Synthesis and Characterization of a *para*-Pyridine Linked NHC Palladium Complexes and their Studies for Heck-Mizoroki Coupling Reaction

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Glenn P. A. Yap,[d] *Shih-Sheng Sun*a and Tiow-Gan Ong*a*

Supporting Information

Table S1. Crystal data and structure refinement for **2a**.

Empirical formula	$C_{36}H_{38}Ag_2Cl_2N_6$
Formula weight	841.36
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 9.9245(4) Å α = 90 °.
	b = 16.8820(7) Å β= 94.389(2) °.
	c = 20.6772(9) Å γ= 90 °.
Volume	3454.2(3) $Å^3$
Z, Calculated density	4, 1.641 mg/m^3
Absorption coefficient	1.324 mm^{-1}
F(000)	1969
Crystal size	0.30 x 0.30 x 0.25 mm
θ range for data collection	1.56 to 27.10 °
Limiting indices	-11≤h≤12, -21≤k≤20, -26≤l≤26
Reflections collected / unique	29460 / 7633 [R(int) = 0.0480]
Completeness to θ= 25.00	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7633 / 0 / 421
Goodness-of-fit on F^2	1.092
Final R indices [I>2σ(*I*)]	R1 = 0.0416, wR2 = 0.138
R indices (all data)	R1 = 0.0595, wR2 = 0.1146
Absolute structure parameter	0.021(11)
Largest diff. peak and hole	2.128 and -1.336 $e.Å^{-3}$

Table S2. Crystal data and structure refinement for **2b**.

Empirical formula	$C_{12}H_{15}$ Ag Cl N_3
Formula weight	344.59
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P2(1)/n
Unit cell dimensions	a =9.786(2) Å α = 90 °.
	b = 11.594(2) Å β = 109.01(3) °.
	c = 12.312(6) Å γ = 90 °.
Volume	1320.7(5) $Å^3$
Z, Calculated density	4, 1.733 mg/m^3
Absorption coefficient	1.709 mm^{-1}
F(000)	688
Crystal size	0.25 x 0.20 x 0.10 mm
θ range for data collection	2.32 to 27.10 °
Limiting indices	-12≤h≤12, -13≤k≤14, -15≤l≤15
Reflections collected / unique	10945 / 2920 [R(int) = 0.0335]
Completeness to θ= 25.00	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2920 / 0 / 156
Goodness-of-fit on F^2	1.025
Final R indices [I>2σ(*I*)]	R1 = 0.0249, wR2 = 0.0525
R indices (all data)	R1 = 0.0327, wR2 = 0.0558
Largest diff. peak and hole	0.458 and -0.414 e.$Å^{-3}$

Table S3. Crystal data and structure refinement for **3a-CO_3**

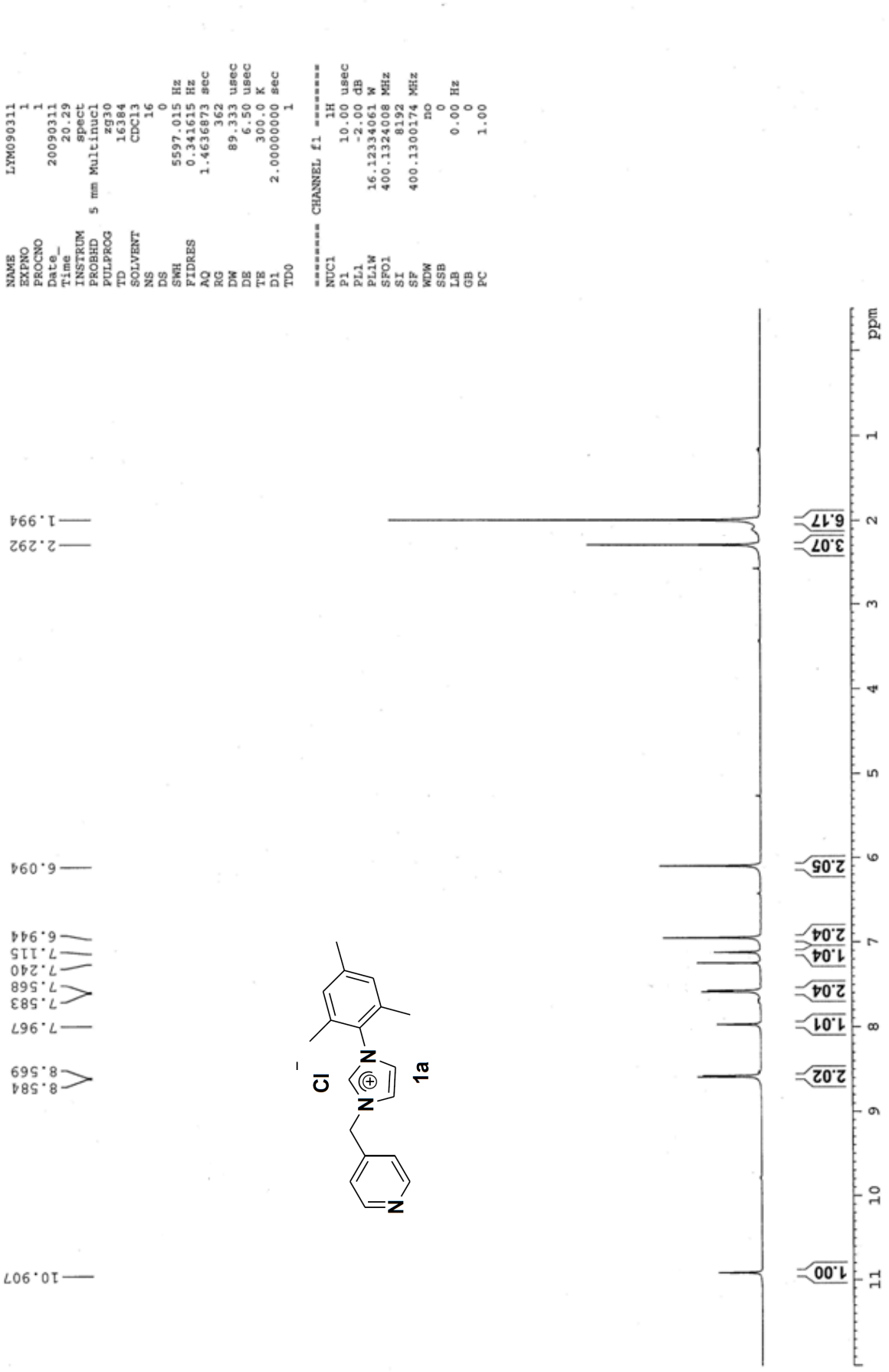
Empirical formula	$C_{38}H_{42}Cl_2N_6O_3Pd$
Formula weight	808.08
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a =12.7736(4) Å α = 90 °.
	b = 19.7296(7) Å β = 102.0670 (10) °.
	c = 14.8140(5) Å γ = 90 °.
Volume	2441,1(2) $Å^3$
Z, Calculated density	4, 1.470 mg/m^3
Absorption coefficient	0.701 mm^{-1}
F(000)	1664
Crystal size	0.20 x 0.20 x 0.18 mm
θ range for data collection	1.92 to 27.09 °
Limiting indices	-13≤h≤16, -24≤k≤25, -18≤l≤17
Reflections collected / unique	30770 / 8034 [R(int) = 0.0353]
Completeness to θ= 25.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8034 / 0 / 457
Goodness-of-fit on F^2	1.024
Final R indices [I>2σ(*I*)]	R1 = 0.0333, wR2 = 0.0851
R indices (all data)	R1 = 0.0430, wR2 = 0.0910
Largest diff. peak and hole	0.728 and -0.751 e.$Å^{-3}$

Table S4. Crystal data and structure refinement for **3a**.

Empirical formula	$C_{36}H_{38}Cl_2N_6Pd$
Formula weight	732.02
Temperature	296 (2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pbcn
Unit cell dimensions	a =15.7750(9) Å α = 90 °.
	b = 12.1317(8) Å β = 90 °.
	c = 17.5570(12) Å γ = 90 °.
Volume	3360.0(4) $Å^3$
Z, Calculated density	4, 1.447 mg/m^3
Absorption coefficient	0.747 mm^{-1}
F(000)	1504
Crystal size	0.10 x 0.08 x 0.08 mm
θ range for data collection	2.12 to 27.03 °
Limiting indices	$-20\leq h\leq 20$, $-15\leq k\leq 15$, $-22\leq l\leq 22$
Reflections collected / unique	27361 / 3688 [R(int) = 0.0661]
Completeness to θ= 25.00	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3688 / 0 / 207
Goodness-of-fit on F^2	1.051
Final R indices [$I>2\sigma(I)$]	R1 = 0.0292, wR2 = 0.0623
R indices (all data)	R1 = 0.0478, wR2 = 0.0670
Largest diff. peak and hole	0.505 and -0.575 $e.Å^{-3}$

Table S5. Crystal data and structure refinement for **3b**.

Empirical formula	$C_{24}H_{30}Cl_2N_6$ Pd
Formula weight	579.84
Temperature	100 (2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a =7.2059(4) Å α = 80.801(3) °.
	b = 8.5398(4) Å β = 76.925(2) °.
	c = 10.6540(5) Å γ = 87.557(2) °.
Volume	630.39(5) $Å^3$
Z, Calculated density	1, 1.527 mg/m^3
Absorption coefficient	0.972 mm^{-1}
F(000)	296
Crystal size	0.20 x 0.18 x 0.18 mm
θ range for data collection	1.99 to 27.10 °
Limiting indices	$-7\leq h\leq 9$, $-10\leq k\leq 10$, $-12\leq l\leq 13$
Reflections collected / unique	10135 / 2772 [R(int) = 0.0197]
Completeness to θ= 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2772 / 0 / 153
Goodness-of-fit on F^2	1.002
Final R indices [$I>2\sigma(I)$]	R1 = 0.0190, wR2 = 0.0534
R indices (all data)	R1 = 0.0195, wR2 = 0.0539
Largest diff. peak and hole	0.535 and -0.224 $e.Å^{-3}$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SI 8192
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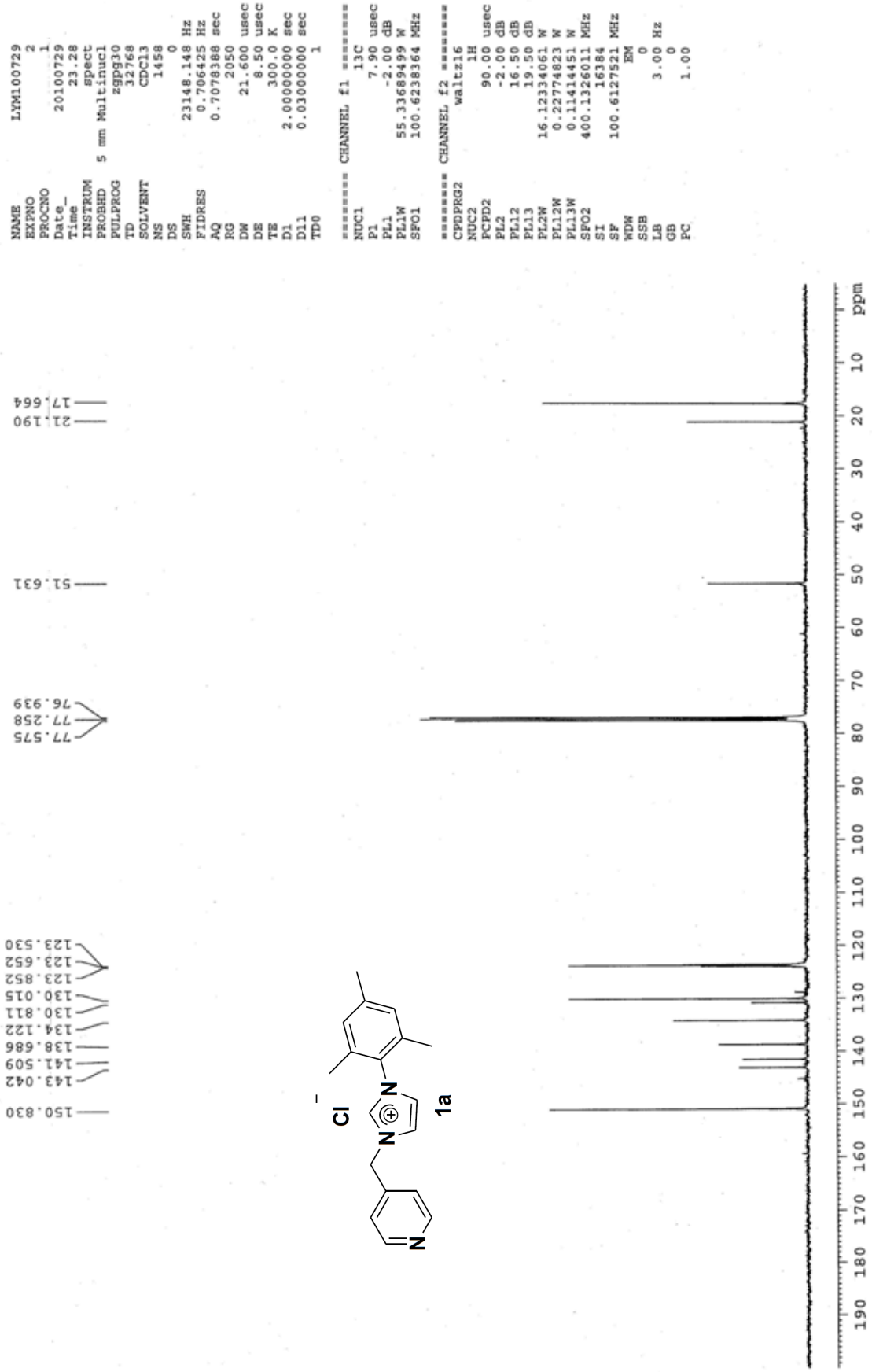
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FIDRES 0.706425 Hz
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TE 300.0 K
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NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 16.50 dB
PL13 19.50 dB
PL2W 16.12334061 W
PL12W 0.22774823 W
PL13W 0.11414451 W
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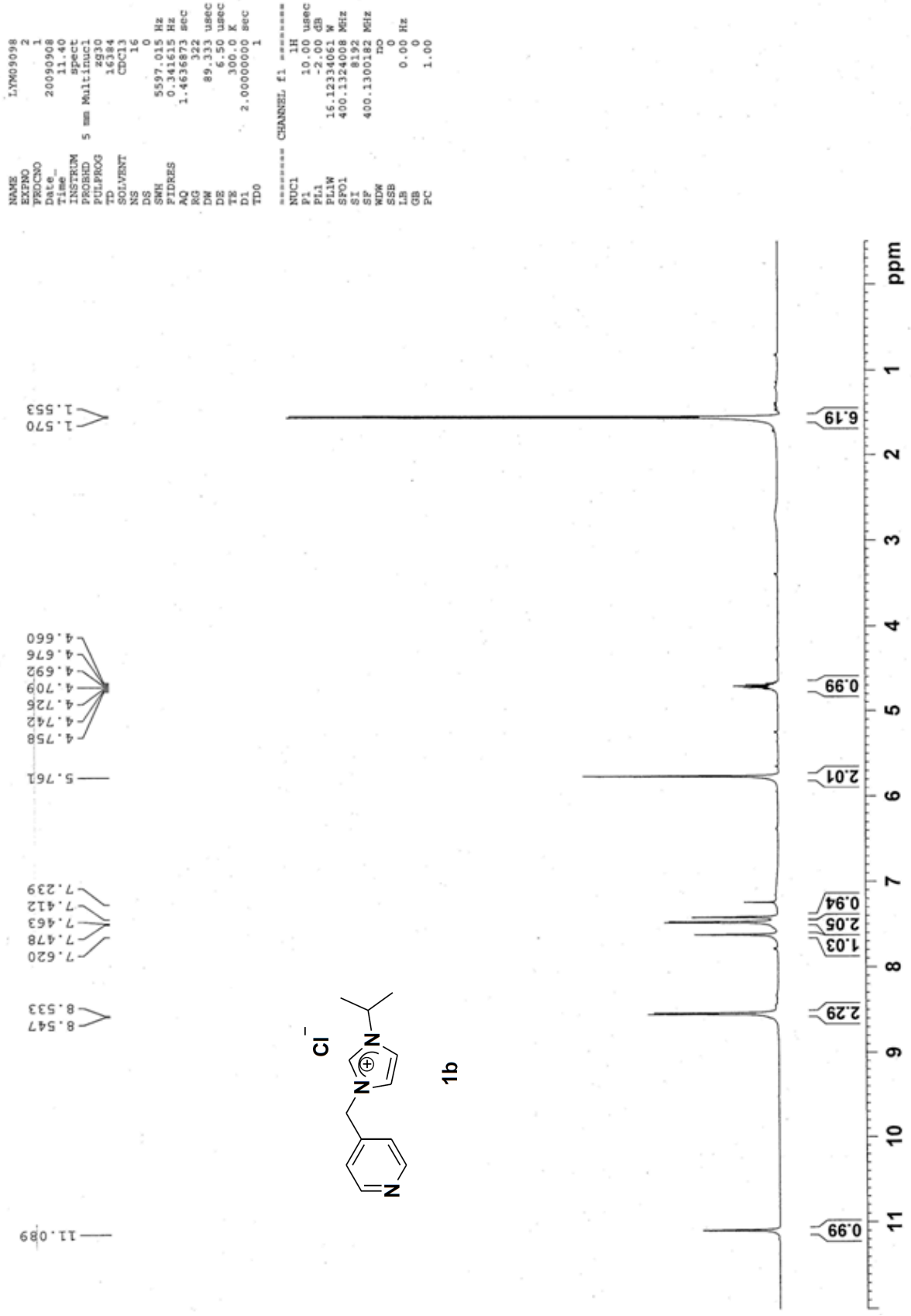

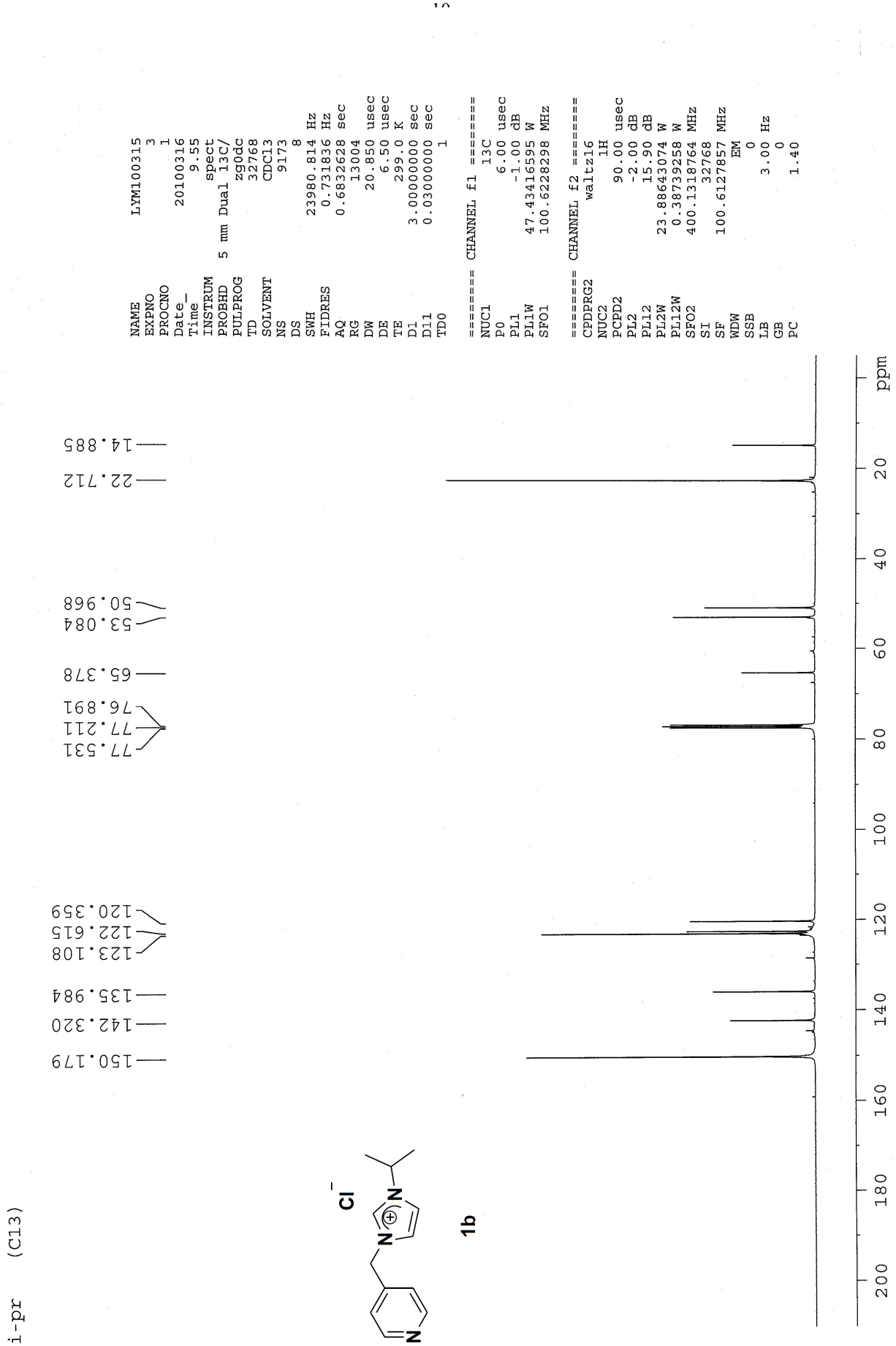
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D11 0.03000000 sec
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P0 6.00 usec
PL1 -1.00 dB
PL1W 47.43416595 W
SFO1 100.6228298 MHz
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CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.90 dB
PL2W 23.88643074 W
PL12W 0.38739258 W
SFO2 400.1318764 MHz
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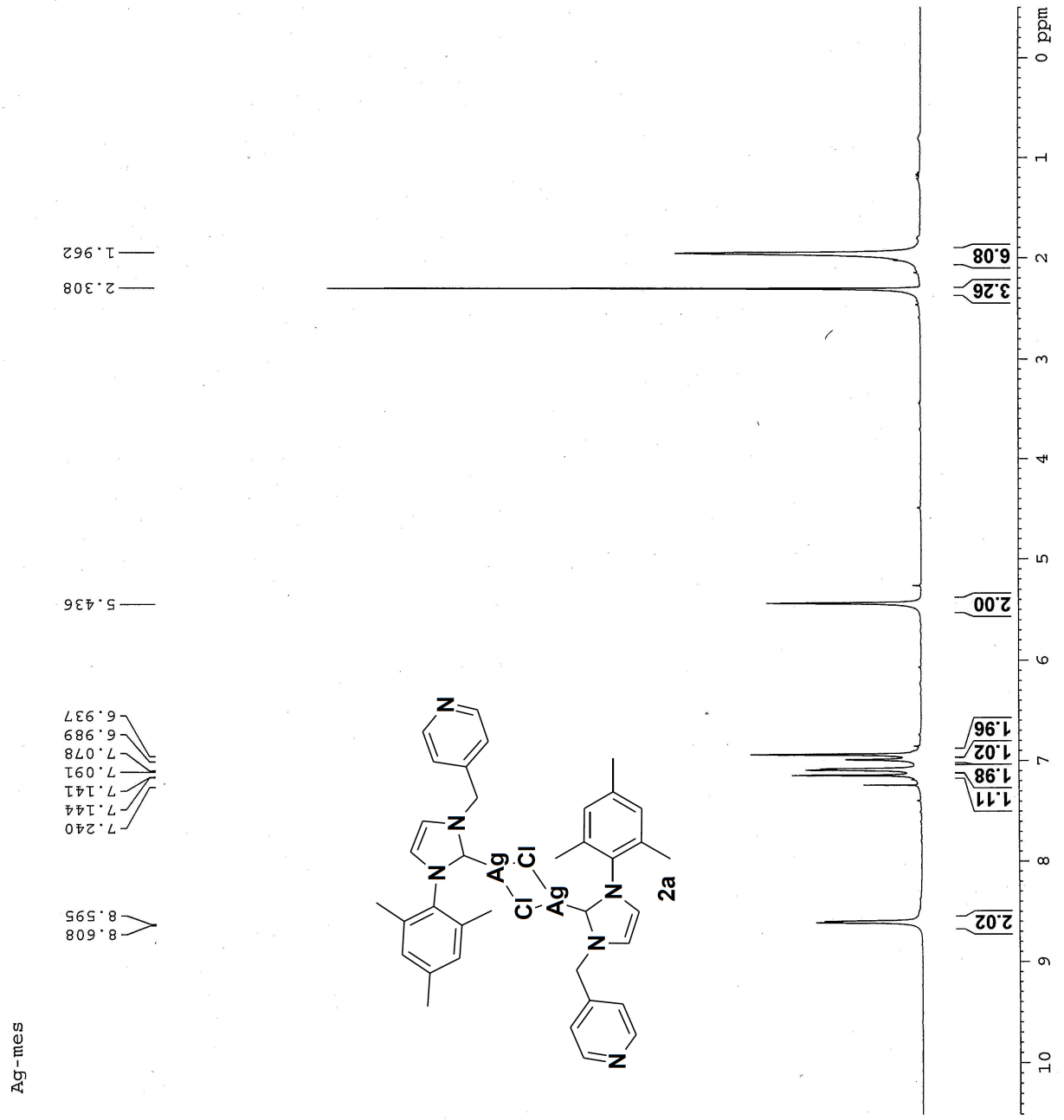
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SOLVENT CDCl3
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FIDRES 0.341615 Hz
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RG 322
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DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
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NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300174 MHz
WDW no
SSB 0
LB 0.00 Hz
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7.141
7.144
7.240
8.595
8.608
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1.96
1.02
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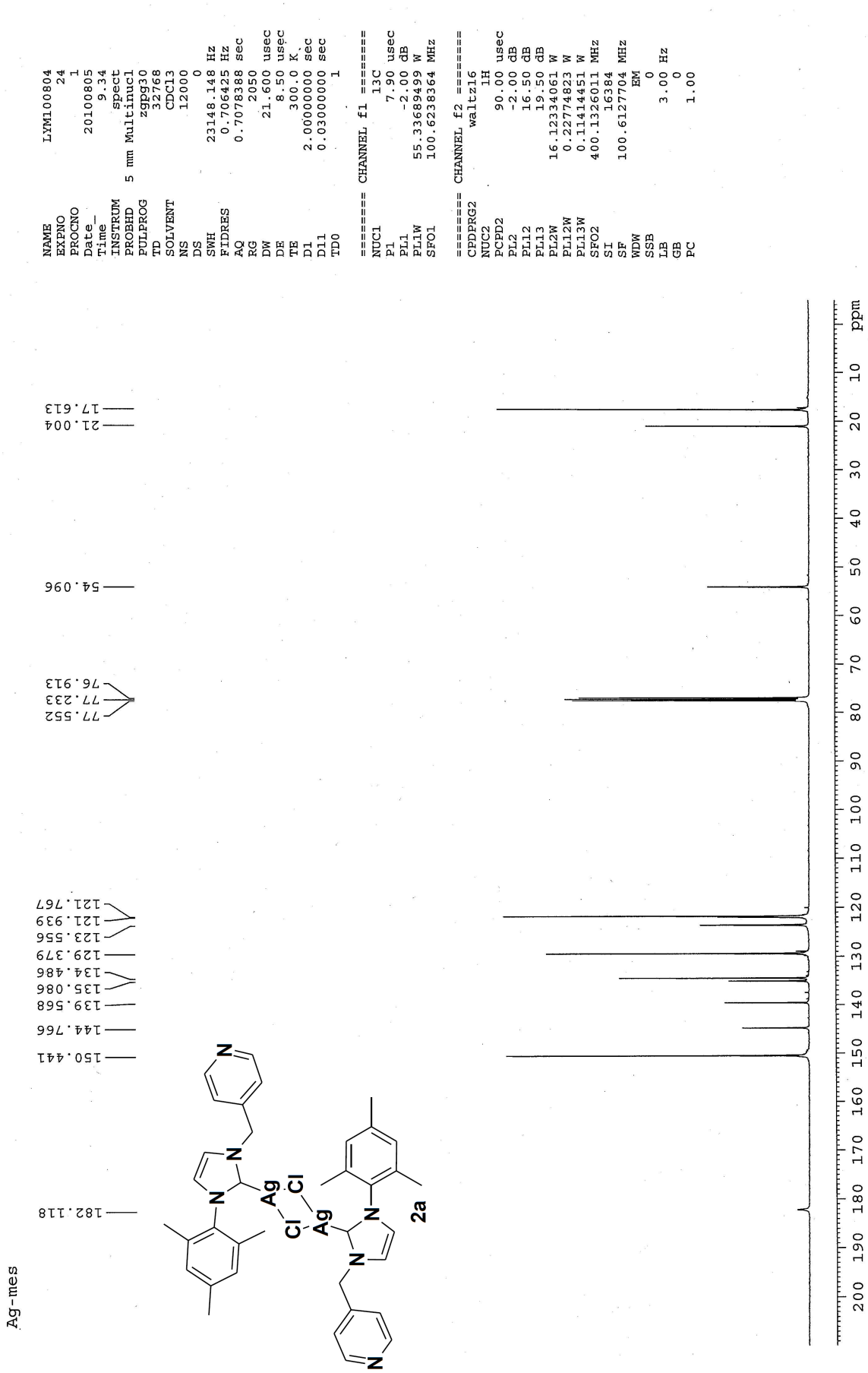
Ag
Cl
Cl
Ag
2a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FIDRES 0.706425 Hz
AQ 0.7078388 sec
RG 2050
DW 21.600 usec
DE 8.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 16.50 dB
PL13 19.50 dB
PL2W 16.12334061 W
PL12W 0.22774823 W
PL13W 0.11414451 W
SFO2 400.1326011 MHz
SI 16384
SF 100.6127704 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
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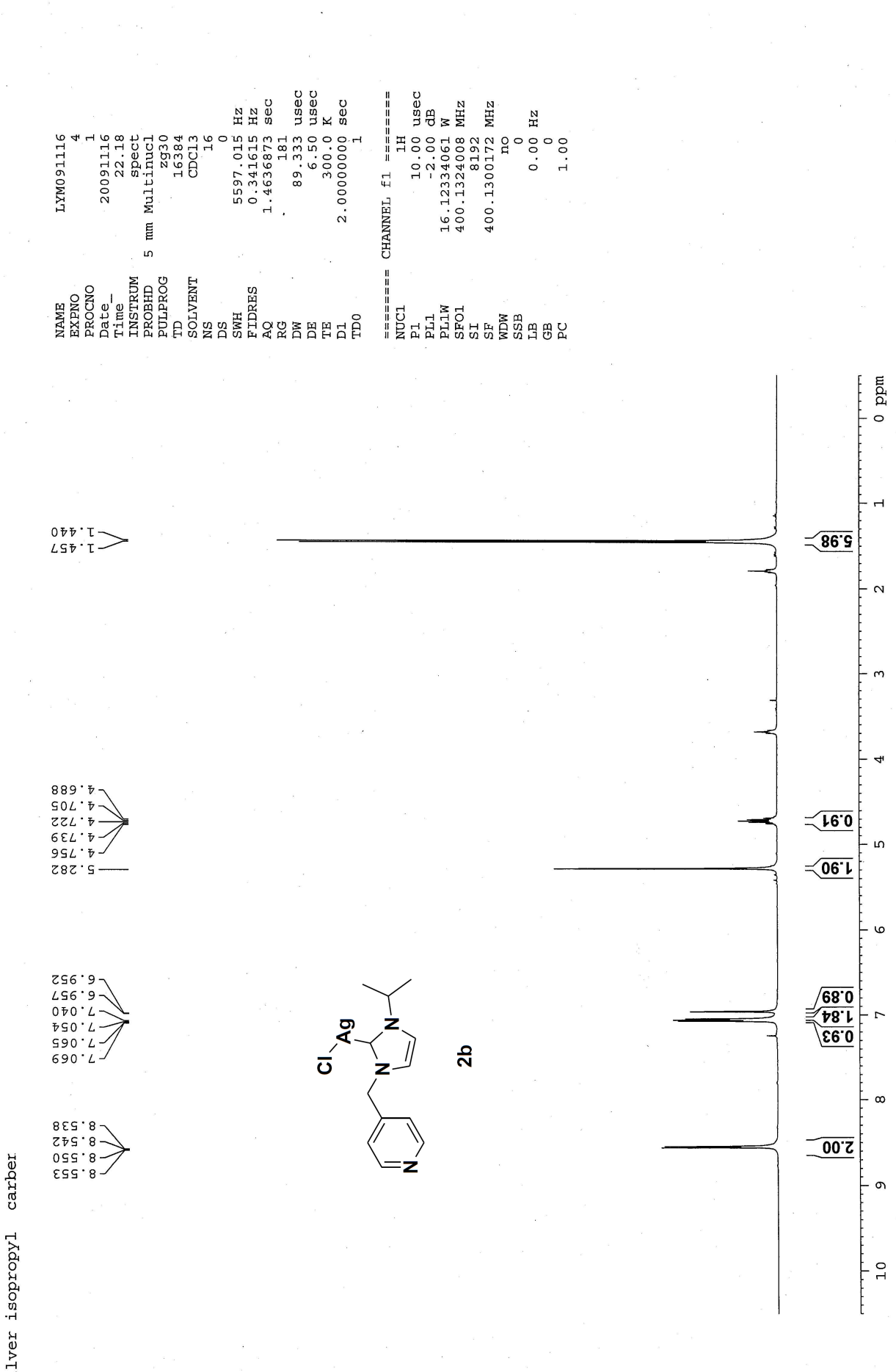
Ag
Cl
Cl
Ag
2a
ppm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SOLVENT CDCl3
NS 16
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FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 181
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300172 MHz
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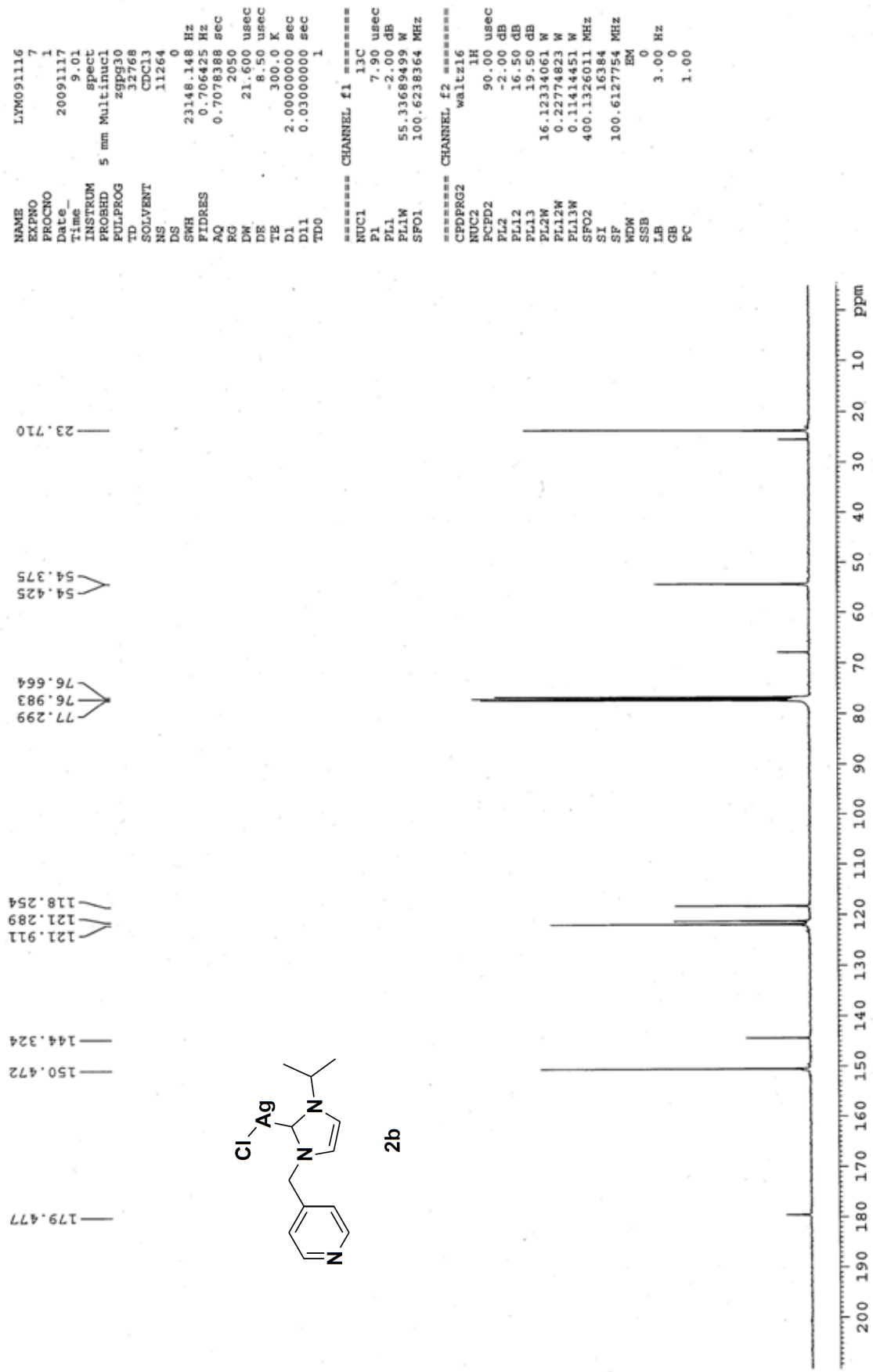
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FIDRES 0.706425 Hz
AQ 0.7078388 sec
RG 2050
DW 21.600 usec
DE 8.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 16.50 dB
PL13 19.50 dB
PL2W 16.12334061 W
PL12W 0.22774823 W
PL13W 0.11414451 W
SFO2 400.1326011 MHz
SI 16384
SF 100.6127754 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
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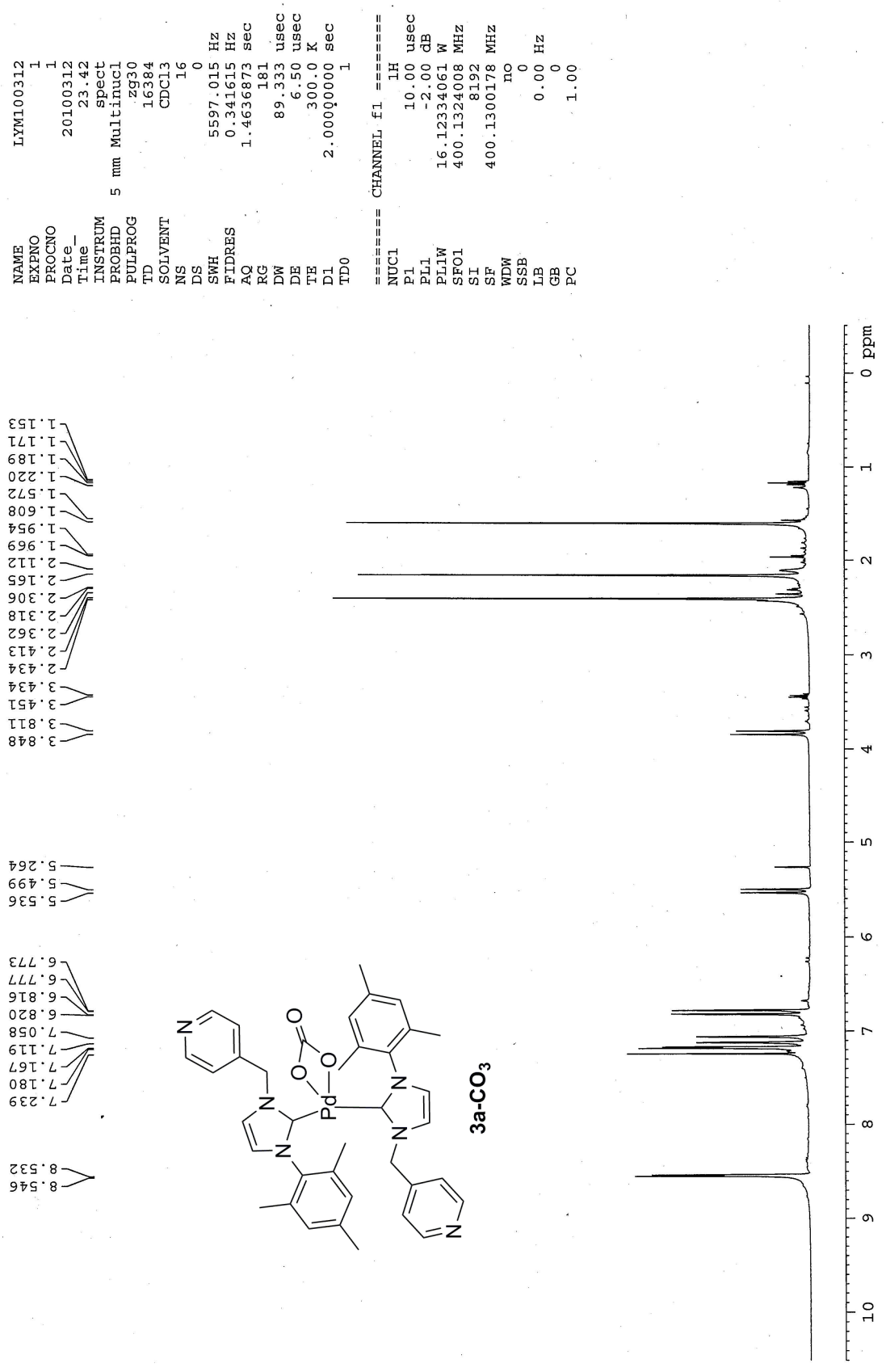
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AQ 1.4636873 sec
RG 181
DW 89.333 usec
DE 6.50 usec
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D1 2.00000000 sec
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NUC1 1H
P1 10.00 usec
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SI 8192
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LB 0.00 Hz
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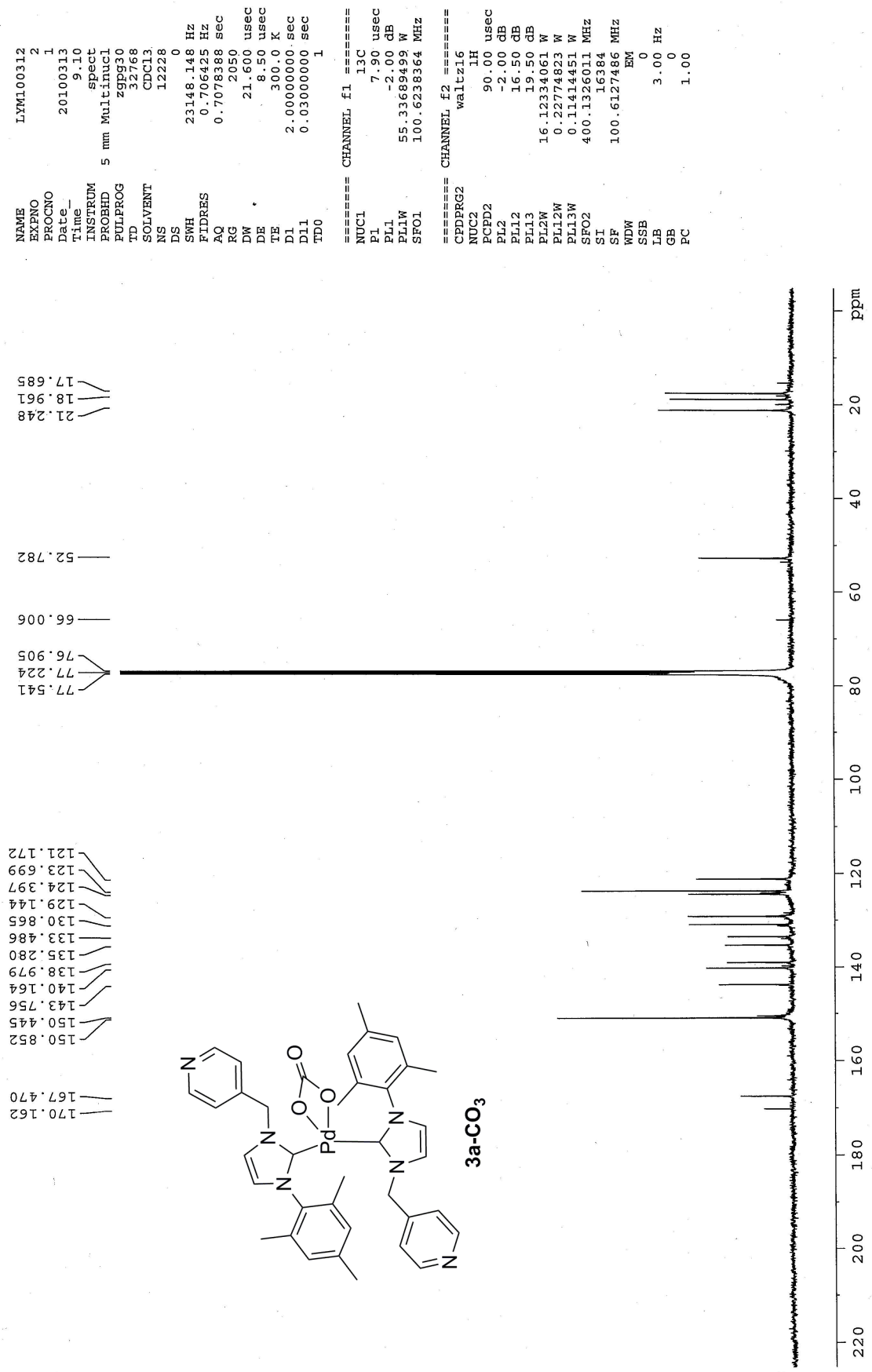
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AQ 0.7078388 sec
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DW 21.600 usec
DE 8.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 16.50 dB
PL13 19.50 dB
PL2W 16.12334061 W
PL12W 0.22774823 W
PL13W 0.11414451 W
SFO2 400.1326011 MHz
SI 16384
SF 100.6127486 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
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77.224
77.541
121.172
123.699
124.397
129.144
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133.486
135.280
138.979
140.164
143.756
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Pd
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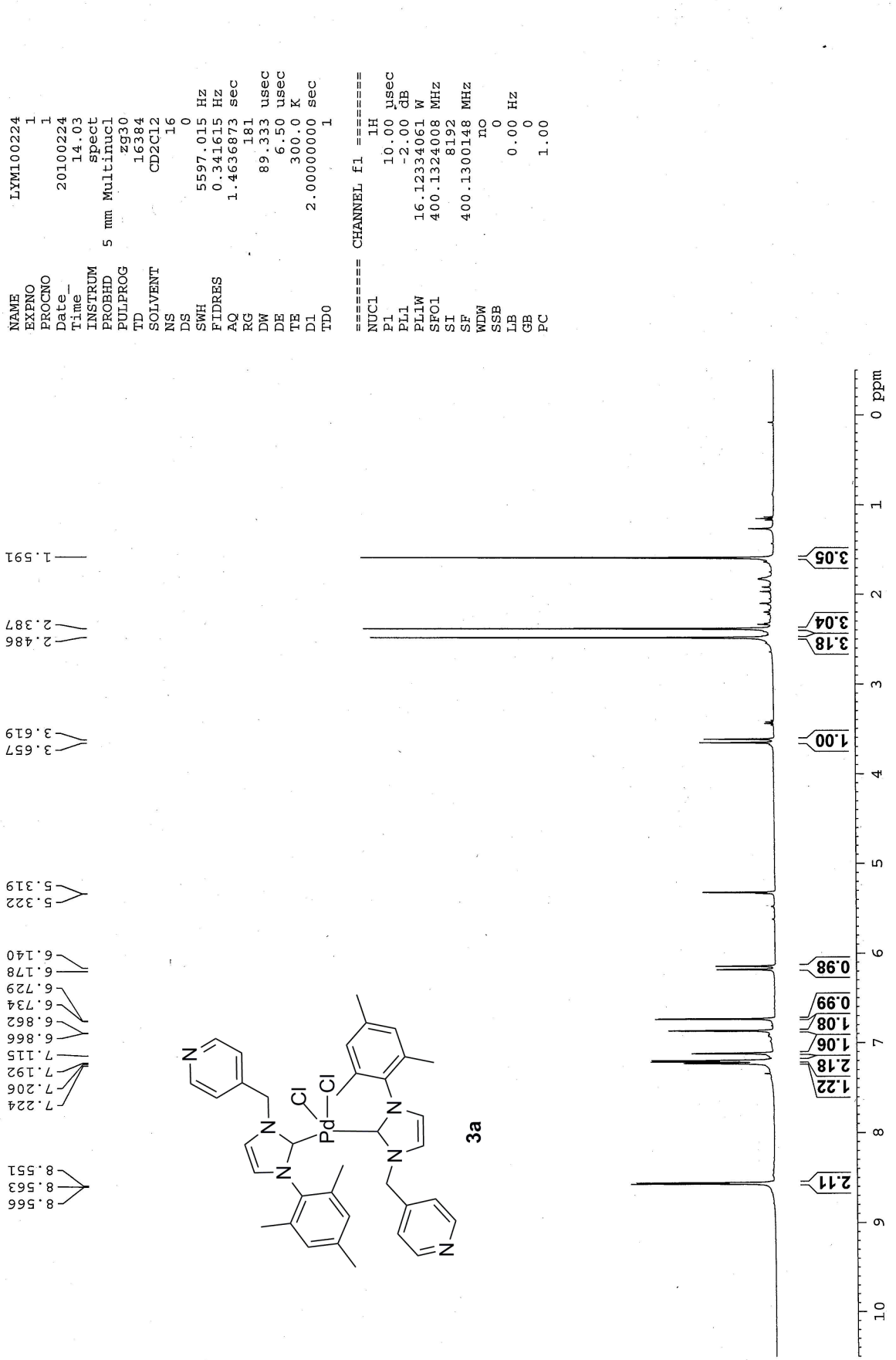
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SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 181
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300148 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
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2.486
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3.657
5.319
5.322
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7.224
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3.18
1.00
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0.99
1.08
1.06
2.18
1.22
2.11
Cl
Cl
Pd
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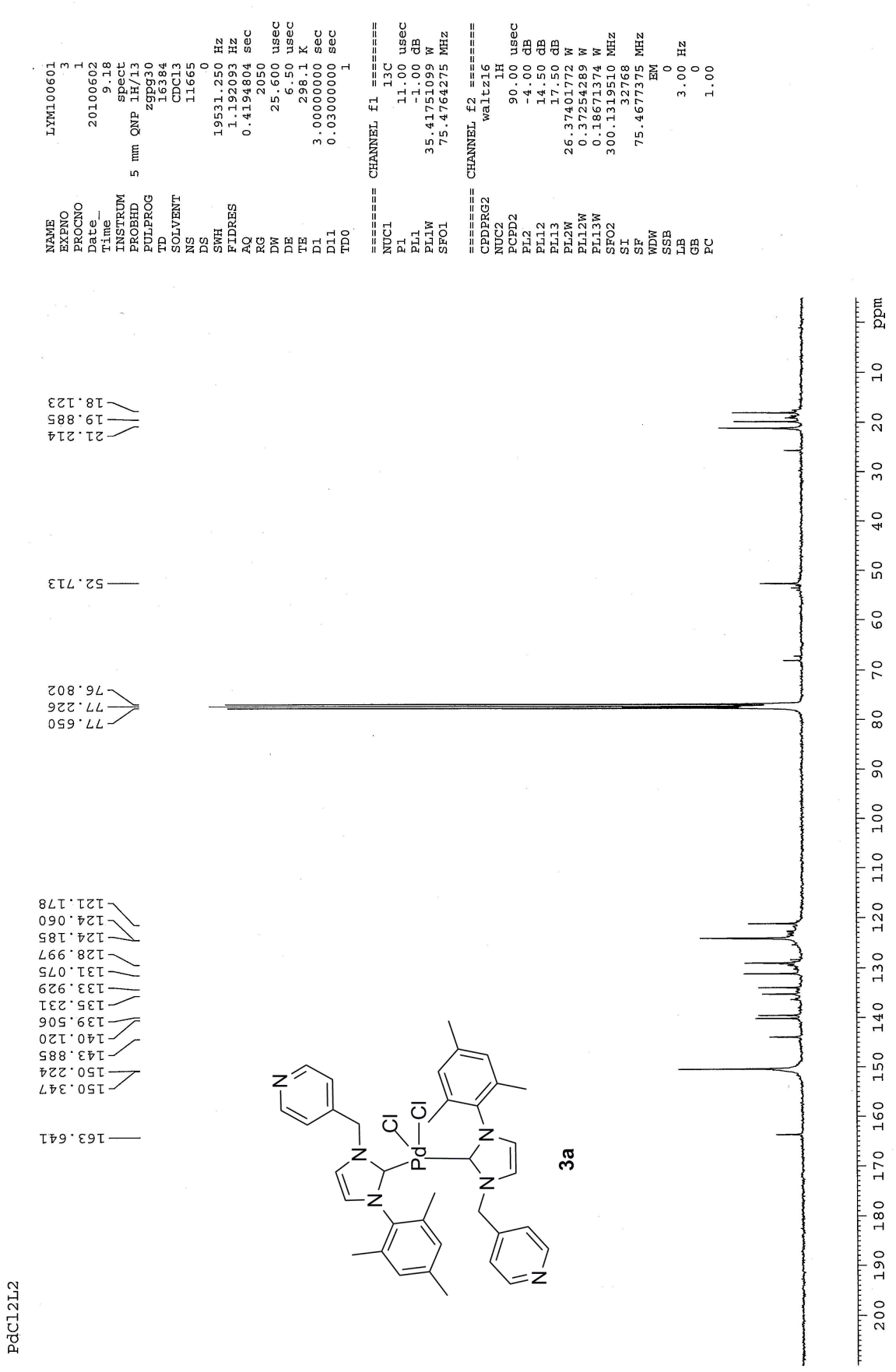
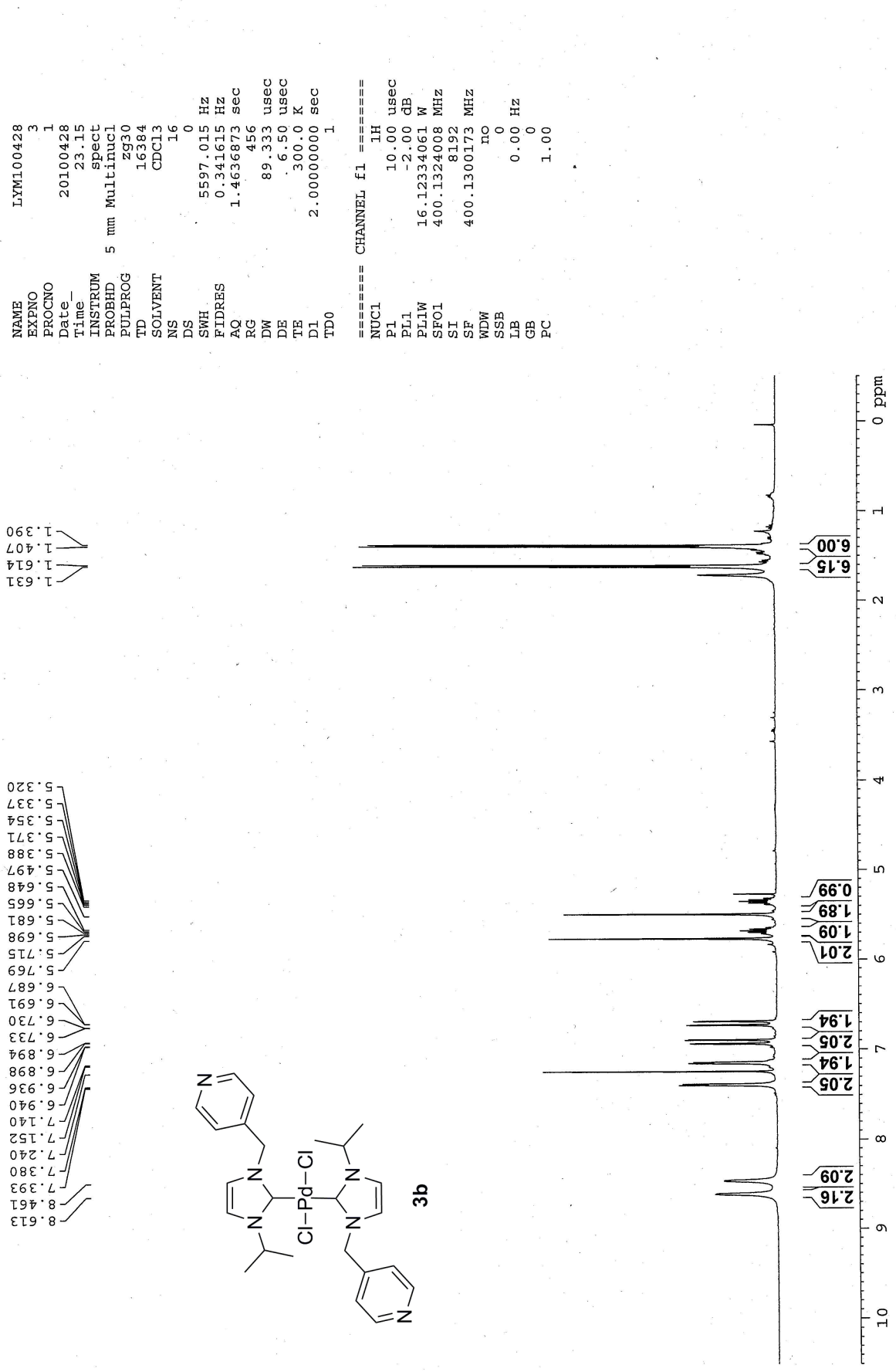
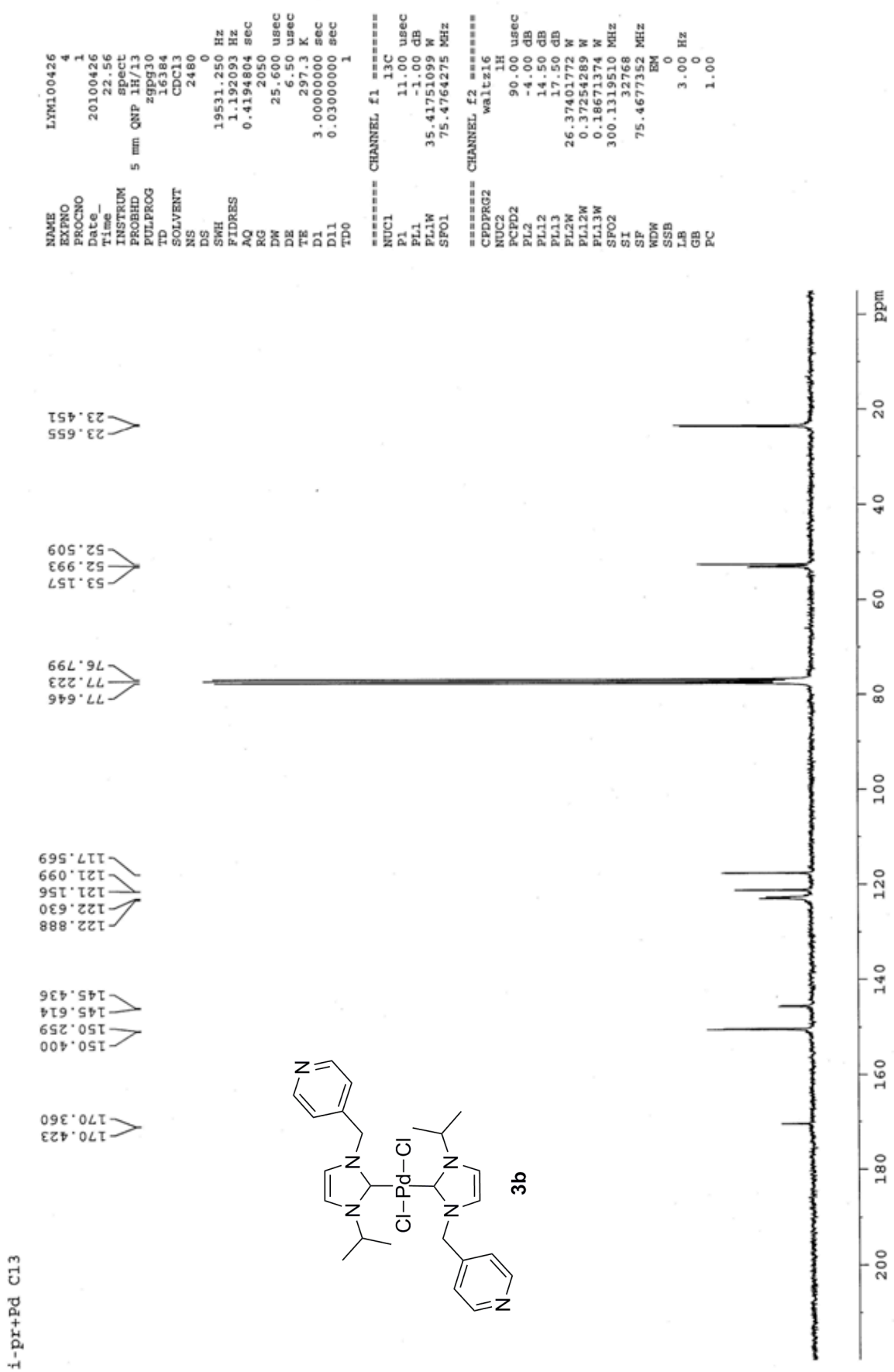
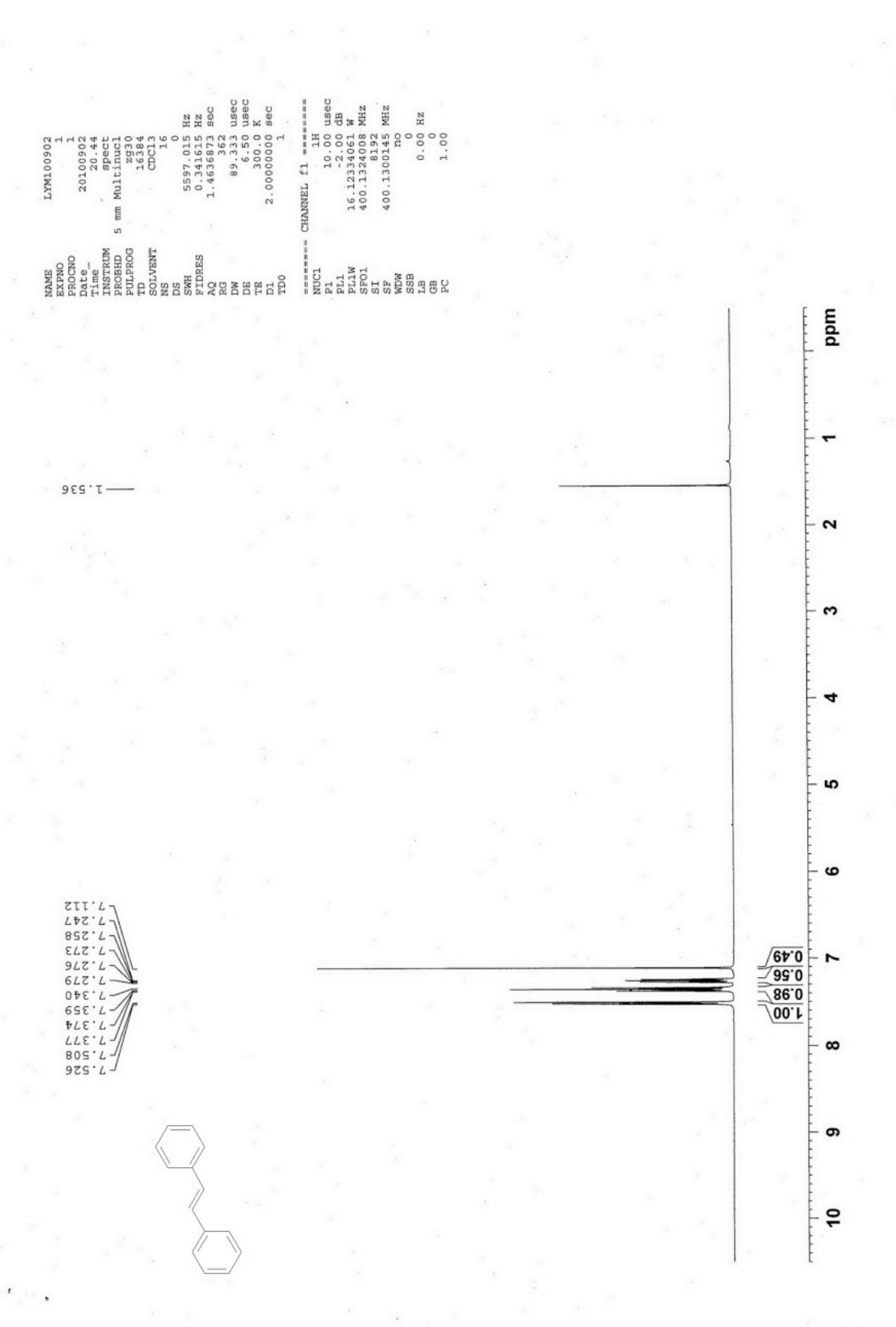
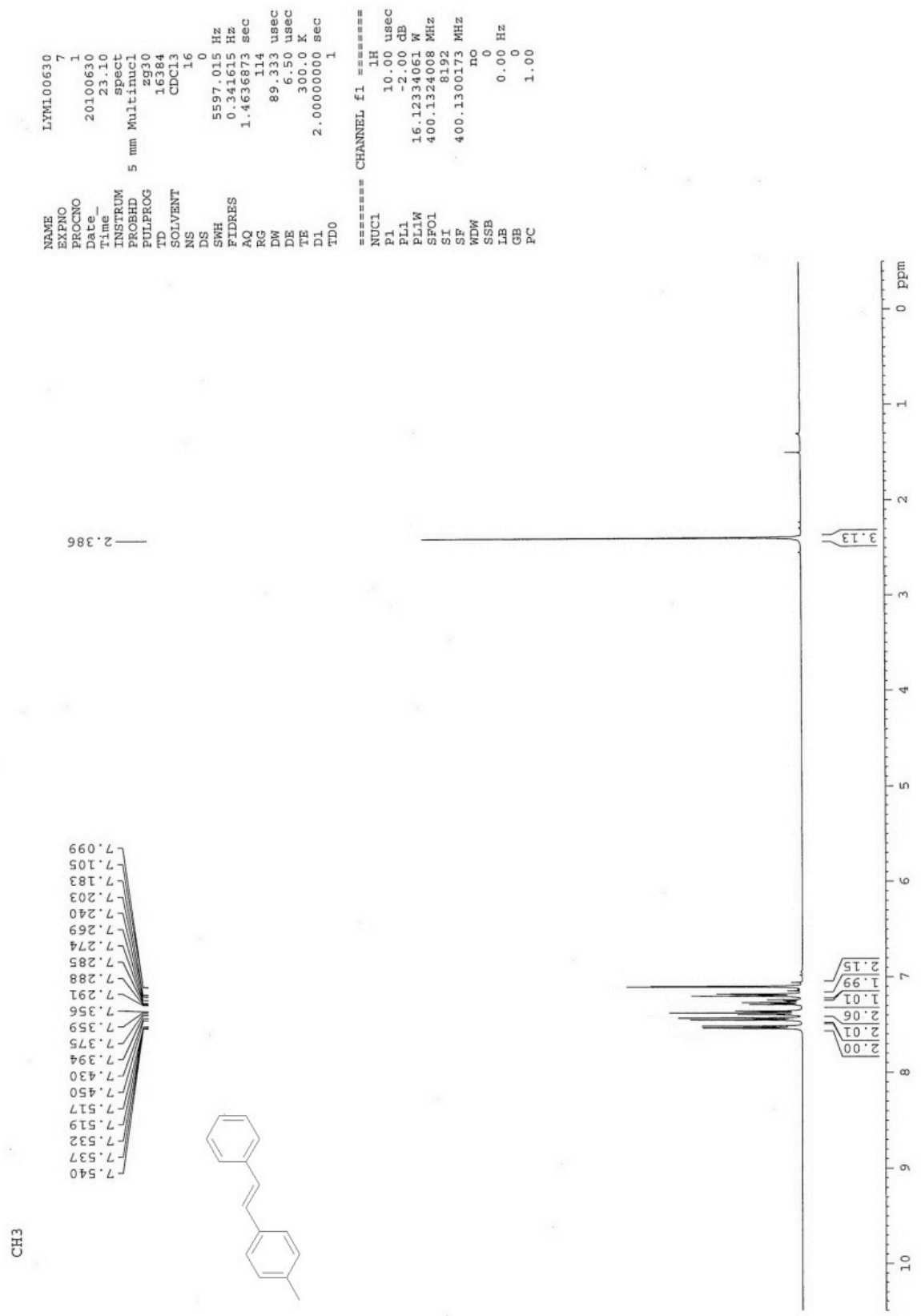
3a
0 ppm

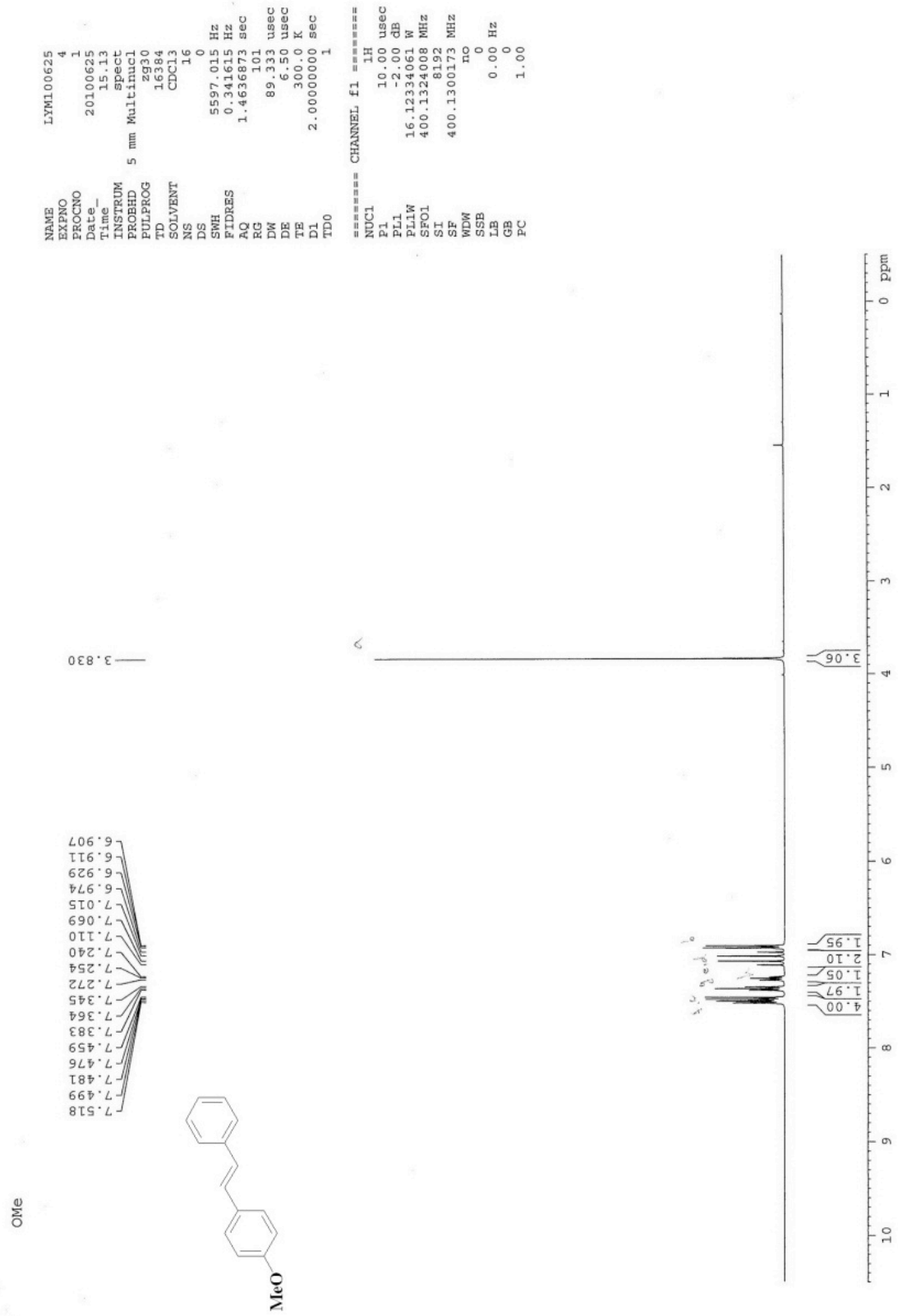

NAME LYM100601
EXPNO 3
PROCNO 1
Date_ 20100602
Time_ 9.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 11665
DS 0
SWH 19531.250 Hz
FIDRES 1.192093 Hz
AQ 0.4194804 sec
RG 2050
DW 25.600 usec
DE 6.50 usec
TE 298.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
PL1W 35.41751099 W
SFO1 75.4764275 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 14.50 dB
PL13 17.50 dB
PL2W 26.37401772 W
PL12W 0.37254289 W
PL13W 0.18671374 W
SFO2 300.1319510 MHz
SI 32768
SF 75.4677375 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
21.214
19.885
18.123
52.713
77.650
77.226
76.802
163.641
150.347
150.224
143.885
140.120
139.506
135.231
133.929
131.075
128.997
124.185
124.060
121.178
PdCl2L2
3a
ppm

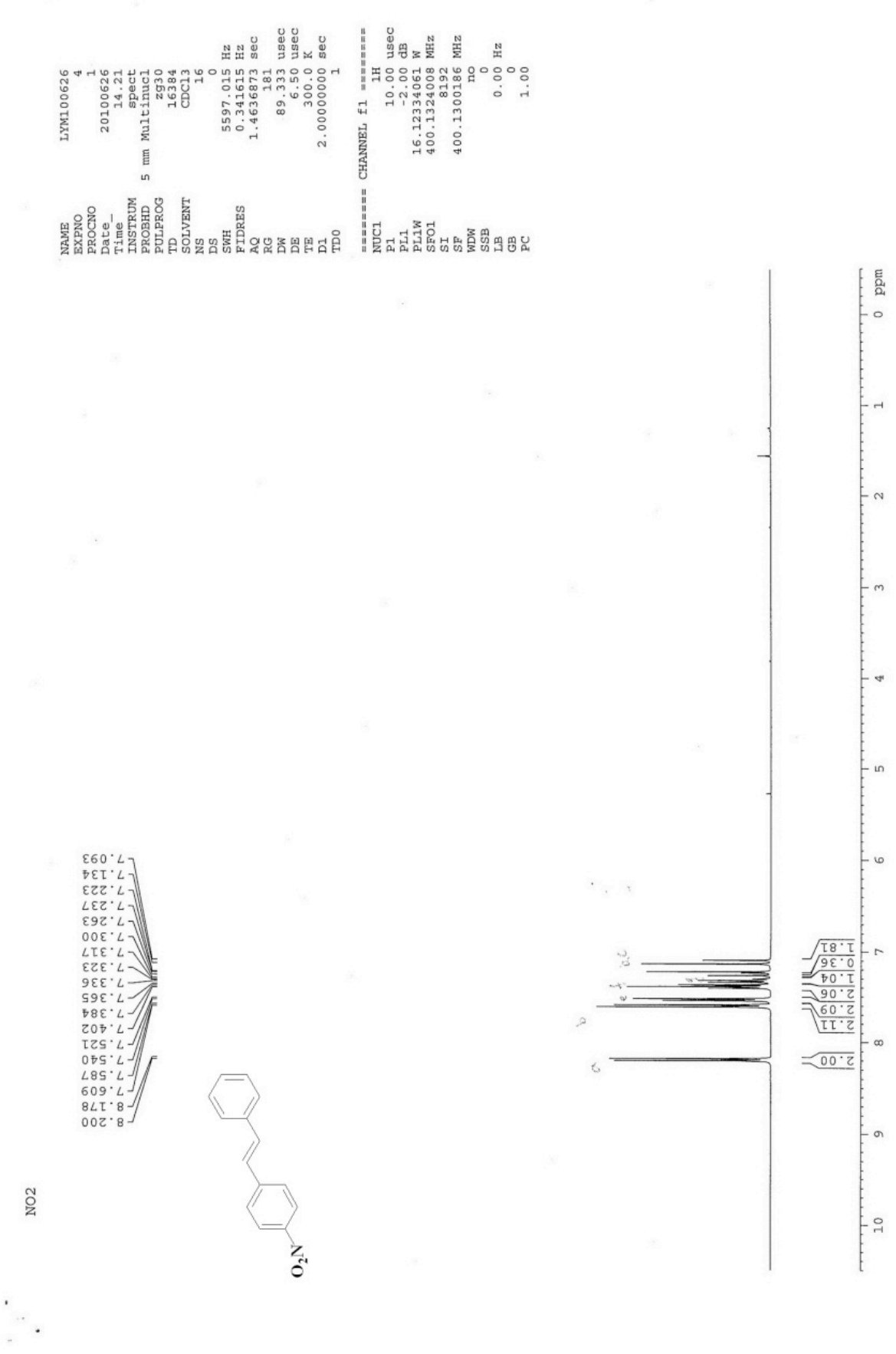


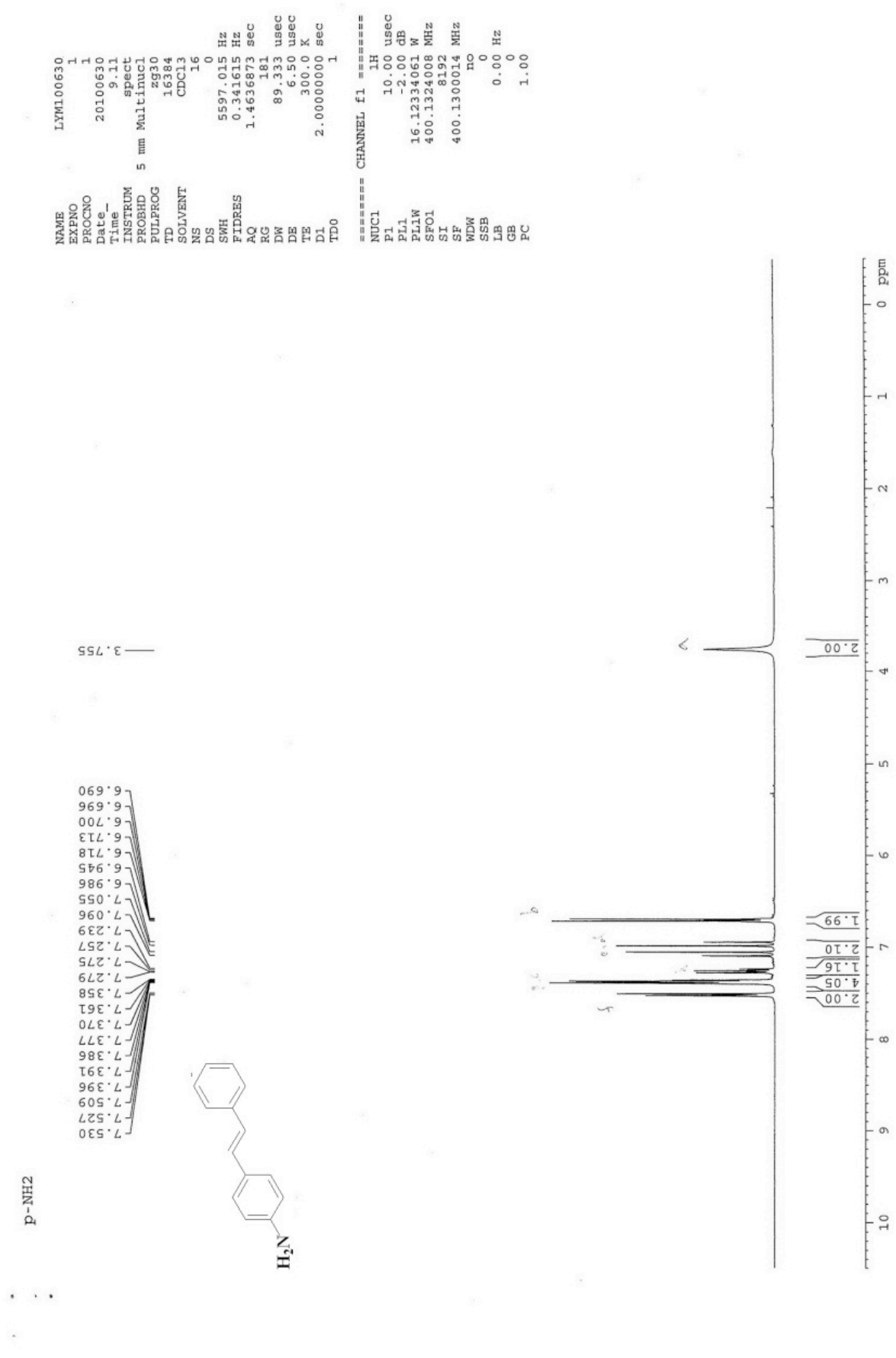

i-pr+Pd C13
NAME LYM100426
EXPNO 4
PROCNO 1
Date_ 20100426
Time_ 22.56
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 2480
DS 0
SWH 19531.250 Hz
FIDRES 1.192093 Hz
AQ 0.4194804 sec
RG 2050
DW 25.600 usec
DE 6.50 usec
TE 297.3 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
PL1W 35.41751099 W
SFO1 75.4764275 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 14.50 dB
PL13 17.50 dB
PL2W 26.37401772 W
PL12W 0.37254289 W
PL13W 0.18671374 W
SFO2 300.1319510 MHz
SI 32768
SF 75.4677352 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
23.655
23.451
52.509
52.993
53.157
76.799
77.223
77.646
117.569
121.099
121.156
122.630
122.888
145.436
145.614
150.259
150.400
170.360
170.423
Cl–Pd–Cl
3b
ppm
200
180
160
140
120
100
80
60
40
20

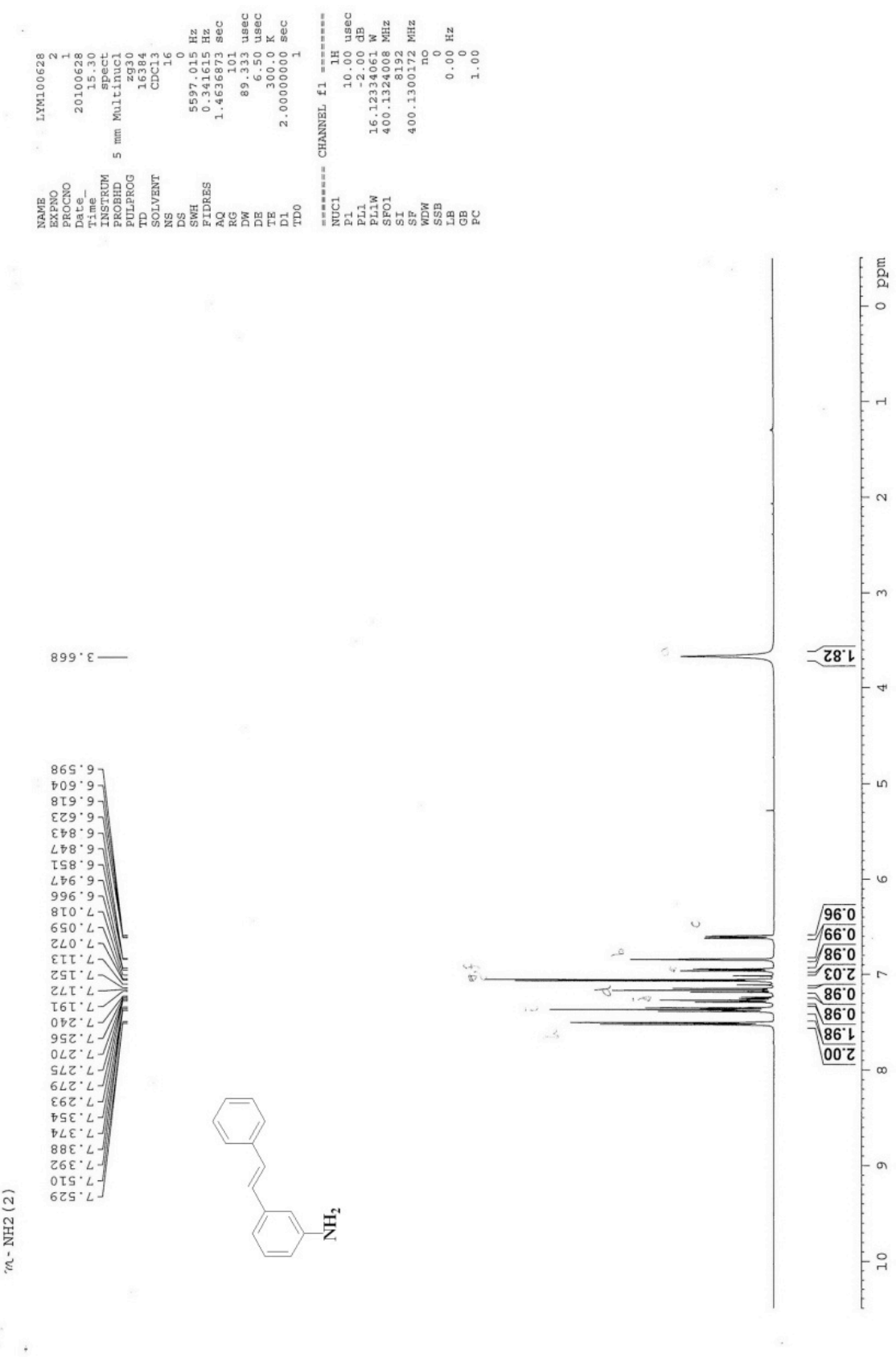

NAME LYM100902
EXPNO 1
PROCNO 1
Date_ 20100902
Time 20.44
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 362
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300145 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.536
7.526
7.508
7.377
7.374
7.359
7.340
7.279
7.276
7.273
7.258
7.247
7.112
1.00
0.98
0.56
0.49
ppm

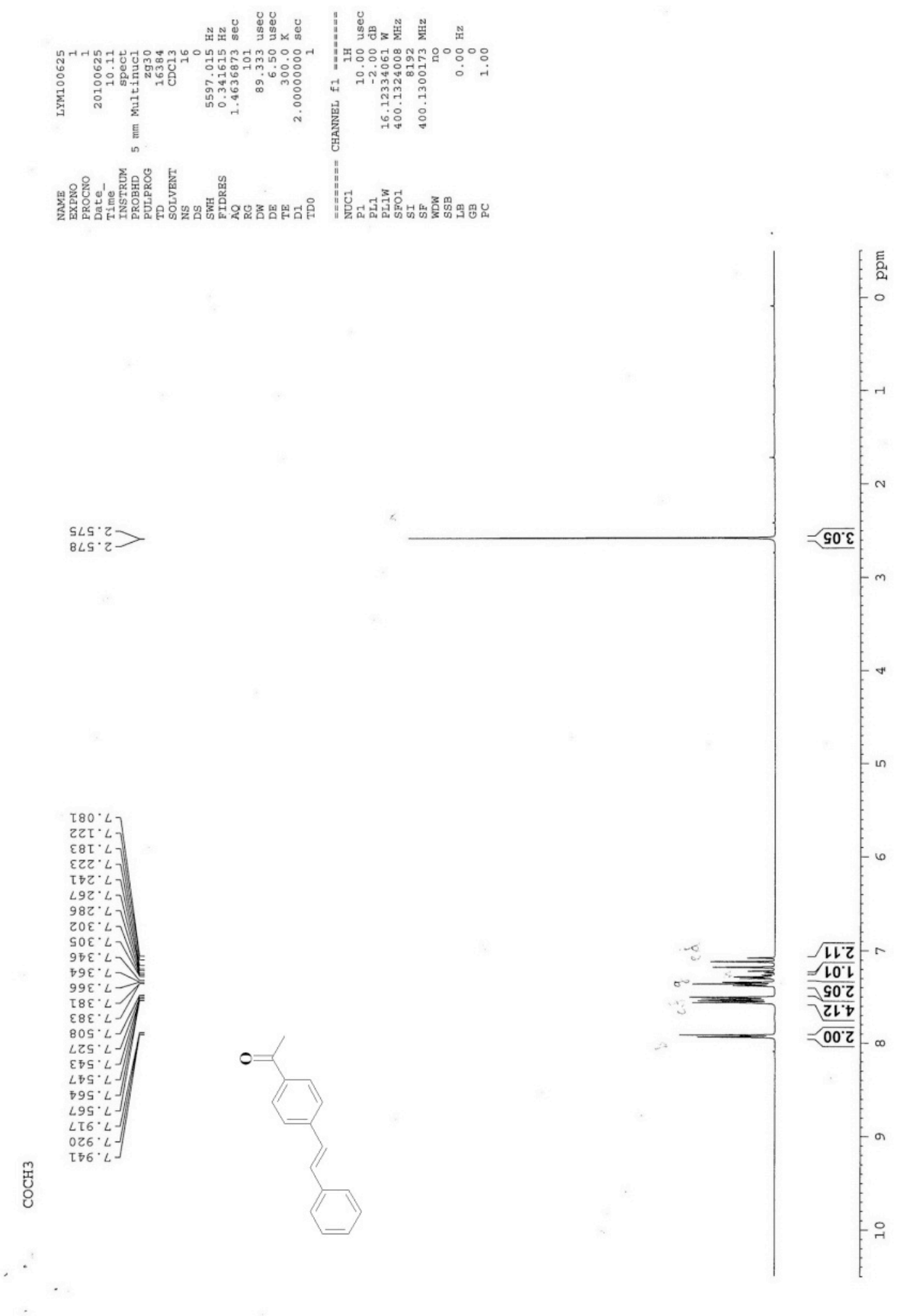

NAME LYM100630
EXPNO 7
PROCNO 1
Date_ 20100630
Time 23.10
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 114
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300173 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
2.386
7.540
7.537
7.532
7.519
7.517
7.450
7.430
7.394
7.375
7.359
7.356
7.291
7.288
7.285
7.274
7.269
7.240
7.203
7.183
7.105
7.099
3.13
2.15
1.99
1.01
2.06
2.01
2.00
CH3
ppm

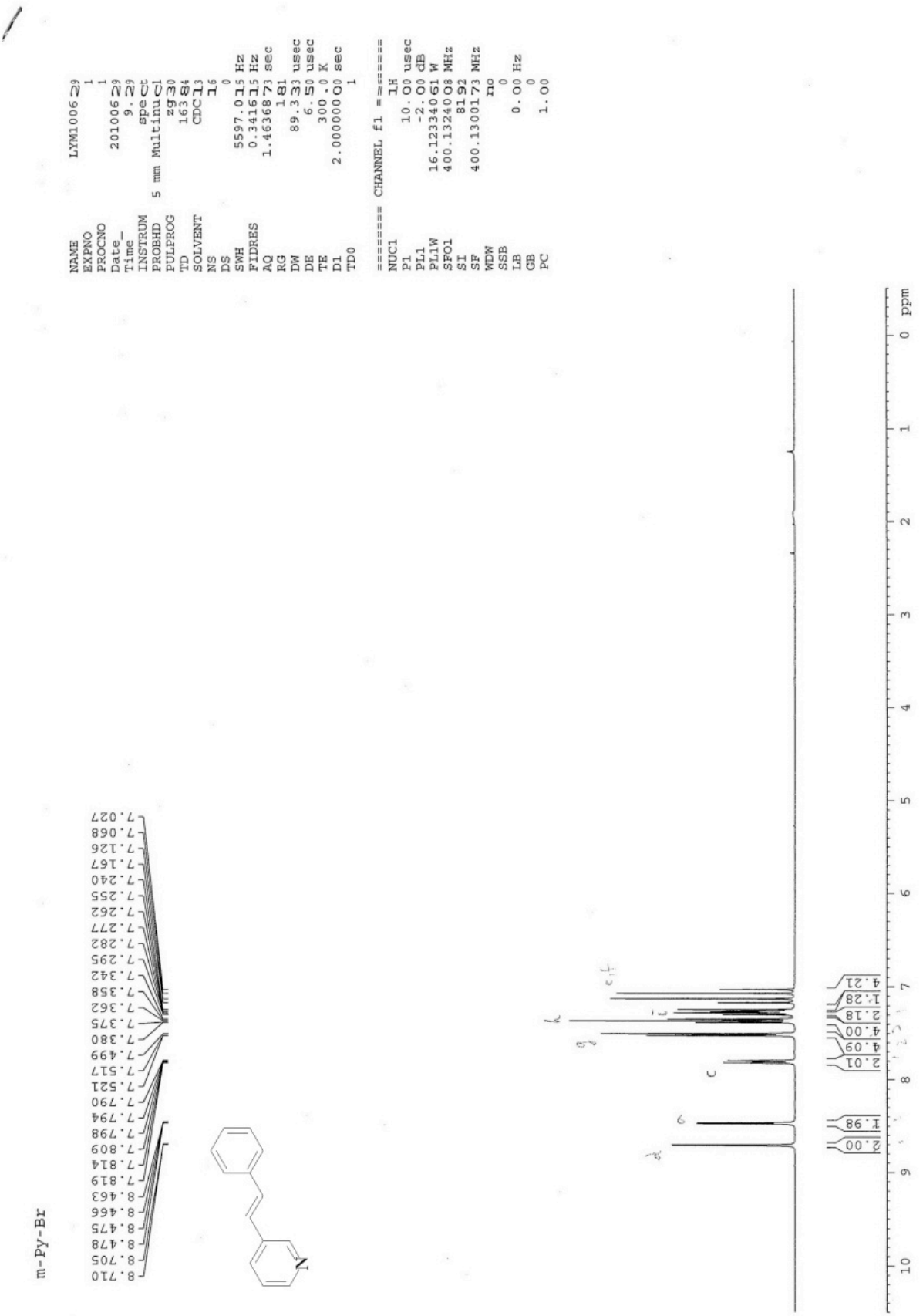

NAME LYM100625
EXPNO 4
PROCNO 1
Date_ 20100625
Time_ 15.13
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 101
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300173 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
3.830
7.518
7.499
7.481
7.476
7.459
7.383
7.364
7.345
7.272
7.254
7.240
7.110
7.069
7.015
6.974
6.929
6.911
6.907
3.06
1.95
2.10
1.05
1.97
4.00
OMe
MeO
ppm

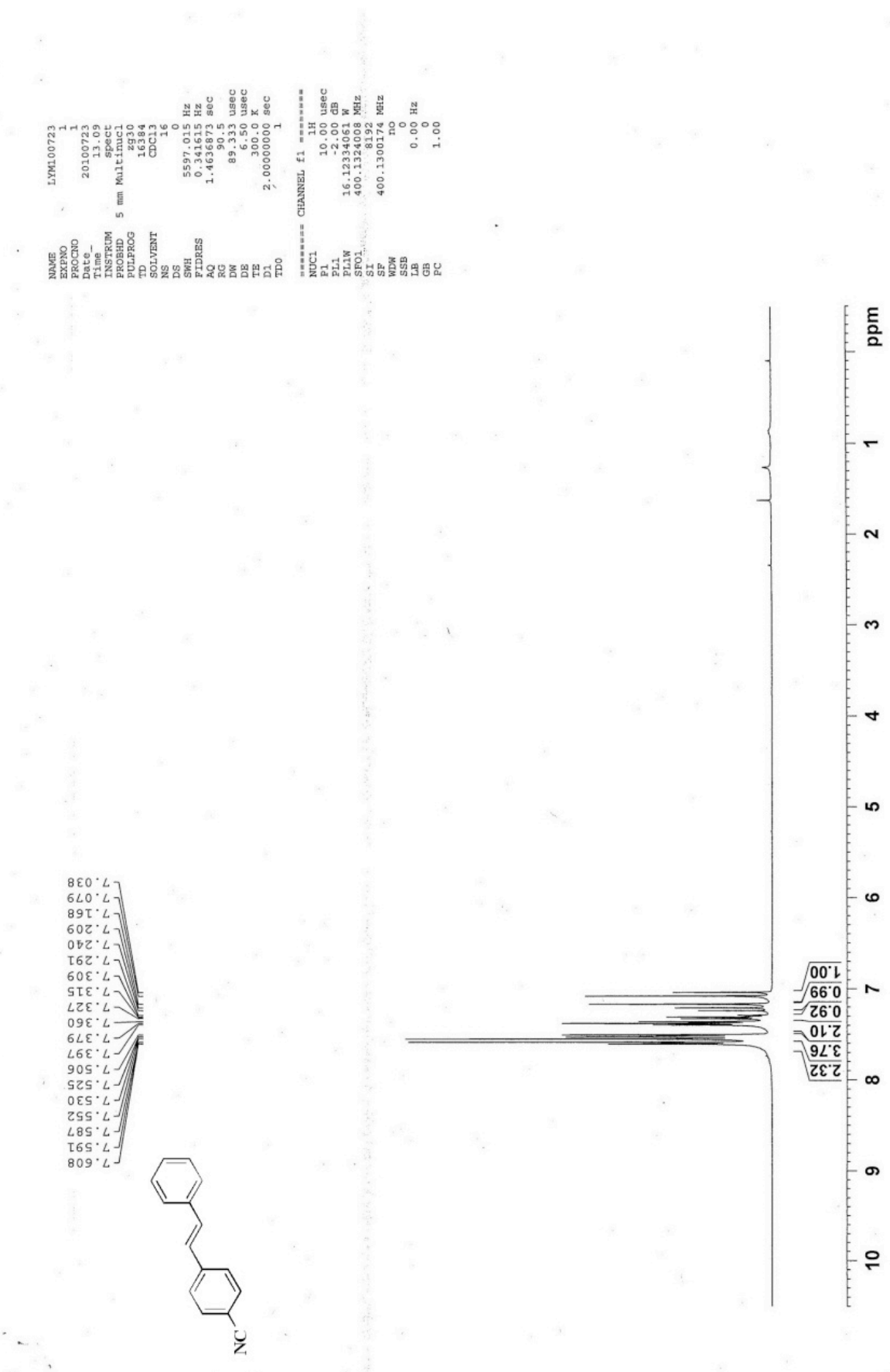

NAME LYM100626
EXPNO 4
PROCNO 1
Date_ 20100626
Time_ 14.21
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 181
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300186 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.200
8.178
7.609
7.587
7.540
7.521
7.402
7.384
7.365
7.336
7.323
7.317
7.300
7.263
7.237
7.223
7.134
7.093
NO2
O2N
2.00
2.11
2.09
2.06
1.04
0.36
1.81
ppm

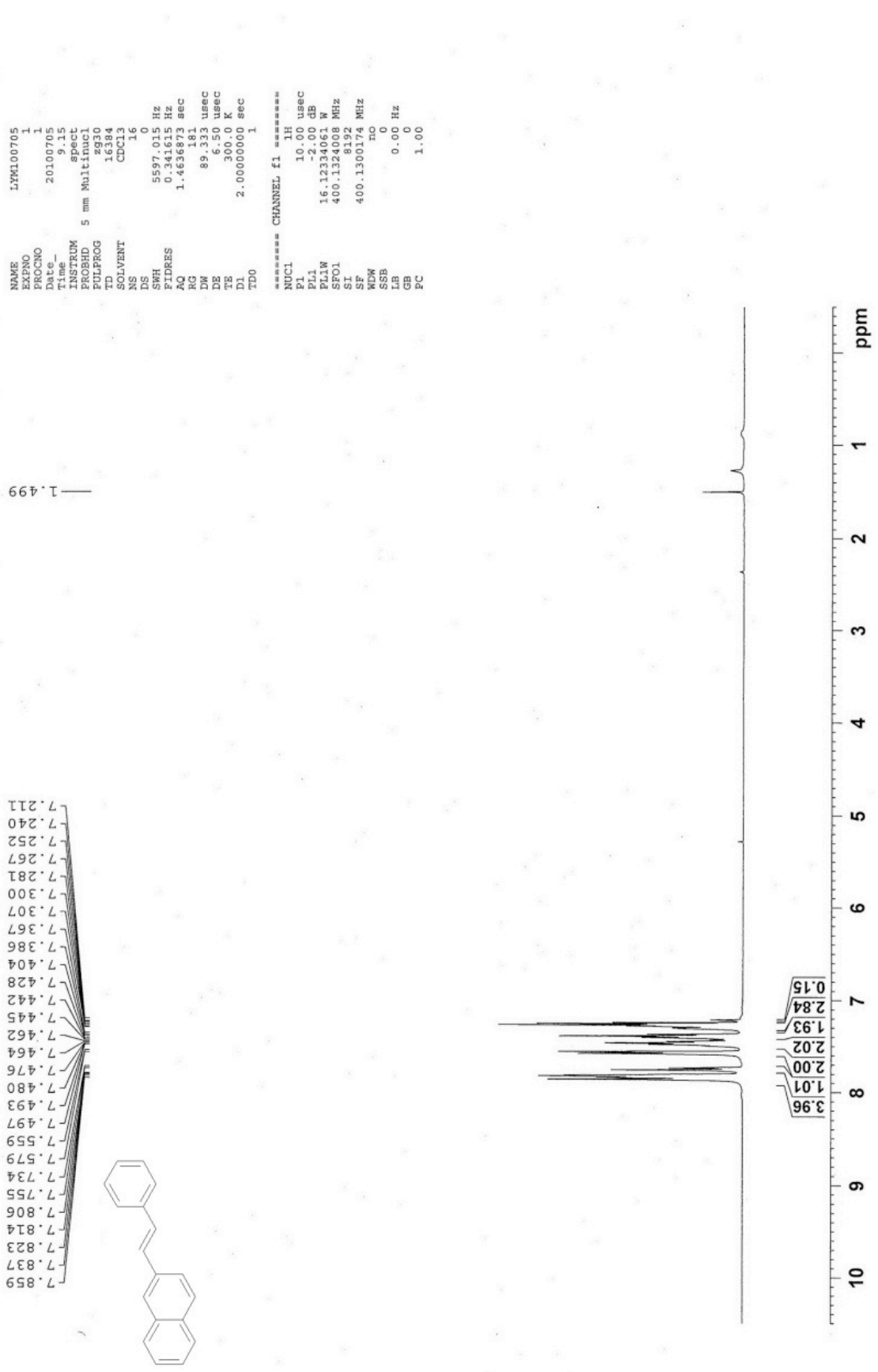

NAME LYM100630
EXPNO 1
PROCNO 1
Date_ 20100630
Time_ 9.11
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 181
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300014 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
3.755
7.530
7.527
7.509
7.396
7.391
7.386
7.377
7.370
7.361
7.358
7.279
7.275
7.257
7.239
7.096
7.055
6.986
6.945
6.718
6.713
6.700
6.696
6.690
p-NH2
H_2N
2.00
1.99
2.10
1.16
4.05
2.00
ppm

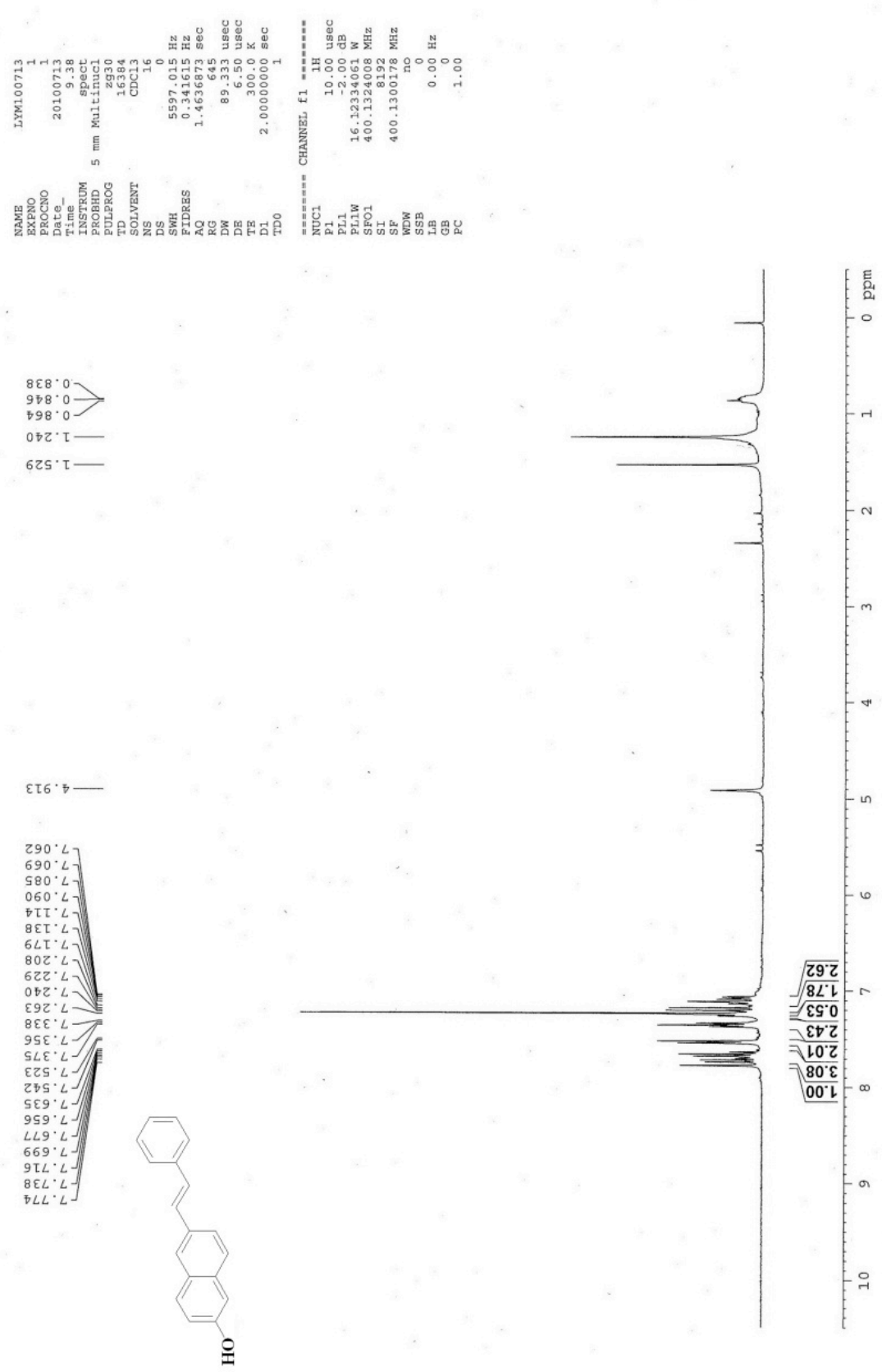

NAME LYM100628
EXPNO 2
PROCNO 1
Date_ 20100628
Time_ 15.30
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 101
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300172 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
3.668
7.529
7.510
7.392
7.388
7.374
7.354
7.293
7.279
7.275
7.270
7.256
7.240
7.191
7.172
7.152
7.113
7.072
7.059
7.018
6.966
6.947
6.851
6.847
6.843
6.623
6.618
6.604
6.598
m- NH2 (2)
NH2
1.82
0.96
0.99
0.98
2.03
0.98
0.98
1.98
2.00
ppm

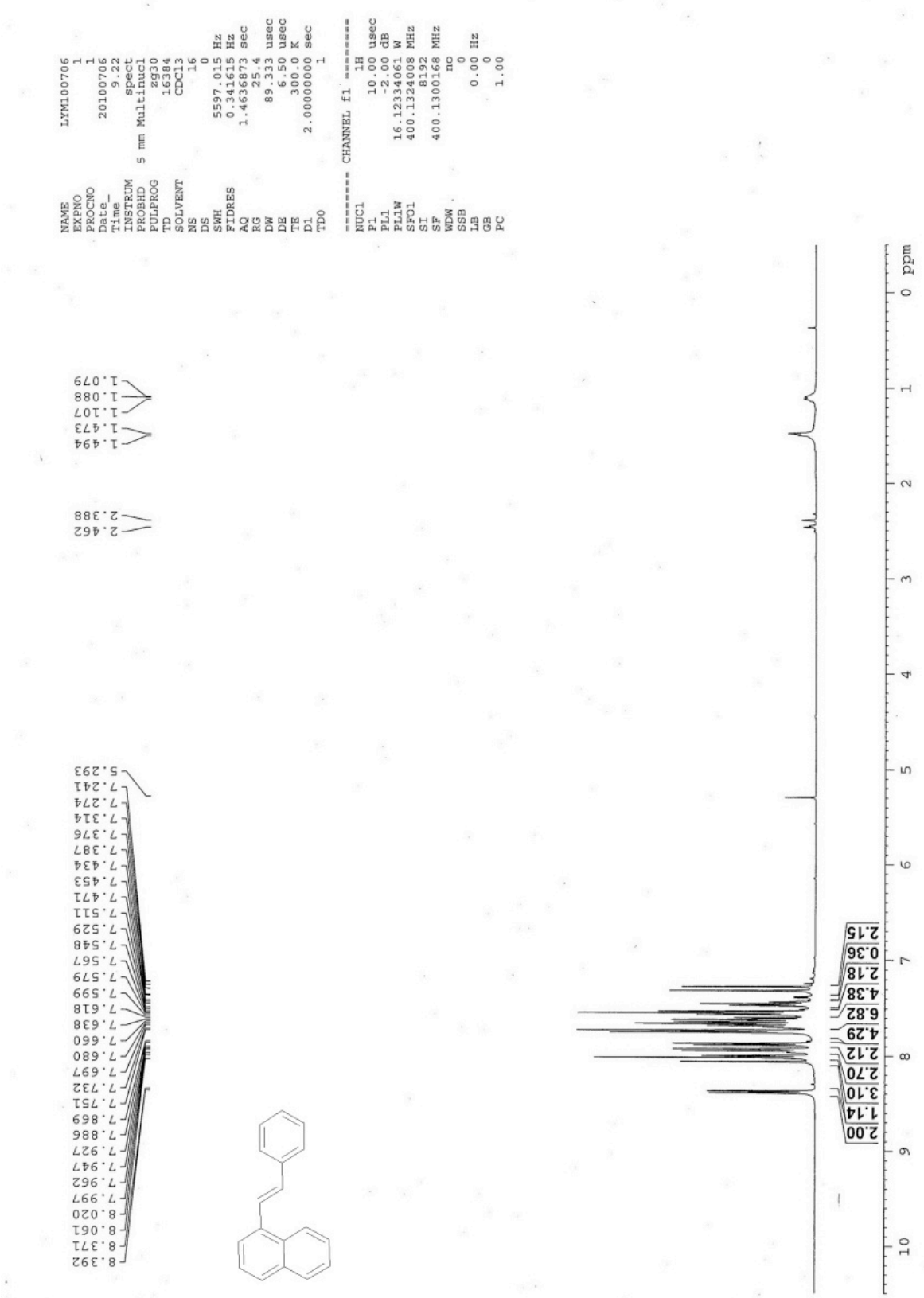

NAME LYM100625
EXPNO 1
PROCNO 1
Date_ 20100625
Time_ 10.11
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 101
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300173 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
2.578
2.575
7.941
7.920
7.917
7.567
7.564
7.547
7.543
7.527
7.508
7.383
7.381
7.366
7.364
7.346
7.305
7.302
7.286
7.267
7.241
7.223
7.183
7.122
7.081
COCH3
3.05
2.00
4.12
2.05
1.01
2.11
ppm

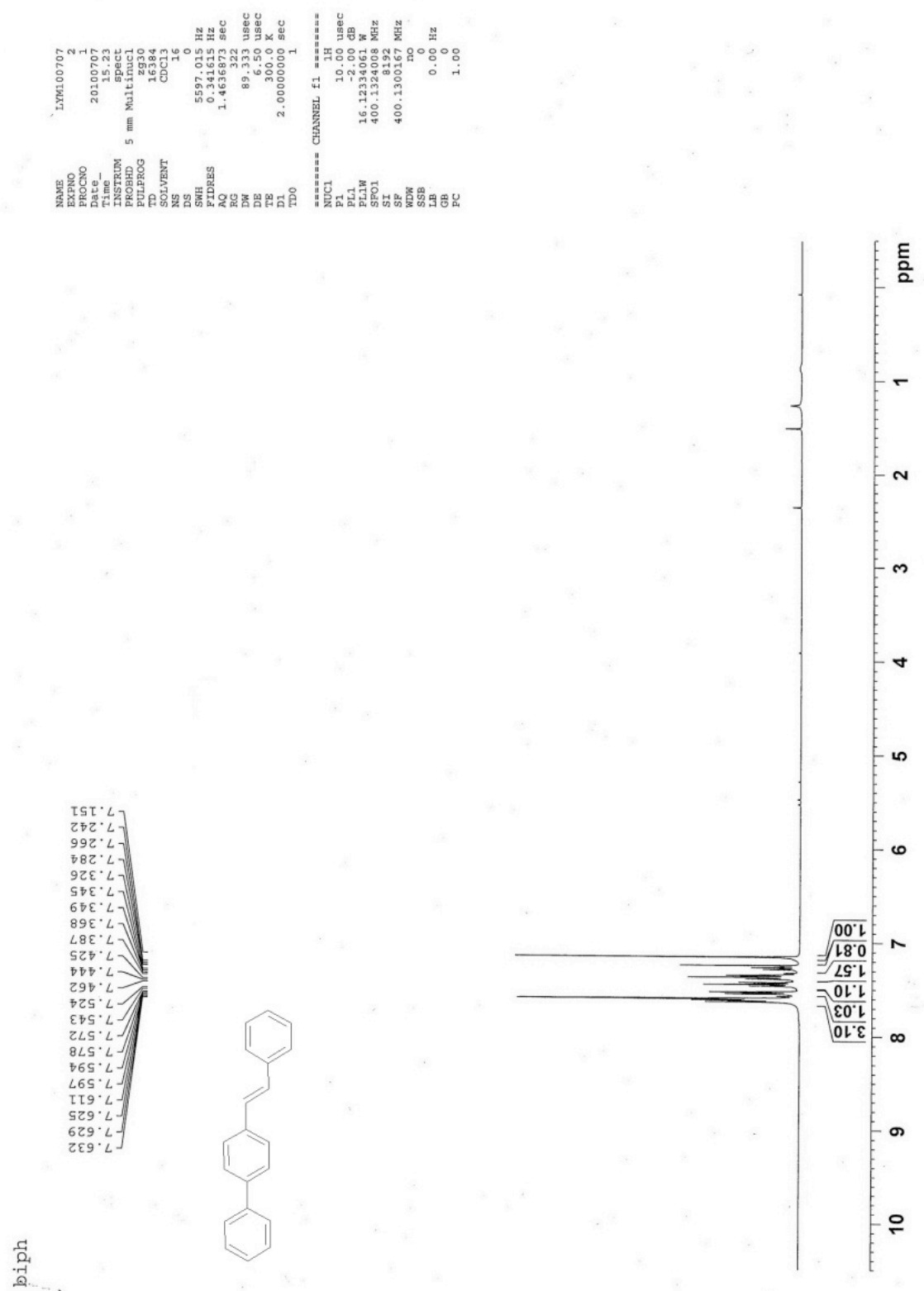

NAME LYM1006-29
EXPNO 1
PROCNO 1
Date_ 20100629
Time_ 9.29
INSTRUM spect
PROBHD 5 mm Multinu<1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.463687 sec
RG 181
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300173 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
m-Py-Br
8.710
8.705
8.478
8.475
8.463
8.466
7.819
7.814
7.809
7.798
7.794
7.790
7.521
7.517
7.499
7.380
7.375
7.362
7.358
7.342
7.295
7.282
7.277
7.262
7.255
7.240
7.167
7.126
7.068
7.027
2.00
1.98
2.01
4.09
4.00
2.18
1.28
4.21
ppm

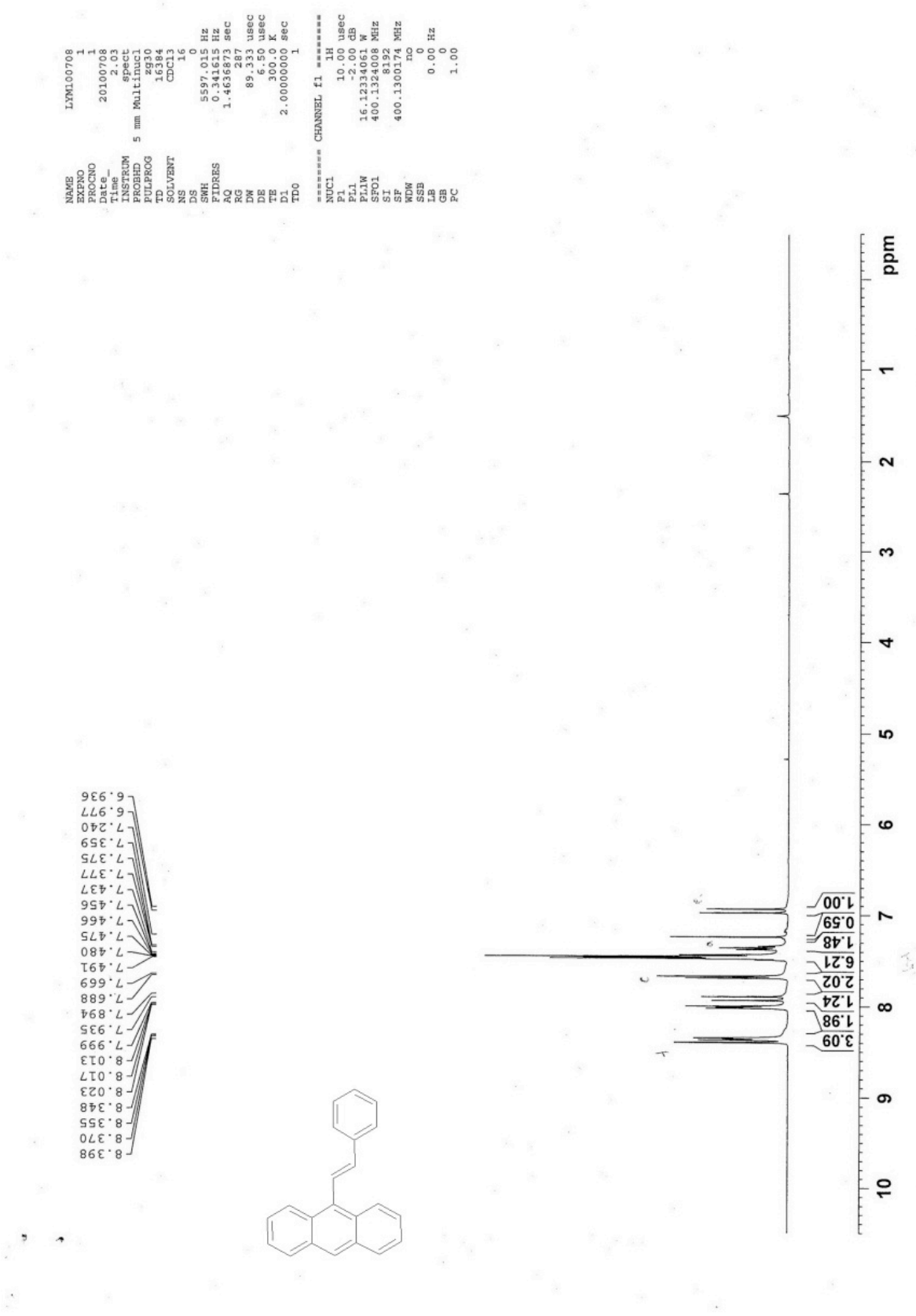

NAME LYM100723
EXPNO 1
PROCNO 1
Date_ 20100723
Time_ 13.09
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 90.5
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300174 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.608
7.591
7.587
7.552
7.530
7.525
7.506
7.397
7.379
7.360
7.327
7.315
7.309
7.291
7.240
7.209
7.168
7.079
7.038
NC
2.32
3.76
2.10
0.92
0.99
1.00
ppm

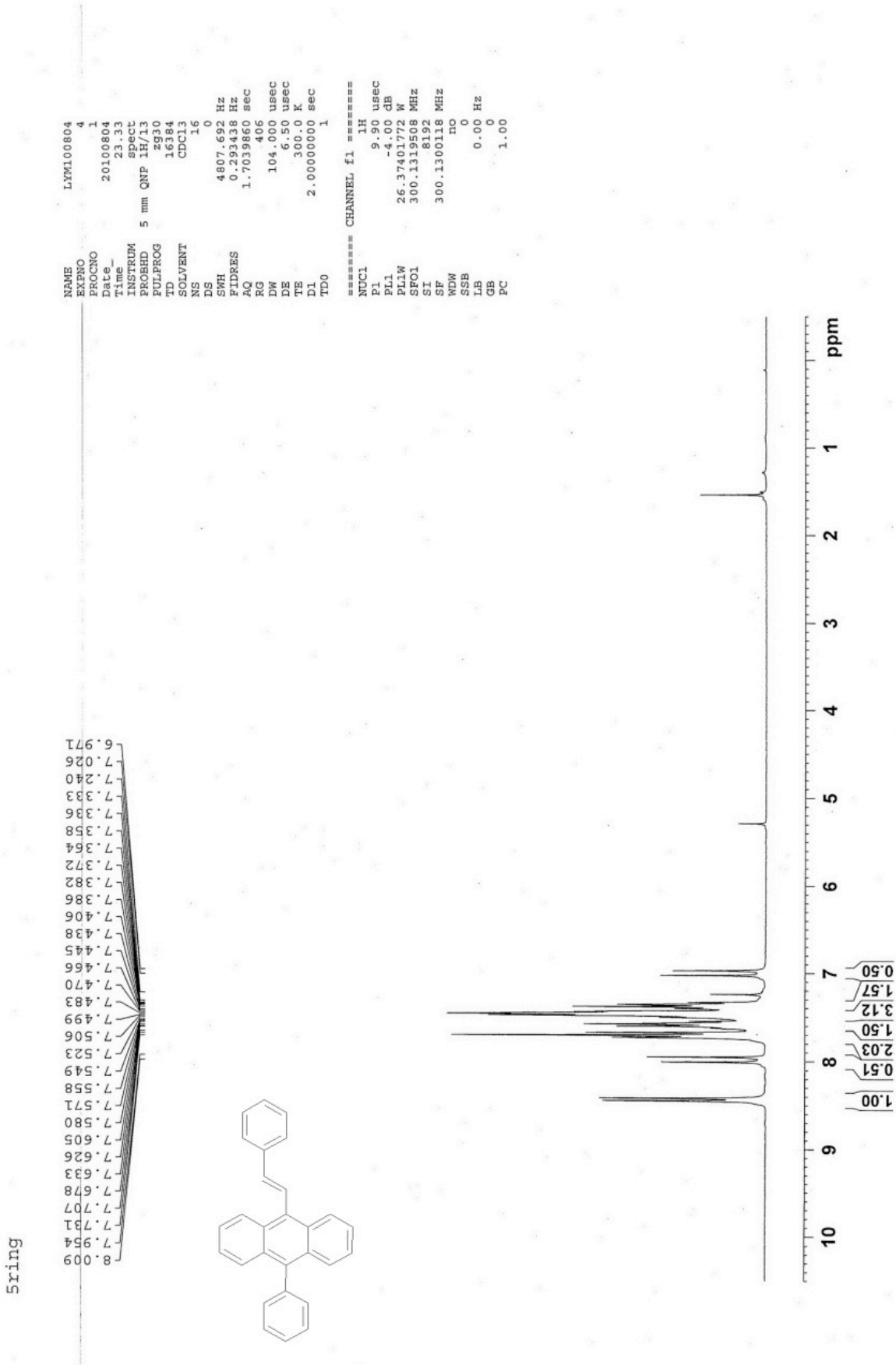

NAME LYM100705
EXPNO 1
PROCNO 1
Date_ 20100705
Time_ 9.15
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.3416153 Hz
AQ 1.4636873 sec
RG 181
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300174 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.499
7.859
7.837
7.823
7.814
7.806
7.755
7.734
7.579
7.559
7.497
7.493
7.480
7.476
7.464
7.462
7.445
7.442
7.428
7.404
7.386
7.367
7.307
7.300
7.281
7.267
7.252
7.240
7.211
3.96
1.01
2.00
2.02
1.93
2.84
0.15
ppm
1
2
3
4
5
6
7
8
9
10

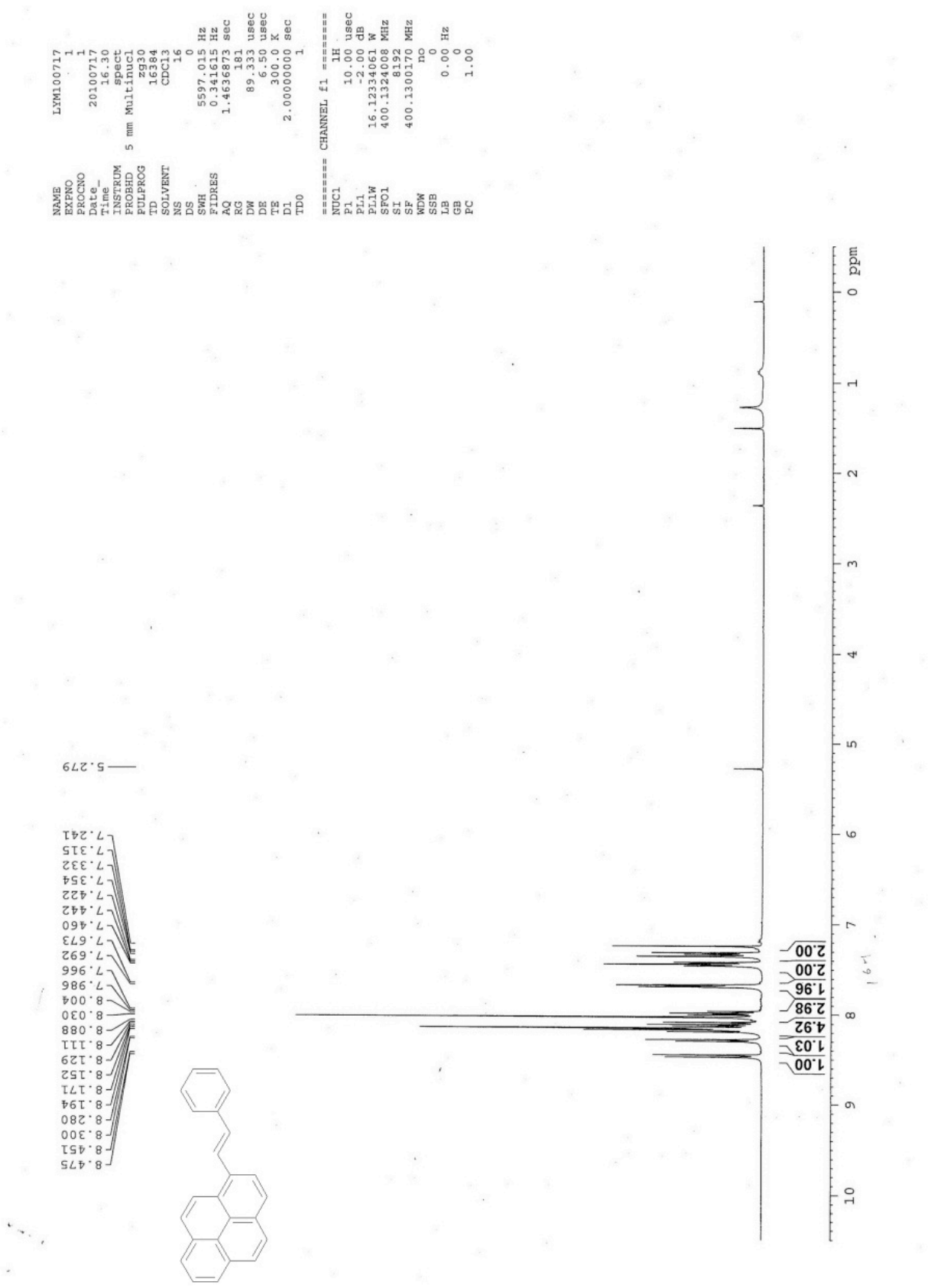

NAME LYM100713
EXPNO 1
PROCNO 1
Date_ 20100713
Time 9.38
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 645
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300178 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
0.838
0.846
0.864
1.240
1.529
4.913
7.062
7.069
7.085
7.090
7.114
7.138
7.179
7.208
7.229
7.240
7.263
7.338
7.356
7.375
7.523
7.542
7.635
7.656
7.677
7.699
7.716
7.738
7.774
1.00
3.08
2.01
2.43
0.53
1.78
2.62
HO
ppm

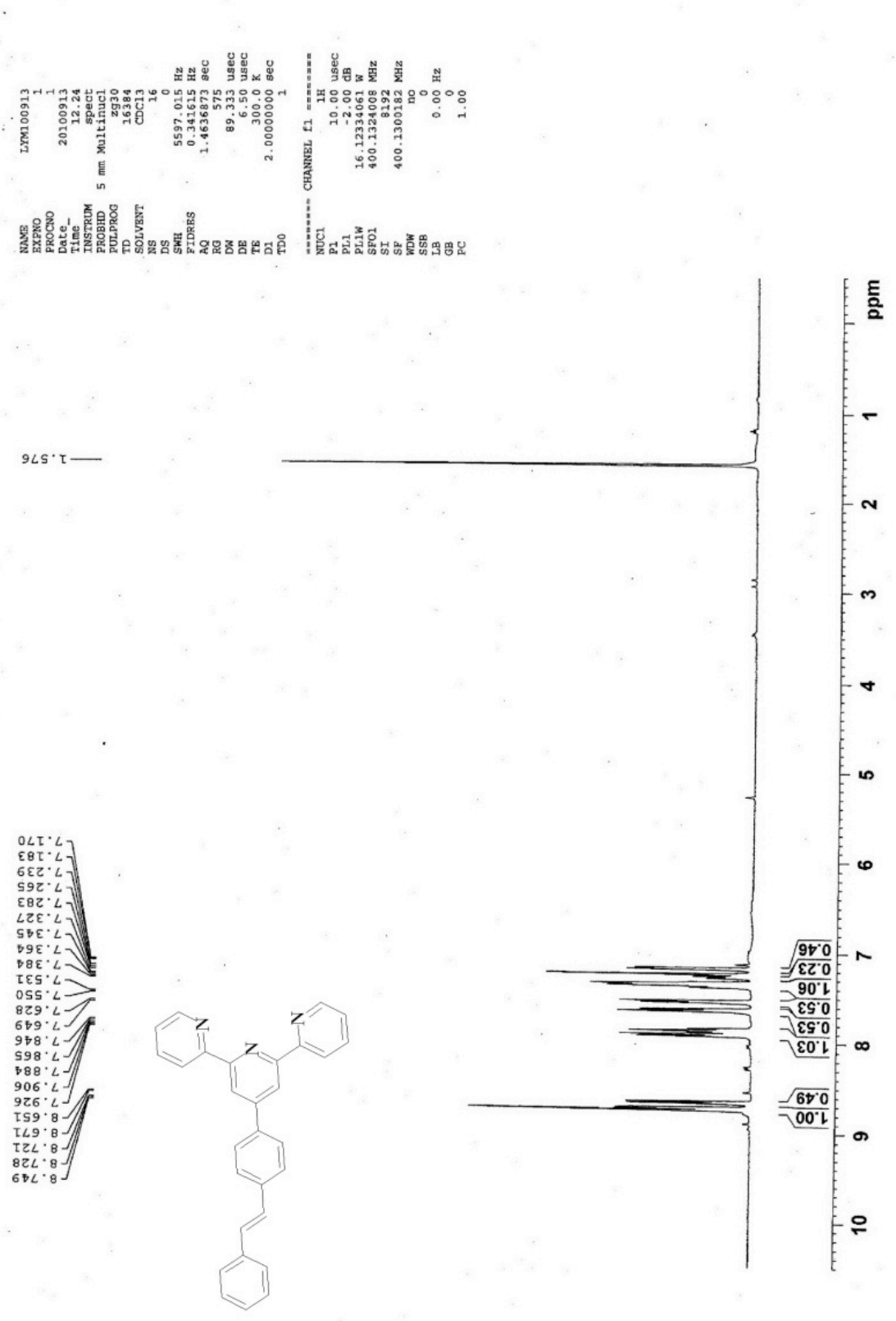

NAME LYM100706
EXPNO 1
PROCNO 1
Date_ 20100706
Time 9.22
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 25.4
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300168 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.079
1.088
1.107
1.473
1.494
2.388
2.462
5.293
7.241
7.274
7.314
7.376
7.387
7.434
7.453
7.471
7.511
7.529
7.548
7.567
7.579
7.599
7.618
7.638
7.660
7.680
7.697
7.732
7.751
7.869
7.886
7.927
7.947
7.962
7.997
8.020
8.061
8.371
8.392
2.00
1.14
3.10
2.70
2.12
4.29
6.82
4.38
2.18
0.36
2.15
0 ppm

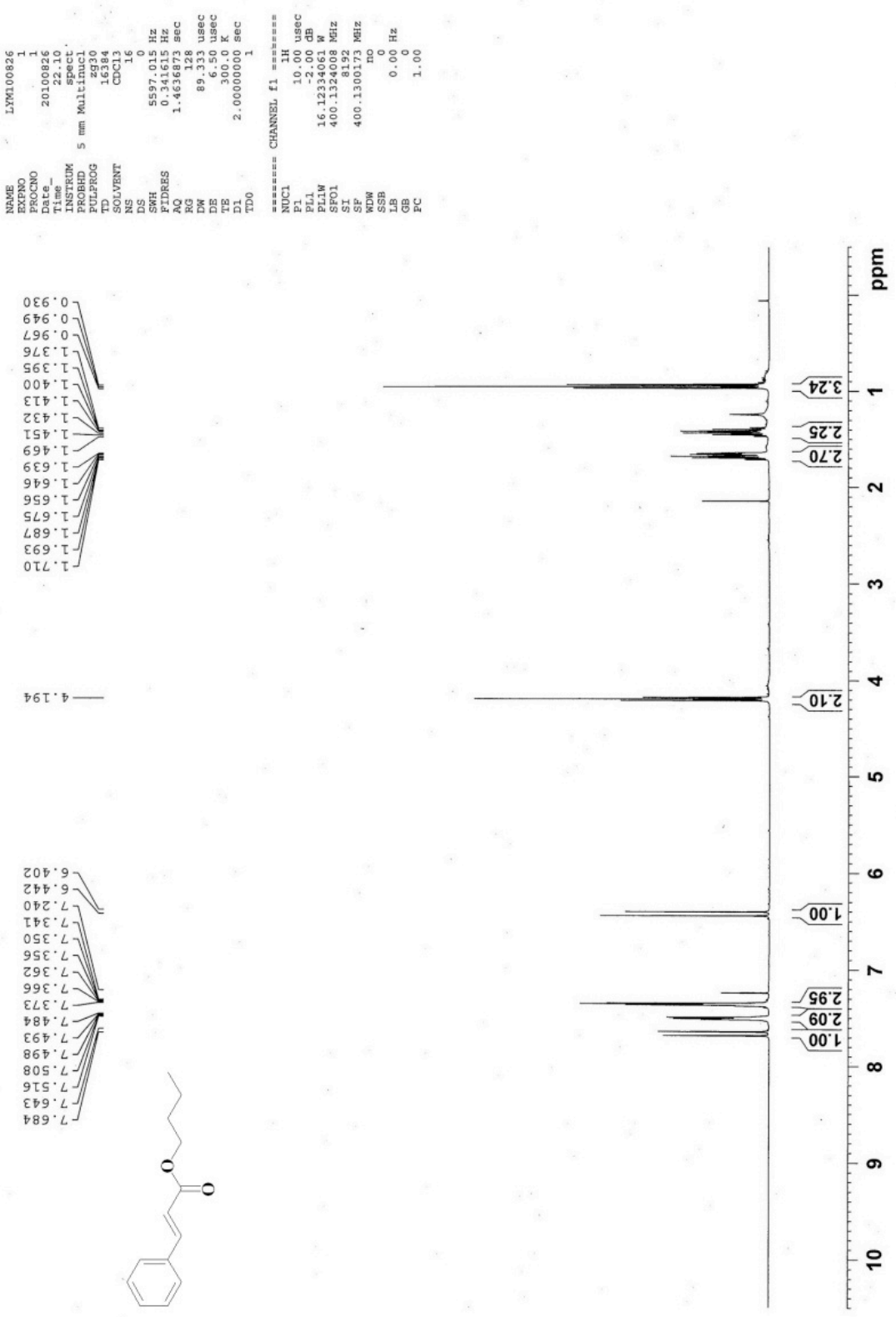

NAME LYM100707
EXPNO 2
PROCNO 1
Date_ 20100707
Time 15.23
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 322
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300167 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.151
7.242
7.266
7.284
7.326
7.345
7.349
7.368
7.387
7.425
7.444
7.462
7.524
7.543
7.572
7.578
7.594
7.597
7.611
7.625
7.629
7.632
3.10
1.03
1.10
1.57
0.81
1.00
ppm
biph

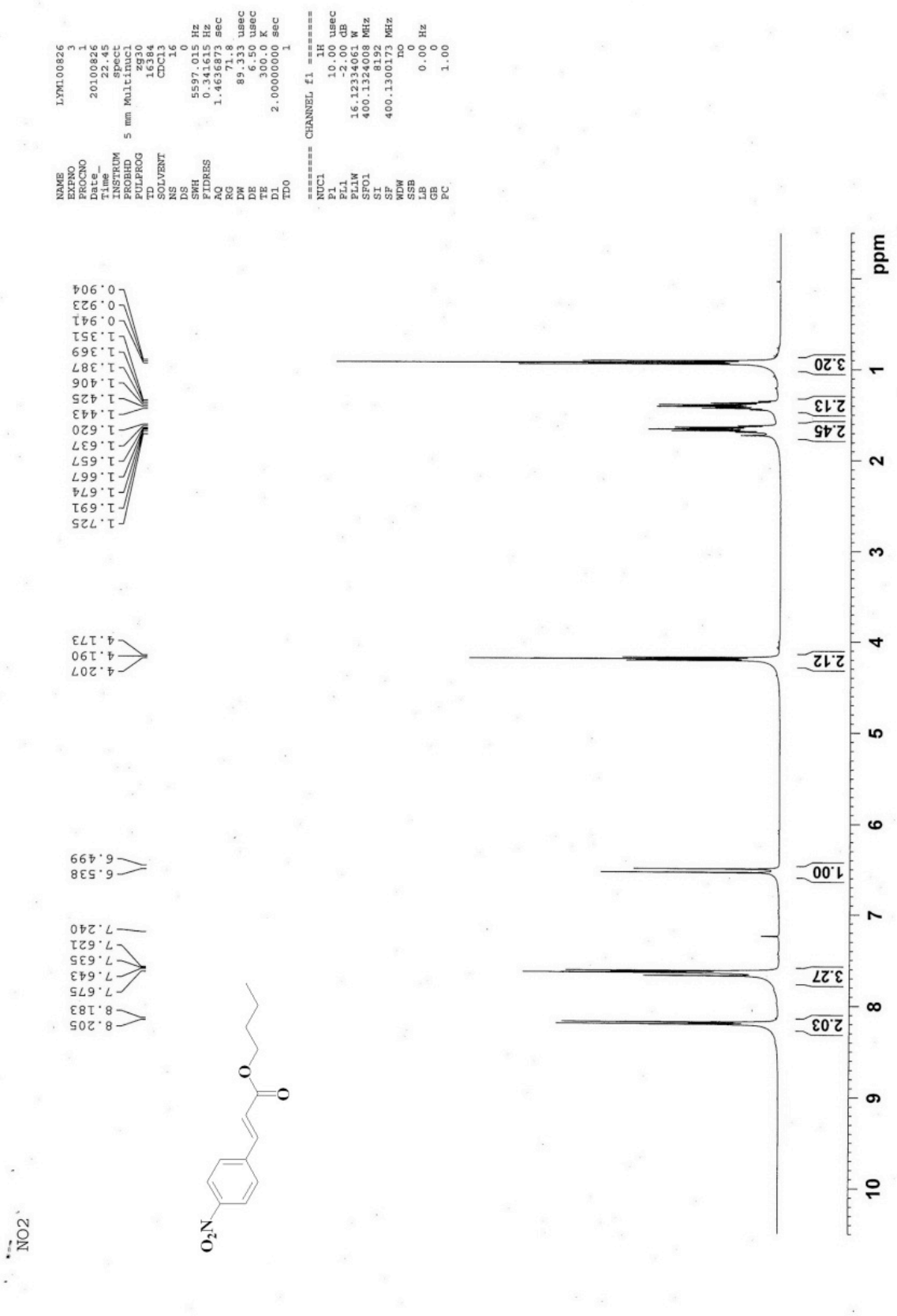

NAME LYM100708
EXPNO 1
PROCNO 1
Date_ 20100708
Time_ 2.03
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 287
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300174 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.398
8.370
8.355
8.348
8.023
8.017
8.013
7.999
7.935
7.894
7.688
7.669
7.491
7.480
7.475
7.466
7.456
7.437
7.377
7.375
7.359
7.240
6.977
6.936
3.09
1.98
1.24
2.02
6.21
1.48
0.59
1.00
ppm

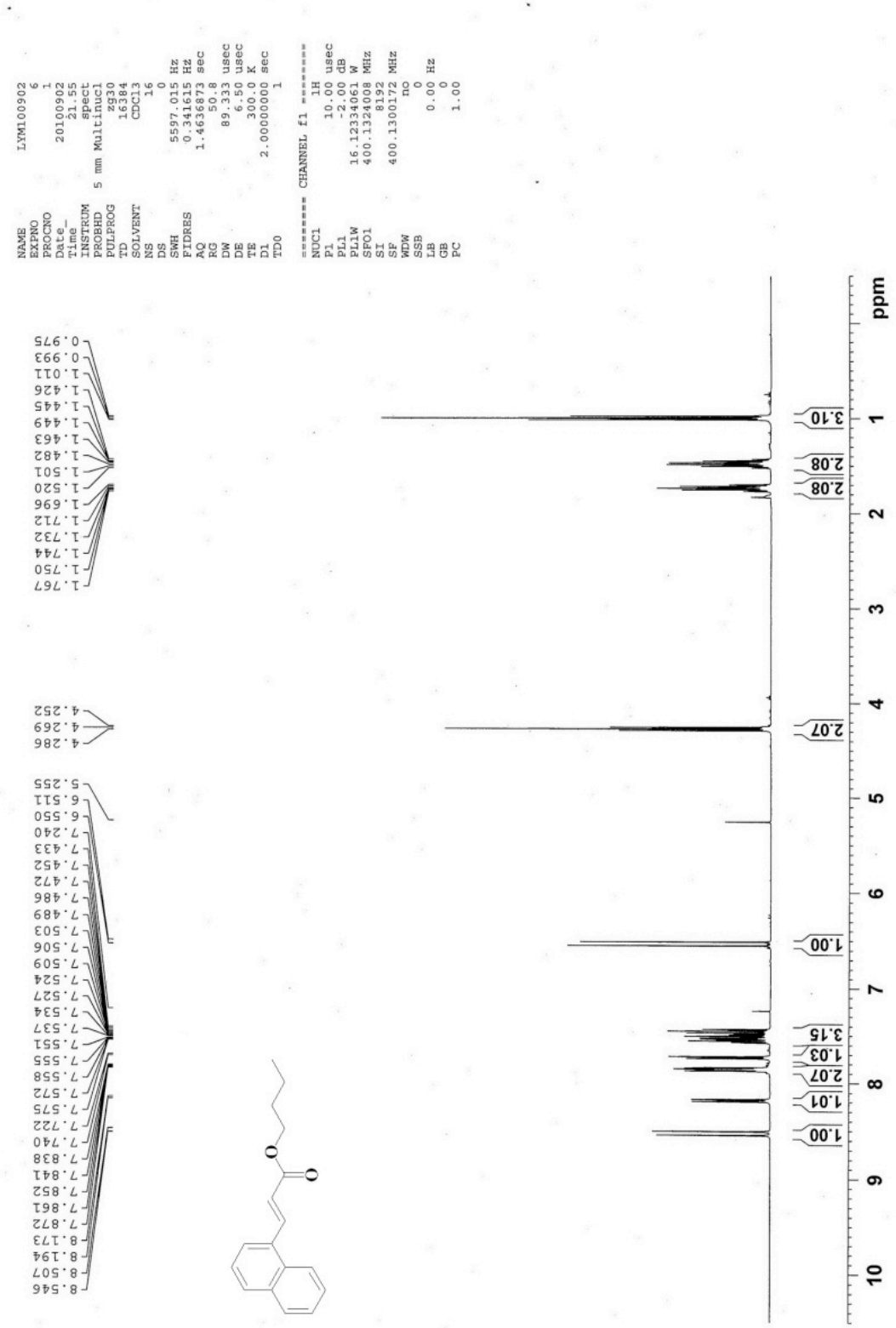

5ring
ppm
1.00
0.51
2.03
1.50
3.12
1.57
0.50


NAME LYM100717
EXPNO 1
PROCNO 1
Date_ 20100717
Time 16.30
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 181
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
5.279
7.241
7.315
7.332
7.354
7.422
7.442
7.460
7.673
7.692
7.966
7.986
8.004
8.030
8.088
8.111
8.129
8.152
8.171
8.194
8.280
8.300
8.451
8.475
1.00
1.03
4.92
2.98
1.96
2.00
2.00
0 ppm


NAME LZM100913
EXPNO 1
PROCNO 1
Date_ 20100913
Time_ 12.24
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 575
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300182 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.576
8.749
8.728
8.721
8.671
8.651
7.926
7.906
7.884
7.865
7.846
7.649
7.628
7.550
7.531
7.384
7.364
7.345
7.327
7.283
7.265
7.239
7.183
7.170
0.46
0.23
1.06
0.53
0.53
1.03
0.49
1.00
ppm


NAME LYM100826
EXPNO 1
PROCNO 1
Date_ 20100826
Time_ 22.10
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 128
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300173 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.684
7.643
7.516
7.508
7.498
7.493
7.484
7.473
7.366
7.362
7.356
7.350
7.341
7.240
6.442
6.402
4.194
1.710
1.693
1.687
1.675
1.656
1.646
1.639
1.469
1.451
1.432
1.413
1.400
1.395
1.376
0.967
0.949
0.930
3.24
2.25
2.70
2.10
1.00
2.95
2.09
1.00
ppm


NAME LYM100826
EXPNO 3
PROCNO 1
Date_ 20100826
Time_ 22.45
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 71.8
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PLIW 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300173 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
0.904
0.923
0.941
1.351
1.369
1.387
1.406
1.425
1.443
1.620
1.637
1.657
1.667
1.674
1.691
1.725
4.173
4.190
4.207
6.499
6.538
7.240
7.621
7.635
7.643
7.675
8.183
8.205
NO2
O2N
O
O
3.20
2.13
2.45
2.12
1.00
3.27
2.03
ppm


NAME LYM100902
EXPNO 6
PROCNO 1
Date_ 20100902
Time 21.55
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 50.8
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1324008 MHz
SI 8192
SF 400.1300172 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
0.975
0.993
1.011
1.426
1.445
1.449
1.463
1.482
1.501
1.520
1.696
1.712
1.732
1.744
1.750
1.767
4.252
4.269
4.286
5.255
6.511
6.550
7.240
7.433
7.452
7.472
7.486
7.489
7.503
7.506
7.509
7.524
7.527
7.534
7.537
7.551
7.555
7.558
7.572
7.575
7.722
7.740
7.838
7.841
7.852
7.861
7.872
8.173
8.194
8.507
8.546
3.10
2.08
2.08
2.07
1.00
3.15
1.03
2.07
1.01
1.00
ppm