.416
2.419
2.426
2.429
2.441
2.443
2.451
2.454
3.504
3.514
3.521
3.526
3.532
3.537
3.544
3.554
3.967
3.971
3.982
3.985
3.988
4.000
4.003
4.622
5.307
6.763
6.780
6.942
6.959
Me
N
Cl
H
N
O
H
32
ppm
3.044
1.121
1.099
1.115
1.099
1.003
1.019
1.005
1.000

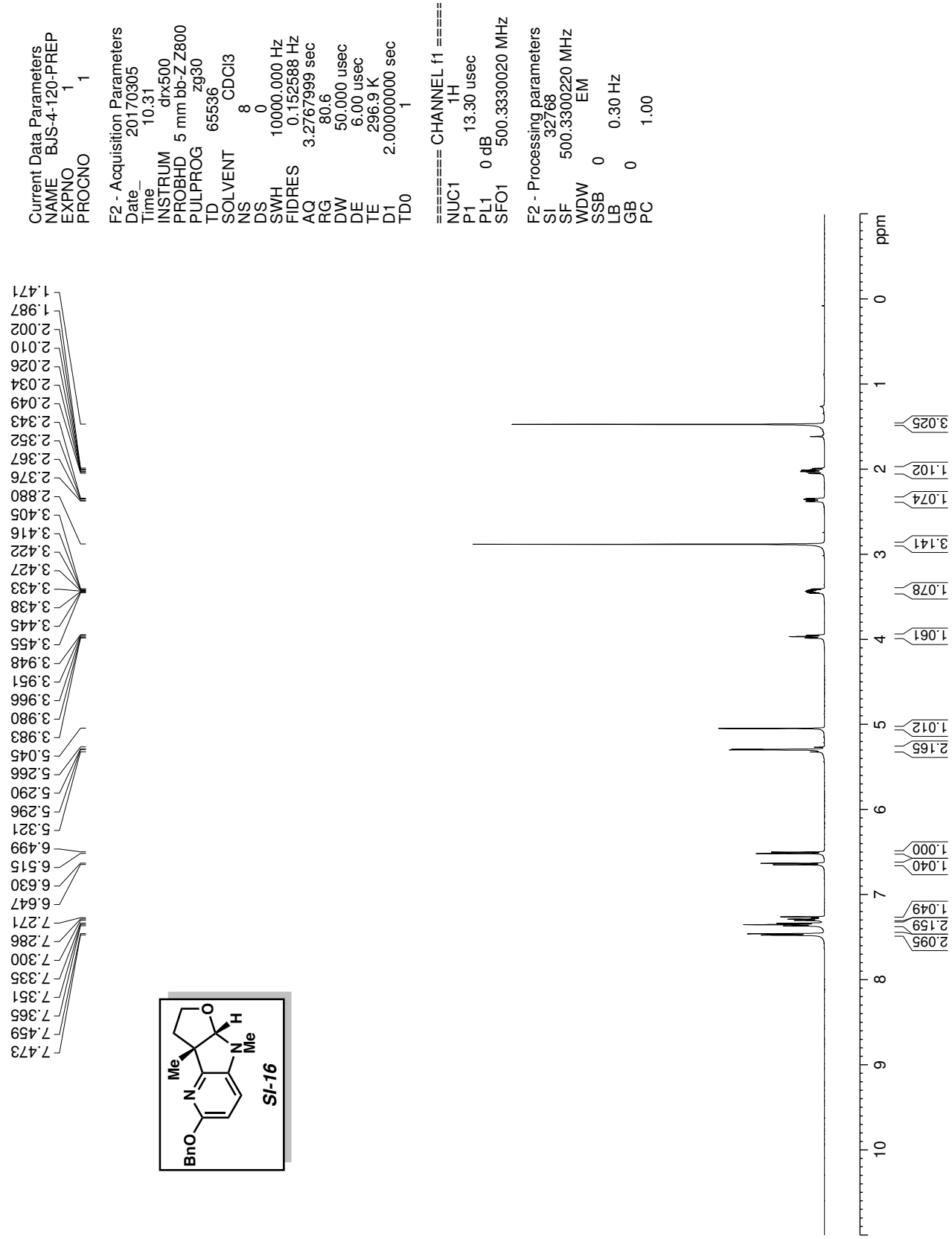

Current Data Parameters
NAME BJS-4-072-PROTON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170328
Time_ 9.00
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 37
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 6.00 usec
TE 296.8 K
D1 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 500.3300221 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.952
7.941
6.615
6.604
5.330
4.512
4.004
4.001
3.986
3.971
3.968
3.877
3.567
3.556
3.549
3.544
3.539
3.534
3.527
3.516
2.465
2.456
2.441
2.432
2.117
2.102
2.093
2.078
2.070
2.055
1.529
Me
OMe
34
1.000
1.019
1.005
0.928
1.118
3.128
1.061
1.094
1.182
3.139
ppm

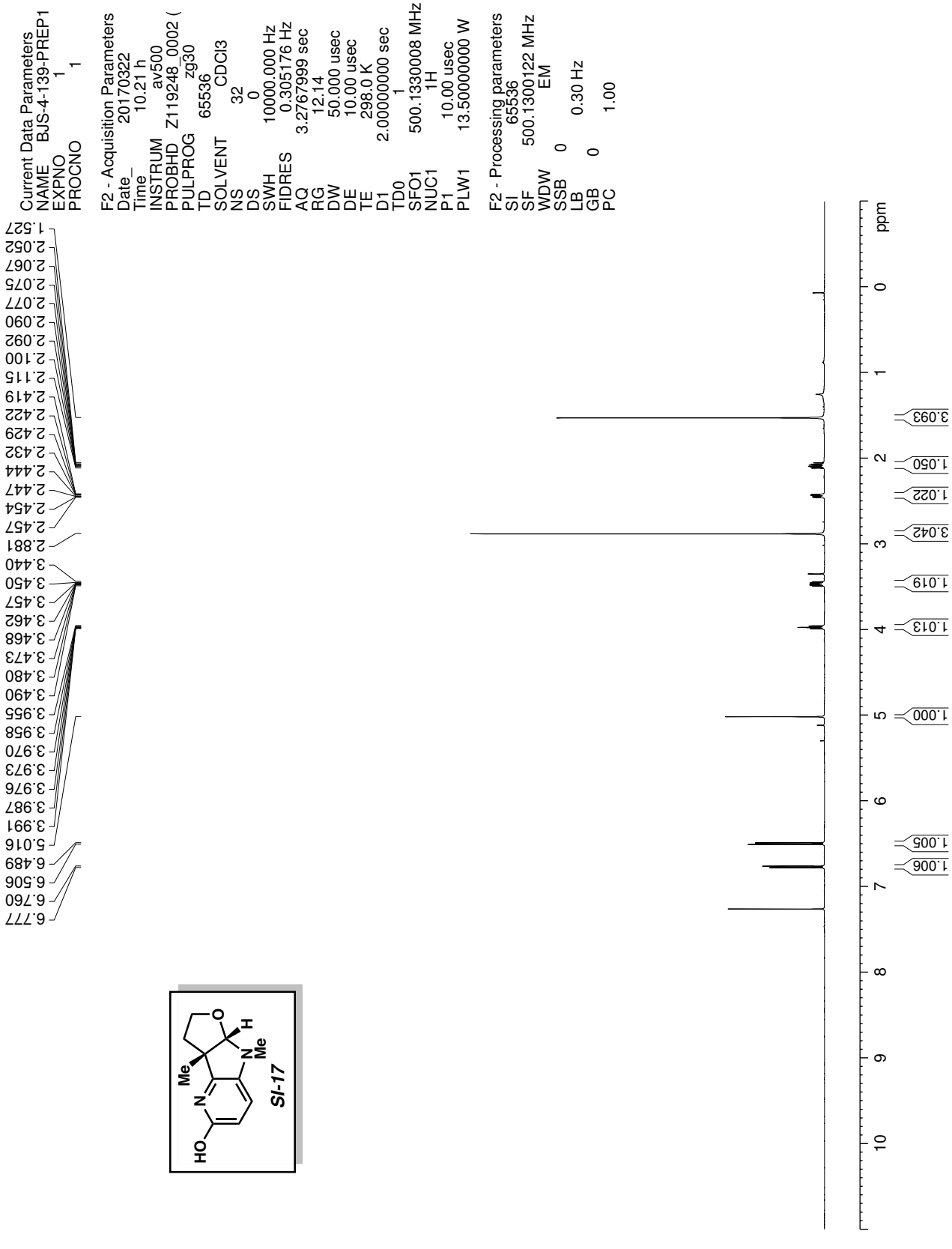

Current Data Parameters
NAME BJS-3-299-CRUDE
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161121
Time_ 13.50 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 12.14
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
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
1.468
2.042
2.057
2.065
2.066
2.079
2.081
2.089
2.103
2.141
2.144
2.152
2.155
2.166
2.169
2.176
2.179
3.520
3.530
3.537
3.542
3.548
3.552
3.559
3.570
3.950
3.953
3.964
3.970
3.982
3.985
3.986
4.476
5.337
6.703
6.713
7.634
7.644
Me
OMe
38
ppm
3.161
1.062
1.095
1.058
4.324
0.905
1.029
1.053
1.000

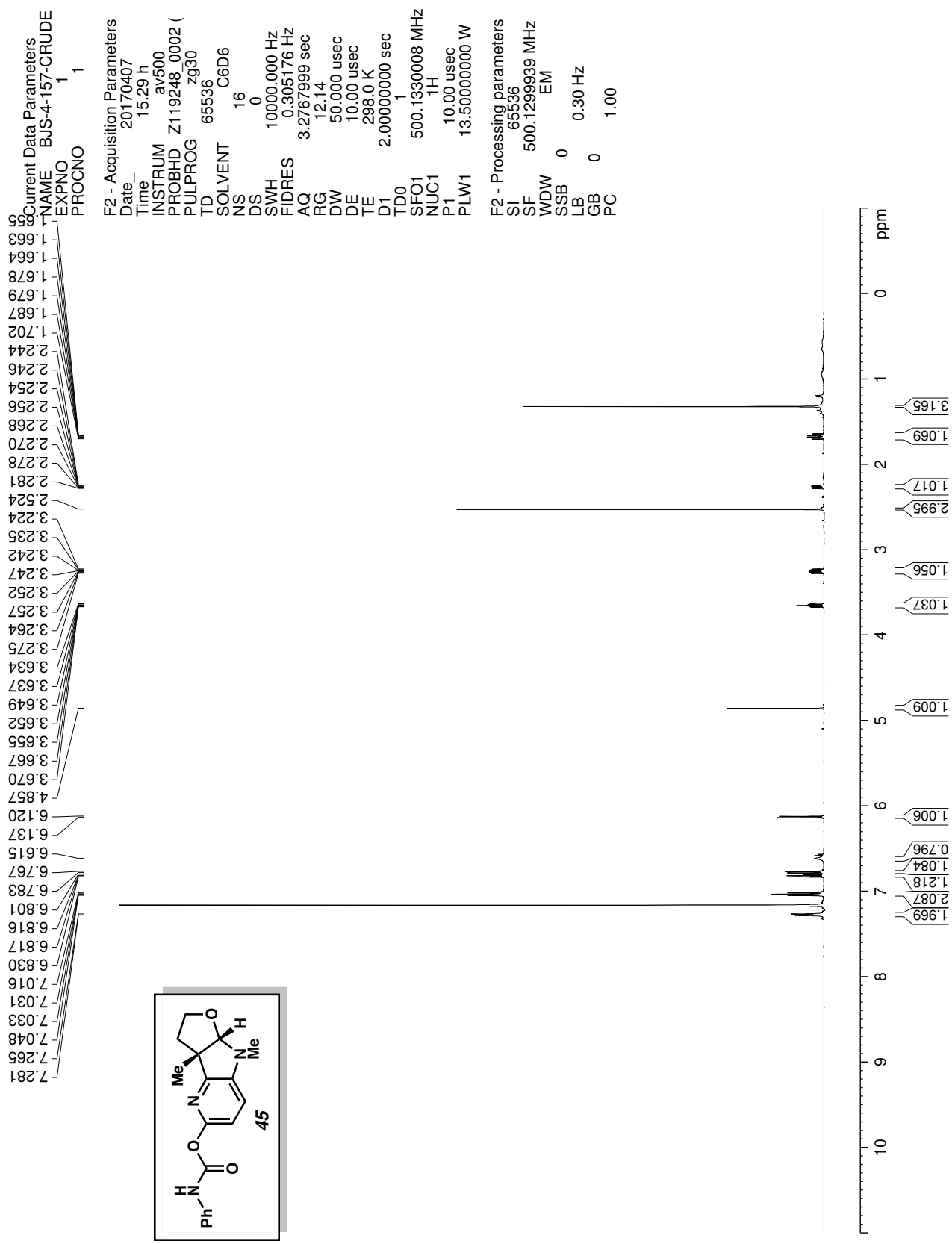

Current Data Parameters
NAME BJS-4-057-PREP
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170119
Time_ 13.05
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 161.3
DW 50.000 usec
DE 6.00 usec
TE 297.2 K
D1 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 500.3300223 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.566
7.561
6.969
6.964
5.306
5.111
3.988
3.985
3.974
3.971
3.967
3.957
3.953
3.779
3.611
3.601
3.594
3.589
3.583
3.579
3.572
3.561
2.131
2.127
2.119
2.117
2.107
2.103
2.095
2.091
2.077
2.069
2.054
2.045
2.031
1.470
Me
MeO
H
N
O
40
1.008
1.000
1.024
0.988
1.124
3.131
1.098
2.321
3.181
ppm

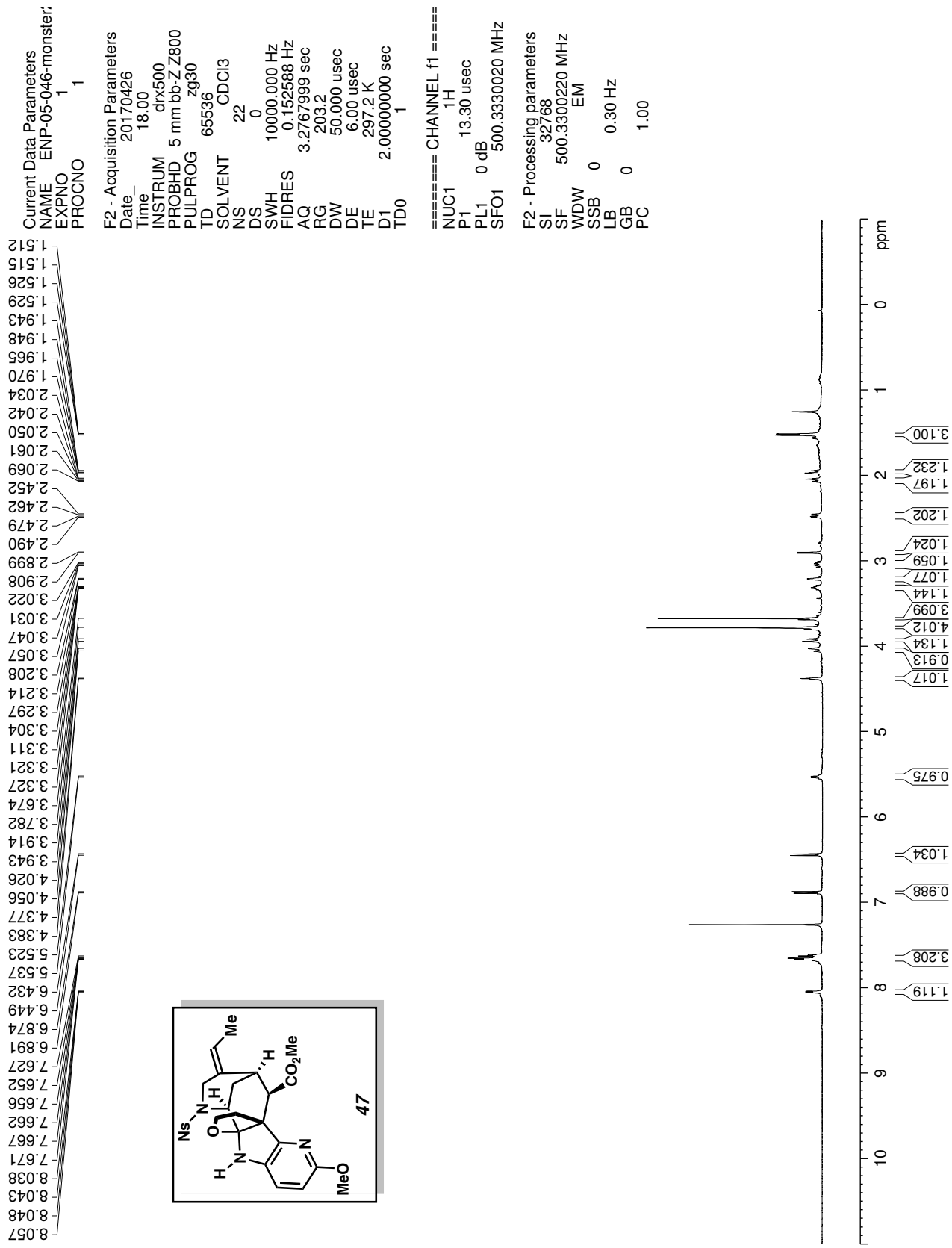

Current Data Parameters
NAME BJS-4-164-PREPPRC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170420
Time_ 11.07 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 12.14
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
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
1.521
2.059
2.074
2.081
2.083
2.096
2.098
2.106
2.120
2.412
2.415
2.422
2.425
2.436
2.439
2.447
2.450
3.502
3.512
3.520
3.524
3.530
3.535
3.542
3.553
3.969
3.972
3.984
3.987
3.990
4.001
4.005
4.587
5.310
6.786
6.789
6.802
6.804
6.916
6.926
6.932
6.942
7.941
7.944
7.951
7.954
Me
N
H
N
H
O
42
ppm
0
1
2
3
4
5
6
7
8
9
10
3.150
1.097
1.066
1.079
1.082
0.934
1.010
1.033
1.024
1.000

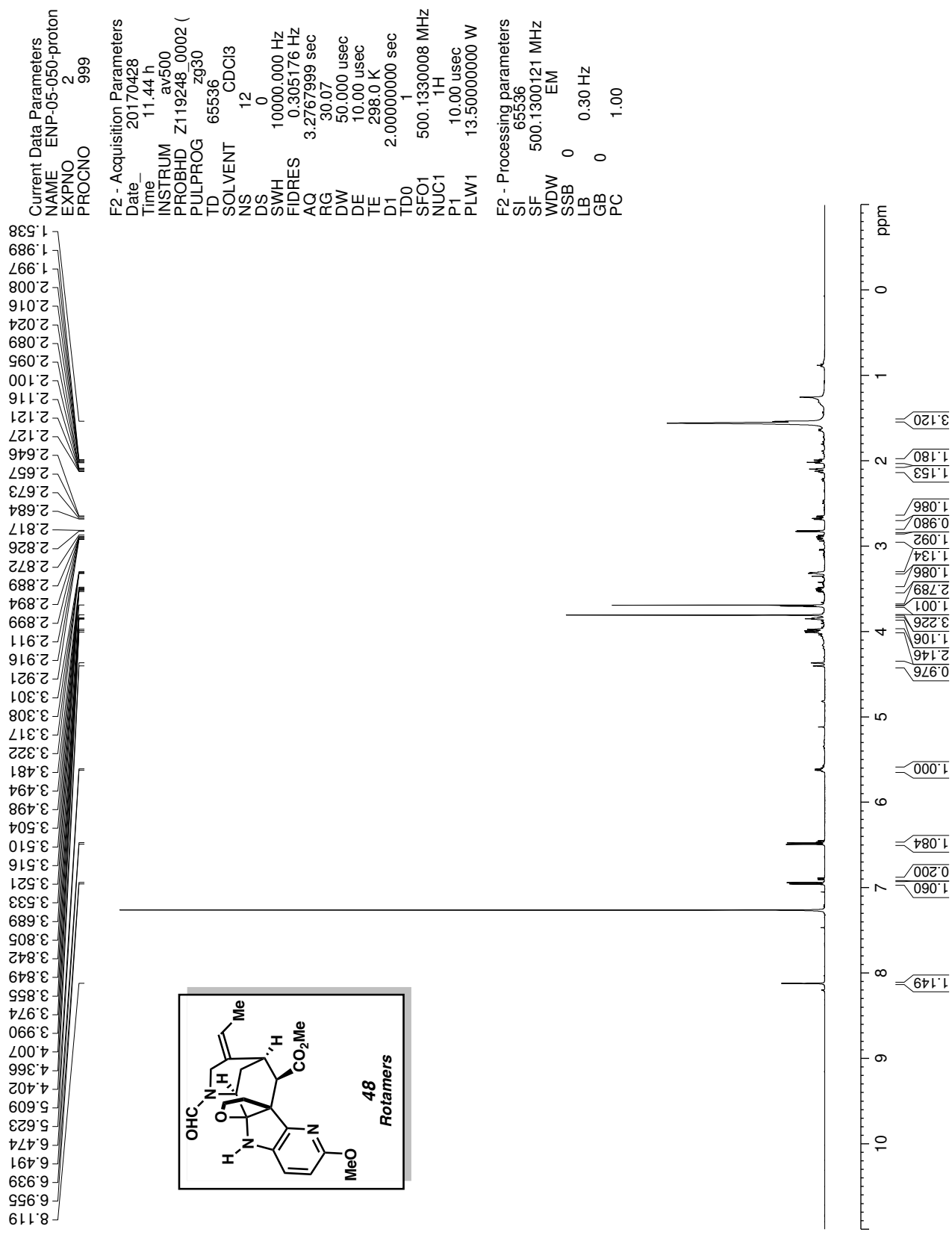

Current Data Parameters
NAME BJS-4-101-PREP2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170220
Time_ 9.25
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 143.7
DW 50.000 usec
DE 6.00 usec
TE 297.1 K
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 500.3300221 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
2.026
2.034
2.035
2.049
2.050
2.058
2.073
2.371
2.374
2.382
2.385
2.395
2.398
2.406
2.409
3.504
3.514
3.521
3.526
3.532
3.536
3.543
3.554
3.950
3.954
3.965
3.968
3.971
3.983
3.986
4.251
5.275
5.304
5.311
6.479
6.495
6.862
6.879
7.275
7.286
7.290
7.294
7.305
7.339
7.354
7.368
7.459
7.474
Me
N
O
H
N
BnO
44
3.162
1.201
1.121
1.121
1.106
0.852
0.953
0.950
1.180
1.079
1.092
1.144
2.290
2.168
ppm


Current Data Parameters
NAME BJS-4-120-PREP
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170305
Time_ 10.31
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 80.6
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 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.471
1.987
2.002
2.010
2.026
2.034
2.049
2.343
2.352
2.367
2.376
2.880
3.405
3.416
3.422
3.427
3.433
3.438
3.445
3.455
3.948
3.951
3.966
3.980
3.983
5.045
5.266
5.290
5.296
5.321
6.499
6.515
6.630
6.647
7.271
7.286
7.300
7.335
7.351
7.365
7.459
7.473
3.025
1.102
1.074
3.141
1.078
1.061
1.012
2.165
1.000
1.040
1.049
2.159
2.095
BnO
N
Me
Me
N
H
O
SI-16
ppm

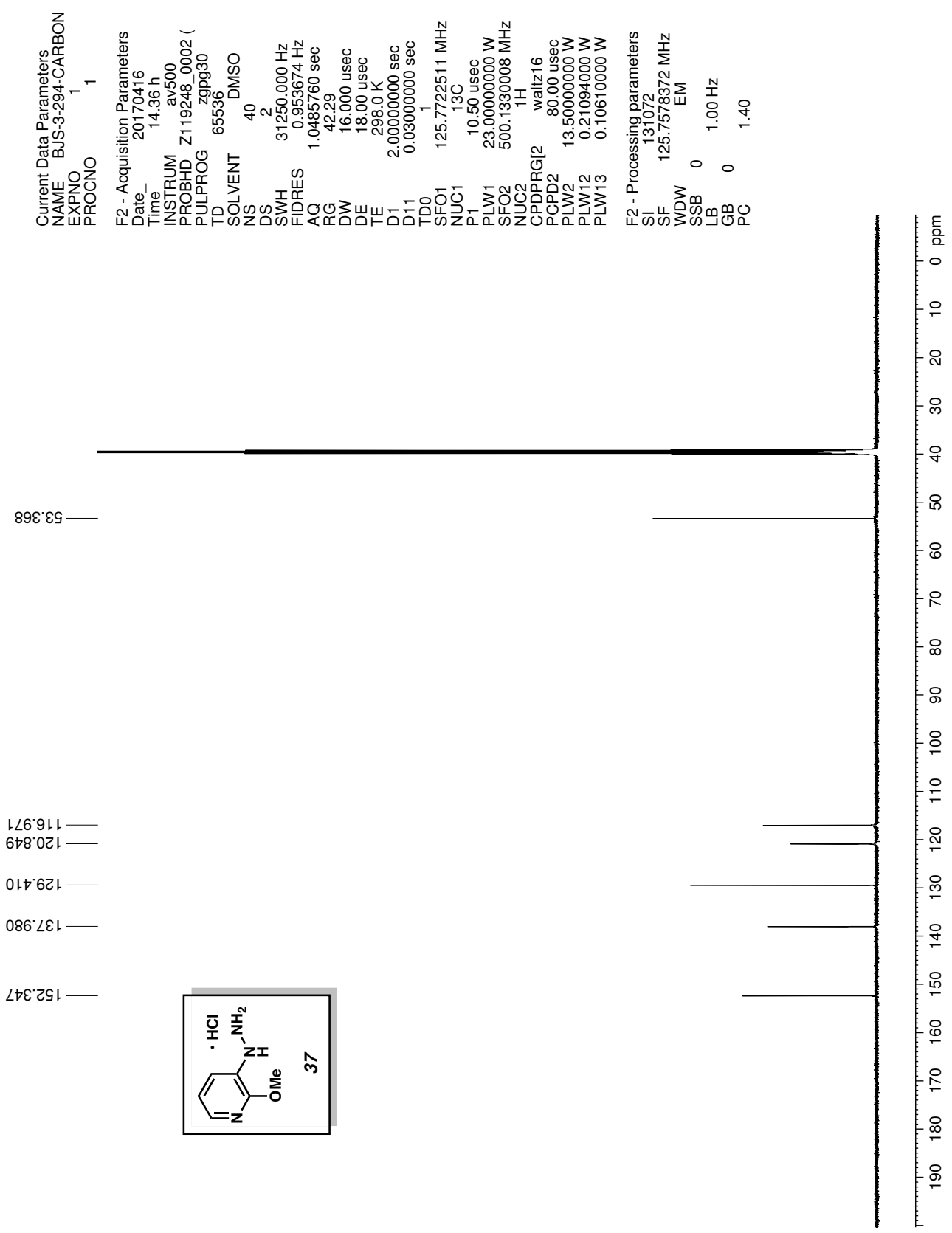

Current Data Parameters
NAME BJS-4-139-PREP1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170322
Time_ 10.21 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 12.14
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
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
1.527
2.052
2.067
2.075
2.077
2.090
2.092
2.100
2.115
2.419
2.422
2.429
2.432
2.444
2.447
2.454
2.457
2.881
3.440
3.450
3.457
3.462
3.468
3.473
3.480
3.490
3.955
3.958
3.970
3.973
3.976
3.987
3.991
5.016
6.489
6.506
6.760
6.777
HO
N
Me
Me
N
H
O
SI-17
3.093
1.050
1.022
3.042
1.019
1.013
1.000
1.005
1.006
ppm

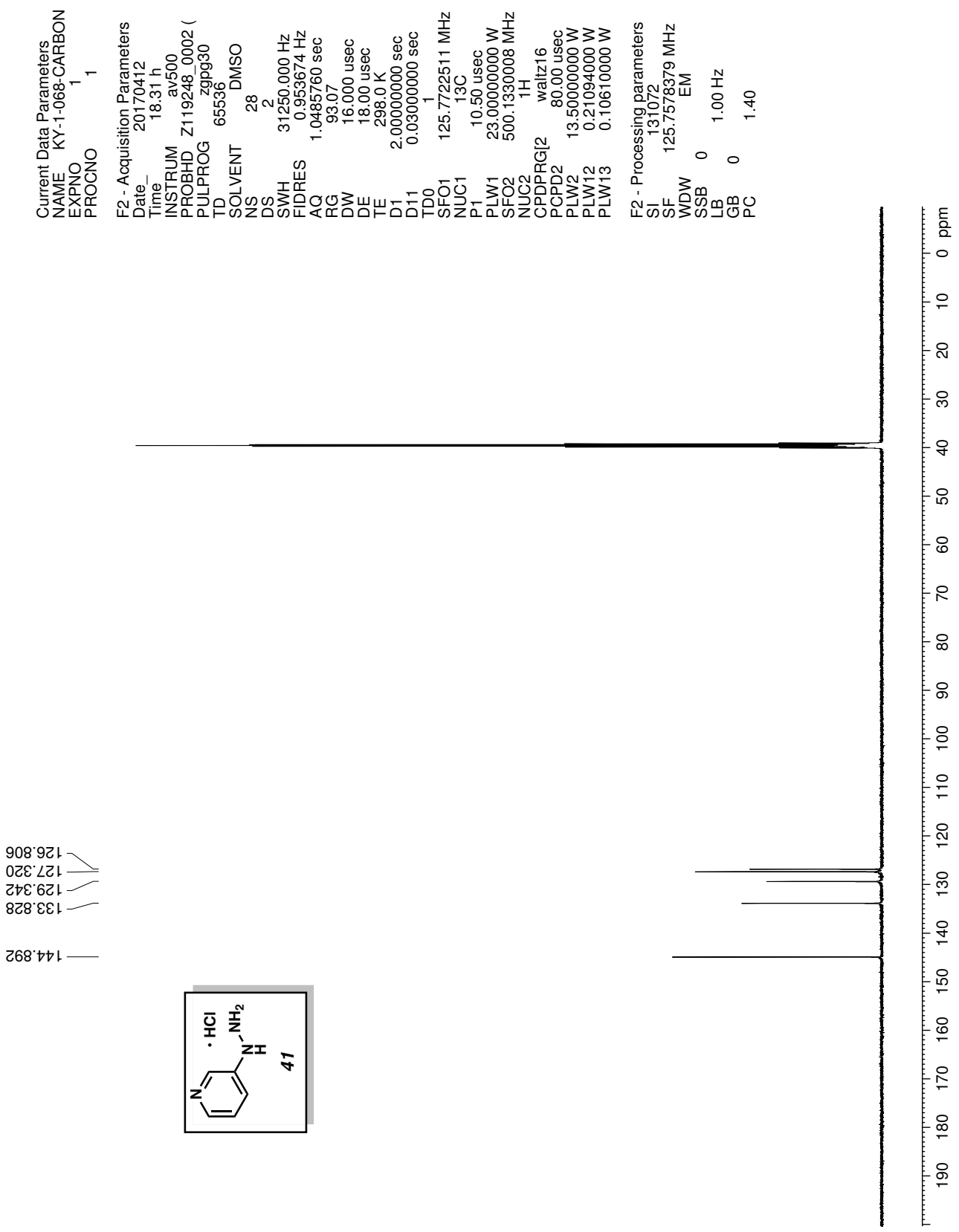

Current Data Parameters
NAME BJS-4-157-CRUDE
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170407
Time_ 15.29 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 12.14
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1299939 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.281
7.265
7.048
7.033
7.031
7.016
6.830
6.817
6.816
6.801
6.783
6.767
6.615
6.137
6.120
4.857
3.670
3.667
3.655
3.652
3.649
3.637
3.634
3.275
3.264
3.257
3.252
3.247
3.242
3.235
3.224
2.524
2.281
2.278
2.270
2.268
2.256
2.254
2.246
2.244
1.702
1.687
1.679
1.678
1.664
1.663
1.655
Me
N
Me
H
O
O
O
N
H
Ph
45
ppm
0
1
2
3
4
5
6
7
8
9
10
3.165
1.069
1.017
2.995
1.056
1.037
1.009
1.006
0.796
1.084
1.218
2.087
1.969

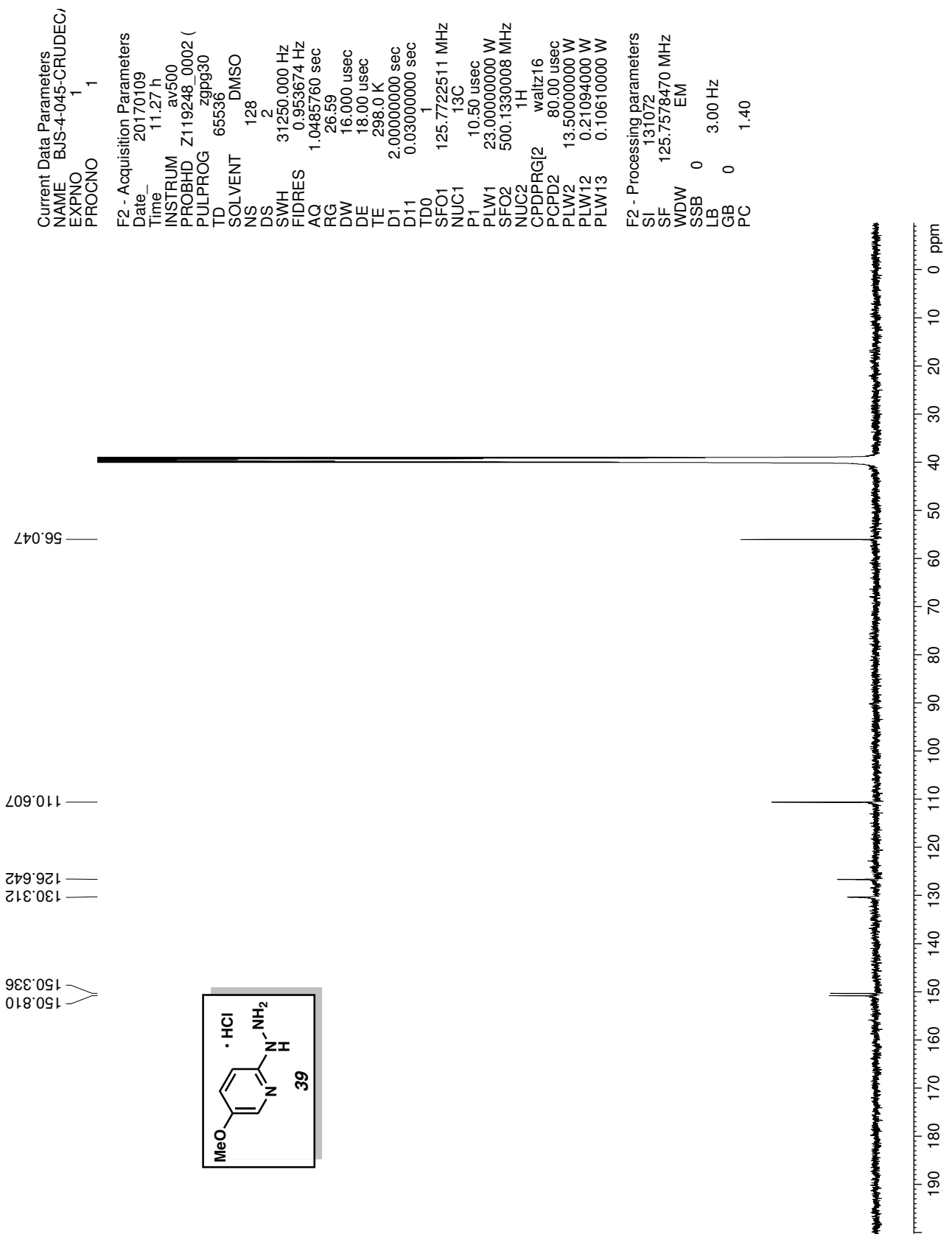

Current Data Parameters
NAME ENP-05-046-monster
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170426
Time_ 18.00
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 22
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 203.2
DW 50.000 usec
DE 6.00 usec
TE 297.2 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 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ns
Me
H
CO2Me
MeO
47
ppm
3.100
1.197
1.232
1.202
1.024
1.059
1.077
1.144
3.099
4.012
1.134
0.913
1.017
0.975
1.034
0.988
3.208
1.119

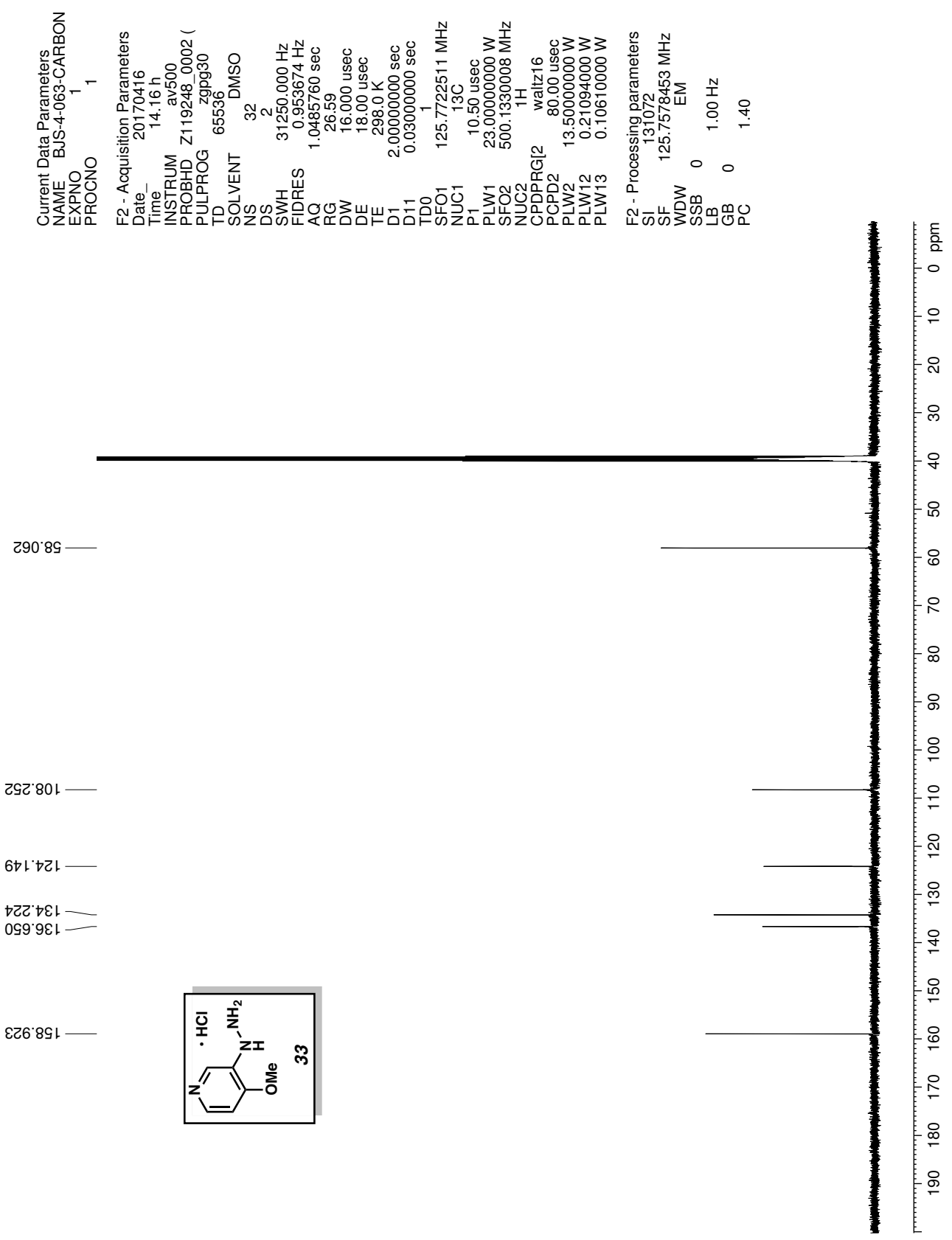

Current Data Parameters
NAME ENP-05-050-proton
EXPNO 2
PROCNO 999
F2 - Acquisition Parameters
Date_ 20170428
Time_ 11.44 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 30.07
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OHC
Me
H
CO2Me
MeO
48
Rotamers
ppm
0.976
2.146
1.106
3.226
1.001
2.789
1.086
1.134
1.092
0.980
1.086
1.153
1.180
3.120
1.000
1.084
0.200
1.060
1.149

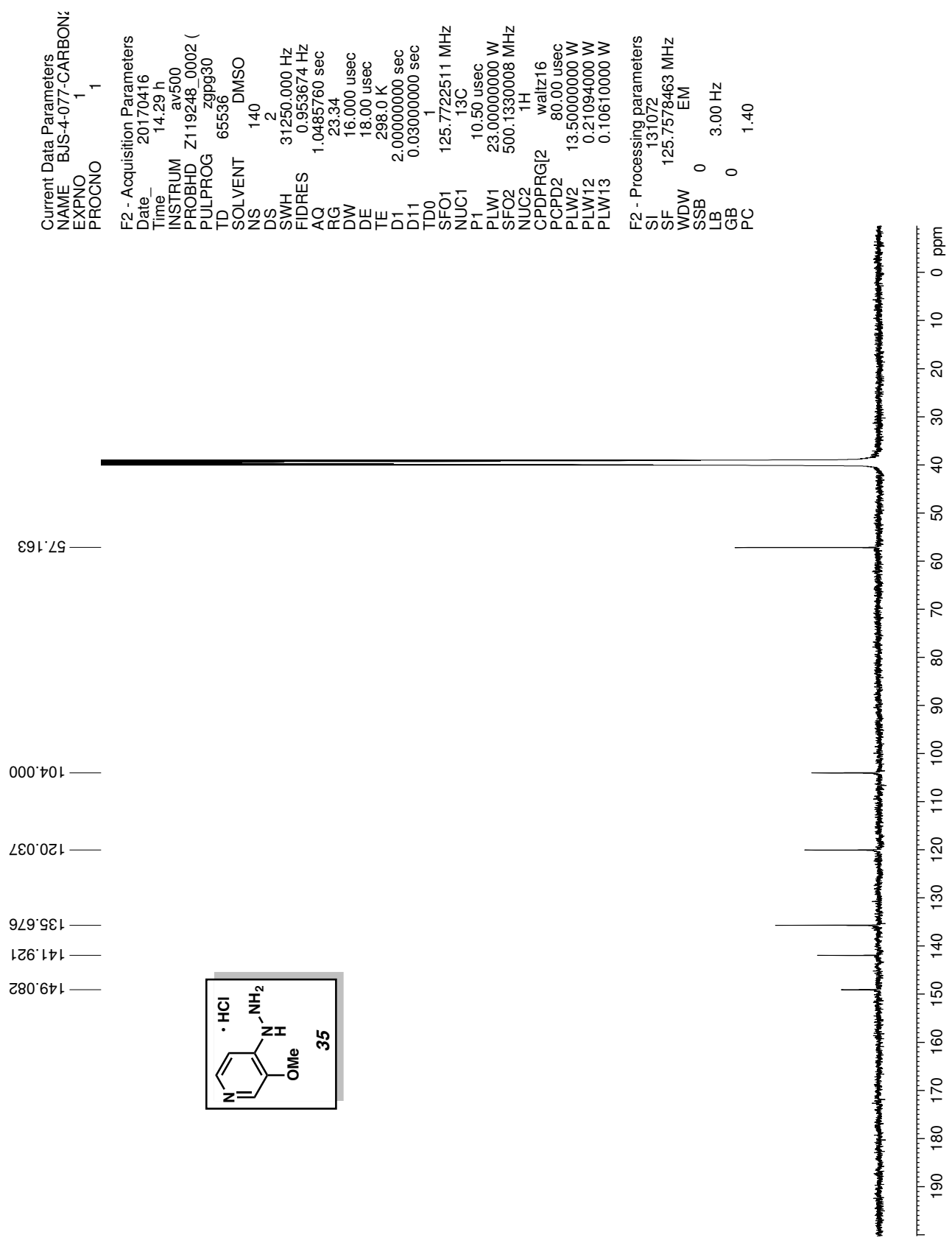
^{13}C NMR Spectra

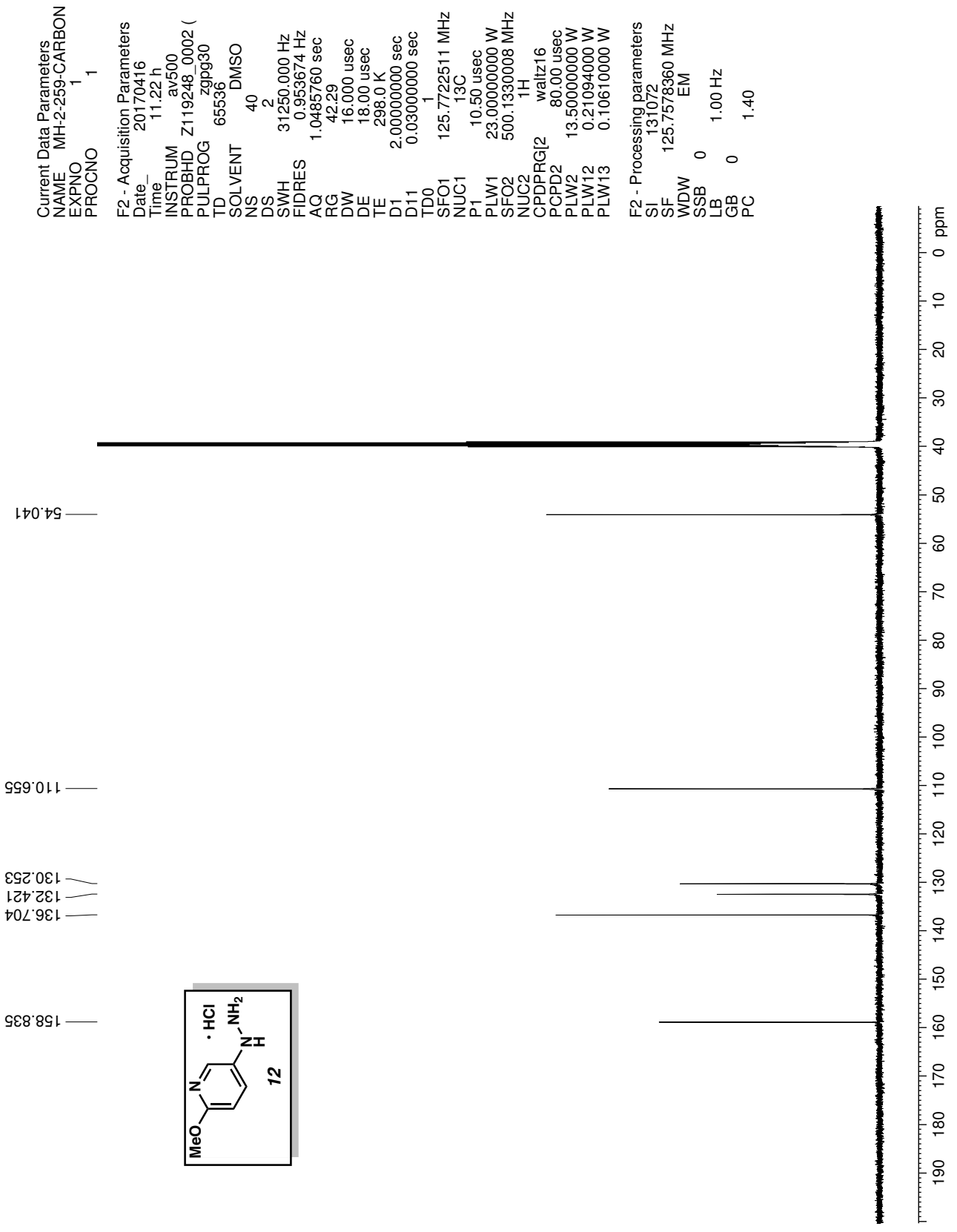

Current Data Parameters
NAME BJS-3-294-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170416
Time_ 14.36 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 40
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 42.29
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578372 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
53.368
116.971
120.849
129.410
137.980
152.347
· HCl
NH2
N
H
OMe
N
37
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

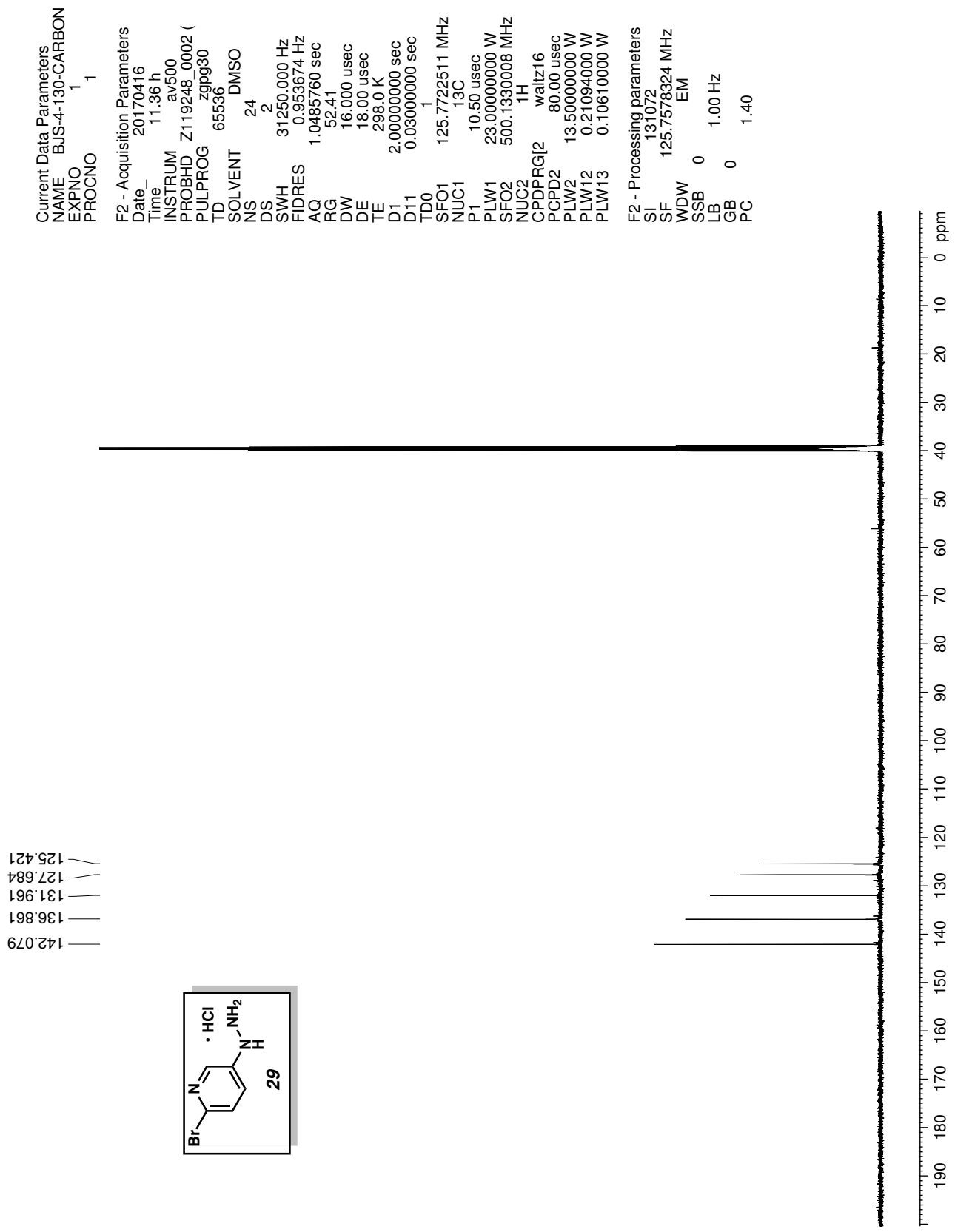

Current Data Parameters
NAME KY-1-068-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170412
Time_ 18.31 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 28
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 93.07
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578379 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
144.892
133.828
129.342
127.320
126.806
· HCl
NH2
N
H
41
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

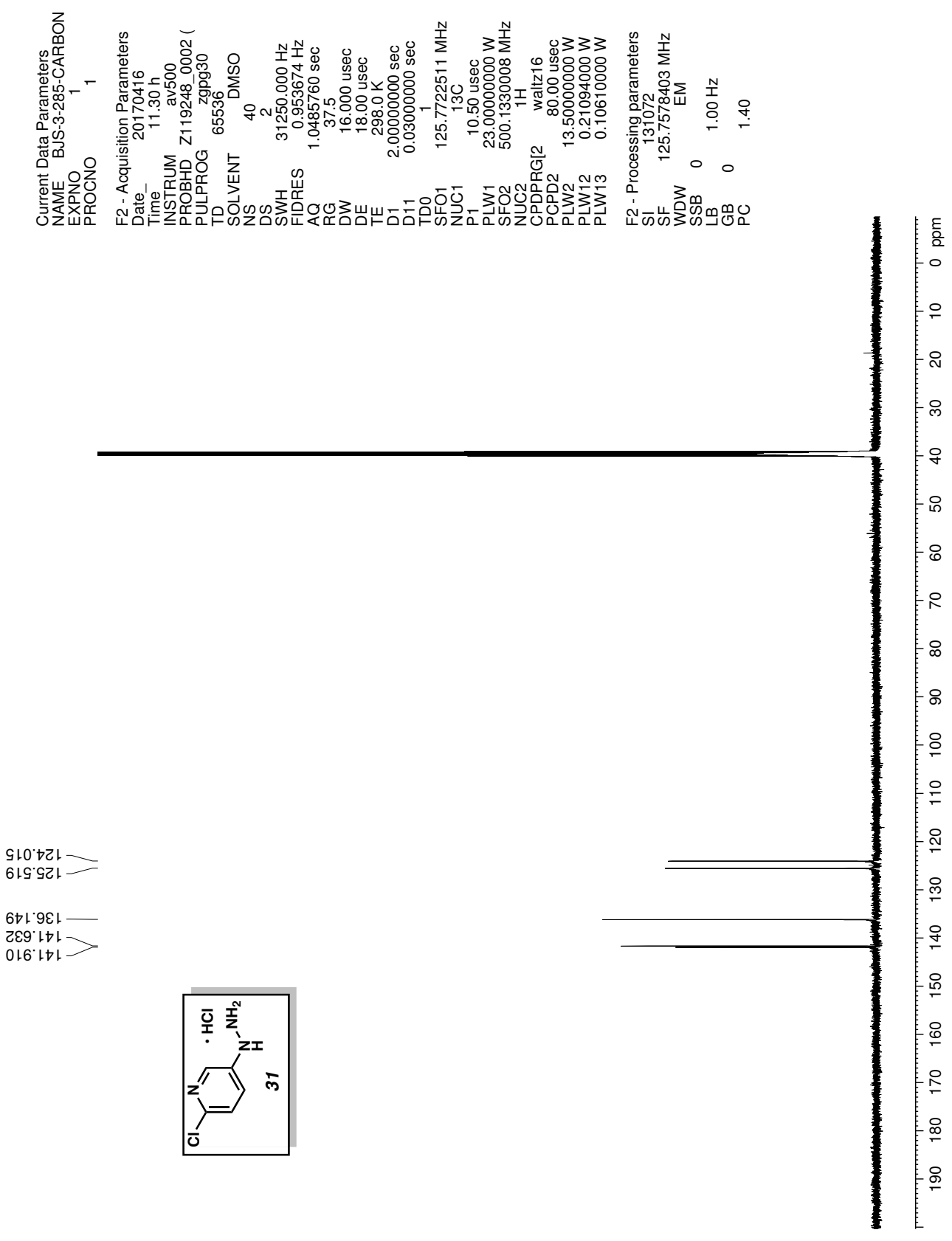

Current Data Parameters
NAME BJS-4-045-CRUDEC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170109
Time 11.27 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 26.59
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578470 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
150.810
150.336
130.312
126.642
110.607
56.047
MeO
· HCl
NH2
N
H
N
39
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

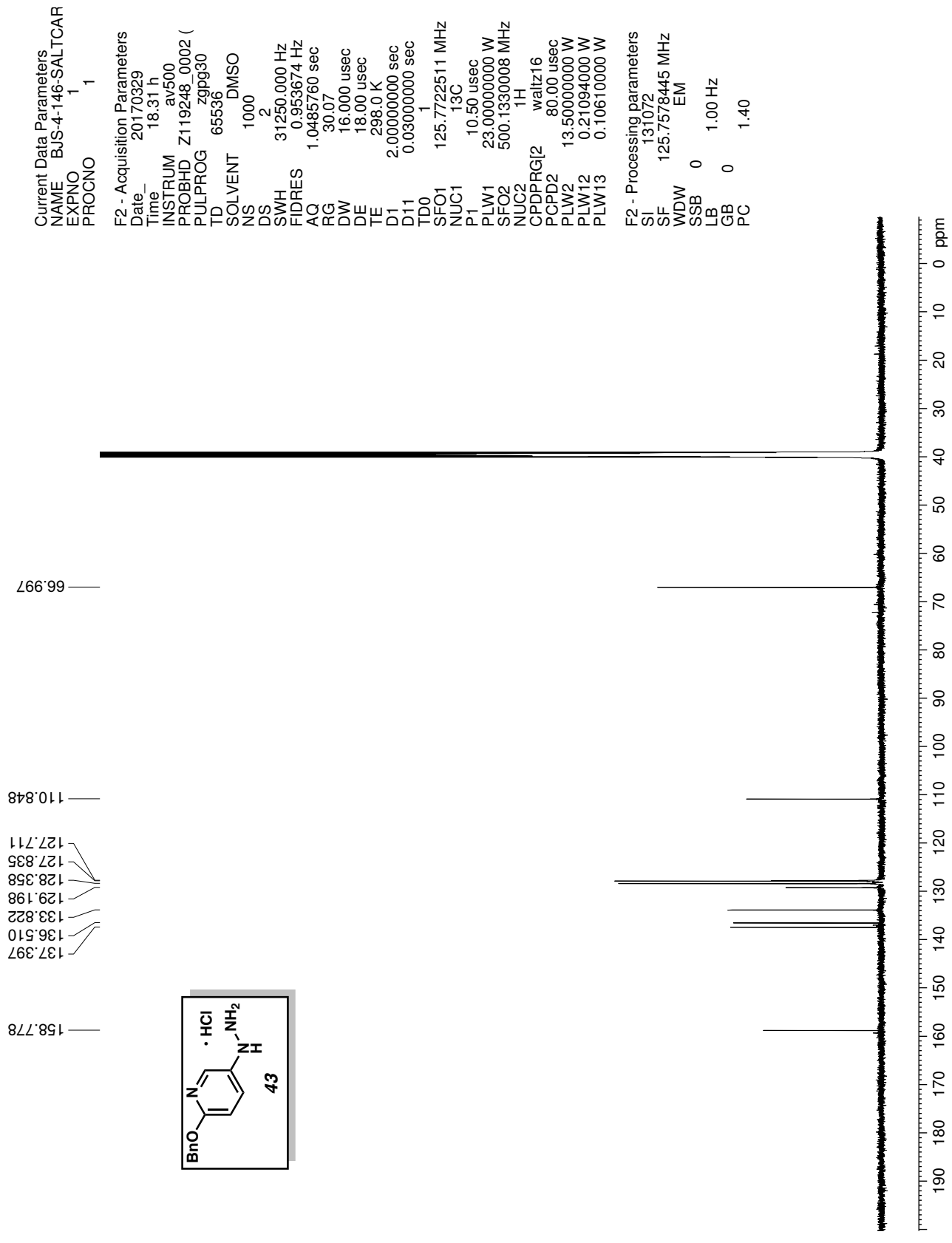

Current Data Parameters
NAME BJS-4-063-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170416
Time_ 14.16 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 26.59
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578453 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
158.923
136.650
134.224
124.149
108.252
58.062
· HCl
NH2
N
H
N
OMe
33
ppm

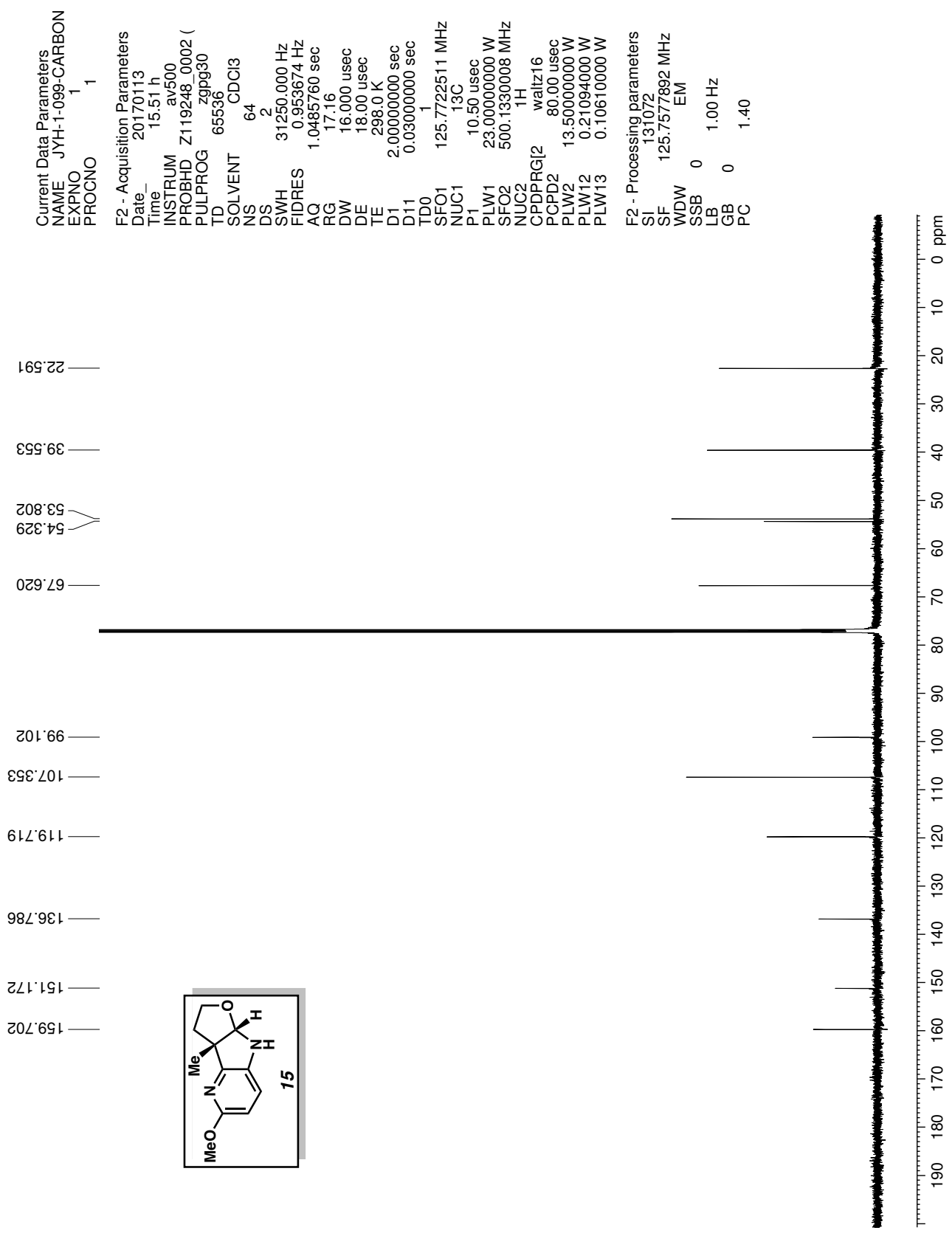

Current Data Parameters
NAME BJS-4-077-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170416
Time 14.29 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 140
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 23.34
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578463 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
149.082
141.921
135.676
120.037
104.000
57.163
· HCl
NH2
N
H
OMe
N
35
ppm

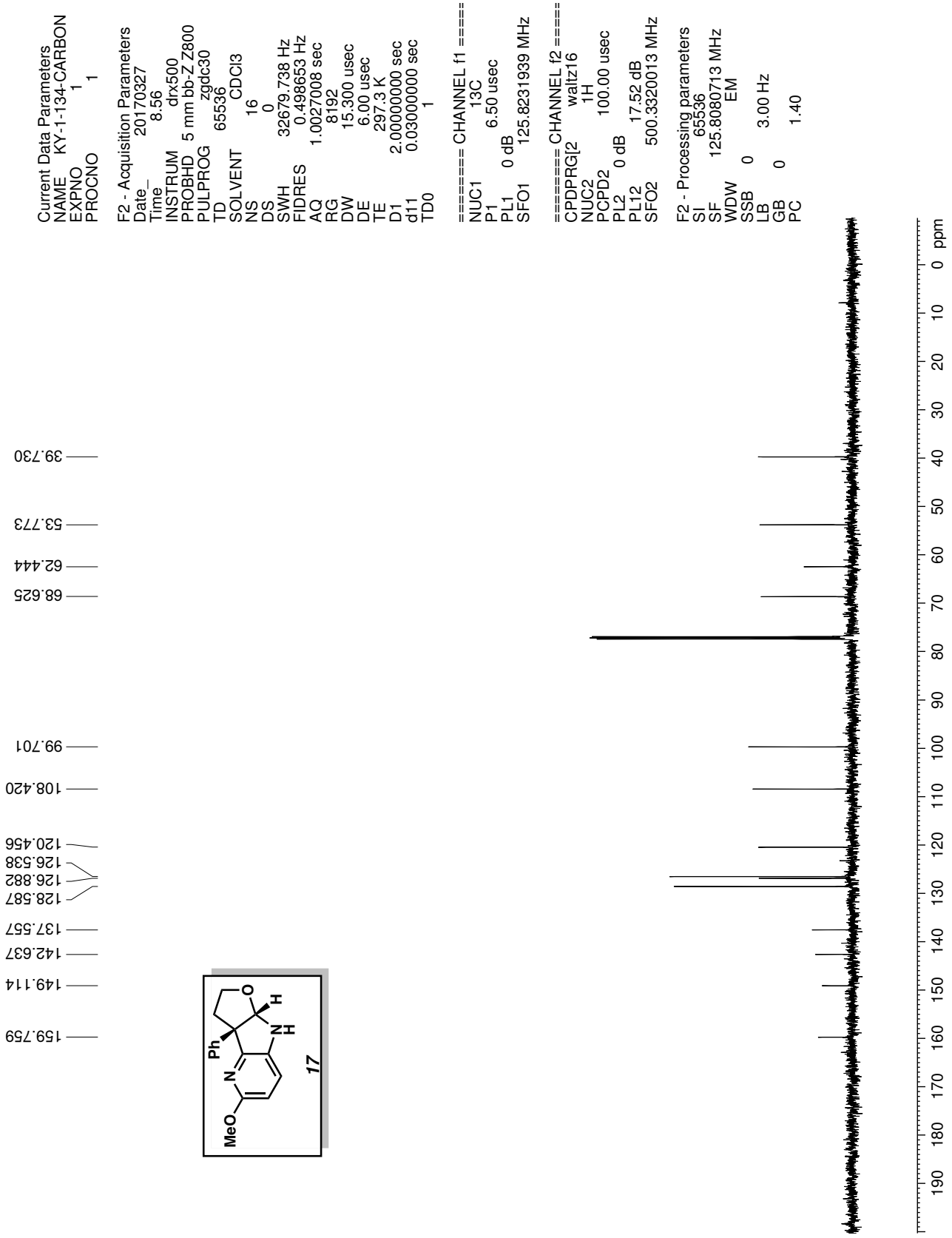

Current Data Parameters
NAME MH-2-259-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170416
Time_ 11.22 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 40
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 42.29
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578360 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
158.835
136.704
132.421
130.253
110.655
54.041
MeO
N
· HCl
NH2
N
H
12
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

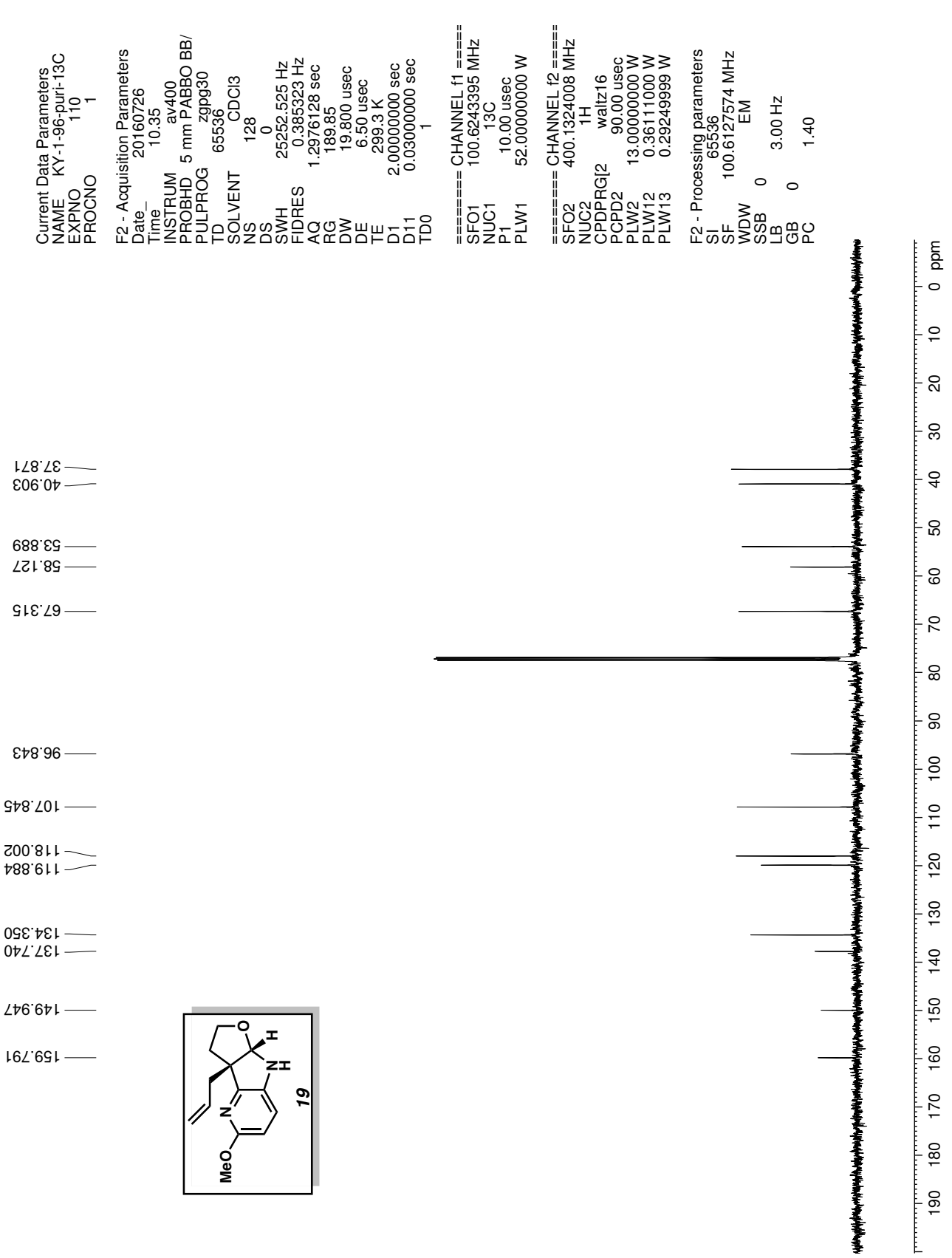

Current Data Parameters
NAME BJS-4-130-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170416
Time_ 11.36 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 24
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 52.41
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578324 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
142.079
136.861
131.961
127.684
125.421
Br
N
· HCl
NH2
N
H
29
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

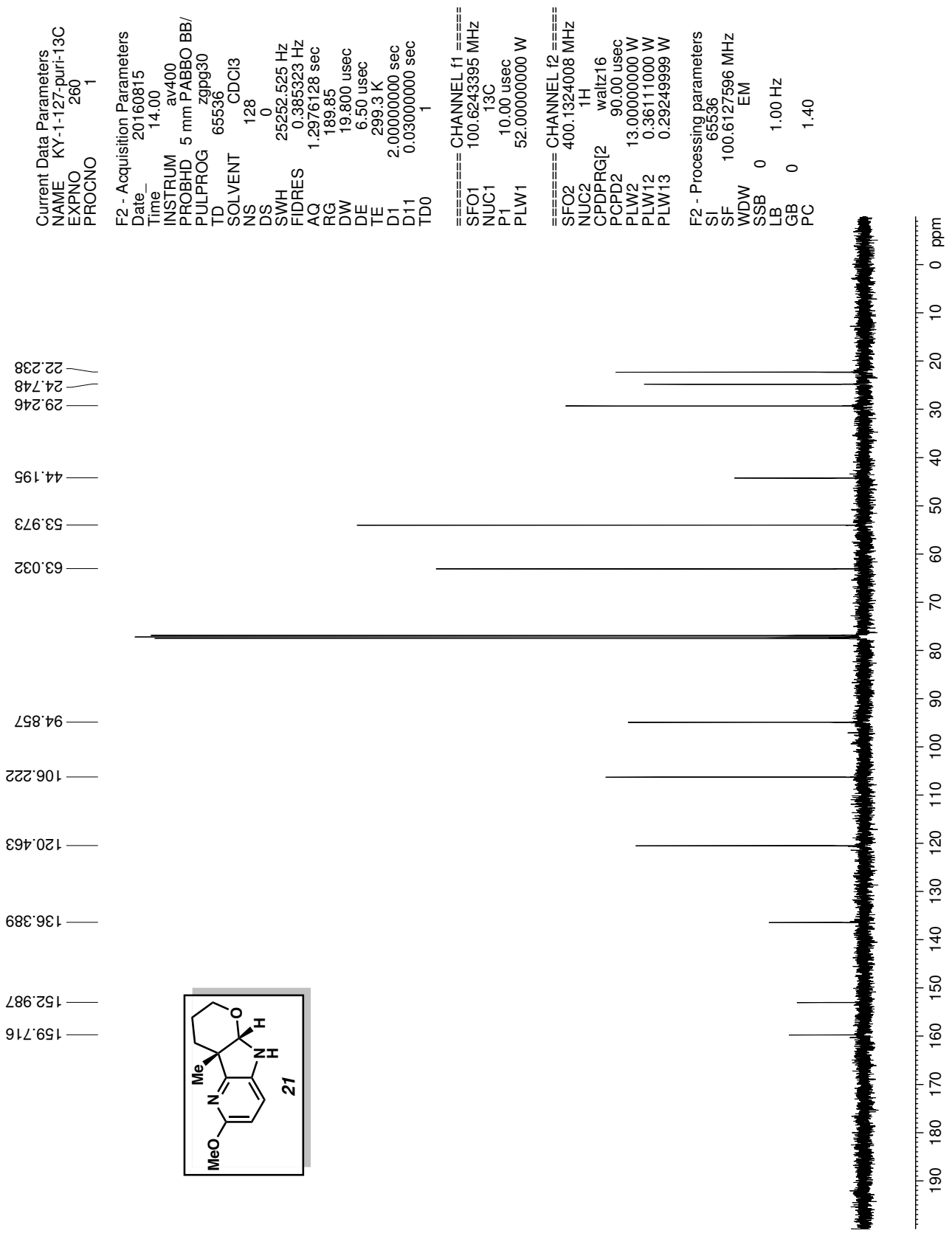

Current Data Parameters
NAME BJS-3-285-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170416
Time_ 11.30 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 40
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 37.5
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578403 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
141.910
141.632
136.149
125.519
124.015
· HCl
31
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

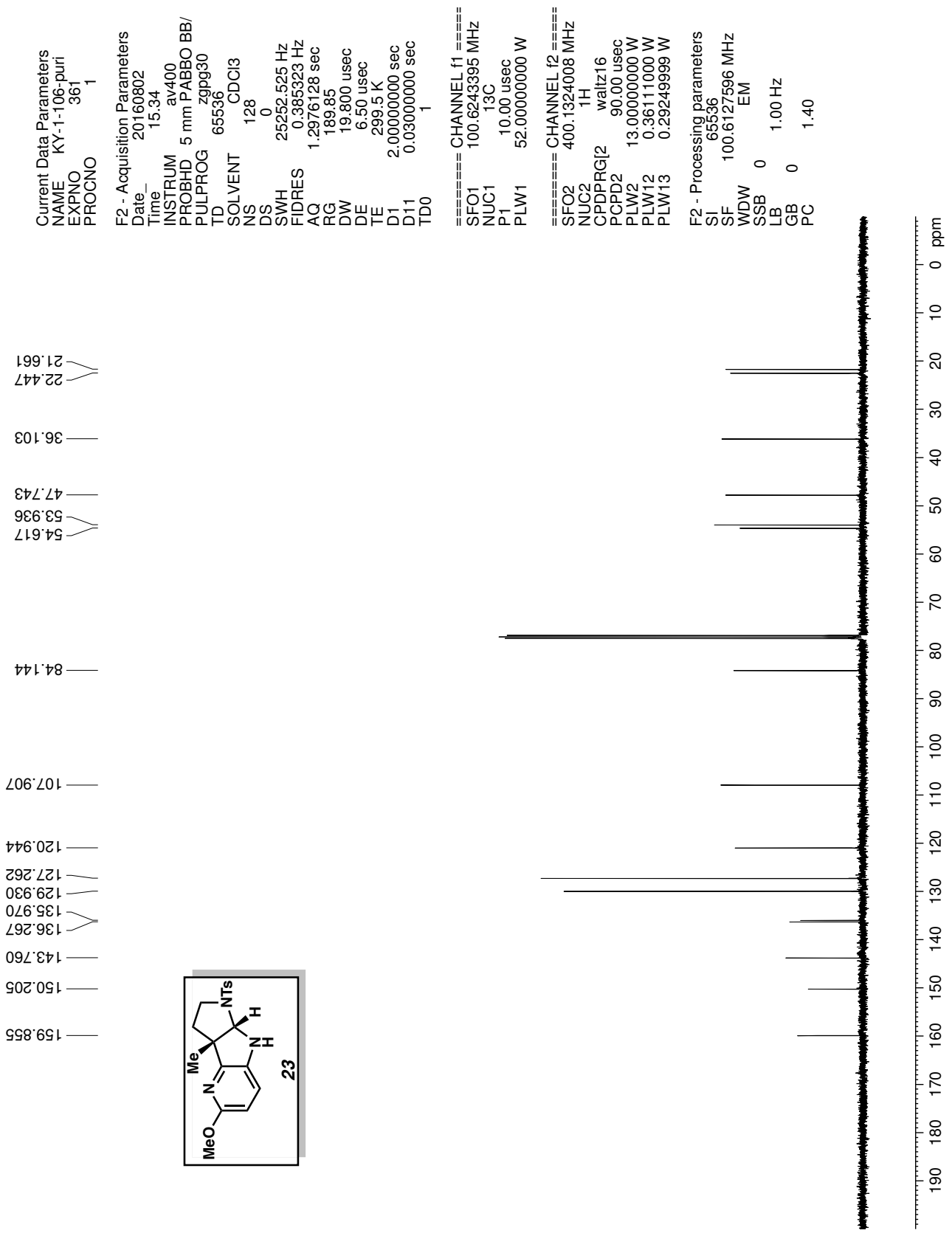

Current Data Parameters
NAME BJS-4-146-SALTCAR
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170329
Time_ 18.31 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1000
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 30.07
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7578445 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
66.997
110.848
127.711
127.835
128.358
129.198
133.822
136.510
137.397
158.778
BnO
N
· HCl
NH2
N
H
43
ppm

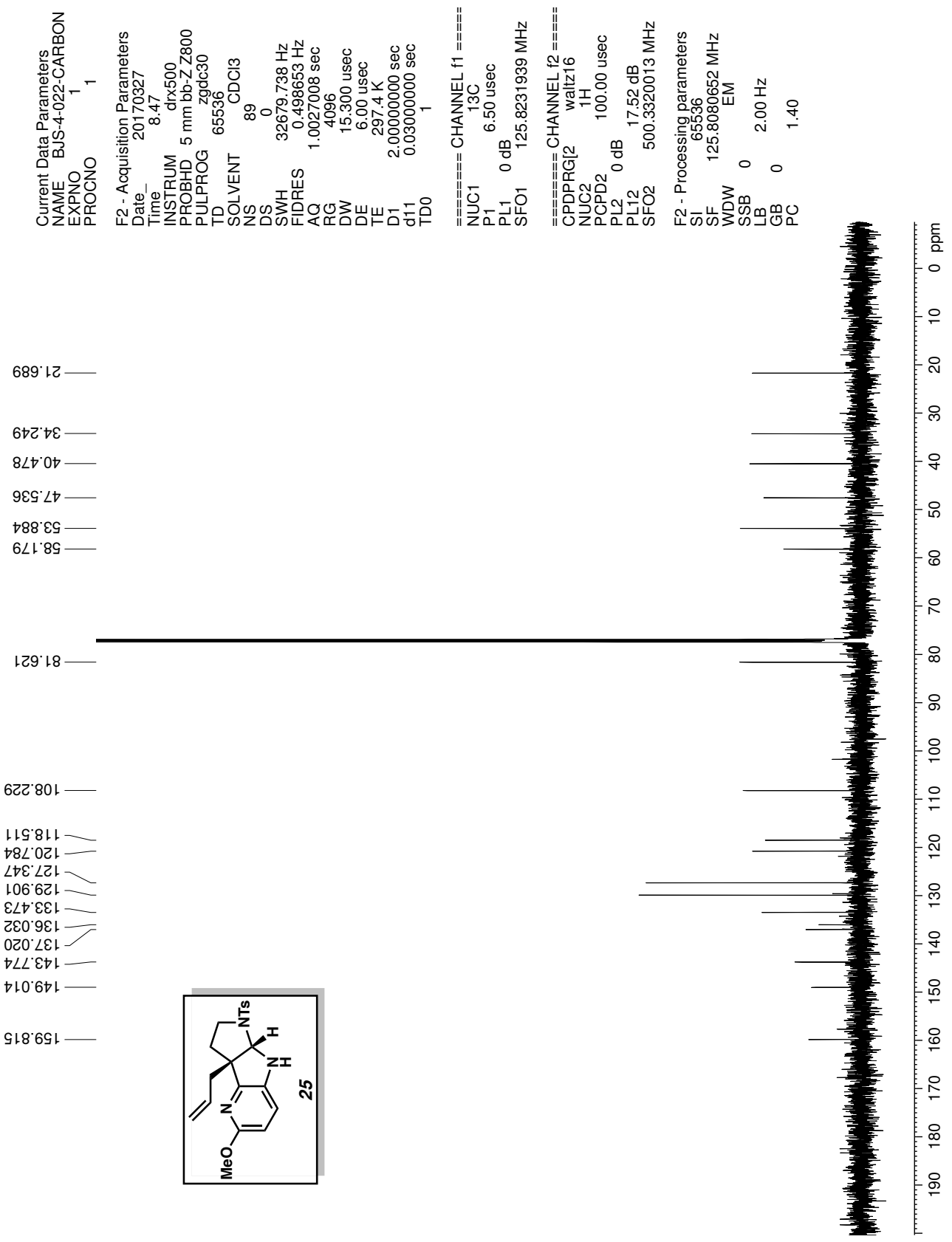

Current Data Parameters
NAME JYH-1-099-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170113
Time_ 15.51 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 17.16
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7577892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.591
39.553
53.802
54.329
67.620
99.102
107.353
119.719
136.786
151.172
159.702
Me
MeO
N
O
H
N
H
15
0 ppm

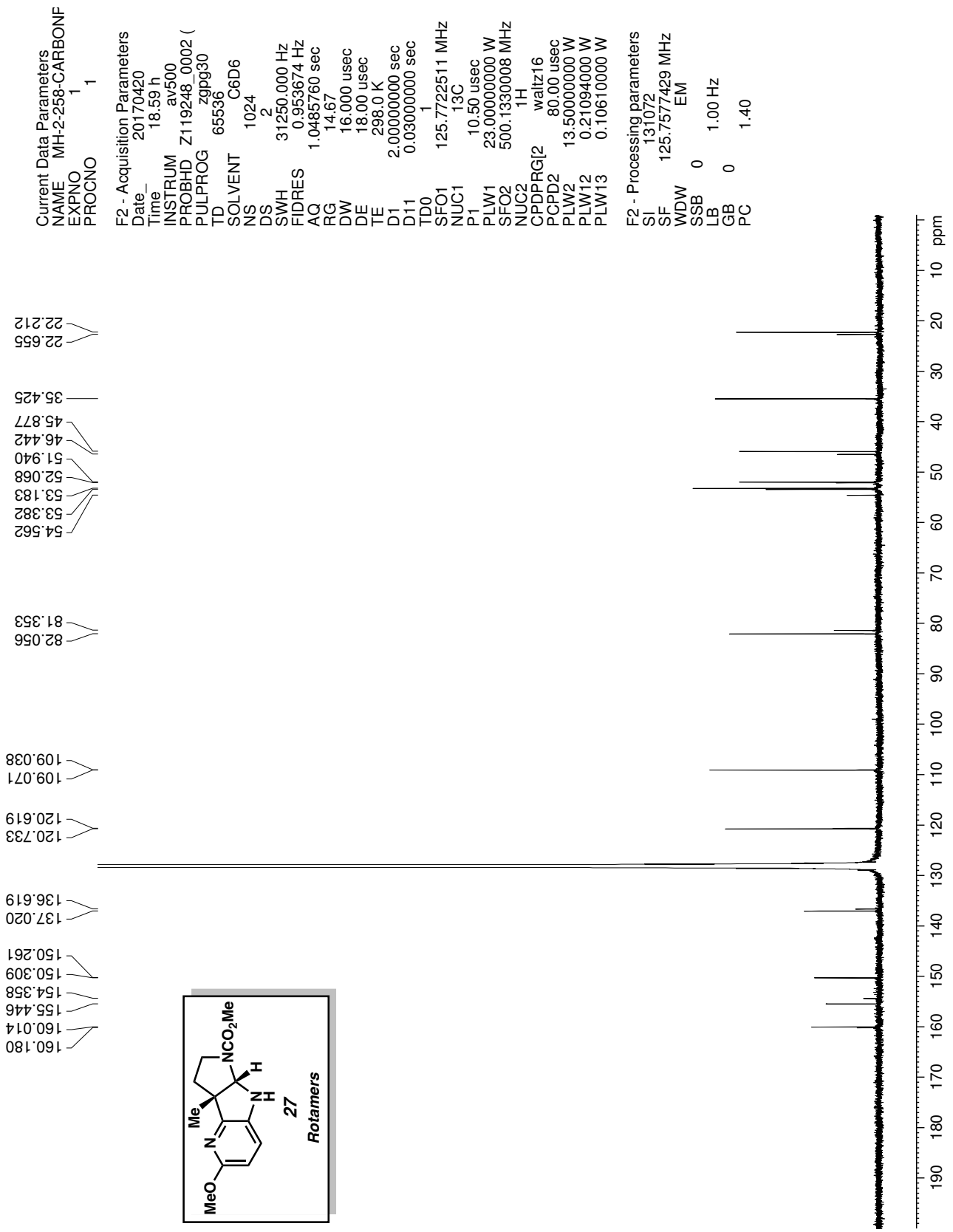

Current Data Parameters
NAME KY-1-134-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170327
Time 8.56
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 8192
DW 15.300 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 =====
NUC1 13C
P1 6.50 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 125.8080713 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
39.730
53.773
62.444
68.625
99.701
108.420
120.456
126.538
126.882
128.587
137.557
142.637
149.114
159.759
MeO
Ph
N
H
O
17
0 ppm

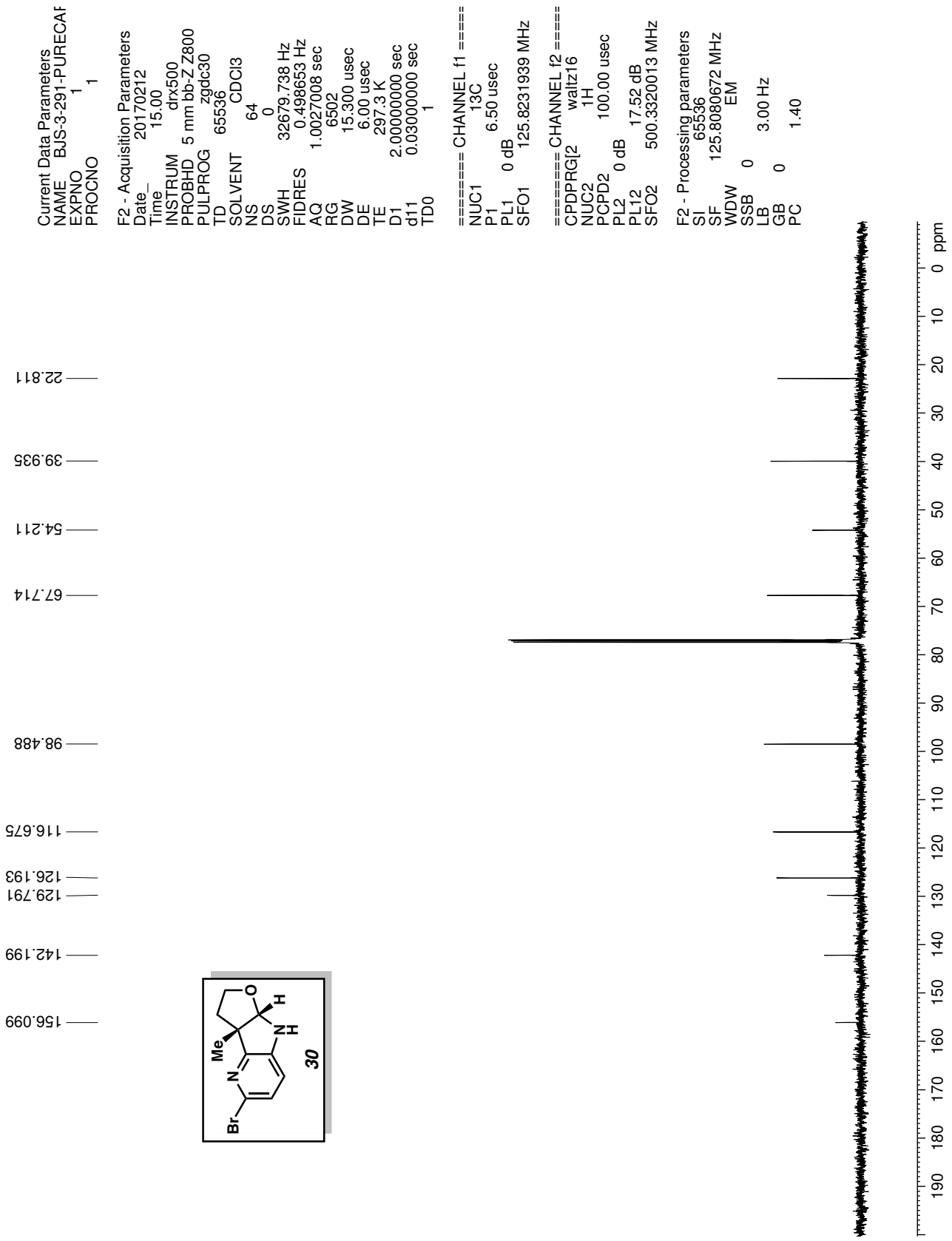

Current Data Parameters
NAME KY-1-96-puri-13C
EXPNO 110
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160726
Time 10.35
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 189.85
DW 19.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =====
SFO1 100.6243395 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W
======== CHANNEL f2 =====
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W
F2 - Processing parameters
SI 65536
SF 100.6127574 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
159.791
149.947
137.740
134.350
119.884
118.002
107.845
96.843
67.315
58.127
53.889
40.903
37.871
MeO
19
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

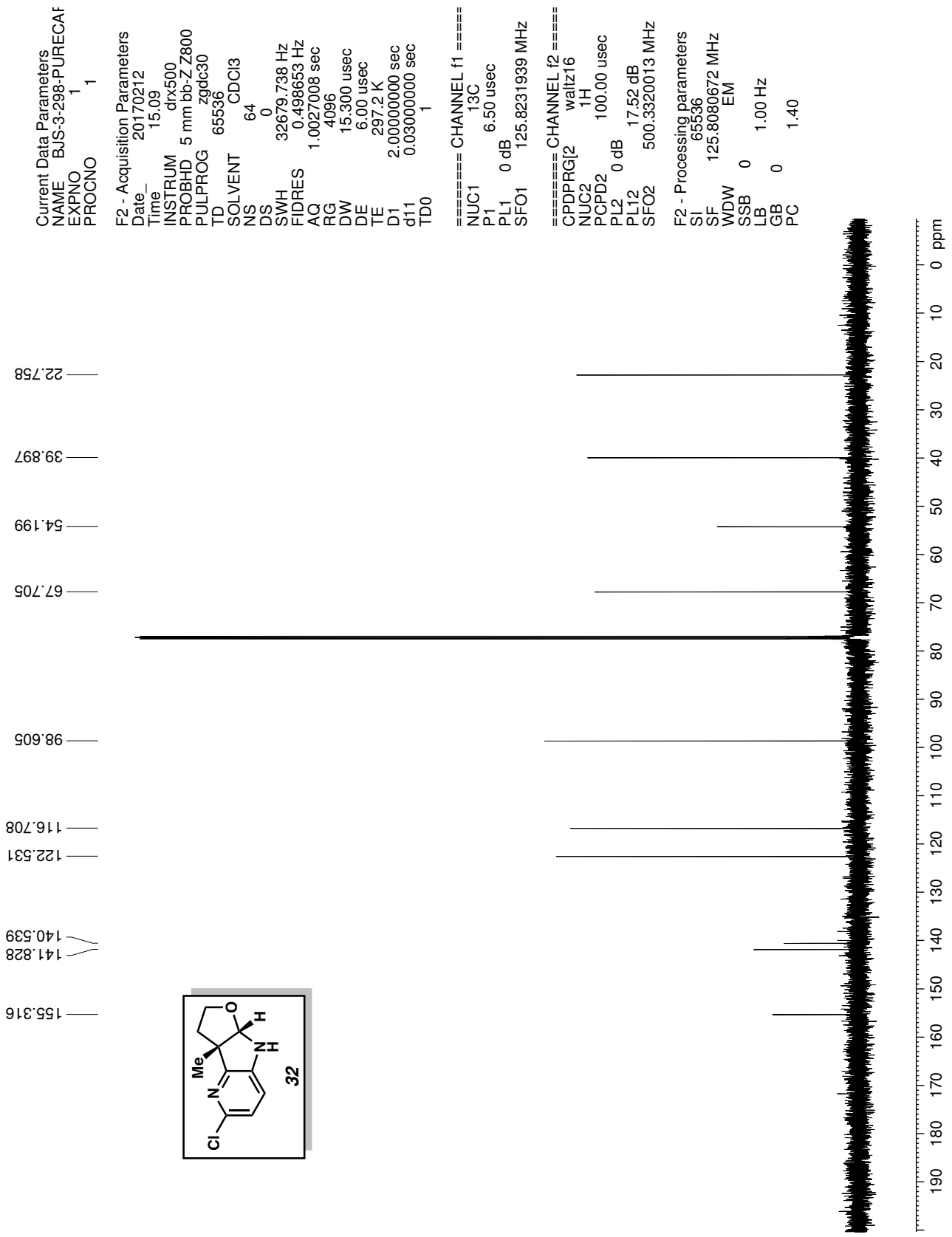

Current Data Parameters
NAME KY-1-127-puri-13C
EXPNO 260 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160815
Time_ 14.00
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 189.85
DW 19.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =====
SFO1 100.6243395 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W
======== CHANNEL f2 =====
SFO2 400.1324008 MHz
NUC2 1H
CPDPRGI2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W
F2 - Processing parameters
SI 65536
SF 100.6127596 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.238
24.748
29.246
44.195
53.973
63.032
94.857
106.222
120.463
136.389
152.987
159.716
Me
MeO
N
N
H
O
H
21
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

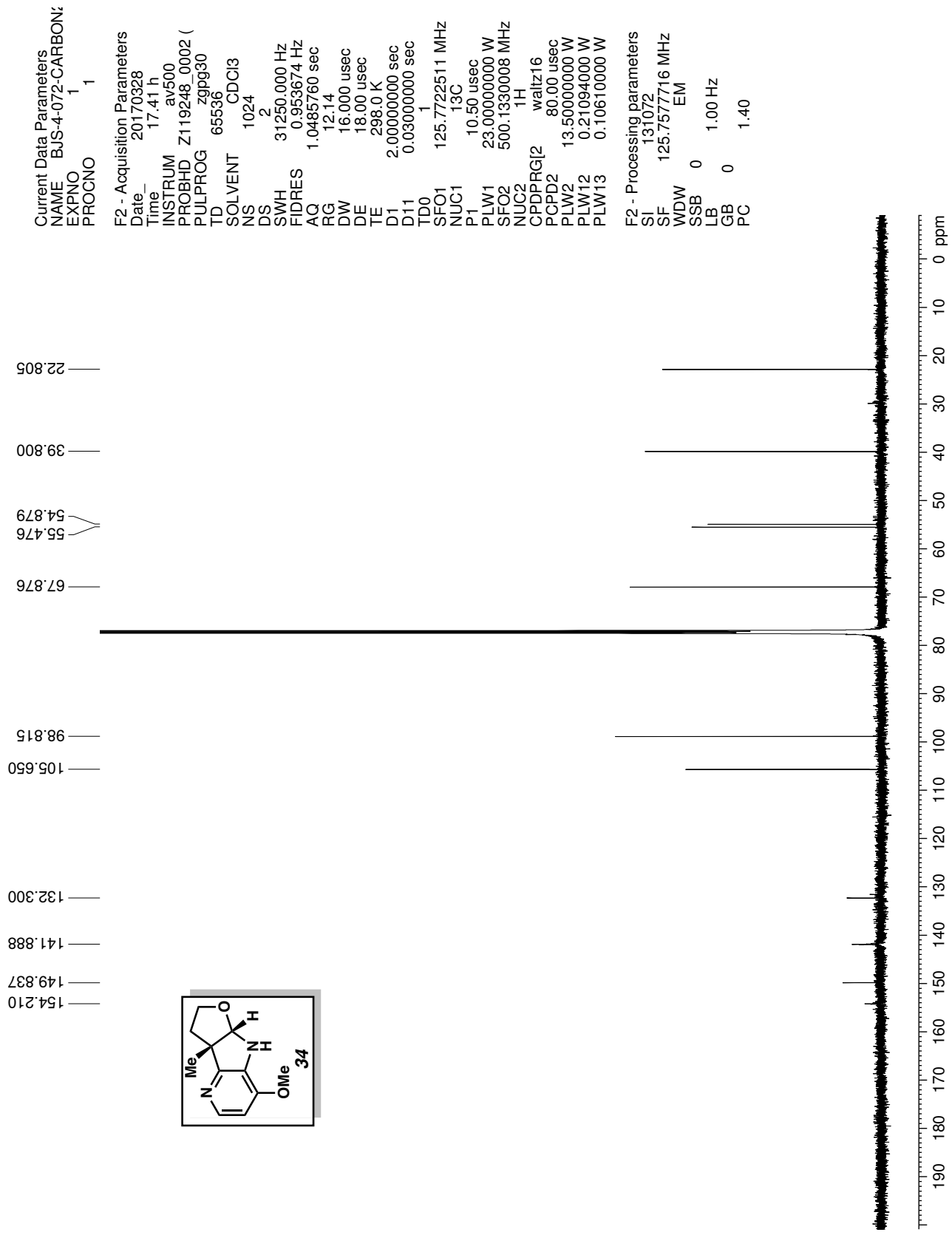

Current Data Parameters
NAME KY-1-106-puri
EXPNO 361
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160802
Time_ 15.34
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 189.85
DW 19.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =====
SFO1 100.6243395 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W
======== CHANNEL f2 =====
SFO2 400.1324008 MHz
NUC2 1H
CPDPRGI2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W
F2 - Processing parameters
SI 65536
SF 100.6127596 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
159.855
150.205
143.760
136.267
135.970
129.930
127.262
120.944
107.907
84.144
54.617
53.936
47.743
36.103
22.447
21.661
Me
MeO
N
NTs
H
N
H
23
0 ppm

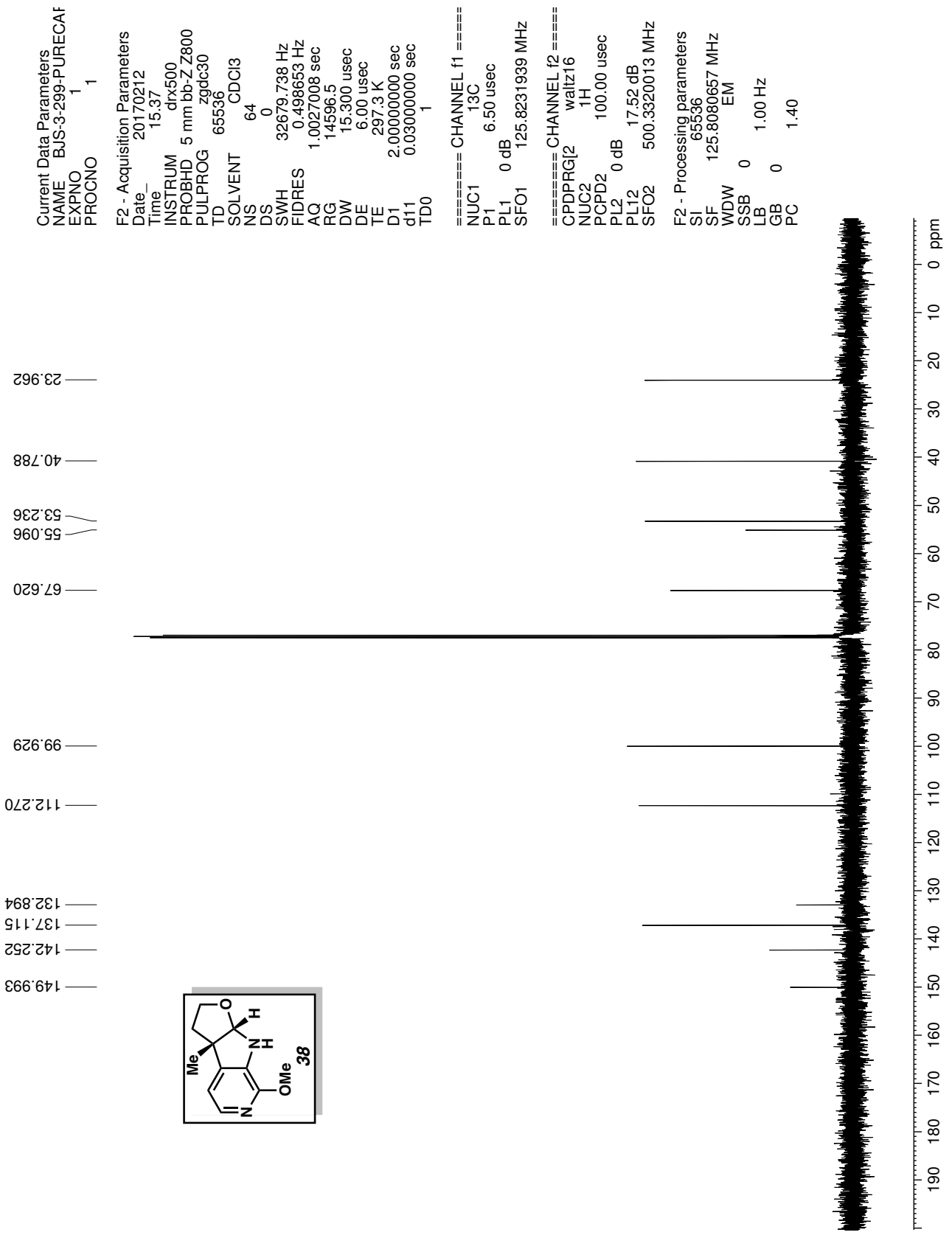

Current Data Parameters
NAME BJS-4-022-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170327
Time_ 8.47
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 89
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 =====
NUC1 13C
P1 6.50 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 125.8080652 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
159.815
149.014
143.774
137.020
136.032
133.473
129.901
127.347
120.784
118.511
108.229
81.621
58.179
53.884
47.536
40.478
34.249
21.689
MeO
N
H
NTs
25
ppm

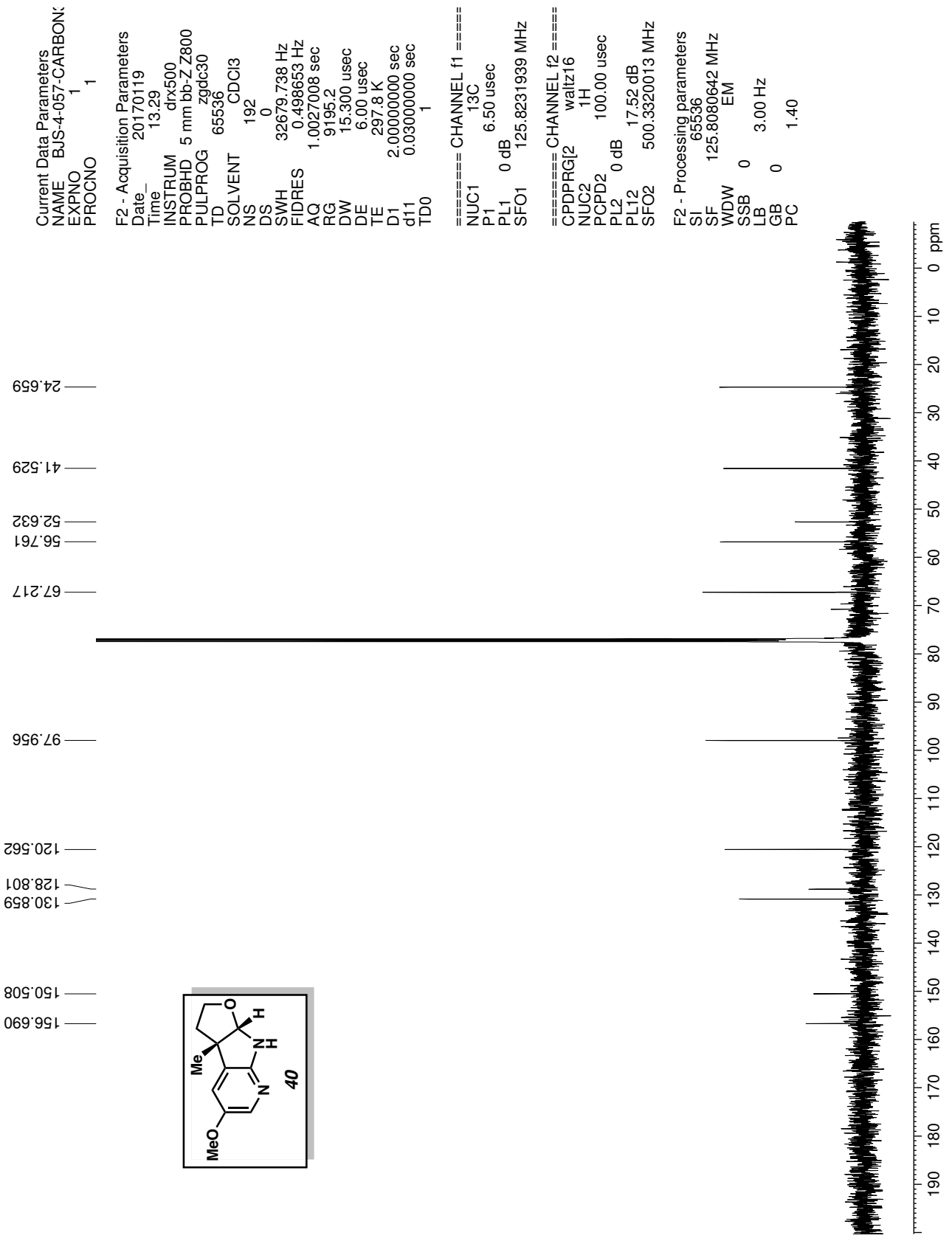

Current Data Parameters
NAME MH-2-258-CARBONF
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170420
Time_ 18.59 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 1024
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 14.67
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7577429 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.212
22.655
35.425
45.877
46.442
51.940
52.068
53.183
53.382
54.562
81.353
82.056
109.038
109.071
120.619
120.733
136.619
137.020
150.261
150.309
154.358
155.446
160.014
160.180
MeO
Me
N
H
N
NCO2Me
27
Rotamers
ppm

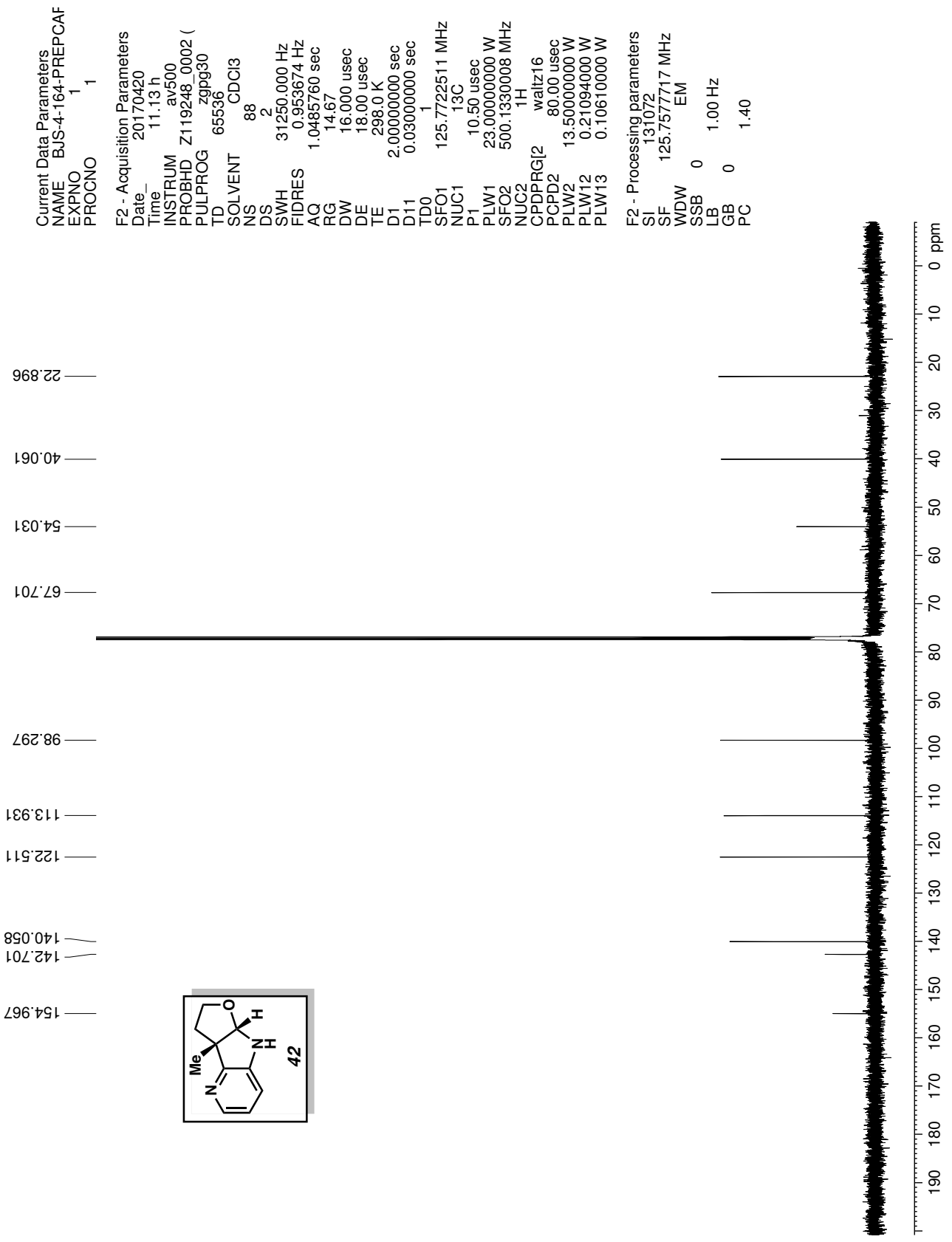

Current Data Parameters
NAME BJS-3-291-PURECAF
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170212
Time 15.00
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 6502
DW 15.300 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 =====
NUC1 13C
P1 6.50 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 125.8080672 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
156.099
142.199
129.791
126.193
116.675
98.488
67.714
54.211
39.935
22.811
Me
N
Br
O
H
N
H
30
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Current Data Parameters
NAME BJS-3-298-PURECAF
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170212
Time_ 15.09
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 6.50 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 125.8080672 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
155.316
141.828
140.539
122.531
116.708
98.605
67.705
54.199
39.897
22.758
Me
N
Cl
O
H
N
H
32
0 ppm


Current Data Parameters
NAME BJS-4-072-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170328
Time_ 17.41 h
INSTRUM av500
PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 12.14
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7577716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.805
39.800
54.879
55.476
67.876
98.815
105.650
132.300
141.888
149.837
154.210
0 ppm
Me
OMe
34


Current Data Parameters
NAME BJS-3-299-PURECAF
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170212
Time_ 15.37
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 14596.5
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 6.50 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 125.8080657 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
149.993
142.252
137.115
132.894
112.270
99.929
67.620
55.096
53.236
40.788
23.962
Me
OMe
38
ppm


Current Data Parameters
NAME BJS-4-057-CARBON
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170119
Time_ 13.29
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 192
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 9195.2
DW 15.300 usec
DE 6.00 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 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 125.8080642 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
156.690
150.508
130.859
128.801
120.562
97.956
67.217
56.761
52.632
41.529
24.659
Me
MeO
40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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SOLVENT CDCl3
NS 88
DS 2
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FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 14.67
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
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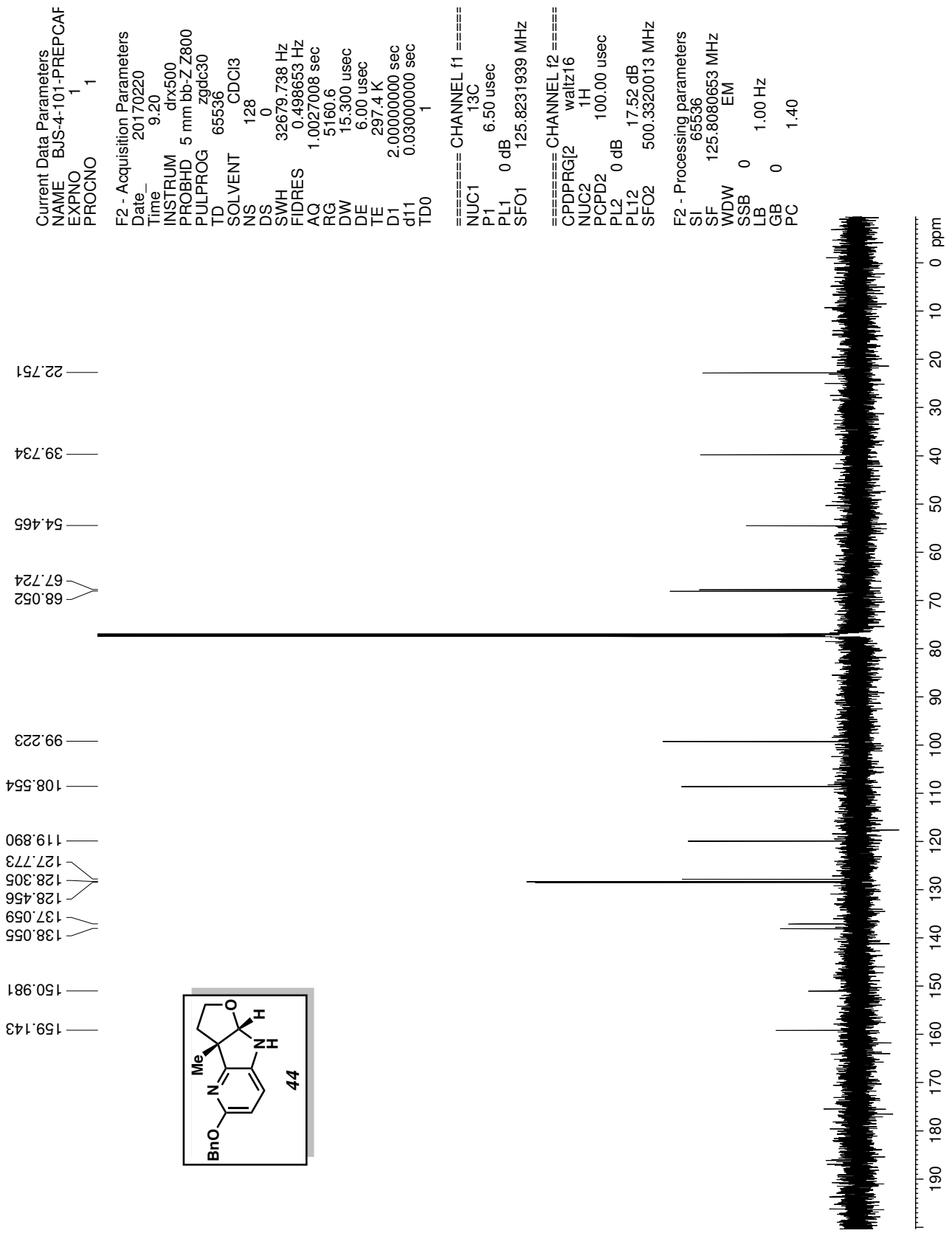
SF 125.7577717 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
154.967
142.701
140.058
122.511
113.931
98.297
67.701
54.031
40.061
22.896
Me
N
H
N
H
O
42
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
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FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 5160.6
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 6.50 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 125.8080653 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
159.143
150.981
138.055
137.059
128.456
128.305
127.773
119.890
108.554
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67.724
54.465
39.734
22.751
Me
N
BnO
O
H
N
44
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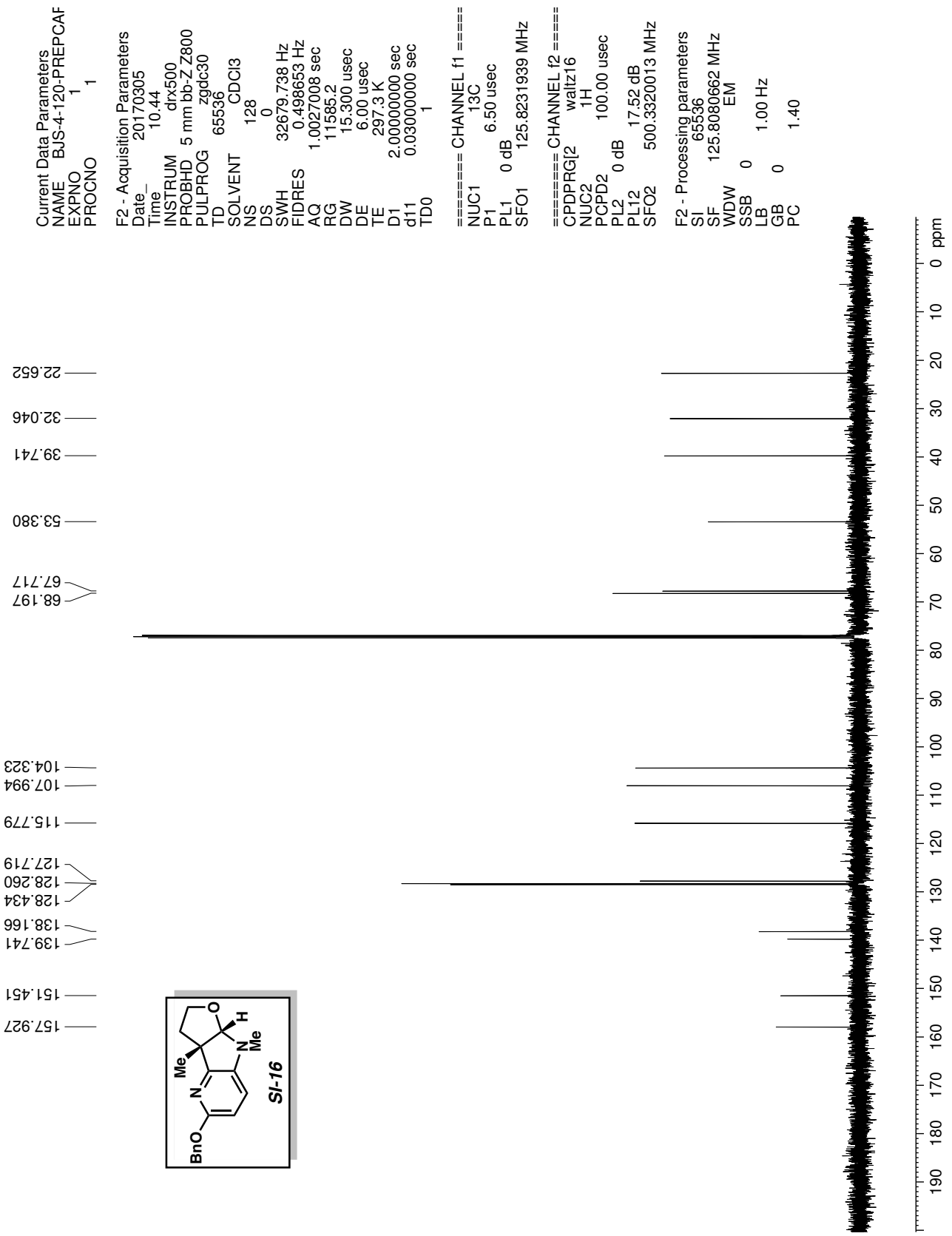
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PROCNO 1
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PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027008 sec
RG 11585.2
DW 15.300 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 =====
NUC1 13C
P1 6.50 usec
PL1 0 dB
SFO1 125.8231939 MHz
======== CHANNEL f2 =====
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NUC2 1H
PCPD2 100.00 usec
PL2 0 dB
PL12 17.52 dB
SFO2 500.3320013 MHz
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.652
32.046
39.741
53.380
67.717
68.197
104.323
107.994
115.779
127.719
128.260
128.434
138.166
139.741
151.451
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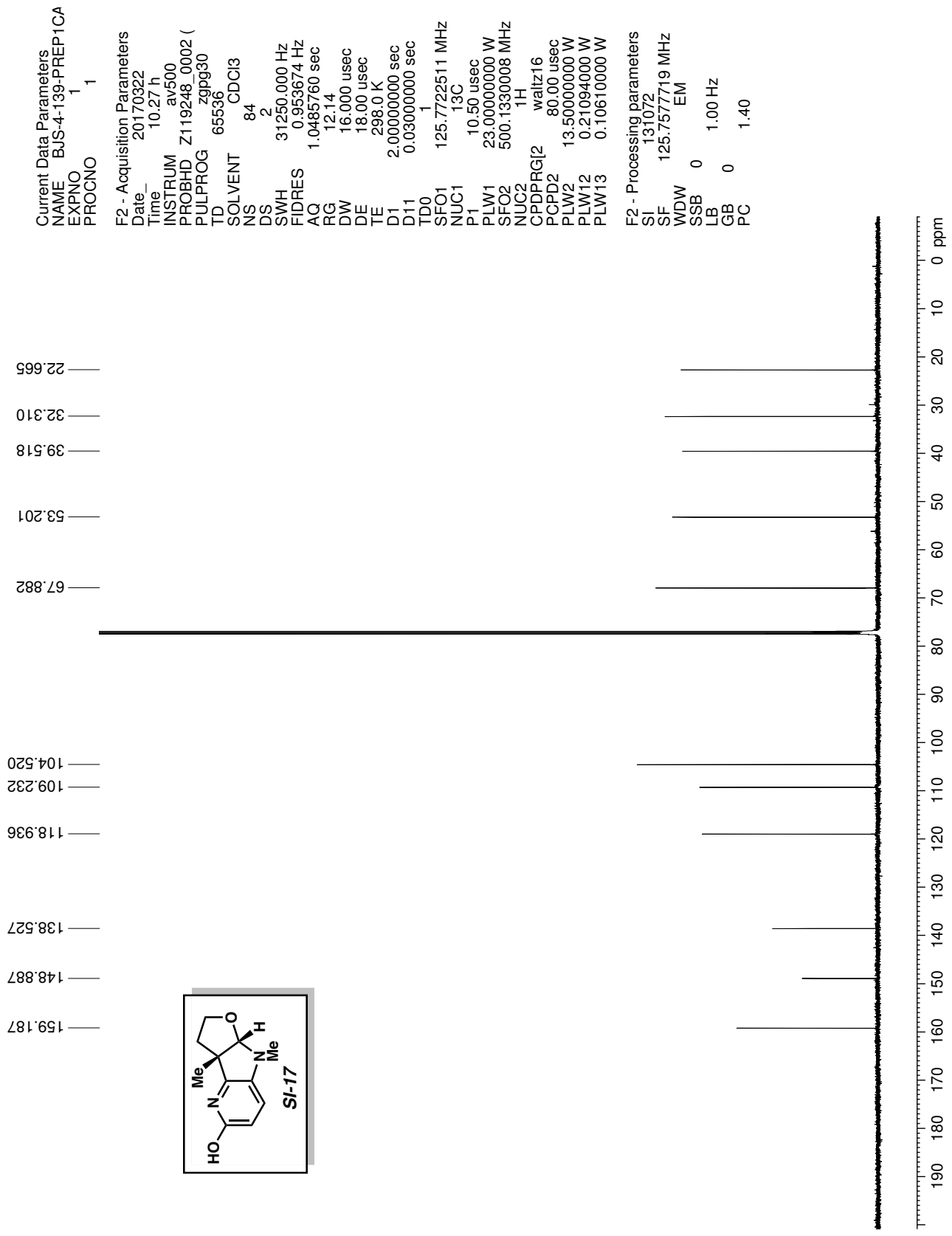
O
H
N
Me
N
BnO
0 ppm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Time_ 10.27 h
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PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 84
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 12.14
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
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SF 125.7577719 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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32.310
39.518
53.201
67.882
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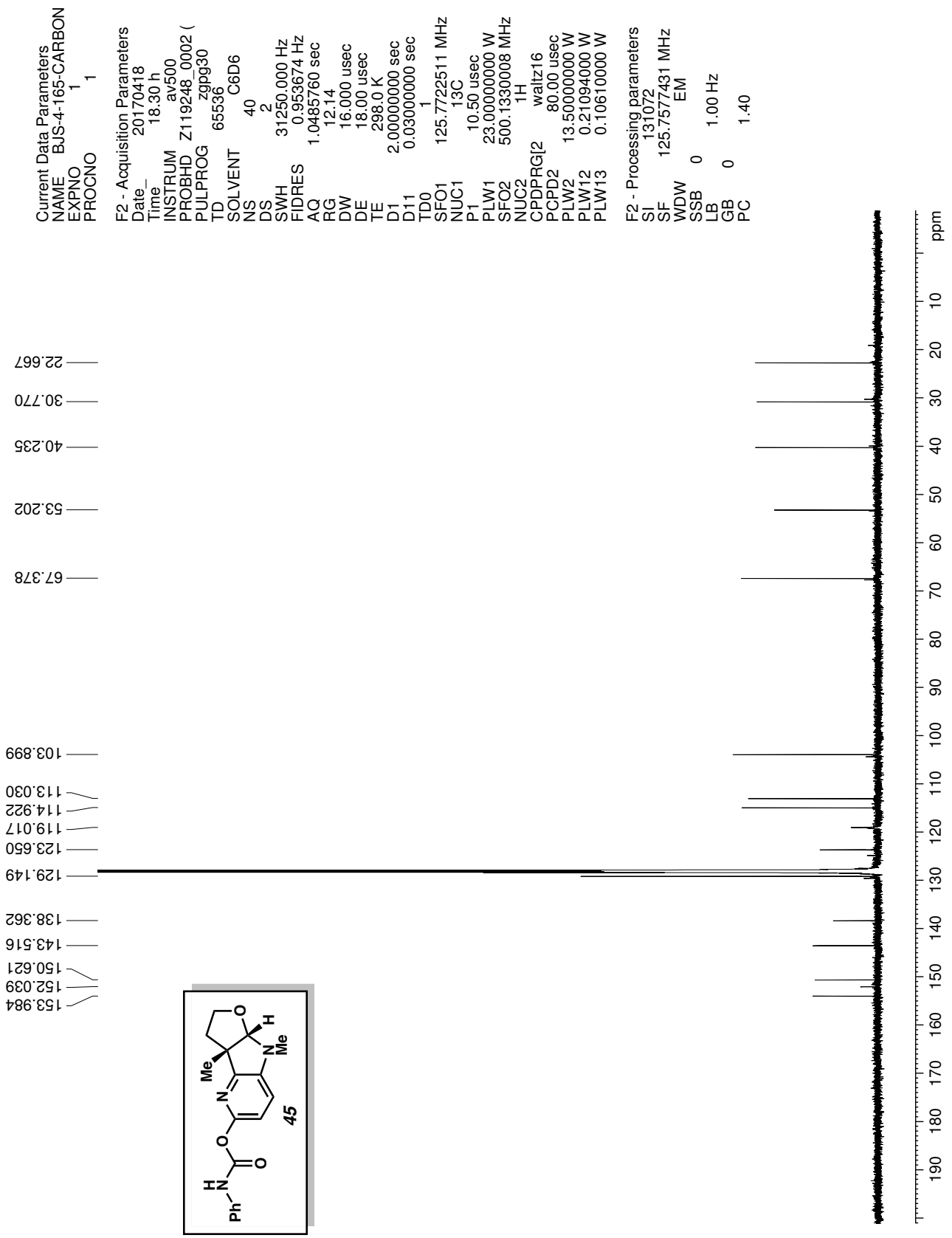
138.527
148.887
159.187
Me
N
Me
N
H
O
HO
SI-17
0 ppm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PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 40
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 12.14
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
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SF 125.7577431 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.667
30.770
40.235
53.202
67.378
103.899
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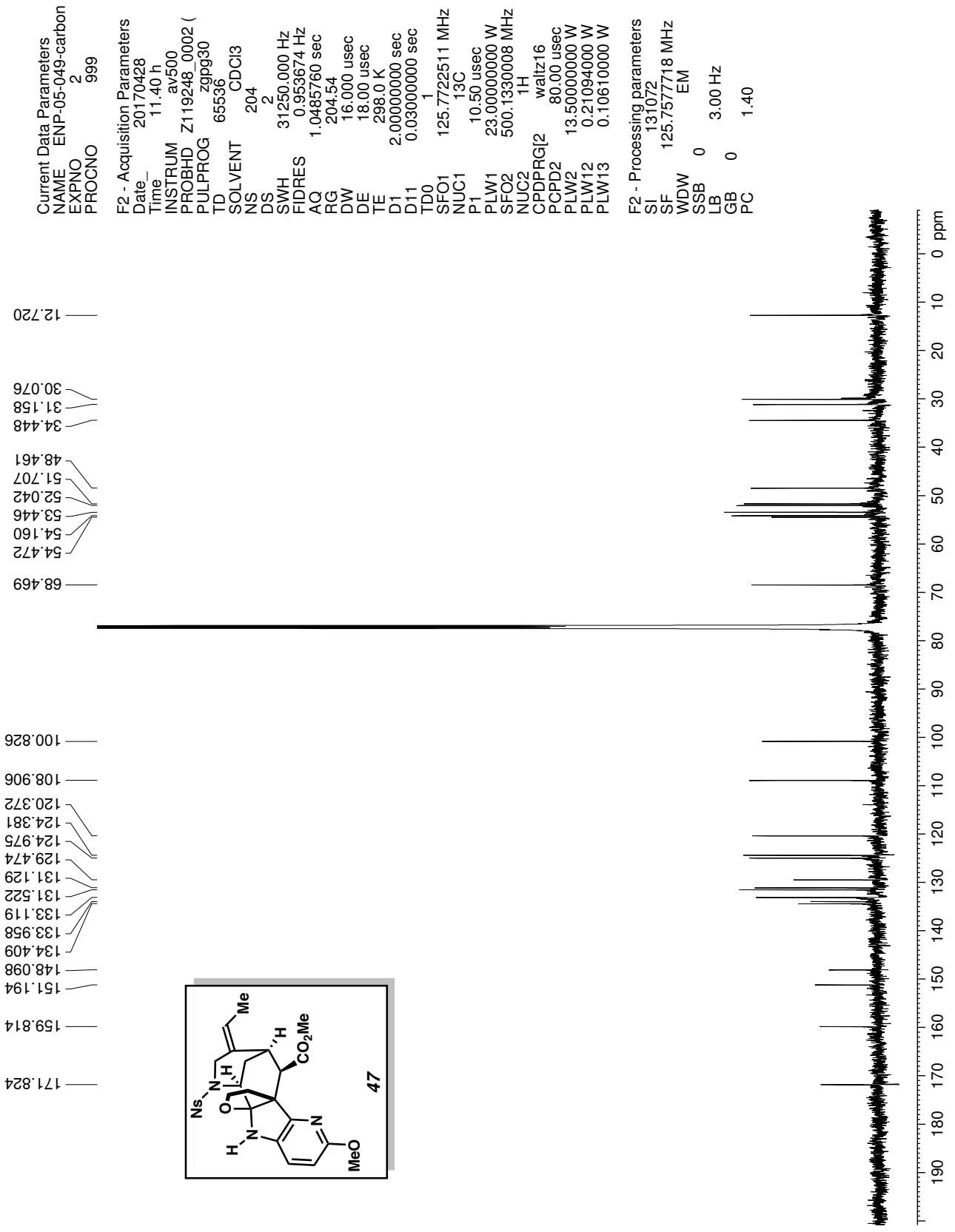
129.149
138.362
143.516
150.621
152.039
153.984
ppm
45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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 204
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 204.54
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
SI 131072
SF 125.7577718 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
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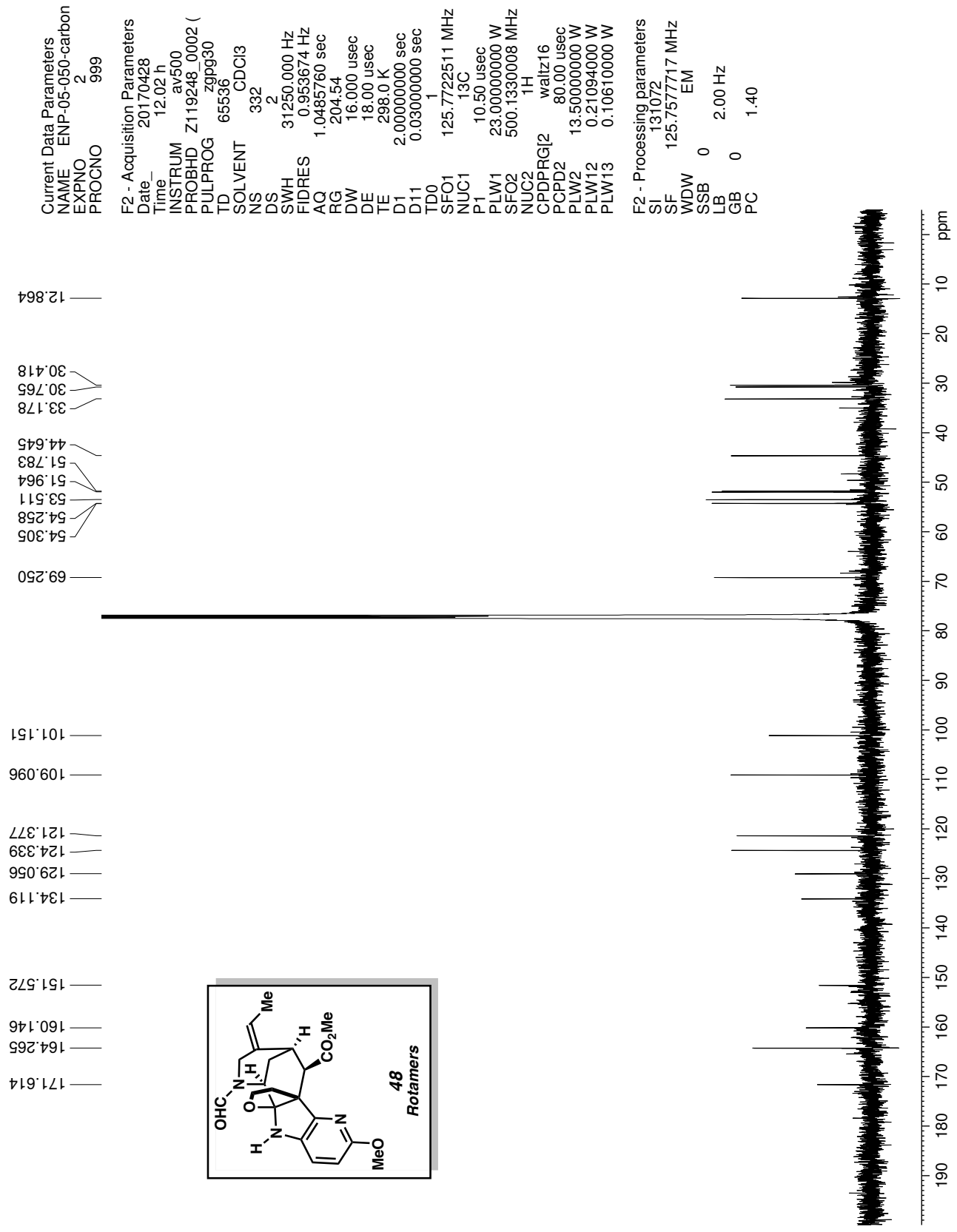
30.076
31.158
34.448
48.461
51.707
52.042
53.446
54.160
54.472
68.469
100.826
108.906
120.372
124.381
124.975
129.474
131.129
131.522
133.119
133.958
134.409
148.098
151.194
159.814
171.824
Me
H
CO2Me
Ns
N
H
O
N
H
N
MeO
47
0 ppm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Time 12.02 h
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PROBHD Z119248_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 332
DS 2
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 204.54
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7722511 MHz
NUC1 13C
P1 10.50 usec
PLW1 23.00000000 W
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.10610000 W
F2 - Processing parameters
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WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
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30.418
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51.783
51.964
53.511
54.258
54.305
69.250
101.151
109.096
121.377
124.339
129.056
134.119
151.572
160.146
164.265
171.614
OHC
Me
H
CO2Me
MeO
48
Rotamers
ppm

Part II: Computational Section

Full computational details

Ab initio calculations were performed with Gaussion 09.[1] Geometries were optimized and their vibrational frequencies obtained at the MP2/6-31G(d) level of theory, with the SMD solvation model for water.[2] MP2 energies were corrected using the "spin-component-scaled" (SCS) approach, pioneered by Grimme,[3] such as

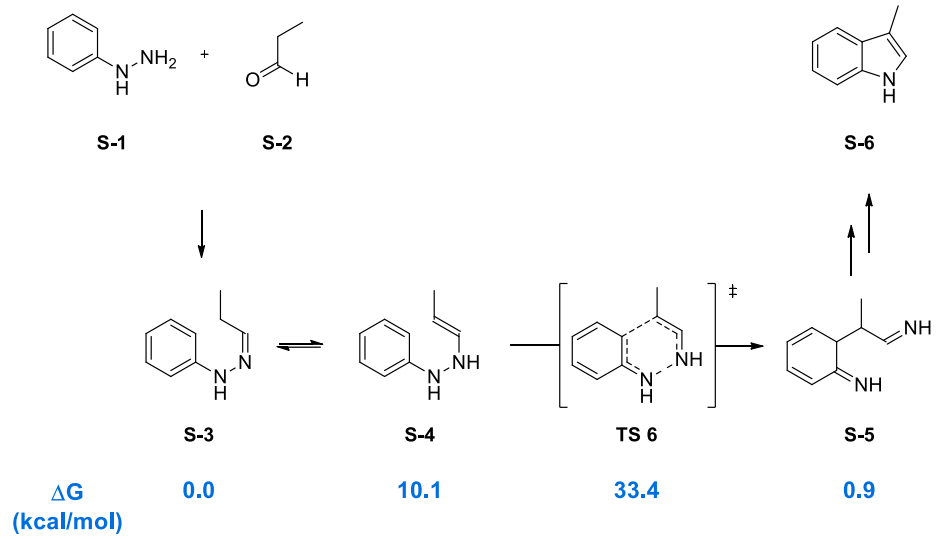
$$E(\text{SCS-MP2}) = E(\text{SCF}) + 1.2*(\alpha\beta) + (1/3)*(\alpha\alpha+\beta\beta)$$

where αα, ββ, and αβ are the "alpha-alpha", "beta-beta" and "alpha-beta" spin contributions, respectively, found in the Gaussian output. In the case of closed-shell calculations such as those used in the current study, αα and ββ are identical. This SCS-MP2 correction was found to greatly improve the performance of MP2 calculations, notably for sigmatropic rearrangements.[4] This SCS-MP2/6-31G(d)/SMD(water)//MP2/6-31G(d)/SMD(water) method was also chosen as we have previously shown that it accurately reproduces experimental rates of Fischer indolization reactions.[5] Normal mode frequency analysis was used to confirm that stationary points were either minima (no imaginary frequency) or saddle-points (TS, one (1) imaginary frequency) on the potential energy surface. All saddle-points were further analyzed with the Intrinsic Reaction Coordinate (IRC) tools to verify that they connected the expected minima. ZPE, enthalpy and free energy corrections were obtained using a standard state of 1 atmosphere of pressure and 298 K. Free energies were computed using Truhlar's quasiharmonic oscillator approximation, setting all frequencies below 100 cm^{-1} to 100 cm^{-1}.[6] The free energies reported in this study are thus obtained by adding the quasiharmonic free energy corrections to the SCS-MP2 electronic energies. Reported structures are the result of extensive conformation sampling on all evaluated compounds. Structures were illustrated using CYLview.[7] To obtain atomic charges, natural bond orbital (NBO) analysis (pop=nbo keyword in Gaussian 09) was performed at the MP2/6-311+G(d,p) level (gas phase) on the MP2/6-31G(d)/SMD(water)-optimized structures.

Additional figures and discussion

To study the effects of protonation and substituents on the barriers of the [3,3] sigmatropic rearrangement typical of Fischer indolization reactions, we chose a model system based on the combination of aryl/pyridyl hydrazines with propanal **S-2**. We have previously shown that in the case of aryl hydrazines, the [3,3]-rearrangement is the rate-limiting step of the reaction and occurs with the substrates being monoprotonated.[5]

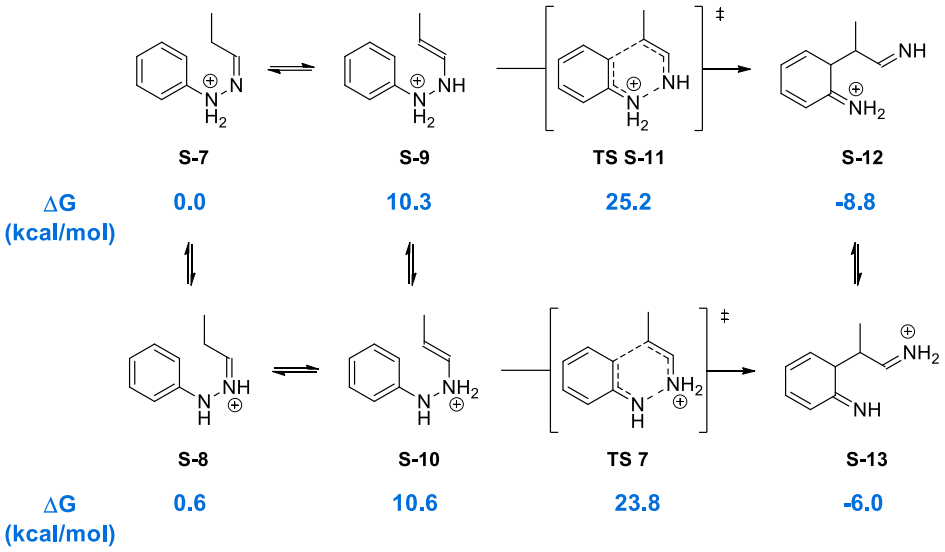
Scheme S-1: Thermal (unprotonated) Fischer indolization reaction of our model system.



In the thermal Fischer indolization reaction (**Scheme S-1**), hydrazone **S-3** (formed from the condensation of aryl hydrazine **S-1** with propanal **S-2**) first tautomerizes to ene-hydrazine **S-4**, which can then undergo a [3,3]-sigmatropic rearrangement to form diimine **S-5**. This intermediate then rearomatizes and goes on to form the indole product **S-6**. When all compounds are neutral, reaching **TS 6** from the hydrazone costs 33.4 kcal/mol. This barrier is much higher than what is known experimentally for such reactions.[5]

In the acid-catalyzed (monoprotonated) reaction (**Scheme S-2**), two pathways are available to the substrates. The hydrazone with its α nitrogen protonated (**S-7**) is the global minimum of the system, but **TS 7** has the smallest barrier for the rearrangement. In this case, the activation free energy of the reaction is then 23.8 kcal/mol, which is in agreement with experimental rates.[5]

Scheme S-2: Acid-catalyzed (monoprotonated) Fischer indolization reaction of our model system.

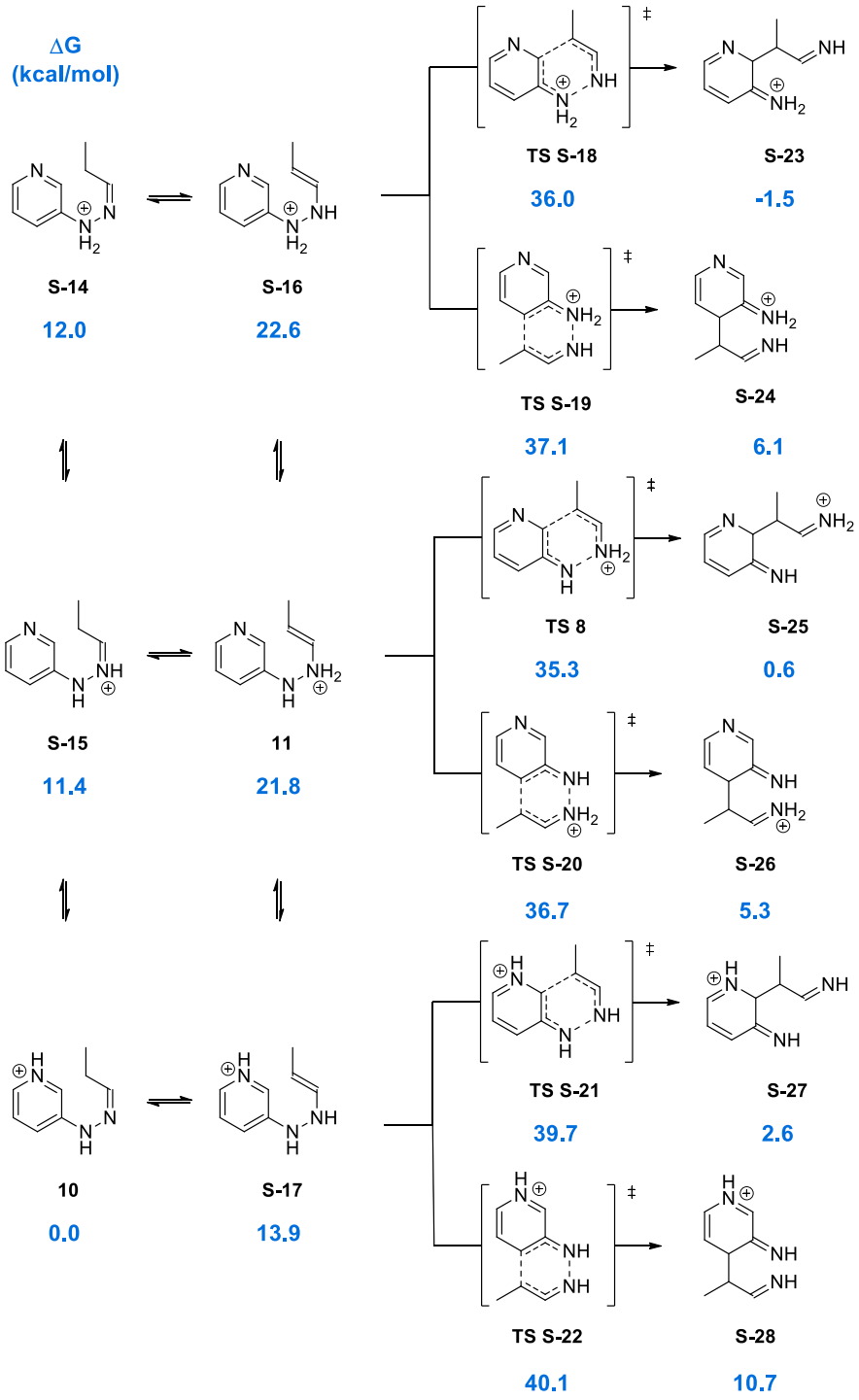


Therefore, all other systems that we studied were singly protonated. For all pyridyl hydrazines, three different nitrogen atoms can be protonated on any intermediate or transition state. Moreover, in most cases the [3,3]-rearrangement can occur on two different carbons, meaning two transition states and two diimine products are possible for each protonation state. The full pathway for the parent pyridyl hydrazine is presented below in **Scheme S-3**.

Relative free energies for all other computed systems can be found in **Table S-1**. In all cases the global minimum is the hydrazone protonated at the pyridine nitrogen. Moreover, in all but one case, the most favored transition state goes through protonation at the β-nitrogen of the hydrazone.

The free energy for the pathway of α-methylpyridine hydrazone is found in **Scheme S-4**. Once again, the hydrazone protonated at the pyridine nitrogen is the global minimum of the system, and because of the increased basicity of the methyl-substituted ene-hydrazine α nitrogen, the best transition state goes through with protonation of the α-nitrogen.

Scheme S-3: Full pathway for the reaction of protonated 3-pyridylhydrazine. Free energies in kcal/mol.



Scheme S-4: Productive pathway for the reaction of methyl-substituted protonated 3-pyridylhydrazine. Free energies in kcal/mol.

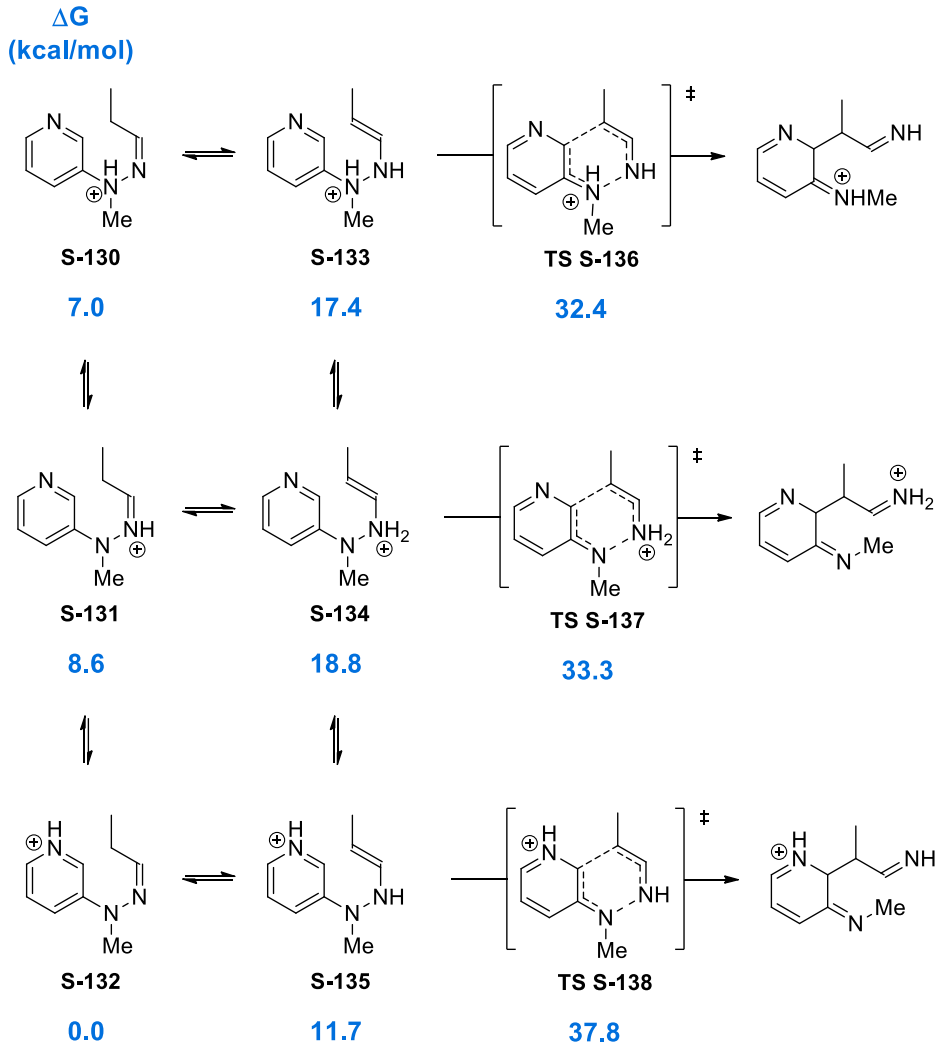
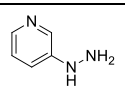
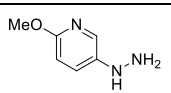
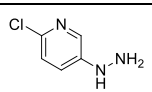
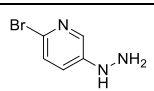
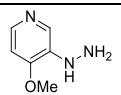
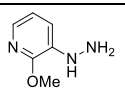
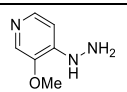
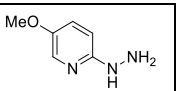
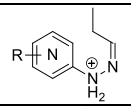
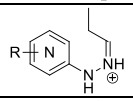
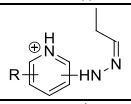
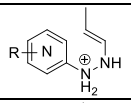
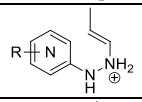
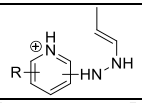
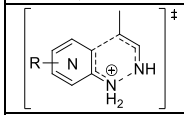
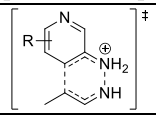
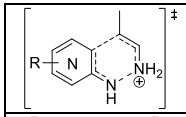
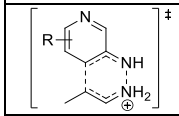
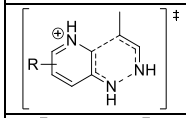
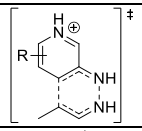
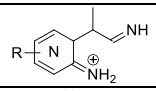
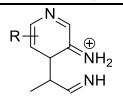
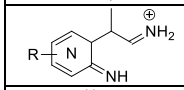
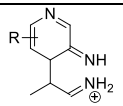
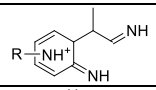
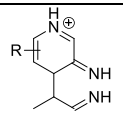


Table S-1: Compound numbers and relative free energies (kcal/mol) for each possible intermediate or transition state on the potential energy pathways of different monoprotonated pyridyl hydrazones formed by pyridyl hydrazines and propanal.

	 41		 12		 31		 29		 33		 37		 35		 39	
	cmpd #	Δ*G*	cmpd #	Δ*G*	cmpd #	Δ*G*	cmpd #	Δ*G*	cmpd #	Δ*G*	cmpd #	Δ*G*	cmpd #	Δ*G*	cmpd #	Δ*G*
	**S-14**	12.0	**S-29**	6.5	**S-46**	4.8	**S-64**	4.5	**S-82**	13.0	**S-94**	4.2	**S-106**	17.4	**S-118**	10.2
	**S-15**	11.4	**S-30**	5.7	**S-47**	2.9	**S-65**	2.1	**S-83**	12.0	**S-95**	3.4	**S-107**	15.4	**S-119**	8.6
	**10**	0.0	**S-31**	0.0	**S-48**	0.0	**S-66**	0.0	**S-84**	0.0	**S-96**	0.0	**S-108**	0.0	**S-120**	0.0
	**S-16**	22.6	**S-32**	16.5	**S-49**	15.4	**S-67**	14.8	**S-85**	23.1	**S-97**	15.8	**S-109**	28.2	**S-121**	21.8
	**11**	21.8	**S-33**	14.9	**S-50**	12.5	**S-68**	12.1	**S-86**	20.1	**S-98**	11.5	**S-110**	23.7	**S-122**	18.8
	**S-17**	13.9	**S-34**	13.9	**S-51**	14.3	**S-69**	14.2	**S-87**	14.6	**S-99**	12.8	**S-111**	15.3	**S-123**	13.3
	**S-18**	36.0	**S-35**	27.8	**S-52**	28.6	**S-70**	27.9	**S-88**	35.5	**S-100**	**25.6**	**S-112**	42.0	**S-124**	35.2
	**S-19**	37.1	**S-36**	32.4	**S-53**	30.5	**S-71**	29.7	–	**–**	–	–	–	**–**	–	**–**

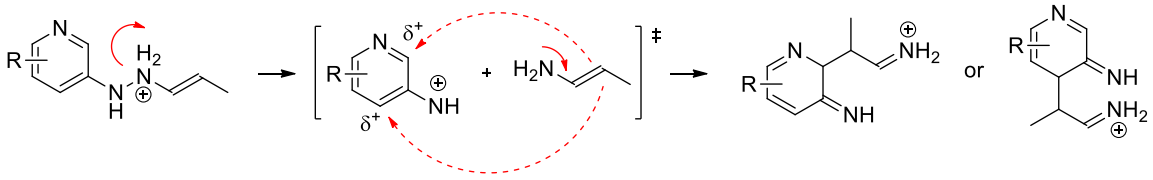
	**8**	**35.3**	**9**	**26.3**	**S-54**	**27.6**	**S-72**	**26.8**	**S-89**	**34.5**	**S-101**	25.8	**S-113**	**40.3**	**S-125**	**32.2**
	**S-20**	36.7	**S-37**	31.2	**S-55**	29.1	**S-73**	28.4	–	–	–	–	–	–	–	–
	**S-21**	39.7	**S-38**	35.9	**S-56**	39.6	**S-74**	40.0	**S-90**	37.7	**S-102**	35.3	**S-114**	45.0	**S-126**	41.7
	**S-22**	40.1	**S-39**	40.0	**S-57**	40.5	**S-75**	40.5	–	–	–	–	–	–	–	–
	**S-23**	-1.5	**S-40**	-10.2	**S-58**	-8.8	**S-76**	-9.3	**S-91**	-0.1	**S-103**	-4.3	**S-115**	5.5	**S-127**	0.7
	**S-24**	6.1	**S-41**	8.3	**S-59**	0.6	**S-77**	-0.4	–	–	–	–	–	–	–	–
	**S-25**	0.6	**S-42**	-9.2	**S-60**	-8.7	**S-78**	-9.3	**S-92**	0.5	**S-104**	-5.9	**S-116**	7.0	**S-128**	1.4
	**S-26**	5.3	**S-43**	2.7	**S-61**	-1.6	**S-79**	-2.5	–	–	–	–	–	–	–	–
	**S-27**	2.6	**S-44**	-6.7	**S-62**	1.8	**S-80**	2.6	**S-93**	0.0	**S-105**	0.7	**S-117**	11.3	**S-129**	10.0
	**S-28**	10.7	**S-45**	-4.3	**S-63**	-7.3	**S-81**	-8.6	–	–	–	–	–	–	–	–

Origin of regioselectivity

Fischer indolization reactions with aza-substituted substrates are regioselective. The calculations support these results. In the case of the 2-methoxy-5-hydrazinylpyridine, the [3,3]-rearrangement at the 6-position is favored by 4.9 kcal/mol over the rearrangement at the 4-position of the pyridine ring.

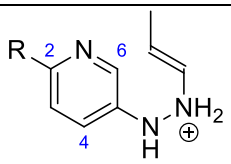
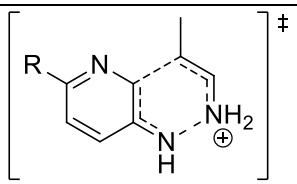
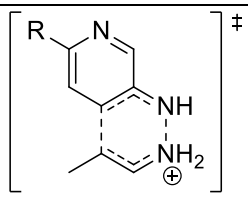
The [3,3] rearrangements are, for all but one aza-substituted system, favored by protonation at the β nitrogen. In the only case where the α-protonated TS is favored, it is only 0.2 kcal/mol lower than the β-protonated TS. We propose the following explanation for the regioselectivity (Scheme S-4). In the transition state, N–N bond cleavage creates two "pieces" of the substrate: a neutral enamine piece and a cationic aromatic ring. This ring is attacked at either the carbon alpha or gamma from the pyridine nitrogen.

Scheme S-4: Schematic representation of a [3,3] sigmatropic rearrangement happening with the β-nitrogen of the ene-hydrazine protonated.



The preference for attack at either position can be predicted from the extent of positive charge on these carbons, before or at the transition state. Using NBO analysis, we calculated the charge at these carbons for the aza-substituted substrate and those with a substituent at the 2-position. We also calculated the same charges for the two transition states leading to regioisomeric products. These data are listed below in Table S-2.

Table S-2: Relative free energies (in kcal/mol, from their respective global minima) and NBO charges of the β-protonated ene-hydrazine and transition states, for the various 2-substituted 5-pyridylhydrazines.

										
entry	**R**	**ΔG**	**z (C4)**	**z (C6)**	**ΔG**	**z (C4)**	**z (C6)**	**ΔG**	**z (C4)**	**z (C6)**
1	H	21.8	-0.132	+0.108	35.3	-0.082	+0.164	36.7	-0.061	+0.182
2	OMe	14.9	-0.110	+0.146	26.3	-0.075	+0.212	31.2	-0.021	+0.225
3	Cl	12.5	-0.127	+0.123	27.6	-0.072	+0.178	29.1	-0.051	+0.207
4	Br	12.1	-0.132	+0.117	26.8	-0.073	+0.177	28.4	-0.053	+0.205

For the unsubstituted case (entry 1), the positive charge at C-6 is much greater than that of C-4, both in the ene-hydrazine and in the transition states. Even more important is that this difference is very similar in both transition states, even though they lead to different products. The greater positive charge at C-6 is presumably caused by the proximity of the pyridine nitrogen, which acts as an electronegative element.

For the methoxy-substituted substrate (entry 2), the difference between the partial positive charge at the C-6 and C-4 positions is even greater. Thus, the regioselectivity would be predicted to be higher, which is what the calculated activation barriers predict. The increased difference is attributed to the methoxy substituent at the 2-position. Indeed, this group is located at the *meta* position of both C-4 and C-6 and as such provides a strong electron-withdrawing effect. For C-6, both the pyridine nitrogen and 2-methoxy combine to make attack at this position much easier than at C-4.

For the halogenated substrates (entries 3 and 4), the same explanation is true. The electronegative substituents make the charge at C-6 more positive, in line with these substrates being slightly more regioselective than the unsubstituted case. Once again, the extent of positive charge do not vary significantly if the TS happens at C-4 or C-6, and are very similar to that observed in the ene-hydrazine intermediate.

Therefore, for these Fischer indolization reactions with aza-substituted compounds, analysis of the charges on the reactant are a good way to determine which will be the most favored regiosiomer formed during the [3,3]-rearrangement.

Cartesian coordinates, energies and vibrational frequencies

These geometries and thermal corrections were obtained at the MP2/6-31G(d)/SMD(water) level of theory. Energies were corrected with the SCS-MP2 method. Charges associated with each structure are +1, unless otherwise specified.

Phenyl hydrazine (S-1)

S-3
Charge: 0

C	3.33631	-0.40947	-0.24650
C	0.87491	0.83583	0.20608
C	2.17482	-1.17414	-0.15639
C	3.28002	0.98183	-0.11473
C	2.04443	1.59417	0.10111
C	0.93311	-0.55705	0.06600
N	-0.20779	-1.39067	0.24622
N	-1.43527	-0.78214	-0.23399
C	-2.09994	-0.25072	0.73186
C	-3.38459	0.47177	0.49535
H	2.22041	-2.25630	-0.26892
H	4.28869	-0.90470	-0.42214
H	4.18517	1.57882	-0.18936
H	1.98364	2.67553	0.20279
H	-0.07425	1.33556	0.37291
H	-1.73568	-0.31830	1.76162
H	-4.15297	-0.01066	1.11390
H	-0.08022	-2.22599	-0.32920
H	-3.27220	1.48220	0.91038
C	-3.82955	0.53802	-0.95856
H	-3.08285	1.04393	-1.57532
H	-3.98543	-0.46205	-1.37016
H	-4.77006	1.09011	-1.03741

There are no imaginary frequencies.

SCF energy: -456.652627 hartree
αα/ββ: -0.19286032 hartree
αβ: -1.08691 hartree
SCS-MP2 energy: -458.0854918 hartree
zero-point correction: +0.197432 hartree
enthalpy correction: +0.209010 hartree
free energy correction: +0.160136 hartree
quasiharmonic free energy correction: +0.161979 hartree

S-4
Charge: 0

C	2.82298	-0.19133	0.90330
C	0.78579	-0.33010	-1.00534
C	1.86758	0.82328	0.83043
C	2.76056	-1.28543	0.03564
C	1.73831	-1.34637	-0.91579
C	0.84501	0.76158	-0.12680
N	-0.05655	1.84912	-0.26436
N	-1.43295	1.52271	-0.51510
C	-1.94901	0.47531	0.28660
C	-2.71700	-0.52880	-0.16446
H	1.90742	1.66903	1.51572
H	3.61017	-0.13186	1.65166
H	3.49969	-2.07993	0.09873
H	1.68057	-2.19068	-1.59931
H	0.00567	-0.38056	-1.76038
H	-1.53442	1.31389	-1.50917
H	-1.74378	0.60420	1.34924
H	-2.88857	-0.62056	-1.23784
H	-0.03031	2.44344	0.56448
C	-3.38551	-1.52285	0.73496
H	-3.09802	-2.54832	0.47767
H	-3.11708	-1.34474	1.78073
H	-4.47716	-1.46835	0.65345

There are no imaginary frequencies.

SCF energy: -456.638210 hartree
αα/ββ: -0.19319933 hartree
αβ: -1.08509 hartree
SCS-MP2 energy: -458.069116 hartree
zero-point correction: +0.197432 hartree
enthalpy correction: +0.209071 hartree
free energy correction: +0.160423 hartree
quasiharmonic free energy correction: +0.161753 hartree

TS 6
Charge: 0

C	-1.32280	1.27061	0.80076
C	-1.47974	-1.21303	-0.50421
C	-0.33841	0.28552	1.04763
C	-2.30505	1.04114	-0.14700
C	-2.38329	-0.21115	-0.80072
C	-0.48621	-1.02006	0.49617
N	0.40112	-2.03315	0.71971
N	1.87813	-1.53454	-0.50608
C	2.12678	-0.24682	-0.17597
C	1.36742	0.83692	-0.57591

H	0.36329	0.42531	1.86780
H	-1.26209	2.23001	1.30908
H	-3.04554	1.80760	-0.36369
H	-3.15793	-0.38155	-1.54491
H	-1.55001	-2.18962	-0.97976
H	1.20128	-1.54535	-1.28164
H	2.88780	-0.09585	0.59280
H	0.64065	0.68007	-1.37539
H	0.98344	-1.78508	1.53207
C	1.73642	2.25060	-0.25756
H	0.84231	2.85328	-0.07090
H	2.38586	2.30230	0.62144
H	2.26541	2.71027	-1.10153

1 imaginary frequency: –302.89 cm^{-1}.

SCF energy: -456.557954 hartree
αα/ββ: -0.20316385 hartree
αβ: -1.11535 hartree
SCS-MP2 energy: -458.0318145 hartree
zero-point correction: +0.196115 hartree
enthalpy correction: +0.206855 hartree
free energy correction: +0.161388 hartree
quasiharmonic free energy correction: +0.161570 hartree

S-5
Charge: 0

C	-1.22158	1.32230	0.60837
C	-1.59925	-1.27039	-0.51750
C	-0.10330	0.33126	0.74976
C	-2.28763	1.05681	-0.17761
C	-2.43846	-0.24652	-0.81073
C	-0.53793	-1.09101	0.47125
N	0.01187	-2.14384	0.99119
N	2.62129	-1.14641	-0.85767
C	2.20272	-0.23036	-0.05804
C	1.04071	0.69650	-0.26010
H	0.32775	0.38210	1.76004
H	-1.11589	2.28889	1.09480
H	-3.06968	1.79880	-0.31925
H	-3.25936	-0.39714	-1.50859
H	-1.74897	-2.26576	-0.92940
H	2.00703	-1.16829	-1.68361
H	2.75831	-0.09350	0.87595
H	0.64403	0.55289	-1.27478
H	0.71534	-1.84595	1.68118
C	1.51178	2.14226	-0.08720
H	0.71232	2.84827	-0.32233
H	1.84334	2.31965	0.94129
H	2.35126	2.34669	-0.75913

There are no imaginary frequencies.

SCF energy: -456.645429 hartree
αα/ββ: -0.19044504 hartree
αβ: -1.09402 hartree
SCS-MP2 energy: -458.0852191 hartree
zero-point correction: +0.198401 hartree
enthalpy correction: +0.209665 hartree
free energy correction: +0.162498 hartree
quasiharmonic free energy correction: +0.163153 hartree

S-7

C	-2.87754	-0.96957	0.63133
C	-1.31137	1.11992	-0.40334
C	-1.72361	-1.27296	-0.09306
C	-3.24634	0.36215	0.84169
C	-2.46984	1.40215	0.32149
C	-0.97493	-0.21607	-0.59911
N	0.26356	-0.51915	-1.32369
N	1.39917	-0.53303	-0.39555
C	2.21445	0.43997	-0.60590
C	3.41513	0.61700	0.25550
H	0.40571	0.15018	-2.10333
H	-1.42017	-2.30229	-0.27044
H	-3.48472	-1.77563	1.03338
H	-4.14617	0.59088	1.40630
H	-2.76096	2.43609	0.48377
H	-0.69302	1.91514	-0.81375
H	2.06050	1.16360	-1.41208
H	4.28624	0.62351	-0.41208
H	0.21216	-1.46426	-1.73607
H	3.35649	1.63243	0.66863
C	3.58245	-0.41388	1.36117
H	2.73033	-0.40353	2.04470
H	3.67975	-1.42156	0.95025
H	4.48436	-0.19158	1.93674

There are no imaginary frequencies.

SCF energy: -457.109498 hartree
αα/ββ: -0.19043871 hartree
αβ: -1.08457 hartree
SCS-MP2 energy: -458.5379371 hartree
zero-point correction: +0.212249 hartree
enthalpy correction: +0.223867 hartree
free energy correction: +0.174869 hartree
quasiharmonic free energy correction: +0.176568 hartree

S-8

C	3.32961	-0.45293	0.46450
C	1.03503	0.82112	-0.51100
C	2.13259	-1.16283	0.37034
C	3.38485	0.89216	0.08799
C	2.23468	1.52531	-0.38939
C	0.99080	-0.51894	-0.11497

N	-0.20340	-1.28703	-0.29765
N	-1.35175	-0.56114	0.07903
C	-2.39422	-0.53626	-0.67410
C	-3.63513	0.17858	-0.31941
H	2.07726	-2.20597	0.67600
H	4.21827	-0.95260	0.84166
H	4.31685	1.44462	0.17173
H	2.27049	2.56986	-0.68812
H	0.14971	1.31146	-0.90852
H	-2.31993	-1.09106	-1.60594
H	-3.86501	0.81974	-1.18039
H	-0.18158	-2.13238	0.28158
H	-4.42528	-0.58498	-0.31332
C	-3.60910	0.96845	0.97972
H	-3.44451	0.31572	1.84141
H	-2.82974	1.73558	0.96372
H	-4.57041	1.46746	1.11610
H	-1.32472	-0.04815	0.97233

There are no imaginary frequencies.

SCF energy: -457.117319 hartree
αα/ββ: -0.18961699 hartree
αβ: -1.07735 hartree
SCS-MP2 energy: -458.5365466 hartree
zero-point correction: +0.211617 hartree
enthalpy correction: +0.223164 hartree
free energy correction: +0.174762 hartree
quasiharmonic free energy correction: +0.176079 hartree

S-9

C	1.80085	-1.38117	0.89678
C	1.67111	0.85899	-0.79264
C	0.88072	-0.36792	1.17352
C	2.64215	-1.28396	-0.21487
C	2.58102	-0.16614	-1.05313
C	0.84893	0.73514	0.32490
N	-0.14453	1.78167	0.56667
N	-1.42079	1.63538	-0.16436
C	-2.07036	0.42701	0.22299
C	-2.37064	-0.54659	-0.64772
H	0.22610	-0.42156	2.04033
H	1.85388	-2.24828	1.54919
H	3.35525	-2.07691	-0.42342
H	3.24173	-0.09057	-1.91216
H	1.61070	1.73822	-1.43074
H	-1.14232	1.58172	-1.15172
H	-2.39115	0.40909	1.26261
H	-2.01537	-0.46298	-1.67523
H	0.22758	2.71004	0.30911
C	-3.20754	-1.73396	-0.29601
H	-2.67074	-2.66233	-0.51712
H	-3.47329	-1.72897	0.76459
H	-4.13174	-1.74903	-0.88365
H	-0.39089	1.83379	1.56913

SCF energy: -457.090831 hartree
αα/ββ: -0.19133648 hartree
αβ: -1.08604 hartree
SCS-MP2 energy: -458.5216367 hartree
zero-point correction: +0.212245 hartree
enthalpy correction: +0.223886 hartree
free energy correction: +0.174923 hartree
quasiharmonic free energy correction: +0.176622 hartree

There are no imaginary frequencies.

S-10

C	-2.82540	-0.37189	-0.95221
C	-1.17351	0.81594	0.96986
C	-1.72887	-1.07587	-0.45531
C	-3.11545	0.91073	-0.47526
C	-2.29388	1.49803	0.48995
C	-0.89831	-0.46875	0.49329
N	0.20304	-1.22490	1.02481
N	1.25362	-1.38882	0.00693
C	1.89479	-0.15614	-0.44600
C	3.14681	0.11425	-0.07227
H	-1.51687	-2.08791	-0.79619
H	-3.46898	-0.83596	-1.69511
H	-3.97992	1.44923	-0.85477
H	-2.51488	2.49492	0.86273
H	-0.51610	1.27301	1.70701
H	1.95099	-2.03180	0.41481
H	1.26293	0.46748	-1.06741
H	3.68228	-0.59700	0.55659
H	0.66430	-0.68392	1.76546
C	3.86608	1.35517	-0.48326
H	4.77507	1.09887	-1.03621
H	3.23787	1.99114	-1.11108
H	4.17334	1.92250	0.40084
H	0.81984	-1.89338	-0.78162

There are no imaginary frequencies.

SCF energy: -457.092823 hartree
αα/ββ: -0.19080449 hartree
αβ: -1.08457 hartree
SCS-MP2 energy: -458.521506 hartree
zero-point correction: +0.212874 hartree
enthalpy correction: +0.224506 hartree
free energy correction: +0.175632 hartree
quasiharmonic free energy correction: +0.177040 hartree

TS S-11

C	-1.34550	1.21663	0.86828

C	-1.47239	-1.20155	-0.57895
C	-0.36821	0.22357	1.09061
C	-2.31867	1.02149	-0.09678
C	-2.38562	-0.19319	-0.81712
C	-0.50962	-1.02425	0.44149
N	0.47981	-1.96200	0.61136
N	1.97815	-1.40932	-0.46438
C	2.14146	-0.11307	-0.10978
C	1.36461	0.91744	-0.59614
H	0.33709	0.32204	1.91239
H	-1.29470	2.14789	1.42496
H	-3.06038	1.79356	-0.28327
H	-3.15429	-0.32985	-1.57285
H	-1.51927	-2.14776	-1.11400
H	1.38999	-1.44084	-1.31115
H	2.83906	0.07830	0.70524
H	0.67645	0.69373	-1.41418
H	0.96697	-1.97862	1.51244
C	1.60793	2.35032	-0.27887
H	0.66110	2.88472	-0.15840
H	2.21068	2.46583	0.62539
H	2.13786	2.82354	-1.11532
H	0.31985	-2.89771	0.22351

1 imaginary frequency: -287.3 cm^{-1}.

SCF energy: -457.038603 hartree
αα/ββ: -0.19896648 hartree
αβ: -1.10513 hartree
SCS-MP2 energy: -458.4973999 hartree
zero-point correction: +0.210714 hartree
enthalpy correction: +0.221483 hartree
free energy correction: +0.175962 hartree
quasiharmonic free energy correction: +0.176247 hartree

TS 7

C	-1.52070	1.06853	0.88462
C	-1.31337	-1.32010	-0.59401
C	-0.44786	0.18995	1.12813
C	-2.42654	0.78617	-0.12647
C	-2.32240	-0.41580	-0.86274
C	-0.39701	-1.06590	0.46294
N	0.60840	-1.96807	0.66910
N	2.00777	-1.22280	-0.41857
C	2.15437	0.10090	-0.12650
C	1.23301	1.00623	-0.59095
H	0.22556	0.36717	1.96490
H	-1.60183	1.99011	1.45471
H	-3.24342	1.47302	-0.33411
H	-3.03944	-0.62365	-1.65282
H	-1.23697	-2.26067	-1.13504
H	1.54622	-1.47038	-1.29916
H	2.87742	0.33978	0.64706
H	0.55224	0.69305	-1.38282
H	1.09918	-1.71358	1.54047
C	1.32390	2.46313	-0.29055
H	0.32745	2.88397	-0.13228
H	1.94401	2.65376	0.58825
H	1.76309	2.98205	-1.15047
H	2.77298	-1.85723	-0.16915

1 imaginary frequency: –348.55 cm^{-1}.

SCF energy: -457.035454 hartree
αα/ββ: -0.19937008 hartree
αβ: -1.10869 hartree
SCS-MP2 energy: -458.4987894 hartree
zero-point correction: +0.210125 hartree
enthalpy correction: +0.221070 hartree
free energy correction: +0.175054 hartree
quasiharmonic free energy correction: +0.175375 hartree

S-12

C	-0.25254	-1.52838	-0.28687
C	-2.15100	0.57349	-0.03794
C	0.17814	-0.17521	-0.75030
C	-1.51195	-1.78804	0.13186
C	-2.47209	-0.71984	0.23881
C	-0.82226	0.90268	-0.45906
N	-0.53259	2.15645	-0.70504
N	0.61912	0.43650	1.86995
C	1.68153	0.45849	1.15015
C	1.61857	0.19559	-0.32516
H	0.19609	-0.23529	-1.85627
H	0.46521	-2.33685	-0.38916
H	-1.80899	-2.79496	0.40852
H	-3.48416	-0.95248	0.56169
H	-2.87482	1.37660	0.07705
H	0.85942	0.63606	2.84856
H	2.67906	0.66364	1.55511
H	1.90723	1.12147	-0.84185
H	0.38709	2.45775	-1.01900
C	2.65419	-0.85748	-0.73202
H	3.65911	-0.46621	-0.54947
H	2.54271	-1.78058	-0.15867
H	2.56656	-1.08981	-1.79728
H	-1.23571	2.88208	-0.57046

There are no imaginary frequencies.

SCF energy: -457.124712 hartree
αα/ββ: -0.18845583 hartree
αβ: -1.08463 hartree
SCS-MP2 energy: -458.5519034 hartree
zero-point correction: +0.211699 hartree
enthalpy correction: +0.223055 hartree
free energy correction: +0.176371 hartree

quasiharmonic free energy correction: +0.176583 hartree

S-13

C	-1.32307	-1.36312	-0.48485
C	-1.94240	1.34152	0.22421
C	-0.24922	-0.33532	-0.68727
C	-2.56420	-1.01596	-0.08636
C	-2.88541	0.36762	0.23830
C	-0.55162	1.01341	-0.06615
N	0.45680	1.79759	0.13420
N	3.29178	0.28688	0.00640
C	2.18808	0.12221	-0.64028
C	1.13307	-0.84326	-0.23222
H	-0.19038	-0.15755	-1.77691
H	-1.08557	-2.39250	-0.74843
H	-3.34464	-1.76665	0.00612
H	-3.91075	0.61330	0.50593
H	3.45328	-0.14418	0.91604
H	2.12189	0.60726	-1.60946
H	1.34935	-1.73705	-0.84177
H	0.14182	2.70799	0.49570
C	1.17230	-1.22195	1.24498
H	2.10896	-1.72197	1.51017
H	1.05129	-0.33806	1.87644
H	0.35883	-1.91791	1.46255
H	-2.17925	2.36392	0.51347
H	4.01987	0.90128	-0.35627

There are no imaginary frequencies.

SCF energy: -457.120322 hartree
αα/ββ: -0.18792143 hartree
αβ: -1.08544 hartree
SCS-MP2 energy: -458.5481343 hartree
zero-point correction: +0.212146 hartree
enthalpy correction: +0.223361 hartree
free energy correction: +0.176713 hartree
quasiharmonic free energy correction: +0.177275 hartree

3-pyridylhydrazine (41)

S-14

C	-1.33703	1.13633	-0.37962
C	-1.73559	-1.23913	-0.08485
C	-3.20597	0.25790	0.84897
C	-2.49420	1.35556	0.36230
C	-0.98252	-0.18918	-0.59472
N	0.24412	-0.49549	-1.32715
N	1.38203	-0.51870	-0.39905
C	2.20626	0.44607	-0.61397
C	3.41029	0.60971	0.24493
H	0.38440	0.17656	-2.10566
H	-1.44542	-2.27286	-0.26362
H	-4.10880	0.40870	1.43474
H	-2.84030	2.36392	0.56541
H	-0.74174	1.95469	-0.77795
H	2.05797	1.16937	-1.42141
H	4.27960	0.60684	-0.42495
H	0.18622	-1.43964	-1.74318
H	3.36325	1.62584	0.65772
C	3.56825	-0.42297	1.35036
H	2.71844	-0.40220	2.03651
H	3.65224	-1.43188	0.93956
H	4.47443	-0.21108	1.92308
N	-2.84861	-1.02495	0.63753

There are no imaginary frequencies.

SCF energy: -473.102350 hartree
αα/ββ: -0.19623821 hartree
αβ: -1.1048809 hartree
SCS-MP2 energy: -474.5590326 hartree
zero-point correction: +0.201149 hartree
enthalpy correction: +0.212480 hartree
free energy correction: +0.164269 hartree
quasiharmonic free energy correction: +0.165494 hartree

S-15

C	-1.94397	1.28991	0.02793
C	-1.38985	-1.05228	-0.16556
C	-3.60503	-0.43080	-0.19691
C	-3.28076	0.92069	-0.07544
C	-0.98322	0.27698	-0.01289
N	0.39338	0.60714	0.01558
N	1.15963	-0.24921	0.80299
C	2.44268	-0.33647	0.69665
C	3.23049	0.45360	-0.27003
H	0.57201	1.57627	0.29612
H	-0.66039	-1.85663	-0.23806
H	-4.64300	-0.74556	-0.26715
H	-4.06558	1.67062	-0.04666
H	-1.64592	2.32999	0.14198
H	2.90914	-1.02644	1.39549
H	3.41625	1.43412	0.19215
H	2.61218	0.64276	-1.15413
C	4.54936	-0.22752	-0.62271
H	4.37456	-1.18659	-1.11569
H	5.11982	0.40859	-1.30279
H	5.15135	-0.39926	0.27308
N	-2.68396	-1.41335	-0.24067
H	0.65802	-0.82462	1.49420

There are no imaginary frequencies.

SCF energy: -473.107576 hartree
αα/ββ: -0.196319439 hartree

αβ: -1.1003748 hartree
SCS-MP2 energy: -474.5589054 hartree
zero-point correction: +0.200138 hartree
enthalpy correction: +0.211601 hartree
free energy correction: +0.162984 hartree
quasiharmonic free energy correction: +0.164406 hartree

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C	2.10474	-1.25190	0.01629
C	1.08163	0.93386	-0.09124
C	3.45797	0.73728	0.09357
C	3.35070	-0.64810	0.10469
C	0.93977	-0.46286	-0.07995
N	-0.28458	-1.05410	-0.20729
N	-1.41524	-0.27059	-0.10584
C	-2.52517	-0.91112	0.05249
C	-3.82526	-0.18397	0.15215
H	-0.35890	-2.05031	0.01571
H	2.01334	-2.33539	0.02943
H	-2.54094	-2.00513	0.12279
H	-4.27837	-0.44010	1.11906
H	-4.50150	-0.60175	-0.60504
C	-3.72611	1.32702	-0.00312
H	-3.31159	1.59524	-0.97802
H	-4.71848	1.77748	0.08342
H	-3.08553	1.76195	0.76801
N	2.32019	1.45436	-0.00139
H	2.39847	2.47534	-0.00704
H	0.25666	1.62954	-0.15786
H	4.25018	-1.24880	0.18278
H	4.38443	1.29307	0.15908

There are no imaginary frequencies.

SCF energy: -473.115264 hartree
αα/ββ: -0.197668102 hartree
αβ: -1.1080868 hartree
SCS-MP2 energy: -474.5767469 hartree
zero-point correction: +0.199710 hartree
enthalpy correction: +0.211292 hartree
free energy correction: +0.162699 hartree
quasiharmonic free energy correction: +0.164019 hartree

S-16

C	-1.58901	0.76195	-0.90467
C	-0.93306	-0.24223	1.20433
C	-2.49512	-1.31144	-0.09699
C	-2.44937	-0.31837	-1.07740
C	-0.83954	0.77870	0.26522
N	0.13409	1.84422	0.47618
N	1.43968	1.64782	-0.19415
C	2.02022	0.41633	0.23394
C	2.28067	-0.59184	-0.61015
H	0.33986	1.96314	1.48249
H	-0.34771	-0.21266	2.12156
H	-3.15550	-2.16629	-0.21614
H	-3.07514	-0.39448	-1.96084
H	-1.51100	1.56151	-1.63826
H	1.20160	1.59395	-1.19206
H	2.31378	0.40282	1.28144
H	1.95281	-0.50824	-1.64678
H	-0.23099	2.75102	0.13991
C	3.03023	-1.82340	-0.21619
H	3.96455	-1.90828	-0.78122
H	3.27024	-1.81602	0.85040
H	2.43864	-2.71814	-0.43590
N	-1.76109	-1.28725	1.03324

There are no imaginary frequencies.

SCF energy: -473.083541 hartree
αα/ββ: -0.197202704 hartree
αβ: -1.1064938 hartree
SCS-MP2 energy: -474.5428021 hartree
zero-point correction: +0.201510 hartree
enthalpy correction: +0.212796 hartree
free energy correction: +0.164806 hartree
quasiharmonic free energy correction: +0.166092 hartree

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C	-1.07854	-0.51828	-1.21352
C	-0.90742	-0.57808	1.19269
C	-2.62471	0.60875	0.23693
C	-2.20221	0.28641	-1.05366
C	-0.41605	-0.94581	-0.06176
N	0.74172	-1.77840	-0.19545
N	1.92296	-0.93307	-0.48770
C	2.27060	0.01616	0.56611
C	1.93725	1.31054	0.52468
H	0.96468	-2.20768	0.71095
H	-0.40502	-0.91950	2.09660
H	-3.50241	1.23268	0.38638
H	-2.75550	0.65017	-1.91422
H	-0.71767	-0.81124	-2.19711
H	2.70022	-1.59182	-0.65468
H	2.77208	-0.46014	1.40054
H	2.23398	1.88058	1.40291
H	1.73714	-0.47432	-1.39179
C	1.22838	2.07525	-0.54563
H	1.79511	2.98103	-0.78012
H	1.07866	1.51452	-1.47026
H	0.24604	2.39074	-0.17756
N	-2.00627	0.18078	1.35647

There are no imaginary frequencies.

SCF energy: -473.083890 hartree
αα/ββ: -0.197669903 hartree
αβ: -1.1074871 hartree
SCS-MP2 energy: -474.5446544 hartree
zero-point correction: +0.201857 hartree
enthalpy correction: +0.212953 hartree
free energy correction: +0.165695 hartree
quasiharmonic free energy correction: +0.166686 hartree

S-17

C	1.51315	0.07905	1.31911
C	1.05287	-0.50344	-0.97504
C	2.99355	0.78456	-0.44208
C	2.65867	0.74605	0.90536
C	0.68831	-0.56078	0.37511
N	-0.41119	-1.29183	0.78714
N	-1.37720	-1.53746	-0.20738
C	-2.39134	-0.55778	-0.32932
C	-2.34040	0.70056	0.13675
H	-0.80938	-0.94633	1.66708
H	1.24191	0.05001	2.37193
H	-1.75980	-2.47235	-0.07545
H	-3.23590	-0.91341	-0.91703
H	-1.48388	1.04430	0.71323
C	-3.43493	1.69290	-0.11850
H	-3.06112	2.56391	-0.66831
H	-4.24376	1.24492	-0.70335
H	-3.86071	2.06634	0.81934
N	2.17515	0.16061	-1.31206
H	0.48497	-0.95882	-1.77499
H	2.41951	0.18915	-2.30630
H	3.29888	1.24426	1.62501
H	3.86261	1.28198	-0.85334

There are no imaginary frequencies.

SCF energy: -473.098235 hartree
αα/ββ: -0.197450702 hartree
αβ: -1.10504 hartree
SCS-MP2 energy: -474.5559168 hartree
zero-point correction: +0.200572 hartree
enthalpy correction: +0.211915 hartree
free energy correction: +0.164062 hartree
quasiharmonic free energy correction: +0.165281 hartree

TS S-18

C	-1.53394	-1.13471	-0.60403
C	-0.39887	0.22295	1.07405
C	-2.20328	1.10627	-0.03623
C	-2.37636	-0.06192	-0.80733
C	-0.56253	-1.01312	0.41169
N	0.39575	-1.98123	0.57957
N	1.91953	-1.45873	-0.46855
C	2.12442	-0.17495	-0.09191
C	1.40618	0.89227	-0.58959
H	0.30048	0.30544	1.90343
H	-2.87423	1.95024	-0.17898
H	-3.16593	-0.10402	-1.55121
H	-1.63183	-2.06310	-1.16259
H	1.34771	-1.46290	-1.32732
H	2.81002	-0.02193	0.74081
H	0.72216	0.70477	-1.42055
H	0.87199	-2.02278	1.48651
C	1.67978	2.30883	-0.23585
H	0.73978	2.84571	-0.07568
H	2.30362	2.38872	0.65754
H	2.19223	2.80193	-1.07138
H	0.20801	-2.90756	0.17989
N	-1.26334	1.25593	0.90251

1 imaginary frequency: –287.93 cm $^{-1}$.

SCF energy: -473.033458 hartree
αα/ββ: -0.204538007 hartree
αβ: -1.1250785 hartree
SCS-MP2 energy: -474.5199109 hartree
zero-point correction: +0.199024 hartree
enthalpy correction: +0.209672 hartree
free energy correction: +0.164306 hartree
quasiharmonic free energy correction: +0.164588 hartree

TS S-19

C	1.30243	1.27066	0.80878
C	1.55250	-1.09350	-0.57196
C	0.36038	0.25651	1.07250
C	2.26896	1.05345	-0.15299
C	0.56486	-0.98710	0.43723
N	-0.34835	-1.99235	0.59630
N	-1.90619	-1.48563	-0.47127
C	-2.12076	-0.21148	-0.08541
C	-1.41419	0.87163	-0.57772
H	-0.33750	0.34037	1.90203
H	1.24731	2.22153	1.32902
H	2.99730	1.82417	-0.38875
H	1.66245	-2.02965	-1.11855
H	-1.32313	-1.47908	-1.32273
H	-2.80480	-0.06917	0.75073
H	-0.73964	0.69776	-1.41915
H	-0.84084	-2.05566	1.49239
C	-1.73414	2.28151	-0.23378
H	-0.81940	2.87424	-0.14224
H	-2.31249	2.35067	0.69061
H	-2.32048	2.72412	-1.04930
H	-0.13254	-2.90564	0.18146
N	2.40359	-0.11399	-0.85152

1 imaginary frequency: –252.36 cm^{-1}.

SCF energy: -473.030379 hartree
αα/ββ: -0.204906085 hartree
αβ: -1.1259987 hartree
SCS-MP2 energy: -474.5181815 hartree
zero-point correction: +0.199022 hartree
enthalpy correction: +0.209667 hartree
free energy correction: +0.164290 hartree
quasiharmonic free energy correction: +0.164555 hartree

TS 8

C	-1.37622	-1.29270	-0.59112
C	-0.44338	0.20384	1.08060
C	-2.32020	0.85757	-0.06074
C	-2.33394	-0.33093	-0.82403
C	-0.42975	-1.06336	0.44015
N	0.55746	-1.98305	0.64687
N	1.96967	-1.25059	-0.44108
C	2.13882	0.06057	-0.12605
C	1.22730	0.98997	-0.57380
H	0.22593	0.38036	1.92162
H	-3.08817	1.61080	-0.22539
H	-3.09954	-0.46961	-1.58169
H	-1.35660	-2.23387	-1.13571
H	1.50289	-1.47955	-1.32441
H	2.85973	0.27402	0.65692
H	0.55236	0.70677	-1.38219
H	1.05291	-1.73885	1.51898
C	1.34159	2.43848	-0.24552
H	0.35008	2.87140	-0.09386
H	1.95323	2.60096	0.64447
H	1.80228	2.96081	-1.09185
H	2.71620	-1.90785	-0.19223
N	-1.42664	1.12564	0.89255

1 imaginary frequency: –357.39 cm^{-1}.

SCF energy: -473.029812 hartree
αα/ββ: -0.205144369 hartree
αβ: -1.1281928 hartree
SCS-MP2 energy: -474.5204063 hartree
zero-point correction: +0.198491 hartree
enthalpy correction: +0.209266 hartree
free energy correction: +0.163541 hartree
quasiharmonic free energy correction: +0.163855 hartree

TS S-20

C	1.49707	1.08755	0.82727
C	1.36290	-1.25797	-0.58905
C	0.42715	0.21242	1.10076
C	2.39311	0.75625	-0.16901
C	0.41807	-1.04884	0.45682
N	-0.53971	-1.99957	0.64091
N	-1.99269	-1.23741	-0.42742
C	-2.13914	0.06839	-0.10050
C	-1.22936	0.99429	-0.56903
H	-0.24047	0.39438	1.94101
H	1.59675	2.02703	1.36244
H	3.21866	1.41871	-0.41568
H	1.32323	-2.19311	-1.14647
H	-1.53192	-1.47066	-1.31252
H	-2.84157	0.28812	0.69749
H	-0.57666	0.70412	-1.39293
H	-1.03948	-1.78838	1.51880
C	-1.34001	2.44566	-0.25224
H	-0.34904	2.89702	-0.16207
H	-1.90632	2.61510	0.66588
H	-1.85288	2.94715	-1.08132
H	-2.73353	-1.89363	-0.16043
N	2.33161	-0.40478	-0.89125

1 imaginary frequency: –328.85 cm^{-1}.

SCF energy: -473.027140 hartree
αα/ββ: -0.205228808 hartree
αβ: -1.1289403 hartree
SCS-MP2 energy: -474.5186876 hartree
zero-point correction: +0.198867 hartree
enthalpy correction: +0.209493 hartree
free energy correction: +0.164206 hartree
quasiharmonic free energy correction: +0.164406 hartree

TS S-21

C	-1.55351	-1.20092	-0.44071
C	-0.25131	0.30374	0.95458
C	-2.20939	1.09287	-0.16056
C	-2.40552	-0.15939	-0.75236
C	-0.50081	-1.02357	0.49047
N	0.35269	-2.05700	0.71173
N	1.79163	-1.59351	-0.54505
C	2.10495	-0.33381	-0.18183
C	1.38850	0.79382	-0.56641
H	0.39204	0.50975	1.80393
H	-1.08077	2.17903	1.13121
H	-2.85344	1.94905	-0.32697
H	-3.23201	-0.28998	-1.44182
H	-1.70640	-2.19191	-0.86217
H	1.11779	-1.56642	-1.32352
H	2.85700	-0.23769	0.60271
H	0.67558	0.68498	-1.38750
H	0.95510	-1.83264	1.51651
C	1.83265	2.18023	-0.22811
H	0.97696	2.84137	-0.06101
H	2.46947	2.18706	0.66028
H	2.40098	2.59701	-1.06771

N	-1.20228	1.25802	0.69984

1 imaginary frequency: –264.93 cm $^{-1}$.

SCF energy: -473.018260 hartree
αα/ββ: -0.206752453 hartree
αβ: -1.1316291 hartree
SCS-MP2 energy: -474.5140498 hartree
zero-point correction: +0.199037 hartree
enthalpy correction: +0.209629 hartree
free energy correction: +0.164478 hartree
quasiharmonic free energy correction: +0.164537 hartree

TS S-22

C	1.14892	1.36346	0.74498
C	1.56511	-1.12069	-0.41987
C	0.22499	0.32174	0.99785
C	2.18984	1.16303	-0.12786
C	0.50978	-0.99315	0.50725
N	-0.27376	-2.08742	0.68713
N	-1.76871	-1.61929	-0.55431
C	-2.10173	-0.37725	-0.16494
C	-1.43005	0.77678	-0.56162
H	-0.47928	0.42992	1.81939
H	1.02165	2.34014	1.19977
H	2.92877	1.90707	-0.39688
H	3.13128	-0.21704	-1.32911
H	1.80627	-2.06139	-0.90424
H	-1.09925	-1.56335	-1.33552
H	-2.83886	-0.30734	0.63637
H	-0.72768	0.68649	-1.39301
H	-0.89188	-1.92137	1.49389
C	-1.91738	2.14756	-0.22419
H	-1.08581	2.85270	-0.14732
H	-2.48209	2.14939	0.71180
H	-2.57496	2.50547	-1.02554
N	2.35031	-0.07752	-0.68127

1 imaginary frequency: –208.85 cm^{-1}.

SCF energy: -473.015197 hartree
αα/ββ: -0.206856213 hartree
αβ: -1.1333961 hartree
SCS-MP2 energy: -474.5131765 hartree
zero-point correction: +0.198783 hartree
enthalpy correction: +0.209350 hartree
free energy correction: +0.164278 hartree
quasiharmonic free energy correction: +0.164372 hartree

S-23

C	-1.72879	1.18934	0.50915
C	-0.01449	-0.23298	-0.73164
C	-2.26303	-0.94687	-0.54722
C	-2.62686	0.20476	0.26701
C	-0.41289	1.04609	-0.05257
N	0.44692	2.01644	0.03352
N	2.75132	0.56686	-0.59264
C	2.43189	-0.53922	-0.02171
C	1.02365	-1.04248	0.09478
H	0.46499	0.03145	-1.68279
H	-3.03850	-1.67666	-0.77333
H	-3.63727	0.26413	0.66138
H	-1.97259	2.08209	1.07932
H	3.76748	0.70152	-0.56119
H	3.18091	-1.20467	0.42070
H	1.02554	-2.04138	-0.36110
C	0.62867	-1.19577	1.56678
H	1.30203	-1.90351	2.05826
H	0.69345	-0.23996	2.09515
H	-0.39154	-1.58132	1.65157
N	-1.08846	-1.16661	-1.04999
H	0.20664	2.88791	0.50966
H	1.40147	1.86639	-0.34142

There are no imaginary frequencies.

SCF energy: -473.119293 hartree
αα/ββ: -0.194637184 hartree
αβ: -1.1098708 hartree
SCS-MP2 energy: -474.5808961 hartree
zero-point correction: +0.200543 hartree
enthalpy correction: +0.211427 hartree
free energy correction: +0.165739 hartree
quasiharmonic free energy correction: +0.165818 hartree

S-24

C	0.00201	-0.26039	-0.73104
C	1.74963	1.15459	0.48251
C	2.39722	-0.87718	-0.45140
C	1.17885	-1.15015	-0.95761
C	0.40620	1.01519	-0.06804
N	-0.42239	2.00531	0.03782
N	-2.73994	0.61409	-0.60406
C	-2.46358	-0.51636	-0.05898
C	-1.06947	-1.05191	0.08436
H	1.97579	2.05014	1.06102
H	1.00720	-2.06527	-1.51831
H	-0.45585	-0.00767	-1.69918
H	-3.75247	0.77615	-0.59463
H	-3.24080	-1.17439	0.34425
H	-1.08876	-2.05821	-0.35611
C	-0.69989	-1.19126	1.56532
H	0.31151	-1.59577	1.66783
H	-0.75180	-0.22558	2.07698
H	-1.39464	-1.87571	2.06005
N	2.68786	0.27124	0.30797

H	3.24103	-1.54112	-0.60348
H	-0.14629	2.87458	0.50203
H	-1.38927	1.87325	-0.32330

There are no imaginary frequencies.

SCF energy: -473.104261 hartree
αα/ββ: -0.194964158 hartree
αβ: -1.1113761 hartree
SCS-MP2 energy: -474.5678884 hartree
zero-point correction: +0.199764 hartree
enthalpy correction: +0.210753 hartree
free energy correction: +0.164663 hartree
quasiharmonic free energy correction: +0.164927 hartree

S-25

C	-1.68820	1.18043	0.59288
C	-0.04194	-0.20344	-0.77436
C	-2.28968	-0.89926	-0.52380
C	-2.60459	0.21296	0.36917
C	-0.39960	1.09726	-0.07973
N	0.46325	2.06134	-0.12048
N	2.78908	0.57542	-0.33413
C	2.39336	-0.61304	-0.04982
C	0.97606	-1.05555	0.02147
H	0.13410	2.87564	0.41308
H	0.42191	0.05476	-1.73452
H	-3.08839	-1.60490	-0.75207
H	-3.58918	0.24617	0.82742
H	-1.89585	2.04514	1.22067
H	3.16280	-1.34833	0.17580
H	0.97225	-2.04765	-0.44734
C	0.60764	-1.23853	1.50360
H	1.28055	-1.95972	1.97514
H	0.67761	-0.29051	2.04301
H	-0.41312	-1.62186	1.57780
N	-1.14704	-1.11781	-1.09295
H	3.78850	0.78887	-0.34475
H	2.09356	1.34478	-0.47776

There are no imaginary frequencies.

SCF energy: -473.115811 hartree
αα/ββ: -0.194397138 hartree
αβ: -1.1106933 hartree
SCS-MP2 energy: -474.5782411 hartree
zero-point correction: +0.201042 hartree
enthalpy correction: +0.211863 hartree
free energy correction: +0.166155 hartree
quasiharmonic free energy correction: +0.166484 hartree

S-26

C	0.01708	-0.23271	-0.77588
C	1.71435	1.13239	0.56571
C	2.40957	-0.84093	-0.43392
C	1.21984	-1.09990	-1.00411
C	0.40175	1.06315	-0.09902
N	-0.41547	2.06449	-0.11983
N	-2.79278	0.61121	-0.36113
C	-2.43174	-0.58520	-0.06319
C	-1.02578	-1.06020	0.02332
H	1.90000	1.99369	1.21073
H	1.09355	-1.98352	-1.62533
H	-0.42770	0.01402	-1.75047
H	-3.22401	-1.29638	0.16104
H	-1.04469	-2.06352	-0.42268
H	-0.03281	2.86828	0.39637
C	-0.66383	-1.21822	1.51031
H	0.35270	-1.61309	1.58869
H	-0.72010	-0.25765	2.02905
H	-1.34611	-1.91877	1.99896
N	2.66589	0.26399	0.41816
H	3.26721	-1.48588	-0.59560
H	-3.78552	0.85337	-0.38098
H	-2.08332	1.36135	-0.50957

There are no imaginary frequencies.

SCF energy: -473.107655 hartree
αα/ββ: -0.194254502 hartree
αβ: -1.1109801 hartree
SCS-MP2 energy: -474.5703342 hartree
zero-point correction: +0.200747 hartree
enthalpy correction: +0.211659 hartree
free energy correction: +0.165643 hartree
quasiharmonic free energy correction: +0.166067 hartree

S-27

C	2.31296	-0.09554	0.18891
C	-0.09604	-0.23432	-0.64992
C	0.94491	1.88936	-0.00724
C	2.16511	1.23384	0.39788
C	1.25705	-0.88074	-0.44414
N	1.51381	-2.10717	-0.76325
N	-2.72021	0.72506	-0.73995
C	-2.52303	-0.27347	0.04509
C	-1.14616	-0.80277	0.33009
H	0.69373	-2.53036	-1.22189
H	-0.44013	-0.42720	-1.67257
H	3.23480	-0.61160	0.44489
H	-3.33648	-0.78746	0.56780
H	-1.16831	-1.88473	0.13597
H	-3.72196	0.93846	-0.79500
C	-0.78822	-0.58400	1.80322
H	0.14777	-1.08864	2.05706
H	-0.69221	0.48105	2.03366

H	-1.57772	-0.99742	2.43719
N	-0.04227	1.22513	-0.51316
H	-0.92649	1.68669	-0.77717
H	0.82324	2.96548	0.07758
H	2.94491	1.84045	0.84367

There are no imaginary frequencies.

SCF energy: -473.114570 hartree
αα/ββ: -0.193395507 hartree
αβ: -1.1087983 hartree
SCS-MP2 energy: -474.5740583 hartree
zero-point correction: +0.200596 hartree
enthalpy correction: +0.211687 hartree
free energy correction: +0.165218 hartree
quasiharmonic free energy correction: +0.165462 hartree

S-28

C	-0.30630	-0.01897	-0.89197
C	1.94302	0.53430	0.18680
C	1.34578	-1.75365	-0.16638
C	0.15273	-1.42938	-0.68726
C	0.76049	0.99062	-0.54409
N	0.76576	2.24608	-0.85128
N	-0.26599	0.28277	1.86831
C	-1.43284	0.36175	1.33842
C	-1.62675	0.30839	-0.14615
H	2.65640	1.24813	0.58754
H	-2.34688	0.48358	1.93134
H	-1.92026	1.31874	-0.46990
H	-0.07698	2.46694	-1.40168
C	-2.76615	-0.64624	-0.50891
H	-2.89193	-0.69720	-1.59427
H	-2.57928	-1.65425	-0.12910
H	-3.70275	-0.28815	-0.07181
N	2.21505	-0.72957	0.27424
H	-0.33810	0.35118	2.89062
H	-0.53353	0.09856	-1.96228
H	3.08044	-1.00883	0.74709
H	-0.49562	-2.23609	-1.01482
H	1.72500	-2.75836	-0.03442

There are no imaginary frequencies.

SCF energy: -473.097839 hartree
αα/ββ: -0.193901387 hartree
αβ: -1.1114166 hartree
SCS-MP2 energy: -474.5608065 hartree
zero-point correction: +0.200246 hartree
enthalpy correction: +0.211380 hartree
free energy correction: +0.164958 hartree
quasiharmonic free energy correction: +0.165190 hartree

2-methoxy-5-hydrazinylpyridine (12)

S-29

C	0.42460	0.82206	0.84885
C	1.09628	-1.34163	-0.00601
C	2.62689	0.36043	0.02879
C	1.70669	1.26639	0.59186
C	0.13737	-0.51011	0.54065
N	-1.21039	-1.02242	0.76128
N	-2.11476	-0.55176	-0.29892
C	-3.05946	0.19077	0.16258
C	-4.07581	0.74944	-0.76701
H	-1.55206	-0.76370	1.70671
H	0.87272	-2.37984	-0.24506
H	2.01188	2.28532	0.80572
H	-0.32996	1.47816	1.27663
H	-3.16241	0.40950	1.23014
H	-4.07981	1.83819	-0.64164
H	-1.20944	-2.05492	0.70856
H	-3.79152	0.52330	-1.79774
C	-5.46127	0.18464	-0.44019
H	-5.47839	-0.89910	-0.58113
H	-5.74069	0.40419	0.59388
H	-6.20985	0.63047	-1.09960
N	2.34830	-0.91137	-0.26272
O	3.86654	0.85293	-0.21681
C	4.82864	-0.06779	-0.77474
H	4.48626	-0.44966	-1.73769
H	5.73315	0.52454	-0.90178
H	5.01211	-0.89620	-0.08874

There are no imaginary frequencies.

SCF energy: -586.995478 hartree
αα/ββ: -0.236958033 hartree
αβ: -1.329402075 hartree
SCS-MP2 energy: -588.7487325 hartree
zero-point correction: +0.234563 hartree
enthalpy correction: +0.248427 hartree
free energy correction: +0.194545 hartree
quasiharmonic free energy correction: +0.195921 hartree

S-30

C	0.18827	-0.62482	0.61272
C	1.21628	1.44070	-0.07636
C	2.50705	-0.44678	0.04662
C	1.41648	-1.23792	0.44991
C	0.08748	0.74712	0.33819
N	-1.14800	1.43554	0.56750
N	-2.16192	0.90397	-0.26658
C	-3.24593	0.42405	0.23130
C	-4.30505	-0.17190	-0.60412

H	-1.05253	2.42426	0.31086
H	1.16212	2.50527	-0.29954
H	1.55682	-2.29657	0.64414
H	-0.67962	-1.19065	0.94480
H	-3.33912	0.47153	1.31386
H	-4.03104	-0.12267	-1.66122
H	-5.20499	0.43555	-0.44902
C	-4.57278	-1.61389	-0.15616
H	-4.85853	-1.64806	0.89788
H	-5.38971	-2.02760	-0.75086
H	-3.68645	-2.23550	-0.30179
N	2.42767	0.85753	-0.21109
O	3.70240	-1.09128	-0.07902
C	4.82850	-0.27609	-0.45987
H	5.00270	0.51425	0.27253
H	5.67277	-0.96386	-0.48129
H	4.67585	0.16413	-1.44692
H	-1.99353	0.87799	-1.28340

There are no imaginary frequencies.

SCF energy: -587.003720 hartree
αα/ββ: -0.23632319 hartree
αβ: -1.323372571 hartree
SCS-MP2 energy: -588.7493159 hartree
zero-point correction: +0.233921 hartree
enthalpy correction: +0.247986 hartree
free energy correction: +0.193080 hartree
quasiharmonic free energy correction: +0.195127 hartree

S-31

C	1.10592	1.43678	0.03537
C	0.42876	-0.86956	0.05665
C	2.75814	-0.30401	0.01455
C	2.43716	1.05688	0.01171
C	0.07170	0.47892	0.05791
N	-1.24103	0.88348	0.14963
N	-2.22293	-0.05620	-0.09802
C	-3.40569	0.41364	-0.32077
C	-4.55385	-0.51206	-0.53712
H	-1.43789	1.85366	-0.11056
H	0.85099	2.49426	0.03028
H	-3.59669	1.49337	-0.33031
H	-4.17554	-1.53756	-0.58694
H	-5.01812	-0.28076	-1.50339
C	-5.59814	-0.37752	0.57433
H	-5.97493	0.64768	0.63603
H	-6.44673	-1.04079	0.38486
H	-5.16465	-0.64152	1.54293
N	1.74317	-1.19083	0.03394
H	3.21807	1.80718	-0.00959
O	3.97022	-0.87962	-0.00408
C	5.10971	0.01641	-0.00823
H	5.09843	0.63608	-0.90664
H	5.10720	0.63277	0.89252
H	5.97536	-0.64189	-0.01385
H	-0.27129	-1.69354	0.06985
H	1.99723	-2.18403	0.03220

There are no imaginary frequencies.

SCF energy: -587.000374 hartree
αα/ββ: -0.238013401 hartree
αβ: -1.331968104 hartree
SCS-MP2 energy: -588.7574113 hartree
zero-point correction: +0.232875 hartree
enthalpy correction: +0.247047 hartree
free energy correction: +0.192685 hartree
quasiharmonic free energy correction: +0.194218 hartree

S-32

C	0.38884	1.67312	-0.81510
C	0.26004	0.26369	1.14985
C	2.10710	0.12508	-0.19777
C	1.62102	1.10901	-1.08055
C	-0.28254	1.23983	0.33218
N	-1.61597	1.75210	0.61599
N	-2.72512	1.07472	-0.09737
C	-2.74148	-0.30896	0.24754
C	-2.55303	-1.28451	-0.65218
H	-1.83521	1.67764	1.62378
H	-0.25748	-0.07344	2.04608
H	2.20911	1.40086	-1.94441
H	-0.03841	2.43621	-1.46212
H	-2.48808	1.18641	-1.09062
H	-3.00551	-0.50513	1.28469
H	-2.28654	-1.01337	-1.67413
H	-1.68769	2.75414	0.37332
C	-2.72752	-2.73563	-0.34069
H	-3.54445	-3.16600	-0.92968
H	-2.94821	-2.88857	0.71921
H	-1.82011	-3.29378	-0.59330
N	1.46121	-0.29310	0.89224
O	3.31774	-0.40149	-0.50955
C	3.82859	-1.42032	0.37615
H	3.17390	-2.29335	0.37838
H	4.80159	-1.67992	-0.03767
H	3.93830	-1.03359	1.39031

There are no imaginary frequencies.

SCF energy: -586.976568 hartree
αα/ββ: -0.238074202 hartree
αβ: -1.331132527 hartree
SCS-MP2 energy: -588.7326432 hartree
zero-point correction: +0.234316 hartree
enthalpy correction: +0.248349 hartree
free energy correction: +0.193701 hartree

quasiharmonic free energy correction: +0.195740 hartree

S-33

C	0.19792	-1.56001	-0.88061
C	0.25111	-0.34550	1.19654
C	2.05265	-0.20736	-0.20769
C	1.45071	-1.04931	-1.16087
C	-0.41970	-1.19392	0.32474
N	-1.70734	-1.73038	0.63949
N	-2.75196	-0.97327	-0.09851
C	-2.82050	0.44807	0.21366
C	-2.26622	1.34101	-0.60978
H	-1.92393	-1.54499	1.62677
H	-0.20583	-0.05043	2.14008
H	1.97914	-1.29521	-2.07650
H	-0.30342	-2.23187	-1.57397
H	-2.56807	-1.12983	-1.10212
H	-3.28634	0.65960	1.17016
H	-1.81130	0.99629	-1.53826
H	-3.64105	-1.45075	0.11615
C	-2.24606	2.80577	-0.32623
H	-2.74841	3.35519	-1.12829
H	-2.73663	3.03557	0.62255
H	-1.21221	3.16337	-0.28487
N	1.48799	0.13789	0.94947
O	3.29215	0.25871	-0.52604
C	3.91238	1.14414	0.42778
H	4.04917	0.64749	1.38976
H	4.87879	1.38877	-0.01059
H	3.31835	2.05017	0.55912

There are no imaginary frequencies.

SCF energy: -586.978911 hartree
αα/ββ: -0.238235296 hartree
αβ: -1.33152506 hartree
SCS-MP2 energy: -588.7355646 hartree
zero-point correction: +0.234603 hartree
enthalpy correction: +0.248641 hartree
free energy correction: +0.193867 hartree
quasiharmonic free energy correction: +0.196041 hartree

S-34

C	0.61308	-0.47057	1.38833
C	0.16769	-0.80435	-0.94524
C	2.29343	0.04938	-0.24384
C	1.88529	-0.00992	1.09233
C	-0.27269	-0.87614	0.37195
N	-1.51706	-1.41166	0.69630
N	-2.46306	-1.35743	-0.35018
C	-3.23614	-0.17406	-0.41693
C	-2.93774	1.00335	0.15631
H	-1.88026	-1.02183	1.57326
H	0.28864	-0.51409	2.42583
H	-3.04522	-2.19264	-0.31084
H	-4.11074	-0.28967	-1.05489
H	-2.05009	1.10629	0.77709
C	-3.78285	2.22694	-0.03445
H	-3.21166	3.03622	-0.50314
H	-4.64822	2.01290	-0.66878
H	-4.15025	2.61002	0.92394
N	1.41900	-0.34875	-1.18890
H	2.55084	0.30345	1.88748
O	3.46824	0.45998	-0.74294
C	4.44577	0.93978	0.21421
H	4.71469	0.14231	0.90874
H	5.30472	1.22183	-0.39010
H	4.05357	1.80721	0.74772
H	-0.42327	-1.08604	-1.80602
H	1.73408	-0.29744	-2.16331

There are no imaginary frequencies.

SCF energy: -586.982836 hartree
αα/ββ: -0.237984489 hartree
αβ: -1.329266291 hartree
SCS-MP2 energy: -588.7366119 hartree
zero-point correction: +0.233773 hartree
enthalpy correction: +0.247659 hartree
free energy correction: +0.194050 hartree
quasiharmonic free energy correction: +0.195593 hartree

TS S-35

C	0.12586	-1.91245	-0.57728
C	0.16381	-0.12406	1.07417
C	-1.76264	-0.51488	-0.09484
C	-1.18000	-1.58060	-0.83171
C	0.80155	-1.20953	0.44954
N	2.15076	-1.39735	0.65034
N	3.10560	-0.15682	-0.38472
C	2.51610	1.03065	-0.07556
C	1.33790	1.46060	-0.63603
H	0.64516	0.39172	1.90222
H	-1.76821	-2.09453	-1.58507
H	0.62392	-2.72070	-1.10861
H	2.68487	-0.51199	-1.25735
H	2.95665	1.58147	0.75455
H	0.91766	0.87603	-1.45741
H	2.52664	-1.13000	1.56648
C	0.70257	2.77007	-0.33573
H	-0.36934	2.63217	-0.15646
H	1.15749	3.24852	0.53507
H	0.79874	3.43931	-1.19918
H	2.55398	-2.27528	0.30160
N	-1.13963	0.17562	0.85333
O	-3.04983	-0.24020	-0.39714

C	-3.65421	0.86947	0.30471
H	-3.11026	1.79287	0.09764
H	-4.66661	0.92591	-0.09123
H	-3.67479	0.68018	1.37867

1 imaginary frequency: –343.70 cm^{-1}.

SCF energy: -586.930851 hartree
αα/ββ: -0.245037419 hartree
αβ: -1.349284632 hartree
SCS-MP2 energy: -588.7133508 hartree
zero-point correction: +0.232041 hartree
enthalpy correction: +0.245423 hartree
free energy correction: +0.193613 hartree
quasiharmonic free energy correction: +0.194402 hartree

TS S-36

C	1.10898	0.23249	0.87616
C	-0.03874	-1.81974	-0.56509
C	-0.24064	-0.06708	1.10516
C	1.77909	-0.48550	-0.10933
C	-0.79573	-1.18966	0.45282
N	-2.11385	-1.50292	0.61152
N	-3.15246	-0.20095	-0.43805
C	-2.57497	0.96690	-0.08417
C	-1.38093	1.42120	-0.61096
H	-0.77299	0.40460	1.92747
H	1.57979	1.03570	1.42898
H	-0.47518	-2.63806	-1.13677
H	-2.69380	-0.54093	-1.29776
H	-3.02824	1.49632	0.75367
H	-0.95693	0.86820	-1.45205
H	-2.55479	-1.28413	1.50910
C	-0.78549	2.74520	-0.29712
H	0.30278	2.66359	-0.20766
H	-1.19830	3.16889	0.62167
H	-0.98522	3.43714	-1.12547
H	-2.45369	-2.37522	0.19130
N	1.21741	-1.49615	-0.82714
O	3.07402	-0.29071	-0.46131
C	3.77651	0.76762	0.22065
H	3.81935	0.57155	1.29473
H	4.78056	0.75760	-0.19928
H	3.29830	1.73188	0.02947

1 imaginary frequency: –243.26 cm^{-1}.

SCF energy: -586.920304 hartree
αα/ββ: -0.246145276 hartree
αβ: -1.351913833 hartree
SCS-MP2 energy: -588.7066975 hartree
zero-point correction: +0.232372 hartree
enthalpy correction: +0.245507 hartree
free energy correction: +0.194444 hartree
quasiharmonic free energy correction: +0.195105 hartree

TS 9

C	0.15195	-1.88535	-0.56901
C	0.14457	-0.12324	1.09750
C	-1.75894	-0.51654	-0.09576
C	-1.14918	-1.56085	-0.84529
C	0.82843	-1.19061	0.47421
N	2.14400	-1.46467	0.71088
N	3.03205	-0.19376	-0.36877
C	2.51195	1.04903	-0.12038
C	1.28592	1.38630	-0.62828
H	0.61140	0.39407	1.93494
H	-1.72276	-2.06540	-1.61661
H	0.66475	-2.68359	-1.10045
H	2.79186	-0.63895	-1.26047
H	3.00298	1.61791	0.66301
H	0.86154	0.77120	-1.42269
H	2.42327	-0.98702	1.58169
C	0.62753	2.69068	-0.33849
H	-0.43626	2.53597	-0.13436
H	1.09074	3.19199	0.51457
H	0.69965	3.34309	-1.21577
H	4.00303	-0.36676	-0.08846
N	-1.16300	0.16083	0.87665
O	-3.04248	-0.25232	-0.41791
C	-3.67628	0.83535	0.29261
H	-3.13837	1.76875	0.11749
H	-4.68005	0.88890	-0.12507
H	-3.71901	0.62294	1.36147

1 imaginary frequency: –347.83 cm^{-1}.

SCF energy: -586.931865 hartree
αα/ββ: -0.245185255 hartree
αβ: -1.350289396 hartree
SCS-MP2 energy: -588.7156691 hartree
zero-point correction: +0.231963 hartree
enthalpy correction: +0.245355 hartree
free energy correction: +0.193389 hartree
quasiharmonic free energy correction: +0.194400 hartree

TS S-37

C	1.13389	0.22526	0.89490
C	-0.05128	-1.80332	-0.53934
C	-0.21863	-0.06118	1.13050
C	1.78112	-0.48648	-0.10599
C	-0.81532	-1.17514	0.48839
N	-2.09655	-1.58553	0.66127
N	-3.05960	-0.25303	-0.45256
C	-2.57873	0.97232	-0.13557
C	-1.33730	1.35950	-0.59461

H	-0.73792	0.42002	1.95754
H	1.62434	1.01527	1.45063
H	-0.50180	-2.62114	-1.10074
H	-2.74503	-0.69134	-1.32304
H	-3.10473	1.50542	0.65062
H	-0.88970	0.79111	-1.41010
H	-2.46150	-1.14776	1.52108
C	-0.74496	2.68918	-0.27839
H	0.33864	2.60528	-0.15714
H	-1.18085	3.12115	0.62517
H	-0.92735	3.36896	-1.11873
H	-4.02227	-0.48646	-0.19220
N	1.19820	-1.48924	-0.82406
O	3.07064	-0.30269	-0.48194
C	3.79489	0.75115	0.18353
H	3.86414	0.55266	1.25573
H	4.78764	0.73803	-0.26238
H	3.31487	1.71714	0.00599

1 imaginary frequency: –262.08 cm^{-1}.

SCF energy: -586.920586 hartree
αα/ββ: -0.246066751 hartree
αβ: -1.353290118 hartree
SCS-MP2 energy: -588.7085786 hartree
zero-point correction: +0.232308 hartree
enthalpy correction: +0.245457 hartree
free energy correction: +0.194218 hartree
quasiharmonic free energy correction: +0.195093 hartree

TS S-38

C	-0.28650	-1.77471	-0.29964
C	0.46130	0.08992	1.04784
C	-1.77538	0.04062	0.18799
C	-1.51607	-1.18246	-0.46667
C	0.71387	-1.20547	0.53181
N	1.93847	-1.80264	0.57240
N	2.88066	-0.85387	-0.77207
C	2.74846	0.43781	-0.38138
C	1.62371	1.21287	-0.60923
H	1.06153	0.53507	1.83423
H	-1.04542	1.46133	1.43099
H	-2.27547	-1.63995	-1.08860
H	-0.07616	-2.72946	-0.77655
H	2.16748	-1.06962	-1.48314
H	3.50305	0.79745	0.31996
H	0.89965	0.85747	-1.34587
H	2.49750	-1.38446	1.32912
C	1.55176	2.65539	-0.22051
H	0.55067	2.92020	0.13410
H	2.27865	2.88880	0.56195
H	1.76219	3.28737	-1.09085
N	-0.82203	0.57798	0.96167
O	-2.90554	0.74104	0.16756
C	-4.03964	0.15598	-0.53067
H	-4.28572	-0.81041	-0.08935
H	-4.84813	0.86559	-0.37426
H	-3.81409	0.06226	-1.59345

1 imaginary frequency: –363.36 cm^{-1}.

SCF energy: -586.911492 hartree
αα/ββ: -0.246815652 hartree
αβ: -1.353665743 hartree
SCS-MP2 energy: -588.7004347 hartree
zero-point correction: +0.232058 hartree
enthalpy correction: +0.245351 hartree
free energy correction: +0.193761 hartree
quasiharmonic free energy correction: +0.194480 hartree

TS S-39

C	1.01478	0.35296	0.83351
C	-0.08939	-1.90118	-0.38078
C	-0.35632	0.05722	1.01378
C	1.75476	-0.41776	-0.03825
C	-0.89435	-1.18406	0.52604
N	-2.16461	-1.61898	0.68966
N	-3.11063	-0.29029	-0.61265
C	-2.60233	0.87723	-0.20715
C	-1.33143	1.34810	-0.55815
H	-0.88086	0.55699	1.82548
H	1.45930	1.21004	1.32457
H	1.74064	-2.06526	-1.25701
H	-0.42498	-2.80691	-0.87584
H	-2.51576	-0.67747	-1.35933
H	-3.15832	1.40288	0.57111
H	-0.82475	0.83869	-1.38104
H	-2.58778	-1.10366	1.47404
C	-0.87505	2.73417	-0.23679
H	0.21456	2.78310	-0.16633
H	-1.31706	3.09396	0.69608
H	-1.18095	3.40671	-1.04720
N	1.16203	-1.51202	-0.61446
O	3.04207	-0.29709	-0.40563
C	3.74015	0.85420	0.12699
H	3.79654	0.78737	1.21516
H	4.73517	0.80092	-0.30851
H	3.23519	1.77305	-0.17912

1 imaginary frequency: –76.93 cm^{-1}.

SCF energy: -586.895067 hartree
αα/ββ: -0.248378355 hartree
αβ: -1.360679754 hartree
SCS-MP2 energy: -588.6934683 hartree
zero-point correction: +0.231522 hartree
enthalpy correction: +0.244792 hartree
free energy correction: +0.193345 hartree

quasiharmonic free energy correction: +0.194051 hartree

S-40

C	-0.31709	2.07438	0.35809
C	0.43074	-0.18017	-0.58887
C	-1.83258	0.21886	-0.06636
C	-1.56217	1.55788	0.45489
C	0.70864	1.25690	-0.23662
N	1.88917	1.74912	-0.45806
N	3.27831	-0.62599	-0.84564
C	2.63964	-1.35461	-0.00099
C	1.19012	-1.16897	0.33822
H	0.80564	-0.34069	-1.60812
H	-2.38032	2.11953	0.89590
H	4.25094	-0.94151	-0.92198
H	3.12021	-2.18151	0.53264
H	0.71520	-2.14077	0.14724
C	1.02418	-0.84854	1.82692
H	1.44443	-1.65871	2.42944
H	1.54121	0.07803	2.09370
H	-0.03505	-0.74966	2.08120
N	-0.96836	-0.58549	-0.58259
O	-3.14721	-0.09308	0.01892
C	-3.52171	-1.39242	-0.48850
H	-4.59756	-1.44991	-0.33432
H	-3.28137	-1.47061	-1.54998
H	-3.01288	-2.18083	0.06818
H	2.10711	2.71773	-0.21479
H	-0.07419	3.07858	0.69593
H	2.62189	1.12169	-0.84308

There are no imaginary frequencies.

SCF energy: -587.016481 hartree
αα/ββ: -0.235987213 hartree
αβ: -1.334754421 hartree
SCS-MP2 energy: -588.7755111 hartree
zero-point correction: +0.233791 hartree
enthalpy correction: +0.247278 hartree
free energy correction: +0.195532 hartree
quasiharmonic free energy correction: +0.196050 hartree

S-41

C	-0.62376	-0.11874	-0.50613
C	0.73982	1.70948	0.62973
C	1.79756	-0.25822	0.00238
C	0.70757	-0.79065	-0.58838
C	-0.47747	1.29699	-0.06399
N	-1.42255	2.16546	-0.23748
N	-3.44205	0.29715	-0.61561
C	-3.02205	-0.50245	0.29928
C	-1.57720	-0.87258	0.48984
H	0.77853	-1.75096	-1.08711
H	-1.11418	-0.13978	-1.48847
H	-4.46469	0.36481	-0.57443
H	-3.70603	-1.00758	0.98944
H	-1.29121	-0.60452	1.51702
C	-1.46366	-2.39599	0.34461
H	-2.21702	-2.87809	0.97459
H	-1.63459	-2.69905	-0.69272
H	-0.48165	-2.74966	0.66336
N	1.80768	0.97173	0.67120
O	2.98176	-0.95255	0.03572
C	4.13250	-0.17033	-0.35706
H	4.33341	0.62355	0.36357
H	4.96535	-0.87215	-0.37855
H	3.97693	0.25657	-1.35199
H	-1.33313	3.12398	0.11040
H	-2.29989	1.84850	-0.68527
H	0.75260	2.67925	1.12603

There are no imaginary frequencies.

SCF energy: -586.981986 hartree
αα/ββ: -0.235948766 hartree
αβ: -1.337566479 hartree
SCS-MP2 energy: -588.744365 hartree
zero-point correction: +0.232716 hartree
enthalpy correction: +0.246440 hartree
free energy correction: +0.193732 hartree
quasiharmonic free energy correction: +0.194460 hartree

S-42

C	0.55932	2.33606	0.22330
C	0.79425	-0.02805	-0.68855
C	-1.30631	0.80302	0.00181
C	-0.74580	2.07892	0.44804
C	1.38855	1.35211	-0.46257
N	2.59096	1.68049	-0.81084
N	-0.02083	-2.81197	-0.48655
C	1.09792	-2.44718	0.03009
C	1.48131	-1.03048	0.26985
H	3.03504	0.89029	-1.30128
H	1.05215	-0.33638	-1.71066
H	-1.40651	2.78906	0.93605
H	1.01356	3.28436	0.49993
H	1.78197	-3.23447	0.33948
H	2.56045	-0.97688	0.07749
C	1.24224	-0.72632	1.75811
H	1.68803	0.23827	2.01112
H	0.17188	-0.70202	1.97795
H	1.70816	-1.49229	2.38454
N	-0.65834	-0.15548	-0.56395
O	-2.64204	0.72964	0.20920
C	-3.27360	-0.50644	-0.19047
H	-2.83312	-1.34964	0.34500

H	-4.32051	-0.38560	0.08199
H	-3.17437	-0.65526	-1.26705
H	-0.24225	-3.80256	-0.60526
H	-0.70794	-2.08512	-0.75125

There are no imaginary frequencies.

SCF energy: -587.015259 hartree
αα/ββ: -0.235524481 hartree
αβ: -1.334440916 hartree
SCS-MP2 energy: -588.7736044 hartree
zero-point correction: +0.233824 hartree
enthalpy correction: +0.247658 hartree
free energy correction: +0.194413 hartree
quasiharmonic free energy correction: +0.195718 hartree

S-43

C	-0.48106	-0.19148	-0.65756
C	0.39090	1.91291	0.49184
C	1.88367	0.22334	-0.02537
C	0.97252	-0.56977	-0.62528
C	-0.69095	1.24766	-0.25287
N	-1.79129	1.85235	-0.55872
N	-3.44164	-0.41116	-0.62176
C	-2.72298	-1.30599	-0.04362
C	-1.26714	-1.19163	0.23407
H	0.16243	2.87152	0.96182
H	1.24307	-1.52311	-1.06611
H	-0.84871	-0.30414	-1.68719
H	-3.23422	-2.20924	0.28391
H	-0.86491	-2.19050	0.01830
H	-1.79950	2.81526	-0.19546
C	-1.08770	-0.93524	1.74047
H	-0.01892	-0.89855	1.96791
H	-1.55363	0.00930	2.03396
H	-1.53893	-1.74207	2.32408
N	1.59684	1.45711	0.59819
O	3.22694	-0.01057	0.08609
C	3.68752	-1.24536	-0.48526
H	3.48038	-1.27549	-1.55889
H	4.76234	-1.26119	-0.31154
H	3.21455	-2.09862	0.00948
H	-4.44201	-0.57113	-0.75660
H	-3.03362	0.50772	-0.89492

There are no imaginary frequencies.

SCF energy: -586.994127 hartree
αα/ββ: -0.235704553 hartree
αβ: -1.337106981 hartree
SCS-MP2 energy: -588.7557917 hartree
zero-point correction: +0.234390 hartree
enthalpy correction: +0.247701 hartree
free energy correction: +0.196323 hartree
quasiharmonic free energy correction: +0.196852 hartree

S-44

C	0.47269	2.33509	0.17210
C	0.84209	-0.05017	-0.66188
C	-1.37166	0.77149	0.01537
C	-0.82824	2.06348	0.40110
C	1.35122	1.36104	-0.47087
N	2.54086	1.73597	-0.80893
N	0.11730	-2.75811	-0.68259
C	1.11098	-2.45067	0.07352
C	1.52093	-1.02613	0.32009
H	3.03469	0.95629	-1.26720
H	1.07151	-0.37449	-1.68315
H	0.89560	3.30531	0.41931
H	1.70830	-3.20338	0.59890
H	2.59740	-0.96157	0.10512
H	-0.00505	-3.77608	-0.71046
C	1.30087	-0.66363	1.79186
H	1.73376	0.31343	2.02218
H	0.23493	-0.64738	2.03846
H	1.78480	-1.40719	2.43168
N	-0.61834	-0.14568	-0.52732
O	-2.66145	0.62067	0.21850
C	-3.27595	-0.65173	-0.14435
H	-2.80990	-1.45727	0.42505
H	-4.31963	-0.53729	0.13383
H	-3.17708	-0.81126	-1.21930
H	-1.51257	2.77101	0.85618
H	-0.96150	-1.09332	-0.74828

There are no imaginary frequencies.

SCF energy: -587.013410 hartree
αα/ββ: -0.234846639 hartree
αβ: -1.333613131 hartree
SCS-MP2 energy: -588.7703102 hartree
zero-point correction: +0.234264 hartree
enthalpy correction: +0.247779 hartree
free energy correction: +0.195862 hartree
quasiharmonic free energy correction: +0.196363 hartree

S-45

C	-0.67028	-0.50509	-0.94811
C	-0.36396	1.42052	0.55513
C	1.56616	0.18261	-0.09050
C	0.81249	-0.72105	-0.75385
C	-0.98079	0.94469	-0.73259
N	-1.64488	1.76899	-1.45534
N	-0.80232	0.48009	1.63909
C	-1.24555	-0.71793	1.45200
C	-1.47318	-1.30159	0.10558

H	-1.50497	-1.28133	2.34656
H	-1.09740	-2.33149	0.13920
H	-1.96033	1.28085	-2.30525
C	-2.98691	-1.33834	-0.16158
H	-3.50585	-1.90790	0.61418
H	-3.40121	-0.32709	-0.19031
H	-3.16178	-1.82169	-1.12605
N	1.06347	1.40532	0.39560
H	-0.68959	0.81386	2.60318
H	-0.98803	-0.81607	-1.95048
H	1.24510	-1.63791	-1.13551
O	2.90040	0.11238	0.18022
C	3.57650	-1.06030	-0.30879
H	3.50061	-1.11865	-1.39737
H	4.61597	-0.93608	-0.01034
H	3.15966	-1.96170	0.14733
H	-0.71037	2.41147	0.84585
H	1.57427	1.73274	1.21803

There are no imaginary frequencies.

SCF energy: -587.013421 hartree
αα/ββ: -0.236359282 hartree
αβ: -1.332810981 hartree
SCS-MP2 energy: -588.770367 hartree
zero-point correction: +0.237176 hartree
enthalpy correction: +0.249799 hartree
free energy correction: +0.200021 hartree
quasiharmonic free energy correction: +0.200293 hartree

2-chloro-5-hydrazinylpyridine (31)

S-46

C	0.53370	0.46706	1.07868
C	0.97498	-1.42446	-0.36949
C	2.60548	0.14136	-0.05768
C	1.82094	0.91122	0.80444
C	0.13147	-0.72150	0.47897
N	-1.22394	-1.21720	0.69756
N	-2.12863	-0.67253	-0.32921
C	-2.91135	0.23198	0.14583
C	-3.89526	0.89063	-0.75275
H	-1.54354	-0.99596	1.66043
H	0.65828	-2.35219	-0.84081
H	2.20255	1.82598	1.24470
H	-0.12736	1.02093	1.74096
H	-2.89583	0.52580	1.19936
H	-3.69435	1.96810	-0.73362
H	-1.25294	-2.24526	0.59280
H	-3.74967	0.53292	-1.77531
C	-5.32312	0.62027	-0.27050
H	-5.54240	-0.45032	-0.29261
H	-5.46756	0.98264	0.75092
H	-6.03770	1.13194	-0.91968
N	2.22046	-0.99484	-0.63974
Cl	4.22084	0.67929	-0.41603

There are no imaginary frequencies.

SCF energy: -932.000836 hartree
αα/ββ: -0.215991747 hartree
αβ: -1.19843316 hartree
SCS-MP2 energy: -933.5829503 hartree
zero-point correction: +0.190747 hartree
enthalpy correction: +0.203367 hartree
free energy correction: +0.151109 hartree
quasiharmonic free energy correction: +0.153150 hartree

S-47

C	-0.23226	-0.53929	0.23713
C	-1.24520	1.63557	0.00850
C	-2.58364	-0.21257	-0.00540
C	-1.50585	-1.08644	0.13441
C	-0.10133	0.85053	0.16420
N	1.15852	1.48563	0.34330
N	2.18465	0.82324	-0.35776
C	3.23905	0.40608	0.25031
C	4.32074	-0.31512	-0.44472
H	1.13789	2.45620	0.01348
H	-1.16868	2.71952	-0.05258
H	-1.65662	-2.16017	0.17749
H	0.63299	-1.18425	0.36837
H	3.28289	0.59775	1.32018
H	5.24254	0.25258	-0.27306
H	4.13028	-0.35404	-1.52039
C	4.46298	-1.72294	0.15033
H	3.55082	-2.30303	-0.00737
H	5.29140	-2.23536	-0.34306
H	4.67131	-1.67698	1.22178
N	-2.48323	1.11463	-0.06796
Cl	-4.19550	-0.87253	-0.11339
H	2.06204	0.66137	-1.36887

There are no imaginary frequencies.

SCF energy: -932.012450 hartree
αα/ββ: -0.215407191 hartree
αβ: -1.19186088 hartree
SCS-MP2 energy: -933.5862879 hartree
zero-point correction: +0.190972 hartree
enthalpy correction: +0.203549 hartree
free energy correction: +0.151626 hartree
quasiharmonic free energy correction: +0.153429 hartree

S-48

C	1.07658	1.66622	0.01349

C	0.35340	-0.63836	-0.04728
C	2.68245	-0.11637	0.00697
C	2.39437	1.24560	0.03044
C	0.02158	0.72576	-0.02753
N	-1.26740	1.14223	-0.06860
N	-2.28977	0.22397	-0.02942
C	-3.48136	0.72152	0.01439
C	-4.68609	-0.15772	0.04772
H	-1.47562	2.14075	0.01058
H	0.84597	2.72861	0.03457
H	-3.64107	1.80588	0.02791
H	-5.32576	0.12487	-0.79890
H	-5.26270	0.10160	0.94542
C	-4.39539	-1.65167	0.01688
H	-3.79379	-1.95546	0.87704
H	-5.33276	-2.21379	0.04132
H	-3.85461	-1.93062	-0.89083
N	1.65564	-0.98983	-0.02912
H	3.20610	1.96450	0.06251
Cl	4.27393	-0.74881	0.02193
H	-0.36597	-1.44575	-0.07621
H	1.86096	-1.99529	-0.04675

There are no imaginary frequencies.

SCF energy: -932.000118 hartree
αα/ββ: -0.217825269 hartree
αβ: -1.20325254 hartree
SCS-MP2 energy: -933.5892379 hartree
zero-point correction: +0.189441 hartree
enthalpy correction: +0.202369 hartree
free energy correction: +0.150056 hartree
quasiharmonic free energy correction: +0.151738 hartree

S-49

C	-0.53173	1.50379	0.84189
C	-0.18253	0.30831	-1.23536
C	-2.09081	-0.06933	-0.04027
C	-1.74489	0.83898	0.96362
C	0.23870	1.22719	-0.28290
N	1.55170	1.84496	-0.41674
N	2.64857	1.15693	0.30007
C	2.77039	-0.18283	-0.17487
C	2.58632	-1.24962	0.61580
H	1.54048	2.81756	-0.06616
Cl	-3.59811	-0.92781	0.09433
H	-2.39889	1.01686	1.81047
H	-0.20357	2.22101	1.59082
H	2.34863	1.15863	1.28267
H	3.11491	-0.25977	-1.20403
H	2.23764	-1.09283	1.63703
H	1.83931	1.89613	-1.40891
C	2.87501	-2.65213	0.18896
H	1.99064	-3.28339	0.32313
H	3.17819	-2.69228	-0.86054
H	3.67549	-3.08637	0.79740
N	-1.35575	-0.33976	-1.11832
H	0.41064	0.09623	-2.12177

There are no imaginary frequencies.

SCF energy: -931.982269 hartree
αα/ββ: -0.217078149 hartree
αβ: -1.20000026 hartree
SCS-MP2 energy: -933.5669881 hartree
zero-point correction: +0.191456 hartree
enthalpy correction: +0.203974 hartree
free energy correction: +0.152414 hartree
quasiharmonic free energy correction: +0.154043 hartree

S-50

C	0.30344	-1.29279	-0.98920
C	0.21852	-0.53267	1.29454
C	2.05401	-0.04199	0.03396
C	1.54768	-0.68547	-1.09745
C	-0.37554	-1.20734	0.22926
N	-1.64634	-1.84366	0.37097
N	-2.68258	-1.04006	-0.31501
C	-2.82460	0.32824	0.17165
C	-2.31571	1.34423	-0.52922
H	-1.93250	-1.83292	1.35772
H	-0.28902	-0.45646	2.25411
H	2.11340	-0.72157	-2.02257
H	-0.13334	-1.82491	-1.83154
H	-2.45302	-1.05868	-1.32179
H	-3.31248	0.39447	1.13812
H	-1.83455	1.14257	-1.48597
H	-3.56134	-1.57071	-0.20453
C	-2.37886	2.76149	-0.06753
H	-2.89871	3.37810	-0.80712
H	-2.89531	2.84686	0.89124
H	-1.36678	3.16505	0.03860
N	1.43562	0.03697	1.21049
Cl	3.61430	0.73077	-0.06750

There are no imaginary frequencies.

SCF energy: -931.987062 hartree
αα/ββ: -0.217156569 hartree
αβ: -1.200118 hartree
SCS-MP2 energy: -933.5719746 hartree
zero-point correction: +0.191632 hartree
enthalpy correction: +0.204130 hartree
free energy correction: +0.152673 hartree
quasiharmonic free energy correction: +0.154347 hartree

S-51

C	-0.59395	-0.78266	1.38423
C	-0.28014	-0.47725	-0.98477
C	-2.34920	0.13398	0.03169
C	-1.87512	-0.26820	1.27634
C	0.22847	-0.90624	0.24564
N	1.46578	-1.50273	0.33793
N	2.34702	-1.25358	-0.73053
C	3.19752	-0.13264	-0.56507
C	3.00445	0.89074	0.28182
H	1.89612	-1.41317	1.26449
H	-0.21685	-1.09655	2.35469
H	2.87192	-2.10395	-0.93060
H	4.03230	-0.14594	-1.26364
H	2.15459	0.89241	0.96138
C	3.92661	2.07127	0.33545
H	4.35634	2.19425	1.33561
H	4.74987	1.95931	-0.37638
H	3.39739	3.00105	0.09852
N	-1.53414	0.01928	-1.03578
H	-2.51273	-0.17417	2.14879
Cl	-3.91919	0.76801	-0.22079
H	0.26735	-0.51035	-1.91717
H	-1.87251	0.32611	-1.95556

There are no imaginary frequencies.

SCF energy: -931.983287 hartree
αα/ββ: -0.217501529 hartree
αβ: -1.19991461 hartree
SCS-MP2 energy: -933.5681856 hartree
zero-point correction: +0.190632 hartree
enthalpy correction: +0.203159 hartree
free energy correction: +0.151896 hartree
quasiharmonic free energy correction: +0.153422 hartree

S-52

C	-0.13007	-1.83848	-0.54017
C	0.26721	-0.08369	1.10235
C	-1.77231	-0.22311	0.08676
C	-1.40240	-1.33683	-0.69640
C	0.70576	-1.24387	0.42978
N	2.02719	-1.60636	0.51916
N	3.01534	-0.40298	-0.58257
C	2.60030	0.81274	-0.15530
C	1.42992	1.40820	-0.57689
H	0.85591	0.34257	1.91096
H	-2.09791	-1.77353	-1.40522
H	0.21601	-2.69880	-1.10906
H	2.45996	-0.66723	-1.41075
H	3.17503	1.26148	0.65394
H	0.87603	0.92948	-1.38763
H	2.51531	-1.40933	1.39926
C	1.01052	2.77530	-0.17467
H	-0.06297	2.79531	0.03580
H	1.56280	3.12512	0.70071
H	1.18725	3.46883	-1.00638
H	2.29569	-2.50709	0.10547
N	-1.00508	0.37945	0.97859
Cl	-3.38229	0.40710	-0.10272

1 imaginary frequency: –305.46 cm^{-1}.

SCF energy: -931.932621 hartree
αα/ββ: -0.224487874 hartree
αβ: -1.21859575 hartree
SCS-MP2 energy: -933.5445945 hartree
zero-point correction: +0.188941 hartree
enthalpy correction: +0.200833 hartree
free energy correction: +0.151838 hartree
quasiharmonic free energy correction: +0.152636 hartree

S-53

C	0.98900	0.43121	0.98362
C	0.21887	-1.75767	-0.50312
C	-0.33193	-0.03520	1.12813
C	1.80016	-0.20649	0.06580
C	-0.68237	-1.22414	0.44905
N	-1.96458	-1.68963	0.50025
N	-3.01740	-0.47548	-0.63491
C	-2.64121	0.73498	-0.17940
C	-1.47070	1.36939	-0.56374
H	-0.96220	0.35064	1.92526
H	1.33839	1.28884	1.54869
H	-0.06605	-2.62694	-1.09429
H	-2.42552	-0.71994	-1.44390
H	-3.24334	1.16077	0.62262
H	-0.89660	0.92021	-1.37700
H	-2.50114	-1.53050	1.35804
C	-1.12624	2.75759	-0.16449
H	-0.05013	2.86096	0.00115
H	-1.66995	3.06732	0.73108
H	-1.38771	3.43579	-0.98738
H	-2.16494	-2.58927	0.04959
N	1.44435	-1.27798	-0.67904
Cl	3.42700	0.35681	-0.17253

1 imaginary frequency: –239.29 cm^{-1}.

SCF energy: -931.928467 hartree
αα/ββ: -0.224961795 hartree
αβ: -1.21977927 hartree
SCS-MP2 energy: -933.5421766 hartree
zero-point correction: +0.189404 hartree
enthalpy correction: +0.201114 hartree
free energy correction: +0.152710 hartree

quasiharmonic free energy correction: +0.153264 hartree

S-54

C	-0.10379	-1.81350	-0.53078
C	0.24076	-0.07003	1.12294
C	-1.77967	-0.22645	0.08439
C	-1.37581	-1.32395	-0.70945
C	0.72757	-1.22331	0.45735
N	2.01135	-1.66606	0.58839
N	2.93800	-0.44493	-0.55428
C	2.60990	0.82782	-0.20044
C	1.38810	1.34295	-0.56566
H	0.81462	0.36488	1.93943
H	-2.05602	-1.75833	-1.43495
H	0.26038	-2.66722	-1.09733
H	2.54070	-0.82532	-1.42049
H	3.24394	1.29063	0.54950
H	0.82146	0.83784	-1.34826
H	2.41946	-1.24285	1.43724
C	0.95593	2.71399	-0.17419
H	-0.11040	2.72165	0.06441
H	1.52482	3.08368	0.68174
H	1.10793	3.39261	-1.02130
H	3.89760	-0.76117	-0.37792
N	-1.03887	0.37500	0.99516
Cl	-3.40093	0.37355	-0.12247

1 imaginary frequency: –373.51 cm^{-1}.

SCF energy: -931.930216 hartree
αα/ββ: -0.225138456 hartree
αβ: -1.2218867 hartree
SCS-MP2 energy: -933.5465723 hartree
zero-point correction: +0.189293 hartree
enthalpy correction: +0.201115 hartree
free energy correction: +0.152380 hartree
quasiharmonic free energy correction: +0.153019 hartree

S-55

C	1.02577	0.40913	1.01263
C	0.19381	-1.73015	-0.50511
C	-0.29704	-0.04202	1.16532
C	1.80981	-0.21693	0.06320
C	-0.70205	-1.21052	0.47215
N	-1.94443	-1.75941	0.54410
N	-2.94027	-0.50358	-0.59670
C	-2.64786	0.75833	-0.20739
C	-1.43948	1.32375	-0.56348
H	-0.91768	0.35566	1.96616
H	1.40334	1.24589	1.59151
H	-0.11417	-2.58547	-1.10426
H	-2.51433	-0.86681	-1.45589
H	-3.29524	1.18922	0.55028
H	-0.86017	0.85041	-1.35620
H	-2.41100	-1.39281	1.38838
C	-1.06854	2.70924	-0.16292
H	0.00532	2.78296	0.02503
H	-1.61988	3.03206	0.72273
H	-1.30183	3.38740	-0.99217
H	-3.88258	-0.86544	-0.41804
N	1.42005	-1.26502	-0.69925
Cl	3.44202	0.32694	-0.19417

1 imaginary frequency: –317.28 cm^{-1}.

SCF energy: -931.925784 hartree
αα/ββ: -0.22533628 hartree
αβ: -1.22313144 hartree
SCS-MP2 energy: -933.5437659 hartree
zero-point correction: +0.188868 hartree
enthalpy correction: +0.200723 hartree
free energy correction: +0.151848 hartree
quasiharmonic free energy correction: +0.152609 hartree

S-56

C	-0.10270	-1.89153	-0.38963
C	0.37360	0.03181	1.01209
C	-1.78320	-0.23968	0.03570
C	-1.37725	-1.41246	-0.61250
C	0.78640	-1.23198	0.49199
N	2.06030	-1.69534	0.59691
N	2.95254	-0.56273	-0.68268
C	2.62938	0.68172	-0.26666
C	1.42612	1.31258	-0.55634
H	0.87775	0.51026	1.84553
H	-1.26196	1.23702	1.34951
H	-2.07006	-1.92050	-1.27425
H	0.22314	-2.81651	-0.85990
H	2.30992	-0.85250	-1.43404
H	3.28612	1.11636	0.48818
H	0.80690	0.88073	-1.34657
H	2.52916	-1.23309	1.38895
C	1.14502	2.72786	-0.16684
H	0.08446	2.87348	0.05967
H	1.74222	3.02717	0.69826
H	1.38779	3.39124	-1.00507
N	-0.94596	0.38769	0.86730
Cl	-3.35105	0.41230	-0.15694

1 imaginary frequency: –299.81 cm^{-1}.

SCF energy: -931.904610 hartree
αα/ββ: -0.226948479 hartree
αβ: -1.22605935 hartree
SCS-MP2 energy: -933.5271802 hartree
zero-point correction: +0.189022 hartree

enthalpy correction: +0.200736 hartree
free energy correction: +0.152414 hartree
quasiharmonic free energy correction: +0.152771 hartree

S-57

C	0.90202	0.56080	0.91921
C	0.18760	-1.80968	-0.34435
C	-0.42636	0.08432	1.04040
C	1.78275	-0.09909	0.09853
C	-0.75475	-1.21387	0.51645
N	-1.96545	-1.81392	0.59315
N	-2.95977	-0.62873	-0.74053
C	-2.67530	0.59591	-0.27990
C	-1.48208	1.28038	-0.53716
H	-1.04258	0.49405	1.83764
H	1.21771	1.46899	1.42235
H	2.05470	-1.74849	-1.12385
H	0.00220	-2.74711	-0.85916
H	-2.27268	-0.89404	-1.46210
H	-3.35447	0.99642	0.47448
H	-0.84942	0.89062	-1.33766
H	-2.50178	-1.38169	1.35906
C	-1.28780	2.71069	-0.14992
H	-0.23008	2.94271	-0.00533
H	-1.84177	2.95556	0.76001
H	-1.65628	3.34962	-0.96146
N	1.39107	-1.26096	-0.51113
Cl	3.39630	0.40834	-0.18082

1 imaginary frequency: –106.05 cm^{-1}.

SCF energy: -931.899516 hartree
αα/ββ: -0.227116933 hartree
αβ: -1.22878032 hartree
SCS-MP2 energy: -933.5254637 hartree
zero-point correction: +0.188882 hartree
enthalpy correction: +0.200640 hartree
free energy correction: +0.152179 hartree
quasiharmonic free energy correction: +0.152566 hartree

S-58

C	-0.50568	1.89738	0.49175
C	0.50563	-0.16334	-0.62895
C	-1.80153	-0.03485	-0.18451
C	-1.70027	1.26348	0.47131
C	0.62143	1.24893	-0.12811
N	1.75024	1.87611	-0.24423
N	3.37164	-0.31000	-0.81784
C	2.78891	-1.18727	-0.08186
C	1.32025	-1.17378	0.22615
H	0.91784	-0.19041	-1.64572
H	-2.58131	1.70657	0.92447
H	4.37239	-0.51941	-0.89543
H	3.33343	-2.01986	0.37564
H	0.94145	-2.16006	-0.07287
C	1.08856	-1.01217	1.73189
H	1.56045	-1.83987	2.26852
H	1.51842	-0.07647	2.10103
H	0.01875	-1.02552	1.96020
N	-0.84687	-0.70235	-0.72004
Cl	-3.40848	-0.70779	-0.25358
H	1.85460	2.83299	0.10052
H	2.55786	1.36817	-0.65623
H	-0.37866	2.87978	0.93949

There are no imaginary frequencies.

SCF energy: -932.017564 hartree
αα/ββ: -0.214634779 hartree
αβ: -1.20402912 hartree
SCS-MP2 energy: -933.6054888 hartree
zero-point correction: +0.190619 hartree
enthalpy correction: +0.202735 hartree
free energy correction: +0.153600 hartree
quasiharmonic free energy correction: +0.153930 hartree

S-59

C	-0.55080	-0.18360	-0.64690
C	0.59238	1.79659	0.49408
C	1.87097	-0.01439	-0.16539
C	0.84796	-0.70209	-0.70618
C	-0.60035	1.20752	-0.10716
N	-1.68783	1.90761	-0.15065
N	-3.42366	-0.15421	-0.79668
C	-2.88656	-1.10828	-0.12418
C	-1.41834	-1.19037	0.17423
H	1.00142	-1.67271	-1.16930
H	-0.96438	-0.16253	-1.66664
H	-4.43501	-0.30128	-0.87916
H	-3.47436	-1.93735	0.28371
H	-1.10008	-2.18827	-0.15711
C	-1.16890	-1.09297	1.68281
H	-0.09900	-1.17473	1.89647
H	-1.54161	-0.14714	2.08698
H	-1.68325	-1.90878	2.19841
N	1.75915	1.22427	0.46978
Cl	3.49390	-0.63005	-0.20677
H	-1.71507	2.85929	0.22653
H	-2.53969	1.46045	-0.55303
H	0.50293	2.76579	0.98321

There are no imaginary frequencies.

SCF energy: -931.999838 hartree
αα/ββ: -0.214691424 hartree
αβ: -1.20526296 hartree

SCS-MP2 energy: -933.5892812 hartree
zero-point correction: +0.189576 hartree
enthalpy correction: +0.201806 hartree
free energy correction: +0.152132 hartree
quasiharmonic free energy correction: +0.152808 hartree

S-60

C	0.92248	2.08870	0.22244
C	-0.35671	-0.06830	0.45337
C	1.93638	-0.09169	0.03634
C	2.05679	1.35477	0.19866
C	-0.35913	1.39945	0.10205
N	-1.48302	1.94340	-0.21712
N	-3.84846	-0.14320	-0.60721
C	-2.83244	-0.10162	0.18543
C	-1.56392	-0.80645	-0.13411
H	-1.37735	2.95929	-0.34618
H	-0.42383	-0.12154	1.55394
H	3.04141	1.80845	0.24963
H	0.94498	3.17601	0.25805
H	-3.00155	0.30241	1.17955
H	-1.45654	-0.86258	-1.22361
C	-1.68420	-2.22349	0.45098
H	-0.76338	-2.77256	0.25057
H	-1.84381	-2.18206	1.53262
H	-2.51992	-2.75575	-0.00997
N	0.86816	-0.79575	0.09836
Cl	3.43785	-0.91831	-0.32784
H	-4.74574	0.25652	-0.33416
H	-3.77014	-0.53627	-1.54624

There are no imaginary frequencies.

SCF energy: -932.021051 hartree
αα/ββ: -0.213456711 hartree
αβ: -1.20112577 hartree
SCS-MP2 energy: -933.6047064 hartree
zero-point correction: +0.190397 hartree
enthalpy correction: +0.202926 hartree
free energy correction: +0.152359 hartree
quasiharmonic free energy correction: +0.153383 hartree

S-61

C	-0.54539	-0.15878	-0.69984
C	0.57332	1.74299	0.59016
C	1.86385	-0.01367	-0.15044
C	0.86517	-0.66529	-0.76896
C	-0.60097	1.24570	-0.14593
N	-1.65761	1.96722	-0.32589
N	-3.50541	-0.12869	-0.55090
C	-2.84959	-1.14297	-0.11328
C	-1.38130	-1.18197	0.11727
H	0.46018	2.66888	1.15659
H	1.04698	-1.59384	-1.30334
H	-0.95013	-0.13474	-1.72160
H	-3.42576	-2.03440	0.12661
H	-1.07422	-2.18167	-0.21765
H	-1.56041	2.88620	0.12675
C	-1.13147	-1.10066	1.63329
H	-0.05804	-1.18495	1.82295
H	-1.49718	-0.15426	2.04013
H	-1.63799	-1.92078	2.14904
N	1.73768	1.17214	0.59538
Cl	3.49762	-0.60979	-0.21090
H	-4.51932	-0.18981	-0.66468
H	-3.02797	0.77908	-0.73328

There are no imaginary frequencies.

SCF energy: -932.006092 hartree
αα/ββ: -0.213937865 hartree
αβ: -1.20434742 hartree
SCS-MP2 energy: -933.5939341 hartree
zero-point correction: +0.190707 hartree
enthalpy correction: +0.202915 hartree
free energy correction: +0.153127 hartree
quasiharmonic free energy correction: +0.153946 hartree

S-62

C	-0.49168	2.23494	0.17375
C	0.86130	0.24038	-0.66478
C	-1.51078	0.06459	-0.08319
C	-1.57905	1.44682	0.33392
C	0.74123	1.72737	-0.41911
N	1.69179	2.56744	-0.66538
N	1.23727	-2.54178	-0.72211
C	2.04058	-1.88278	0.03498
C	1.84436	-0.42157	0.32548
H	2.48902	2.08000	-1.09964
H	1.22180	0.06553	-1.68531
H	-0.52126	3.28623	0.44818
H	2.89730	-2.34661	0.53387
H	2.80810	0.07766	0.15096
H	1.52467	-3.52404	-0.78562
C	1.45223	-0.22798	1.79386
H	1.44827	0.83194	2.06108
H	0.46366	-0.65089	1.99709
H	2.17698	-0.73607	2.43616
N	-0.43453	-0.45186	-0.58141
Cl	-2.89805	-0.91452	0.04921
H	-2.50776	1.81408	0.75573
H	-0.34476	-1.45815	-0.83612

There are no imaginary frequencies.

SCF energy: -931.999493 hartree

αα/ββ: -0.214243095 hartree
αβ: -1.20476436 hartree
SCS-MP2 energy: -933.588039 hartree
zero-point correction: +0.190294 hartree
enthalpy correction: +0.202455 hartree
free energy correction: +0.152941 hartree
quasiharmonic free energy correction: +0.153394 hartree

S-63

C	-0.78814	-0.25378	-1.05046
C	-0.16194	1.19124	0.84432
C	1.55167	-0.04891	-0.23406
C	0.66412	-0.66716	-1.03431
C	-0.89924	1.12195	-0.46618
N	-1.49619	2.16635	-0.90729
N	-0.66067	0.06762	1.70205
C	-1.25500	-0.99352	1.26792
C	-1.62188	-1.19925	-0.15624
H	-0.35598	2.11482	1.38854
H	-1.53475	-1.73114	2.01741
H	-1.37546	-2.23977	-0.40066
H	-1.92134	1.94584	-1.81869
C	-3.14016	-1.00623	-0.30363
H	-3.68306	-1.68195	0.36272
H	-3.42639	0.02277	-0.07078
H	-3.42344	-1.23056	-1.33489
N	1.24803	1.05063	0.58352
H	-0.45180	0.13573	2.70520
H	-1.18756	-0.27410	-2.07091
H	0.98116	-1.48725	-1.67019
Cl	3.22468	-0.50337	-0.19905
H	1.82428	1.12465	1.42409

There are no imaginary frequencies.

SCF energy: -932.022699 hartree
αα/ββ: -0.214936135 hartree
αβ: -1.20157843 hartree
SCS-MP2 energy: -933.6078839 hartree
zero-point correction: +0.194386 hartree
enthalpy correction: +0.205504 hartree
free energy correction: +0.158705 hartree
quasiharmonic free energy correction: +0.158800 hartree

2-bromo-5-hydrazinylpyridine (29)

S-64

C	0.21292	-0.31355	1.09112
C	-0.23424	1.56723	-0.37119
C	-1.90259	0.07615	0.06376
C	-1.10482	-0.71118	0.89826
C	0.62667	0.84657	0.44488
N	2.00851	1.29622	0.58835
N	2.86310	0.61594	-0.39903
C	3.64337	-0.24860	0.14930
C	4.57187	-1.03859	-0.70069
H	2.34069	1.15137	1.56071
H	0.09257	2.47253	-0.87818
H	-1.49518	-1.60173	1.37914
H	0.88726	-0.88058	1.72863
H	3.66424	-0.41960	1.23020
H	4.32036	-2.09738	-0.56688
H	2.07794	2.30796	0.38714
H	4.41459	-0.78051	-1.75107
C	6.02329	-0.79375	-0.28050
H	6.29437	0.25560	-0.42250
H	6.17645	-1.05190	0.77088
H	6.69370	-1.40845	-0.88596
N	-1.50957	1.18348	-0.56372
Br	-3.71486	-0.45493	-0.22003

There are no imaginary frequencies.

SCF energy: -3042.406749 hartree
αα/ββ: -0.214254722 hartree
αβ: -1.18483132 hartree
SCS-MP2 energy: -3043.971383 hartree
zero-point correction: +0.190463 hartree
enthalpy correction: +0.203226 hartree
free energy correction: +0.150186 hartree
quasiharmonic free energy correction: +0.152122 hartree

S-65

C	-0.46485	-0.37351	-0.33270
C	0.41534	1.84190	0.02497
C	1.85762	0.07865	-0.03354
C	0.83772	-0.85070	-0.23982
C	-0.67769	1.00076	-0.19083
N	-1.97534	1.56449	-0.35775
N	-2.94765	0.83341	0.35494
C	-3.93989	0.27994	-0.24887
C	-4.94567	-0.53012	0.46273
H	-2.00744	2.53000	-0.01350
H	0.27371	2.91479	0.14121
H	1.05118	-1.90997	-0.33804
H	-1.28896	-1.06042	-0.50938
H	-3.98930	0.42481	-1.32575
H	-5.91975	-0.06572	0.26978
H	-4.75946	-0.51602	1.53960
C	-4.93552	-1.96214	-0.09027
H	-3.96833	-2.43794	0.08790
H	-5.70956	-2.54386	0.41437
H	-5.13971	-1.96845	-1.16353
N	1.68249	1.39204	0.09577
Br	3.65949	-0.55789	0.07898
H	-2.82363	0.72083	1.37241

There are no imaginary frequencies.

SCF energy: -3042.418290 hartree
αα/ββ: -0.213704996 hartree
αβ: -1.17844415 hartree
SCS-MP2 energy: -3043.974893 hartree
zero-point correction: +0.190092 hartree
enthalpy correction: +0.202999 hartree
free energy correction: +0.148876 hartree
quasiharmonic free energy correction: +0.151785 hartree

S-66

C	0.26722	1.82539	-0.00316
C	-0.34005	-0.51457	-0.03898
C	1.95986	0.12440	-0.00338
C	1.60481	1.47119	0.00888
C	-0.74051	0.83271	-0.02605
N	-2.04862	1.17893	-0.04785
N	-3.01749	0.20367	-0.01827
C	-4.23592	0.63063	0.02636
C	-5.38516	-0.32041	0.05621
H	-2.31146	2.16651	0.00596
H	-0.01616	2.87520	0.00843
H	-4.45812	1.70347	0.04556
H	-6.05266	-0.06002	-0.77570
H	-5.96303	-0.11485	0.96714
C	-5.00565	-1.79285	-0.01049
H	-4.37531	-2.07826	0.83521
H	-5.90774	-2.41017	0.01308
H	-4.46164	-2.01940	-0.93080
N	0.97760	-0.80129	-0.02704
H	2.37555	2.23461	0.02896
Br	3.73820	-0.47859	0.01400
H	-1.01786	-1.35736	-0.05704
H	1.22356	-1.79690	-0.03512

There are no imaginary frequencies.

SCF energy: -3042.405515 hartree
αα/ββ: -0.216025344 hartree
αβ: -1.18946842 hartree
SCS-MP2 energy: -3043.976894 hartree
zero-point correction: +0.189008 hartree
enthalpy correction: +0.202197 hartree
free energy correction: +0.148484 hartree
quasiharmonic free energy correction: +0.150416 hartree

S-67

C	0.21541	-1.70418	-0.78711
C	0.50391	-0.37551	1.21974
C	-1.46604	-0.25410	0.07645
C	-1.06305	-1.17057	-0.89858
C	0.98633	-1.29448	0.29591
N	2.35772	-1.77069	0.41400
N	3.36615	-0.98324	-0.33148
C	3.37402	0.36102	0.14595
C	3.07118	1.40971	-0.63186
H	2.43994	-2.74464	0.07716
Br	-3.21389	0.50373	-0.05716
H	-1.71849	-1.45575	-1.71452
H	0.59539	-2.42103	-1.51189
H	3.03923	-1.01159	-1.30524
H	3.73613	0.46633	1.16654
H	2.71222	1.22865	-1.64544
H	2.66718	-1.77576	1.40111
C	3.23653	2.82906	-0.19518
H	2.29080	3.37236	-0.29043
H	3.56994	2.88575	0.84440
H	3.97041	3.34620	-0.82246
N	-0.73300	0.14477	1.11378
H	1.09748	-0.06282	2.07543

There are no imaginary frequencies.

SCF energy: -3042.387916 hartree
αα/ββ: -0.215377769 hartree
αβ: -1.18650334 hartree
SCS-MP2 energy: -3043.955305 hartree
zero-point correction: +0.190579 hartree
enthalpy correction: +0.203381 hartree
free energy correction: +0.150145 hartree
quasiharmonic free energy correction: +0.152351 hartree

S-68

C	-0.43342	-1.21933	-1.08443
C	-0.38931	-0.79651	1.28719
C	1.44736	-0.28597	0.04038
C	0.85599	-0.70627	-1.15329
C	-1.06928	-1.25676	0.15979
N	-2.37556	-1.82146	0.27127
N	-3.37376	-0.91567	-0.32992
C	-3.41337	0.42929	0.23504
C	-2.94310	1.46216	-0.46758
H	-2.64690	-1.87695	1.26038
H	-0.86337	-0.81720	2.26658
H	1.38956	-0.65463	-2.09643
H	-0.93439	-1.58662	-1.97772
H	-3.18172	-0.88772	-1.34447
H	-3.81068	0.46230	1.24385
H	-2.56004	1.29125	-1.47330
H	-4.28117	-1.39608	-0.22099
C	-2.92824	2.85976	0.05457
H	-3.52310	3.51123	-0.59307
H	-3.32738	2.91055	1.07017
H	-1.90510	3.24839	0.05661

N	0.87175	-0.32415	1.23925
Br	3.22936	0.40875	-0.02531

There are no imaginary frequencies.

SCF energy: -3042.393237 hartree
αα/ββ: -0.215377435 hartree
αβ: -1.18641675 hartree
SCS-MP2 energy: -3043.960522 hartree
zero-point correction: +0.191317 hartree
enthalpy correction: +0.203999 hartree
free energy correction: +0.151272 hartree
quasiharmonic free energy correction: +0.153293 hartree

S-69

C	0.16059	-0.98485	1.38694
C	0.39729	-0.59710	-0.98099
C	-1.68003	-0.14378	0.09941
C	-1.15314	-0.54906	1.32222
C	0.96582	-1.01269	0.22924
N	2.24731	-1.50646	0.27838
N	3.08400	-1.14961	-0.79487
C	3.84441	0.03051	-0.59933
C	3.58774	0.99562	0.29771
H	2.68594	-1.42201	1.20148
H	0.58020	-1.30018	2.33955
H	3.66941	-1.94809	-1.03691
H	4.65688	0.11817	-1.31831
H	2.76043	0.89227	0.99693
C	4.39978	2.25281	0.38378
H	4.84766	2.36886	1.37678
H	5.20666	2.25233	-0.35514
H	3.77919	3.13854	0.20815
N	-0.88752	-0.18608	-0.99133
H	-1.76999	-0.52039	2.21408
Br	-3.43762	0.48097	-0.11655
H	0.92108	-0.57686	-1.92723
H	-1.26205	0.10983	-1.89913

There are no imaginary frequencies.

SCF energy: -3042.388491 hartree
αα/ββ: -0.215695744 hartree
αβ: -1.18609736 hartree
SCS-MP2 energy: -3043.955605 hartree
zero-point correction: +0.189940 hartree
enthalpy correction: +0.202694 hartree
free energy correction: +0.150409 hartree
quasiharmonic free energy correction: +0.151761 hartree

TS S-70

C	0.58001	-1.88205	-0.54741
C	0.87470	-0.13203	1.12341
C	-1.15896	-0.39341	0.12828
C	-0.72681	-1.46613	-0.68019
C	1.38575	-1.24432	0.42075
N	2.73196	-1.50508	0.48628
N	3.61142	-0.20575	-0.60298
C	3.09768	0.96617	-0.16043
C	1.87791	1.46009	-0.57331
H	1.44493	0.31891	1.93230
H	-1.39837	-1.93909	-1.38888
H	0.97522	-2.70697	-1.13631
H	3.07660	-0.50548	-1.43262
H	3.63703	1.45500	0.64987
H	1.36589	0.93513	-1.38347
H	3.21449	-1.28600	1.36431
C	1.33355	2.78023	-0.16579
H	0.25997	2.70158	0.02969
H	1.84144	3.17227	0.71854
H	1.45758	3.49308	-0.99084
H	3.06706	-2.37368	0.05243
N	-0.42917	0.24238	1.02674
Br	-2.96927	0.18523	-0.05877

1 imaginary frequency: –295.13 cm^{-1}.

SCF energy: -3042.338230 hartree
αα/ββ: -0.222840152 hartree
αβ: -1.20518171 hartree
SCS-MP2 energy: -3043.933008 hartree
zero-point correction: +0.188170 hartree
enthalpy correction: +0.200377 hartree
free energy correction: +0.149617 hartree
quasiharmonic free energy correction: +0.151013 hartree

TS S-71

C	0.40193	0.31490	1.03690
C	-0.46897	-1.81092	-0.48796
C	-0.94793	-0.07101	1.14899
C	1.18744	-0.36229	0.12433
C	-1.35596	-1.22831	0.44861
N	-2.66808	-1.60656	0.46225
N	-3.60305	-0.31871	-0.68169
C	-3.15955	0.86151	-0.20636
C	-1.94318	1.42055	-0.56242
H	-1.57198	0.34800	1.93446
H	0.78929	1.14351	1.61999
H	-0.79429	-2.65814	-1.09041
H	-3.01045	-0.59315	-1.48063
H	-3.74954	1.31872	0.58734
H	-1.38311	0.93886	-1.36706
H	-3.21446	-1.42036	1.30866
C	-1.50924	2.77718	-0.14212
H	-0.42870	2.80479	0.02512
H	-2.03296	3.10942	0.75728

H	-1.72409	3.48316	-0.95509
H	-2.91679	-2.48712	-0.00283
N	0.78763	-1.40484	-0.63685
Br	3.00555	0.16896	-0.10008

1 imaginary frequency: –243.97 cm^{-1}.

SCF energy: -3042.334292 hartree
αα/ββ: -0.223302651 hartree
αβ: -1.20632677 hartree
SCS-MP2 energy: -3043.930753 hartree
zero-point correction: +0.188592 hartree
enthalpy correction: +0.200573 hartree
free energy correction: +0.150782 hartree
quasiharmonic free energy correction: +0.151570 hartree

TS S-72

C	0.58990	-1.85193	-0.53602
C	0.85066	-0.11895	1.14486
C	-1.16857	-0.38208	0.13140
C	-0.71405	-1.44038	-0.68798
C	1.39852	-1.22665	0.44909
N	2.71062	-1.58665	0.55039
N	3.53517	-0.28156	-0.58213
C	3.11982	0.95912	-0.20777
C	1.86041	1.38542	-0.56048
H	1.41005	0.33770	1.95971
H	-1.37583	-1.90604	-1.41114
H	0.99724	-2.67266	-1.12190
H	3.15692	-0.67852	-1.44939
H	3.72608	1.45673	0.54285
H	1.33245	0.84291	-1.34563
H	3.10468	-1.15487	1.40176
C	1.32145	2.71474	-0.15909
H	0.25601	2.63709	0.07074
H	1.85402	3.12060	0.70375
H	1.42544	3.41016	-0.99992
H	4.51643	-0.53126	-0.41817
N	-0.45662	0.24724	1.04477
Br	-2.98504	0.17855	-0.07051

1 imaginary frequency: –377.54 cm^{-1}.

SCF energy: -3042.335550 hartree
αα/ββ: -0.223525107 hartree
αβ: -1.20865108 hartree
SCS-MP2 energy: -3043.934948 hartree
zero-point correction: +0.188431 hartree
enthalpy correction: +0.200593 hartree
free energy correction: +0.150244 hartree
quasiharmonic free energy correction: +0.151215 hartree

TS S-73

C	0.43188	0.28880	1.07862
C	-0.48810	-1.77129	-0.50009
C	-0.91794	-0.08810	1.19309
C	1.19507	-0.36217	0.12792
C	-1.37384	-1.21770	0.46806
N	-2.64979	-1.68918	0.50035
N	-3.53309	-0.35894	-0.64231
C	-3.16885	0.87790	-0.23206
C	-1.91929	1.36566	-0.55832
H	-1.53490	0.33359	1.98466
H	0.84144	1.09154	1.68323
H	-0.83113	-2.59720	-1.12119
H	-3.11148	-0.73848	-1.49653
H	-3.80369	1.34267	0.51613
H	-1.35671	0.85999	-1.34353
H	-3.11444	-1.30903	1.33980
C	-1.46055	2.71884	-0.13911
H	-0.38326	2.72140	0.04328
H	-1.98715	3.06379	0.75317
H	-1.65448	3.42152	-0.95821
H	-4.50175	-0.65902	-0.49104
N	0.76692	-1.37167	-0.66250
Br	3.01597	0.15818	-0.11164

1 imaginary frequency: –324.66 cm^{-1}.

SCF energy: -3042.331460 hartree
αα/ββ: -0.223701809 hartree
αβ: -1.20978488 hartree
SCS-MP2 energy: -3043.932336 hartree
zero-point correction: +0.188295 hartree
enthalpy correction: +0.200357 hartree
free energy correction: +0.150405 hartree
quasiharmonic free energy correction: +0.151162 hartree

TS S-74

C	0.58694	-1.93814	-0.38952
C	0.96734	0.00282	1.02020
C	-1.18623	-0.40126	0.08398
C	-0.72084	-1.53935	-0.58445
C	1.44889	-1.23120	0.48117
N	2.74770	-1.61912	0.56589
N	3.55371	-0.40171	-0.71345
C	3.15060	0.80965	-0.27603
C	1.90515	1.36229	-0.55249
H	1.45443	0.50330	1.85110
H	-0.72751	1.09688	1.40694
H	-1.38872	-2.08958	-1.23830
H	0.96020	-2.83796	-0.87338
H	2.92214	-0.72574	-1.45991
H	3.78217	1.27887	0.47953
H	1.31057	0.89556	-1.34223

H	3.19955	-1.13516	1.35483
C	1.53653	2.75408	-0.15343
H	0.46650	2.83646	0.05986
H	2.10564	3.08037	0.72074
H	1.75096	3.43663	-0.98408
N	-0.37507	0.27429	0.90517
Br	-2.95573	0.19922	-0.08729

1 imaginary frequency: –275.14 cm^{-1}.

SCF energy: -3042.308813 hartree
αα/ββ: -0.225247944 hartree
αβ: -1.21260379 hartree
SCS-MP2 energy: -3043.914103 hartree
zero-point correction: +0.188491 hartree
enthalpy correction: +0.200470 hartree
free energy correction: +0.150707 hartree
quasiharmonic free energy correction: +0.151402 hartree

TS S-75

C	0.33130	0.44632	0.96834
C	-0.50072	-1.86648	-0.33249
C	-1.02501	0.05071	1.05902
C	1.18648	-0.26195	0.15981
C	-1.42310	-1.21620	0.50955
N	-2.67425	-1.73333	0.54689
N	-3.55190	-0.48018	-0.77957
C	-3.20354	0.72250	-0.30126
C	-1.97028	1.33715	-0.53725
H	-1.63195	0.49128	1.84671
H	0.68561	1.33068	1.48831
H	1.37959	-1.92501	-1.07042
H	-0.73448	-2.78603	-0.86005
H	-2.87431	-0.77562	-1.49798
H	-3.86869	1.15372	0.44851
H	-1.34656	0.91190	-1.32700
H	-3.19821	-1.28061	1.30927
C	-1.69133	2.74812	-0.13328
H	-0.62403	2.90775	0.03895
H	-2.25015	3.02351	0.76486
H	-1.99402	3.41625	-0.94849
N	0.73995	-1.39467	-0.46797
Br	2.98965	0.20081	-0.10408

1 imaginary frequency: –95.35 cm^{-1}.

SCF energy: -3042.305746 hartree
αα/ββ: -0.225260596 hartree
αβ: -1.21452832 hartree
SCS-MP2 energy: -3043.913354 hartree
zero-point correction: +0.188533 hartree
enthalpy correction: +0.200402 hartree
free energy correction: +0.151117 hartree
quasiharmonic free energy correction: +0.151488 hartree

S-76

C	0.26540	2.03285	0.47036
C	1.06623	-0.13970	-0.61243
C	-1.20736	0.20370	-0.12019
C	-0.98025	1.50481	0.49819
C	1.31908	1.26753	-0.14832
N	2.50059	1.78101	-0.29585
N	3.90130	-0.54786	-0.85453
C	3.25816	-1.35555	-0.08970
C	1.80457	-1.20087	0.25055
H	1.45011	-0.22591	-1.63682
H	-1.80637	2.03816	0.95752
H	4.87703	-0.84792	-0.95090
H	3.73464	-2.22708	0.37095
H	1.33219	-2.15570	-0.01470
C	1.62475	-0.98499	1.75681
H	2.03695	-1.83879	2.30164
H	2.14472	-0.08247	2.09137
H	0.56397	-0.89974	2.01030
N	-0.33347	-0.55772	-0.66412
Br	-3.03299	-0.38244	-0.13327
H	2.70200	2.73162	0.02357
H	3.24908	1.18637	-0.70625
H	0.48792	3.01216	0.88744

There are no imaginary frequencies.

SCF energy: -3042.422815 hartree
αα/ββ: -0.212953594 hartree
αβ: -1.19066621 hartree
SCS-MP2 energy: -3043.993584 hartree
zero-point correction: +0.189957 hartree
enthalpy correction: +0.202412 hartree
free energy correction: +0.151654 hartree
quasiharmonic free energy correction: +0.152209 hartree

S-77

C	-1.12200	-0.16463	-0.62813
C	-0.15093	1.92655	0.47656
C	1.26997	0.20174	-0.10805
C	0.31365	-0.57852	-0.64646
C	-1.28670	1.22928	-0.11904
N	-2.42636	1.83827	-0.18658
N	-3.98862	-0.35135	-0.83233
C	-3.39337	-1.25855	-0.14414
C	-1.93133	-1.21988	0.19188
H	0.54460	-1.54705	-1.08094
H	-1.50938	-0.19153	-1.65837
H	-4.98256	-0.57845	-0.94027
H	-3.92304	-2.13197	0.25049

H	-1.52843	-2.19645	-0.10946
C	-1.73076	-1.07264	1.70412
H	-0.66383	-1.06642	1.94641
H	-2.18653	-0.15029	2.07583
H	-2.19508	-1.91468	2.22494
N	1.05726	1.44527	0.48791
Br	3.09223	-0.34677	-0.11046
H	-2.53380	2.79362	0.16591
H	-3.23546	1.31427	-0.58648
H	-0.32169	2.90030	0.93468

There are no imaginary frequencies.

SCF energy: -3042.406199 hartree
αα/ββ: -0.212972145 hartree
αβ: -1.19160844 hartree
SCS-MP2 energy: -3043.978111 hartree
zero-point correction: +0.188852 hartree
enthalpy correction: +0.201400 hartree
free energy correction: +0.150084 hartree
quasiharmonic free energy correction: +0.151047 hartree

S-78

C	0.08394	2.28892	0.24290
C	-0.96153	0.01181	0.51116
C	1.32961	0.22963	0.13759
C	1.29360	1.68500	0.25503
C	-1.11294	1.46131	0.11834
N	-2.28053	1.87105	-0.24094
N	-4.35244	-0.47440	-0.75280
C	-3.40780	-0.30145	0.10825
C	-2.05273	-0.87661	-0.09511
H	-2.28511	2.88842	-0.39858
H	-1.05343	-0.02298	1.61049
H	2.22038	2.24745	0.30660
H	-0.01193	3.37273	0.25036
H	-3.69104	0.10076	1.07637
H	-1.86799	-0.98072	-1.17076
C	-2.06138	-2.26407	0.56882
H	-1.06991	-2.70990	0.47912
H	-2.31625	-2.18173	1.62958
H	-2.78870	-2.91645	0.07933
N	0.34721	-0.58618	0.20665
Br	3.07622	-0.50939	-0.20592
H	-5.30646	-0.17374	-0.55555
H	-4.16169	-0.87558	-1.67202

There are no imaginary frequencies.

SCF energy: -3042.426476 hartree
αα/ββ: -0.211796062 hartree
αβ: -1.187765 hartree
SCS-MP2 energy: -3043.992991 hartree
zero-point correction: +0.189619 hartree
enthalpy correction: +0.202438 hartree
free energy correction: +0.150314 hartree
quasiharmonic free energy correction: +0.151723 hartree

S-79

C	-1.12002	-0.13967	-0.69034
C	-0.17878	1.85216	0.60553
C	1.25624	0.19536	-0.08900
C	0.32703	-0.53851	-0.72487
C	-1.29100	1.26513	-0.16105
N	-2.38904	1.90670	-0.38871
N	-4.07591	-0.32621	-0.58470
C	-3.35510	-1.27842	-0.11124
C	-1.88966	-1.20925	0.13171
H	-0.37665	2.76877	1.16402
H	0.58790	-1.45451	-1.24788
H	-1.50472	-0.16255	-1.71962
H	-3.86954	-2.20071	0.15154
H	-1.50933	-2.18938	-0.18586
H	-2.37596	2.83677	0.05189
C	-1.65983	-1.08818	1.64837
H	-0.58467	-1.09051	1.84834
H	-2.09778	-0.16522	2.03733
H	-2.10990	-1.93536	2.17262
N	1.02577	1.37064	0.64624
Br	3.08934	-0.33039	-0.11843
H	-5.08229	-0.46092	-0.70204
H	-3.66314	0.60774	-0.78979

There are no imaginary frequencies.

SCF energy: -3042.411994 hartree
αα/ββ: -0.212287682 hartree
αβ: -1.19095983 hartree
SCS-MP2 energy: -3043.982671 hartree
zero-point correction: +0.189944 hartree
enthalpy correction: +0.202400 hartree
free energy correction: +0.151359 hartree
quasiharmonic free energy correction: +0.152279 hartree

S-80

C	-0.55175	-2.35241	0.16995
C	-1.42121	-0.09958	-0.66127
C	0.93119	-0.47392	-0.09946
C	0.69127	-1.83647	0.31464
C	-1.64444	-1.57269	-0.40284
N	-2.76645	-2.17240	-0.63176
N	-1.09278	2.69521	-0.70403
C	-2.07310	2.25107	-0.00038
C	-2.22498	0.78852	0.31363
H	-3.43883	-1.51522	-1.05411
H	-1.72921	0.14153	-1.68568

H	-0.75995	-3.38351	0.44442
H	-2.83102	2.90837	0.43652
H	-3.27690	0.52108	0.14317
H	-1.13929	3.71501	-0.79742
C	-1.89247	0.53417	1.78721
H	-2.10663	-0.50247	2.06065
H	-0.84180	0.75077	2.00214
H	-2.50624	1.18405	2.41735
N	-0.00047	0.28105	-0.58155
Br	2.66078	0.23548	0.02941
H	1.51420	-2.41327	0.72185
H	0.11919	1.29272	-0.82576

There are no imaginary frequencies.

SCF energy: -3042.403175 hartree
αα/ββ: -0.212536753 hartree
αβ: -1.19115832 hartree
SCS-MP2 energy: -3043.974256 hartree
zero-point correction: +0.189627 hartree
enthalpy correction: +0.202033 hartree
free energy correction: +0.151096 hartree
quasiharmonic free energy correction: +0.151872 hartree

S-81

C	-1.30221	-0.30918	-1.03253
C	-0.82063	1.27663	0.79155
C	0.99711	0.10763	-0.18805
C	0.17547	-0.61856	-0.96761
C	-1.52416	1.08323	-0.52524
N	-2.19196	2.05270	-1.03125
N	-1.25639	0.16611	1.69955
C	-1.77381	-0.95238	1.31366
C	-2.08670	-1.26367	-0.10404
H	-1.09233	2.21018	1.28307
H	-2.02509	-1.66416	2.09751
H	-1.75597	-2.29468	-0.28091
H	-2.58171	1.74902	-1.93467
C	-3.61041	-1.19712	-0.29838
H	-4.11699	-1.88829	0.38043
H	-3.98339	-0.18620	-0.11440
H	-3.84479	-1.48163	-1.32708
N	0.60235	1.22607	0.56117
H	-1.07873	0.30359	2.70166
H	-1.67524	-0.41132	-2.05810
H	0.55873	-1.44933	-1.55089
Br	2.85807	-0.26158	-0.08973
H	1.15699	1.39434	1.40171

There are no imaginary frequencies.

SCF energy: -3042.429096 hartree
αα/ββ: -0.213216957 hartree
αβ: -1.18795741 hartree
SCS-MP2 energy: -3043.99679 hartree
zero-point correction: +0.193313 hartree
enthalpy correction: +0.204856 hartree
free energy correction: +0.156176 hartree
quasiharmonic free energy correction: +0.156567 hartree

3-hydrazinyl-4-methoxypyridine (33)

S-82

C	0.98179	0.60678	-0.26164
C	2.16001	-1.48440	0.11330
C	3.14349	0.47674	0.76141
C	2.07357	1.25338	0.32009
C	1.05774	-0.78906	-0.35501
N	-0.07691	-1.50302	-0.91927
N	-1.17182	-1.53398	0.06677
C	-2.20264	-0.87970	-0.33939
C	-3.36401	-0.70399	0.57021
H	0.18270	-2.48557	-1.11050
H	2.19589	-2.56941	0.03228
H	3.99980	0.96853	1.21580
H	2.10805	2.33075	0.43478
H	-2.24914	-0.41252	-1.32664
H	-4.26539	-1.03937	0.04576
H	-0.37550	-1.07794	-1.81811
H	-3.23048	-1.32191	1.46174
C	-3.49751	0.77721	0.94310
H	-2.60818	1.12000	1.47891
H	-3.62415	1.39647	0.05070
H	-4.36798	0.92183	1.58789
N	3.21580	-0.86658	0.67078
O	-0.13780	1.17874	-0.75416
C	-0.26630	2.61143	-0.59394
H	-0.24074	2.87488	0.46522
H	0.52792	3.12525	-1.13903
H	-1.23659	2.85372	-1.02220

There are no imaginary frequencies.

SCF energy: -586.986479 hartree
αα/ββ: -0.237782978 hartree
αβ: -1.33159 hartree
SCS-MP2 energy: -588.742906 hartree
zero-point correction: +0.234822 hartree
enthalpy correction: +0.248545 hartree
free energy correction: +0.195542 hartree
quasiharmonic free energy correction: +0.196474 hartree

S-83

C	1.40039	0.53443	-0.10605
C	1.52608	-1.87276	-0.18980
C	3.21391	-0.71380	0.83398

C	2.60500	0.51866	0.59317
C	0.84244	-0.69874	-0.48425
N	-0.34925	-0.72540	-1.26862
N	-1.41867	-0.06750	-0.65506
C	-2.59922	-0.54775	-0.47711
C	-3.69810	0.27898	0.06996
H	-0.63926	-1.68745	-1.47521
H	1.10079	-2.82937	-0.49001
H	4.15989	-0.74367	1.36898
H	3.08649	1.43076	0.92692
H	-2.75748	-1.59253	-0.74297
H	-4.49065	0.30459	-0.68720
H	-3.35097	1.30337	0.23456
C	-4.23574	-0.34186	1.36305
H	-3.46017	-0.36395	2.13215
H	-5.07350	0.25510	1.73021
H	-4.58822	-1.36185	1.19042
N	2.70860	-1.90226	0.45554
O	0.67748	1.63941	-0.44723
C	1.17437	2.91503	0.01933
H	2.16168	3.11325	-0.40237
H	0.45564	3.64555	-0.34634
H	1.21121	2.93055	1.11062
H	-1.19468	0.91348	-0.42852

There are no imaginary frequencies.

SCF energy: -586.991395 hartree
αα/ββ: -0.237843809 hartree
αβ: -1.32841 hartree
SCS-MP2 energy: -588.7440496 hartree
zero-point correction: +0.234537 hartree
enthalpy correction: +0.248480 hartree
free energy correction: +0.193730 hartree
quasiharmonic free energy correction: +0.196014 hartree

S-84

C	1.79587	0.42016	0.02055
C	0.60961	-1.67975	-0.14202
C	2.96055	-1.66652	0.24816
C	2.98185	-0.28029	0.23391
C	0.57656	-0.28742	-0.16520
N	-0.56224	0.42461	-0.42894
N	-1.76601	-0.25337	-0.42286
C	-2.82102	0.48997	-0.35866
C	-4.17802	-0.12486	-0.37288
H	-0.56018	1.41584	-0.17680
H	-2.74268	1.58062	-0.28091
H	-4.07724	-1.20226	-0.53491
H	-4.74092	0.28890	-1.21861
C	-4.93265	0.15853	0.92800
H	-5.02025	1.23492	1.10271
H	-5.94124	-0.26184	0.88548
H	-4.40977	-0.28489	1.77999
N	1.79095	-2.30406	0.06244
H	-0.26455	-2.30183	-0.27444
H	3.92641	0.22773	0.38508
H	3.83762	-2.28203	0.40382
O	1.66664	1.76230	-0.02243
C	2.87278	2.54971	0.12337
H	3.57221	2.31448	-0.68120
H	2.54054	3.58269	0.04732
H	3.32681	2.36800	1.09958
H	1.78805	-3.32620	0.07644

There are no imaginary frequencies.

SCF energy: -587.001250 hartree
αα/ββ: -0.238695775 hartree
αβ: -1.3337053 hartree
SCS-MP2 energy: -588.7608269 hartree
zero-point correction: +0.232804 hartree
enthalpy correction: +0.247107 hartree
free energy correction: +0.192071 hartree
quasiharmonic free energy correction: +0.193728 hartree

S-85

C	-1.33858	-0.23921	0.03066
C	-0.29809	1.70550	-0.98226
C	-1.82827	2.00638	0.69364
C	-2.05204	0.63815	0.84691
C	-0.46624	0.33347	-0.90273
N	0.30684	-0.56489	-1.74529
N	1.40137	-1.29414	-1.06965
C	2.28245	-0.36398	-0.44348
C	2.53427	-0.38138	0.87266
H	0.73839	-0.04675	-2.52941
H	0.39011	2.13304	-1.70924
H	-2.37149	2.70361	1.32650
H	-2.75735	0.28673	1.59146
H	0.92107	-1.86175	-0.36159
H	2.80374	0.29224	-1.13751
H	1.97308	-1.06802	1.50752
H	-0.30085	-1.28788	-2.16585
C	3.57930	0.46786	1.52109
H	4.36392	-0.15172	1.96841
H	4.04344	1.14332	0.79745
H	3.14209	1.06539	2.32759
N	-0.97659	2.55815	-0.19303
O	-1.39230	-1.59178	0.03168
C	-2.30802	-2.20788	0.96929
H	-2.19790	-3.27728	0.80295
H	-2.02846	-1.95089	1.99281
H	-3.33136	-1.89316	0.75659

There are no imaginary frequencies.

SCF energy: -586.968952 hartree

αα/ββ: -0.238388049 hartree
αβ: -1.3323005 hartree
SCS-MP2 energy: -588.7266379 hartree
zero-point correction: +0.234848 hartree
enthalpy correction: +0.248830 hartree
free energy correction: +0.194516 hartree
quasiharmonic free energy correction: +0.196428 hartree

S-86

C	-1.02269	0.57691	-0.12797
C	-1.15746	-1.78933	-0.56579
C	-2.48346	-0.89224	1.06986
C	-1.97055	0.39060	0.87602
C	-0.59437	-0.54936	-0.85248
N	0.31337	-0.37841	-1.93446
N	1.58017	0.20777	-1.46150
C	2.23523	-0.50954	-0.37354
C	2.23791	0.00923	0.85673
H	0.57130	-1.29274	-2.32385
H	-0.83065	-2.66563	-1.12431
H	-3.23651	-1.05345	1.83745
H	-2.33651	1.21176	1.48194
H	2.18460	0.26770	-2.29599
H	2.65061	-1.46698	-0.67004
H	1.77799	0.98327	1.02424
H	1.33942	1.17451	-1.17797
C	2.86056	-0.67808	2.02563
H	2.11113	-0.84802	2.80515
H	3.29540	-1.63830	1.73853
H	3.64407	-0.04940	2.45992
N	-2.10445	-1.97959	0.37274
O	-0.43176	1.75742	-0.46978
C	-0.74308	2.90663	0.35146
H	-0.46481	2.71636	1.39010
H	-0.14316	3.71588	-0.05970
H	-1.80502	3.14846	0.27569

There are no imaginary frequencies.

SCF energy: -586.970618 hartree
αα/ββ: -0.239351198 hartree
αβ: -1.3346039 hartree
SCS-MP2 energy: -588.7317102 hartree
zero-point correction: +0.234832 hartree
enthalpy correction: +0.248702 hartree
free energy correction: +0.195177 hartree
quasiharmonic free energy correction: +0.196596 hartree

S-87

C	1.37010	0.43731	-0.15351
C	0.47996	-1.80320	-0.22866
C	2.49116	-1.36387	0.96699
C	2.42686	-0.02072	0.63423
C	0.36838	-0.46745	-0.59124
N	-0.63947	-0.00903	-1.42616
N	-1.82691	-0.77318	-1.36736
C	-2.76953	-0.34618	-0.40044
C	-2.52669	0.45167	0.65230
H	-0.80337	0.99630	-1.31113
H	-2.23474	-0.81914	-2.30013
H	-3.74997	-0.79150	-0.56135
H	-1.53973	0.88378	0.80575
C	-3.58080	0.78665	1.66470
H	-3.74933	1.86777	1.71987
H	-4.53227	0.30752	1.41515
H	-3.28833	0.45767	2.66818
N	1.52697	-2.19450	0.53197
H	-0.23875	-2.55899	-0.51482
H	3.20437	0.64259	0.99324
H	3.27890	-1.79798	1.57001
O	1.17368	1.71266	-0.54446
C	2.11783	2.70363	-0.07295
H	3.11820	2.47847	-0.44786
H	1.76235	3.64484	-0.48643
H	2.11159	2.73995	1.01818
H	1.58393	-3.18261	0.78940

There are no imaginary frequencies.

SCF energy: -586.983667 hartree
αα/ββ: -0.238674184 hartree
αβ: -1.3311917 hartree
SCS-MP2 energy: -588.7402132 hartree
zero-point correction: +0.234347 hartree
enthalpy correction: +0.248160 hartree
free energy correction: +0.194572 hartree
quasiharmonic free energy correction: +0.196435 hartree

TS S-88

C	1.05676	0.31891	-0.24060
C	-1.02294	0.80772	-1.40567
C	-0.04905	2.43800	-0.13364
C	1.01893	1.62183	0.24738
C	0.05637	-0.06512	-1.17012
N	0.02580	-1.36084	-1.59494
N	-0.93284	-2.41167	-0.24241
C	-0.93123	-1.61905	0.85554
C	-1.84306	-0.58973	0.91642
H	-1.82448	0.48928	-2.07087
H	-0.08594	3.46130	0.23182
H	1.76965	2.00573	0.92868
H	-0.19057	-3.11805	-0.14229
H	-0.16017	-1.70417	1.62391
H	-2.63175	-0.57255	0.16485
H	-0.59318	-1.57793	-2.38064
C	-1.87256	0.42163	1.99524

H	-2.87387	0.48315	2.43597
H	-1.13778	0.20383	2.77440
H	-1.65497	1.41856	1.58200
H	0.92345	-1.85540	-1.61603
N	-1.06246	2.06660	-0.94785
O	1.97616	-0.62634	0.02659
C	3.02167	-0.27522	0.96725
H	2.58210	-0.01118	1.93104
H	3.62781	-1.17378	1.05798
H	3.61753	0.54946	0.57203

1 imaginary frequency: –119.98 cm^{-1}.

SCF energy: -586.918797 hartree
αα/ββ: -0.245943734 hartree
αβ: -1.3515755 hartree
SCS-MP2 energy: -588.7046501 hartree
zero-point correction: +0.231605 hartree
enthalpy correction: +0.245026 hartree
free energy correction: +0.193228 hartree
quasiharmonic free energy correction: +0.194189 hartree

TS S-89

C	1.08414	0.09112	-0.29157
C	-0.89770	0.94513	-1.39106
C	0.41652	2.38836	-0.20928
C	1.31867	1.39035	0.15593
C	-0.00983	-0.13925	-1.18299
N	-0.31383	-1.35497	-1.70241
N	-1.41304	-2.13873	-0.19515
C	-1.20682	-1.37836	0.90303
C	-1.81771	-0.14626	0.98877
H	-1.76970	0.77105	-2.02084
H	0.59542	3.40958	0.11977
H	2.15643	1.64125	0.79734
H	-2.26995	-1.99502	-0.73294
H	-0.40992	-1.68924	1.57124
H	-2.64466	0.06201	0.31202
H	0.48143	-1.98127	-1.50909
C	-1.53646	0.82156	2.07284
H	-2.45653	1.05029	2.62073
H	-0.77758	0.44683	2.76336
H	-1.18268	1.76878	1.64028
H	-1.05797	-3.09832	-0.20920
N	-0.68534	2.19746	-0.96871
O	1.83792	-0.98996	-0.01818
C	2.95581	-0.81033	0.88256
H	2.60417	-0.44754	1.85075
H	3.39305	-1.80126	0.98611
H	3.68091	-0.11772	0.45036

1 imaginary frequency: 140.79 cm^{-1}.

SCF energy: -586.915712 hartree
αα/ββ: -0.246487949 hartree
αβ: -1.3552454 hartree
SCS-MP2 energy: -588.7063317 hartree
zero-point correction: +0.231567 hartree
enthalpy correction: +0.245004 hartree
free energy correction: +0.193078 hartree
quasiharmonic free energy correction: +0.194157 hartree

TS S-90

C	-1.39117	0.11970	0.14737
C	0.81448	0.64973	1.01649
C	-0.50279	2.34692	0.00692
C	-1.52223	1.44493	-0.26667
C	-0.25022	-0.27925	0.92126
N	-0.12867	-1.58461	1.26834
N	0.86230	-2.29046	-0.23234
C	1.95038	-1.48740	-0.27481
C	1.97009	-0.22459	-0.84531
H	1.65785	0.47880	1.67739
H	1.33343	2.63839	0.84027
H	-0.55345	3.39257	-0.27559
H	-2.38778	1.79860	-0.81270
H	0.15290	-1.94339	-0.89337
H	2.79586	-1.80403	0.33775
H	1.13447	0.05346	-1.49166
H	0.67495	-1.68448	1.90400
C	3.21002	0.60378	-0.93950
H	2.98577	1.66521	-0.79455
H	3.95224	0.29068	-0.20063
H	3.64875	0.50277	-1.93904
N	0.59136	1.95548	0.66939
O	-2.28549	-0.84478	-0.08734
C	-3.46646	-0.49140	-0.84979
H	-3.18041	-0.12650	-1.83809
H	-4.02723	-1.41937	-0.93557
H	-4.05093	0.25803	-0.31301

1 imaginary frequency: –313.05 cm^{-1}.

SCF energy: -586.909624 hartree
αα/ββ: -0.2474896 hartree
αβ: -1.356016 hartree
SCS-MP2 energy: -588.7018363 hartree
zero-point correction: +0.232243 hartree
enthalpy correction: +0.245467 hartree
free energy correction: +0.194140 hartree
quasiharmonic free energy correction: +0.194750 hartree

S-91

C	1.51199	-0.13973	-0.12058
C	-0.86460	0.60163	-0.69469
C	0.88028	2.17661	-0.50033

C	1.86297	1.17762	-0.12791
C	0.15297	-0.47955	-0.48641
N	-0.17846	-1.72755	-0.61066
N	-2.93816	-1.39394	-0.56691
C	-2.99682	-0.43408	0.28561
C	-1.93311	0.61316	0.43554
H	-1.38898	0.37843	-1.63326
H	1.22312	3.20904	-0.55210
H	2.86523	1.50571	0.12546
H	-3.77525	-1.98188	-0.49737
H	-3.84518	-0.31245	0.96745
H	-2.44292	1.57912	0.32432
C	-1.31817	0.56199	1.83798
H	-2.09620	0.72356	2.58944
H	-0.85259	-0.40880	2.03230
H	-0.56601	1.34806	1.95310
N	-0.36516	1.96384	-0.79760
O	2.27864	-1.21174	0.15822
C	3.65742	-0.93713	0.50069
H	3.70285	-0.32711	1.40542
H	4.10276	-1.91386	0.67590
H	4.15610	-0.43213	-0.32951
H	0.51176	-2.46379	-0.44980
H	-1.16900	-1.94950	-0.83022

There are no imaginary frequencies.

SCF energy: -586.998660 hartree
αα/ββ: -0.236992775 hartree
αβ: -1.3388257 hartree
SCS-MP2 energy: -588.7632461 hartree
zero-point correction: +0.233663 hartree
enthalpy correction: +0.247161 hartree
free energy correction: +0.195383 hartree
quasiharmonic free energy correction: +0.195980 hartree

S-92

C	1.49818	-0.16163	-0.12597
C	-0.85118	0.62702	-0.73860
C	0.92060	2.16260	-0.48765
C	1.87436	1.14297	-0.08429
C	0.15043	-0.50131	-0.59986
N	-0.22440	-1.70344	-0.88899
N	-2.93256	-1.45280	-0.31072
C	-2.97562	-0.34737	0.34240
C	-1.88090	0.65526	0.41709
H	0.53508	-2.37303	-0.71440
H	-1.40267	0.45251	-1.67067
H	1.29014	3.18788	-0.52655
H	2.86383	1.45815	0.22805
H	-3.88578	-0.14196	0.90245
H	-2.38583	1.62685	0.34411
C	-1.24114	0.56403	1.81337
H	-1.99554	0.72129	2.58905
H	-0.77951	-0.41478	1.96858
H	-0.48097	1.34331	1.91109
N	-0.31982	1.98990	-0.82341
O	2.24539	-1.24694	0.17927
C	3.60544	-0.98551	0.58549
H	3.61820	-0.38651	1.49921
H	4.04123	-1.96560	0.76918
H	4.14597	-0.47236	-0.21347
H	-3.73281	-2.08810	-0.28854
H	-2.05804	-1.74413	-0.80232

There are no imaginary frequencies.

SCF energy: -587.000028 hartree
αα/ββ: -0.236400902 hartree
αβ: -1.3380148 hartree
SCS-MP2 energy: -588.7632464 hartree
zero-point correction: +0.234514 hartree
enthalpy correction: +0.247956 hartree
free energy correction: +0.196115 hartree
quasiharmonic free energy correction: +0.196984 hartree

S-93

C	1.63076	0.07474	-0.13777
C	-0.86059	-0.18923	-0.70317
C	0.14801	1.96606	-0.14479
C	1.43381	1.40697	0.10055
C	0.53491	-0.76375	-0.67926
N	0.68814	-1.97430	-1.09072
N	-3.53835	0.57674	-0.45663
C	-3.17490	-0.41473	0.27657
C	-1.73997	-0.84390	0.38328
H	1.67026	-2.25189	-0.96062
H	-1.30821	-0.40257	-1.67934
H	-3.87944	-0.99424	0.88282
H	-1.69839	-1.92087	0.16946
H	-4.55232	0.71392	-0.38266
C	-1.22804	-0.61345	1.80858
H	-0.23364	-1.04826	1.94365
H	-1.18334	0.45393	2.04439
H	-1.90394	-1.09021	2.52435
N	-0.86913	1.26321	-0.54715
O	2.76787	-0.59959	0.01925
C	3.92057	0.14268	0.49339
H	3.71235	0.55575	1.48199
H	4.72199	-0.59043	0.54350
H	4.16489	0.93448	-0.21697
H	-0.02081	3.03162	-0.01457
H	2.21259	2.06656	0.46143
H	-1.79698	1.68697	-0.67416

There are no imaginary frequencies.

SCF energy: -587.004633 hartree

αα/ββ: -0.235448926 hartree
αβ: -1.3348763 hartree
SCS-MP2 energy: -588.7634505 hartree
zero-point correction: +0.234257 hartree
enthalpy correction: +0.247945 hartree
free energy correction: +0.195101 hartree
quasiharmonic free energy correction: +0.196342 hartree

3-hydrazinyl-2-methoxypyridine (37)

S-94

C	-2.15599	-1.50924	0.12570
C	-0.99678	0.57912	-0.26509
C	-3.05301	0.62509	0.74335
C	-3.18988	-0.75670	0.68770
C	-1.05946	-0.82060	-0.35640
N	0.08355	-1.52337	-0.92115
N	1.17694	-1.54198	0.06588
C	2.19887	-0.87069	-0.33532
C	3.35597	-0.68348	0.57746
H	0.37753	-1.09594	-1.82029
H	-3.83532	1.24072	1.17944
H	-4.08033	-1.23691	1.07865
H	-2.20212	-2.59388	0.05905
H	2.24163	-0.39943	-1.32052
H	3.22546	-1.30186	1.46917
H	-0.16744	-2.50837	-1.11004
H	4.26153	-1.01197	0.05574
C	3.47632	0.79905	0.94916
H	3.59948	1.41837	0.05633
H	2.58317	1.13488	1.48296
H	4.34426	0.95172	1.59553
N	-1.97571	1.29671	0.27557
O	0.11569	1.15890	-0.76992
C	0.23679	2.59075	-0.59596
H	1.19930	2.83816	-1.03944
H	-0.56907	3.10836	-1.11726
H	0.22599	2.84564	0.46437

There are no imaginary frequencies.

SCF energy: -586.993586 hartree
αα/ββ: -0.2378149 hartree
αβ: -1.3308925 hartree
SCS-MP2 energy: -588.7492003 hartree
zero-point correction: +0.234309 hartree
enthalpy correction: +0.248135 hartree
free energy correction: +0.194763 hartree
quasiharmonic free energy correction: +0.195843 hartree

S-95

C	-1.57618	-1.88460	-0.16579
C	-1.39256	0.51004	-0.10933
C	-3.23257	-0.47053	0.83802
C	-2.79846	-1.74383	0.49913
C	-0.85187	-0.74108	-0.46941
N	0.34837	-0.80163	-1.23794
N	1.41617	-0.12281	-0.64878
C	2.60038	-0.59144	-0.46440
C	3.69546	0.26250	0.04831
H	0.63573	-1.77114	-1.40866
H	-4.17220	-0.32049	1.36307
H	-3.39369	-2.61401	0.75654
H	-1.18467	-2.86275	-0.43782
H	2.76439	-1.64241	-0.70084
H	3.34066	1.29022	0.17063
H	4.48555	0.26352	-0.71186
C	4.24255	-0.29746	1.36494
H	4.60378	-1.32082	1.23580
H	5.07610	0.32212	1.70317
H	3.46969	-0.29333	2.13708
N	-2.53628	0.65459	0.54485
O	-0.64130	1.59719	-0.45843
C	-1.12279	2.88718	-0.01511
H	-2.10870	3.08943	-0.43401
H	-1.16048	2.92614	1.07433
H	-0.39259	3.59758	-0.39831
H	1.18525	0.86277	-0.44671

There are no imaginary frequencies.

SCF energy: -586.998324 hartree
αα/ββ: -0.2379585 hartree
αβ: -1.3280047 hartree
SCS-MP2 energy: -588.7505687 hartree
zero-point correction: +0.234394 hartree
enthalpy correction: +0.248185 hartree
free energy correction: +0.194614 hartree
quasiharmonic free energy correction: +0.195972 hartree

S-96

C	0.78214	-1.66370	0.33689
C	1.79874	0.42875	-0.29783
C	3.13051	-1.55057	-0.21239
C	2.02047	-2.27993	0.18542
C	0.64505	-0.28690	0.07936
N	-0.51797	0.41214	0.21879
N	-1.69471	-0.28648	0.39560
C	-2.77309	0.41581	0.27512
C	-4.11020	-0.21890	0.44295
H	-0.56076	1.35097	-0.18684
H	-0.08829	-2.23665	0.63638
H	-2.72981	1.48278	0.02765
H	-4.64791	0.29872	1.24680
H	-3.97458	-1.26034	0.74953
C	-4.92541	-0.13678	-0.85013

H	-4.42727	-0.68549	-1.65428
H	-5.91994	-0.56776	-0.70505
H	-5.04865	0.90196	-1.17022
N	2.96484	-0.22697	-0.43855
O	1.76492	1.74707	-0.60660
C	2.04326	2.61216	0.54160
H	3.06938	2.45412	0.87827
H	1.91402	3.62588	0.16837
H	1.33540	2.40411	1.34575
H	2.12940	-3.34211	0.37537
H	4.12545	-1.94954	-0.36265
H	3.77036	0.33640	-0.73322

There are no imaginary frequencies.

SCF energy: -586.993508 hartree
αα/ββ: -0.2387697 hartree
αβ: -1.3336819 hartree
SCS-MP2 energy: -588.7531061 hartree
zero-point correction: +0.232367 hartree
enthalpy correction: +0.246821 hartree
free energy correction: +0.191422 hartree
quasiharmonic free energy correction: +0.193133 hartree

S-97

C	-1.68785	1.86202	-0.14010
C	-1.45184	-0.54468	-0.10919
C	-3.50427	0.36802	0.32602
C	-3.03465	1.66718	0.17706
C	-0.90494	0.73419	-0.28976
N	0.50760	0.82590	-0.61803
N	1.36115	0.55751	0.55639
C	2.72867	0.74849	0.18180
C	3.63852	-0.23293	0.24104
H	0.73205	1.78488	-0.93329
H	-4.54759	0.18173	0.56641
H	-3.70508	2.51057	0.30215
H	-1.26359	2.85456	-0.27467
H	1.19586	-0.43706	0.75318
H	2.97959	1.77731	-0.06856
H	3.31233	-1.23995	0.50222
H	0.74764	0.18254	-1.39598
C	5.09813	-0.01635	0.00199
H	5.45970	-0.67575	-0.79365
H	5.30227	1.01921	-0.28293
H	5.67934	-0.24837	0.90071
N	-2.73125	-0.73510	0.18958
O	-0.58533	-1.57755	-0.25377
C	-1.12639	-2.90776	-0.06631
H	-1.52264	-3.01717	0.94373
H	-1.90533	-3.10909	-0.80208
H	-0.27674	-3.57034	-0.21800

There are no imaginary frequencies.

SCF energy: -586.976089 hartree
αα/ββ: -0.2375531 hartree
αβ: -1.3298342 hartree
SCS-MP2 energy: -588.7302588 hartree
zero-point correction: +0.234484 hartree
enthalpy correction: +0.248631 hartree
free energy correction: +0.193986 hartree
quasiharmonic free energy correction: +0.195519 hartree

S-98

C	1.15886	-1.81534	-0.55690
C	1.03839	0.54469	-0.13391
C	2.50114	-0.71447	1.09715
C	2.14251	-1.87973	0.43439
C	0.59111	-0.58307	-0.85337
N	-0.32370	-0.40655	-1.92872
N	-1.57189	0.21618	-1.45864
C	-2.25632	-0.49095	-0.38217
C	-2.24896	0.01216	0.85457
H	-0.60402	-1.32002	-2.30402
H	3.25633	-0.72435	1.87879
H	2.61262	-2.82362	0.69110
H	0.83322	-2.70467	-1.09289
H	-1.29910	1.17197	-1.16352
H	-2.70276	-1.42982	-0.69273
H	-1.75750	0.96775	1.03787
H	-2.16912	0.30383	-2.29567
C	-2.90496	-0.66781	2.00955
H	-3.67088	-0.01822	2.44451
H	-3.36978	-1.60888	1.70627
H	-2.16921	-0.87281	2.79355
N	1.94908	0.49290	0.82844
O	0.44671	1.72980	-0.47148
C	0.75358	2.86860	0.36667
H	0.16136	3.68160	-0.04905
H	0.46211	2.67123	1.39916
H	1.81644	3.10545	0.31519

There are no imaginary frequencies.

SCF energy: -586.978022 hartree
αα/ββ: -0.2393746 hartree
αβ: -1.3339335 hartree
SCS-MP2 energy: -588.7383253 hartree
zero-point correction: +0.234775 hartree
enthalpy correction: +0.248544 hartree
free energy correction: +0.195528 hartree
quasiharmonic free energy correction: +0.196618 hartree

S-99

C	-0.37643	-1.82640	-0.26412

C	-1.35246	0.37210	-0.14146
C	-2.42997	-1.46653	0.93809
C	-1.43785	-2.31663	0.50494
C	-0.31338	-0.47479	-0.59554
N	0.65621	0.08609	-1.41358
N	1.87915	-0.61773	-1.43151
C	2.81405	-0.22787	-0.44245
C	2.54769	0.46521	0.67646
H	0.77611	1.09088	-1.24883
H	0.41404	-2.48616	-0.60493
H	2.27254	-0.56677	-2.37011
H	3.81167	-0.61187	-0.64899
H	1.54306	0.83407	0.87420
C	3.59619	0.75758	1.70743
H	3.33840	0.31176	2.67473
H	4.56945	0.36208	1.40176
H	3.70369	1.83529	1.87184
N	-2.34487	-0.14742	0.59960
H	-1.49023	-3.36795	0.76490
H	-3.28709	-1.74925	1.53551
O	-1.28367	1.66576	-0.46519
C	-2.35536	2.54777	-0.03442
H	-2.40251	2.57537	1.05597
H	-2.07645	3.52336	-0.42365
H	-3.30254	2.22217	-0.46964
H	-3.08901	0.47177	0.93354

There are no imaginary frequencies.

SCF energy: -586.978813 hartree
αα/ββ: -0.2386184 hartree
αβ: -1.3308202 hartree
SCS-MP2 energy: -588.7348761 hartree
zero-point correction: +0.233544 hartree
enthalpy correction: +0.247552 hartree
free energy correction: +0.193395 hartree
quasiharmonic free energy correction: +0.195286 hartree

TS S-100

C	-0.21340	2.28859	-0.83325
C	1.03159	-0.10155	-0.28663
C	-0.85194	1.11873	-1.23728
C	0.98570	2.18683	-0.13788
C	-0.13533	-0.11170	-1.14418
N	-0.53063	-1.23558	-1.71184
N	-2.03342	-2.04248	0.13533
C	-1.46039	-1.18275	0.95249
C	-1.65400	0.22529	0.93101
H	-1.77319	1.14147	-1.81587
H	-0.67953	3.25700	-0.98136
H	1.51195	3.07800	0.19380
H	-2.71385	-1.53220	-0.44838
H	-0.71384	-1.58070	1.64291
H	-2.53557	0.58211	0.39591
H	-1.29801	-1.23661	-2.38243
C	-1.09249	1.08506	1.98990
H	-1.91048	1.50482	2.58903
H	-0.40323	0.53639	2.63595
H	-0.55902	1.95644	1.57199
H	0.02167	-2.08440	-1.61151
N	1.59829	1.00440	0.15699
O	1.55959	-1.30998	-0.06928
C	2.76001	-1.35425	0.74783
H	2.55844	-0.92711	1.73024
H	2.99428	-2.41343	0.82576
H	3.56539	-0.81174	0.25269

1 imaginary frequency: –77.04 cm^{-1}.

SCF energy: -586.924442 hartree
αα/ββ: -0.2459435 hartree
αβ: -1.3528196 hartree
SCS-MP2 energy: -588.7117878 hartree
zero-point correction: +0.230075 hartree
enthalpy correction: +0.243649 hartree
free energy correction: +0.192266 hartree
quasiharmonic free energy correction: +0.192559 hartree

TS S-101

C	-0.77593	2.03722	-0.97290
C	1.07609	0.14339	-0.27457
C	-1.01813	0.70545	-1.33080
C	0.36612	2.32637	-0.24883
C	0.02405	-0.25580	-1.19450
N	-0.09388	-1.47238	-1.73070
N	-1.30098	-2.31112	0.06963
C	-1.15549	-1.34995	0.96035
C	-1.83520	-0.12510	0.83540
H	-1.87281	0.44125	-1.95150
H	-1.49925	2.81741	-1.18877
H	0.59735	3.34581	0.05087
H	-2.04727	-2.27407	-0.62402
H	-0.38709	-1.49053	1.71651
H	-2.72706	-0.10738	0.21238
H	0.73808	-2.01785	-1.46218
C	-1.64790	0.92466	1.86460
H	-2.61037	1.16056	2.32882
H	-0.93542	0.60615	2.62882
H	-1.27279	1.85764	1.41710
H	-0.82029	-3.20393	0.18396
N	1.27418	1.38284	0.13464
O	1.93311	-0.83907	0.06007
C	3.02457	-0.47319	0.93734
H	3.56919	-1.40146	1.09859
H	3.66201	0.27012	0.45742
H	2.63652	-0.08479	1.87991

1 imaginary frequency: –72.94 cm^{-1}.

SCF energy: -586.916960 hartree
αα/ββ: -0.2471778 hartree
αβ: -1.3586791 hartree
SCS-MP2 energy: -588.7121601 hartree
zero-point correction: +0.230867 hartree
enthalpy correction: +0.244366 hartree
free energy correction: +0.192697 hartree
quasiharmonic free energy correction: +0.193354 hartree

TS S-102

C	0.55407	2.01721	0.71901
C	-1.35661	0.05824	0.16808
C	0.80997	0.66629	1.06987
C	-0.59817	2.33071	0.05969
C	-0.20697	-0.30975	0.93933
N	-0.07698	-1.62642	1.24516
N	0.98251	-2.25587	-0.23331
C	2.03185	-1.40169	-0.26113
C	2.00497	-0.15141	-0.85540
H	1.65562	0.43692	1.71360
H	1.28283	2.79433	0.92063
H	-0.88496	3.32130	-0.27064
H	-2.35633	1.60318	-0.71850
H	0.27281	-1.94587	-0.91223
H	2.88026	-1.67164	0.36920
H	1.15545	0.08282	-1.50062
H	0.71039	-1.72789	1.89998
C	3.20815	0.72656	-0.96228
H	2.93095	1.78003	-0.86508
H	3.94941	0.47752	-0.19844
H	3.67082	0.60225	-1.94858
N	-1.51727	1.33408	-0.19845
O	-2.24112	-0.88148	-0.12600
C	-3.43169	-0.51782	-0.87940
H	-3.97111	-1.45344	-0.99868
H	-4.02979	0.19576	-0.30899
H	-3.14866	-0.11594	-1.85400

1 imaginary frequency: –326.59 cm^{-1}.

SCF energy: -586.907518 hartree
αα/ββ: -0.2468446 hartree
αβ: -1.3554003 hartree
SCS-MP2 energy: -588.6985614 hartree
zero-point correction: +0.232170 hartree
enthalpy correction: +0.245342 hartree
free energy correction: +0.194111 hartree
quasiharmonic free energy correction: +0.194809 hartree

S-103

C	0.87273	0.62735	-0.68476
C	-1.50637	-0.12645	-0.13673
C	-1.09378	2.13246	-0.45875
C	0.21346	1.96651	-0.73373
C	-0.12349	-0.46864	-0.50055
N	0.20490	-1.71063	-0.64405
N	2.94912	-1.36689	-0.58482
C	3.02591	-0.40380	0.26277
C	1.95324	0.63021	0.44340
H	0.84059	2.82257	-0.96607
H	1.39785	0.43951	-1.63318
H	3.79011	-1.95144	-0.53839
H	3.89249	-0.27580	0.92004
H	2.45694	1.60302	0.36367
C	1.34020	0.52809	1.84495
H	0.57474	1.29791	1.98042
H	0.88927	-0.45535	2.00901
H	2.11387	0.67738	2.60340
N	-1.97050	1.08179	-0.12154
H	-1.56228	3.11059	-0.48308
O	-2.23895	-1.21014	0.16789
C	-3.62162	-0.96419	0.52616
H	-4.14406	-0.48695	-0.30342
H	-4.03182	-1.95138	0.72615
H	-3.66923	-0.33547	1.41590
H	-0.48678	-2.45087	-0.50179
H	1.20343	-1.92175	-0.85959

There are no imaginary frequencies.

SCF energy: -586.997176 hartree
αα/ββ: -0.2369193 hartree
αβ: -1.3385296 hartree
SCS-MP2 energy: -588.7613578 hartree
zero-point correction: +0.232596 hartree
enthalpy correction: +0.246374 hartree
free energy correction: +0.193638 hartree
quasiharmonic free energy correction: +0.194581 hartree

S-104

C	0.87247	0.66249	-0.72267
C	-1.47891	-0.14948	-0.14800
C	-1.13138	2.11093	-0.45888
C	0.17250	1.98844	-0.76272
C	-0.11520	-0.47850	-0.64435
N	0.24024	-1.66553	-1.00099
N	2.96107	-1.40020	-0.33787
C	2.98070	-0.32983	0.37294
C	1.88112	0.66685	0.45799
H	0.76006	2.86691	-1.01682
H	1.44537	0.53787	-1.65180
H	3.87223	-0.15592	0.97218
H	2.38885	1.64055	0.43985
H	-0.52932	-2.33309	-0.86574
C	1.20722	0.51763	1.83374

H	0.43409	1.28363	1.93531
H	0.75302	-0.47134	1.94154
H	1.93644	0.65527	2.63661
N	-1.97538	1.04003	-0.07376
H	-1.62995	3.07510	-0.48496
O	-2.17589	-1.25029	0.19859
C	-3.53689	-1.02718	0.63382
H	-3.92507	-2.02080	0.84837
H	-3.54873	-0.40626	1.53061
H	-4.11309	-0.54995	-0.15978
H	3.75942	-2.03807	-0.32021
H	2.11251	-1.66977	-0.87665

There are no imaginary frequencies.

SCF energy: -587.004665 hartree
αα/ββ: -0.2359875 hartree
αβ: -1.3365826 hartree
SCS-MP2 energy: -588.7658891 hartree
zero-point correction: +0.234181 hartree
enthalpy correction: +0.247731 hartree
free energy correction: +0.195775 hartree
quasiharmonic free energy correction: +0.196437 hartree

S-105

C	1.13068	0.20559	-0.87132
C	-1.35127	0.06336	-0.24818
C	-0.18739	2.14035	-0.00849
C	0.97773	1.62356	-0.41682
C	-0.18904	-0.51215	-0.98103
N	-0.29646	-1.57971	-1.69041
N	0.33908	-0.67407	1.64988
C	1.56339	-0.92198	1.35125
C	2.11764	-0.62072	-0.00699
H	2.26178	-1.38093	2.06093
H	2.23822	-1.58519	-0.52316
H	-1.25377	-1.95101	-1.62918
C	3.49498	0.03553	0.09987
H	3.88440	0.26819	-0.89561
H	3.45310	0.95921	0.68331
H	4.19660	-0.64503	0.59098
N	-1.35381	1.33647	0.06862
H	0.13989	-0.96430	2.61457
H	1.56323	0.22069	-1.88099
H	1.84185	2.27895	-0.45538
H	-0.34431	3.16873	0.29112
O	-2.37399	-0.73291	-0.09690
C	-3.57080	-0.24316	0.58296
H	-3.30363	0.07849	1.59062
H	-4.01429	0.56473	-0.00016
H	-4.23201	-1.10411	0.61430
H	-2.17628	1.75374	0.50963

There are no imaginary frequencies.

SCF energy: -586.994394 hartree
αα/ββ: -0.2355573 hartree
αβ: -1.3363799 hartree
SCS-MP2 energy: -588.7550881 hartree
zero-point correction: +0.233842 hartree
enthalpy correction: +0.247491 hartree
free energy correction: +0.195274 hartree
quasiharmonic free energy correction: +0.196159 hartree

4-hydrazinyl-3-methoxypyridine (35)

S-106

C	0.98536	0.59008	-0.26629
C	2.15981	-1.49927	0.11431
C	2.07702	1.24566	0.31891
C	1.06016	-0.80460	-0.35894
N	-0.08350	-1.50775	-0.92876
N	-1.17316	-1.53602	0.06041
C	-2.20404	-0.87888	-0.33990
C	-3.36225	-0.70555	0.57408
H	0.17029	-2.49012	-1.12716
H	2.21427	-2.58254	0.04342
H	2.08898	2.32569	0.42161
H	-2.25376	-0.40867	-1.32549
H	-4.26492	-1.04139	0.05206
H	-0.37958	-1.07184	-1.82317
H	-3.22518	-1.32457	1.46432
C	-3.49679	0.77494	0.94931
H	-2.60672	1.11821	1.48357
H	-3.62654	1.39524	0.05809
H	-4.36596	0.91734	1.59635
O	-0.13321	1.16757	-0.76476
C	-0.26703	2.59719	-0.58754
H	-1.23913	2.84060	-1.01127
H	-0.24085	2.84988	0.47456
H	0.52314	3.12242	-1.12807
C	3.19266	-0.75024	0.67605
H	4.08123	-1.24498	1.05713
N	3.15966	0.59209	0.78295

There are no imaginary frequencies.

SCF energy: -586.977953 hartree
αα/ββ: -0.238656252 hartree
αβ: -1.3345712 hartree
SCS-MP2 energy: -588.7385426 hartree
zero-point correction: +0.234512 hartree
enthalpy correction: +0.248283 hartree
free energy correction: +0.195102 hartree
quasiharmonic free energy correction: +0.196101 hartree

S-107

C	-1.37094	0.52923	-0.11527
C	-1.68274	-1.85519	-0.11449
C	-2.61259	0.64324	0.51344
C	-0.88106	-0.75676	-0.40304
N	0.33883	-0.92183	-1.11527
N	1.41415	-0.20271	-0.59985
C	2.60963	-0.65044	-0.43947
C	3.71174	0.23626	-0.00427
H	0.60706	-1.90771	-1.19926
H	-1.33716	-2.86187	-0.33692
H	-3.01631	1.61626	0.77344
H	2.77923	-1.70859	-0.63628
H	3.34719	1.26255	0.09894
H	4.46840	0.22202	-0.79768
C	4.32376	-0.27183	1.30494
H	4.69097	-1.29526	1.19415
H	5.16410	0.36731	1.58489
H	3.58593	-0.24960	2.11031
O	-0.56309	1.57418	-0.47494
C	-0.97185	2.89745	-0.05971
H	-0.17397	3.55523	-0.39831
H	-1.91375	3.17019	-0.53981
H	-1.06586	2.94318	1.02729
N	-3.39090	-0.42008	0.80632
C	-2.92251	-1.63903	0.48386
H	-3.56442	-2.48287	0.72299
H	1.17815	0.79049	-0.43856

There are no imaginary frequencies.

SCF energy: -586.986776 hartree
αα/ββ: -0.238331993 hartree
αβ: -1.3298323 hartree
SCS-MP2 energy: -588.7414628 hartree
zero-point correction: +0.234289 hartree
enthalpy correction: +0.248192 hartree
free energy correction: +0.194068 hartree
quasiharmonic free energy correction: +0.195747 hartree

S-108

C	-1.77362	0.43076	0.02726
C	-0.65860	-1.72706	-0.06838
C	-2.98581	-0.22115	0.14843
C	-0.57076	-0.32454	-0.07877
N	0.59174	0.35466	-0.18772
N	1.78729	-0.32261	-0.27830
C	2.83491	0.43043	-0.35577
C	4.19210	-0.17520	-0.43770
H	0.58174	1.37753	-0.18036
H	2.75060	1.52299	-0.34292
H	4.68687	0.19696	-1.34302
H	4.09259	-1.26049	-0.53213
C	5.03435	0.18794	0.78821
H	4.57807	-0.20738	1.69988
H	6.04063	-0.23021	0.69714
H	5.12482	1.27296	0.89326
H	0.23252	-2.33576	-0.15055
O	-1.60549	1.77593	0.00255
C	-2.80489	2.58034	0.04412
H	-2.45546	3.60904	-0.01051
H	-3.44363	2.34978	-0.81187
H	-3.34266	2.41332	0.98050
C	-1.89137	-2.33163	0.05064
H	-2.02795	-3.40618	0.06430
N	-3.00468	-1.58019	0.15569
H	-3.94359	0.27380	0.23815
H	-3.90887	-2.04616	0.24180

There are no imaginary frequencies.

SCF energy: -587.008733 hartree
αα/ββ: -0.237610018 hartree
αβ: -1.3307522 hartree
SCS-MP2 energy: -588.7640424 hartree
zero-point correction: +0.232738 hartree
enthalpy correction: +0.247101 hartree
free energy correction: +0.191395 hartree
quasiharmonic free energy correction: +0.193800 hartree

S-109

C	-0.99163	-0.58419	0.24839
C	-1.28182	1.81617	0.04631
C	-1.90963	-0.72812	-0.80122
C	-0.69844	0.72001	0.66146
N	0.28959	0.89875	1.71903
N	1.65708	1.22312	1.25691
C	2.12779	0.20612	0.37138
C	2.40274	0.45062	-0.91744
H	0.36527	0.03682	2.28573
H	-1.05263	2.83018	0.36504
H	-2.18825	-1.71053	-1.16798
H	1.54099	2.10368	0.74106
H	2.32619	-0.74855	0.85141
H	2.17417	1.43608	-1.32449
H	0.01001	1.65928	2.36042
C	3.04552	-0.54547	-1.82715
H	4.02529	-0.19090	-2.16481
H	3.18007	-1.50841	-1.32696
H	2.43278	-0.69793	-2.72142
O	-0.36585	-1.58322	0.91830
C	-0.70205	-2.93675	0.53319
H	-0.44012	-3.10939	-0.51284
H	-0.09873	-3.56879	1.18154
H	-1.76474	-3.12439	0.70080
N	-2.49003	0.32198	-1.41287
C	-2.17782	1.56269	-0.99031

H	-2.66786	2.38528	-1.50301

There are no imaginary frequencies.

SCF energy: -586.958781 hartree
αα/ββ: -0.239494444 hartree
αβ: -1.3359873 hartree
SCS-MP2 energy: -588.7216287 hartree
zero-point correction: +0.234586 hartree
enthalpy correction: +0.248535 hartree
free energy correction: +0.194397 hartree
quasiharmonic free energy correction: +0.196330 hartree

S-110

C	-1.00233	0.57961	-0.15771
C	-1.27430	-1.78964	-0.46265
C	-1.96681	0.51284	0.85090
C	-0.63141	-0.60753	-0.81336
N	0.28599	-0.55226	-1.89773
N	1.56099	0.04779	-1.48185
C	2.21847	-0.60894	-0.35771
C	2.28209	0.00641	0.82491
H	0.52074	-1.50206	-2.20832
H	-1.01131	-2.72344	-0.95425
H	-2.27056	1.40300	1.39230
H	2.15658	0.04631	-2.32498
H	2.59093	-1.60148	-0.58901
H	1.86417	1.00761	0.92659
H	1.33581	1.03406	-1.25422
C	2.92076	-0.60754	2.02533
H	2.19523	-0.67962	2.84177
H	3.30544	-1.60619	1.80539
H	3.74523	0.01976	2.37805
O	-0.35622	1.71312	-0.56781
C	-0.58406	2.91421	0.20413
H	-0.32260	2.74899	1.25162
H	0.07408	3.66001	-0.23724
H	-1.62531	3.23059	0.11381
C	-2.24795	-1.75317	0.53338
H	-2.76548	-2.66371	0.82380
N	-2.59413	-0.63214	1.19299

There are no imaginary frequencies.

SCF energy: -586.966168 hartree
αα/ββ: -0.23975087 hartree
αβ: -1.3359893 hartree
SCS-MP2 energy: -588.729189 hartree
zero-point correction: +0.234903 hartree
enthalpy correction: +0.248762 hartree
free energy correction: +0.195097 hartree
quasiharmonic free energy correction: +0.196750 hartree

S-111

C	-1.38120	0.44207	-0.15221
C	-0.51239	-1.82160	-0.19701
C	-2.47115	-0.00823	0.57225
C	-0.36786	-0.47320	-0.54792
N	0.65792	-0.00356	-1.31838
N	1.82980	-0.77846	-1.35568
C	2.82938	-0.36661	-0.43799
C	2.64045	0.40344	0.64519
H	0.80664	1.00841	-1.26422
H	2.18229	-0.79786	-2.31243
H	3.80064	-0.79954	-0.67022
H	1.65785	0.81839	0.86182
C	3.74732	0.72460	1.60375
H	3.51146	0.37501	2.61501
H	4.68567	0.25544	1.29360
H	3.91375	1.80539	1.67074
H	-3.28037	0.61875	0.92281
O	-1.16501	1.72832	-0.51841
C	-2.12610	2.70328	-0.05532
H	-1.75796	3.65805	-0.42450
H	-3.11263	2.49107	-0.47415
H	-2.16372	2.70691	1.03661
N	-2.55274	-1.32809	0.87799
C	-1.61805	-2.22909	0.52102
H	-1.79056	-3.25479	0.82382
H	0.24332	-2.54290	-0.48145
H	-3.36358	-1.64603	1.41168

There are no imaginary frequencies.

SCF energy: -586.987534 hartree
αα/ββ: -0.238034144 hartree
αβ: -1.3294062 hartree
SCS-MP2 energy: -588.7415109 hartree
zero-point correction: +0.233774 hartree
enthalpy correction: +0.247762 hartree
free energy correction: +0.193766 hartree
quasiharmonic free energy correction: +0.195588 hartree

TS S-112

C	-1.36878	0.18013	0.13262
C	0.78527	0.62930	1.16479
C	-1.42426	1.52064	-0.22212
C	-0.28400	-0.25537	0.93995
N	-0.13636	-1.59443	1.18300
N	0.97569	-2.27364	-0.24491
C	2.00455	-1.39901	-0.27025
C	1.94758	-0.16965	-0.90055
H	1.60882	0.34126	1.81328
H	-2.25666	1.91916	-0.79168
H	0.27808	-1.97941	-0.94547
H	2.86814	-1.64981	0.34478

H	1.06873	0.04444	-1.51340
H	0.46143	-1.86923	1.96843
C	3.11973	0.73357	-1.03886
H	2.81194	1.78116	-0.98512
H	3.87843	0.53124	-0.27920
H	3.56774	0.58299	-2.02982
H	-0.97024	-2.18175	1.07308
O	-2.27387	-0.78153	-0.17040
C	-3.41440	-0.37251	-0.95991
H	-3.08490	0.01986	-1.92456
H	-3.99929	-1.27915	-1.09943
H	-3.99809	0.37672	-0.42061
C	0.60894	1.97950	0.78872
H	1.37594	2.71063	1.02925
N	-0.44889	2.41444	0.10725

1 imaginary frequency: –269.50 cm^{-1}.

SCF energy: -586.909713 hartree
αα/ββ: -0.246699343 hartree
αβ: -1.3532931 hartree
SCS-MP2 energy: -588.698131 hartree
zero-point correction: +0.232390 hartree
enthalpy correction: +0.245674 hartree
free energy correction: +0.194155 hartree
quasiharmonic free energy correction: +0.194847 hartree

TS S-113

C	-1.35045	0.12383	0.13450
C	0.72055	0.68395	1.26003
C	-1.46458	1.46728	-0.20808
C	-0.26710	-0.28489	0.97274
N	-0.04861	-1.57735	1.33767
N	1.11303	-2.18672	-0.07569
C	2.11646	-1.28043	-0.25099
C	1.88219	-0.14049	-0.97384
H	1.55163	0.41660	1.90766
H	-2.29438	1.82782	-0.80711
H	0.39757	-2.24395	-0.80980
H	3.00805	-1.43083	0.34884
H	0.95548	-0.07100	-1.54506
H	-0.85967	-2.14015	1.03555
C	2.91632	0.90364	-1.20069
H	2.47792	1.90090	-1.10270
H	3.75183	0.80062	-0.50503
H	3.29362	0.81646	-2.22640
H	1.35640	-3.09135	0.33851
O	-2.21273	-0.86417	-0.21751
C	-3.35865	-0.47799	-1.00617
H	-3.04020	-0.05356	-1.96123
H	-3.91216	-1.40050	-1.17094
H	-3.97342	0.23872	-0.45660
N	-0.55380	2.40812	0.15468
C	0.50416	2.01357	0.87759
H	1.22150	2.78447	1.14717

1 imaginary frequency: –352.63 cm^{-1}.

SCF energy: -586.905149 hartree
αα/ββ: -0.247119758 hartree
αβ: -1.3585053 hartree
SCS-MP2 energy: -588.7001019 hartree
zero-point correction: +0.231717 hartree
enthalpy correction: +0.245174 hartree
free energy correction: +0.192953 hartree
quasiharmonic free energy correction: +0.194097 hartree

TS S-114

C	-1.39315	0.12223	0.14537
C	0.85317	0.50961	1.02324
C	-1.46148	1.45310	-0.22515
C	-0.27361	-0.36169	0.90417
N	-0.12255	-1.64503	1.28044
N	0.94599	-2.28665	-0.32981
C	1.99749	-1.45753	-0.28732
C	1.99516	-0.15465	-0.78800
H	1.65062	0.23756	1.70717
H	-2.28035	1.92159	-0.75331
H	0.25205	-1.89051	-0.98272
H	2.83584	-1.77559	0.33442
H	1.18835	0.11078	-1.47599
H	-0.96579	-2.17515	1.01879
C	3.24297	0.66871	-0.85012
H	3.01626	1.73743	-0.86661
H	3.90210	0.45310	-0.00461
H	3.78566	0.43637	-1.77465
O	-2.35209	-0.79190	-0.09922
C	-3.50430	-0.35151	-0.85550
H	-3.19173	0.01752	-1.83516
H	-4.12456	-1.23835	-0.96392
H	-4.04221	0.42413	-0.30578
N	-0.40743	2.26944	0.08993
C	0.69777	1.87541	0.70976
H	1.44768	2.63079	0.91303
H	-0.49334	3.25906	-0.15955

1 imaginary frequency: –254.15 cm^{-1}.

SCF energy: -586.895213 hartree
αα/ββ: -0.248444455 hartree
αβ: -1.3604148 hartree
SCS-MP2 energy: -588.6933404 hartree
zero-point correction: +0.232185 hartree
enthalpy correction: +0.245396 hartree
free energy correction: +0.193999 hartree
quasiharmonic free energy correction: +0.194845 hartree

S-115

C	1.51112	-0.13669	-0.11882
C	-0.85136	0.57802	-0.68099
C	1.87377	1.17789	-0.14871
C	0.15452	-0.49981	-0.45599
N	-0.17127	-1.75278	-0.54737
N	-2.93907	-1.40211	-0.59515
C	-3.03388	-0.42284	0.23082
C	-1.96964	0.62094	0.40780
H	-1.34743	0.38659	-1.64541
H	2.88574	1.48779	0.08491
H	-3.77985	-1.98730	-0.54918
H	-3.91098	-0.28175	0.87135
H	-2.47747	1.58654	0.27523
C	-1.40453	0.57754	1.83165
H	-2.20908	0.73812	2.55483
H	-0.94340	-0.39137	2.04386
H	-0.65794	1.36495	1.97143
O	2.29530	-1.20275	0.16638
C	3.67266	-0.91448	0.49521
H	3.72323	-0.28864	1.38923
H	4.12485	-1.88555	0.68493
H	4.16683	-0.42189	-0.34552
C	-0.22971	1.93532	-0.74117
H	-0.89999	2.75578	-0.99728
N	1.00450	2.22986	-0.49208
H	0.52581	-2.48051	-0.38144
H	-1.15945	-1.98088	-0.76449

There are no imaginary frequencies.

SCF energy: -586.997441 hartree
αα/ββ: -0.236306265 hartree
αβ: -1.3347987 hartree
SCS-MP2 energy: -588.7567369 hartree
zero-point correction: +0.233238 hartree
enthalpy correction: +0.246941 hartree
free energy correction: +0.194448 hartree
quasiharmonic free energy correction: +0.195315 hartree

S-116

C	1.49606	-0.15774	-0.13414
C	-0.84195	0.61845	-0.72296
C	1.88694	1.14352	-0.08954
C	0.14504	-0.51505	-0.57882
N	-0.23048	-1.72530	-0.82864
N	-2.95085	-1.43890	-0.34396
C	-3.01651	-0.32262	0.28780
C	-1.90775	0.66276	0.40620
H	0.53762	-2.38536	-0.65709
H	-1.37134	0.49304	-1.67879
H	2.88333	1.43663	0.21899
H	-3.95135	-0.09687	0.79719
H	-2.40150	1.64159	0.34454
C	-1.29875	0.53275	1.81390
H	-2.06547	0.68958	2.57748
H	-0.86035	-0.45815	1.95721
H	-0.52274	1.29195	1.94255
O	2.25645	-1.24323	0.16910
C	3.61502	-0.97506	0.56896
H	3.63134	-0.37382	1.48167
H	4.05638	-1.95269	0.75378
H	4.15301	-0.46132	-0.23194
N	1.05213	2.22172	-0.46467
C	-0.17999	1.96659	-0.75545
H	-0.81366	2.80934	-1.03567
H	-3.75830	-2.06555	-0.35255
H	-2.05296	-1.74676	-0.78499

There are no imaginary frequencies.

SCF energy: -586.993797 hartree
αα/ββ: -0.236071281 hartree
αβ: -1.3367736 hartree
SCS-MP2 energy: -588.7553061 hartree
zero-point correction: +0.233936 hartree
enthalpy correction: +0.247507 hartree
free energy correction: +0.195183 hartree
quasiharmonic free energy correction: +0.196294 hartree

S-117

C	1.62602	-0.05931	-0.15681
C	-0.84905	0.00415	-0.70828
C	1.63809	1.29608	-0.08865
C	0.35386	-0.80438	-0.27032
N	0.25623	-2.07533	-0.09853
N	-1.57412	0.31268	1.83753
C	-2.37104	-0.44936	1.18004
C	-2.18165	-0.62952	-0.29598
H	1.18779	-2.45281	0.11986
H	-0.81387	0.03314	-1.81579
H	-3.21728	-0.97275	1.63705
H	-2.10607	-1.70259	-0.50048
H	-1.85039	0.36220	2.82544
C	-3.38517	-0.08071	-1.06979
H	-4.29521	-0.59990	-0.75482
H	-3.53263	0.98903	-0.89518
H	-3.25069	-0.24580	-2.14236
H	2.50910	1.92664	0.01817
O	2.71023	-0.85571	-0.07536
C	3.97851	-0.19660	0.13675
H	3.95899	0.36035	1.07666
H	4.71147	-0.99900	0.18270
H	4.19875	0.47190	-0.69883
C	-0.74890	1.42821	-0.31011
N	0.40729	1.98389	-0.12613
H	-1.61033	2.08704	-0.30967

H	0.43866	2.98818	0.06896

There are no imaginary frequencies.

SCF energy: -586.989022 hartree
αα/ββ: -0.235468189 hartree
αβ: -1.3355961 hartree
SCS-MP2 energy: -588.7487161 hartree
enthalpy correction: +0.247761 hartree
free energy correction: +0.195664 hartree
quasiharmonic free energy correction: +0.196441 hartree

2-hydrazinyl-5-methoxypyridine (39)

S-118

C	1.04053	-1.47422	-0.30925
C	2.54159	0.34332	0.12773
C	2.29942	-0.89565	-0.47722
C	0.11843	-0.78172	0.45599
N	-1.24115	-1.30694	0.62076
N	-2.13043	-0.71026	-0.38380
C	-2.90258	0.18616	0.12228
C	-3.85522	0.91205	-0.75857
H	-1.57316	-1.13477	1.58763
H	3.05271	-1.40772	-1.06519
H	0.79638	-2.43415	-0.75630
H	-2.89923	0.42824	1.18904
H	-3.61743	1.98049	-0.69484
H	-1.25572	-2.32665	0.45876
H	-3.70899	0.59183	-1.79350
C	-5.29781	0.67525	-0.30502
H	-5.55591	-0.38464	-0.37460
H	-5.44211	0.99962	0.72917
H	-5.98487	1.24038	-0.93952
O	3.70413	1.04289	0.05707
C	4.74178	0.48934	-0.77784
H	4.39313	0.39283	-1.80903
H	5.55896	1.20641	-0.72499
H	5.06979	-0.48013	-0.39489
C	1.52140	0.94780	0.88514
H	1.70346	1.90674	1.36343
N	0.31225	0.39783	1.04718

There are no imaginary frequencies.

SCF energy: -586.987213 hartree
αα/ββ: -0.238030299 hartree
αβ: -1.332850124 hartree
SCS-MP2 energy: -588.74532 hartree
zero-point correction: +0.233910 hartree
enthalpy correction: +0.247923 hartree
free energy correction: +0.192855 hartree
quasiharmonic free energy correction: +0.195285 hartree

S-119

C	0.82023	1.62533	-0.00681
C	2.79295	0.24555	0.03137
C	2.19768	1.51587	0.08324
C	0.08960	0.44226	-0.14614
N	-1.32590	0.50645	-0.31123
N	-1.95865	-0.67853	-0.01915
C	-3.23182	-0.83068	0.12019
C	-4.18790	0.29749	0.03223
H	-1.76572	1.29827	0.16574
H	2.82589	2.39492	0.19869
H	0.32318	2.59053	0.03857
H	-3.54397	-1.85407	0.30718
H	-4.00168	0.82603	-0.91300
H	-3.95262	1.01457	0.83182
C	-5.63547	-0.16620	0.13425
H	-5.81943	-0.65536	1.09389
H	-6.30646	0.69159	0.05294
H	-5.87688	-0.86791	-0.66774
O	4.15534	0.21503	0.13486
C	4.77186	-1.08554	0.10208
H	4.57900	-1.58373	-0.85177
H	5.83858	-0.89743	0.21277
H	4.41515	-1.70482	0.92951
N	0.63050	-0.77141	-0.20789
C	1.97486	-0.87841	-0.11091
H	2.37085	-1.88668	-0.15688
H	-1.30216	-1.47579	0.01041

There are no imaginary frequencies.

SCF energy: -586.993574 hartree
αα/ββ: -0.238219938 hartree
αβ: -1.328954619 hartree
SCS-MP2 energy: -588.7471328 hartree
zero-point correction: +0.233089 hartree
enthalpy correction: +0.247089 hartree
free energy correction: +0.192806 hartree
quasiharmonic free energy correction: +0.194466 hartree

S-120

C	1.07905	1.79185	0.05301
C	2.80013	0.08472	0.03573
C	2.40920	1.44177	0.05860
C	0.09963	0.78086	0.01446
N	-1.23448	1.03936	0.05461
N	-2.09942	-0.01831	-0.14163
C	-3.33969	0.29443	-0.31478
C	-4.36216	-0.77163	-0.49929
H	-1.55074	1.99785	-0.11594
H	0.76778	2.83139	0.07064
H	-3.66423	1.34051	-0.31320

H	-3.85986	-1.74195	-0.55158
H	-4.86885	-0.60445	-1.45747
C	-5.39192	-0.75308	0.63356
H	-5.88809	0.21959	0.69659
H	-6.15766	-1.51520	0.46526
H	-4.91099	-0.95514	1.59457
H	3.18098	2.20644	0.08279
O	4.13764	-0.15574	0.04939
C	4.53228	-1.54181	0.00547
H	4.17120	-2.01352	-0.91250
H	5.62037	-1.52871	0.01738
H	4.15217	-2.07492	0.88116
C	1.82093	-0.89185	-0.00121
N	0.51262	-0.49927	-0.01122
H	1.98619	-1.96038	-0.02616
H	-0.21502	-1.21961	-0.05220

There are no imaginary frequencies.

SCF energy: -587.006561 hartree
αα/ββ: -0.237073384 hartree
αβ: -1.329621258 hartree
SCS-MP2 energy: -588.7601554 hartree
zero-point correction: +0.232700 hartree
enthalpy correction: +0.246907 hartree
free energy correction: +0.192551 hartree
quasiharmonic free energy correction: +0.193844 hartree

S-121

C	-0.89410	-1.15115	0.36889
C	-2.77300	0.27774	-0.05246
C	-2.24542	-1.01559	0.05352
C	-0.16672	0.01123	0.56615
N	1.26301	-0.07177	0.86103
N	2.03344	-0.39089	-0.34803
C	3.42171	-0.48148	-0.01836
C	4.35267	0.29607	-0.58687
H	1.58016	0.81704	1.29064
H	-2.85317	-1.89953	-0.10228
H	-0.43225	-2.12989	0.46398
H	1.87354	0.41203	-0.96793
H	3.66281	-1.29542	0.66223
H	4.03467	1.09114	-1.26196
H	1.45060	-0.82989	1.53773
C	5.82055	0.10814	-0.37526
H	6.31833	-0.16388	-1.31217
H	6.01580	-0.67857	0.35848
H	6.28161	1.03659	-0.02342
O	-4.06288	0.58153	-0.35303
C	-4.95129	-0.52876	-0.59475
H	-5.02979	-1.16059	0.29334
H	-5.91575	-0.07532	-0.81601
H	-4.60794	-1.11555	-1.45027
N	-0.63158	1.25778	0.47157
C	-1.93065	1.38138	0.16743
H	-2.33209	2.38833	0.09012

There are no imaginary frequencies.

SCF energy: -586.969404 hartree
αα/ββ: -0.238151547 hartree
αβ: -1.332457622 hartree
SCS-MP2 energy: -588.7271208 hartree
zero-point correction: +0.234156 hartree
enthalpy correction: +0.248359 hartree
free energy correction: +0.192384 hartree
quasiharmonic free energy correction: +0.195536 hartree

S-122

C	-1.07109	1.40426	0.07115
C	-2.77775	-0.28275	0.00867
C	-2.42184	1.07203	-0.00182
C	-0.14033	0.37253	0.15954
N	1.24436	0.66258	0.36996
N	2.07689	-0.36121	-0.23234
C	3.42756	-0.31553	0.31439
C	4.45935	-0.01848	-0.47555
H	1.51293	1.54965	-0.06667
H	-3.16486	1.85882	-0.07372
H	-0.75111	2.44269	0.05397
H	1.59713	-1.25332	-0.00671
H	3.46614	-0.53576	1.37477
H	4.28167	0.18908	-1.53051
H	2.08889	-0.28007	-1.26530
C	5.86753	0.03959	0.01567
H	6.29150	1.03071	-0.17273
H	5.92556	-0.17172	1.08586
H	6.48590	-0.68623	-0.52135
O	-4.05339	-0.76929	-0.06090
C	-5.10463	0.20756	-0.17522
H	-4.98300	0.80364	-1.08345
H	-6.02526	-0.37113	-0.23120
H	-5.12840	0.85879	0.70262
C	-1.76454	-1.24590	0.08216
H	-2.01918	-2.30290	0.07637
N	-0.46359	-0.92676	0.16971

There are no imaginary frequencies.

SCF energy: -586.975350 hartree
αα/ββ: -0.238152611 hartree
αβ: -1.331599539 hartree
SCS-MP2 energy: -588.7320379 hartree
zero-point correction: +0.234273 hartree
enthalpy correction: +0.248341 hartree
free energy correction: +0.193781 hartree
quasiharmonic free energy correction: +0.195654 hartree

S-123

C	0.53361	-1.30857	1.16390
C	2.36431	0.00386	0.26678
C	1.81233	-0.80966	1.27941
C	-0.22890	-0.98623	0.02854
N	-1.47874	-1.50791	-0.21931
N	-2.21900	-0.81760	-1.19906
C	-3.10912	0.17035	-0.69835
C	-3.03389	0.75960	0.50425
H	-2.00328	-1.73149	0.63317
H	0.09809	-1.93369	1.93708
H	-2.69640	-1.49718	-1.79032
H	-3.85591	0.45746	-1.43553
H	-2.26673	0.46503	1.21812
C	-3.97850	1.84454	0.92498
H	-3.43953	2.76867	1.16107
H	-4.70280	2.06506	0.13551
H	-4.53243	1.55875	1.82574
H	2.41854	-1.03781	2.15184
O	3.63252	0.44178	0.47175
C	4.18705	1.29293	-0.55231
H	3.59182	2.20388	-0.65615
H	5.18907	1.53761	-0.20579
H	4.23891	0.76044	-1.50553
N	0.33208	-0.20779	-0.90874
C	1.59212	0.30678	-0.84352
H	1.89084	0.92201	-1.68152
H	-0.26474	0.01853	-1.71402

There are no imaginary frequencies.

SCF energy: -586.986842 hartree
αα/ββ: -0.237625724 hartree
αβ: -1.328652851 hartree
SCS-MP2 energy: -588.7396426 hartree
zero-point correction: +0.233058 hartree
enthalpy correction: +0.247031 hartree
free energy correction: +0.193263 hartree
quasiharmonic free energy correction: +0.194603 hartree

TS S-124

C	0.25449	-0.06444	1.09870
C	-1.77923	-0.47073	-0.08735
C	-1.10507	-1.52150	-0.77497
C	0.79148	-1.19360	0.45103
N	2.12196	-1.48560	0.59576
N	3.10939	-0.21746	-0.47232
C	2.55610	0.96539	-0.11239
C	1.34894	1.42193	-0.59798
H	0.79748	0.39712	1.91904
H	-1.64454	-2.06989	-1.54442
H	2.63118	-0.55074	-1.32291
H	3.04546	1.49737	0.70315
H	0.88633	0.86124	-1.41389
H	2.56413	-1.26498	1.49220
C	0.78357	2.76197	-0.28760
H	-0.30330	2.70449	-0.17189
H	1.22502	3.18785	0.61692
H	0.97987	3.44176	-1.12655
H	2.44252	-2.36794	0.18178
O	-3.06962	-0.29689	-0.45698
C	-3.78500	0.76682	0.20617
H	-3.30561	1.72939	0.00970
H	-4.78438	0.74853	-0.22398
H	-3.83543	0.57993	1.28154
N	0.14638	-1.87802	-0.53421
C	-1.10262	0.24924	0.88578
H	-1.56180	1.05808	1.44220

1 imaginary frequency: –282.80 cm^{-1}.

SCF energy: -586.916572 hartree
αα/ββ: -0.246578738 hartree
αβ: -1.353362083 hartree
SCS-MP2 energy: -588.7049923 hartree
zero-point correction: +0.232142 hartree
enthalpy correction: +0.245327 hartree
free energy correction: +0.194160 hartree
quasiharmonic free energy correction: +0.194792 hartree

TS S-125

C	0.21128	-0.15744	1.15182
C	-1.80098	-0.47392	-0.08760
C	-1.12301	-1.48501	-0.81868
C	0.79770	-1.21606	0.42054
N	2.09353	-1.53714	0.67787
N	3.07109	-0.21991	-0.30881
C	2.55143	1.01817	-0.03275
C	1.38731	1.41550	-0.62503
H	0.75904	0.26578	1.98885
H	-1.66266	-1.99679	-1.61398
H	2.90357	-0.59408	-1.24951
H	3.00198	1.54685	0.80085
H	0.98799	0.81798	-1.44632
H	2.34287	-2.32589	0.05964
C	0.74469	2.72866	-0.34750
H	-0.33576	2.60323	-0.22451
H	1.15911	3.19596	0.54882
H	0.89755	3.39957	-1.20047
H	4.00870	-0.42313	0.04941
O	-3.08764	-0.26763	-0.46268
C	-3.79673	0.77830	0.23311
H	-3.29683	1.73970	0.08776
H	-4.78794	0.79842	-0.21578
H	-3.87174	0.54738	1.29849
N	0.13754	-1.84228	-0.60745

C	-1.12623	0.19110	0.93209
H	-1.59257	0.96557	1.53086

1 imaginary frequency: –316.45 cm^{-1}.

SCF energy: -586.916775 hartree
αα/ββ: -0.246294104 hartree
αβ: -1.356296827 hartree
SCS-MP2 energy: -588.7085273 hartree
zero-point correction: +0.231209 hartree
enthalpy correction: +0.244765 hartree
free energy correction: +0.192325 hartree
quasiharmonic free energy correction: +0.193494 hartree

TS S-126

C	0.32387	0.05790	1.02762
C	-1.76742	-0.45789	-0.06604
C	-1.13795	-1.58167	-0.65330
C	0.89083	-1.16088	0.55833
N	2.16209	-1.57195	0.65972
N	3.05755	-0.29192	-0.60589
C	2.56140	0.89750	-0.21343
C	1.30628	1.38336	-0.55884
H	0.83721	0.56379	1.83968
H	-1.65157	-2.23604	-1.34988
H	2.47852	-0.64851	-1.37964
H	3.13199	1.41978	0.55695
H	0.78133	0.87247	-1.37070
H	2.60448	-1.09704	1.45511
C	0.85953	2.77286	-0.23398
H	1.11120	3.44553	-1.06301
H	-0.22528	2.81672	-0.10040
H	1.34778	3.14519	0.67109
O	-3.05912	-0.30400	-0.42842
C	-3.74278	0.84149	0.12614
H	-3.23672	1.76429	-0.16855
H	-4.74296	0.80445	-0.30022
H	-3.79325	0.76368	1.21453
N	0.11527	-1.87142	-0.33945
C	-1.05315	0.32840	0.82394
H	-1.50258	1.18534	1.31385
H	0.54479	-2.70702	-0.75477

1 imaginary frequency: –207.86 cm^{-1}.

SCF energy: -586.896850 hartree
αα/ββ: -0.248699516 hartree
αβ: -1.360164178 hartree
SCS-MP2 energy: -588.6948467 hartree
zero-point correction: +0.232212 hartree
enthalpy correction: +0.245320 hartree
free energy correction: +0.194179 hartree
quasiharmonic free energy correction: +0.195012 hartree

S-127

C	0.48342	-0.20777	-0.59669
C	-1.88780	0.20756	-0.06550
C	-1.48001	1.48185	0.49117
C	0.67701	1.22459	-0.20295
N	1.80970	1.81079	-0.43628
N	3.32647	-0.50603	-0.87701
C	2.74576	-1.27652	-0.02780
C	1.28764	-1.18453	0.31730
H	0.88799	-0.31914	-1.61261
H	-2.24263	2.06912	1.00191
H	4.31804	-0.75518	-0.95725
H	3.28382	-2.06839	0.50460
H	0.87197	-2.18251	0.11916
C	1.10752	-0.88892	1.80912
H	1.56196	-1.68572	2.40457
H	1.58606	0.05576	2.08476
H	0.04415	-0.83699	2.06123
O	-3.22969	-0.00172	0.04892
C	-3.69646	-1.26075	-0.47024
H	-3.23352	-2.09146	0.06955
H	-4.77252	-1.25871	-0.30677
H	-3.47613	-1.33822	-1.53859
C	-0.95428	-0.61416	-0.59935
N	-0.28260	1.99565	0.43438
H	-1.18469	-1.59905	-0.99332
H	2.57252	1.25243	-0.85721
H	1.94872	2.78094	-0.14933

There are no imaginary frequencies.

SCF energy: -587.006691 hartree
αα/ββ: -0.235548593 hartree
αβ: -1.331342446 hartree
SCS-MP2 energy: -588.7613343 hartree
zero-point correction: +0.233952 hartree
enthalpy correction: +0.247360 hartree
free energy correction: +0.195770 hartree
quasiharmonic free energy correction: +0.196185 hartree

S-128

C	0.47377	-0.19038	-0.64646
C	-1.87903	0.20600	-0.04240
C	-1.44737	1.42922	0.62948
C	0.68421	1.25373	-0.23745
N	1.74967	1.86199	-0.62518
N	3.41952	-0.40017	-0.63033
C	2.71429	-1.29684	-0.03829
C	1.25754	-1.19491	0.24088
H	1.77089	2.81302	-0.23678
H	0.86132	-0.28485	-1.67002
H	-2.19151	1.94943	1.23367

H	3.23749	-2.18881	0.30103
H	0.86102	-2.19496	0.01854
C	1.08404	-0.94994	1.74952
H	1.53815	-1.76175	2.32395
H	1.55415	-0.00849	2.04646
H	0.01737	-0.91310	1.98542
O	-3.22598	0.00956	0.07621
C	-3.72024	-1.20715	-0.51002
H	-3.26063	-2.07599	-0.03026
H	-4.79370	-1.20185	-0.32848
H	-3.51995	-1.22405	-1.58502
N	-0.25569	1.93635	0.57562
C	-0.97489	-0.58396	-0.66003
H	-1.23445	-1.52583	-1.13384
H	4.42164	-0.54846	-0.76588
H	2.99760	0.50752	-0.92064

There are no imaginary frequencies.

SCF energy: -587.002777 hartree
αα/ββ: -0.235551559 hartree
αβ: -1.334526805 hartree
SCS-MP2 energy: -588.7612435 hartree
zero-point correction: +0.234700 hartree
enthalpy correction: +0.247992 hartree
free energy correction: +0.196686 hartree
quasiharmonic free energy correction: +0.197167 hartree

S-129

C	0.53289	-0.21932	-0.61162
C	-1.86939	0.17287	-0.07068
C	-1.51376	1.46867	0.44427
C	0.77536	1.23618	-0.30316
N	1.81680	1.95107	-0.49676
N	3.32949	-0.61508	-0.90655
C	2.76634	-1.25324	0.05631
C	1.30254	-1.14495	0.37547
H	2.52476	1.34943	-0.94332
H	0.94746	-0.40334	-1.61091
H	3.31947	-1.93491	0.71278
H	0.88823	-2.15523	0.24097
H	4.32679	-0.85562	-0.93599
C	1.10747	-0.74982	1.84150
H	1.56695	-1.49754	2.49428
H	1.57468	0.21701	2.05303
H	0.04295	-0.69193	2.08839
H	-2.25718	2.09875	0.92573
O	-3.20269	-0.07022	0.05355
C	-3.63762	-1.35077	-0.44386
H	-3.43234	-1.43288	-1.51455
H	-3.13958	-2.15864	0.09906
H	-4.71007	-1.37779	-0.26193
C	-0.91115	-0.61646	-0.61598
N	-0.30503	1.93118	0.33553
H	-1.14198	-1.59915	-1.01671
H	-0.09363	2.87430	0.68164

There are no imaginary frequencies.

SCF energy: -586.988720 hartree
αα/ββ: -0.235237941 hartree
αβ: -1.334807932 hartree
SCS-MP2 energy: -588.7473148 hartree
zero-point correction: +0.234947 hartree
enthalpy correction: +0.248476 hartree
free energy correction: +0.196472 hartree
quasiharmonic free energy correction: +0.196965 hartree

Nα-methylated hydrazine

S-130

C	1.54052	0.25571	1.11692
C	1.55042	-0.37340	-1.22638
C	3.17095	-1.23002	0.15505
C	2.66261	-0.55413	1.26612
C	0.99780	0.32791	-0.16162
N	-0.18493	1.15251	-0.41528
N	-1.29172	0.65745	0.41607
C	-2.26351	0.19775	-0.29192
C	-3.46331	-0.36529	0.38146
H	-0.42772	1.07189	-1.42147
H	1.11505	-0.30719	-2.22214
H	4.04715	-1.86497	0.25578
H	3.14003	-0.66335	2.23475
H	1.10895	0.79168	1.95712
H	-2.23068	0.18661	-1.38641
H	-3.37661	-0.21829	1.46111
H	-4.33769	0.19294	0.02760
C	-3.62128	-1.84888	0.03664
H	-3.70350	-1.99407	-1.04398
H	-2.76371	-2.42169	0.39885
H	-4.52495	-2.24520	0.50604
N	2.63735	-1.15146	-1.07968
C	0.02759	2.60494	-0.11740
H	0.87979	2.93711	-0.70989
H	-0.88261	3.12889	-0.40629
H	0.22082	2.70855	0.94788

There are no imaginary frequencies.

SCF energy: -512.132264 hartree
αα/ββ: -0.212699658 hartree
αβ: -1.206693003 hartree
SCS-MP2 energy: -513.7220954 hartree
zero-point correction: +0.230105 hartree
enthalpy correction: +0.242790 hartree
free energy correction: +0.191504 hartree

quasiharmonic free energy correction: +0.192973 hartree

S-131

C	-2.19984	1.02515	0.24657
C	-1.26406	-1.08652	-0.44480
C	-3.46752	-1.02096	0.20050
C	-3.40251	0.34773	0.44484
C	-1.10427	0.28505	-0.20405
N	0.17236	0.87229	-0.49607
N	1.16314	0.14897	0.21042
C	2.18473	-0.36434	-0.37958
C	3.25761	-1.05496	0.36087
H	-0.43009	-1.67747	-0.81808
H	-4.39452	-1.56750	0.35384
H	-4.28138	0.88092	0.79506
H	-2.13406	2.09010	0.44182
H	2.23868	-0.23639	-1.45823
H	3.37222	-2.04730	-0.08920
H	2.98347	-1.17602	1.41213
C	4.56674	-0.26560	0.21321
H	4.46864	0.73032	0.65109
H	5.36498	-0.79917	0.73326
H	4.84536	-0.16263	-0.83822
N	-2.41656	-1.74415	-0.24058
H	1.04802	0.06003	1.23345
C	0.32554	2.30161	-0.17035
H	-0.38278	2.85942	-0.78241
H	0.15147	2.50921	0.89145
H	1.33892	2.59378	-0.44558

There are no imaginary frequencies.

SCF energy: -512.137338 hartree
αα/ββ: -0.212176858 hartree
αβ: -1.200282242 hartree
SCS-MP2 energy: -513.7191279 hartree
zero-point correction: +0.229684 hartree
enthalpy correction: +0.242332 hartree
free energy correction: +0.191476 hartree
quasiharmonic free energy correction: +0.192647 hartree

S-132

C	-2.15714	1.04743	0.31703
C	-1.27582	-1.10561	-0.31695
C	-3.59920	-0.88287	0.20232
C	-3.41433	0.46955	0.44778
C	-1.05030	0.26625	-0.08671
N	0.20431	0.79518	-0.26794
N	1.21823	-0.13700	-0.34222
C	2.44913	0.26111	-0.28782
C	3.54005	-0.75459	-0.36962
H	-2.03698	2.09780	0.55549
H	2.74039	1.30382	-0.15634
H	4.16998	-0.52638	-1.23866
H	3.09648	-1.74180	-0.53119
C	4.39968	-0.74890	0.89609
H	3.79733	-1.00745	1.77164
H	5.21261	-1.47570	0.81179
H	4.84193	0.23754	1.06395
N	-2.51574	-1.59978	-0.16164
H	-2.63965	-2.60061	-0.34065
H	-0.50656	-1.80314	-0.61389
H	-4.26084	1.07173	0.75964
H	-4.53764	-1.41529	0.28702
C	0.46923	2.22636	-0.19605
H	-0.43121	2.76880	-0.47624
H	0.79769	2.53681	0.80125
H	1.24105	2.47267	-0.92763

There are no imaginary frequencies.

SCF energy: -512.136041 hartree
αα/ββ: -0.214849679 hartree
αβ: -1.210455137 hartree
SCS-MP2 energy: -513.7318203 hartree
zero-point correction: +0.229078 hartree
enthalpy correction: +0.242087 hartree
free energy correction: +0.190168 hartree
quasiharmonic free energy correction: +0.191596 hartree

S-133

C	-1.32777	0.16018	-1.08285
C	-1.11041	-0.39860	1.26481
C	-2.37455	-1.76104	-0.08270
C	-2.12856	-0.97118	-1.20696
C	-0.82968	0.43399	0.18699
N	0.05853	1.58121	0.40598
N	1.39978	1.42291	-0.19317
C	2.01293	0.22925	0.29086
C	2.42020	-0.75936	-0.51742
H	0.24080	1.66043	1.42130
H	-0.71395	-0.18158	2.25535
H	-2.99312	-2.65088	-0.16434
H	-2.55321	-1.24384	-2.16793
H	-1.10310	0.78621	-1.94257
H	1.22795	1.35272	-1.20352
H	2.20852	0.23445	1.36160
H	2.19227	-0.69838	-1.58187
C	3.20875	-1.93595	-0.03916
H	4.20246	-1.95483	-0.49922
H	3.33336	-1.91258	1.04689
H	2.70909	-2.87058	-0.31380
N	-1.88293	-1.49261	1.14251
C	-0.51431	2.89267	-0.03321
H	-1.48720	3.00258	0.44358
H	0.17613	3.66788	0.29279

H	-0.60719	2.88808	-1.11769

There are no imaginary frequencies.

SCF energy: -512.113277 hartree
αα/ββ: -0.213544162 hartree
αβ: -1.207835007 hartree
SCS-MP2 energy: -513.7050418 hartree
zero-point correction: +0.229651 hartree
enthalpy correction: +0.242656 hartree
free energy correction: +0.189959 hartree
quasiharmonic free energy correction: +0.192520 hartree

S-134

C	-1.06016	0.26154	1.17936
C	-1.37091	0.32680	-1.20901
C	-2.76931	-0.99336	0.04101
C	-2.14533	-0.61302	1.22655
C	-0.66903	0.74219	-0.07129
N	0.40875	1.66747	-0.28128
N	1.54462	0.92269	-0.88411
C	2.09534	-0.17495	-0.09427
C	1.72414	-1.43023	-0.36079
H	-1.09240	0.71571	-2.18783
H	-3.60923	-1.68345	0.05614
H	-2.49378	-1.00969	2.17553
H	-0.55216	0.55790	2.09166
H	2.26576	1.63665	-1.08212
H	2.77424	0.13289	0.69171
H	1.03401	-1.61800	-1.18326
H	1.21549	0.57995	-1.80049
C	2.21997	-2.60577	0.41225
H	2.71953	-3.31416	-0.25567
H	2.91879	-2.30327	1.19558
H	1.37829	-3.13285	0.87302
N	-2.39819	-0.53688	-1.17420
C	0.89718	2.37505	0.91149
H	0.05764	2.95026	1.30183
H	1.28581	1.71875	1.69575
H	1.68036	3.06688	0.59355

There are no imaginary frequencies.

SCF energy: -512.111195 hartree
αα/ββ: -0.214049219 hartree
αβ: -1.208347294 hartree
SCS-MP2 energy: -513.7039112 hartree
zero-point correction: +0.230178 hartree
enthalpy correction: +0.242726 hartree
free energy correction: +0.192304 hartree
quasiharmonic free energy correction: +0.193602 hartree

S-135

C	2.13123	1.13341	-0.11336
C	1.39071	-1.15575	-0.00162
C	3.72971	-0.66893	-0.01324
C	3.44804	0.68647	-0.08408
C	1.06526	0.20950	-0.07743
N	-0.25929	0.59707	-0.17555
N	-1.15437	-0.34610	0.41687
C	-2.40338	-0.37531	-0.25122
C	-3.58614	-0.29192	0.37730
H	1.93829	2.19906	-0.15842
H	-1.28017	-0.10628	1.40877
H	-2.32629	-0.55945	-1.32088
H	-3.60036	-0.09630	1.45011
C	-4.90138	-0.49683	-0.30778
H	-5.56427	0.36093	-0.15205
H	-4.76555	-0.63675	-1.38421
H	-5.42084	-1.37787	0.08564
N	2.68401	-1.52058	0.02417
H	0.65626	-1.94789	0.03281
H	2.88271	-2.52374	0.07840
H	4.26760	1.39656	-0.10763
H	4.72122	-1.10185	0.01992
C	-0.59320	1.99818	0.09458
H	-0.31489	2.29655	1.11356
H	-0.10036	2.64789	-0.62970
H	-1.67089	2.10349	-0.03367

There are no imaginary frequencies.

SCF energy: -512.122937 hartree
αα/ββ: -0.213785707 hartree
αβ: -1.20651874 hartree
SCS-MP2 energy: -513.7132833 hartree
zero-point correction: +0.228863 hartree
enthalpy correction: +0.241807 hartree
free energy correction: +0.190347 hartree
quasiharmonic free energy correction: +0.191741 hartree

TS S-136

C	-0.61740	1.65539	-0.62774
C	0.55574	0.33480	1.05236
C	1.68380	2.02577	-0.00955
C	0.56051	2.35464	-0.79464
C	-0.64169	0.65865	0.37256
N	-1.72176	-0.17897	0.54860
N	-1.33424	-1.74800	-0.50842
C	-0.09409	-2.11672	-0.11410
C	1.06127	-1.51950	-0.57510
H	0.52880	-0.36858	1.88238
H	2.60752	2.58778	-0.12707
H	0.63180	3.15430	-1.52555
H	-1.50108	1.90150	-1.20843

H	-1.24640	-1.16427	-1.35556
H	-0.04048	-2.83135	0.70704
H	0.97258	-0.81148	-1.40244
H	-1.71998	-0.67785	1.44649
C	2.42864	-1.96005	-0.19599
H	3.07043	-1.09113	-0.02242
H	2.41638	-2.58907	0.69757
H	2.87374	-2.52826	-1.02244
N	1.69427	1.06388	0.91798
C	-3.07964	0.18136	0.09828
H	-3.07569	0.33530	-0.97934
H	-3.73265	-0.65083	0.35165
H	-3.39561	1.08960	0.61448

1 imaginary frequency: –275.19 cm^{-1}.

SCF energy: -512.059803 hartree
αα/ββ: -0.221475179 hartree
αβ: -1.228038875 hartree
SCS-MP2 energy: -513.6810998 hartree
zero-point correction: +0.228536 hartree
enthalpy correction: +0.240632 hartree
free energy correction: +0.192123 hartree
quasiharmonic free energy correction: +0.192522 hartree

TS S-137

C	-1.12806	-1.43628	-0.83533
C	-0.53164	0.00475	1.02287
C	-2.66647	0.10931	0.17371
C	-2.38091	-0.86541	-0.80564
C	-0.17333	-1.04764	0.13983
N	1.08249	-1.59240	0.03349
N	1.89802	-0.24023	-1.09757
C	1.74933	0.97594	-0.51355
C	0.52169	1.60326	-0.55836
H	0.12424	0.29699	1.83695
H	-3.65978	0.55103	0.22376
H	-3.14948	-1.15478	-1.51622
H	-0.86320	-2.20818	-1.55435
H	1.31105	-0.46463	-1.90765
H	2.55569	1.30879	0.13098
H	-0.21038	1.26223	-1.29087
C	0.28193	2.91680	0.10169
H	-0.71914	2.94469	0.53815
H	1.02483	3.11726	0.87666
H	0.33275	3.70997	-0.65317
H	2.84216	-0.63631	-1.15627
N	-1.79073	0.52301	1.08956
C	1.93103	-1.46021	1.22252
H	2.90786	-1.89204	0.99363
H	2.07762	-0.43446	1.57972
H	1.47589	-2.03635	2.03391

1 imaginary frequency: –345.83 cm^{-1}.

SCF energy: -512.054835 hartree
αα/ββ: -0.222037679 hartree
αβ: -1.229912403 hartree
SCS-MP2 energy: -513.678755 hartree
zero-point correction: +0.227525 hartree
enthalpy correction: +0.239600 hartree
free energy correction: +0.191219 hartree
quasiharmonic free energy correction: +0.191562 hartree

TS S-138

C	0.44916	-1.78911	-0.50491
C	-0.55200	-0.08052	0.91052
C	-1.91903	-1.78608	-0.04942
C	-0.80801	-2.32979	-0.70287
C	0.63553	-0.69309	0.38038
N	1.79729	-0.07787	0.67788
N	1.57258	1.62891	-0.47138
C	0.39614	2.15244	-0.10707
C	-0.77689	1.54533	-0.56190
H	-0.50194	0.57822	1.77031
H	-2.55361	-0.37818	1.26751
H	-2.92525	-2.18246	-0.12560
H	-0.95201	-3.18674	-1.35202
H	1.30581	-2.26420	-0.97299
H	2.32288	2.11317	0.04034
H	0.32209	2.91785	0.67071
H	-0.68382	0.85928	-1.40470
C	-2.12938	2.12444	-0.29785
H	-2.90910	1.35824	-0.31962
H	-2.16272	2.64893	0.66049
H	-2.36365	2.84266	-1.09294
N	-1.73806	-0.75113	0.77238
C	2.99219	-0.59802	0.00690
H	3.80637	0.10908	0.17602
H	3.27596	-1.55426	0.45931
H	2.86999	-0.73463	-1.07156

1 imaginary frequency: –121.20 cm^{-1}.

SCF energy: -512.039899 hartree
αα/ββ: -0.22368334 hartree
αβ: -1.235256326 hartree
SCS-MP2 energy: -513.6713288 hartree
zero-point correction: +0.227280 hartree
enthalpy correction: +0.239377 hartree
free energy correction: +0.191124 hartree
quasiharmonic free energy correction: +0.191401 hartree

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