

Iron-Catalyzed Cross-Coupling of Imidoyl Chlorides with Grignard Reagents

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SUPPORTING INFORMATION

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¹³ C NMR	S16-S38
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Supporting information file three (this file)

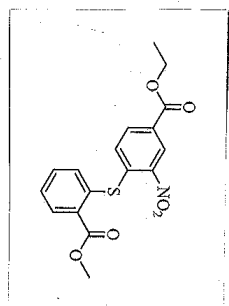
¹ H NMR	S39-S61
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235j18p1
STANDARD 1H OSSERVE

Automation directory: /export/home/robot/auto/auto_30_06_05
File : 235j18p102

Pulse Sequence: s2pul
Solvent: cdcl3
Temp: 28.0 C / 303.1 K
Samp: 235j18p101
File: 235j18p101
Mercury-40088 "hmr"

Relax. delay: 1.000 sec
Pulse: 45.0 degrees
Acq. time: 4.300 sec
Aldn: 8402.0 Hz
R: 8
OSSERVE: H1 400.4405123 MHz
DATA PROCESSING
FT size: 65536
Total time: 0 min, 50 sec



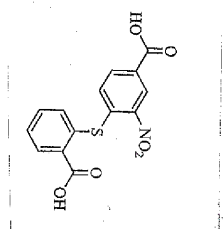
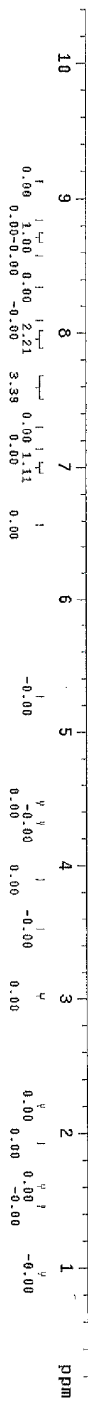
2351191
STANDARD 1H OBSERVE

expl s2pul

```

SAMPLE 4 2005 temp SPECIAL 30.0
date JUN 02 2005 gain not used
solvent CD3OD nom gain 0.020
file export/home/ not used
f2/rf 298.1408 14.100
t1 0.0765/2351191P101- pw90
0.0765/2351191P101- pw90
ACQUISITION 0.0765 14.100
INSTRUMENT spect
PROBHD 13C/1H QNP
NUC1 13C 8 sp 7.8740
NUC2 1H 4 7.844
AT 0.4158 7.816
FB not used 7.795
NS 1.000 7.762
DECOUPLER 13C 7.850
CT TRANSMITTER 8 7.832
UH 400.444 7.828
SFO 333.3 FP 7.826
TPO 58 7.822
PW 7.050 7.816
DECOUPLER C13 SC PLOT 20 7.814
dm 0 vs 11.22 7.810
dof 0 th 7.803
dms 4 c 15.72 7.801
dm 13500 at 7.597
 7.593
 7.590
 7.015
 6.993

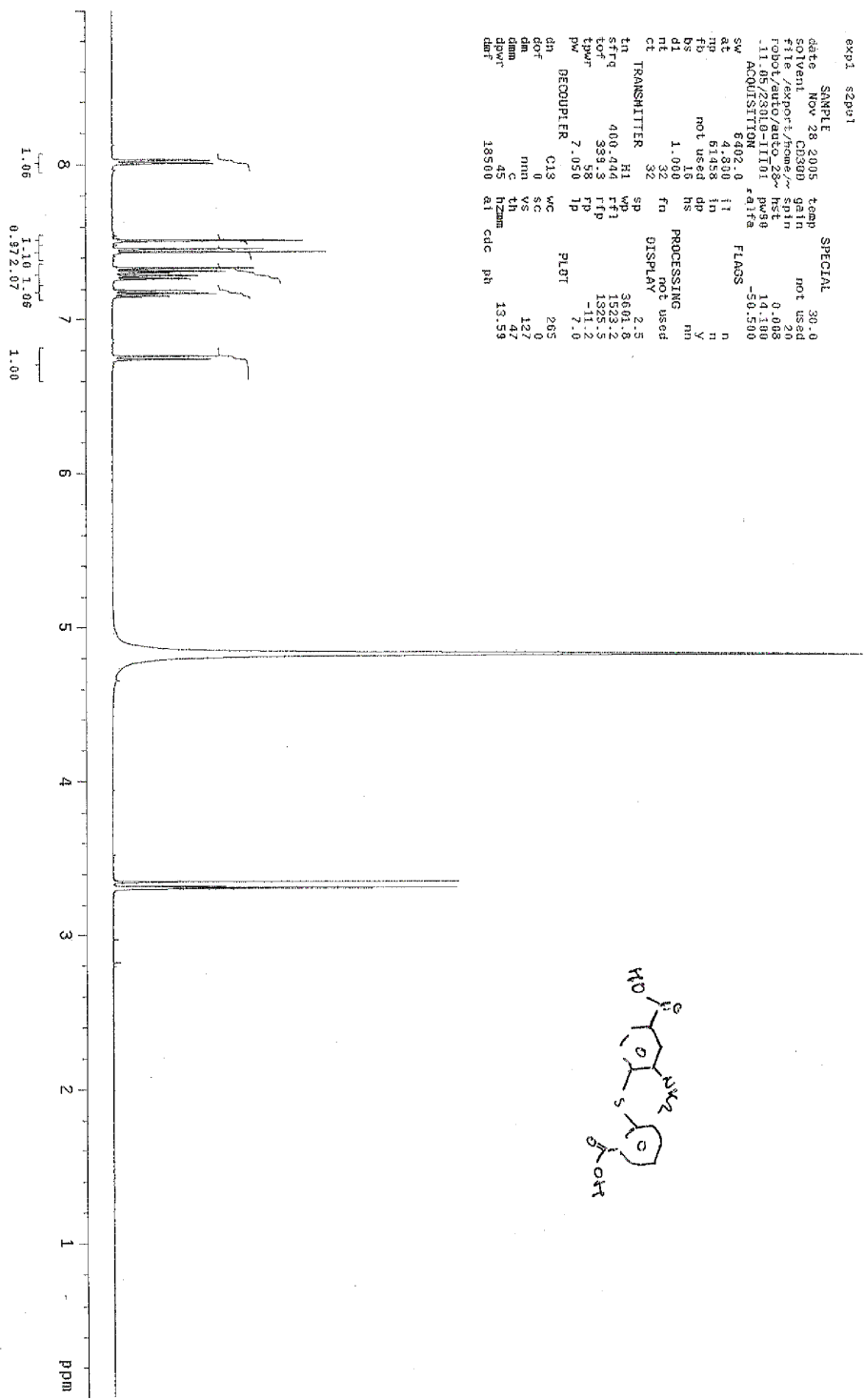
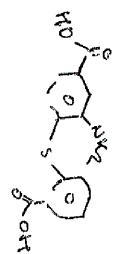
```



2301G-III
STANDARD 1H OBSERVE

exp1 s2prt1

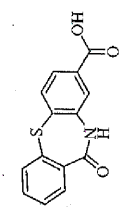
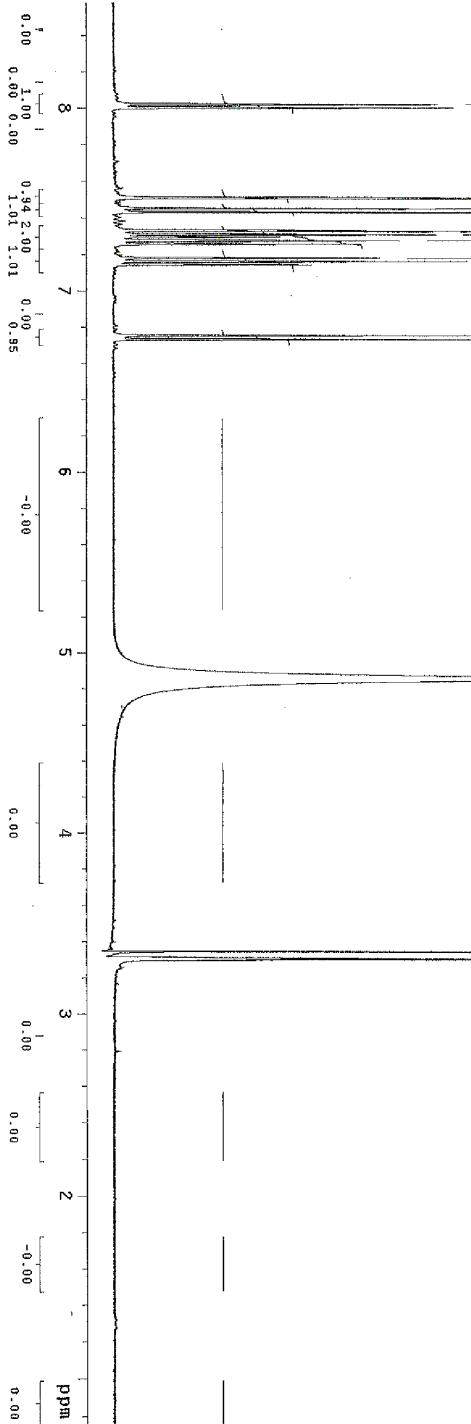
date	Nov 28 2005	temp	30.0	SPECIAL
solvent	Nov 28 2005	gain	not used	
robot	400/400/22	ns1	0.008	
acq	-11.05/2301G-III01	pw98	14.180	
sw	ACQUISITION	faifs	-50.500	
ac	6402.0	f1		
bc	81.000	in		
bs	not used	dp		
d1	1.080	ls	hs	PROCESSING
cl	32	fn	not used	DISP
ct	TRANSMITTER	sp	2.5	
tn	H1	wp	3601.6	
sfreq	400.444	rf1	1523.2	
tor	339.3	rfp	1523.5	
tpwr	2.000	tp	-11.2	
pw	7.000	tp	7.0	
de	DECOUPLER	C13	wc	PLBT
dn	0	sc	265	
dof	0	vs	127	
dm	nm	vs	127	
dmu	45	nm	13.54	
dmr	18500	at	calc	ph



235J1200F 1H OBSERVE
STANDARD 1H OBSERVE

expt s2pnt1

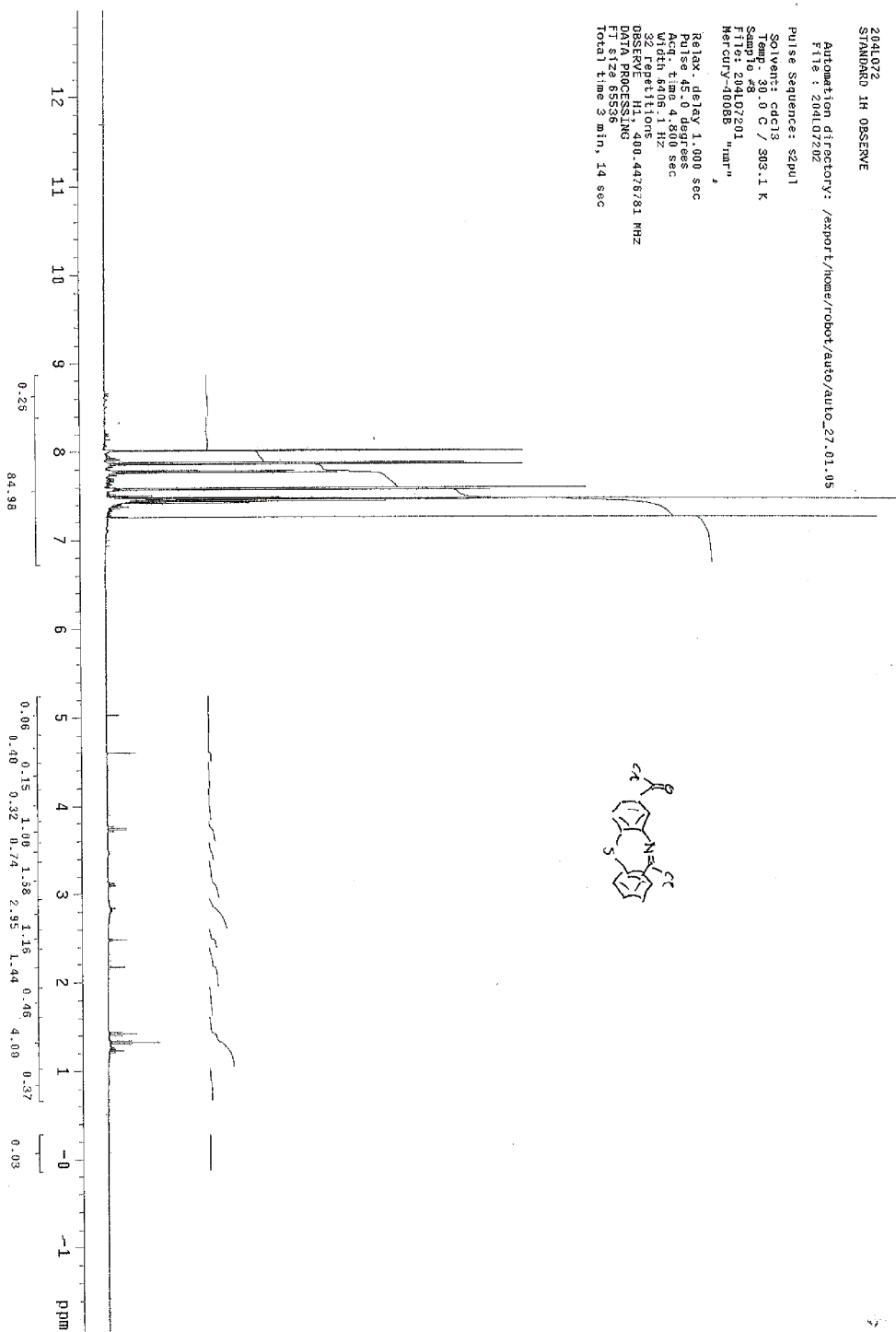
SAMPLE SPECIAL 30.0
date jul 5 2005 temp not used
solvent CD3OD gain 20
file /export/home/~ not used
robot/auto/auto_05-hst 0.008
.07.05/235J1200F 1H 235J1200F
ACQUISITION 1.000 6402.8 0.25 2.50 50.500
SOLVENT 6402.8 0.25 2.50 50.500
sw 6402.8 0.25 2.50 50.500
at 4.805 1.70 7.7 80.7 92.8
np 81538 160 80.7 92.8
hs 16 not used 80.7 92.8
d1 1.000 1.000 80.7 92.8
nl 8 80.7 92.8
nt 8 80.7 92.8
CE TRANSMITTER 8 300 80.7 92.8
in 12.0 1.00 40.5 798.2
strq 12.0 1.00 40.5 798.2
lof 338.3 1.00 40.5 798.2
lpuw 9 7.000 285 0
pw 7.000 285 0
dn decoder C13 SC 0
dof 0 48 0
dm 0 48 0
sm 12mm vdc 11.84
dwr 45 18500
dnf 18500



2041.072
STANDARD IH OBSERVE

Automation directory: /export/home/robot/auto/auto_27.01.05
File : 2041.07202

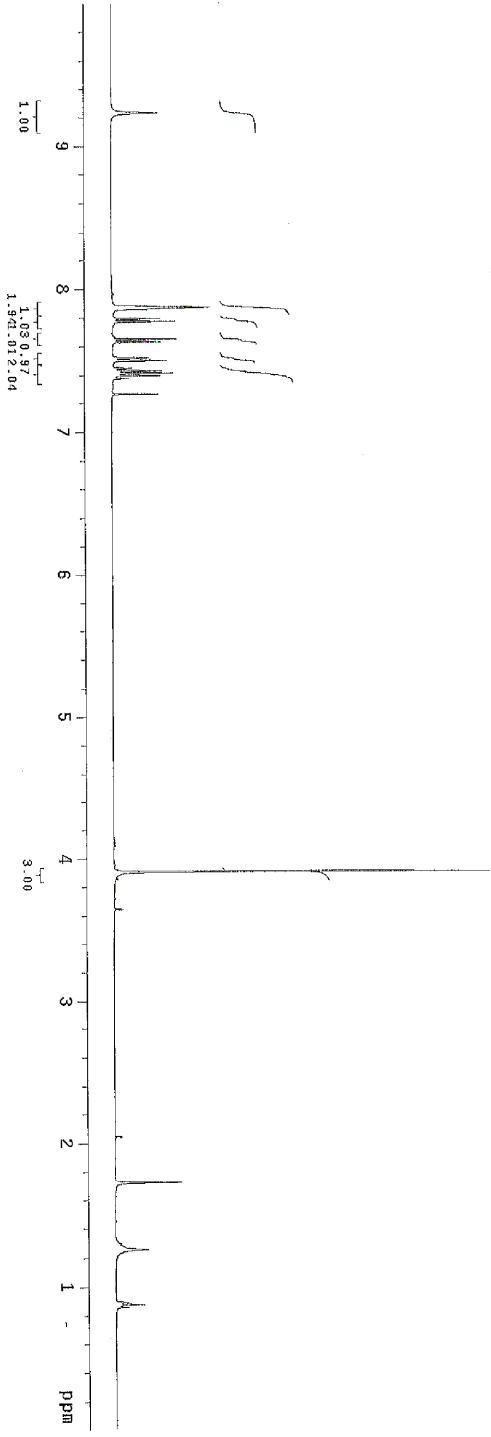
Pulse Sequence: s2pu1
Solvent: cdcl3
Temp: 30.0 C / 303.1 K
Sample #9
File: 2041.07201
Name: 910058 "nmr"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.800 sec
Width 6406.1 Hz
S2 Repeat time 0.004476781 MHz
Observed 111.11111111111111
DATA PROCESSING
FT size 65538
Total time 3 min, 14 sec



2311039
STANDARD IN OBSERVE

expi s2pu1

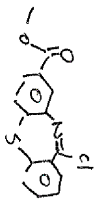
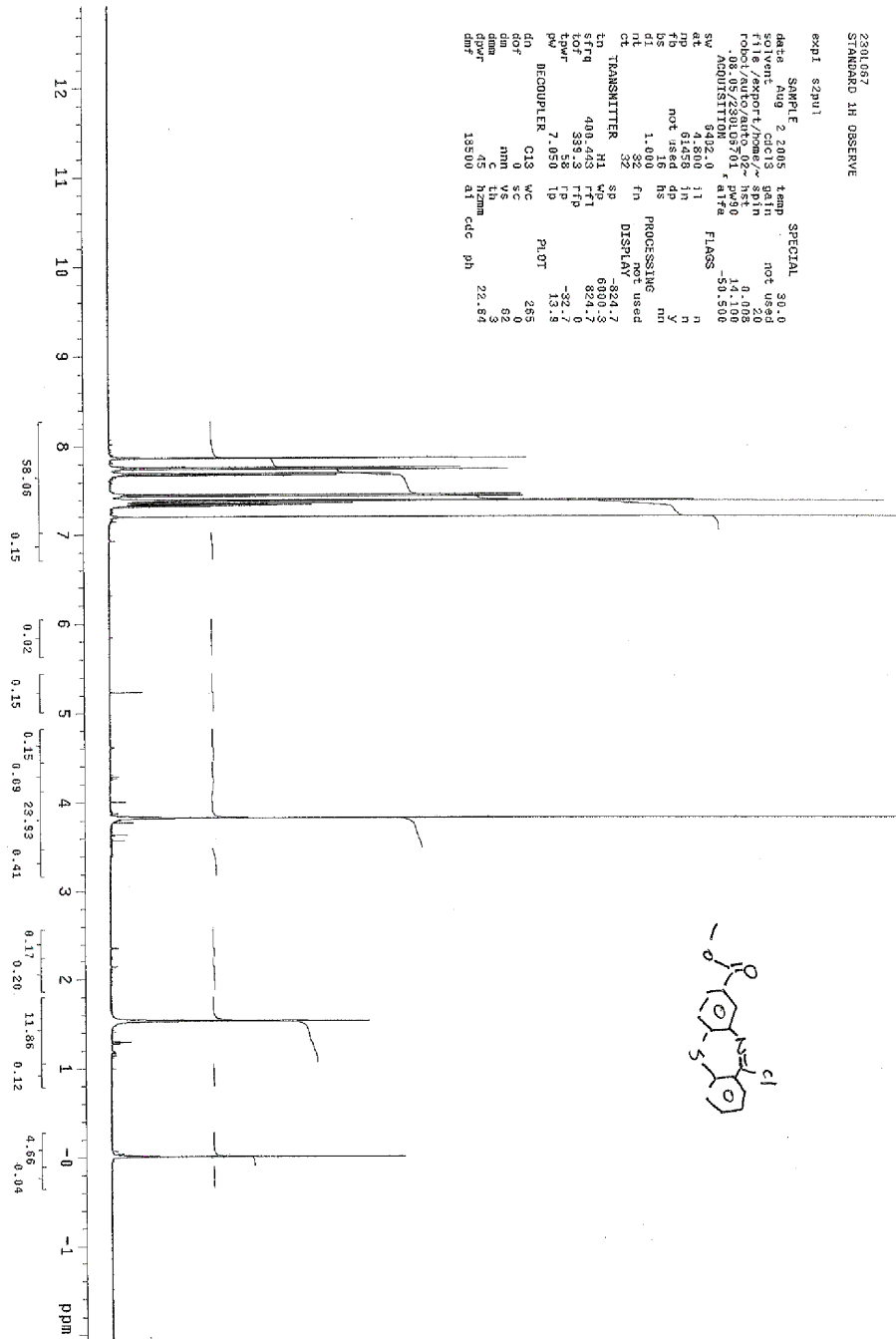
```
SAMPLE 2 2005 temp SPECIAL 30.0  
date Aug 2 2005 gain not used  
solvent cdc13 not used  
file /export/home/~  
robot/auo/auo_02- hst 0.008  
- 5001 f 017a 1.008  
- 50.500  
ACQUISITION 6402.0 017a  
sw 6402.0 11  
at 4.800 11  
np 61438 11  
bs not used 11  
di 1.000 11  
nt 32 11  
ct TRANSMITTER 32 11  
fr not used  
ct DISPLAY 2 1  
fn 3998.4  
in 3203.6  
sfreq 400.443 rfi  
f0r 399.3 rfp 2907.2  
tpur 58 TP -50.9  
pw 7.650 11  
PLOT 265  
dn DECOUPLER C13 WC  
dof 0 SC  
dm 0 SC  
dmn 41  
dpr 45 hzmm  
dprf 18500 ai cdc ph 15.06  
dmf
```



2301057
STANDARD 1H OBSERVE

expi s2pu1

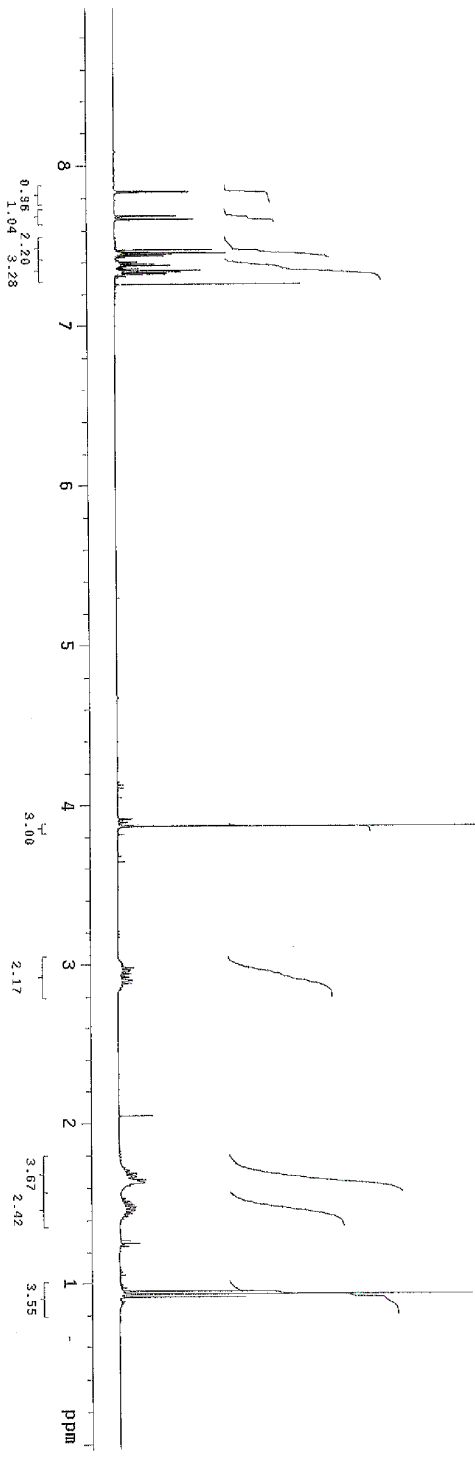
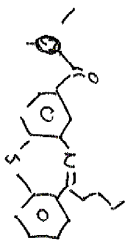
date Aug 2 2005 temp SPECIAL 30.0
solvent cdc13 gain not used
file /export/home/~ spm not used
f2 08.05/230105701 pw90 14.100
ACQUISITION * a1f4 -50.500
SPECIAL FLAGS
sv 3922.0 11 n
ns 61455 in n
fb not used dp y
ds 1.000 ns PROCESSING m
nt 32 fn not used
ct 32 DISPLAY m
td TRANSMITTER H1 SP 824.2
sfreq 400.443 FT1 824.7
lof 339.3 FTp 824.7
tpar 7.050 TP -92.7
pw DECOUPLER C13 WC 265
dn 0 SC 0
dof 0 SC 0
nm 0 SC 0
c th 3
dmm /45 hzmm 22.84
dpr 13500 at cdc ph



2301052
STANDARD 1H OBSERVE

expt s2p01

SAMPLE 21 2005 temp SPECIAL 30.0
date 001 21 2005 cdc13 not used
solvent auto/home/~ sp1n 2.0
file /export/home/~ sp1n 0.008
robot/auto/21~ hst 14.100
-07_05/230105201_ pw90 -50.500
SW ACQUISITION 0.002.0 d178 FLAGS
at 4.800 11 n
np 61456 1n n
fb not used dp y
bs 1.000 1b hs PROCESSING mn
rl 32 fr not used
ct 32 fr DISPLAY
TRANSMITTER M1 SP -12.4
LD M1 W1 398.3
SFR 400.413 738.0
SOT 339.3 17P -27.5
tpwr 58 1P 5.0
pw 7.050 1P
DECOUPLER C13 WC PLOT 265
dd 400.133 1b
dm mmh vs 47
dmm C th 34
dpwr 45 hZmm 13.62
dmf 18300 at cdc ph



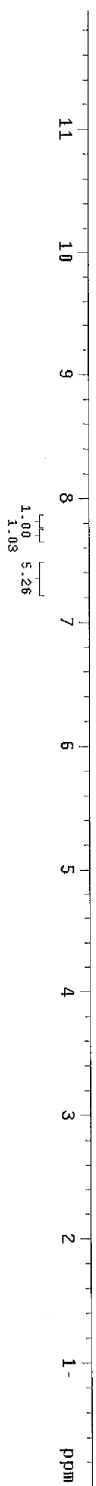
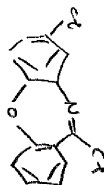
2041017
STANDARD 1H OBSERVE

Archive directory: /export/home/robot/vnmr/sys/data
Sample directory: auto_060ct004

Pulse Sequence: s2pul

Solvent: acetone
File: 204101702
Mercury-400BB "nmr"

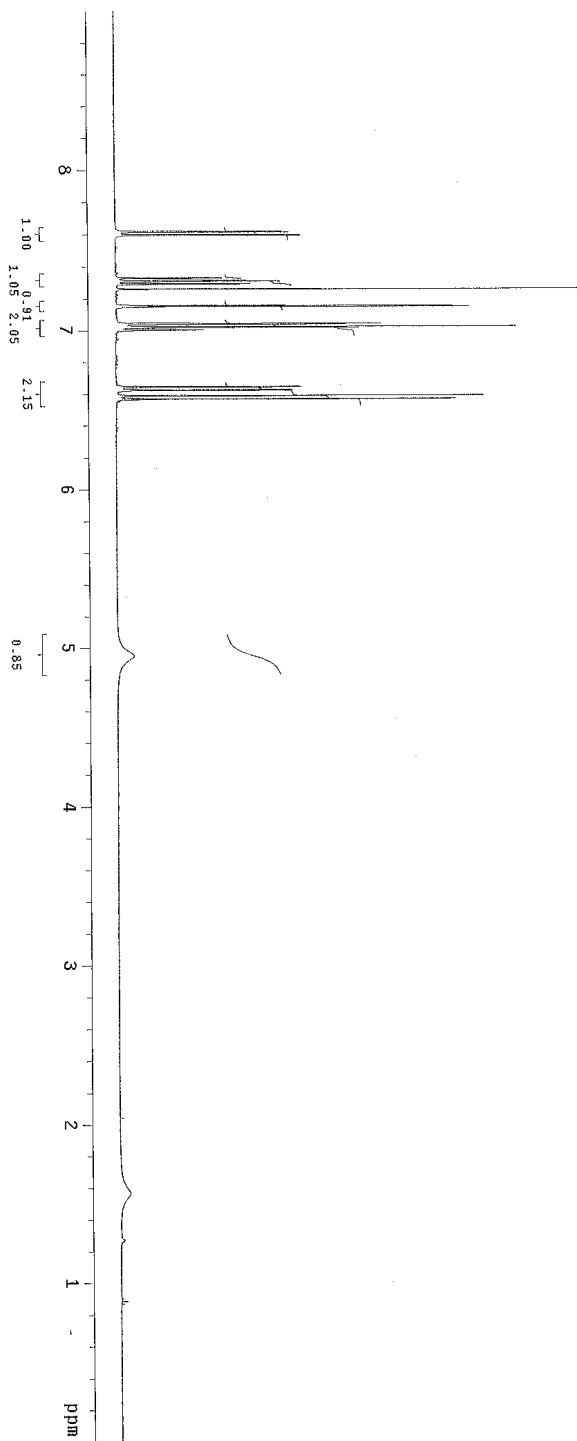
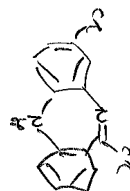
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.800 sec
Width 8406.1 Hz
Sweep rate 400.4497564 MHz
SOLVENT
REPELLIONS
DATA PROCESSING
FI size 65536
Total time 1 min, 37 sec



189J01C1
STANDARD 1H OBSERVE

Archive directory: /export/home/robot/vmr/sys/data
Sample directory: auto_250042304

Pulse Sequence: s2p11
Solvent: CDCl3
Temp: 30.0 C / 303.1 K
File: 189J01C101
Mercury-400BB "nmr"
Relax: delay 1.000 sec
Pulse: 45.0 degrees
Acq: 4.000 sec
Width: 6400.1 Hz
16 Repetitions
OBSERVE: H1, 400.4476780 MHz
DATA PROCESSING
F1 S1 Z50330
Total time 1 min, 37 sec



2301024-I
STANDARD 1H OBSERVE

Automation directory: /export/home/robot/auto/auto_09_08_05
File : 2301024-I02

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 30.0 C / 303.1 K

File: 2301024-I01

Mercury-40088 "mmr"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 4.800 sec

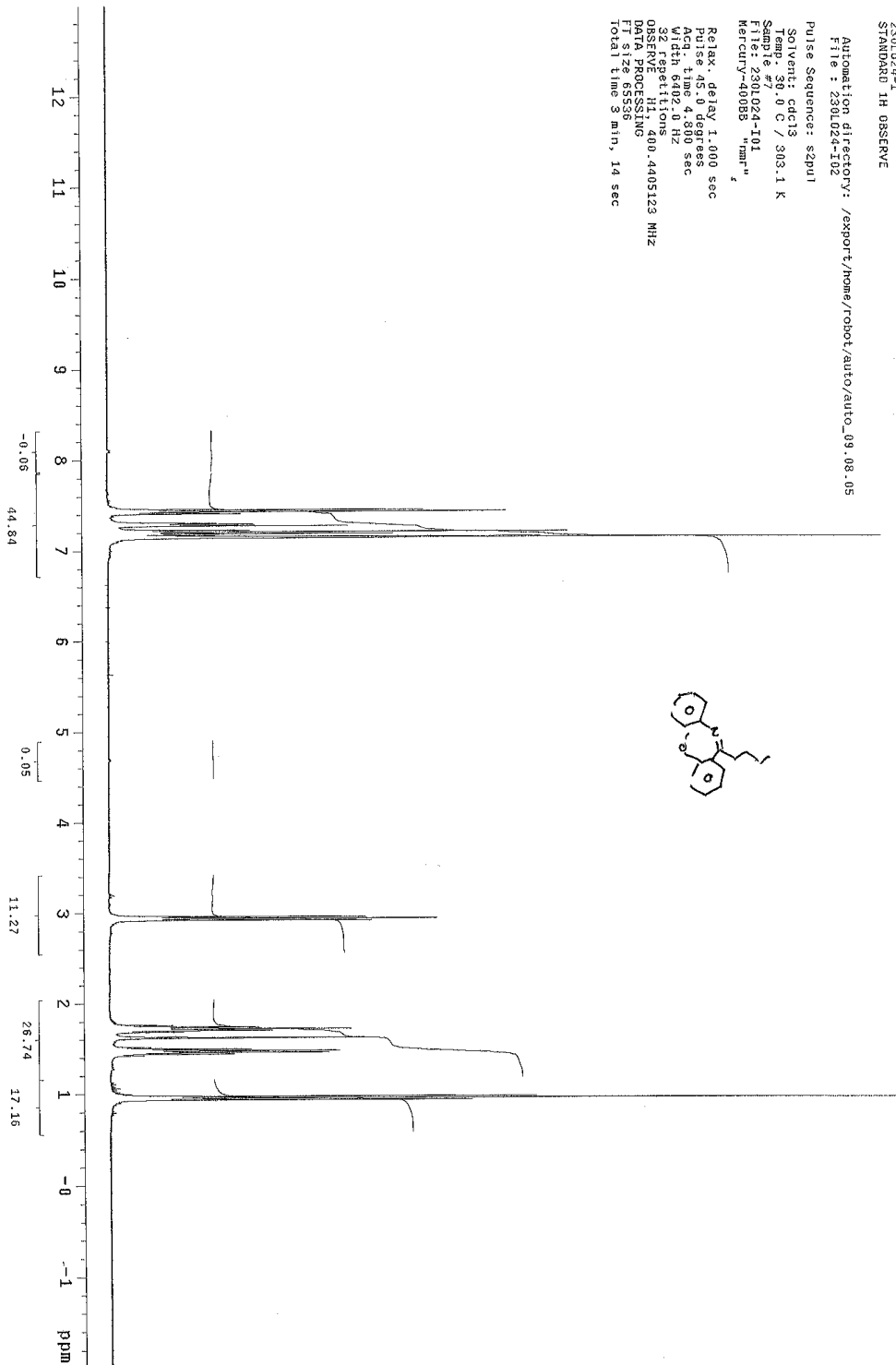
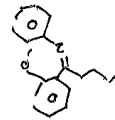
Width 6402.0 Hz

Observed 400.4405123 MHz

DATA PROCESSING

FI size 65536

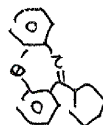
Total time 3 min, 14 sec



230U024-T1
STANDARD 1H OSSEWE

Automation directory: /export/home/robot/autg/autc_10.05.05
File: 230U024-T102

Pulse sequence: szpml
Solvent: cdcl3
Temp: 30.0 C / 303.1 K
Sample #4
File: 230U024-T101
Molecule: 40089 nmf
Pulse delay: 1.000 sec
Pulse: 45.0 degrees
Acq. time: 1.500 sec
Width: 6402.0 Hz
82 repetitions
DDEK: RPOC23100.4405125 MHz
DDEK: RPOC23100.4405125 MHz
FI size: 65536
Total time: 3 min, 14 sec



2301024-111
STANDARD 1H OBSERVE

Automation directory: /export/home/robot/auto/auto_09_08_05

File : 2301024-11102

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp: 30.0 C / 303.1 K

Sample #9

File: 2301024-11101

Mercury-40086 "mm"

Relax. delay: 1.000 sec

Acq. time: 4.380 sec

Width: 6002.0 Hz

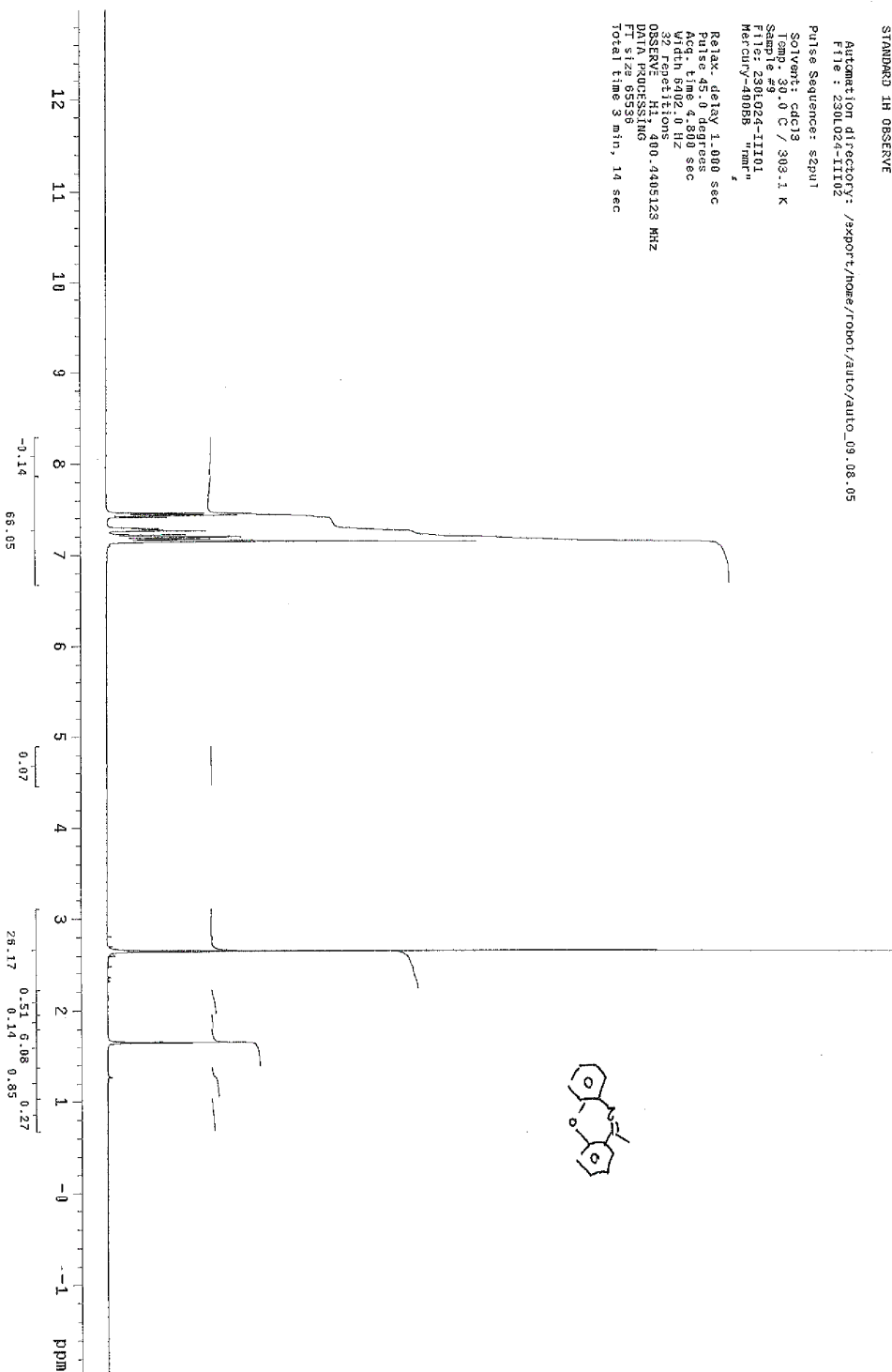
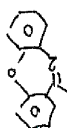
32 Repetitions

OBSERVE: H1, 400.4405123 MHz

PROB: zgpg30

File: 2301024-11101

Total time: 8 min, 14 sec

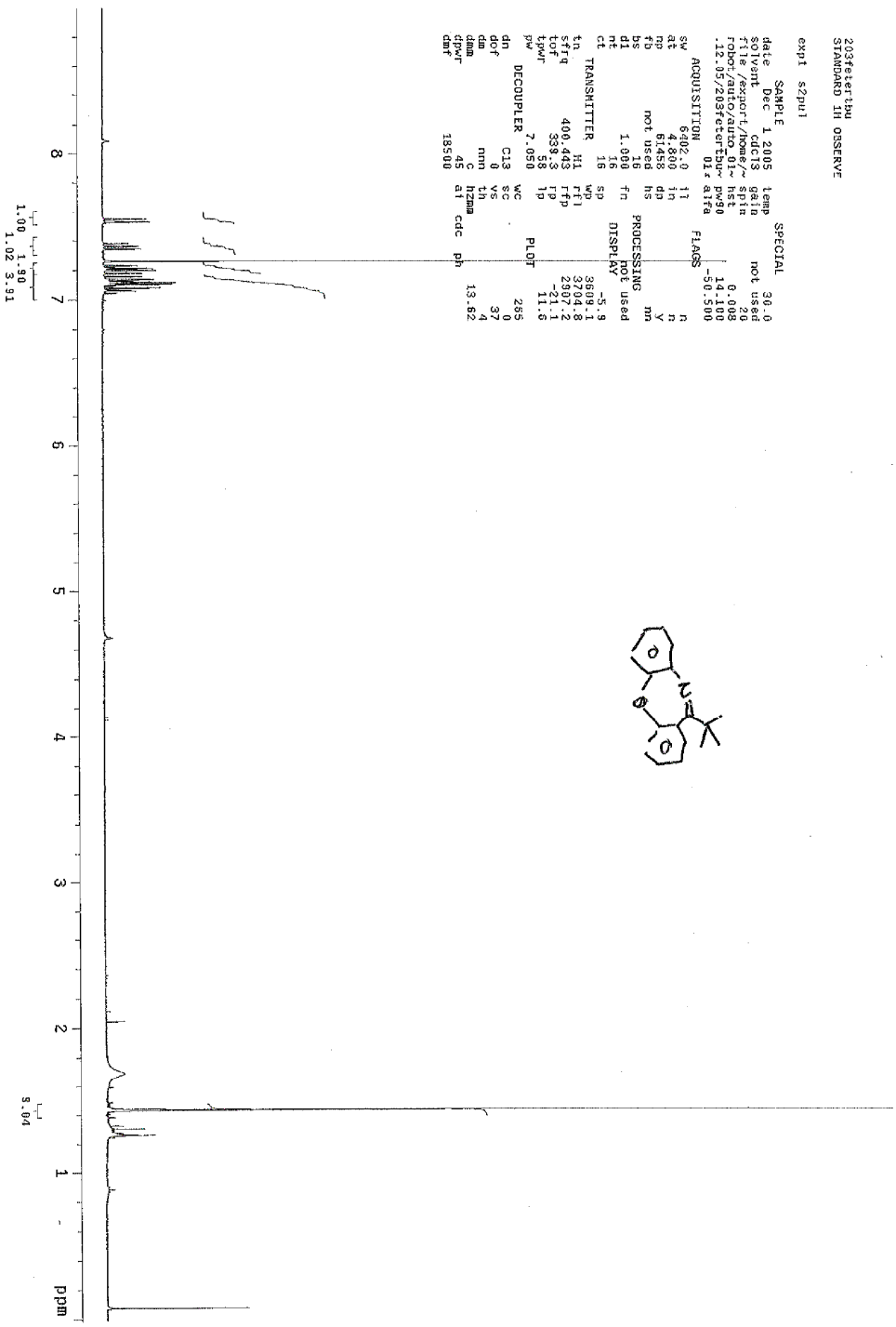
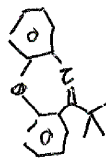


3036437100
STANDARD IN OBSERVE

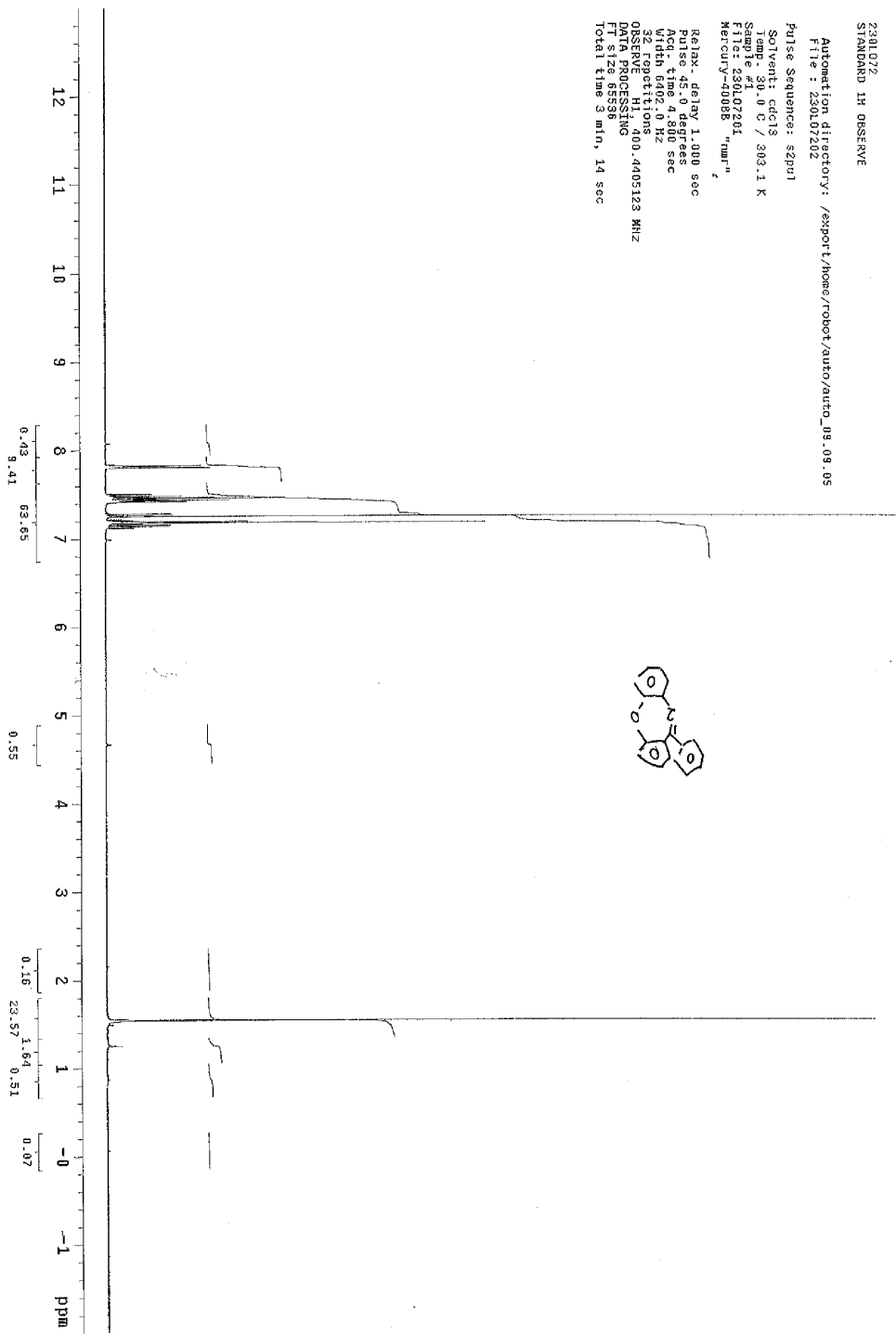
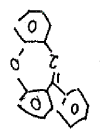
expt szpu1

SAMPLE Dec 1 2005 Temp SPECIAL 39.0
Solvent CDC13 gain not used
Title /EXPORT/ROMS/ SPIN 0.000
Date /2005/12/01 14.100
-12.05/2037eter Ebuw pw90
014 A1FA -50.500

ACQUISITION 014 A1FA
SW 6402.0 11
SI 6402.0 11
F2 61458.0 11
FB not used hs
DS 16 16
DI 1.099 fr DISPLA not used
CT 16
TRANSMITTER M1 WP -5.9
FR 400 M1 FTI 3809.1
FREQ 400.43 FTI 3794.8
SFS 338 FTI 2971.2
LPOW 58 1p 11.6
PLOT 13-62
DECOUPLER C13 WC 285
DN V 37
DNF nmn th 4
DM nm C hzma 13-62
DPM 45 at cdc ph
DMF 18500



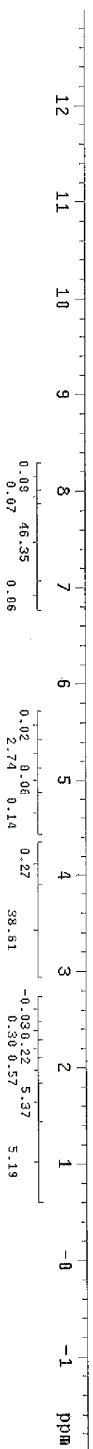
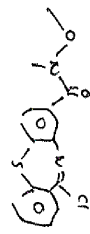
230L072
 STANDARD 1H OBSERVE
 Automation directory: /export/home/robot/auto/auto_09_09_05
 File : 230L07202
 Pulse Sequence: s2pul
 Solvent: cdcl3
 Sample # : 100 / 303.1 K
 F1tc: 230L07201
 Mercury-0008B "nmr"
 Relax - delay 1.000 sec
 Pulse 45.0 degrees
 Width 6002.0 Hz
 32 Repetitions
 OBSERVE HI 100.4405123 MHz
 DATA PROCESSING
 Total Time 3 min, 14 sec



230U.057
STANDARD IH RESERVE

Automation directory: /export/home/robot/auto/auto_20.07.05
File : 230U05702

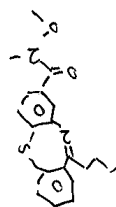
Pulse Sequence: szpui
Solvent: cdcl3
Temp: 30.0 C / 303.1 K
Sample #: 105701
File: 230U05701
Nuc1: 13C
Nuc2: 13C
Relax. delay: 1.000 sec
Pulse: 45.0 degrees
Acq. time: 4.380 sec
Width: 6402.0 Hz
S2: 100.625 MHz
S1: 100.625 MHz
DATA PROCESSING
FT size: 65536
Total time: 3 min, 14 sec



2301081
STANDARD 1H OBSERVE

Automation directory: /export/home/robot/auto/auto_19_09_05
File: 230108102

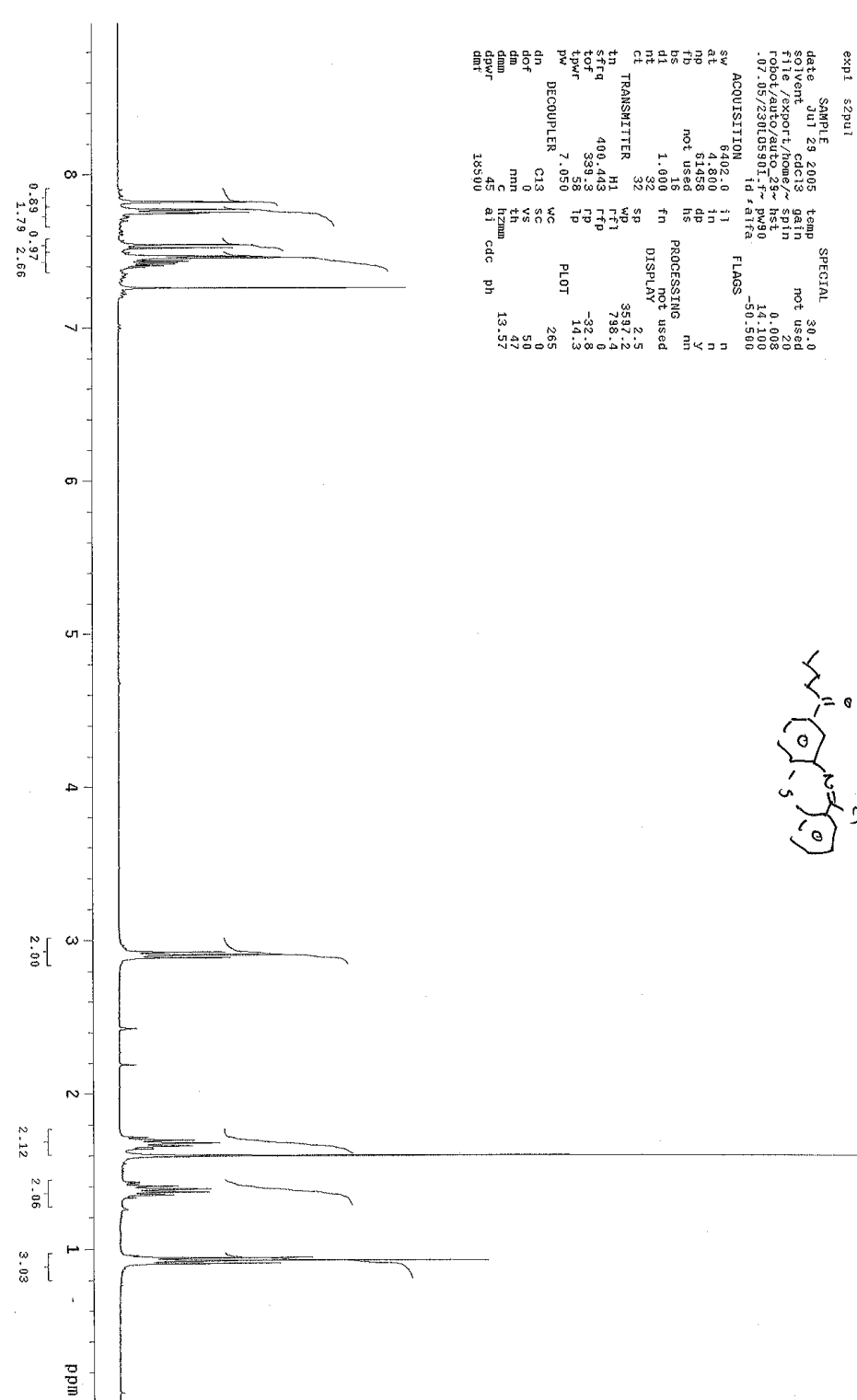
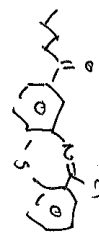
Pulse Sequence: szgnt1
Solvent: cdcl3
Temp: 30.0 C / 303.1 K
Sample #4
File: 230108101 "nmr"
Mercury-400DB "nmr" f
Pulse delay: 1.000 sec
Pulse: 45.0 degrees
Acq. time: 4.800 sec
Width: 6402.0 Hz
S2 repetitions: 00.4405129 MHz
S2: 400.146 MHz
DATA PROCESSING
FT size: 65536
Total time: 3 min, 14 sec



2301059
STANDARD IH OBSERVE

expt s2pu1

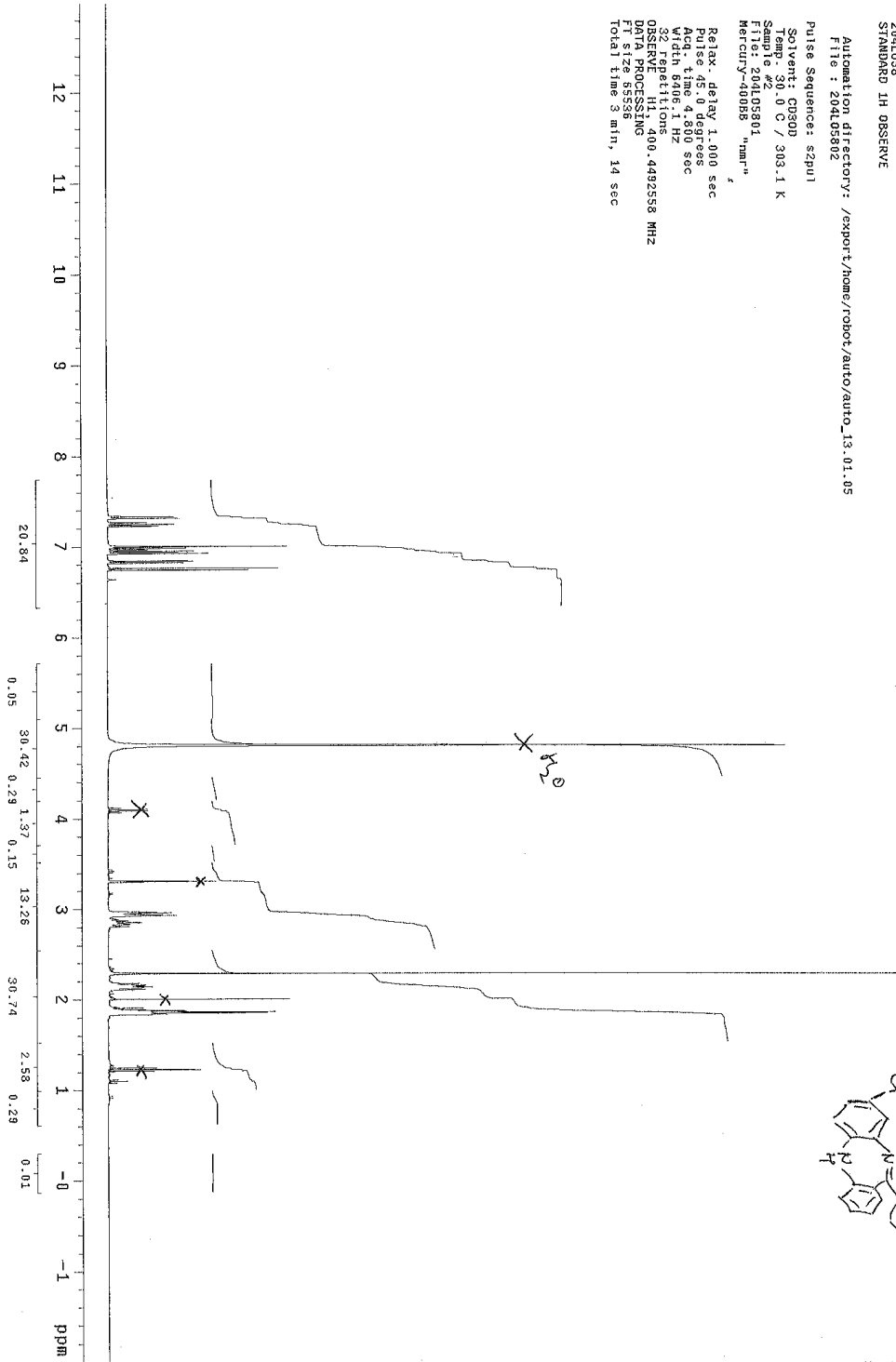
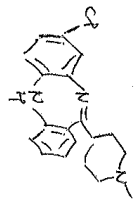
date	Jul 29 2005	temp	30.0
solvent	cdcl3	gain	not used
file	/export/home/~	spin	0.008
tosol	adco/adco_3	hs4	14.108
id	07/09/2301059	id	-50.500
id	atira	flags	
sw	6402.0	fi	n
at	4.800	in	n
fp	01493	dp	y
bs	not used	hs	not used
d1	1.000	fn	not used
nt	32	sp	2.5
ct	TRANSMITTER	wp	3592.2
tn	H1	wp	730.0
stfr	400.443	rfp	-32.8
tof	339.3	tp	14.3
lpwr	58	tp	
pw	7.050	plot	
decoupler	WC		265
dn	C13	vc	50
dnf	vc	th	47
dmm	mn	hzmm	13.57
dpwr	45	ai	cdc
dmt	13500	ph	



204.058
STANDARD 1H OBSERVE

Automation directory: /export/home/robot/auto/auto_13.01.05
File : 204.05802

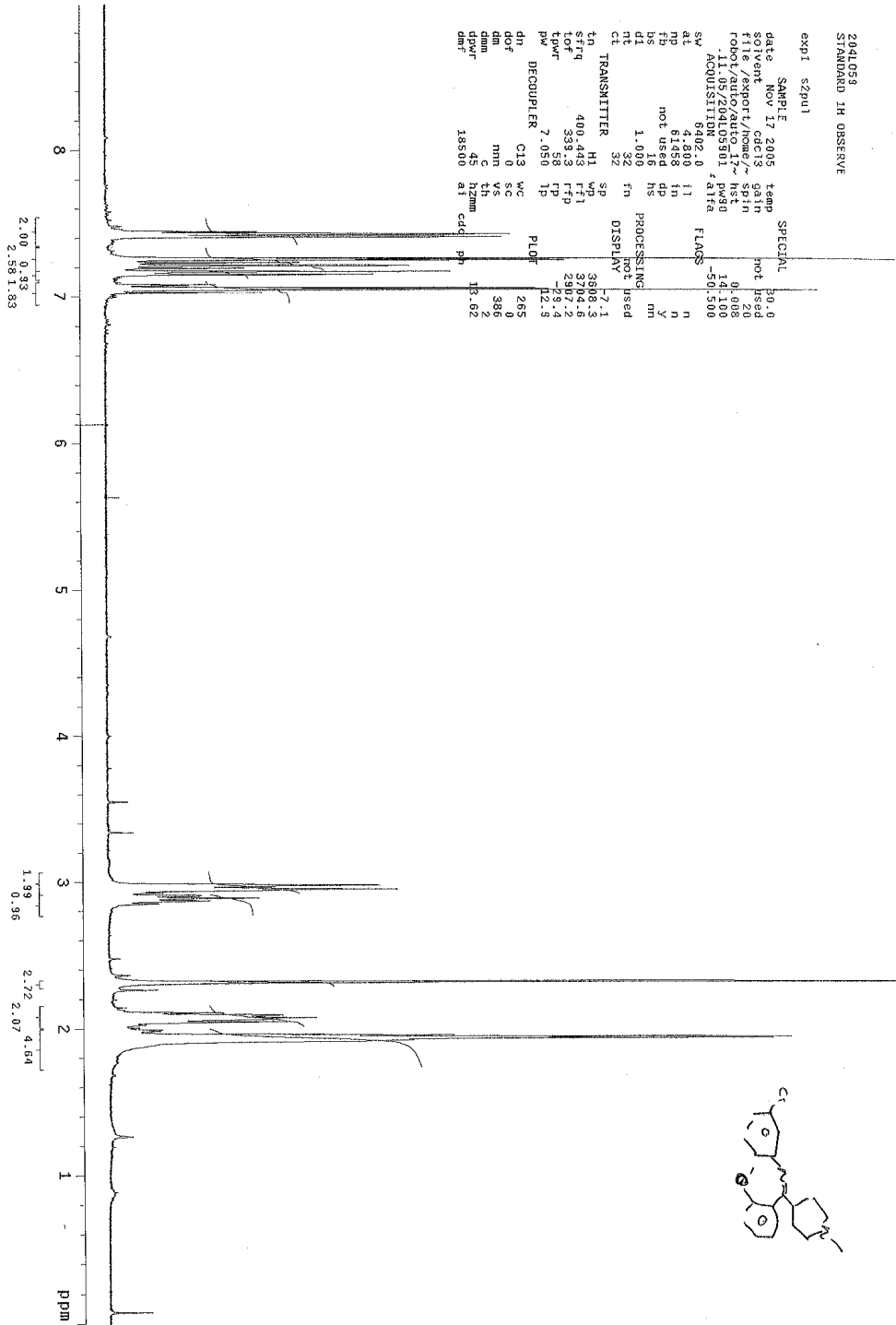
Pulse Sequence: szpu1
Solvent: CD3OD
Temp: 30.0 C / 303.1 K
Sample 42
Date_ 20.05.2011
Mercury-400MHz "nmr"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.800 sec
Width 6406.1 Hz
S2 Repetitions 300.4492558 MHz
S2 Frequency 100.628111 MHz
DATA PROCESSING
FT size 85536
Total time 3 min, 14 sec



2041058
STANDARD 1H OBSERVE

expt1 s2pu1

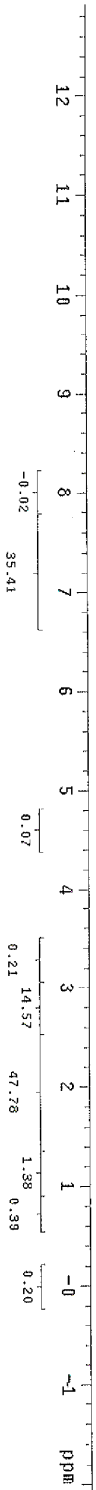
date Nov 17 2005 temp SPECIAL 30.0
solvent H2O cdc13 gain not used
fobol/srbc/4100 17-02-02 01.008
-11.05/204105501 pw30 141.100
ACQUISITION 4178 FLMS -501.500
SW 6402.0 11
AQ 1.000 16
RG 61458 16
FB not used dp
BS 16 hs
DI 1.000 32
RT 32 fn
CL TRANSMITTER 32 fn
IN WP 13.62
STFQ 400.443 FFI 3808.3
TOR 393.3 FFI 3704.6
PW 7.050 1p 292.2
PWR 12.9
DECOUPLER C13 WC PLOFF 265
DR 0 mm 348
DOR 0 mm 348
C th 2
DMM 45 hzmm
DPR 18500 af cdc ph 13.62
DMF



2041060
STANDARD IN OBSERVE

Automation directory: /export/home/robot/auto/auto_17.11.05
File: 204106002

Pulse Sequence: s2gu1
Solvent: cdcl3
Temp: 30.0 C / 303.1 K
Samp: 2.1105001
F1 size 65536
Mercury-400BB "nmr"
Relax. delay: 1.000 sec
Pulse: 45.0 degrees
Acq. time: 4.800 sec
Width: 3402.0 Hz
32 repetitions
DATA PROCESSING
F1 size 65536
Total time: 3 min, 14 sec



2301024-1V
STANDARD IN OBSERVE

Automation directory: /export/home/robot/auto/auto_25_08_05
File: 2301024-1V02

Pulse Sequence: szpu1

Solvent: cdcl3

Temp: 30.0 C / 303.1 K

Sample #7

File: 2301024-1V01

Mercury-40088 "mm" f

Relax delay: 1.000 sec

Pulse delay: 0.000 sec

Acq time: 4.800 sec

Width: 6402.0 Hz

32 repetitions: 0.4405123 MHz

0.0500 PROCESSION

FT size: 65536

Total time: 3 min, 14 sec

