

Supporting Information

Direct Synthesis of *Cis*-Dihalo-Bis(NHC) Complex of Nickel (II) and Catalytic Application in Olefin Addition Polymerization: Effect of Halogen Co-Ligands and Theory Study

Dao Zhang,* Sen Zhou, Zhiming Li, Quanrui Wang and Linhong Weng

P1, **Figure S1.** The ^1H NMR spectrum of $[\text{H}(\mathbf{1a})]\text{Br}$

P2, **Figure S2.** The ^1H NMR spectrum of $[\text{H}(\mathbf{1b})]\text{Br}$

P3, **Figure S3.** The ^1H NMR spectrum of *trans*- $[(\mathbf{1a})_2\text{NiBr}_2]$, **2a**

P4, **Figure S4.** The ^1H NMR spectrum of *trans*- $[(\mathbf{1b})_2\text{NiBr}_2]$, **2b**

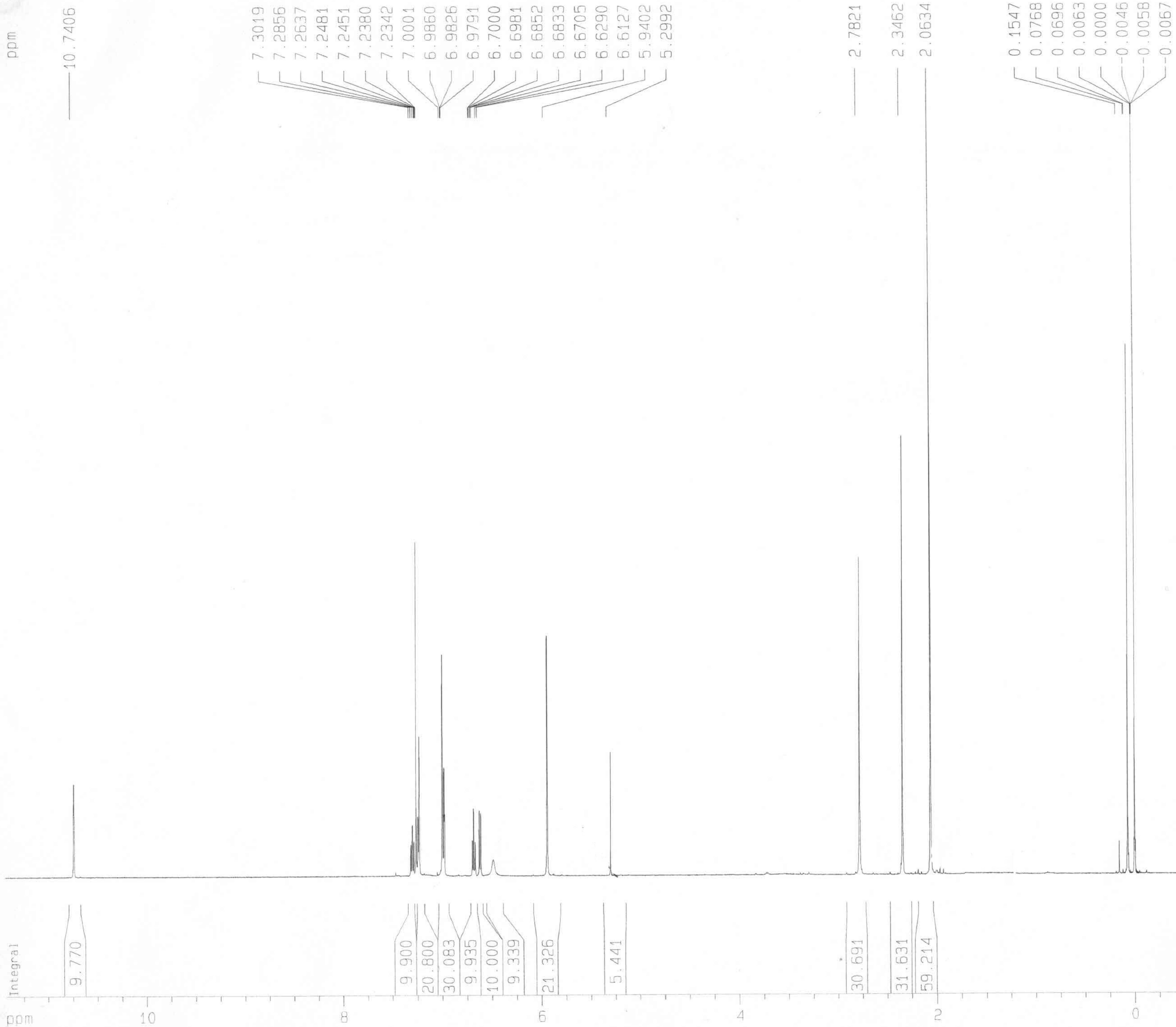
P5, **Figure S5.** The ^1H NMR spectrum of *cis*- $[(\mathbf{1a})_2\text{NiBr}_2]$, **3**

P6, **Figure S6.** The ^1H NMR spectrum of $[(\mathbf{1a})\text{AgBr}]$

P7, **Figure S7.** The ^1H NMR spectrum of $[(\mathbf{1b})\text{AgBr}]$

P8, **Figure S8.** The ^1H NMR spectrum of $[\text{Ag}(\text{PPh}_3)\text{Br}]_4$

周壽 15



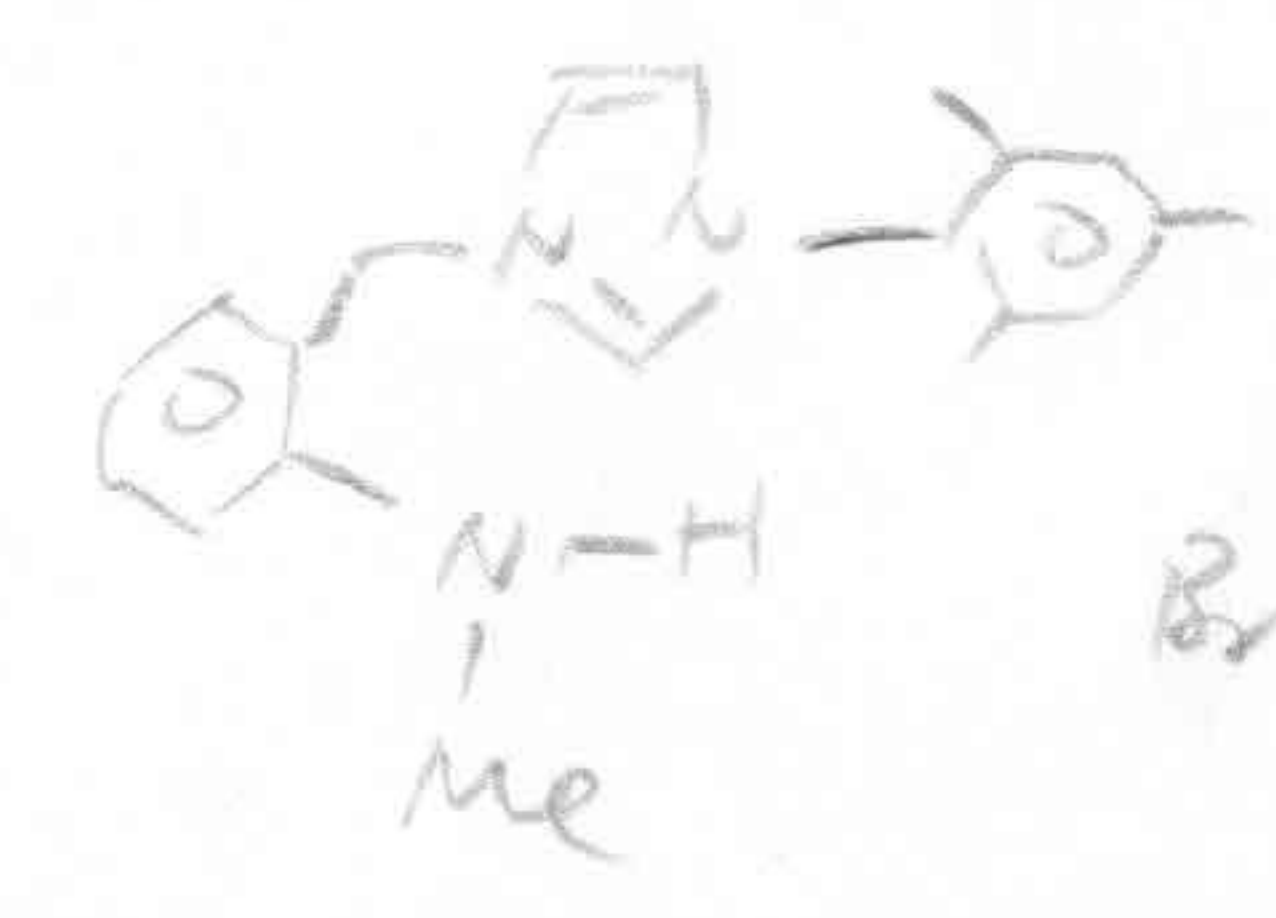
Current Data Parameters
 NAME servzhousen
 EXPNO 17
 PROCNO 1

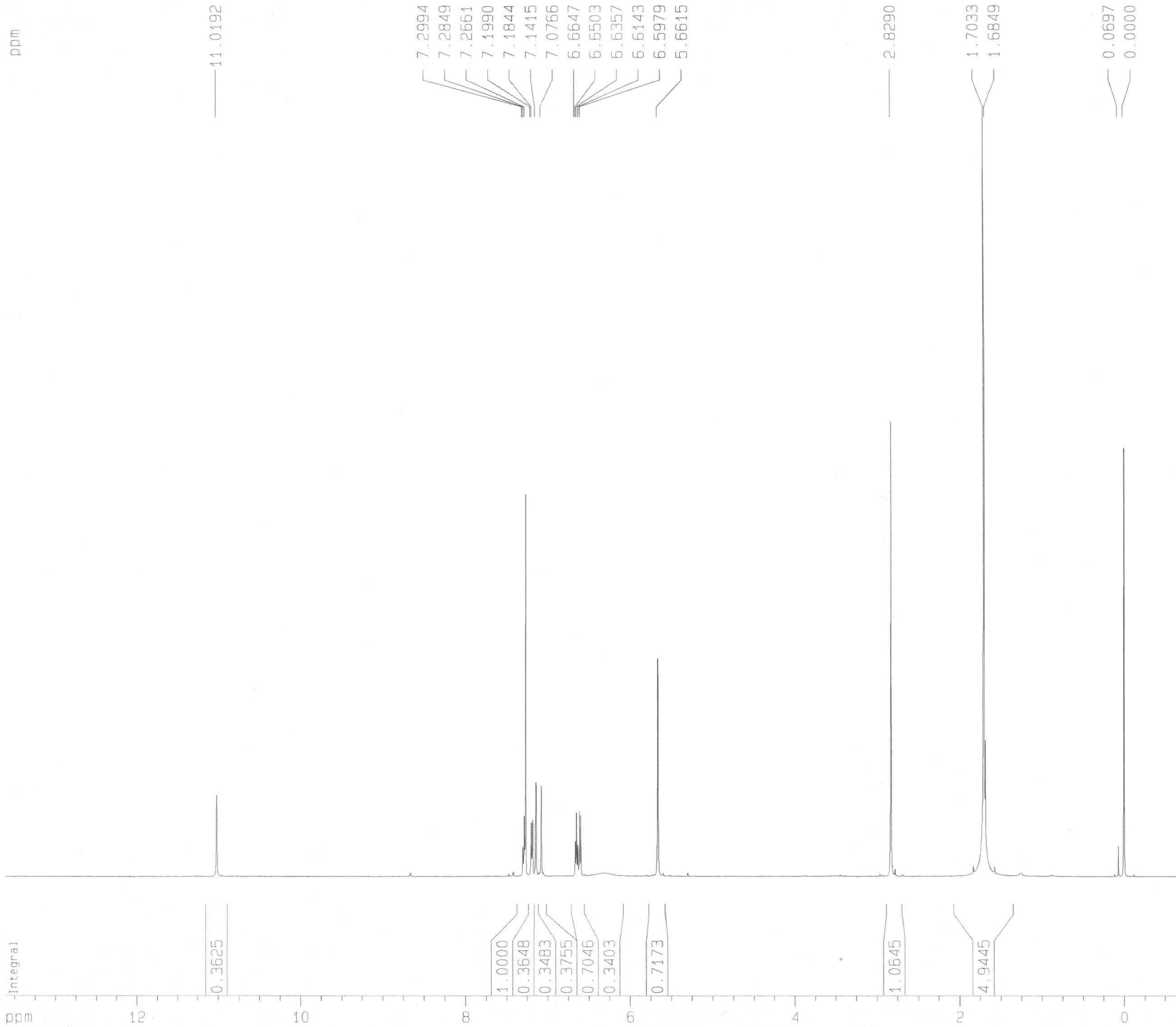
F2 - Acquisition Parameters
 Date_ 20100611
 Time 10.51
 INSTRUM dmx500
 PROBHD 5 mm GNP 1H/13
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 8503.401 Hz
 FIDRES 0.259503 Hz
 AQ 1.9268672 sec
 RG 1024
 DW 58.800 usec
 DE 6.00 usec
 TE 0.0 K
 D1 6.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PL1 3.00 dB
 SF01 500.1337409 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300121 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 22.00 cm
 CY 17.72 cm
 F1P 11.440 ppm
 F1 5721.44 Hz
 F2P -0.472 ppm
 F2 -236.24 Hz
 PPMCM 0.54147 ppm/cm
 HZCM 270.80344 Hz/cm





Current Data Parameters
 NAME servzhausen
 EXPNO 10
 PROCNO 1

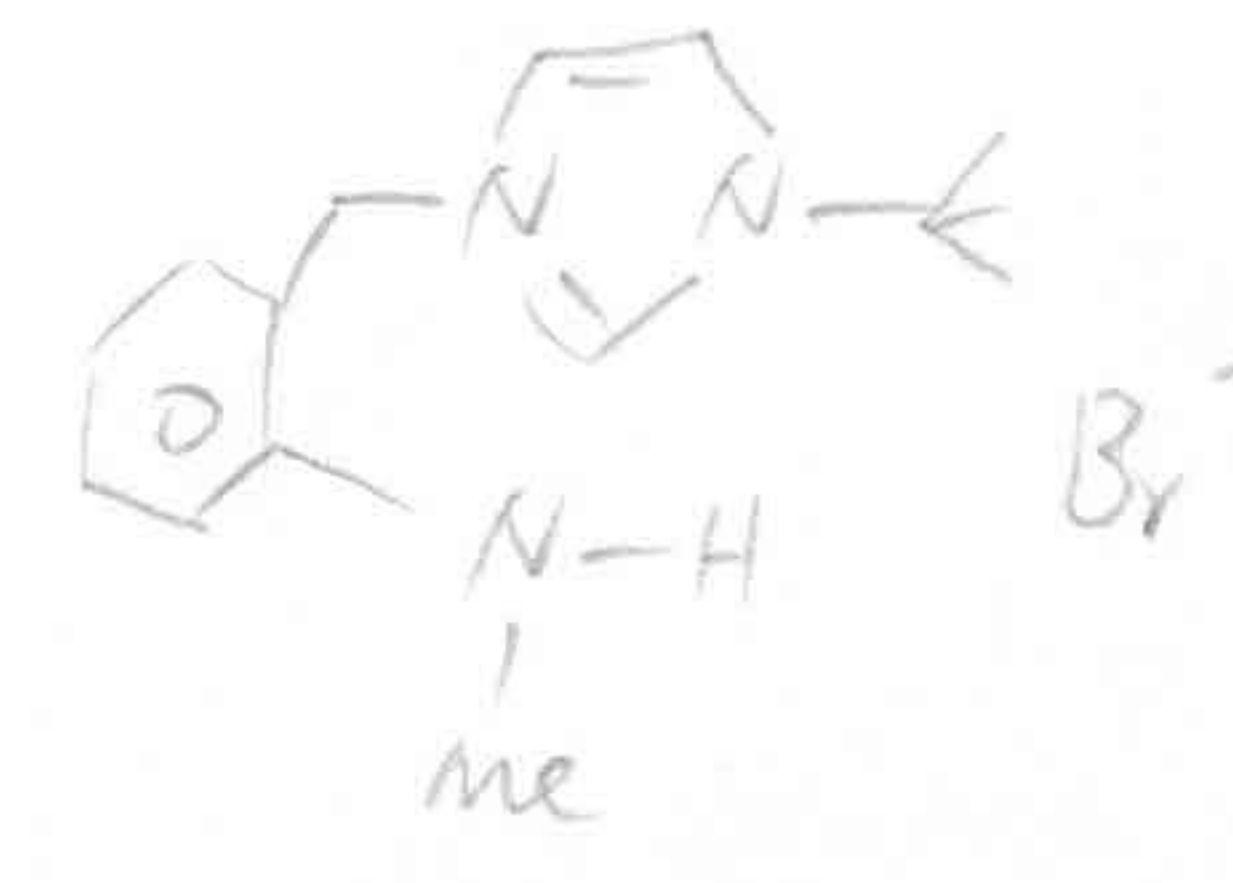
F2 - Acquisition Parameters
 Date_ 20100601
 Time 11.21
 INSTRUM dmx500
 PROBHD 5 mm GNP 1H/13
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8503.401 Hz
 FIDRES 0.259503 Hz
 AQ 1.9268672 sec
 RG 1024
 DW 58.800 usec
 DE 6.00 usec
 TE 0.0 K
 D1 6.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PL1 3.00 dB
 SF01 500.1337409 MHz

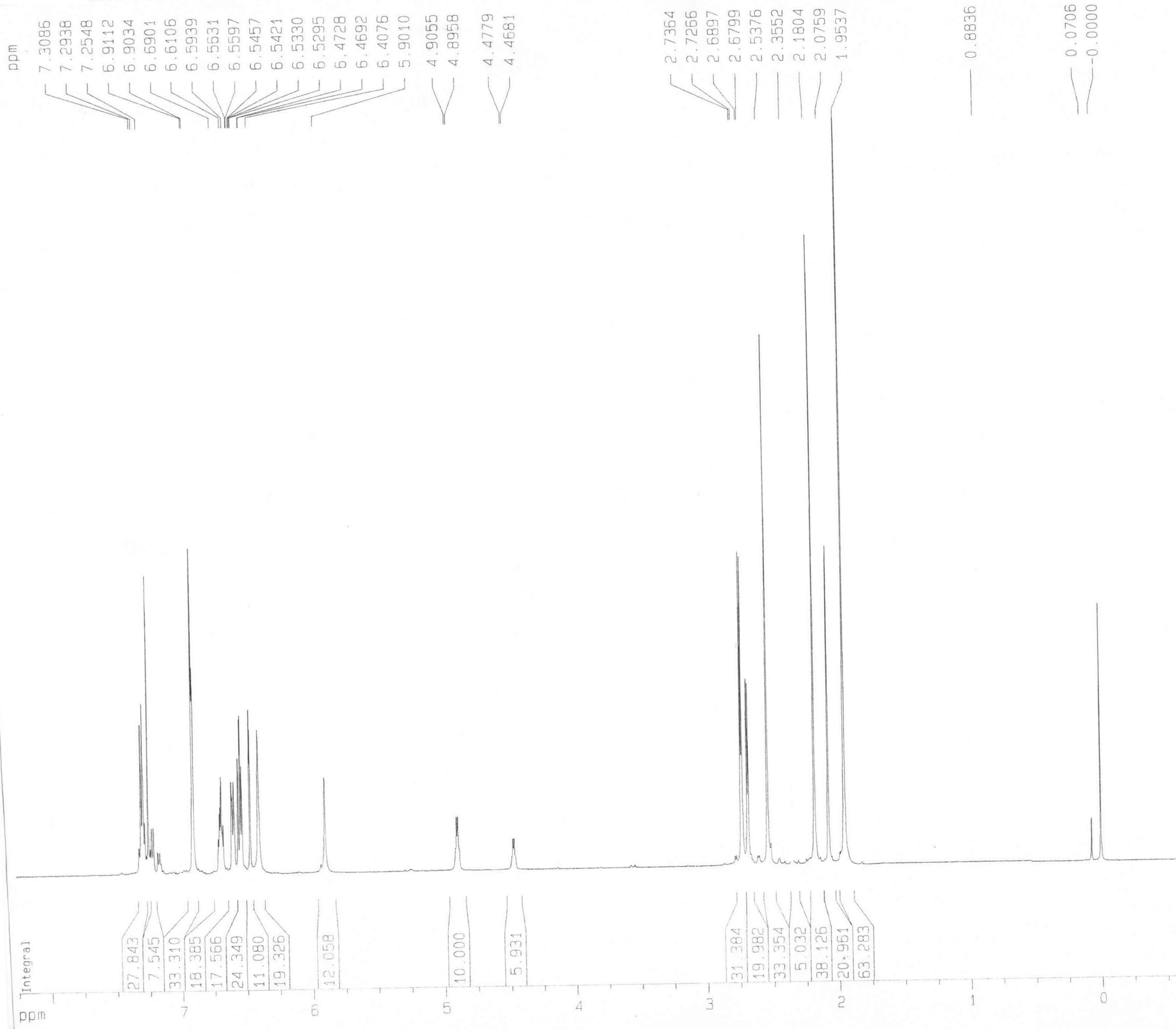
F2 - Processing parameters
 SI 32768
 SF 500.1300110 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 22.00 cm
 CY 29.27 cm
 F1P 13.614 ppm
 F1 6808.75 Hz
 F2P -0.703 ppm
 F2 -351.51 Hz
 PPMCM 0.65076 ppm/cm
 HZCM 325.46640 Hz/cm

10



周壽 1103



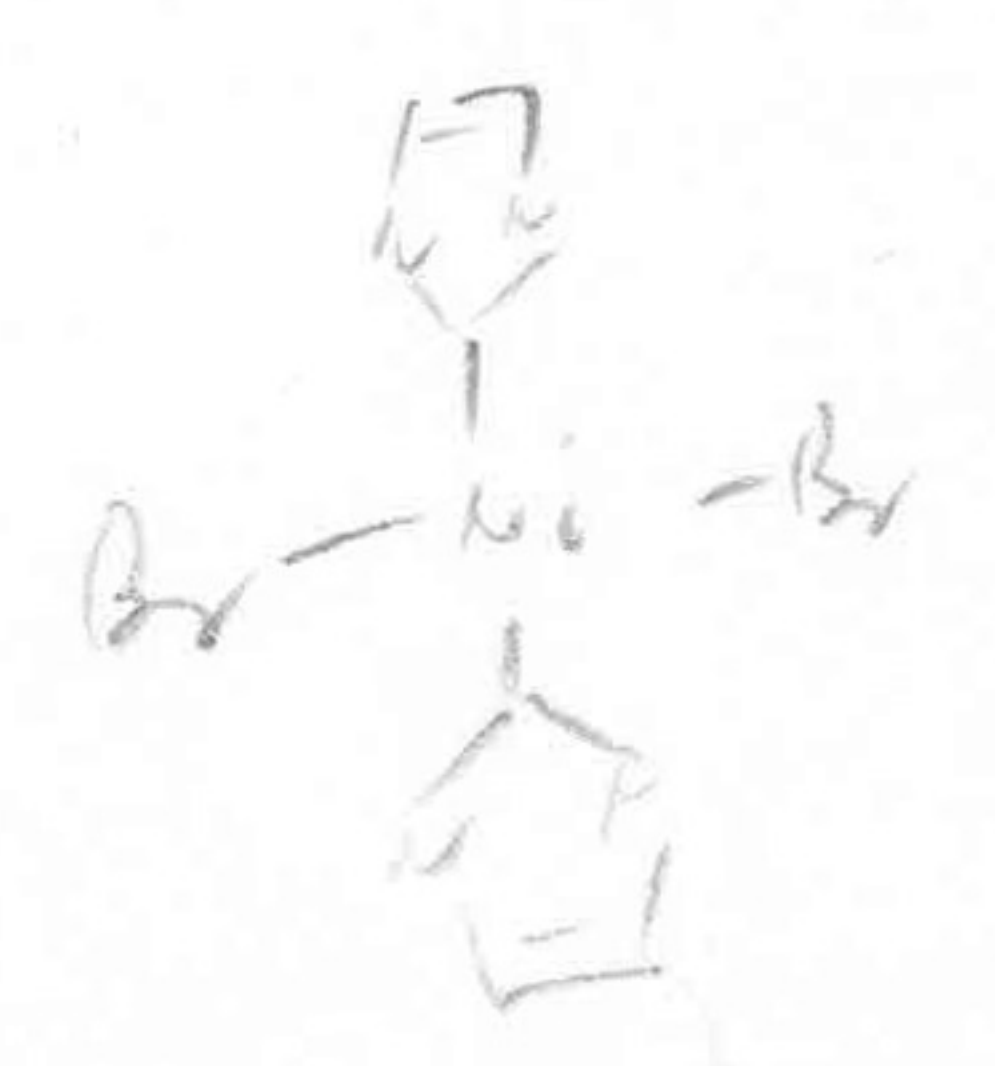
Current Data Parameters
NAME servzhausen
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110302
Time 16.36
INSTRUM dmx500
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 8503.401 Hz
FIDRES 0.259503 Hz
AQ 1.9268672 sec
RG 128
DW 58.800 usec
DE 6.00 usec
TE 0.0 K
D1 6.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

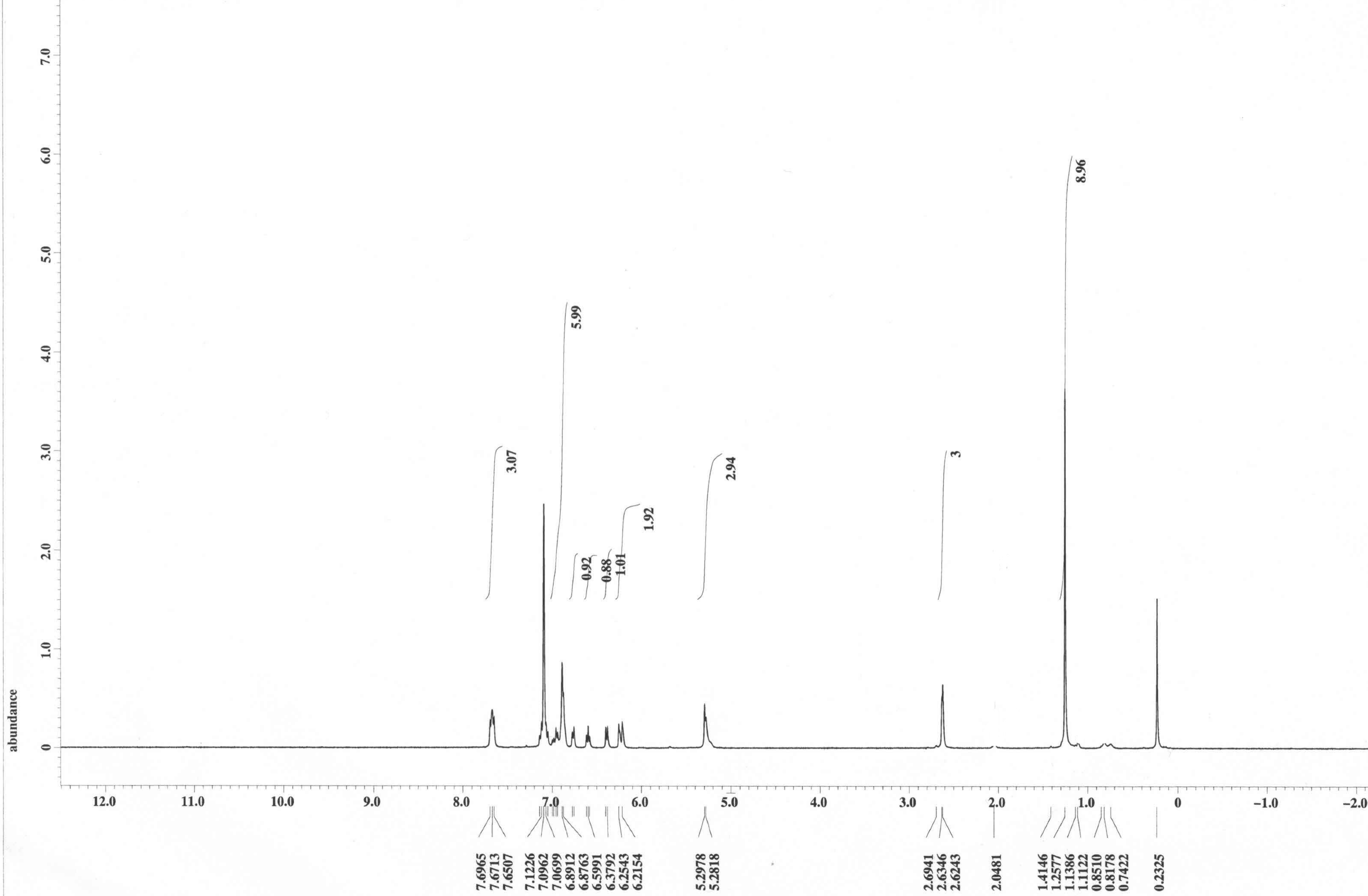
==== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 3.00 dB
SF01 500.1337409 MHz

F2 - Processing parameters
SI 32768
SF 500.1300166 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 3.00

1D NMR plot parameters
CX 22.00 cm
CY 21.34 cm
F1P 8.264 ppm
F1 4133.24 Hz
F2P -0.563 ppm
F2 -281.33 Hz
PPMCM 0.40122 ppm/cm
HZCM 200.66211 Hz/cm



20120728-zhang-02-H-4.jdf
liyinke/20120728-zhang-02-H



X : parts per Million : 1H

Proton Standard



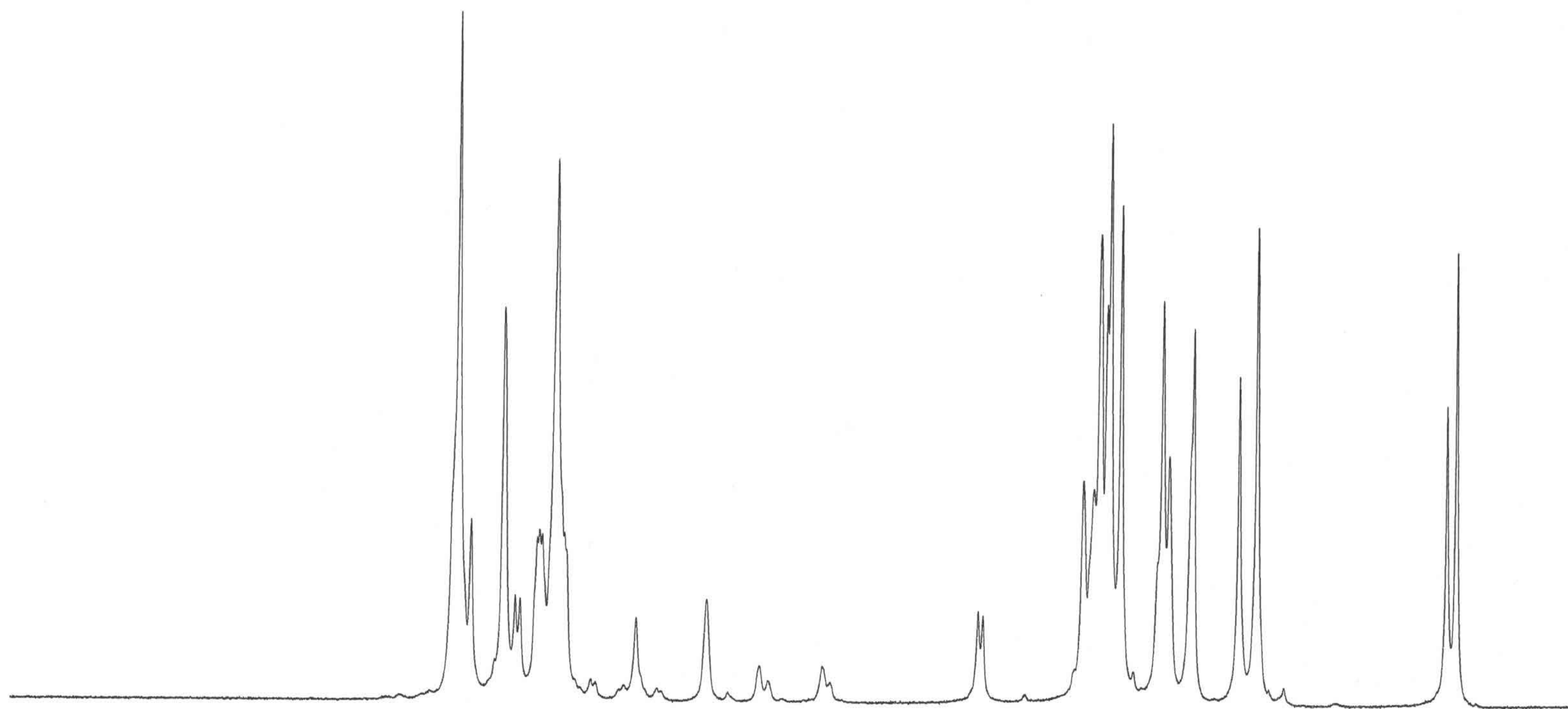
7.263
7.172
6.933
6.851
6.816
6.675
6.550
5.970
5.457
5.074
4.614
3.479
3.444
2.717
2.597
2.548
2.523
2.445
2.139
2.092
1.917
1.585
1.456
0.073
0.003

Current Data Parameters
NAME liyinle
EXPNO 2013013101
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130131
Time_ 9.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 51.14
DW 78.200 usec
DE 6.50 usec
TE 293.4 K
D1 6.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W

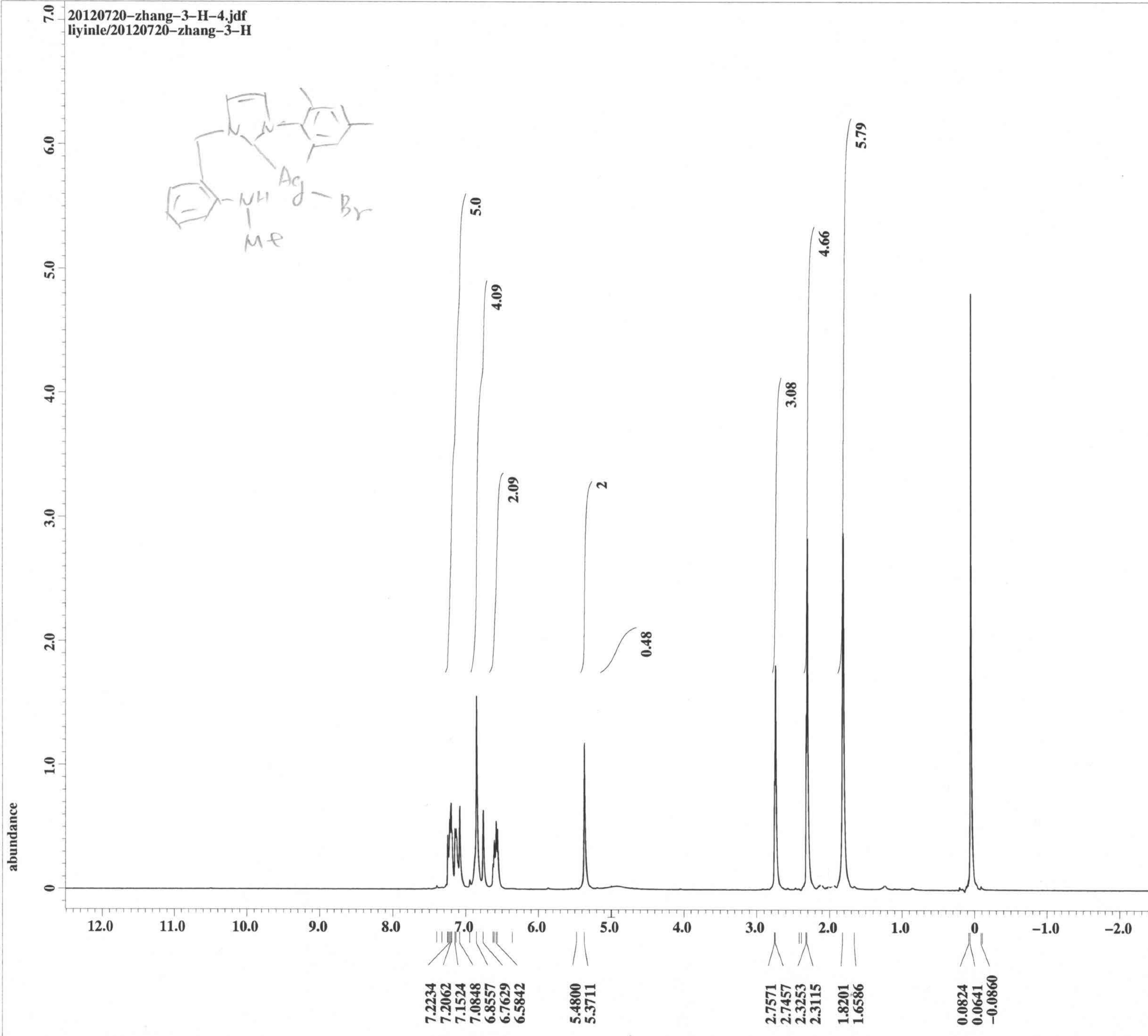
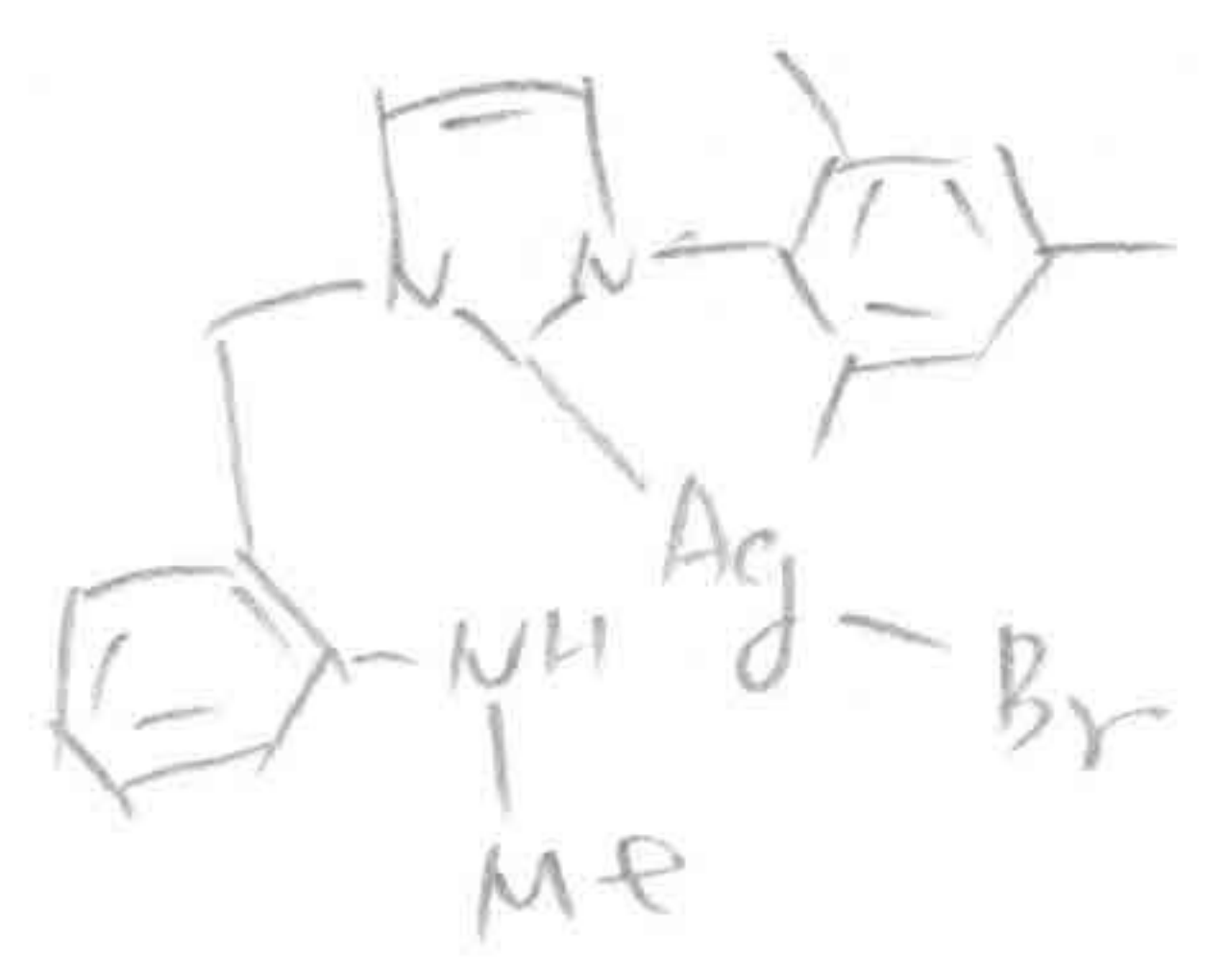
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00



10 9 8 7 6 5 4 3 2 1 0 ppm

7.45
4.26
9.28
0.92
0.95
0.45
0.47
1.00
14.41
4.86
2.98
5.00

20120720-zhang-3-H-4.jdf
liylnle/20120720-zhang-3-H



X : parts per Million : 1H



----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sexp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 ppm

Derived from: 20120720-zhang-3-H-1.jdf

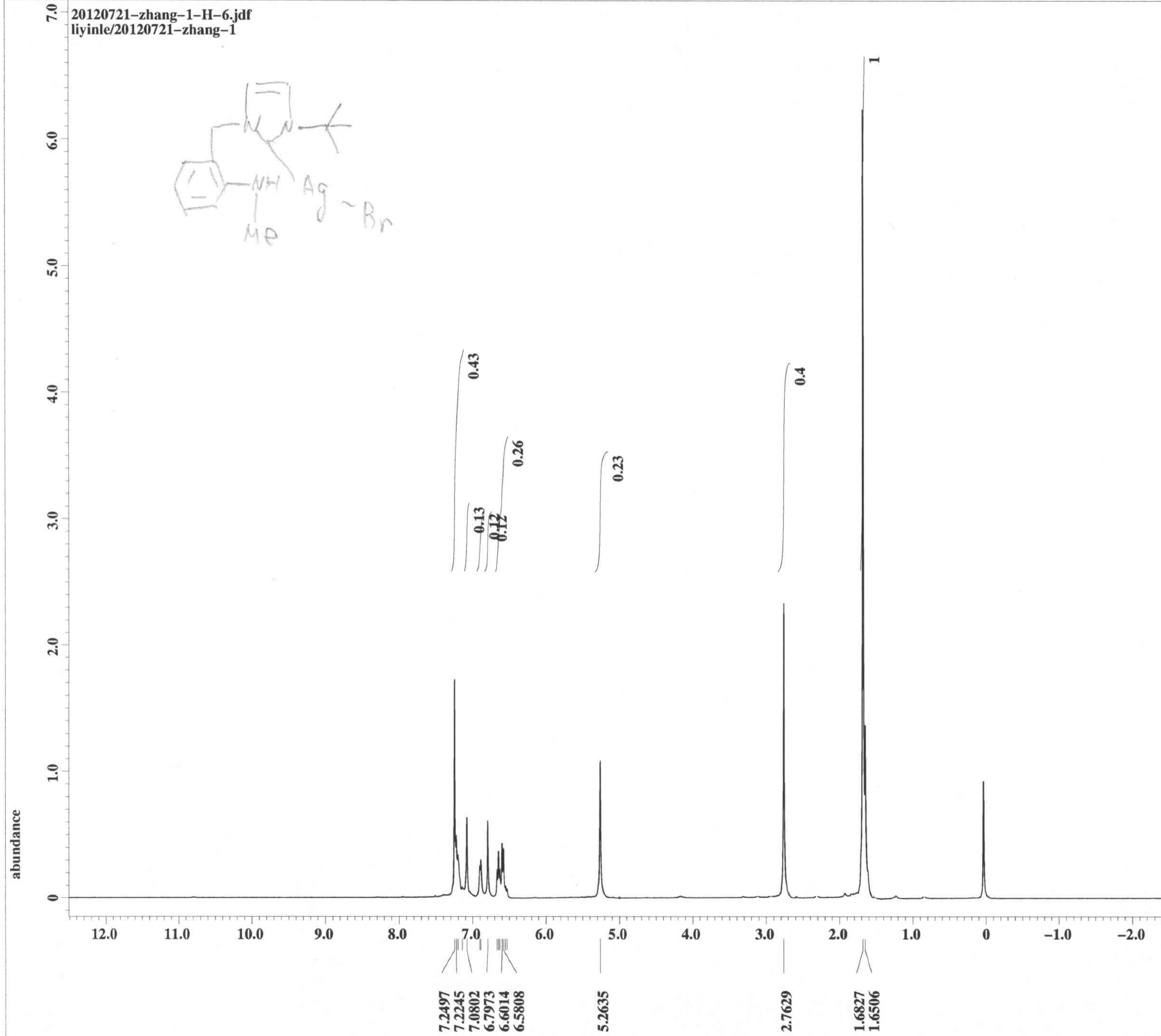
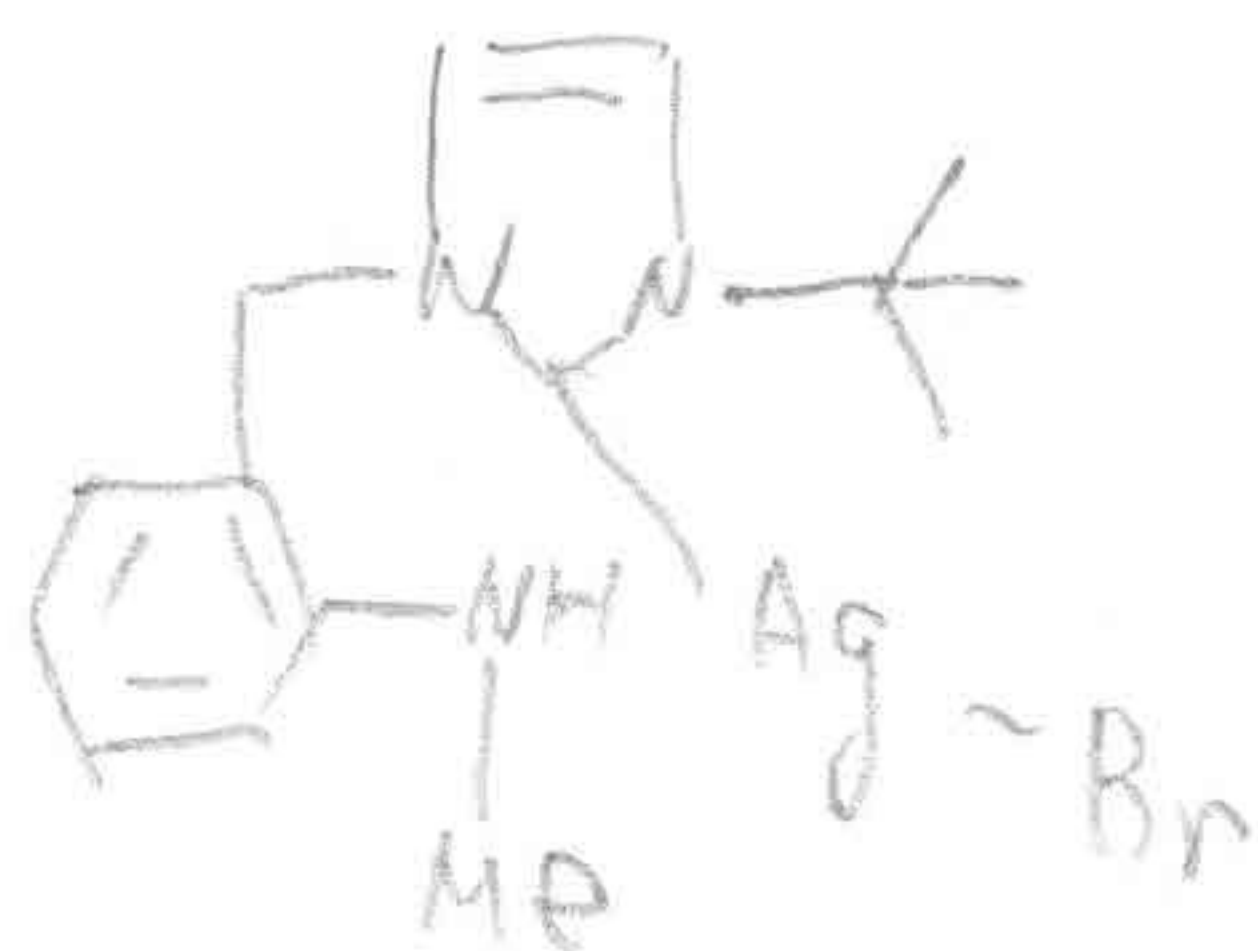
Filename = 20120720-zhang-3-H-4.
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = liylnle/20120720-zhan
 Solvent = CHLOROFORM-D
 Creation_time = 20-JUL-2012 15:00:30
 Revision_time = 20-JUL-2012 15:24:36
 Current_time = 20-JUL-2012 15:28:44

Comment = liylnle/20120720-zhan
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA400
 Spectrometer = DELTA2_NMR

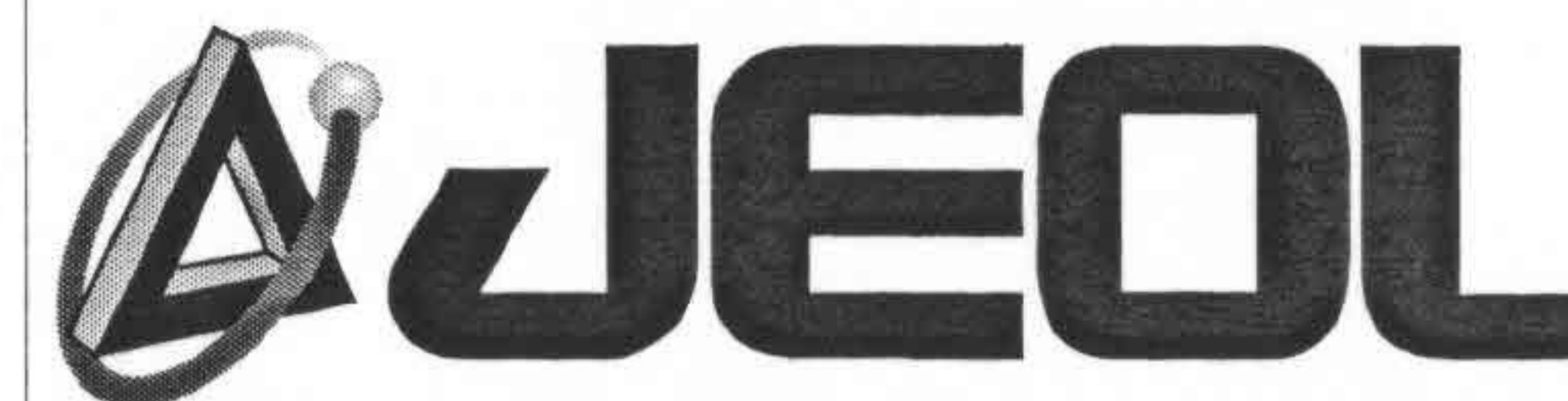
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 2.18365952[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685[Hz]
 X_sweep = 7.5030012[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 10.6[us]
 X_acq_time = 2.18365952[s]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.3[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 7.18365952[s]
 Temp_get = 23.7[dc]

20120721-zhang-1-H-6.jdf
liyine/20120721-zhang-1



X : parts per Million : 1H



---- PROCESSING PARAMETERS ----

dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
ppm

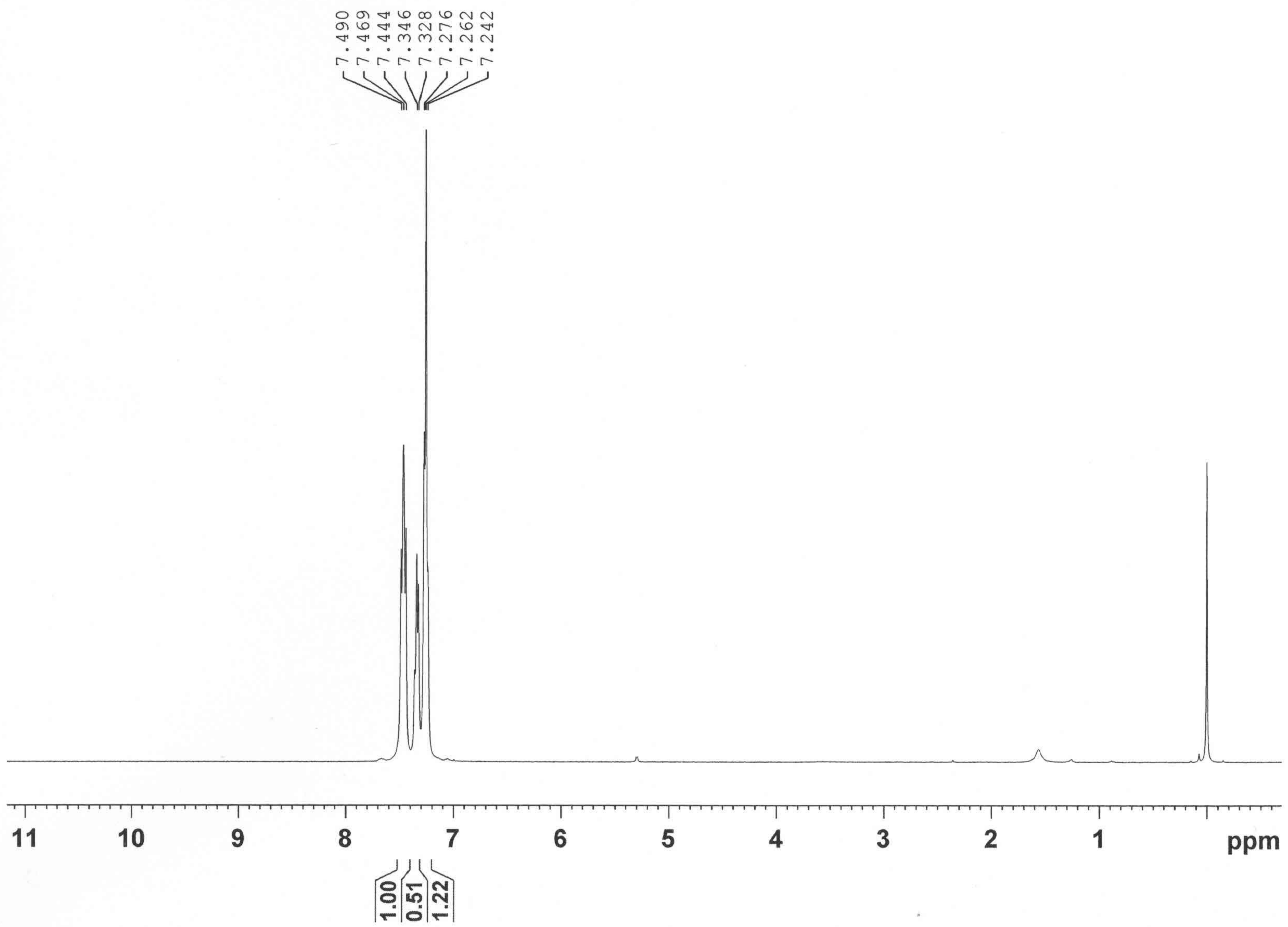
Filename = 20120721-zhang-1-H-6.
Author = delta
Experiment = single_pulse.ex2
Sample_id = liyine/20120721-zhan
Solvent = CHLOROFORM-D
Creation_time = 21-JUL-2012 12:58:08
Revision_time = 25-JUL-2012 11:02:46
Current_time = 25-JUL-2012 11:02:57

Comment = liyine/20120721-zhan
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.6[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 4.5[dB]
X_pulse = 5.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get = 23.9[dc]

Proton Standard



Current Data Parameters
NAME liyinle
EXPNO 2013013105
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130131
Time_ 11.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 51.14
DW 78.200 usec
DE 6.50 usec
TE 294.0 K
D1 6.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W

F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00