Copper-mediated Tandem Reaction through Isocyanides N-H Bond Insertion: Efficient Access to Unsymmetrical Tetrasubstituted Ureas

Xiaomei Huang,[a] Shuguang Xu,[a] Qitao Tan,[a] Mingchun Gao,[a] Minjie Li,[a] and Bin Xu*[a,b]

[a]Department of Chemistry, College of Sciences, Shanghai University, Shanghai 200444, China
[b]State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China
Tel: (+86) 21-66132830; Fax: (+86) 21-66134594; E-mail: xubin@shu.edu.cn

Supporting Information

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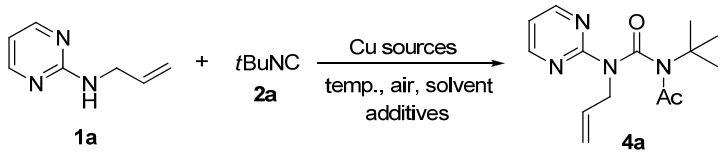
1. General Information

All reagents and metal catalysts were obtained from commercial sources without further purification, and commercially available solvents were purified before use. All new compounds were fully characterized. All melting points were taken on a WRS-1A or a WRS-1B Digital Melting Point Apparatus without correction. Infrared spectra were obtained using an AVATAR 370 FT-IR spectrometer. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded with a Bruker AV-500 spectrometer operating at 500 MHz and 125 MHz, respectively, with chemical shift values being reported in ppm relative to chloroform (δ = 7.26 ppm), dimethyl sulfoxide (δ = 2.50 ppm), acetone (δ = 2.05 ppm) or TMS (δ = 0.00 ppm) for ^{1}H NMR; chloroform (δ = 77.16 ppm), acetone (δ = 29.84 and 206.26 ppm) or dimethyl sulfoxide (δ = 39.52 ppm) for ^{13}C NMR; and C_6F_6 (δ = -164.9 ppm) for ^{19}F NMR. Mass spectra and high resolution mass spectra were recorded with an Agilent 5975N using an Electron impact (EI) or Electrospray ionization (ESI) techniques. Elemental analyses were carried out on an Elementar Vario EL elemental analyzer. Silica gel plate GF254 were used for thin layer chromatography (TLC) and silica gel H or 300-400 mesh were used for flash column chromatography. Yields refer to chromatographically and spectroscopically pure compounds, unless otherwise indicated.

2. Screening of the Reaction Conditions

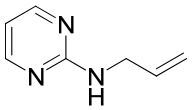
Table S1. Optimization of reaction conditions[a]



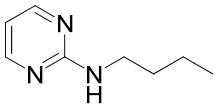
Entry	Cu sources	Solvent	Time [h]	Temp. [°C]	Yield [%][b]
1	CuCl	toluene	36	110	n.d.
2	$Cu(OAc)_2$	toluene	58	110	30[c]
3	$Cu(OAc)_2$	toluene	35	110	67
4	$Cu(OAc)_2·H_2O$	toluene	27	110	65
5	$Cu(OAc)_2·H_2O$	toluene	47	110	51[d]
6	$Cu(OAc)_2·H_2O$	PhCl	24	110	32
7	$Cu(OAc)_2·H_2O$	dioxane	35	110	trace
8	$Cu(OAc)_2·H_2O$	DMF	35	110	trace
9	$Cu(OAc)_2·H_2O$	toluene	59	100	59
10	$Cu(OAc)_2·H_2O$	toluene	36	120	48
11	$Cu(OAc)_2·H_2O$	toluene	24	110	19[e]
12	$Cu(OAc)_2·H_2O$	toluene	40	110	16[f]
13	$Cu(OAc)_2·H_2O$	toluene	39	110	trace[g]
14	--	toluene	24	110	n.d.
15	--	toluene	12	110	n.d.[h]

[a] Reaction conditions: **1a** (0.3 mmol), **2a** (0.9 mmol), Cu source (0.6 mmol), 110 °C, air, solvent (1.5 mL), dried through a calcium chloride tube. n.d. = not detected. [b] Isolated yield. [c] $Cu(OAc)_2·H_2O$ (1.5 equiv). [d] $Cu(OAc)_2·H_2O$ (2.5 equiv). [e] N_2. [f] O_2. [g] $Cu(OAc)_2·H_2O$ (0.2 equiv), NaOAc (2.0 equiv). [h] $Pd(OAc)_2$ (5 mol %), NaOAc (3.0 equiv).

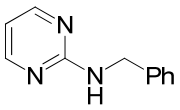
3. Synthesis and characterization for starting materials



Allyl-pyrimidin-2-yl-amine (1a)[1]**:** To an oven-dried flask containing 2-chloro-pyrimidine (1.145 g, 10 mmol) was added allylamine (2.5 mL). The reaction mixture was stirred under reflux for 3 h and monitored by TLC. Upon completion, the mixture was washed with 10% NaOH aqueous solution and extracted with Et_2O (3×30 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel to give **1a** as yellow liquid (1.318 g, 97%). IR (KBr, cm^{-1}): 3264, 1592, 1411, 1362, 919, 801; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.25 (d, J = 5.0 Hz, 2H), 6.50 (t, J = 5.0 Hz, 1H), 5.98-5.91 (m, 2H), 5.26-5.22 (m, 1H), 5.13-5.10 (m, 1H), 4.06-4.04 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 162.1, 158.0, 134.9, 115.7, 110.5, 43.7; LC-MS (ESI) m/z 136.1 [M^+H].

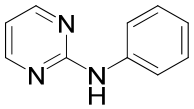


Butyl-pyrimidin-2-yl-amine (1b)[2]**:** To an oven-dried flask containing 2-chloro-pyrimidine (2.2 g, 19.2 mmol), butylamine (1.4 g, 19.2 mmol) and triethylamine (6.0 mL) were added in *n*-butanol (40 mL) and the mixture was stirred at 110 ^{o}C for 18 h and monitored by TLC. Upon completion, the reaction mixture was extracted with ethyl acetate (3×30 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel to give **1b** as yellow liquid (2.3 g, 79%). IR (KBr, cm^{-1}): 3444, 3275, 2871, 1592, 801, 640; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.26 (s, 2H), 6.51 (t, J = 5.0 Hz, 1H), 5.46 (s, 1H), 3.42-3.38 (m, 2H), 1.62-1.56 (m, 2H), 1.45-1.37 (m, 2H), 0.94 (t, J = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 162.3, 157.9, 110.2, 41.2, 31.7, 20.1, 13.8; LC-MS (ESI) m/z 152.1 [M^+H].

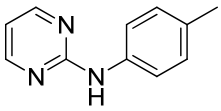


Benzyl-pyrimidin-2-yl-amine (1c)[2]**:** To an oven-dried flask containing 2-chloro-pyrimidine (230.0 mg, 2.0 mmol), benzylamine (107.0 mg, 1.0 mmol) and triethylamine (101.0 mg, 1.0 mmol) were added in ethanol (2 mL) and the mixture was stirred at 78 ^{o}C for 24 h and monitored by TLC. Upon completion, the reaction mixture was extracted with ethyl acetate (3×30 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel to give **1c** as yellow solid (140.6 mg, 76%). M.p. 72-74 ^{o}C; IR (KBr, cm^{-1}): 3241, 2874, 1592, 1261, 667, 537; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.28 (s, 2H), 7.37-7.32 (m, 4H), 7.29-7.26 (m, 1H), 6.58 (t, J = 5.0 Hz, 1H), 6.11 (s, 1H), 4.66 (d, J = 6.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 162.1, 158.0, 139.0, 128.6,

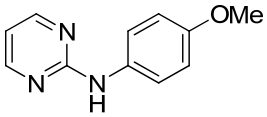
127.6, 127.3, 110.6, 45.5; LC-MS (ESI) m/z 186.1 [M^+H].



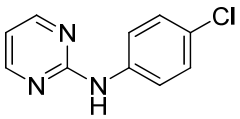
Phenyl-pyrimidin-2-yl-amine (1d)[3]**:** To an oven-dried flask containing aniline (6.975 g, 75 mmol), 2-chloro-pyrimidine (5.725 g, 50 mmol) and acetic acid (50 mL) in 1,4-dioxane (130 mL) was added. The reaction mixture was stirred at 110 ^oC for 23 h and monitored by TLC. Upon completion, the mixture was extracted with CH_2Cl_2 (3×100 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel and then recrystallization to give **1d** as white solid (7.006 g, 82%). M.p. 106-108 ^oC; IR (KBr, cm^{-1}): 3441, 3258, 1613, 1252, 751, 640; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.43 (d, J = 4.8 Hz, 2H), 7.71 (br, 1H), 7.62 (d, 2H), 7.35 (t, J = 8.2 Hz, 2H), 7.07 (t, J = 7.4 Hz, 1H), 6.73 (t, J = 4.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.2, 158.0, 139.4, 129.0, 122.9, 119.8, 112.4; EI-MS m/z (%): 171 (46) [M^+], 170 (100).



Pyrimidin-2-yl-*p*-tolyl-amine (1e)[4]**:** Following the same procedure as for **1d** with 4-methylaniline (321.0 mg, 3 mmol), 2-chloro-pyrimidine (520.0 mg, 4.5 mmol), and acetic acid (270 mg, 4.5 mmol) in 1,4-dioxane (6.0 mL) for 9 h to give **1e** as yellow solid (433.4 mg, 78%). M.p. 124-126 ^oC; IR (KBr, cm^{-1}): 3443, 3259, 1617, 1252, 794, 640, 507; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.40 (d, J = 4.5 Hz, 2H), 7.95 (s, 1H), 7.49 (d, J = 8.5 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 6.67 (t, J = 4.5 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.4, 158.0, 136.7, 132.6, 129.5, 120.3, 112.1, 20.9; EI-MS m/z (%): 185 (58) [M^+], 184 (100).

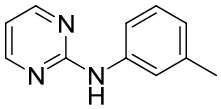


(4-Methoxy-phenyl)-pyrimidin-2-yl-amine (1f)[4]**:** Following the same procedure as for **1d** with 4-methoxyaniline (370.0 mg, 3.0 mmol), 2-chloro-pyrimidine (520.0 mg, 4.5 mmol), and acetic acid (270 mg, 1.5 mmol) in 1,4-dioxane (6.0 mL) for 18 h to give **1f** as orange-red solid (509.0 mg, 84%). M.p. 123-124 ^oC; IR (KBr, cm^{-1}): 3442, 3258, 1617, 1424, 1243, 560; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.37 (d, J = 4.5 Hz, 2H), 7.95 (br, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.16 (d, J = 8.2 Hz, 2H), 6.68 (t, J = 4.8 Hz, 1H), 3.80 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.6, 158.0, 155.9, 132.3, 122.4, 114.2, 111.9, 55.6; LC-MS (ESI) m/z 202.1 [M^+H].

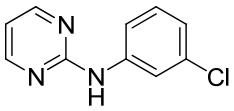


(4-Chloro-phenyl)-pyrimidin-2-yl-amine (1g)[4]**:** Following the same procedure as for **1d** with *p*-chloroaniline (765.4 mg, 6.0 mmol), 2-chloro-pyrimidine (572.5 mg, 5.0 mmol), and acetic acid (300.3 mg, 5.0 mmol) in 1,4-dioxane (12.0 mL) for 29 h to give **1g** as yellow solid (849.3 mg, 83%). M.p. 172-174 ^oC; IR (KBr, cm^{-1}): 3455, 3259, 1616, 1424, 790, 464; ^1H NMR ($CDCl_3$, 500

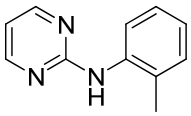
MHz): δ 8.43 (d, *J* = 4.8 Hz, 2H), 7.62 (br, 1H), 7.58 (d, *J* = 8.7 Hz, 2H), 7.30 (d, *J* = 8.7 Hz, 2H), 6.76 (t, *J* = 4.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.7, 158.0, 137.9, 128.9, 127.6, 120.7, 112.8; EI-MS m/z (%): 207 (18) [M^+ (^{37}Cl)], 205 (58) [M^+ (^{35}Cl)], 204 (100).



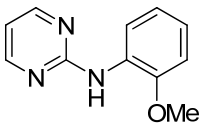
Pyrimidin-2-yl-*m*-tolyl-amine (1h)[4]**:** Following the same procedure as for **1d** with 3-methylaniline (385.7 mg, 3.6 mmol), 2-chloro-pyrimidine (343.5 mg, 3.0 mmol), and acetic acid (180.0 mg, 3.0 mmol) in 1,4-dioxane (7.2 mL) for 18 h to give **1h** as yellow solid (245.0 mg, 44%). M.p. 80-82 ^{o}C; IR (KBr, cm^{-1}): 3314, 1614, 1254, 798, 519, 443; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.43 (d, *J* = 5.0 Hz, 2H), 7.49 (br, 1H), 7.44-7.42 (m, 2H), 7.23 (t, *J* = 8.0 Hz, 1H), 6.89 (d, *J* = 8.0 Hz, 1H), 6.72 (t, *J* = 5.0 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.3, 158.0, 139.3, 138.8, 128.8, 123.8, 120.4, 116.9, 112.3, 21.7; LC-MS (ESI) m/z 186.1 [M^+H].



(3-Chloro-phenyl)-pyrimidin-2-yl-amine (1i)[4]**:** Following the same procedure as for **1d** with *m*-chloroaniline (765.0 mg, 6.0 mmol), 2-chloro-pyrimidine (572.5 mg, 5.0 mmol), and acetic acid (300.3 mg, 5.0 mmol) in 1,4-dioxane (12 mL) for 24 h to give **1i** as yellow solid (906.5 mg, 88%). M.p. 106-108 ^{o}C; IR (KBr, cm^{-1}): 3445, 1617, 1432, 995, 793, 640; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.45 (d, *J* = 4.5 Hz, 2H), 7.86 (s, 1H), 7.73 (br, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.79 (t, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.8, 158.0, 140.8, 134.6, 129.9, 122.5, 119.4, 117.4, 113.0; LC-MS (ESI) m/z 208.1 [M^+H (^{37}Cl)], 206.1 [M^+H (^{35}Cl)].

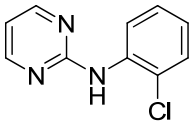


Pyrimidin-2-yl-*o*-tolyl-amine (1j)[3]**:** Following the same procedure as for **1d** with *o*-methylaniline (642.9 mg, 6.0 mmol), 2-chloro-pyrimidine (572.5 mg, 5.0 mmol), and acetic acid (300.3 mg, 5.0 mmol) in 1,4-dioxane (12 mL) for 25 h to give **1j** as white solid (493.3 mg, 53%). M.p. 88-90 ^{o}C; IR (KBr, cm^{-1}): 3444, 3230, 1583, 1257, 752, 639; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.40 (d, *J* = 5.0 Hz, 2H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.22-7.26 (m, 3H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.72 (t, *J* = 5.0 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.6, 158.1, 137.1, 130.6, 129.8, 126.7, 124.3, 122.7, 122.2, 18.2; LC-MS (ESI) m/z 186.1 [M^+H].

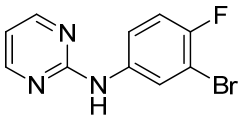


(2-Methoxy-phenyl)-pyrimidin-2-yl-amine (1k)[3]**:** Following the same procedure as for **1d** with *o*-methoxyaniline (738.9 mg, 6.0 mmol), 2-chloro-pyrimidine (572.5 mg, 5.0 mmol), and acetic acid (300.3 mg, 5.0 mmol) in 1,4-dioxane (12 mL) for 18 h to give **1k** as yellow solid (382.7 mg, 38%). M.p. 54-56 ^{o}C; IR (KBr, cm^{-1}): 3385, 2998, 1581, 1245, 749, 583; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.42-8.45 (m, 3H), 8.05 (br, 1H), 7.00-7.01 (m, 2H), 6.90-6.92 (m, 1H), 6.73 (t, *J* = 5.0,

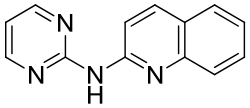
1H), 3.91 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.9, 157.9, 148.0, 129.0, 122.0, 120.9, 118.9, 112.3, 110.0, 55.7; LC-MS (ESI) m/z 202.1 [M^+H].



(2-Chloro-phenyl)-pyrimidin-2-yl-amine (1l)[4]**:** To an oven-dried flask containing 2-phenyl-pyrimidine (872.2 mg, 5.0 mmol), *N*-chlorosuccinimide (815.8 mg, 6.0 mg), $Pd(OAc)_2$ (59.9 mg, 0.25 mmol) were added in HOAc (50 mL). The reaction mixture was stirred at 110 °C for 17 h and monitored by TLC. Upon completion, the reaction mixture was extracted with ethyl acetate (3×30 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel and then recrystallization to give **1l** as white solid (404.4 mg, 39%). M.p. 94-96 °C; IR (KBr, cm^{-1}): 3445, 3226, 1596, 1289, 798, 600; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.47-8.46 (m, 3H), 7.85 (br, 1H), 7.40 (d, *J* = 7.0 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.00 (t, *J* = 5.0 Hz, 1H), 6.81 (t, *J* = 5.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.7, 158.0, 136.0, 129.2, 127.4, 122.9, 122.7, 120.5, 113.3; LC-MS (ESI) m/z 208.1 [M^+H (^{37}Cl)], 206.1 [M^+H (^{35}Cl)].

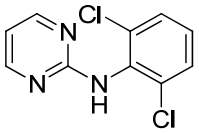


(3-Bromo-4-fluoro-phenyl)-pyrimidin-2-yl-amine (1m): Following the same procedure as for **1d** with 3-bromo-4-fluoro-phenylamine (912.1 mg, 4.8 mmol), 2-chloro-pyrimidine (458.0 mg, 4.0 mmol), and acetic acid (24.2 mg, 4.0 mmol) in 1,4-dioxane (9.6 mL) for 23 h to give **1m** as white solid (701.9 mg, 65%). M.p. 156-158 °C; IR (KBr, cm^{-1}): 3440, 3263, 1614, 1253, 798, 556 cm^{-1}; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.44 (d, *J* = 4.5 Hz, 2H), 7.98 (dd, $^4J_{F\text{-}H}$ = 6.0 Hz, $^4J_{H\text{-}H}$ = 2.5 Hz, 1H), 7.74 (br, 1H), 7.45-7.42 (m, 1H), 7.08 (t, *J* = 8.5 Hz, 1H), 6.78 (t, *J* = 5.0, 1H); ^{19}F NMR ($CDCl_3$, 470 MHz): δ -115.0 (m, Ar-F); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.5, 158.0, 155.0 (d, $^1J_{C\text{-}F}$ = 237.5 Hz), 136.2 (d, $^4J_{C\text{-}F}$ = 3.8 Hz), 124.4, 120.1 (d, $^3J_{C\text{-}F}$ = 6.3 Hz), 116.3 (d, $^2J_{C\text{-}F}$ = 23.8 Hz), 112.9, 108.9 (d, $^2J_{C\text{-}F}$ = 21.3 Hz); EI-MS m/z (%): 269 (62) [M^+ (^{81}Br)], 267 (64) [M^+ (^{79}Br)]; HRMS (EI) calcd for $C_{10}H_6BrFN_3$ [M-H]$^+$ 265.9729, found 265.9728.

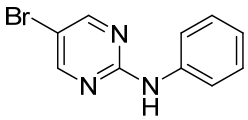


Pyrimidin-2-yl-quinolin-2-yl-amine (1n)[5]**:** To an oven-dried flask containing 2-chloroquinoline (589.0 mg, 3.6 mmol), 2-aminopyrimidine (285.3 mg, 3.0 mg), $Pd_2(dba)_3$ (41.2 mg, 0.045 mmol), DPPF (49.9 mg, 0.09 mmol) and *t*-BuOK (403.9 mg, 3.6 mmol) were added in toluene (30 mL). The reaction mixture was stirred at 80 °C for 27 h and monitored by TLC. Upon completion, the mixture was extracted with ethyl acetate (3×30 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel and then recrystallization to give **1n** as white solid (85 mg, 13%). M.p. 180-182 °C; IR (KBr, cm^{-1}): 3444, 3038, 1610, 1503, 1449, 1427, 1334, 817, 737; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 9.48 (br, 1H), 8.69-8.67 (m, 3H), 8.14 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 8.0

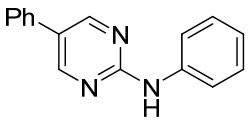
Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.64 (td, *J* = 7.5, 1.5 Hz, 1H), 7.39 (td, *J* = 7.5, 0.5 Hz, 1H), 6.88 (t, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.5, 158.2, 152.4, 138.0, 129.8, 127.5, 127.1, 125.4, 124.2, 114.1, 113.8; LC-MS (ESI) m/z 223.1 [M^+H].



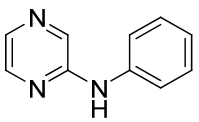
(2,6-Dichloro-phenyl)-pyrimidin-2-yl-amine (1o)[6]**:** Following the same procedure as for **1l** with 2-phenyl-pyrimidine (872.2 mg, 5.0 mmol), *N*-chlorosuccinimide (815.8 mg, 6.0 mg), $Pd(OAc)_2$ (59.9 mg, 0.25 mmol) in HOAc (50 mL) for 17 h to give **1o** as white solid (244.0 mg, 20%). M.p. 172-174 °C; IR (KBr, cm^{-1}): 3453, 3063, 1589, 1519, 1445, 1413, 1250, 784; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.37 (d, *J* = 5.0 Hz, 2H), 7.98 (br, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 8.5, 1H), 6.71 (t, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.6, 158.2, 134.2, 133.9, 128.6, 127.8, 112.7; EI-MS m/z (%): 241 (1) [M^+ (^{37}Cl, ^{35}Cl)], 239 (3) [M^+ (2×^{35}Cl)], 204 (100).



(5-Bromo-pyrimidin-2-yl)-phenyl-amine (1p)[7]**:** To an oven-dried flask containing 5-bromo-2-chloro-pyrimidine (580.2 mg, 3.0 mmol), aniline (279.6 mg, 3.0 mmol) in *n*-butanol (3 mL) were added. The reaction mixture was stirred at 110 °C for 21 h and monitored by TLC. Upon completion, the mixture was filtered through a thin pad of celite, and the residue was purified by recrystallization to give **1p** as yellow solid (418.2 mg, 56%). M.p. 122-124 °C; IR (KBr, cm^{-1}): 3442, 3264, 1608, 1574, 1529, 1448, 1430, 753; ^{1}H NMR (d_6-Acetone, 500 MHz): δ 8.89 (br, 1H), 8.53 (s, 2H), 7.81 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 8.0 Hz, 2H), 7.03 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (d_6-Acetone, 125 MHz): δ 158.8, 158.1, 140.0, 128.6, 122.2, 119.2, 107.8; LC-MS (ESI) m/z 252.0 [M^+H (^{81}Br)], 250.0 [M^+H (^{79}Br)].

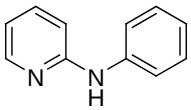


Phenyl-(5-phenyl-pyrimidin-2-yl)-amine (1q)[8]**:** Following the same procedure as for **1p** with 2-chloro-5-phenyl-pyrimidine (190.6 mg, 1.0 mmol) and aniline (186.4 mg, 2.0 mmol) in *n*-butanol (1.0 mL) for 18 h to give **1q** as white solid (137.3 mg, 56%). M.p. 166-168 °C; IR (KBr, cm^{-1}): 3453, 3269, 3029, 1619, 1529, 1451, 756, 698; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.67 (s, 2H), 7.74 (br, 1H), 7.66 (d, *J* = 8.0Hz, 2H), 7.53-7.47 (m, 4H), 7,41-7.36 (m, 3H), 7.09 (t, *J* = 7.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 158.8, 155.9, 139.0, 134.8, 129.3, 129.1, 127.9, 126.1, 125.7, 123.1, 119.7; EI-MS m/z (%): 247 (64) [M^+], 246 (100).

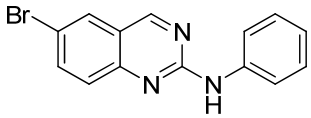


Phenyl-pyrazin-2-yl-amine (1r)[9]**:** Following the same procedure as for **1p** with 2-chloropyrazine (343.5 mg, 3.0 mmol) and aniline (279.6 mg, 3.0 mmol) in *n*-butanol (3.0 mL) for 52 h to give **1r** as yellow solid (245.4 mg, 48%). M.p. 130-132 °C; IR (KBr, cm^{-1}): 3473, 3283,

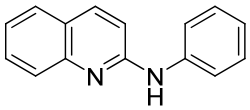
3101, 1626, 1584, 1521, 1498, 1352, 752; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.25 (s, 1H), 8.10 (d, *J* = 1.5 Hz, 1H), 7.96 (d, *J* = 3.0 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.35 (t, *J* = 8.0 Hz, 2H), 7.10 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 152.4, 141.9, 139.2, 134.7, 133.0, 129.4, 123.7, 120.4; EI-MS m/z (%): 171 (72) [M^+], 170 (100).



Phenyl-pyridin-2-yl-amine (1s)[3]**:** To an oven-dried flask containing 2-bromopyridine (4.74 g, 30.0 mmol), aniline (2.794 g, 3.0 mmol) was added. The reaction mixture was stirred at 160 ^{o}C for 7 h and monitored by TLC. Upon completion, saturate $NaHCO_3$ was added, and the reaction mixture was extracted with ethyl acetate (3×30 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel to give **1s** as white solid (4.954 g, 97%). M.p. 106-108 ^{o}C; IR (KBr, cm^{-1}): 3450, 3224, 1590, 1574, 1464, 1444, 1327, 770, 670; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.17 (d, *J* = 4.0 Hz, 1H), 7.51 (td, *J* = 5.5, 2.0 Hz, 1H), 7.36-7.32 (m, 4H), 7.09-7.05 (m, 1H), 6.98 (s, 1H), 6.89 (d, *J* = 8.5 Hz, 1H), 6.75-6.73 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 156.1, 148.2, 140.5, 137.9, 129.3, 122.9, 120.5, 114.9, 108.2; LC-MS (ESI) m/z 171.1 [M^+H].



(6-Bromo-quinazolin-2-yl)-phenyl-amine (1t)[10]**:** Following the same procedure as for **1d** with aniline (139.7 mg, 1.5 mmol), 2,6-dibromoquinazoline (287.9 mg, 1.0 mmol), and acetic acid (60.1 mg, 1.0 mmol) in 1,4-dioxane (3.0 mL) for 22 h to give **1t** as yellow solid (208.0 mg, 70%). M.p. 154-156 ^{o}C; IR (KBr, cm^{-1}): 3442, 3279, 1601, 1583, 1543, 1446, 1353, 747; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 9.02 (s, 1H), 7.88 (d, *J* = 2.0 Hz, 1H), 7.82-7.79 (m, 3H), 7.63 (d, *J* = 9.0 Hz, 1H), 7.55 (br, 1H), 7.39 (t, *J* = 8.0 Hz, 2H), 7.10 (t, *J* = 7.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.9, 156.8, 150.1, 139.2, 137.7, 129.5, 129.0, 128.0, 123.0, 121.7, 119.3, 116.5; EI-MS m/z (%): 301 (1) [M^+ (^{81}Br)], 299 (1) [M^+ (^{79}Br)], 57 (100).



Phenyl-quinolin-2-yl-amine (1u)[9]**:** To an oven-dried flask containing 2-chloroquinoline (327.2 mg, 2.0 mmol), aniline (186.2 mg, 2.0 mmol) were added in ethanol (10 mL). The reaction mixture was stirred under reflux for 10 h and monitored by TLC. Upon completion, the reaction mixture was extracted with ethyl acetate (3×10 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel to give **1u** as white solid (409.2 mg, 93%). M.p. 94-96 ^{o}C; IR (KBr, cm^{-1}): 3404, 3050, 1620, 1597, 1533, 1401, 823, 752; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.95 (d, *J* = 9.0 Hz, 1H), 7.79 (d, *J* = 8.5 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.61 (td, *J* = 8.0, 1.5 Hz, 1H), 7.55 (dd, *J* = 8.5, 1.0 Hz, 2H), 7.37 (t, *J* = 8.5 Hz, 2H), 7.31 (td, *J* = 8.0, 1.0 Hz, 1H), 7.12 (tt, *J* = 7.0, 1.5 Hz, 1H), 7.00 (d, *J* = 9.0 Hz, 1H), 2.50 (br, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 154.5, 147.6,

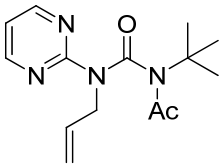
140.2, 137.8, 129.9, 129.3, 127.5, 126.7, 124.2, 123.2, 123.1, 120.6, 111.8; LC-MS (ESI) m/z 221.0 [M^+H].

4. Synthesis of copper carboxylates

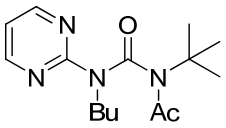
General procedure: To a round-bottom flask, sodium carboxylates was dissolved in water, and aqueous $CuSO_4$ was added. The reaction mixture was stirred at room temperature for 2 h. Upon completion, the reaction mixture filtered and washed with water and then dried in vacuum to give copper complex as copper (II) laurate monohydrate (**3b**),[11] copper (II) phenylacetate (**3c**),[12] copper (II) benzoate monohydrate (**3d**),[13] copper (II) crotonate monohydrate (**3f**),[14] and copper (II) phenylpropionate multihydrate (**3g**).[15]

Copper (II) cinnamate monohydrate (3e)[16]: To a round-bottom flask, A solution of $CuCl_2 \cdot 2H_2O$ in ethanol was added to a solution of cinnamic acid and Et_3N were added in ethanol. The reaction mixture was stirred at room temperature for 2 h. Upon completion, the reaction mixture filtered and washed with water and then dried in vacuum to give copper (II) cinnamate monohydrate (**3e**).

5. Synthesis and characterization of ureas

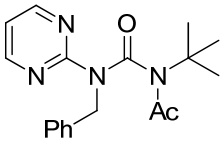


1-Acetyl-3-allyl-1-*tert*-butyl-3-pyrimidin-2-yl-urea (4a): To an oven-dried flask containing **1a** (67.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol) and *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) was added in toluene (3.0 mL). The reaction mixture was stirred at 110 ^oC for 36 h in the presence of air which was dried through a calcium chloride tube and monitored by TLC. Upon completion, the reaction mixture was washed with dilute ammonia and extracted with CH_2Cl_2 (3×10 mL). The combined organic phase was washed with brine and dried over Na_2SO_4. After that, the solid was filtered off through a thin pad of celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel to give **4a** as white solid (89.8 mg, 65%). M.p. 50-52 ^oC; IR (KBr, cm^{-1}): 2979, 2964, 1675, 1568, 1415, 1315, 825; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.69 (d, J = 4.5 Hz, 2H), 7.16 (t, J = 4.5 Hz, 1H), 5.96-5.88 (m, 1H), 5.24 (dd, J = 17.0, 1.0 Hz, 1H) 5.12 (dd, J = 10.0, 1.0 Hz, 1H), 4.68 (m, 2H), 2.18 (s, 3H), 1.23 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.9, 160.2, 158.3, 156.4, 132.0, 118.6, 118.4, 58.3, 50.8, 27.6, 25.3; LC-MS (ESI) m/z 299.1 [M^+Na]; Anal. Calcd. For $C_{14}H_{20}N_4O_2$: C, 60.85; H, 7.30; N, 20.28. Found: C, 60.71; H, 7.29; N, 20.15.

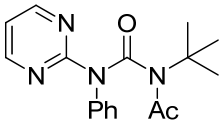


1-Acetyl-3-butyl-1-*tert*-butyl-3-pyrimidin-2-yl-urea (4b): Following the same procedure as for **4a** with **1b** (75.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 66 h to give **4b** as yellow liquid (97.6 mg, 67%). IR (KBr,

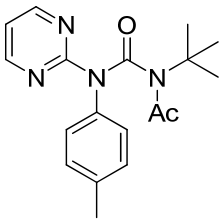
cm^{-1}): 2961, 2933, 1693, 1670, 1565, 1417, 803; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.70 (d, *J* = 4.5 Hz, 2H), 7.16 (t, *J* = 5.0 Hz, 1H), 4.06-4.03 (m, 2H), 2.19 (s, 3H), 1.68-1.54 (m, 2H), 1.36-1.28 (m, 2H), 1.21 (s, 9H), 0.88 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.9, 160.5, 158.3, 156.4, 118.6, 58.0, 48.5, 29.7, 27.5, 25.3, 20.1, 13.7; LC-MS (ESI) m/z 293.1 [M$^+$H]; HRMS (ESI) calcd for $C_{15}H_{24}N_4NaO_2$ [M$^+$Na] 315.1797, found 315.1778.



1-Acetyl-3-benzyl-1-*tert*-butyl-3-pyrimidin-2-yl-urea (4c)[17]: Following the same procedure as for **4a** with **1c** (92.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 19 h to give **4c** as white solid (105.2 mg, 65%). M.p. 46-48 ^{o}C; IR (KBr, cm^{-1}): 2979, 2929, 1694, 1670, 1565, 1416, 1317, 700; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.66 (d, *J* = 5.0 Hz, 2H), 7.35-7.31 (m, 2H), 7.26-7.21 (m, 3H), 7.11 (t, *J* = 5.0 Hz, 1H), 5.37 (A of AB, *J* = 14.5 Hz, 1H), 5.26 (B of AB, *J* = 15.0 Hz, 1H), 2.16 (s, 3H), 1.24 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.9, 160.1, 158.3, 156.9, 136.3, 128.5, 128.3, 127.6, 118.6, 58.4, 51.6, 27.6, 25.4; LC-MS (ESI) m/z 349.1 [M$^+$Na]; Anal. Calcd. For $C_{18}H_{22}N_4O_2$: C, 66.24; H, 6.79; N, 17.17. Found: C, 66.20; H, 6.78; N, 17.28.

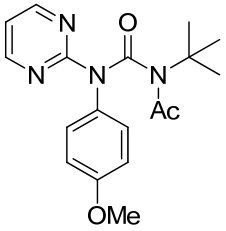


1-Acetyl-1-*tert*-butyl-3-phenyl-3-pyrimidin-2-yl-urea (4d): Following the same procedure as for **4a** with **1d** (85.5 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 25 h to give **4d** as white solid (140.4 mg, 90%). M.p. 82-83 ^{o}C; IR (KBr, cm^{-1}): 2979, 2923, 1704, 1668, 1566, 1512, 1413, 1297, 1021, 763, 734; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.73 (d, *J* = 5.0 Hz, 2H), 7.45-7.42 (m, 2H), 7.36-7.33 (m, 3H), 7.22 (t, *J* = 5.0 Hz, 1H), 2.39 (s, 3H), 1.33 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.1, 160.8, 158.9, 156.2, 140.4, 129.5, 128.0, 127.0, 119.4, 58.8, 27.7, 25.6; EI-MS m/z (%): 312 (1) [M$^+$], 170 (100); Anal. Calcd. For $C_{17}H_{20}N_4O_2$: C, 65.37; H, 6.45; N, 17.94. Found: C, 65.57; H, 6.47; N, 18.14.

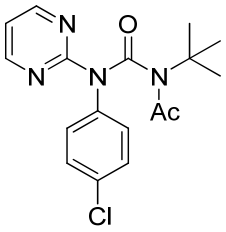


1-Acetyl-1-*tert*-butyl-3-pyrimidin-2-yl-3-p-tolyl-urea (4e)[17]: Following the same procedure as for **4a** with **1e** (92.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 27 h to give **4e** as yellow solid (156.8 mg, 96%). M.p. 110-111 ^{o}C; IR (KBr, cm^{-1}): 3007, 2979, 2924, 1704, 1668, 1565, 1513, 1413, 1298, 763, 734; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.72 (d, *J* = 5.0 Hz, 2H), 7.23 (s, 4H), 7.20 (t, *J* = 5.0Hz, 1H), 2.38 (s, 3H), 2.36 (s, 3H), 1.33 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.1, 160.9, 158.8, 156.3, 138.0, 137.8, 130.0, 126.8, 119.2, 58.7, 27.7, 25.6, 21.2; EI-MS m/z (%): 326 (4) [M$^+$], 184 (100); Anal.

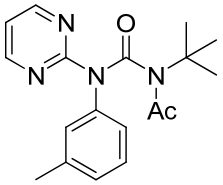
Calcd. For $C_{18}H_{22}N_4O_2$: C, 66.24; H, 6.79; N, 17.17. Found: C, 66.36; H, 6.73; N, 17.27.



1-Acetyl-1-*tert*-butyl-3-(4-methoxy-phenyl)-3-pyrimidin-2-yl-urea (4f)[17]: Following the same procedure as for **4a** with **1f** (100.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 25 h to give **4f** as white solid (145.2 mg, 85%). M.p. 124-126 ^oC; IR (KBr, cm^{-1}): 3010, 2977, 2933, 1699, 1672, 1565, 1510, 1411, 1295, 828; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.72 (d, J = 5.0 Hz, 2H), 7.28 (AA' of AA'BB', J = 9.5 Hz, 2H), 7.20 (t, J = 5.0 Hz, 1H), 6.93 (BB' of AA'BB', J = 9.0 Hz, 2H), 3.80 (s, 3H), 2.38 (s, 3H), 1.32 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.1, 160.9, 159.0, 158.9, 156.4, 133.0, 128.3, 119.3, 114.7, 58.7, 55.5, 27.7, 25.6; LC-MS (ESI) m/z 365.2 [M^+Na]; Anal. Calcd. For $C_{18}H_{22}N_4O_3$: C, 63.14; H, 6.48; N, 16.36. Found: C, 63.26; H, 6.67; N, 16.23.

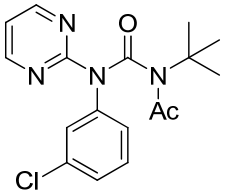


1-Acetyl-1-*tert*-butyl-3-(4-chloro-phenyl)-3-pyrimidin-2-yl-urea (4g): Following the same procedure as for **4a** with **1g** (102.8 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 20 h to give **4g** as yellow solid (124.9 mg, 72%). M.p. 151-152 ^oC; IR (KBr, cm^{-1}): 3007, 2979, 2922, 1705, 1673, 1566, 1490, 1416, 1309, 835; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.72 (d, J = 5.0 Hz, 2H), 7.38 (AA' of AA'BB', J = 8.5 Hz, 2H), 7.27 (BB' of AA'BB', J = 8.5 Hz, 2H), 7.23 (t, J = 4.5 Hz, 1H), 2.36 (s, 3H), 1.31 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.0, 160.5, 159.0, 156.2, 138.8, 133.8, 129.6, 128.4, 119.6, 58.9, 27.7, 25.6; LC-MS (ESI) m/z 371.1 [M^+Na (^{37}Cl)], 369.1 [M^+Na (^{35}Cl)]; Anal. Calcd. For $C_{17}H_{19}ClN_4O_2$: C, 58.87; H, 5.52; N, 16.15. Found: C, 58.84; H, 5.45; N, 15.85.

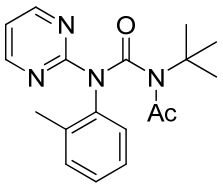


1-Acetyl-1-*tert*-butyl-3-pyrimidin-2-yl-3-*m*-tolyl-urea (4h)[17]: Following the same procedure as for **4a** with **1h** (92.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 22 h to give **4h** as white solid (142.3 mg, 87%). M.p. 76-78 ^oC; IR (KBr, cm^{-1}): 3009, 2968, 2922, 1706, 1673, 1564, 1409, 727; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.73 (d, J = 5.0 Hz, 2H), 7.31 (t, J = 7.5 Hz, 1H), 7.21 (t, J = 5.0 Hz, 1H), 7.16-7.12 (m, 3H), 2.39 (s, 3H), 2.36 (s, 3H), 1.33 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.1, 160.9, 158.9, 156.2, 140.2, 139.5, 129.3, 128.9, 127.5, 124.0, 119.4, 58.8, 27.7, 25.6, 21.4; LC-MS (ESI) m/z 349.1

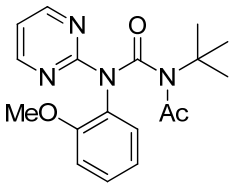
[M^+Na]; Anal. Calcd. For $C_{18}H_{22}N_4O_2$: C, 66.24; H, 6.79; N, 17.17. Found: C, 66.50; H, 6.88; N, 17.35.



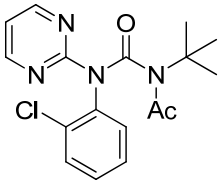
1-Acetyl-1-*tert*-butyl-3-(3-chloro-phenyl)-3-pyrimidin-2-yl-urea (4i)[17]: Following the same procedure as for **4a** with **1i** (102.8 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 25 h to give **4i** as yellow solid (160.4 mg, 93%). M.p. 122-124 ^oC; IR (KBr, cm^{-1}): 2968, 2925, 1709, 1661, 1565, 1411, 1311, 785, 704; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.74 (d, J = 4.5 Hz, 2H), 7.38-7.31 (m, 3H), 7.26-7.24 (m, 2H), 2.37 (s, 3H), 1.32 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.0, 160.4, 159.0, 156.2, 141.3, 134.9, 130.3, 128.2, 127.3, 125.3, 119.7, 58.9, 27.7, 25.6; LC-MS (ESI) m/z 371.1 [M^+Na (^{37}Cl)], 369.1 [M^+Na (^{35}Cl)]; Anal. Calcd. For $C_{17}H_{19}ClN_4O_2$: C, 58.87; H, 5.52; N, 16.15. Found: C, 58.81; H, 5.46; N, 16.01.



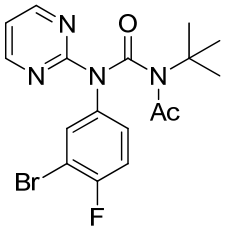
1-Acetyl-1-*tert*-butyl-3-pyrimidin-2-yl-3-*o*-tolyl-urea (4j): Following the same procedure as for **4a** with **1j** (92.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 23 h to give **4j** as white solid (129.8 mg, 80%). M.p. 102-104 ^oC; IR (KBr, cm^{-1}): 3007, 2969, 2925, 1700, 1667, 1566, 1409, 1310, 730; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.70 (d, J = 5.0 Hz, 2H), 7.51 (s, 1H), 7.32-7.26 (m, 3H), 7.17 (t, J = 5.0 Hz, 1H), 2.41 (s, 3H), 2.22 (s, 3H), 1.35 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.2, 160.4, 158.6, 156.2, 139.1, 136.2, 131.4, 128.9, 127.0, 118.9, 58.8, 27.9, 25.7, 18.3; LC-MS (ESI) m/z 349.1 [M^+Na]; Anal. Calcd. For $C_{18}H_{22}N_4O_2$: C, 66.24; H, 6.79; N, 17.17. Found: C, 66.12; H, 6.75; N, 17.04.



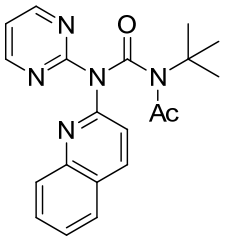
1-Acetyl-1-*tert*-butyl-3-(2-methoxy-phenyl)-3-pyrimidin-2-yl-urea (4k): Following the same procedure as for **4a** with **1k** (100.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 24 h to give **4k** as white solid (129.1 mg, 76%). M.p. 132-133 ^oC; IR (KBr, cm^{-1}): 2972, 2928, 1693, 1671, 1564, 1412, 1313, 750; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.66 (d, J = 5.0 Hz, 2H), 7.39 (d, J = 8.0 Hz, 1H), 7.35 (t, J = 8 Hz, 1H), 7.12 (t, J = 4.5 Hz, 1H), 7.04 (t, J = 7.5 Hz, 1H), 6.98 (d, J = 8.0 Hz, 1H), 3.73 (s, 3H), 2.37 (s, 3H), 1.35 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.2, 160.7, 158.3, 155.9, 155.1, 129.8, 129.3, 129.2, 121.0, 118.5, 112.6, 58.6, 55.8, 27.8, 25.5; LC-MS (ESI) m/z 365.1 [M^+Na]; Anal. Calcd. For $C_{18}H_{22}N_4O_3$: C, 63.14; H, 6.48; N, 16.36. Found: C, 63.09; H, 6.49; N, 16.29.



1-Acetyl-1-*tert*-butyl-3-(2-chloro-phenyl)-3-pyrimidin-2-yl-urea (4l): Following the same procedure as for **4a** with **1l** (102.8 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 21 h to give **4l** as white solid (135.9 mg, 78%). M.p. 132-134 ^oC; IR (KBr, cm^{-1}): 2980, 2915, 1703, 1679, 1567, 1411, 1304, 732; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.68 (d, J = 5.0 Hz, 2H), 7.60 (d, J = 8.0 Hz, 1H), 7.47-7.41 (m, 2H), 7.36 (dt, J = 8.0, 1.5 Hz, 1H), 7.16 (t, J = 5.0 Hz, 1H), 2.39 (s, 3H), 1.37 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.8, 158.5, 158.4, 156.3, 137.8, 132.5, 130.9, 130.6, 129.8, 127.8, 118.7, 58.9, 27.9, 25.7; LC-MS (ESI) m/z 371.1 [M^+Na (^{37}Cl)], 369.1 [M^+Na (^{35}Cl)]; Anal. Calcd. For $C_{17}H_{19}ClN_4O_2$: C, 58.87; H, 5.52; N, 16.15. Found: C, 58.60; H, 5.52; N, 15.92.

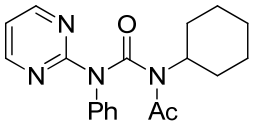


1-Acetyl-3-(3-bromo-4-fluoro-phenyl)-1-*tert*-butyl-3-pyrimidin-2-yl-urea (4m)[17]: Following the same procedure as for **4a** with **1m** (142.6 mg, 0.53 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 22 h to give **4m** as white solid (198.0 mg, 91%). M.p. 88-90 ^oC; IR (KBr, cm^{-1}): 2981, 2925, 1707, 1676, 1566, 1412, 1309, 730; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.74 (d, J = 4.5 Hz, 2H), 7.56 (dd, $^4J_{F\text{-}H}$ = 6.0, $^4J_{H\text{-}H}$ = 3.0 Hz, 1H), 7.33-7.30 (m, 1H), 7.26 (t, J = 5.0 Hz, 1H), 7.18 (t, J = 8.5 Hz, 1H), 2.36 (s, 3H), 1.31 (s, 9H); ^{19}F NMR ($CDCl_3$, 470 MHz): δ -107.2 (m, Ar-F); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.9, 160.3, 159.0, 158.4 (d, $^1J_{C\text{-}F}$ = 247.5 Hz), 156.3, 136.8 (d, $^3J_{C\text{-}F}$ = 3.8 Hz), 132.4, 128.0 (d, $^3J_{C\text{-}F}$ = 7.5 Hz), 119.7, 117.0 (d, $^2J_{C\text{-}F}$ = 23.8 Hz), 109.5 (d, $^2J_{C\text{-}F}$ = 22.5 Hz), 58.9, 27.7, 25.6; LC-MS (ESI) m/z 433.0 [M^+Na (^{81}Br)], 431.0 [M^+Na (^{79}Br)]; Anal. Calcd. For $C_{17}H_{18}BrFN_4O_2$: C, 49.89; H, 4.43; N, 13.69. Found: C, 50.09; H, 4.64; N, 13.77.

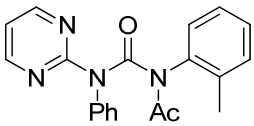


1-Acetyl-1-*tert*-butyl-3-pyrimidin-2-yl-3-quinolin-2-yl-urea (4n): Following the same procedure as for **4a** with **1n** (77.8 mg, 0.35 mmol), $Cu(OAc)_2 \cdot H_2O$ (139.8 mg, 0.7 mmol), *tert*-butyl isocyanide (90 mg, 1.05 mmol) in *m*-xylene at 130 ^oC with O_2 balloon for 11 h to give **4n** as white solid (39.1 mg, 31%) together with recovered **1n** (34.1 mg, 56% conversion). M.p. 148-150 ^oC; IR (KBr, cm^{-1}): 2976, 1688, 1670, 1566, 1404, 765; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.76 (d, J = 5.0 Hz, 2H), 8.25 (d, J = 8.5 Hz, 1H), 7.82 (d, J = 8.0 Hz, 2H), 7.70 (d, J = 9.0 Hz,

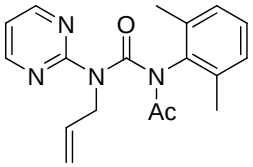
1H), 7.64 (td, *J* = 7.0, 1.5 Hz, 1H), 7.52 (td, *J* = 7.5, 1.0 Hz, 1H), 7.26 (t, *J* = 4.5 Hz, 1H), 2.46 (s, 3H), 1.39 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.2, 160.7, 158.8, 156.5, 152.9, 147.0, 138.4, 130.0, 129.0, 127.4, 127.0, 126.9, 119.4, 118.6, 59.4, 27.9, 25.9; LC-MS (ESI) m/z 364.0 [M^+H]; HRMS (ESI) m/z Calcd. for $C_{20}H_{22}N_5O_2$ [M^+H] 364.1773, found 364.1768.



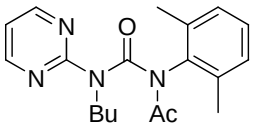
1-Acetyl-1-cyclohexyl-3-phenyl-3-pyrimidin-2-yl-urea (5a)[17]: Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), cyclohexyl isonitrile (163.8 mg, 1.5 mmol) in toluene for 23 h to give **5a** as white solid (134.3 mg, 79%). M.p. 112-114 °C; IR (KBr, cm^{-1}): 2967, 2930, 1707, 1688, 1564, 1410, 1226, 702; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.65 (d, *J* = 4.5 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.25 (d, *J* = 7.5 Hz, 2H), 7.12 (t, *J* = 5.0 Hz, 1H), 3.96-3.91 (m, 1H), 2.30 (s, 3H), 1.74-1.57 (m, 7H), 1.27-1.06 (m, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.9, 161.4, 158.6, 157.1, 140.8, 129.5, 127.8, 127.1, 118.2, 58.3, 30.1, 26.3, 25.4, 24.7; EI-MS m/z (%): 338 (3) [M^+]; HRMS (EI) m/s calcd for $C_{19}H_{22}N_4O_2$ 338.1743, found 338.1742.



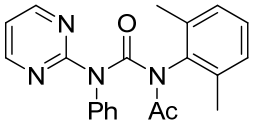
1-Acetyl-3-phenyl-3-pyrimidin-2-yl-1-*o*-tolyl-urea (5c): Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), 2-methylisonitrile (175.7 mg, 1.5 mmol) in toluene for 19 h to give **5c** as yellow liquid (86.3 mg, 50%). IR (KBr, cm^{-1}): 3039, 1702, 1594, 1564, 1410, 1242, 724; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.55 (d, *J* = 4.5 Hz, 2H), 7.29-7.28 (m, 3H), 7.14 (t, *J* = 7.0 Hz, 1H), 7.07-7.04 (m, 3H), 6.99 (t, *J* = 5.0 Hz, 1H), 6.89 (d, *J* = 4.5 Hz, 2H), 2.45 (s, 3H), 1.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 172.9, 161.4, 158.3, 157.1, 139.9, 137.0, 136.7, 130.8, 129.3, 128.3, 128.1, 127.7, 127.6, 126.4, 117.1, 25.0, 17.9; EI-MS m/z (%): 346 (5) [M^+], 170 (100); HRMS (EI): m/s Calcd. for $C_{20}H_{18}N_4O_2$: 346.1430, found: 346.1428.



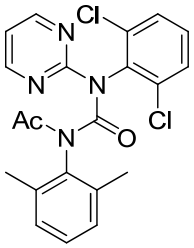
1-Acetyl-3-allyl-1-(2,6-dimethyl-phenyl)-3-pyrimidin-2-yl-urea (5d)[17]: Following the same procedure as for **4a** with **1d** (72.4 mg, 0.54 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), 2,6-xylyl isocyanide (196.8 mg, 1.5 mmol) in toluene for 13 h to give **5d** as white solid (157.8 mg, 90%). M.p. 82-84 °C; IR (KBr, cm^{-1}): 2956, 2916, 1706, 1677, 1562, 1442, 1233, 808, 764; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.53 (d, *J* = 4.5 Hz, 2H), 7.13 (A of ABB', *J* = 7.5 Hz, 1H), 7.06 (BB' of ABB', *J* = 7.5 Hz, 2H), 6.93 (t, *J* = 5.0 Hz, 1H), 6.00-5.92 (m, 1H), 5.27 (dd, *J* = 18.0, 1.5 Hz, 1H), 5.09 (dd, *J* = 10.5, 1.5 Hz, 1H), 4.76 (d, *J* = 5.5 Hz, 2H), 2.31 (s, 6H), 1.88 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 172.6, 160.7, 157.6, 154.1, 137.7, 136.8, 133.5, 128.8, 128.5, 116.9, 116.4, 51.1, 24.8, 18.7; LC-MS (ESI) m/z 325.2 [M^+H]; Anal. Calcd. For $C_{18}H_{20}N_4O_2$: C, 66.65; H, 6.21; N, 17.27. Found: C, 66.65; H, 6.25; N, 16.97.



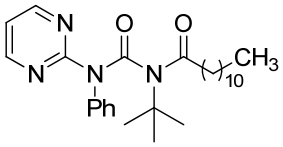
1-Acetyl-3-butyl-1-(2,6-dimethyl-phenyl)-3-pyrimidin-2-yl-urea (5e)[17]: Following the same procedure as for **4a** with **1d** (80.6 mg, 0.53 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), 2,6-xylyl isocyanide (196.8 mg, 1.5 mmol) in toluene for 13 h to give **5e** as white solid (158.1 mg, 88%). M.p. 106-108 ^oC; IR (KBr, cm^{-1}): 2960, 2931, 1702, 1676, 1561, 1423, 1246, 806, 782; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.51 (d, J = 5.0 Hz, 2H), 7.12 (t, J = 7.5 Hz, 1H), 7.04 (d, J = 7.5 Hz, 2H), 6.92 (t, J = 5.0 Hz, 1H), 4.12 (t, J = 7.5 Hz, 2H), 2.30 (s, 6H), 1.90 (s, 3H), 1.62 (quint, J = 7.5 Hz, 2H), 1.33 (sext, J = 7.5 Hz, 2H), 0.88 (t, J = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 172.6, 160.9, 157.6, 154.5, 137.7, 136.8, 128.8, 128.4, 116.2, 49.1, 30.7, 24.8, 20.1, 18.7, 13.9; LC-MS (ESI) m/z 341.2 [M^+H]; Anal. Calcd. For $C_{19}H_{24}N_4O_2$: C, 67.04; H, 7.11; N, 16.46. Found: C, 66.86; H, 7.08; N, 16.19.



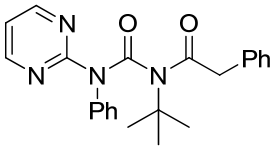
1-Acetyl-1-(2,6-dimethyl-phenyl)-3-phenyl-3-pyrimidin-2-yl-urea (5f): Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), 2,6-xylyl isocyanide (196.8 mg, 1.5 mmol) in toluene for 13 h to give **5f** as white solid (167.2 mg, 93%). M.p. 148-150 ^oC; IR (KBr, cm^{-1}): 2920, 1718, 1684, 1578, 1563, 1419, 1238, 712; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.52 (d, J = 4.5 Hz, 2H), 7.30-7.29 (m, 3H), 7.07 (t, J = 7.5 Hz, 1H), 6.97-6.92 (m, 5H), 2.38 (s, 3H), 2.09 (s, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 173.3, 161.7, 158.0, 156.7, 139.8, 137.2, 136.3, 129.3, 128.5, 128.4, 128.3, 127.9, 116.7, 25.3, 18.5; EI-MS m/z (%): 360 (10) [M^+], 170 (100); Anal. Calcd. For $C_{21}H_{20}N_4O_2$: C, 69.98; H, 5.59; N, 15.55. Found: C, 69.90; H, 5.63; N, 15.29.



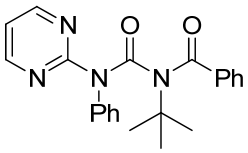
1-Acetyl-3-(2,6-dichloro-phenyl)-1-(2,6-dimethyl-phenyl)-3-pyrimidin-2-yl-urea (5g): Following the same procedure as for **4a** with **1d** (84.0 mg, 0.35 mmol), $Cu(OAc)_2 \cdot H_2O$ (140.0 mg, 0.7 mmol), 2,6-xylyl isocyanide (137.7 mg, 1.1 mmol) in toluene for 14 h to give **5g** as white solid (114.6 mg, 76%). M.p. 196-198 ^oC; IR (KBr, cm^{-1}): 3033, 2917, 1724, 1691, 1565, 1417, 1311, 1234, 782, 772; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.58 (d, J = 5.0 Hz, 2H), 7.29 (m, 2H), 7.19 (t, J = 8.0 Hz, 1H), 7.11 (t, J = 7.5 Hz, 1H), 7.02 (t, J = 4.5 Hz, 1H), 6.98 (d, J = 5.5 Hz, 2H), 2.24 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 172.8, 160.4, 158.0, 137.3, 136.3, 135.7, 129.3, 128.8, 128.7, 128.5, 117.0, 25.1, 18.5; EI-MS m/z (%): 430 [M^+ (^{37}Cl, ^{35}Cl)], 428 [M^+ ($2\times^{35}Cl$)]; HRMS (EI) m/s calcd. for $C_{21}H_{18}Cl_2N_4O_2$ 428.0807, found 428.0804.



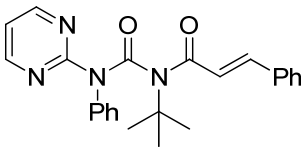
1-*tert*-Butyl-1-dodecanoyl-3-phenyl-3-pyrimidin-2-yl-urea (5i): Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), copper (II) laurate monohydrate (424.1 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 23 h to give **5i** as yellow liquid (144.8 mg, 64%) together with recovered **1d** (22.9 mg, 74% conversion). IR (KBr, cm^{-1}): 2925, 2854, 1701, 1675, 1565, 1409, 722; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.70 (d, *J* = 5.0 Hz, 2H), 7.43 (t, *J* = 8.0 Hz, 2H), 7.35-7.32 (m, 3H), 7.20 (t, *J* = 5.0 Hz, 1H), 2.77-2.74 (m, 1H), 2.59-2.58 (m, 1H), 1.70-1.66 (m, 2H), 1.35-1.25 (m, 25H), 0.87 (t, *J* = 6.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 172.9, 160.9, 158.8, 156.1, 140.4, 129.4, 127.9, 127.0, 119.3, 58.7, 37.4, 31.9, 29.7, 29.7, 29.6, 29.5, 29.4, 29.3, 27.8, 25.1, 22.7, 14.1; LC-MS (ESI) m/z 475.2 [M^+Na]; HRMS (ESI) m/s calcd for $C_{27}H_{41}N_4O_2$ [M^+H] 453.3230, found 453.3222.



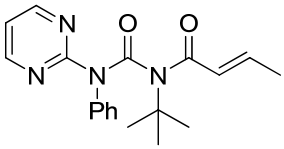
1-*tert*-Butyl-3-phenyl-1-phenylacetyl-3-pyrimidin-2-yl-urea (5j): Following the same procedure as for **4a** with **1d** (51.4 mg, 0.3 mmol), copper (II) phenylacetate monohydrate (250.4 mg, 0.75 mmol), *tert*-butyl isocyanide (74.8 mg, 0.9 mmol) in toluene at 90 °C for 41 h to give **5j** as white solid (66.2 mg, 57%) together with recovered **1d** (5.7 mg, 89% conversion). M.p. 128-130 °C; IR (KBr, cm^{-1}): 2977, 1704, 1674, 1564, 1409, 1320, 720; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.75 (d, *J* = 5.0 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.41 (d, *J* = 8.5 Hz, 2H), 7.38-7.32 (m, 5H), 7.26 (d, *J* = 6.5 Hz, 1H), 7.23 (t, *J* = 5.0 Hz, 1H), 4.25 (d, *J* = 15.5 Hz, 1H), 3.96 (d, *J* = 16.0 Hz, 1H), 1.34 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.7, 160.9, 158.9, 156.1, 140.3, 135.5, 130.0, 129.5, 128.3, 128.1, 127.0, 126.6, 119.5, 59.1, 43.8, 27.8; LC-MS (ESI) m/z 389.1 [M^+H]; Anal. Calcd. For $C_{23}H_{24}N_4O_2$: C, 71.11; H, 6.23; N, 14.42. Found: C, 71.18; H, 6.41; N, 14.44.



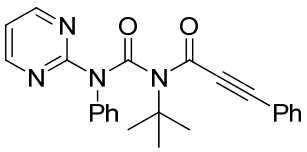
1-Benzoyl-1-*tert*-butyl-3-phenyl-3-pyrimidin-2-yl-urea (5k): Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), copper (II) benzoate monohydrate (323.8 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 33 h to give **5k** as white solid (165.2 mg, 88%). M.p. 110-111 °C; IR (KBr, cm^{-1}): 2983, 1702, 1648, 1565, 1405, 1314, 697; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.56 (d, *J* = 4.5 Hz, 2H), 7.48-7.43 (m, 3H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.28-7.21 (m, 3H), 7.04 (t, *J* = 4.5 Hz, 1H), 6.65 (d, *J* = 6.5 Hz, 2H), 1.70 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.0, 160.4, 158.1, 155.6, 140.3, 138.0, 131.0, 129.1, 128.2, 127.9, 127.7, 127.3, 117.6, 60.4, 28.7; LC-MS (ESI) m/z 375.1 [M^+H]; Anal. Calcd. For $C_{22}H_{22}N_4O_2$: C, 70.57; H, 5.92; N, 14.96. Found: C, 70.83; H, 6.13; N, 14.68.



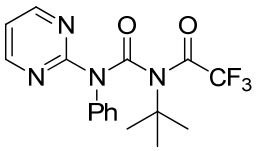
1-*tert*-Butyl-3-phenyl-1-(3-phenyl-acryloyl)-3-pyrimidin-2-yl-urea (5l): Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), copper (II) cinnamate monohydrate (375.9 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 33 h to give **5l** as white solid (157.0 mg, 78%). M.p. 146-148 ^{o}C; IR (KBr, cm^{-1}): 2974, 2930, 1693, 1664, 1567, 1410, 1193, 762, 703; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.70 (d, *J* = 5.0 Hz, 2H), 7.62 (d, *J* = 15.0 Hz, 1H), 7.58 (d, *J* = 6.5 Hz, 2H), 7.42 (t, *J* = 8.0 Hz, 2H), 7.38-7.34 (m, 6H), 7.27 (d, *J* = 14.0 Hz, 1H), 7.16 (t, *J* = 5.0 Hz, 1H), 1.48 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 165.4, 161.0, 158.8, 156.0, 142.0, 140.3, 135.3, 129.7, 129.5, 128.8, 128.2, 128.1, 127.5, 121.7, 119.1, 59.3, 28.0; LC-MS (ESI) m/z 401.1 [M^{+}H]; Anal. Calcd. For $C_{24}H_{24}N_4O_2$: C, 71.98; H, 6.04; N, 13.99. Found: C, 71.85; H, 6.17; N, 13.78.



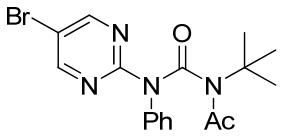
1-But-2-enoyl-1-*tert*-butyl-3-phenyl-3-pyrimidin-2-yl-urea (5m): Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), copper (II) crotonate monohydrate (233.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene at 90 ^{o}C for 26 h to give **5m** as white solid (78.7 mg, 47%). M.p. 116-118 ^{o}C; IR (KBr, cm^{-1}): 2973, 2925, 1689, 1672, 1565, 1407, 1330, 1191, 723; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.69 (d, *J* = 5.0 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.35-7.33 (m, 3H), 7.16 (t, *J* = 4.5 Hz, 1H), 6.84 (dq, *J* = 15.0, 7.5 Hz, 1H), 6.53 (dq, *J* = 15.0, 2.0 Hz, 1H), 1.87 (dd, *J* = 7.0, 2.0 Hz, 3H), 1.40 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 165.5, 160.9, 158.7, 156.1, 141.1, 140.4, 129.4, 128.0, 127.3, 125.7, 119.1, 59.0, 27.9, 18.1; LC-MS (ESI) m/z 339.1 [M^{+}H]; Anal. Calcd. For $C_{19}H_{22}N_4O_2$: C, 67.44; H, 6.55; N, 16.56. Found: C, 67.70; H, 6.42; N, 16.57.



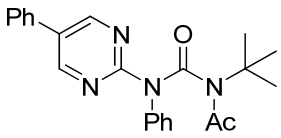
1-*tert*-Butyl-3-phenyl-1-(3-phenyl-propynoyl)-3-pyrimidin-2-yl-urea (5n): Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), copper (II) phenylpropionate multihydrate (851.7 mg, 2.0 mmol), *tert*-butyl isocyanide (249.4 mg, 3.0 mmol) in toluene at 90 ^{o}C for 22 h to give **5n** as white solid (93.5 mg, 47%). M.p. 37-39 ^{o}C; IR (KBr, cm^{-1}): 2981, 2927, 2211, 1703, 1646, 1565, 1407, 691; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.67 (d, *J* = 5.0 Hz, 2H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.40-7.30 (m, 8H), 7.14 (t, *J* = 4.5 Hz, 1H), 1.57 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.8, 158.4, 154.5, 151.8, 140.8, 132.9, 130.1, 129.3, 128.4, 128.0, 127.6, 120.4, 118.7, 88.3, 83.6, 60.1, 27.7; LC-MS (ESI) m/z 399.1 [M^{+}H]; HRMS (ESI) m/s calcd for $C_{24}H_{23}N_4O_2$ [M^{+}H] 399.1821, found 399.1807.



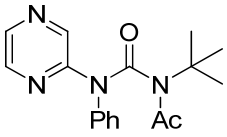
1-*tert*-Butyl-3-phenyl-3-pyrimidin-2-yl-1-(2,2,2-trifluoro-acetyl)-urea (5o): Following the same procedure as for **4a** with **1d** (85.6 mg, 0.5 mmol), copper (II) trifluoroacetate (289.6 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene at 90 ^{o}C for 45 h to give **5o** as white solid (58.2 mg, 32%) together with recovered **1d** (26.6 mg, 69% conversion). M.p. 118-119 ^{o}C; IR (KBr, cm^{-1}): 2977, 2934, 1721, 1695, 1570, 1409, 1325, 1134, 725; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.68 (d, *J* = 5.0 Hz, 2H), 7.46 (t, *J* = 7.0 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.32 (d, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 5.0 Hz, 1H), 1.35 (s, 9H); ^{19}F NMR ($CDCl_3$, 470 MHz): δ -70.74 (s); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.2, 158.5, 157.0 (q, $^{2}J_{C\text{-}F}$ = 36.8 Hz), 151.9, 139.9, 129.6, 128.5, 127.5, 119.0, 116.0 (q, $^{1}J_{C\text{-}F}$ = 287.5 Hz), 61.5, 27.1; LC-MS (ESI) m/z 367.0 [M^{+}H]; Anal. Calcd. For $C_{17}H_{17}F_3N_4O_2$: C, 55.74; H, 4.68; N, 15.29. Found: C, 55.88; H, 4.90; N, 15.20.



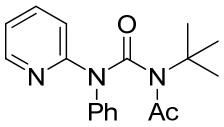
1-Acetyl-3-(5-bromo-pyrimidin-2-yl)-1-*tert*-butyl-3-phenyl-urea (6a)[17]: Following the same procedure as for **4a** with **1p** (125.0 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 21 h to give **6a** as white solid (97.3 mg, 50%). M.p. 94-96 ^{o}C; IR (KBr, cm^{-1}): 2984, 2955, 1705, 1665, 1539, 1412, 1017, 731; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.75 (s, 2H), 7.44 (t, *J* = 8.0 Hz, 2H), 7.36-7.31 (m, 3H), 2.35 (s, 3H), 1.36 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.9, 159.5, 159.1, 156.1, 140.0, 129.6, 128.2, 127.1, 117.9, 59.0, 27.8, 25.5; EI-MS m/z (%): 392 (0.6) [M^{+} (^{81}Br)], 390 (0.6) [M^{+} (^{79}Br)], 251 (100); HRMS (EI) m/z Calcd. for $C_{17}H_{19}BrN_4O_2$ 390.0691, found 390.0695.



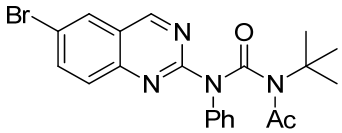
1-Acetyl-1-*tert*-butyl-3-phenyl-3-(5-phenyl-pyrimidin-2-yl)-urea (6b)[17]: Following the same procedure as for **4a** with **1q** (86.6 mg, 0.35 mmol), $Cu(OAc)_2 \cdot H_2O$ (139.8 mg, 0.7 mmol), *tert*-butyl isocyanide (91.9 mg, 1.1 mmol) in toluene for 12 h to give **6b** as yellow liquid (86.4 mg, 64%). IR (KBr, cm^{-1}): 2978, 1705, 1672, 1424, 1302, 1191, 758, 694; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.93 (s, 2H), 7.56 (d, *J* = 7.5 Hz, 2H), 7.52 (t, *J* = 7.5 Hz, 2H), 7.49-7.44 (m, 3H), 7.40 (d, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.0 Hz, 1H), 2.44 (s, 3H), 1.38 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.1, 159.6, 156.6, 156.3, 140.4, 133.1, 132.3, 129.6, 129.5, 129.4, 128.0, 127.0, 126.9, 58.9, 27.8, 25.6; LC-MS (ESI) m/z 411.2 [M^{+}Na]; HRMS (ESI) calcd for $C_{23}H_{24}N_4NaO_2$ [M^{+}Na] 411.1797, found 411.1791.



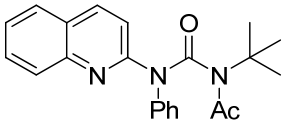
1-Acetyl-1-*tert*-butyl-3-phenyl-3-pyrazin-2-yl-urea (6c)[17]**:** Following the same procedure as for **4a** with **1r** (85.6 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isonitrile (131.3 mg, 1.5 mmol) in toluene for 18 h to give **6c** as yellow solid (93.4 mg, 60%). M.p. 80-82 ^oC; IR (KBr, cm^{-1}): 2979, 1702, 1674, 1405, 1294, 1016, 728; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.57 (s, 1H), 8.47 (s, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 1H) 7.30 (d, *J* = 7.0 Hz, 2H), 2.33 (s, 3H), 1.31 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.6, 156.6, 143.2, 143.0, 142.5, 140.4, 129.8, 128.3, 127.2, 58.9, 27.8, 25.6; LC-MS (ESI) m/z 335.1 [M^+Na]; HRMS (ESI) calcd for $C_{17}H_{20}N_4NaO_2$ [M^+Na] 335.1484, found 335.1483.



1-Acetyl-1-*tert*-butyl-3-phenyl-3-pyridin-2-yl-urea (6d)[17]: Following the same procedure as for **4a** with **1s** (85.1 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 26 h to give **6d** as white solid (110.5 mg, 71%). M.p. 92-94 ^oC; IR (KBr, cm^{-1}): 2961, 2925, 1695, 1665, 1469, 1318, 783, 711; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.52-8.51(m, 1H), 7.72 (dt, *J* = 8.0, 1.5 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.32-7.29 (m, 3H), 7.23-7.21 (m, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 2.37 (s, 3H), 1.31 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.8, 156.5, 154.9, 149.3, 141.4, 138.3, 129.5, 127.6, 126.9, 122.6, 121.6, 58.6, 27.7, 25.7; LC-MS (ESI) m/z 312.1 [M^+H]; Anal. Calcd. For $C_{18}H_{21}N_3O_2$: C, 69.43; H, 6.80; N, 13.49. Found: C, 69.26; H, 6.78; N, 13.31.

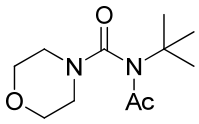


1-Acetyl-3-(6-bromo-quinazolin-2-yl)-1-*tert*-butyl-3-phenyl-urea (6e): Following the same procedure as for **4a** with **1t** (150.1 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 24 h to give **6e** as yellow liquid (90.9 mg, 41%). IR (KBr, cm^{-1}): 2977, 2927, 1700, 1669, 1569, 1420, 836; ^1H NMR ($CDCl_3$, 500 MHz): δ 9.28 (s, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.99 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.86 (d, *J* = 9.0 Hz, 1H), 7.45-7.39 (m, 4H), 7.34 (t, *J* = 7.5 Hz, 1H), 2.47 (s, 3H), 1.31 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.0, 161.4, 157.1, 156.3, 149.7, 140.3, 138.7, 129.9, 129.4, 129.3, 128.0, 127.1, 123.8, 122.3, 58.8, 27.8, 25.8; LC-MS (ESI) m/z 465.1 [M^+Na (^{81}Br)], 463.1 [M^+Na (^{79}Br)]; HRMS (ESI) calcd for $C_{21}H_{21}BrN_4NaO_2$ [M^+Na] 463.0746, found 463.0738.



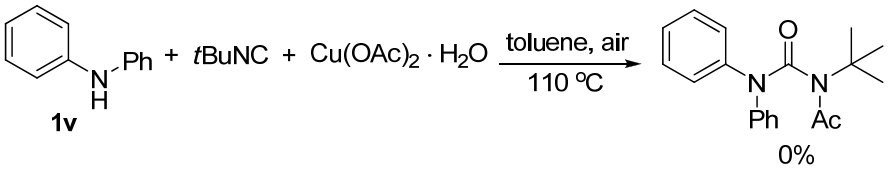
1-Acetyl-1-*tert*-butyl-3-phenyl-3-quinolin-2-yl-urea (6f): Following the same procedure as for **4a** with **1u** (110.1 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 18 h to give **6f** as yellow solid (122.6 mg, 68%). M.p. 90-92 ^oC; IR (KBr, cm^{-1}): 2978, 2928, 1698, 1669, 1593, 1501, 1296, 1193, 824, 756; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.13 (d, *J* = 8.5 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.74 (td, *J* = 7.0, 1.0 Hz, 1H), 7.57 (td, *J* = 8.0, 1.0 Hz, 1H), 7.42 (t, *J* = 7.0 Hz, 2H), 7.37 (d, *J* = 7.5 Hz,

2H), 7.32 (t, J = 8.0 Hz, 1H), 7.12 (d, J = 8.5 Hz, 1H), 2.47 (s, 3H), 1.31 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.7, 156.6, 153.1, 146.9, 141.0, 138.7, 130.5, 129.5, 129.2, 127.8, 127.4, 127.3, 127.0, 126.6, 119.1, 58.6, 27.9, 25.9; LC-MS (ESI) m/s 384.0 [M^+Na]; HRMS (ESI) calcd for $C_{22}H_{23}N_3NaO_2$ [M^+Na] 384.1688, found 384.1679.

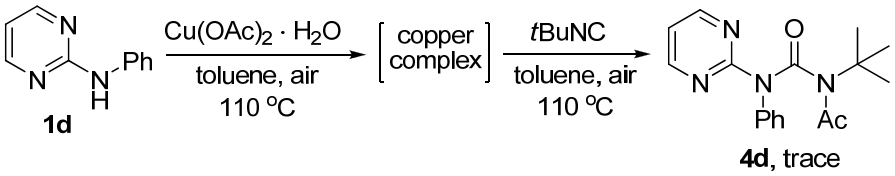


***N*-acetyl-*N*-*tert*-butylmorpholine-4-carboxamide (6g):** Following the same procedure as for **4a** with morpholine (43.6 mg, 0.5 mmol), $Cu(OAc)_2·H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol) in toluene for 22 h to give **6g** as pale yellow oil (79.7 mg, 70%). IR (KBr, cm^{-1}): 2967, 2924, 2856, 1681, 1426, 1364, 1317, 1273, 1220, 1196, 1117, 1027, 597; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 3.73-3.53 (m, 8H), 2.00 (s, 3H), 1.45 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 168.7, 156.3, 66.7, 66.4, 57.9, 47.1, 43.8, 28.1, 24.0; LC-MS (ESI) m/s 251.1 [M^+Na]; HRMS (ESI) calcd for $C_{11}H_{20}N_2NaO_3$ [M^+Na] 251.1368, found 251.1366.

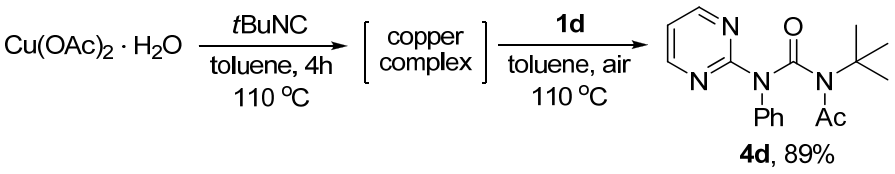
6. Mechanistic Studies



Following the same procedure as for **4a** with **1v** (16.9 mg, 0.1 mmol), $Cu(OAc)_2·H_2O$ (40.0 mg, 0.2 mmol) and *tert*-butyl isocyanide (26 mg, 0.3 mmol) in toluene for 20 h, no desired urea product was detected by TLC and LC-MS.



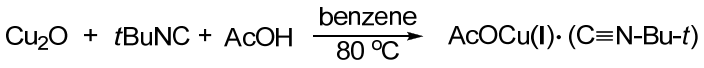
Following the same procedure as for **4a** with **1d** (342.4 mg, 2.0 mmol), $Cu(OAc)_2·H_2O$ (798.6 mg, 4.0 mmol) in toluene for 1 h and monitored by TLC. Upon completion, the reaction mixture filtered and washed with water to give copper complex. Then the given copper complex and *t*BuNC was mixed in toluene and was stirred under 110 °C for 24 h, only trace amount of **4d** was detected which was monitored by TLC.



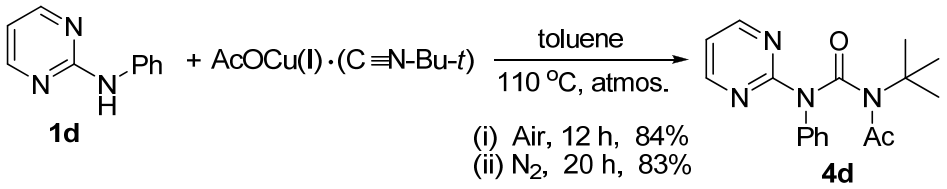
Synthesis of copper complex from $Cu(OAc)_2$ and isocyanide. To an oven-dried flask containing $Cu(OAc)_2·H_2O$ (399.3 mg, 2.0 mmol), *tert*-butyl isocyanide (277.2 mg, 3.0 mmol) was added in

toluene (3.0 mL). The reaction mixture was stirred at 110 °C for 4 h in the presence of air which was dried through a calcium chloride tube. Upon completion, filtrated the reaction and the filtrate was cooled to give a crystal. Filtrated to give the Cu(II) complex, which was used directly for next step without further purification.

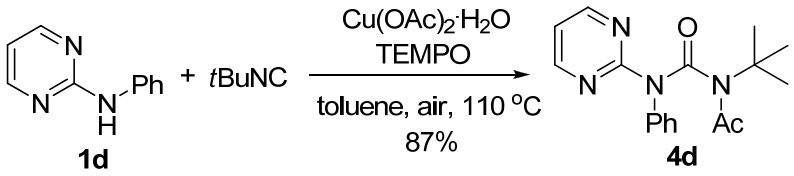
Following the same procedure used for **4a** with **1d** (34.2 mg, 0.2 mmol) and Cu(II) complex (113.1 mg, 0.4 mmol) in toluene (1.8 mL). After 22 h at 110 °C, purification by column chromatography on silica gel yielded **4d** (55.8 mg, 89%) as a white solid.



Synthesis of Cu(I) complex [AcOCu(I)•(C≡N-Bu-*t*)].[18] Under nitrogen, a mixture of acetic acid (17 mmol), Cu_2O (8.5 mmol), and *t*-BuNC (17 mmol) was heated in 12 mL of benzene at 80 °C for 3 h. After filtration, the filtrate was subjected to evaporation in vacuo. Then benzene (10 mL) was added and recrystallization was carried out by warming the mixture up to 80 °C. The procedure was repeated for three times to give Cu(I) complex as a white solid. IR (KBr, cm^{-1}): 2174, 1581, 1562, 1410; ^1H NMR (d_6-DMSO, 500 MHz): δ 1.46 (s, 9H); ^{13}C NMR (d_6-DMSO, 125 MHz): δ 57.1, 29.9.

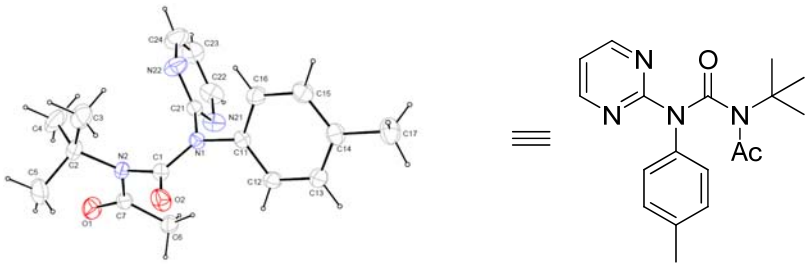


Following the same procedure used for **4a** with **1d** (34.2 mg, 0.2 mmol) and above prepared [AcOCu(I)•(C≡N-Bu-*t*)] (82.3 mg, 0.4 mmol) in toluene (1.2 mL) under air or N_2 atmosphere. After stirred at 110 °C, purification by column chromatography on silica gel yielded **4d** as a white solid in 84% and 83% yield, respectively.

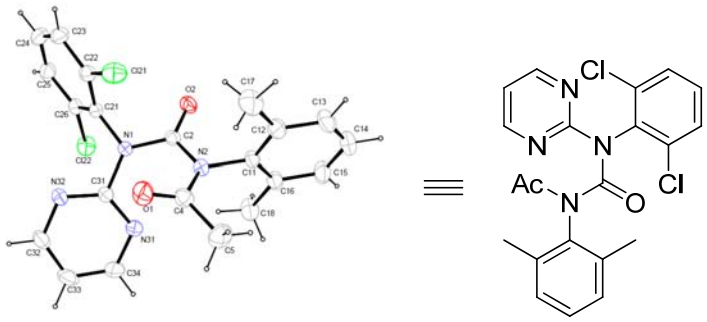


Following the same procedure as for **4a** with **1d** (85.5 mg, 0.5 mmol), $Cu(OAc)_2 \cdot H_2O$ (199.7 mg, 1.0 mmol), *tert*-butyl isocyanide (131.3 mg, 1.5 mmol)，TEMPO (78.2 mg, 0.5 mmol) in toluene for 16 h to give **4d** as white solid (135.6 mg, 87%).

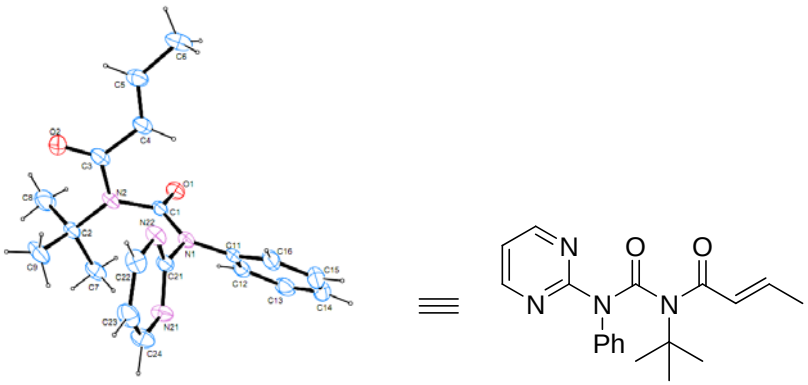
7. X-ray crystal structure for compounds 4e, 5g and 5m



Crystallographic data for **4e**: $C_{18}H_{22}N_4O_2$, M = 326.40, monoclinic, P 21/n (No. 14), a = 10.438 (2) Å, b = 8.222 (1) Å, c = 20.993 (4) Å, β = 94.658(2)°, V = 1795.7 (5) Å^3, Z = 4, Crystal size: 0.30 × 0.25 × 0.20 mm, T = 295 K, ρ_{calcd} = 1.207 g·cm^{-3}, R_1 = 0.0528 (I>4σ(I)), wR_2 = 0.1700 (all data), GOF = 1.046, reflections collected/unique: 4120 / 2824 (Rint = 0.0261), Data: 2824, restraints: 0, parameters: 218. CCDC 882910 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam. ac.uk/data_request/cif



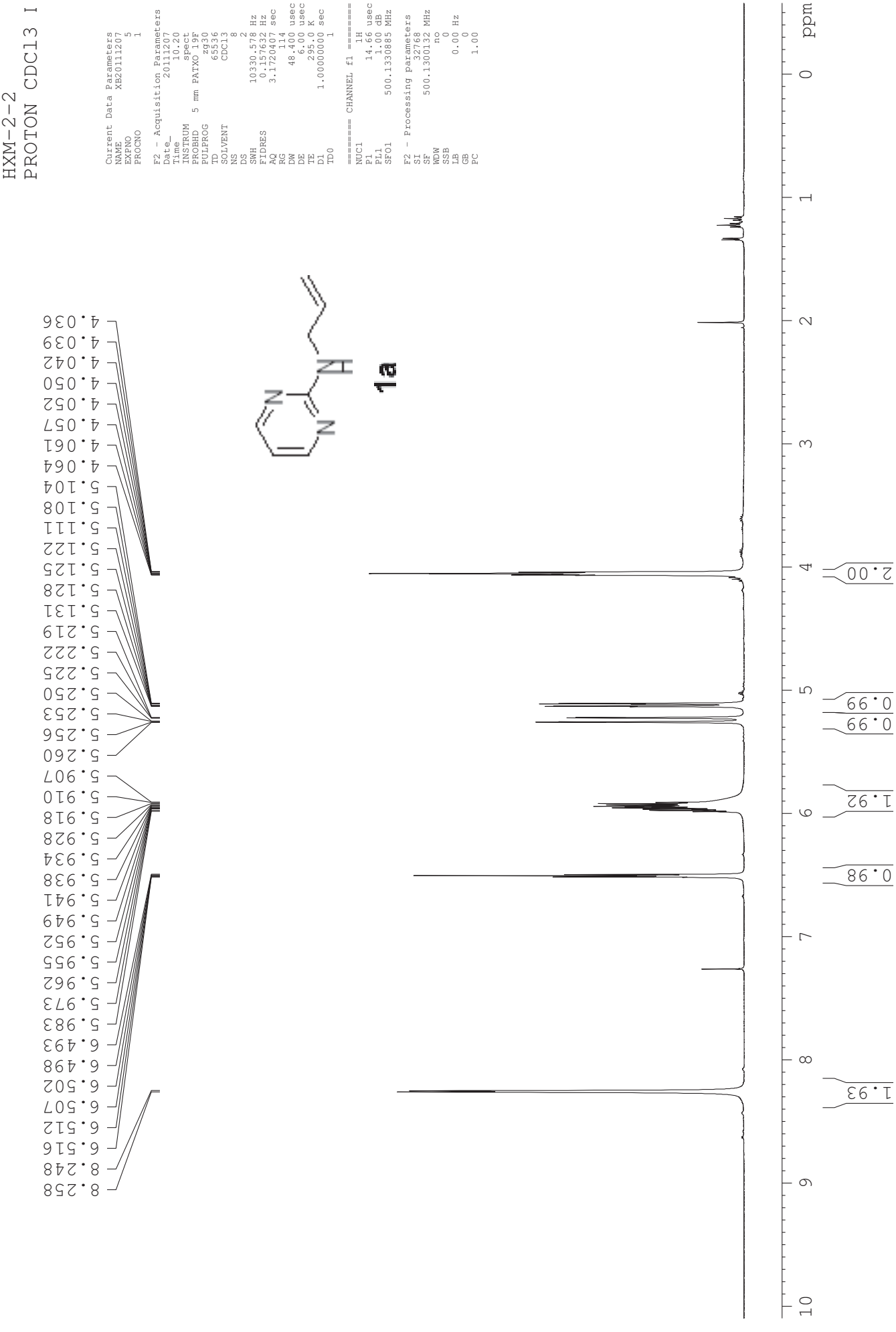
Crystallographic data for **5g**: $C_{21}H_{18}Cl_2N_4O_2$, M= 429.29, monoclinic, P 21/c (No. 14), a = 15.245 (5) Å, b = 8.417 (5) Å, c = 16.508 (5) Å, β = 104.637 (5)°, V = 2049.5 (15) Å^3, Z = 4, Crystal size: 0.30 × 0.25 × 0.20 mm, T = 295 K，ρ_{calcd} = 1.391 g·cm^{-3}, R_1 = 0.0421 (I>4σ(I))，wR_2 = 0.1278 (all data), GOF = 1.041, reflections collected/unique: 4697 / 3685 (Rint = 0.0200), Data: 3685, restraints: 0, parameters: 262. CCDC 883162 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/date_request/cif.



Crystallographic data for **5m**: $C_{19}H_{22}N_4O_2$, M = 338.41, monoclinic, P21/n (No. 14), a = 10.47 (2) Å, b = 13.29 (3) Å, c = 14.71 (3) Å, β = 105.91 (3)°, V = 1969 (8) Å^3, Z = 4, Crystal size: 0.28 × 0.25 × 0.21 mm, T = 295 K, ρ_{calcd} = 1.142 g·cm^{-3}, R_1 = 0.1526 (I>4σ(I)), wR_2 = 0.4040 (all data), GOF = 1.223, reflections collected/unique: 8416 / 3226 (Rint = 0.0637), Data: 3226, restraints: 0, parameters: 227. CCDC 888379 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam. ac.uk/date_request/cif.

8. Reference

[1] S. Jaime-Figueroa, Y. Liu, J. M. Muchowski and D. G. Putman, *Tetrahedron Lett.*, 1998, **39**, 1313.
[2] H. P. L. Steenackers, *J. Med. Chem.*, 2010, **54**, 472.
[3] L. Ackermann and A. V. Lygin, *Org. Lett.*, 2012, **14**, 764.
[4] H. Takeuchi and K. Watanabe, *J. Phys. Org. Chem.*, 1998, 478.
[5] R. Pierre, M. Florence, N. Romain, T. Jamal and G. Gilles, *Int. Patent*, WO 2010/143168A2, 2010.
[6] E. Andre, *DE Patent*, DE 1978/2739659A1, 1978.
[7] G. John, B. S. Armen, M. Allison, K. Tomas, F. K. Chiu, S. Jeongbeob, T. Hongqi, B. James and K. Kevin, *Int. Patent*, WO 2007/146824A2, 2007.
[8] M. Colombo, M. Giglio and I. Peretto, *J. Heterocycl. Chem.*, 2008, **45**, 1077.
[9] J. Chen, Q. Pang, Y. Sun and X. Li, *J. Org. Chem.*, 2011, **76**, 3523.
[10] E. F. DiMauro, J. Newcomb, J. J. Nunes, J. E. Bemis, C. Boucher, J. L. Buchanan, W. H. Buckner, V. J. Cee, L. Chai, H. L. Deak, L. F. Epstein, T. Faust, P. Gallant, S. D. Geuns-Meyer, A. Gore, Y. Gu, B. Henkle, B. L. Hodous, F. Hsieh, X. Huang, J. L. Kim, J. H. Lee, M. W. Martin, C. E. Masse, D. C. McGowan, D. Metz, D. Mohn, K. A. Morgenstern, A. Oliveira-dos-Santos, V. F. Patel, D. Powers, P. E. Rose, S. Schneider, S. A. Tomlinson, Y.-Y. Tudor, S. M. Turci, A. A. Welcher, R. D. White, H. Zhao, L. Zhu and X. Zhu, *J. Med. Chem.*, 2006, **49**, 5671.
[11] R. L. Martin and A. Whitley, *J. Chem. Soc.*, 1958, 1394.
[12] M. Kondo and M. Kubo *J. Phys. Chem.*, 1958, **62**, 1558.
[13] M. H. Borawska, P. Koczoń, J. Piekut, R. Świsłocka and W. Lewandowski, *J. Mol. Struct.*, 2009, **919**, 284.
[14] M. Perec, R. Baggio, R. P. Sartoris, R. C. Santana, O. Peña and R. Calvo, *Inorg. Chem.*, 2009, **49**, 695.
[15] M. T. Rogers, *J. Am. Chem. Soc.*, 1947, ***69***, 1506.
[16] M. D. B. Drew, A. P. Mullins and D. A. Rice, *Polyhedron*, 1994, **13**, 1631.
[17] B. Xu, X. M. Huang, X. H. Hong, G. Y. Qian, T. Fang and X. C. Xu, *Faming Zhuanli Shenqing*, CN 102718719 A 20121010, 2012.
[18] T. Saegusa, I. Murase and Y. Ito, *J. Org. Chem.*, 1973, **38**, 1753.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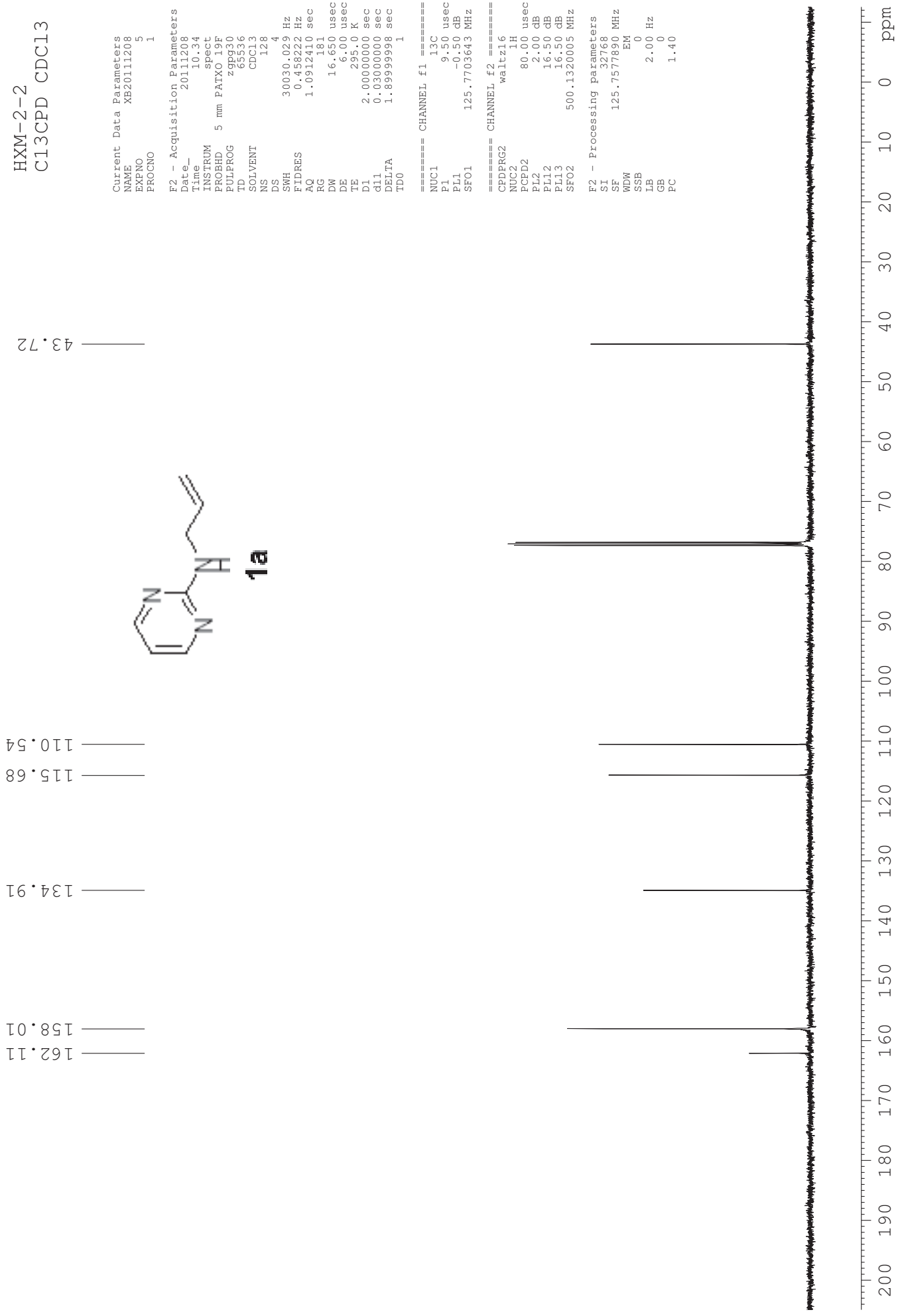
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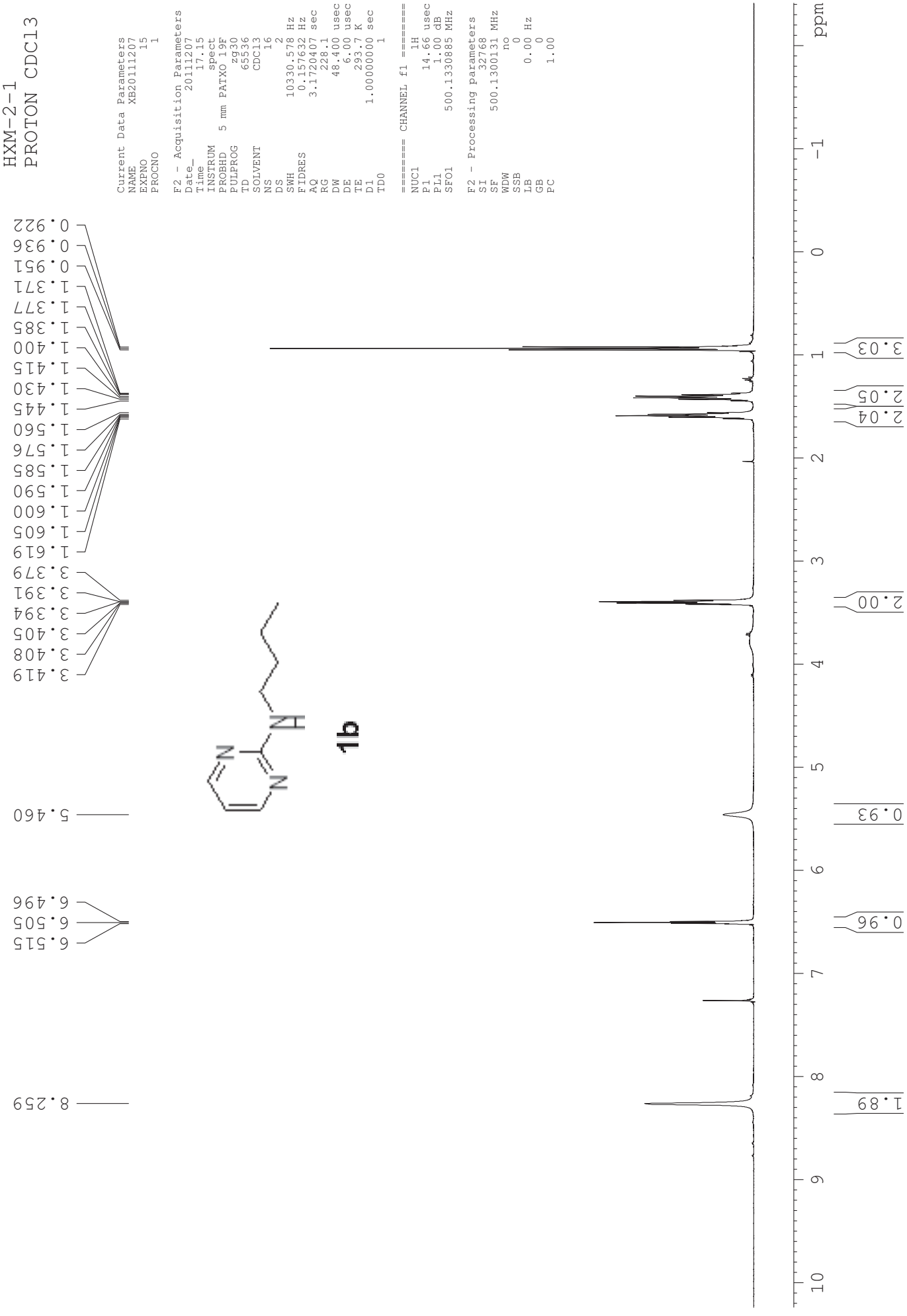
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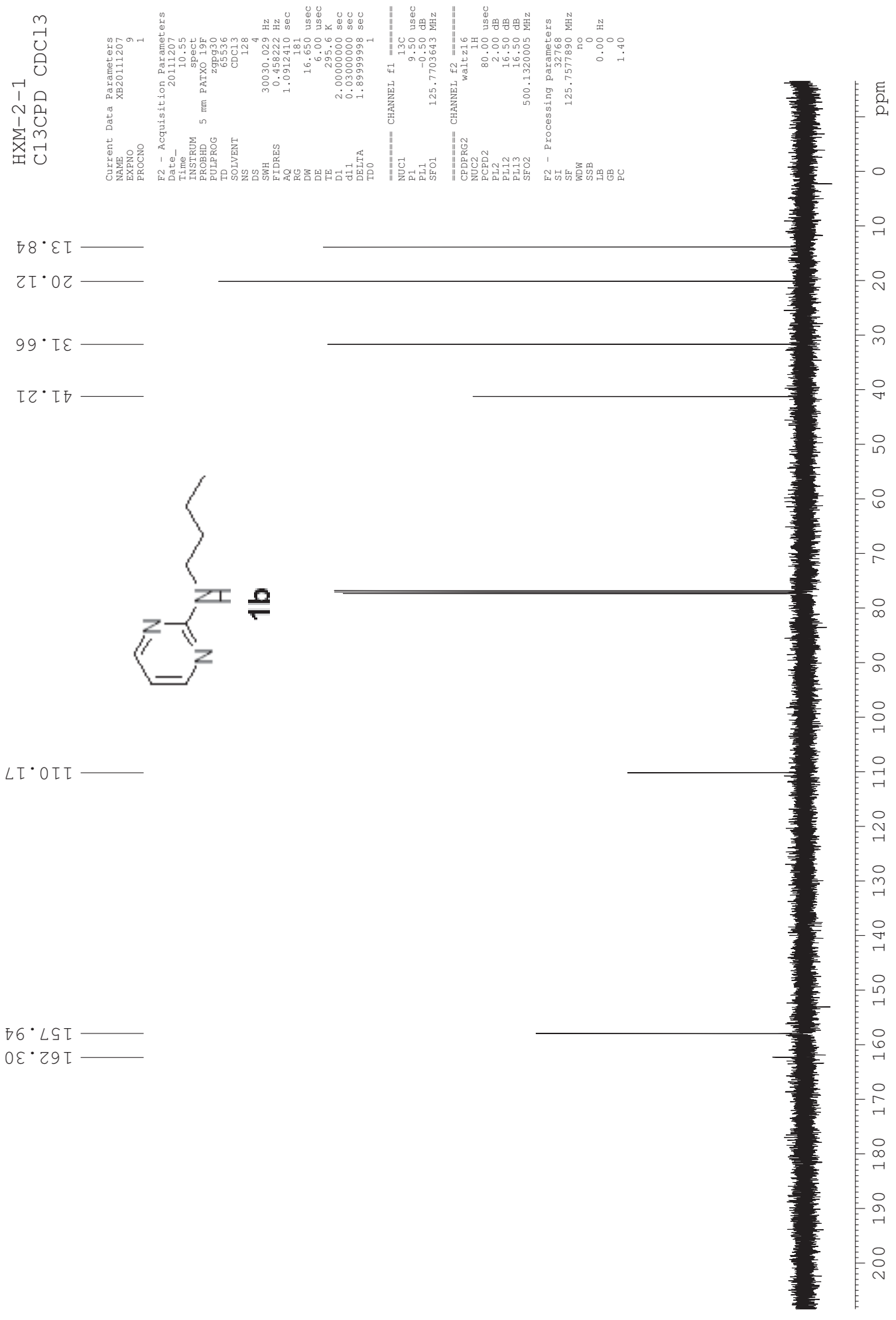
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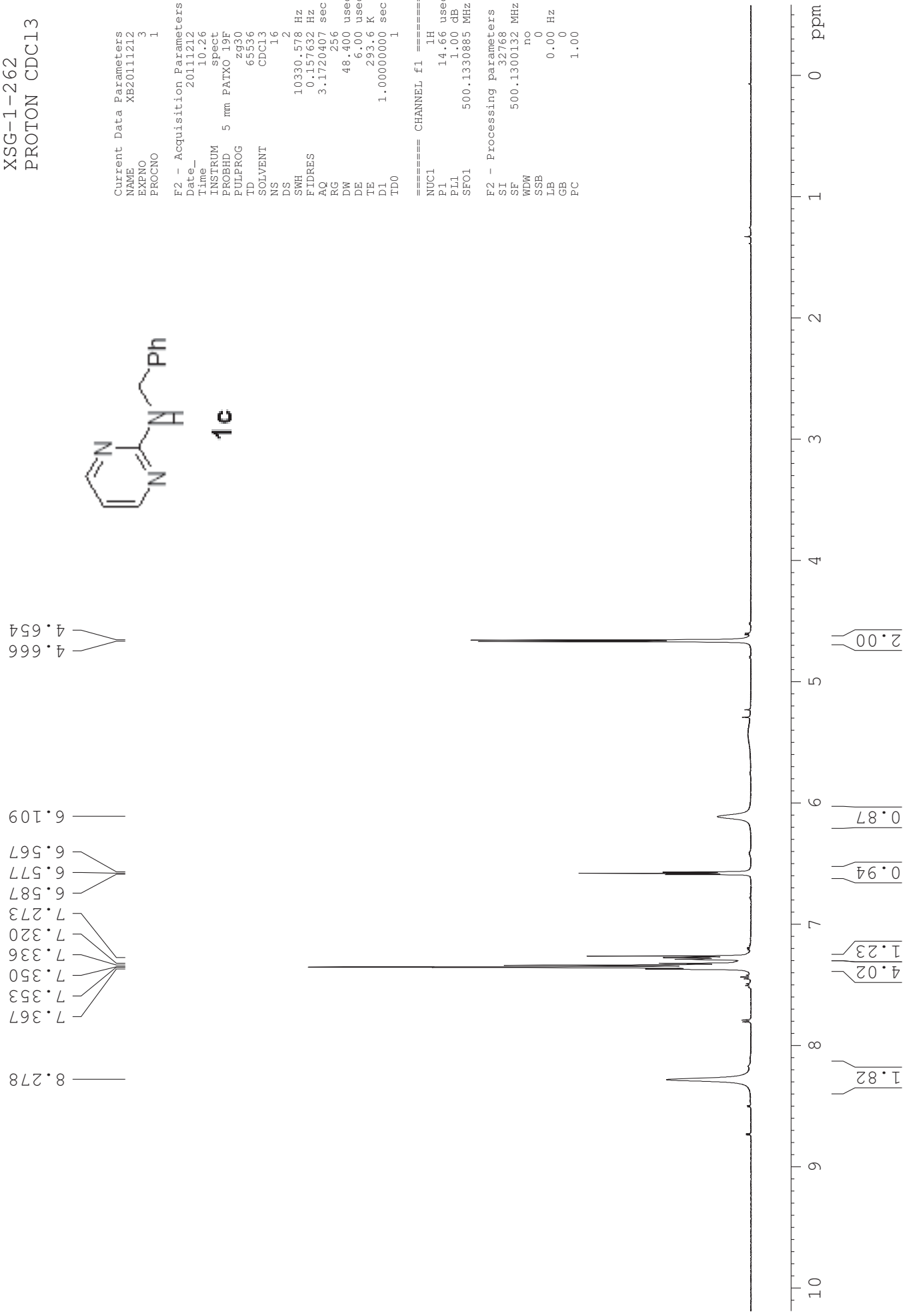
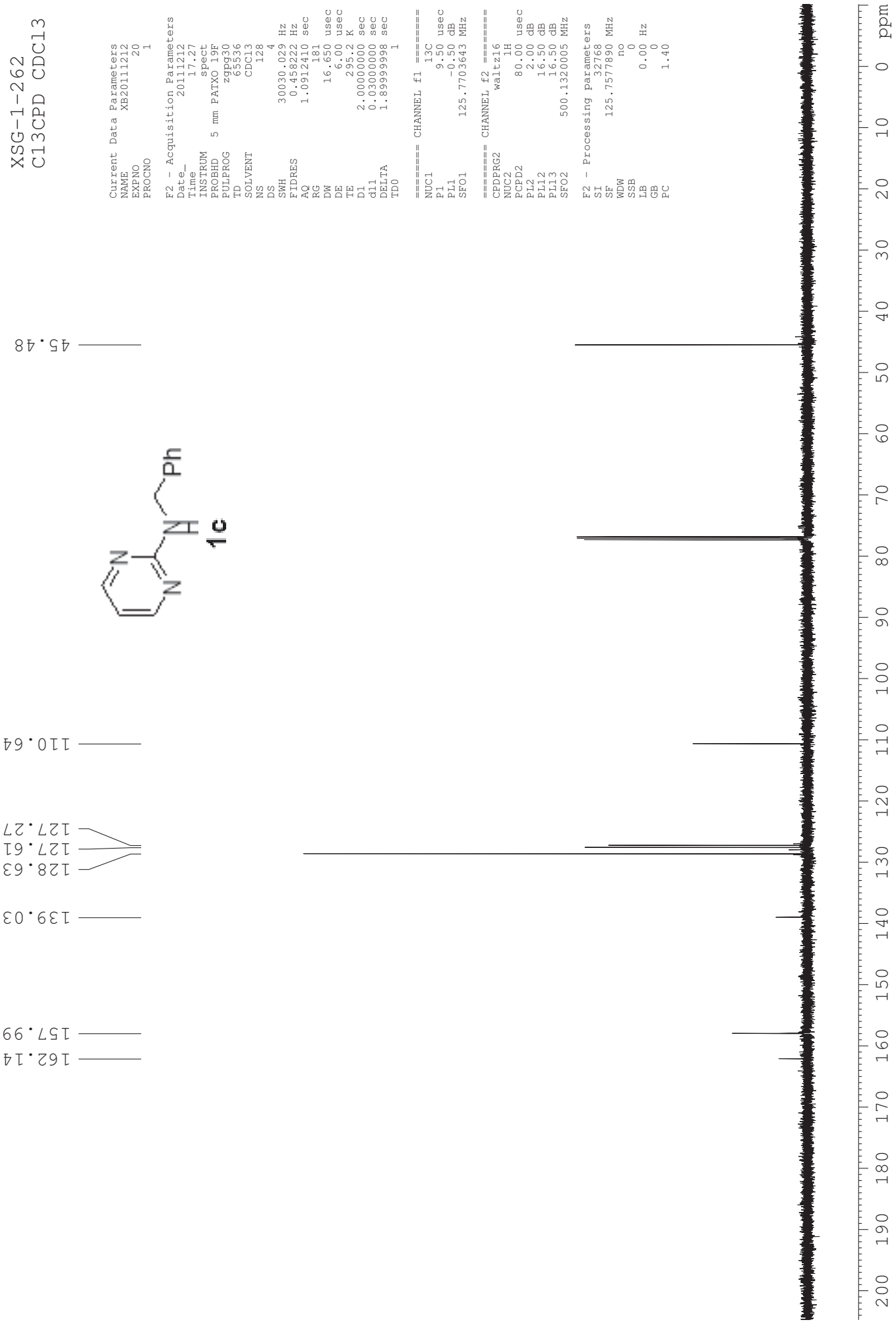
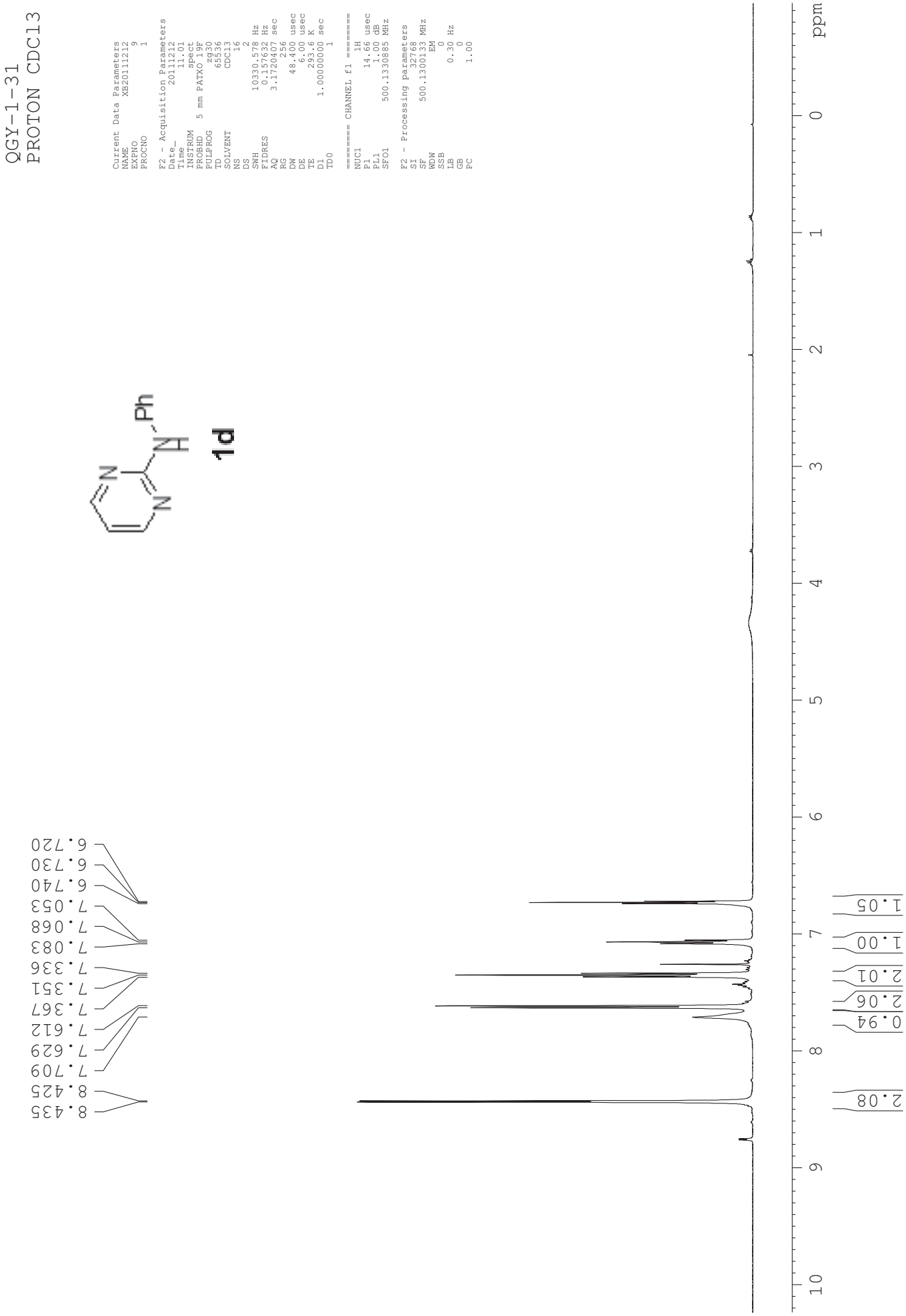
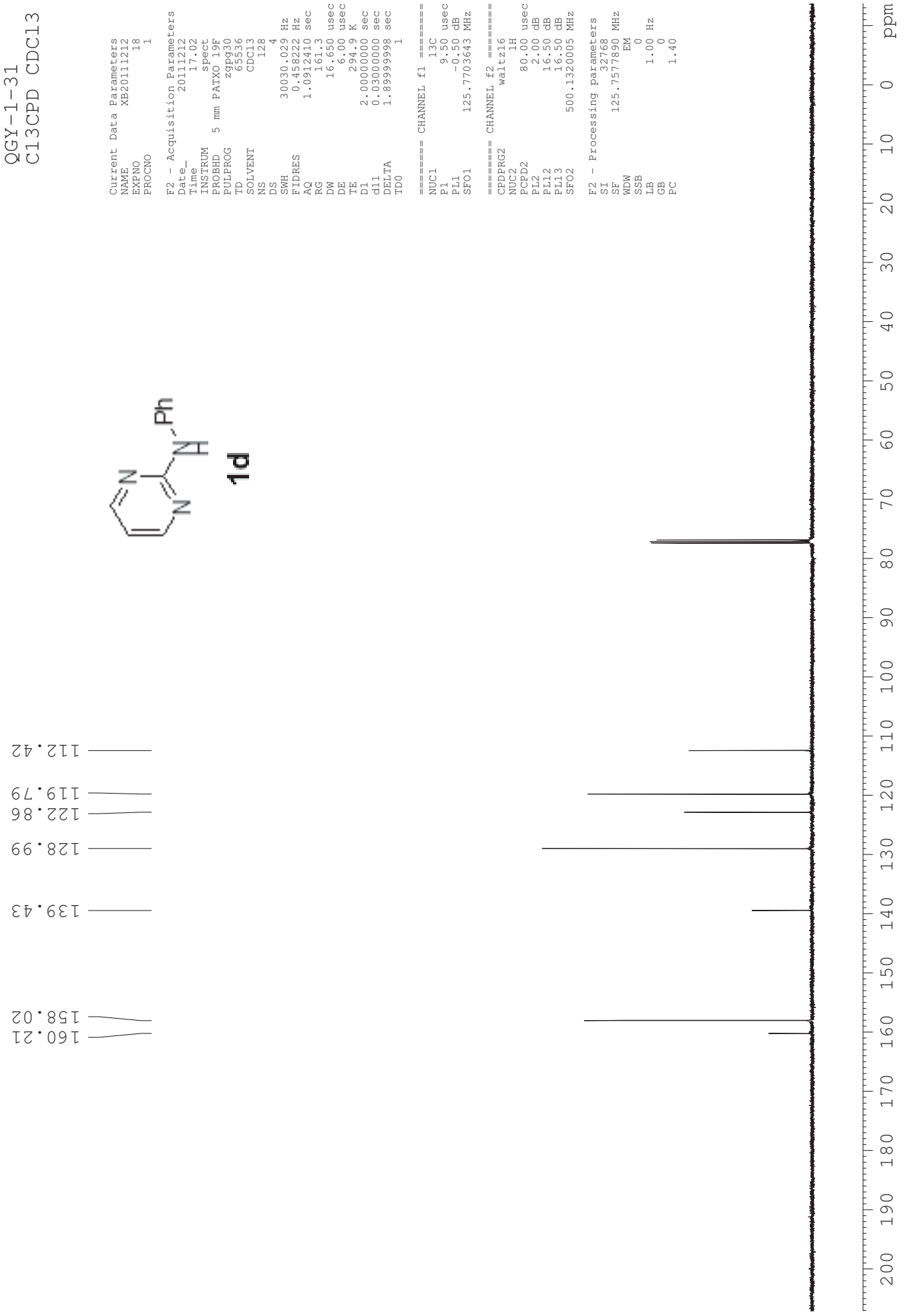
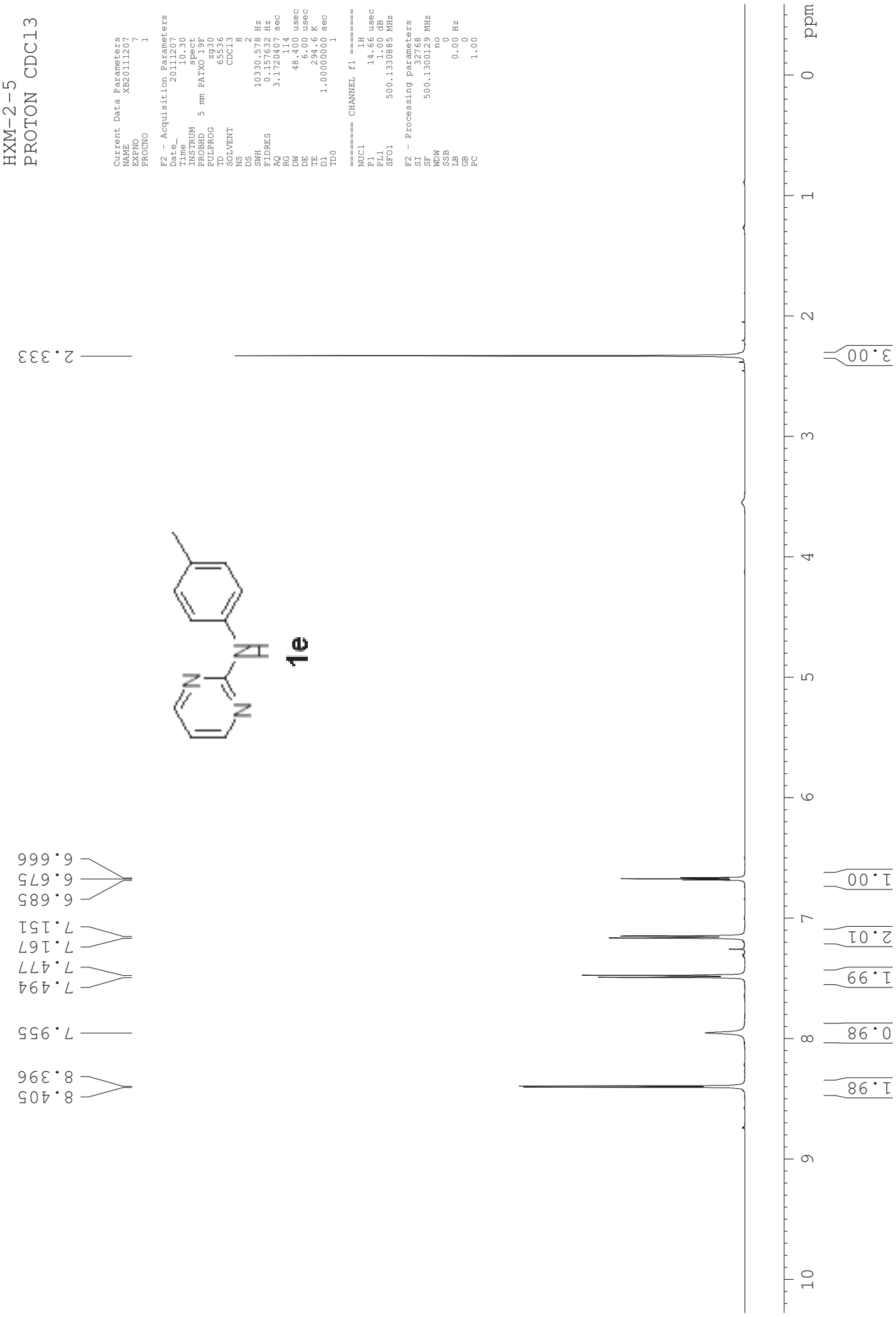
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
13.84
20.12
31.66
41.21
110.17
157.94
162.30
1b
ppm

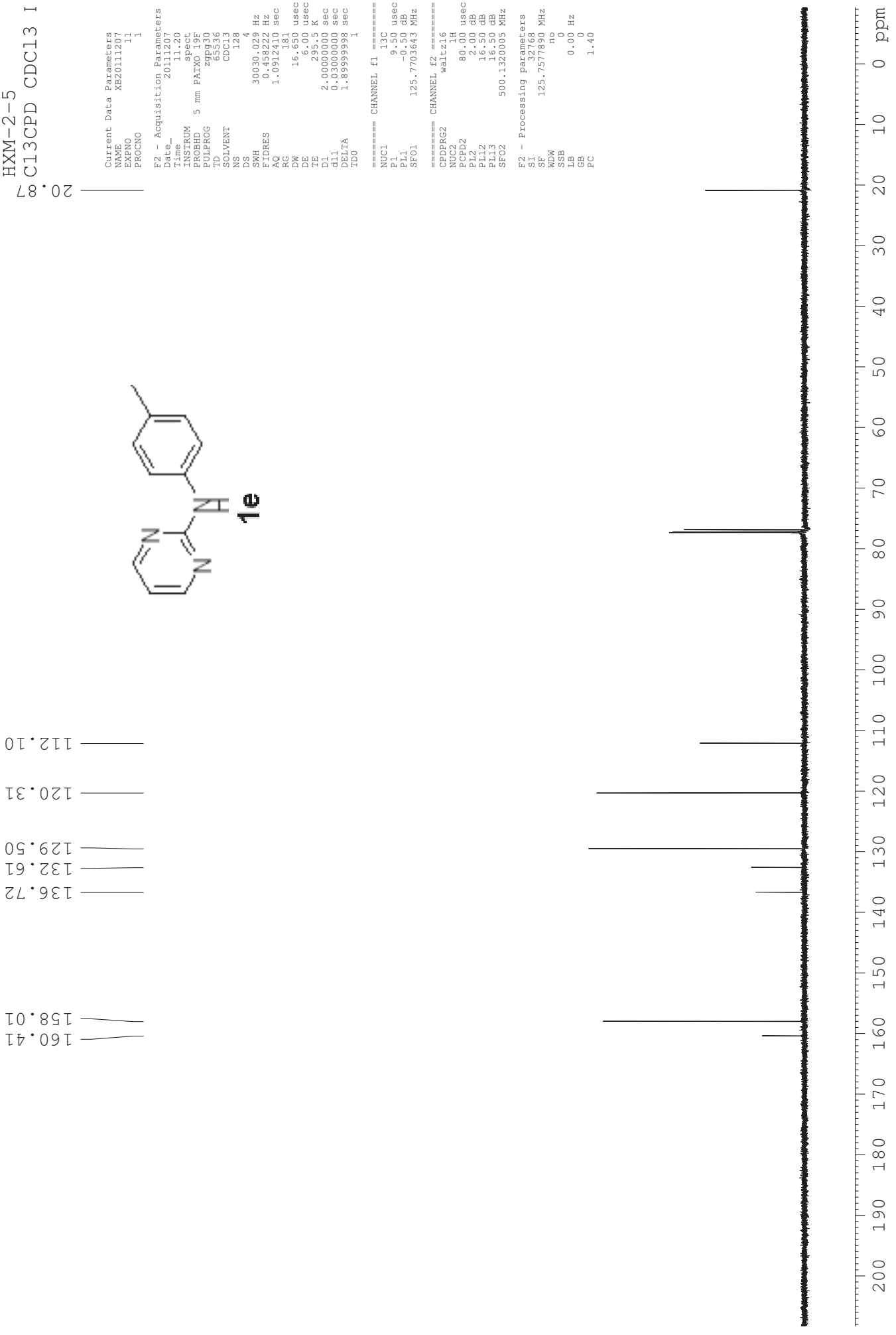

XSG-1-262
PROTON CDC13
Current Data Parameters
NAME XB20111212
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111212
Time_ 10.26
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 256
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ph
N
H
N
1c
8.278
7.367
7.353
7.350
7.336
7.320
7.273
6.587
6.577
6.567
6.109
4.666
4.654
1.82
4.02
1.23
0.94
0.87
2.00
ppm

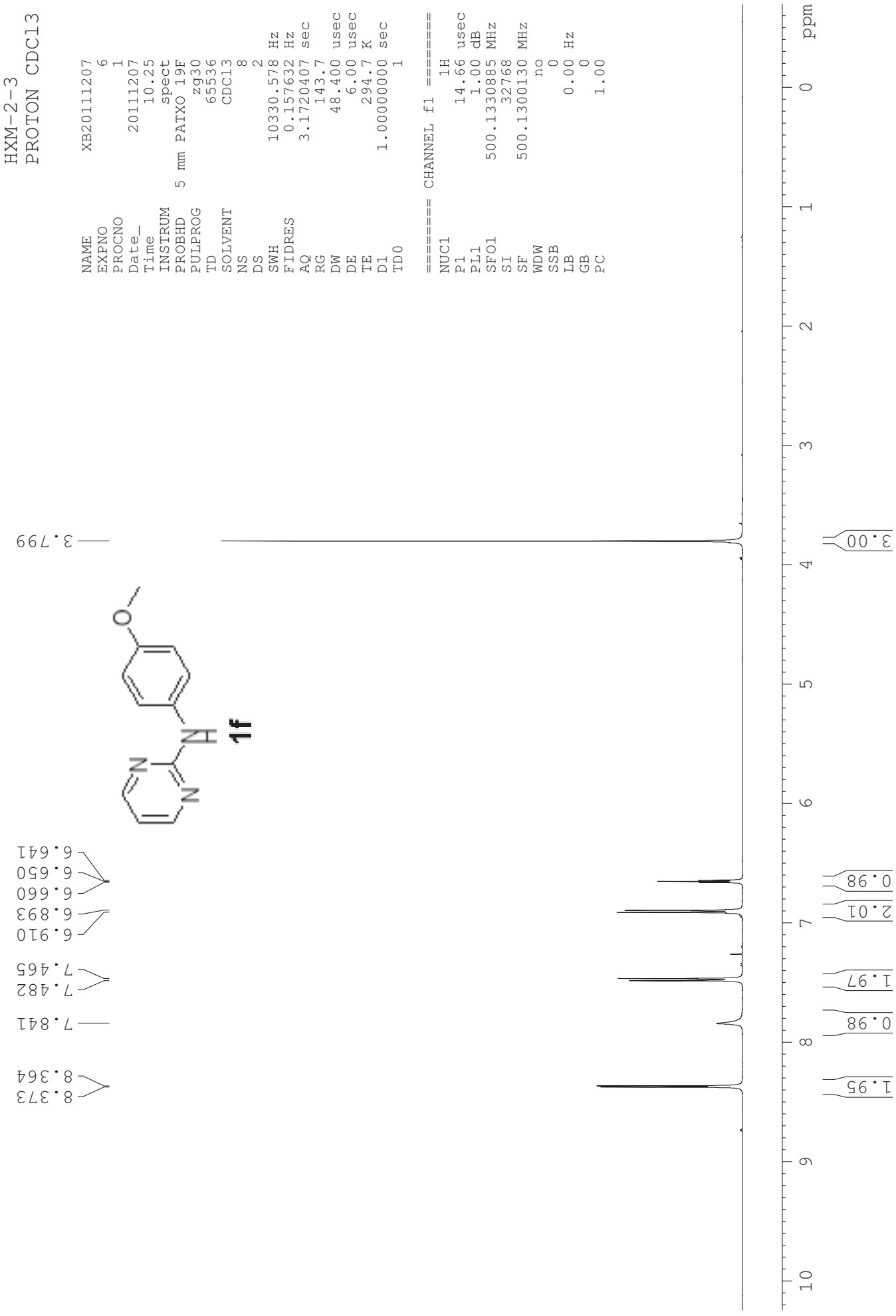

XSG-1-262
C13CPD CDC13
Current Data Parameters
NAME XB20111212
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111212
Time 17.27
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 181
DW 16.650 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
45.48
110.64
127.27
127.61
128.63
139.03
157.99
162.14
Ph
N
H
N
1c
ppm

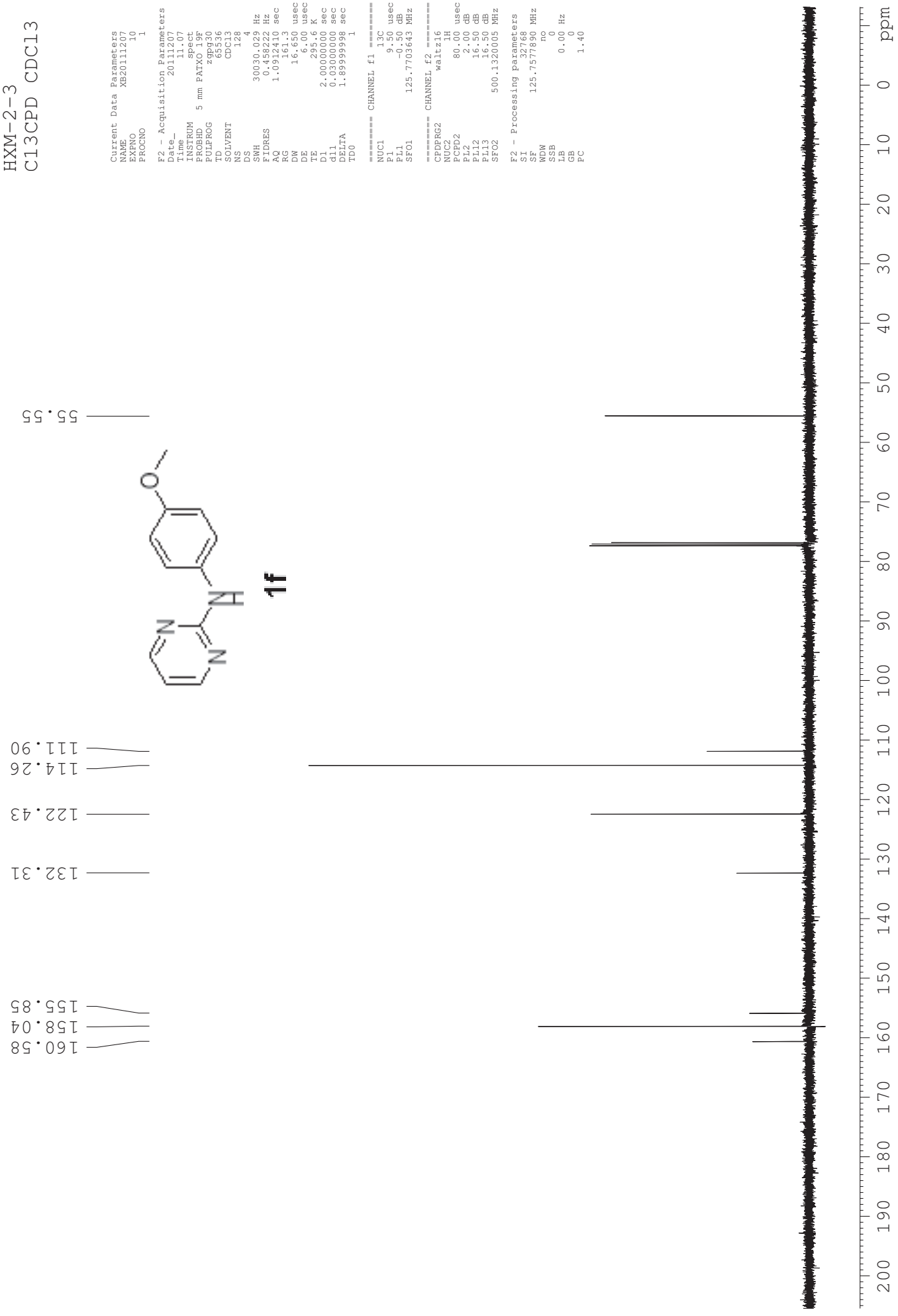

QGY-1-31
PROTON CDC13
Current Data Parameters
NAME XB20111212
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111212
Time 11.01
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 256
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
N
N
H
1d
8.435
8.425
7.709
7.629
7.612
7.367
7.351
7.336
7.083
7.068
7.053
6.740
6.730
6.720
2.08
0.94
2.06
2.01
1.00
1.05
ppm
10
9
8
7
6
5
4
3
2
1
0


QGY-1-31
C13CPD CDCl3
Current Data Parameters
NAME XB20111212
EXPNO 18
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111212
Time 17.02
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
N
H
N
N
1d
160.21
158.02
139.43
128.99
122.86
119.79
112.42
ppm

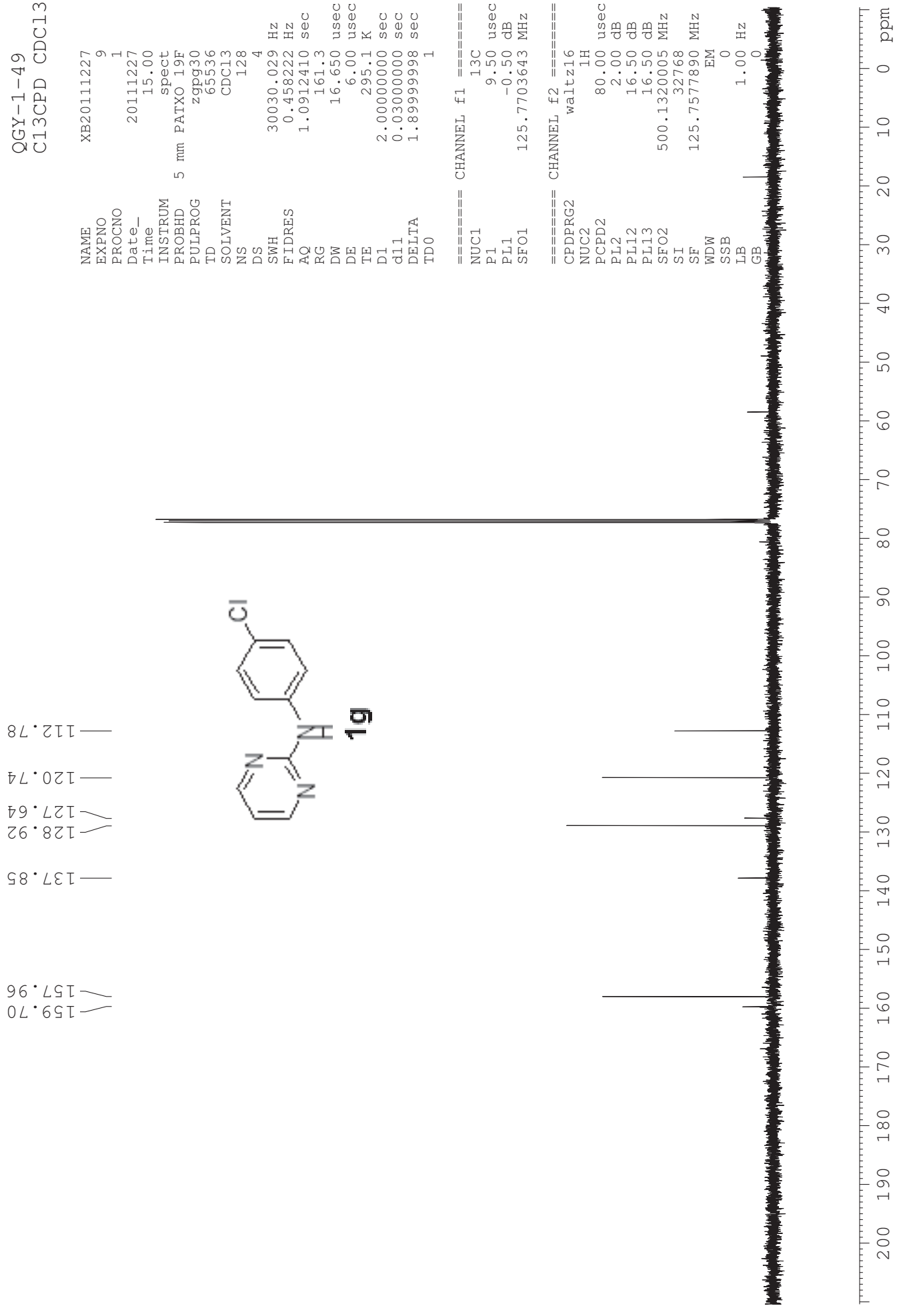

HXM-2-5
PROTON CDCl3
Current Data Parameters
NAME XB20111207
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111207
Time 10.30
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 114
DW 48.400 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
2.333
6.666
6.675
6.685
7.151
7.167
7.477
7.494
7.955
8.396
8.405
1e
3.00
1.00
2.01
1.99
0.98
1.98
ppm

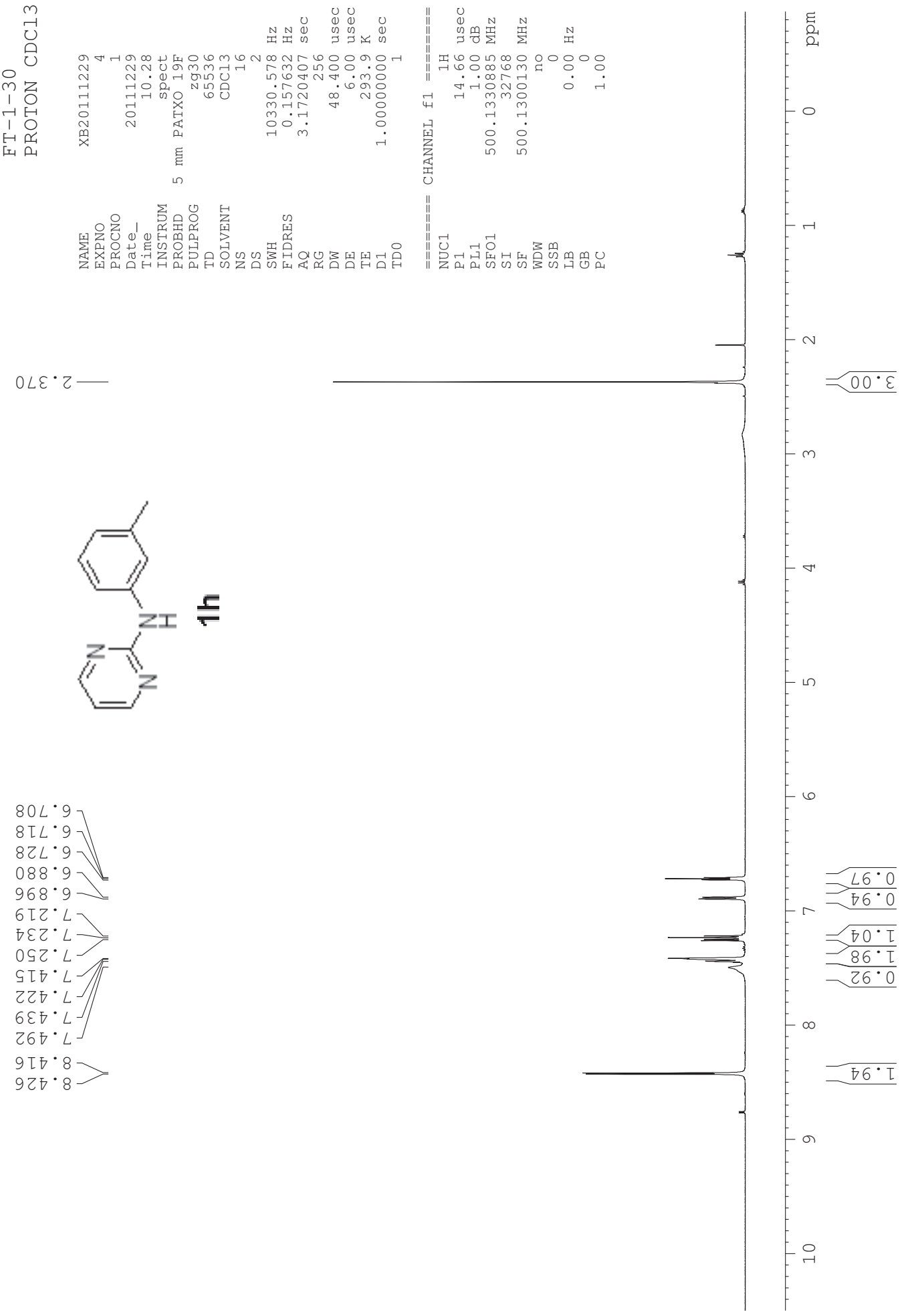

HXM-2-5
C13CPD CDCl3 I
20.87
112.10
120.31
129.50
132.61
136.72
158.01
160.41
1e
Current Data Parameters
NAME XB20111207
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111207
Time_ 11.20
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 181
DW 16.650 usec
DE 6.00 usec
TE 295.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

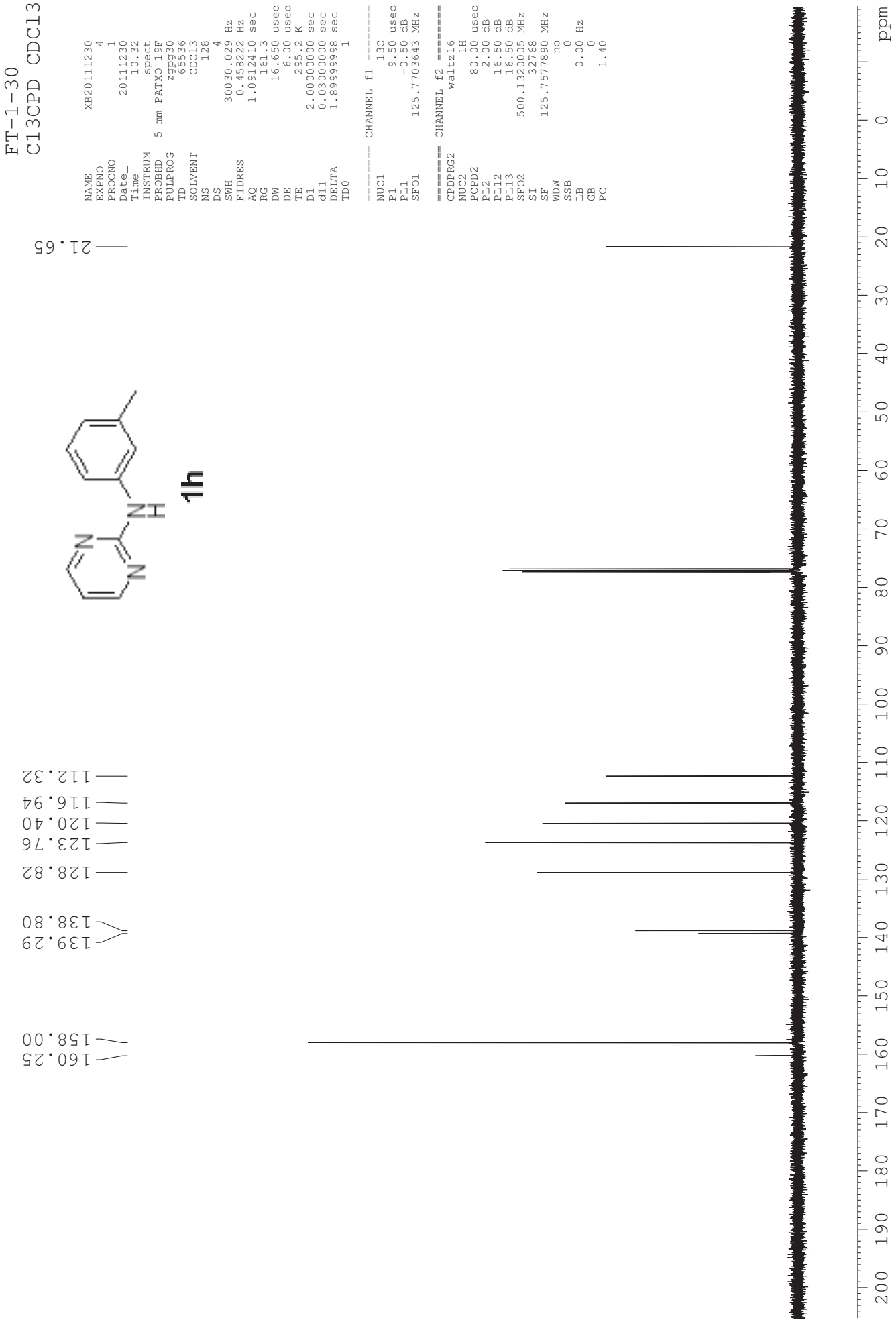

HXM-2-3
PROTON CDC13
NAME XB20111207
EXPNO 6
PROCNO 1
Date_ 20111207
Time 10.25
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 143.7
DW 48.400 usec
DE 6.00 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300130 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1f
3.799
8.373
8.364
7.841
7.482
7.465
6.910
6.893
6.660
6.650
6.641
3.00
0.98
2.01
1.97
0.98
1.95
ppm

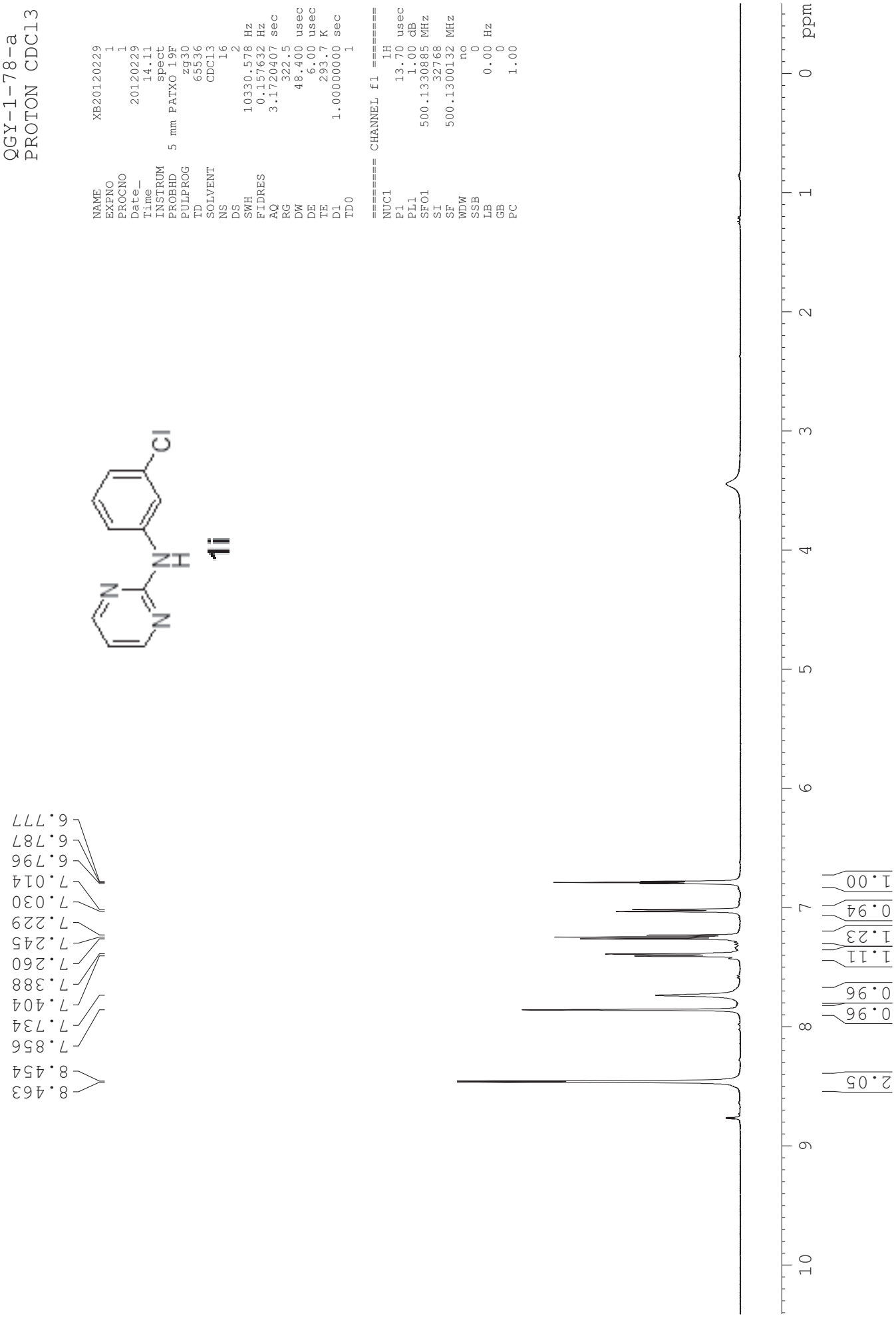

HXM-2-3
C13CPD CDC13
Current Data Parameters
NAME XB20111207
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111207
Time 11.07
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 295.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
55.55
111.90
114.26
122.43
132.31
155.85
158.04
160.58
1f
ppm

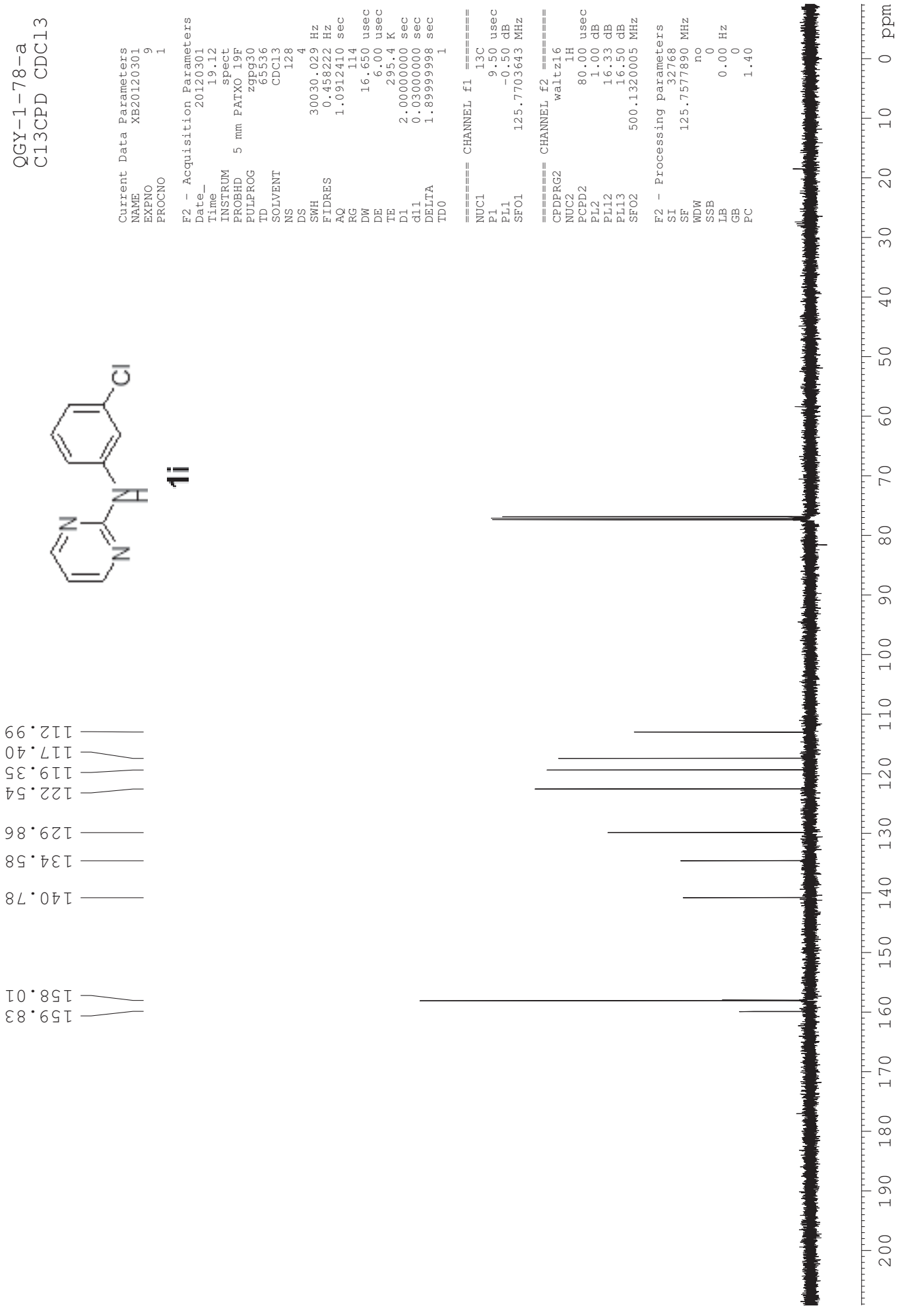

QGY-1-49
PROTON CDC13
NAME XB20111226
EXPNO 3
PROCNO 1
Date_ 20111226
Time 10.23
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
N
H
N
1g
8.434
8.425
7.616
7.588
7.571
7.304
7.287
6.769
6.759
6.749
2.04
0.90
2.09
1.97
1.00
ppm

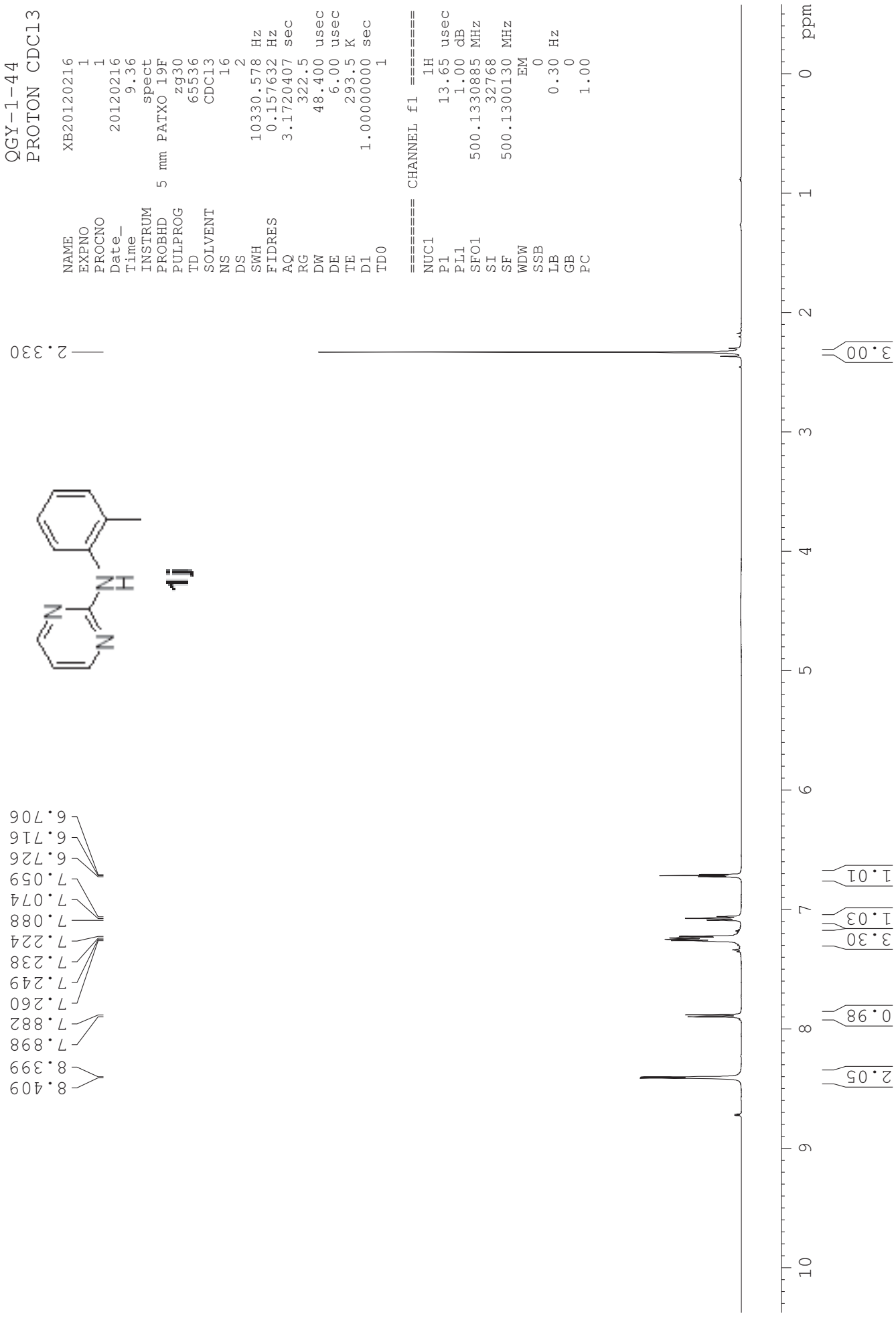

QGY-1-49
C13CPD CDC13
NAME XB20111227
EXPNO 9
PROCNO 1
Date_ 20111227
Time 15.00
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
Cl
N
H
N
19
112.78
120.74
127.64
128.92
137.85
157.96
159.70
ppm

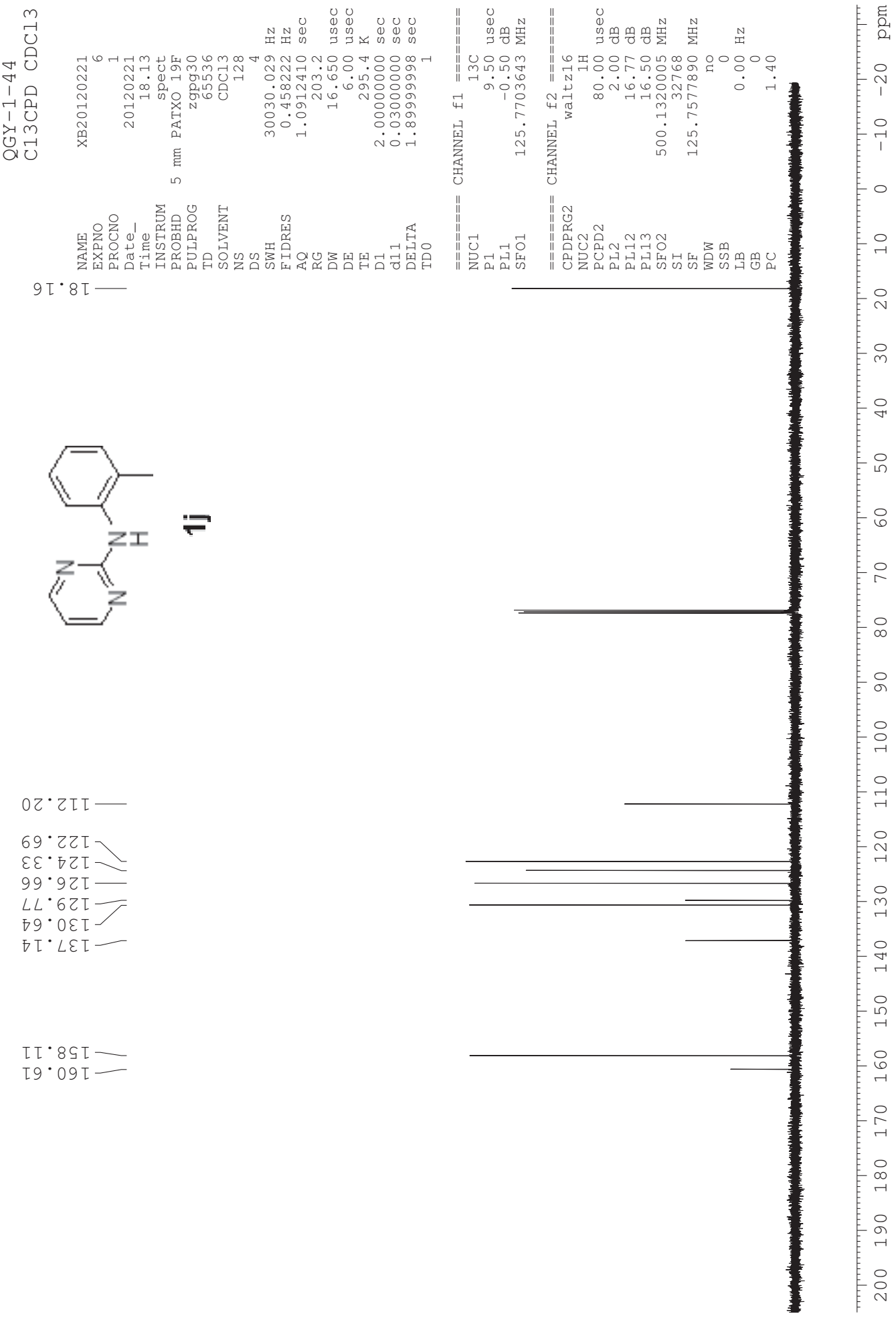

FT-1-30
PROTON CDC13
NAME XB20111229
EXPNO 4
PROCNO 1
Date_ 20111229
Time 10.28
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 256
DW 48.400 usec
DE 6.00 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300130 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
2.370
8.426
8.416
7.492
7.439
7.422
7.415
7.250
7.234
7.219
6.896
6.880
6.728
6.718
6.708
1h
ppm
3.00
1.94
0.92
1.98
1.04
0.94
0.97



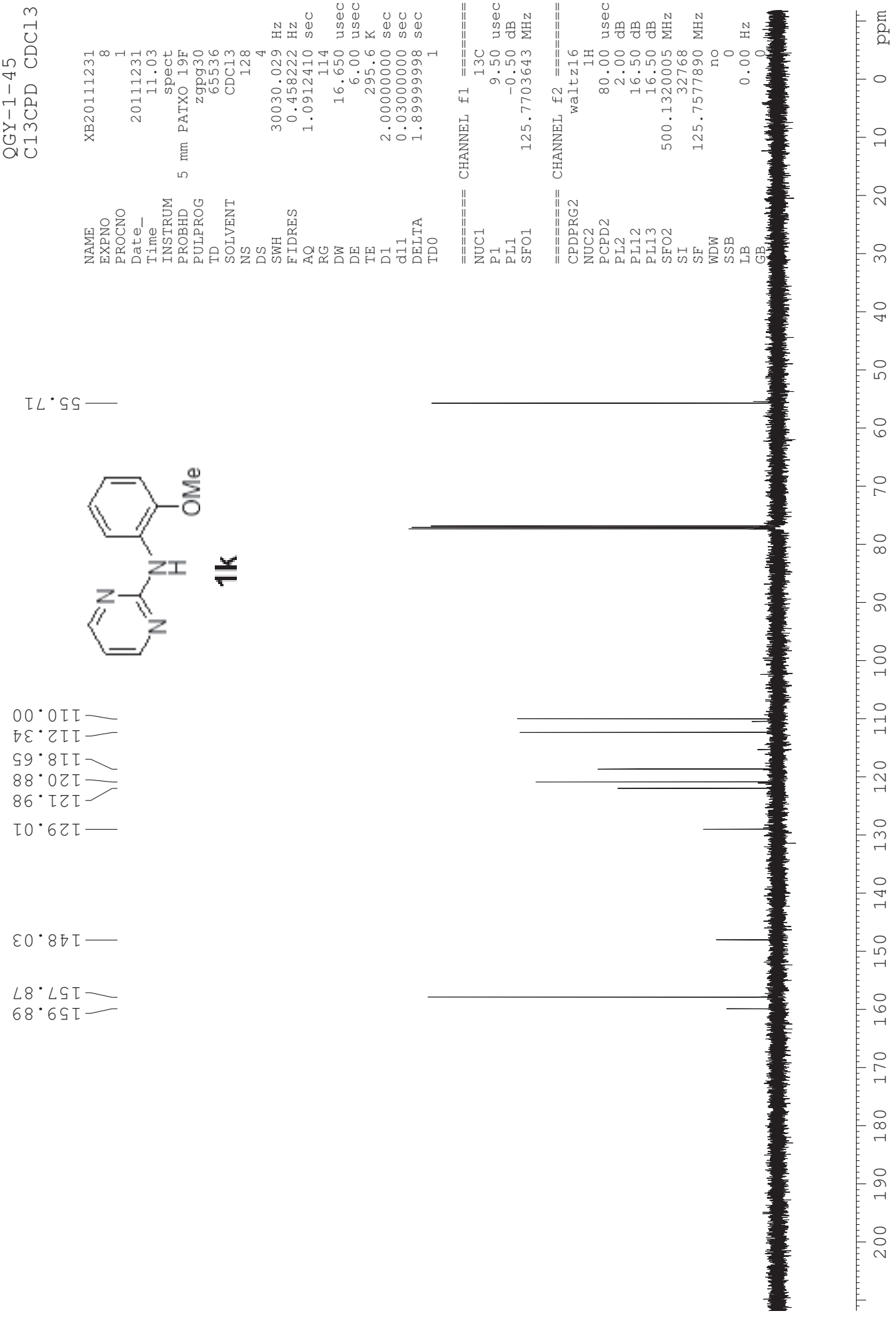

QGY-1-78-a
PROTON CDC13
NAME XB20120229
EXPNO 1
PROCNO 1
Date_ 20120229
Time_ 14.11
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 322.5
DW 48.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
NH
N
N
1i
8.463
8.454
7.856
7.734
7.404
7.388
7.260
7.245
7.229
7.030
7.014
6.796
6.787
6.777
2.05
0.96
0.96
1.11
1.23
0.94
1.00
ppm

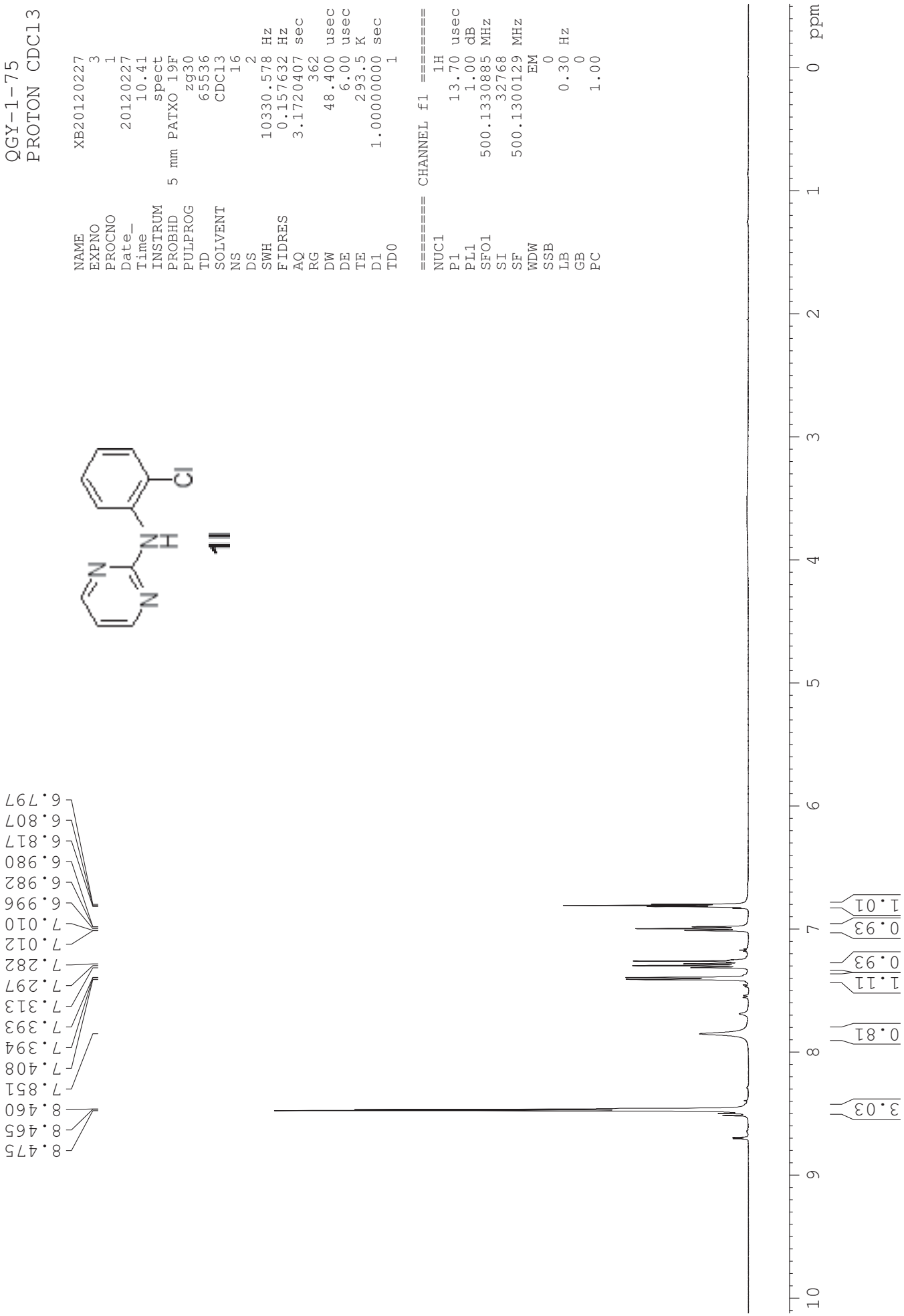

QGY-1-78-a
C13CPD CDC13
Current Data Parameters
NAME XB20120301
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120301
Time 19.12
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
1i
Cl
N
H
N
159.83
158.01
140.78
134.58
129.86
122.54
119.35
117.40
112.99
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

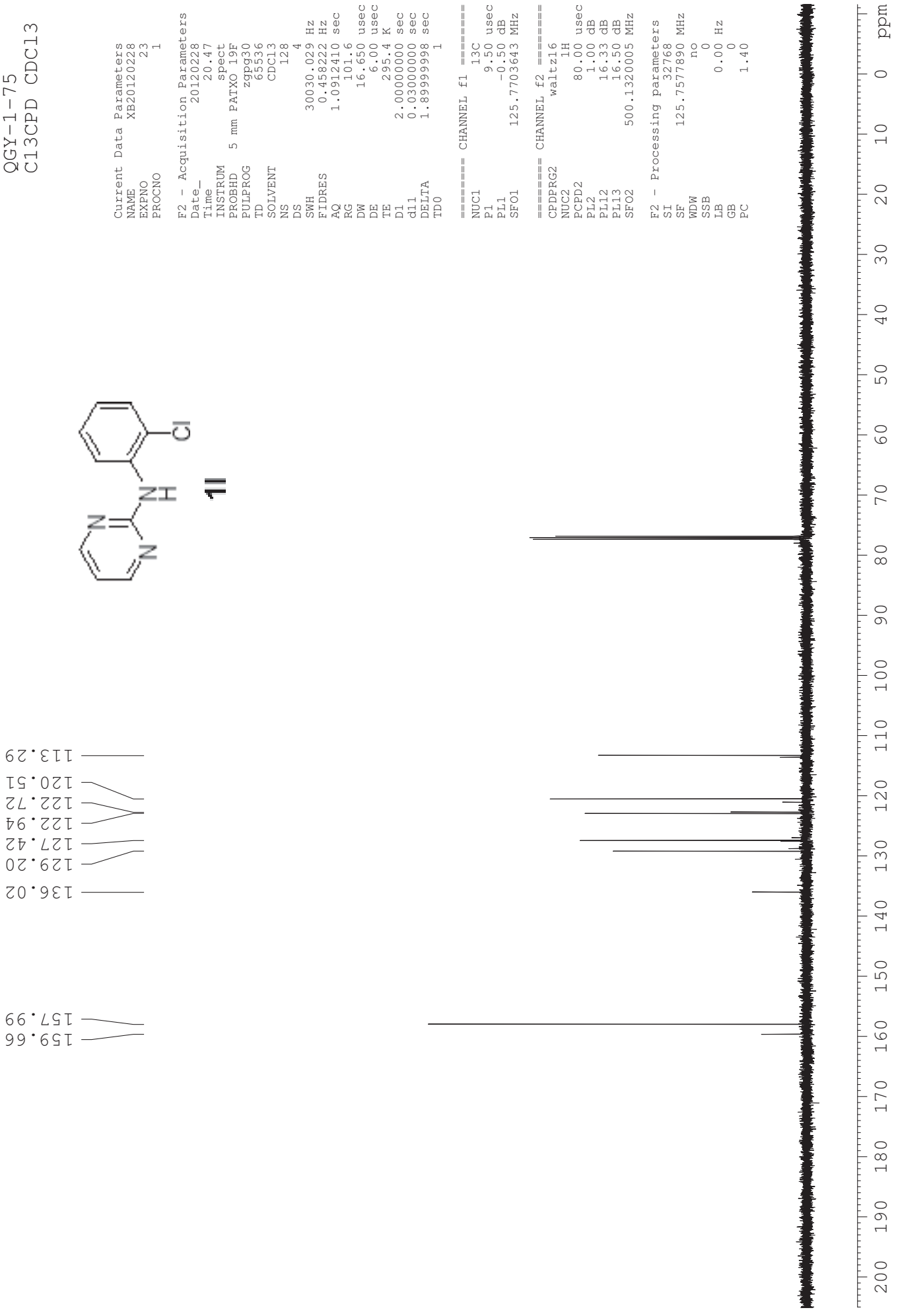


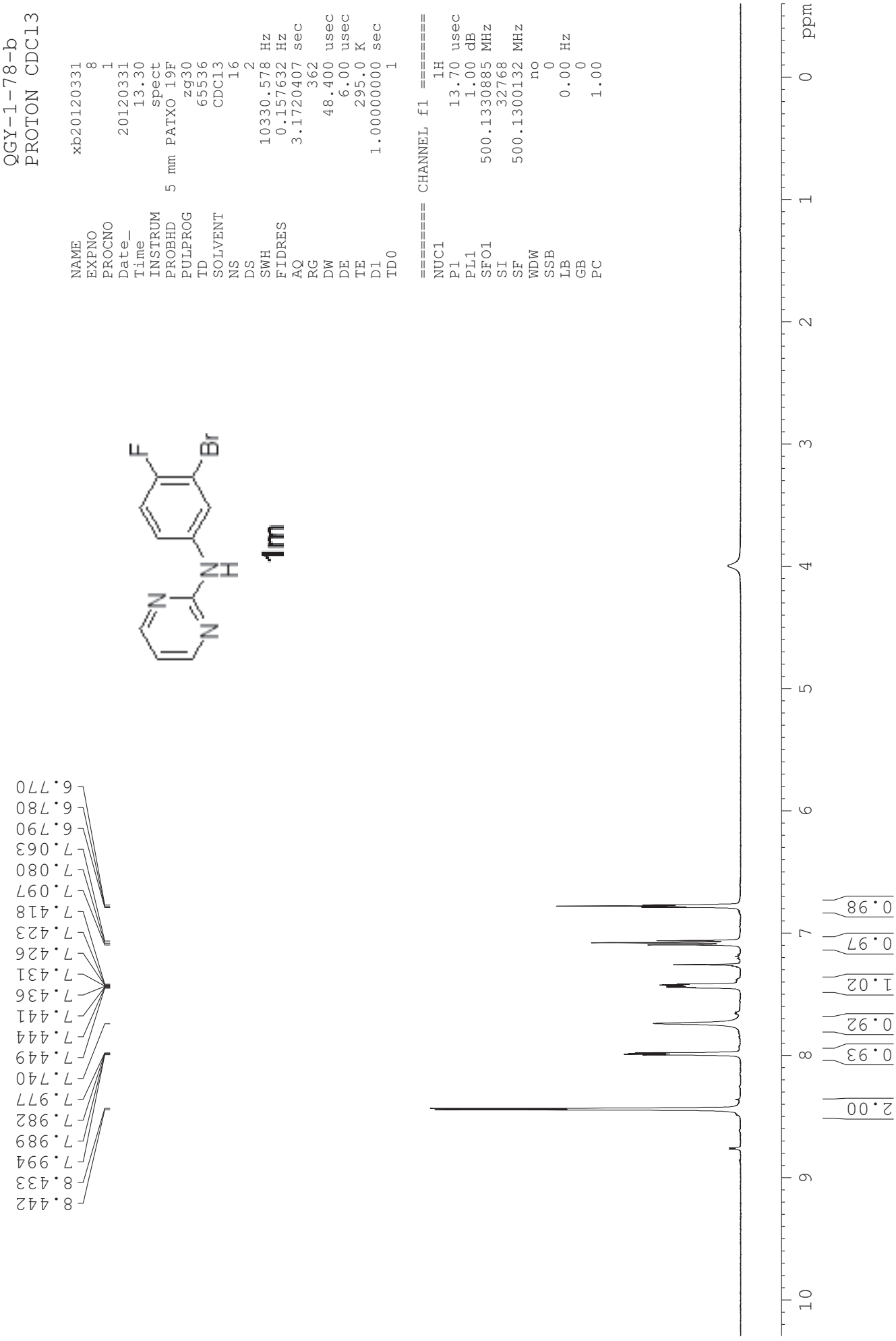

QGY-1-44
C13CPD CDC13
NAME XB20120221
EXPNO 6
PROCNO 1
Date_ 20120221
Time 18.13
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 203.2
DW 16.650 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.77 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
1j
158.16
160.61
158.11
137.14
130.64
129.77
126.66
124.33
122.69
112.20
ppm

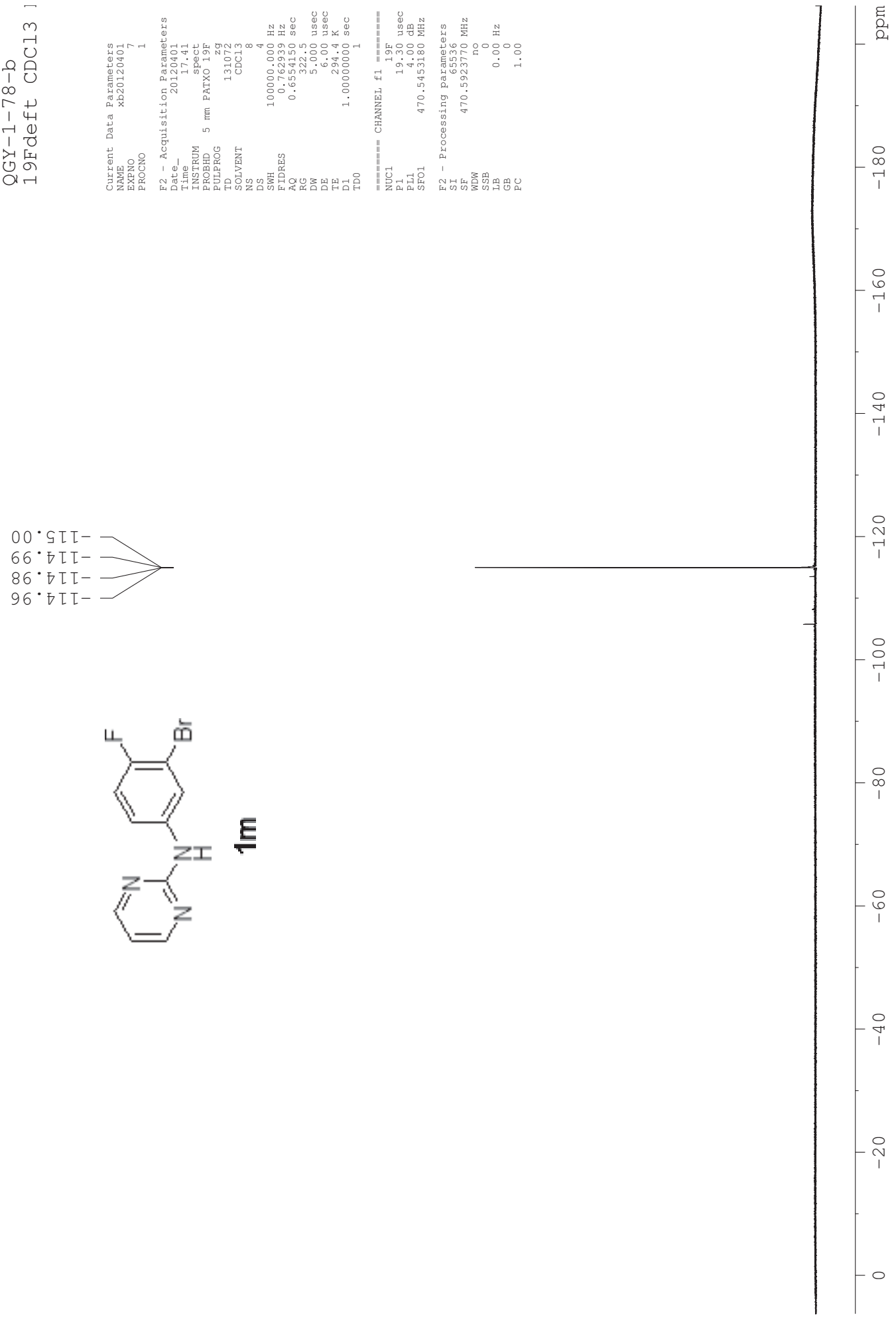

QGY-1-45
PROTON CDC13
NAME XB20111226
EXPNO 2
PROCNO 1
Date_ 20111226
Time 10.17
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300130 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OMe
1k
8.447
8.437
8.421
8.048
7.011
7.005
6.997
6.995
6.918
6.911
6.909
6.904
6.899
6.741
6.731
6.721
3.906
3.00
2.06
1.11
1.04
0.86
2.98
ppm

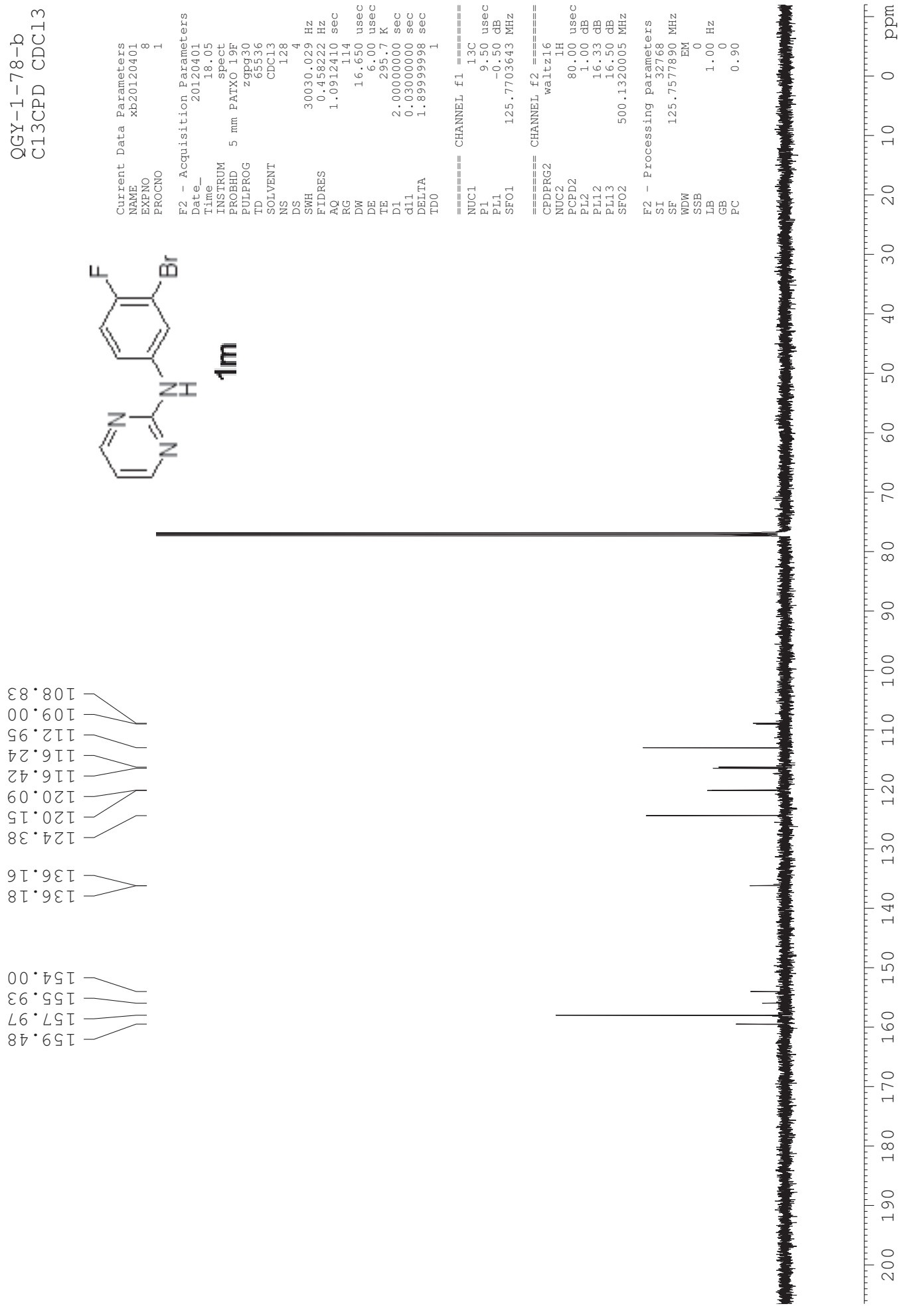

QGY-1-45
C13CPD CDC13
NAME XB20111231
EXPNO 8
PROCNO 1
Date_ 20111231
Time 11.03
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 295.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
55.71
110.00
112.34
118.65
120.88
121.98
129.01
148.03
157.87
159.89
OMe
N
H
N
N
1k
ppm

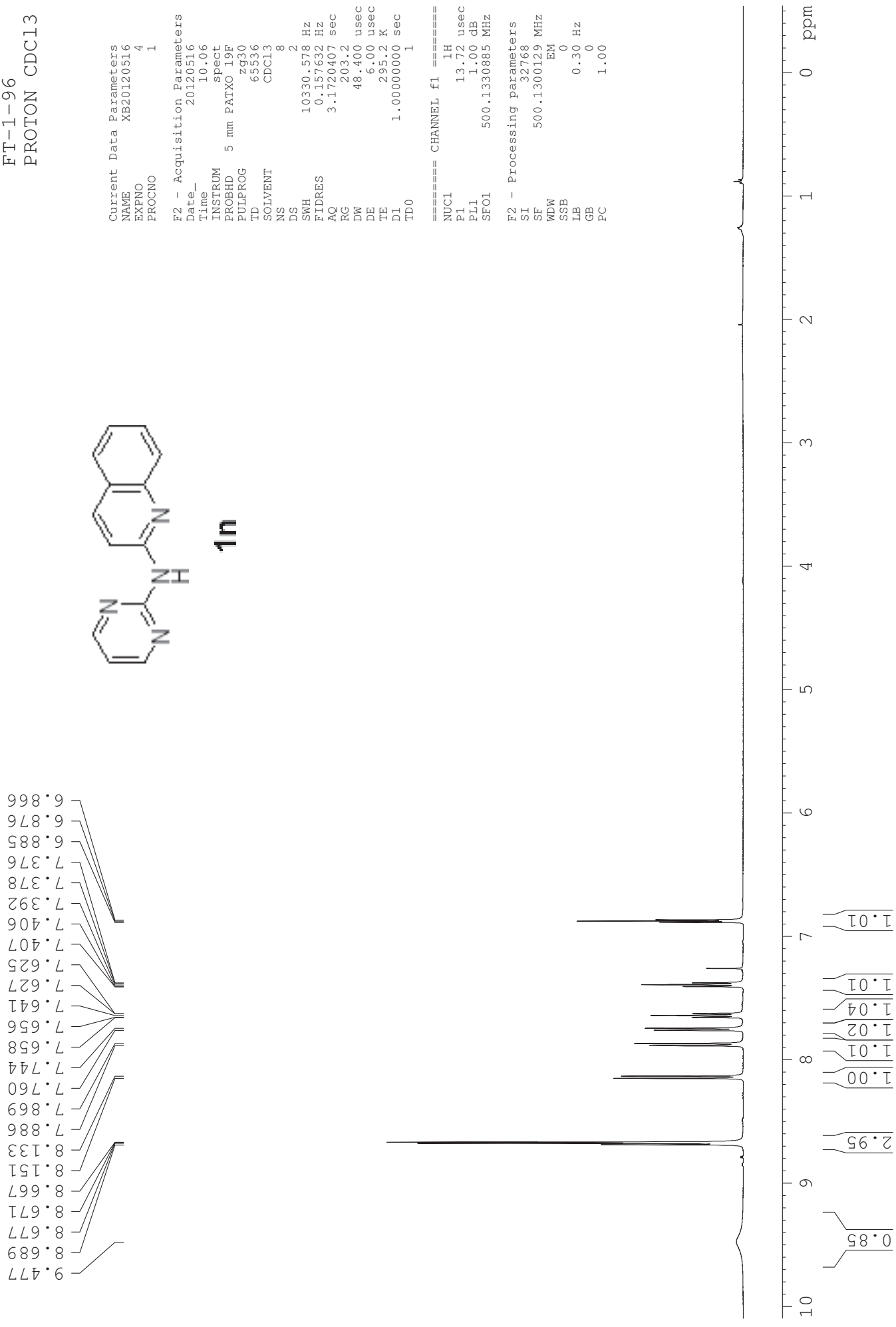

QGY-1-75
PROTON CDC13
NAME XB20120227
EXPNO 3
PROCNO 1
Date_ 20120227
Time 10.41
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 362
DW 48.400 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
NH
N
N
8.475
8.465
8.460
7.851
7.408
7.394
7.393
7.313
7.297
7.282
7.012
7.010
6.996
6.982
6.980
6.817
6.807
6.797
3.03
0.81
1.11
0.93
0.93
1.01
ppm

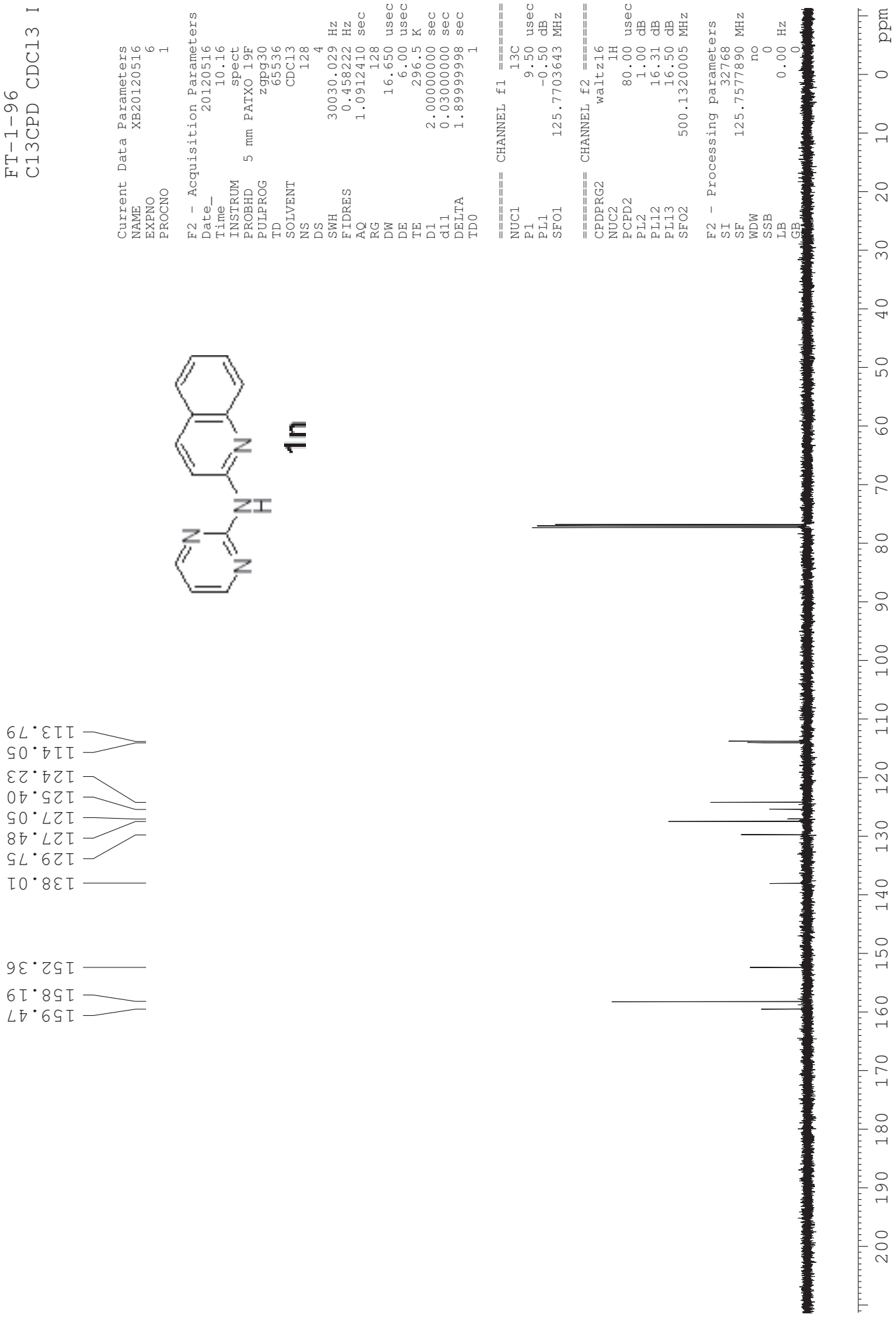

QGY-1-75
C13CPD CDC13
Current Data Parameters
NAME XB20120228
EXPNO 23
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120228
Time 20.47
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 101.6
DW 16.650 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
Cl
NH
N
N
1l
113.29
120.51
122.72
122.94
127.42
129.20
136.02
157.99
159.66
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

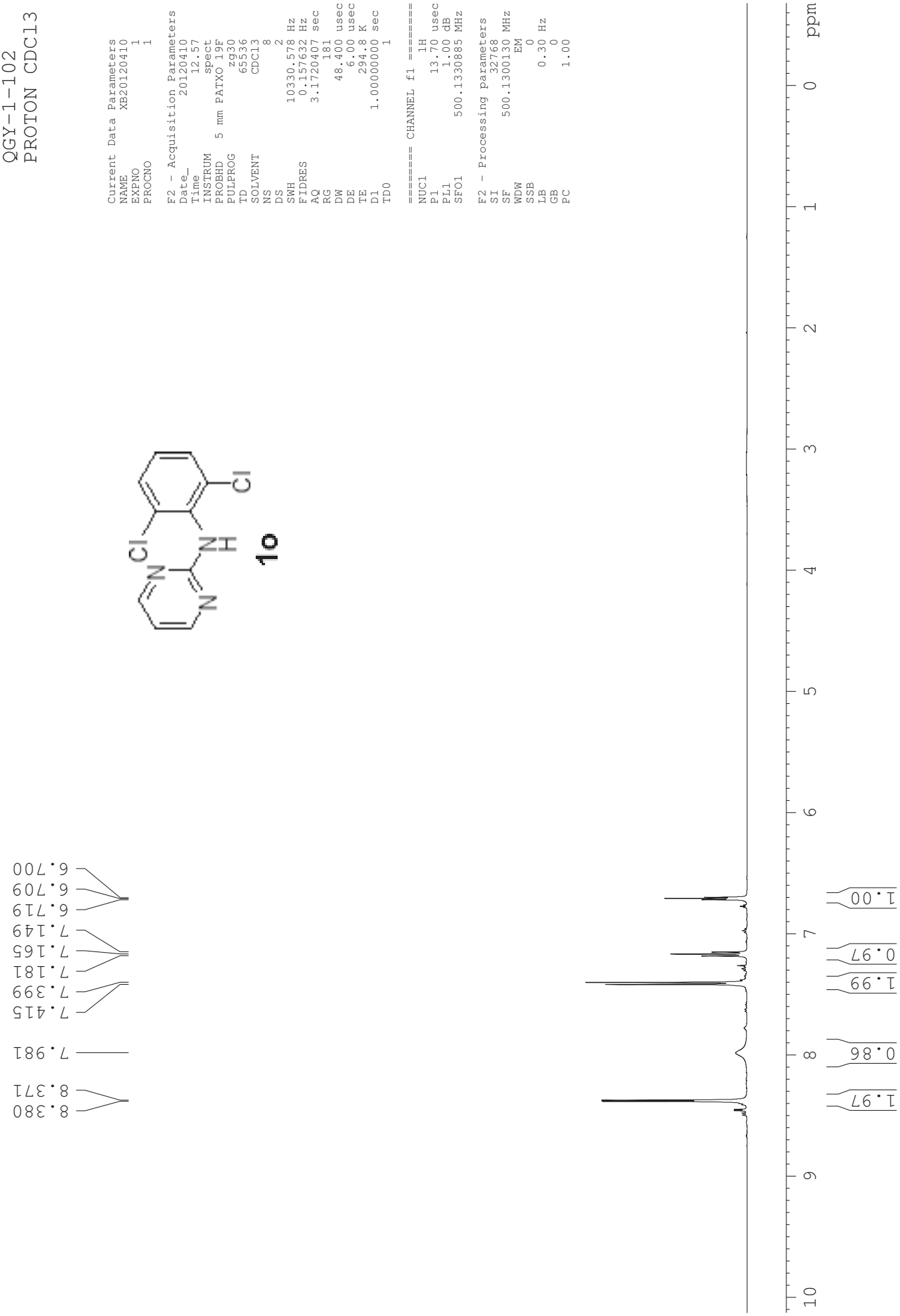

QGY-1-78-b
PROTON CDC13
NAME xb20120331
EXPNO 8
PROCNO 1
Date_ 20120331
Time 13.30
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 362
DW 48.400 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
F
Br
N
H
N
N
1m
8.442
8.433
7.994
7.989
7.982
7.977
7.740
7.449
7.444
7.441
7.436
7.431
7.426
7.423
7.418
7.097
7.080
7.063
6.790
6.780
6.770
ppm
0 1 2 3 4 5 6 7 8 9 10
2.00
0.93
0.92
1.02
0.97
0.98

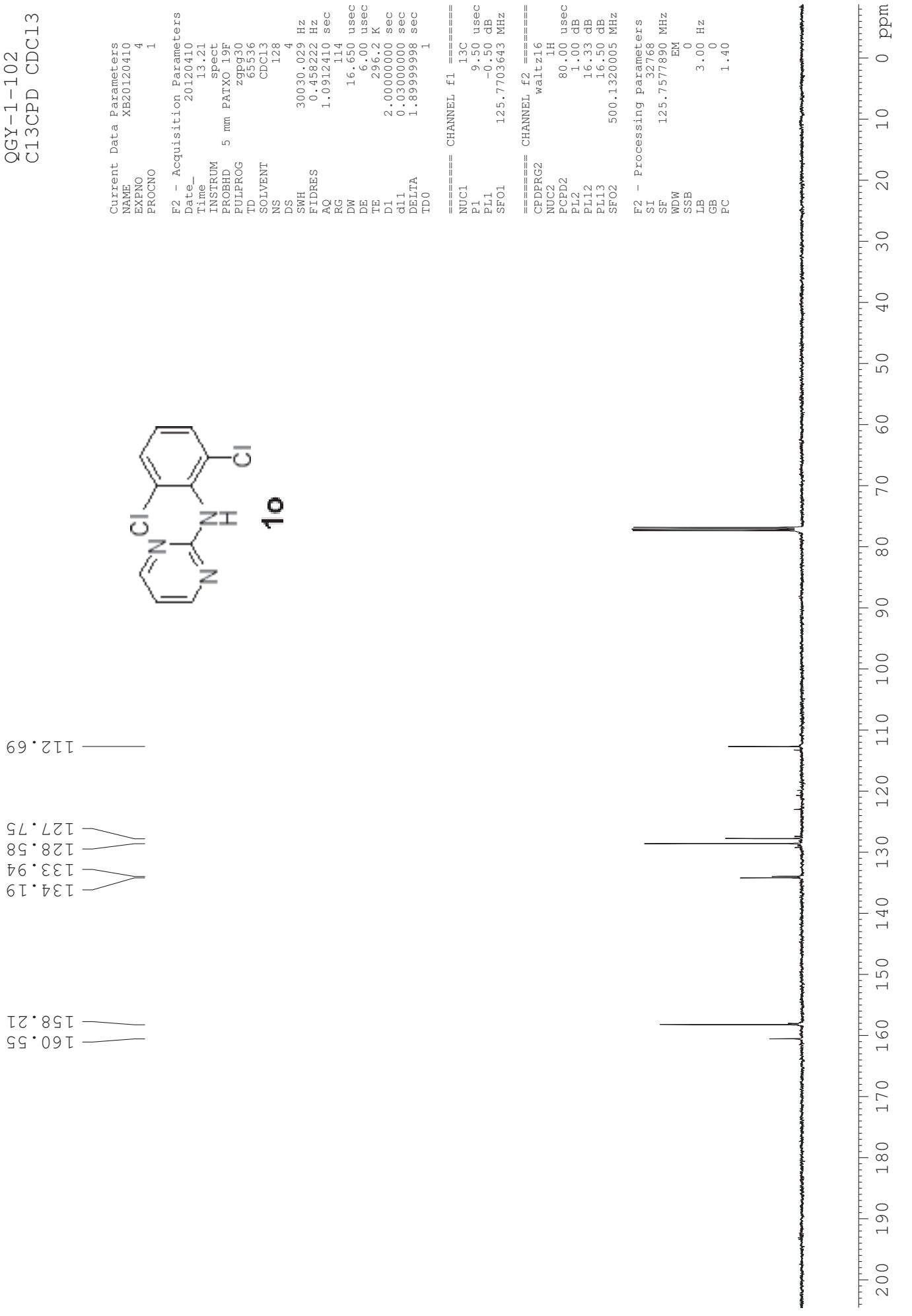

QGY-1-78-b
19Fdeft CDCl3
Current Data Parameters
NAME xb20120401
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120401
Time 17.41
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg
TD 131072
SOLVENT CDCl3
NS 8
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554150 sec
RG 322.5
DW 5.000 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 19.30 usec
PL1 4.00 dB
SFO1 470.5453180 MHz
F2 - Processing parameters
SI 65536
SF 470.5923770 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
-114.96
-114.98
-114.99
-115.00
F
Br
N
H
N
N
1m
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

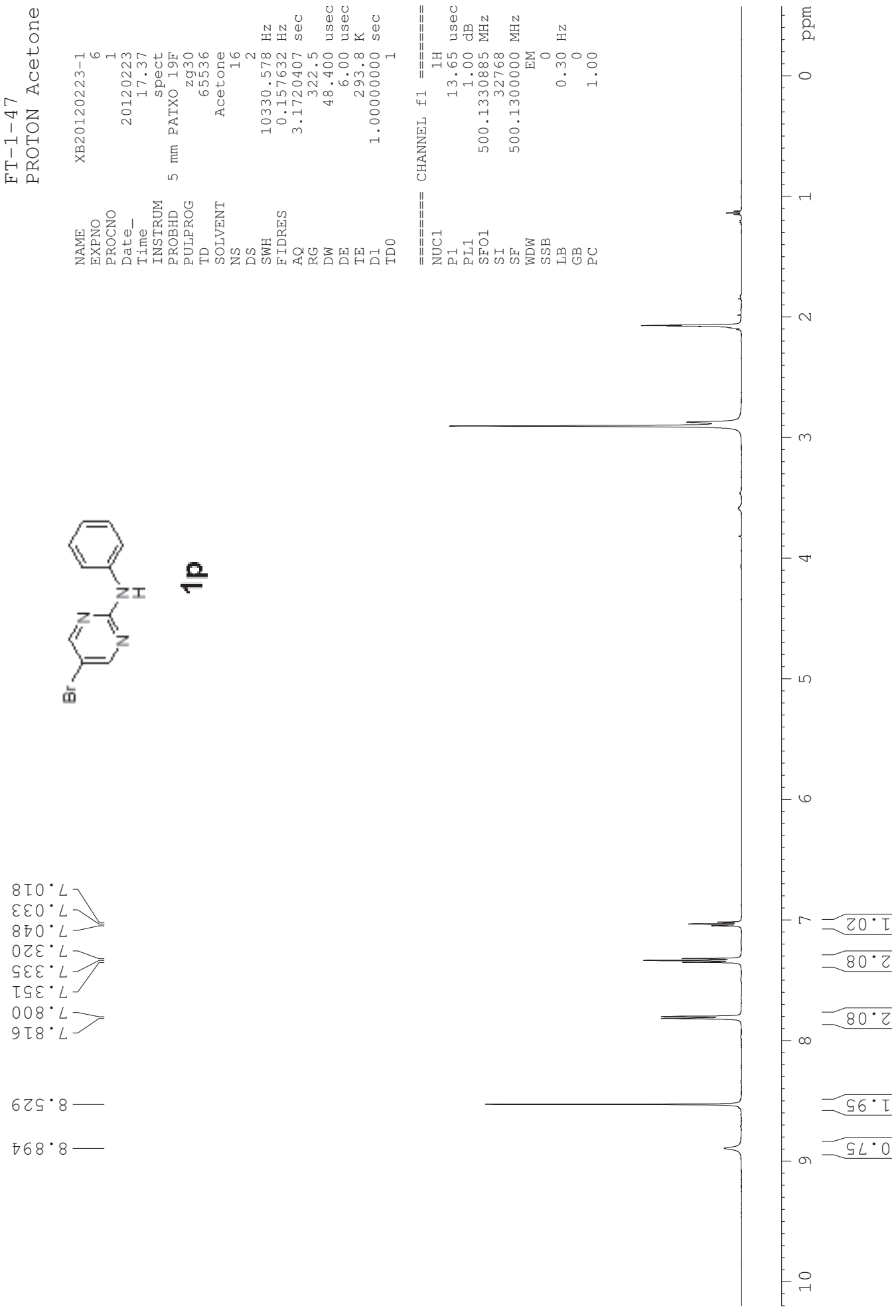

QGY-1-78-b
C13CPD CDC13
Current Data Parameters
NAME xb20120401
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120401
Time 18.05
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 295.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.90
1m
F
Br
N
H
N
N
159.48
157.97
155.93
154.00
136.18
136.16
124.38
120.15
120.09
116.42
116.24
112.95
109.00
108.83
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

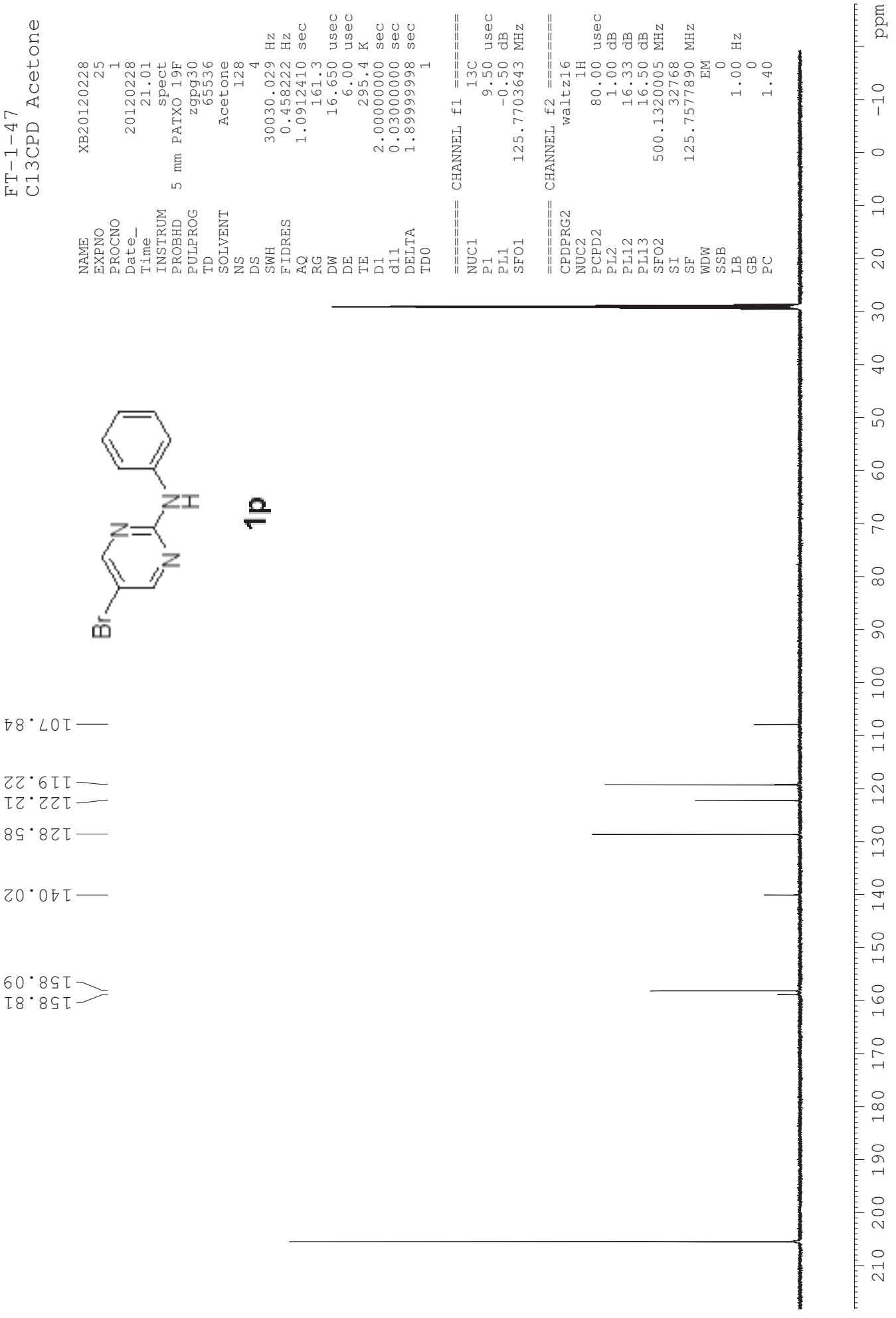

FT-1-96
PROTON CDCl3
Current Data Parameters
NAME XB20120516
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120516
Time 10.06
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1n
N
NH
N
N
9.477
8.689
8.677
8.671
8.667
8.151
8.133
7.886
7.869
7.760
7.744
7.658
7.656
7.641
7.627
7.625
7.407
7.406
7.392
7.378
7.376
6.885
6.876
6.866
0.85
2.95
1.00
1.01
1.04
1.02
1.01
1.01
ppm

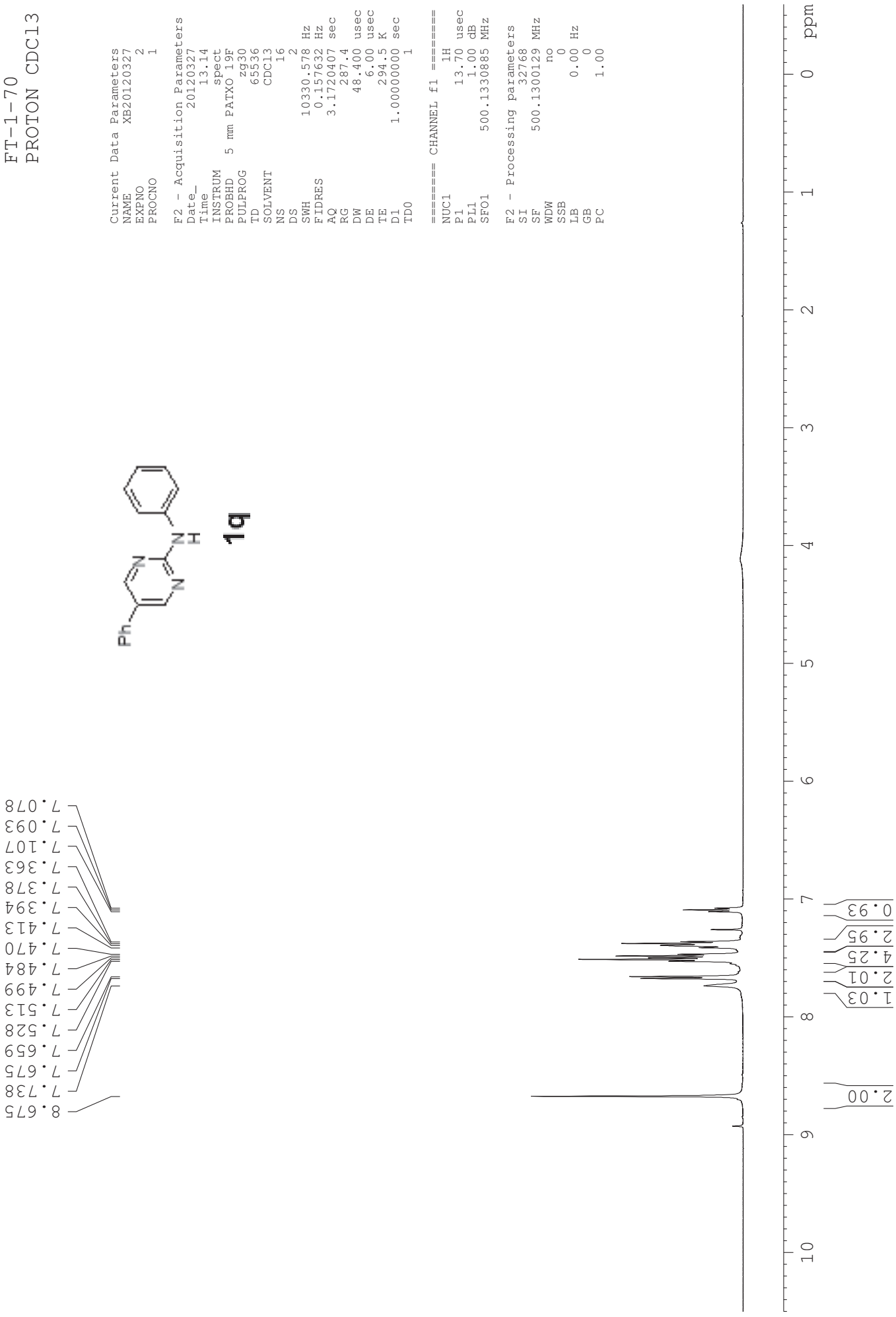

FT-1-96
C13CPD CDC13 I
Current Data Parameters
NAME XB20120516
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120516
Time_ 10.16
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 128
DW 16.650 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
1n
N
NH
N
N
159.47
158.19
152.36
138.01
129.75
127.48
127.05
125.40
124.23
114.05
113.79
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

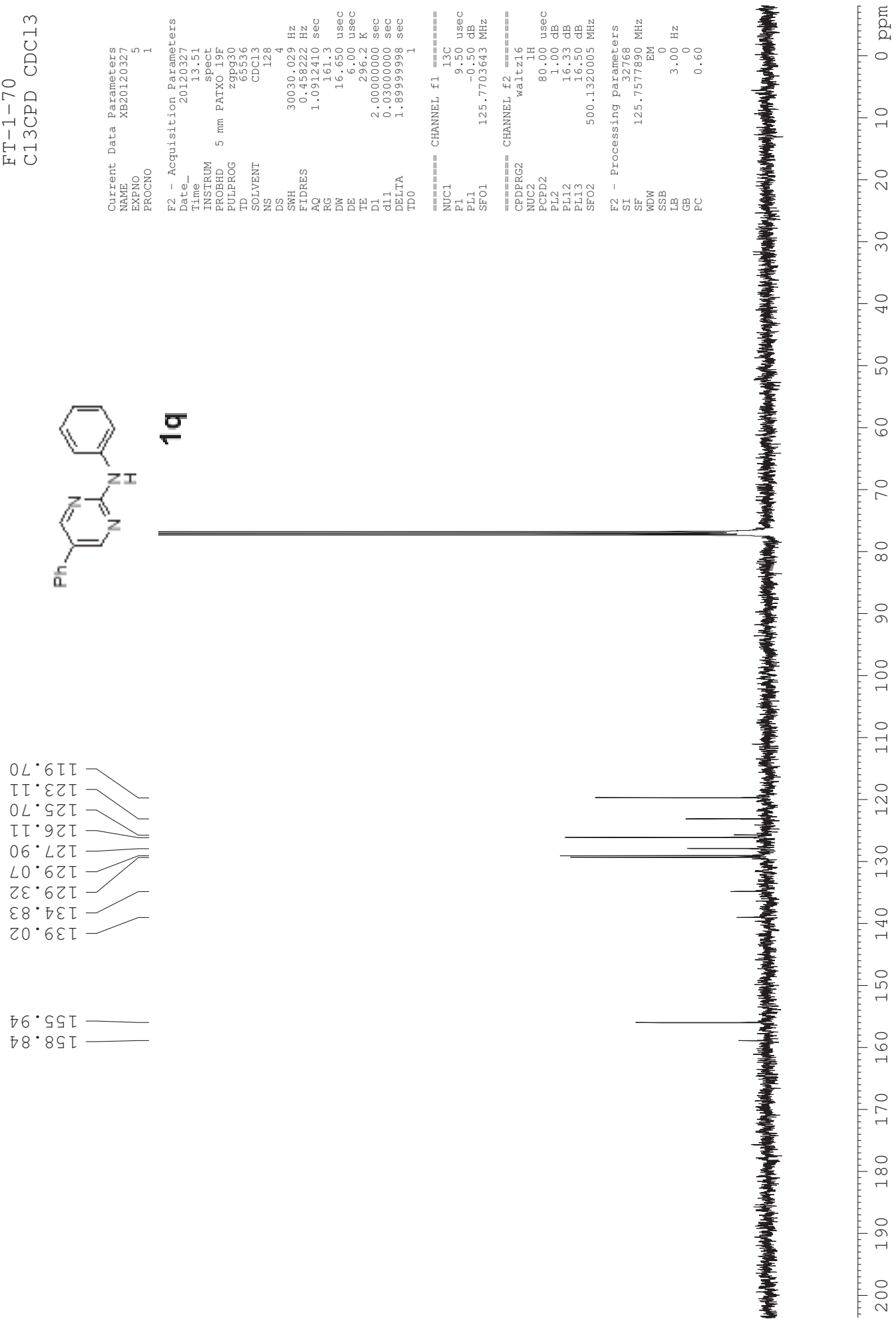

QGY-1-102
PROTON CDC13
Current Data Parameters
NAME XB20120410
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120410
Time_ 12.57
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
NH
N
N
Cl
1o
8.380
8.371
7.981
7.415
7.399
7.181
7.165
7.149
6.719
6.709
6.700
1.00
0.97
1.99
0.86
1.97
ppm

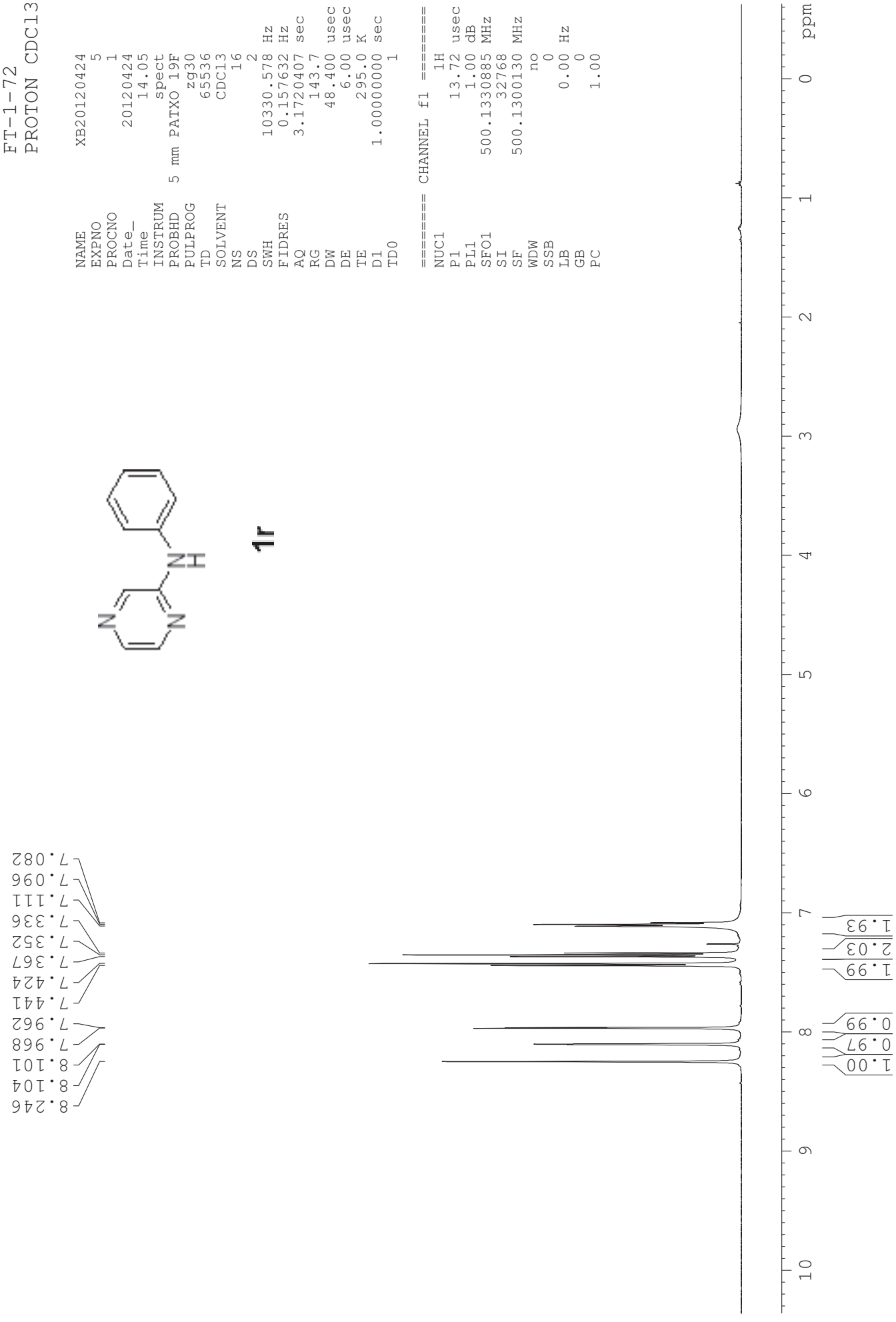

QGY-1-102
C13CPD CDC13
Current Data Parameters
NAME XB20120410
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120410
Time 13.21
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
Cl
NH
N
N
Cl
1o
112.69
127.75
128.58
133.94
134.19
158.21
160.55
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

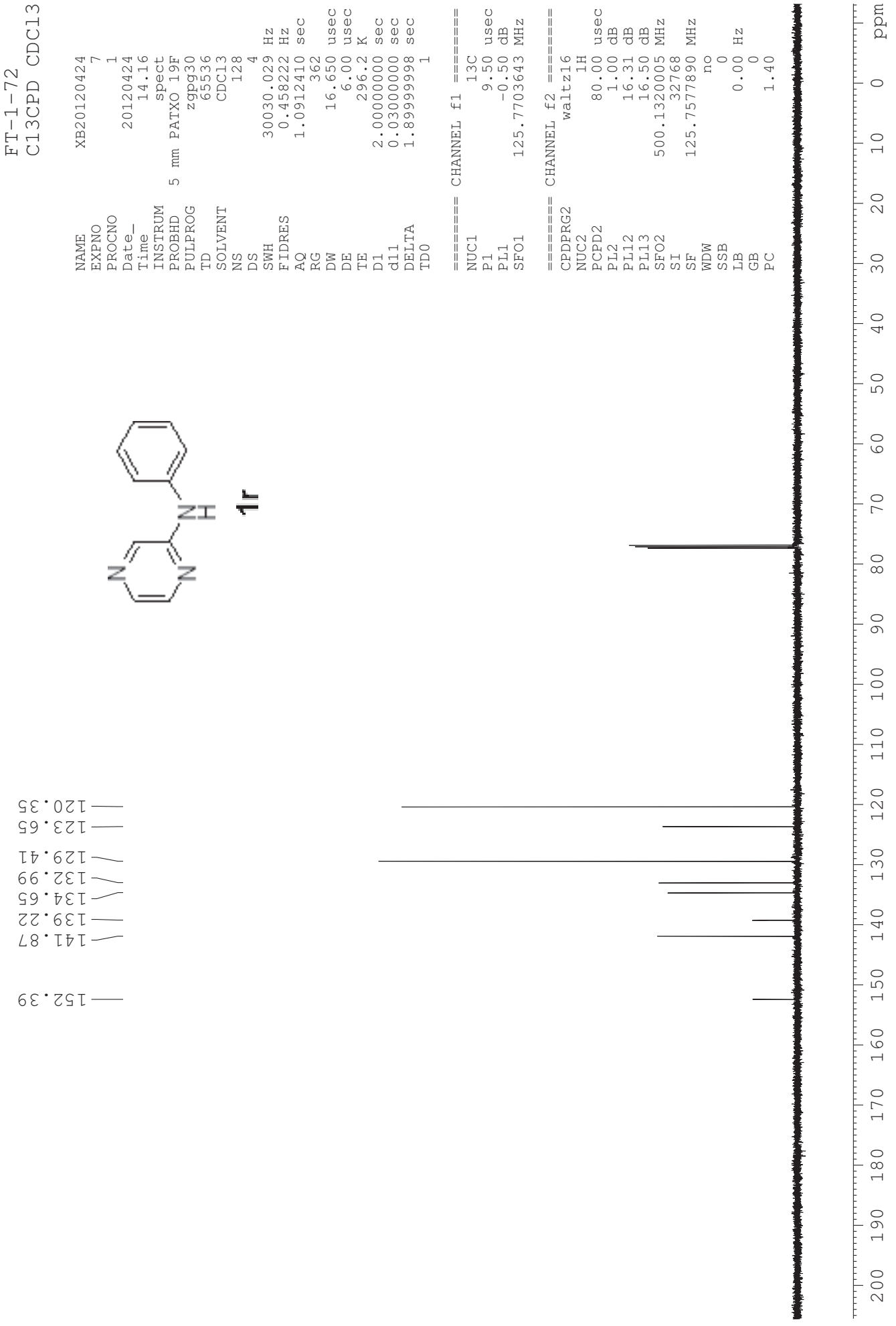

FT-1-47
PROTON Acetone
NAME XB20120223-1
EXPNO 6
PROCNO 1
Date_ 20120223
Time 17.37
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 322.5
DW 48.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.65 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1p
Br
N
H
N
N
8.894
8.529
7.816
7.800
7.351
7.335
7.320
7.048
7.033
7.018
0.75
1.95
2.08
2.08
1.02
ppm

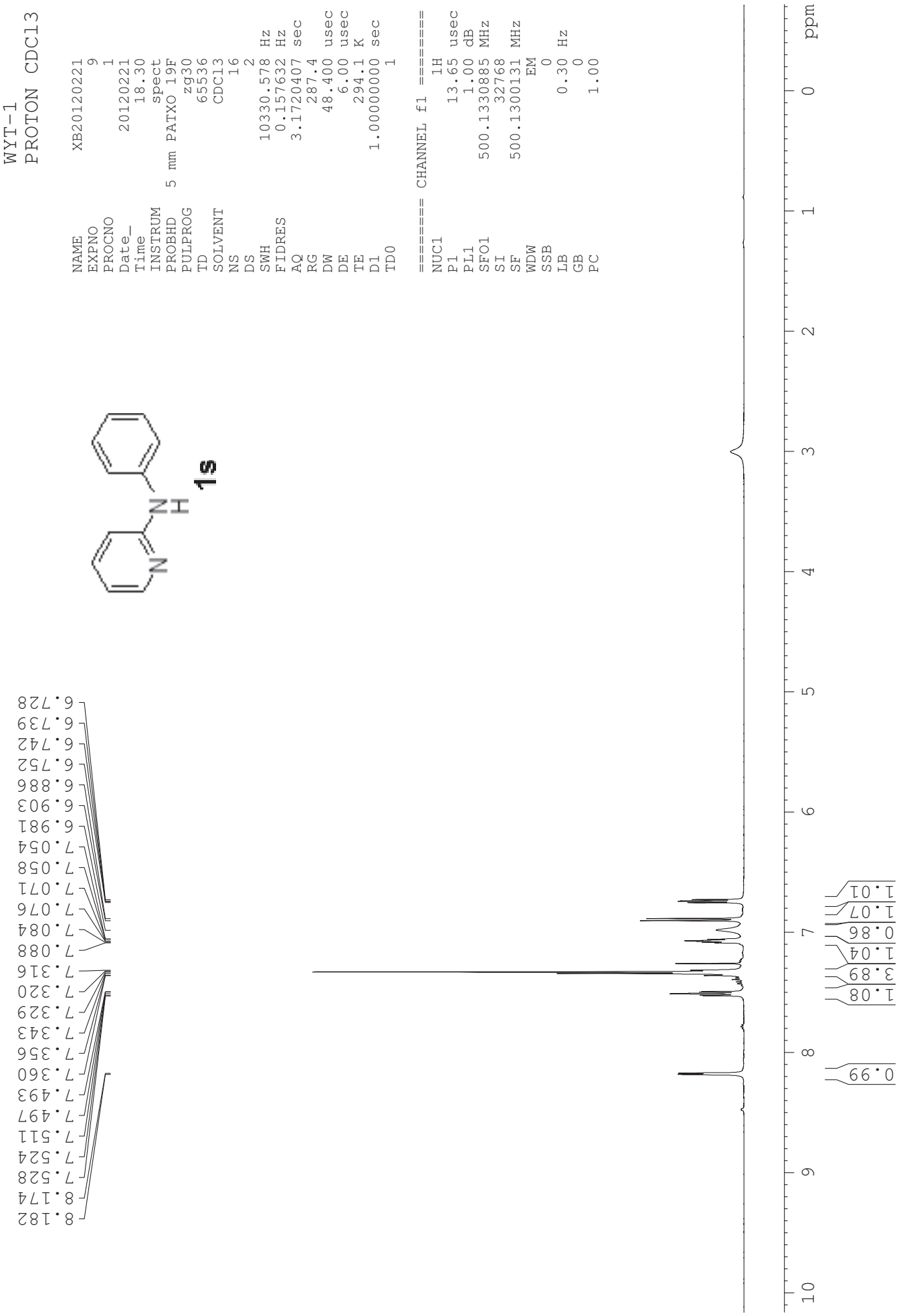

FT-1-47
C13CPD Acetone
NAME XB20120228
EXPNO 25
PROCNO 1
Date_ 20120228
Time 21.01
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1p
Br
N
NH
N
158.81
158.09
140.02
128.58
122.21
119.22
107.84
ppm

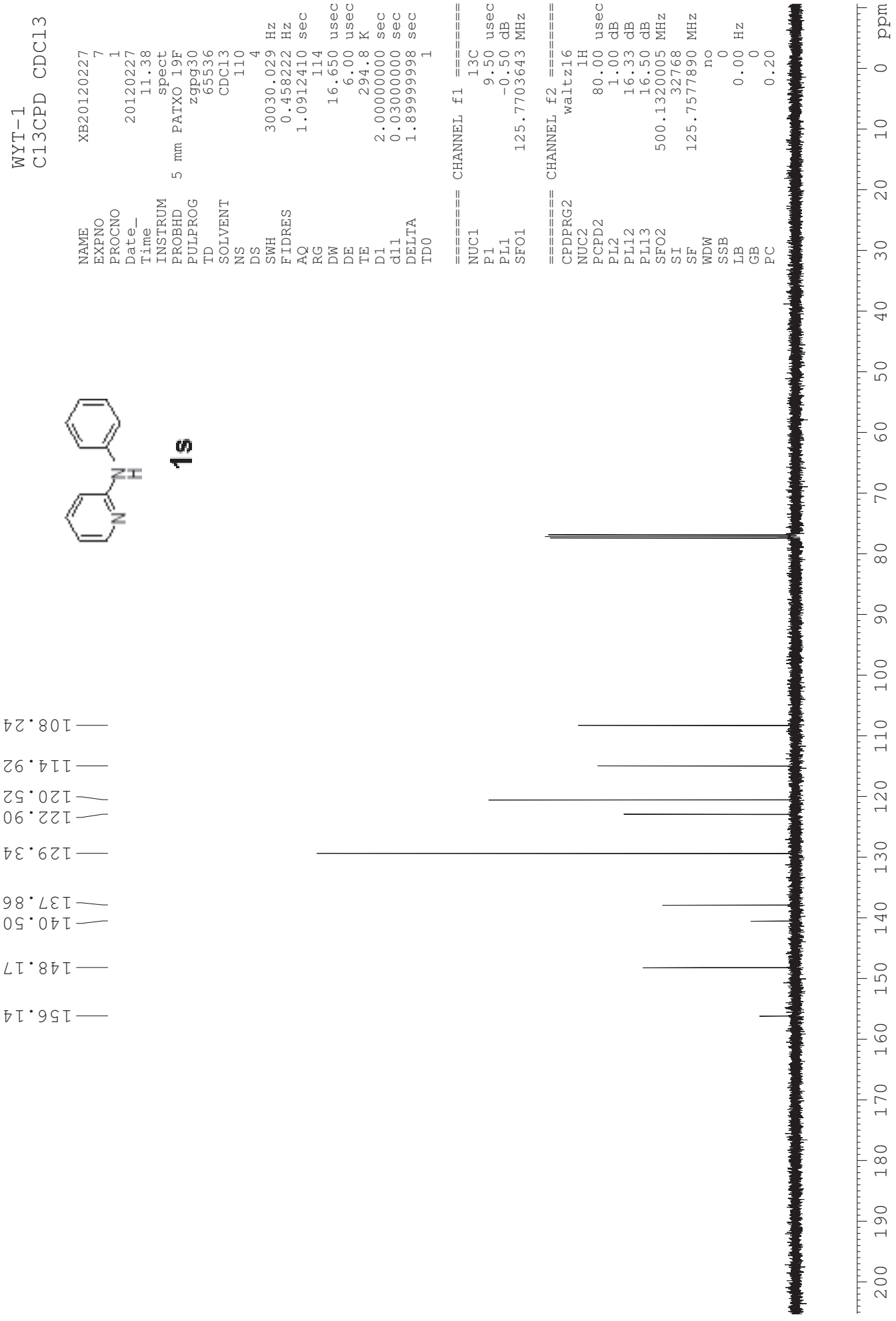

FT-1-70
PROTON CDC13
Current Data Parameters
NAME XB20120327
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120327
Time 13.14
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1q
Ph
N
H
8.675
7.738
7.675
7.659
7.528
7.513
7.499
7.484
7.470
7.413
7.394
7.378
7.363
7.107
7.093
7.078
0.93
2.95
4.25
2.01
1.03
2.00
ppm

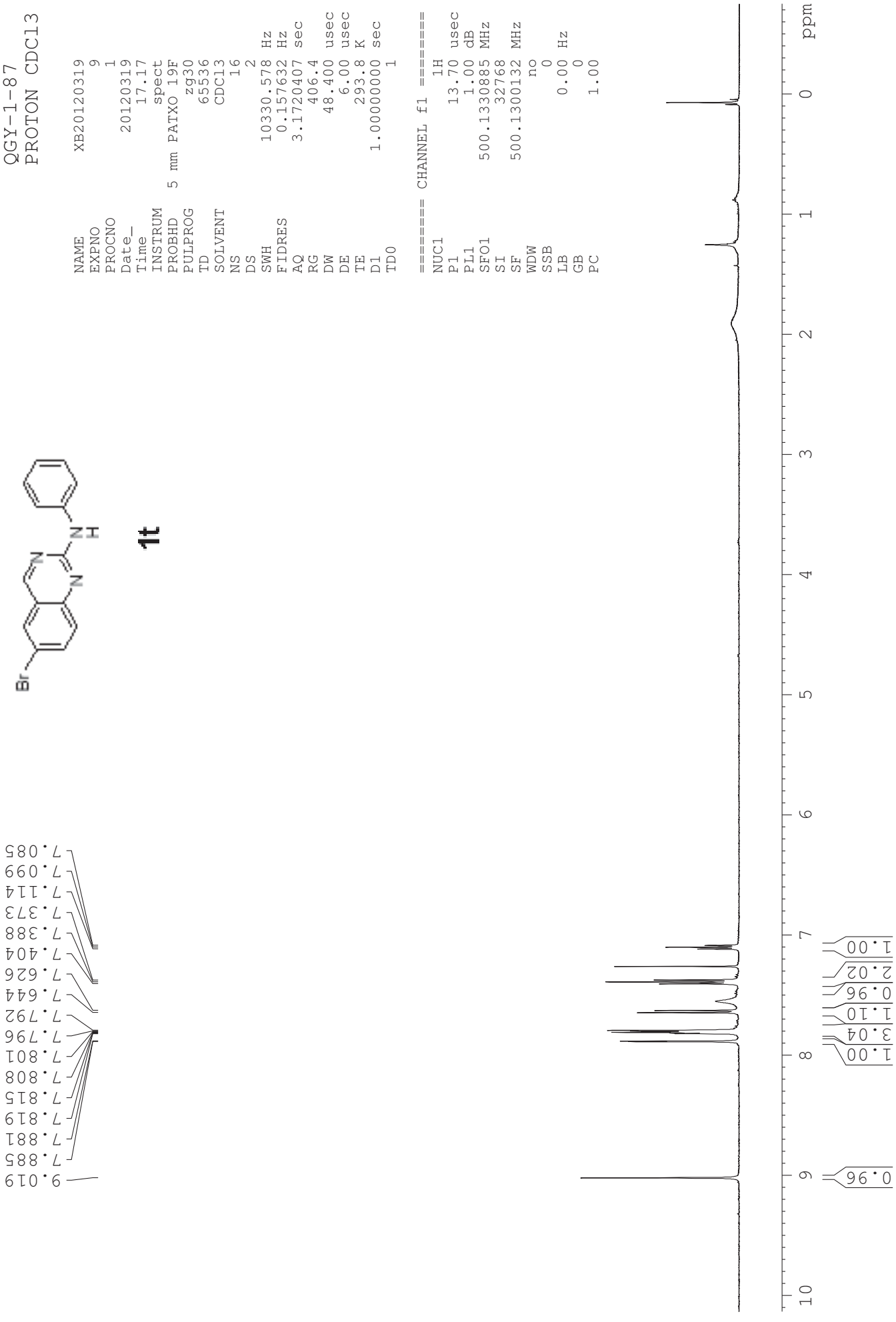

FT-1-70
C13CPD CDCl3
Current Data Parameters
NAME XB20120327
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120327
Time_ 13.51
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.60
1q
Ph
N
H
158.84
155.94
139.02
134.83
129.32
129.07
127.90
126.11
125.70
123.11
119.70
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

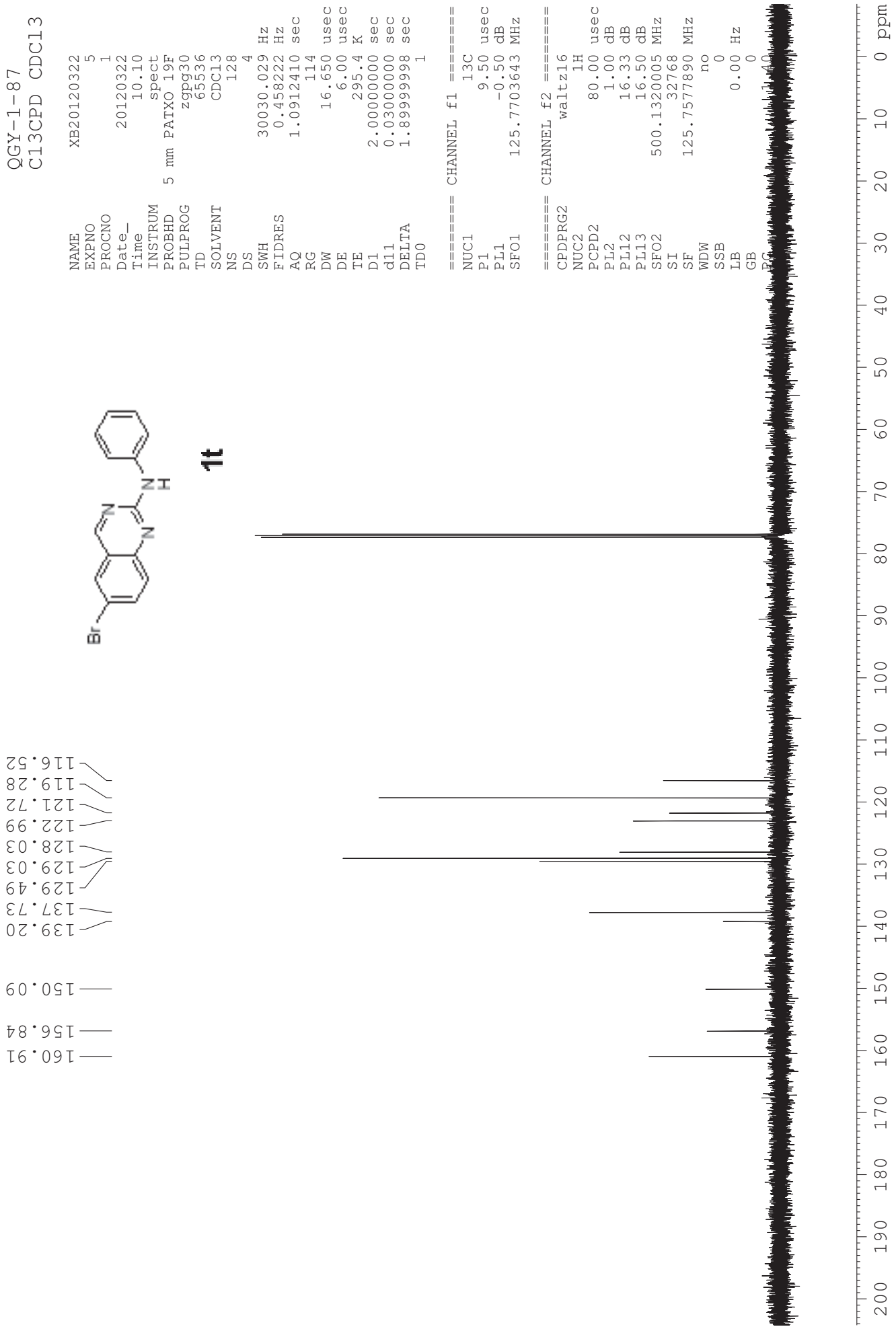

FT-1-72
PROTON CDC13
NAME XB20120424
EXPNO 5
PROCNO 1
Date_ 20120424
Time 14.05
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.17204407 sec
RG 143.7
DW 48.400 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300130 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1r
8.246
8.104
8.101
7.968
7.962
7.441
7.424
7.367
7.352
7.336
7.111
7.096
7.082
1.00
0.97
0.99
1.99
2.03
1.93
ppm

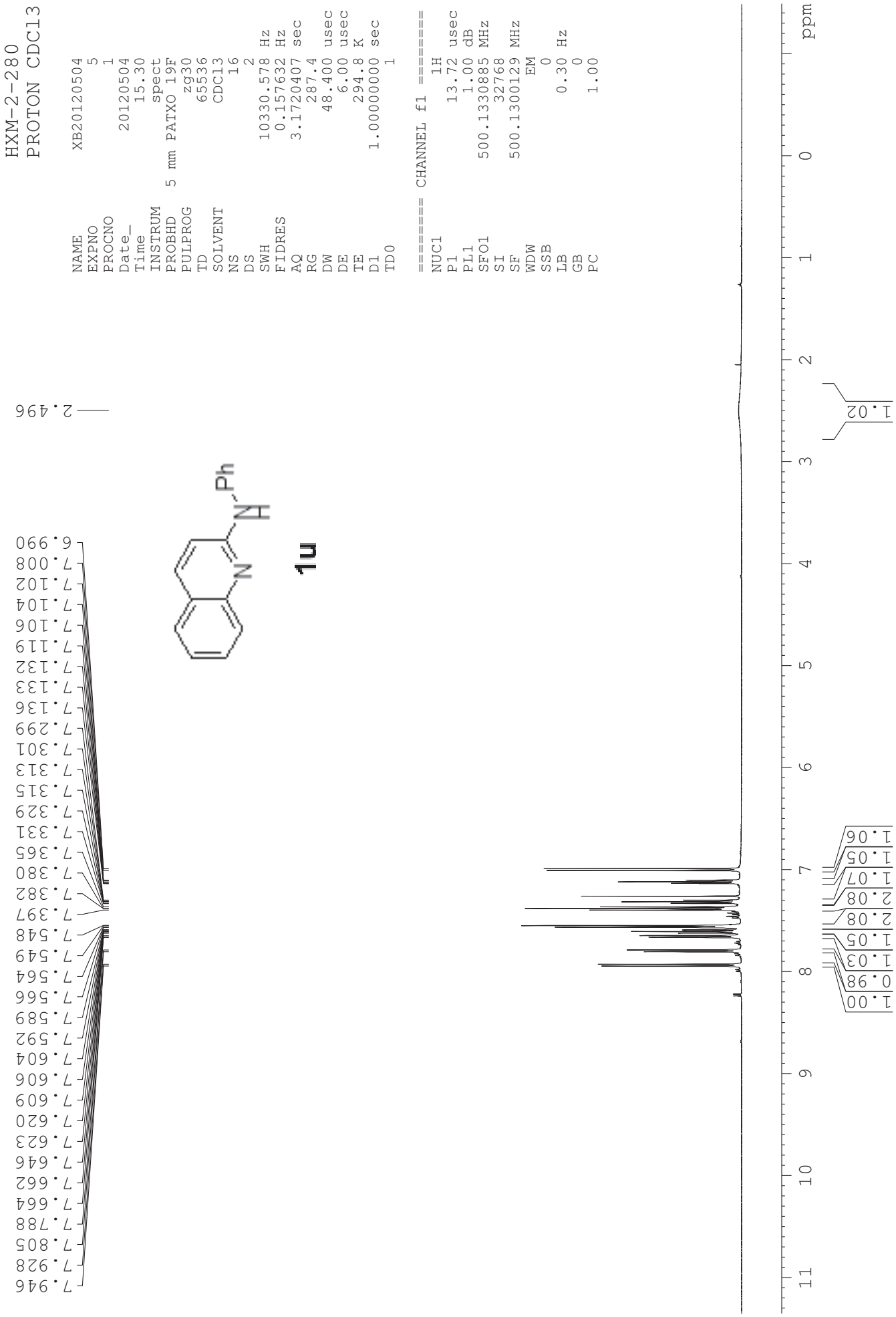

FT-1-72
C13CPD CDC13
NAME XB20120424
EXPNO 7
PROCNO 1
Date_ 20120424
Time 14.16
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 362
DW 16.650 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
========== CHANNEL f1 ==========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
1r
152.39
141.87
139.22
134.65
132.99
129.41
123.65
120.35
ppm

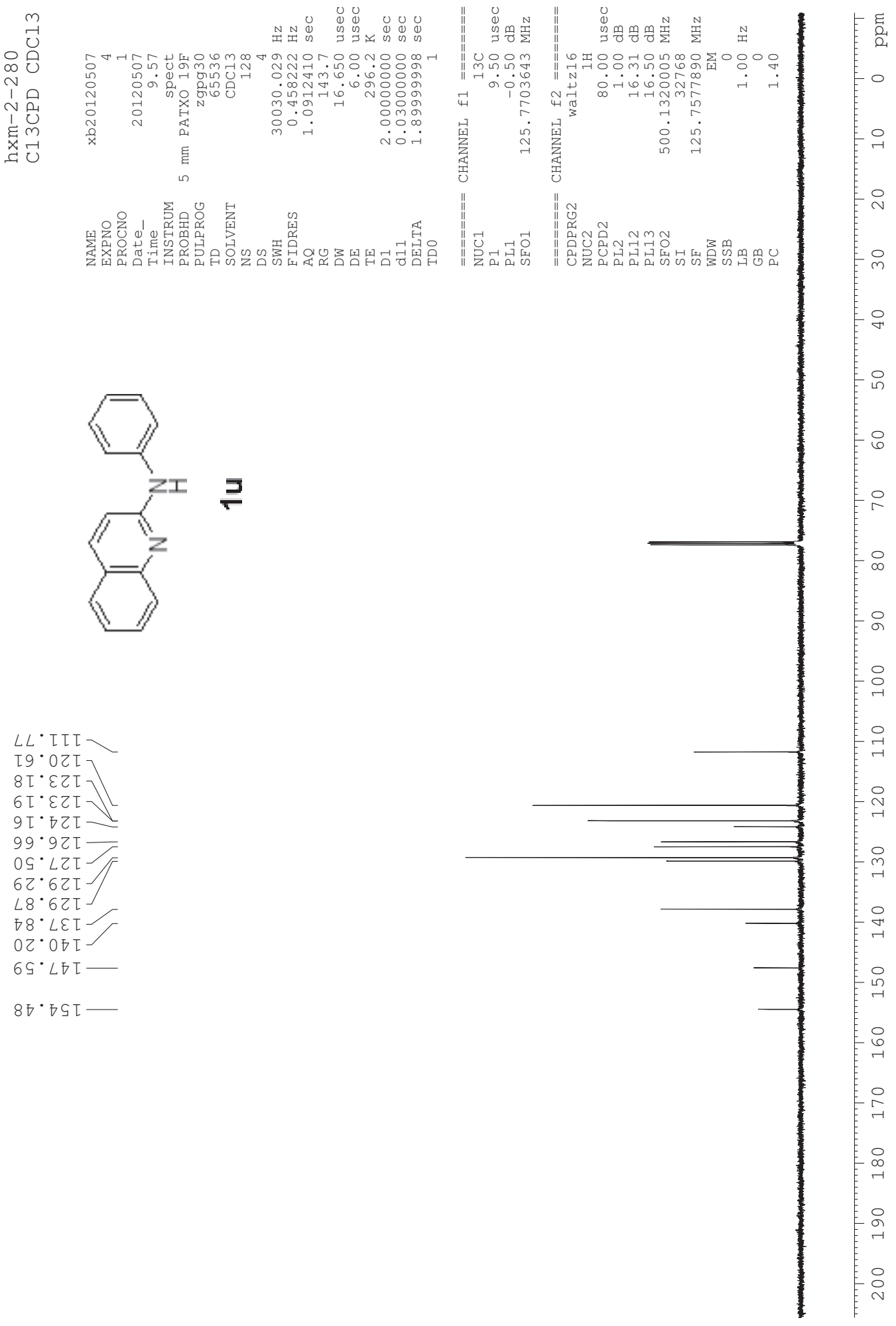

WYT-1
PROTON CDC13
NAME XB20120221
EXPNO 9
PROCNO 1
Date_ 20120221
Time 18.30
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.65 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
NH
N
8.182
8.174
7.528
7.524
7.511
7.497
7.493
7.360
7.356
7.343
7.329
7.320
7.316
7.088
7.084
7.076
7.071
7.058
7.054
6.981
6.903
6.886
6.752
6.742
6.739
6.728
0.99
1.08
3.89
1.04
0.86
1.07
1.01
ppm

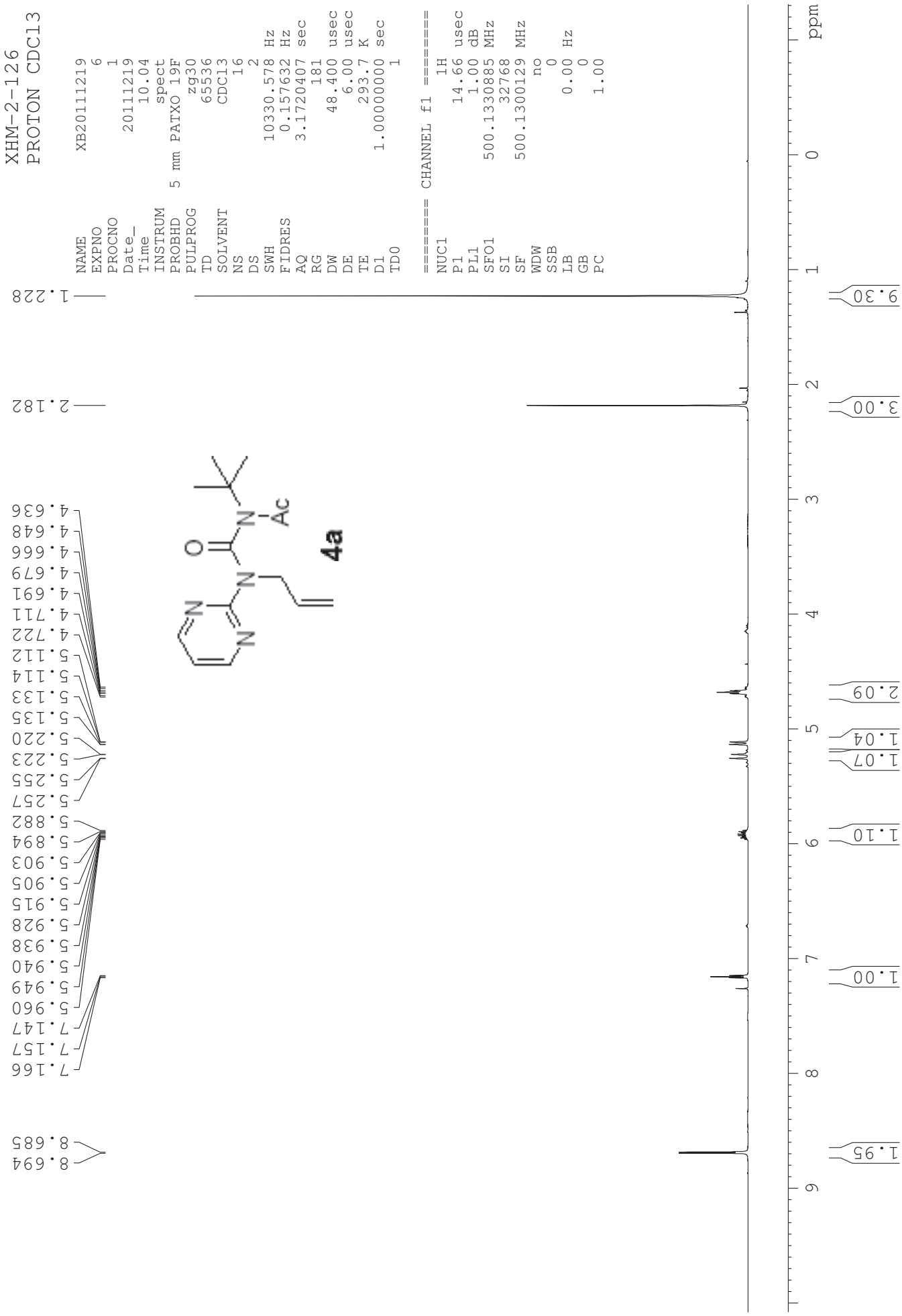

WYT-1
C13CPD CDC13
NAME XB20120227
EXPNO 7
PROCNO 1
Date_ 20120227
Time 11.38
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 110
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20
19
156.14
148.17
140.50
137.86
129.34
122.90
120.52
114.92
108.24
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

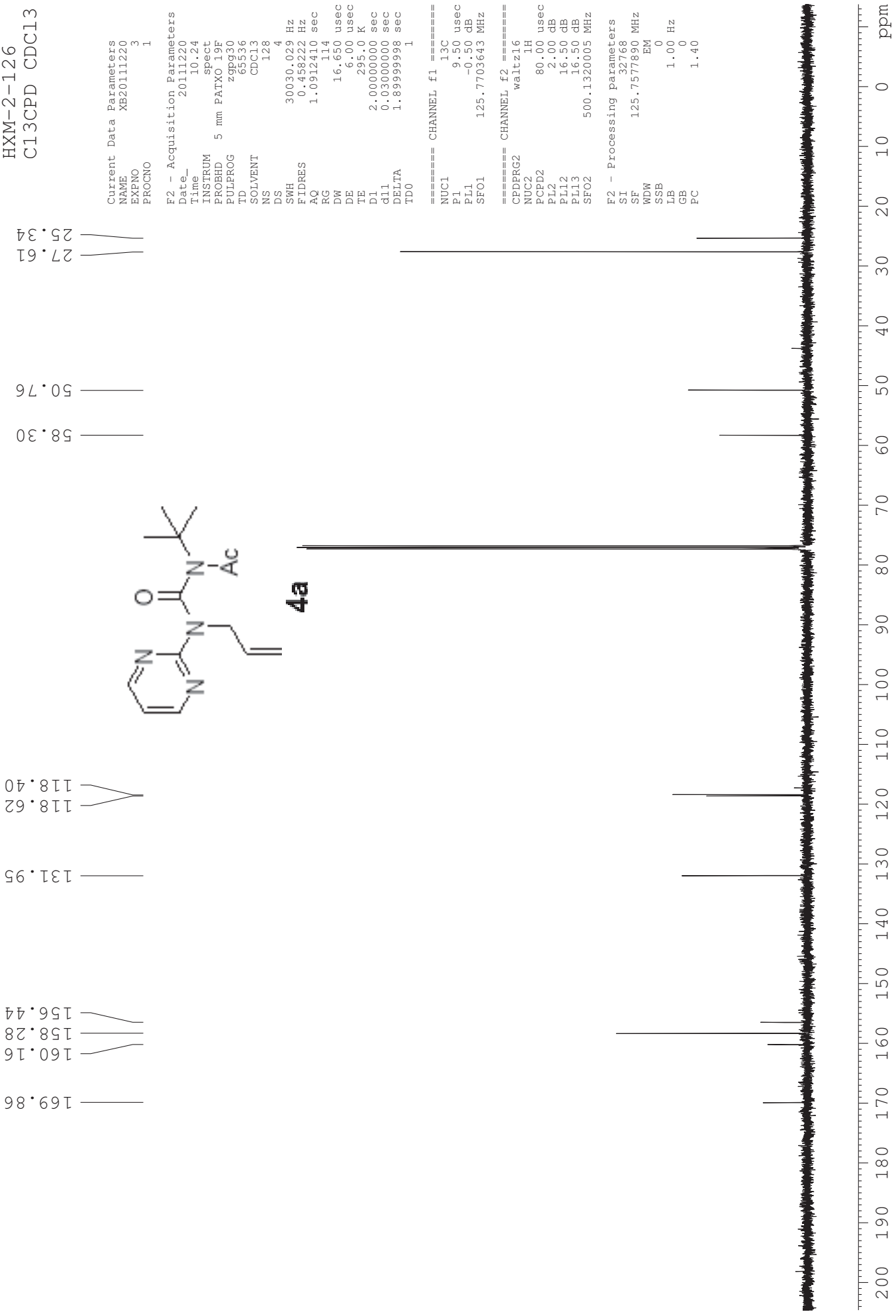

QGY-1-87
PROTON CDC13
NAME XB20120319
EXPNO 9
PROCNO 1
Date_ 20120319
Time 17.17
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 406.4
DW 48.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1t
Br
N
H
N
9.019
7.885
7.881
7.819
7.815
7.808
7.801
7.796
7.792
7.644
7.626
7.404
7.388
7.373
7.114
7.099
7.085
0.96
1.00
3.04
1.10
0.96
2.02
1.00
ppm
0
1
2
3
4
5
6
7
8
9
10

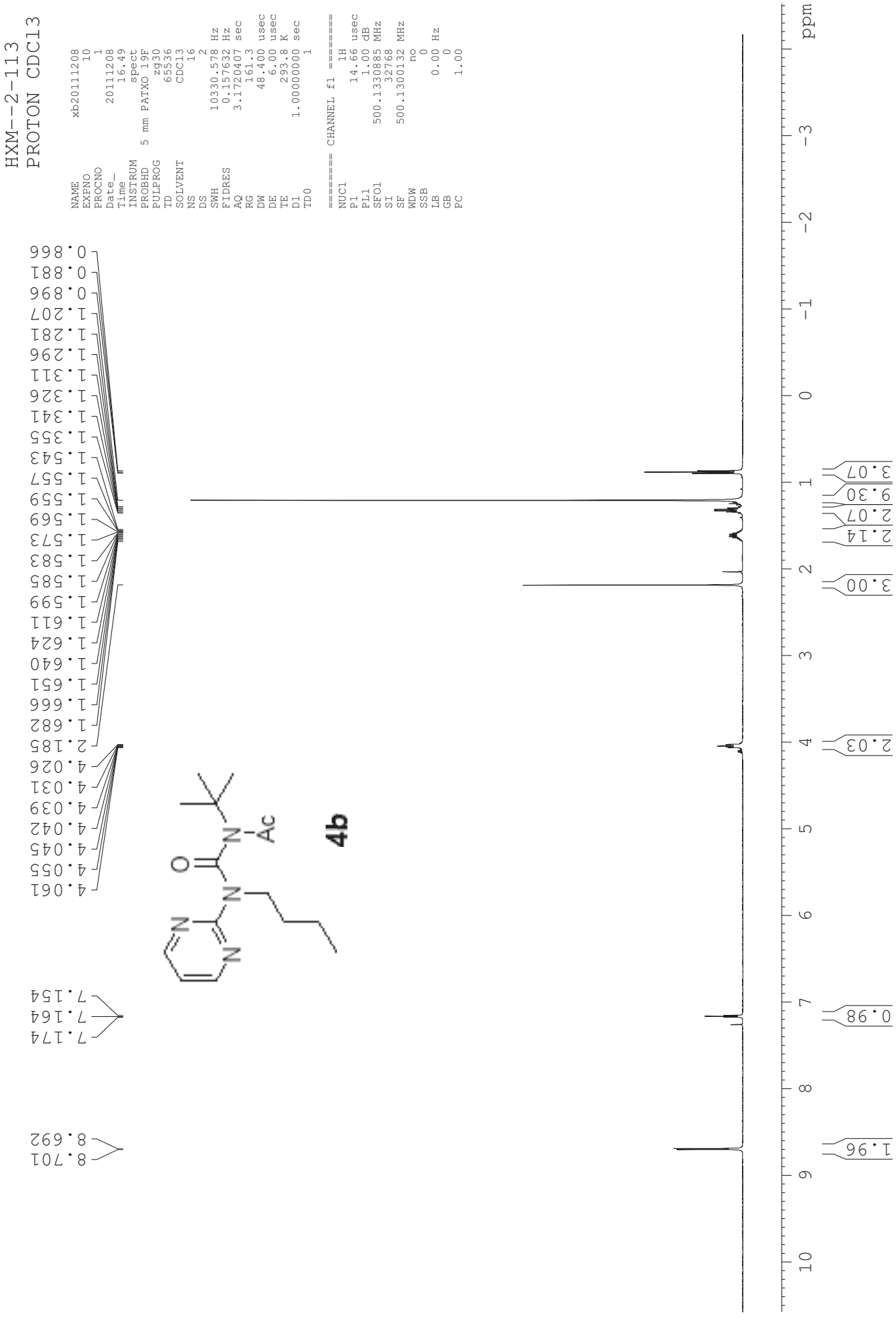

QGY-1-87
C13CPD CDCl3
NAME XB20120322
EXPNO 5
PROCNO 1
Date_ 20120322
Time 10.10
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
1t
Br
N
H
160.91
156.84
150.09
139.20
137.73
129.49
129.03
128.03
122.99
121.72
119.28
116.52
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

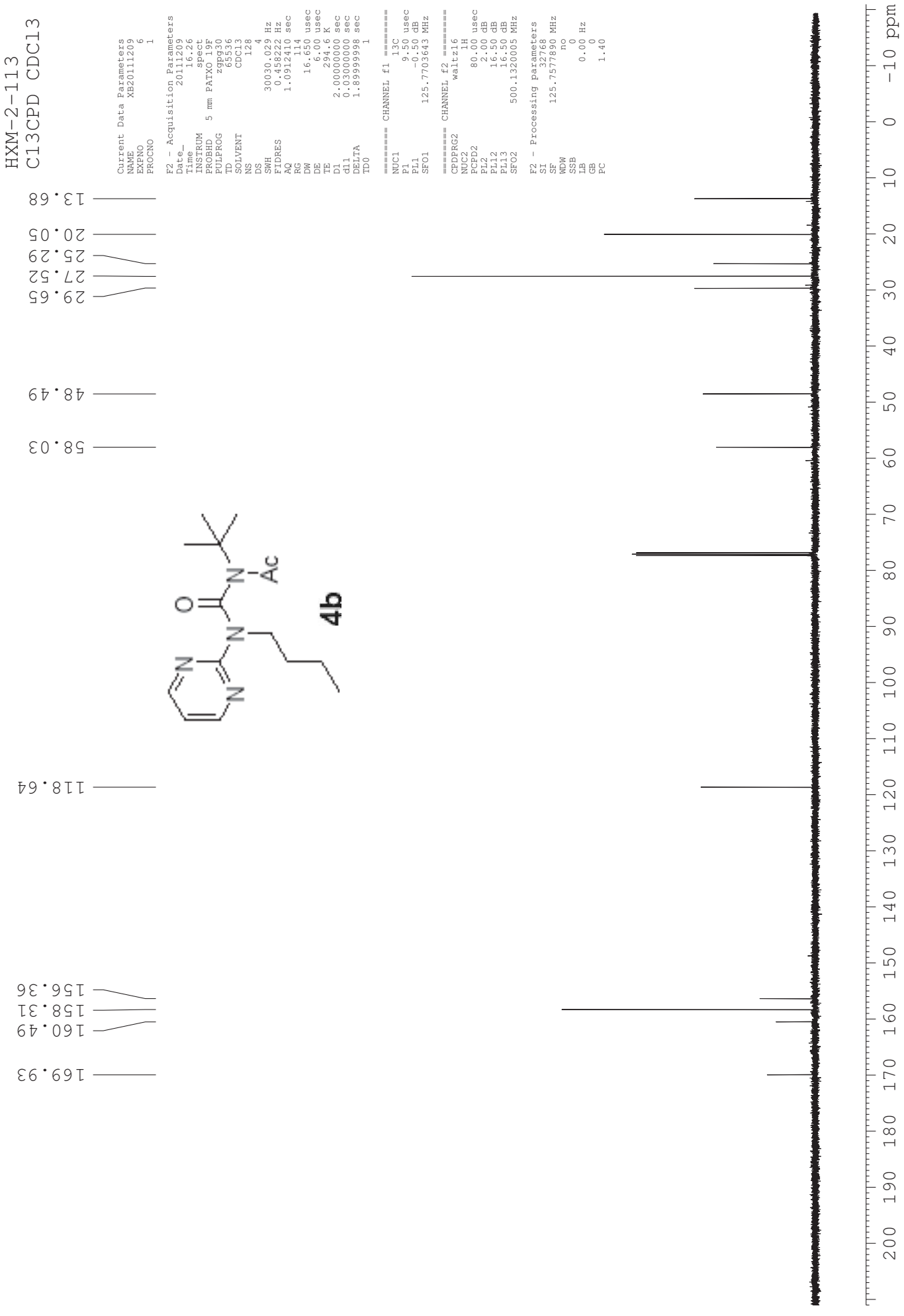

HXM-2-280
PROTON CDC13
NAME XB20120504
EXPNO 5
PROCNO 1
Date_ 20120504
Time 15.30
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
2.496
1u
Ph
N
H
7.946
7.928
7.805
7.788
7.664
7.662
7.646
7.623
7.620
7.609
7.606
7.604
7.592
7.589
7.566
7.564
7.549
7.548
7.397
7.382
7.380
7.365
7.331
7.329
7.315
7.313
7.301
7.299
7.136
7.133
7.132
7.119
7.106
7.104
7.102
7.008
6.990
1.02
1.00
0.98
1.03
1.05
2.08
2.08
1.07
1.05
1.06
ppm

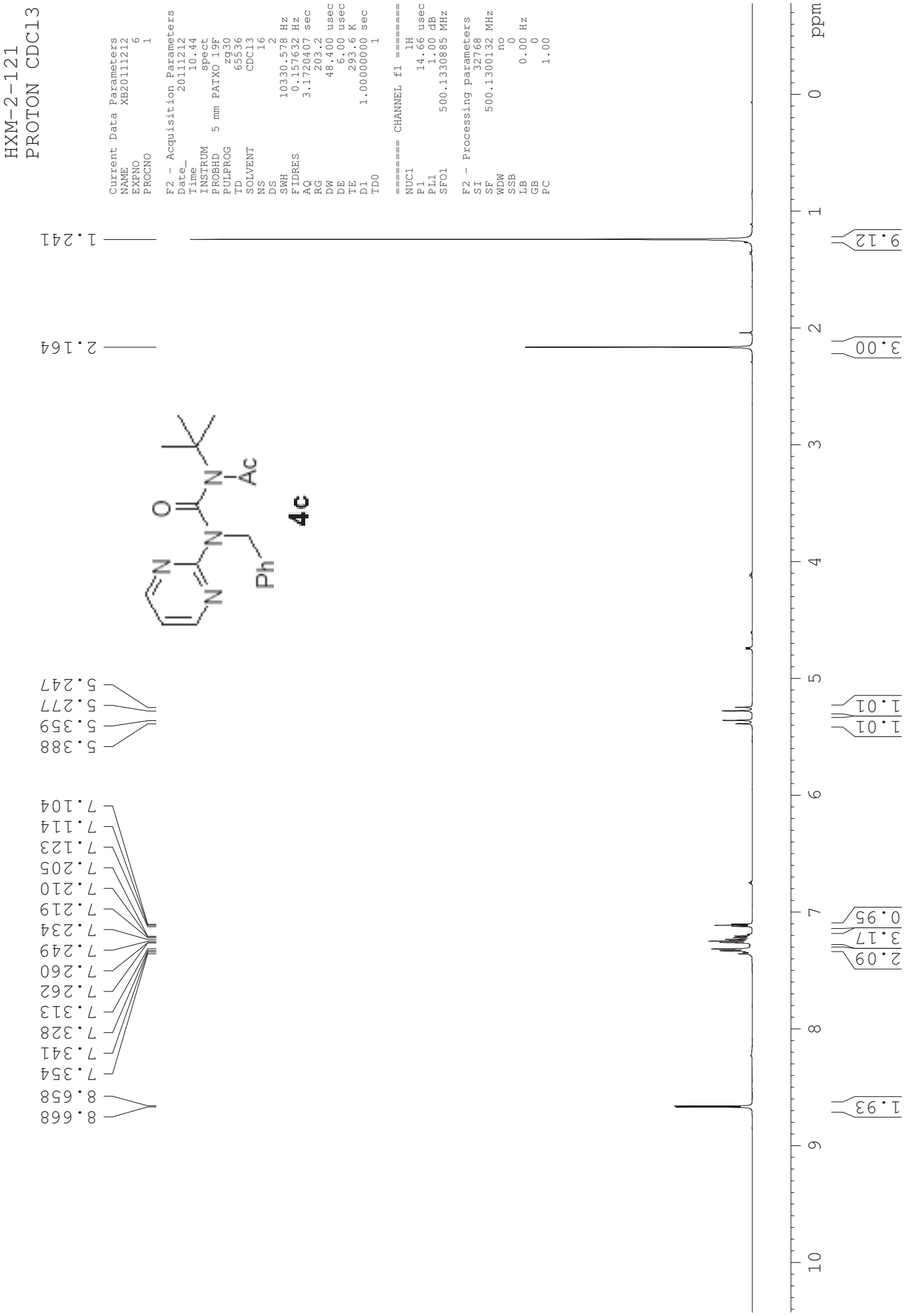

hxm-2-280
C13CPD CDC13
NAME xb20120507
EXPNO 4
PROCNO 1
Date_ 20120507
Time 9.57
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1u
NH
N
154.48
147.59
140.20
137.84
129.87
129.29
127.50
126.66
124.16
123.19
123.18
120.61
111.77
ppm

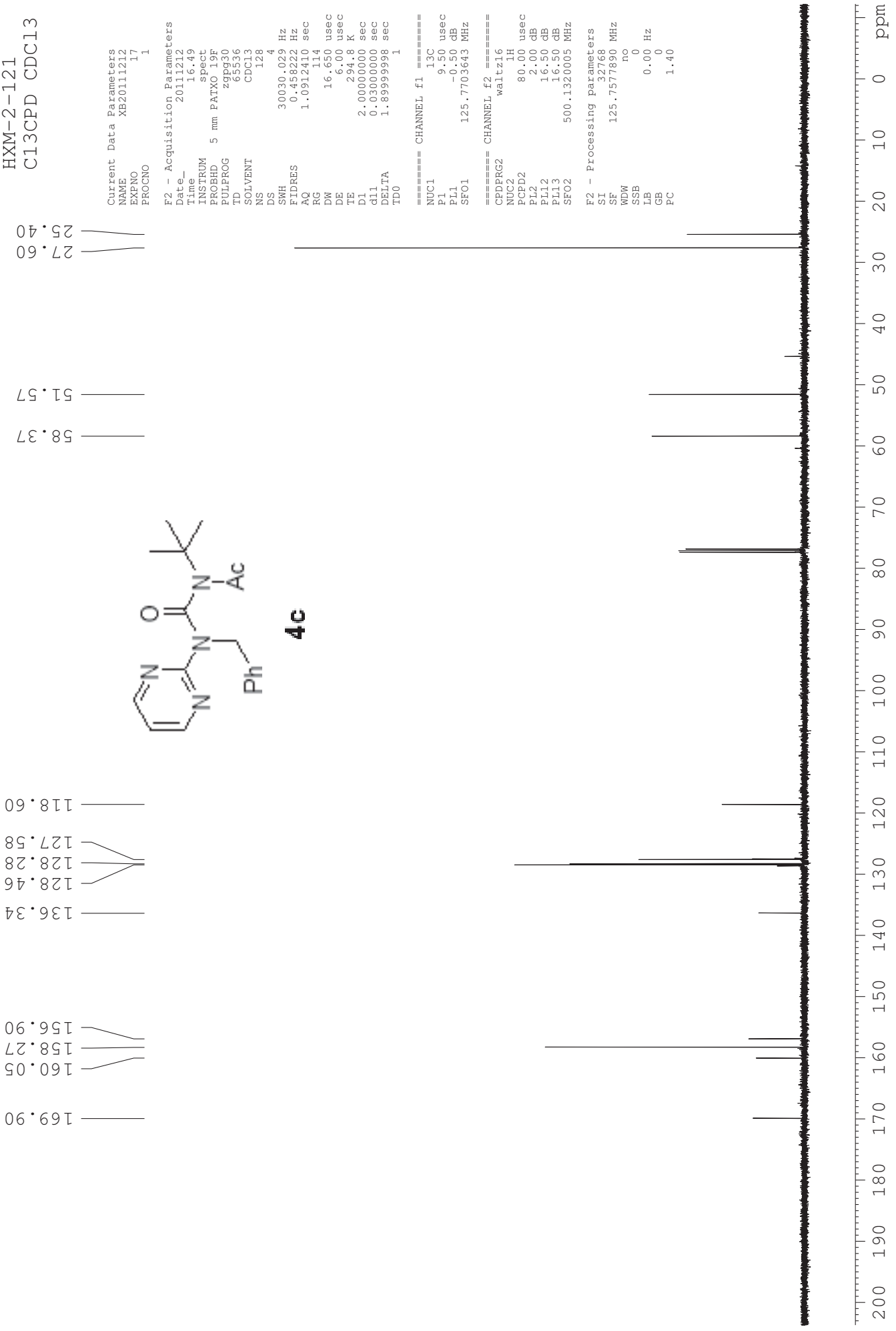

XHM-2-126
PROTON CDC13
NAME XB20111219
EXPNO 6
PROCNO 1
Date_ 20111219
Time 10.04
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.228
2.182
4.636
4.648
4.666
4.679
4.691
4.711
4.722
5.112
5.114
5.133
5.135
5.220
5.223
5.255
5.257
5.882
5.894
5.903
5.905
5.915
5.928
5.938
5.940
5.949
5.960
7.147
7.157
7.166
8.685
8.694
4a
9.30
3.00
2.09
1.04
1.07
1.10
1.00
1.95
ppm

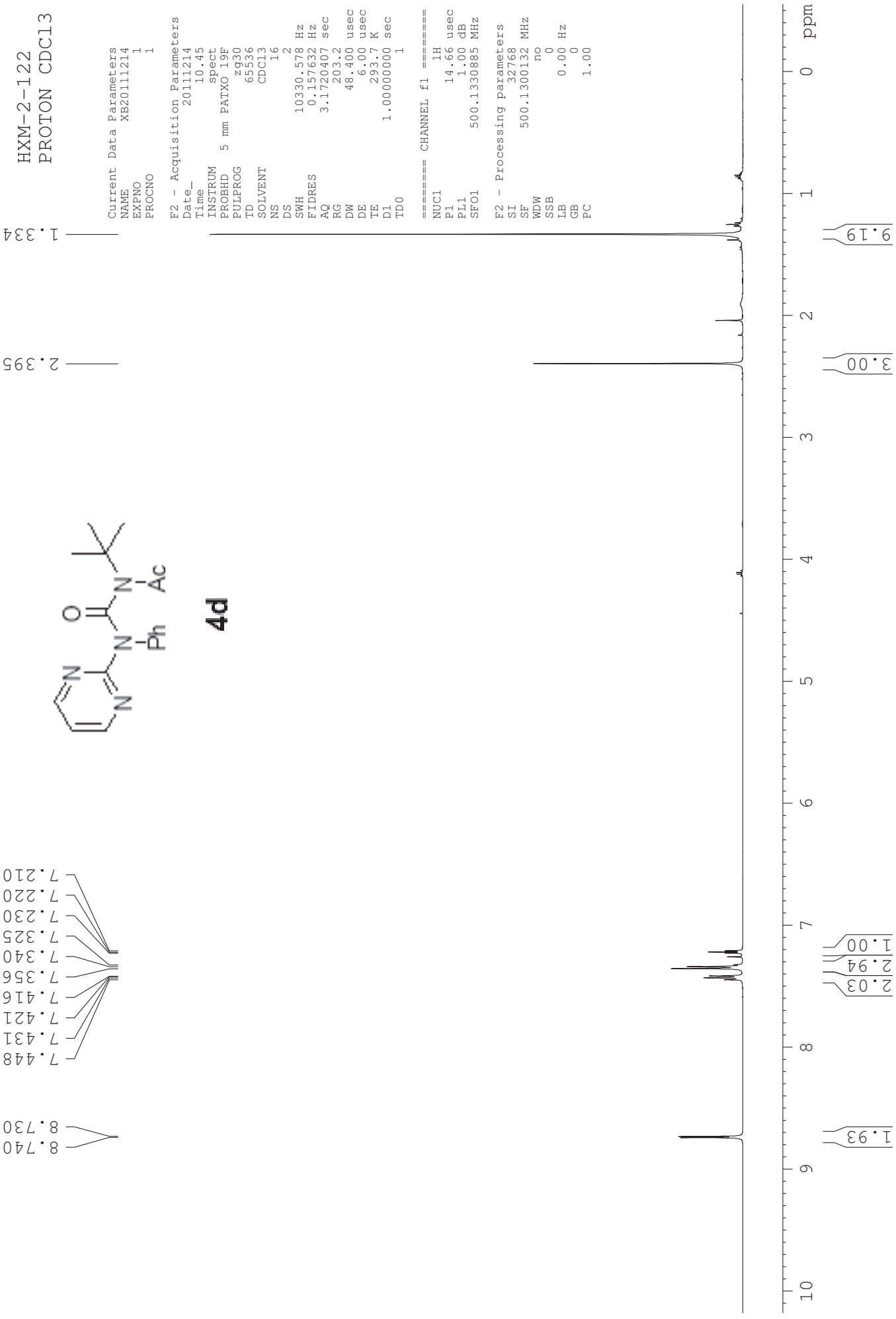

HXM-2-126
C13CPD CDC13
Current Data Parameters
NAME XB20111220
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111220
Time 10.24
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 295.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
25.34
27.61
50.76
58.30
118.40
118.62
131.95
156.44
158.28
160.16
169.86
4a
Ac
N
O
ppm

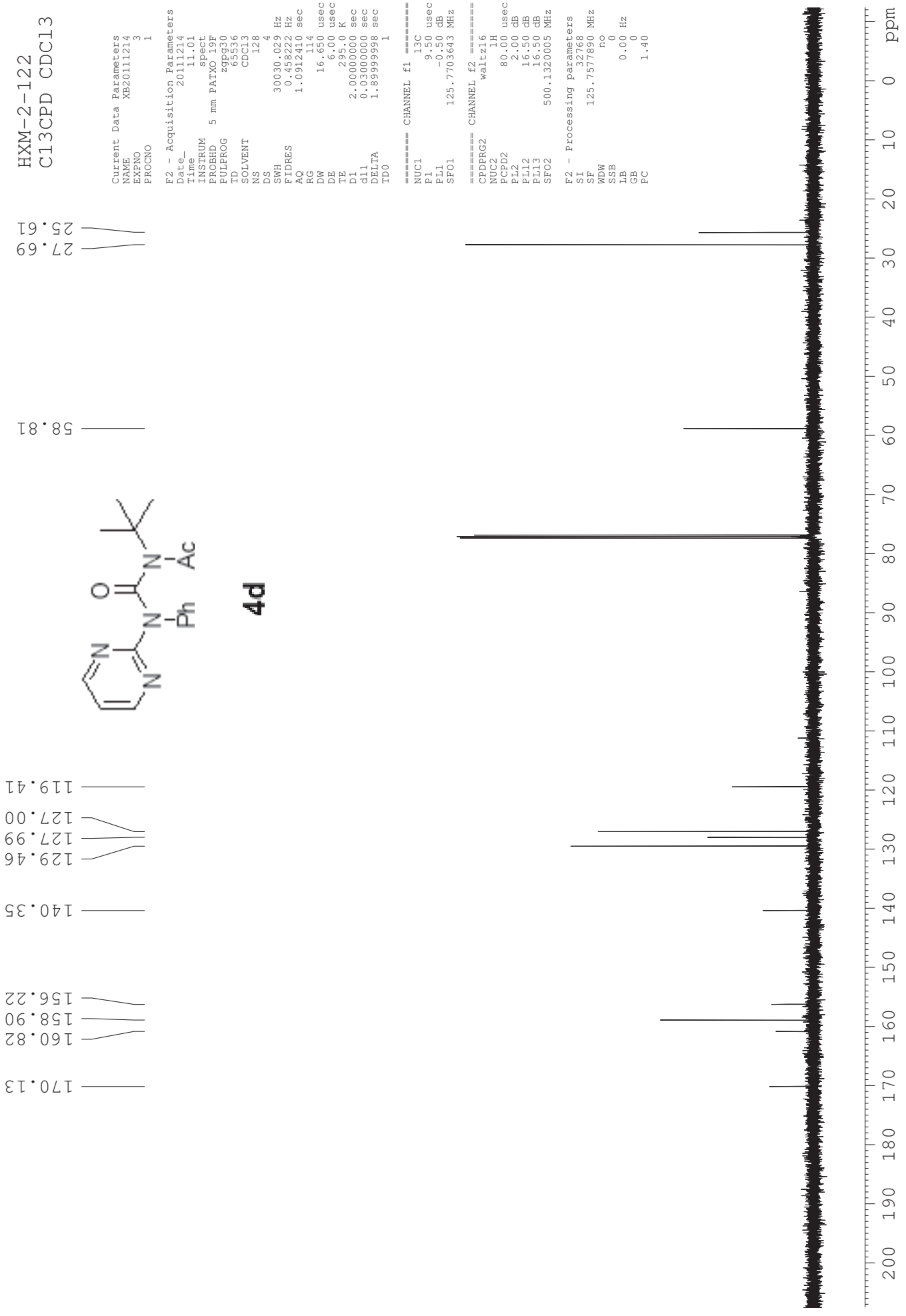

HXM--2-113
PROTON CDC13
NAME xb20111208
EXPNO 10
PROCNO 1
Date_ 20111208
Time 16.49
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 161.3
DW 48.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
4b
Ac
ppm

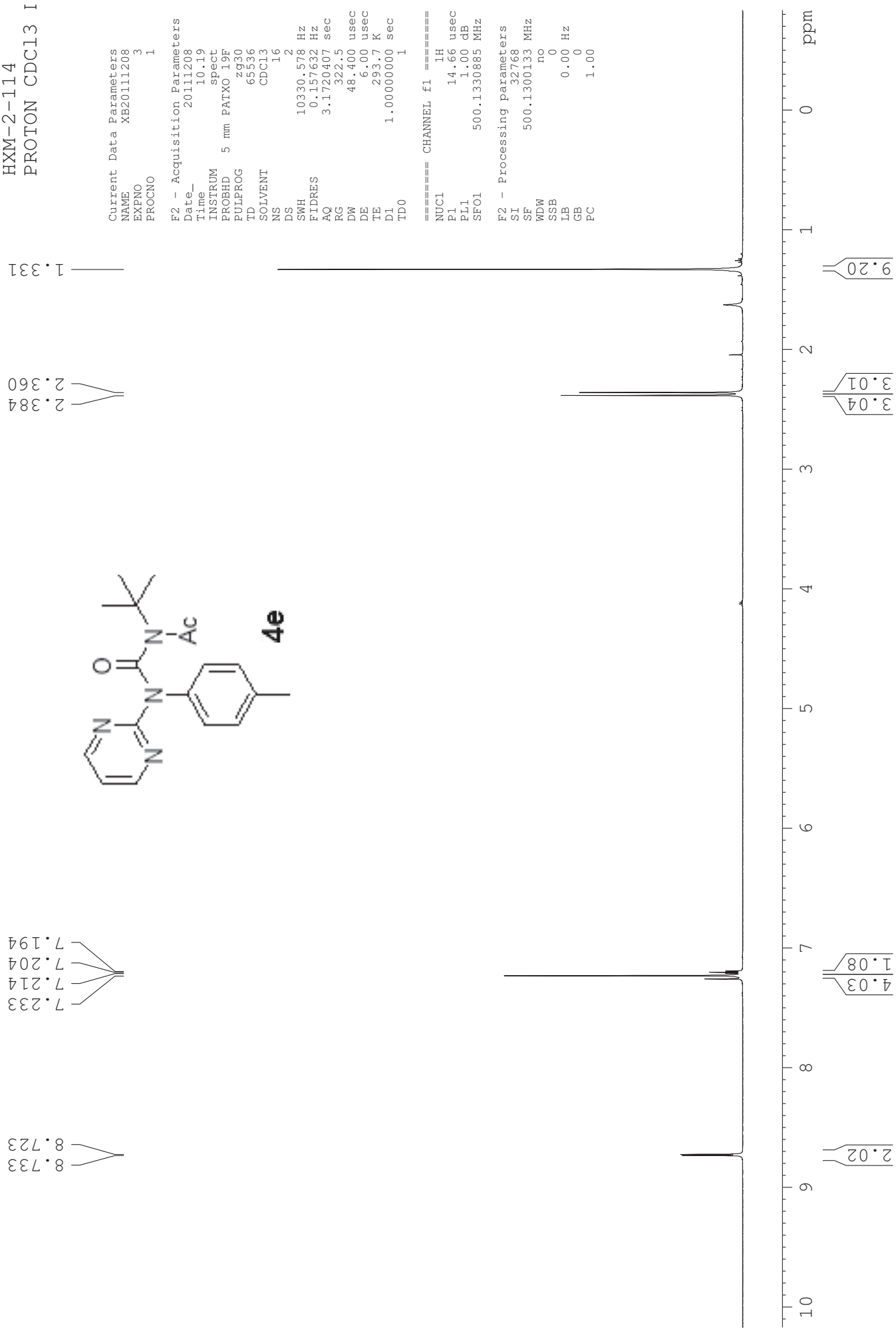

HXM-2-113
C13CPD CDCl3
Current Data Parameters
NAME XB20111209
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111209
Time 16.26
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 294.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
13.68
20.05
25.29
27.52
29.65
48.49
58.03
118.64
156.36
158.31
160.49
169.93
O
N
Ac
N
N
N
4b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 ppm

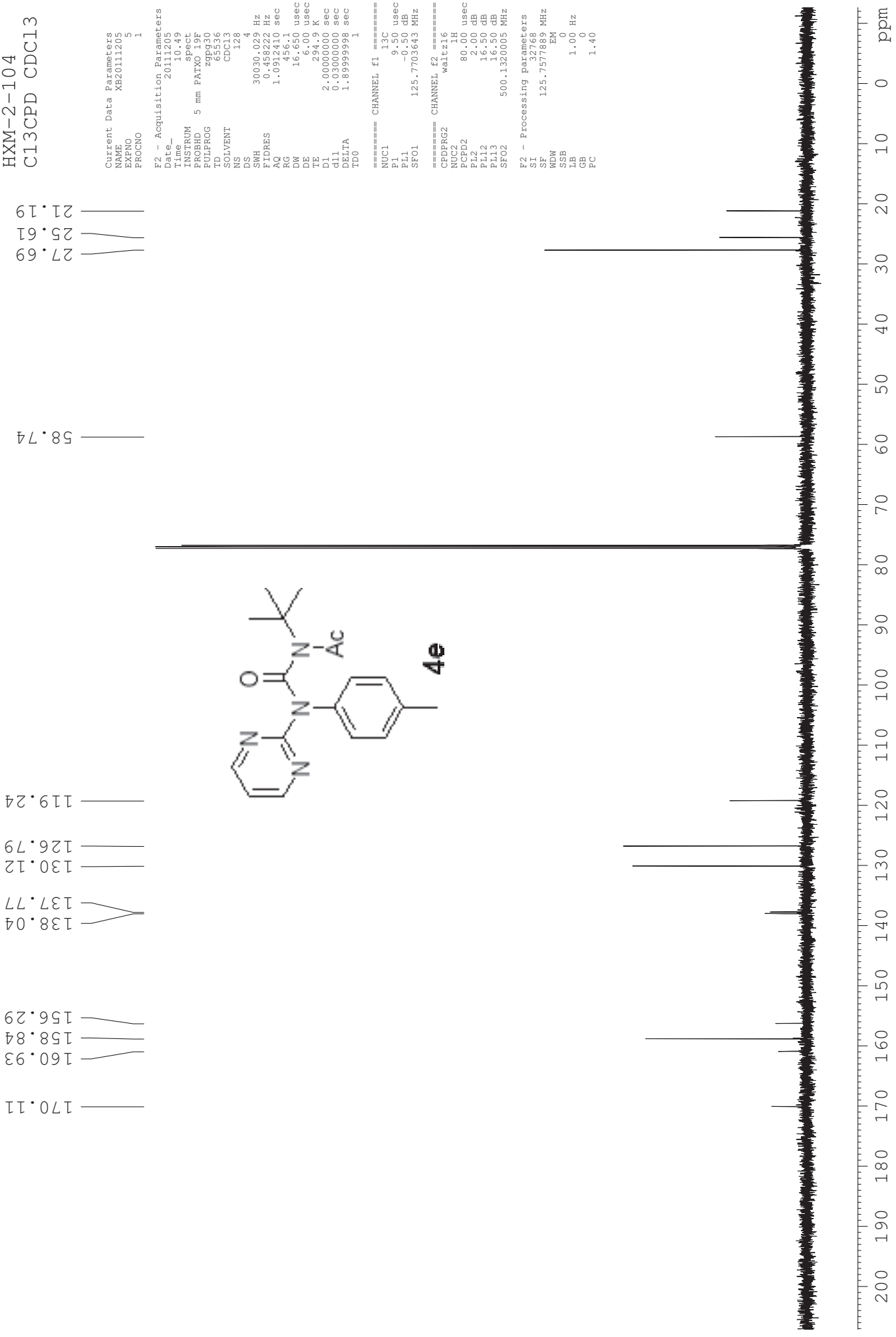

HXM-2-121
PROTON CDC13
Current Data Parameters
NAME XB20111212
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111212
Time 10.44
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.241
2.164
5.388
5.359
5.277
5.247
7.104
7.114
7.123
7.205
7.210
7.219
7.234
7.249
7.260
7.262
7.313
7.328
7.341
7.354
8.658
8.668
9.12
3.00
1.01
1.01
0.95
3.17
2.09
1.93
ppm
4c
N
N
O
N
Ac
Ph

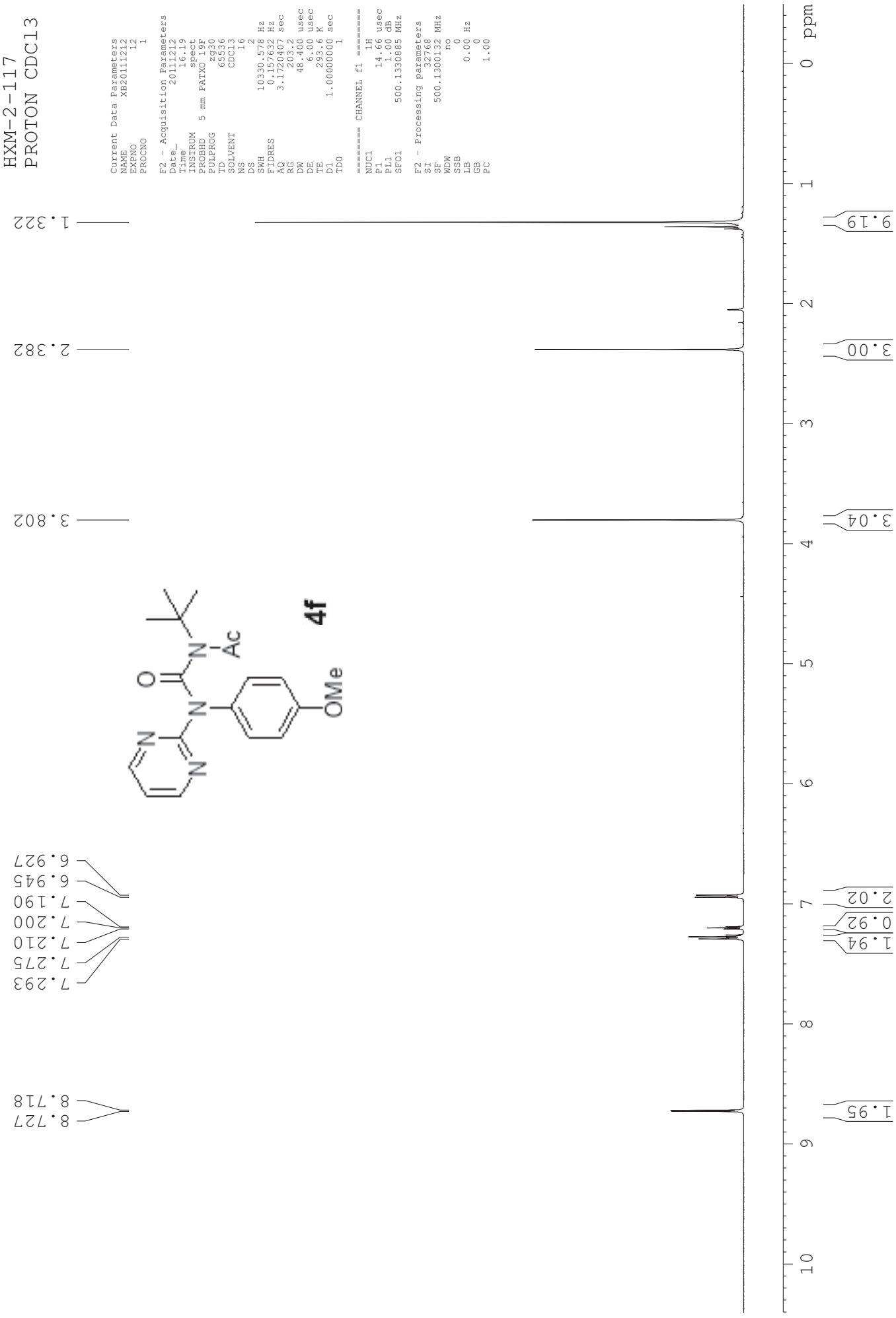

HXM-2-121
C13CPD CDC13
Current Data Parameters
NAME XB20111212
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111212
Time 16.49
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
25.40
27.60
51.57
58.37
118.60
127.58
128.28
128.46
136.34
156.90
158.27
160.05
169.90
N
Ac
O
N
N
Ph
4c
ppm

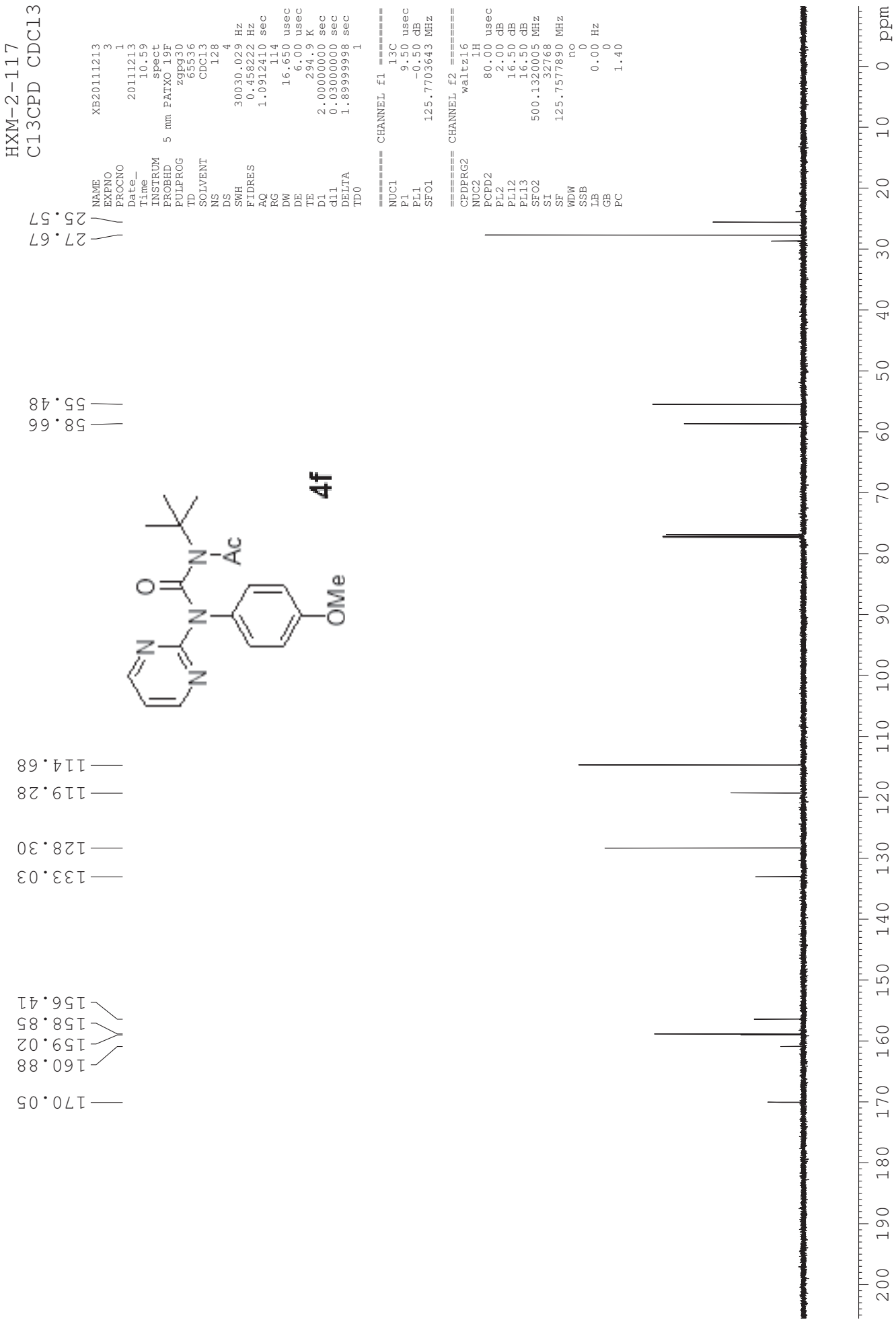

HXM-2-122
PROTON CDCl3
Current Data Parameters
NAME XB20111214
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111214
Time 10.45
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.334
2.395
7.210
7.220
7.230
7.325
7.340
7.356
7.416
7.421
7.431
7.448
8.730
8.740
9.19
3.00
1.00
2.94
2.03
1.93
ppm
4d
N
N
N
Ph
O
N
Ac

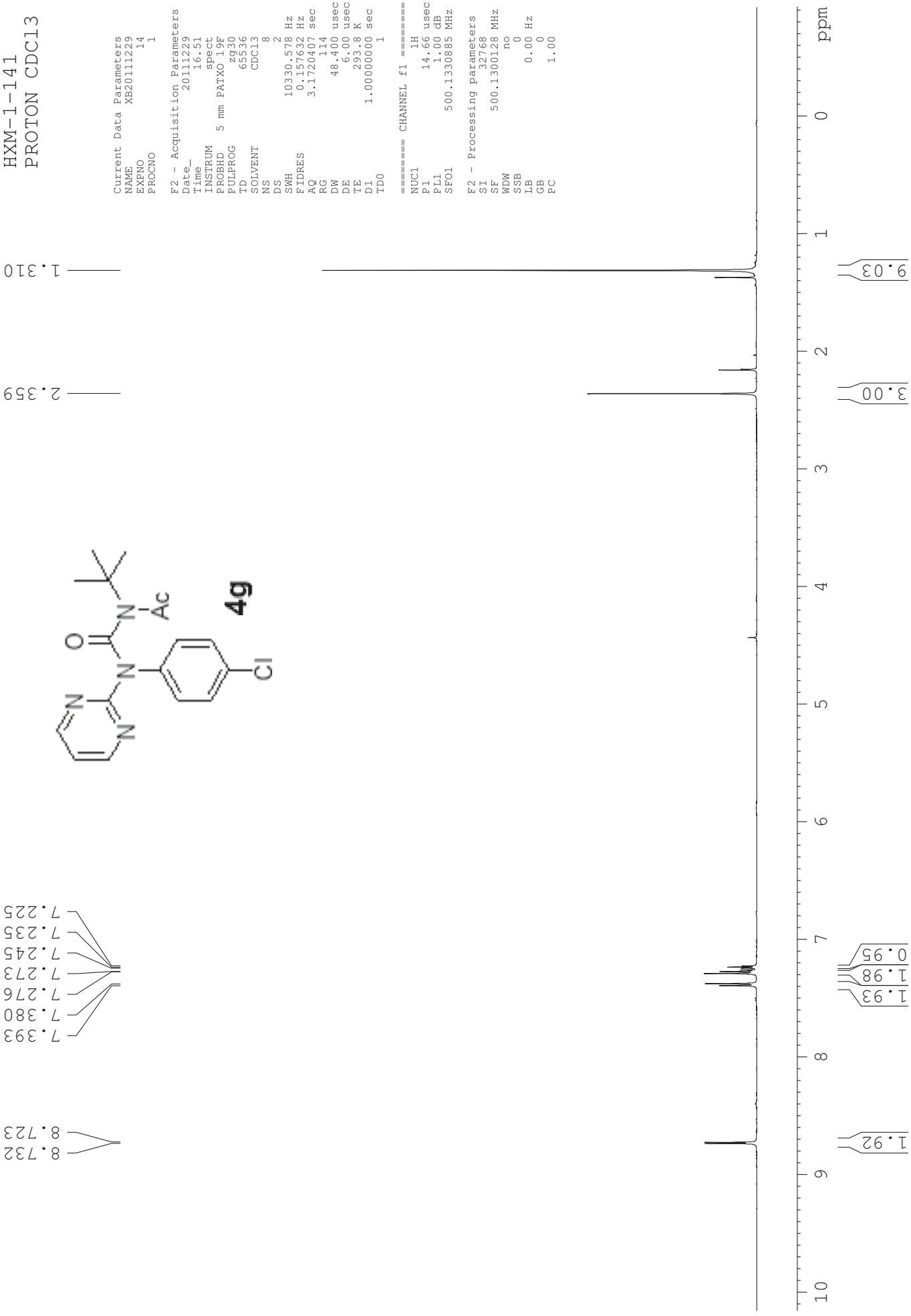

HXM-2-122
C13CPD CDCl3
4d
Ac
Ph
O
N
N
N
N
Current Data Parameters
NAME XB20111214
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111214
Time_ 11.01
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 295.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
25.61
27.69
58.81
119.41
127.00
127.99
129.46
140.35
156.22
158.90
160.82
170.13
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

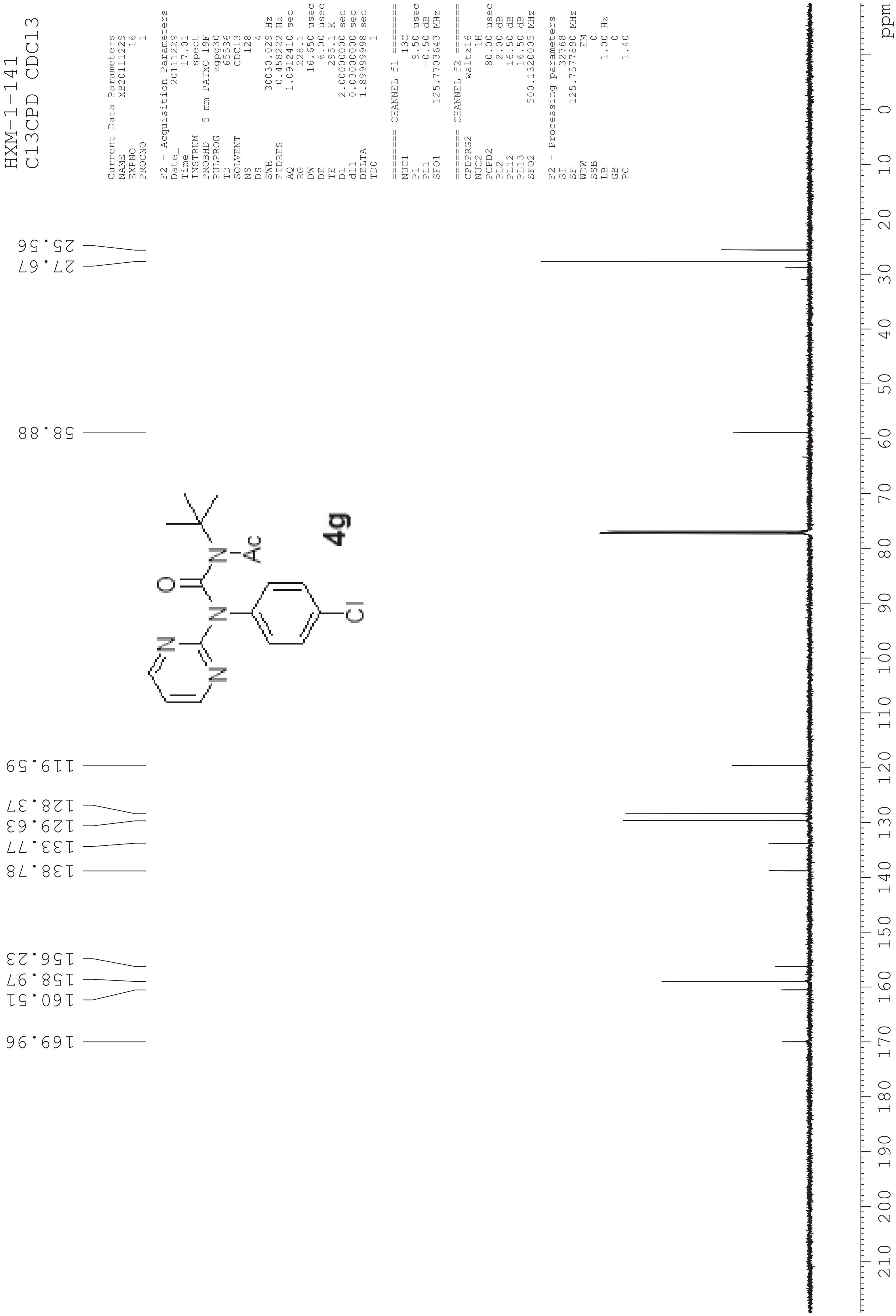

HXM-2-114
PROTON CDCl3 I
Current Data Parameters
NAME XB20111208
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111208
Time 10.19
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 322.5
DW 48.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300133 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.331
2.384
2.360
7.233
7.214
7.204
7.194
8.733
8.723
9.20
3.04
3.01
4.03
1.08
2.02
ppm
4e

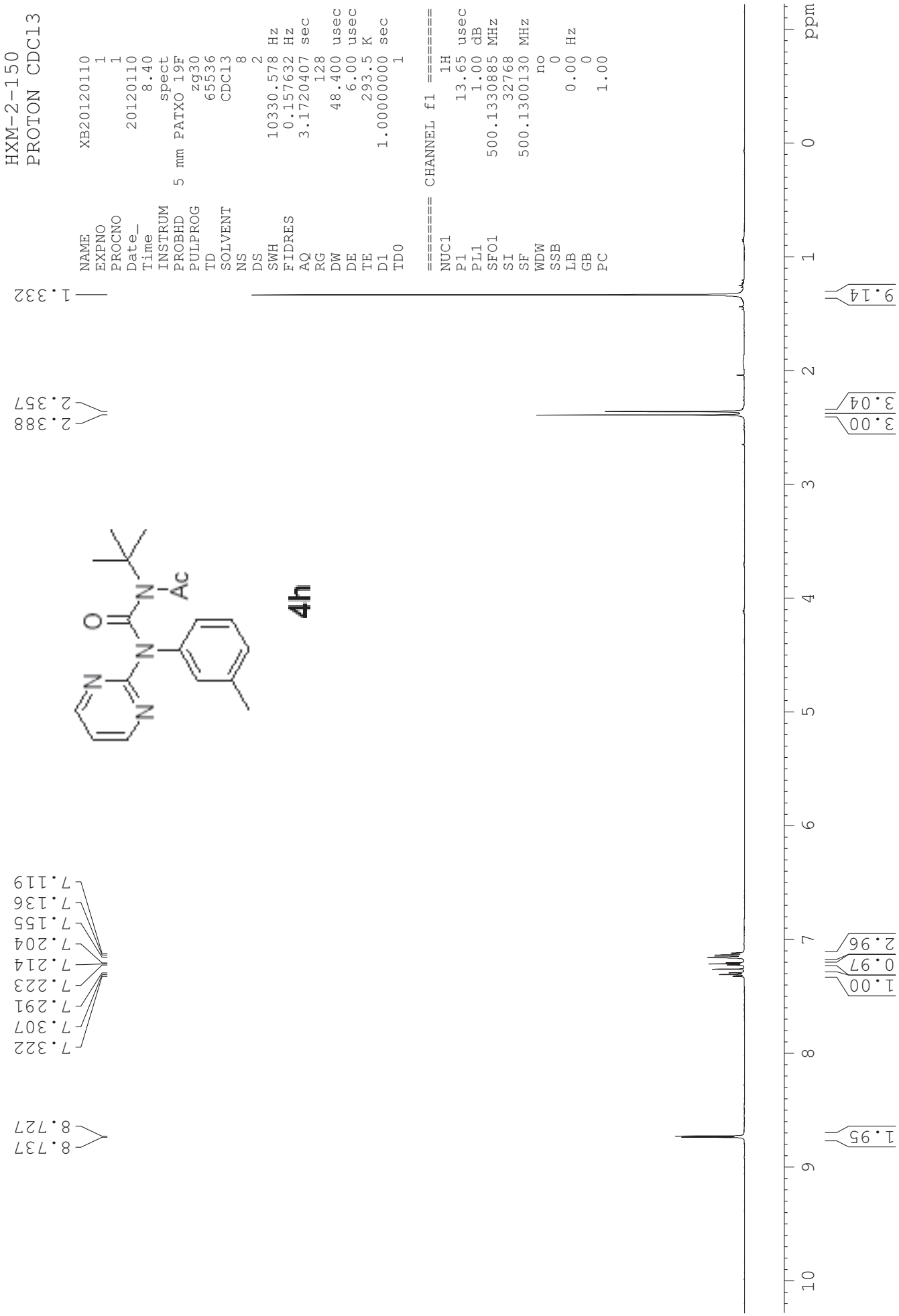

HXM-2-104
C13CPD CDCl3
Current Data Parameters
NAME XB20111205
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111205
Time_ 10.49
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 456.1
DW 16.650 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577889 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
21.19
25.61
27.69
58.74
119.24
126.79
130.12
137.77
138.04
156.29
158.84
160.93
170.11
4e
ppm

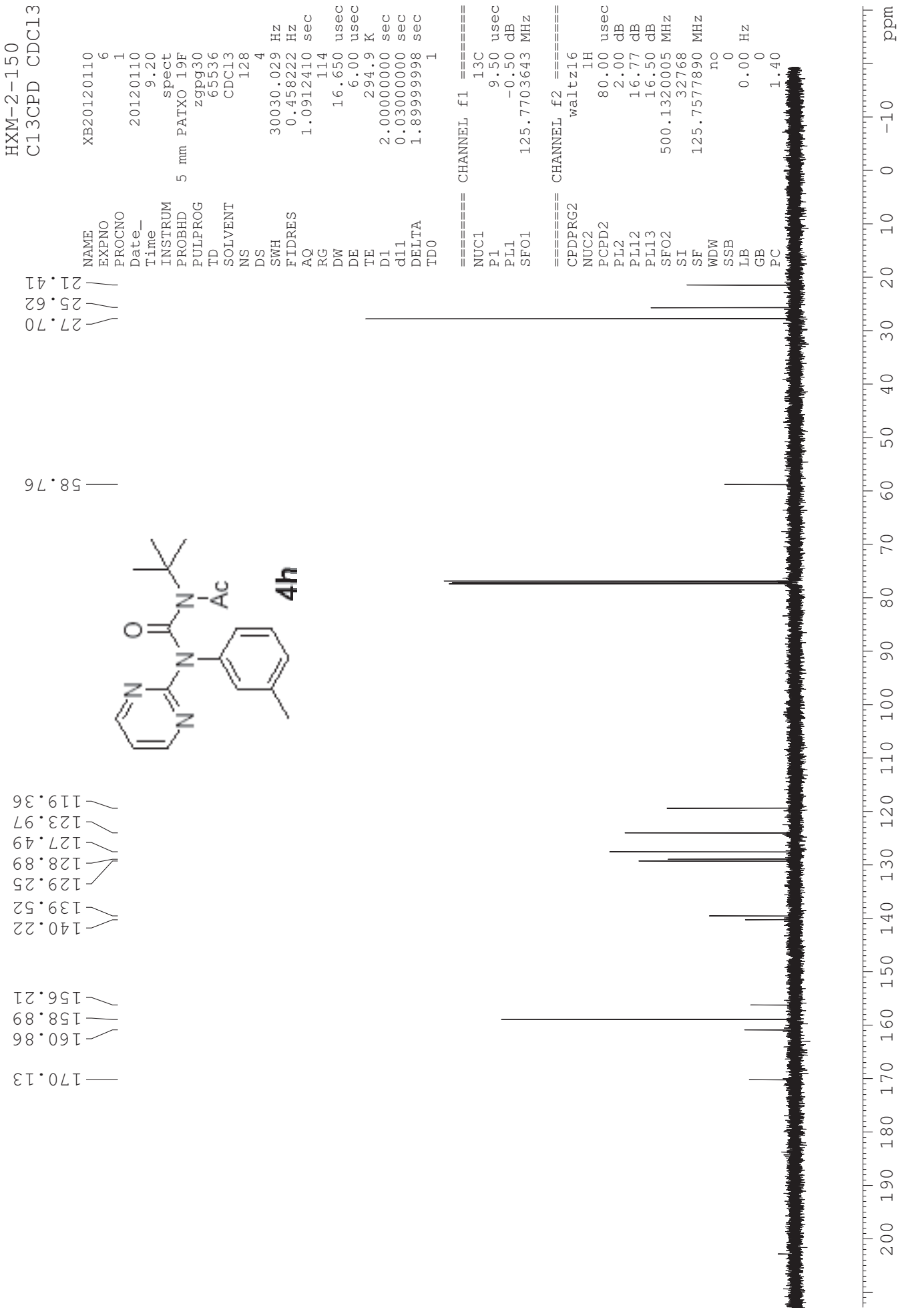

HXM-2-117
PROTON CDC13
Current Data Parameters
NAME XB20111212
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111212
Time 16.19
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.322
2.382
3.802
6.927
6.945
7.190
7.200
7.210
7.275
7.293
8.718
8.727
9.19
3.00
3.04
2.02
0.92
1.94
1.95
ppm
4f
N
Ac
O
N
N
N
OMe

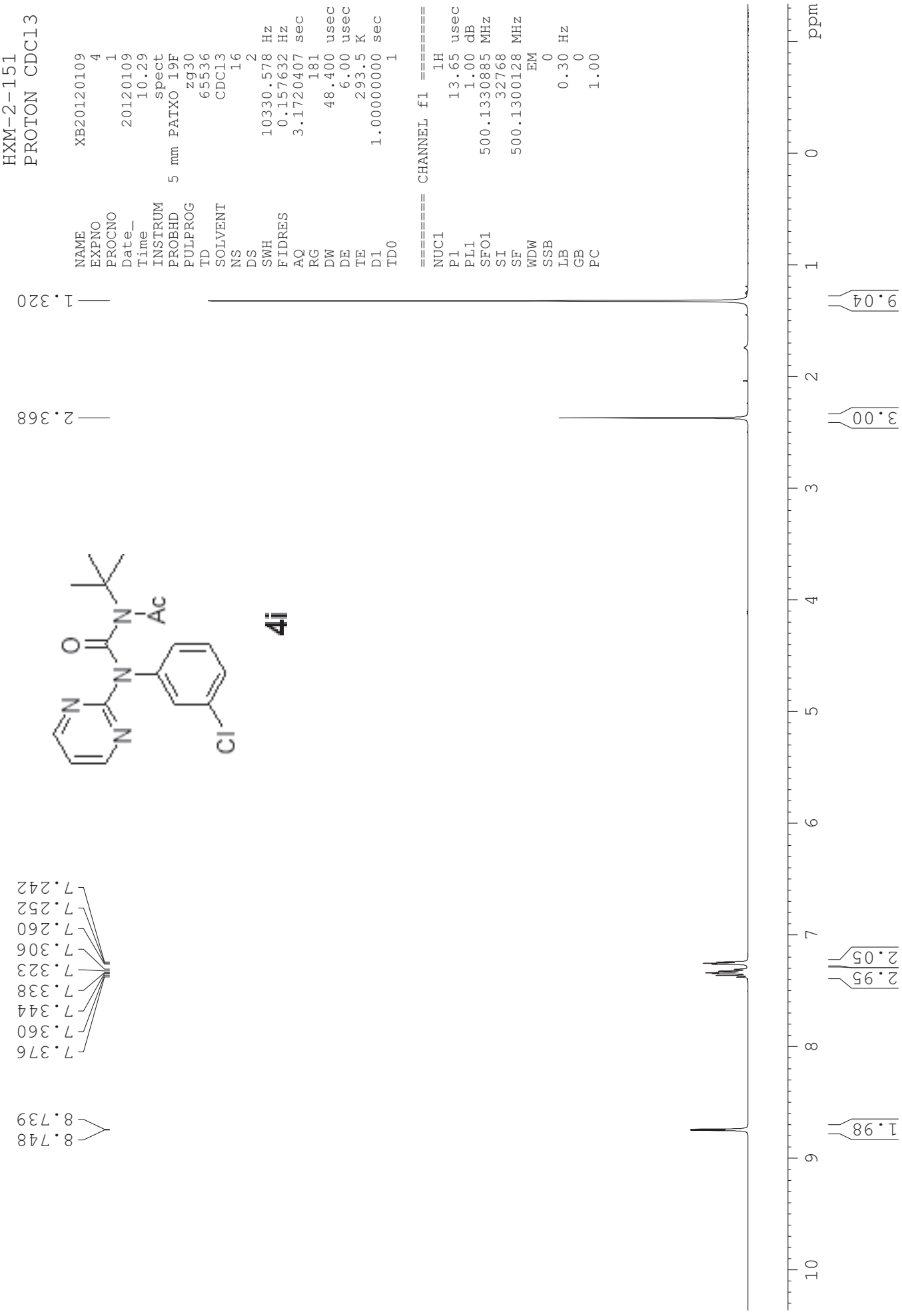

HXM-2-117
C13CPD CDCl3
NAME XB20111213
EXPNO 3
PROCNO 1
Date_ 20111213
Time 10.59
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
4f
N
Ac
O
N
OMe
N
N
25.57
27.67
55.48
58.66
114.68
119.28
128.30
133.03
156.41
158.85
159.02
160.88
170.05
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

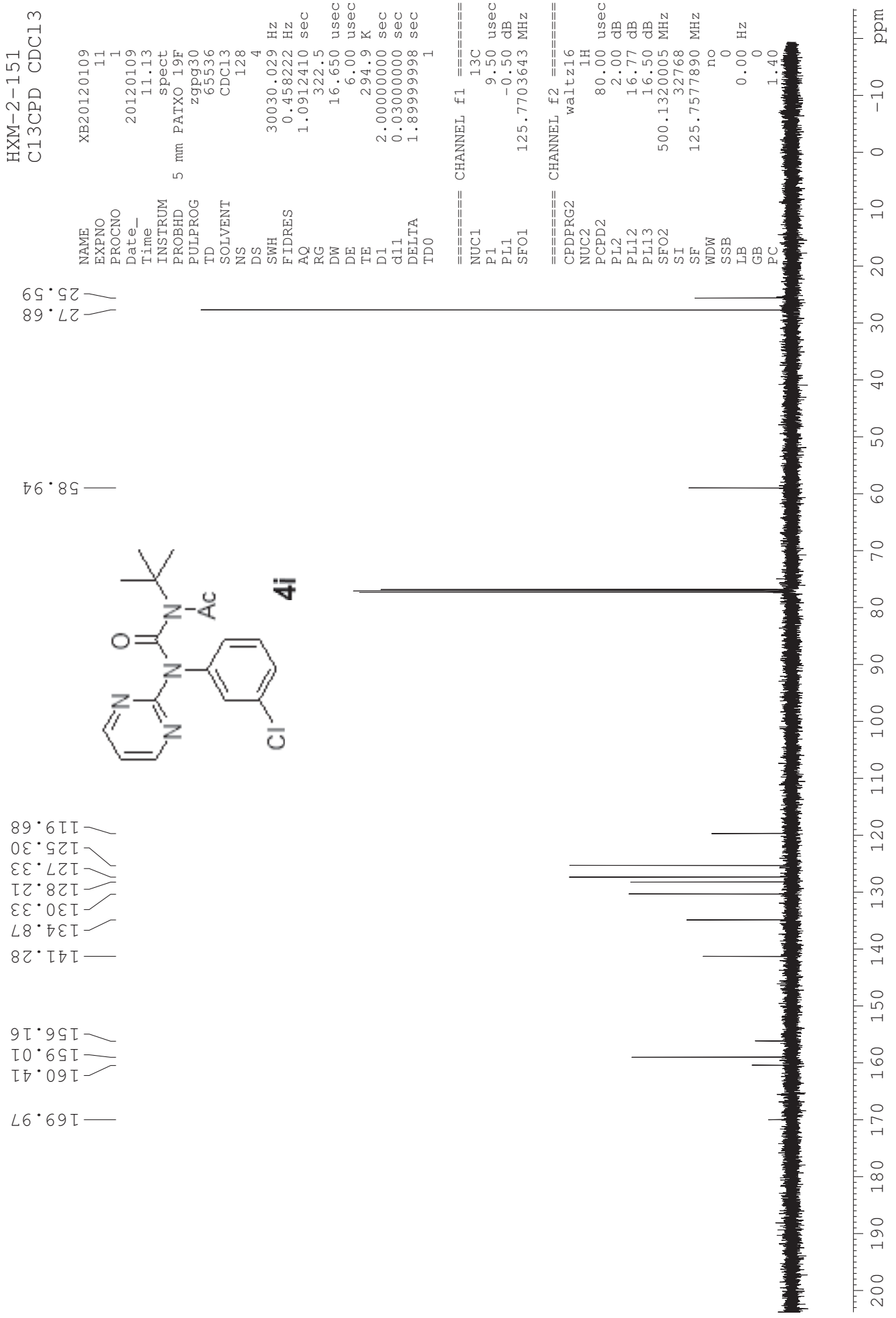

HXM-1-141
PROTON CDCl3
Current Data Parameters
NAME XB20111229
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111229
Time 16.51
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 114
DW 48.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.66 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300128 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.310
2.359
7.393
7.380
7.276
7.273
7.245
7.235
7.225
8.732
8.723
9.03
3.00
1.92
1.93
1.98
0.95
ppm
4g
Ac
N
O
Cl

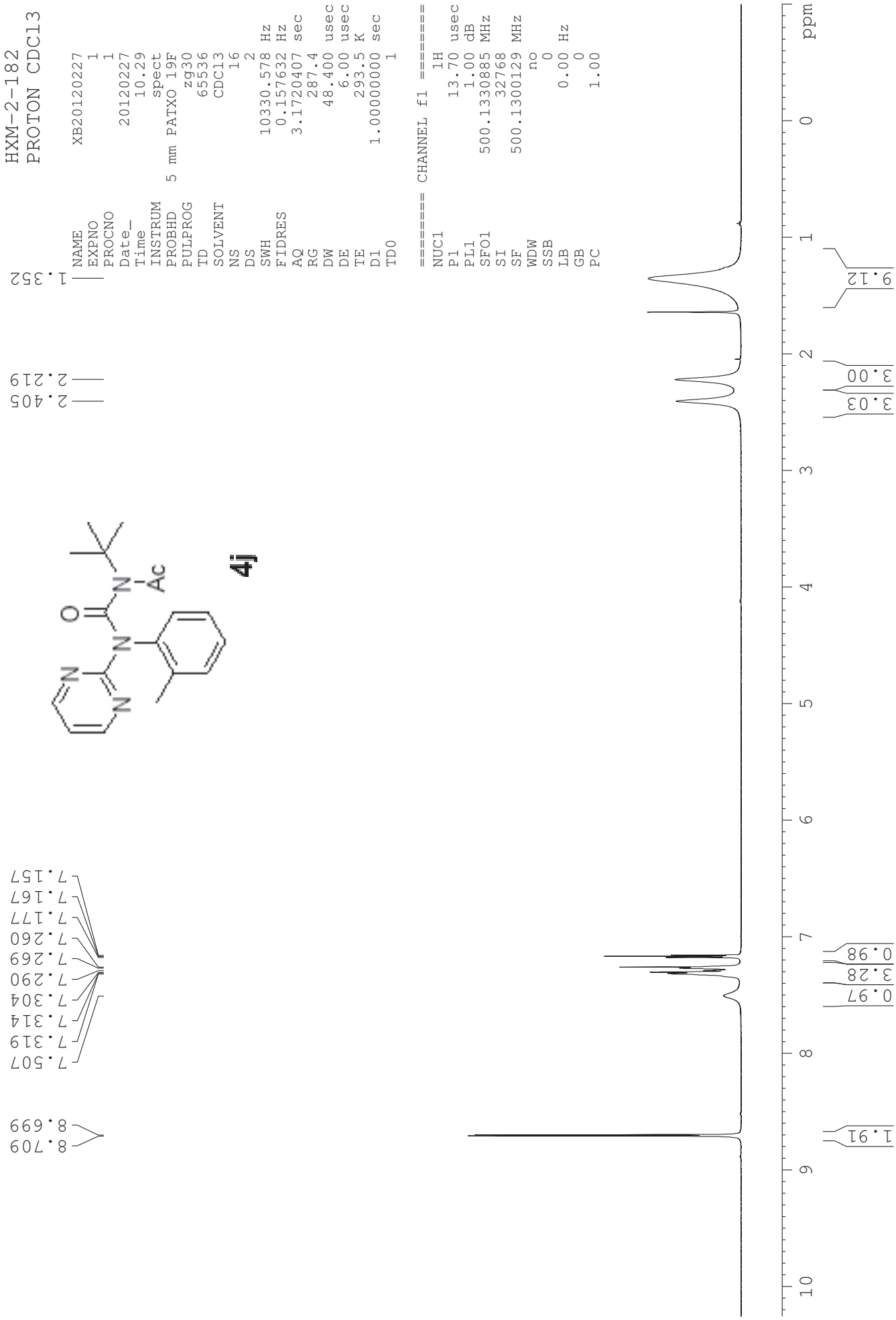

HXM-1-141
C13CPD CDCl3
25.56
27.67
58.88
119.59
128.37
129.63
133.77
138.78
156.23
158.97
160.51
169.96
4g
Current Data Parameters
NAME XB20111229
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111229
Time 17.01
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 228.1
DW 16.650 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210


HXM-2-150
PROTON CDC13
NAME XB20120110
EXPNO 1
PROCNO 1
Date_ 20120110
Time 8.40
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.65 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300130 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
4h
Ac
O
N
N
N
1.332
2.388
2.357
7.322
7.307
7.291
7.223
7.214
7.204
7.155
7.136
7.119
8.737
8.727
9.14
3.00
3.04
1.00
0.97
2.96
1.95
ppm

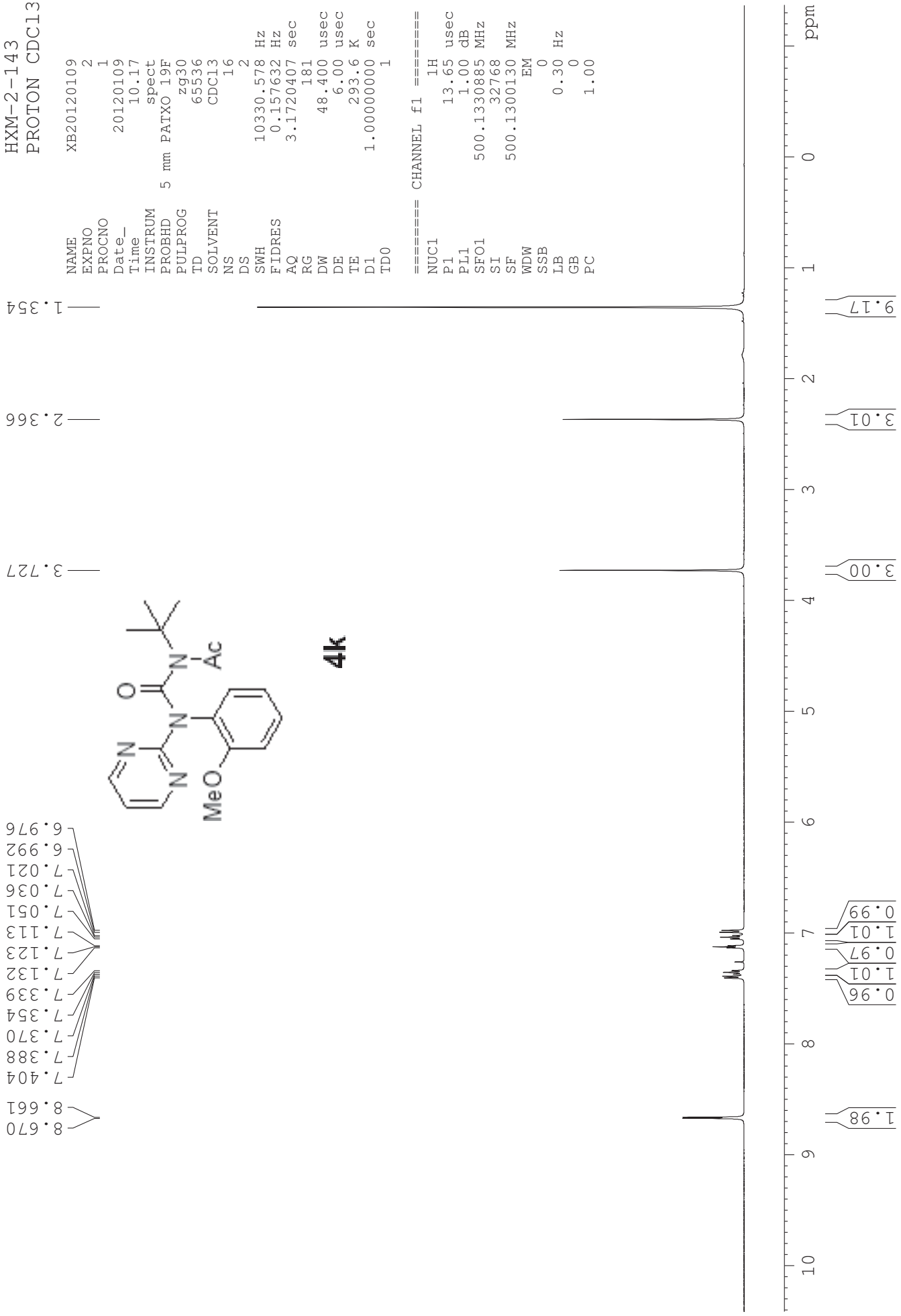

HXM-2-150
C13CPD CDC13
NAME XB20120110
EXPNO 6
PROCNO 1
Date_ 20120110
Time 9.20
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.77 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
21.41
25.62
27.70
58.76
119.36
123.97
127.49
128.89
129.25
139.52
140.22
156.21
158.89
160.86
170.13
4h
Ac
O
N
N
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

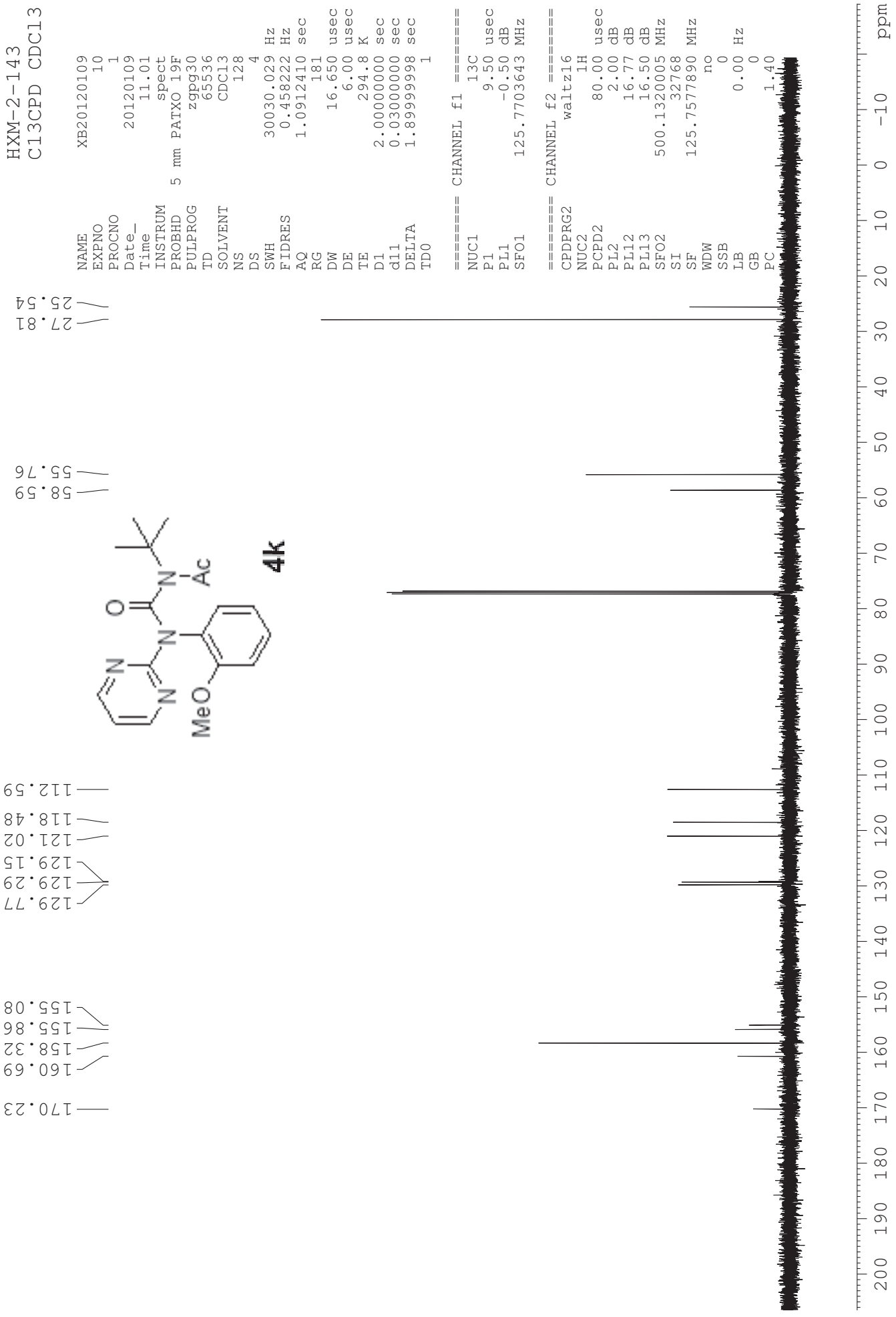

HXM-2-151
PROTON CDCl3
NAME XB20120109
EXPNO 4
PROCNO 1
Date_ 20120109
Time 10.29
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.65 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.320
2.368
8.748
8.739
7.376
7.360
7.344
7.338
7.323
7.306
7.260
7.252
7.242
9.04
3.00
2.95
2.05
1.98
ppm
4i
Ac
O
N
N
N
N
Cl

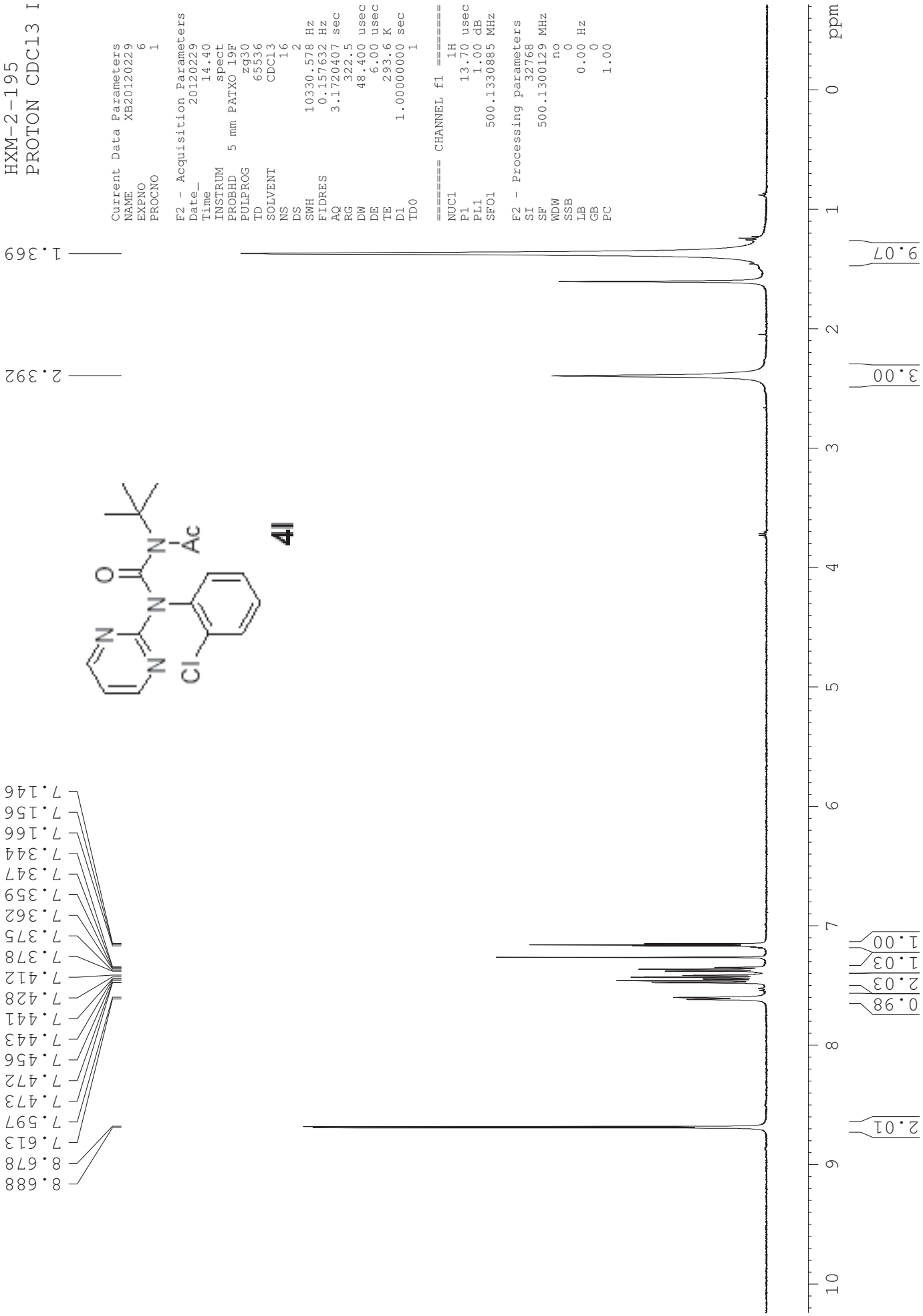

HXM-2-151
C13CPD CDC13
NAME XB20120109
EXPNO 11
PROCNO 1
Date_ 20120109
Time 11.13
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 322.5
DW 16.650 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.77 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
25.59
27.68
58.94
119.68
125.30
127.33
128.21
130.33
134.87
141.28
156.16
159.01
160.41
169.97
4i
Ac
N
O
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

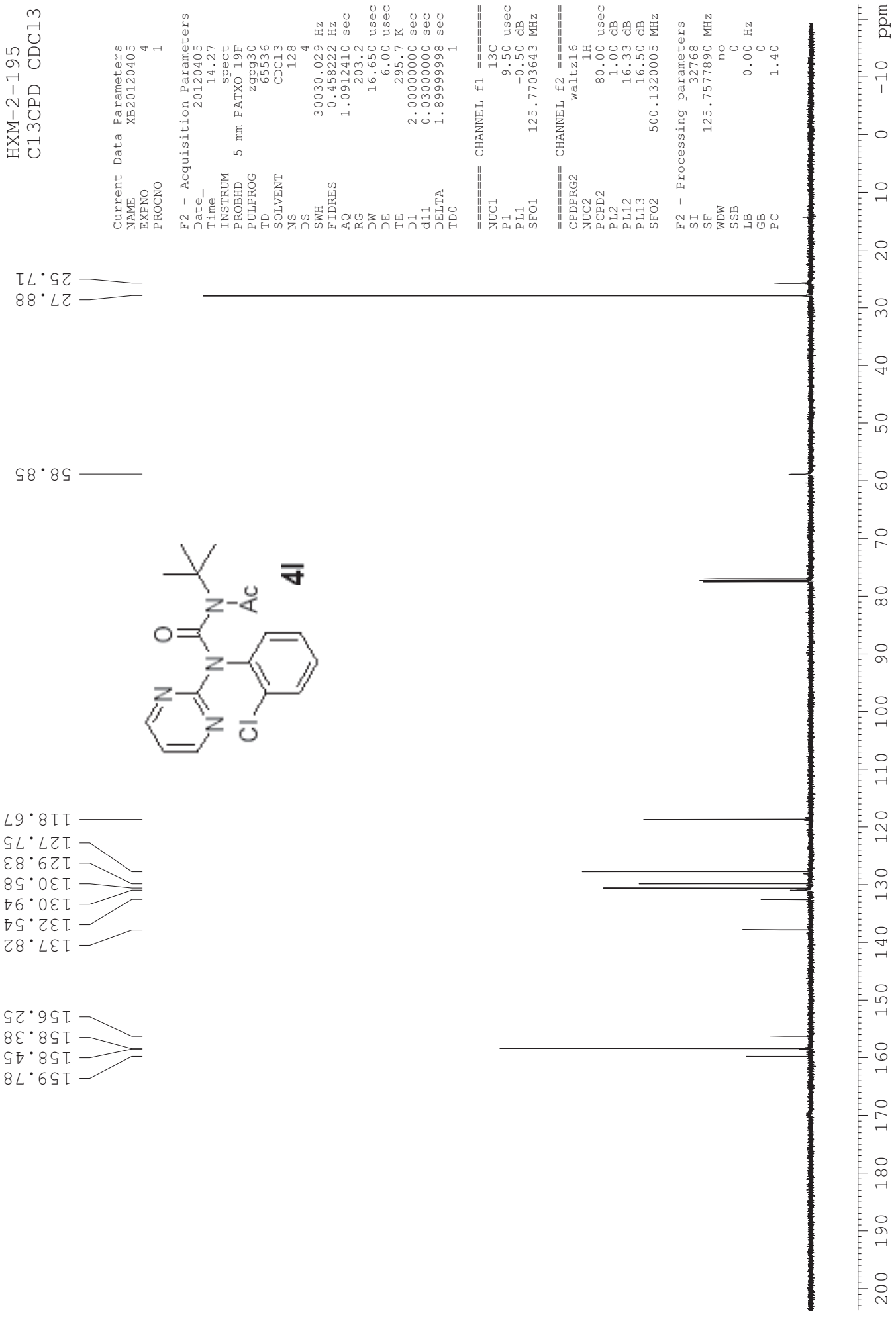

HXM-2-182
PROTON CDC13
NAME XB20120227
EXPNO 1
PROCNO 1
Date_ 20120227
Time 10.29
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.352
2.219
2.405
7.157
7.167
7.177
7.260
7.269
7.290
7.304
7.314
7.319
7.507
8.699
8.709
4j
Ac
ppm
9.12
3.00
3.03
0.98
3.28
0.97
1.91

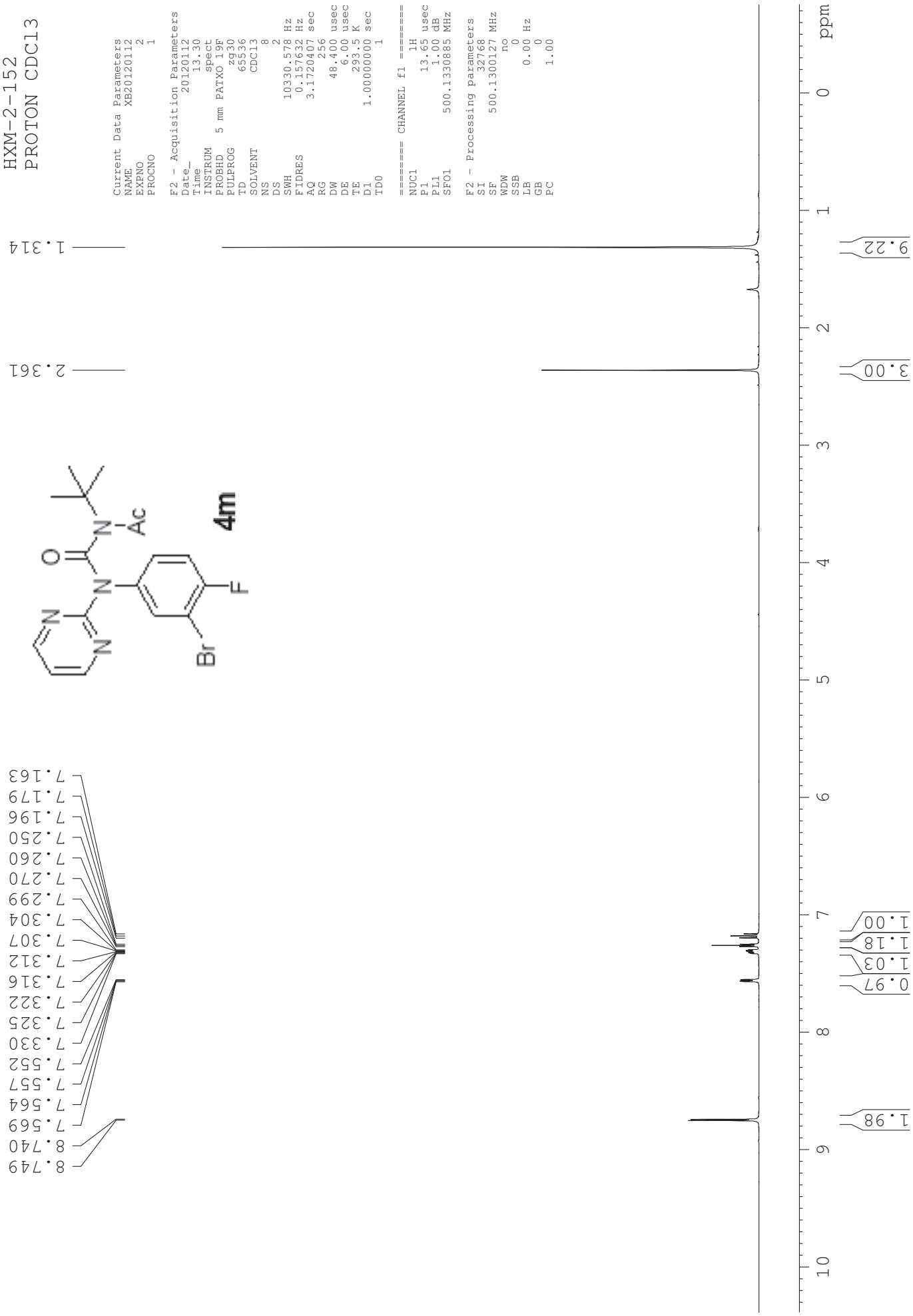

HXM-2-182
C13CPD CDC13
NAME XB20120316
EXPNO 12
PROCNO 1
Date_ 20120316
Time 18.11
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40
18.28
25.65
27.86
58.78
118.91
126.96
128.86
131.43
136.18
139.12
156.21
158.62
160.41
170.19
4j
N
Ac
O
N
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 ppm

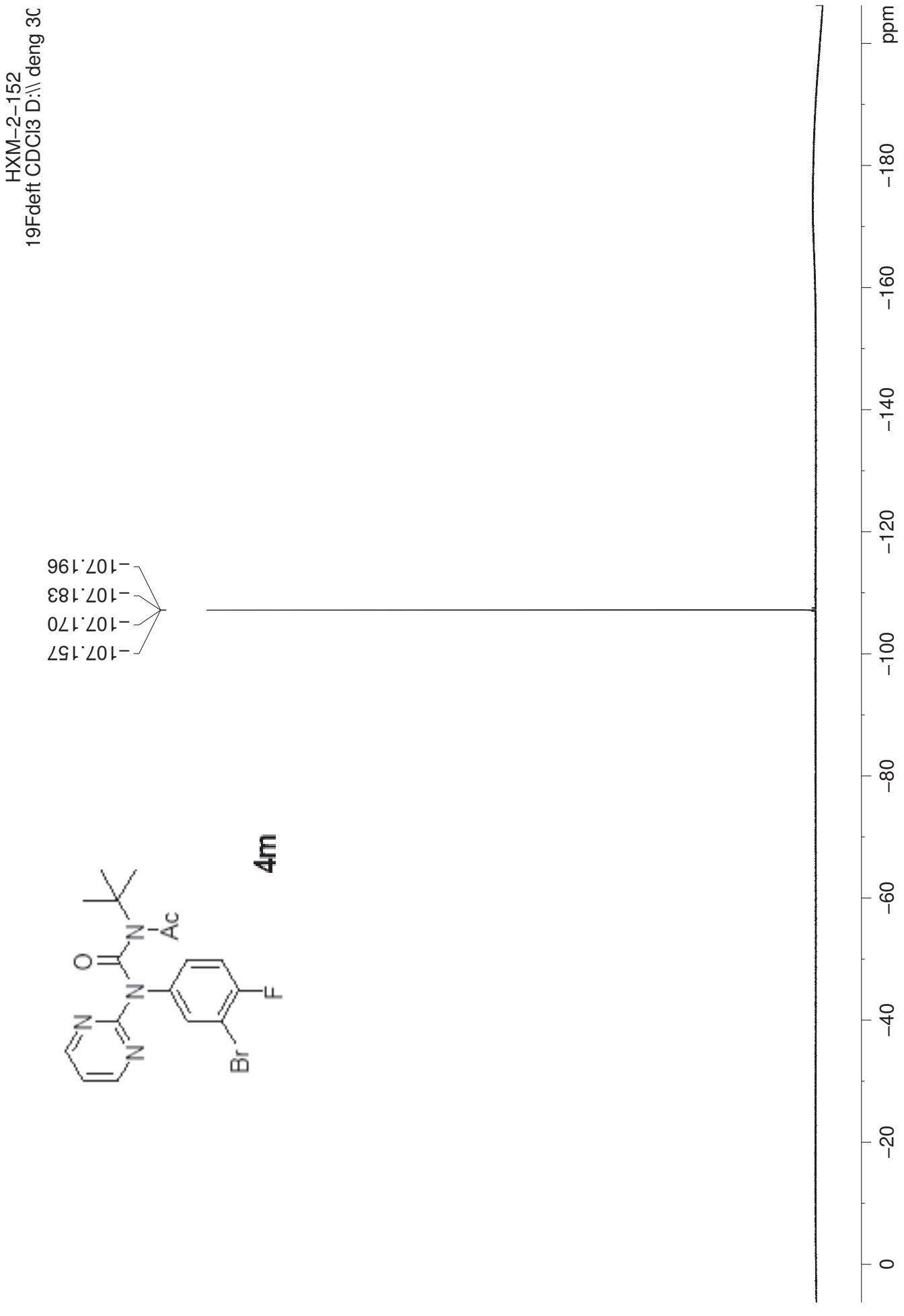

HXM-2-143
PROTON CDC13
NAME XB20120109
EXPNO 2
PROCNO 1
Date_ 20120109
Time 10.17
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.65 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.354
2.366
3.727
8.670
8.661
7.404
7.388
7.370
7.354
7.339
7.132
7.123
7.113
7.051
7.036
7.021
6.992
6.976
9.17
3.01
3.00
1.98
0.99
1.01
0.97
1.01
0.96
ppm
4k
N
Ac
O
N
N
N
MeO

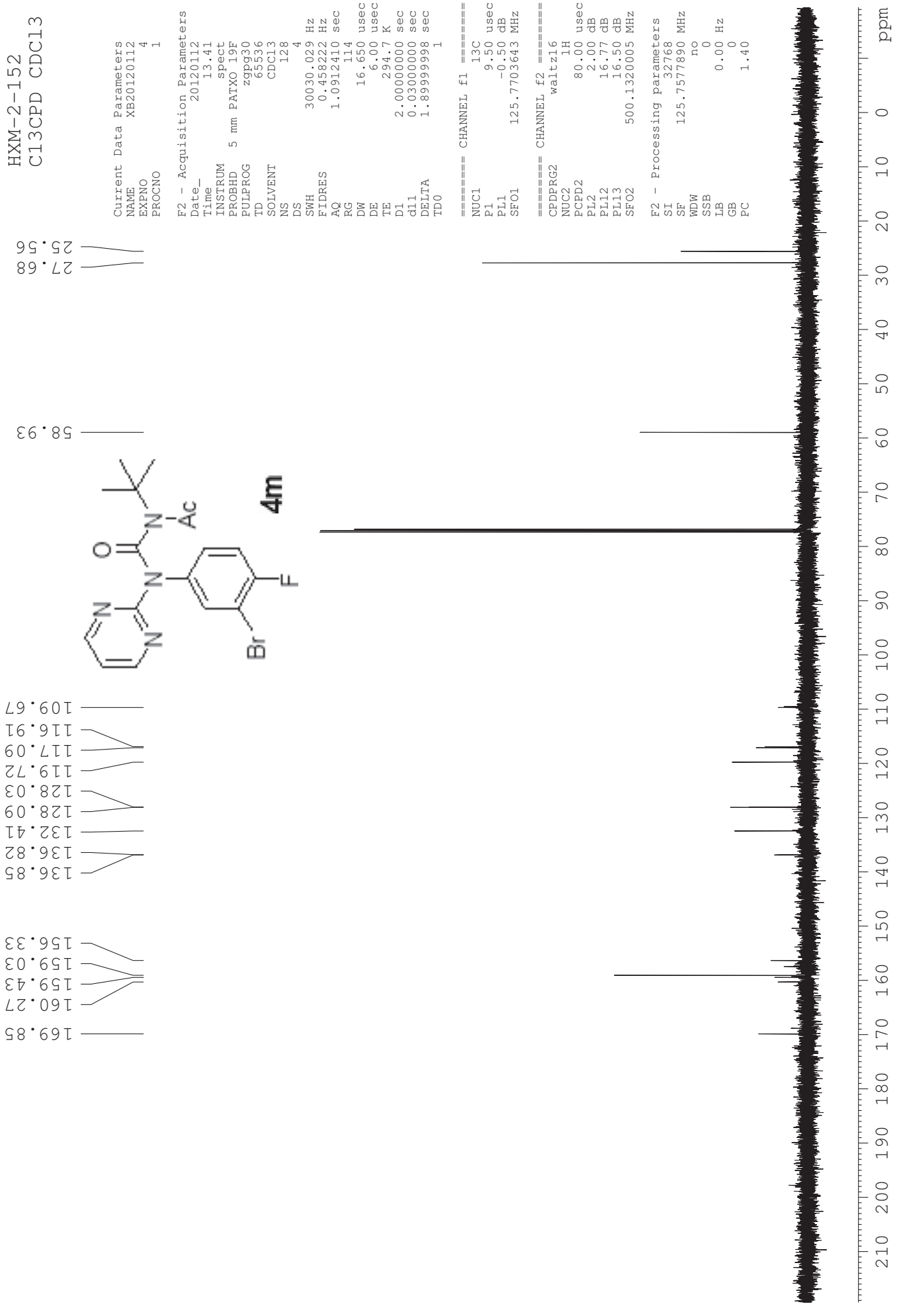

HXM-2-143
C13CPD CDCl3
NAME XB20120109
EXPNO 10
PROCNO 1
Date_ 20120109
Time 11.01
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 181
DW 16.650 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.77 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
25.54
27.81
55.76
58.59
112.59
118.48
121.02
129.15
129.29
129.77
155.08
155.86
158.32
160.69
170.23
4k
N
N
N
O
Ac
MeO
ppm

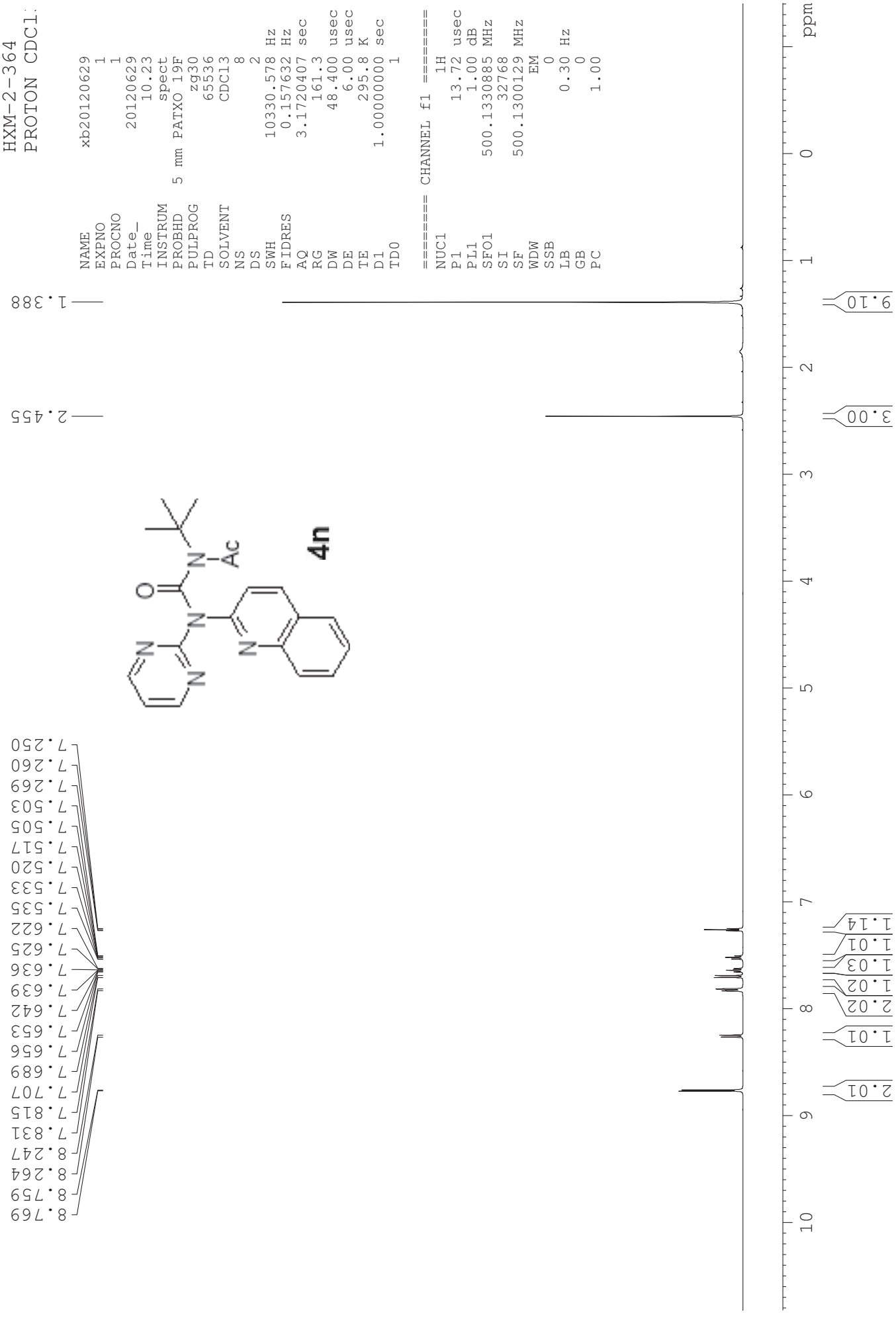

HXM-2-195
PROTON CDCl3 I
Current Data Parameters
NAME XB20120229
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120229
Time 14.40
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 322.5
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.369
2.392
7.146
7.156
7.166
7.344
7.347
7.359
7.362
7.375
7.378
7.412
7.428
7.441
7.443
7.456
7.472
7.473
7.597
7.613
8.678
8.688
9.07
3.00
1.00
1.03
2.03
0.98
2.01
ppm
0
1
2
3
4
5
6
7
8
9
10
N
Ac
O
N
N
N
Cl
4l

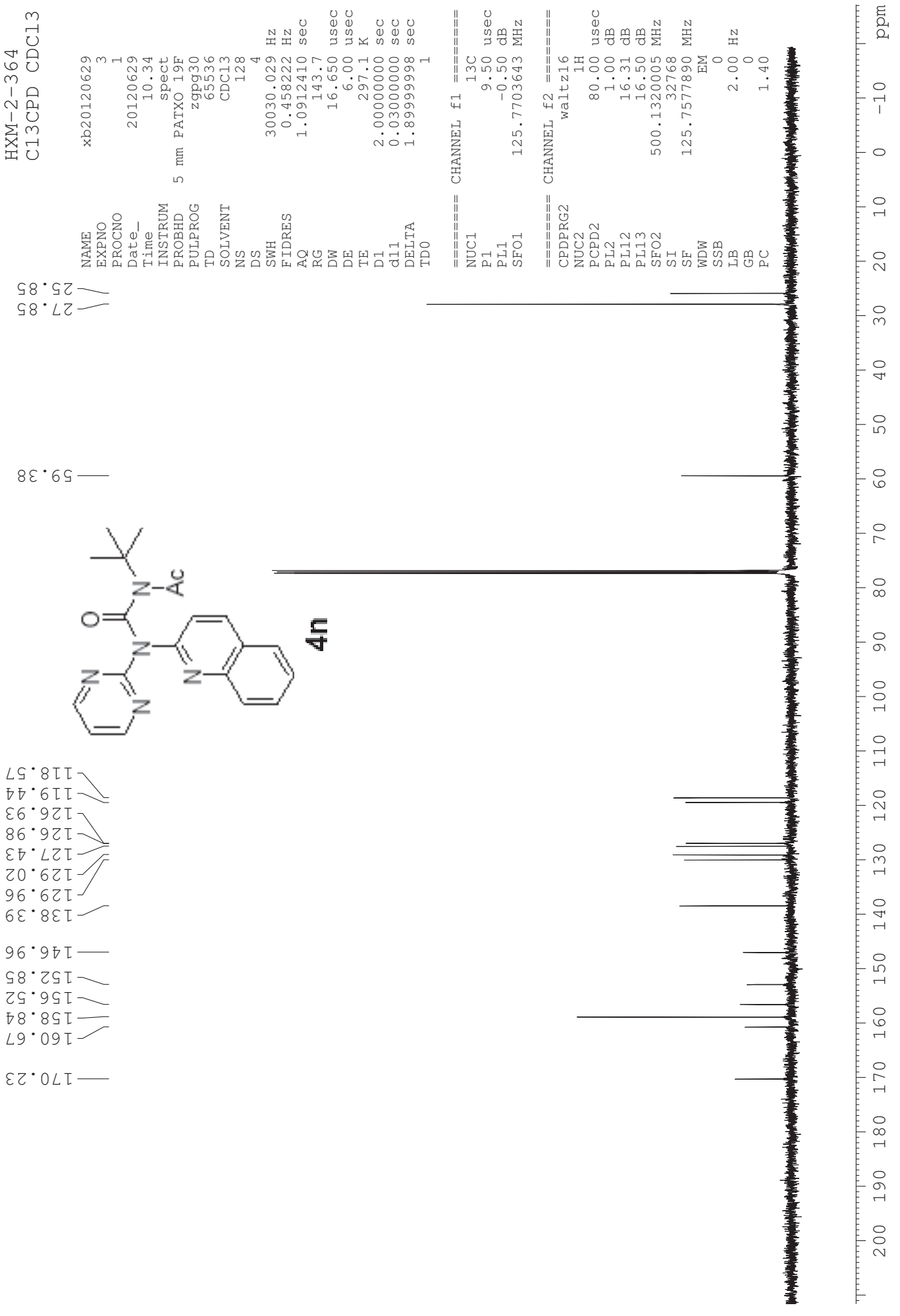

HXM-2-195
C13CPD CDC13
Current Data Parameters
NAME XB20120405
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120405
Time 14.27
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 203.2
DW 16.650 usec
DE 6.00 usec
TE 295.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
25.71
27.88
58.85
118.67
127.75
129.83
130.58
130.94
132.54
137.82
156.25
158.38
158.45
159.78
4l
Ac
N
O
Cl
ppm

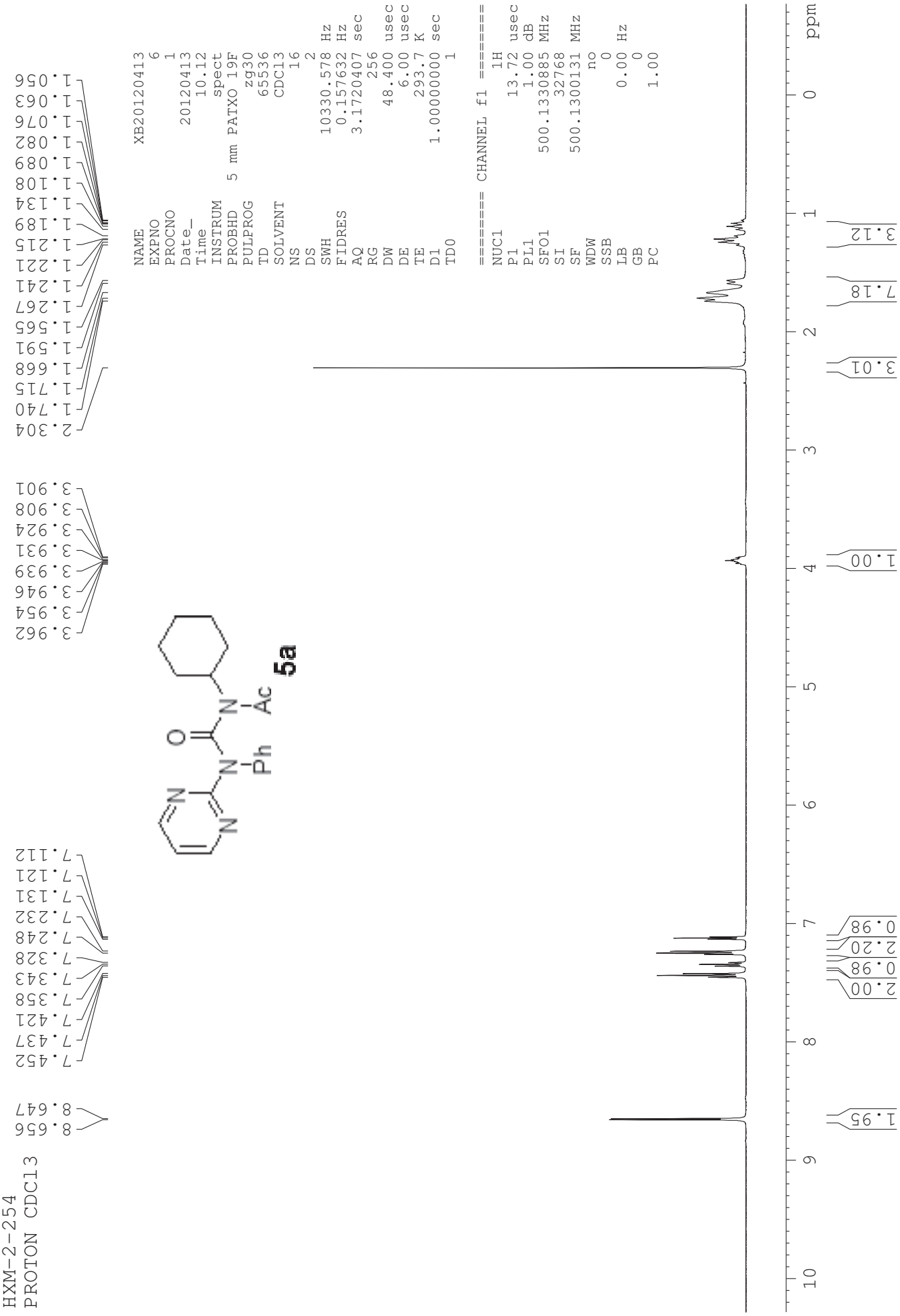

HXM-2-152
PROTON CDC13
Current Data Parameters
NAME XB20120112
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120112
Time 13.30
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 256
DW 48.400 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.65 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300127 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.314
2.361
7.163
7.179
7.196
7.250
7.260
7.270
7.299
7.304
7.307
7.312
7.316
7.322
7.325
7.330
7.552
7.557
7.564
7.569
8.740
8.749
9.22
3.00
1.98
1.00
1.18
1.03
0.97
ppm
4m
Ac
O
N
Br
F

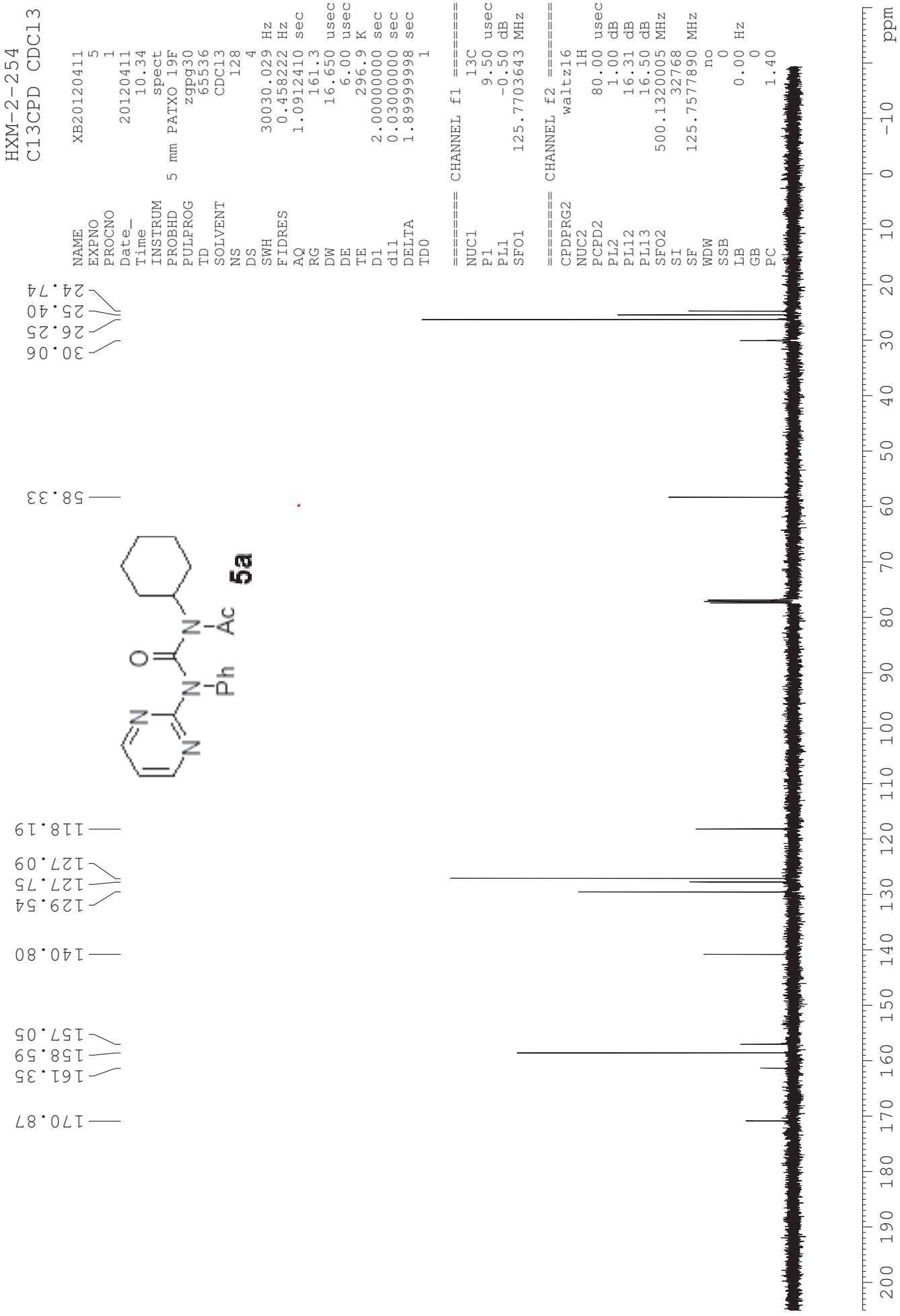

HXM-2-152
19Fdeft CDCl3 D:\\ deng 3C
-107.157
-107.170
-107.183
-107.196
4m
Ac
N
O
N
N
N
Br
F
ppm
0
-20
-40
-60
-80
-100
-120
-140
-160
-180

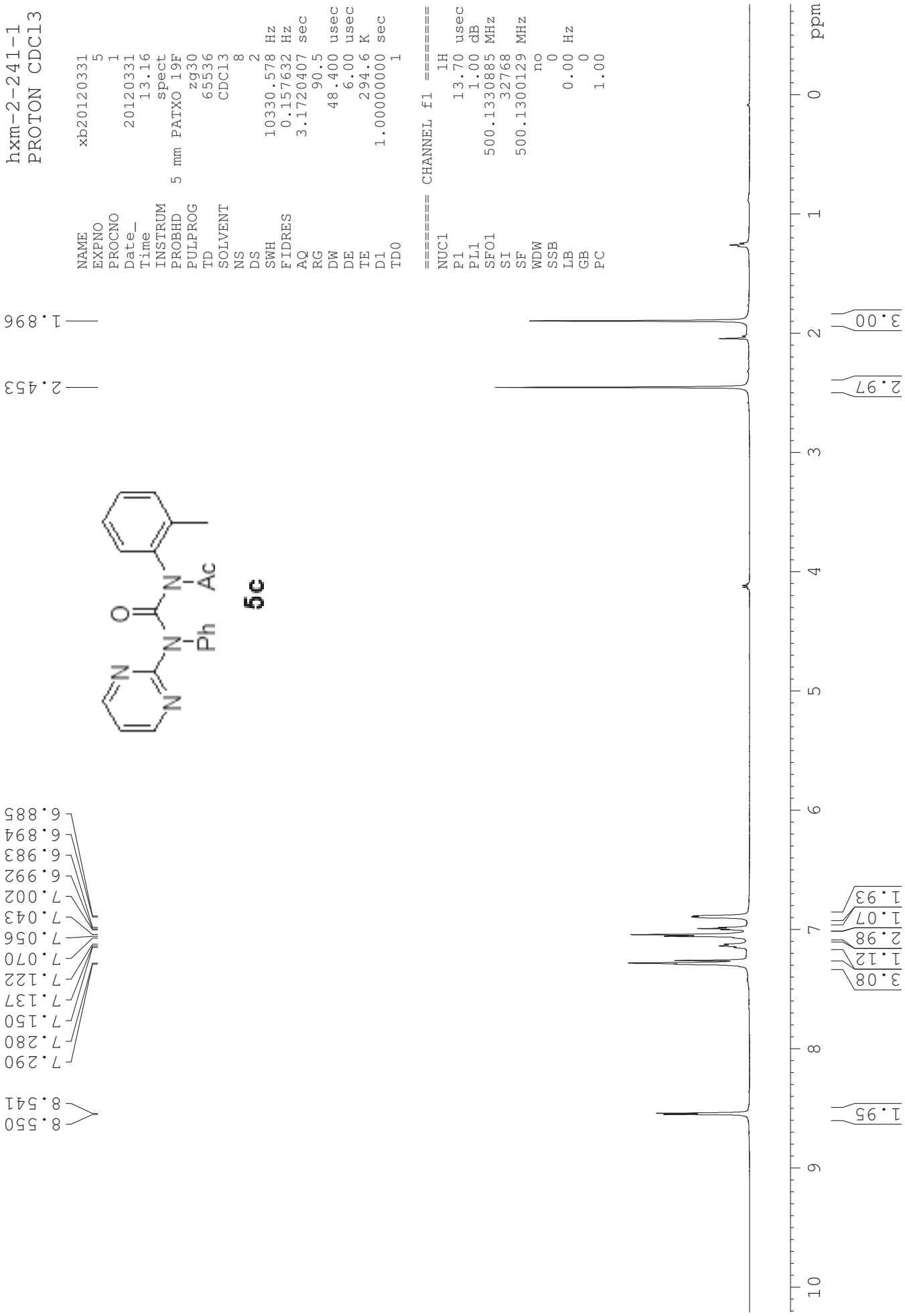

HXM-2-152
C13CPD CDCl3
Current Data Parameters
NAME XB20120112
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120112
Time 13.41
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 294.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.77 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
27.68
25.56
58.93
109.67
116.91
117.09
119.72
128.03
128.09
132.41
136.82
136.85
156.33
159.03
159.43
160.27
169.85
4m
Ac
O
N
N
N
N
Br
F
ppm

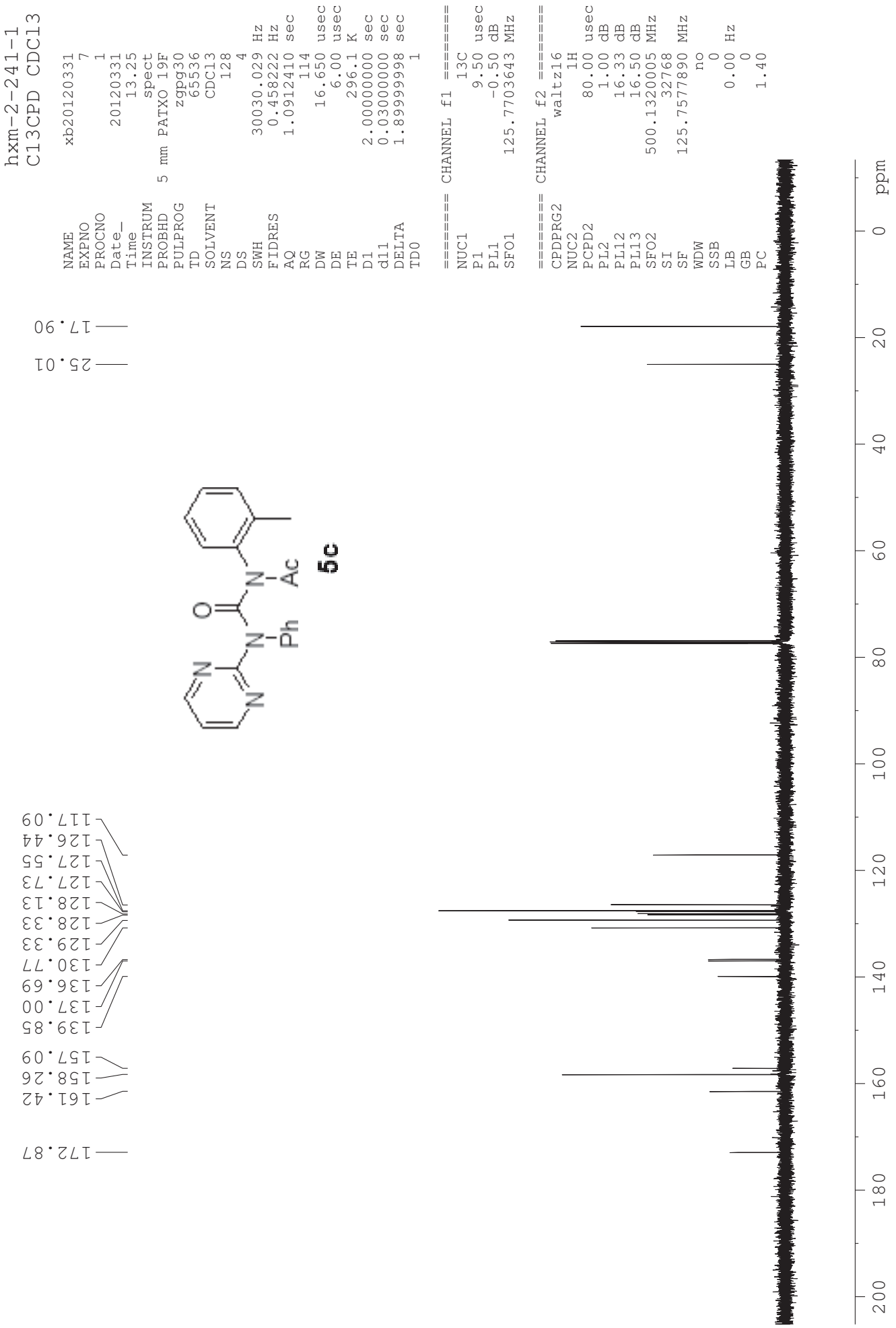

HXM-2-364
PROTON CDCl3
NAME xb20120629
EXPNO 1
PROCNO 1
Date_ 20120629
Time_ 10.23
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 161.3
DW 48.400 usec
DE 6.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.388
2.455
7.250
7.260
7.269
7.503
7.505
7.517
7.520
7.533
7.535
7.622
7.625
7.636
7.639
7.642
7.653
7.656
7.689
7.707
7.815
7.831
8.247
8.264
8.759
8.769
Ac
O
4n
ppm
9.10
3.00
2.01
1.01
2.02
1.02
1.03
1.01
1.14

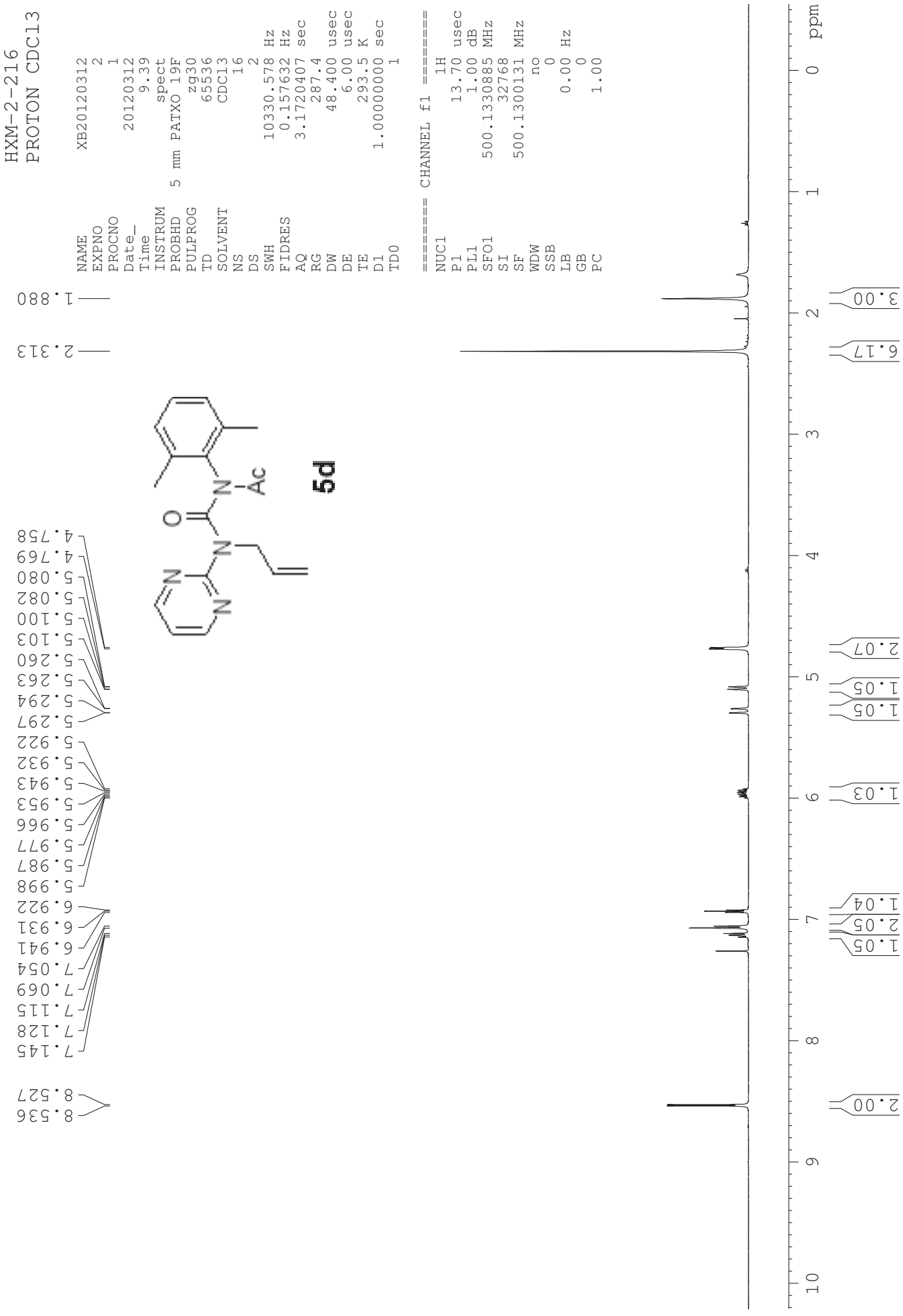

HXM-2-364
C13CPD CDC13
NAME xb20120629
EXPNO 3
PROCNO 1
Date_ 20120629
Time 10.34
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
25.85
27.85
59.38
118.57
119.44
126.93
126.98
127.43
129.02
129.96
138.39
146.96
152.85
156.52
158.84
160.67
170.23
4n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

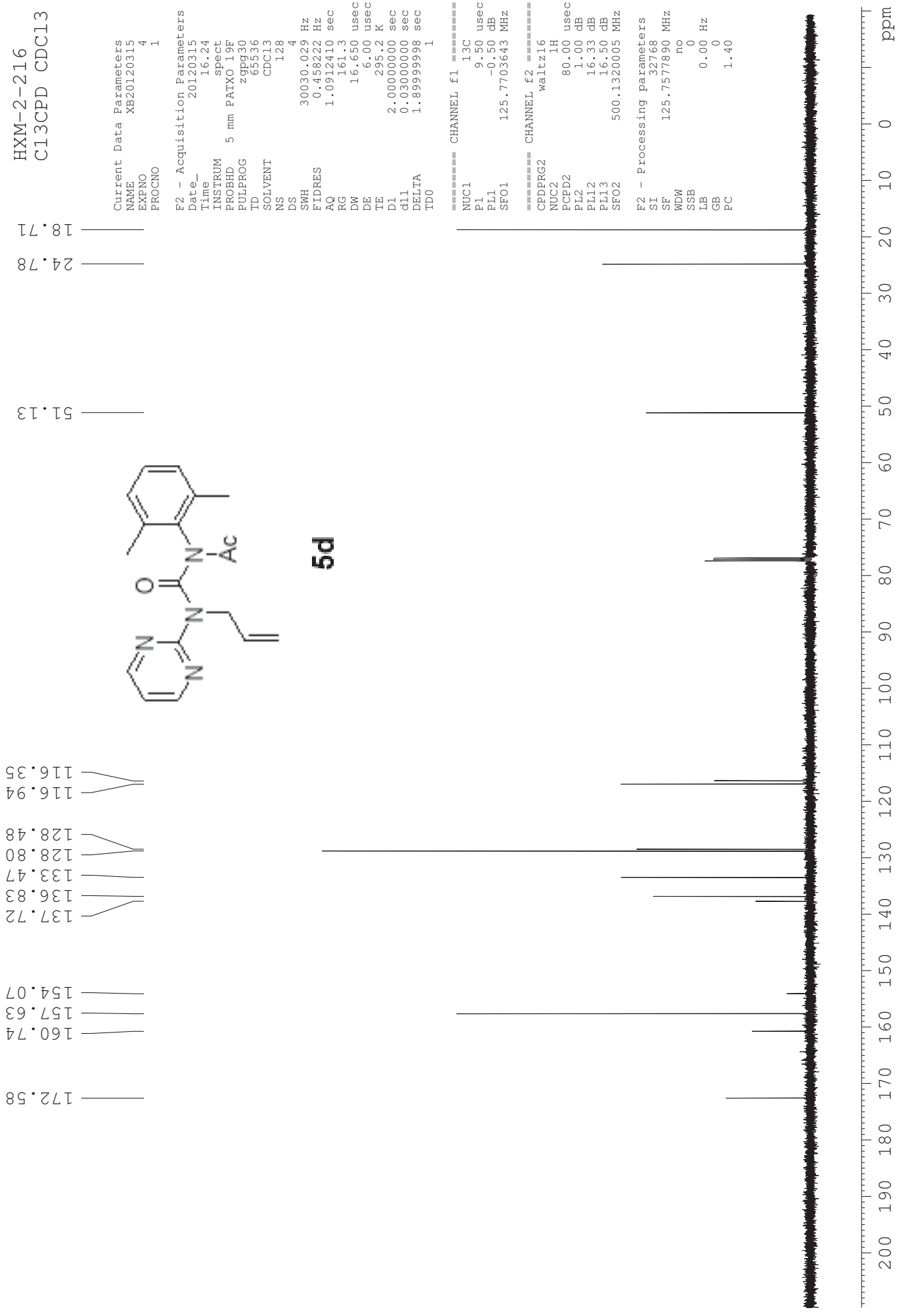

HXM-2-254
PROTON CDC13
NAME XB20120413
EXPNO 6
PROCNO 1
Date_ 20120413
Time 10.12
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 256
DW 48.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300131 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
5a
Ac
Ph
O
N
ppm
1.95
0.98
2.20
0.98
2.00
1.00
3.01
7.18
3.12

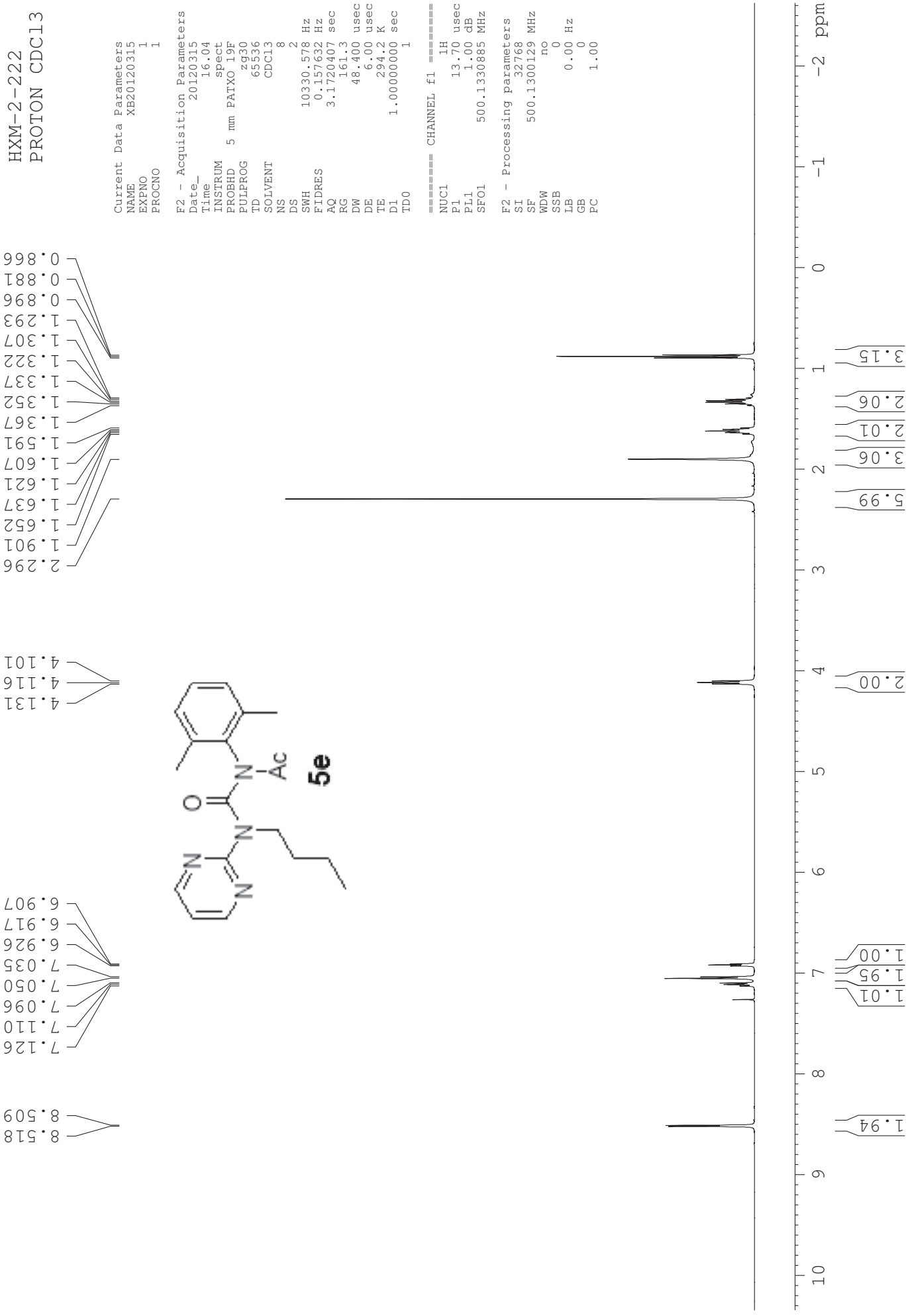

HXM-2-254
C13CPD CDC13
NAME XB20120411
EXPNO 5
PROCNO 1
Date_ 20120411
Time 10.34
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
24.74
25.40
26.25
30.06
58.33
118.19
127.09
127.75
129.54
140.80
157.05
158.59
161.35
170.87
5a
Ac
Ph
N
O
ppm


hxm-2-241-1
PROTON CDC13
NAME xb20120331
EXPNO 5
PROCNO 1
Date_ 20120331
Time 13.16
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 90.5
DW 48.400 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.896
2.453
8.550
8.541
7.290
7.280
7.150
7.137
7.122
7.070
7.056
7.043
7.002
6.992
6.983
6.894
6.885
3.00
2.97
1.95
3.08
1.12
2.98
1.07
1.93
ppm
5c
N
N
O
N
Ph
N
Ac

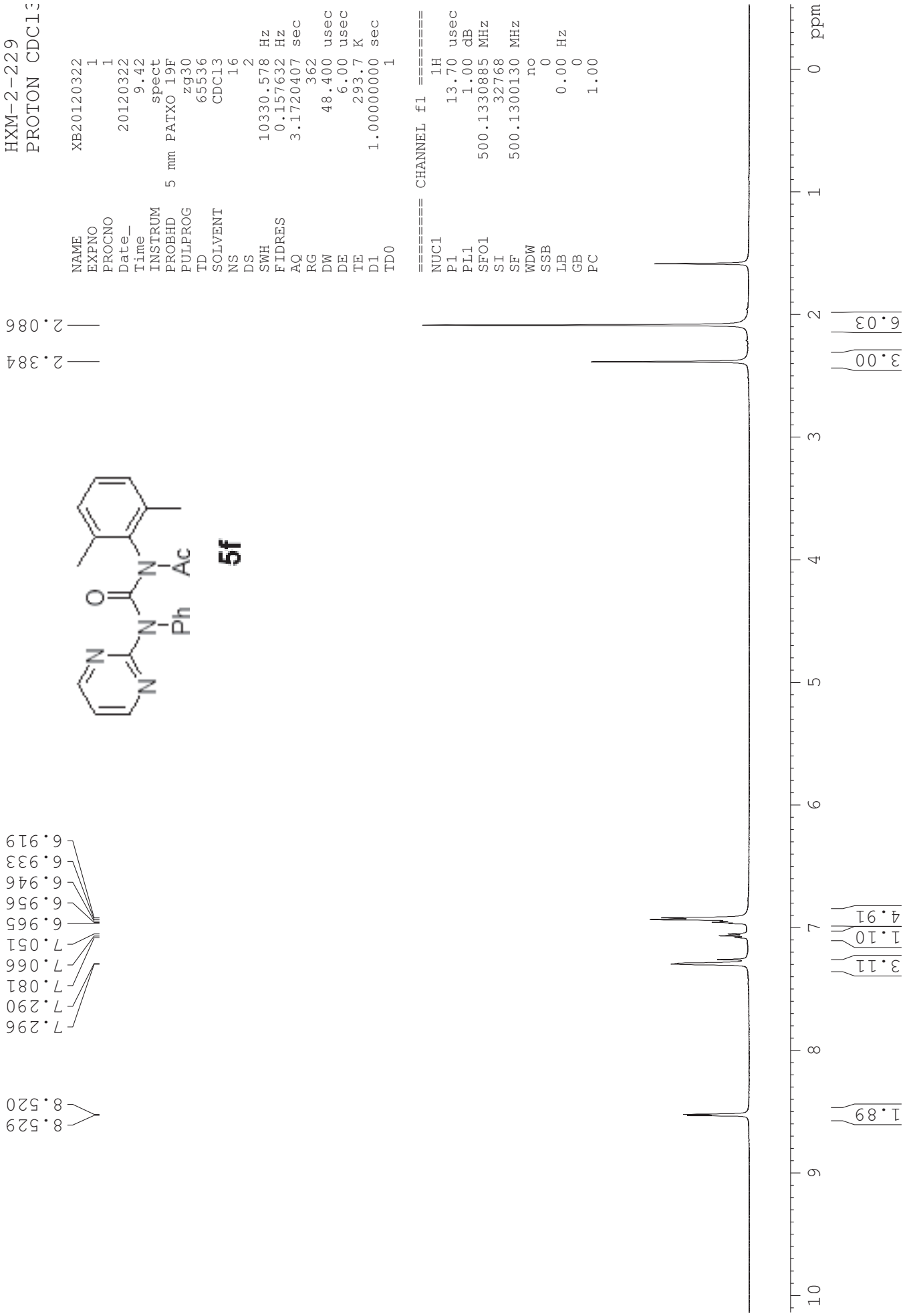

hxm-2-241-1
C13CPD CDC13
NAME xb20120331
EXPNO 7
PROCNO 1
Date_ 20120331
Time 13.25
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 296.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
5c
Ac
Ph
O
N
N
N
N
172.87
161.42
158.26
157.09
139.85
137.00
136.69
130.77
129.33
128.33
128.13
127.73
127.55
126.44
117.09
25.01
17.90
ppm
0
20
40
60
80
100
120
140
160
180
200


HXM-2-216
PROTON CDC13
NAME XB20120312
EXPNO 2
PROCNO 1
Date_ 20120312
Time 9.39
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300131 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.880
2.313
4.758
4.769
5.080
5.082
5.100
5.103
5.260
5.263
5.294
5.297
5.922
5.932
5.943
5.953
5.966
5.977
5.987
5.998
6.922
6.931
6.941
7.054
7.069
7.115
7.128
7.145
8.527
8.536
Ac
5d
ppm
3.00
6.17
2.07
1.05
1.05
1.03
1.04
2.05
1.05
2.00

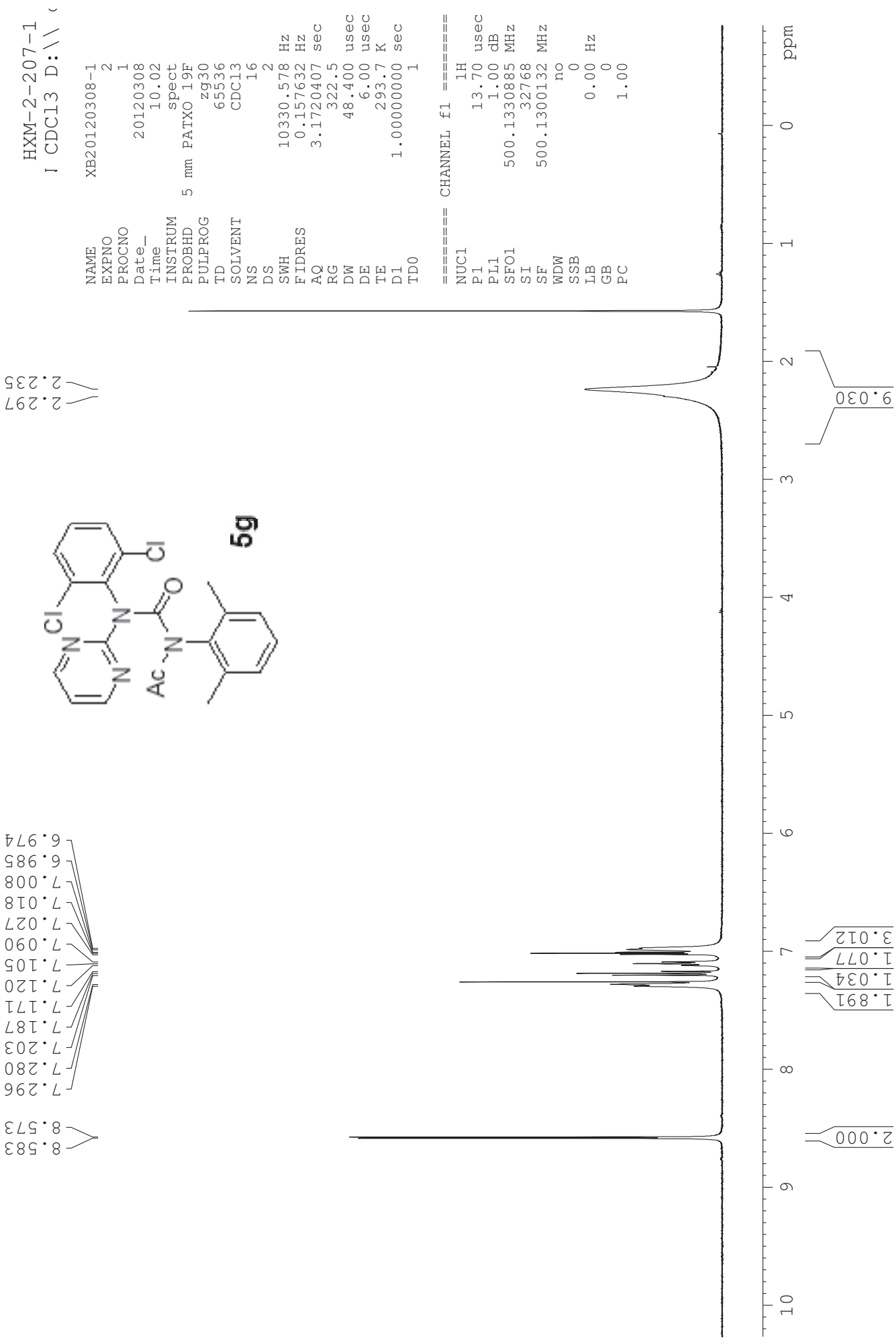

HXM-2-216
C13CPD CDC13
Current Data Parameters
NAME XB20120315
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120315
Time 16.24
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
18.71
24.78
51.13
116.35
116.94
128.48
128.80
133.47
136.83
137.72
154.07
157.63
160.74
172.58
N
Ac
O
N
N
N
5d
ppm

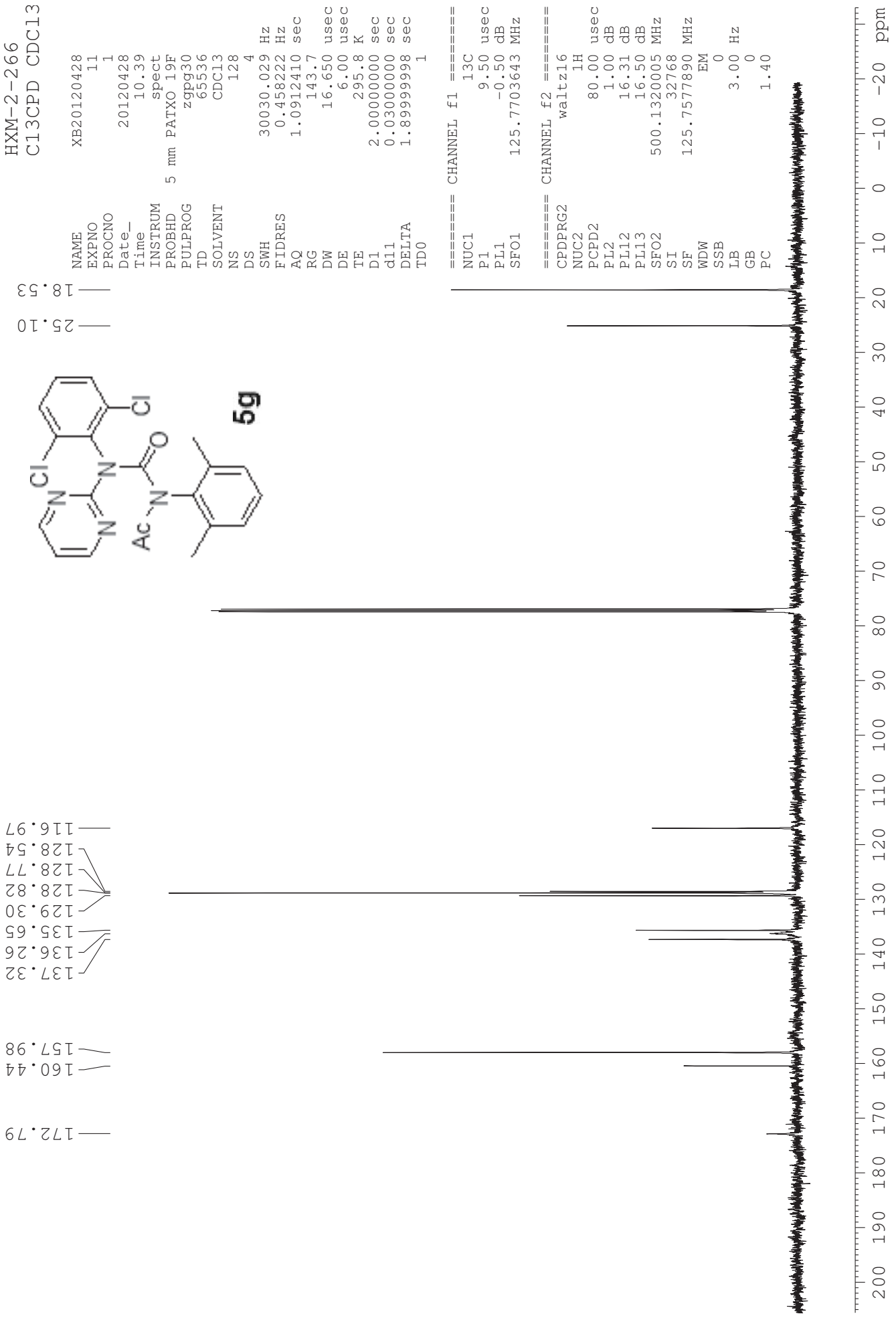

HXM-2-222
PROTON CDCl3
Current Data Parameters
NAME XB20120315
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120315
Time 16.04
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 161.3
DW 48.400 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
0.866
0.881
0.896
1.293
1.307
1.322
1.337
1.352
1.367
1.591
1.607
1.621
1.637
1.652
1.901
2.296
4.101
4.116
4.131
6.907
6.917
6.926
7.035
7.050
7.096
7.110
7.126
8.509
8.518
3.15
2.06
2.01
3.06
5.99
2.00
1.00
1.95
1.01
1.94
ppm
5e
N
Ac
O
N
N
N

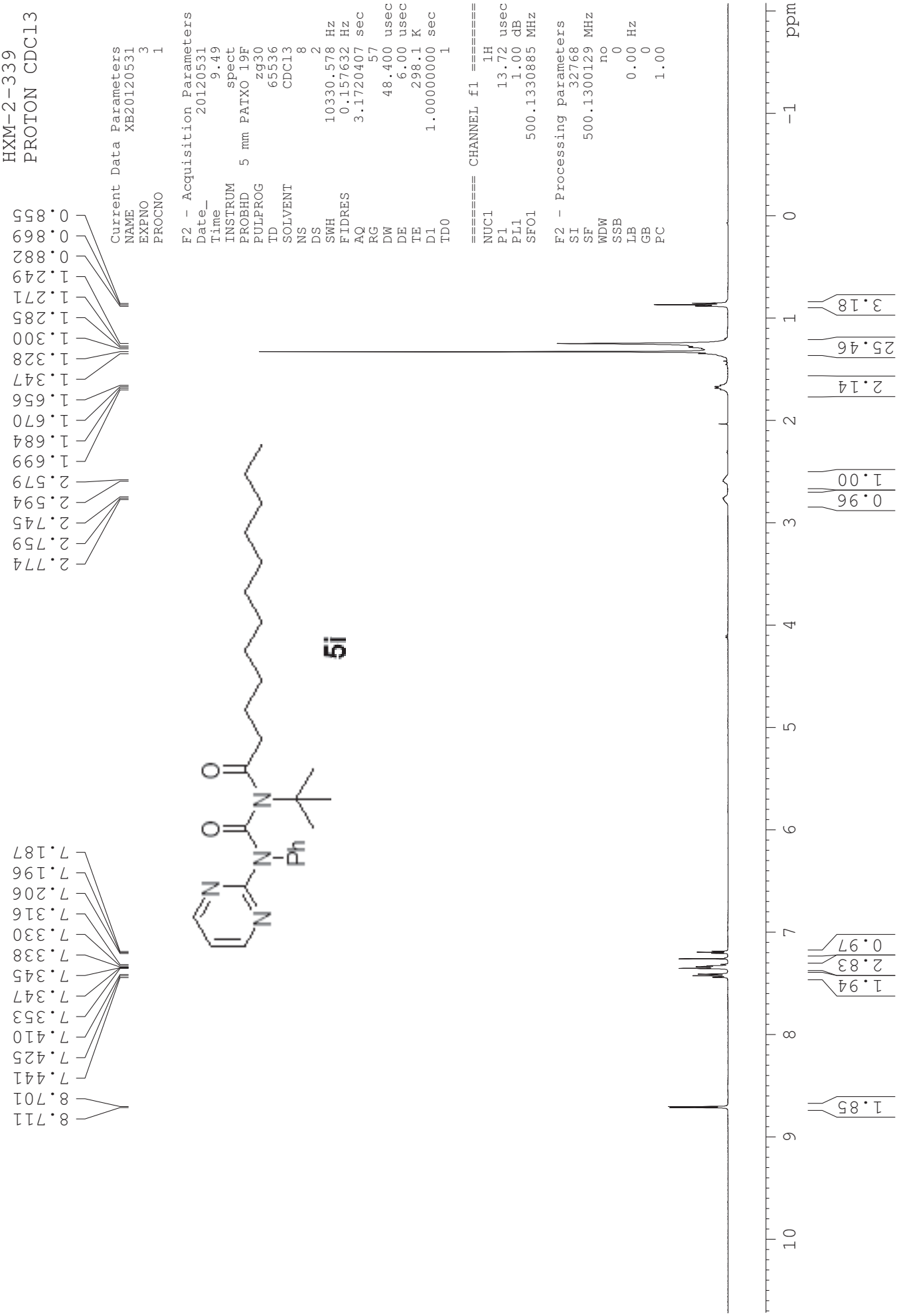

HXM-2-222
C13CPD CDC13
Current Data Parameters
NAME XB20120315
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120315
Time 16.36
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
13.87
18.73
20.07
24.78
30.74
49.05
116.24
128.37
128.76
136.80
137.69
154.47
157.60
160.88
172.56
5e
Ac
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


HXM-2-229
PROTON CDCl3
NAME XB20120322
EXPNO 1
PROCNO 1
Date_ 20120322
Time 9.42
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 362
DW 48.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300130 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
2.086
2.384
6.919
6.933
6.946
6.956
6.965
7.051
7.066
7.081
7.290
7.296
8.520
8.529
5f
N
Ac
O
N
Ph
N
N
ppm
0
1
2
3
4
5
6
7
8
9
10
6.03
3.00
4.91
1.10
3.11
1.89

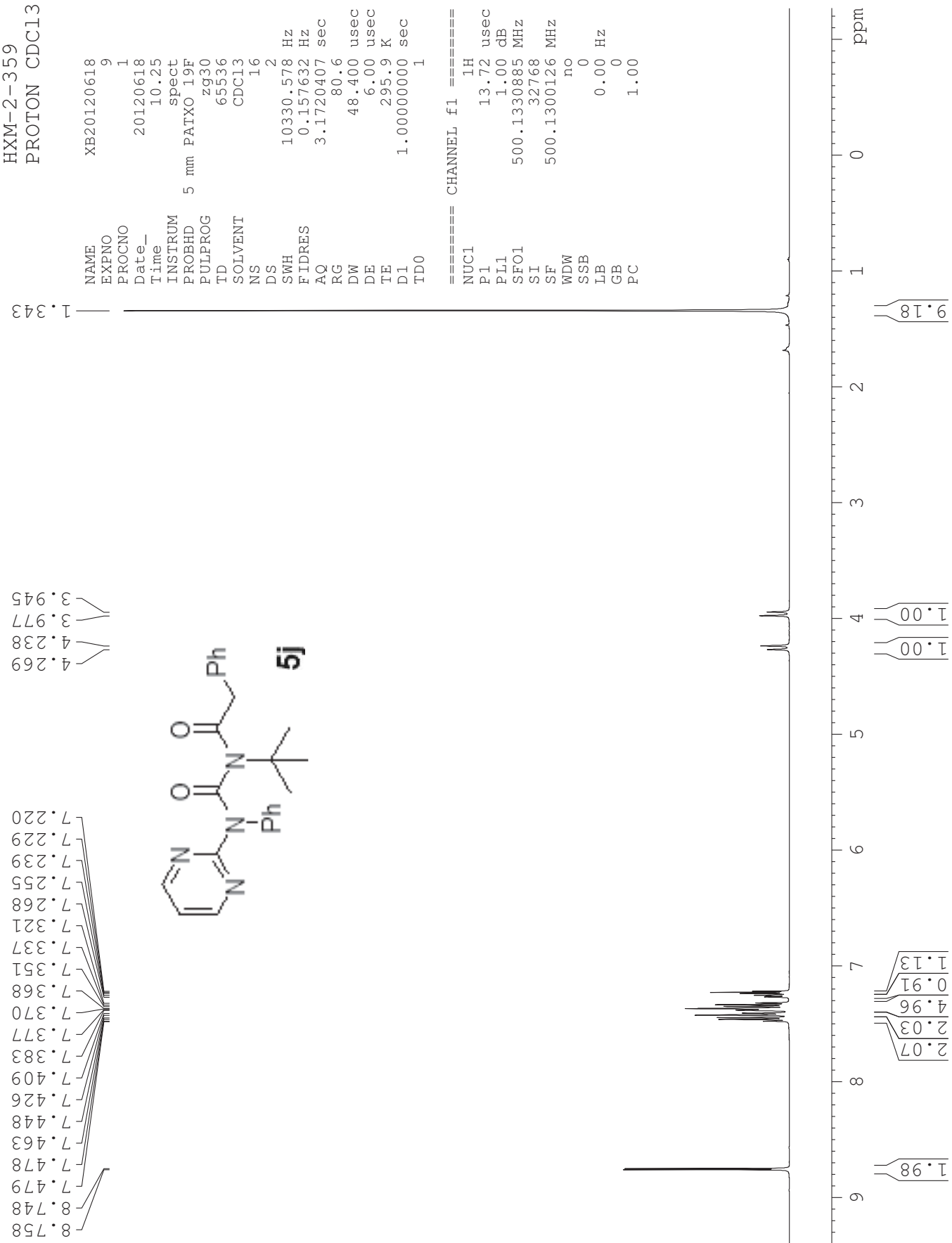

HXM-2-229
C13CPD CDC13
NAME XB20120322
EXPNO 8
PROCNO 1
Date_ 20120322
Time 10.28
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 59
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
18.45
25.27
116.66
127.88
128.32
128.42
128.48
129.30
136.28
137.16
139.84
156.70
157.97
161.66
173.30
5f
Ph
Ac
O
N
N
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 ppm


HXM-2-207-1
1 CDC13 D:\\
NAME XB20120308-1
EXPNO 2
PROCNO 1
Date_ 20120308
Time 10.02
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 322.5
DW 48.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
5g
Cl
Cl
N
N
N
O
N
Ac
2.297
2.235
6.974
6.985
7.008
7.018
7.027
7.090
7.105
7.120
7.171
7.187
7.203
7.280
7.296
8.573
8.583
9.030
2.000
1.891
1.034
1.077
3.012
ppm

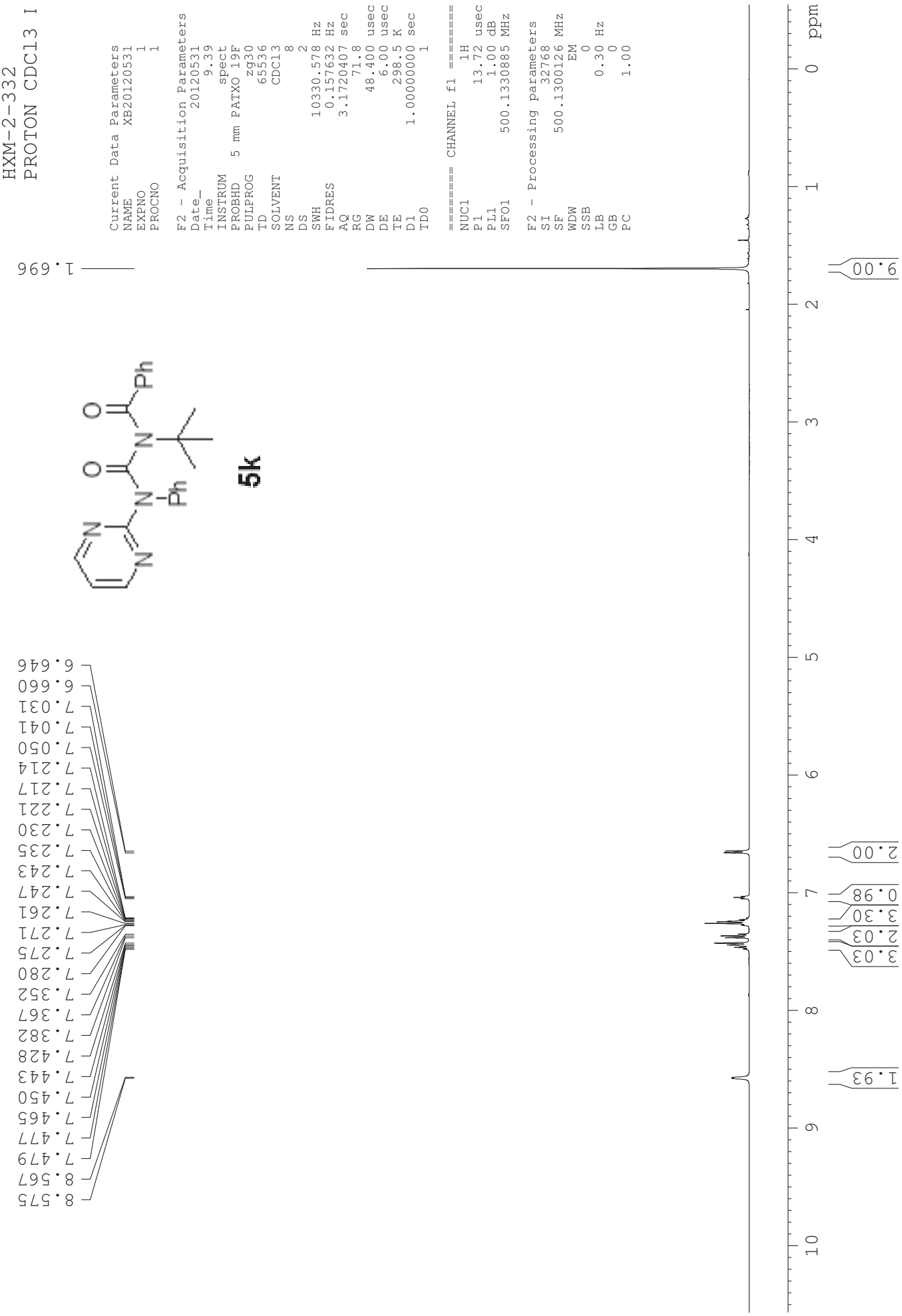

HXM-2-266
C13CPD CDC13
NAME XB20120428
EXPNO 11
PROCNO 1
Date_ 20120428
Time 10.39
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
18.53
25.10
116.97
128.54
128.77
128.82
129.30
135.65
136.26
137.32
157.98
160.44
172.79
5g
Cl
Cl
N
N
N
O
Ac
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 ppm


HXM-2-339
PROTON CDCl3
Current Data Parameters
NAME XB20120531
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 9.49
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 57
DW 48.400 usec
DE 6.00 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
0.855
0.869
0.882
1.249
1.271
1.285
1.300
1.328
1.347
1.656
1.670
1.684
1.699
2.579
2.594
2.745
2.759
2.774
7.187
7.196
7.206
7.316
7.330
7.338
7.345
7.347
7.353
7.410
7.425
7.441
8.701
8.711
5i
Ph
ppm
3.18
25.46
2.14
1.00
0.96
1.94
2.83
0.97
1.85

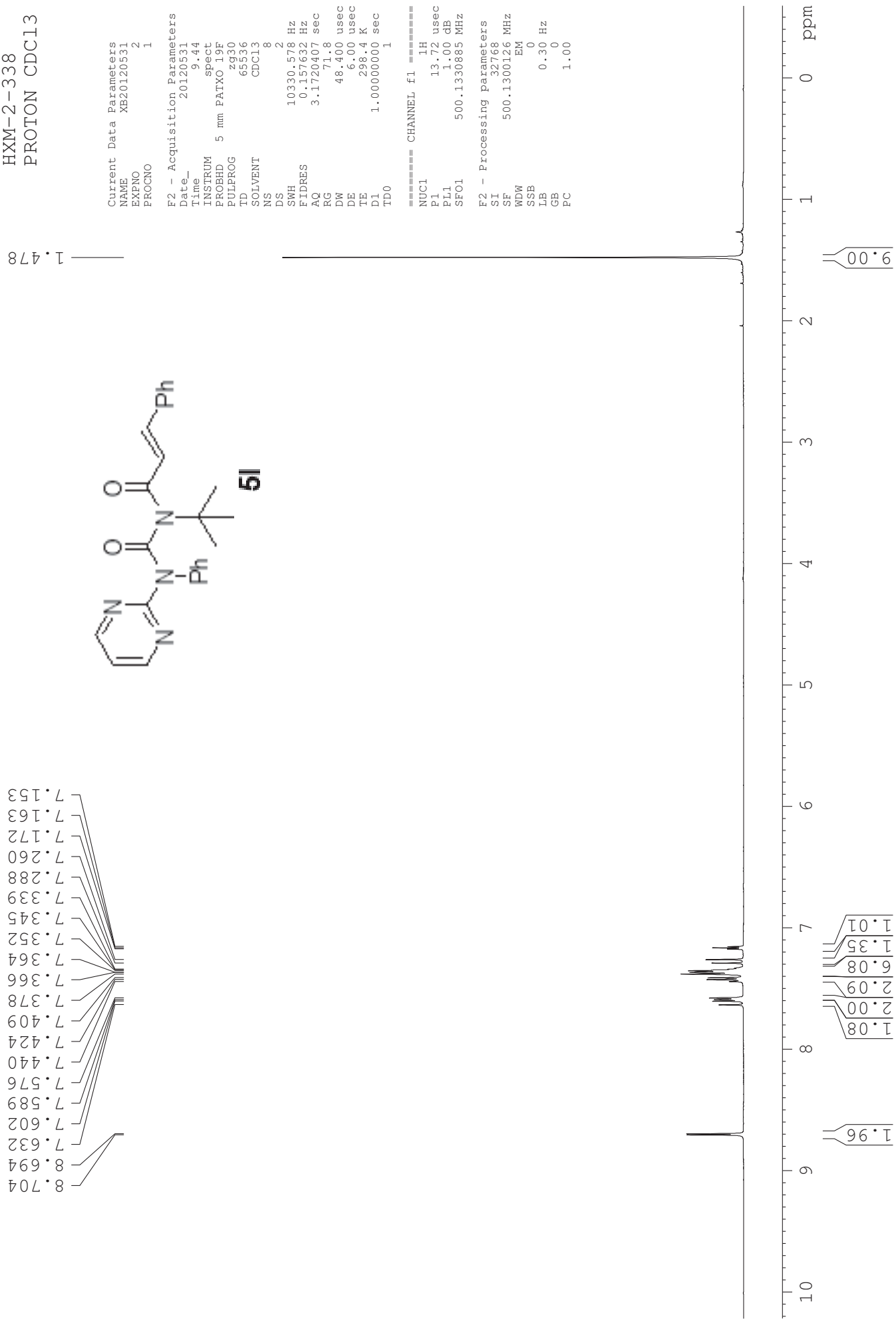

HXM-2-339
C13CPD CDC13
Current Data Parameters
NAME XB20120531
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 10.59
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 128
DW 16.650 usec
DE 6.00 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
14.13
22.69
25.07
27.76
29.33
29.36
29.55
29.56
29.64
29.70
31.92
37.37
58.68
119.32
127.00
127.91
129.42
140.43
156.10
158.78
160.86
172.92
5i
Ph
ppm
0
20
40
60
80
100
120
140
160
180
200

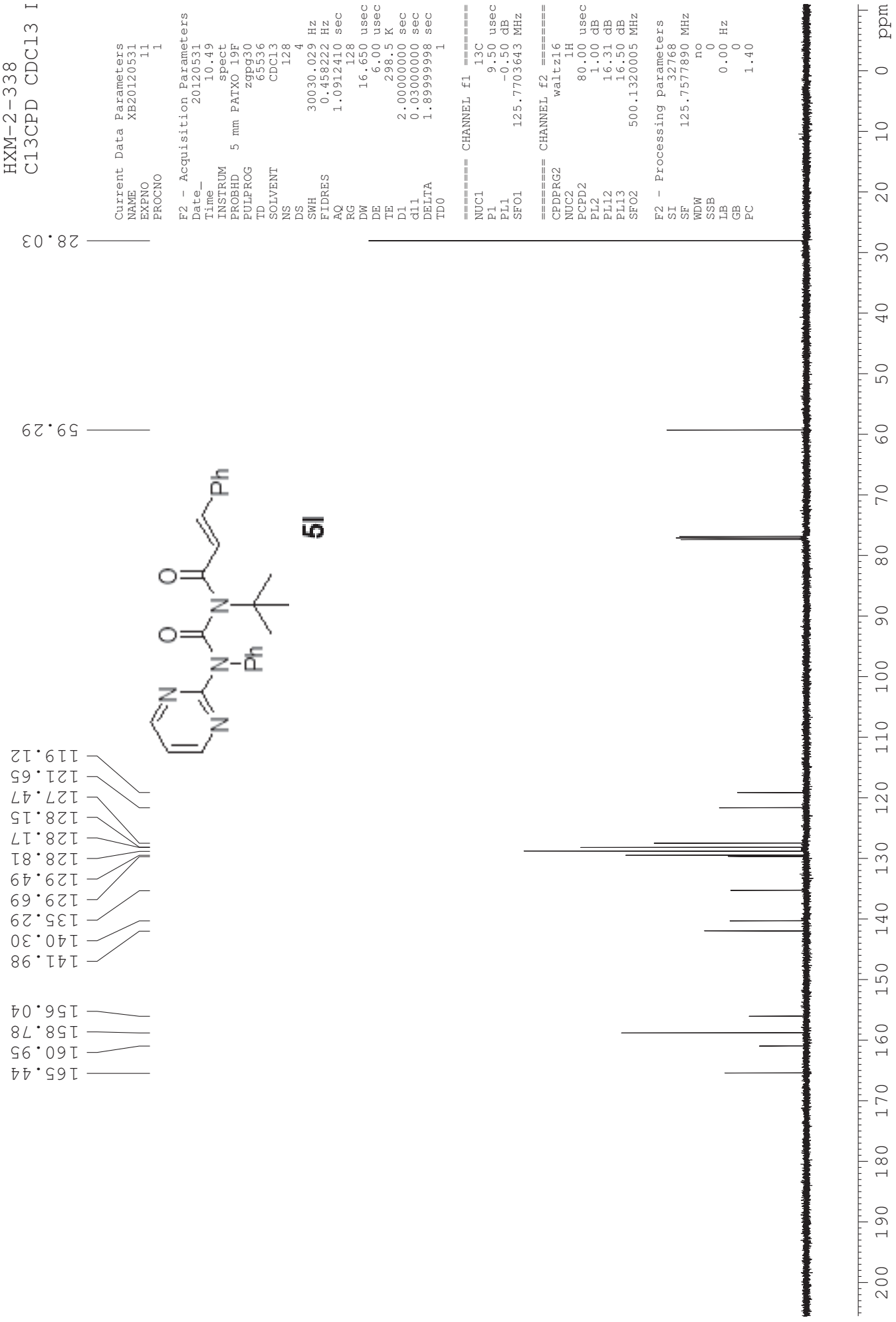

HXM-2-359
PROTON CDC13
NAME XB20120618
EXPNO 9
PROCNO 1
Date_ 20120618
Time 10.25
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 80.6
DW 48.400 usec
DE 6.00 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
5j
Ph
O
N
O
N
Ph
N
N
1.343
9.18
1.00
1.00
1.98
1.13
0.91
4.96
2.03
2.07
4.269
4.238
3.977
3.945
7.220
7.229
7.239
7.255
7.268
7.321
7.337
7.351
7.368
7.370
7.377
7.383
7.409
7.426
7.448
7.463
7.478
7.479
8.748
8.758
ppm

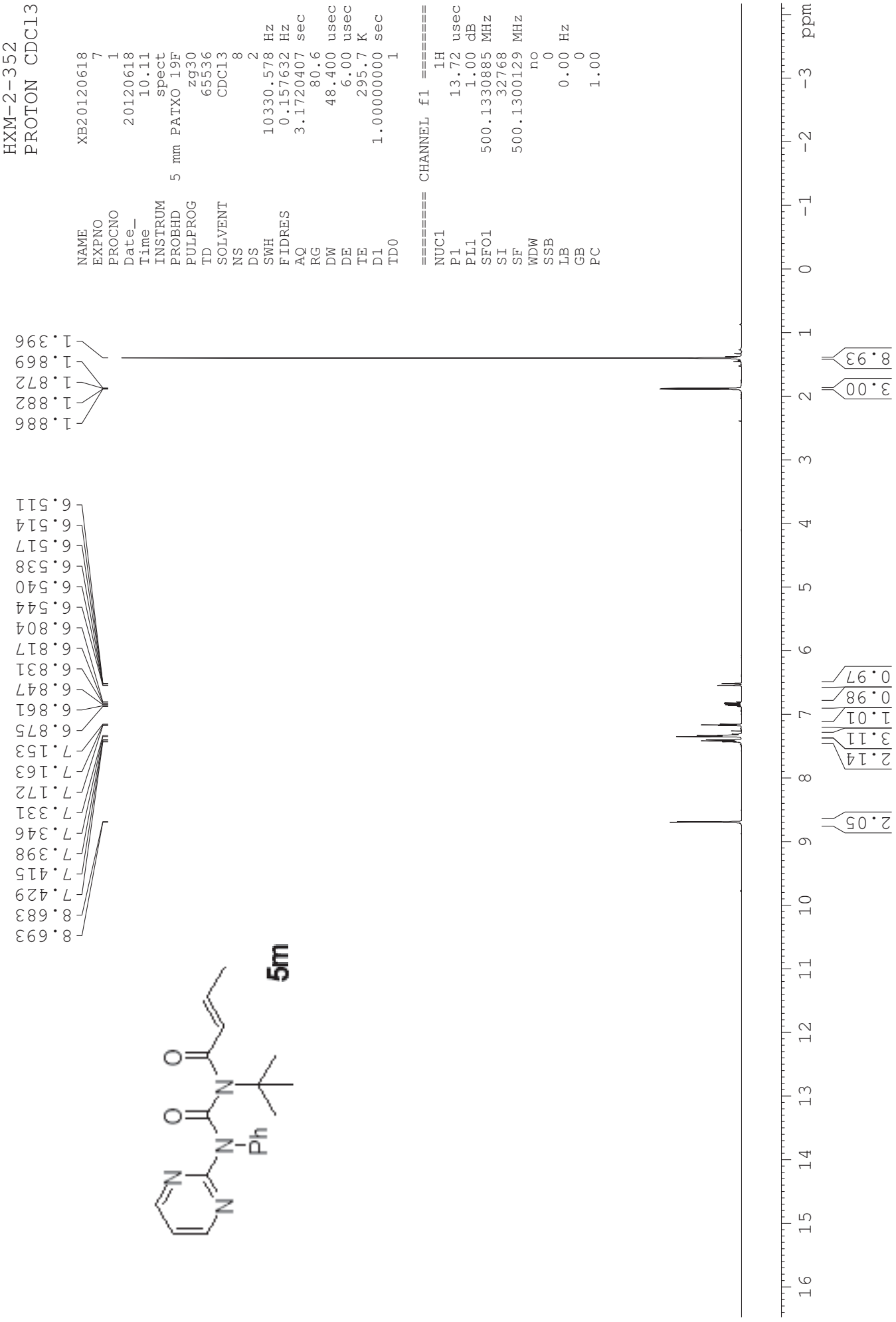

HXM-2-359
C13CPD CDCl3
NAME XB20120618
EXPNO 10
PROCNO 1
Date_ 20120618
Time 10.34
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
27.75
43.78
59.12
119.54
126.63
127.03
128.07
128.27
129.52
130.04
135.51
140.33
156.06
158.91
160.87
170.73
5j
Ph
O
N
O
N
Ph
N
N
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


HXM-2-332
PROTON CDC13 I
Current Data Parameters
NAME XB20120531
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 9.39
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 298.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.696
5k
8.575
8.567
7.479
7.477
7.465
7.450
7.443
7.428
7.382
7.367
7.352
7.280
7.275
7.271
7.261
7.247
7.243
7.235
7.230
7.221
7.217
7.214
7.050
7.041
7.031
6.660
6.646
9.00
2.00
0.98
3.30
2.03
3.03
1.93
ppm

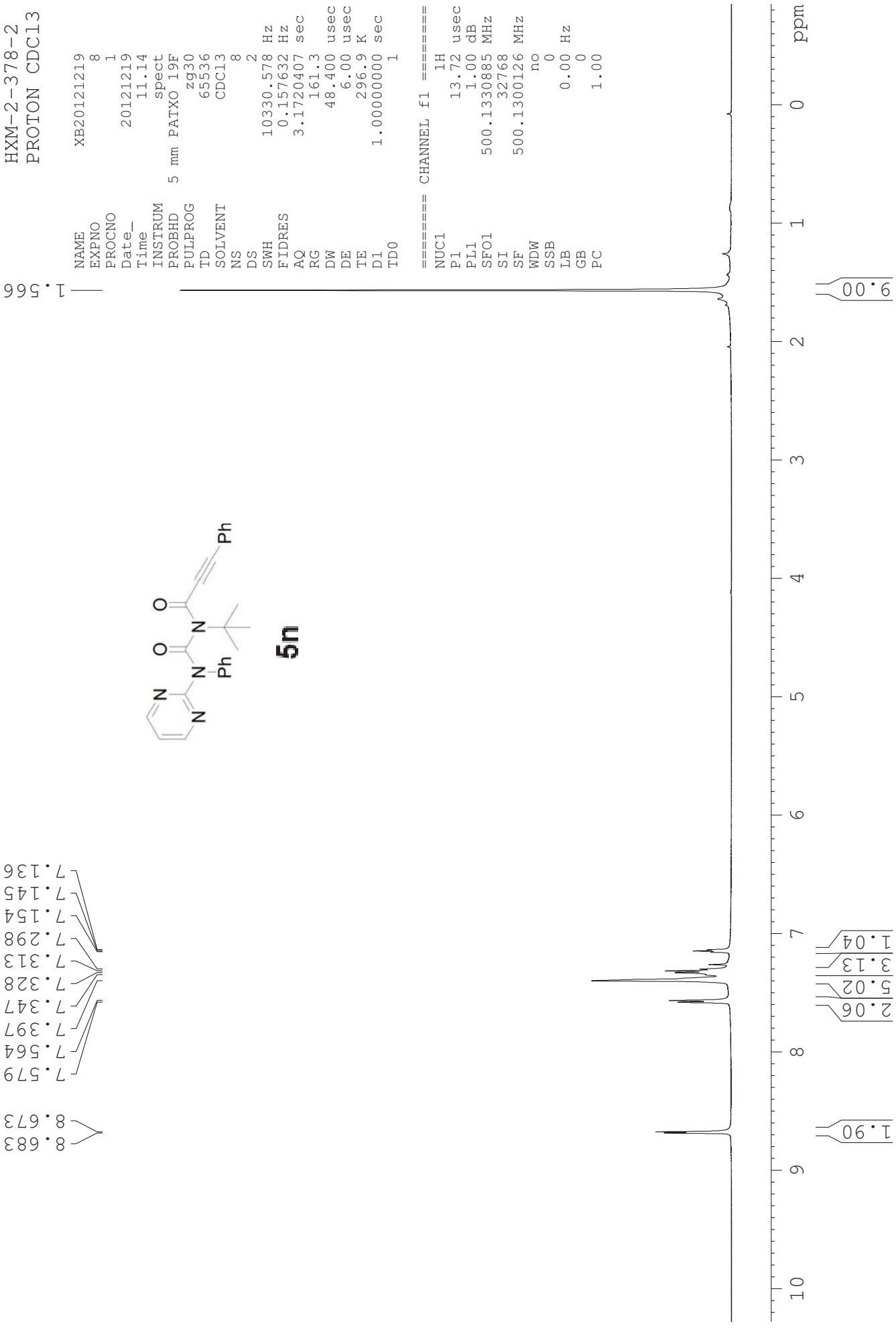

HXM-2-332
C13CPD CDCl3 I
Current Data Parameters
NAME XB20120531
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 10.36
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 287.4
DW 16.650 usec
DE 6.00 usec
TE 298.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
28.71
60.37
117.62
127.29
127.67
127.92
128.17
129.05
130.96
138.01
140.27
155.61
158.05
160.44
170.03
5k
Ph
Ph
ppm


HXM-2-338
PROTON CDC13
Current Data Parameters
NAME XB20120531
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 9.44
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.478
9.00
1.96
1.08
2.00
2.09
6.08
1.35
1.01
8.704
8.694
7.632
7.602
7.589
7.576
7.440
7.424
7.409
7.378
7.366
7.364
7.352
7.345
7.339
7.288
7.260
7.172
7.163
7.153
ppm
0
1
2
3
4
5
6
7
8
9
10
Ph
O
N
O
N
N
Ph
5l


HXM-2-338
C13CPD CDCl3 I
Current Data Parameters
NAME XB20120531
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 10.49
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 128
DW 16.650 usec
DE 6.00 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
28.03
59.29
119.12
121.65
127.47
128.15
128.17
128.81
129.49
129.69
135.29
140.30
141.98
156.04
158.78
160.95
165.44
5l
Ph
O
N
O
N
Ph
N
N
ppm


HXM-2-352
PROTON CDC13
NAME XB20120618
EXPNO 7
PROCNO 1
Date_ 20120618
Time 10.11
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 80.6
DW 48.400 usec
DE 6.00 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.396
1.869
1.872
1.882
1.886
8.693
8.683
7.429
7.415
7.398
7.346
7.331
7.172
7.163
7.153
6.875
6.861
6.847
6.831
6.817
6.804
6.544
6.540
6.538
6.517
6.514
6.511
3.00
8.93
2.14
3.11
1.01
0.98
0.97
2.05
ppm
5m
O
N
O
N
Ph
N
N


HXM-2-352
C13CPD CDC13
NAME XB20120618
EXPNO 8
PROCNO 1
Date_ 20120618
Time 10.19
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 296.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
18.13
27.90
59.00
119.07
125.70
127.28
127.99
129.40
140.40
141.12
156.06
158.72
160.88
165.49
5m
Ph
ppm
0
20
40
60
80
100
120
140
160
180
200


HXM-2-378-2
PROTON CDC13
NAME XB20121219
EXPNO 8
PROCNO 1
Date_ 20121219
Time 11.14
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 161.3
DW 48.400 usec
DE 6.00 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.566
9.00
1.90
2.06
5.02
3.13
1.04
8.683
8.673
7.579
7.564
7.397
7.347
7.328
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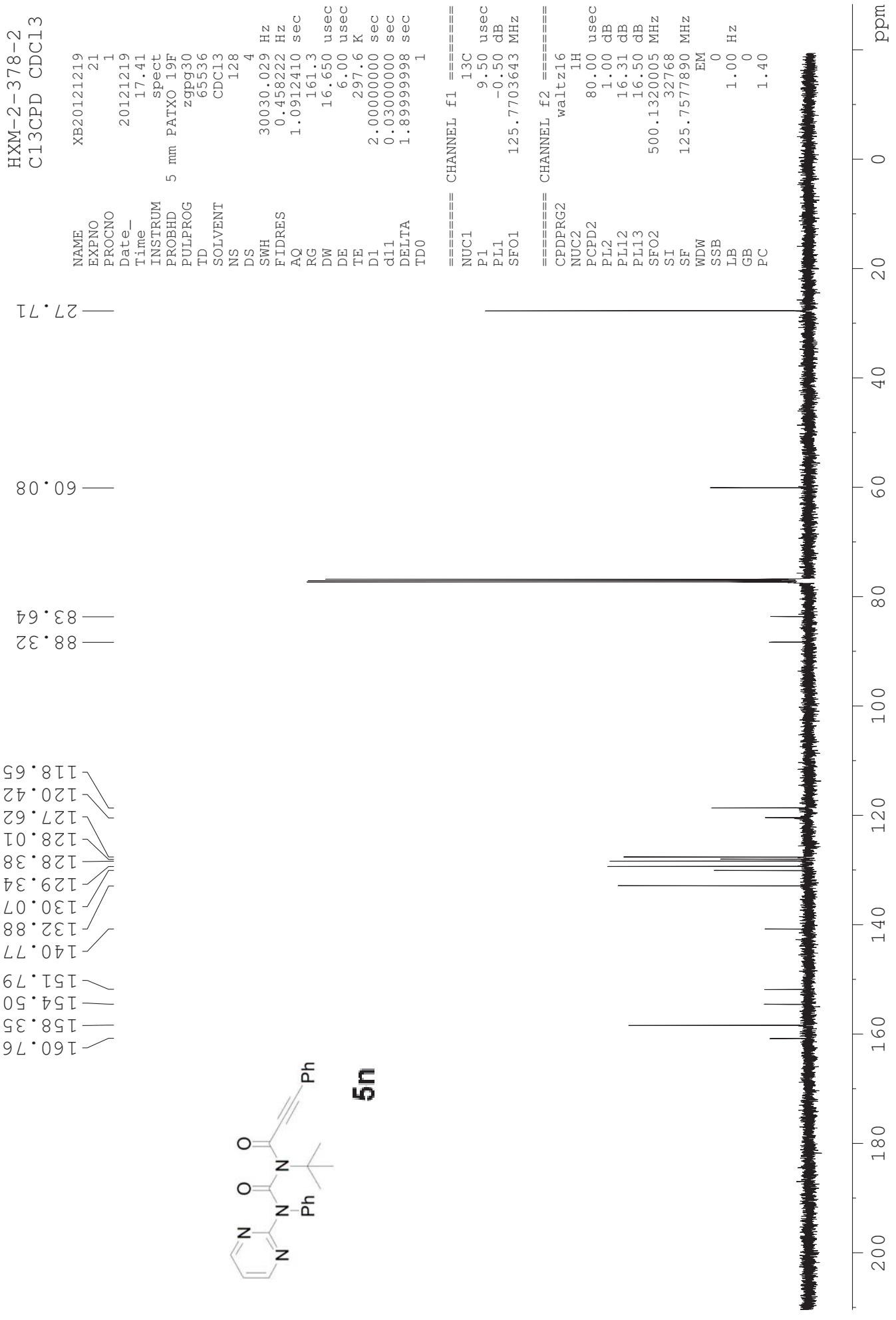
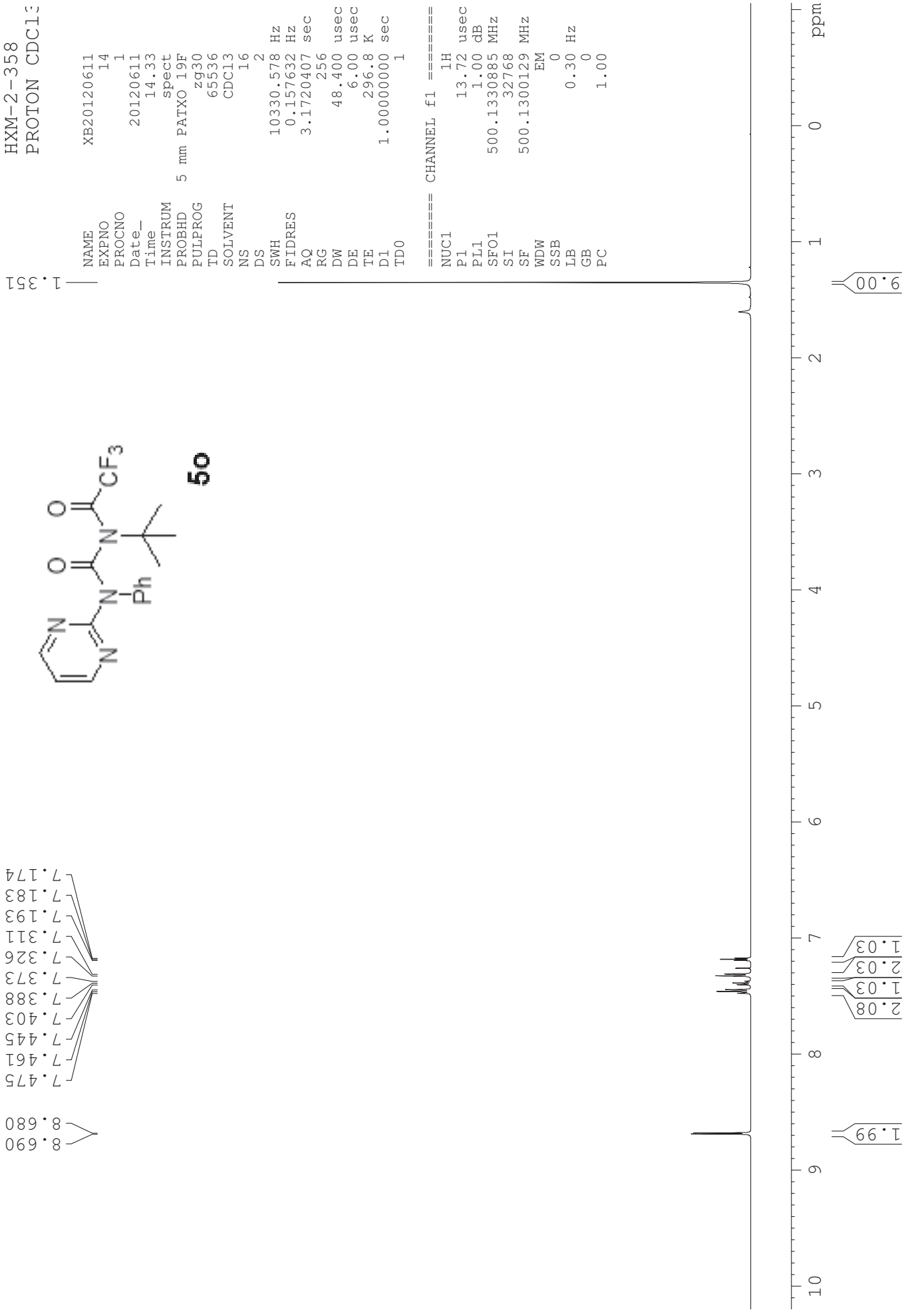
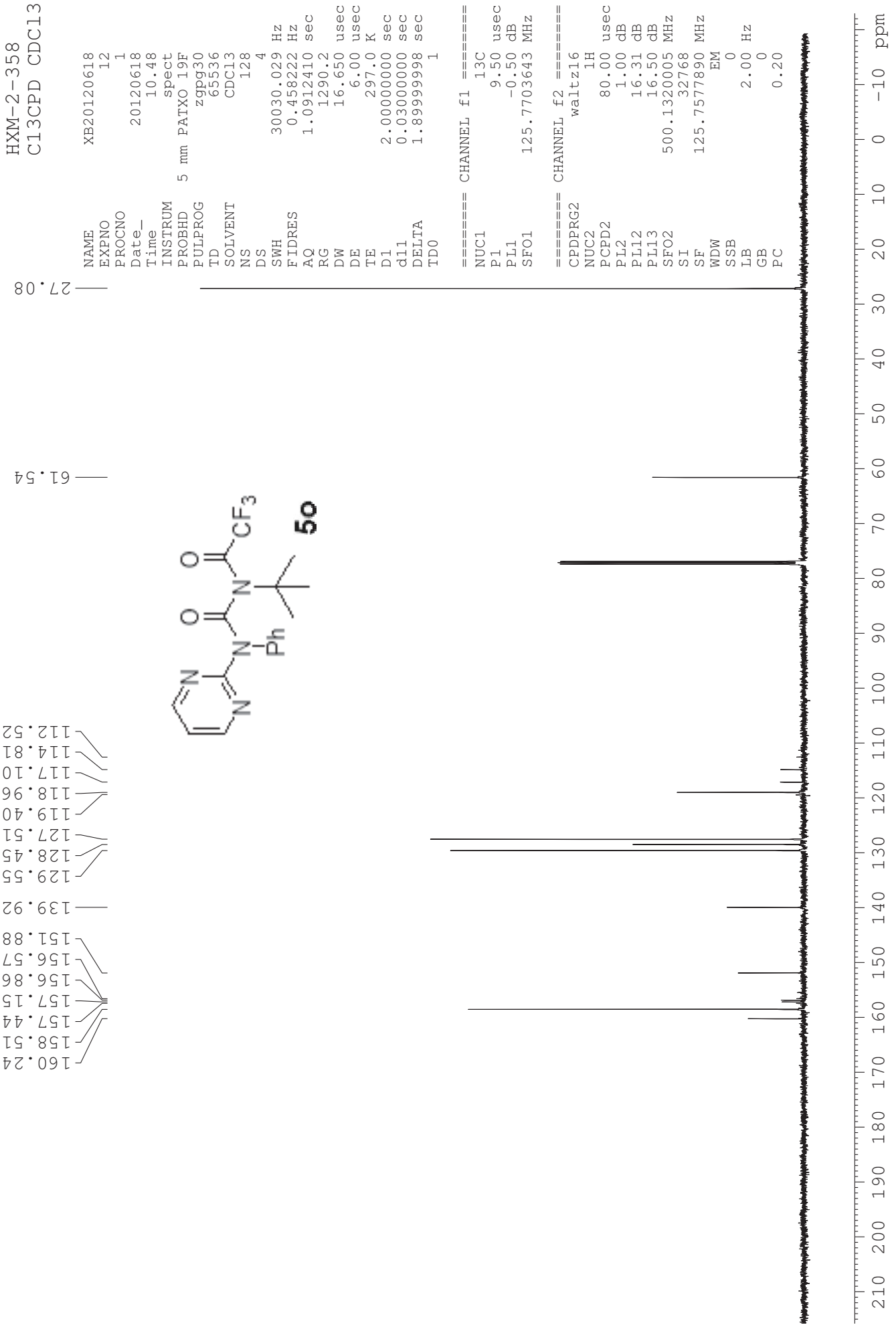
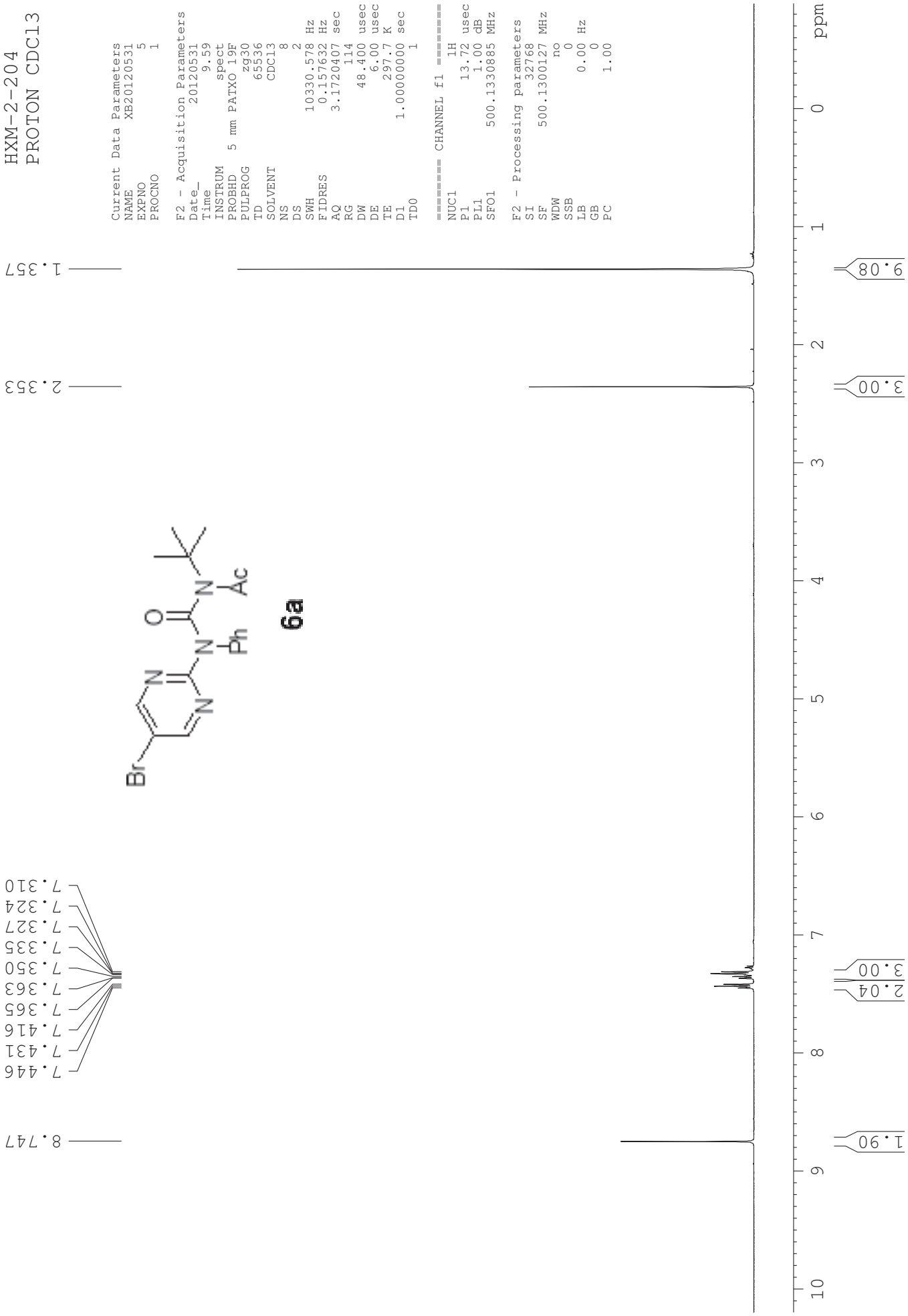
7.298
7.154
7.145
7.136
5n
Ph
Ph
ppm

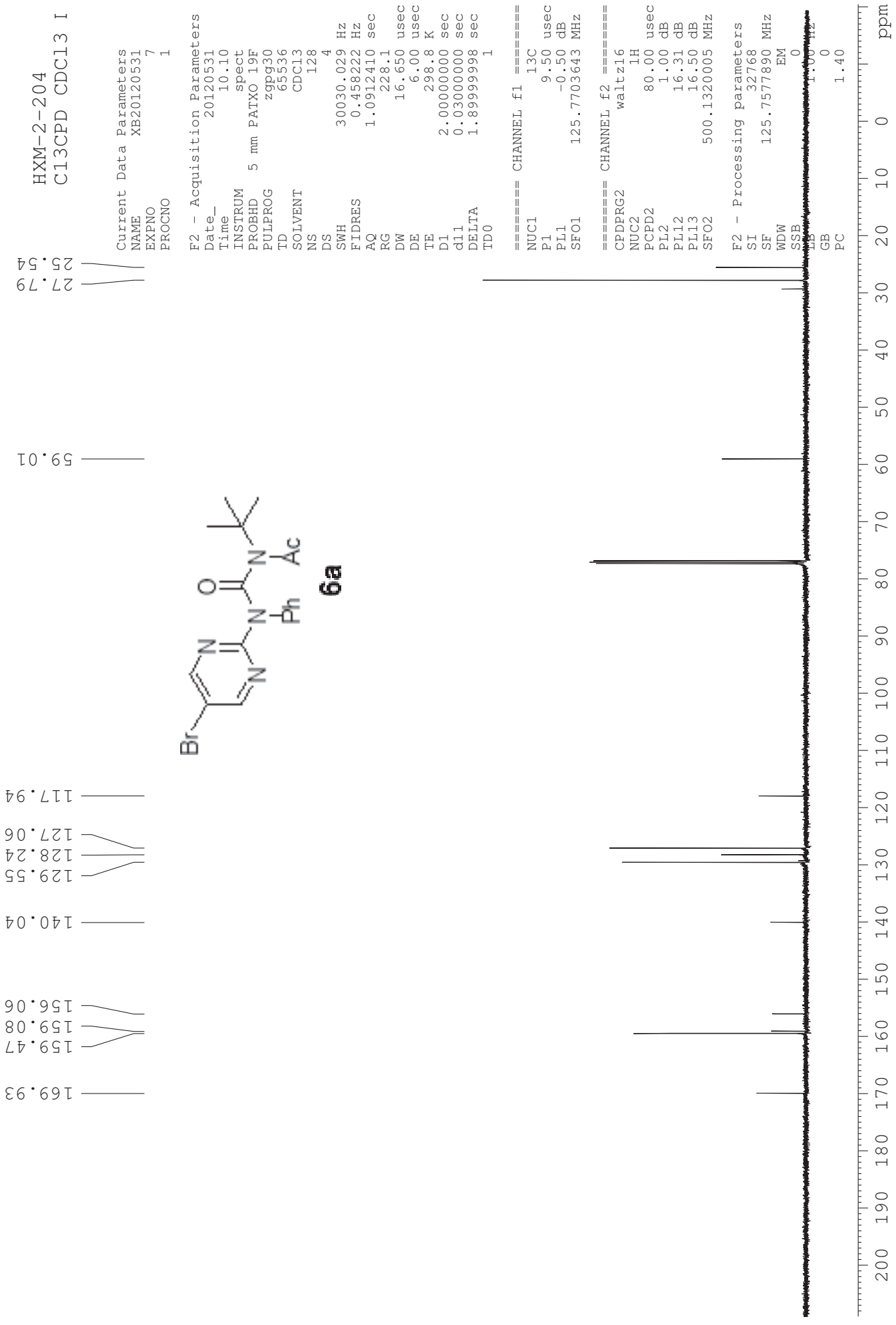

HXM-2-378-2
C13CPD CDC13
NAME XB20121219
EXPNO 21
PROCNO 1
Date_ 20121219
Time 17.41
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
27.71
60.08
83.64
88.32
118.65
120.42
127.62
128.01
128.38
129.34
130.07
132.88
140.77
151.79
154.50
158.35
160.76
5n
Ph
O
N
O
N
Ph
N
N
ppm
0
20
40
60
80
100
120
140
160
180
200


HXM-2-358
PROTON CDCl3
NAME XB20120611
EXPNO 14
PROCNO 1
Date_ 20120611
Time 14.33
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 256
DW 48.400 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.351
9.00
2.08
1.03
1.03
2.03
1.03
1.99
8.690
8.680
7.475
7.461
7.445
7.403
7.388
7.373
7.326
7.311
7.193
7.183
7.174
ppm
50

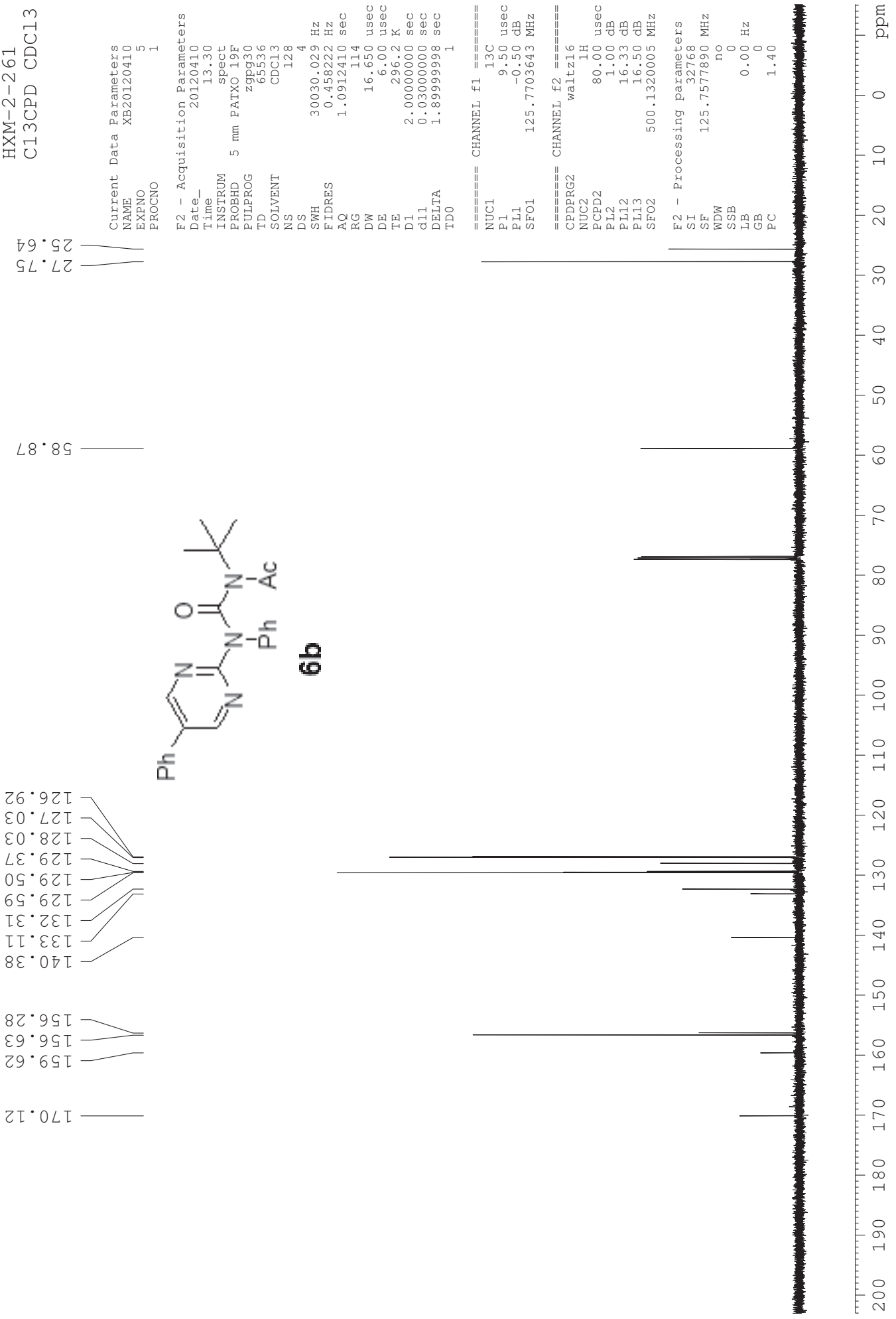
HXM-2-358
left CDCl3 D:\\ den
50
CF3
O
O
N
N
Ph
N
N
-70.743
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

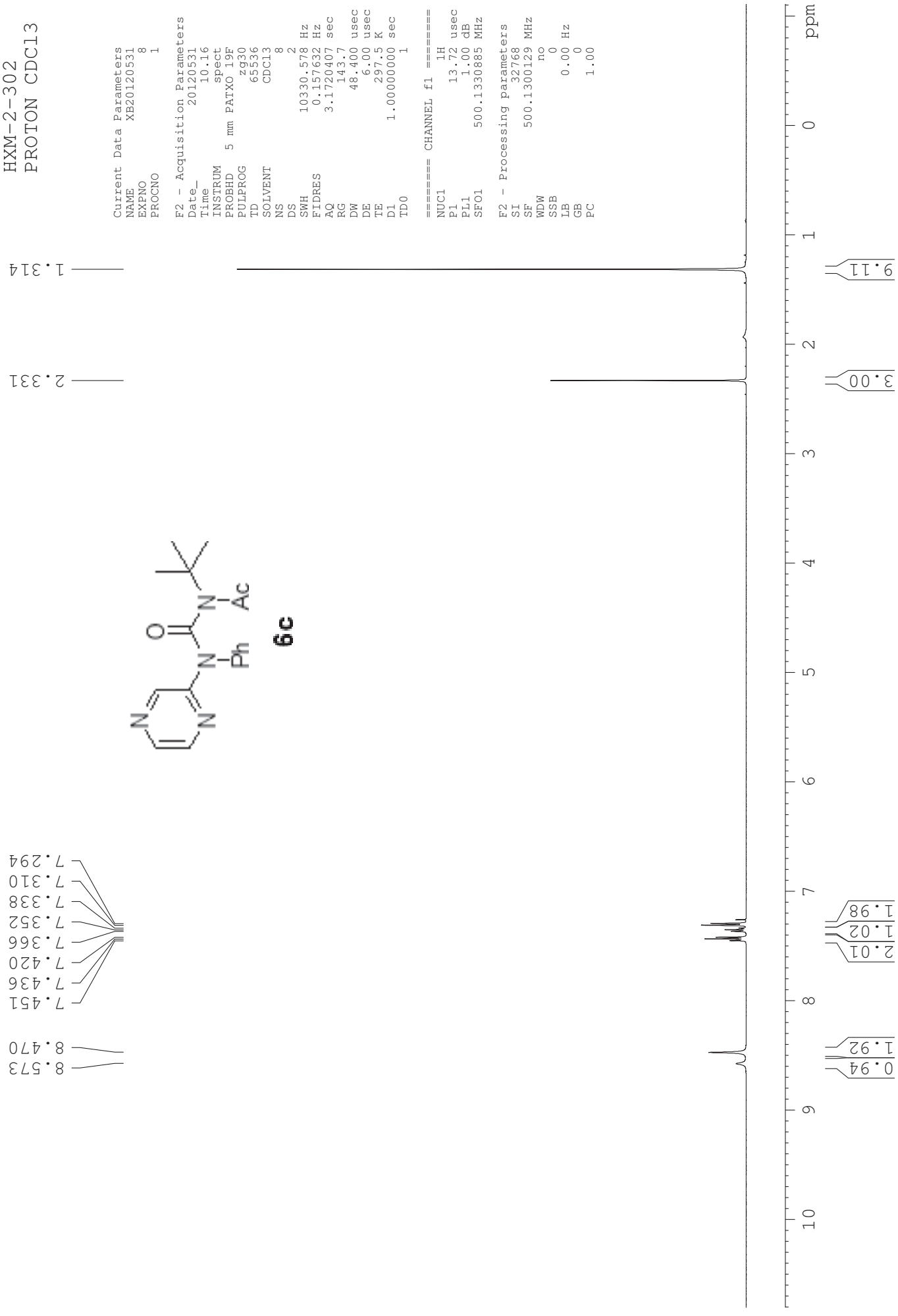

HXM-2-358
C13CPD CDC13
NAME XB20120618
EXPNO 12
PROCNO 1
Date_ 20120618
Time 10.48
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 1290.2
DW 16.650 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 0.20
27.08
61.54
112.52
114.81
117.10
118.96
119.40
127.51
128.45
129.55
139.92
151.88
156.57
156.86
157.15
157.44
158.51
160.24
50
ppm

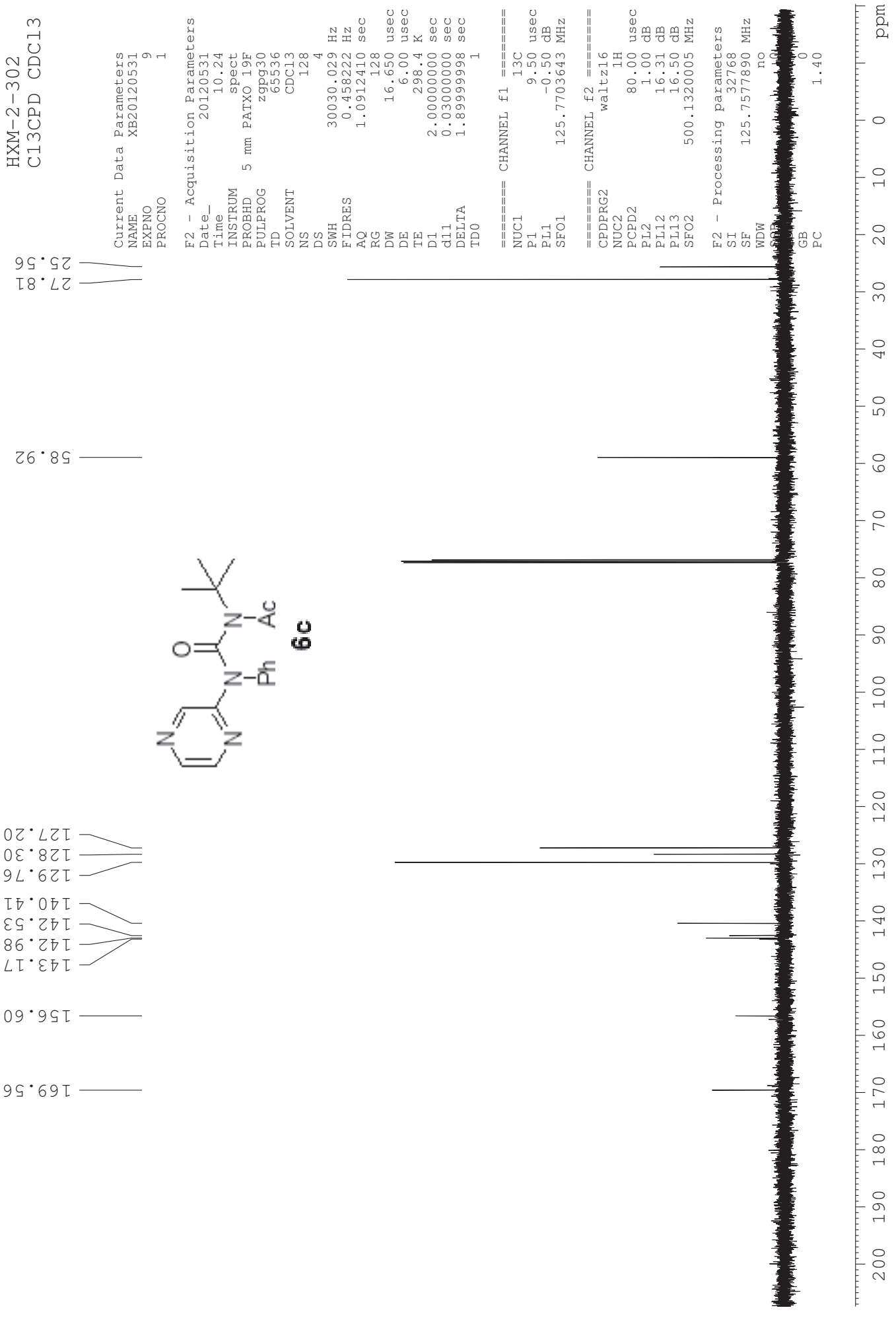

HXM-2-204
PROTON CDCl3
Current Data Parameters
NAME XB20120531
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 9.59
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 114
DW 48.400 usec
DE 6.00 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300127 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.357
2.353
7.310
7.324
7.327
7.335
7.350
7.363
7.365
7.416
7.431
7.446
8.747
9.08
3.00
2.04
3.00
1.90
ppm
Br
N
N
N
Ph
O
N
Ac
6a

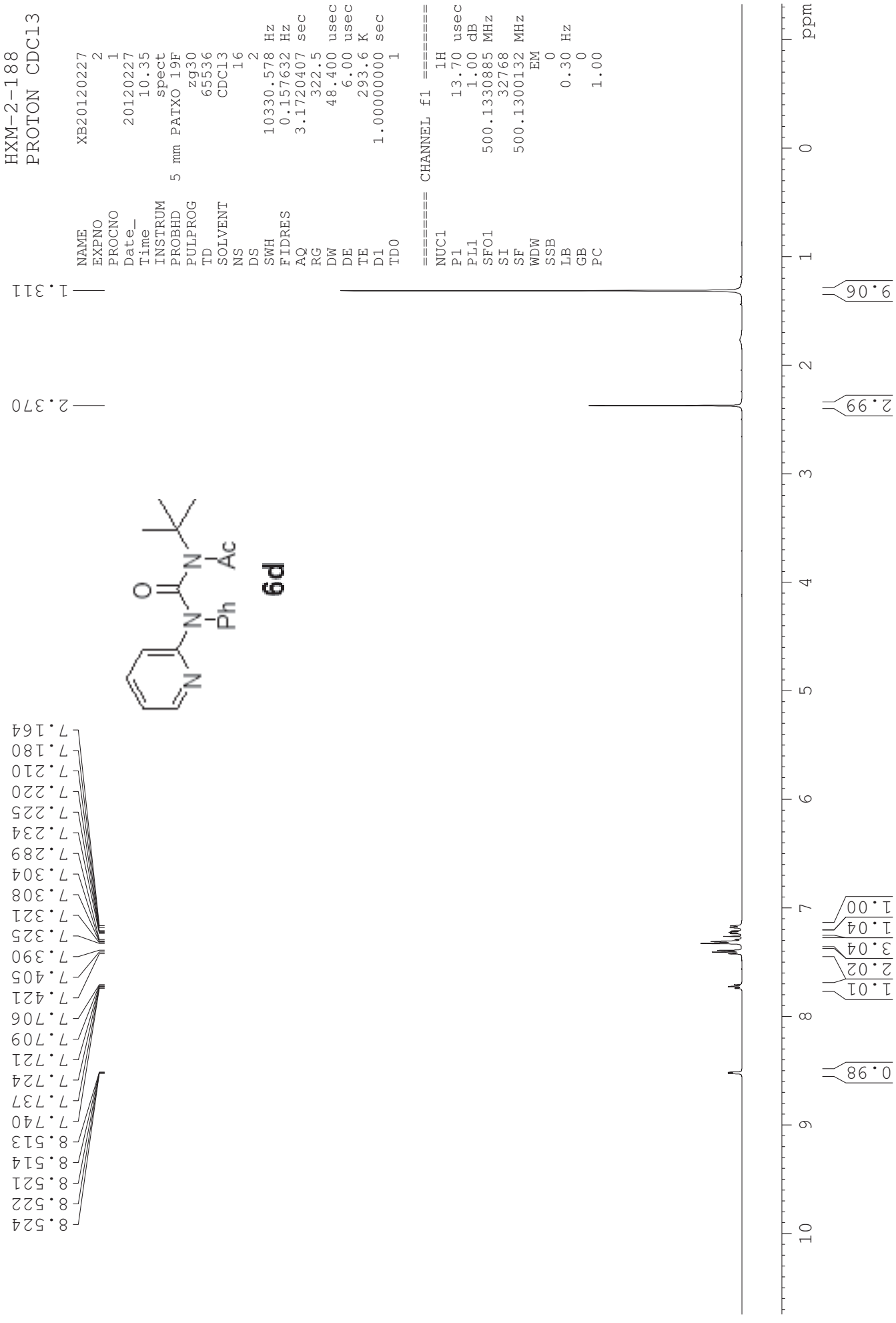

HXM-2-204
C13CPD CDC13 I
Current Data Parameters
NAME XB20120531
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 10.10
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 228.1
DW 16.650 usec
DE 6.00 usec
TE 298.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
25.54
27.79
59.01
117.94
127.06
128.24
129.55
140.04
156.06
159.08
159.47
169.93
Br
N
N
N
O
N
Ph
Ac
6a
ppm

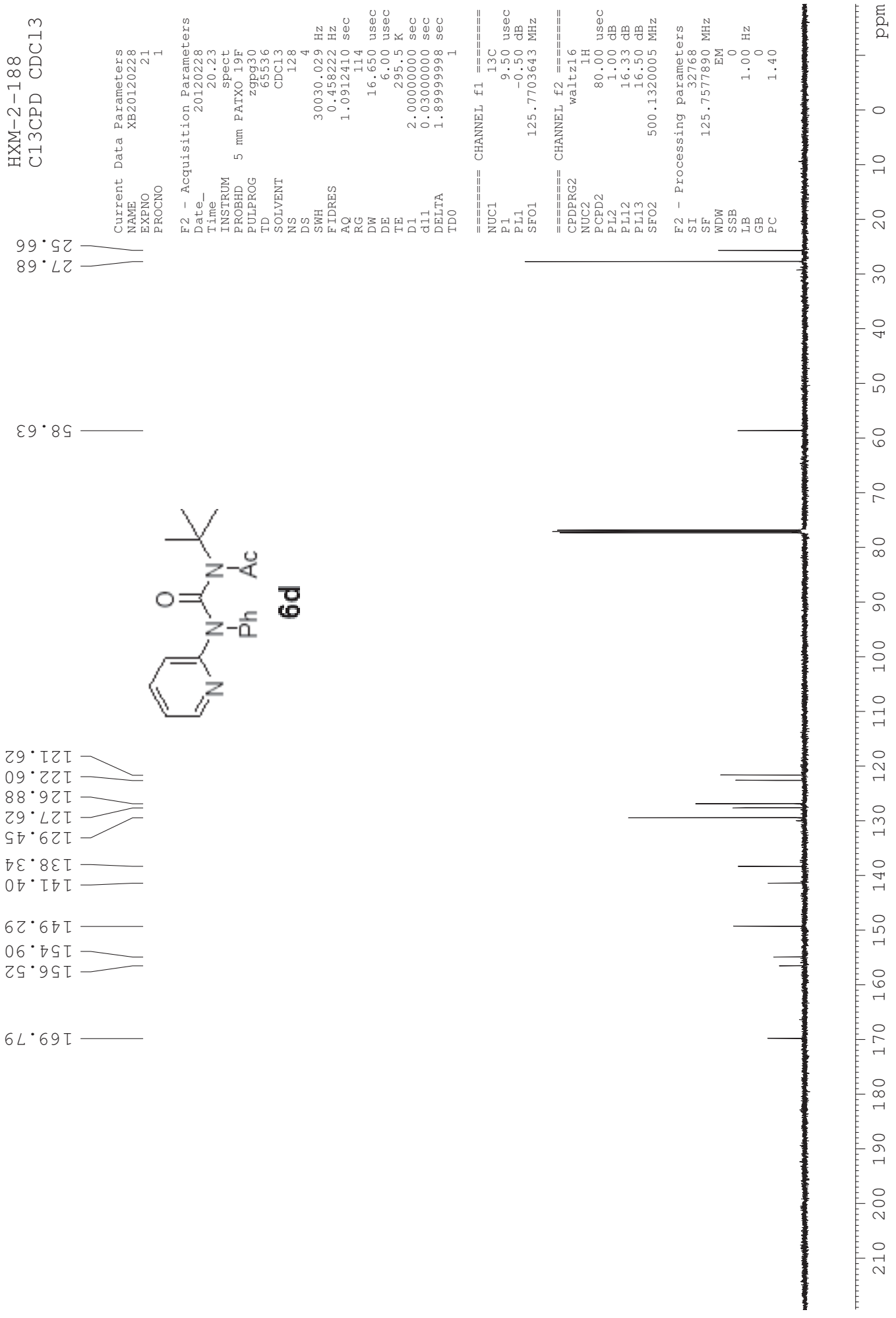

HXM-2-261
PROTON CDC13
NAME XB20120410
EXPNO 2
PROCNO 1
Date_ 20120410
Time 13.02
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.382
2.440
8.927
7.566
7.552
7.530
7.516
7.501
7.485
7.470
7.453
7.438
7.408
7.393
7.368
7.354
7.339
9.14
3.00
1.91
1.95
2.07
3.01
1.97
1.02
ppm
6b

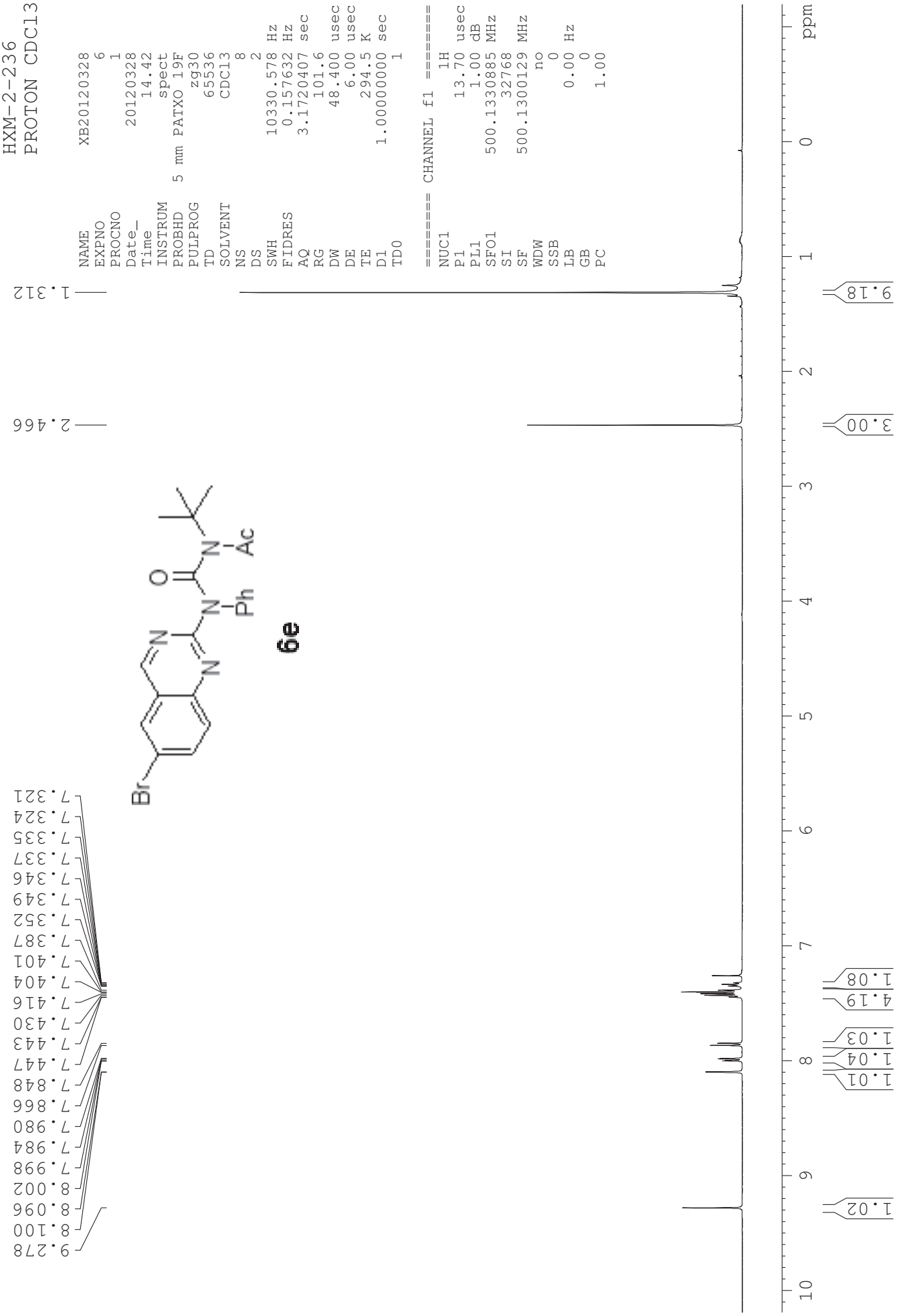

HXM-2-261
C13CPD CDC13
Current Data Parameters
NAME XB20120410
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120410
Time 13.30
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
170.12
159.62
156.63
156.28
140.38
133.11
132.31
129.59
129.50
129.37
128.03
127.03
126.92
58.87
27.75
25.64
Ph
N
N
N
O
N
Ph
Ac
6b
ppm

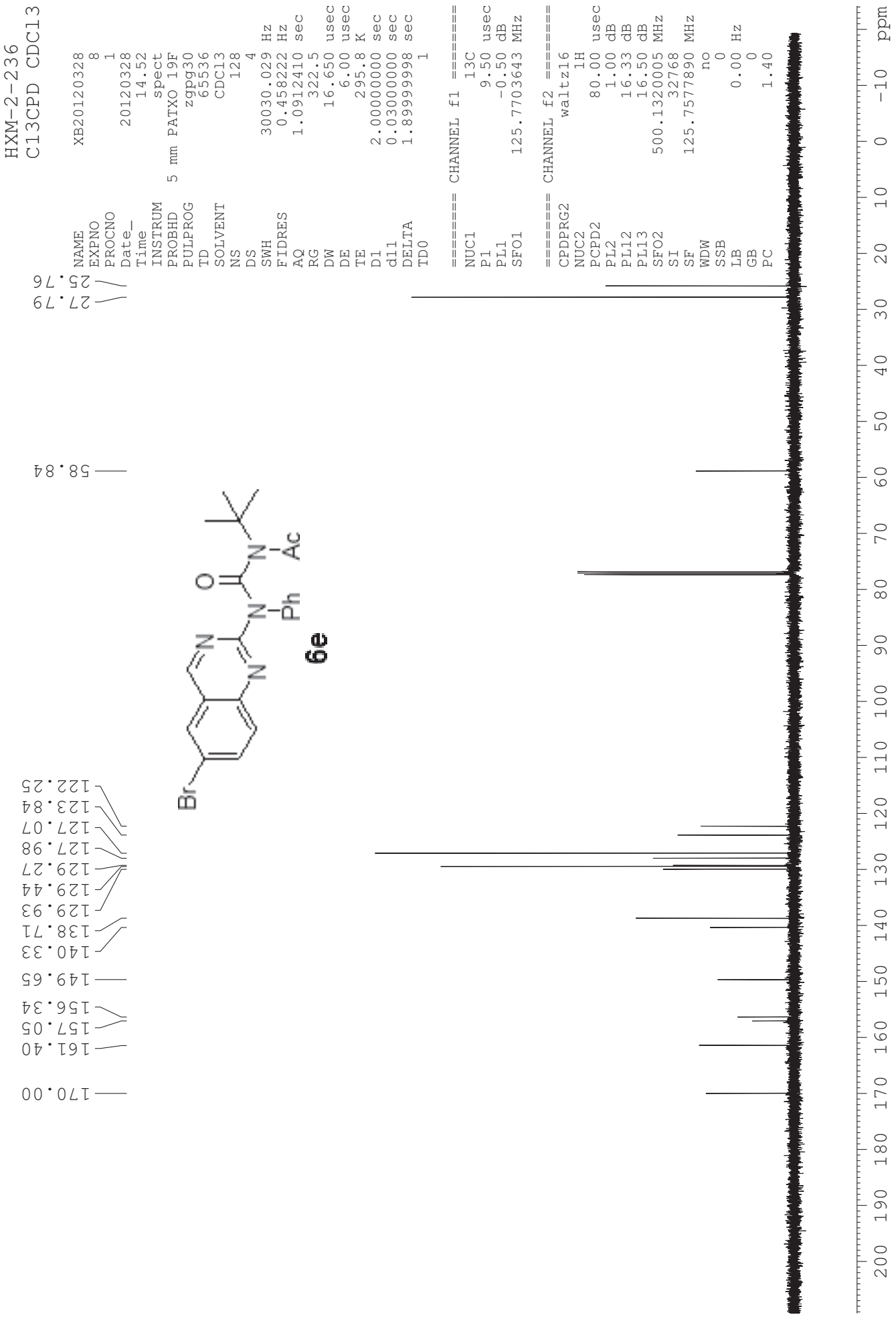

HXM-2-302
PROTON CDCl3
Current Data Parameters
NAME XB20120531
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 10.16
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 143.7
DW 48.400 usec
DE 6.00 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.314
2.331
8.573
8.470
7.451
7.436
7.420
7.366
7.352
7.338
7.310
7.294
9.11
3.00
1.92
0.94
2.01
1.02
1.98
ppm
6c

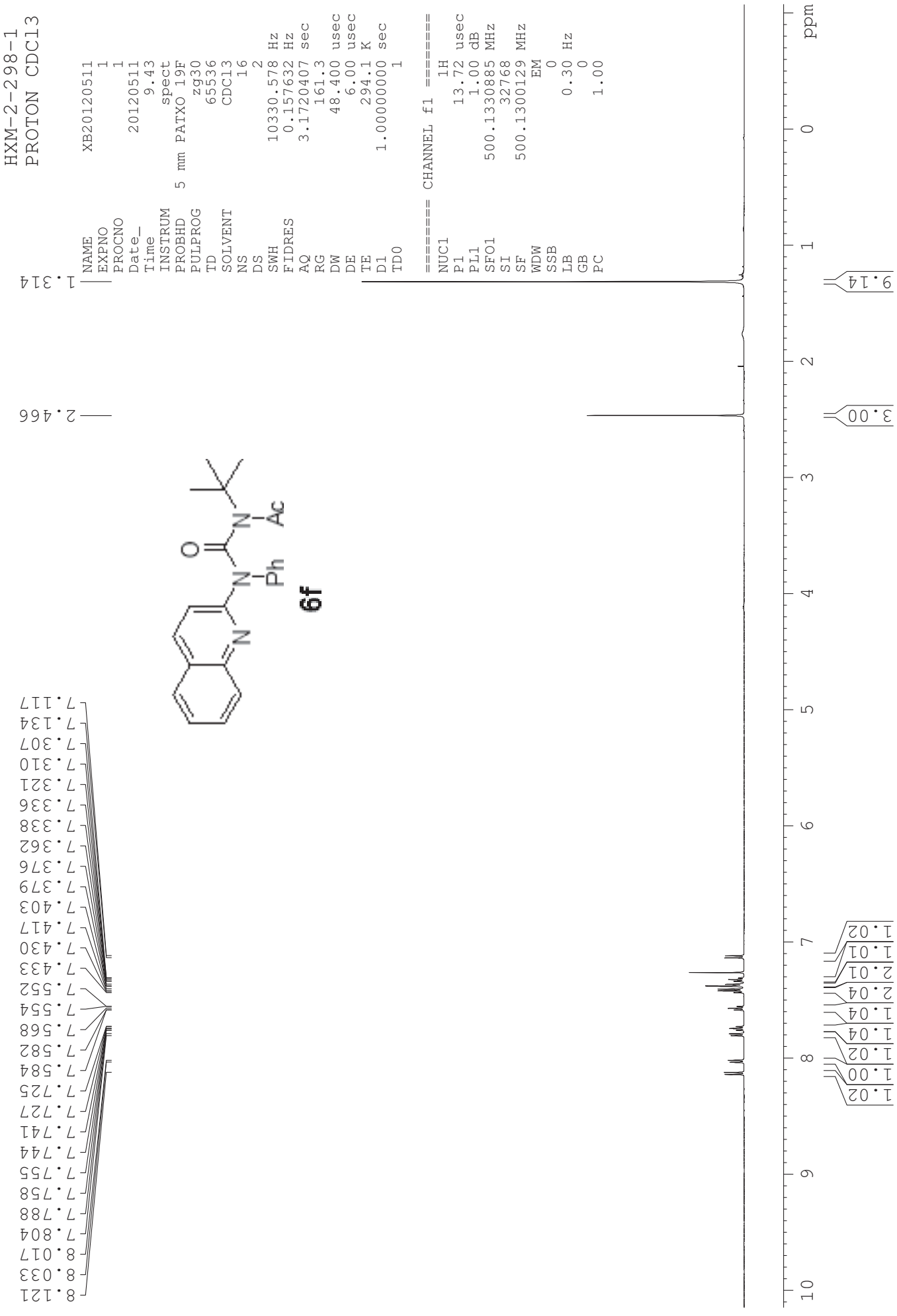

HXM-2-302
C13CPD CDC13
Current Data Parameters
NAME XB20120531
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time 10.24
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 128
DW 16.650 usec
DE 6.00 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0
GB 0
PC 1.40
25.56
27.81
58.92
127.20
128.30
129.76
140.41
142.53
142.98
143.17
156.60
169.56
6c
ppm

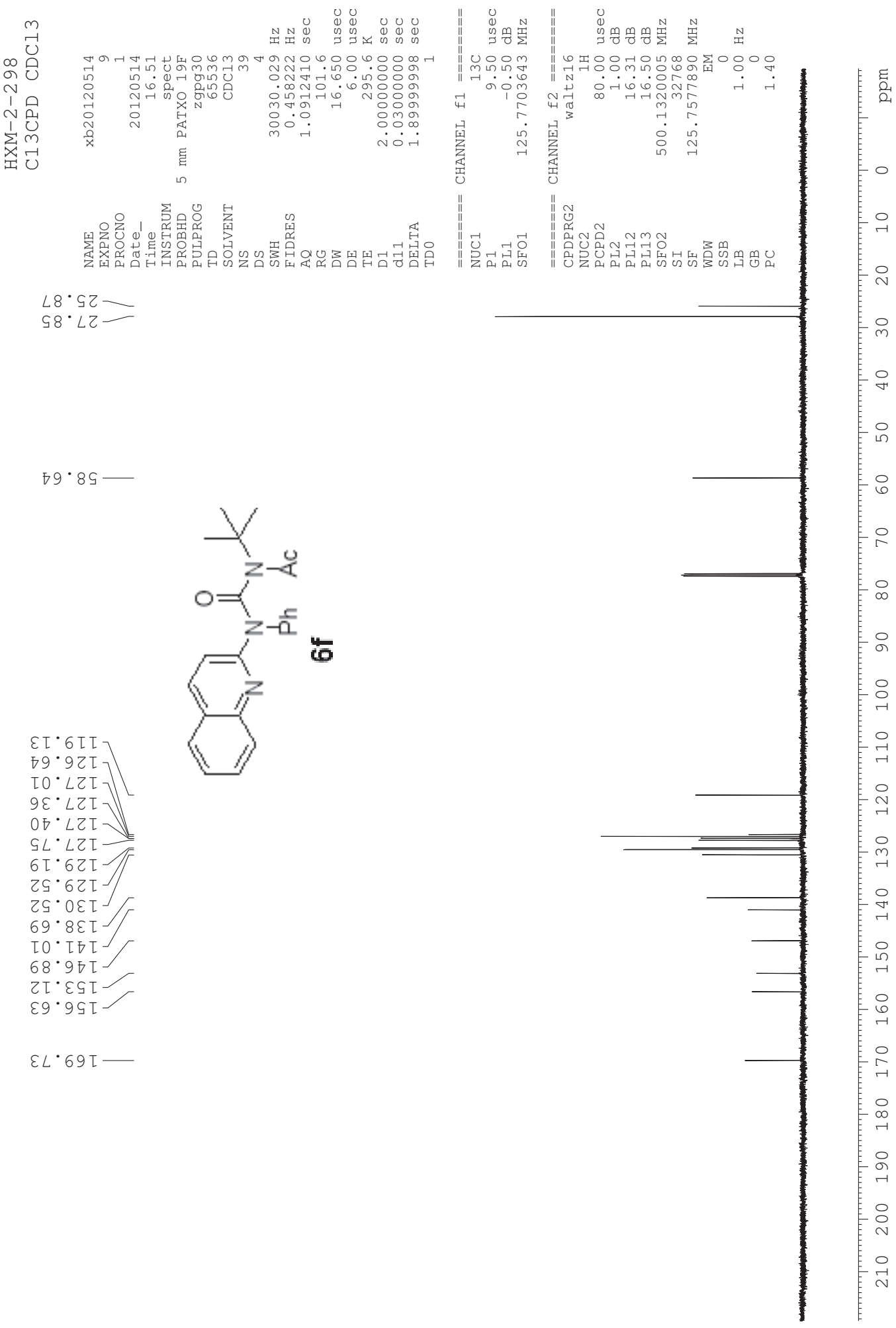

HXM-2-188
PROTON CDC13
NAME XB20120227
EXPNO 2
PROCNO 1
Date_ 20120227
Time 10.35
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 322.5
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.311
2.370
9.06
2.99
1.00
1.04
3.04
2.02
1.01
0.98
ppm
6d
Ac
Ph
O
N
N
N
7.164
7.180
7.210
7.220
7.225
7.234
7.289
7.304
7.308
7.321
7.325
7.390
7.405
7.421
7.706
7.709
7.721
7.724
7.737
7.740
8.513
8.514
8.521
8.522
8.524

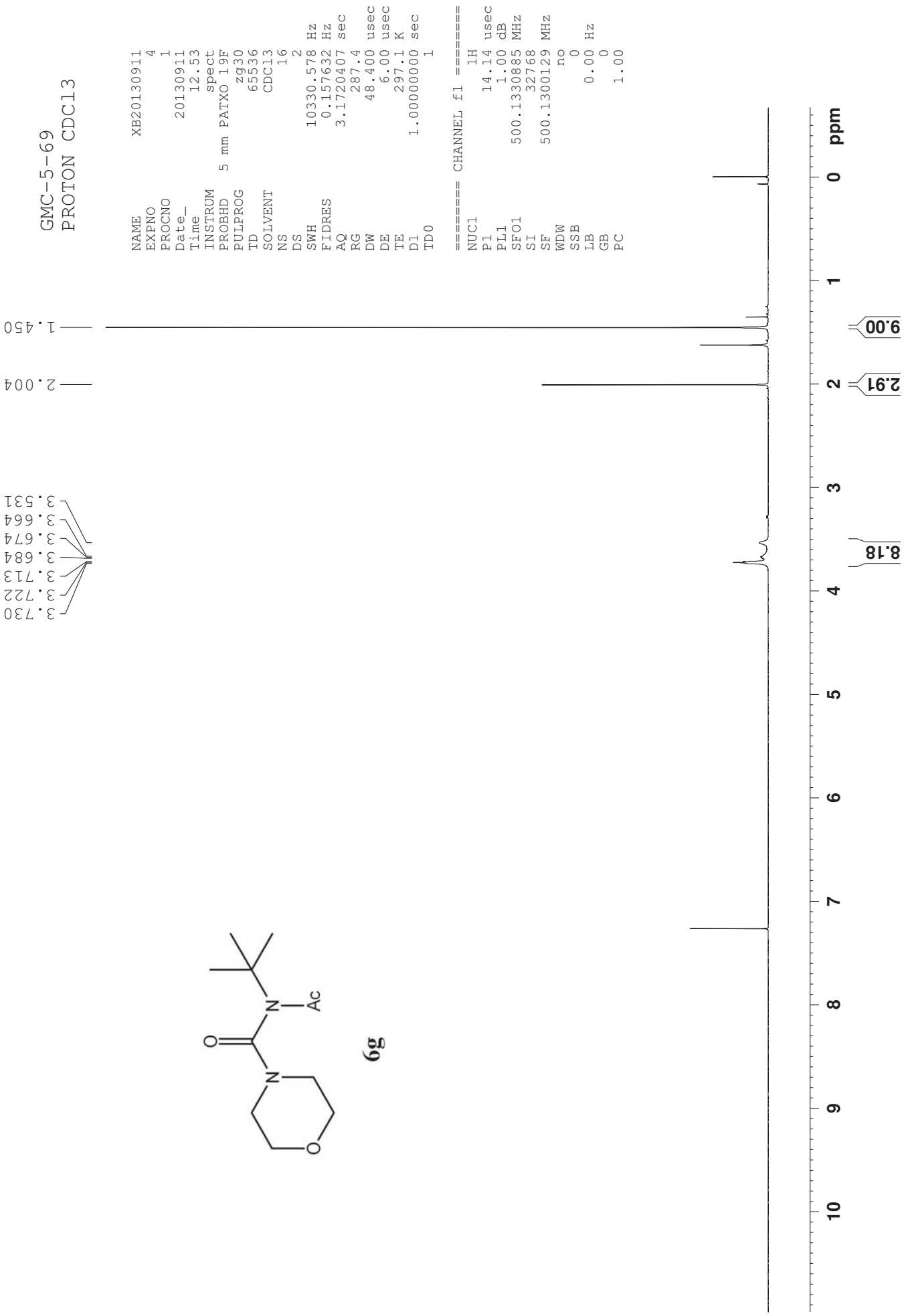

HXM-2-188
C13CPD CDC13
Current Data Parameters
NAME XB20120228
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120228
Time 20.23
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 295.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
25.66
27.68
58.63
121.62
122.60
126.88
127.62
129.45
138.34
141.40
149.29
154.90
156.52
169.79
O
N
Ph
N
N
Ac
6d
ppm

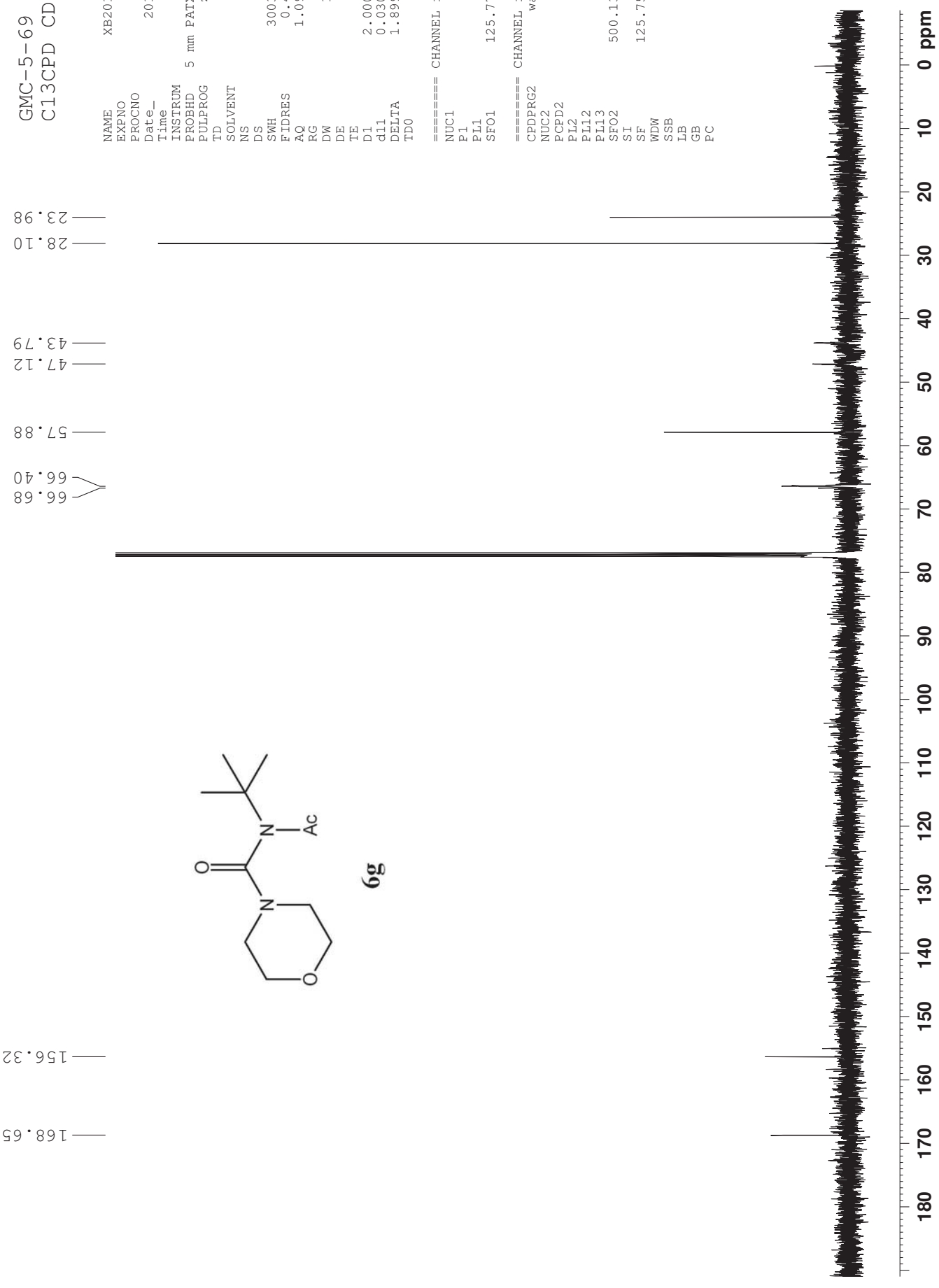

HXM-2-236
PROTON CDC13
NAME XB20120328
EXPNO 6
PROCNO 1
Date_ 20120328
Time 14.42
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 101.6
DW 48.400 usec
DE 6.00 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
6e
Br
N
N
N
Ph
O
N
Ac
1.312
2.466
9.278
8.100
8.096
8.002
7.998
7.984
7.980
7.866
7.848
7.447
7.443
7.430
7.416
7.404
7.401
7.387
7.352
7.349
7.346
7.337
7.335
7.324
7.321
9.18
3.00
1.08
4.19
1.03
1.04
1.01
1.02
ppm


HXM-2-236
C13CPD CDC13
NAME XB20120328
EXPNO 8
PROCNO 1
Date_ 20120328
Time 14.52
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 322.5
DW 16.650 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.33 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
170.00
161.40
157.05
156.34
149.65
140.33
138.71
129.93
129.44
129.27
127.98
127.07
123.84
122.25
58.84
27.79
25.76
Br
N
N
N
Ph
O
N
Ac
6e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


HXM-2-298-1
PROTON CDC13
NAME XB20120511
EXPNO 1
PROCNO 1
Date_ 20120511
Time 9.43
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 161.3
DW 48.400 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
6f
Ac
Ph
ppm
9.14
3.00
1.02
1.01
2.01
2.04
1.04
1.04
1.02
1.00
1.02


HXM-2-298
C13CPD CDCl3
NAME xb20120514
EXPNO 9
PROCNO 1
Date_ 20120514
Time 16.51
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 39
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 101.6
DW 16.650 usec
DE 6.00 usec
TE 295.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
25.87
27.85
58.64
119.13
126.64
127.01
127.36
127.40
127.75
129.19
129.52
130.52
138.69
141.01
146.89
153.12
156.63
169.73
6f
N
O
N
Ph
Ac
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


GMC-5-69
PROTON CDC13
NAME XB20130911
EXPNO 4
PROCNO 1
Date_ 20130911
Time 12.53
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.450
2.004
3.531
3.664
3.674
3.684
3.713
3.722
3.730
9.00
2.91
8.18
ppm
0
1
2
3
4
5
6
7
8
9
10
Ac
N
O
N
O
6g


GMC-5-69
C13CPD CDCl3
NAME XB20130912
EXPNO 2
PROCNO 1
Date_ 20130912
Time 9.53
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 362
DW 16.650 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.05 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577709 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20
23.98
28.10
43.79
47.12
57.88
66.40
66.68
156.32
168.65
N
Ac
O
N
O
6g
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180