

Supporting Information

Direct Diazo-Transfer Reaction on β -lactam:

Synthesis and Preliminary Biological Activities of 6-Triazolylpenicillanic Acids

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¹³C-NMR and ¹H-NMR spectra of compound **12c** (S56-S57)

¹³C-NMR and ¹H-NMR spectra of compound **12d** (S58-S59)

¹³C-NMR and ¹H-NMR spectra of compound **12e** (S60-S61)

¹H-NMR spectra of compound **12f** (S62)

¹H-NMR spectra of compound **12g** (S63)

¹³C-NMR and ¹H-NMR spectra of compound **12h** (S64-S65)

¹H-NMR spectra of compound **12i** (S66)

¹³C-NMR and ¹H-NMR spectra of compound **12j** (S67-S68)

¹H-NMR spectra of compound **12k** (S69)

¹H-NMR spectra of compound **12l** (S70)

¹H NMR of **3a**:

A0-1-23

Pulse Sequence: szpu1

USER: hchen

DATE: Jun 11 2006

File: exp

Solvent: DMSO

Ambient temperature

Mercury-400BB "r2d2"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 37.5 degrees

Acq. time 2.000 sec

Width 3999.8 Hz

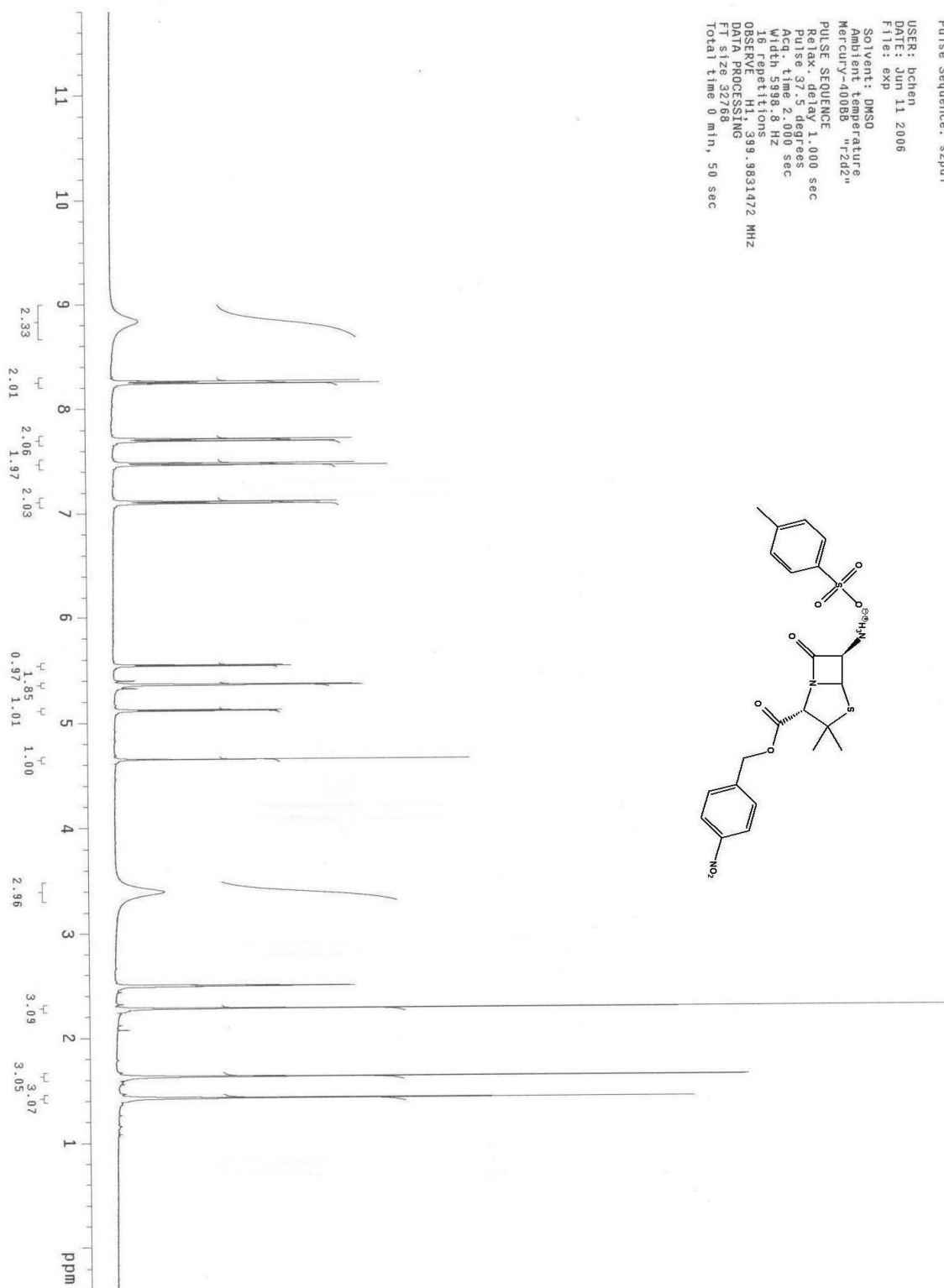
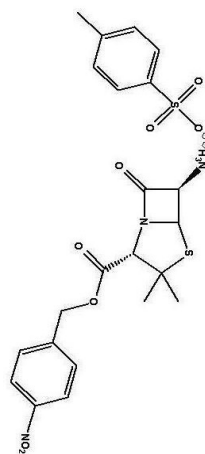
18 repetitions

Observed frequency 99.9831472 MHz

Observed processing

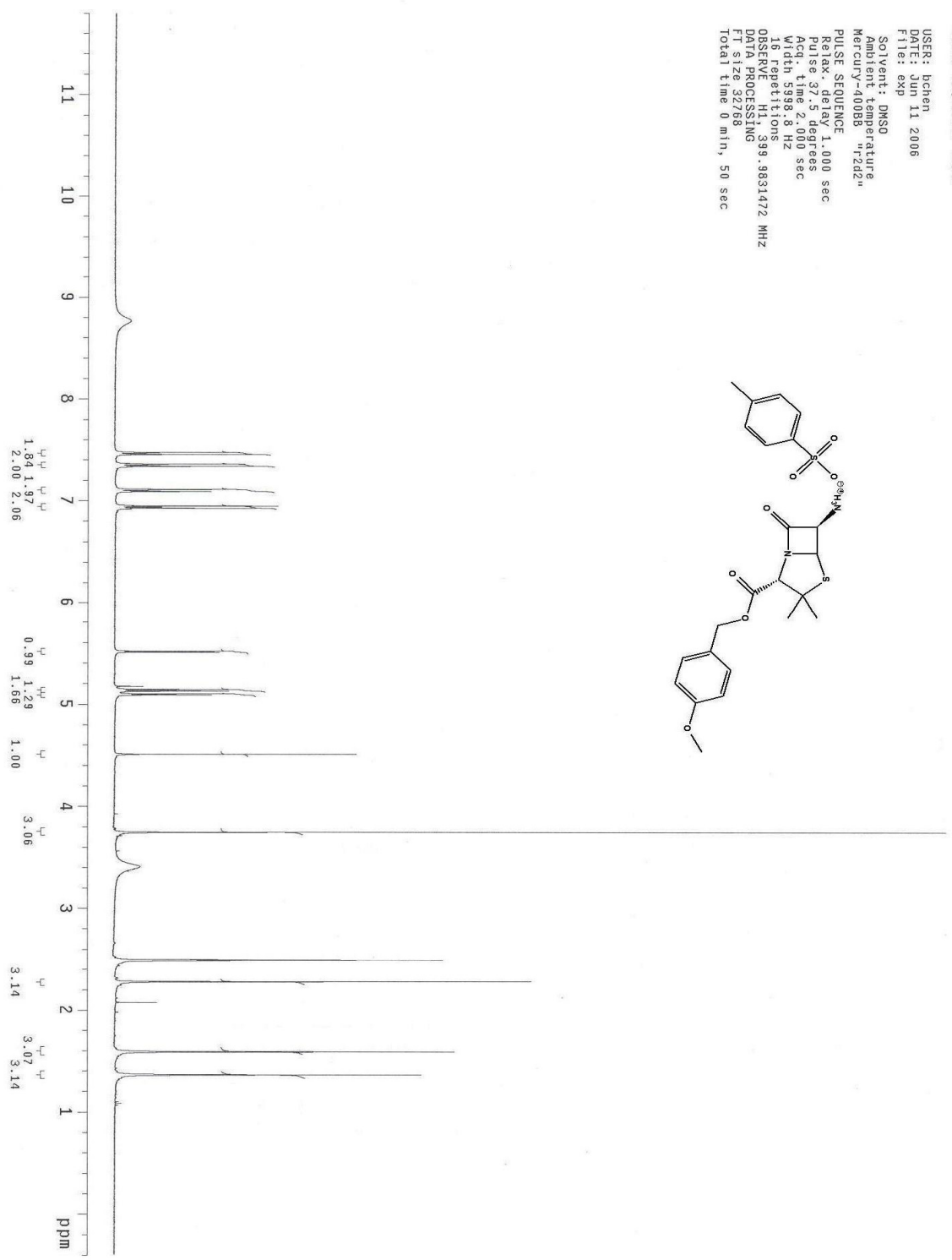
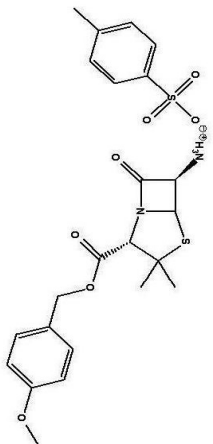
File size 32768

Total time 0 min, 50 sec



¹H NMR of **3b**:

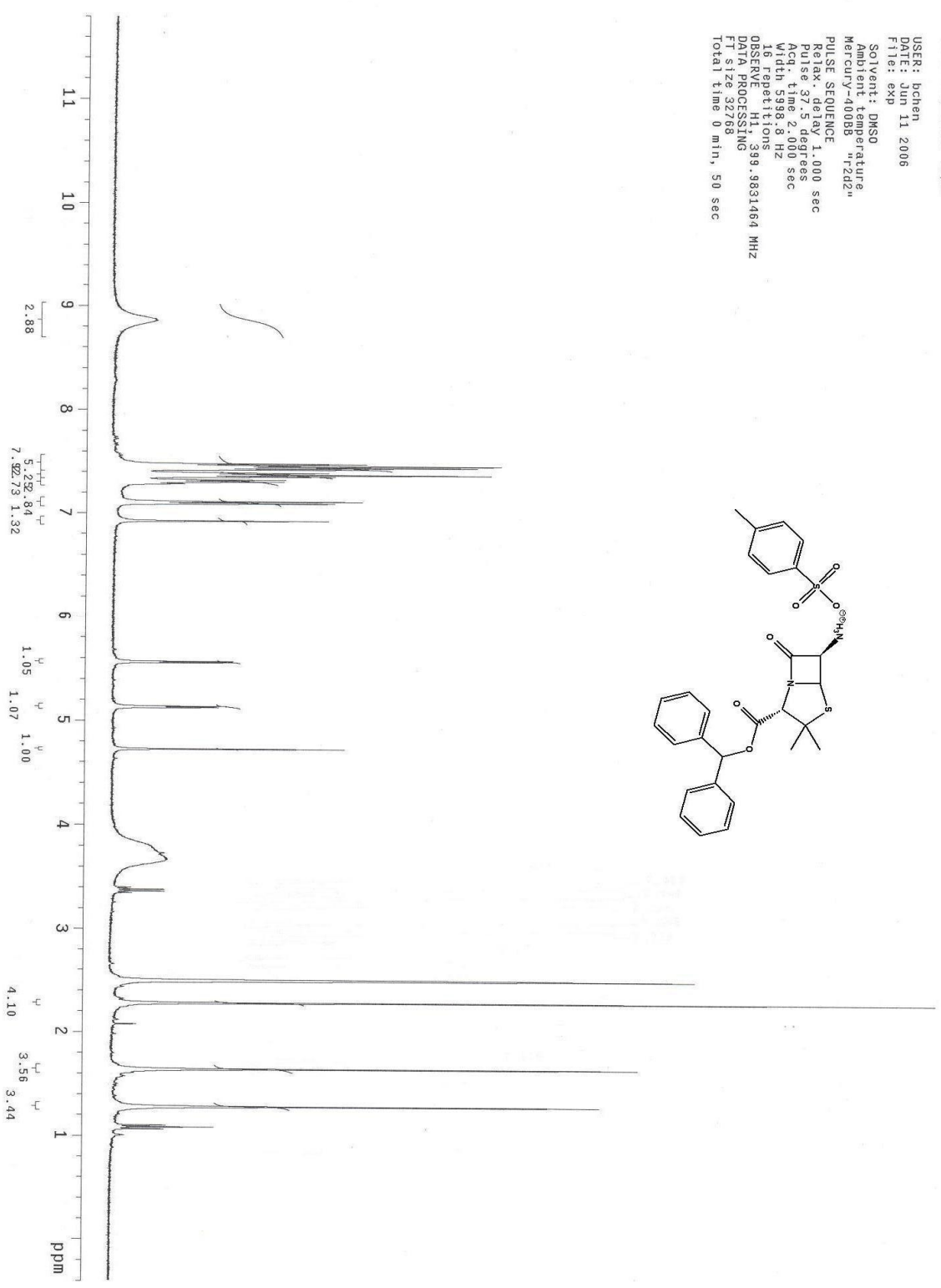
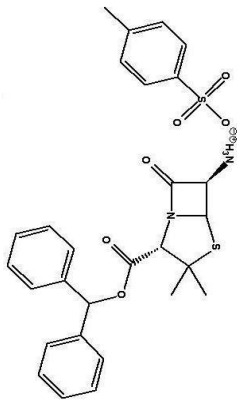
ao-1-60
 Pulse Sequence: s2pu1
 USER: bchen
 DATE: Jun 11 2006
 File: exp
 Solvent: DMSO
 Ambient temperature
 Mercury-400BB "P2D2"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 37.5 degrees
 Acq. time 2.000 sec
 Width 5998.8 Hz
 16 Repetitions
 OBSERVE H1, 399.9831472 MHZ
 DATA PROCESSING
 FT size 32768
 Total time 0 min, 50 sec



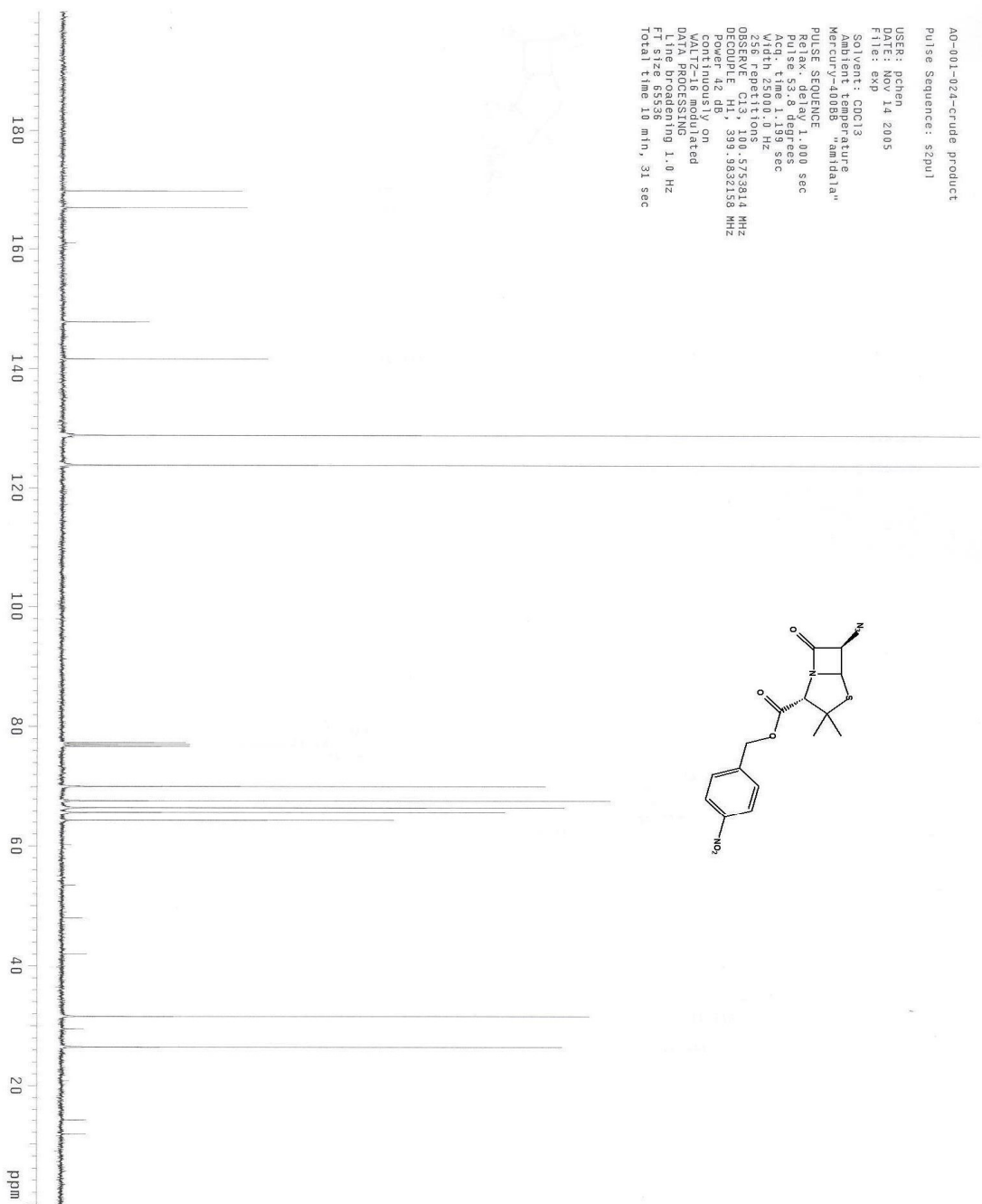
¹H NMR of 3c:

bob-2-140
Pulse Sequence: szpu1

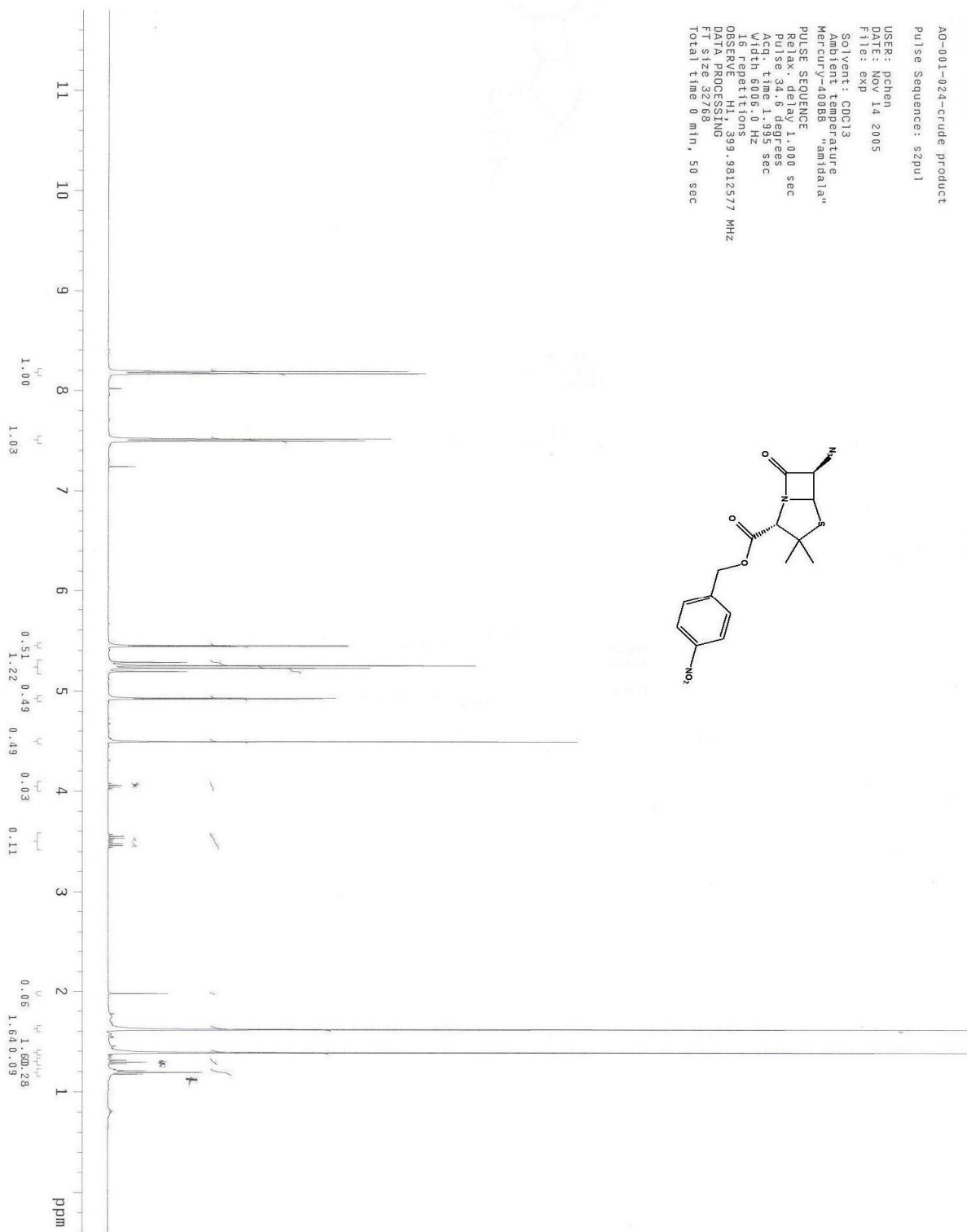
USER: bchen
DATE: Jun 11 2006
File: exp
Solvent: DMSO
Ambient temperature
Mercury-400BB "F242"
PULSE SEQUENCE
Relax: delay 1.000 sec
Pulse: 31.0 deg/sec
Acq: 4.00 sec
Width: 5998.8 Hz
16 Repetitions
OBSERVE: H1 399.9831464 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec



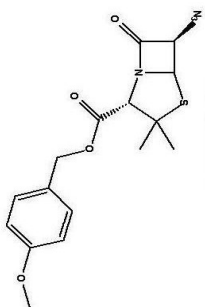
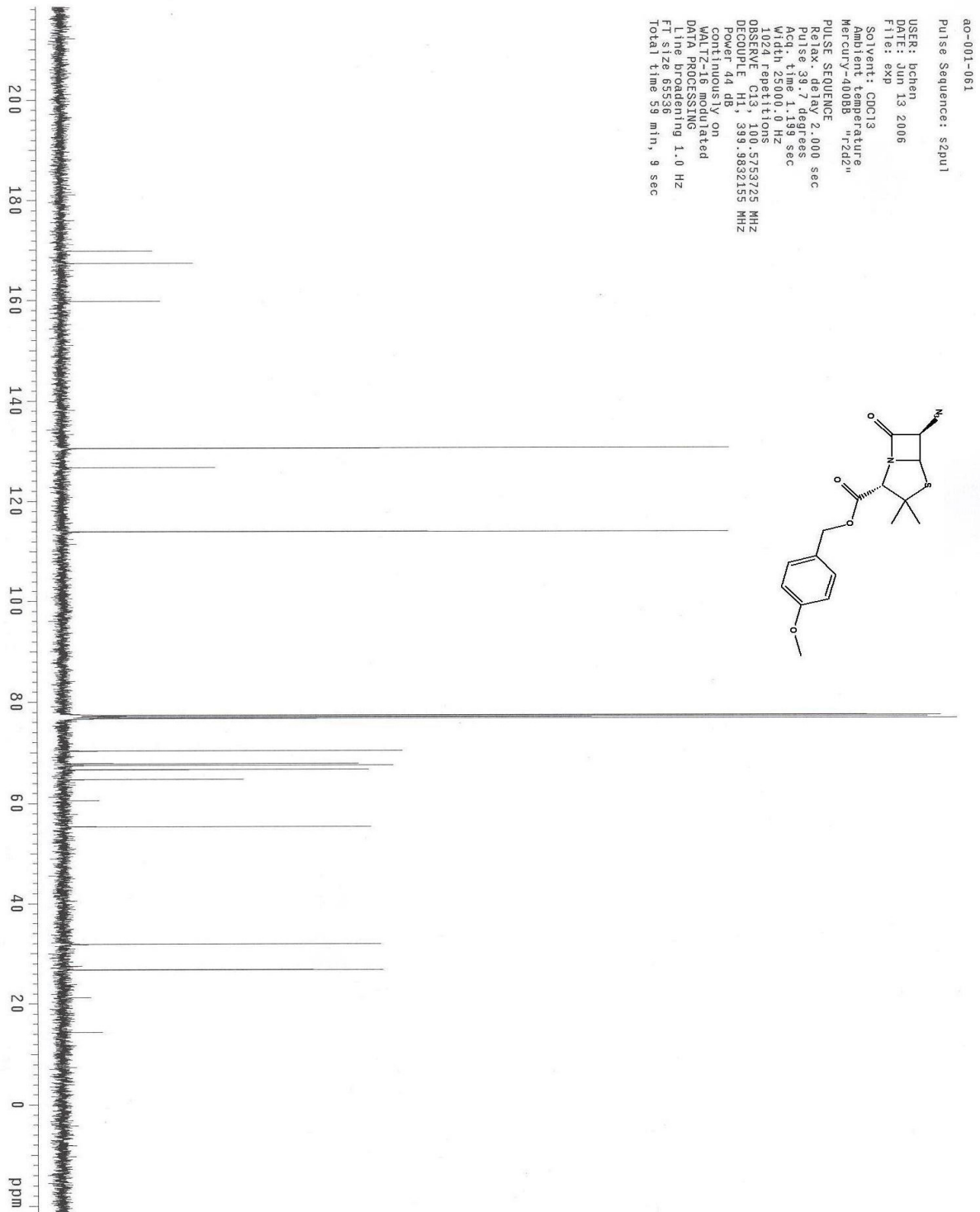
¹³C NMR of 5a:



¹H NMR of 5a:

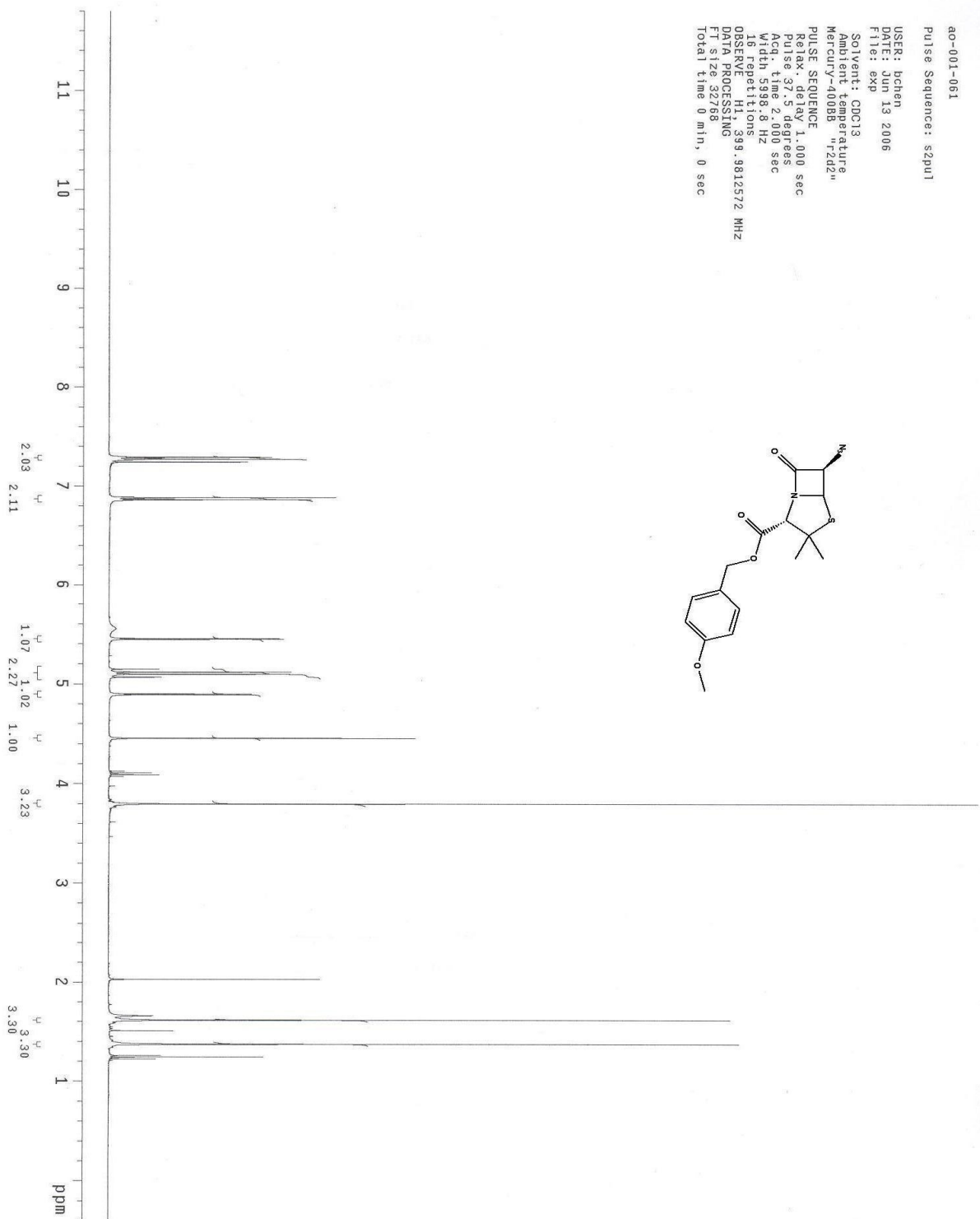


¹³C NMR of 5b:

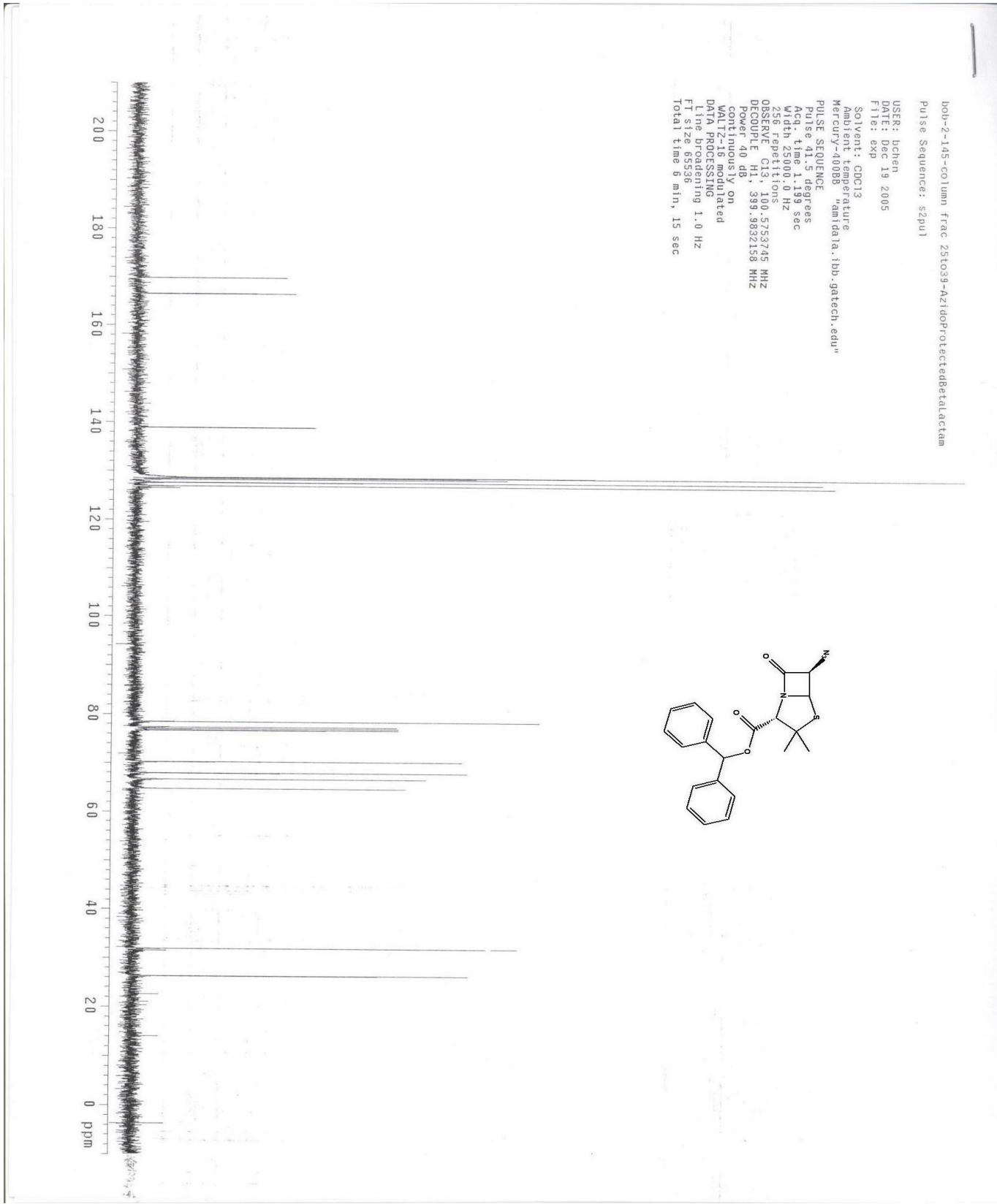


ao-001-081
Pulse Sequence: s2pu1
USER: bchen
DATE: Jun 13 2006
File: exp
Solvent: CDCl3
Ambient temperature
Mercury-400BB "r2d2"
PULSE SEQUENCE
Relax: delay 2.000 sec
Pulse: 39.7 degrees
Acq: time 1.39 sec
1024 repetitions
OBSERVE C13, 100.5753725 MHz
DECUPLE H1, 399.9832155 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 59 min, 9 sec

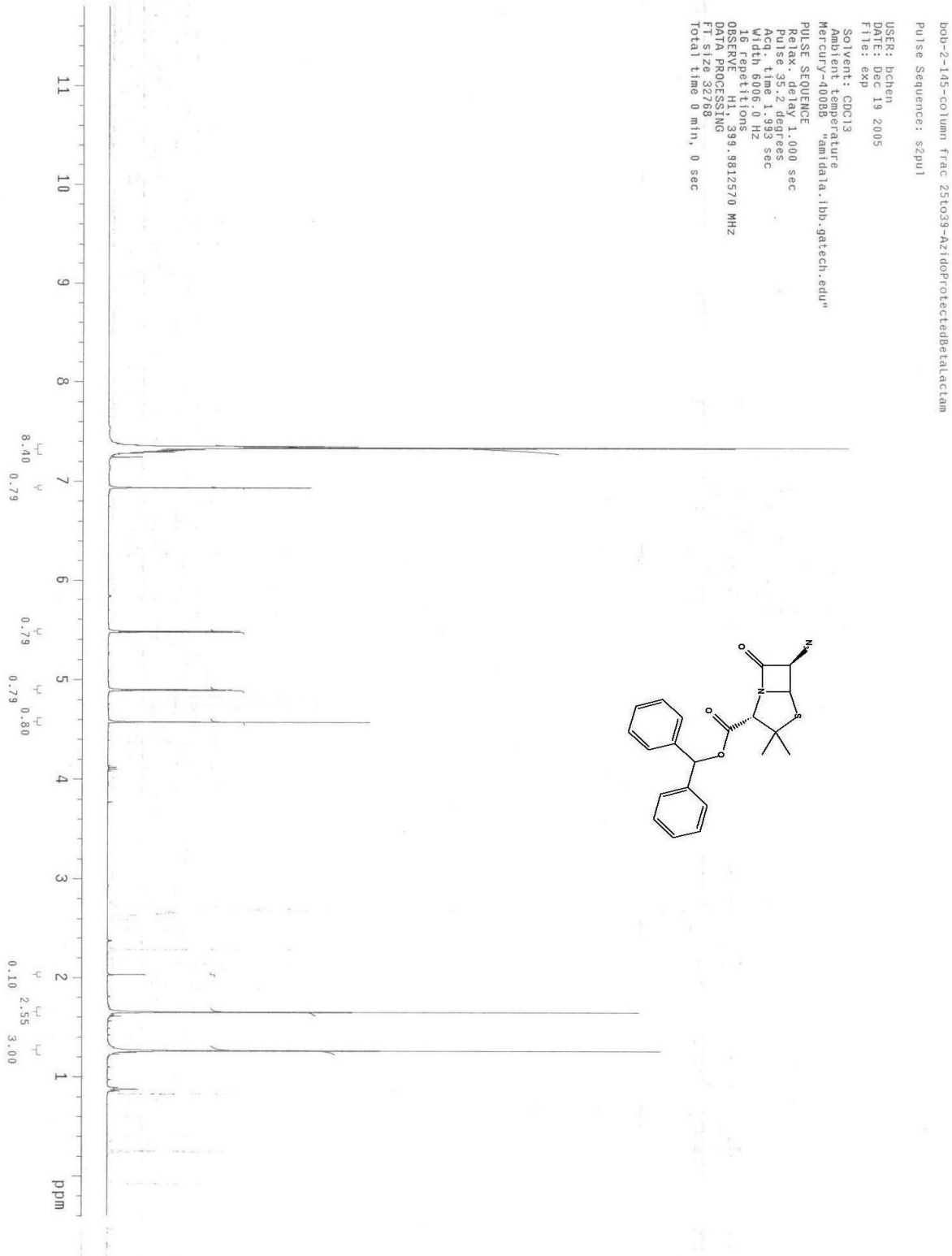
¹H NMR of **5b**:



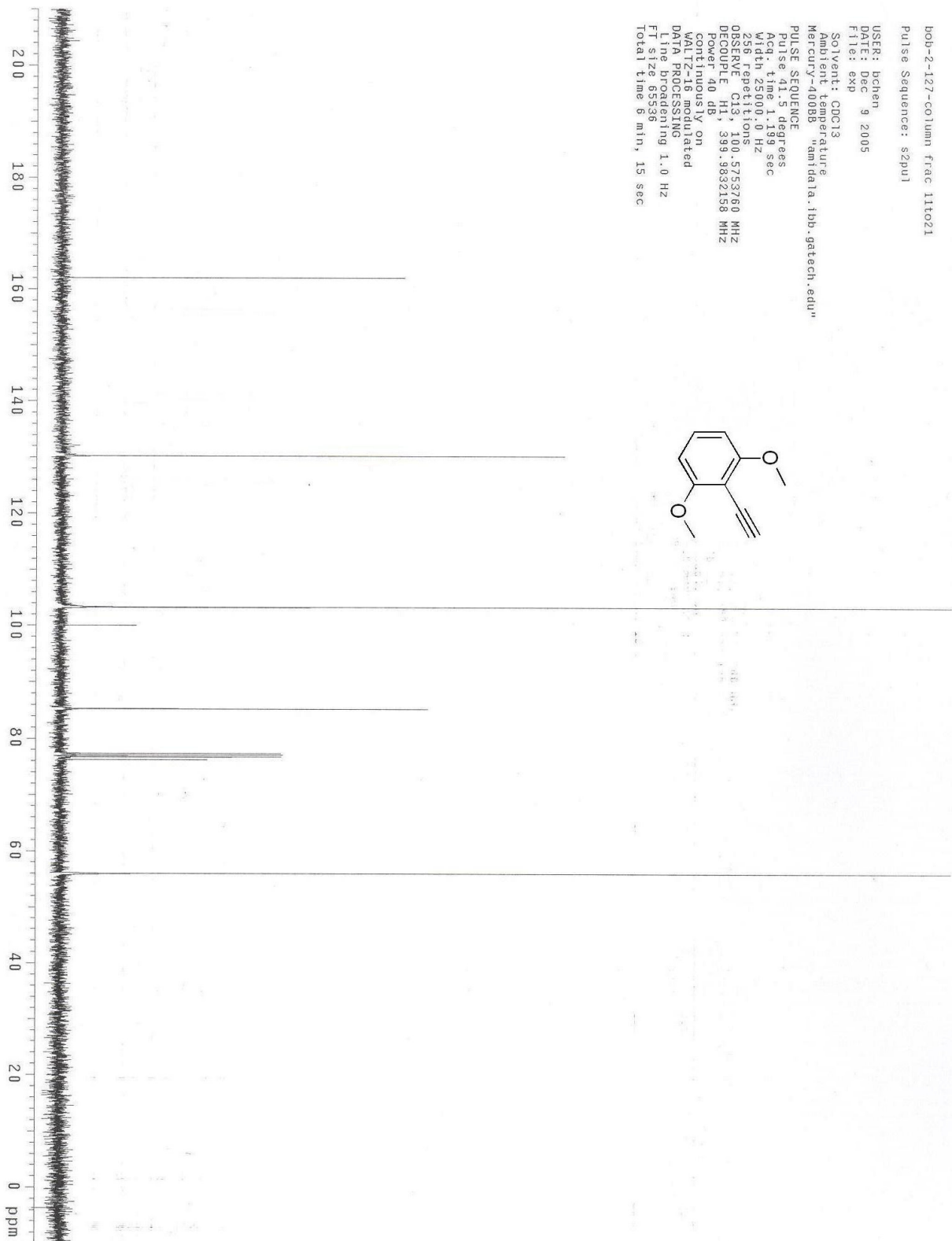
¹³C NMR of 5c:



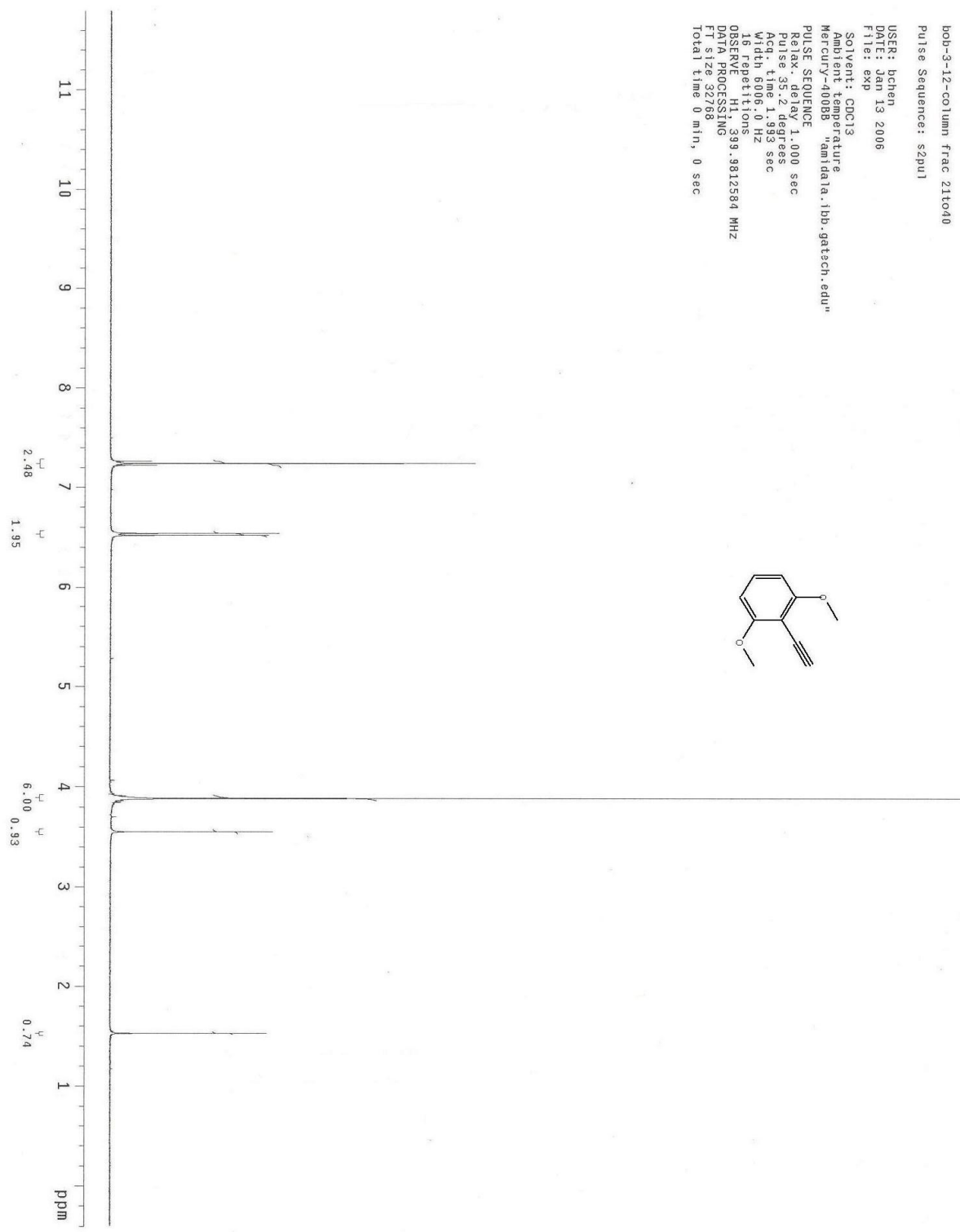
¹H NMR of 5c:



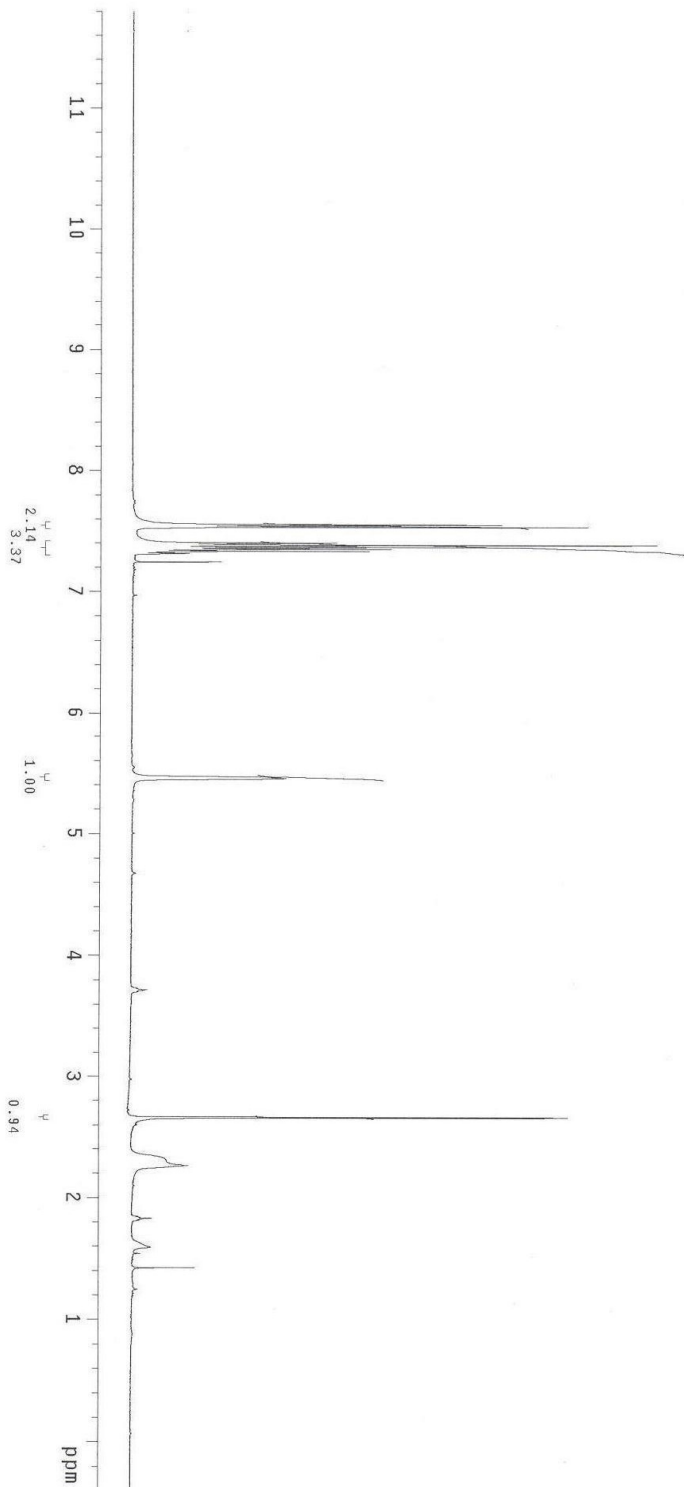
¹³C NMR of 7:



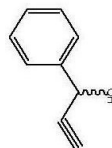
¹H NMR of 7:



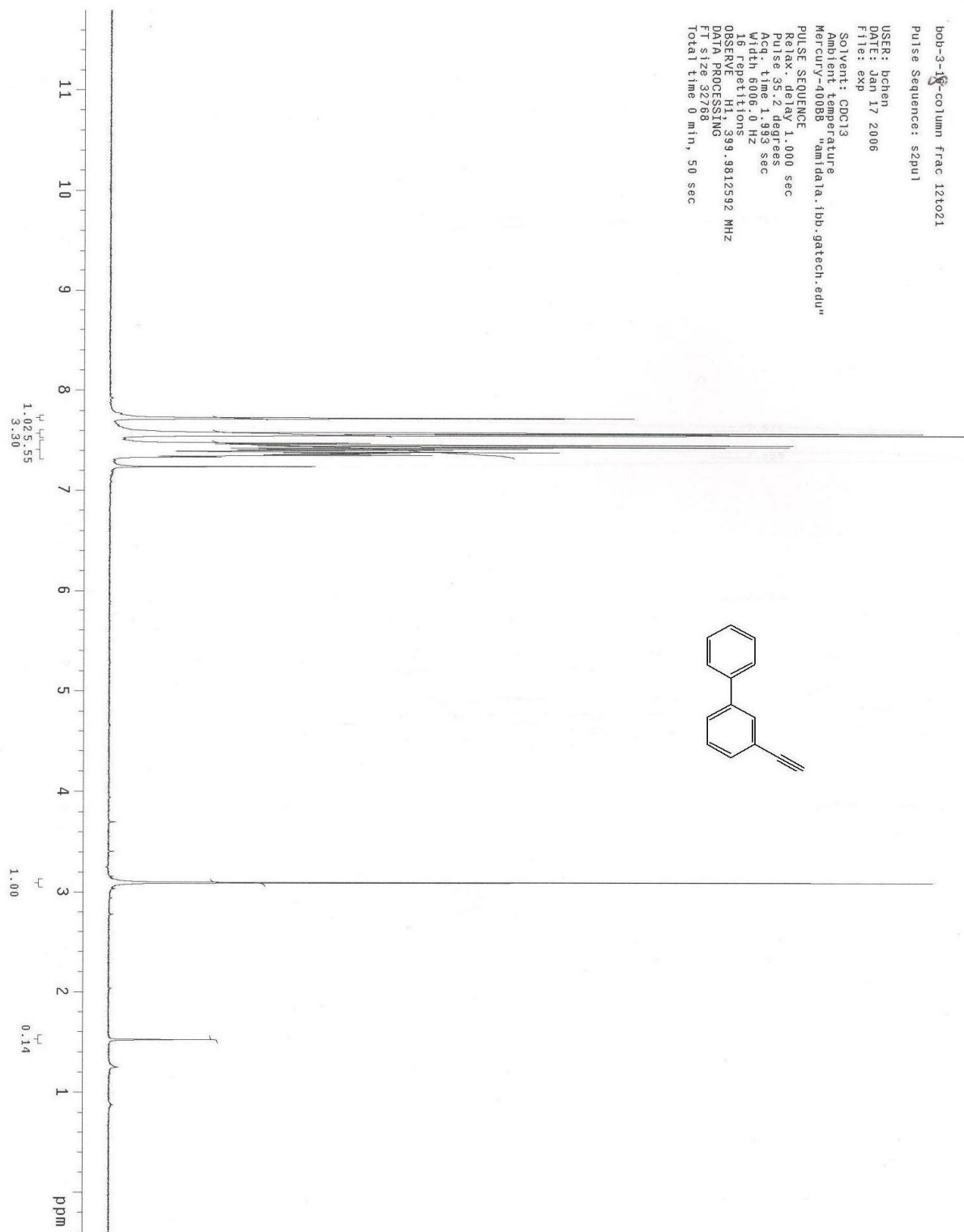
¹H NMR of 10f:



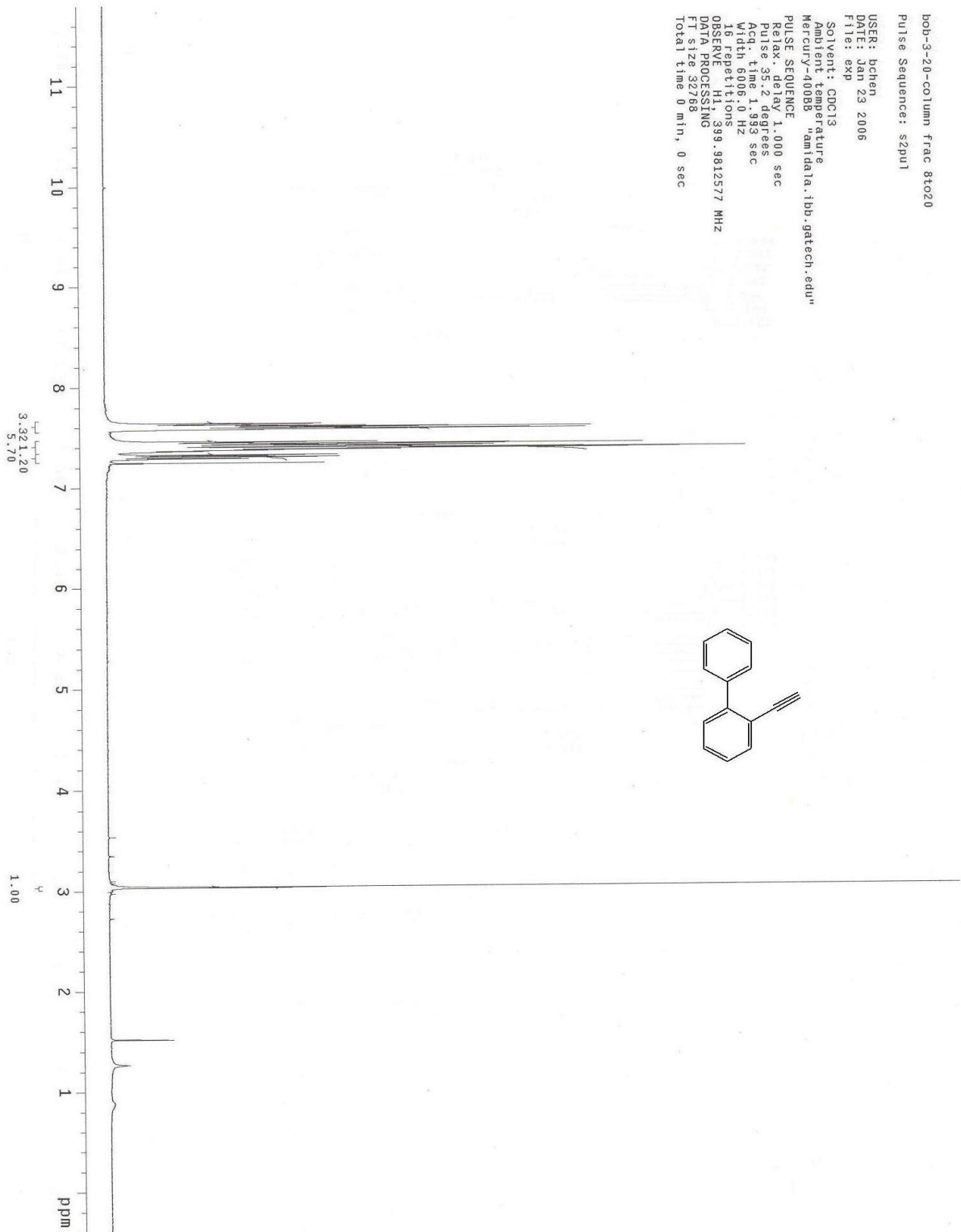
bob-4-29-Benzaldehyde+ethynyl]MgBr
Pulse Sequence: s2pul1
USER: bchen
DATE: Jul 24 2006
File: exp
Solvent: CDCl3
Ambient temperature
Mercury-400BB "r2d2"
PULSE SEQUENCE
Relax: d81
Pulse: 1.000 sec
Acq. time: 2.000 sec
Width: 5998.8 Hz
16 Repetitions
OBSERVE: H1, 399.9747427 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec



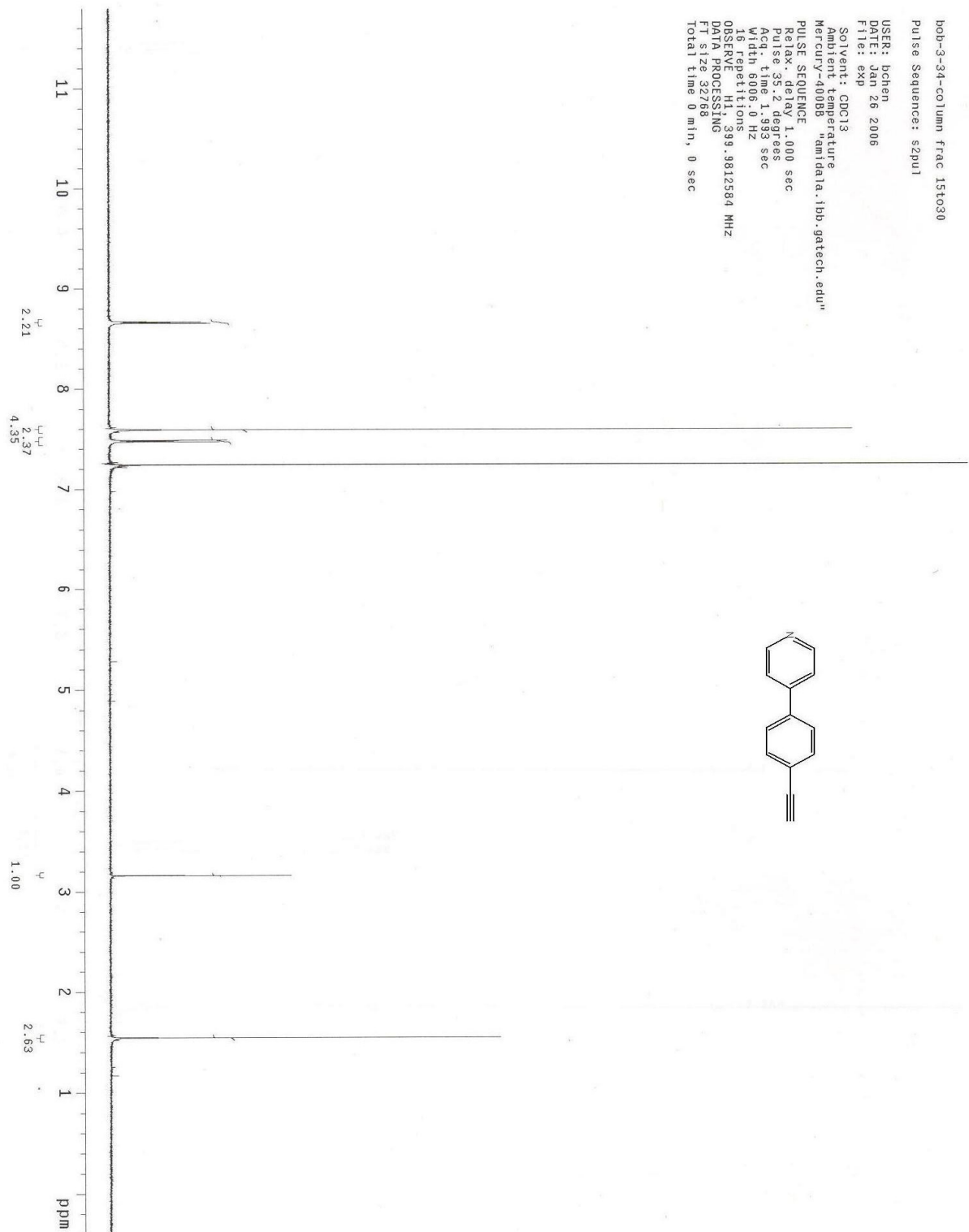
¹H NMR of 10h:



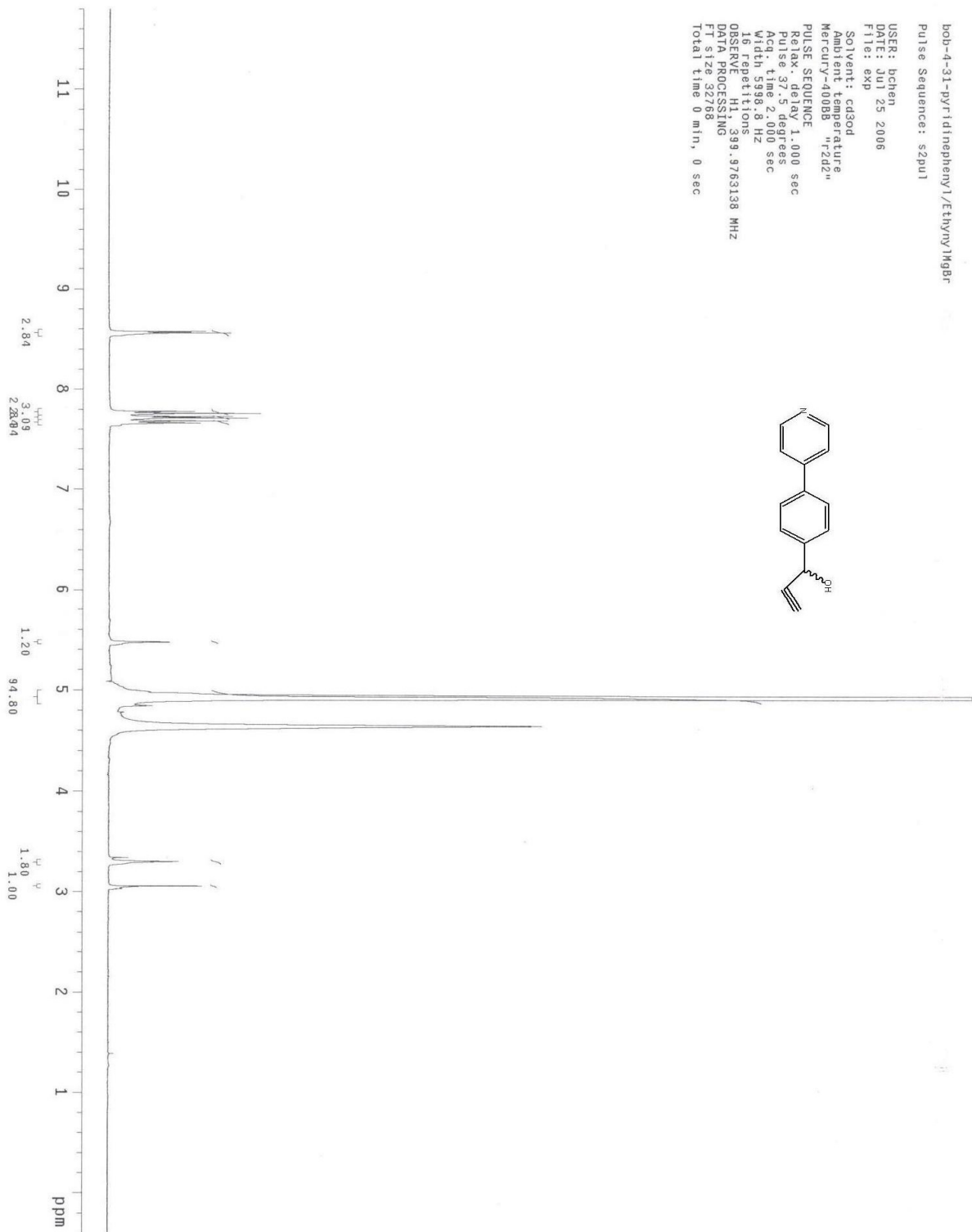
¹H NMR of 10i:



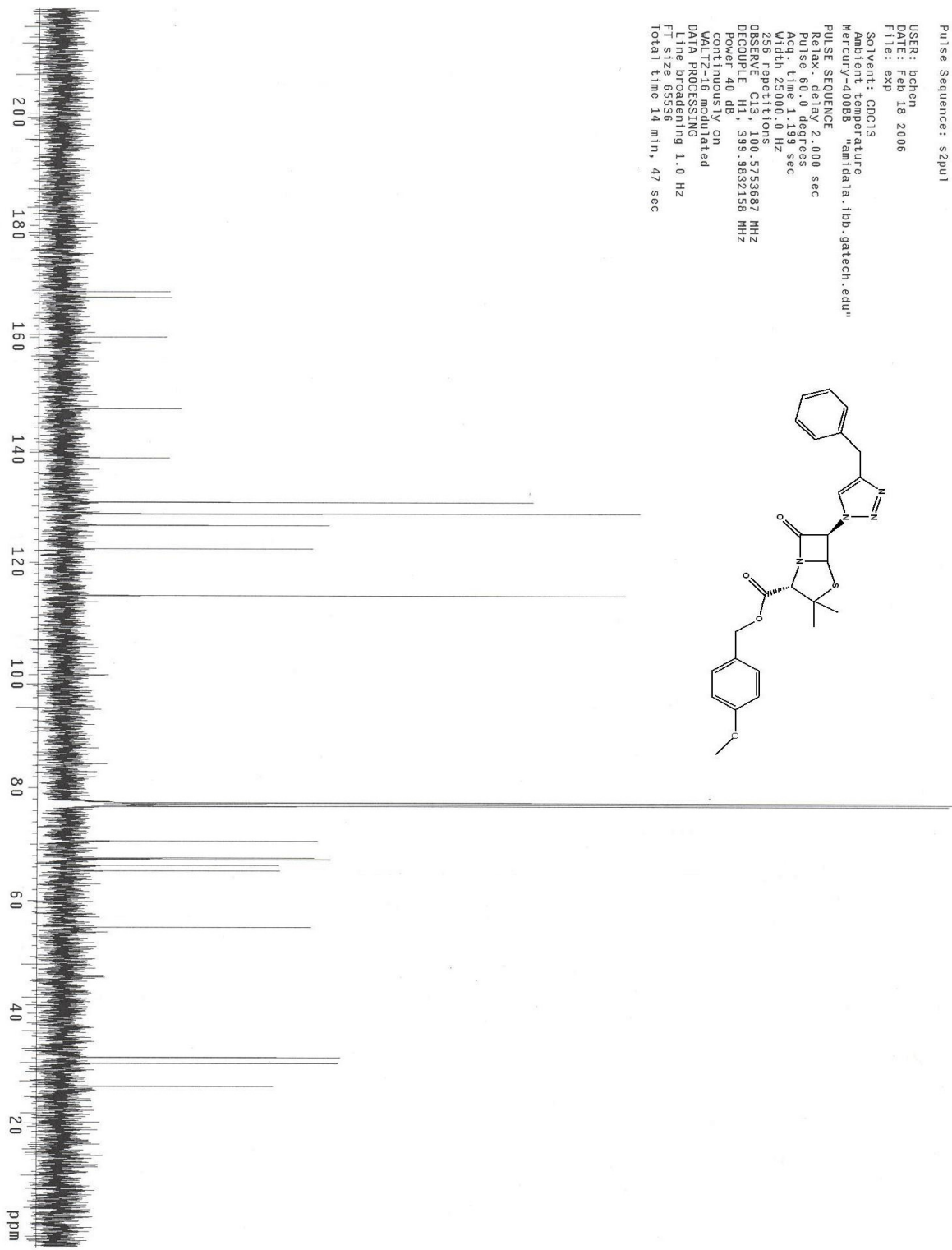
¹H NMR of 10k:



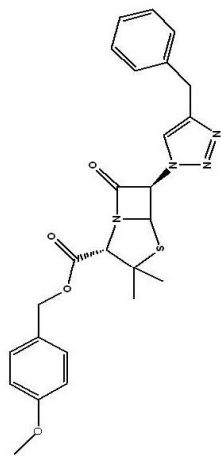
¹H NMR of 10l:



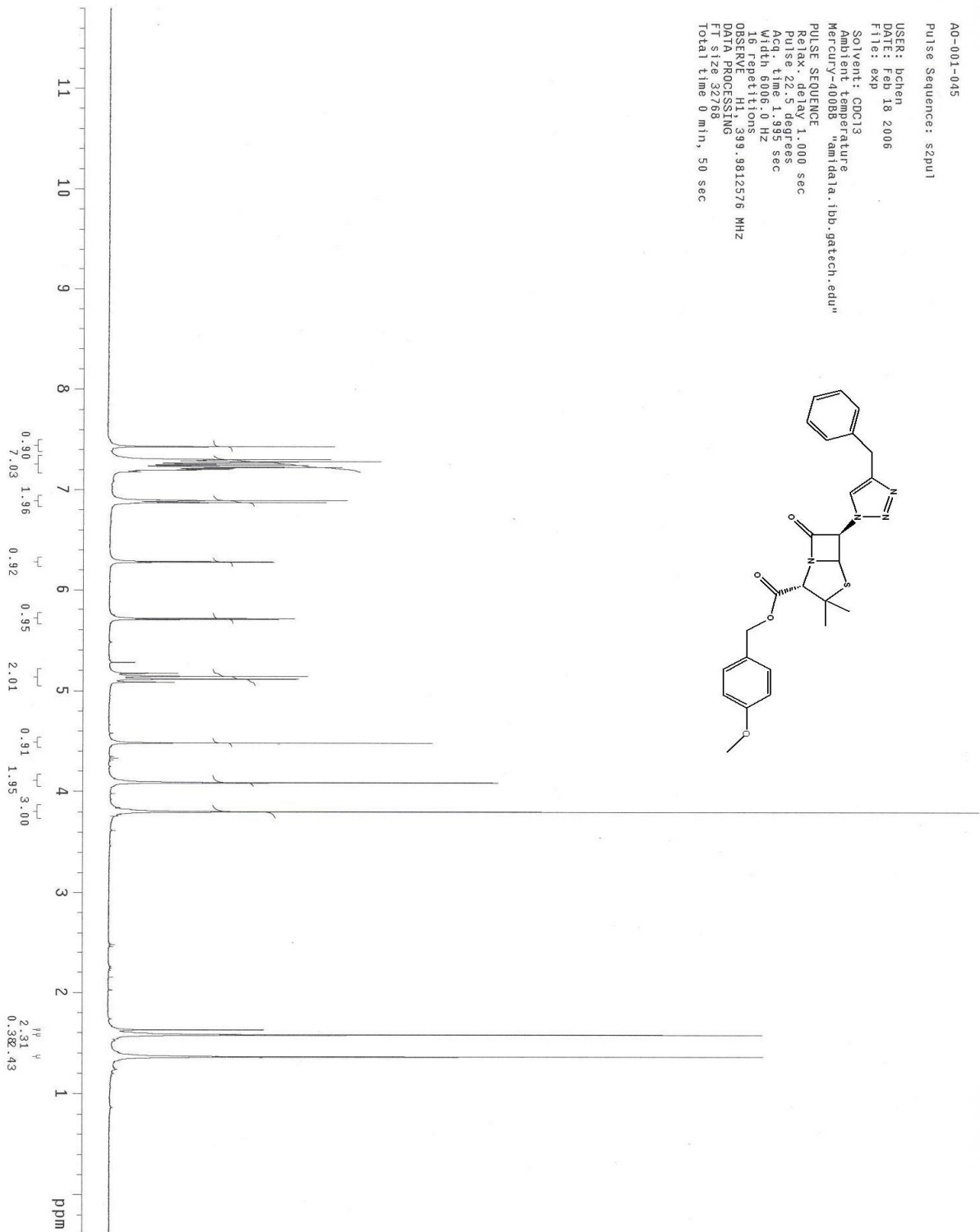
¹³C NMR of 8a:



A0-001-045
Pulse Sequence: s2pu1
USER: bchen
DATE: Feb 18 2006
File: exp
Solvent: CDCl3
Ambient temperature
Mercury-400BB "amidata.lib.gatech.edu"
PULSE SEQUENCE
Relax: delay 2.000 sec
Pulse: 60.0 degrees
Acq: time 1.139 sec
Vd: 120.0 Hz
256 repetitions
OBSERVE C13, 100.5753682 MHz
DECUPLE H1, 399.9832158 MHz
Power: 40 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 14 min, 47 sec

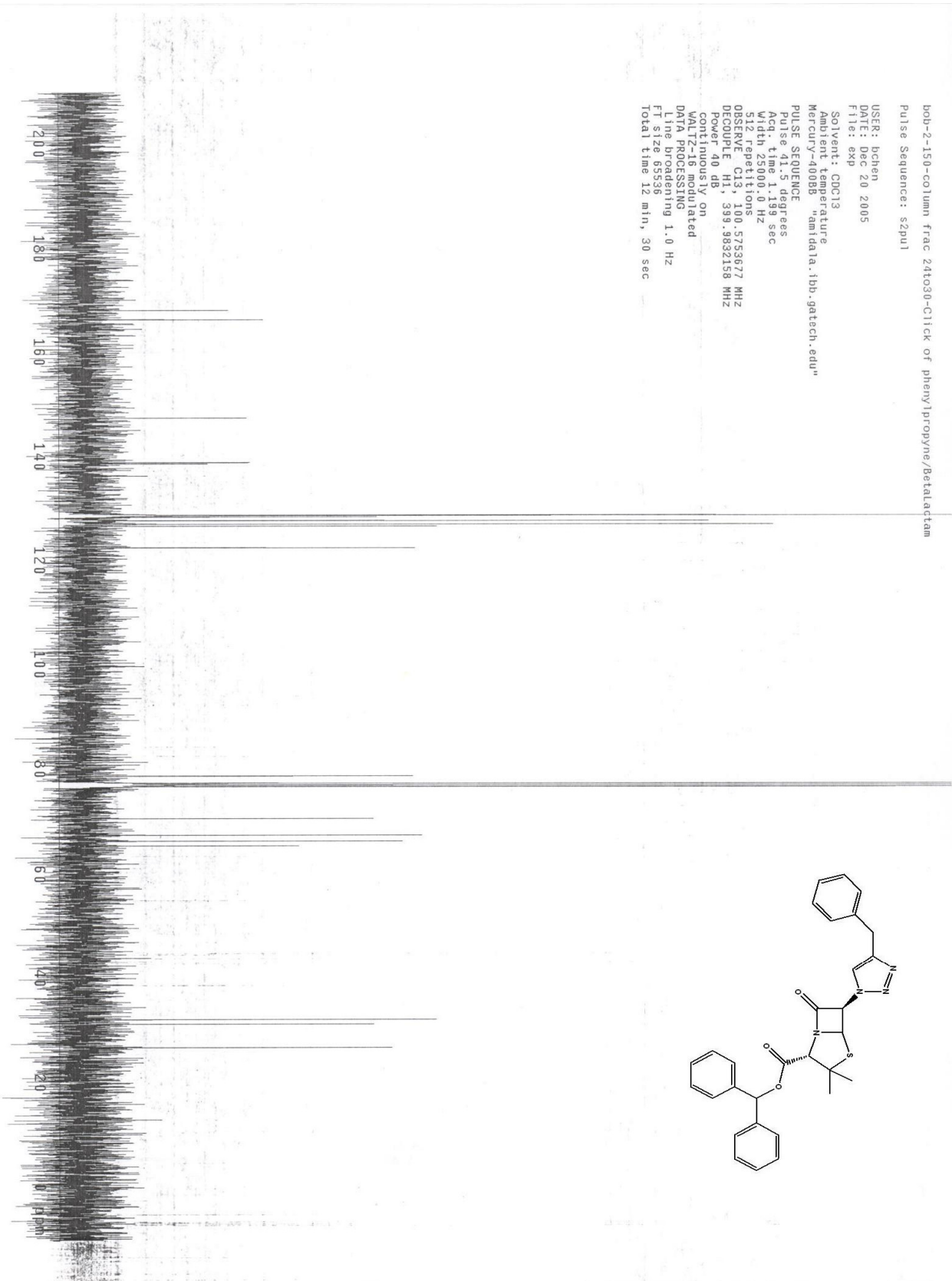


¹H NMR of 8a:

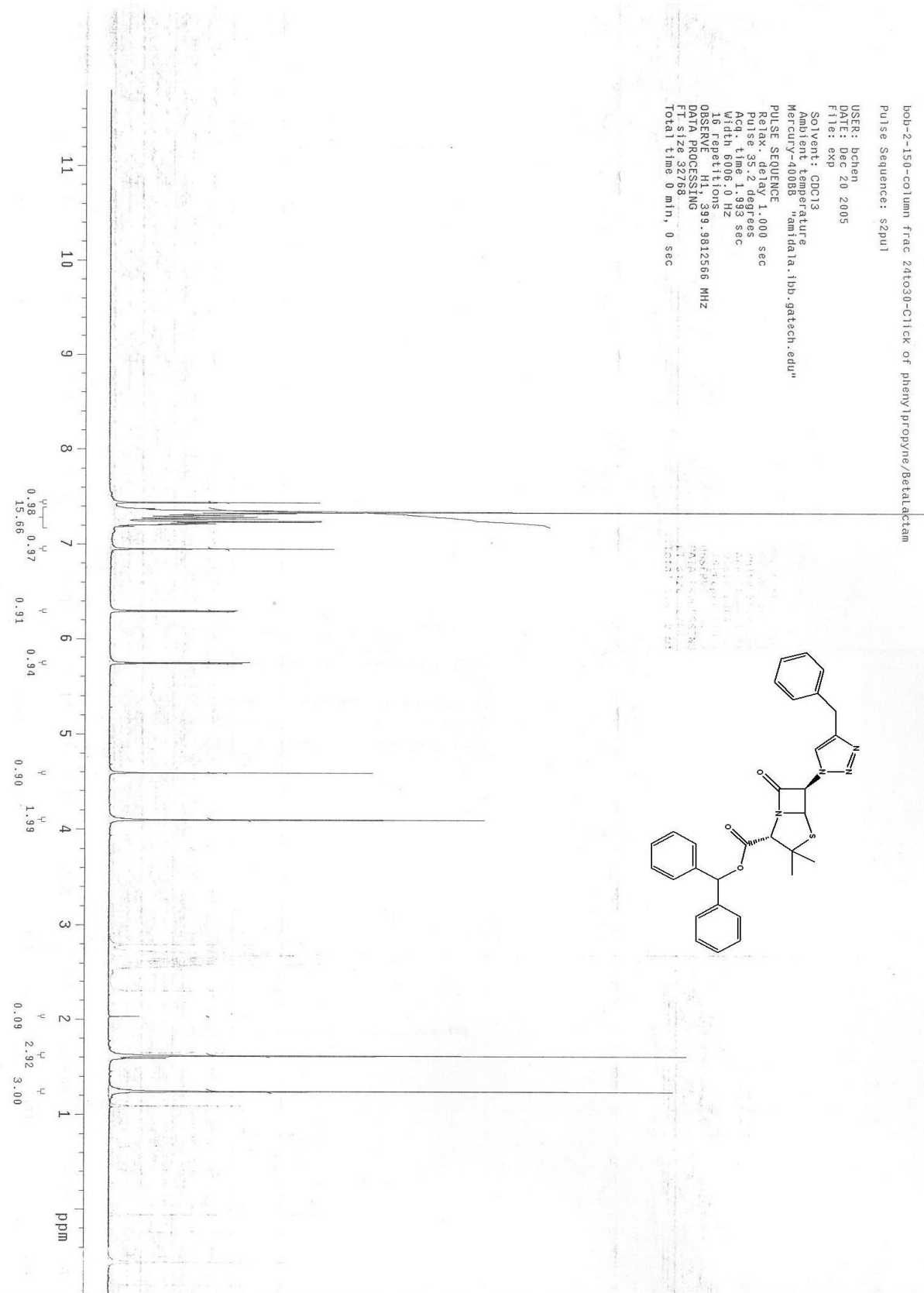


A0-001-045
Pulse Sequence: szpu1
USER: bchen
DATE: Feb 18 2006
File: exp
Solvent: CDCl3
Ambient Temperature
Mercury-400BB "amidata.ibd.gatech.edu"
PULSE SEQUENCE
Pulse, delay 1.000 sec
Relax, delay 1.000 sec
Pulse, delay 1.000 sec
Acq. time 1.935 sec
Width 6006.0 Hz
Nuclei 13C
Observed 13C 99.9812576 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

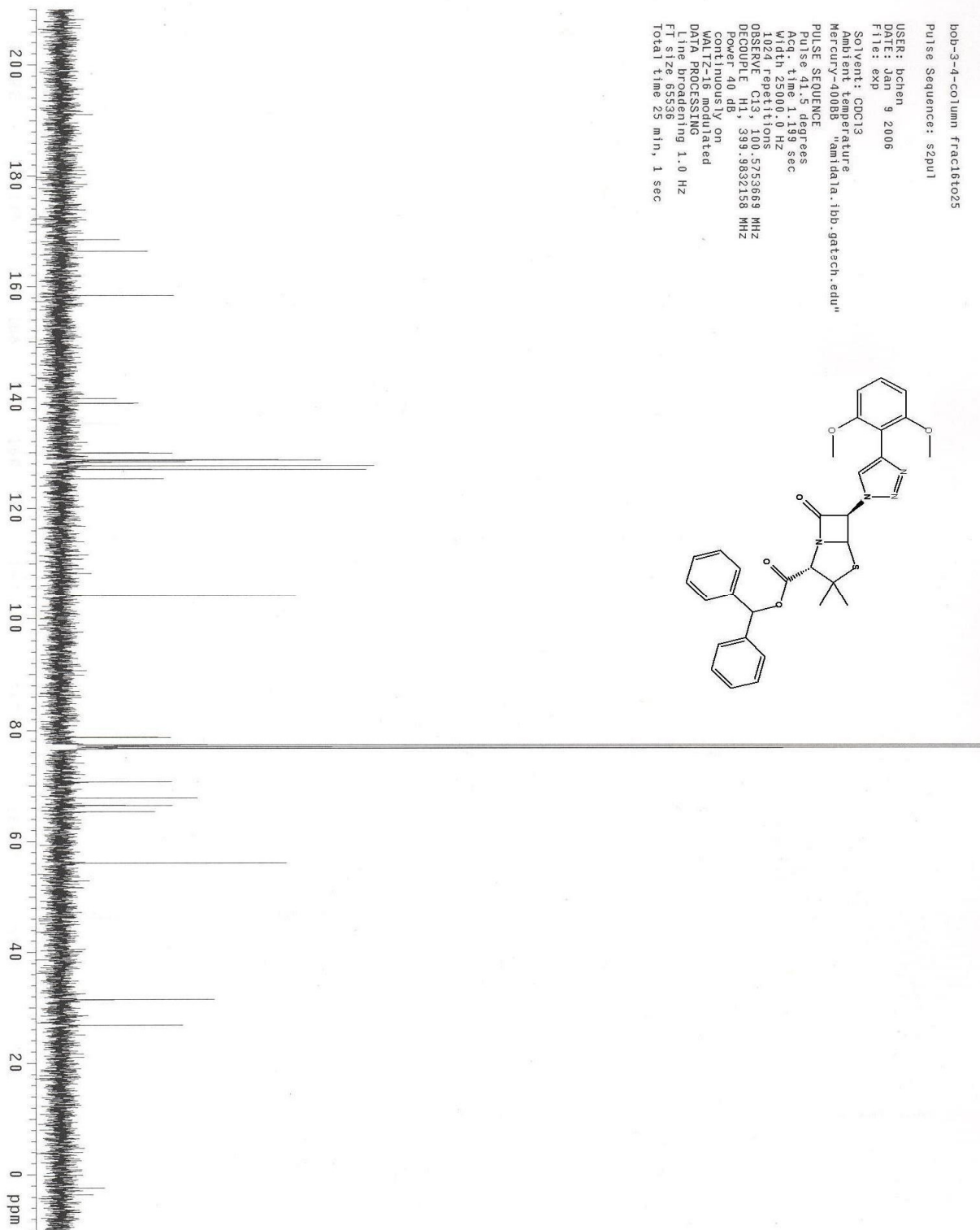
¹³C NMR of 8b:



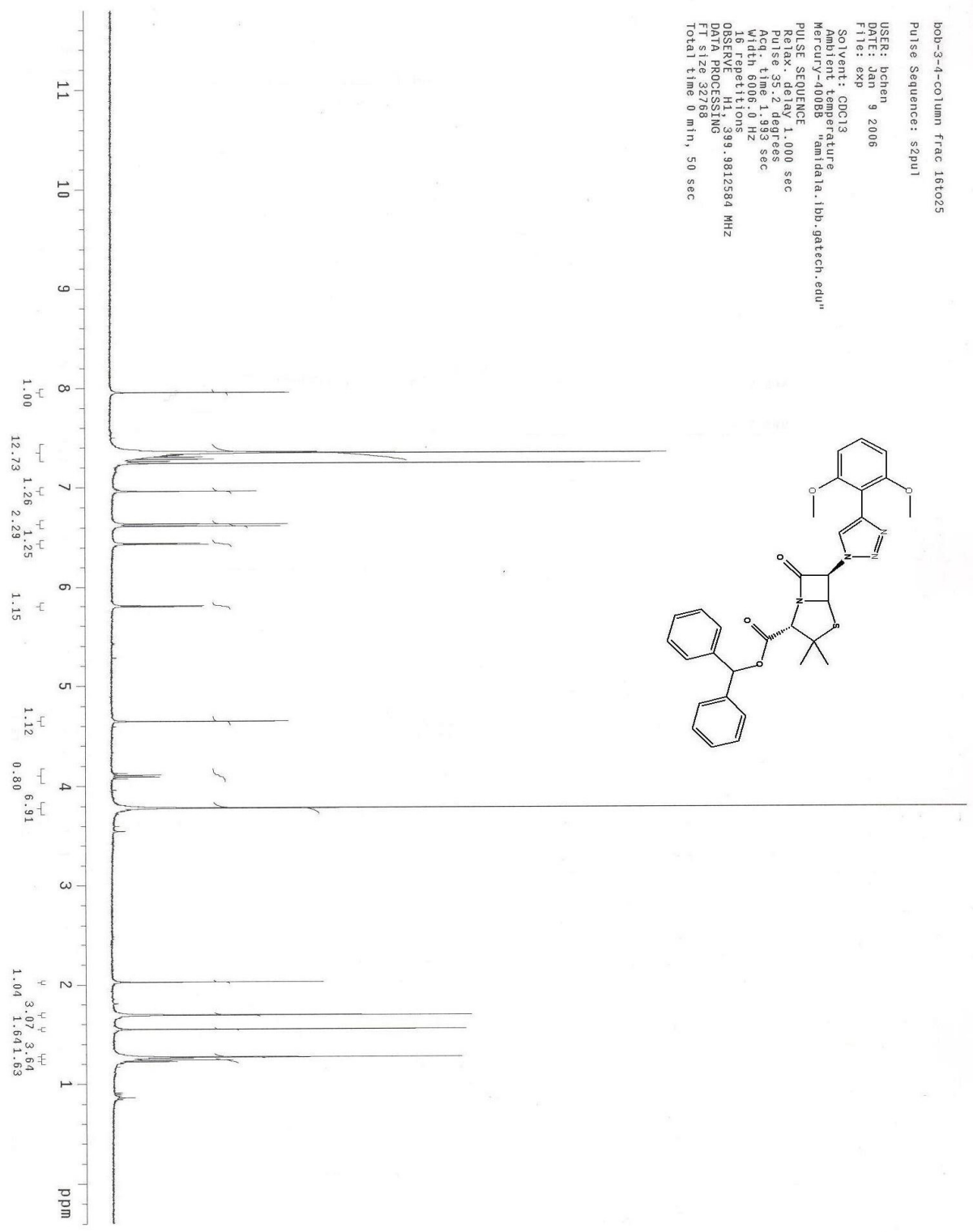
¹H NMR of **8b**:



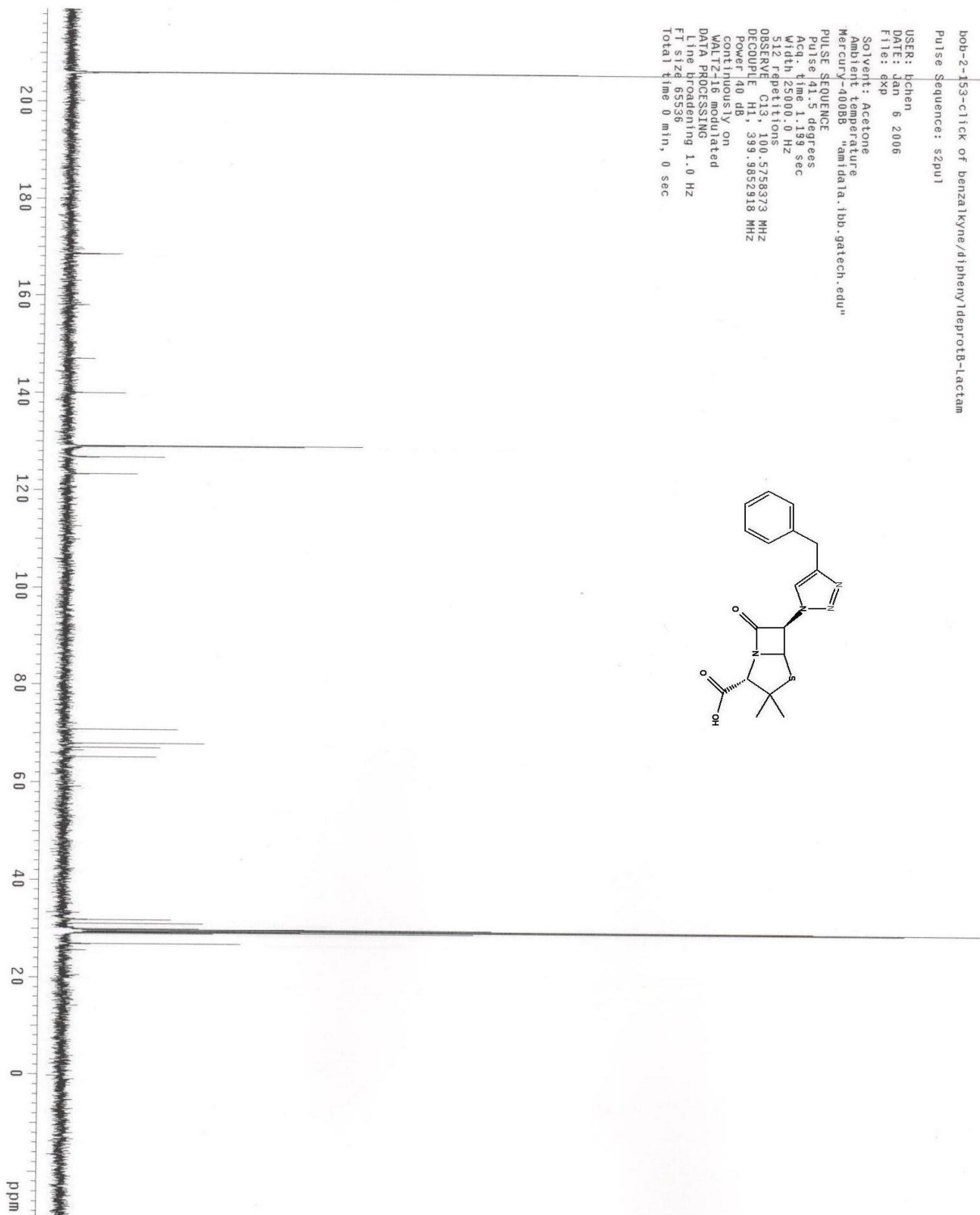
¹³C NMR of 8c:



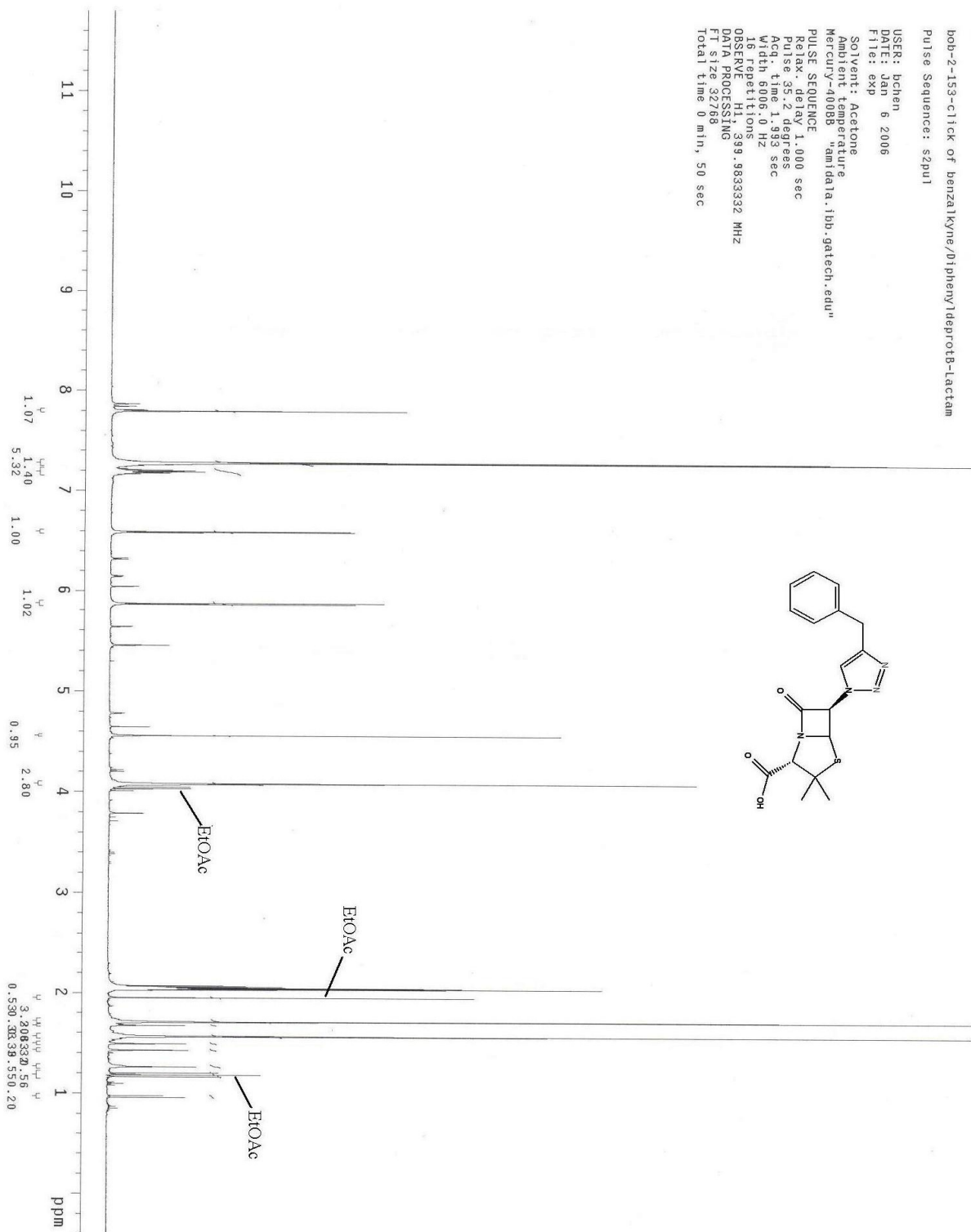
¹H NMR of 8c:



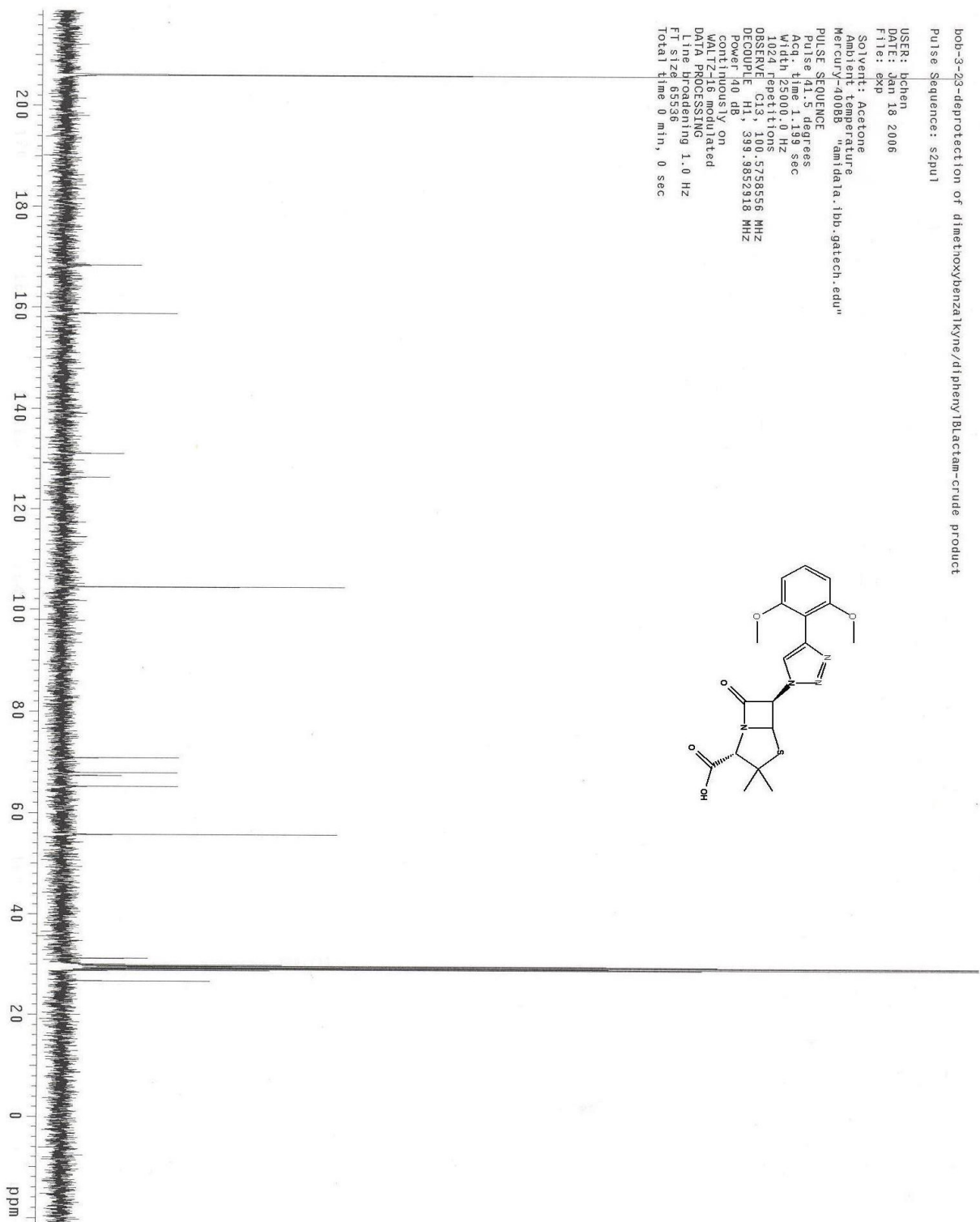
¹³C NMR of 9a:



¹H NMR of 9a:

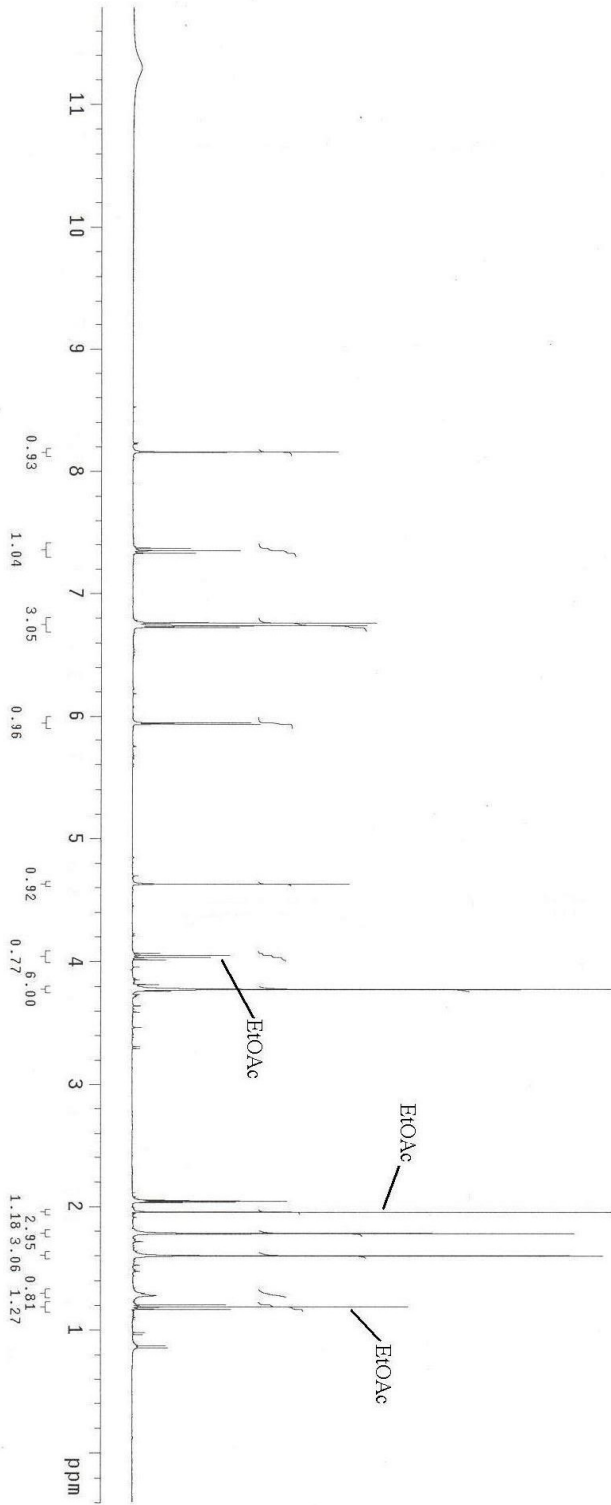
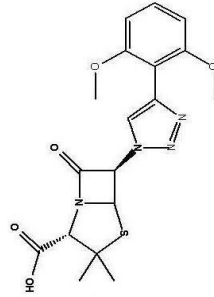


¹³C NMR of 9b:



bob-3-23-deprotection of dimethoxybenzylkyne/diphenylLactam-crude product
Pulse Sequence: s2pu1

USER: bchen
DATE: Jan 18 2006
File: exp
Solvent: Acetone
Ambient temperature
Mercury-400B8 "amidata.lpb.gatech.edu"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 35.2 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 399.9833310 MHz
DATA PROCESSING
F1 size 32768
Total time 0 min, 0 sec

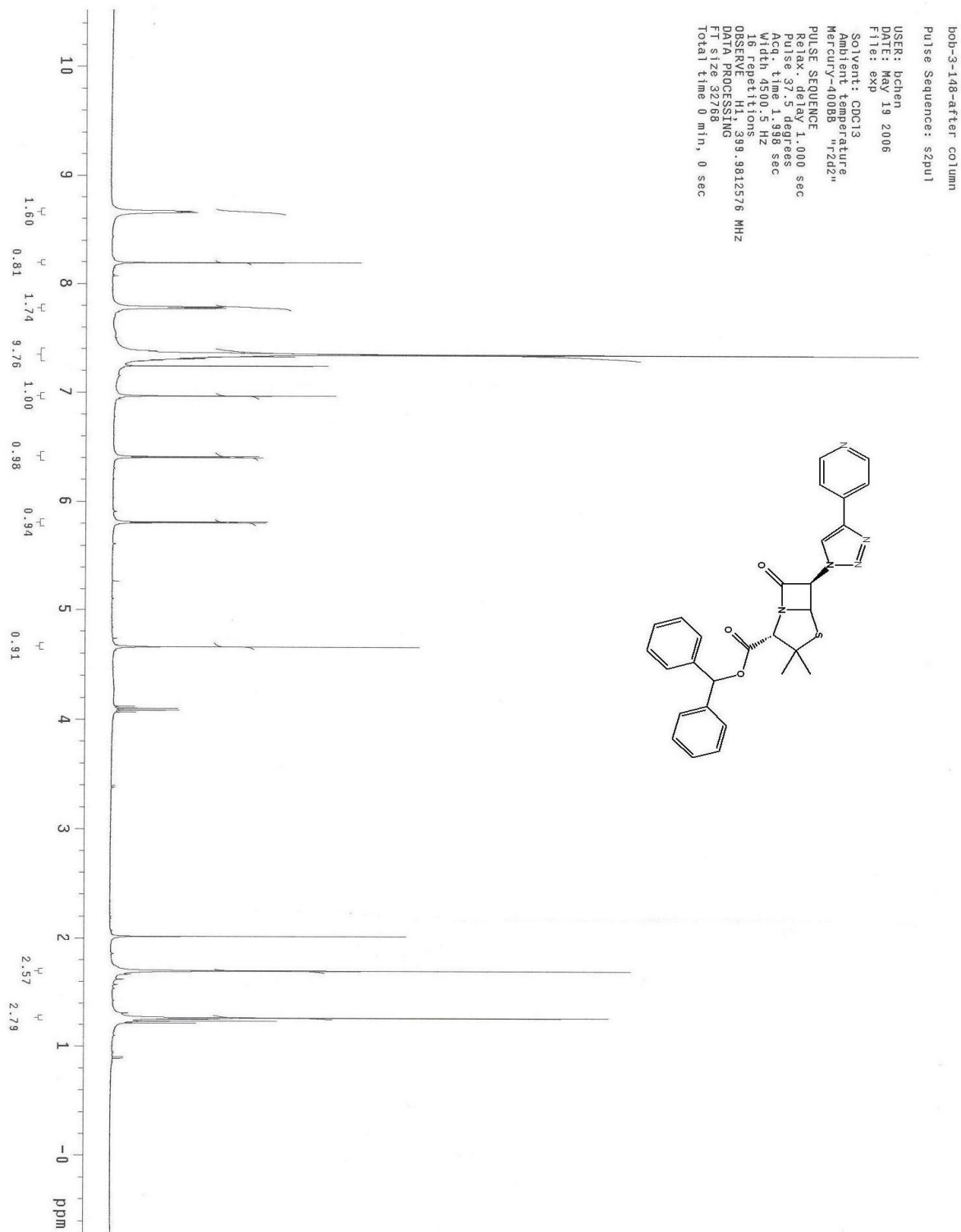


¹H NMR of **9b**:

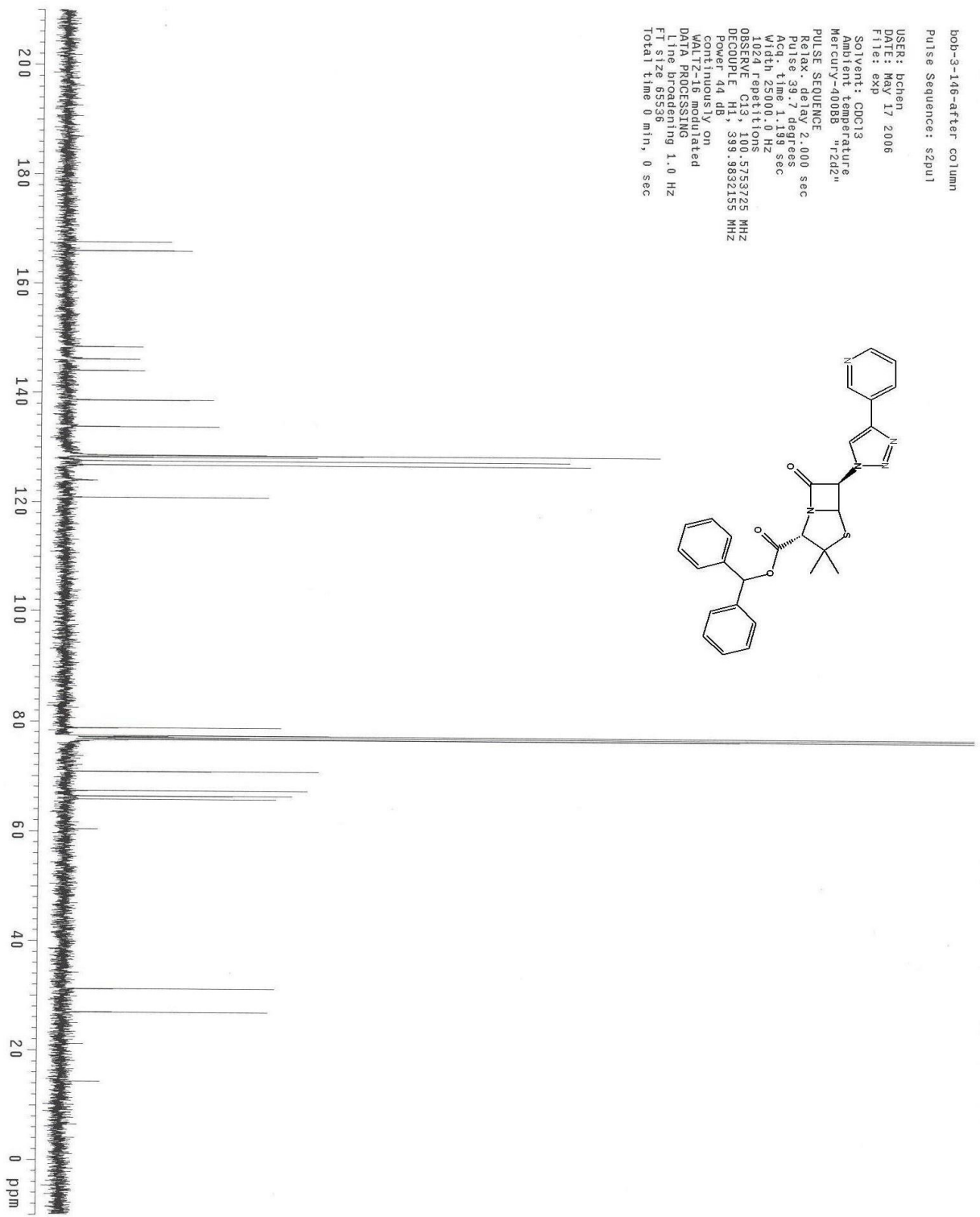
¹³C NMR of 11a:



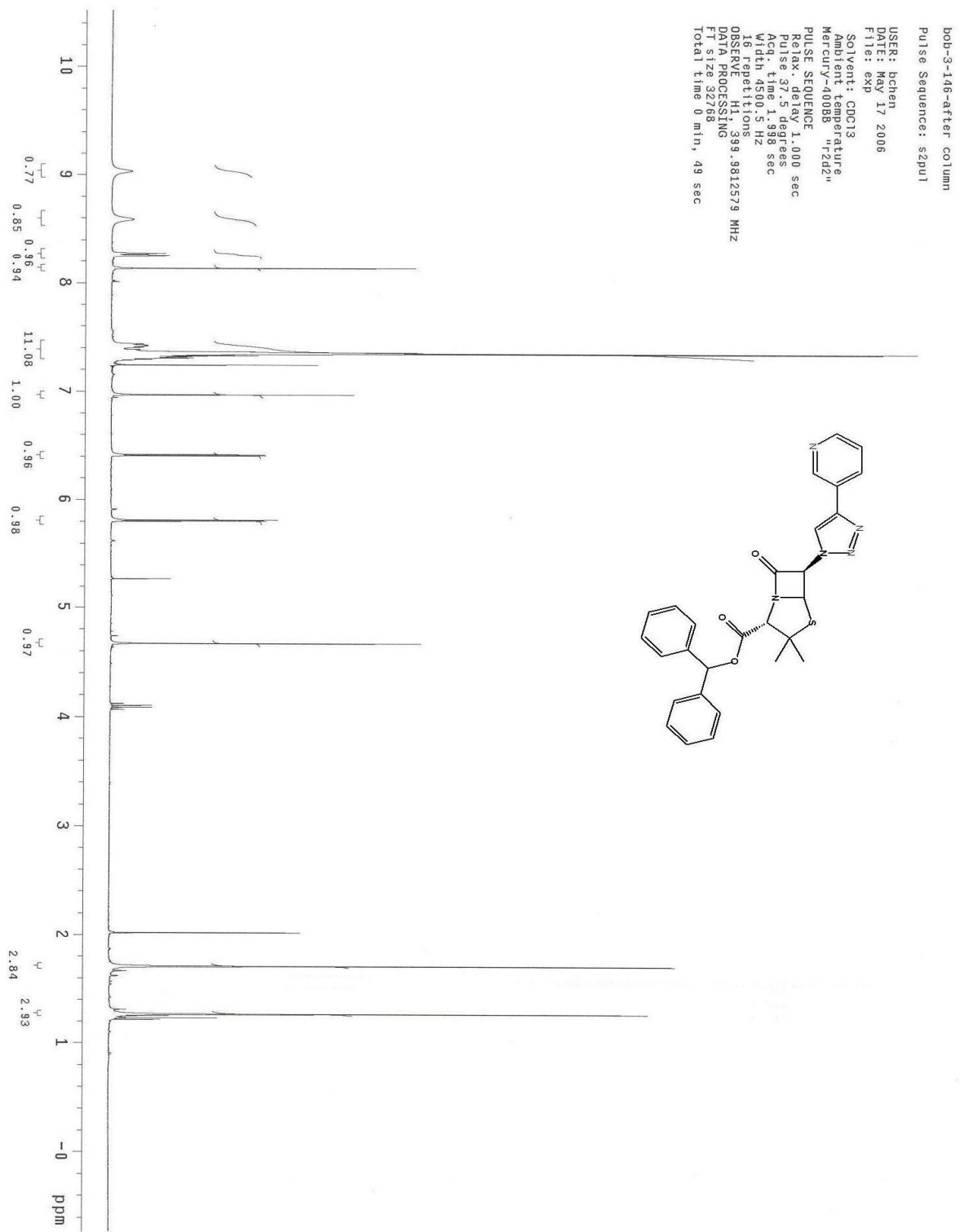
¹H NMR of 11a:



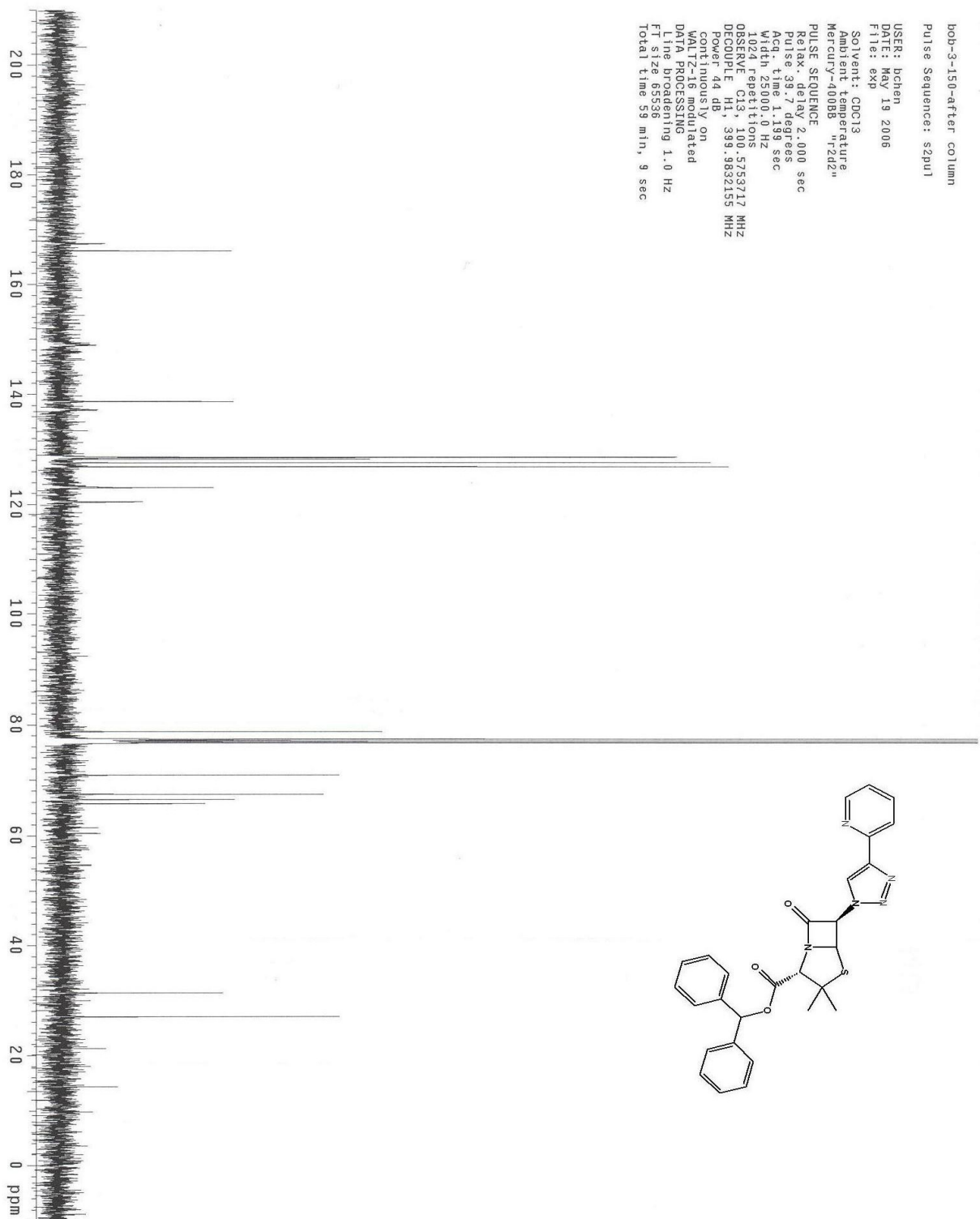
¹³C NMR of 11b:



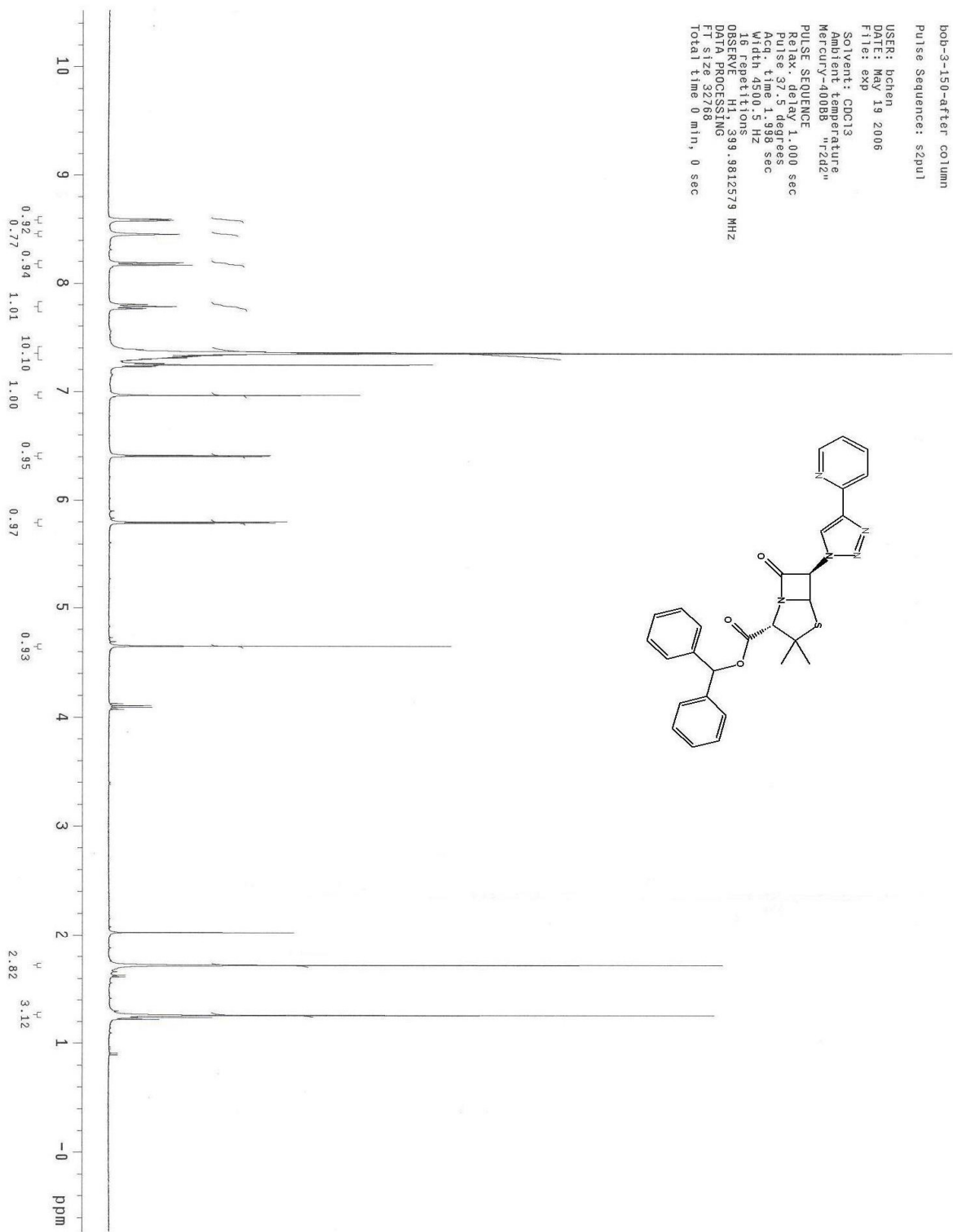
¹H NMR of **11b**:



¹³C NMR of 11c:

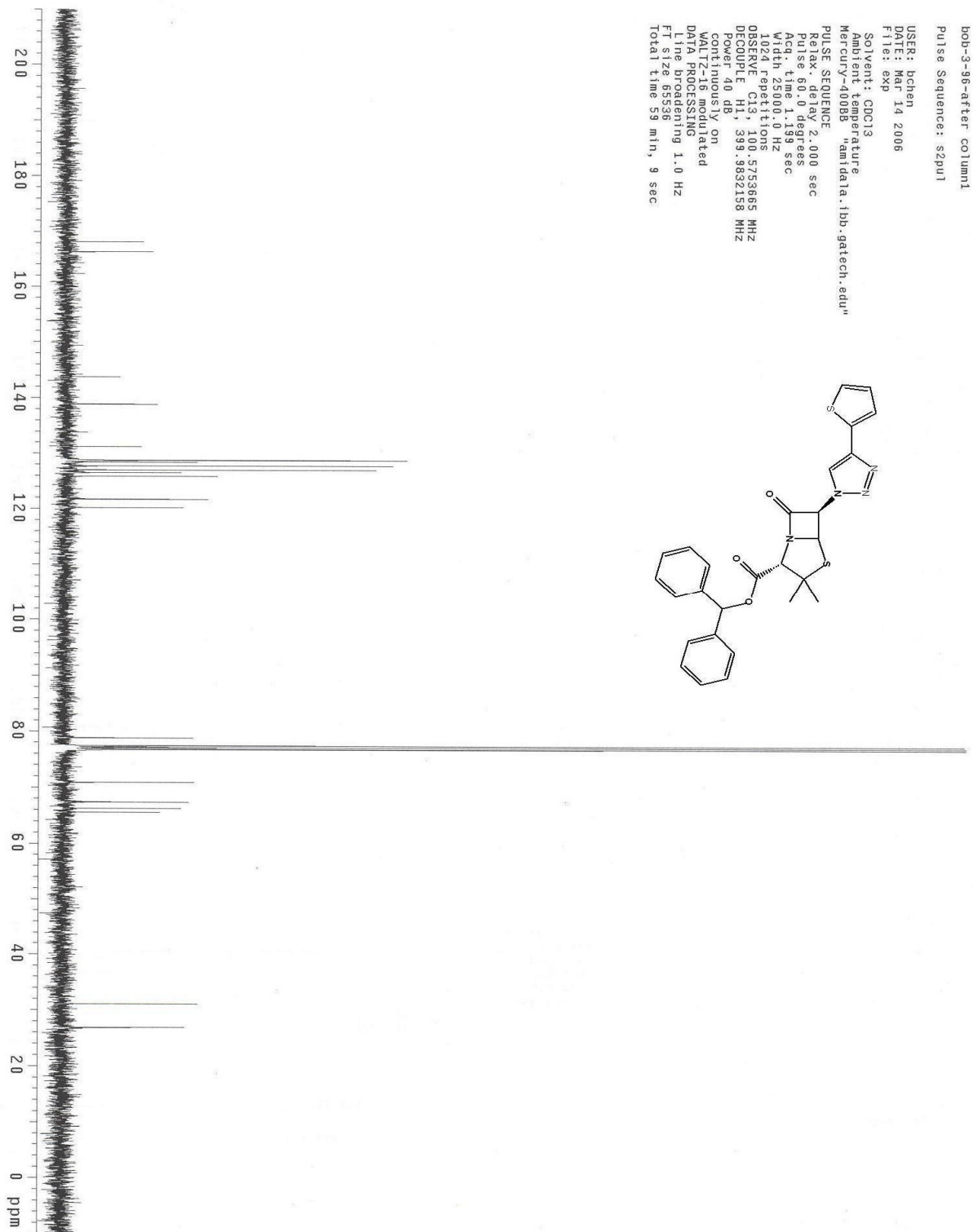


¹H NMR of 11c:

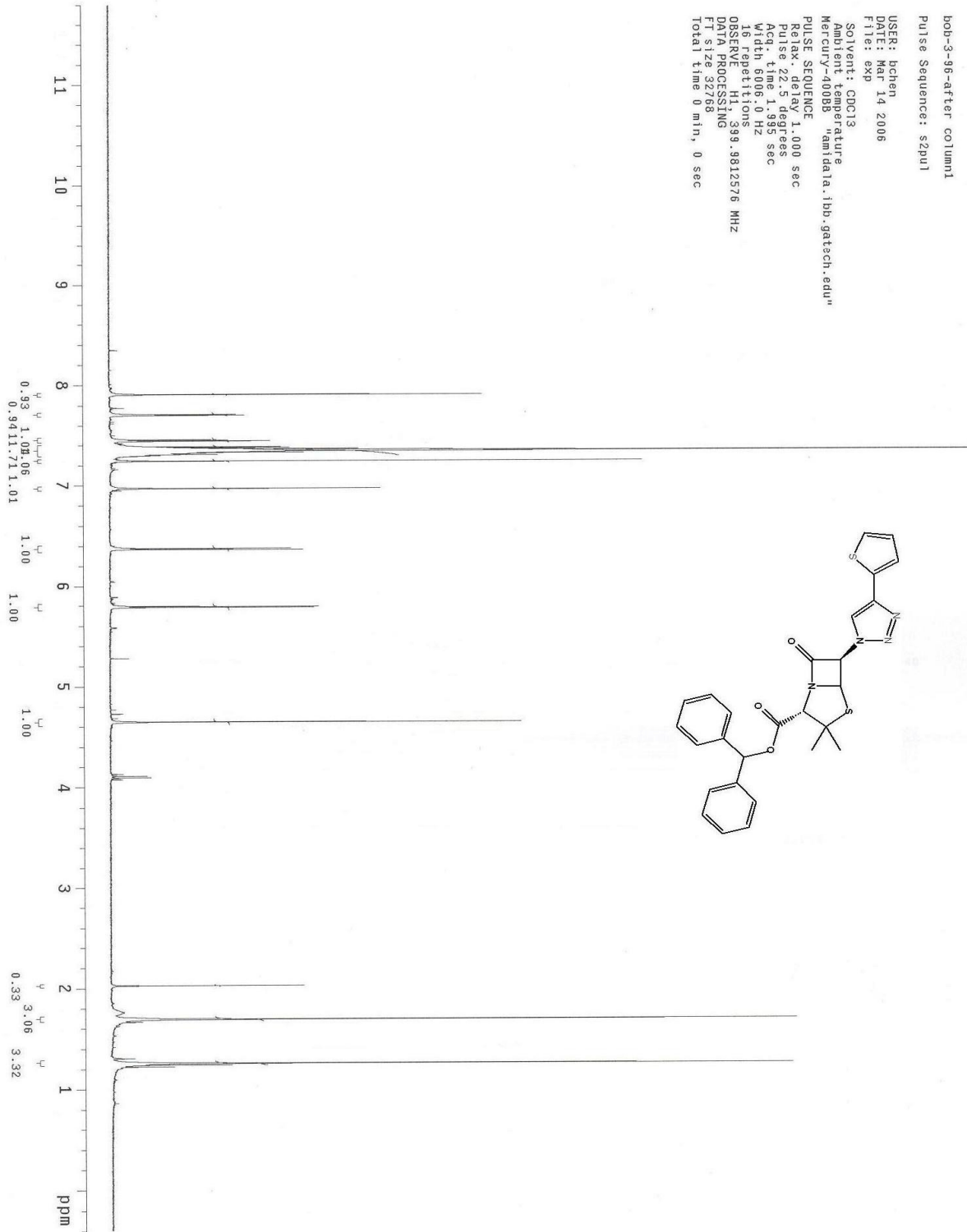


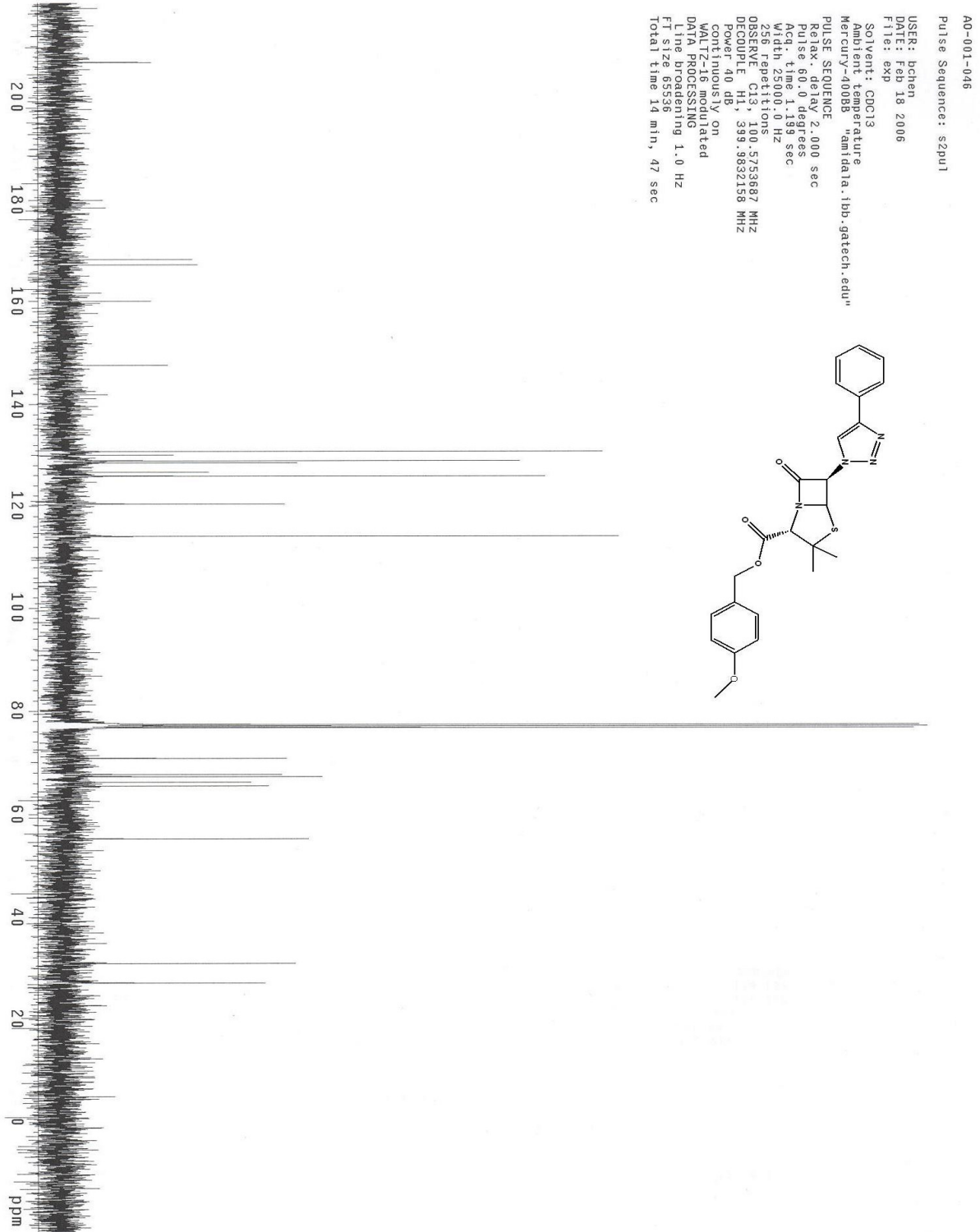
bob-3-150-after column
Pulse Sequence: s2pul
USER: bchen
DATE: May 19 2006
File: exp
Solvent: CDCl3
Ambient temperature
Mercury-400BB "r2d2"
PULSE SEQUENCE
Rf1sk: 491.84 1.000 sec
Pulse: 37.5 degrees
Acq time: 1.998 sec
Width: 4500.5 Hz
16 repetitions
OBSERVE: H1, 399.9812579 MHz
DATA PROCESSING
FT size: 32768
Total time: 0 min, 0 sec

¹³C NMR of 11d:

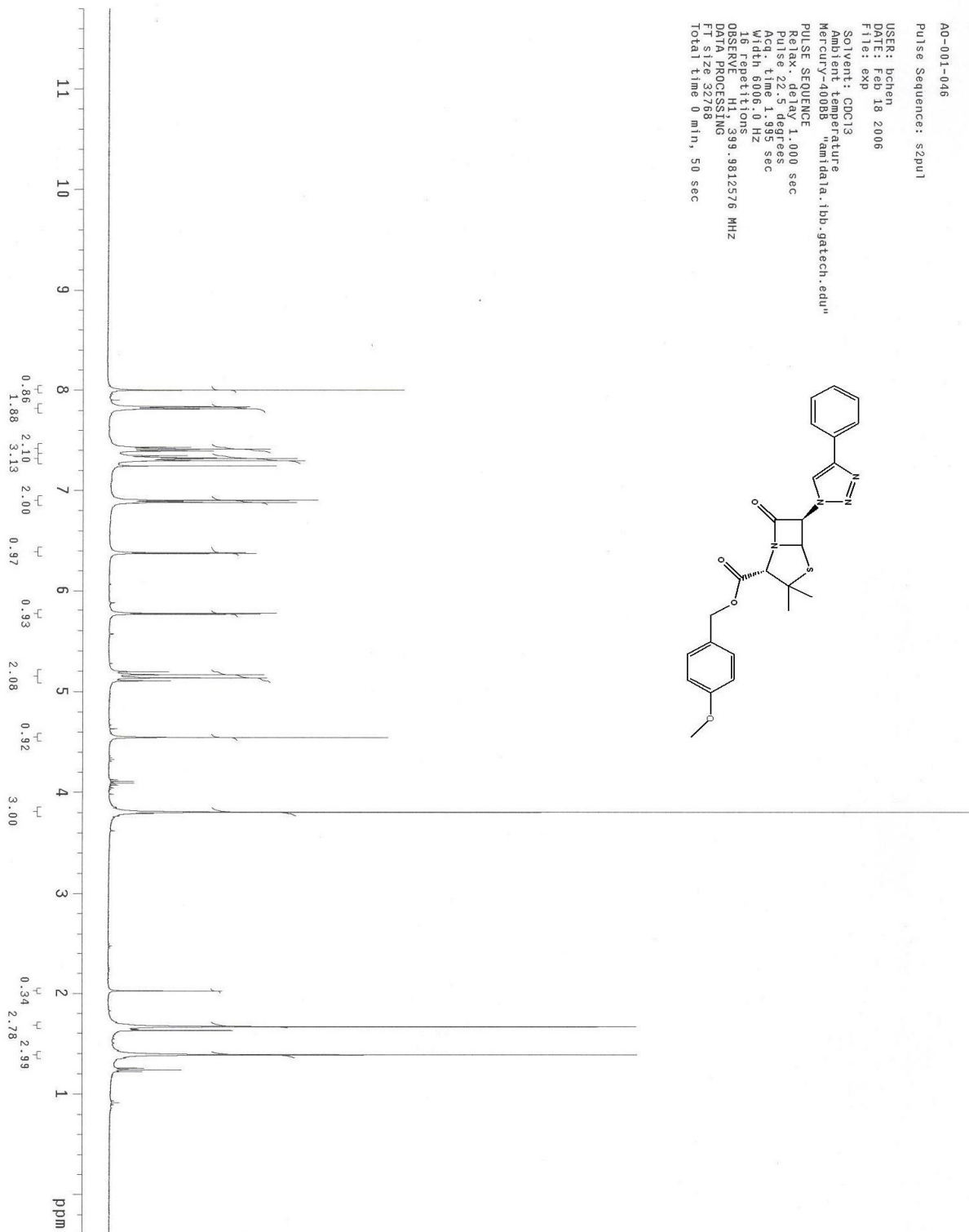


¹H NMR of 11d:

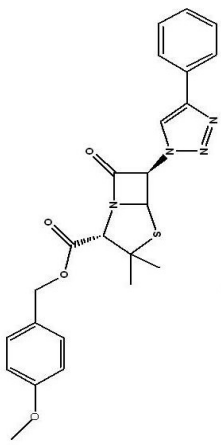




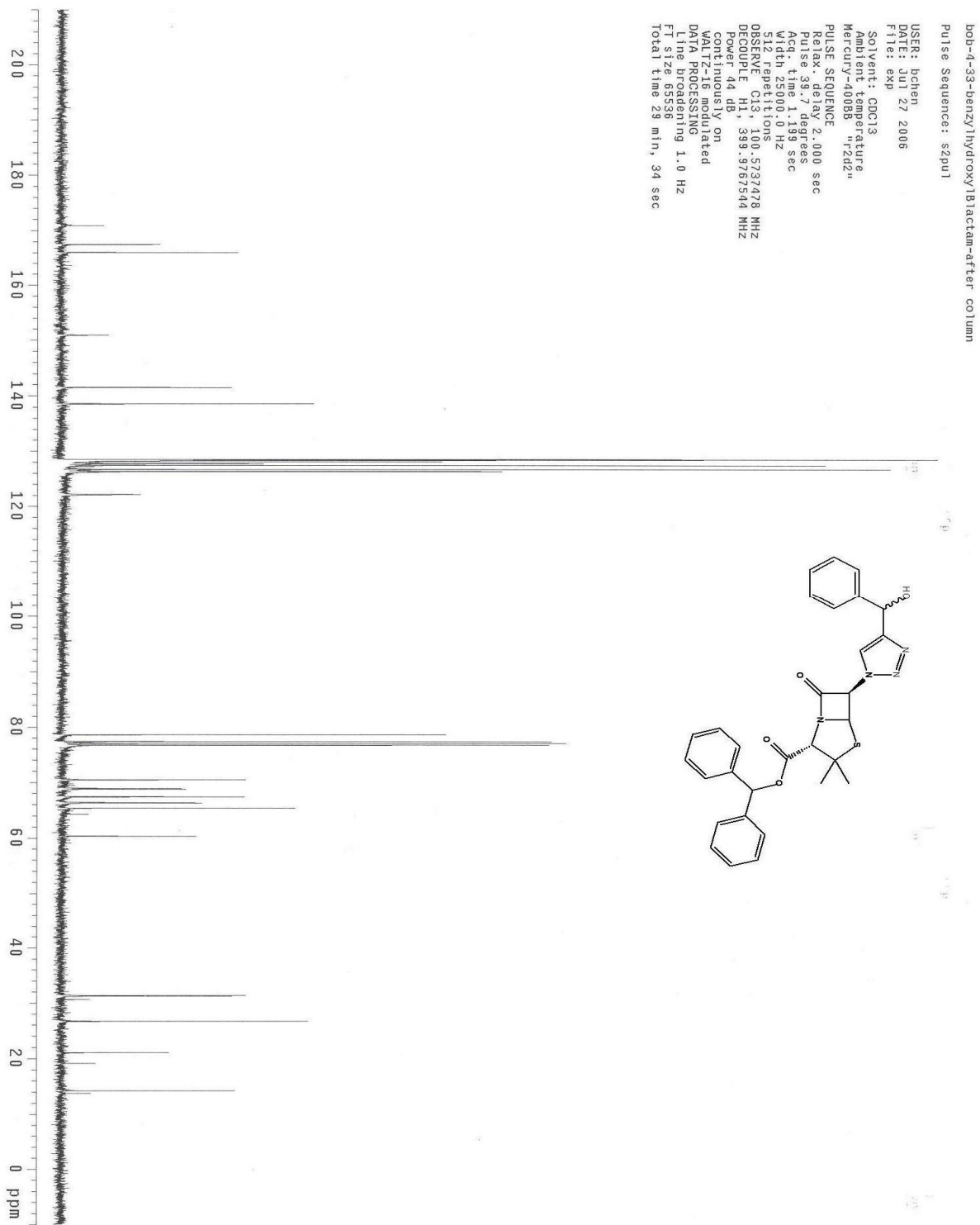
¹H NMR of 11e.



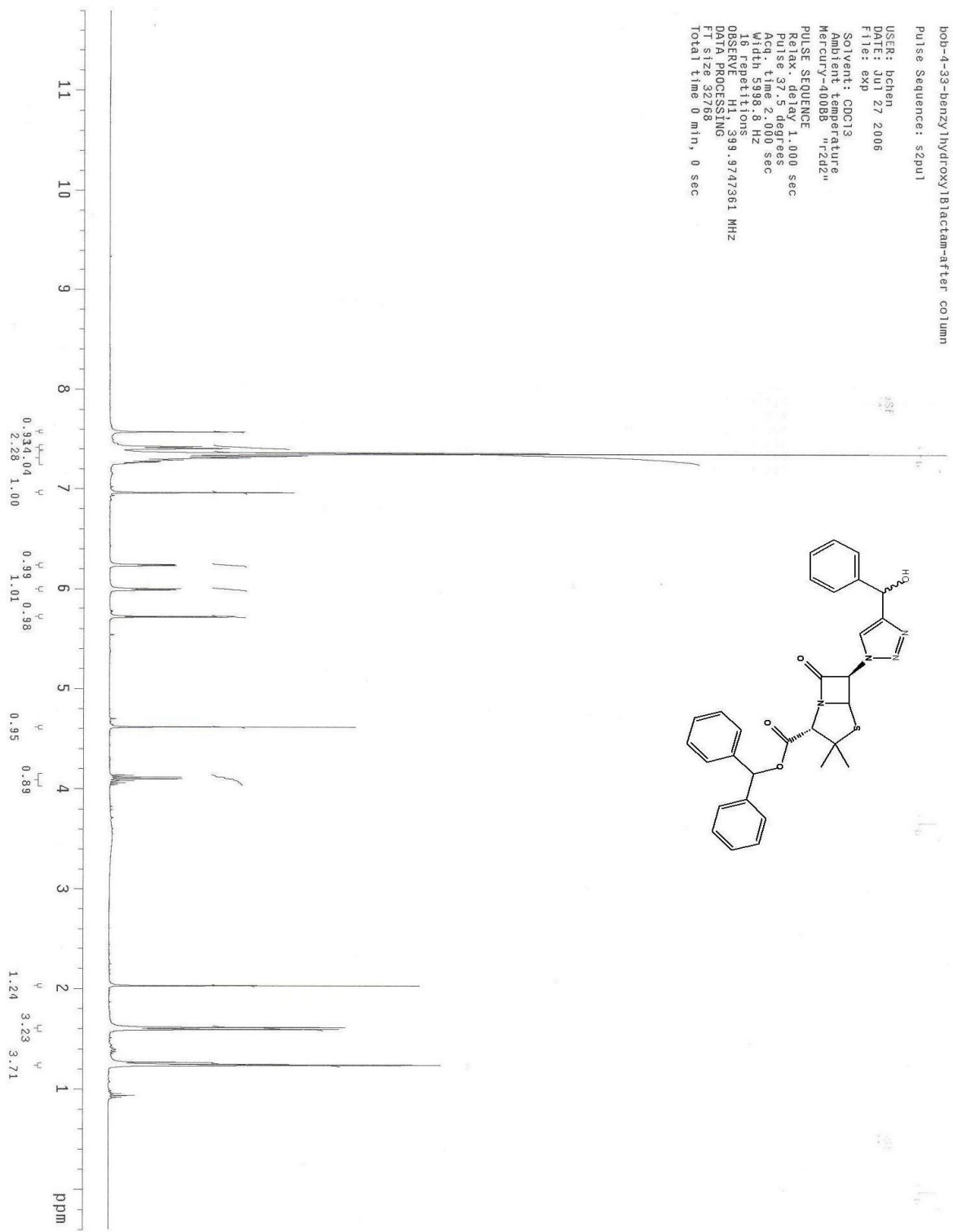
AO-001-046
Pulse Sequence: s2pu1
USER: bchen
DATE: Feb 18 2006
File: exp
SOLVENT: CDCl3
Ambient temperature
Mercury-400BB "amida.la.tib.gatech.edu"
PULSE SEQUENCE
Relax: delay 1.000 sec
Pulse: 22.5 degrees
Acq: time 1.935 sec
Wdth: 100 Hz
16 repetitions
OBSERVE H1 399.9812576 MHZ
DATA PROCESSING
FT size 32788
Total time 0 min, 50 sec



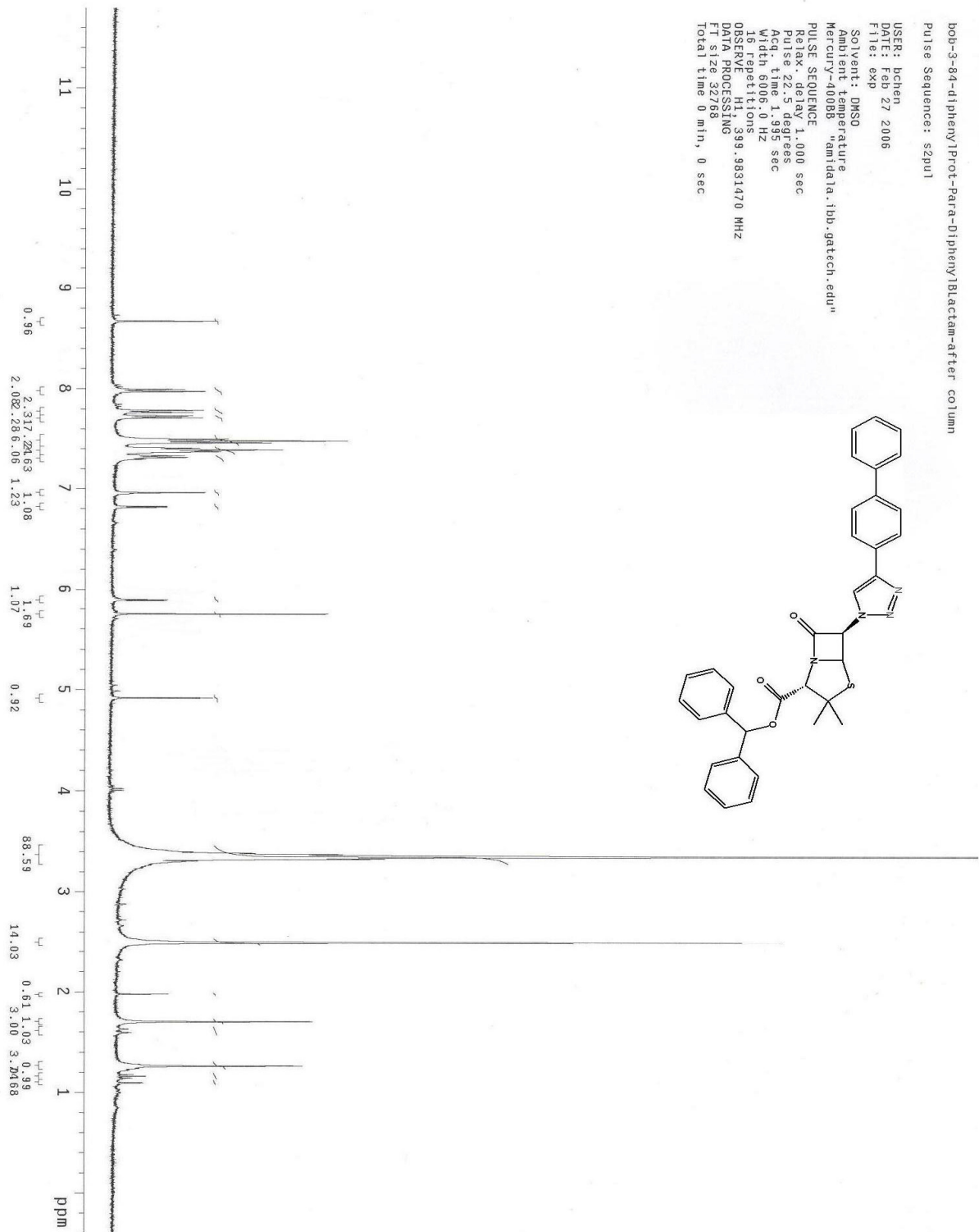
¹³C NMR of 11f:



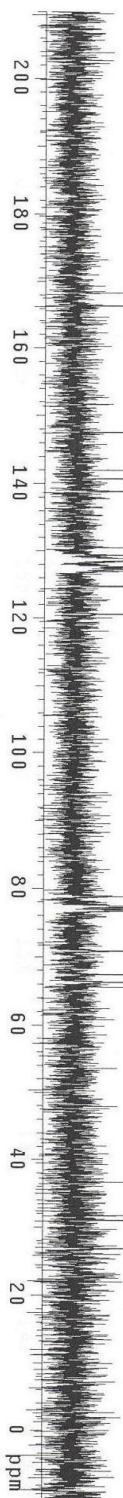
¹H NMR of 11f:



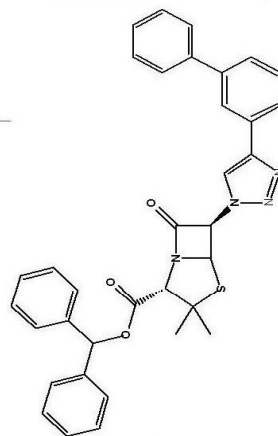
¹H NMR of **11g**:



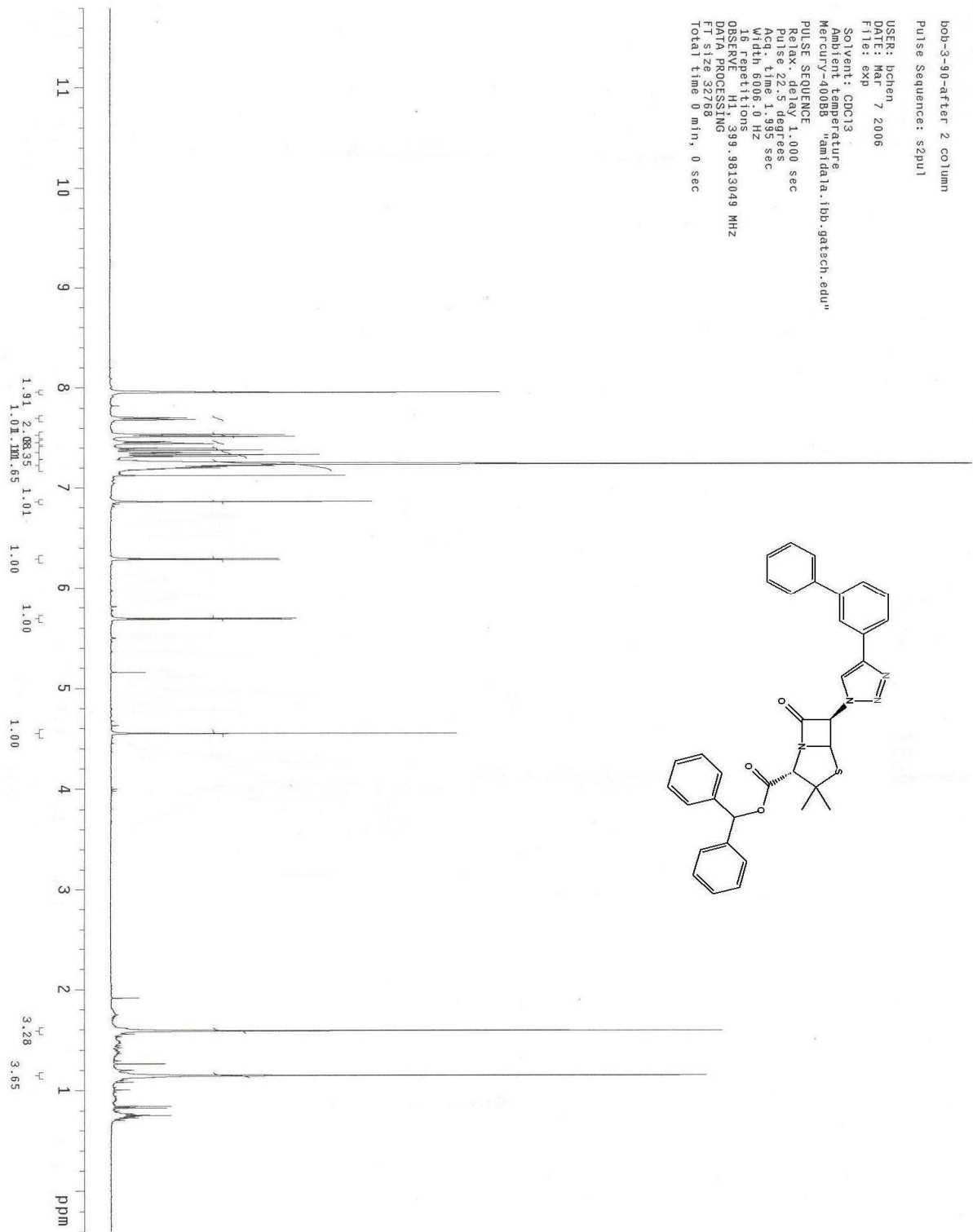
¹³C NMR of 11h:



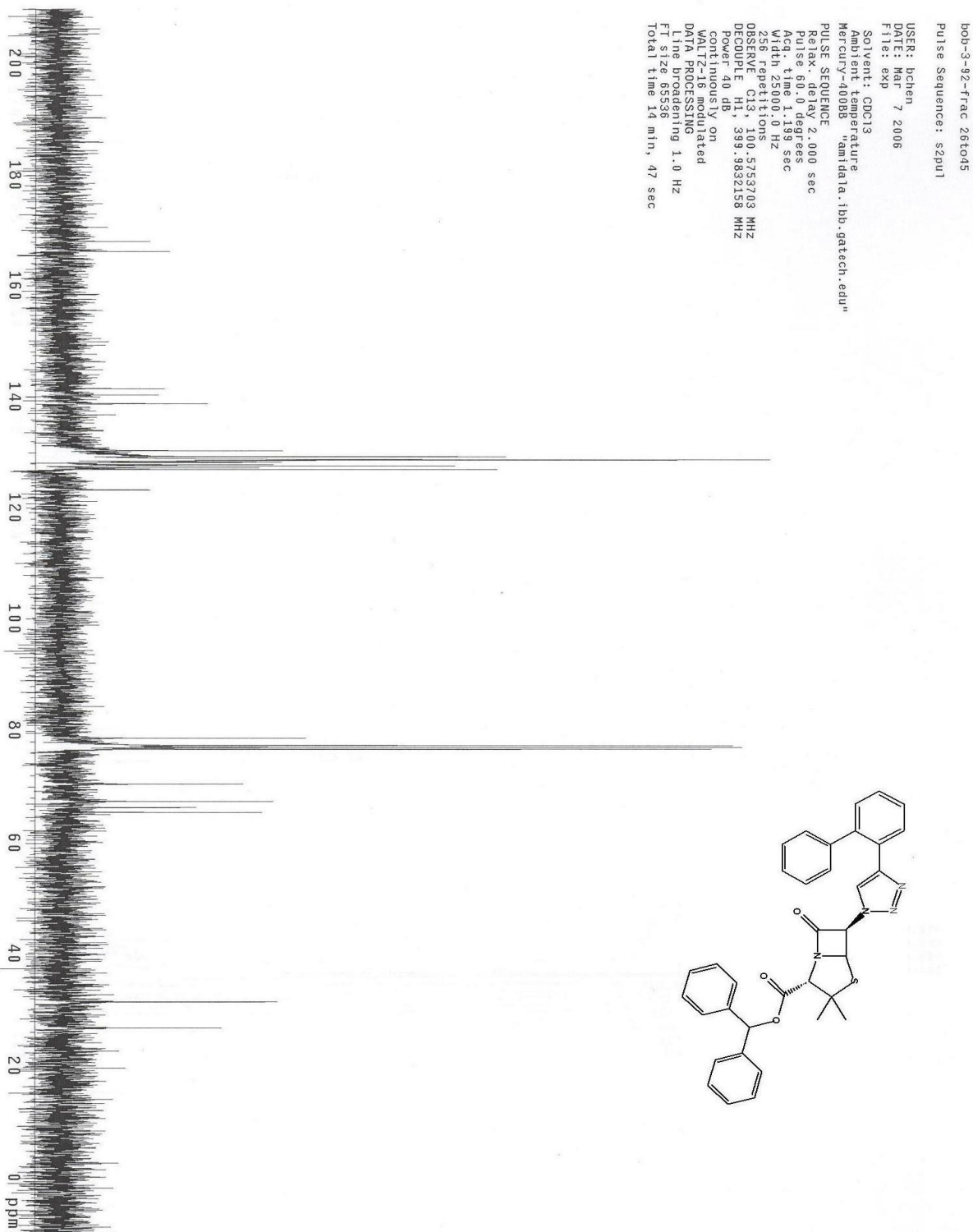
bob-3-90-after 2 column
Pulse Sequence: s2pu1
USER: hchen
DATE: Mar 7 2006
File: exp
Solvent: CDCl3
Ambient temperature
Mercury-400Bb "amidata.ibh.gatech.edu"
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse program
Acq. time 1.199 sec
Width 23000.0 Hz
Spectrum
06SERV03 0 5759695 MHz
DECUPLE H1 399.9822158 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 HZ
FT size 65536
Total time 14 min, 47 sec



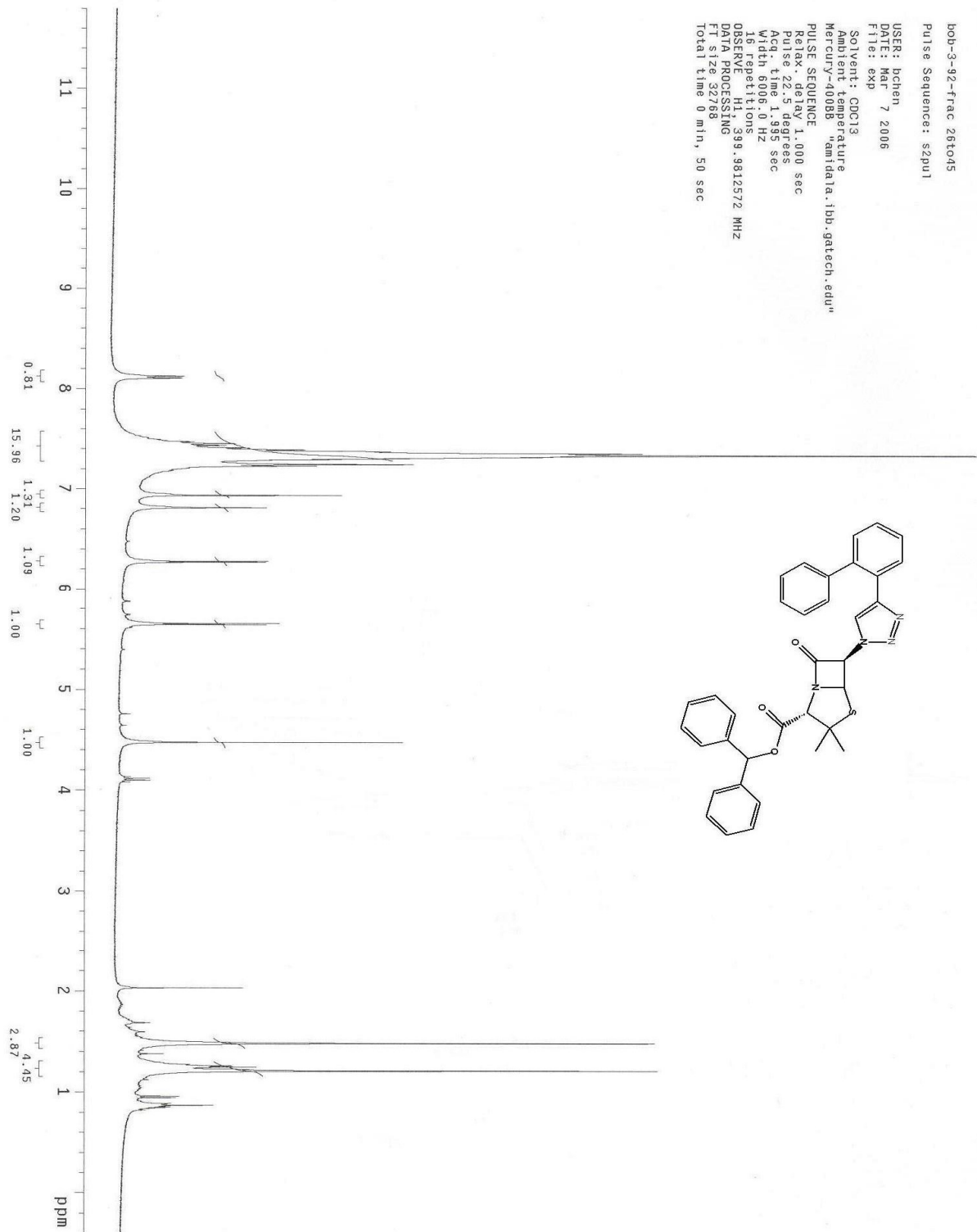
¹H NMR of 11h:



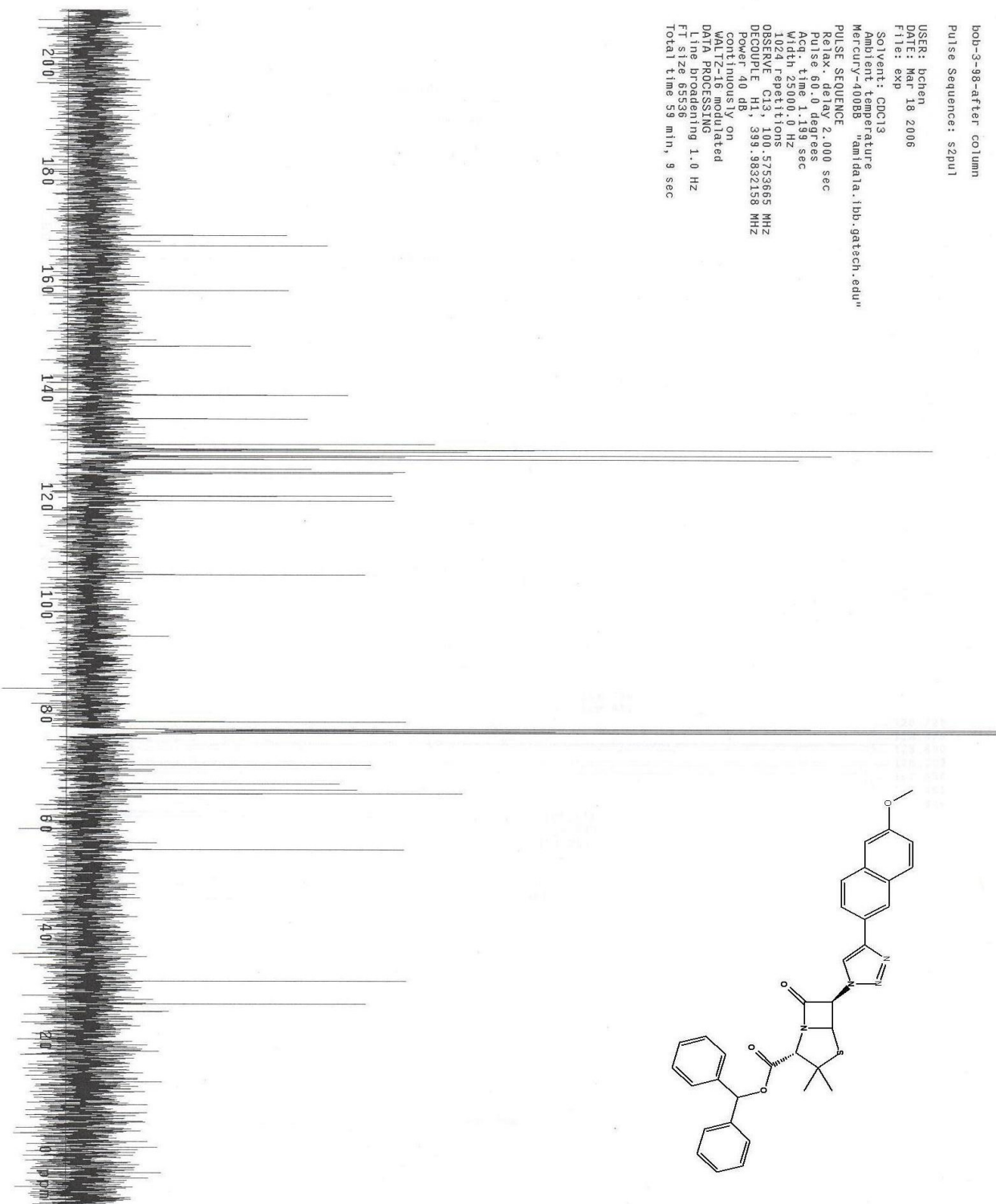
¹³C NMR of 11i:



¹H NMR of **11i**:

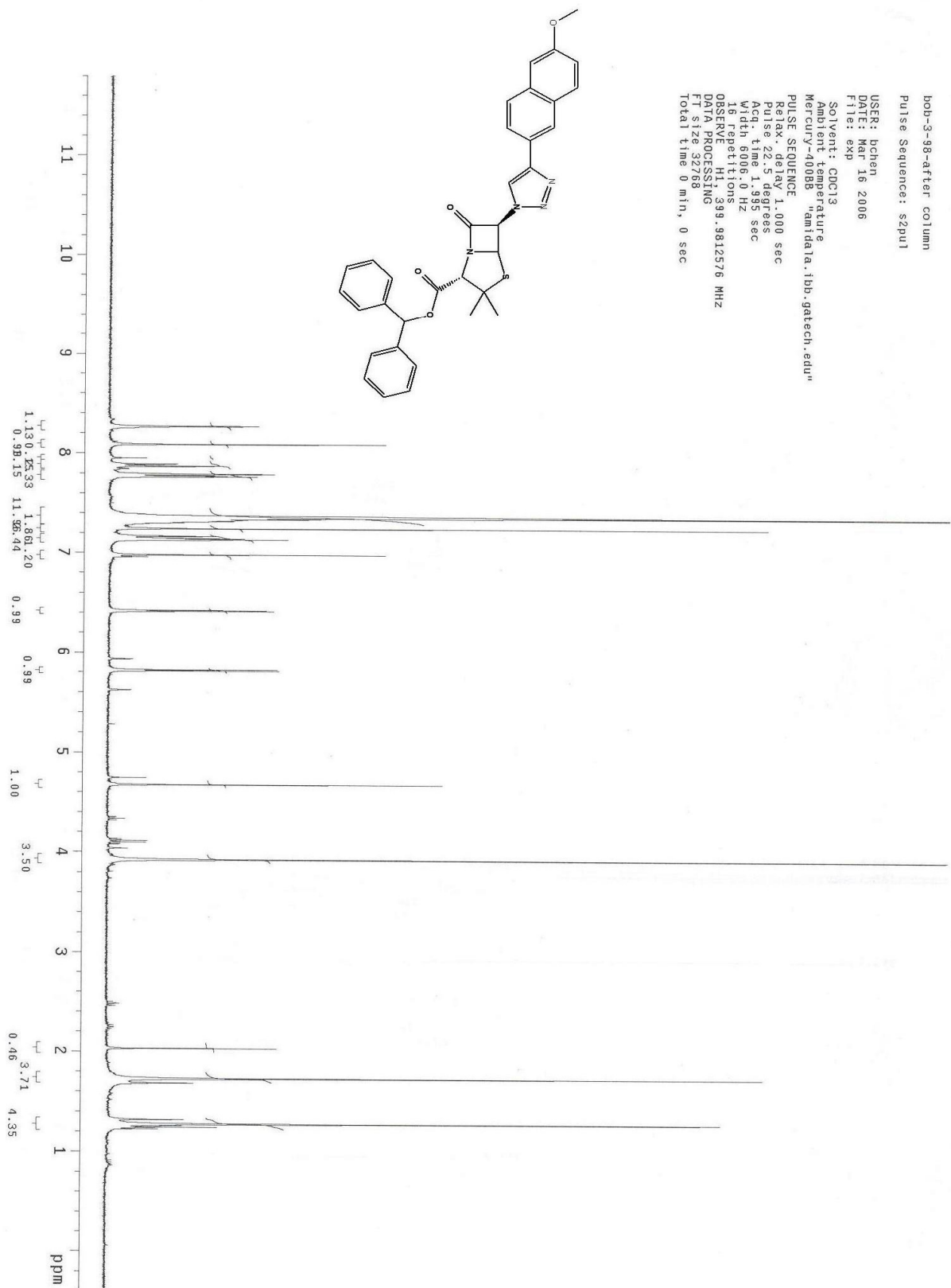


¹³C NMR of 11j:

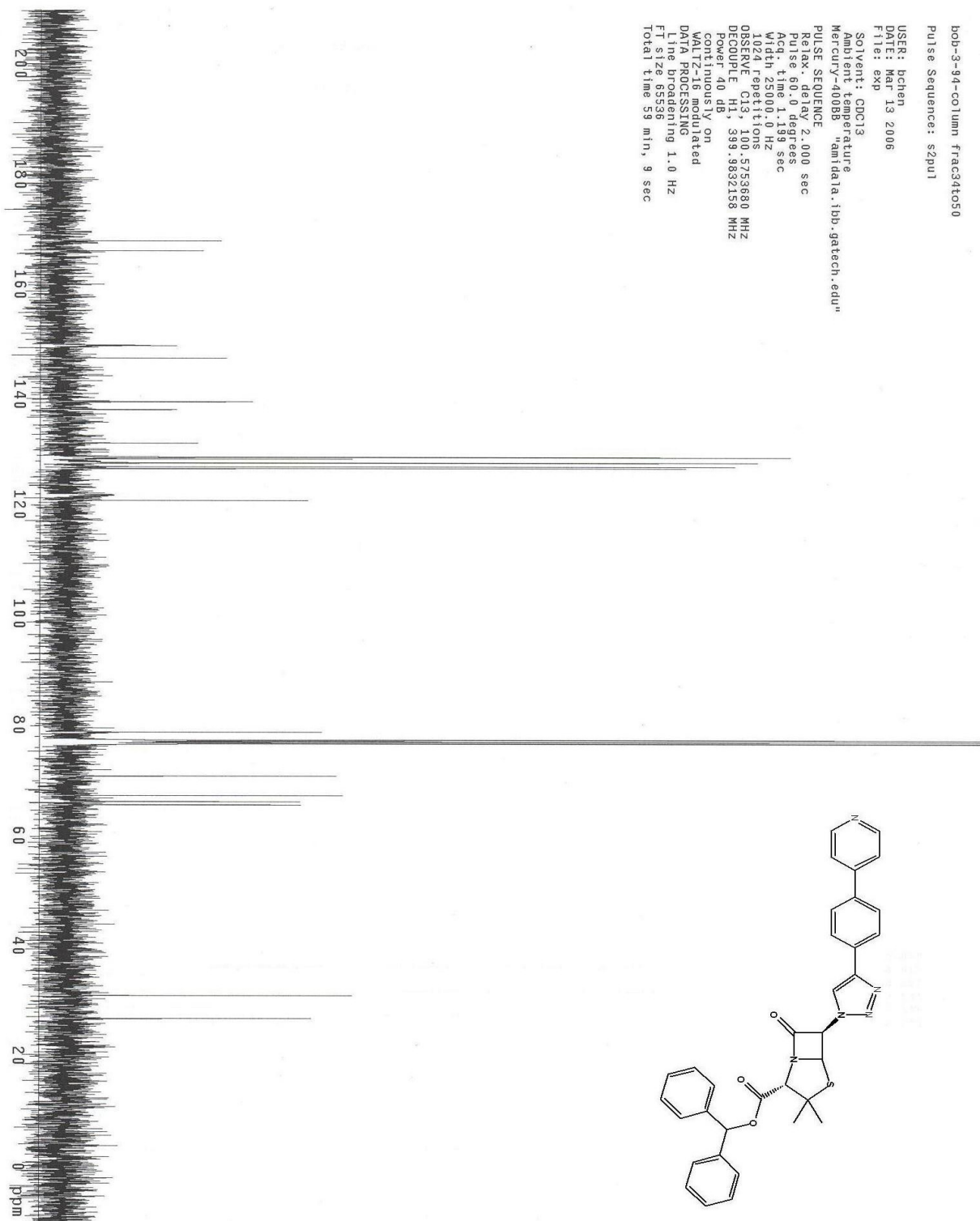


bob-3-98-after column
Pulse Sequence: s2pu1
USER: bchen
DATE: Mar 18 2006
File: exp
Solvent: CDCl3
Ambient temperature
Mercury-400BB "amidata.lib.gatech.edu"
PULSE SEQUENCE
Relax delay/ 2.000 sec
Pulse prog/ zgpg30
Acq. time/ 1.199 sec
Width/ 25000.0 Hz
1024 Repetitions
OBSERVE/ C13, 100.5753665 MHz
DECUPLE/ H1, 399.9832158 MHz
Power/ 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening/ 1.0 Hz
FT size/ 65536
Total time/ 59 min, 9 sec

¹H NMR of 11j:

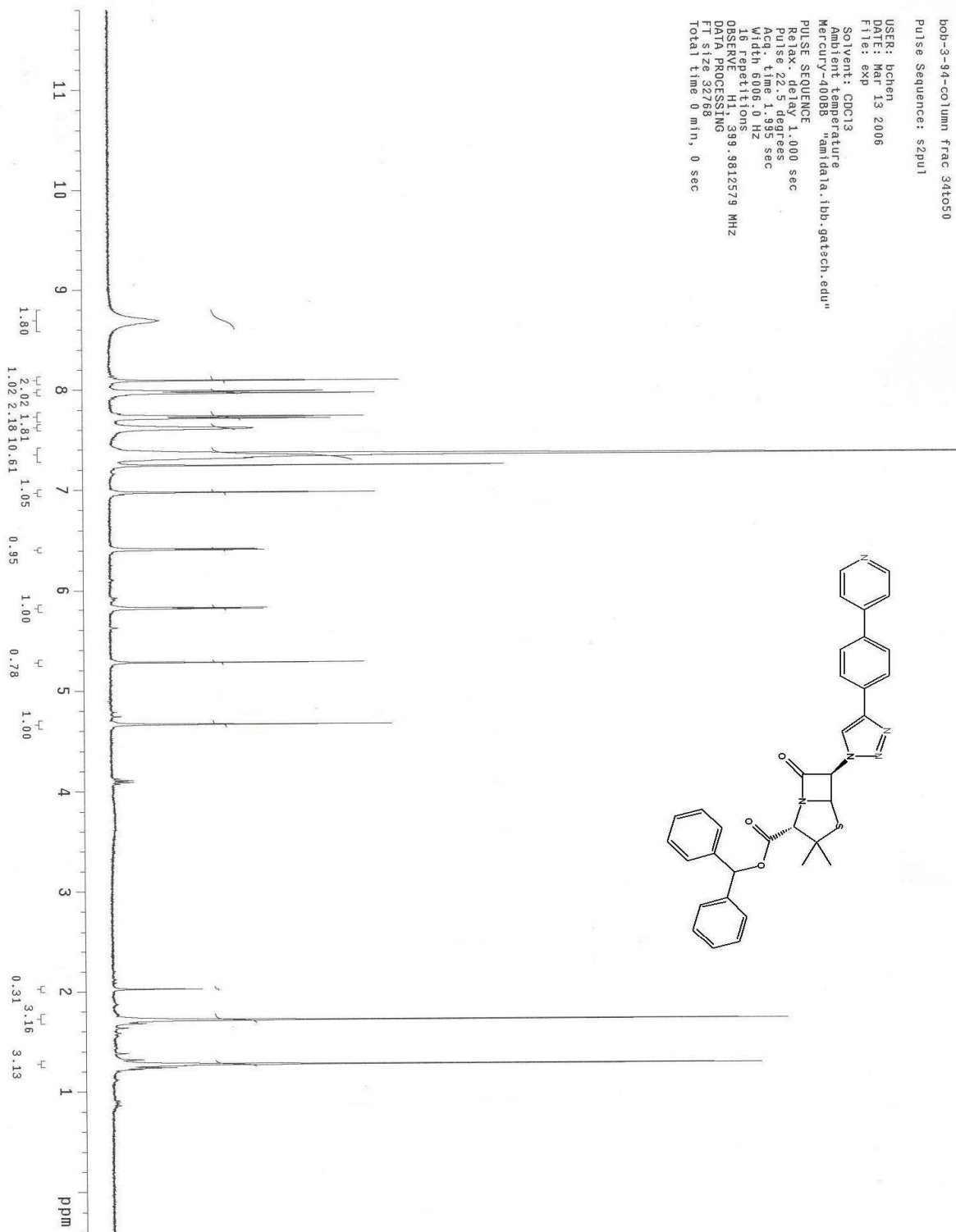


¹³C NMR of 11k:

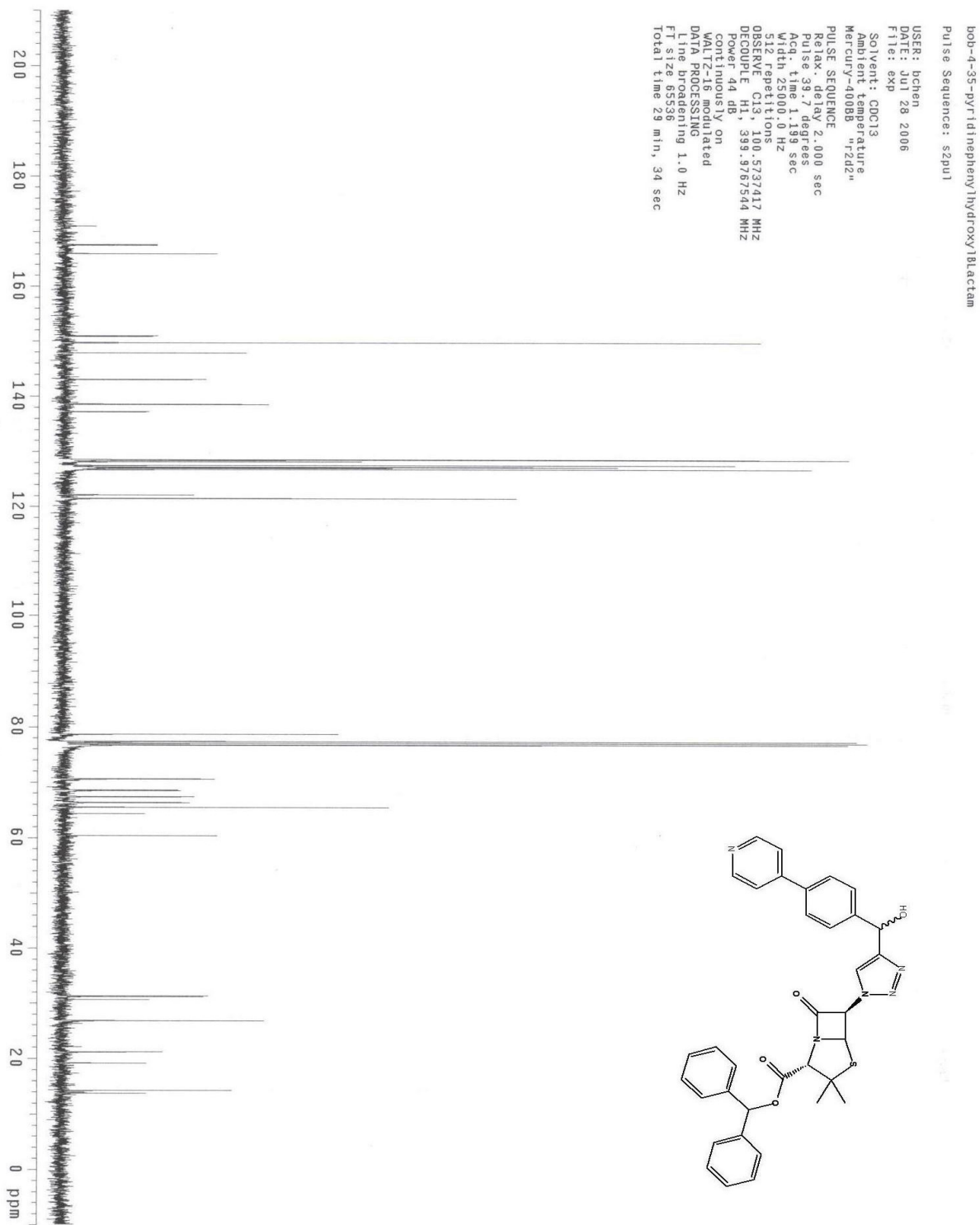


bob-3-94-column frac34to50
Pulse Sequence: s2pu1
USER: bchen
DATE: Mar 13 2006
File: exp
Solvent: CDCl3
Ambient temperature
Mercury-400B8 "amidata.lib.gatech.edu"
PULSE SEQUENCE
Relax: delay 2.000 sec
Pulse 60.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
1024 Repetitions
OBSERVE C13, 100.5753680 MHz
DECUPLE H1, 399.9632156 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
File size 65536
Total time 59 min, 9 sec

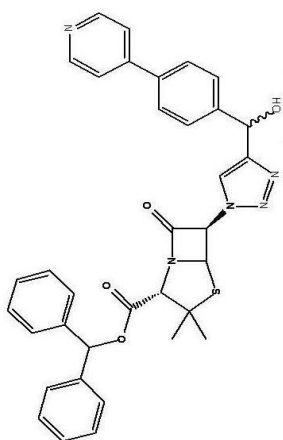
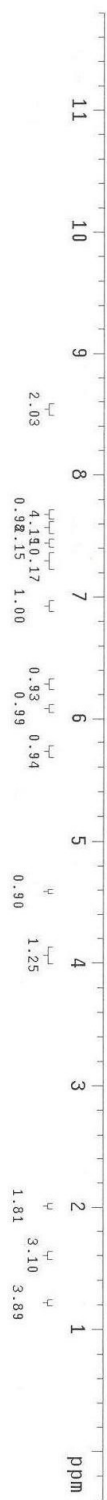
¹H NMR of 11k:



¹³C NMR of 11l:

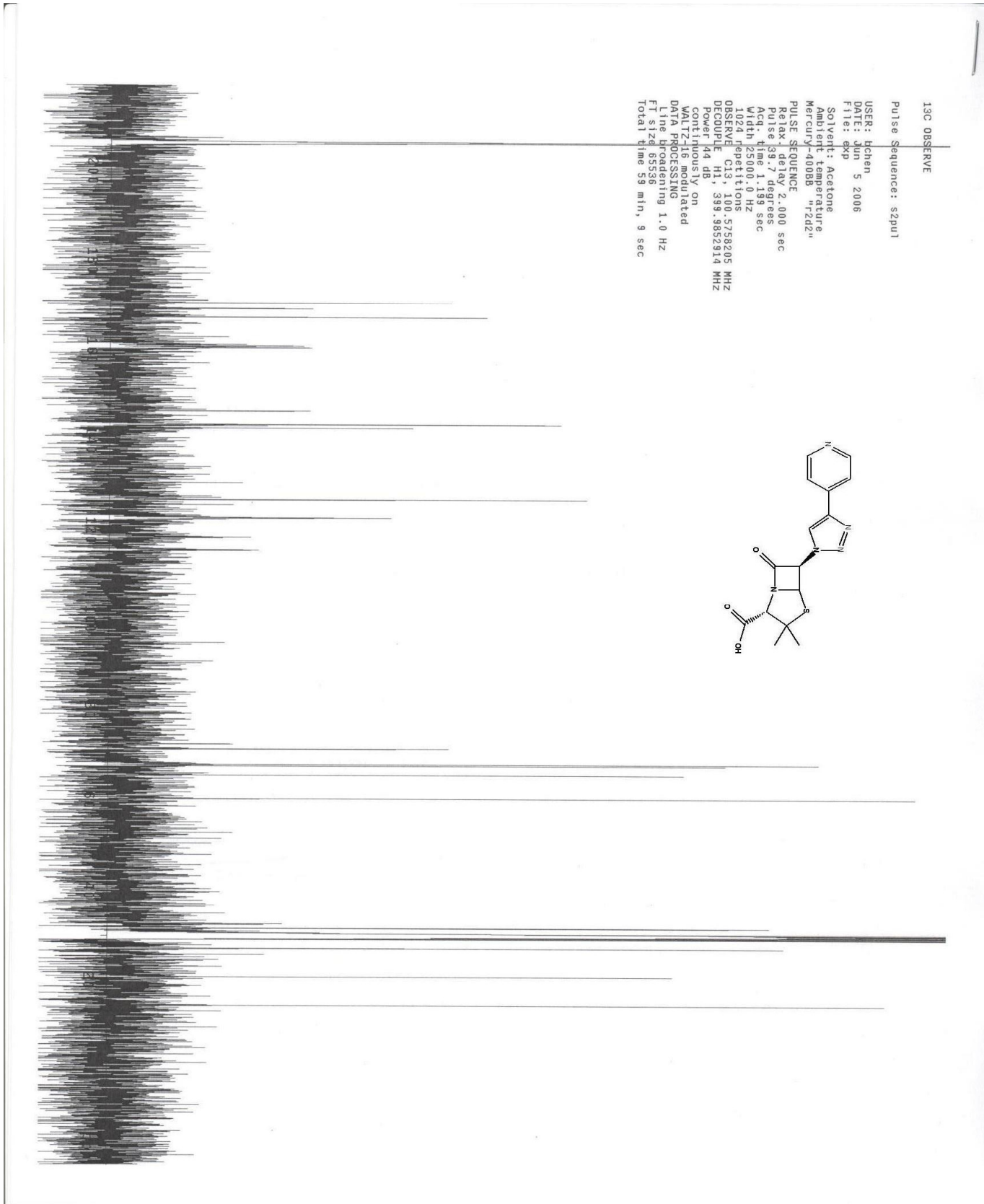


¹H NMR of **11l**:

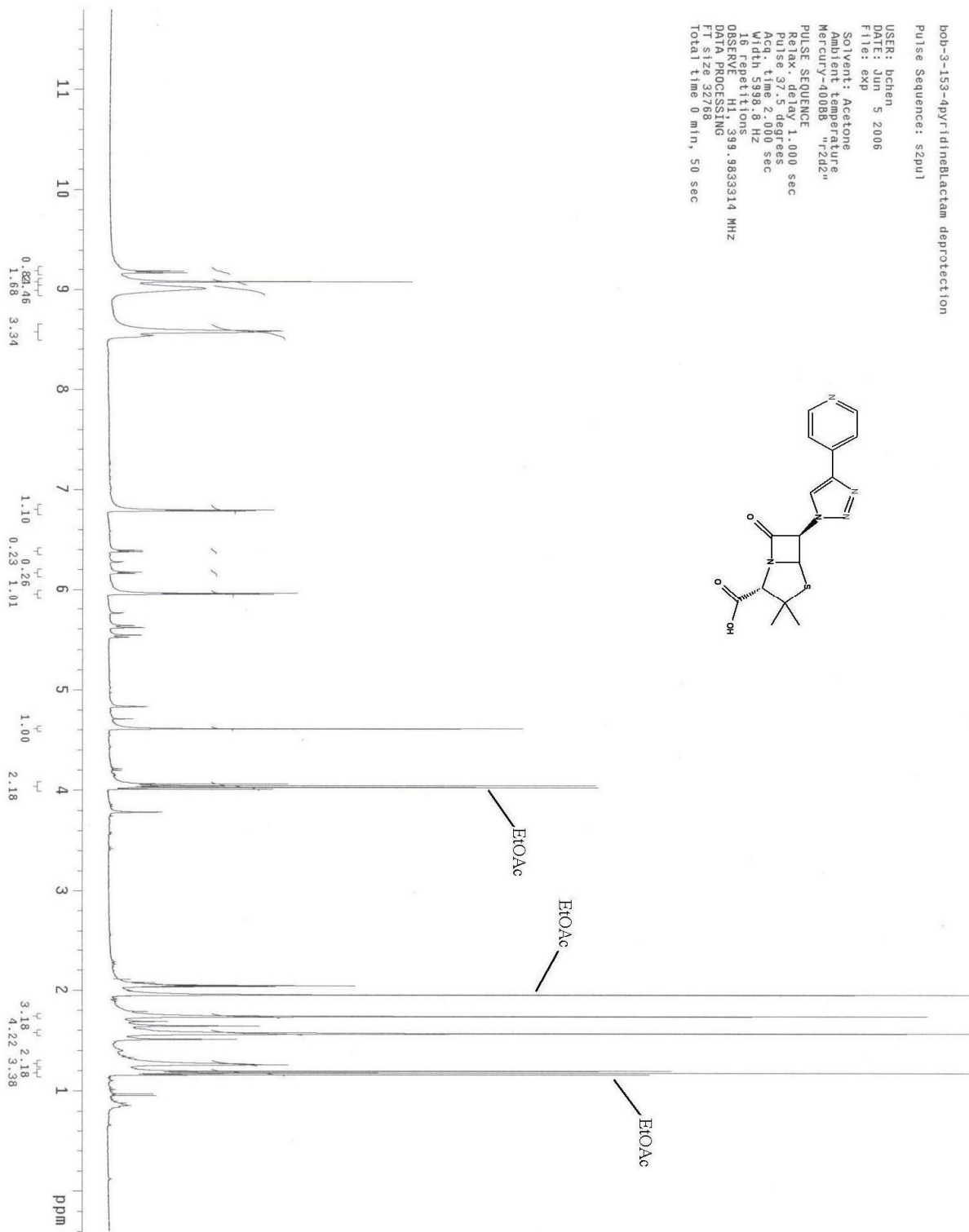


bob-4-35-pyr(1)naphenylhydroxy)lactam
Pulse Sequence: s2pul1
USER: bchen
DATE: Jul 28 2006
File: exp
Solvent: CDCl3
Ambient temperature
Mercury-400BB "242"
PULSE SEQUENCE
Pulse program 1.000 sec
Pulse 37.5 degrees
Acq. time 2.000 sec
Width 5998.8 Hz
16 Repetitions
OBSERVE H1. 399.9747427 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec

¹³C NMR of 12a:

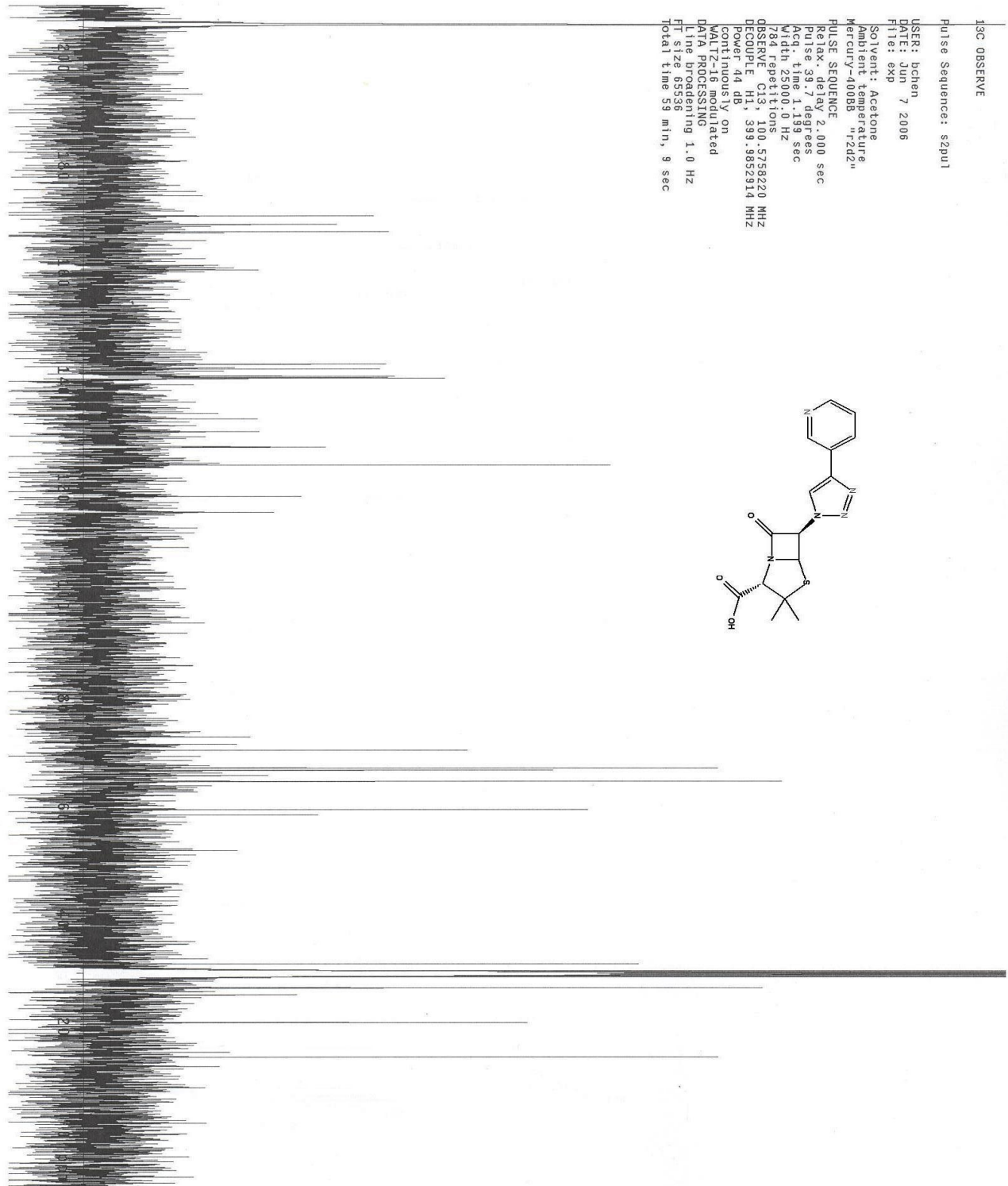


¹H NMR of 12a:

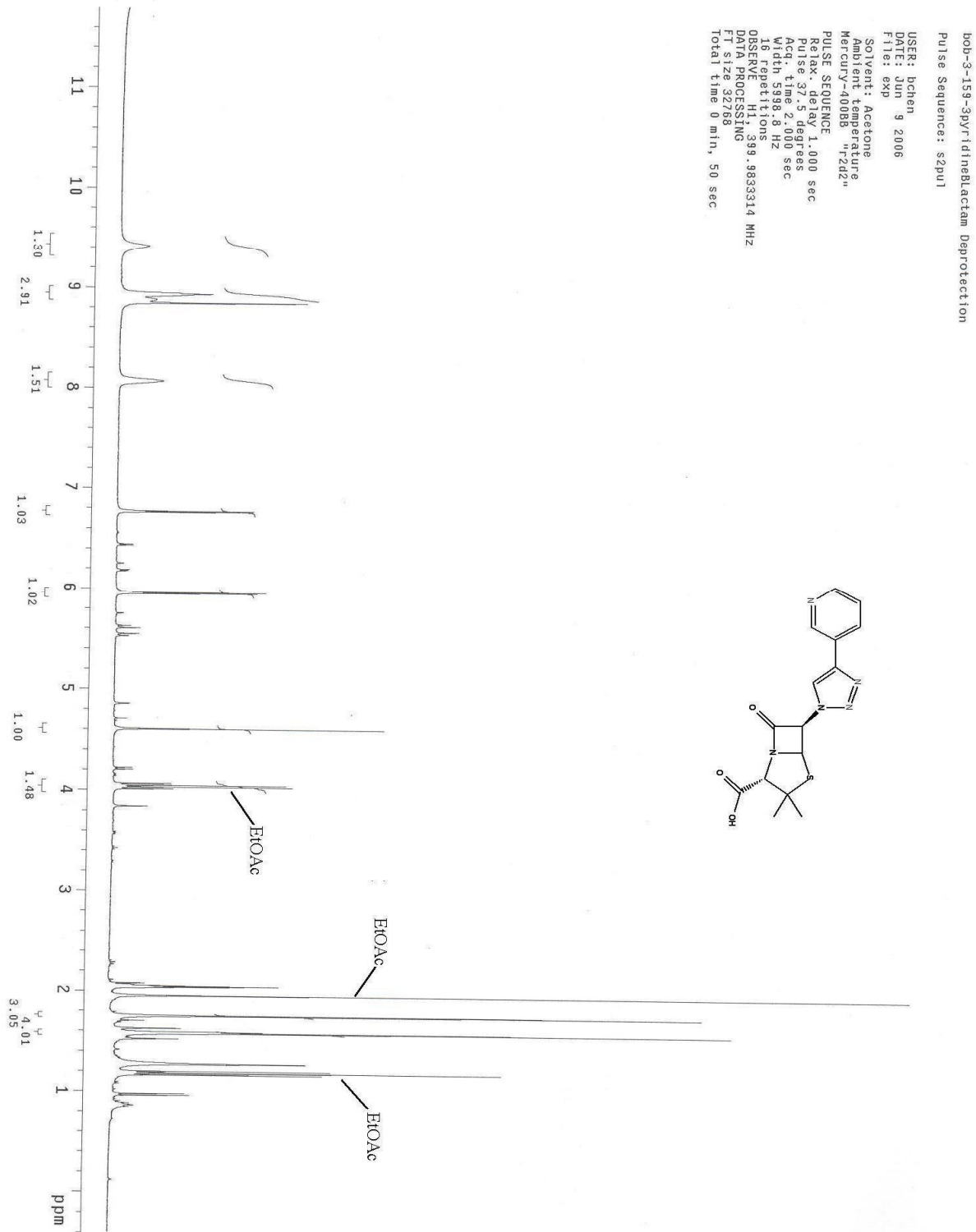


bob-3-153-4pyridineblactam deprotection
Pulse Sequence: szpu1
USER: bchen
DATE: Jun 5 2006
File: exp
Solvent: Acetone
Ambient Temperature
Mercury-400BB "r2d2"
PULSE SEQUENCE
Relax: delay 1.000 sec
Pulse: 37.5 degrees
Acq: time 2.000 sec
Fid: 339.8 Hz
1.000000000
ORSERV: H1 on 39.9833314 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

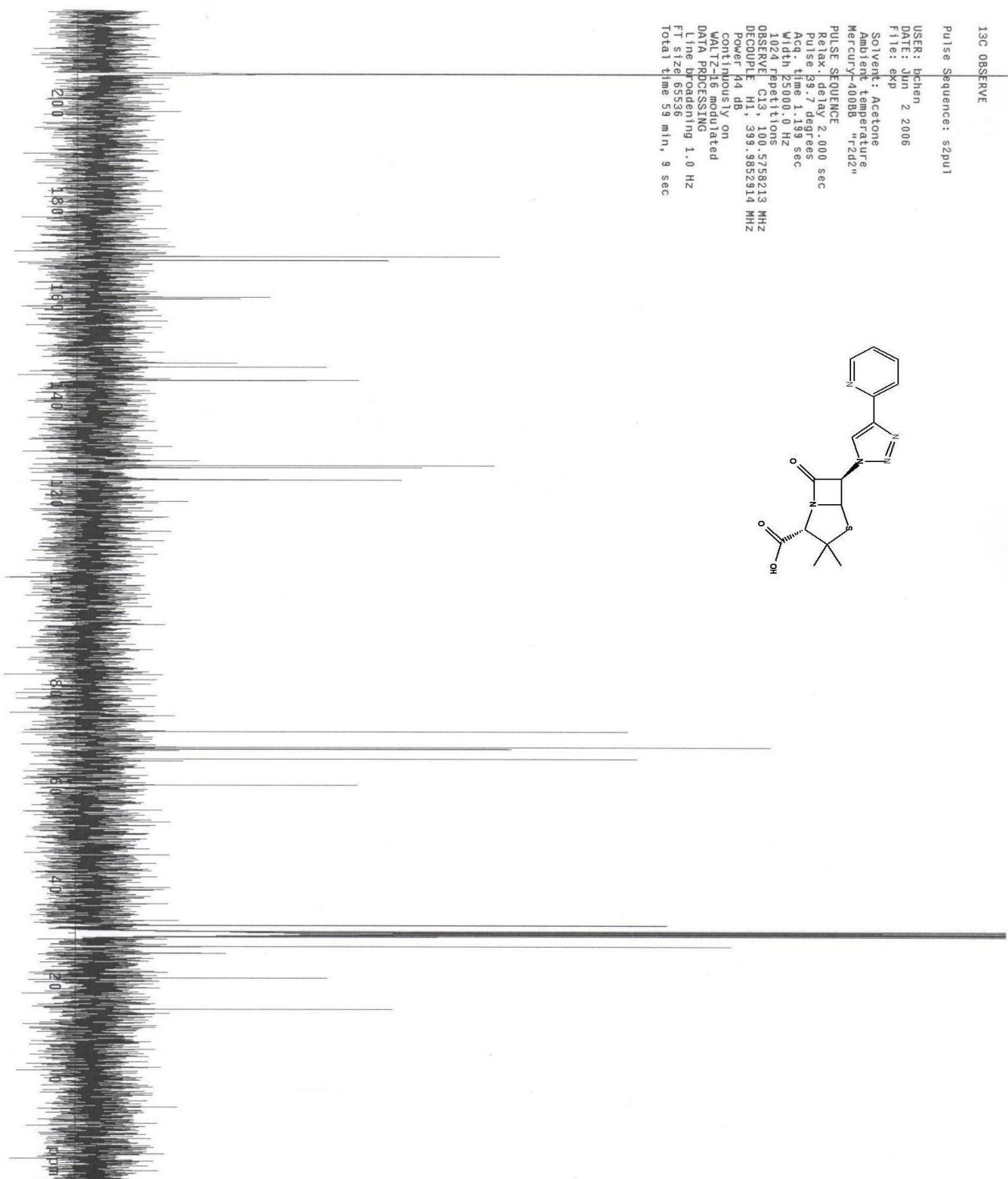
¹³C NMR of 12b:



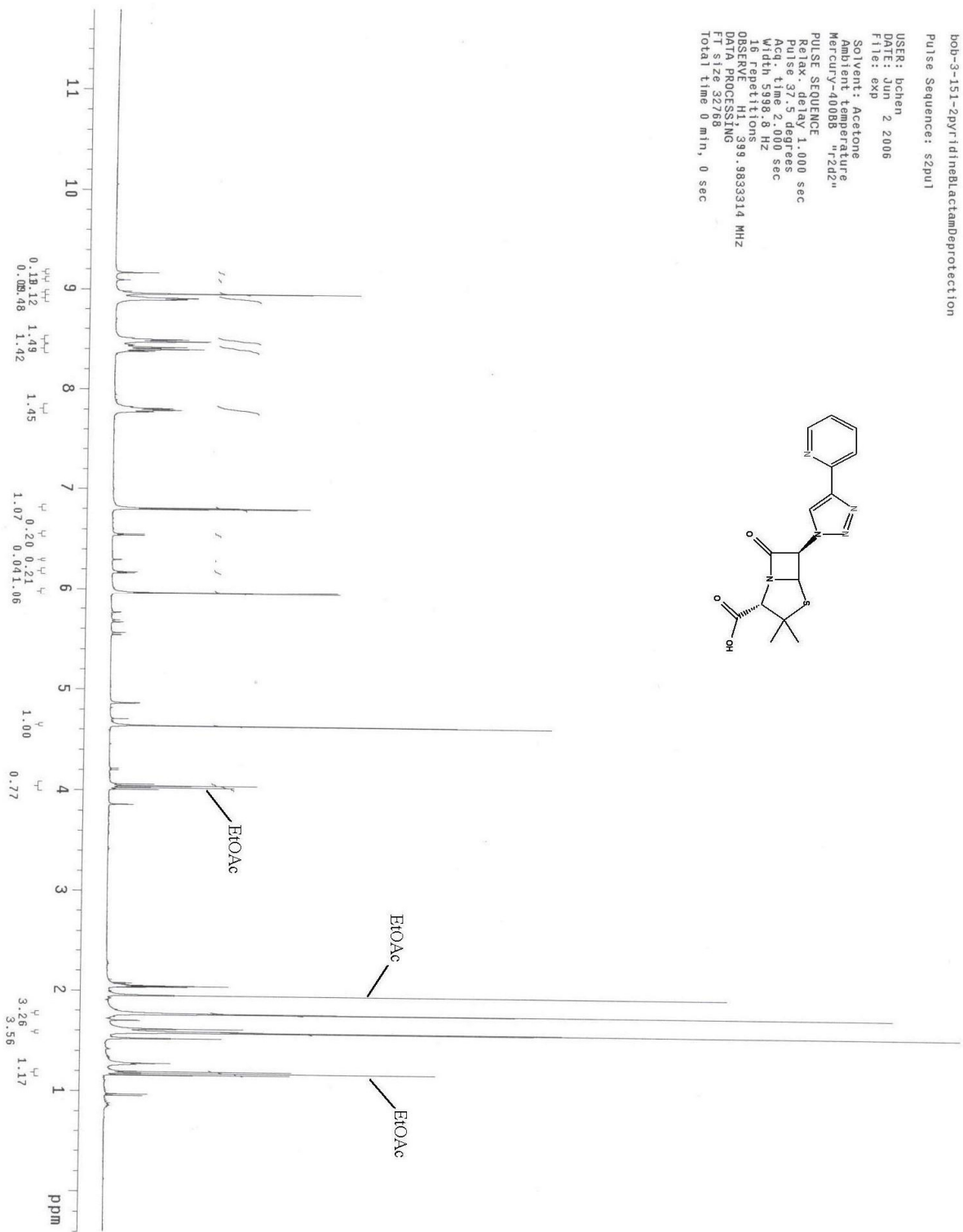
¹H NMR of 12b:



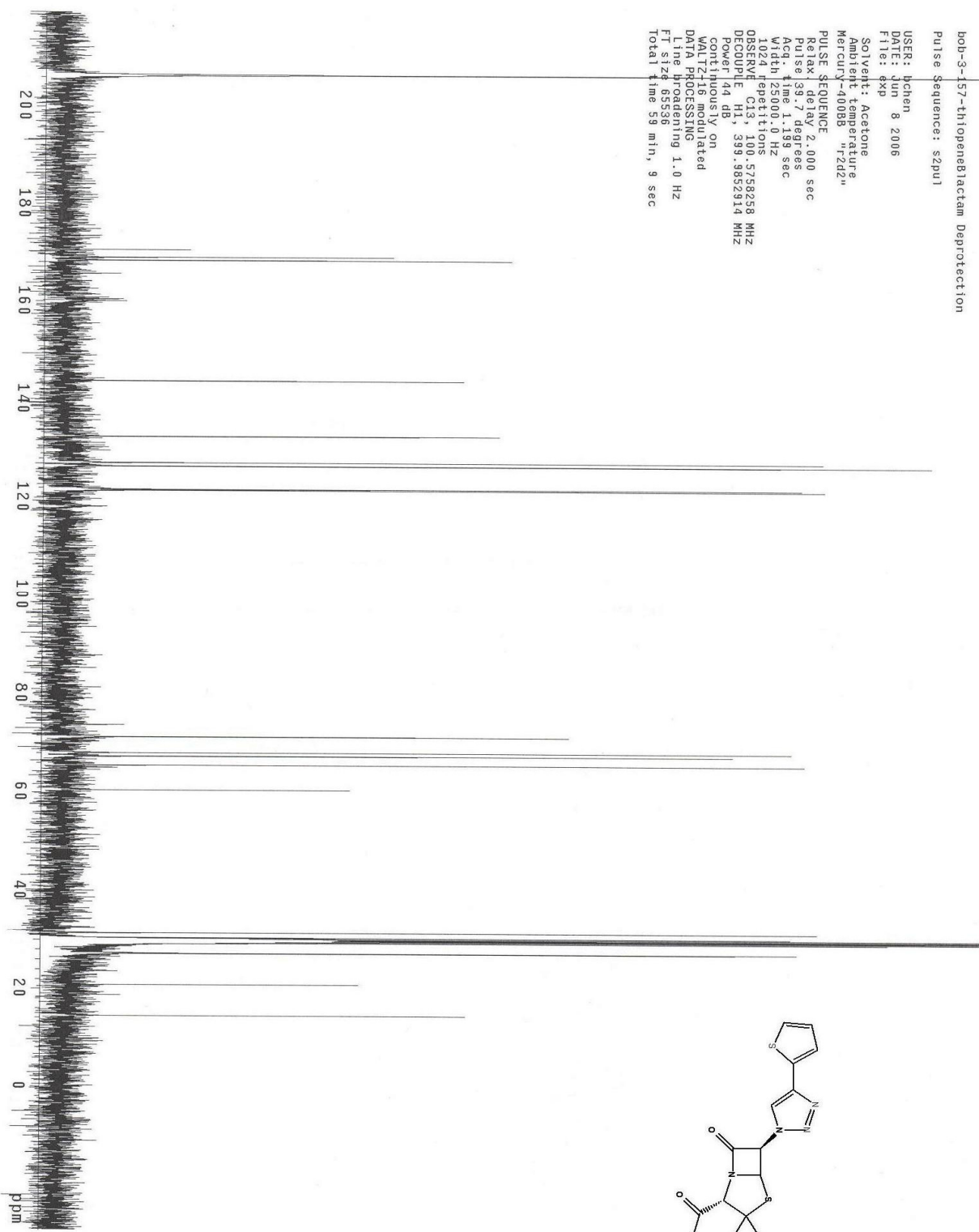
¹³C NMR of 12c:



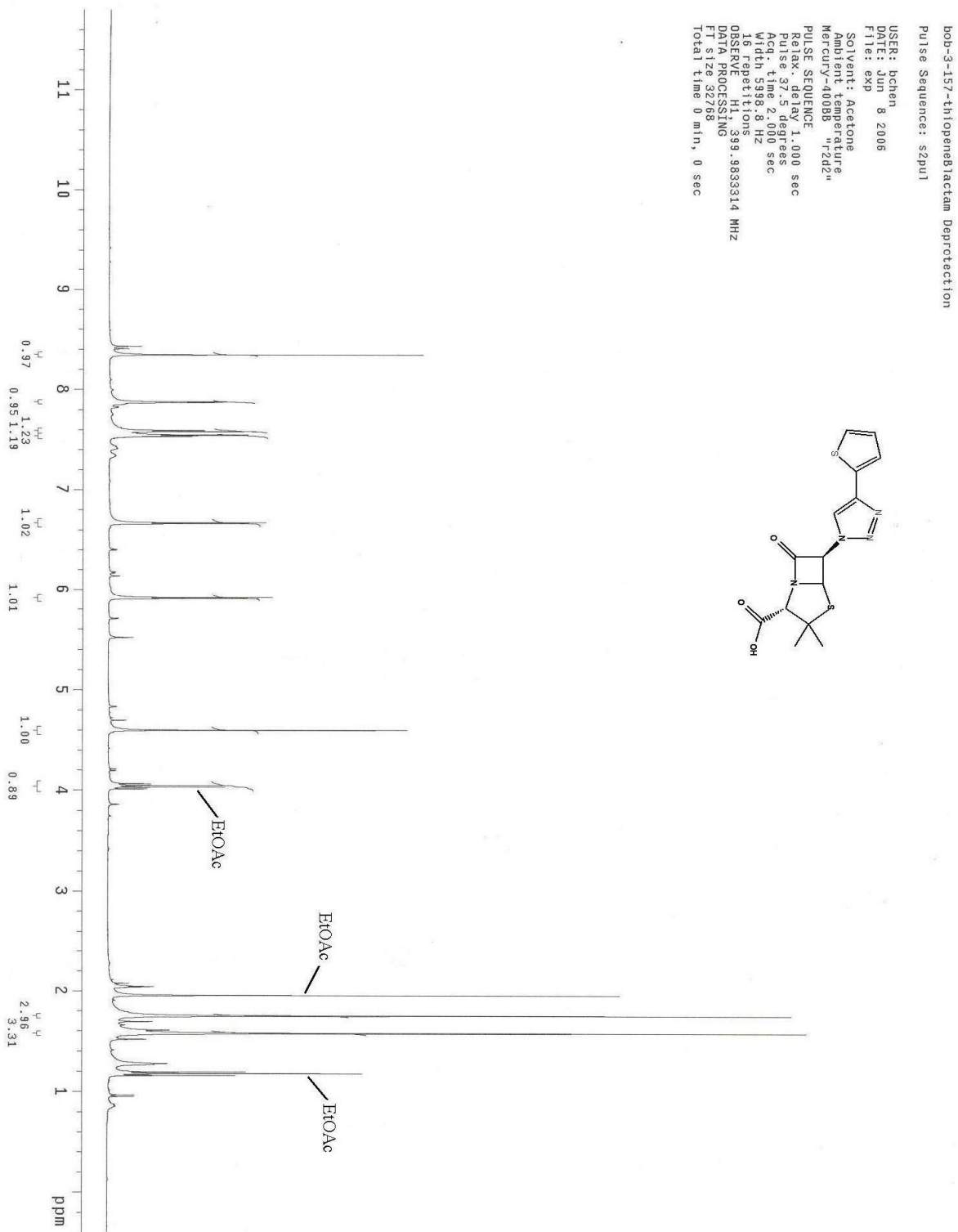
¹H NMR of 12c:



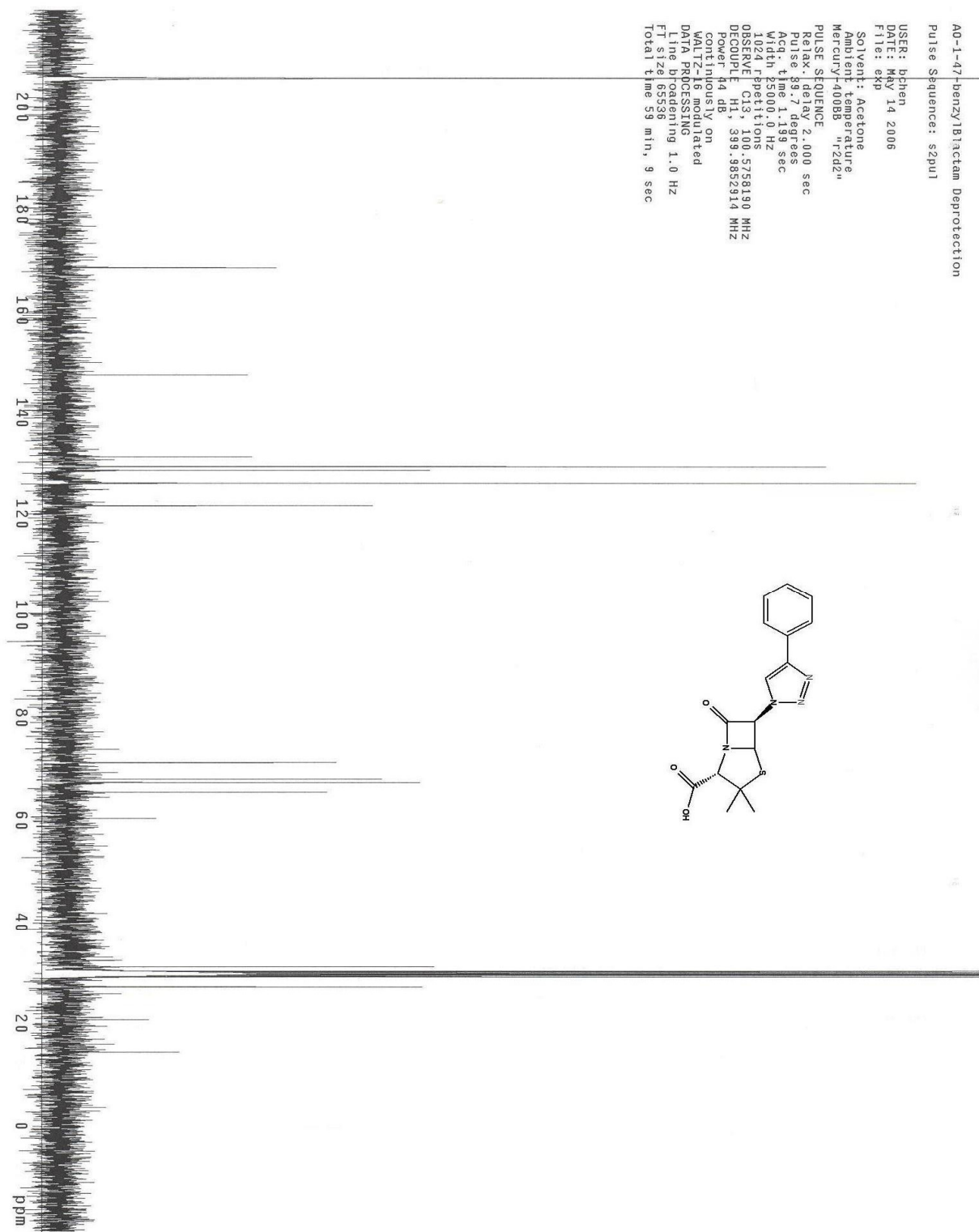
¹³C NMR of 12d:



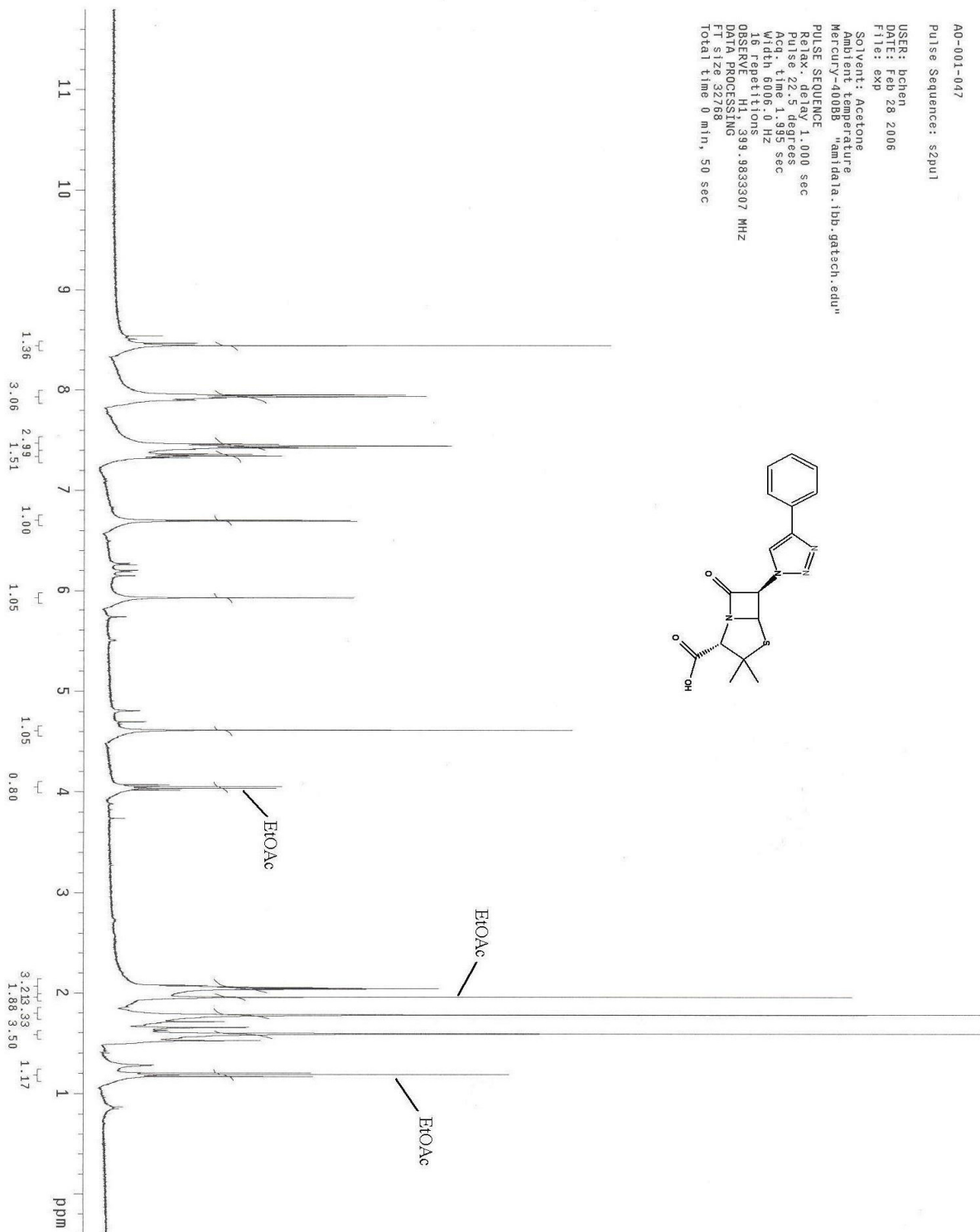
¹H NMR of 12d:



¹³C NMR of 12e:

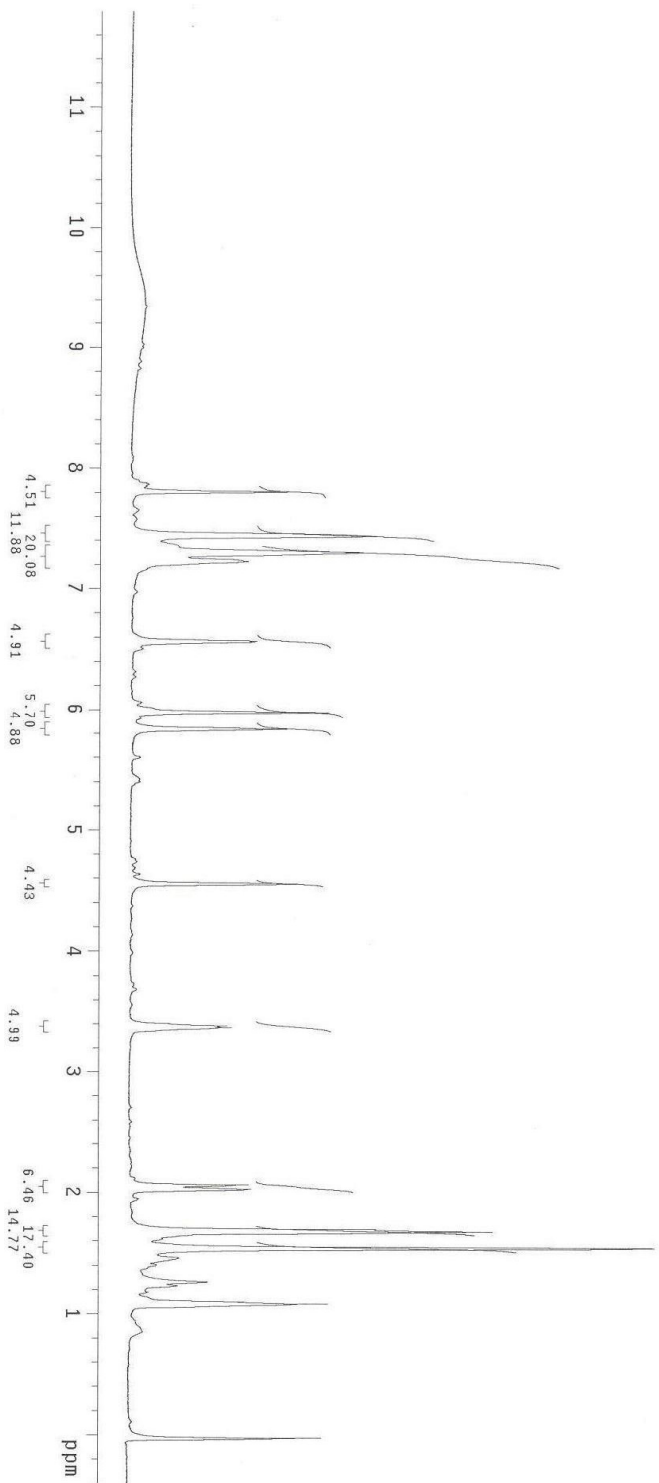


¹H NMR of 12e:

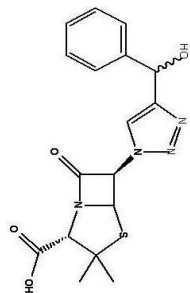


A0-001-047
Pulse Sequence: s2pul1
USER: bchen
DATE: Feb 28 2006
File: exp
Solvent: Acetone
Ambient temperature
Mercury-400BB "amidata.ibv.gatech.edu"
PULSE SEQUENCE
Relax delay 1.000 sec
Pulse 22.5 degrees
Acq time 1.995 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1 399.983307 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

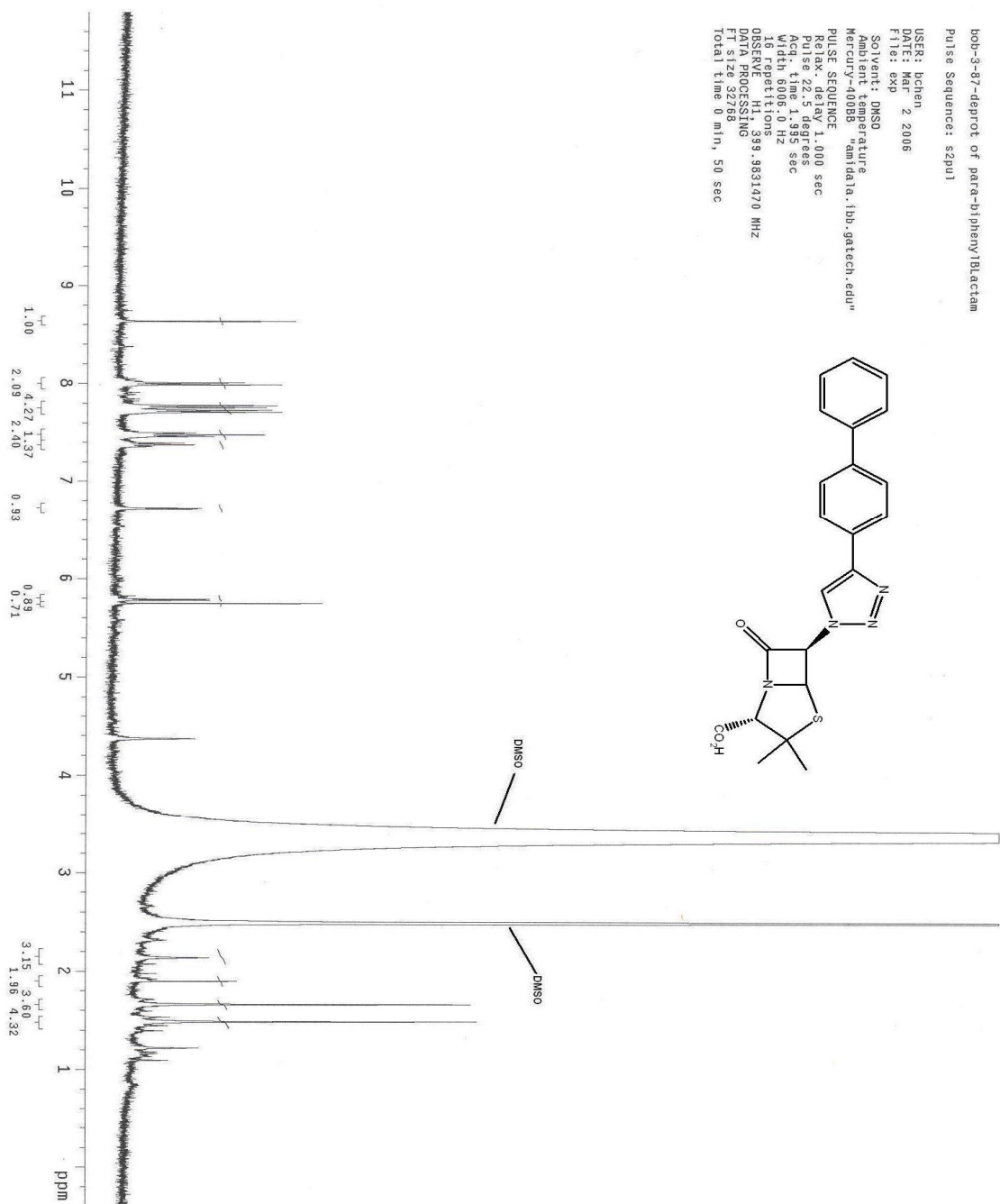
¹H NMR of 12f:



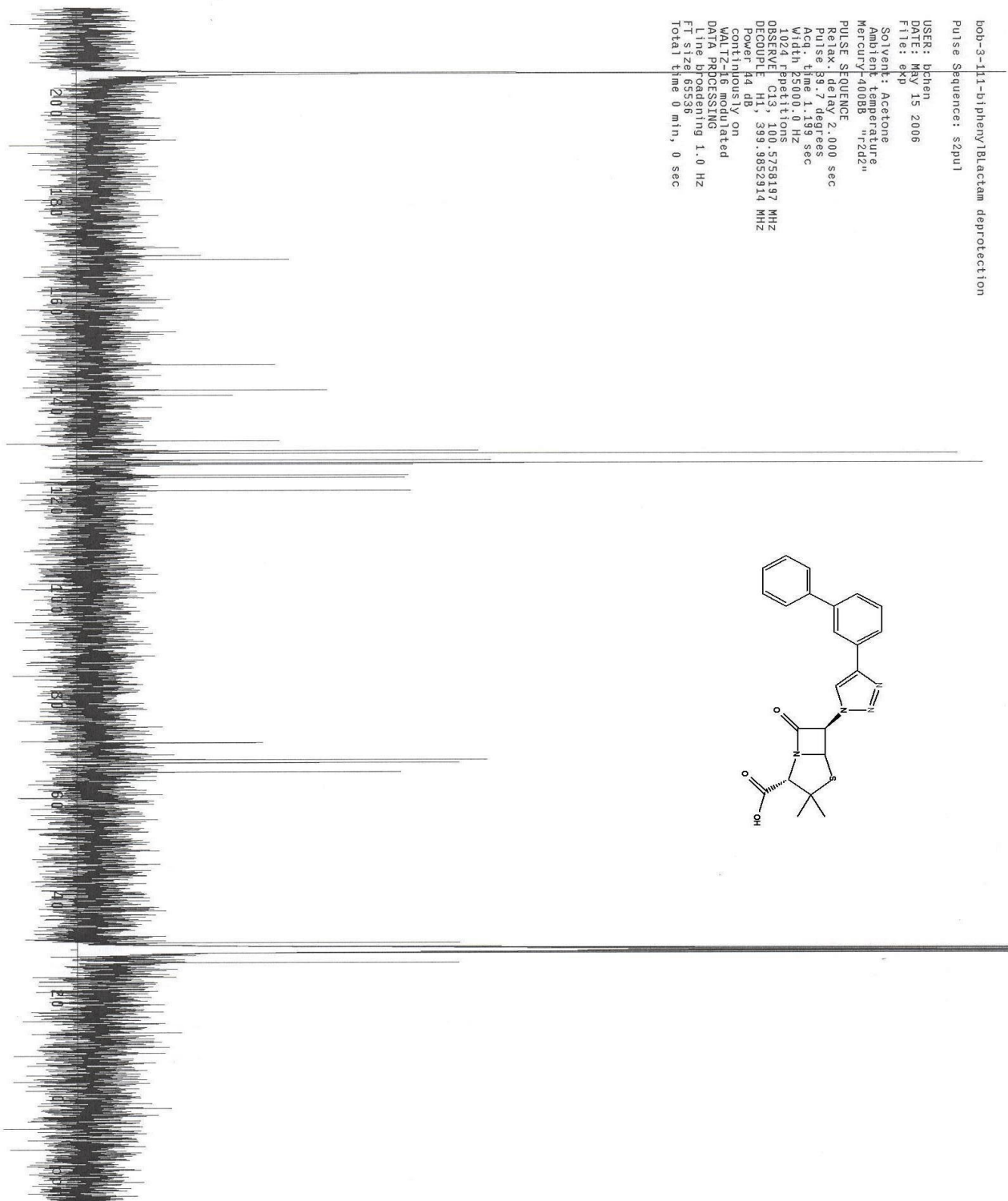
bob-4-39-DeprotBenzylHydroxyBLactam
Pulse Sequence: szpu1
USER: bchen
DATE: Aug 2 2006
File: exp
Solvent: Acetone
Ambient temperature
Mercury-400SB 1202
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.5 degrees
Acq. time 2.000 sec
Width 5395.8 Hz
#8 repetitions
OBSERVED F1 39.9768234 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec



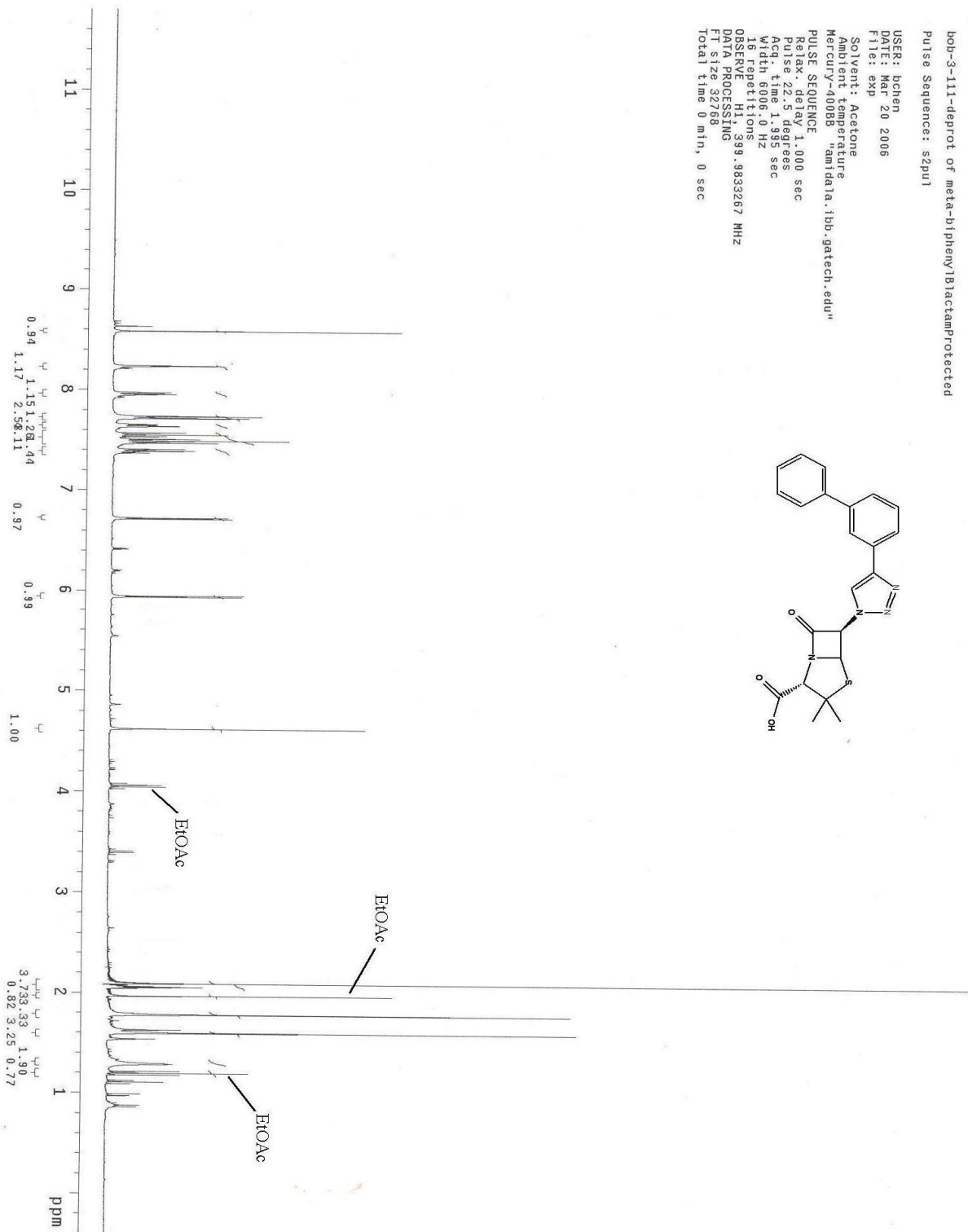
¹H NMR of 12g:



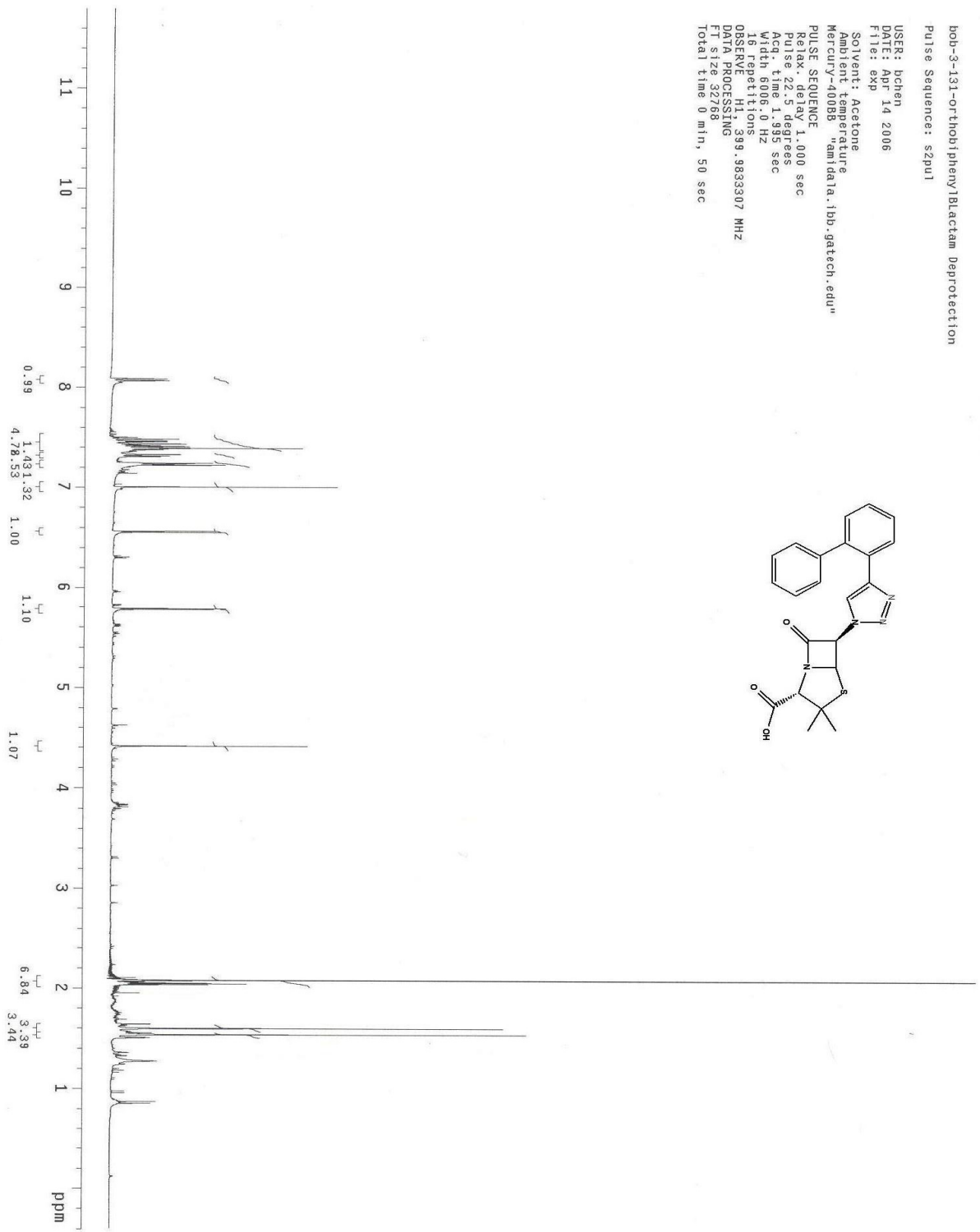
¹³C NMR of 12h:



¹H NMR of 12h:

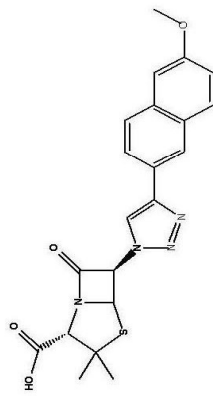
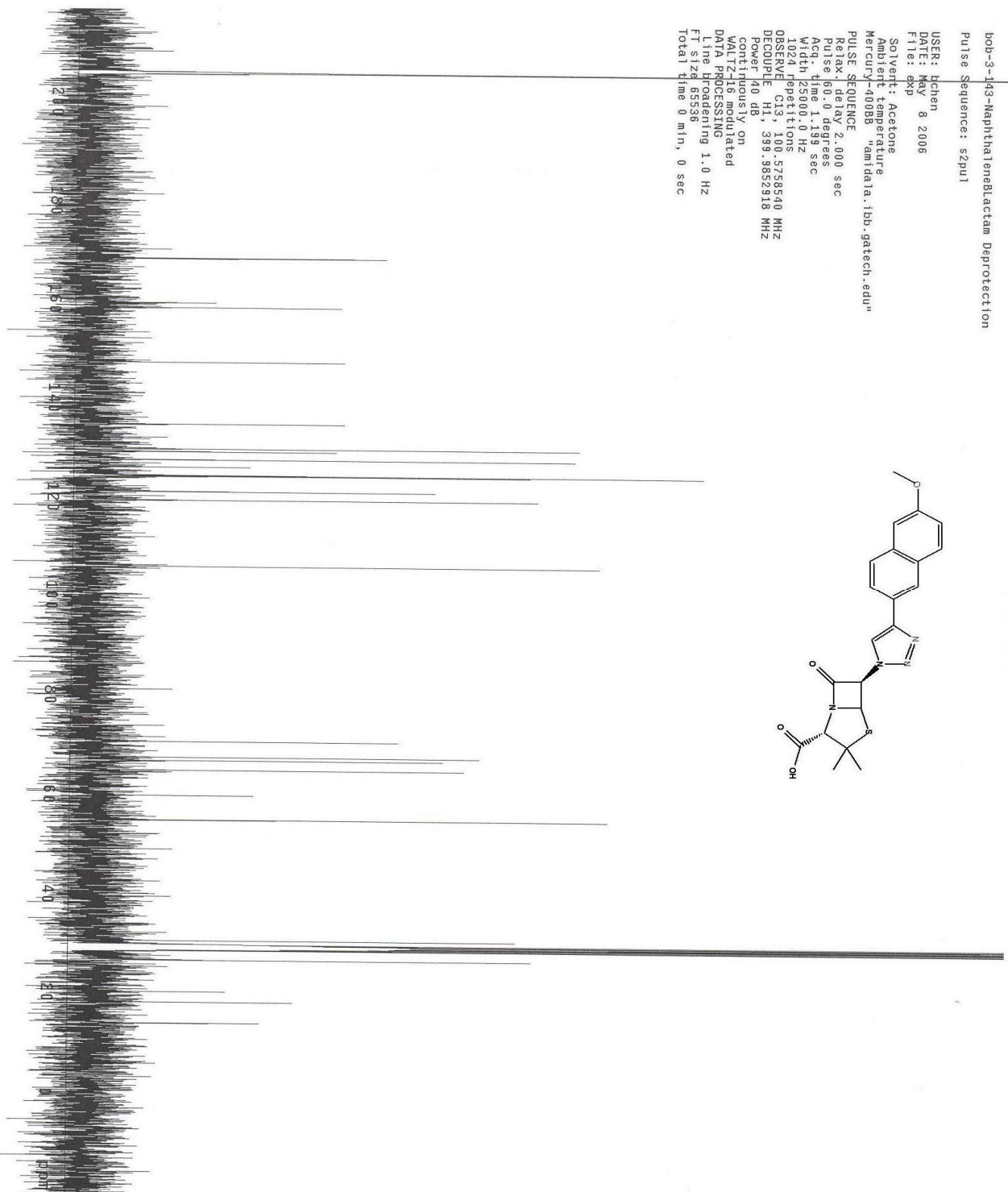


¹H NMR of 12i:



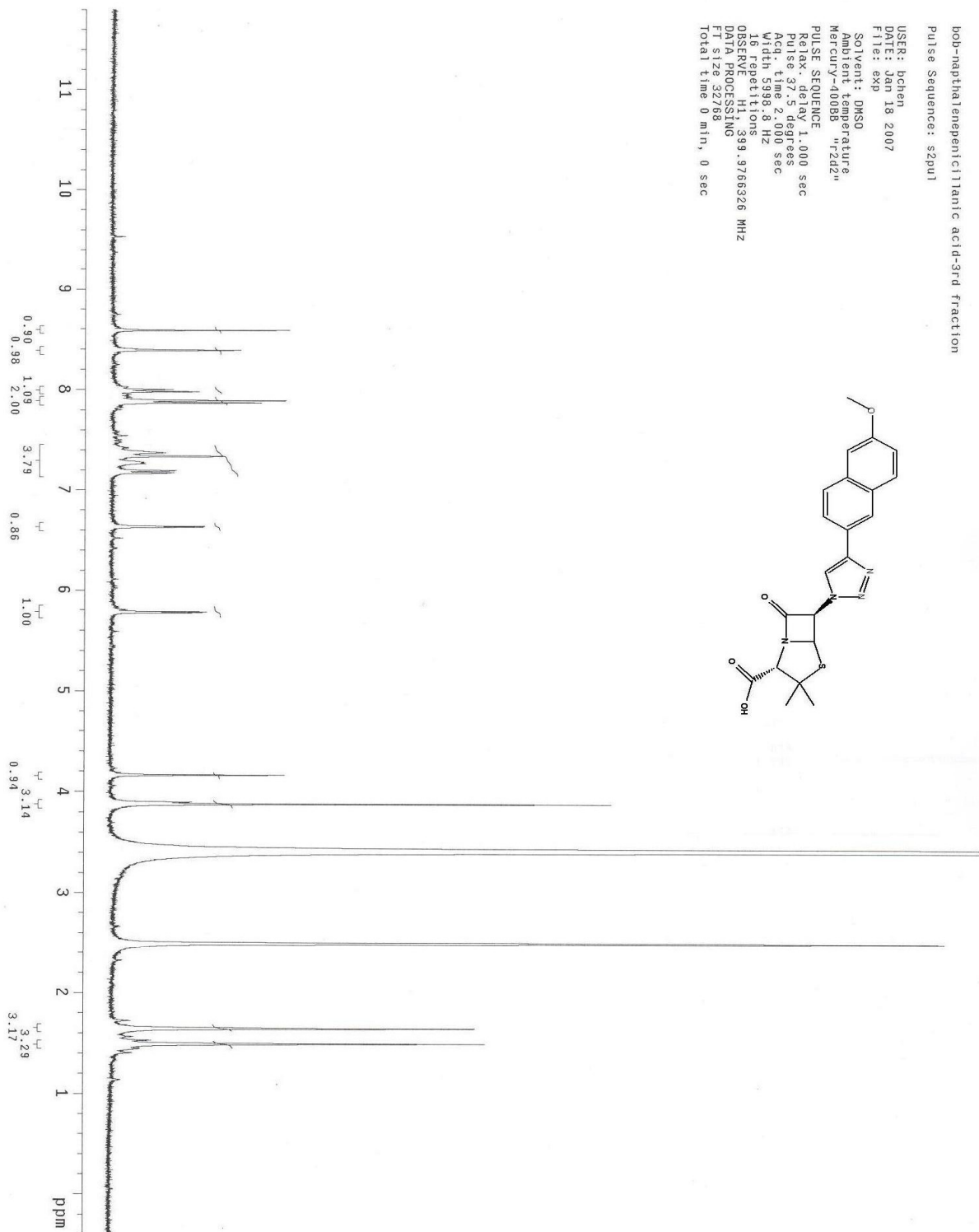
bob-3-131-OrthoIphenylBlactam Deprotection
Pulse Sequence: szpu1
USER: bchen
DATE: Apr 14 2006
File: exp
Solvent: Acetone
Ambient temperature
Mercury-400DB "amdata.ibp.gatech.edu"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 22.5 degrees
Acq. time 1.995 sec
Width 6008.0 Hz
Observed F1
Repetitions 39.9833307 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

¹³C NMR of 12j:

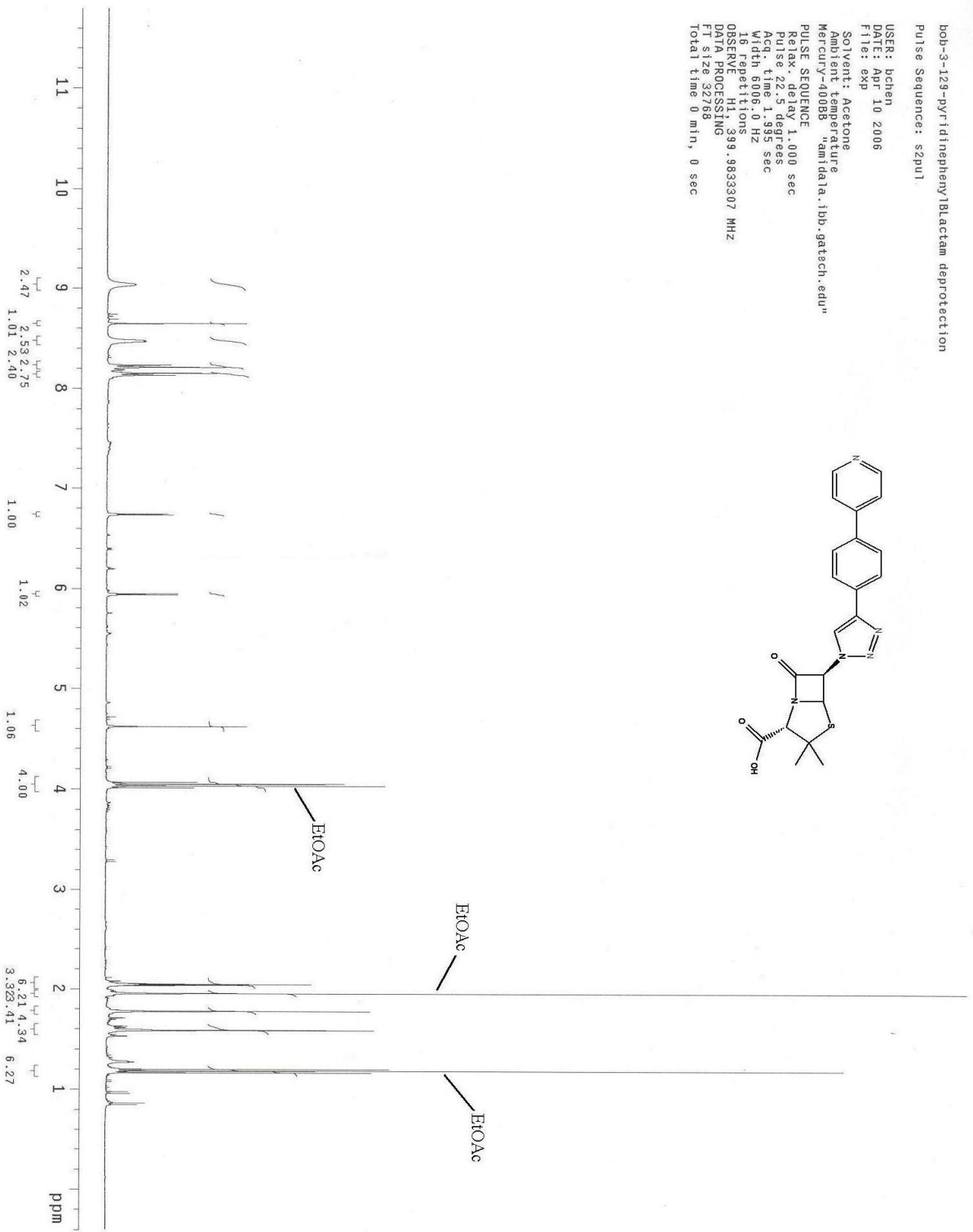


bob-3-143-NaphthaleneBLactam Deprotection
Pulse Sequence: szpu1
USER: hchen
DATE: May 8 2008
File: exp
Solvent: Acetone
Ambient temperature
Mercury-400BB "amida1a.1lb.gatech.edu"
PULSE SEQUENCE
Relax delay 2.000 sec
Pulse 60.0 degrees
Acq. time 1.19 sec
Width 25000.0 Hz
1024 repetitions
OBSERVE C13, 100.5758540 MHz
DECOUPLE H1, 399.9852918 MHz
Power 40 db
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 0 min, 0 sec

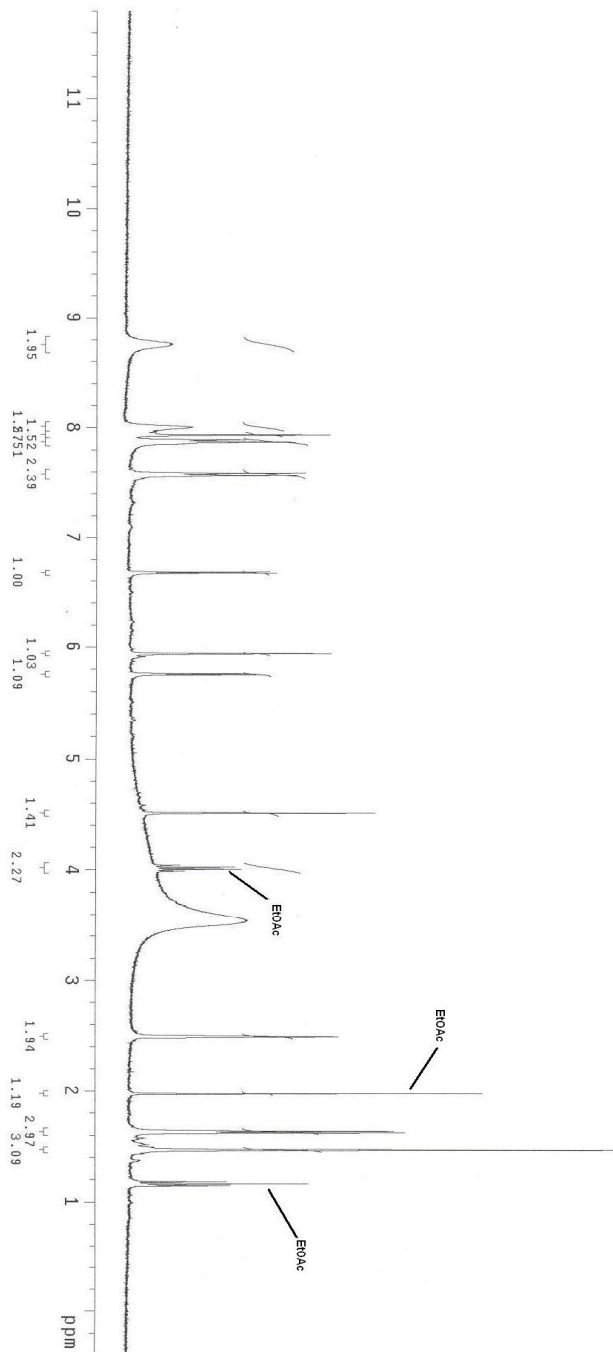
¹H NMR of 12j:



¹H NMR of 12k:



¹H NMR of 12l:



bob453-pyr-1diphenylhydroxy/1betaetamiasat
Pulse Sequence: szpu1
USER: bchen
DATE: Aug 9 2006
File: exp
Solvent: DMSO
Ambient temperature
Mercury-400B8 "r2d2"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.5 degrees
Acq. time 2.000 sec
Width 5398.8 Hz
Spectral width 93.9766329 MHz
Observed 11
DATA PROCESSING
FT size 32788
Total time 0 min, 50 sec

