

SUPPORTING INFORMATION

*Synthesis of Cyclopentenimines from N-Allyl Ynamides via a Tandem Aza-Claisen
Rearrangement–Carbocyclization Sequence.*

authored by

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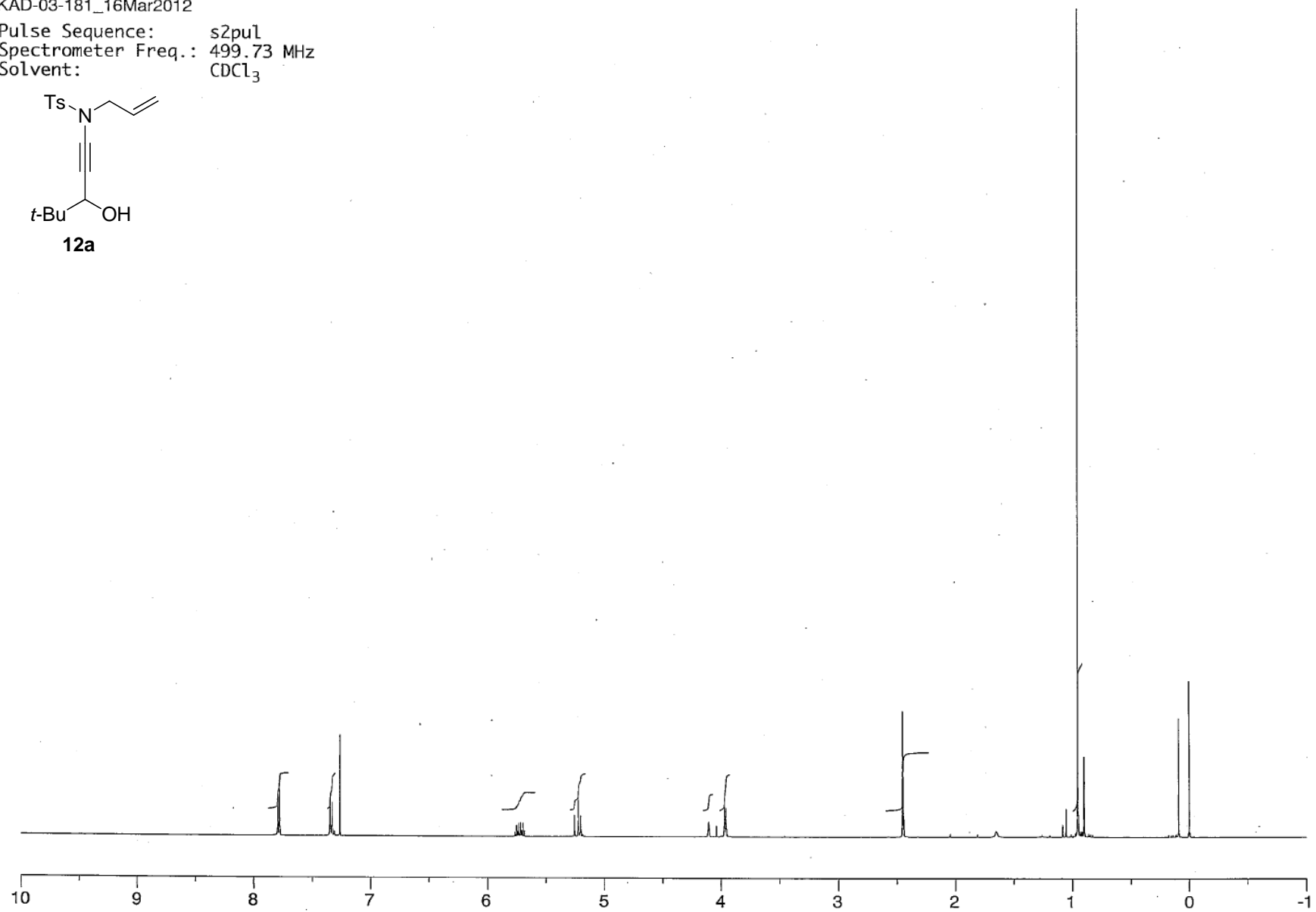
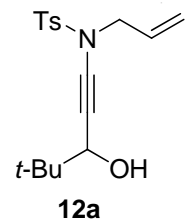
Table of Contents

¹H, ¹³C, ³¹P, gCOSY and NOESY1D spectra

S2-S122

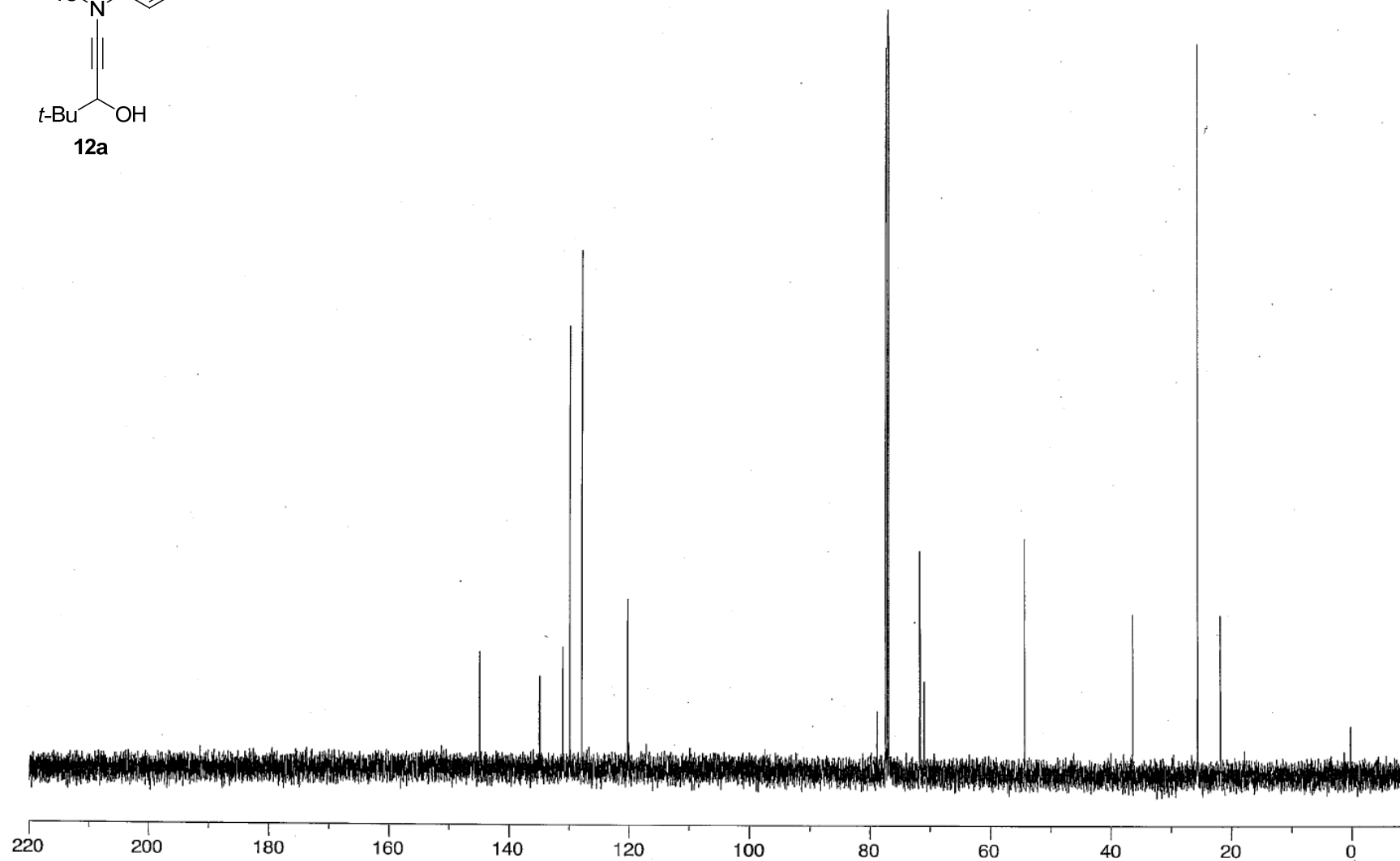
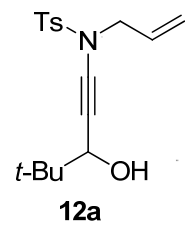
KAD-03-181_16Mar2012

Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃



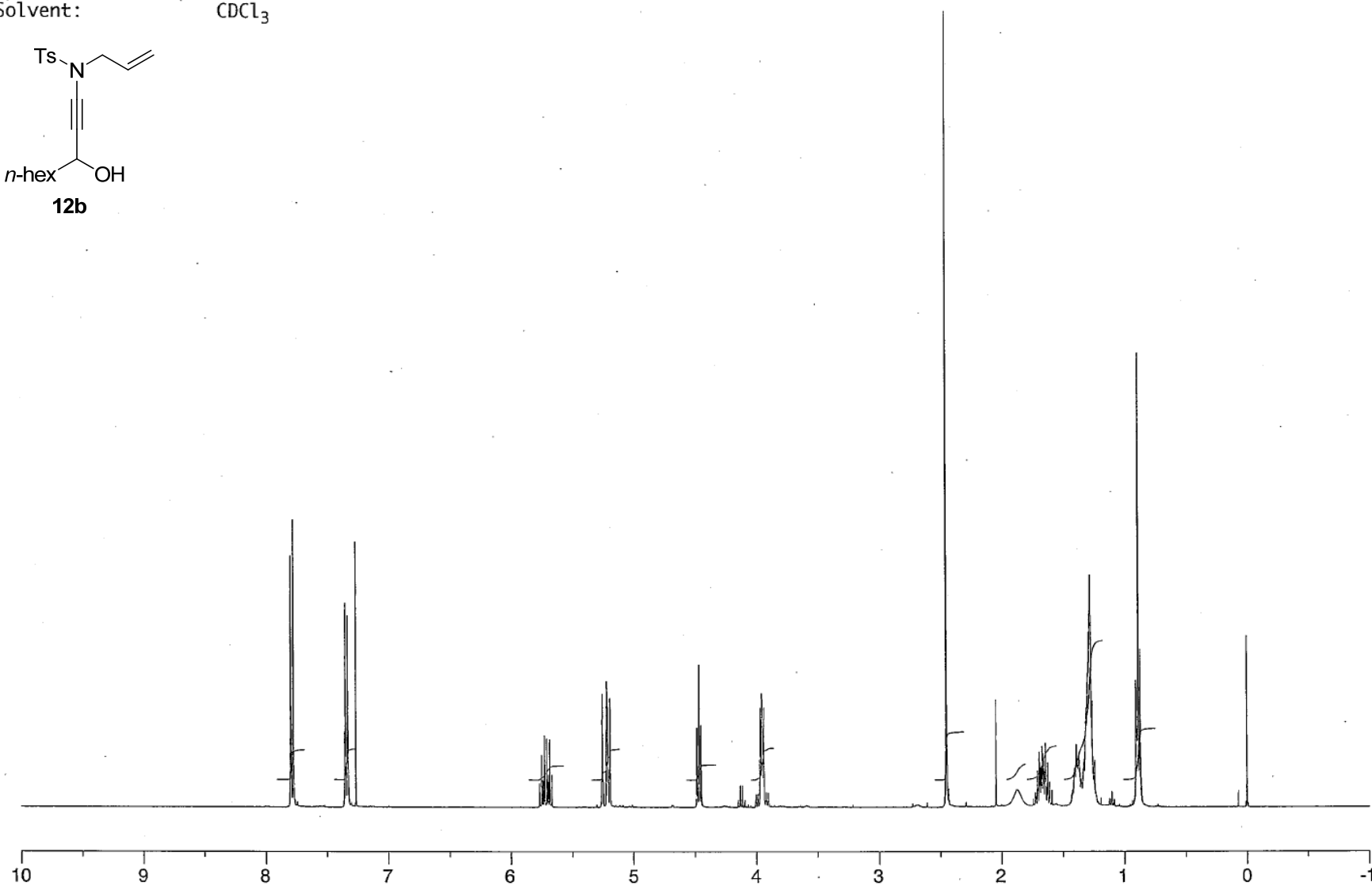
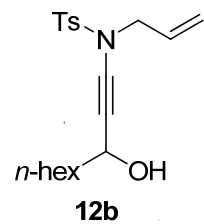
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Pulse Sequence: s2pu1
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃



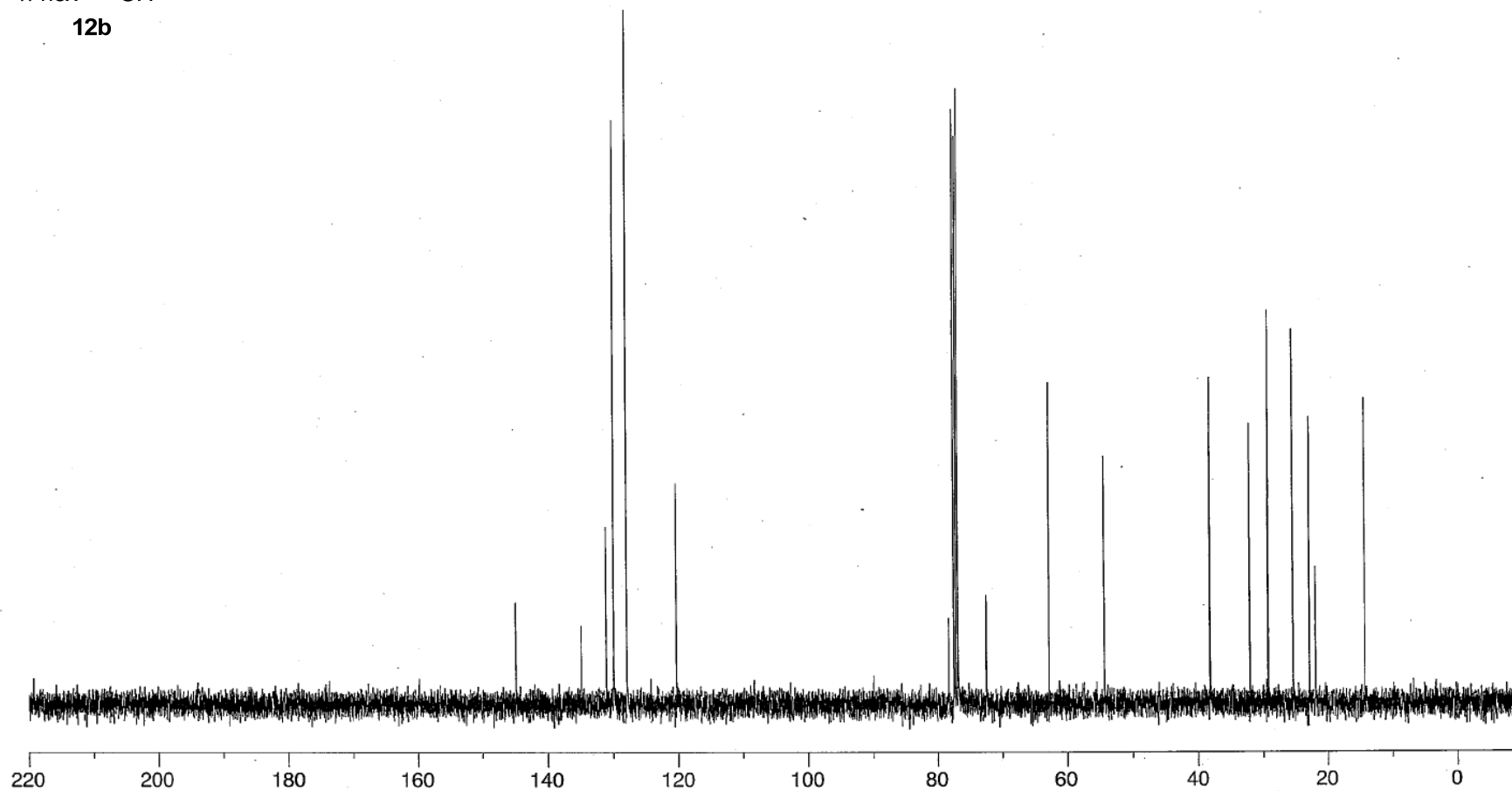
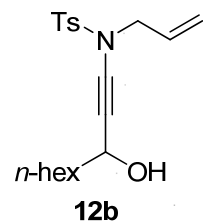
MW-1-132_30Aug2011

Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



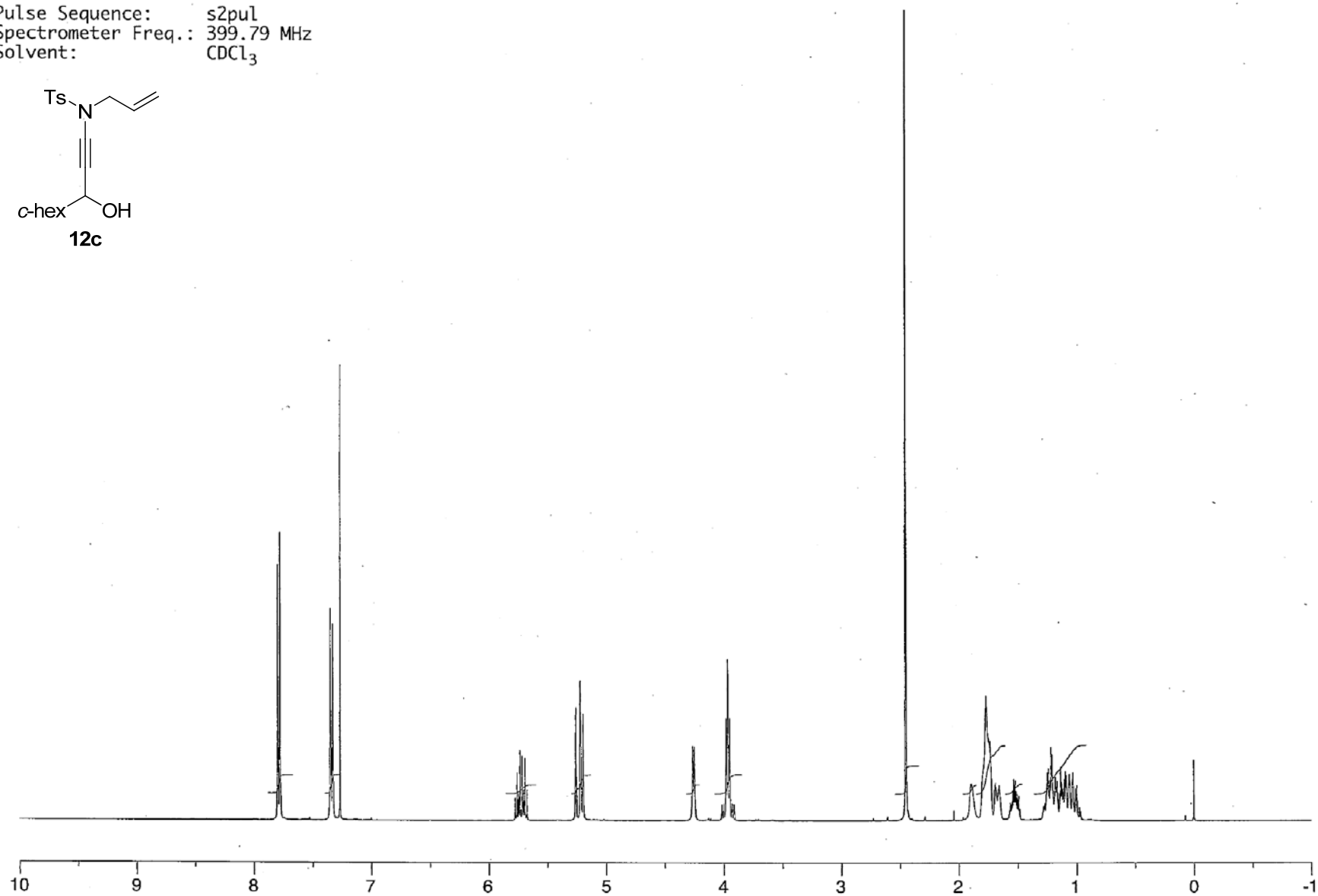
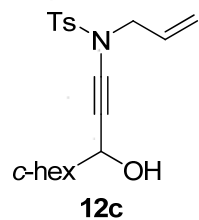
MW-1-132_30Aug2011

Pulse Sequence: s2pul
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃



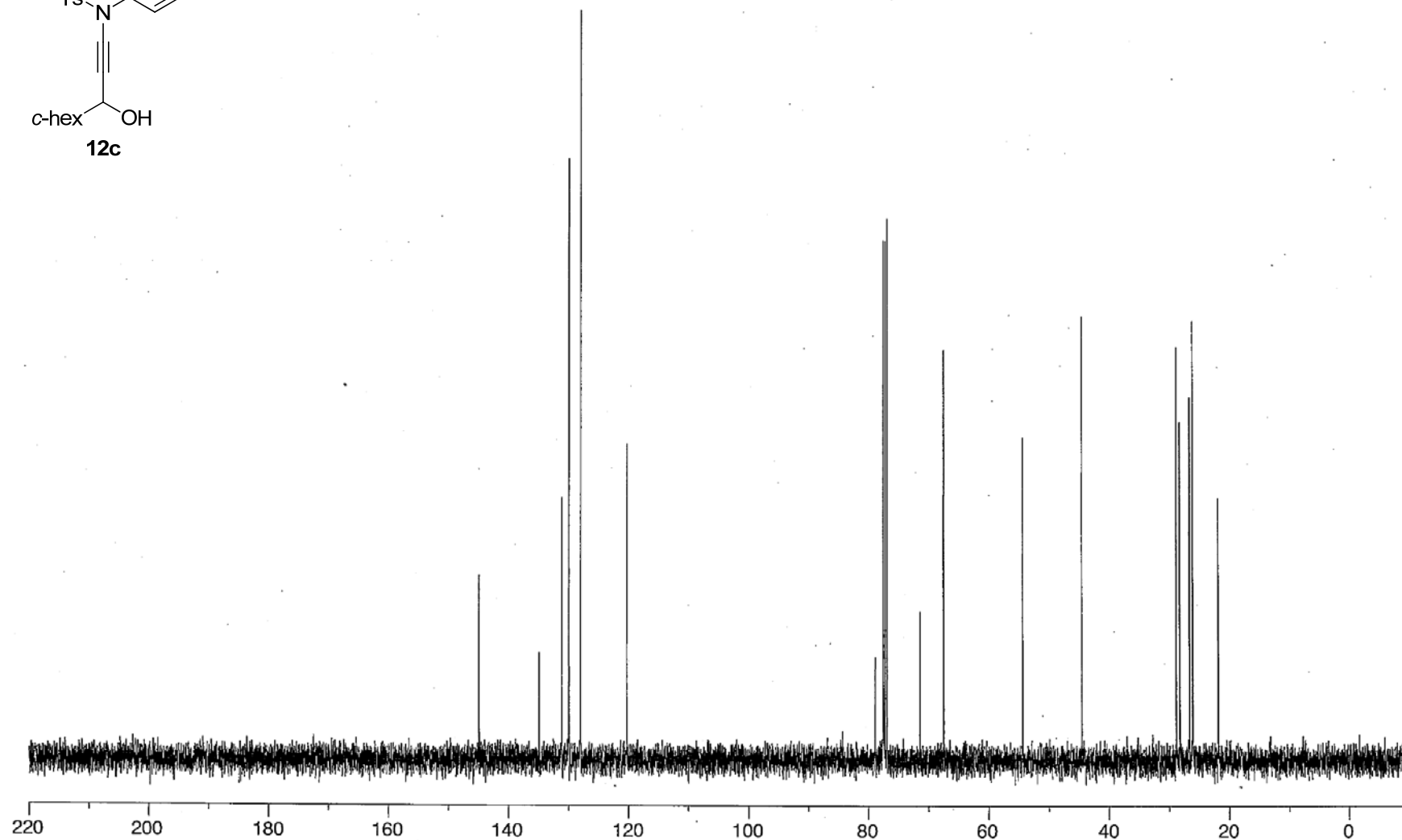
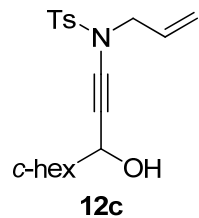
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Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



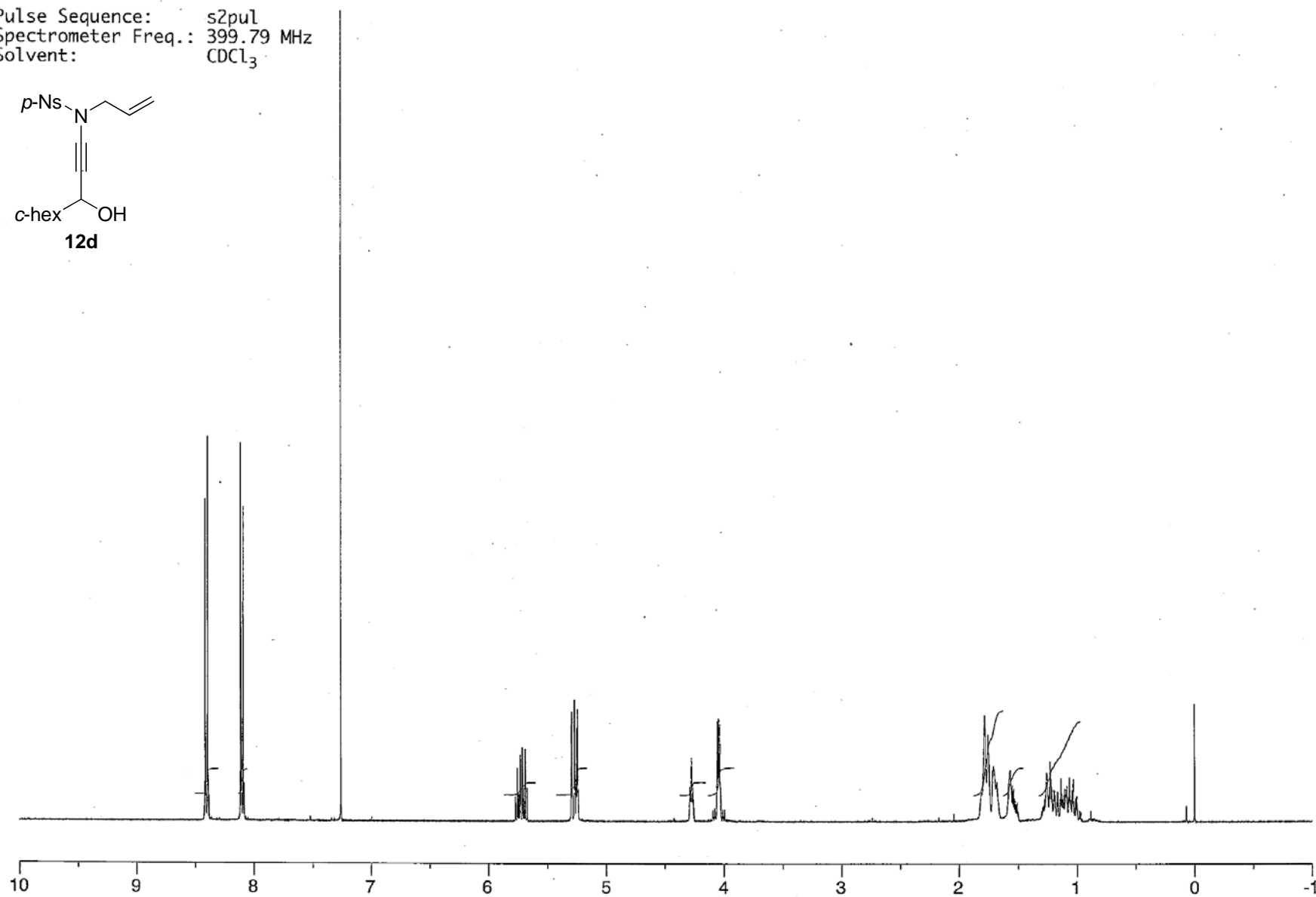
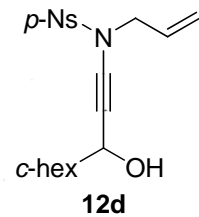
GWM-01-069_01Aug2011

Pulse Sequence: s2pul
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃



gwm-l-65_29Jul2011

Pulse Sequence: s2pu1
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

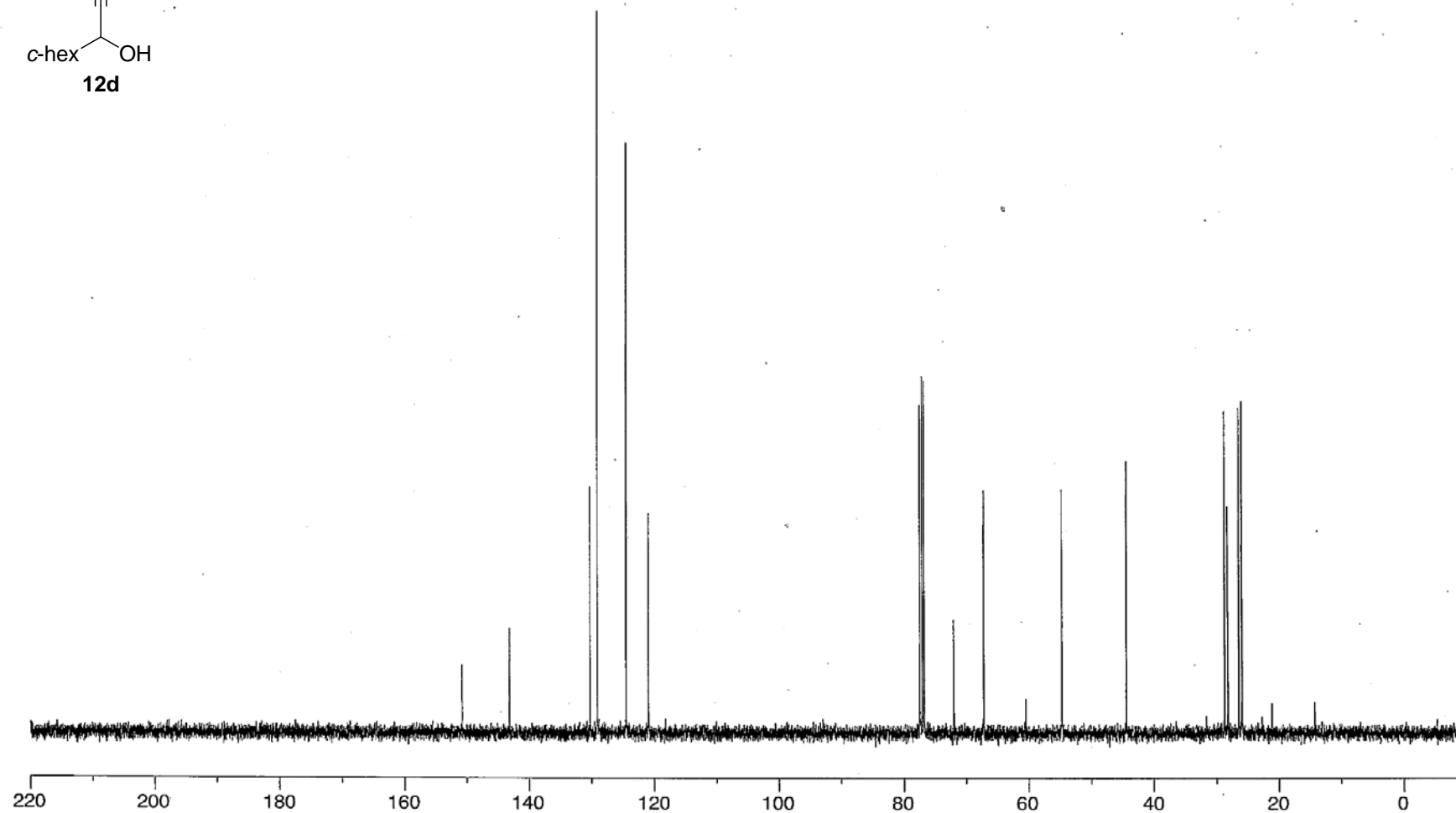
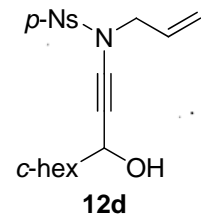


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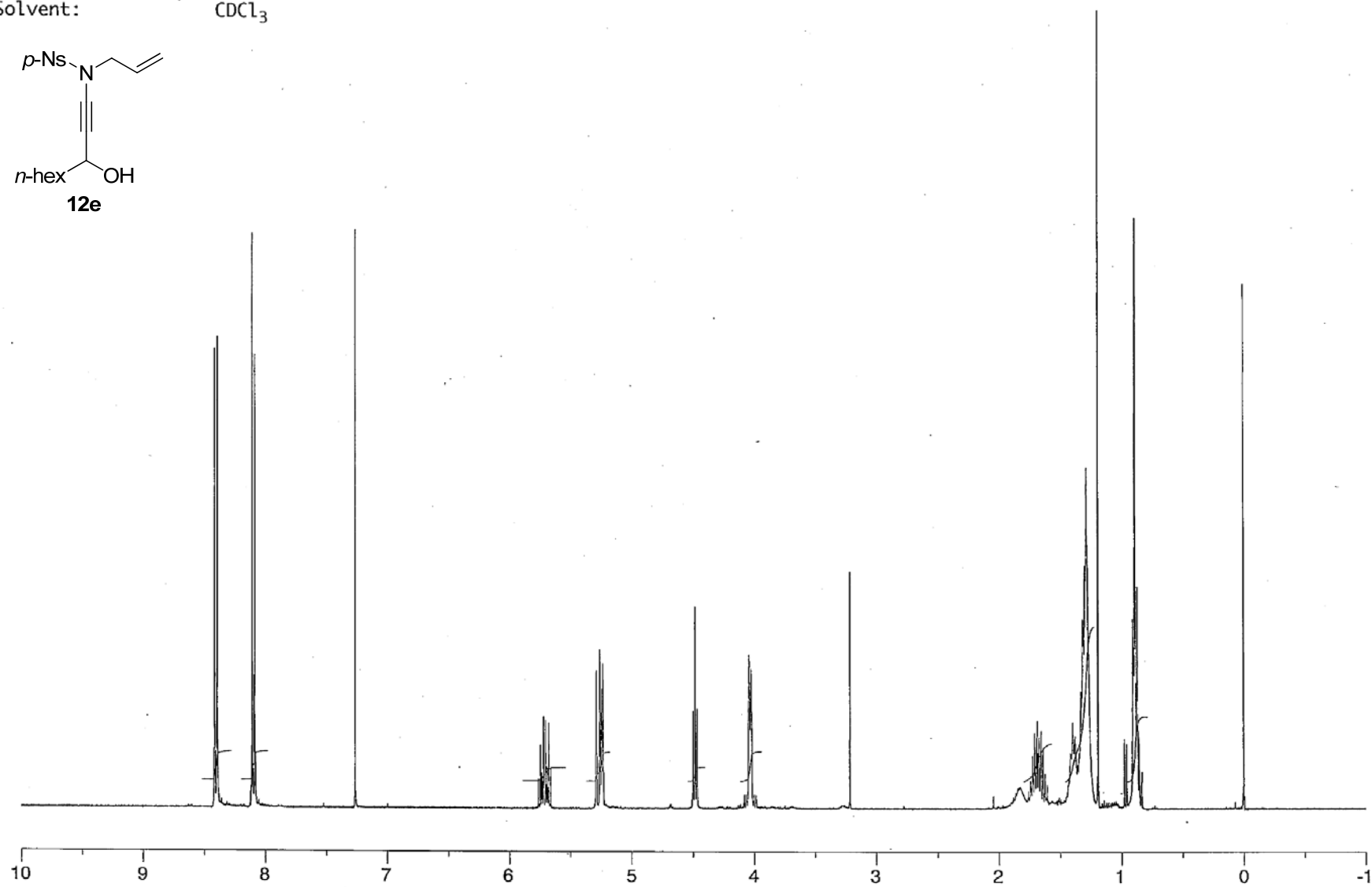
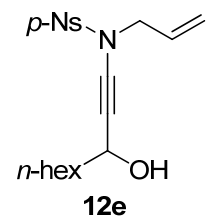
Spectrometer Freq.: 100.54 MHz

Solvent: CDCl₃



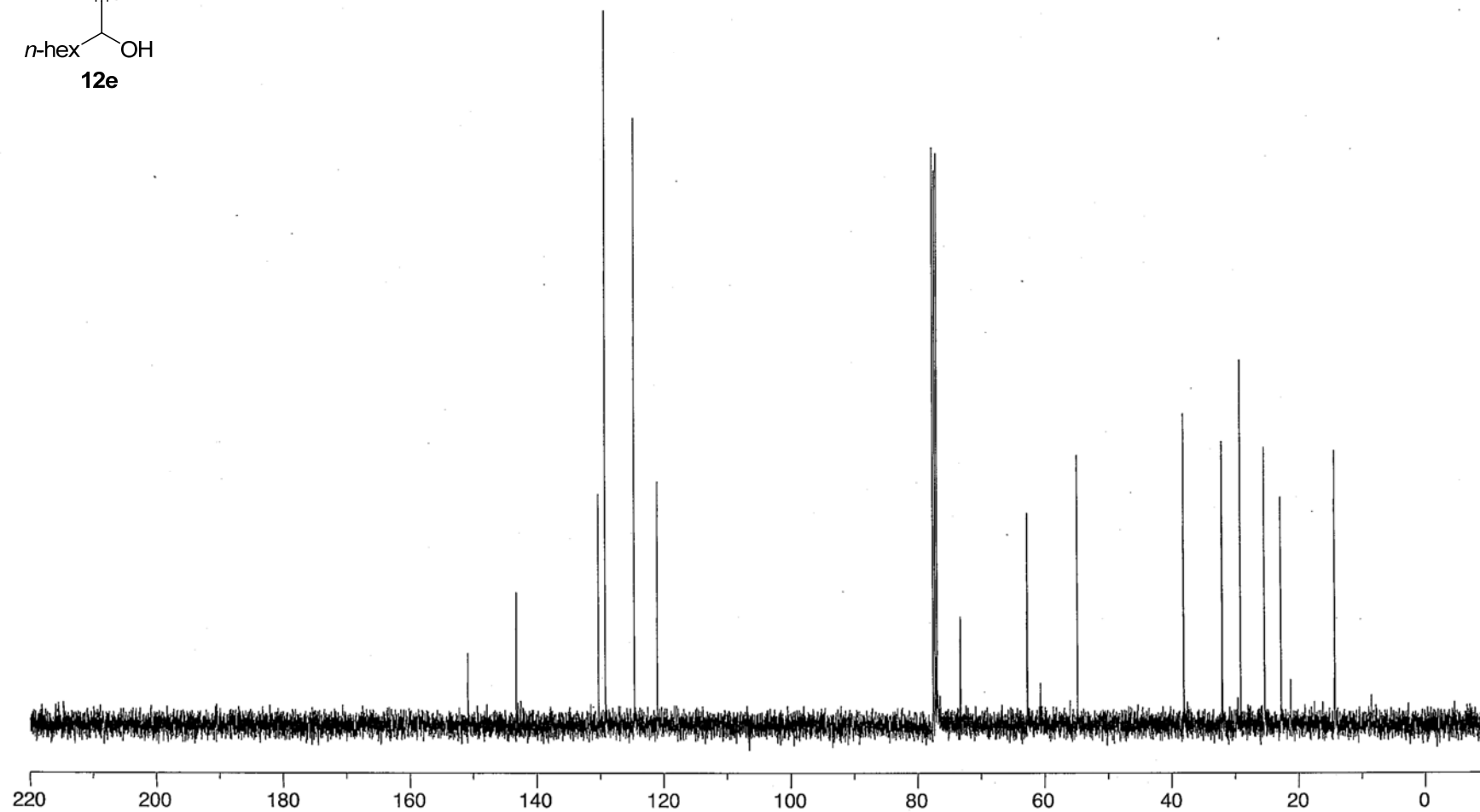
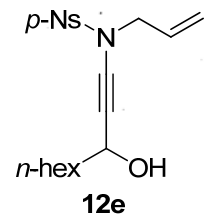
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Pulse Sequence: s2pu1
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



gwm-I-62_15Jul2011

Pulse Sequence: s2pul
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃



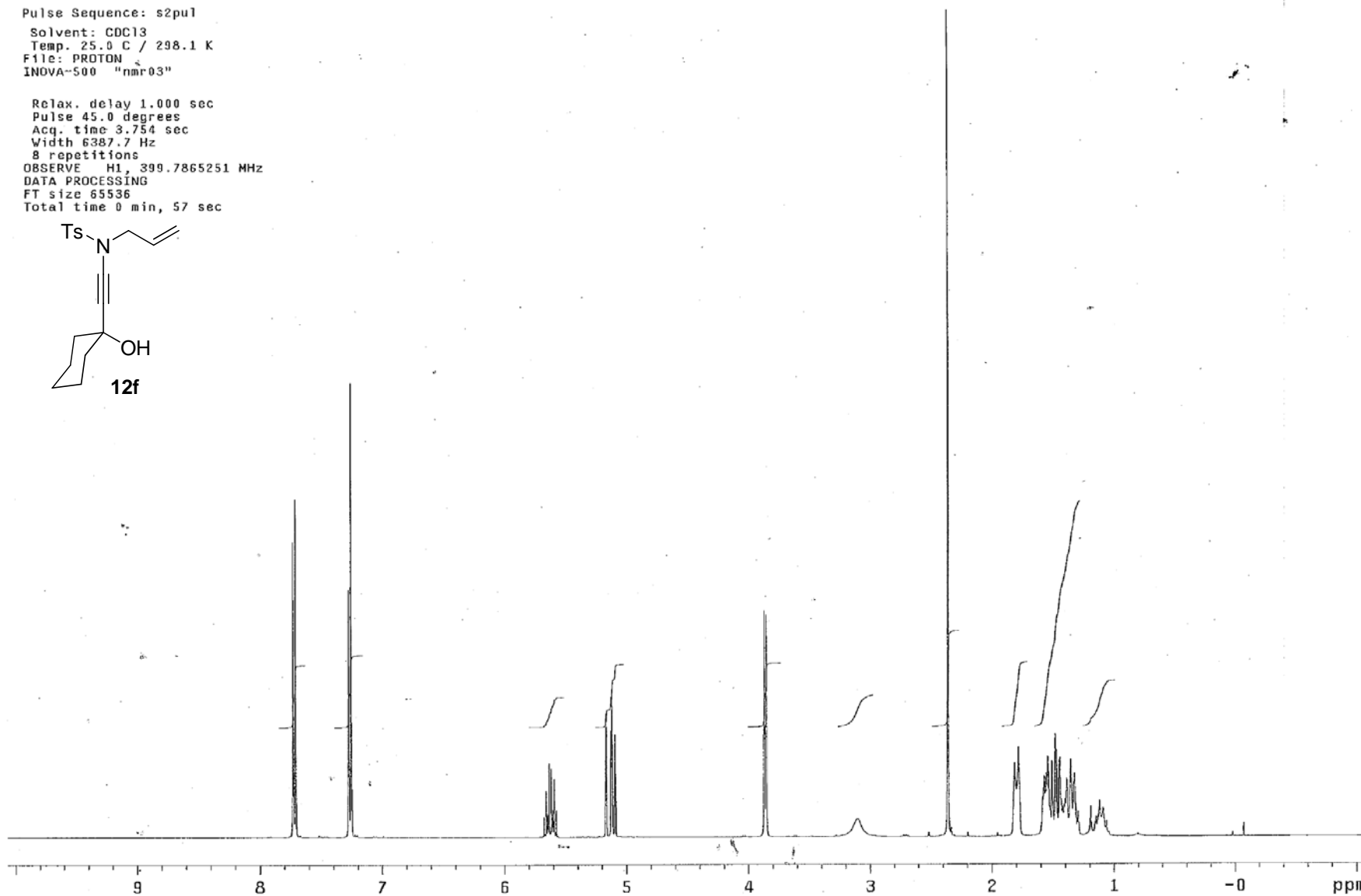
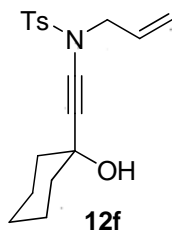
wxn21-1_09Oct2011-14:31:40

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn21-1_09Oct2011-14:31:40

Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865251 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



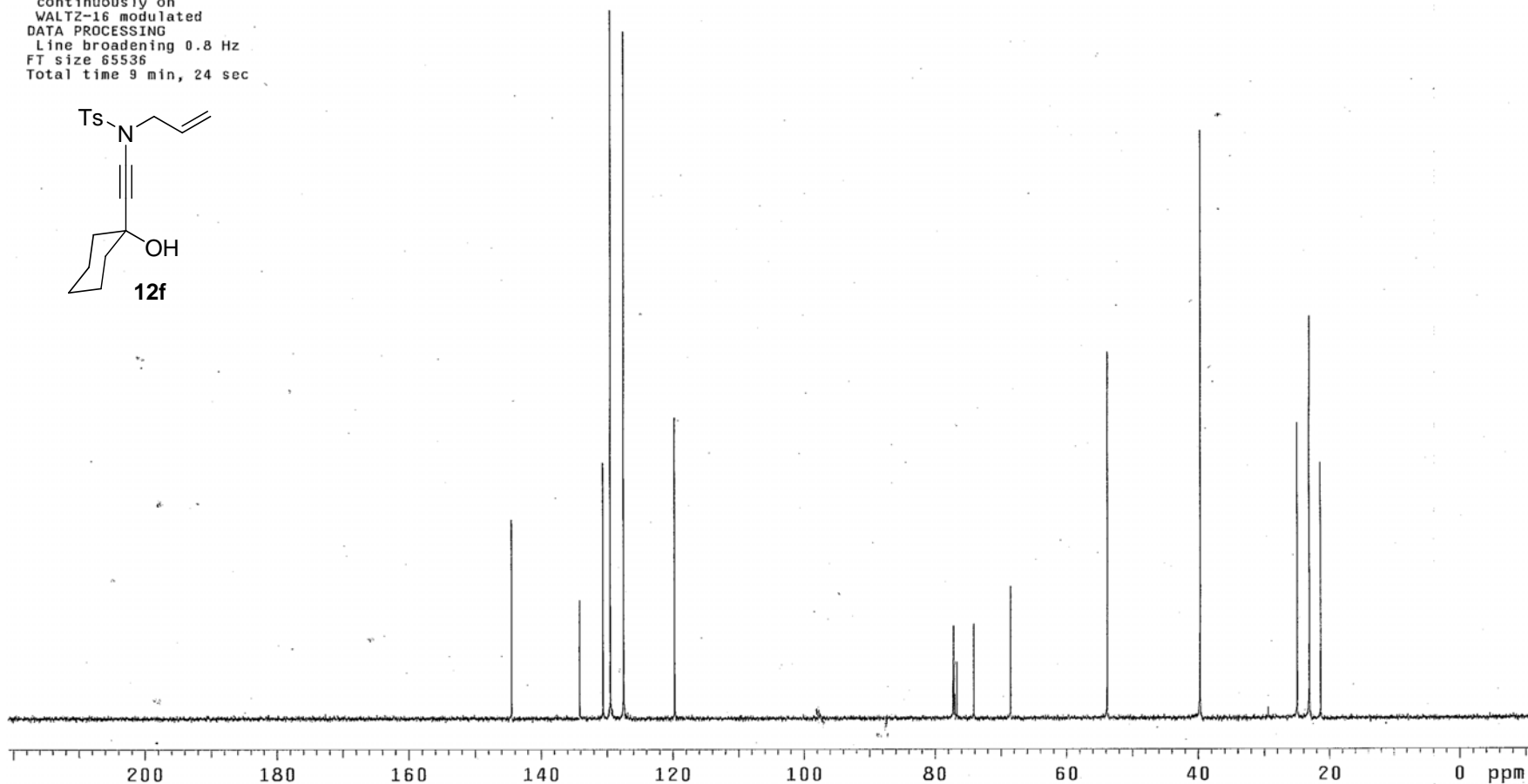
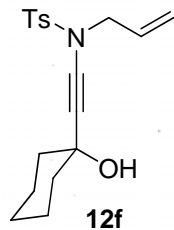
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Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn21-1_09Oct2011-14:31:40

Pulse Sequence: s2pu1

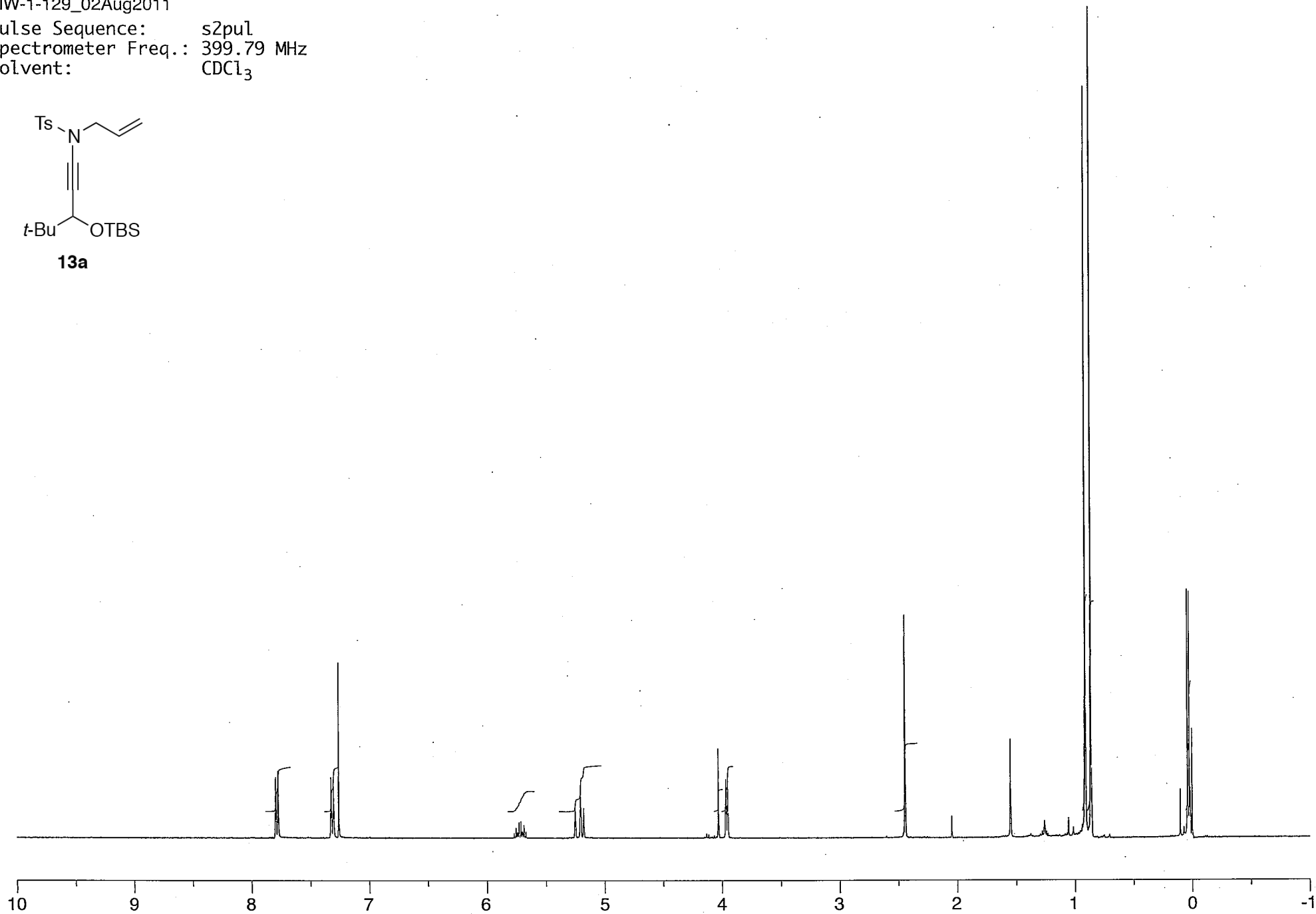
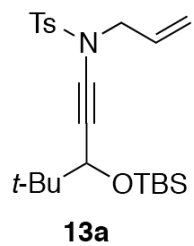
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
54 repetitions
OBSERVE C13, 100.5264253 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 9 min, 24 sec

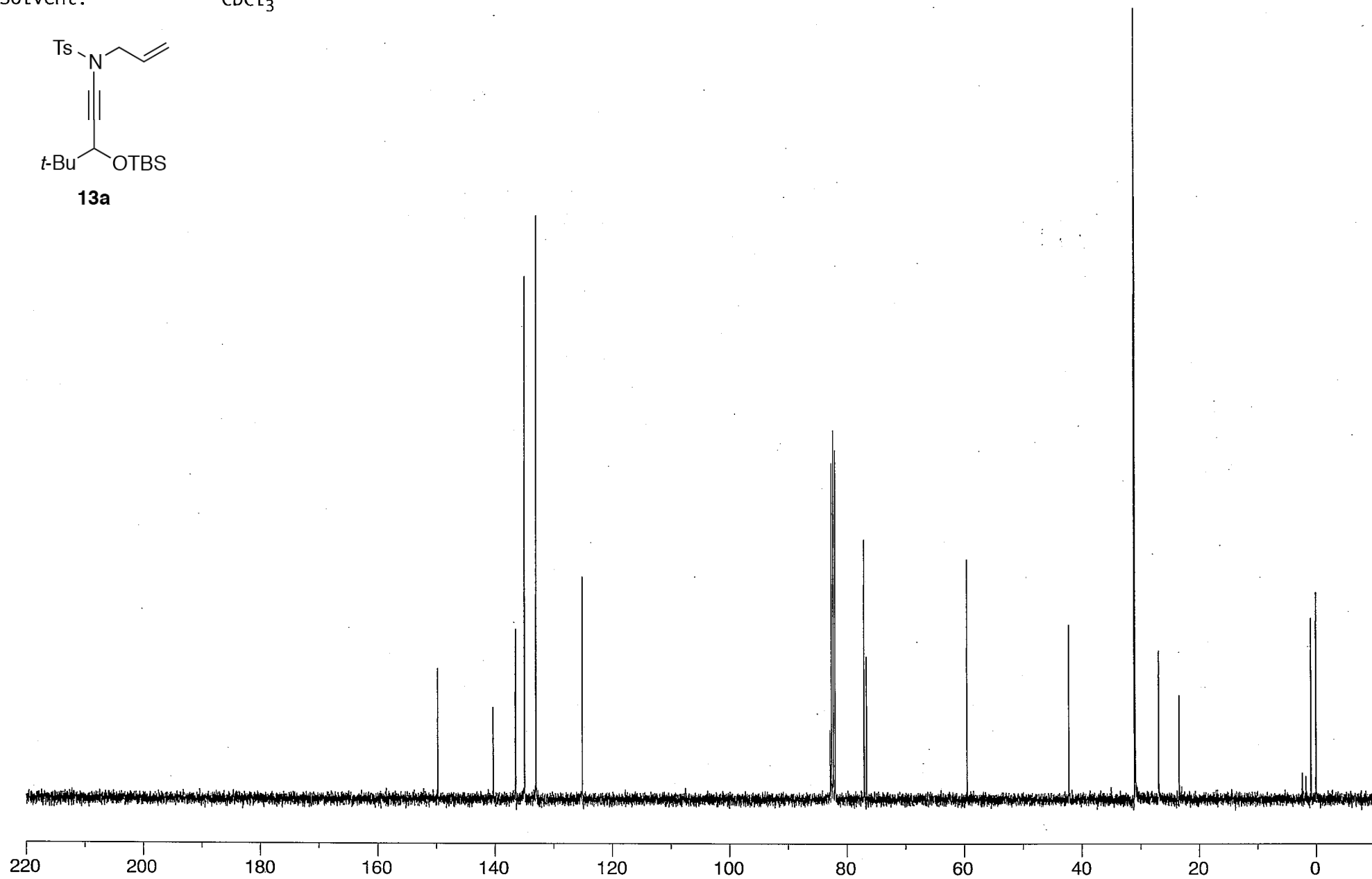
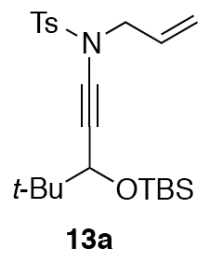


MW-1-129_02Aug2011

Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

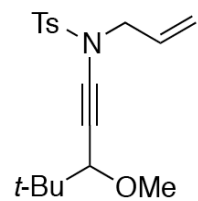


Pulse Sequence: s2pul
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

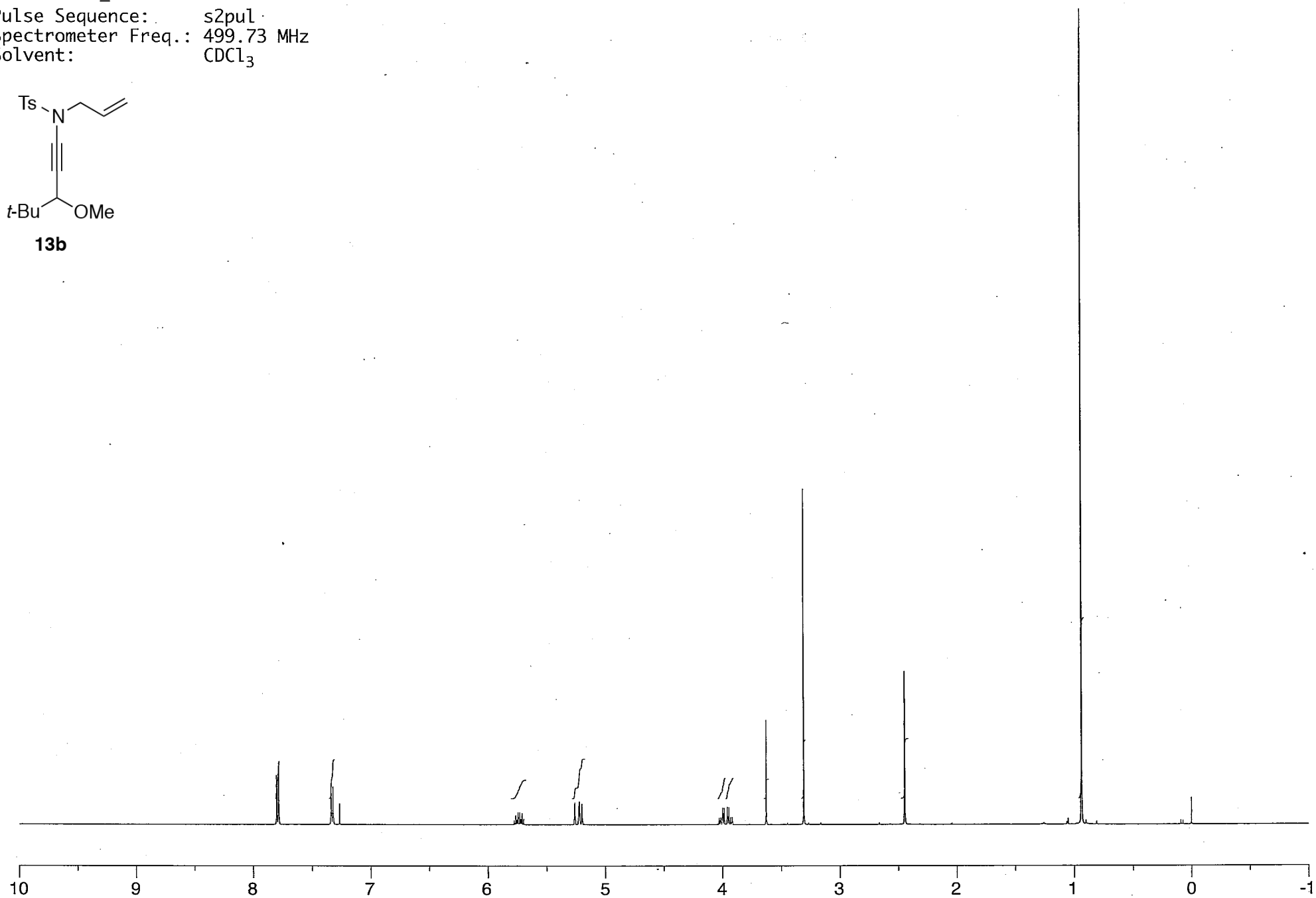


KAD-03-202A_14Oct2011

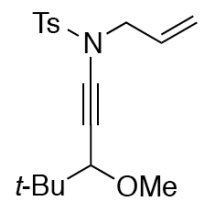
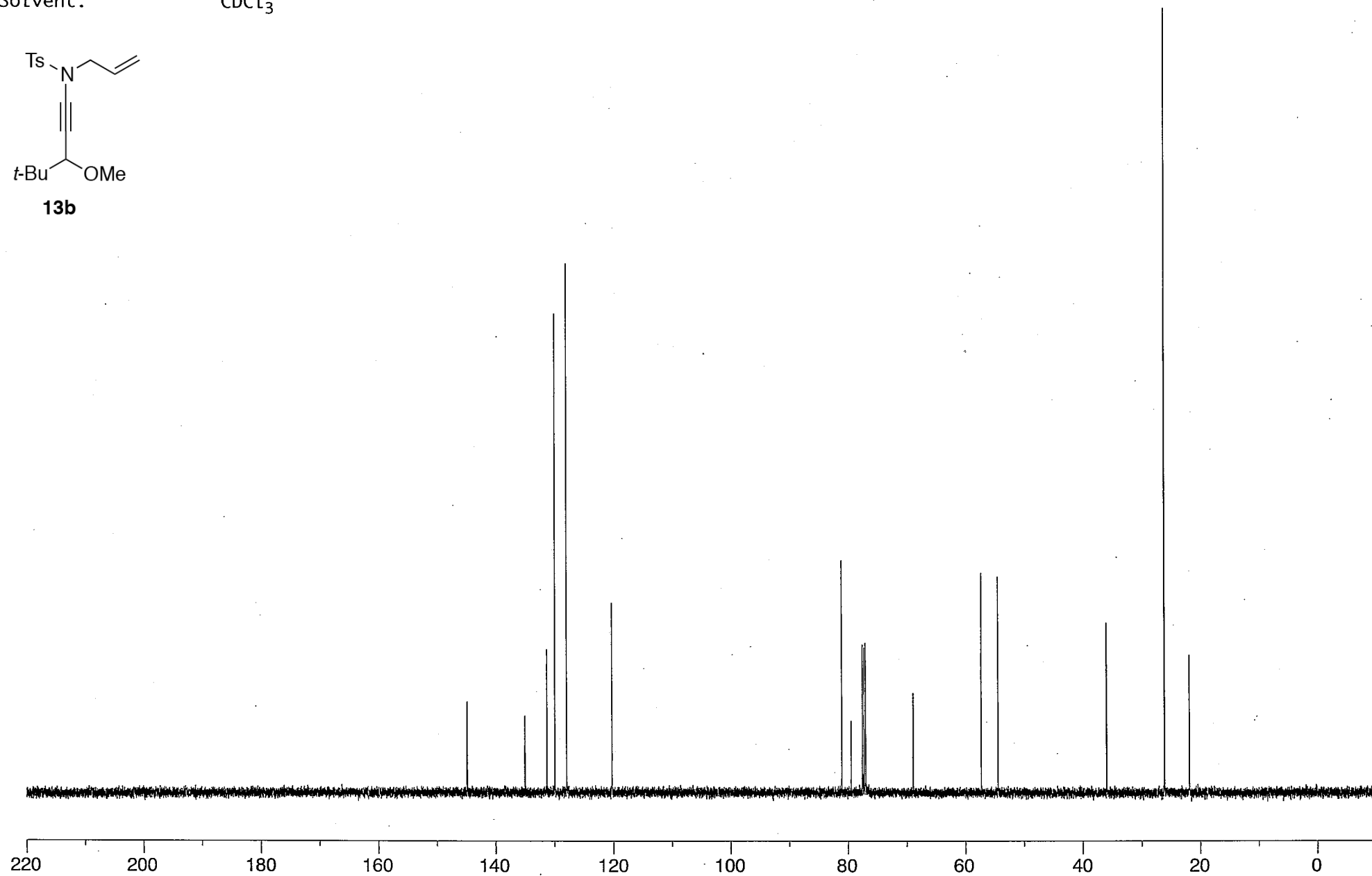
Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃



13b

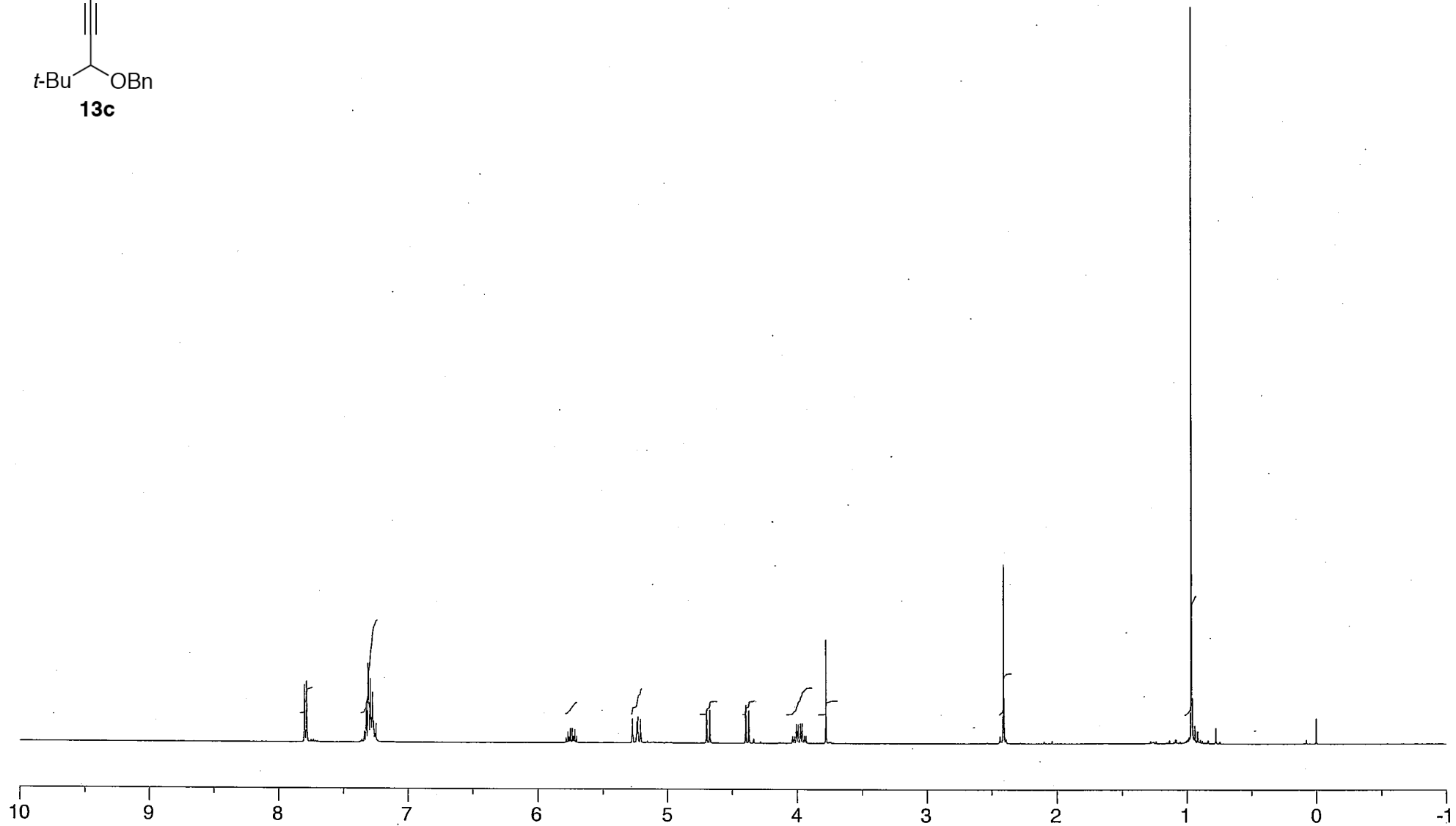
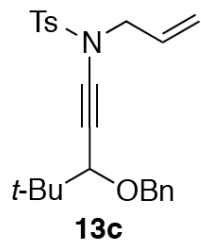


Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃

**13b**

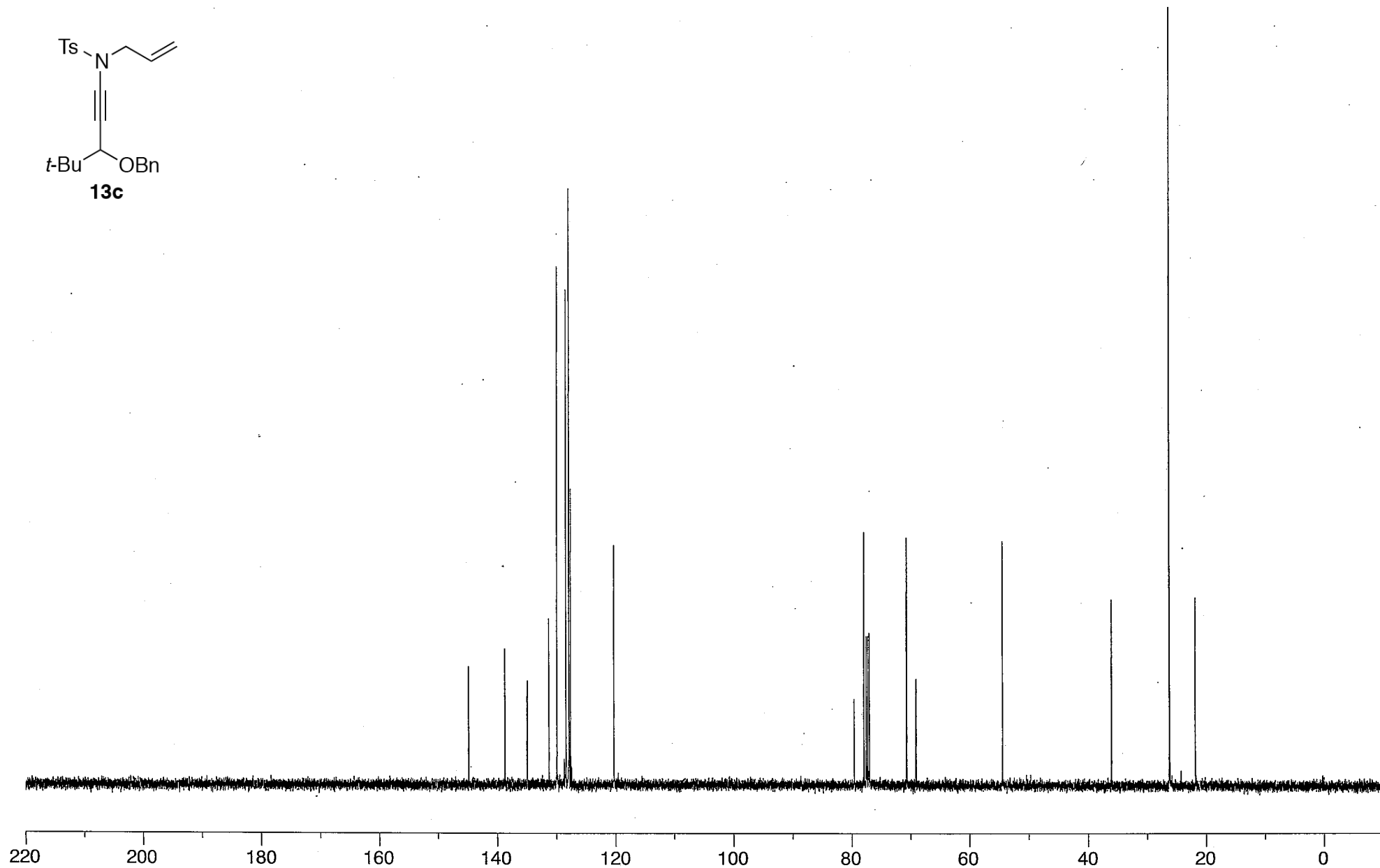
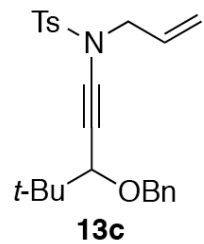
KAD-03-202B_14Oct2011

Pulse Sequence: s2pu1
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃

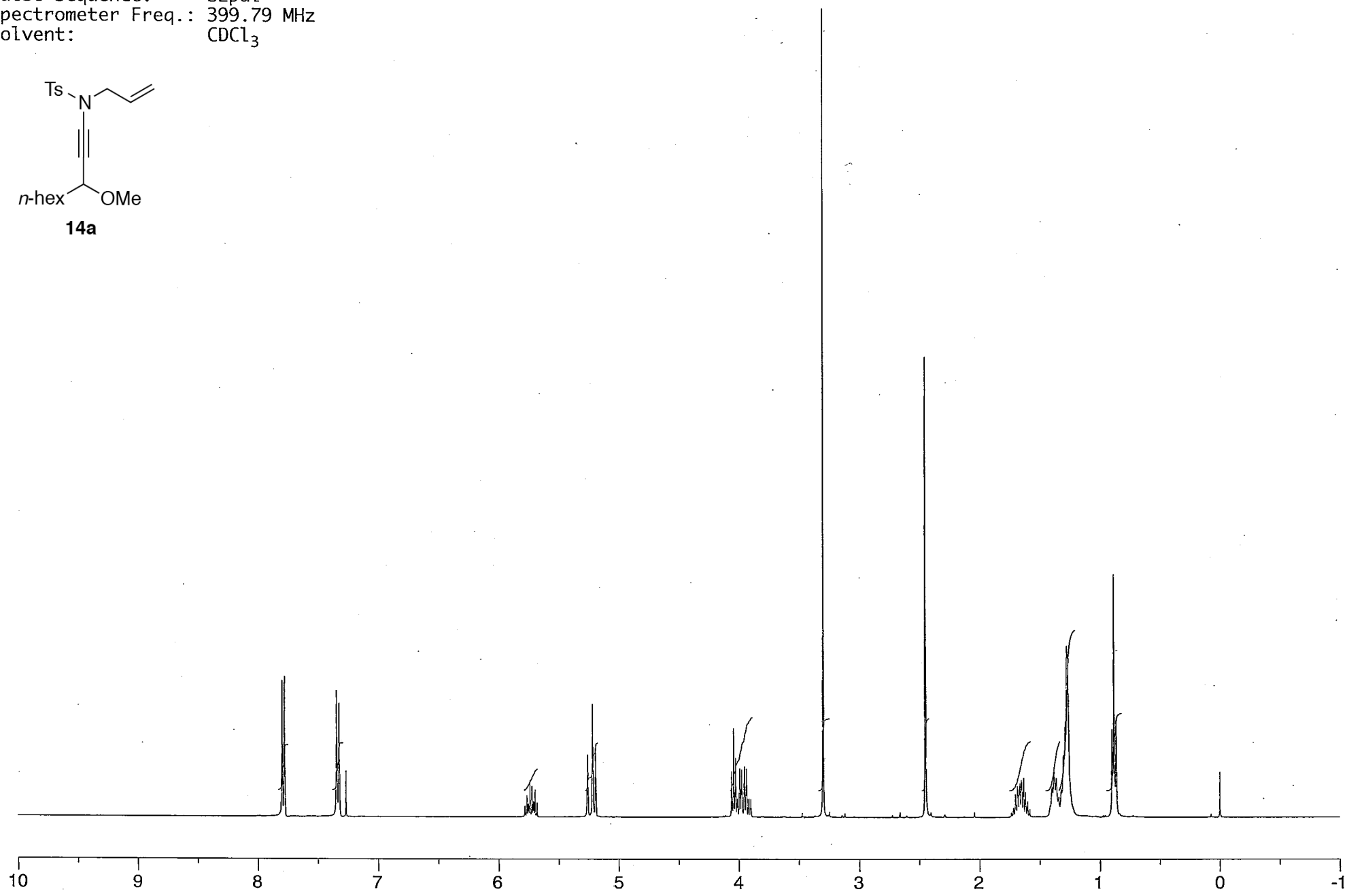
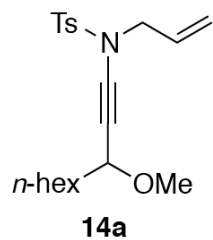


KAD-03-202B_14Oct2011

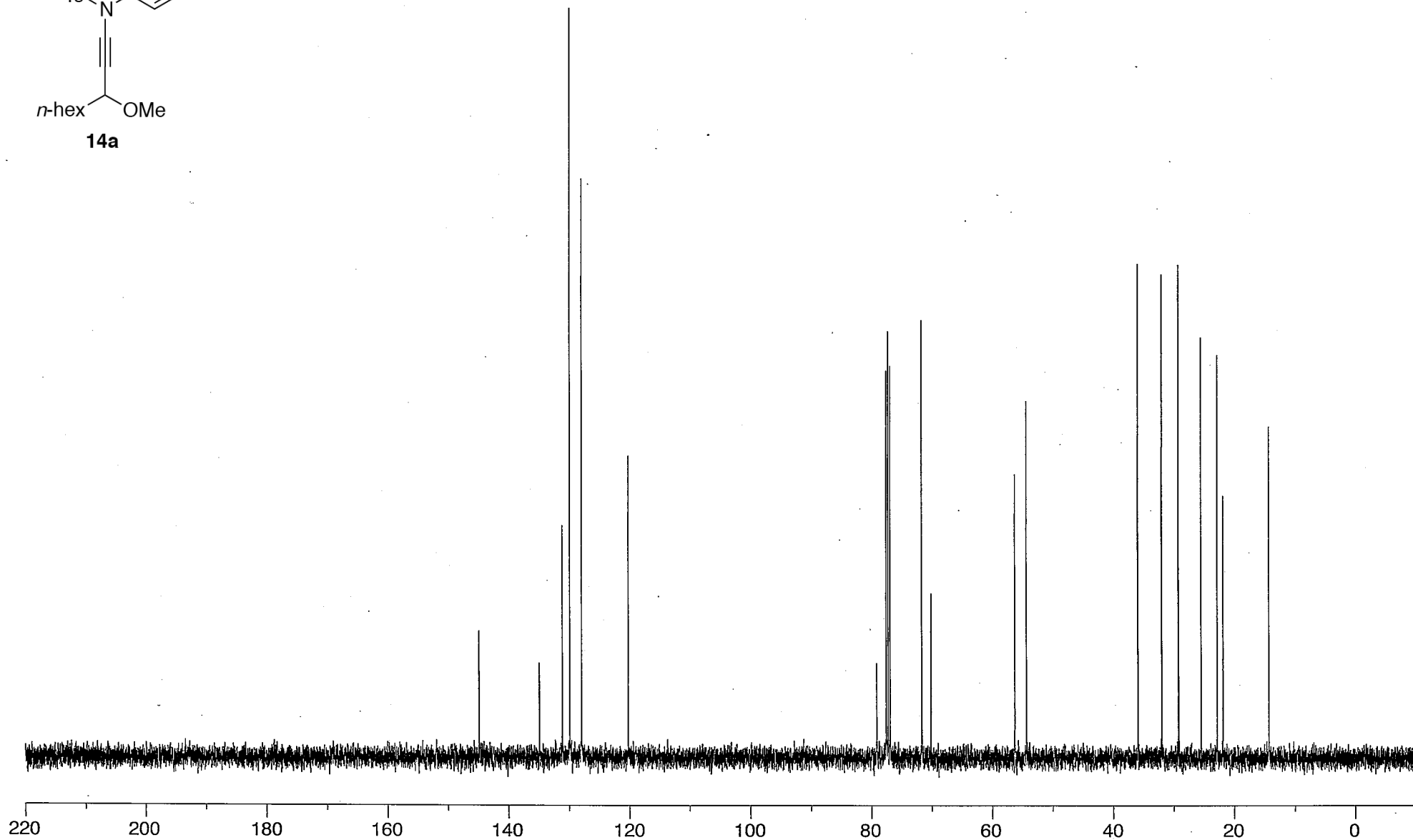
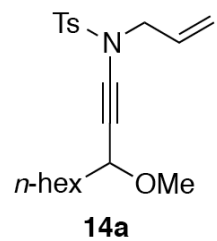
Pulse Sequence: s2pu1
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃



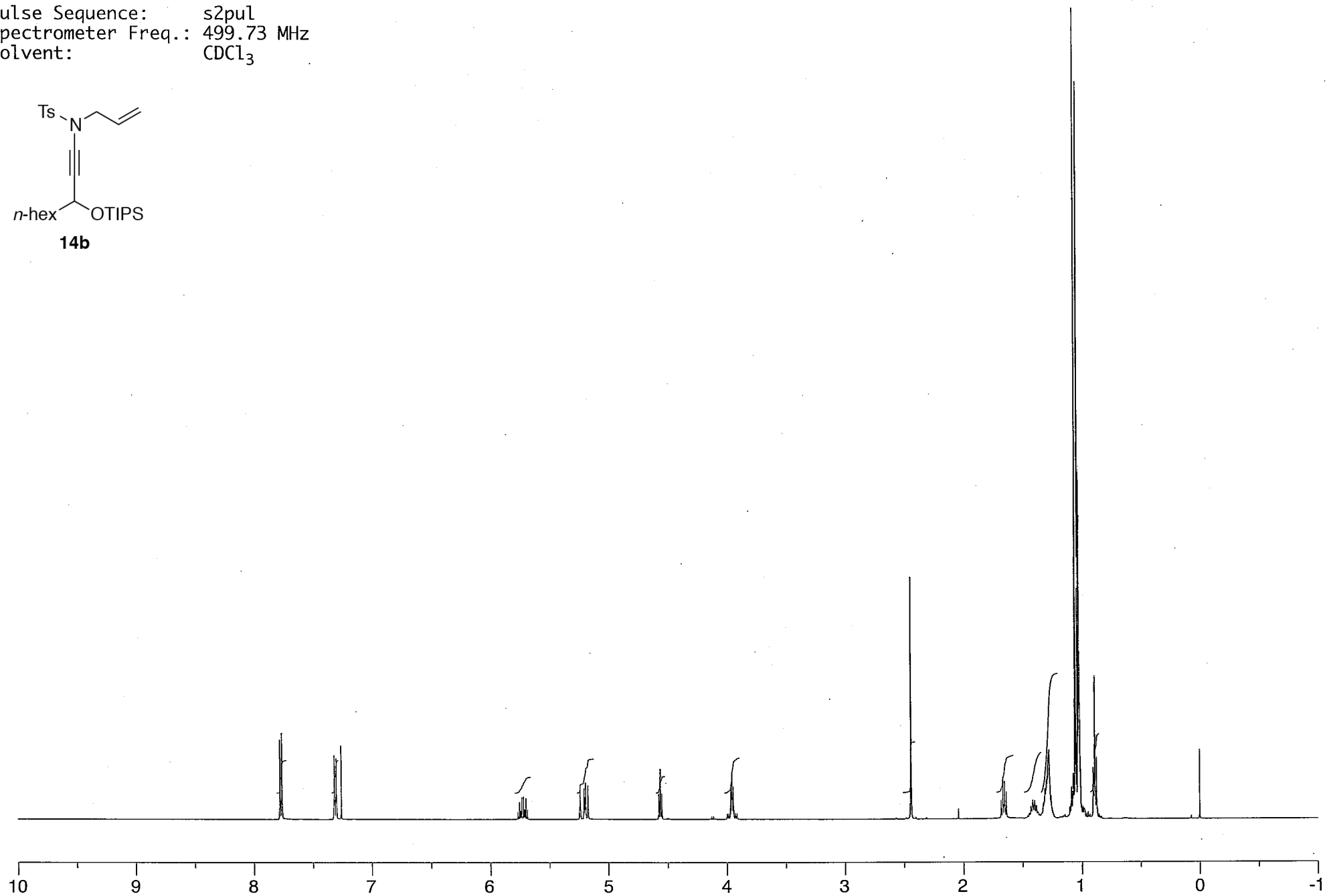
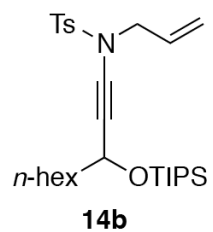
Pulse Sequence: s2pu1
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



Pulse Sequence: s2pul
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

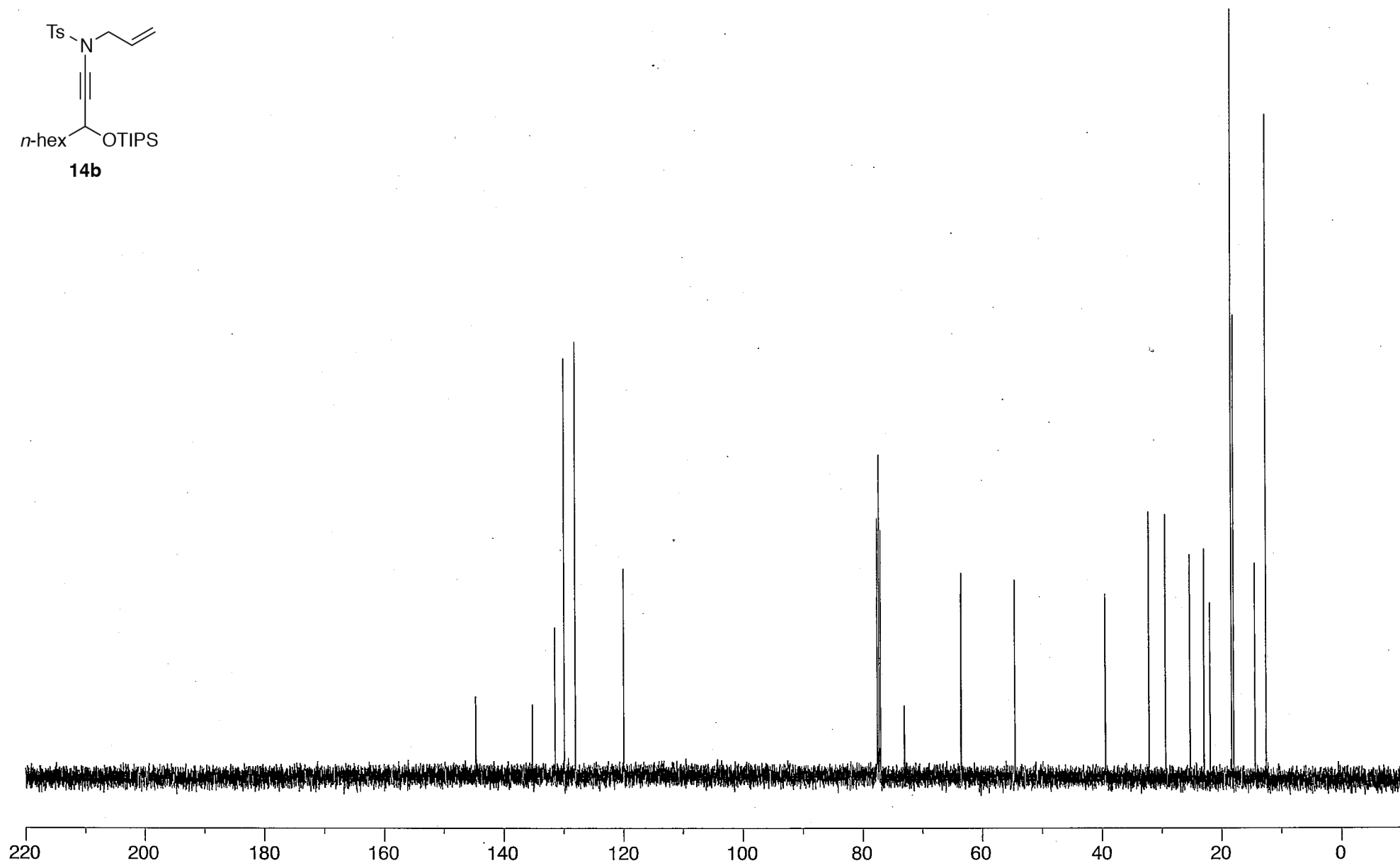
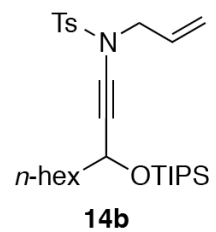


Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃

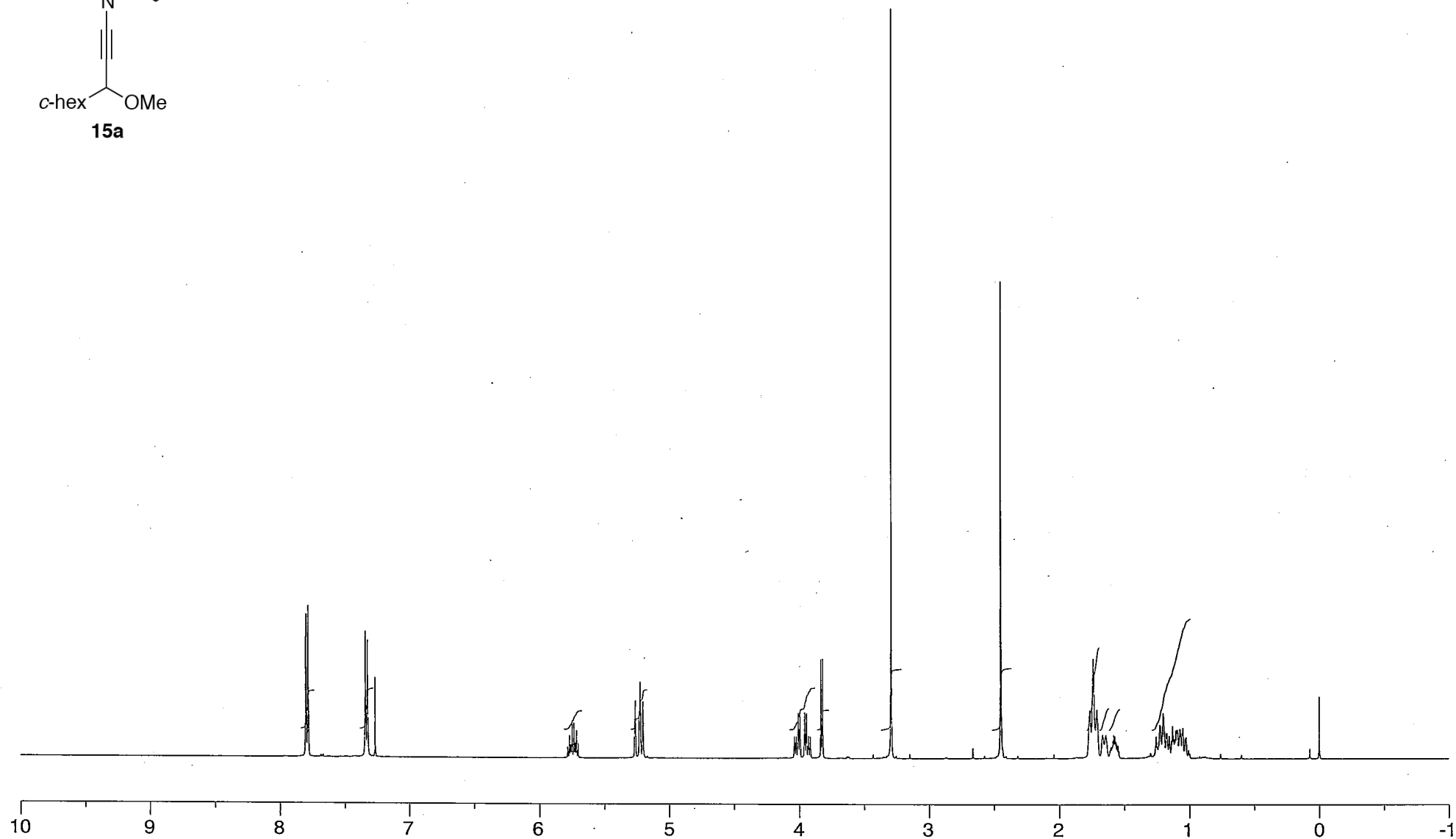
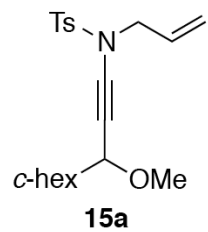


KAD-03-190A_03Oct2011

Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃

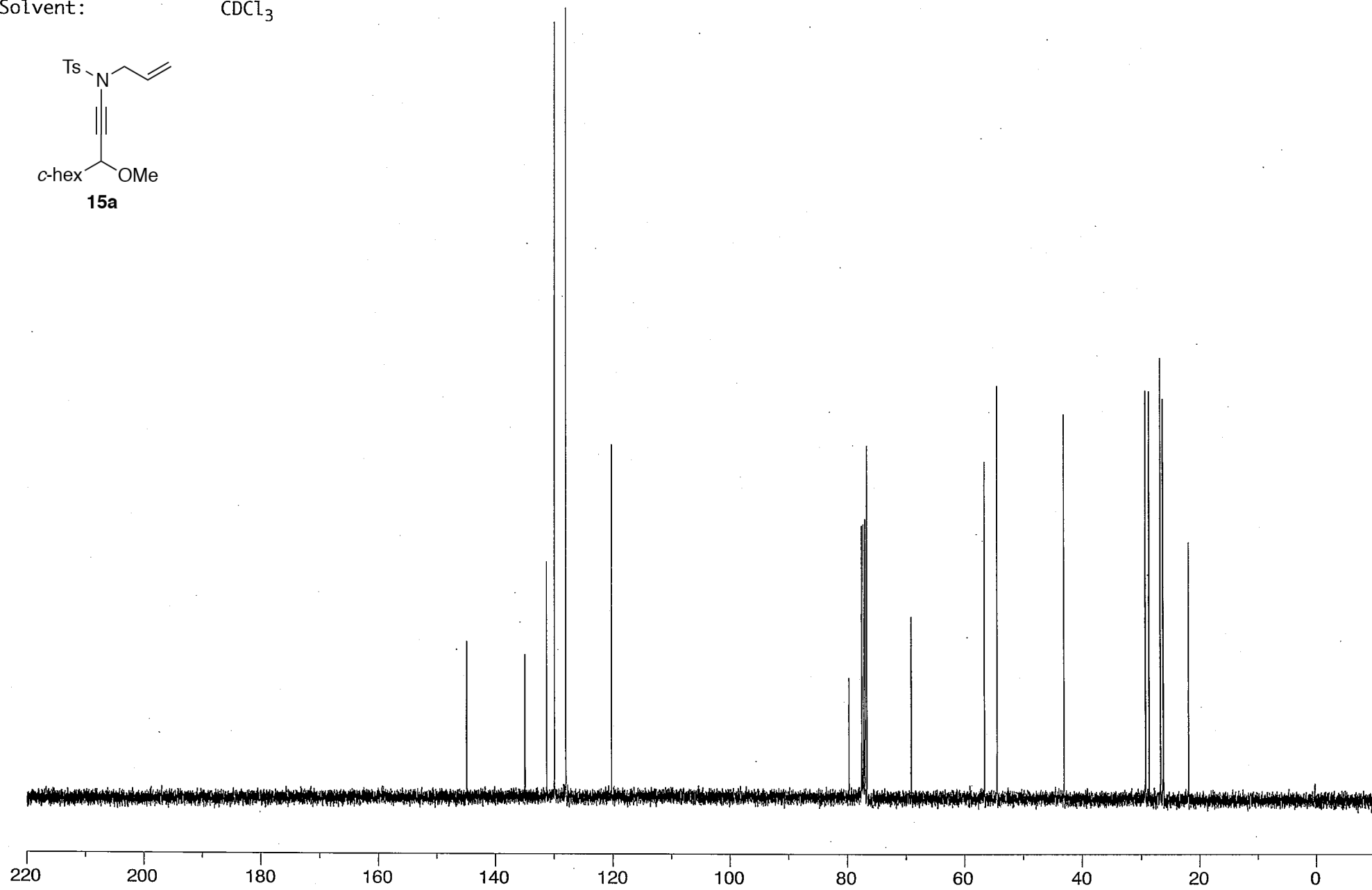
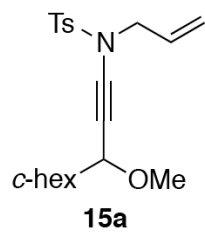


Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃



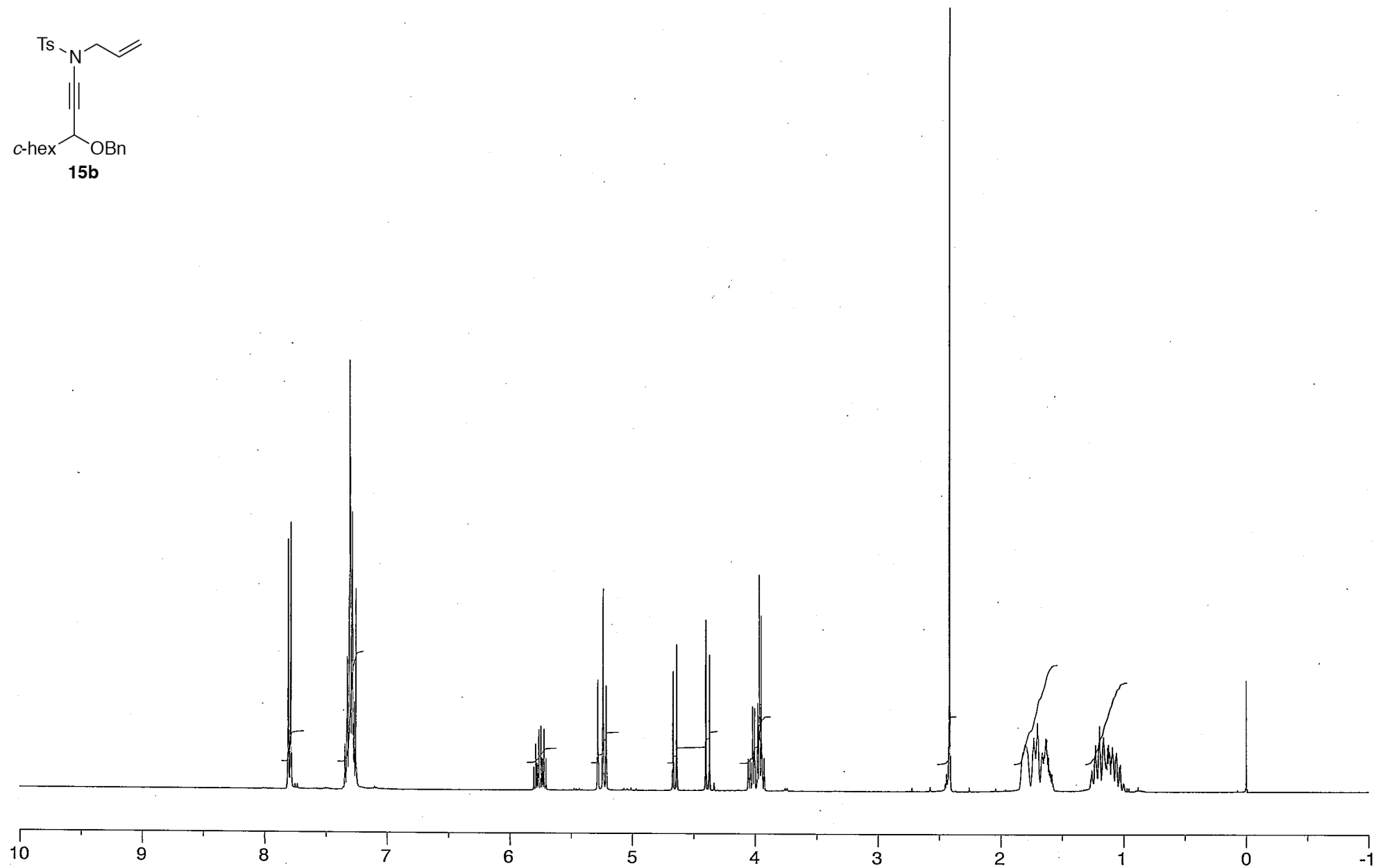
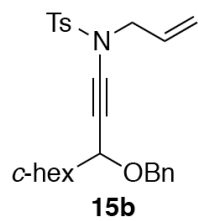
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Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃



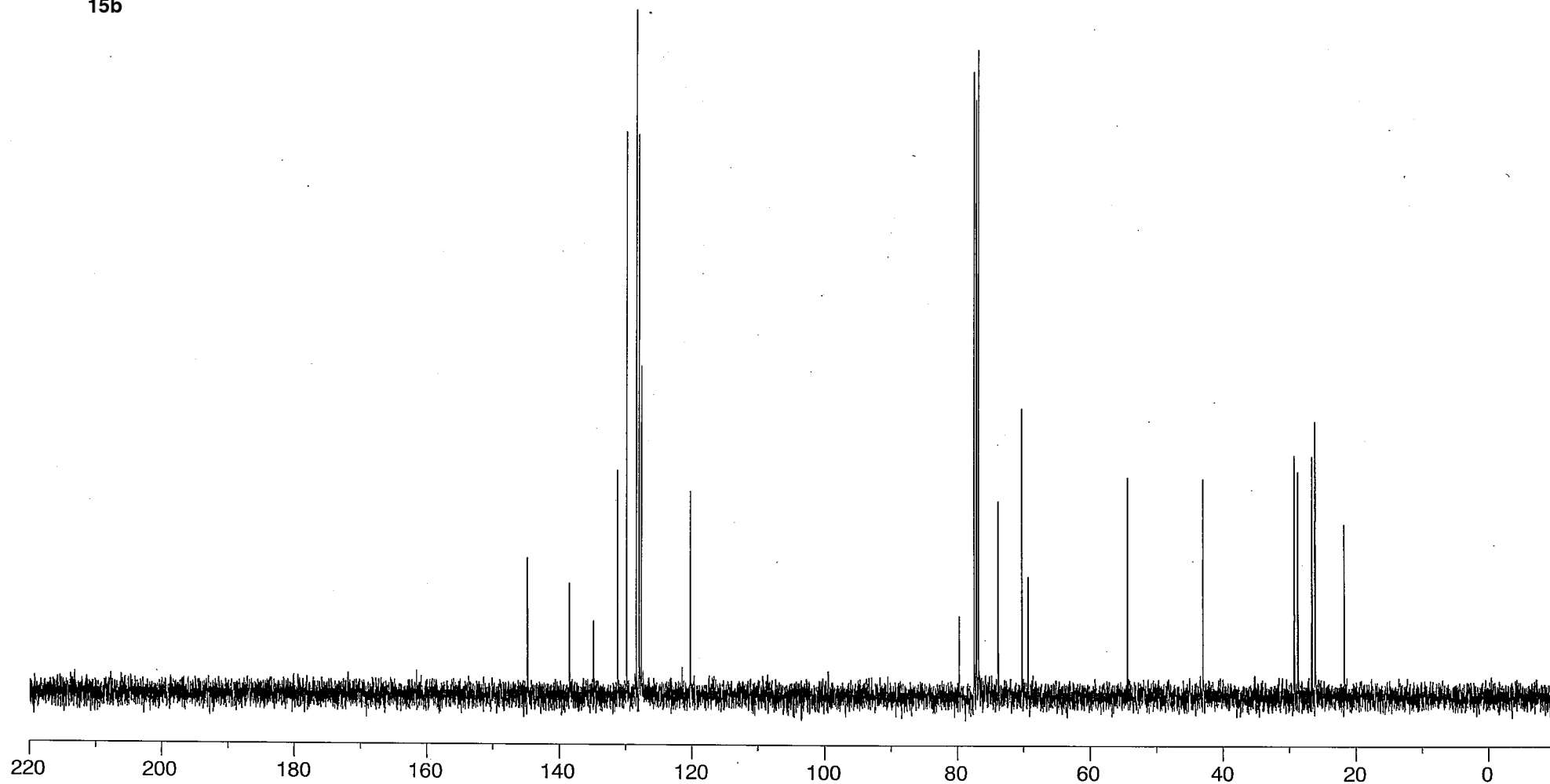
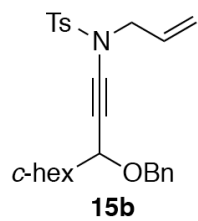
gwm-l-70_01Aug2011

Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



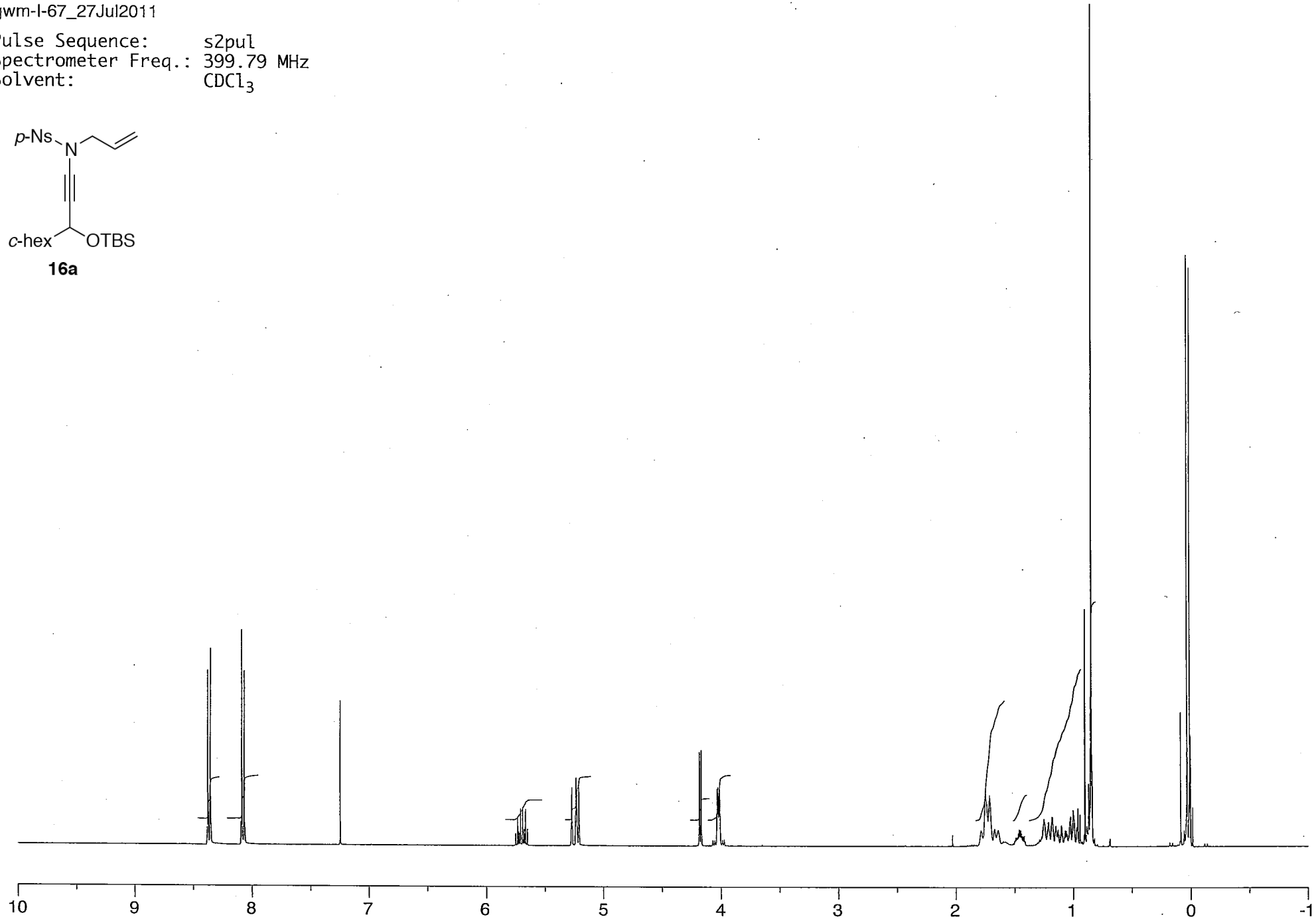
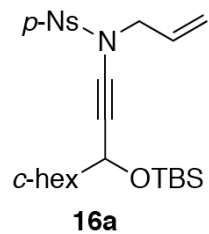
gwm-l-70_01Aug2011

Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

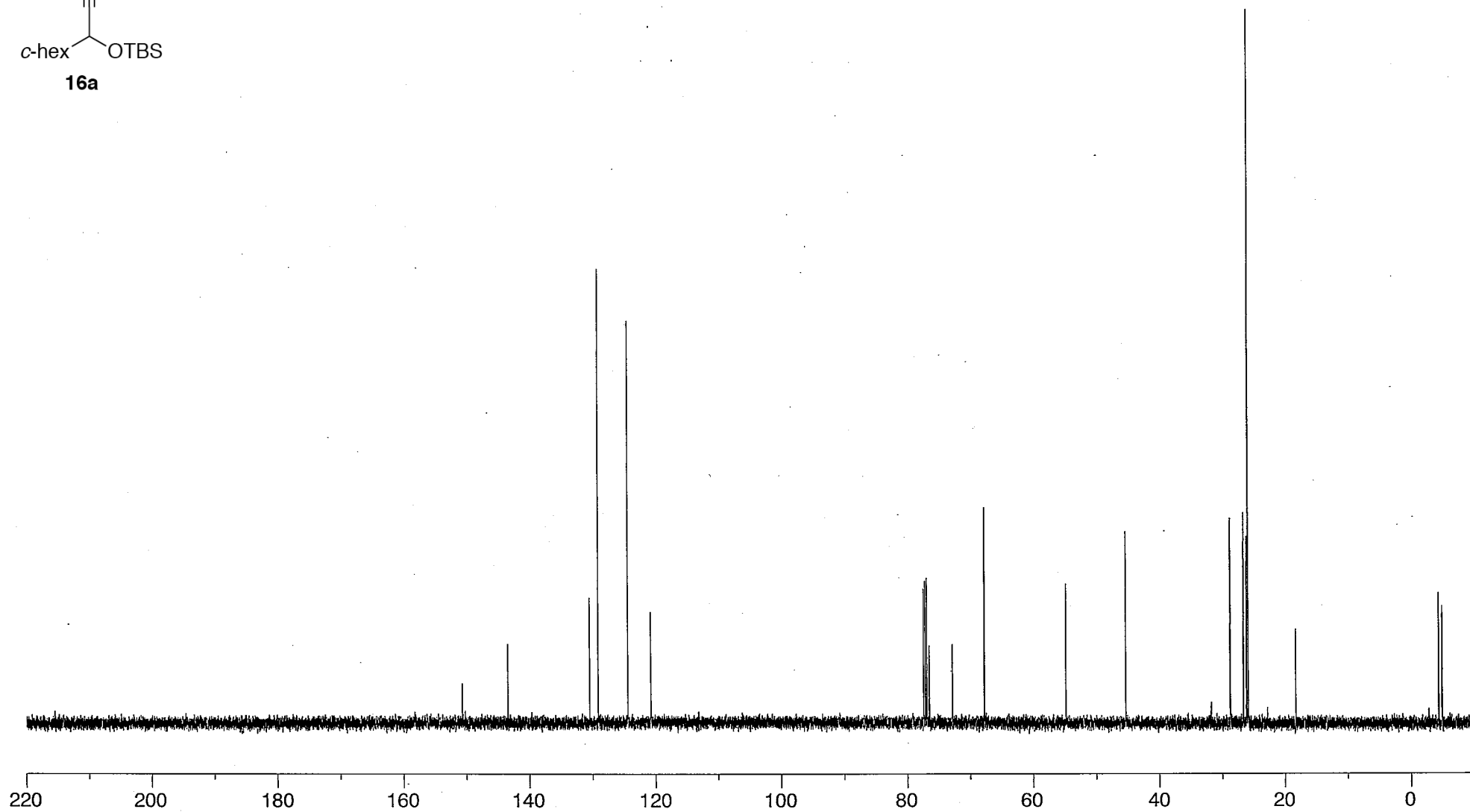
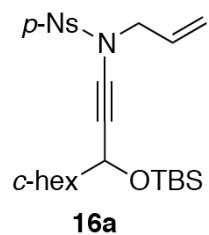


gwm-l-67_27Jul2011

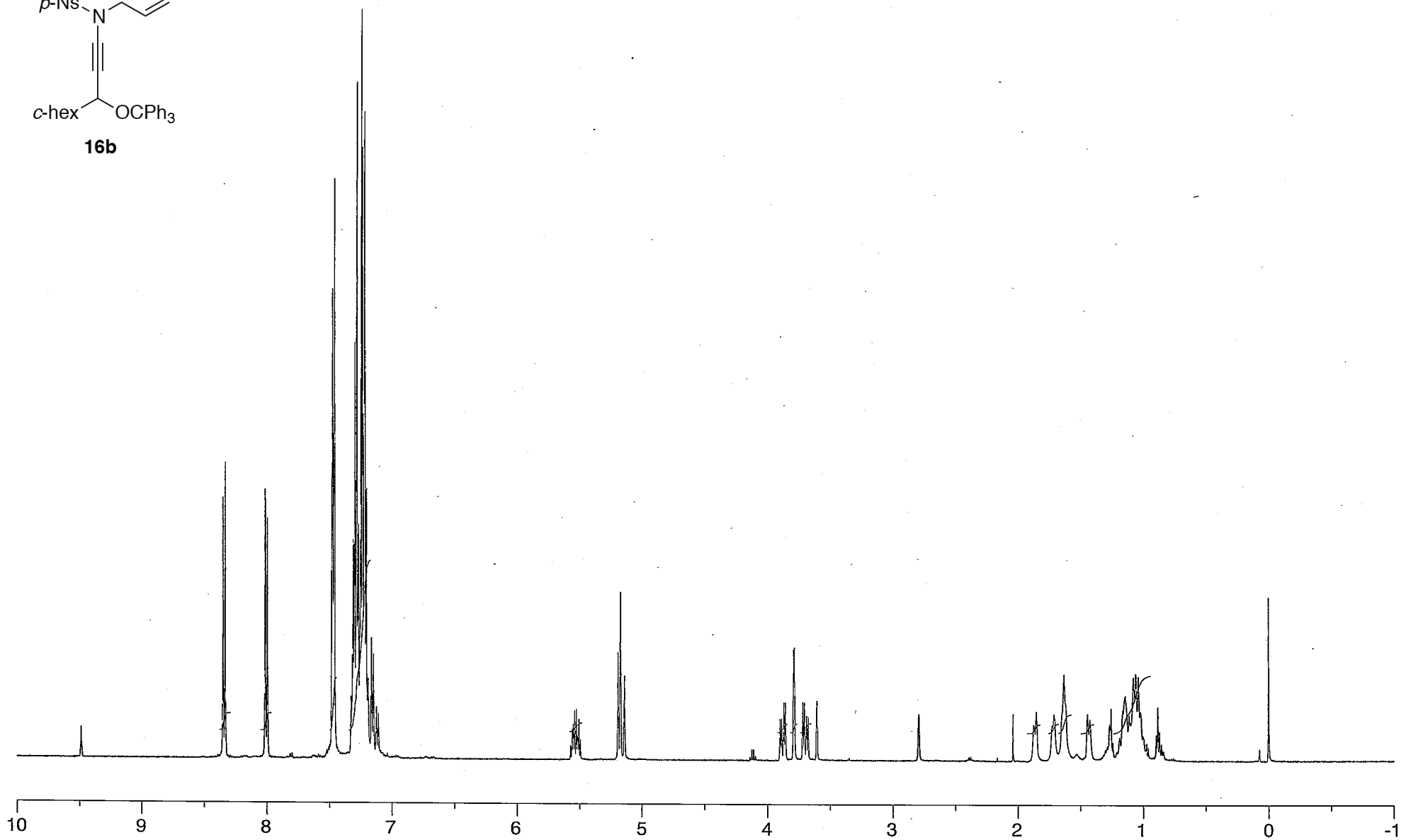
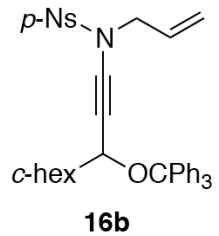
Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃

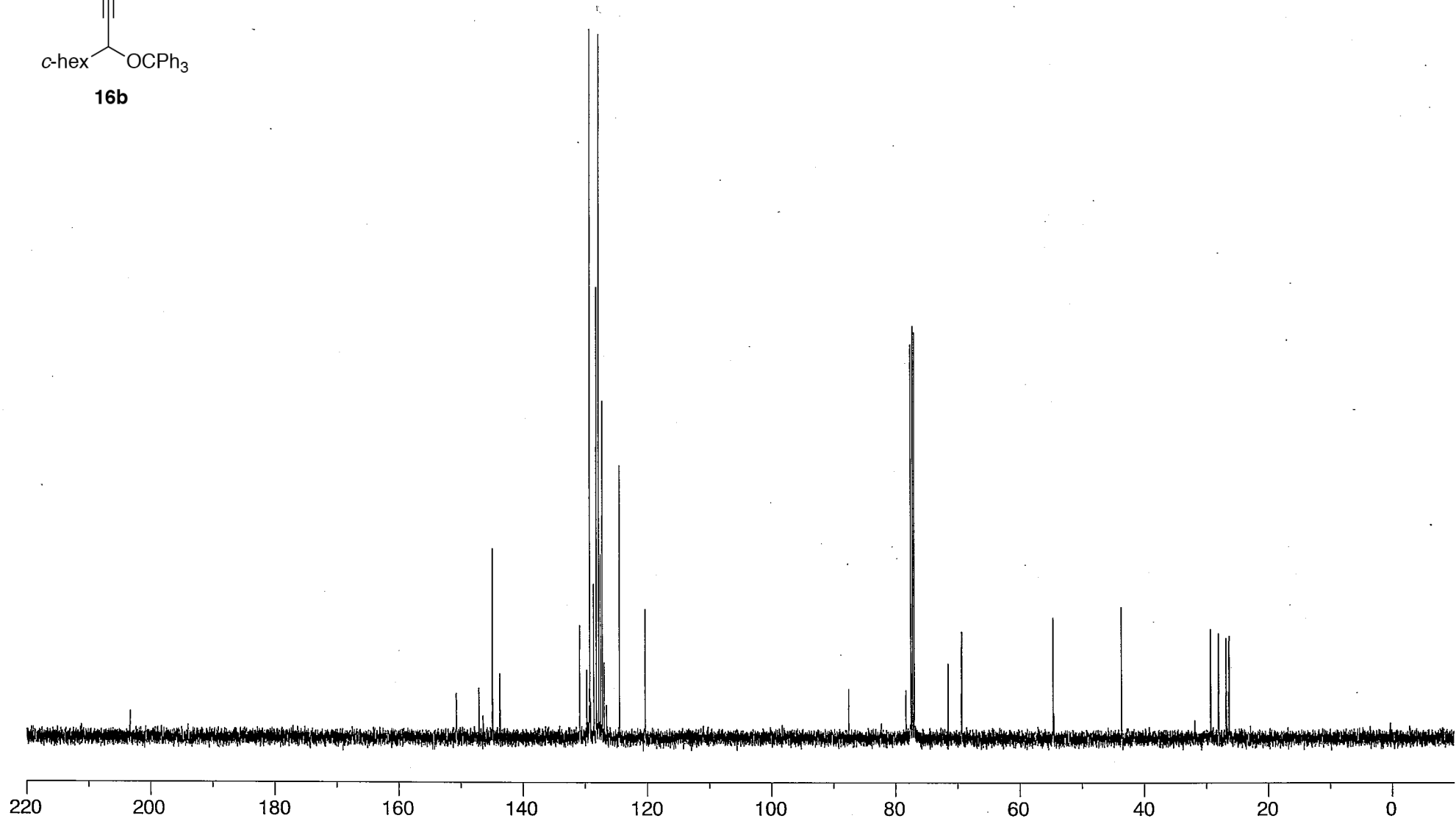
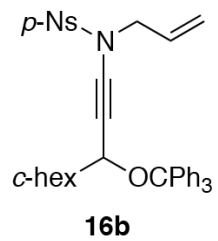


Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃



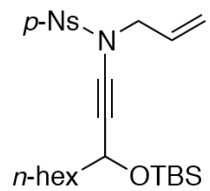
KAD-03-194_08Oct2011

Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃

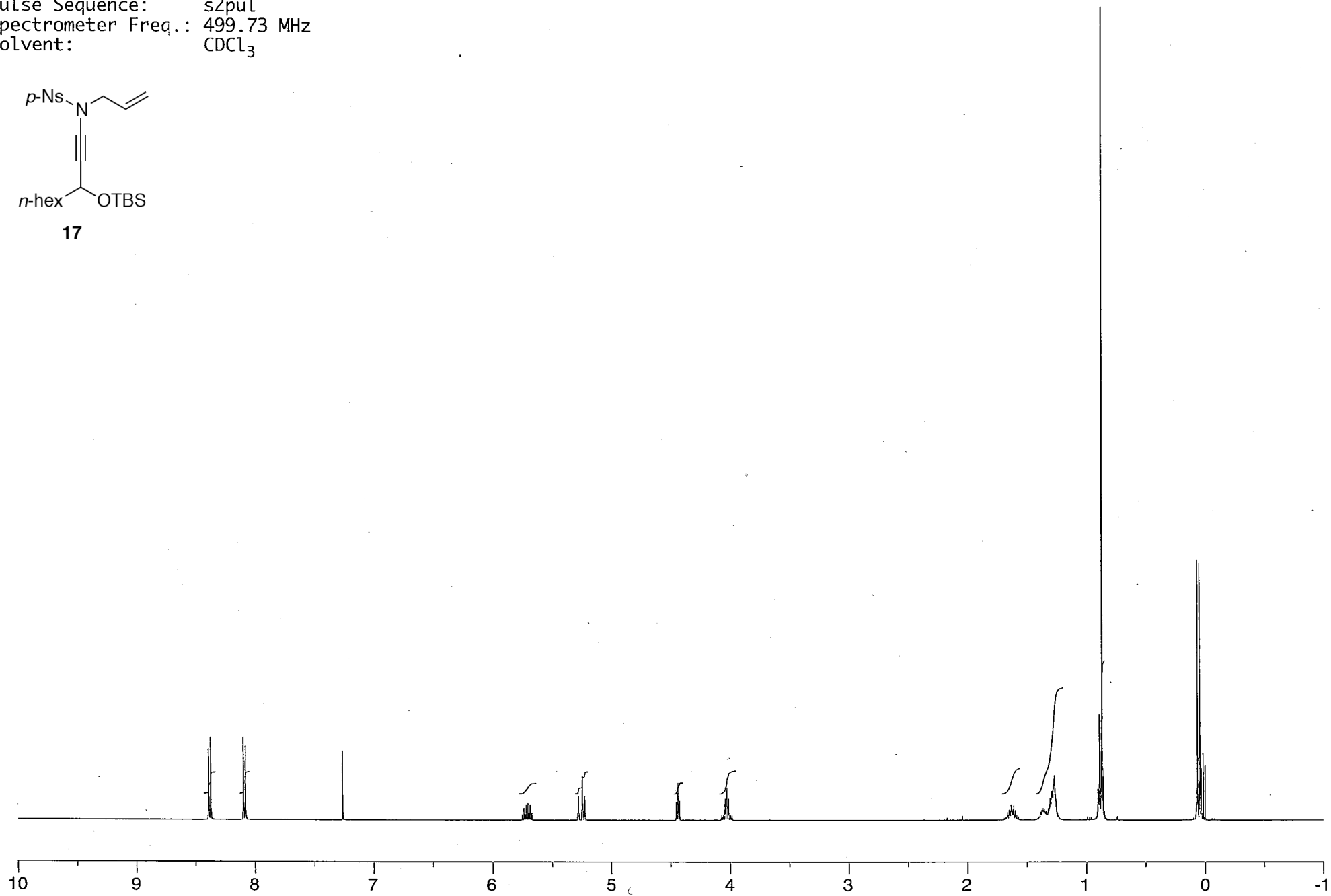


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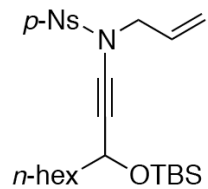
Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃



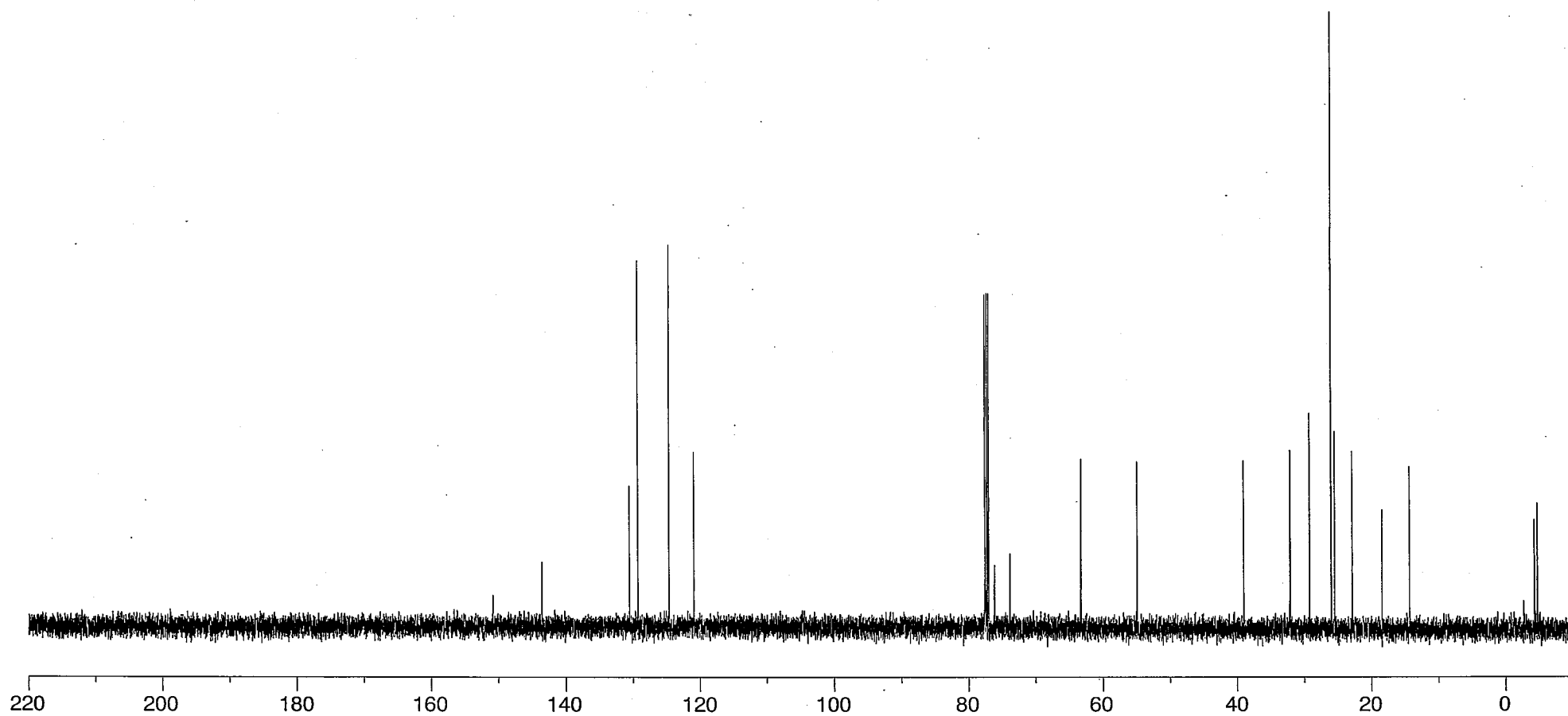
17



Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃



17



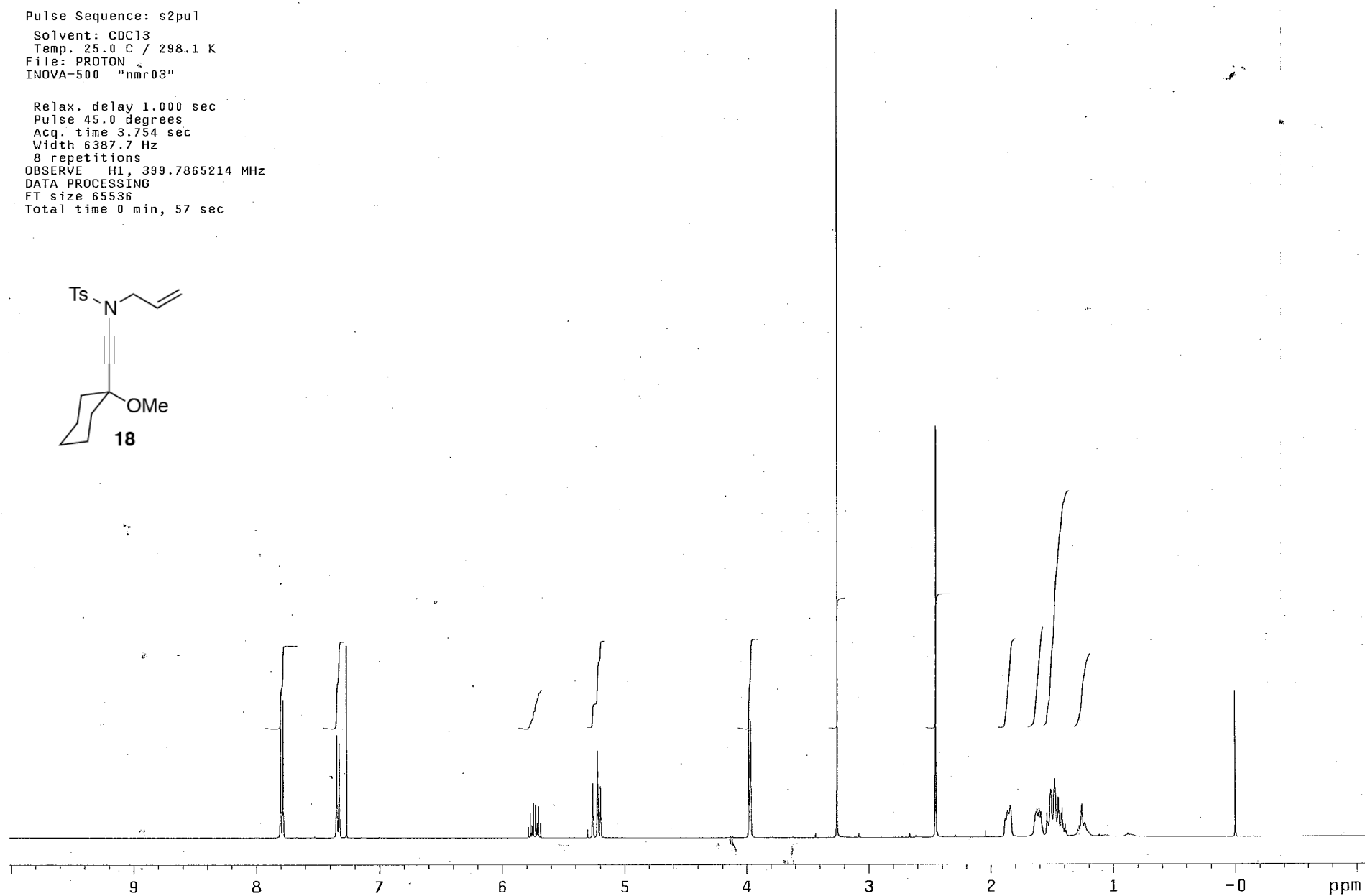
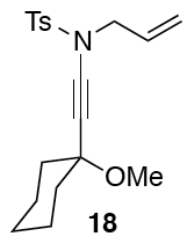
wxn22-1_10Oct2011-16:10:19

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn22-1_10Oct2011-16:10:19

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865214 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



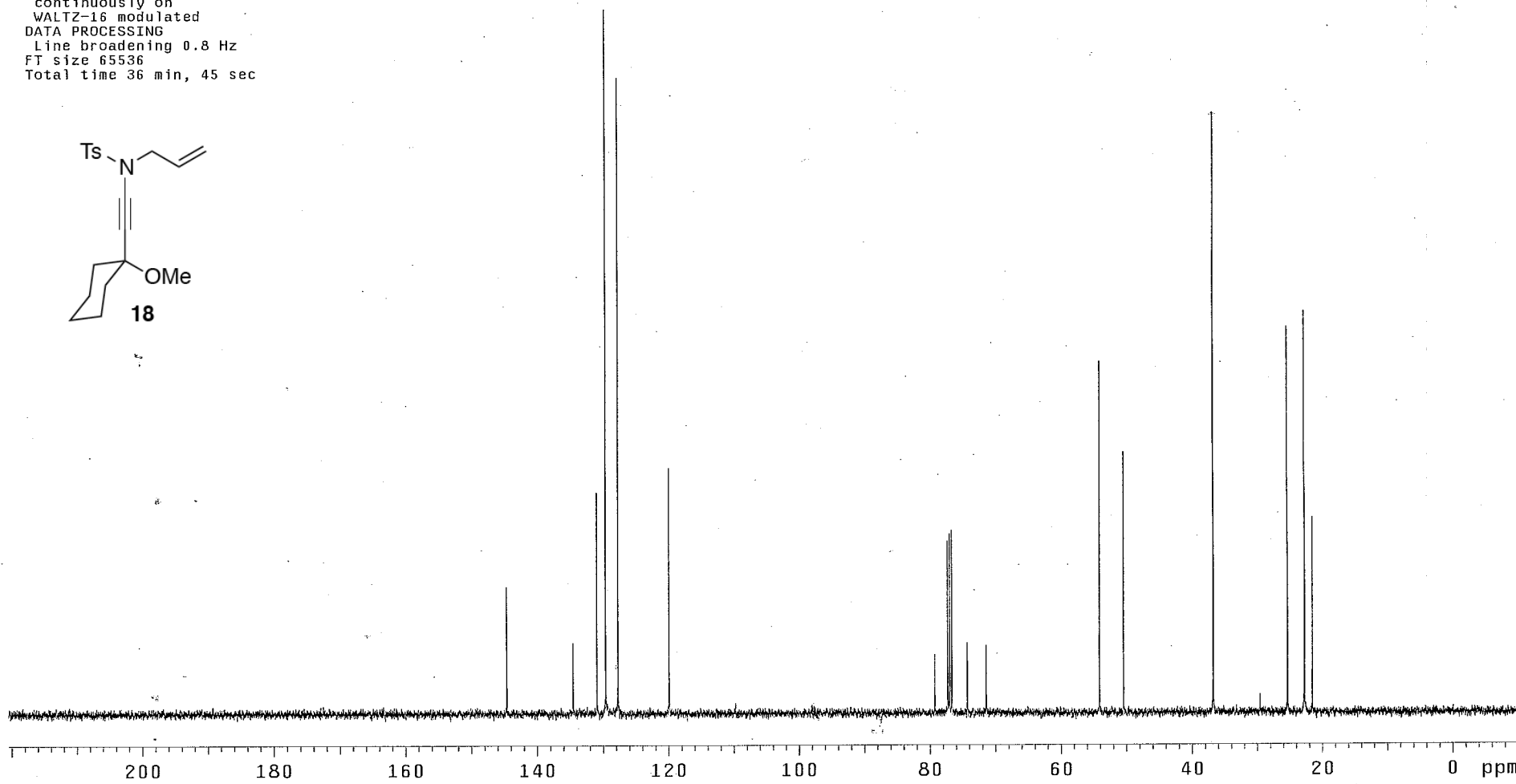
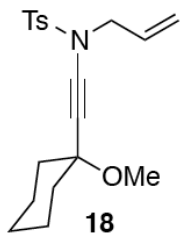
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Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn22-1_10Oct2011-17:25:08

Pulse Sequence: s2pul

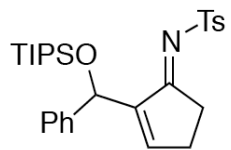
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INNOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
174 repetitions
OBSERVE C13, 100.5264076 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 36 min, 45 sec

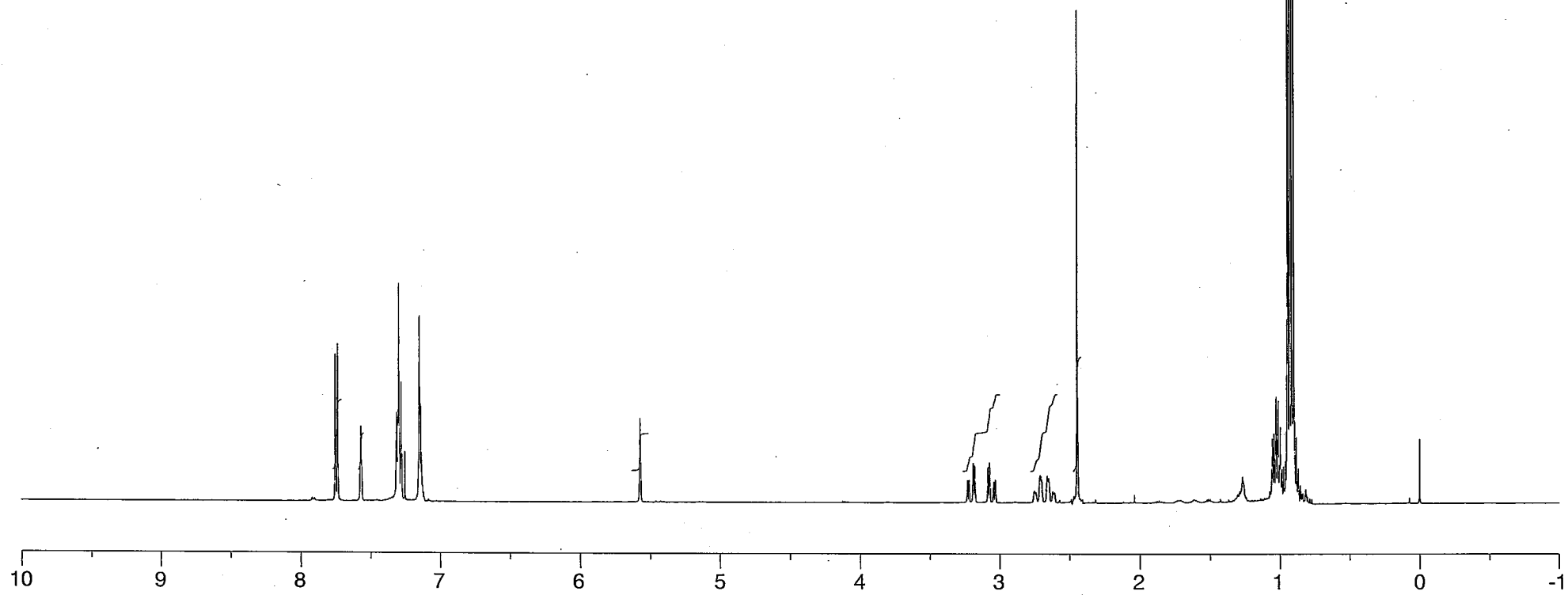


KAD-03-047B

Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃

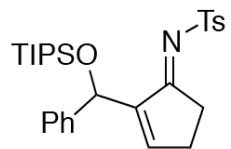


8

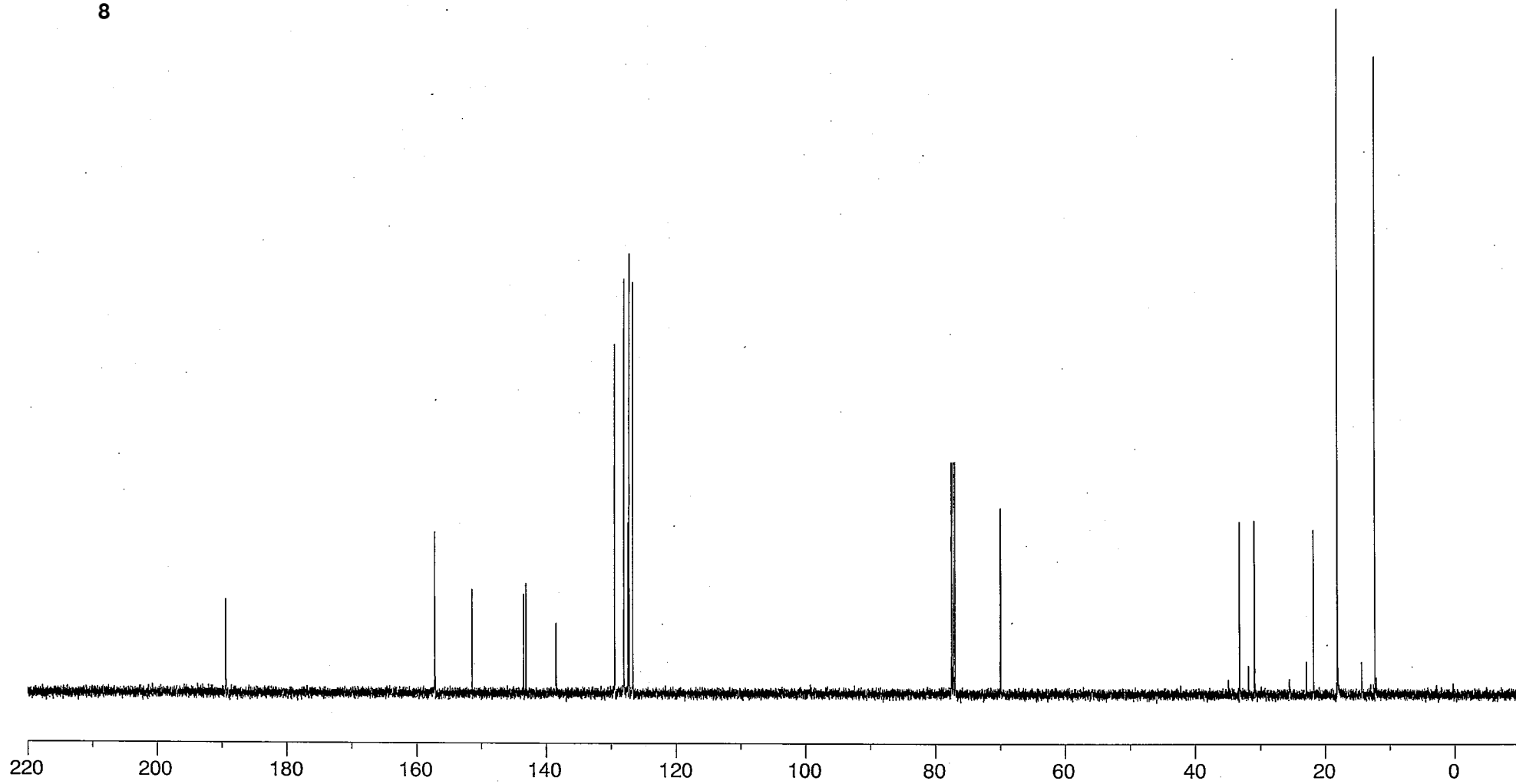


KAD-03-047B

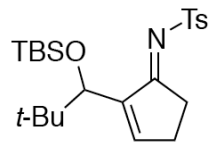
Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃



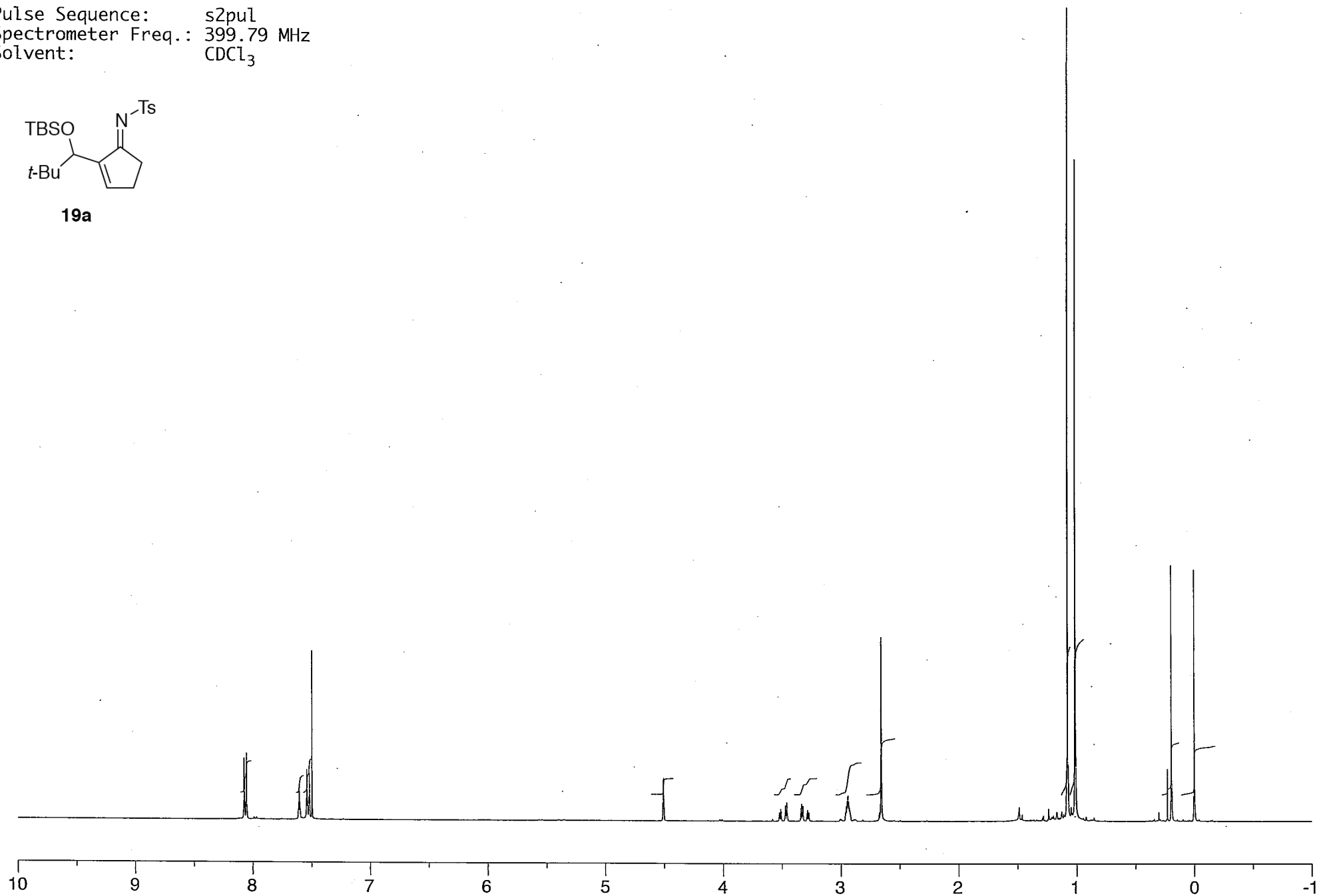
8



Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

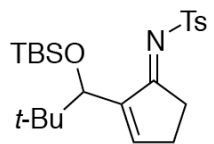


19a

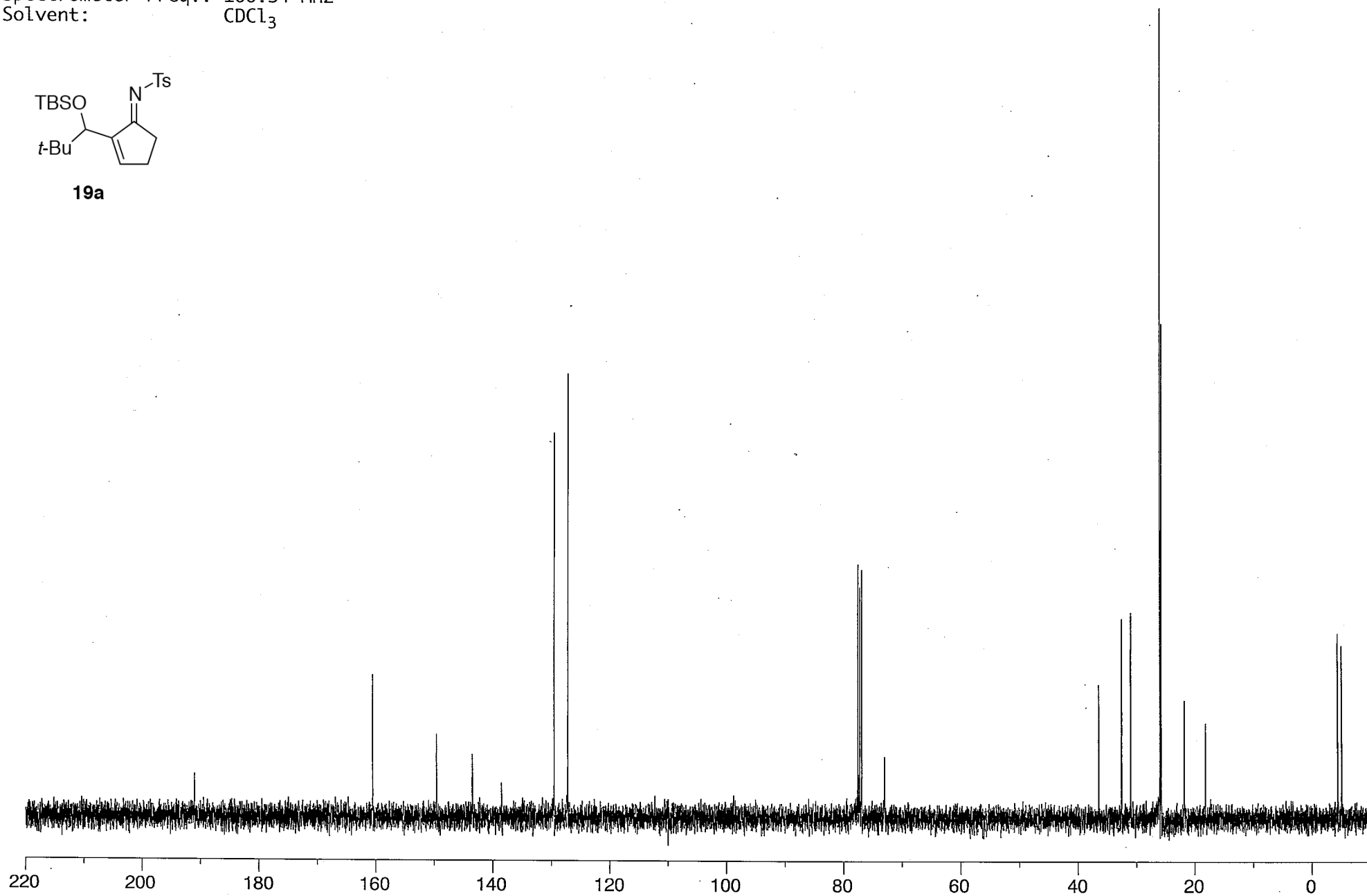


MW-1-130redo_03Apr2012

Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

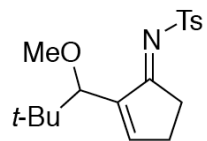


19a

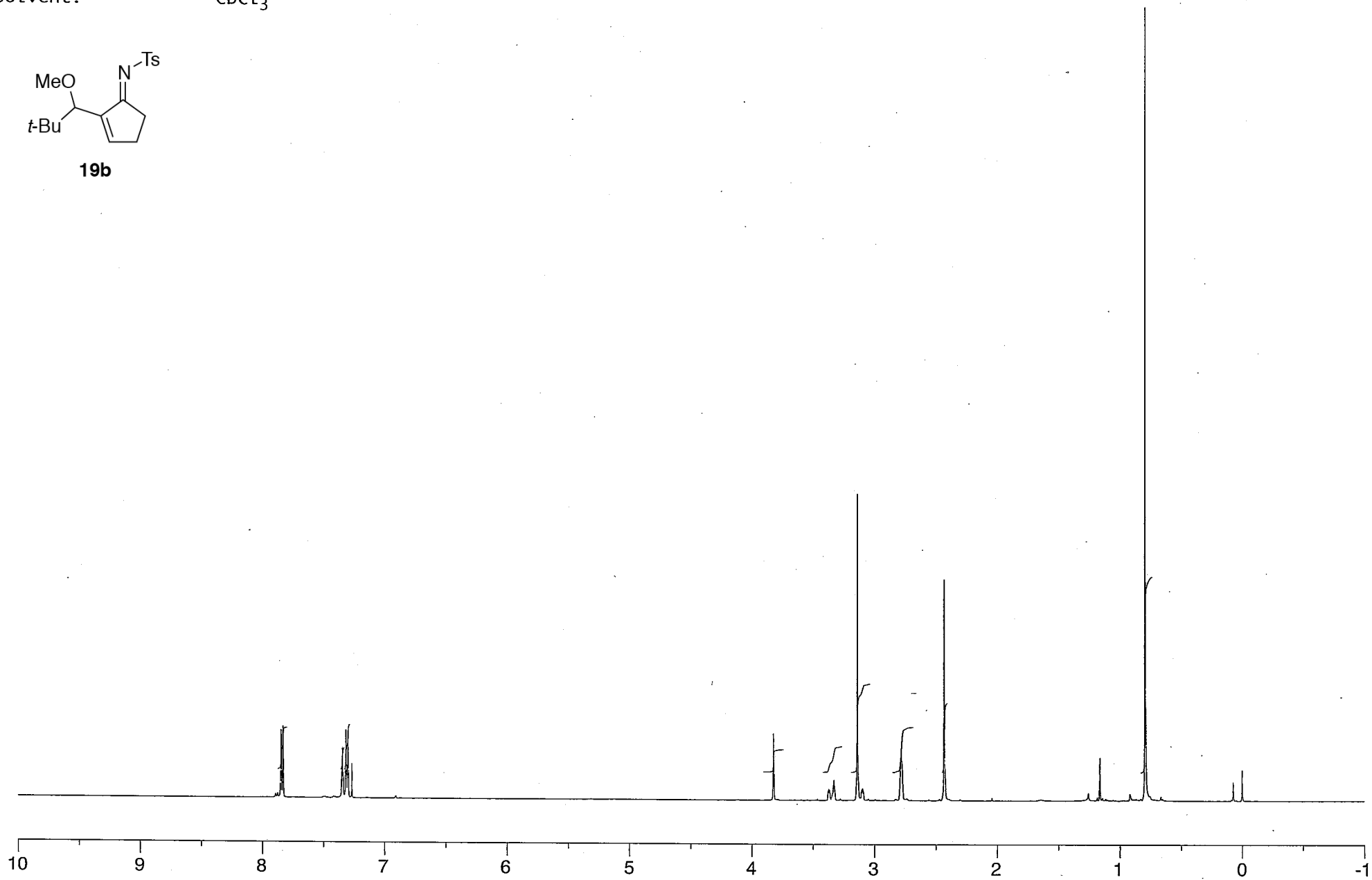


KAD-03-203_15Oct2011

Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃

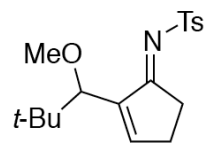


19b

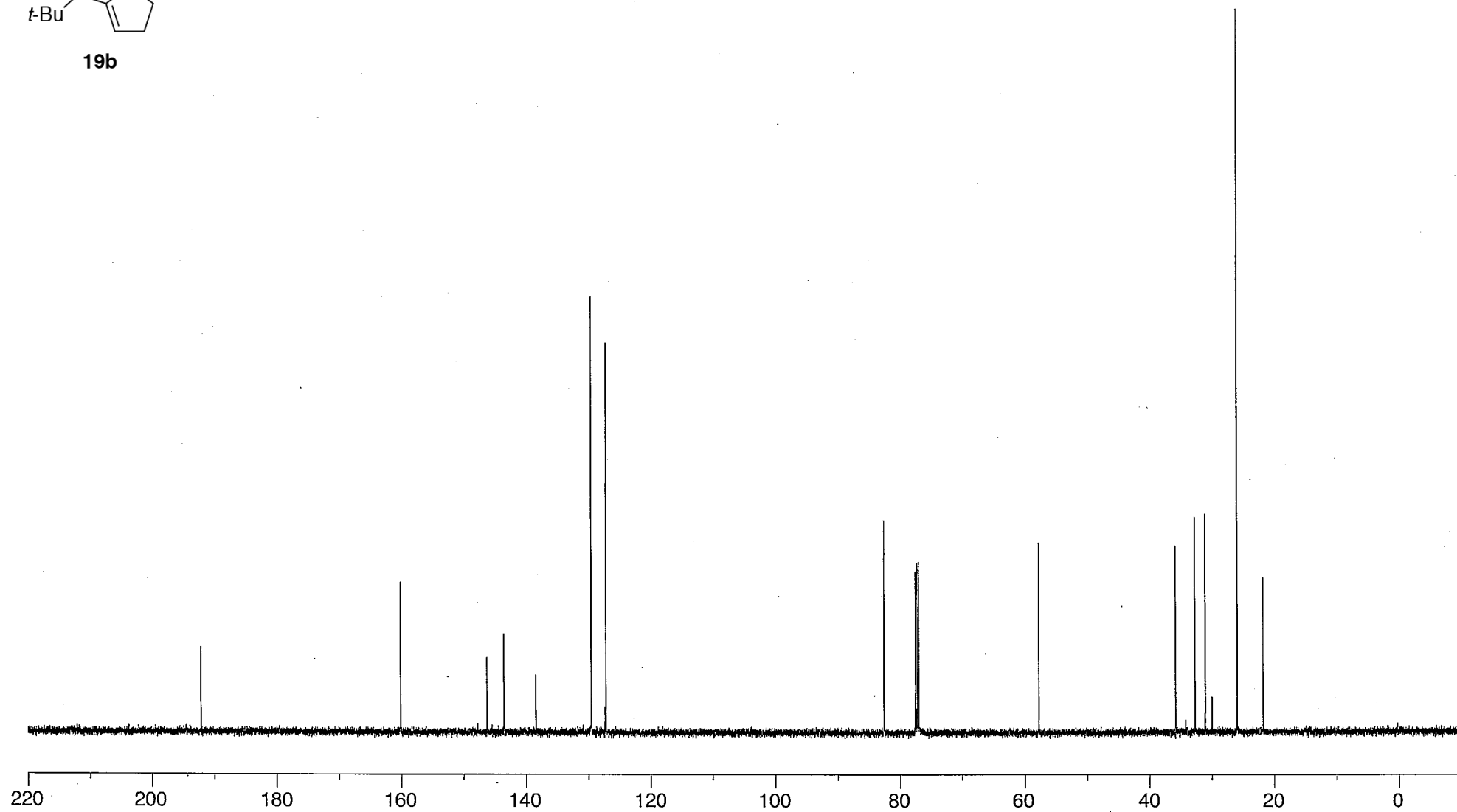


KAD-03-203_15Oct2011

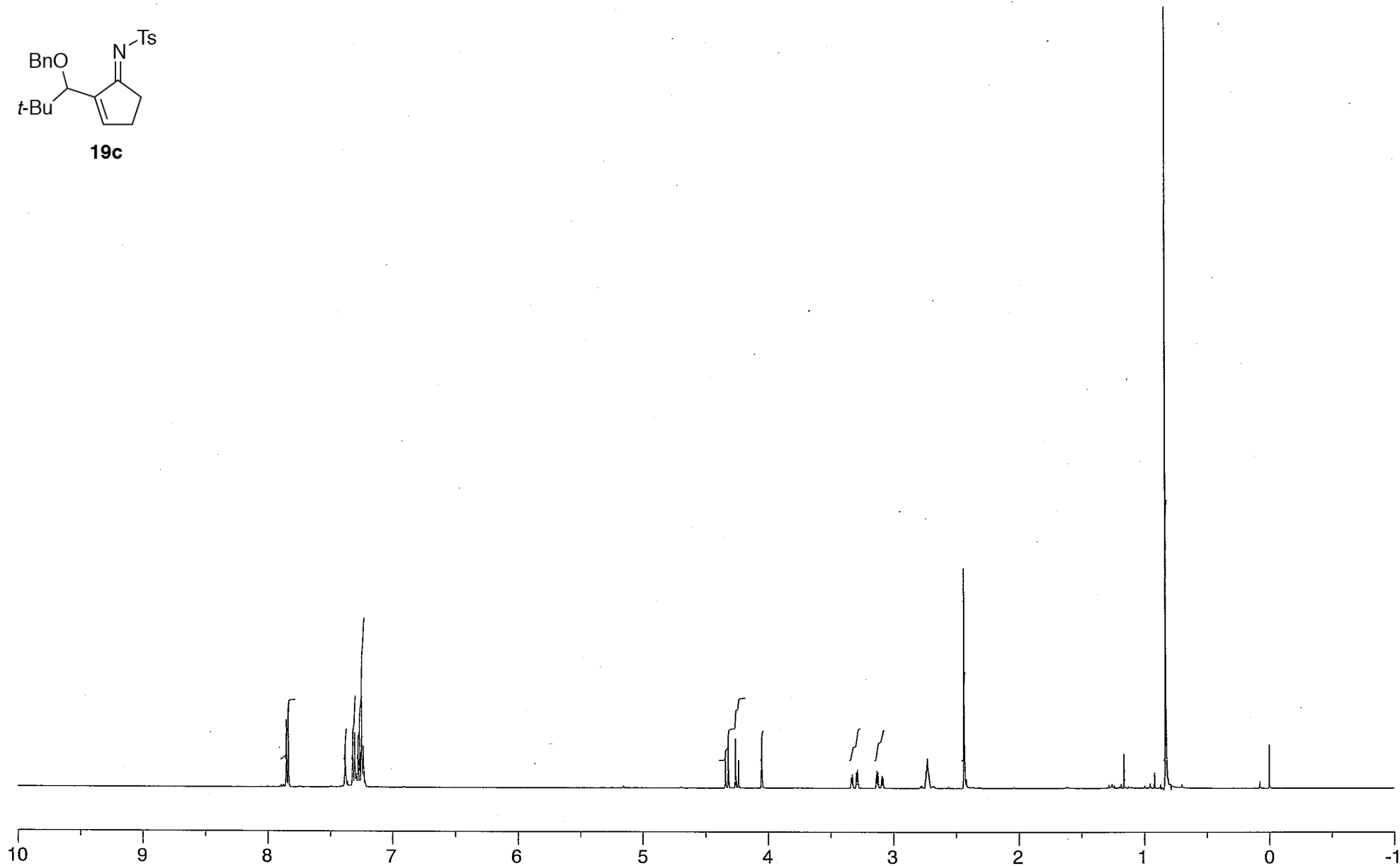
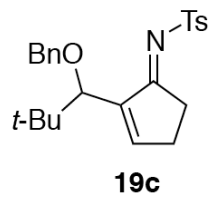
Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃



19b

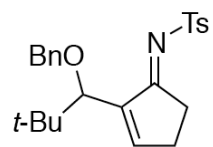


Pulse Sequence: s2pu1
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃

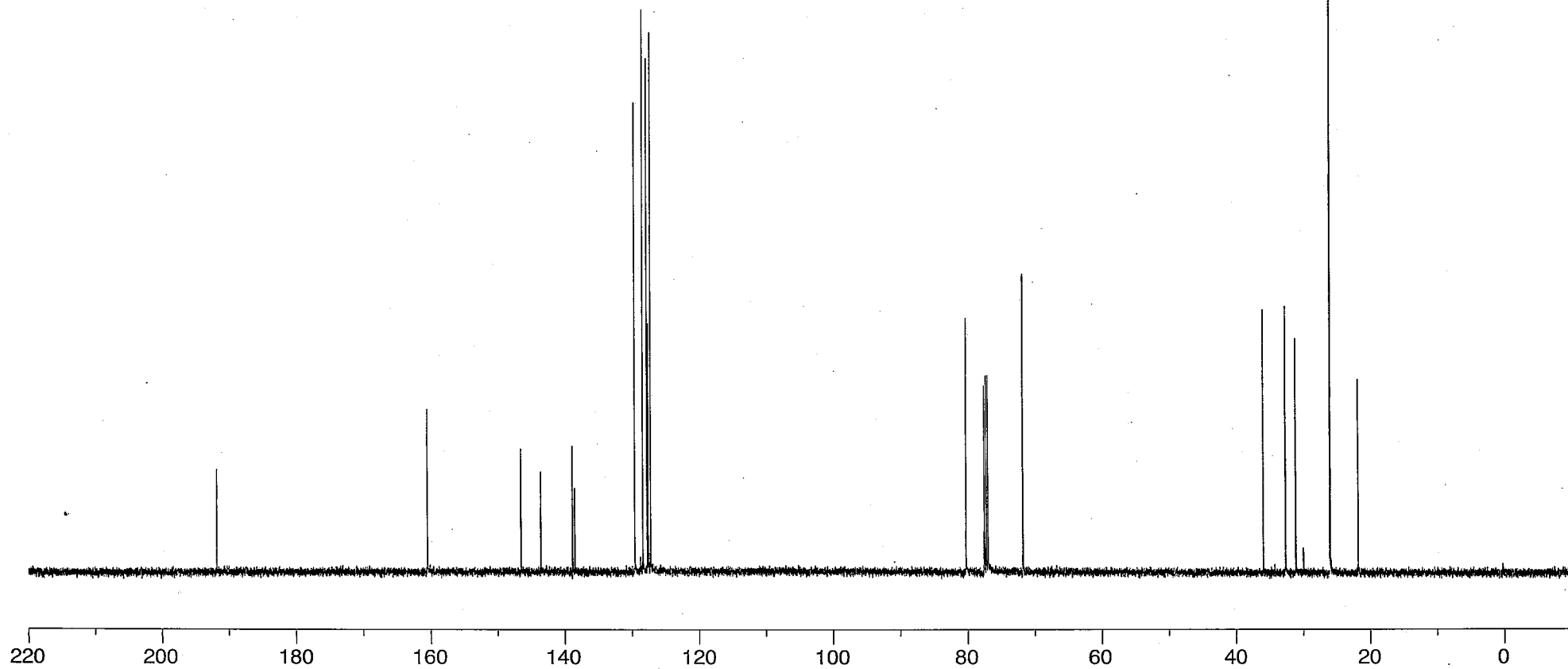


KAD-02-204__15Oct2011

Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃

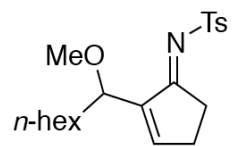


19c

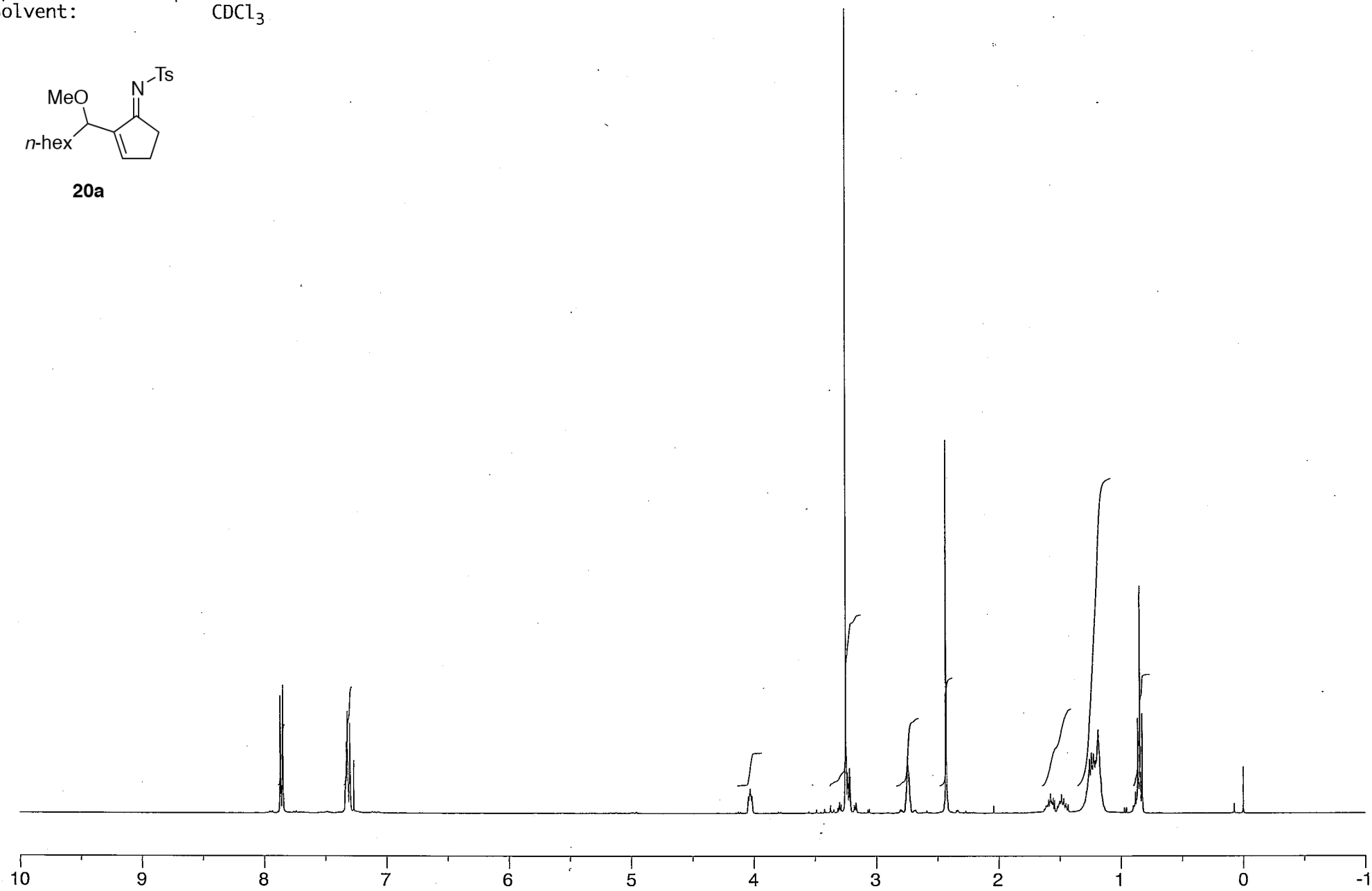


KAD-03-193_04Oct2011

Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

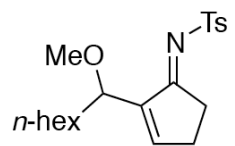


20a

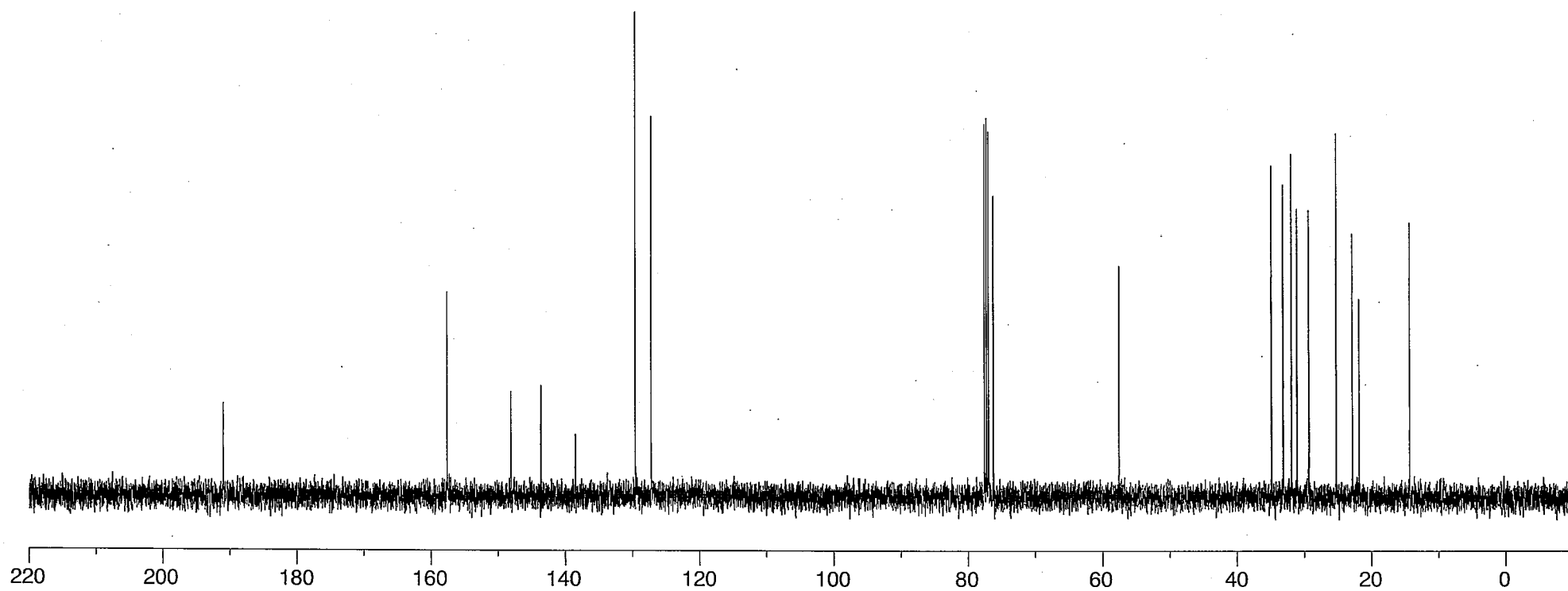


KAD-03-193_04Oct2011

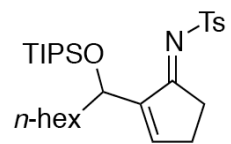
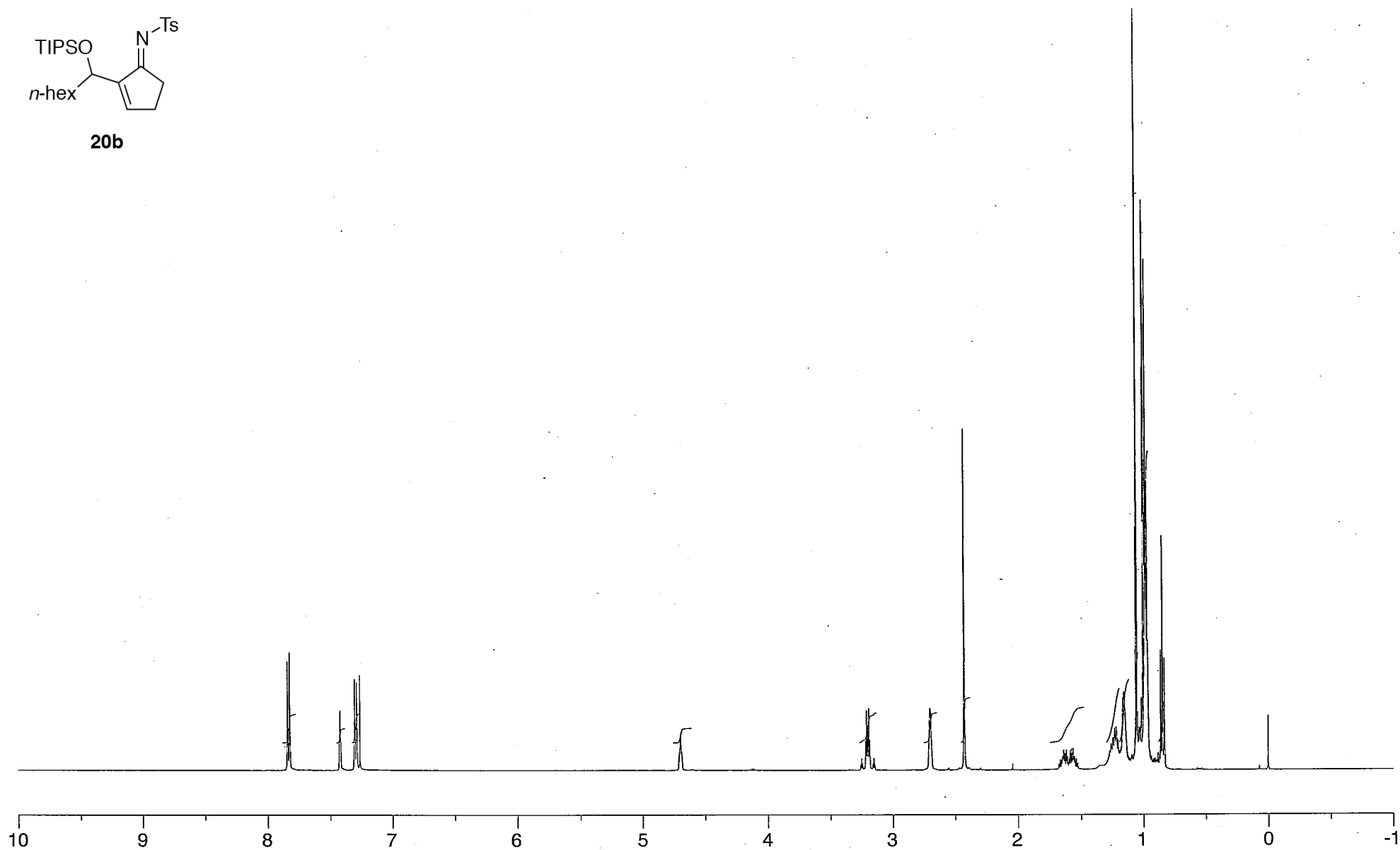
Pulse Sequence: s2pul
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃



20a

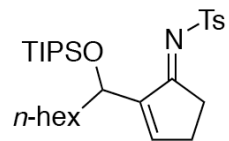


Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃

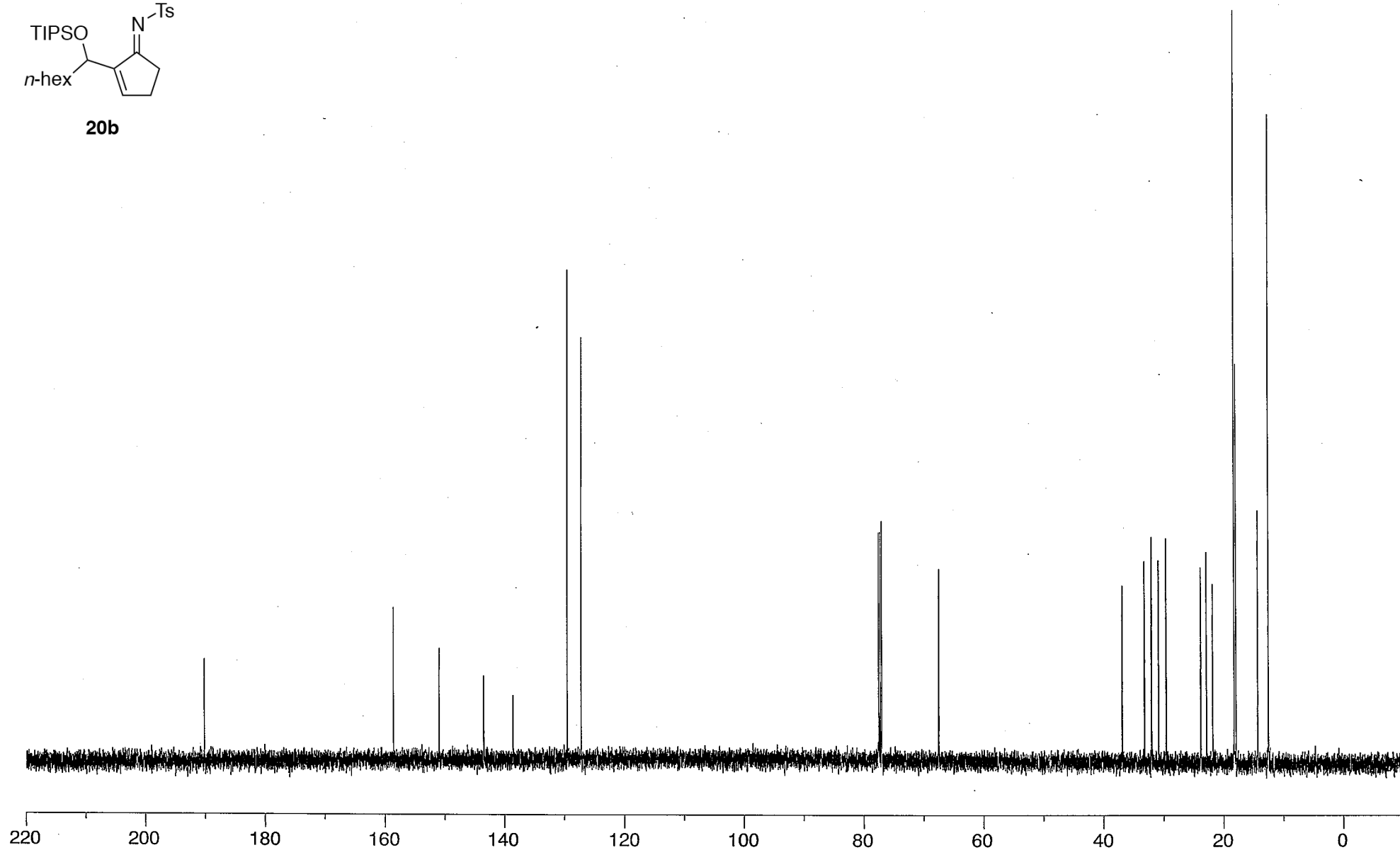
**20b**

KAD-03-192_04Oct2011

Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃

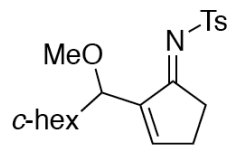


20b

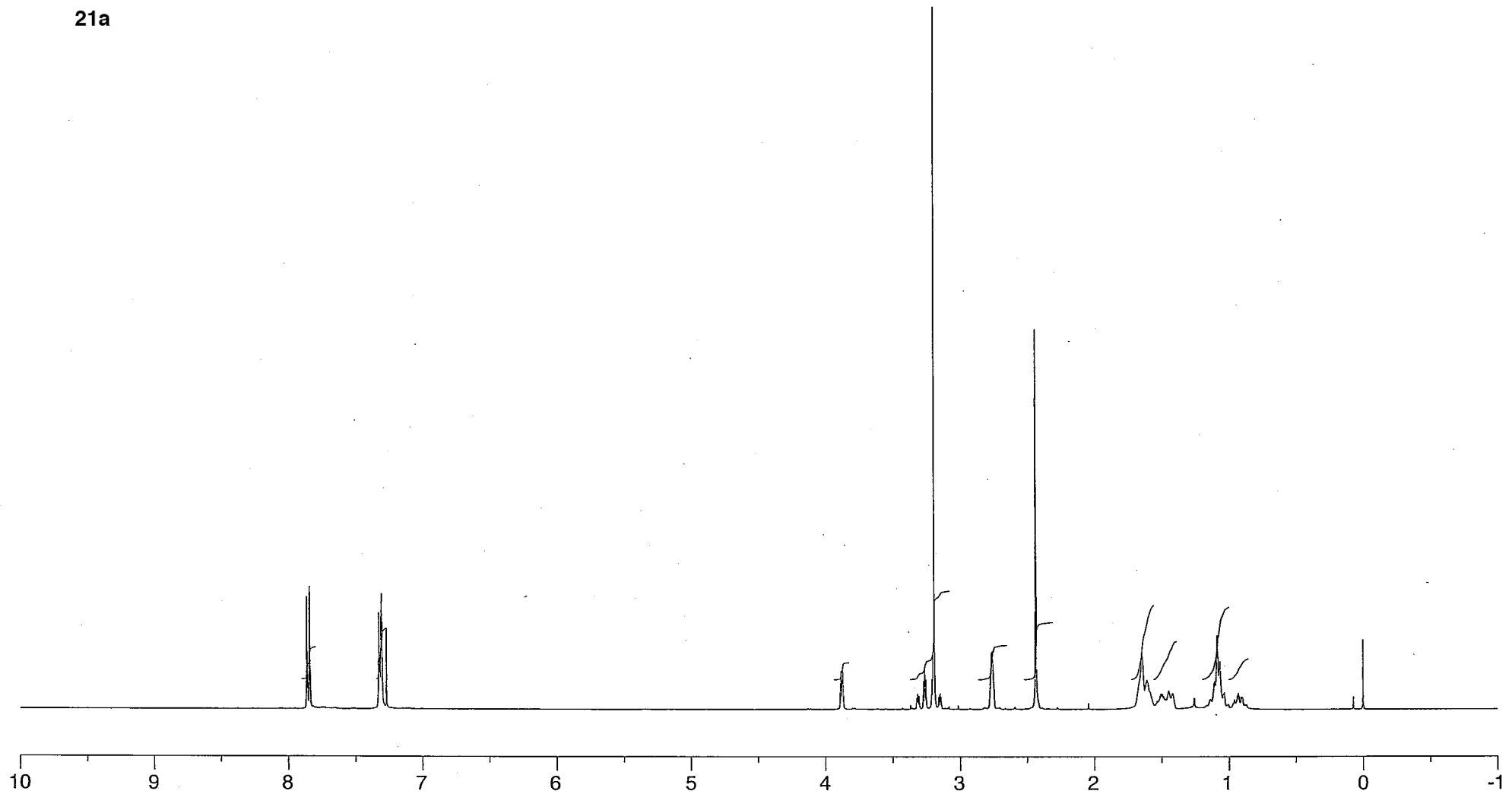


KAD-03-213_24Oct2011

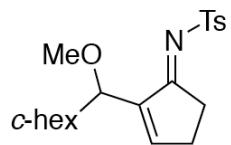
Pulse Sequence: s2pu1
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



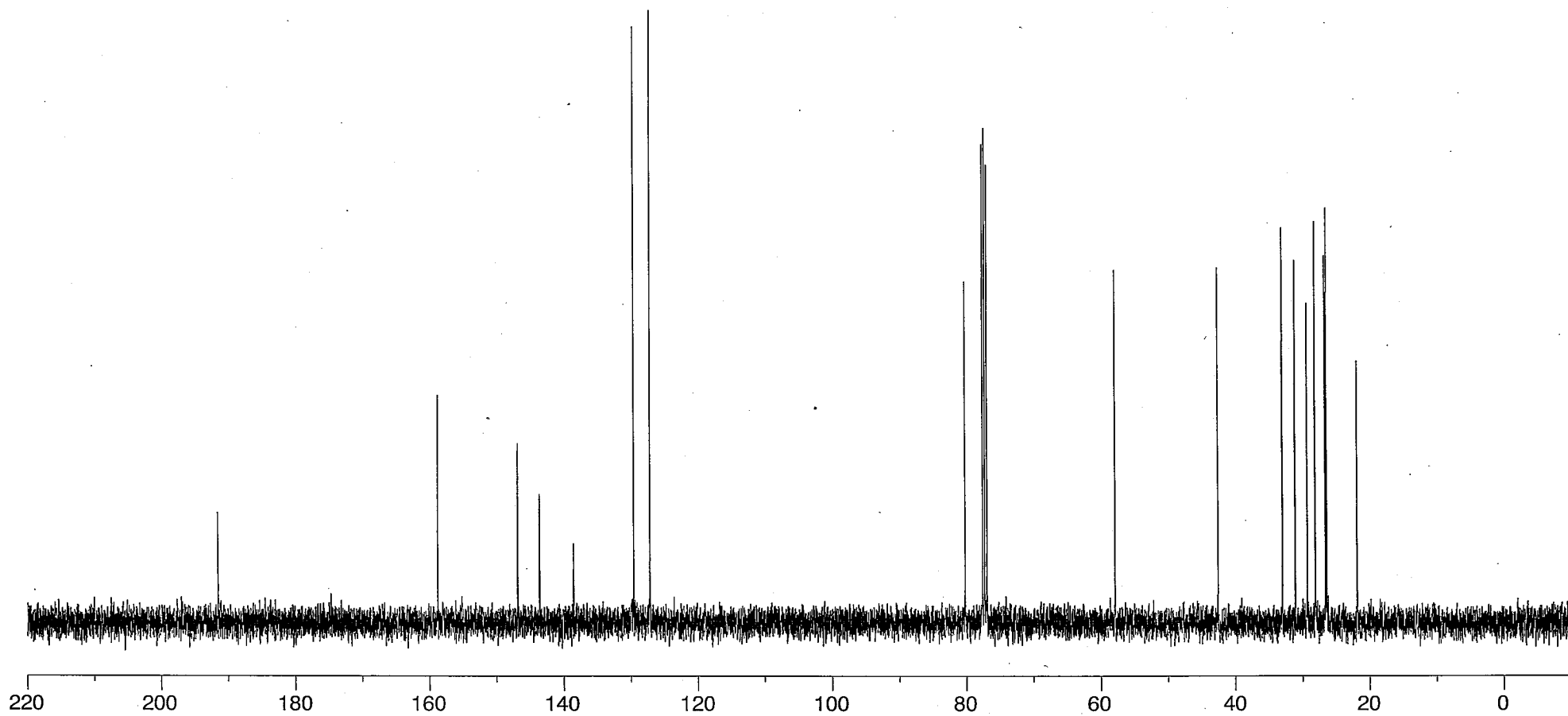
21a



Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

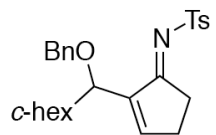


21a

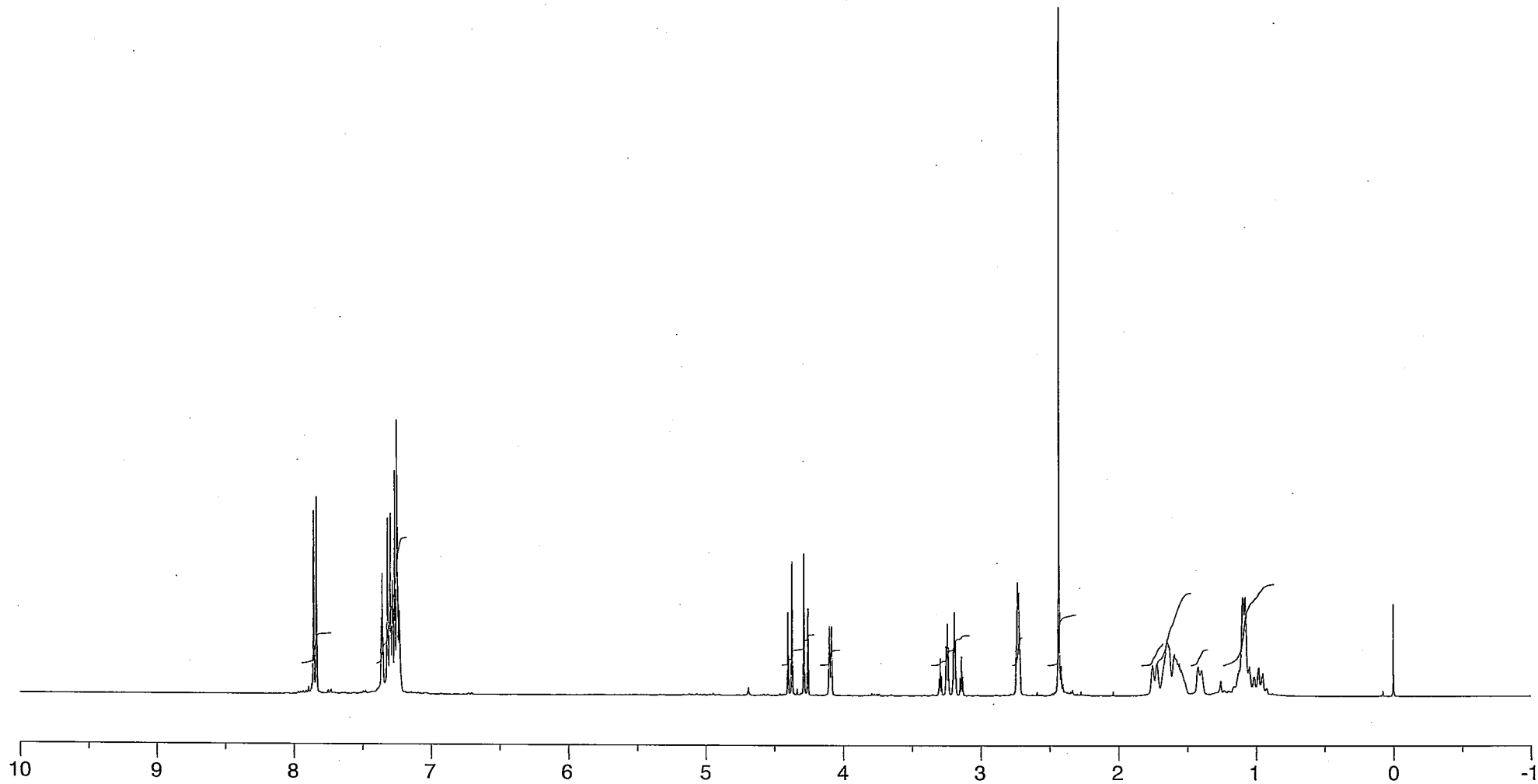


KAD-03-214_24Oct2011

Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

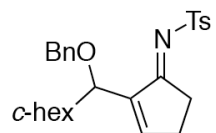


21b

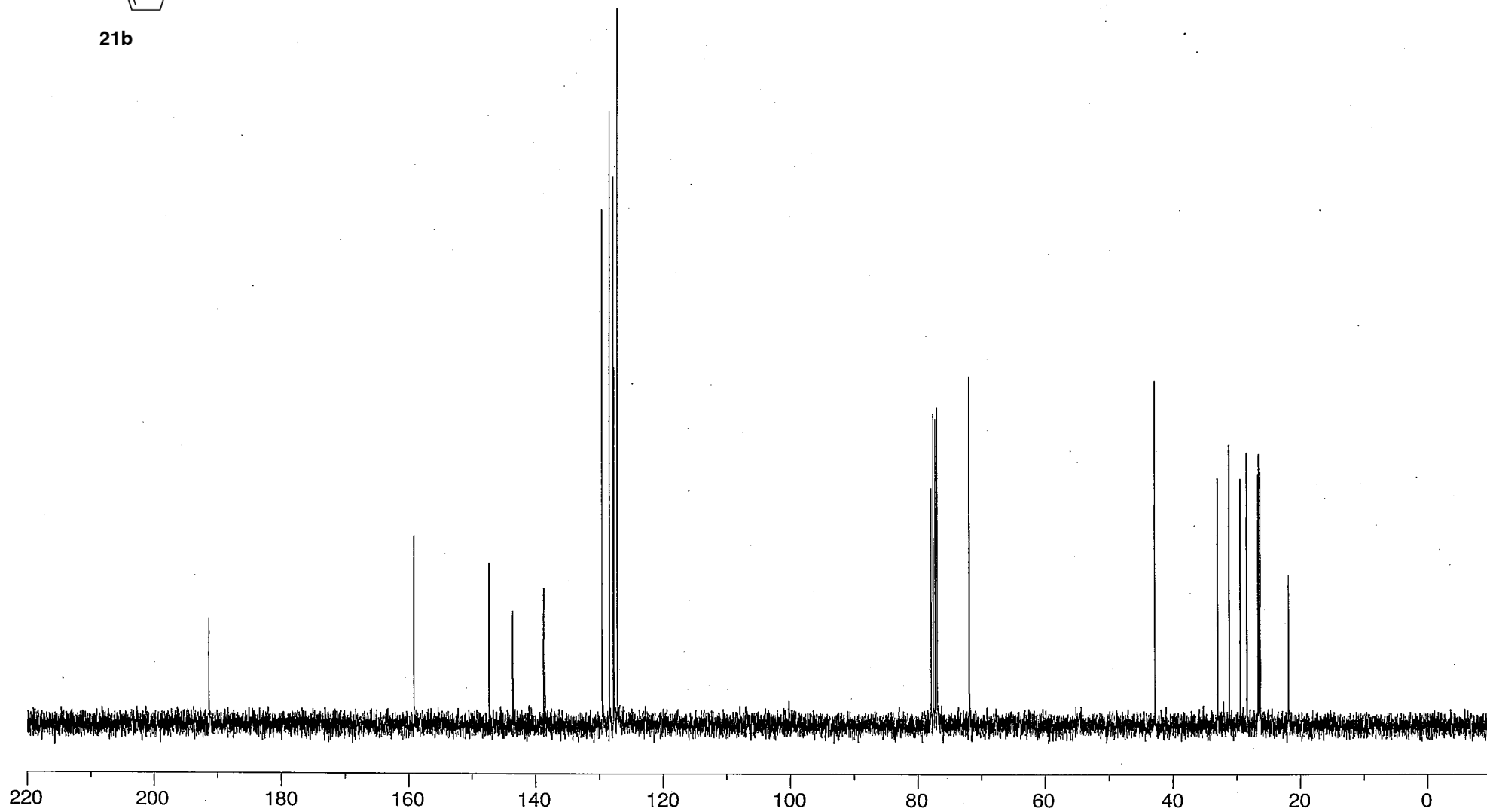


KAD-03-214_24Oct2011

Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

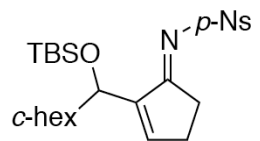


21b

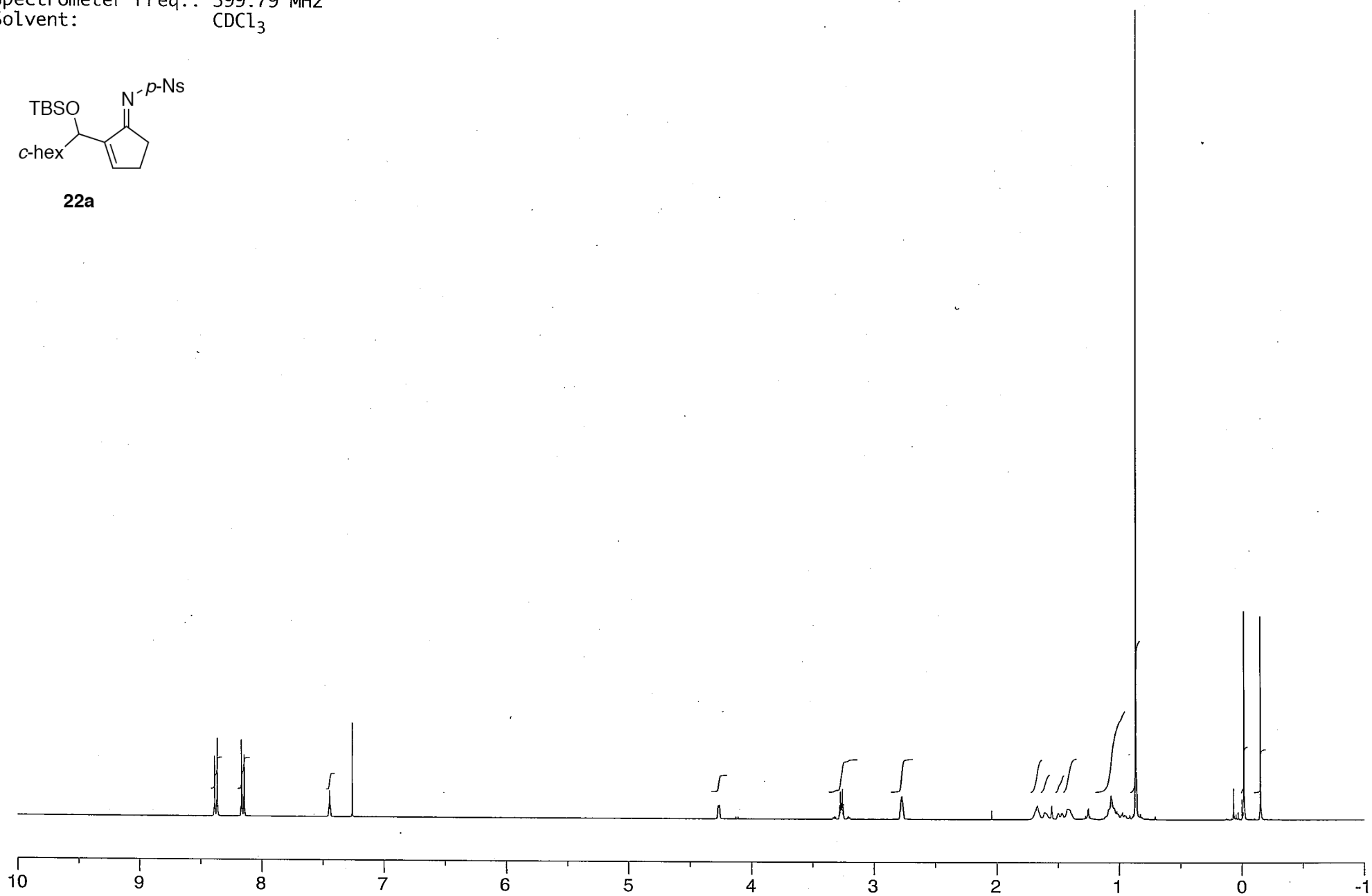


gwm-l-68_28Jul2011

Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

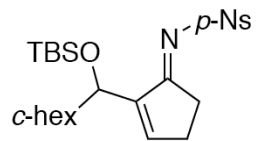


22a

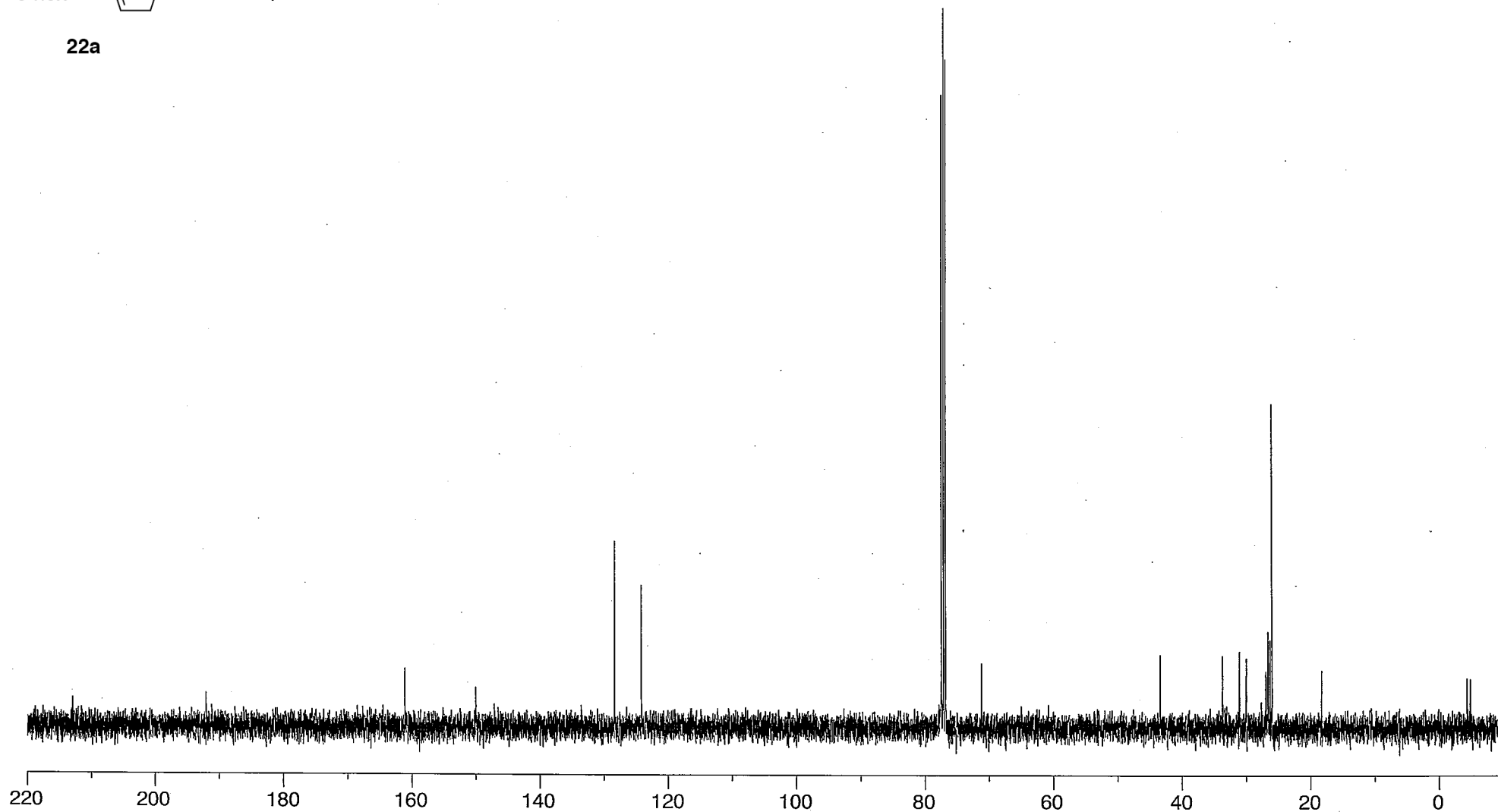


gwm-l-68_28Jul2011

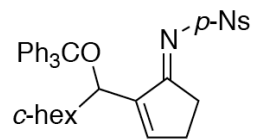
Pulse Sequence: s2pul
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃



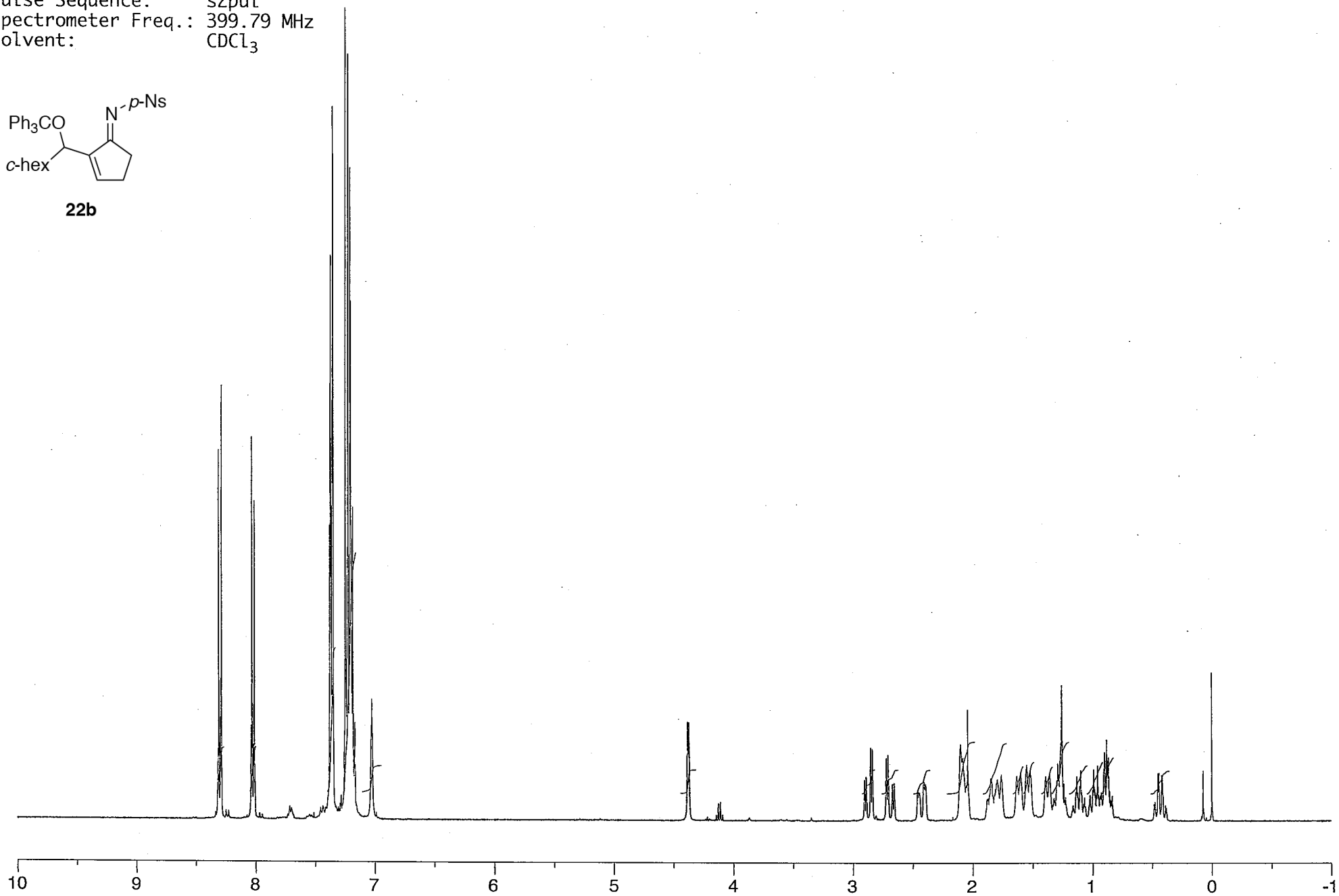
22a



Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



22b

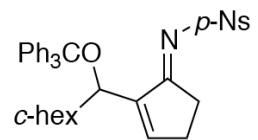


KAD-03-199_11Oct2011

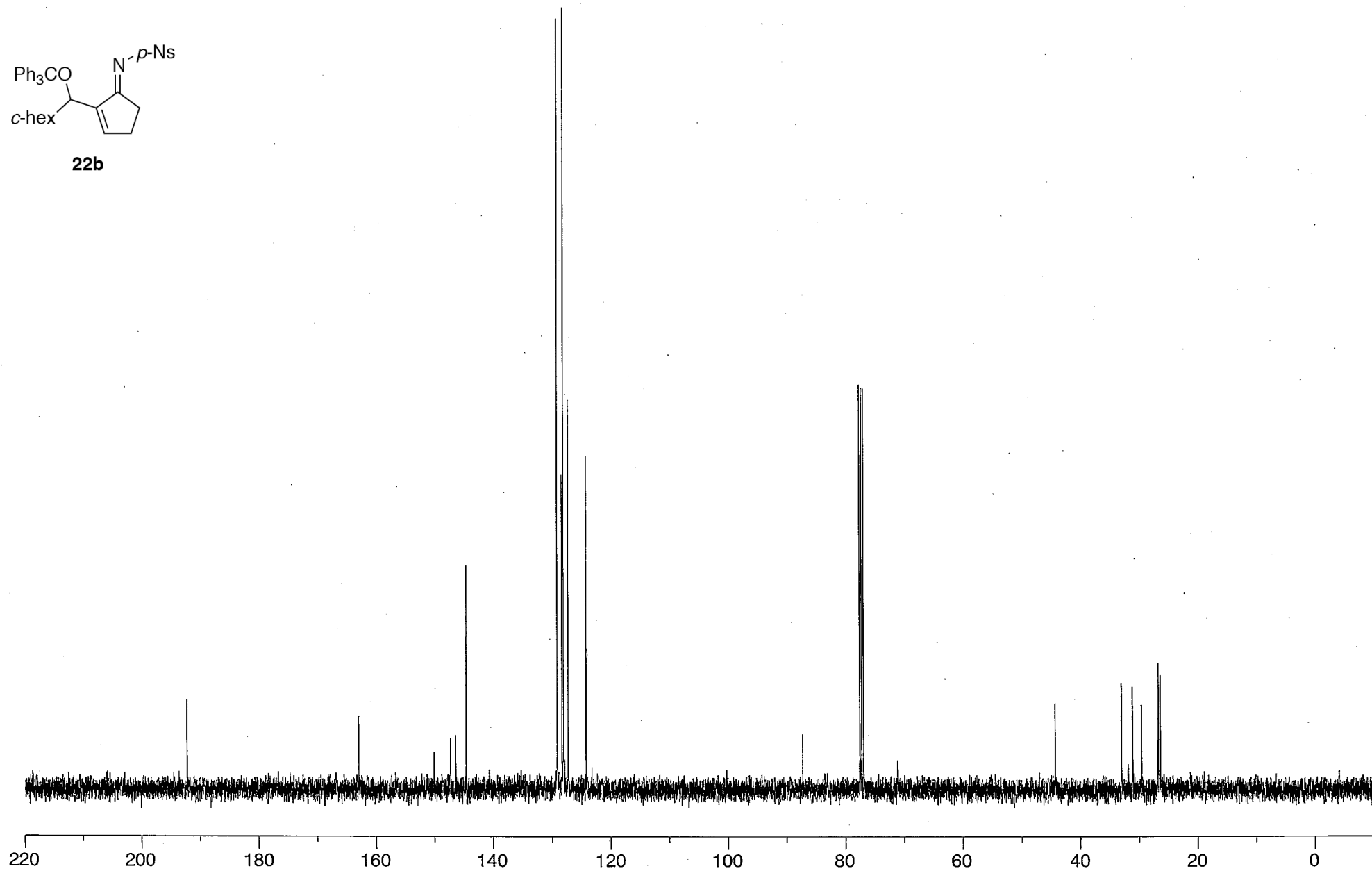
Pulse Sequence: s2pul

Spectrometer Freq.: 100.54 MHz

Solvent: CDCl₃

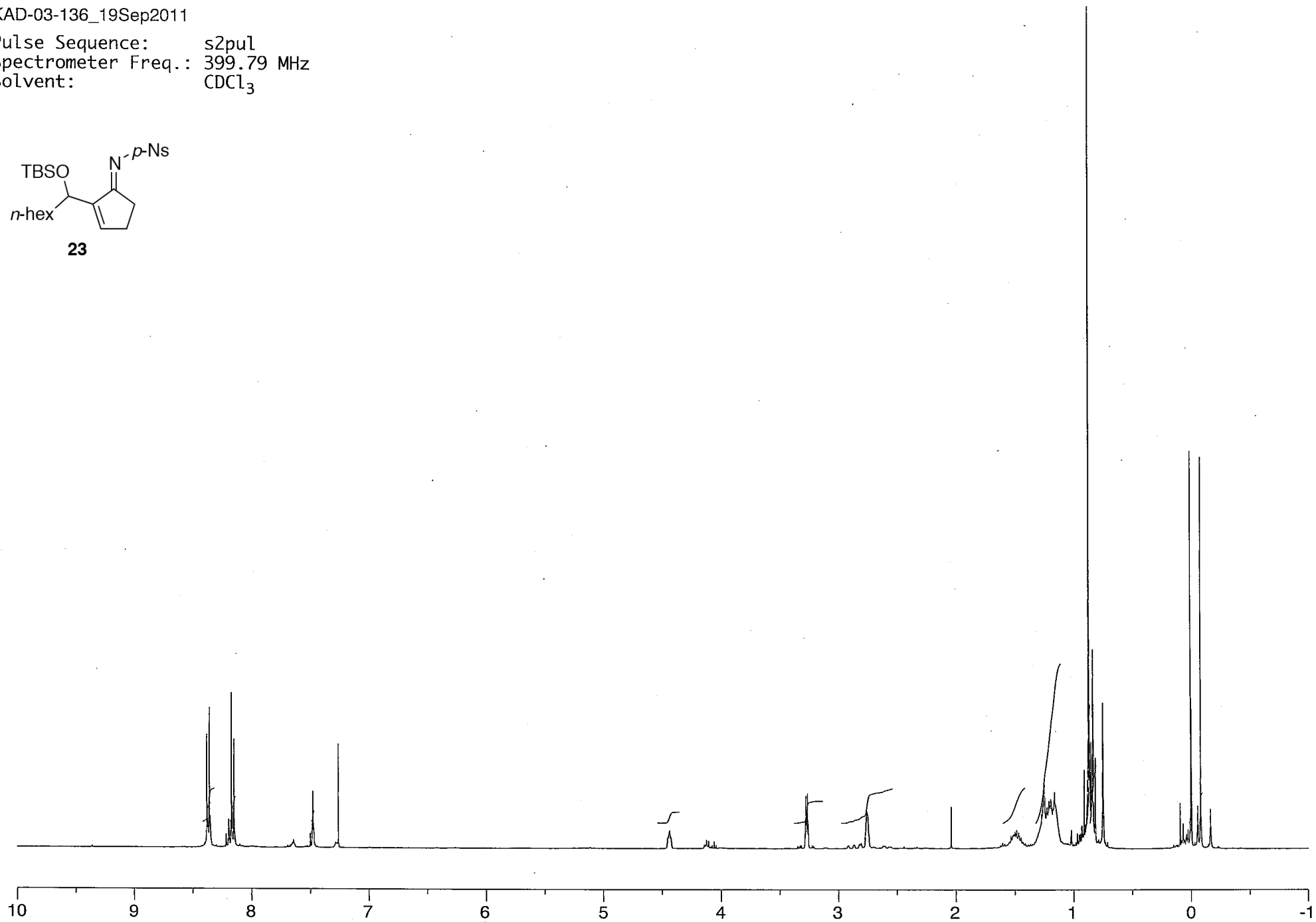
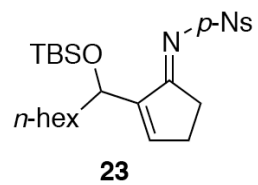


22b

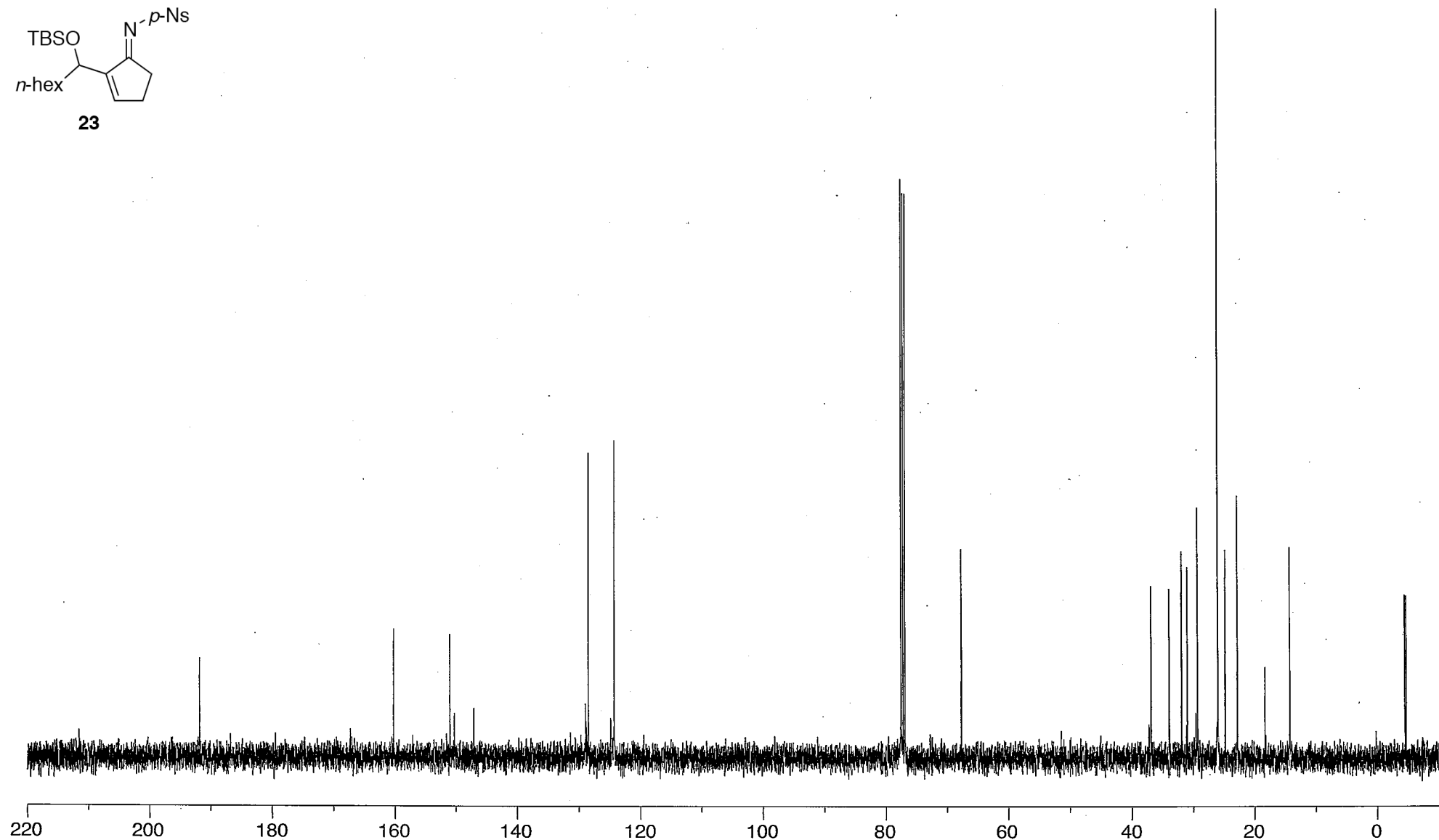
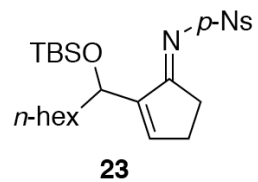


KAD-03-136_19Sep2011

Pulse Sequence: s2pu1
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃



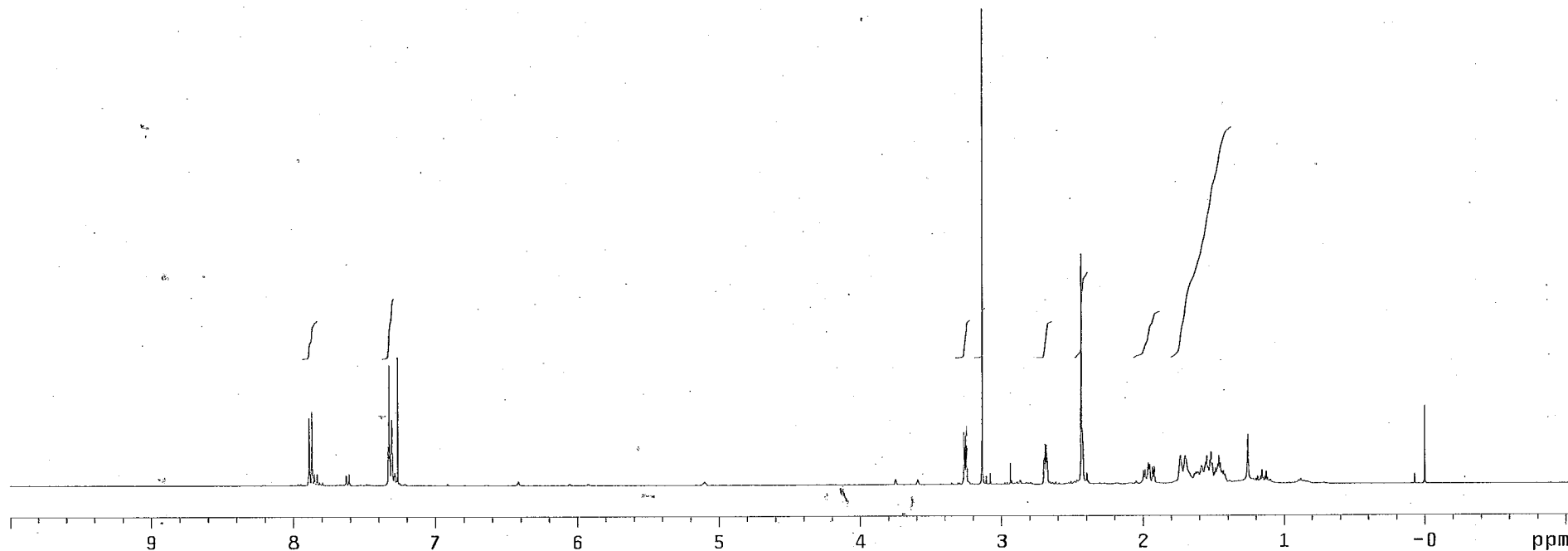
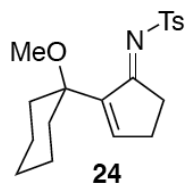
wxn28-1_13Oct2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn28-1_13Oct2011

Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865222 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



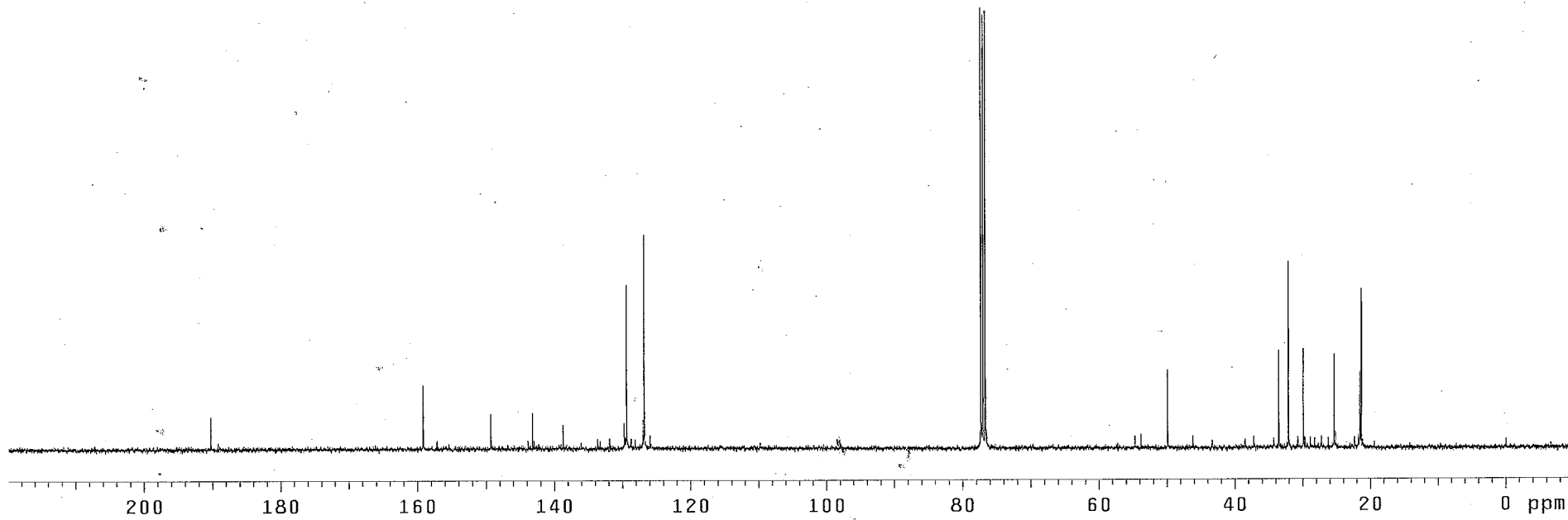
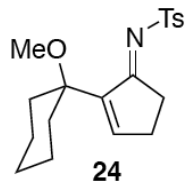
wxn25-28-1_03Nov2011-22:16:52

Archive directory: /export/home/xiaona/vnmrSYS/data
Sample directory: wxn25-28-1_03Nov2011-22:16:52

Pulse Sequence: s2pu1

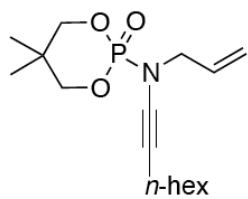
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
5000 repetitions
OBSERVE C13, 100.5264022 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec

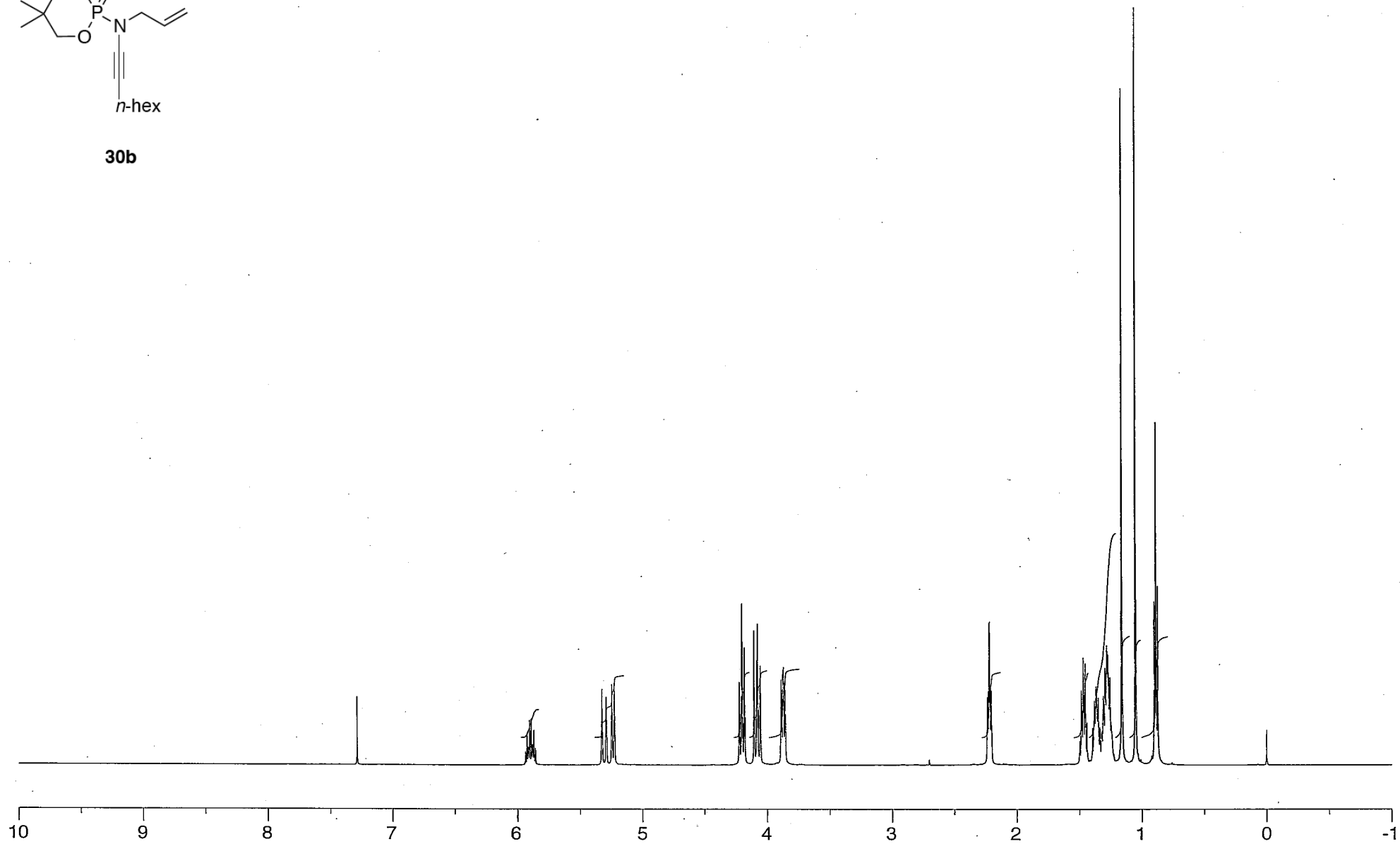


KAD-03-086_23Apr2012

Pulse Sequence: s2pu1
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃

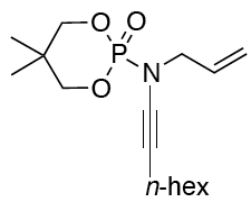


30b

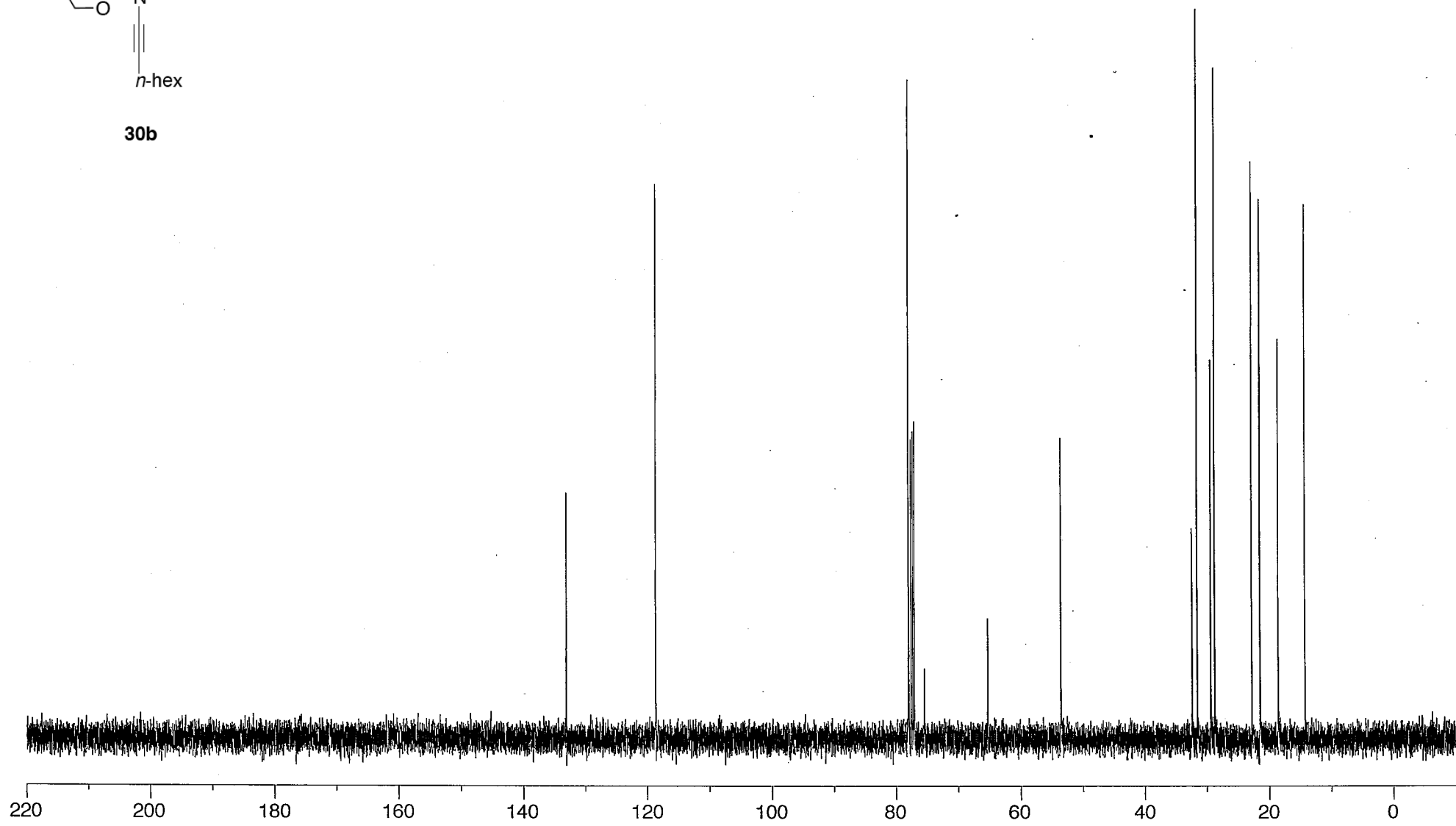


KAD-03-086_23Apr2012

Pulse Sequence: s2pul
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃

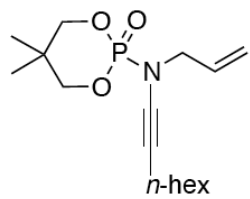


30b

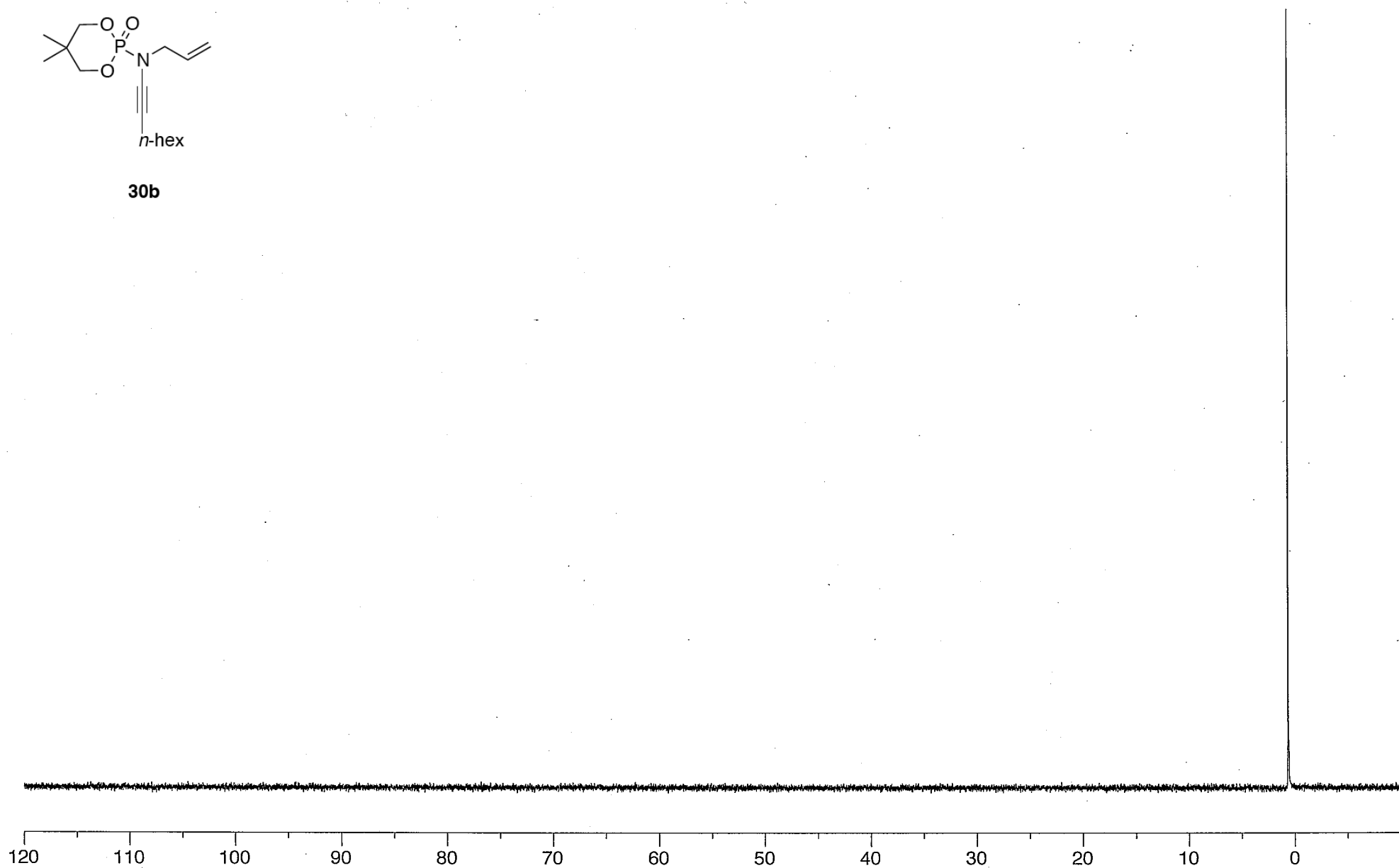


KAD-03-086_23May2011

Pulse Sequence: s2pul
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



30b



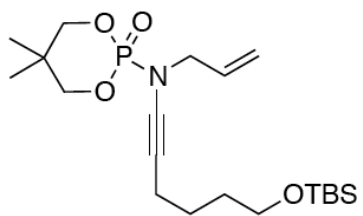
wxn50-2_04Nov2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn50-2_04Nov2011

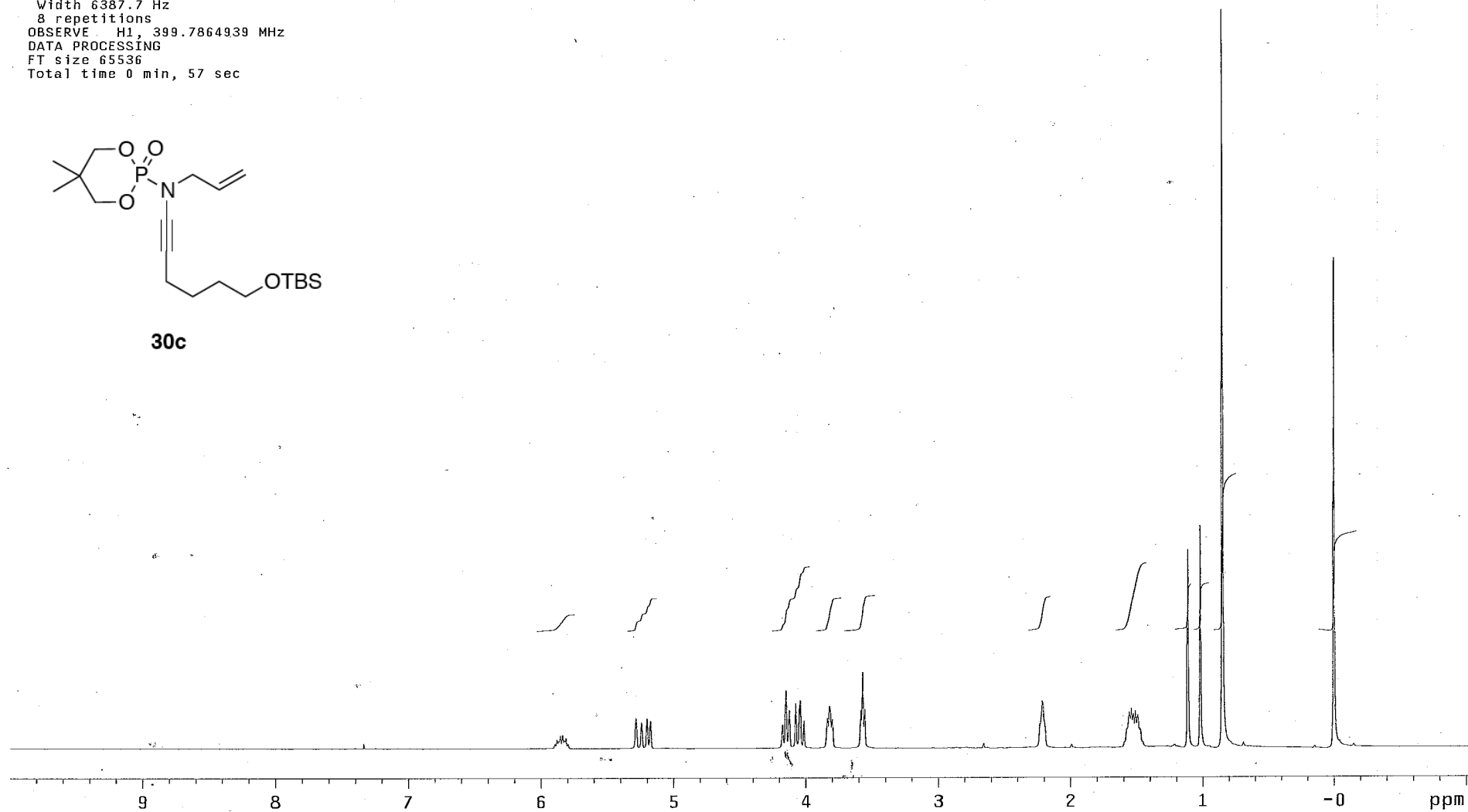
Pulse Sequence: s2pul

Solvent: CDCl3
Temp: 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7864939 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



30c



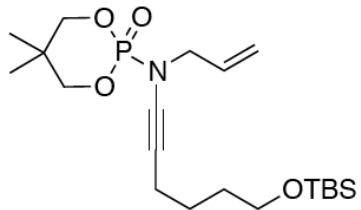
wxn50-2_04Nov2011-12:46:23

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn50-2_04Nov2011-12:46:23

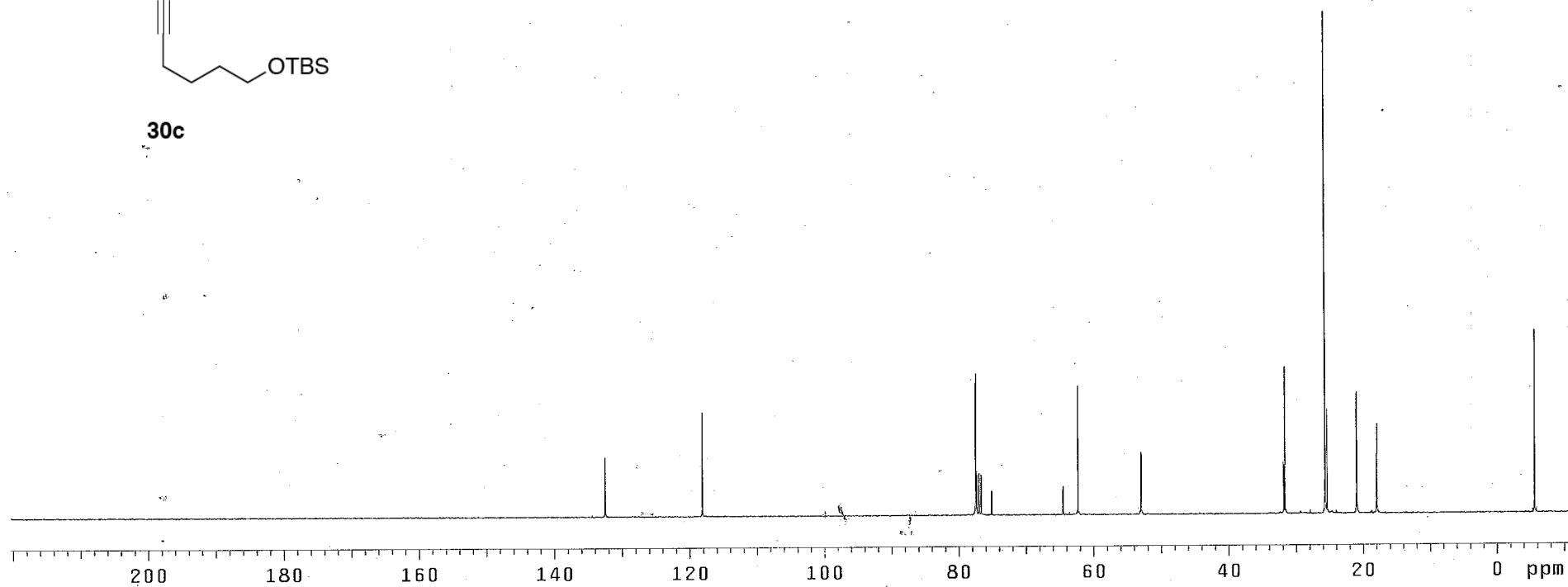
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
314 repetitions
OBSERVE C13, 100.5264199 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 18 min, 49 sec



30c



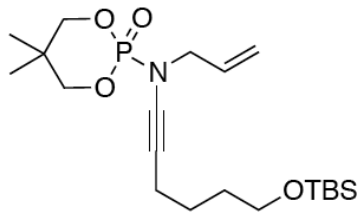
wxn50-2_04Nov2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn50-2_04Nov2011

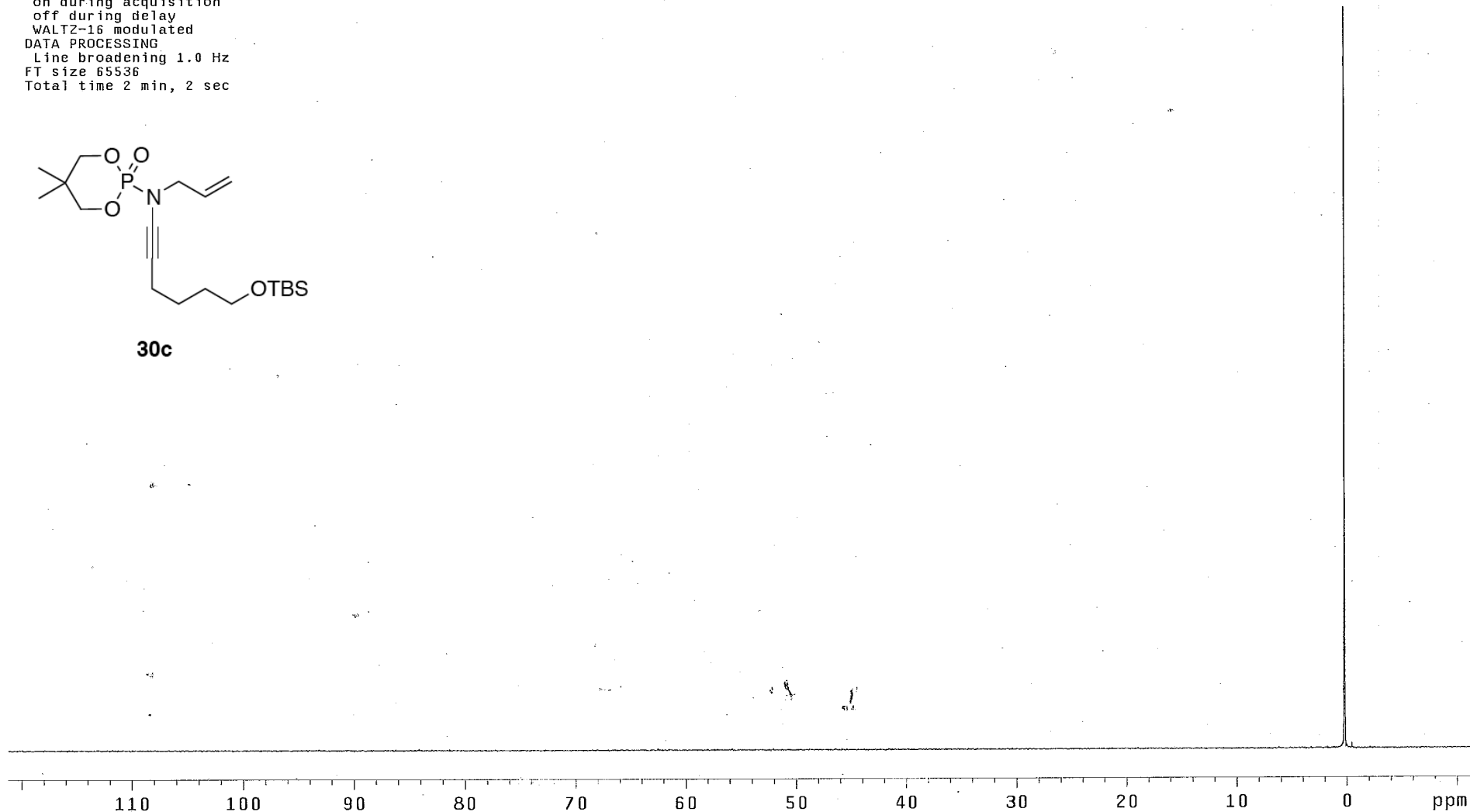
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PHOSPHORUS
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 0.799 sec
Width 35650.6 Hz
64 repetitions
OBSERVE P31, 161.8363711 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 min, 2 sec

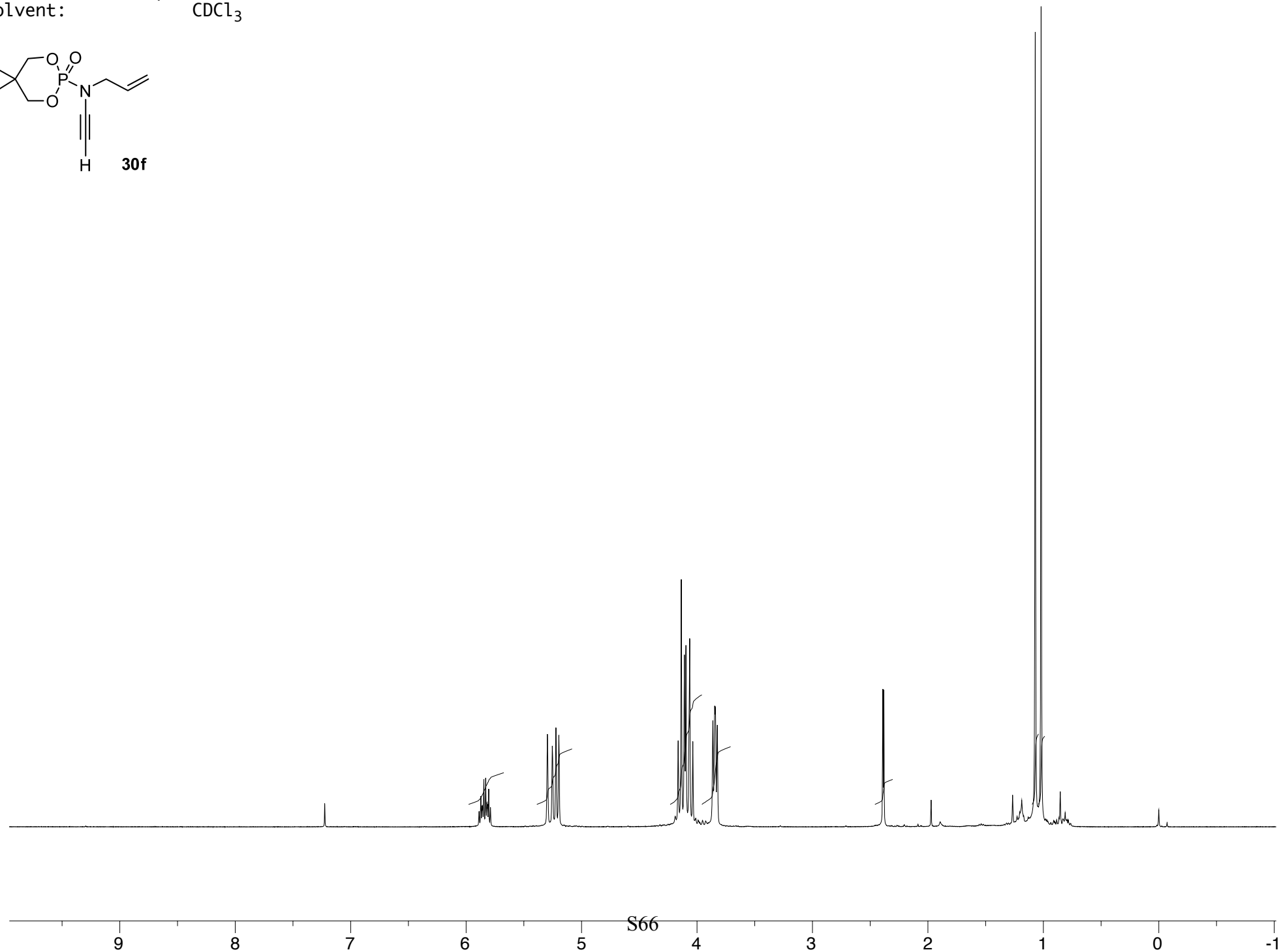
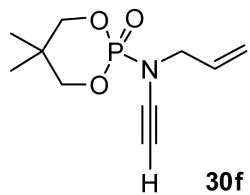


30c



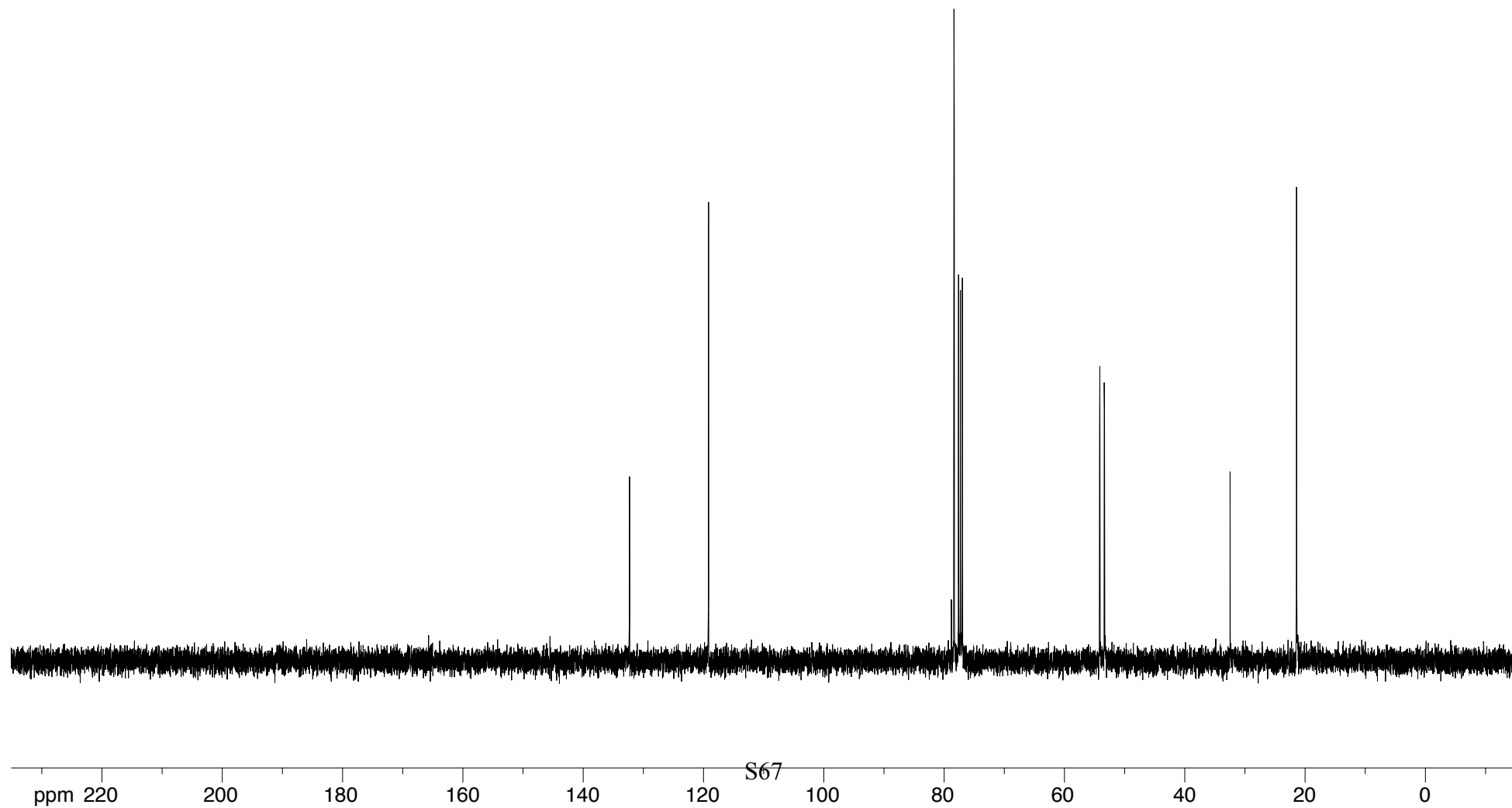
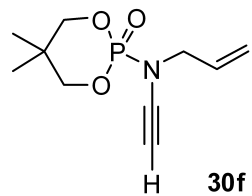
KAD-03-096_26May2011

Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



KAD-03-096_26May2011

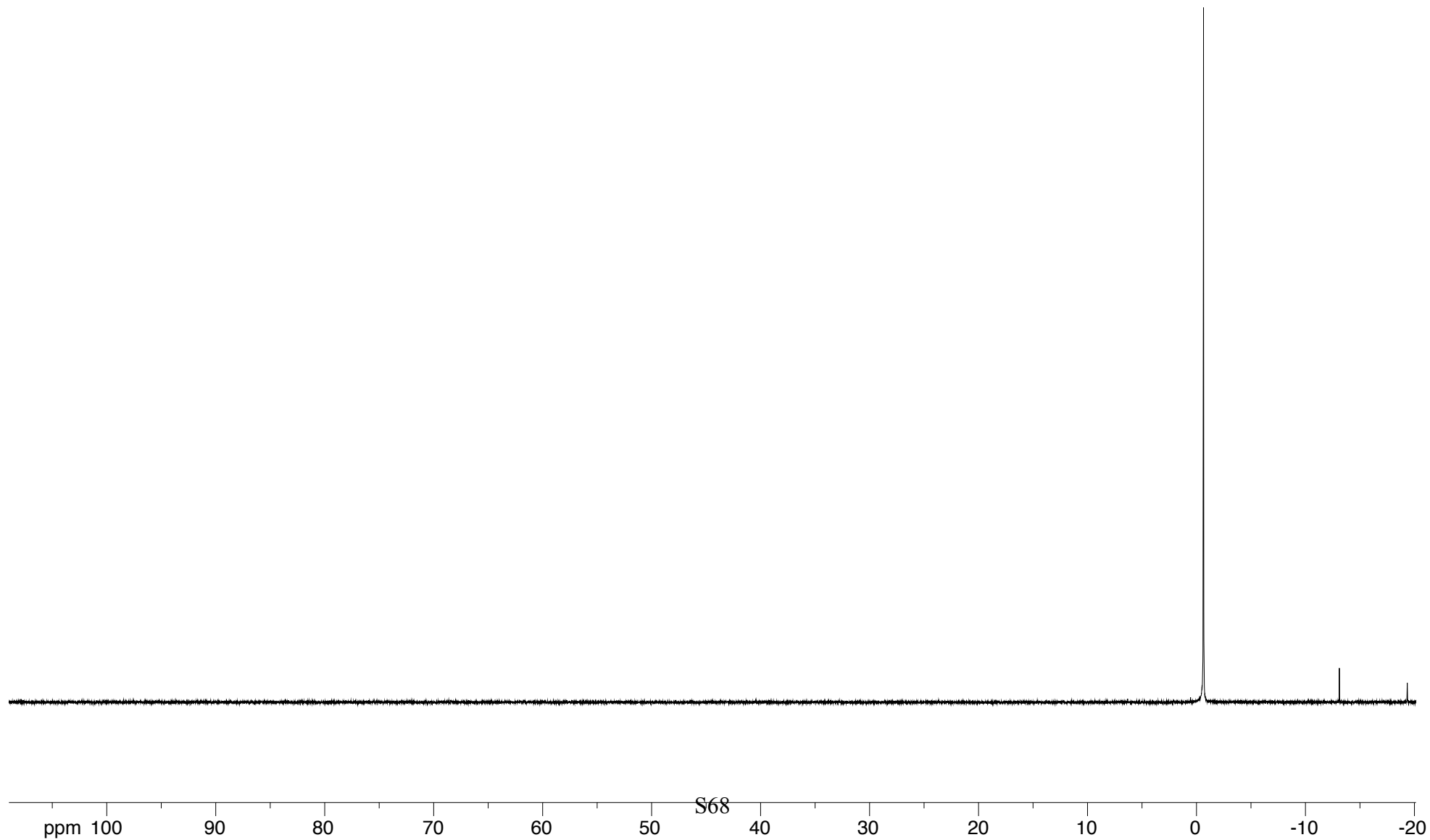
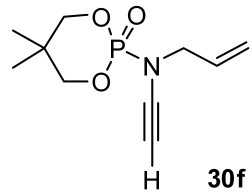
Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃



S67

KAD-03-096_26May2011

Pulse Sequence: s2pul
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



S68

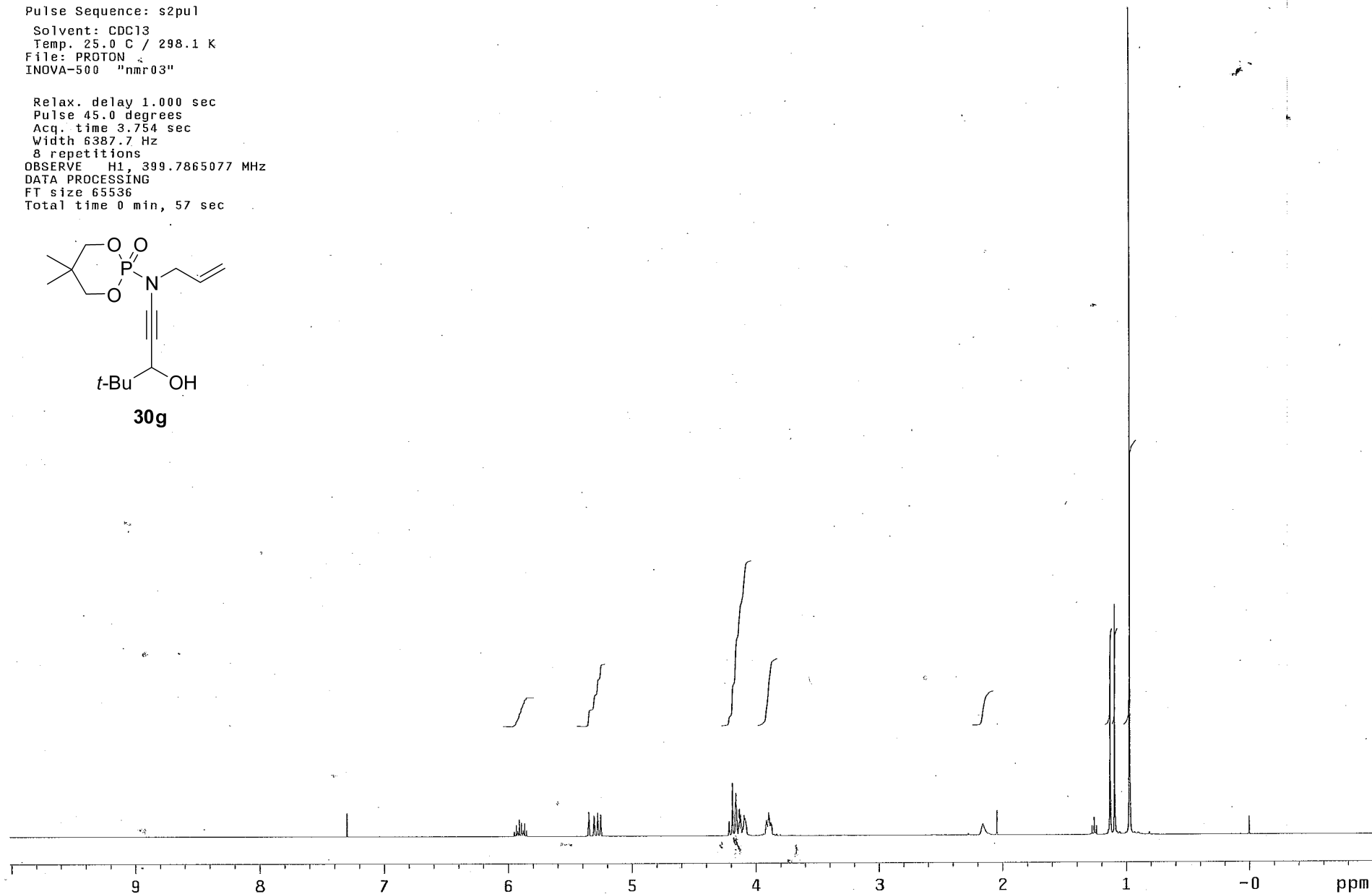
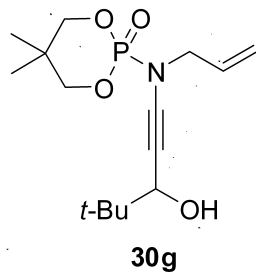
wxn44-1_26Oct2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn44-1_26Oct2011

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865077 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



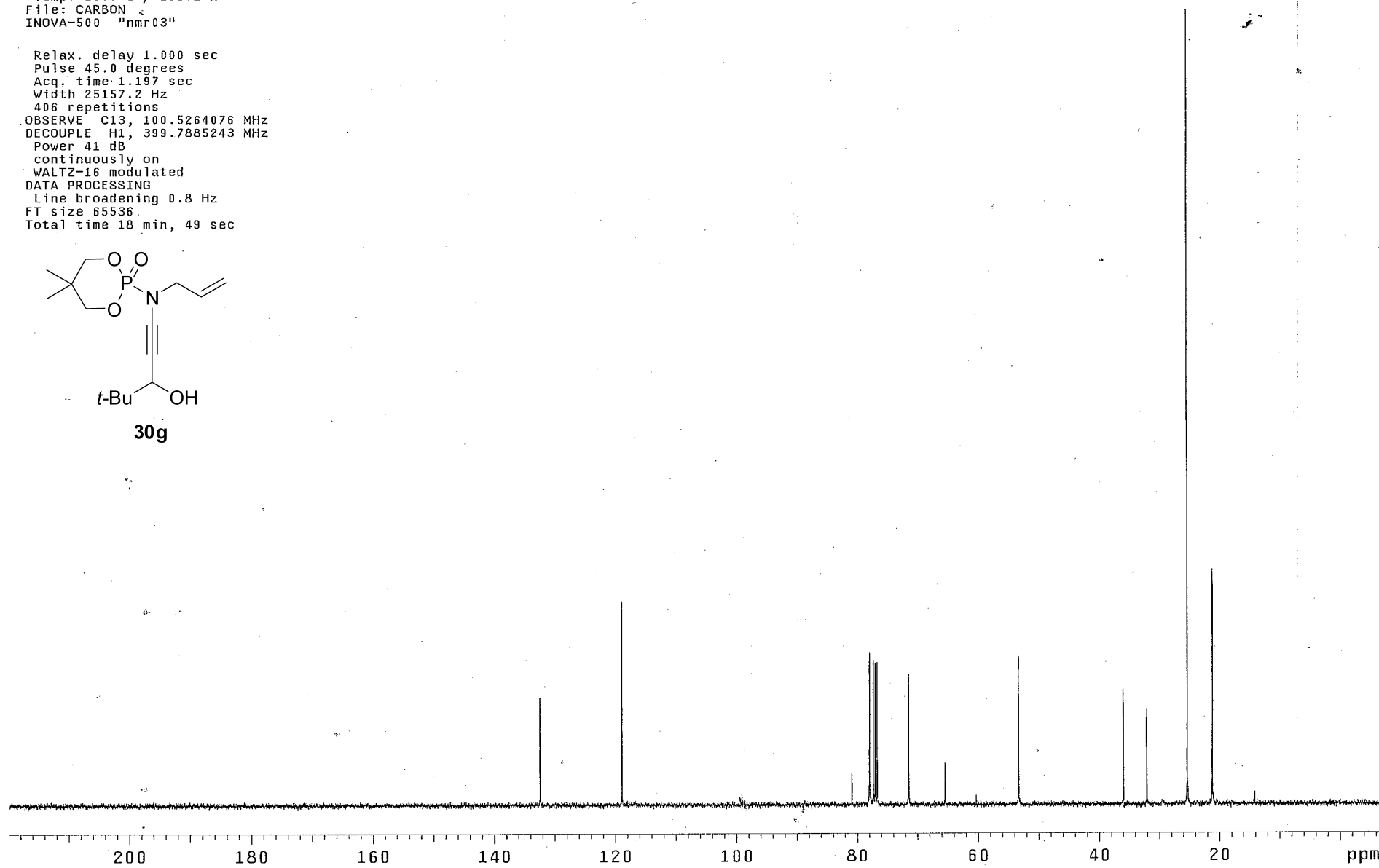
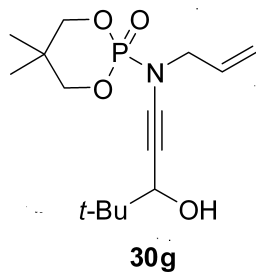
wxn44-1_26Oct2011-17:29:17

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn44-1_26Oct2011-17:29:17

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INNOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
406 repetitions
OBSERVE C13, 100.5264076 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 18 min, 49 sec



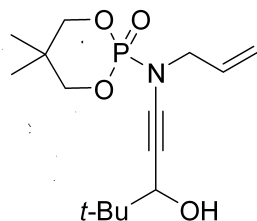
wxn44-1_26Oct2011-17:29:17

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn44-1_26Oct2011-17:29:17

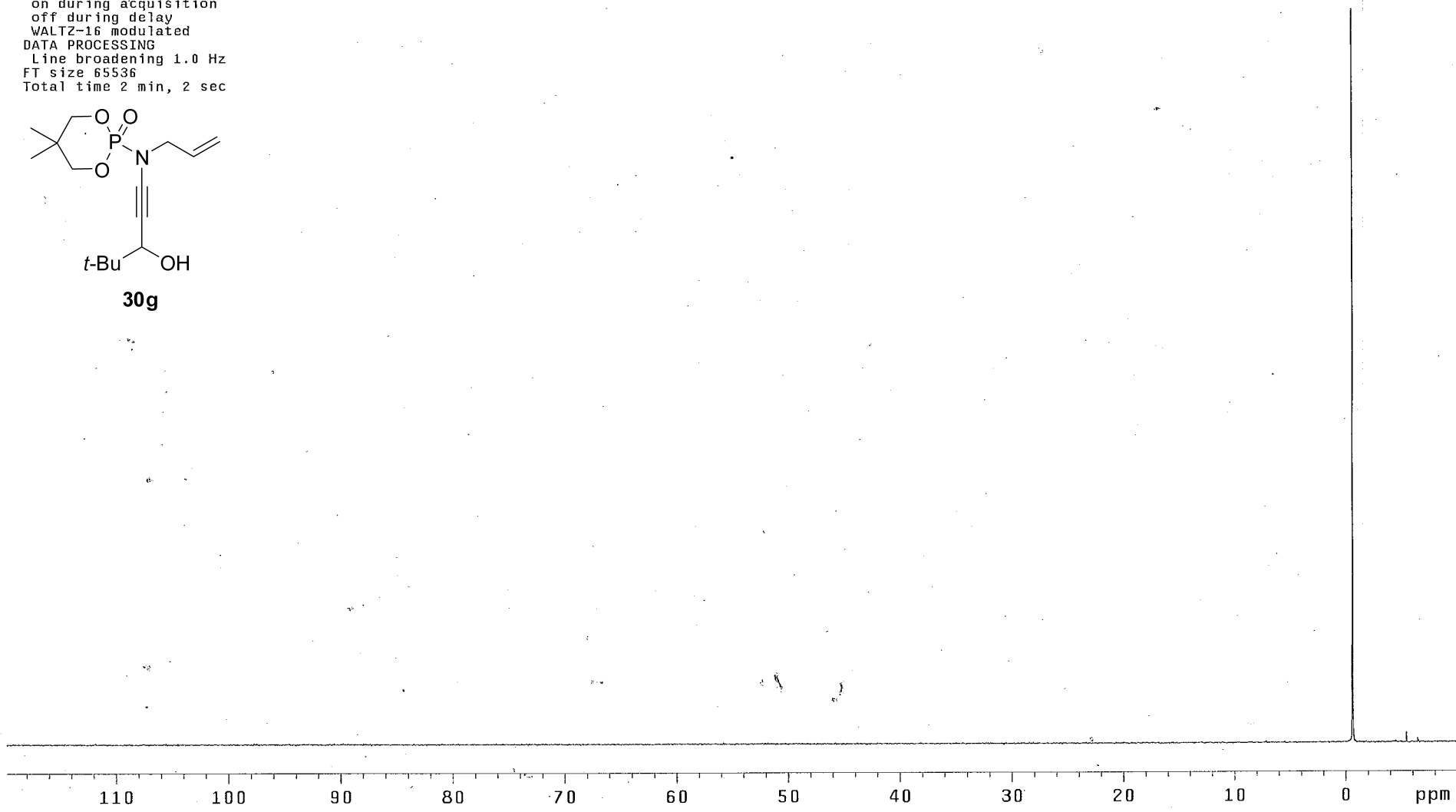
Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PHOSPHORUS
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 0.799 sec
Width 35650.6 Hz
64 repetitions
OBSERVE P31, 161.8363711 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 min, 2 sec



30g



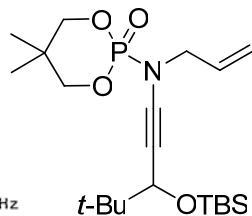
wxn47-1_29Oct2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn47-1_29Oct2011

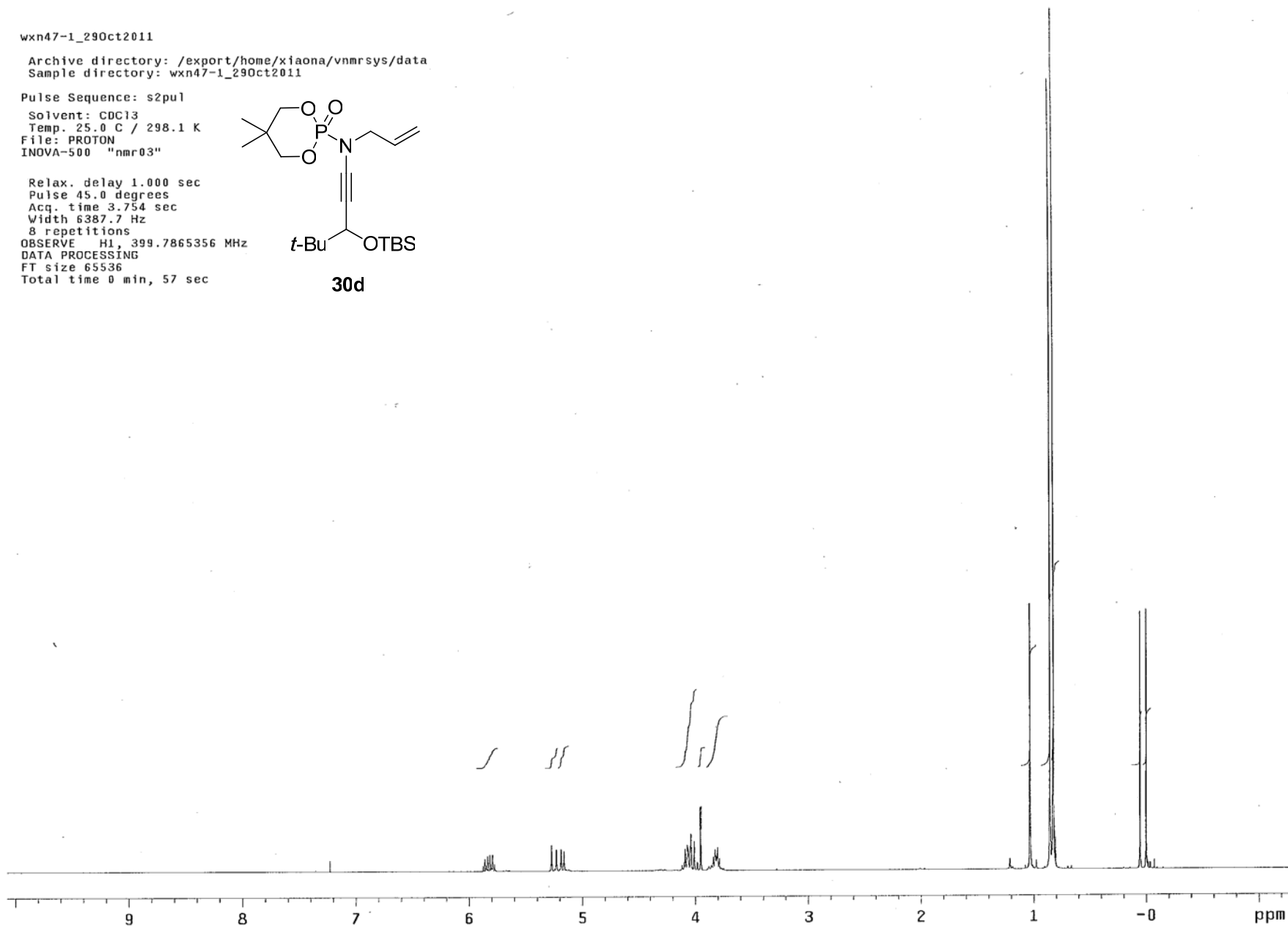
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865356 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



30d



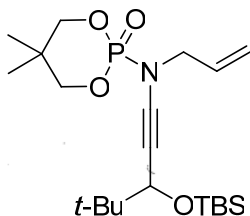
wxn47-1_29Oct2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn47-1_29Oct2011

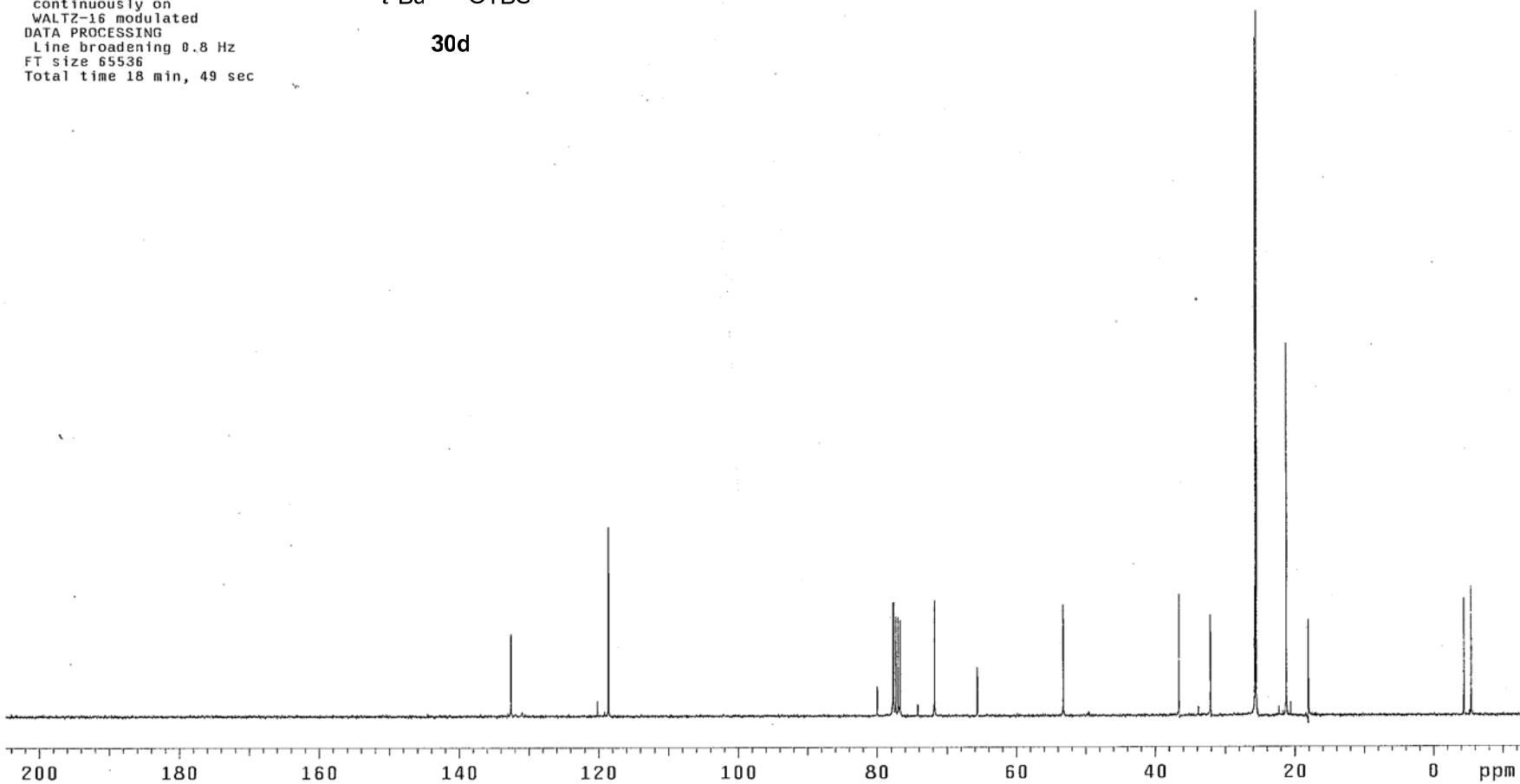
Pulse Sequence: s2pul

Solvent: CDC13
Temp. 25.0 C / 298.1 K
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
436 repetitions
OBSERVE C13, 100.5264076 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 18 min, 49 sec



30d



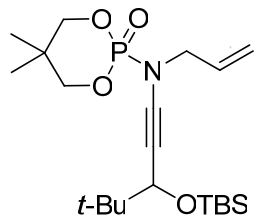
wxn47-1_29Oct2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn47-1_29Oct2011

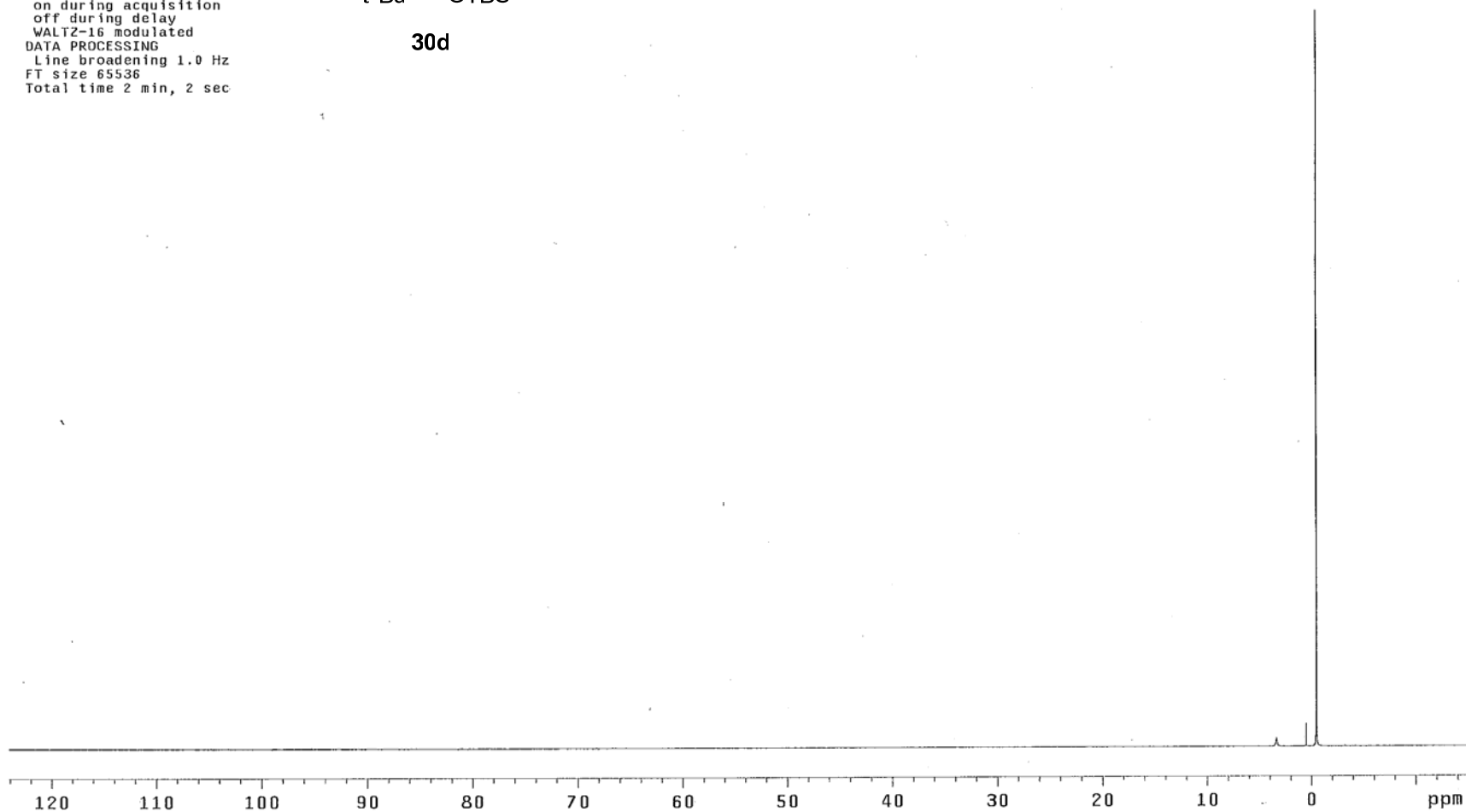
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PHOSPHORUS
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 0.799 sec
Width 35650.6 Hz
64 repetitions
OBSERVE P31, 161.8363711 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 min, 2 sec



30d



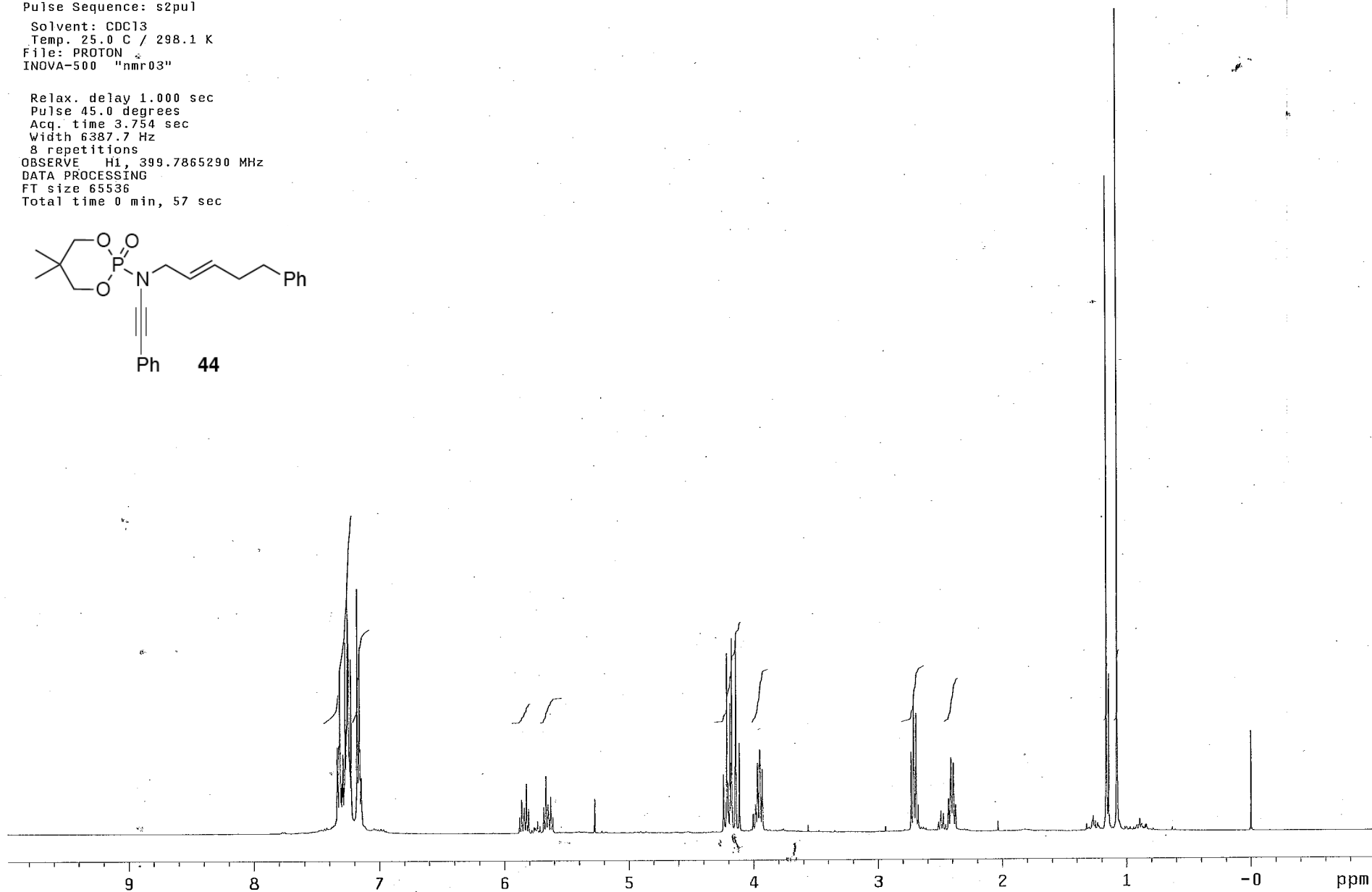
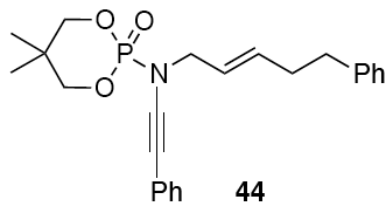
wxn72-1_02Dec2011-14:32:33

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn72-1_02Dec2011-14:32:33

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865290 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



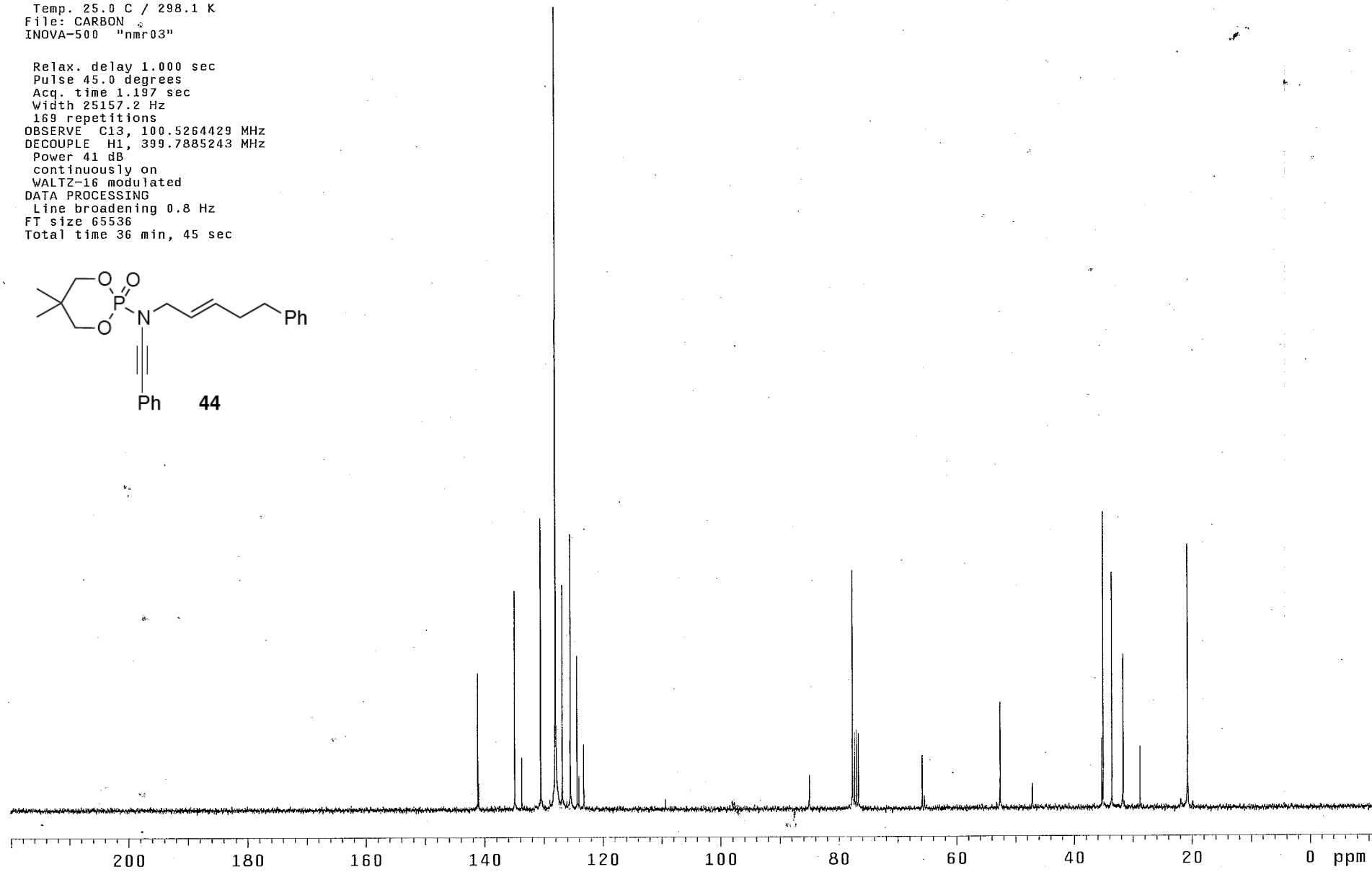
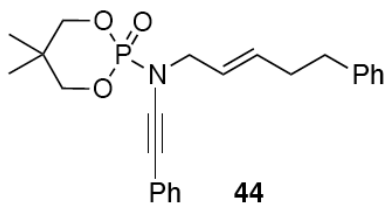
wxn72-1_02Dec2011-14:48:54

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn72-1_02Dec2011-14:48:54

Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
169 repetitions
OBSERVE C13, 100.5264429 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 36 min, 45 sec



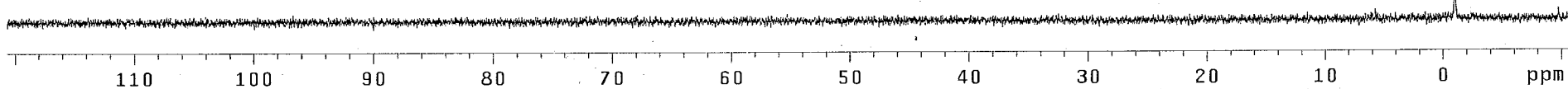
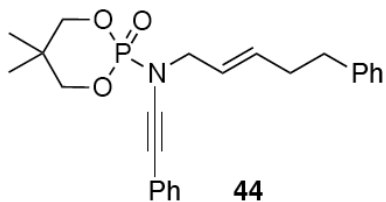
wxn72-1_02Dec2011-10:02:07

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn72-1_02Dec2011-10:02:07

Pulse Sequence: s2pul

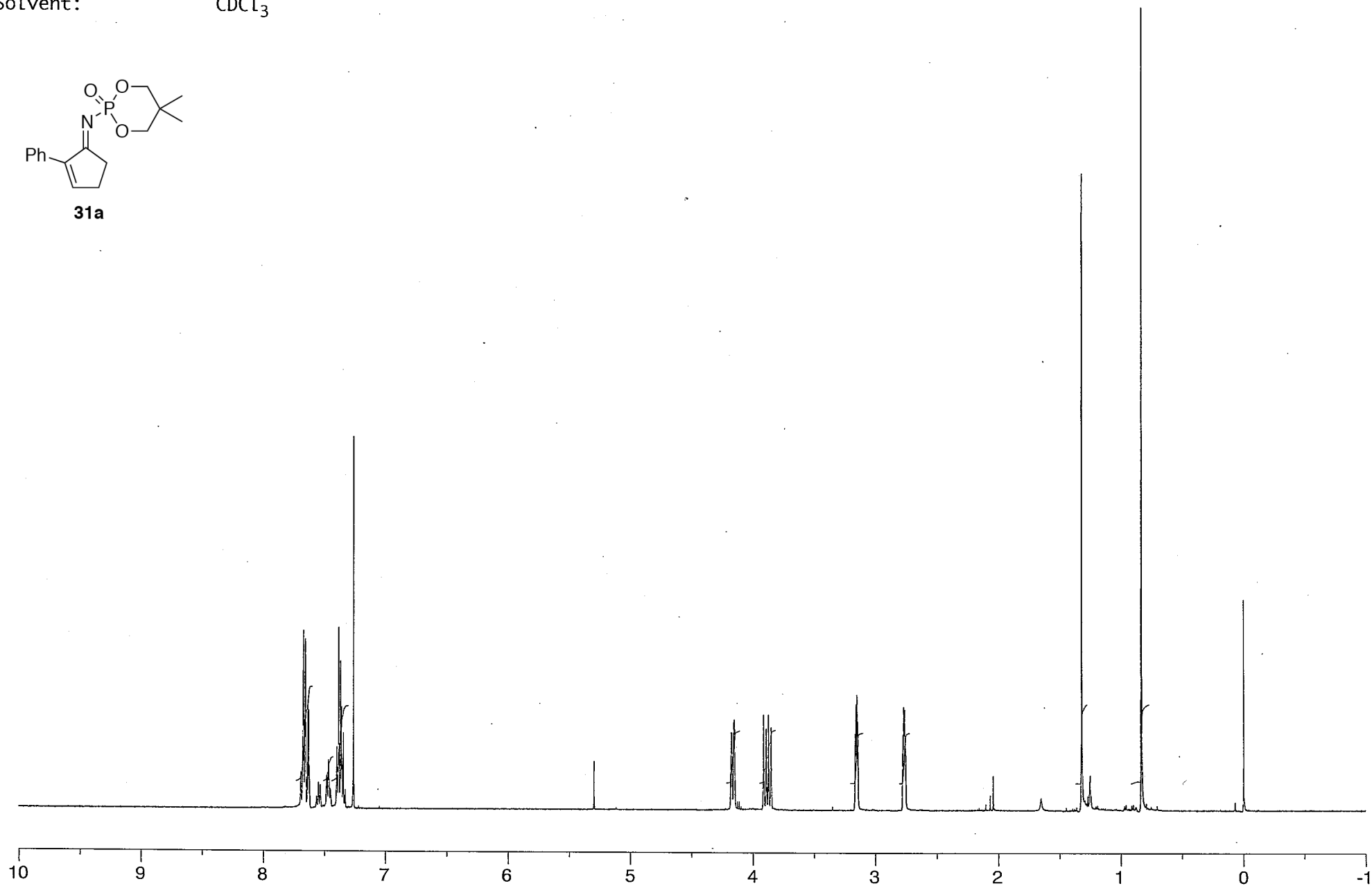
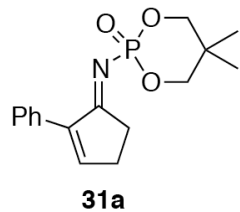
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PHOSPHORUS
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 0.800 sec
Width 35650.6 Hz
64 repetitions
OBSERVE P31, 161.8363711 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 min, 3 sec

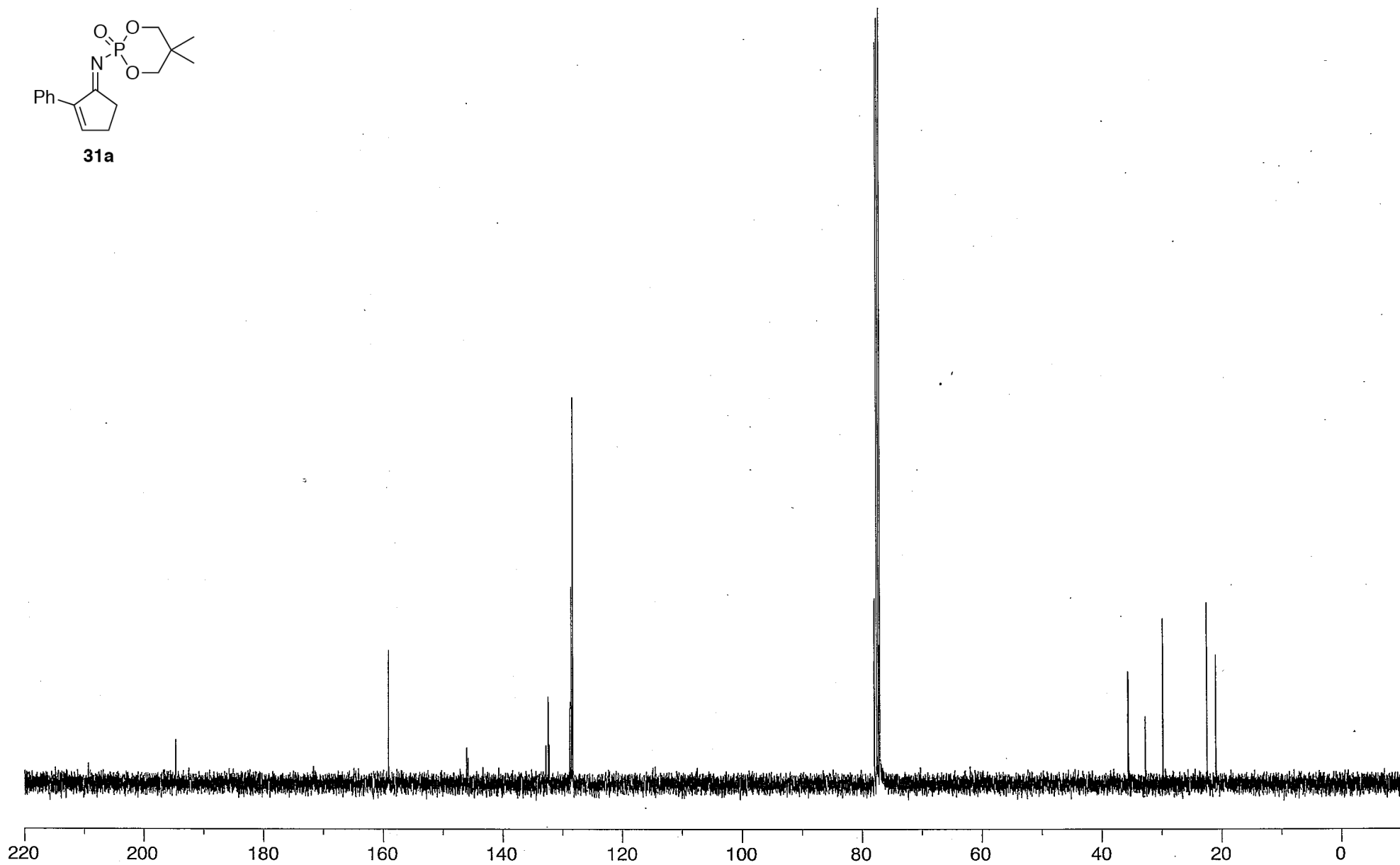
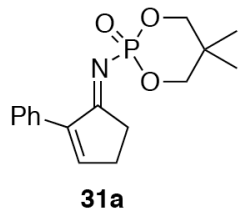


KAD-03-188_04Feb2012

Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃

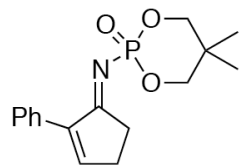


Pulse Sequence: s2pu1
Spectrometer Freq.: 125.67 MHz
Solvent: CDCl₃

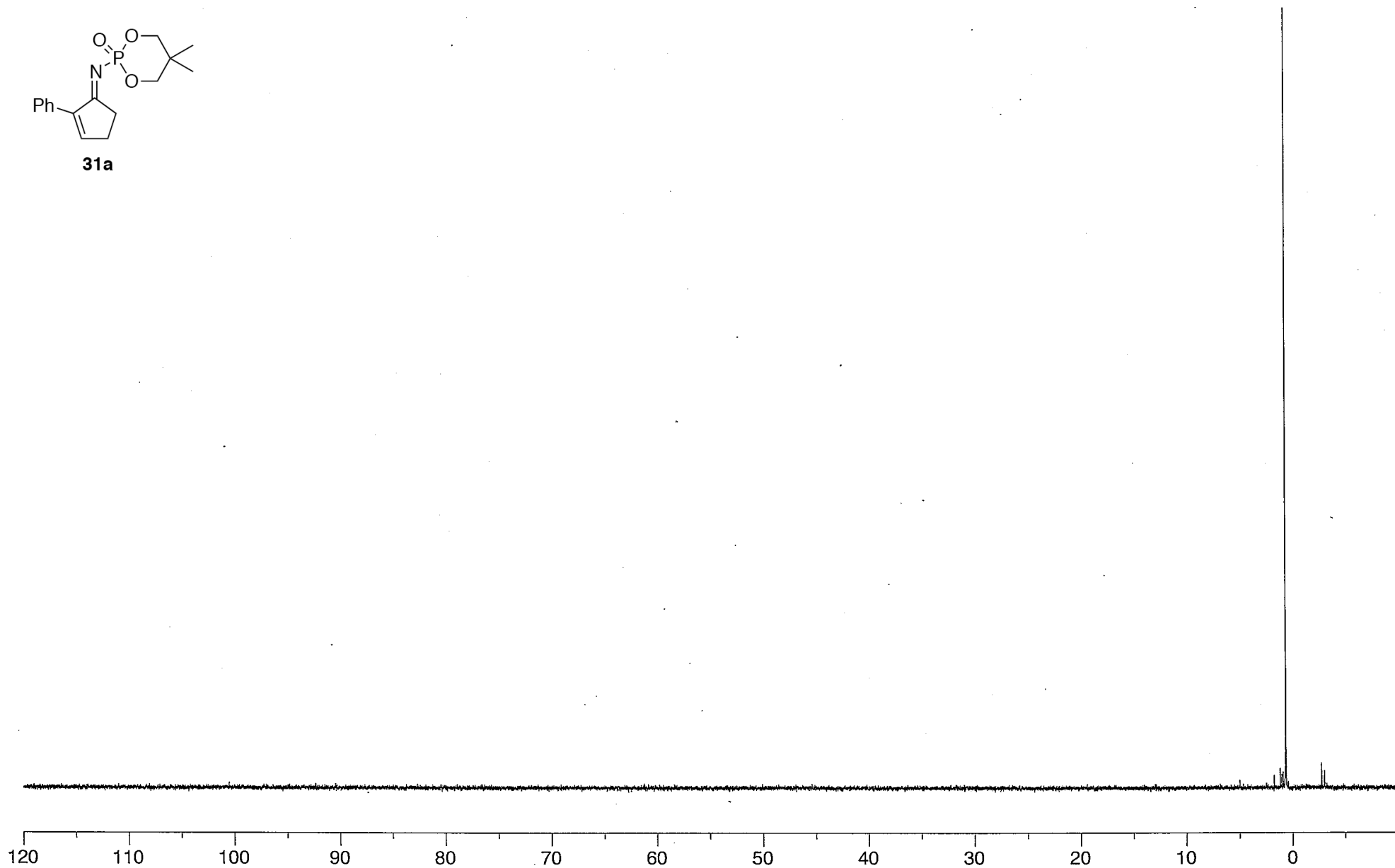


KAD-03-188P_29Sep2011

Pulse Sequence: s2pul
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



31a



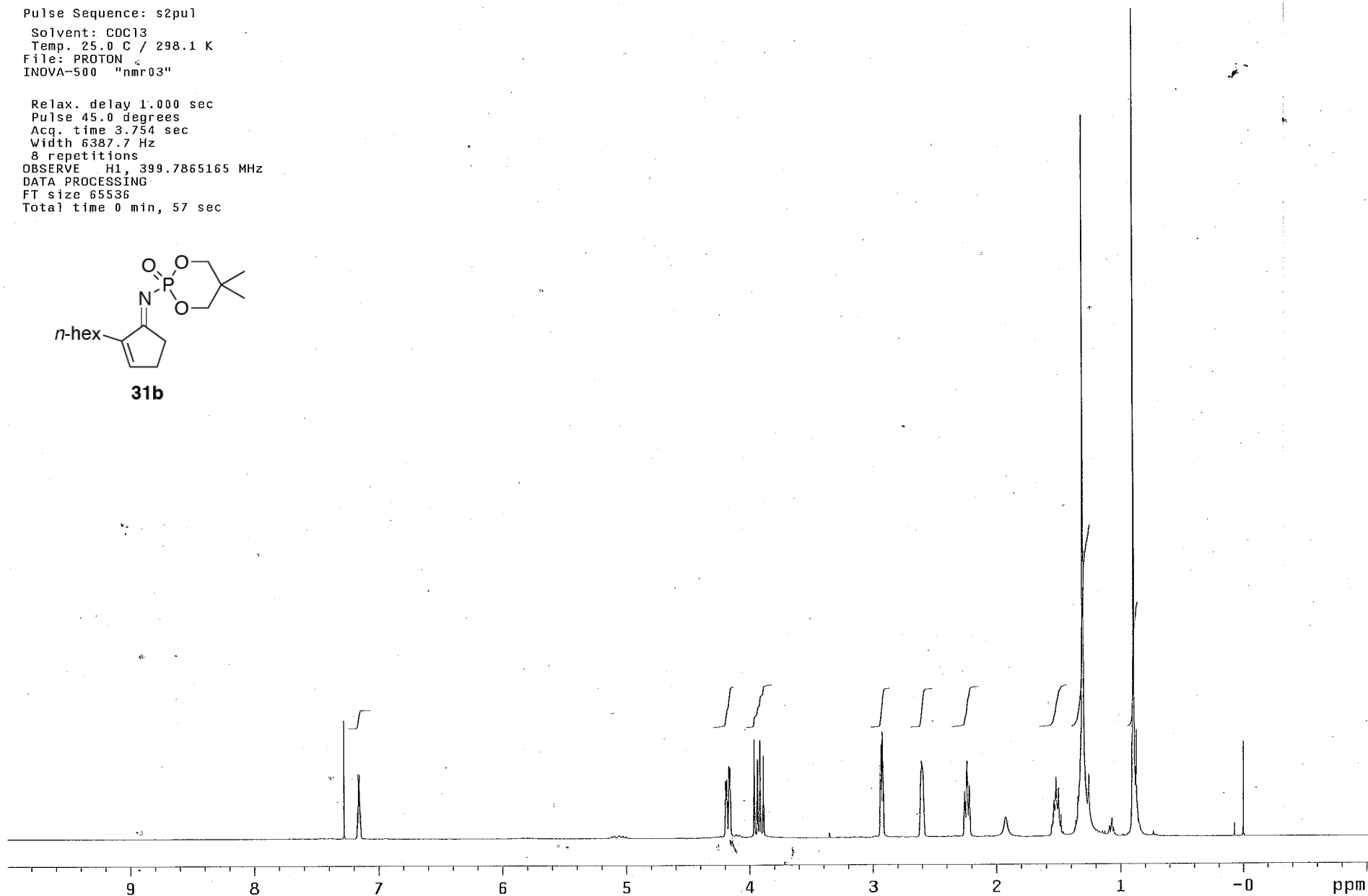
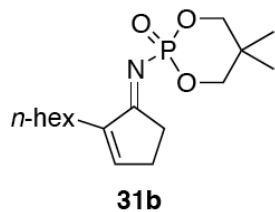
wxn27-1_130ct2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn27-1_130ct2011

Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865165 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



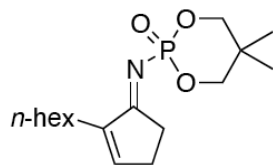
wxn27-1_13Oct2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn27-1_13Oct2011

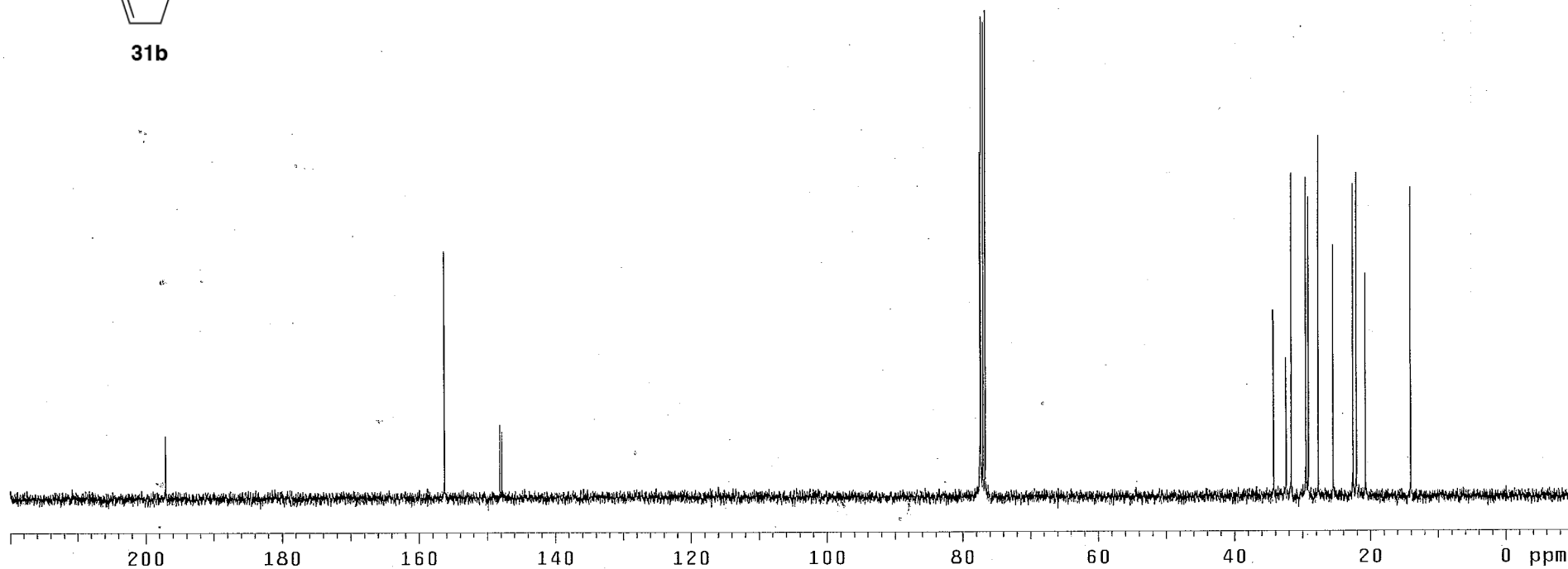
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INNOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
744 repetitions
OBSERVE C13, 100.5264045 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 36 min, 45 sec



31b



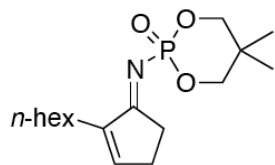
wxn27-1_13Oct2011-11:08:24

Archive directory: /export/home/xiaona/vnmrSYS/data
Sample directory: wxn27-1_13Oct2011-11:08:24

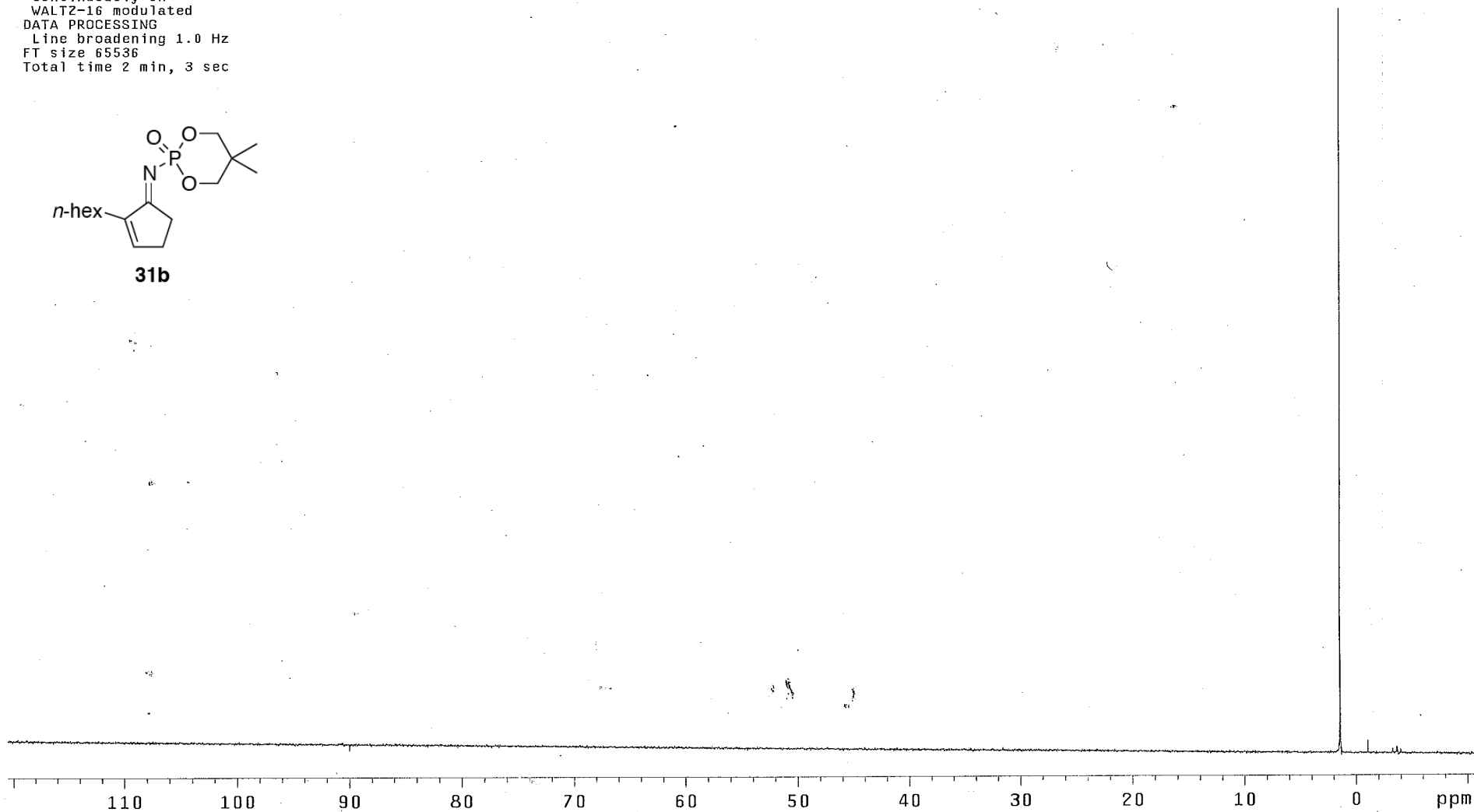
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PHOSPHORUS
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 0.800 sec
Width 35650.6 Hz
64 repetitions
OBSERVE P31, 161.8363711 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 min, 3 sec



31b



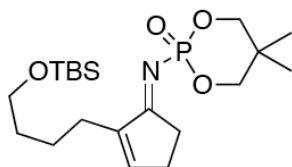
wxn60-2_09Nov2011-18:51:57

Archive directory: /export/home/xiaona/vnmrSYS/data
Sample directory: wxn60-2_09Nov2011-18:51:57

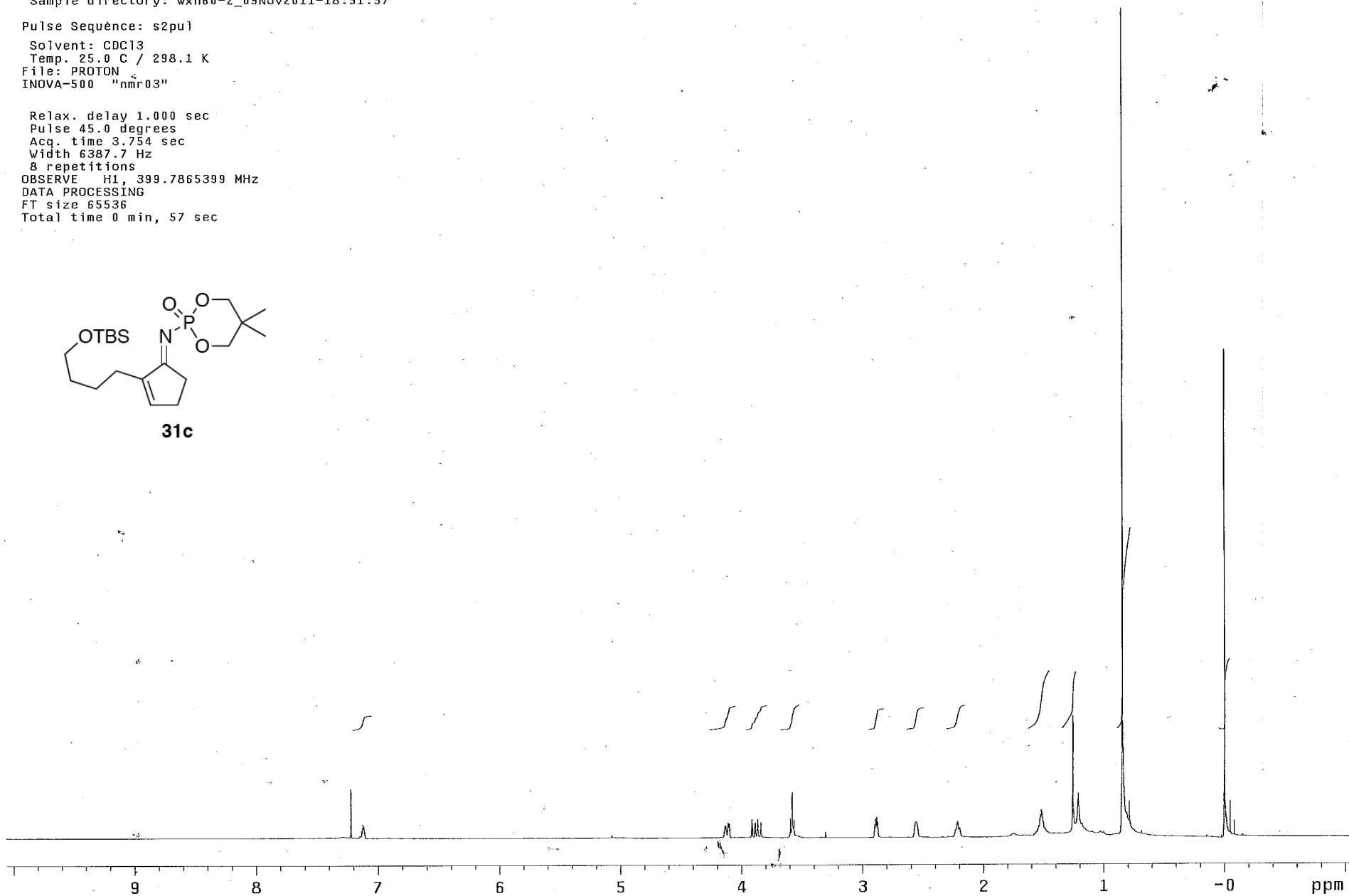
Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865399 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



31c



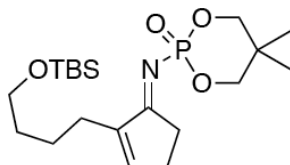
wxn60-2_09Nov2011-20:55:14

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn60-2_09Nov2011-20:55:14

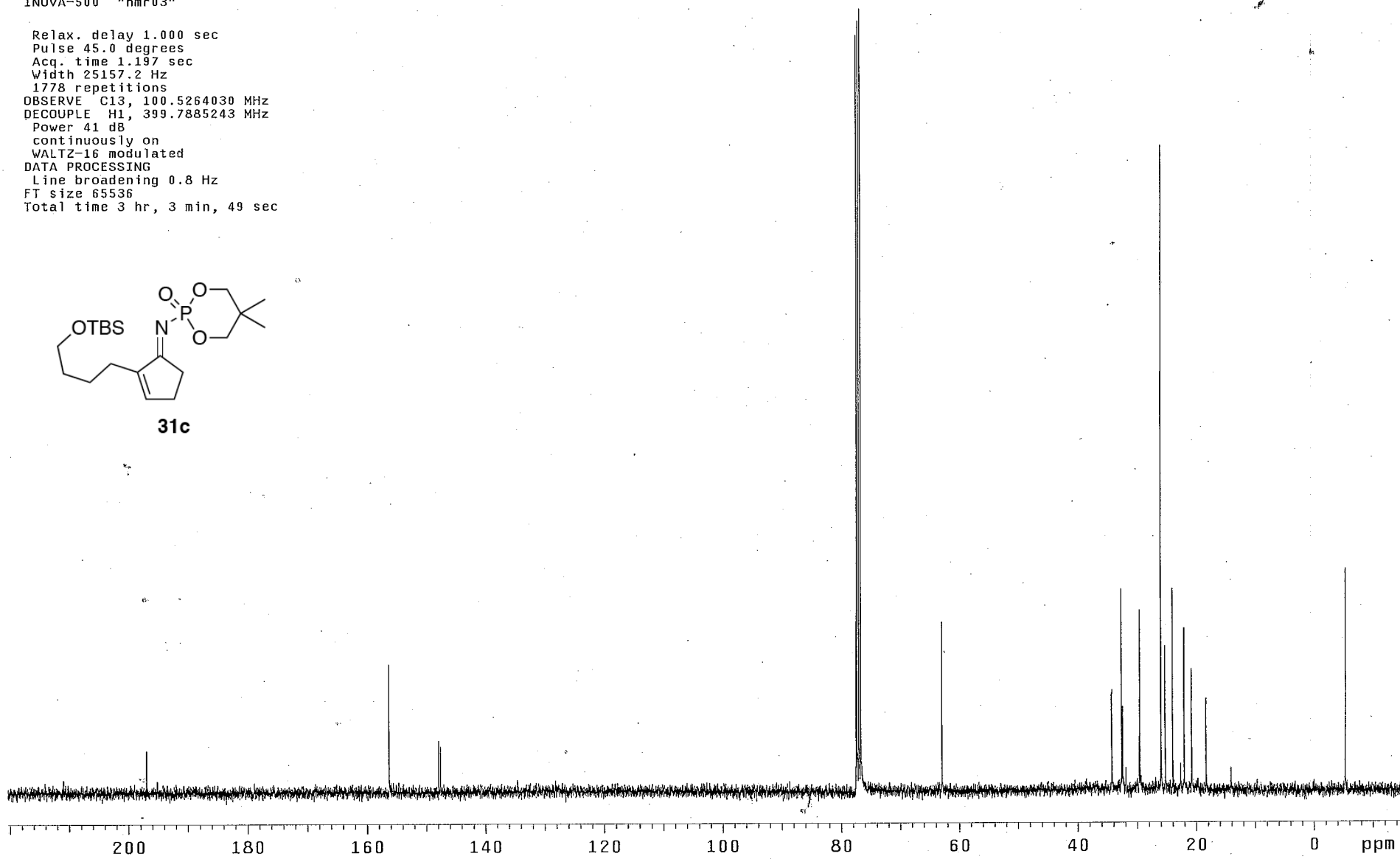
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
1778 repetitions
OBSERVE C13, 100.5264030 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



31c



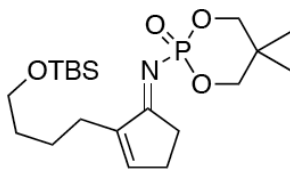
wxn60-2_09Nov2011

Archive directory: /export/home/xiaona/vnmrSYS/data
Sample directory: wxn60-2_09Nov2011

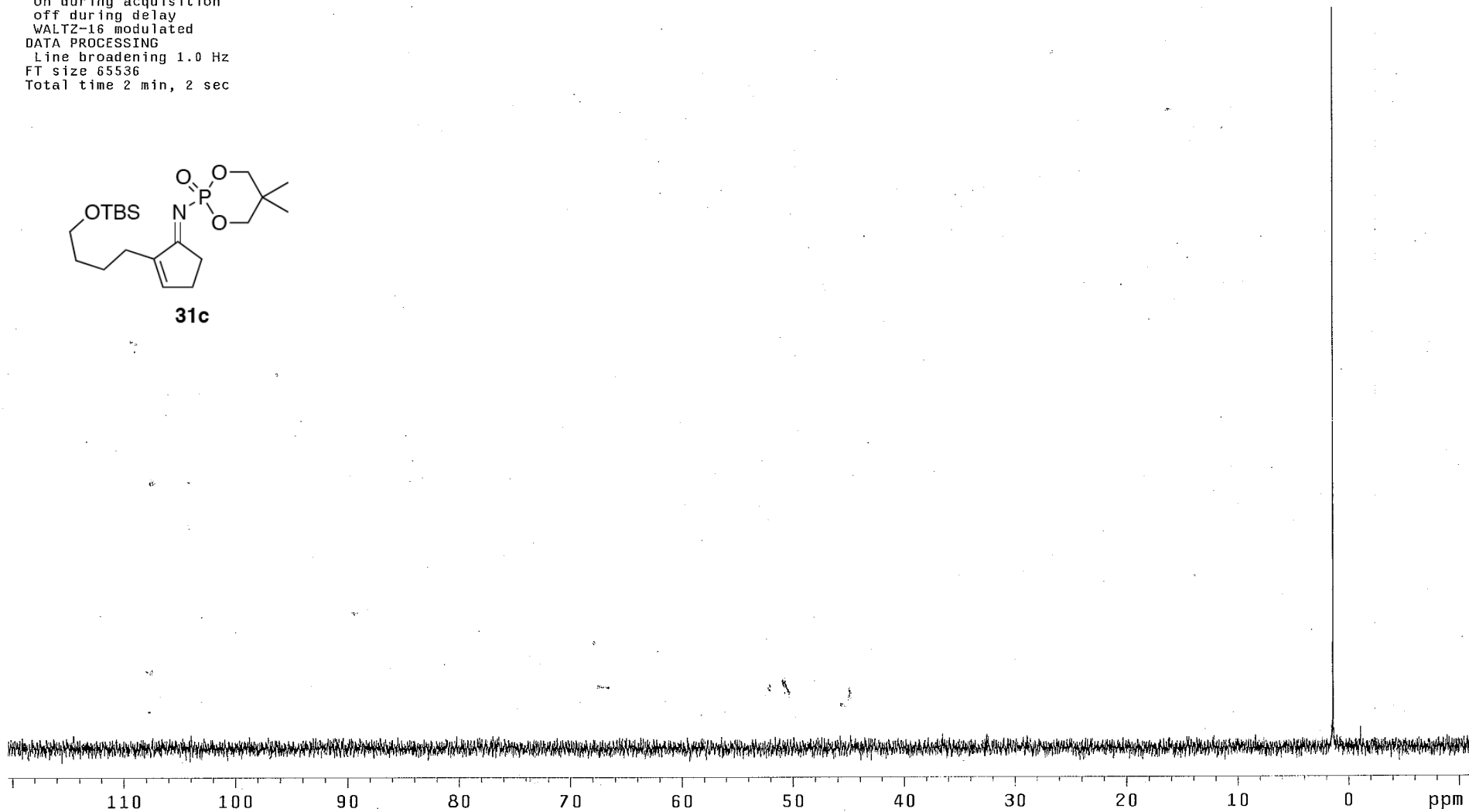
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PHOSPHORUS
INOVA-500 "nmr03"

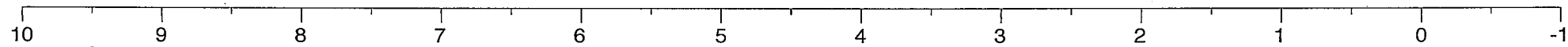
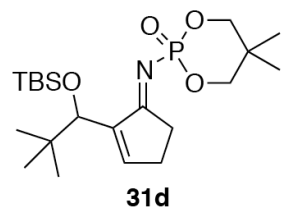
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 0.799 sec
Width 35650.6 Hz
64 repetitions
OBSERVE P31, 161.8363711 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 min, 2 sec



31c

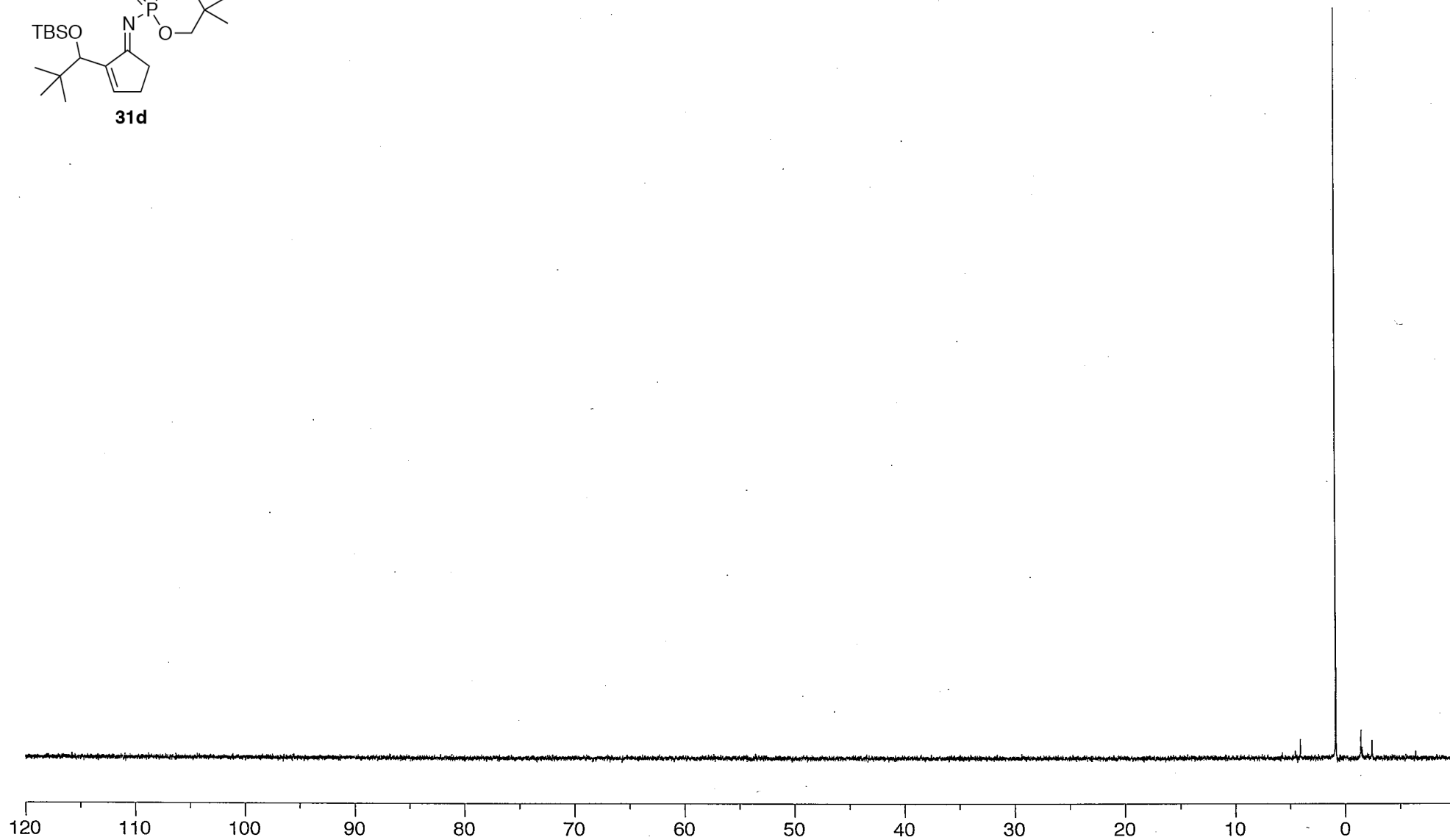
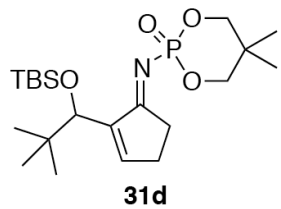


Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



KAD-03-256_24Jan2012

Pulse Sequence: s2pu1
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



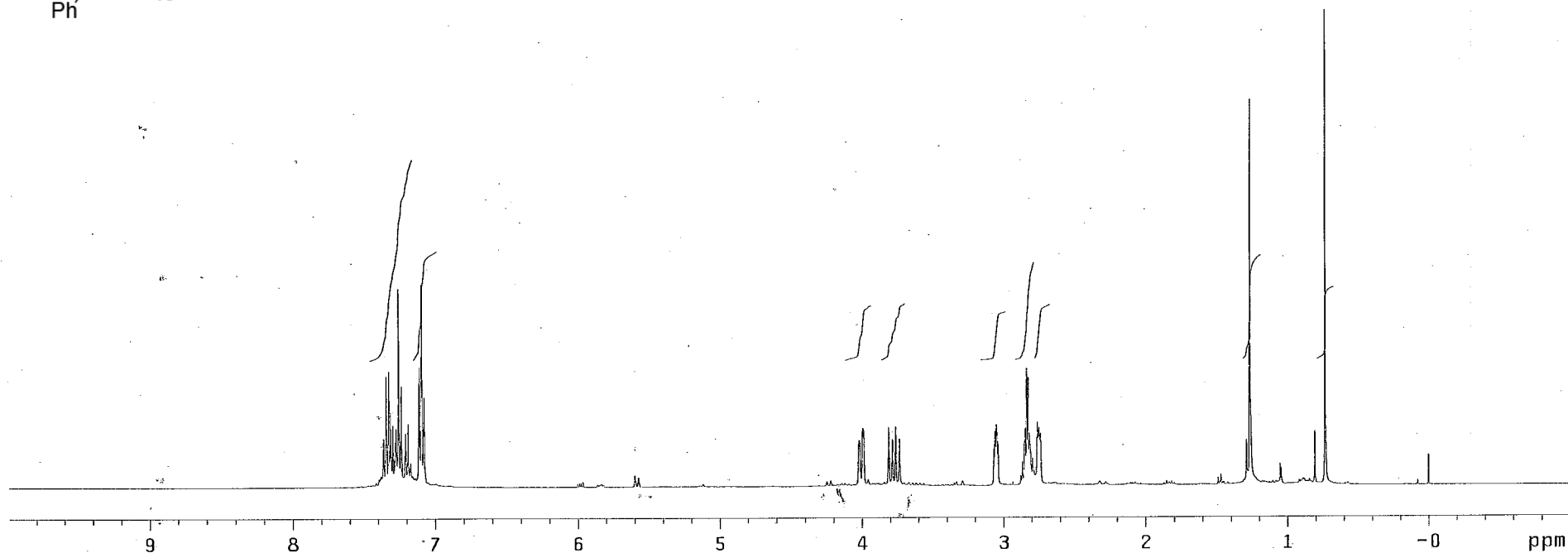
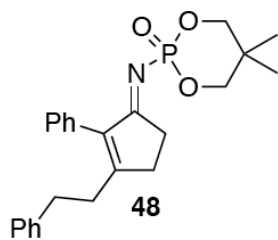
wxn80-a-1_07Dec2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn80-a-1_07Dec2011

Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865241 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



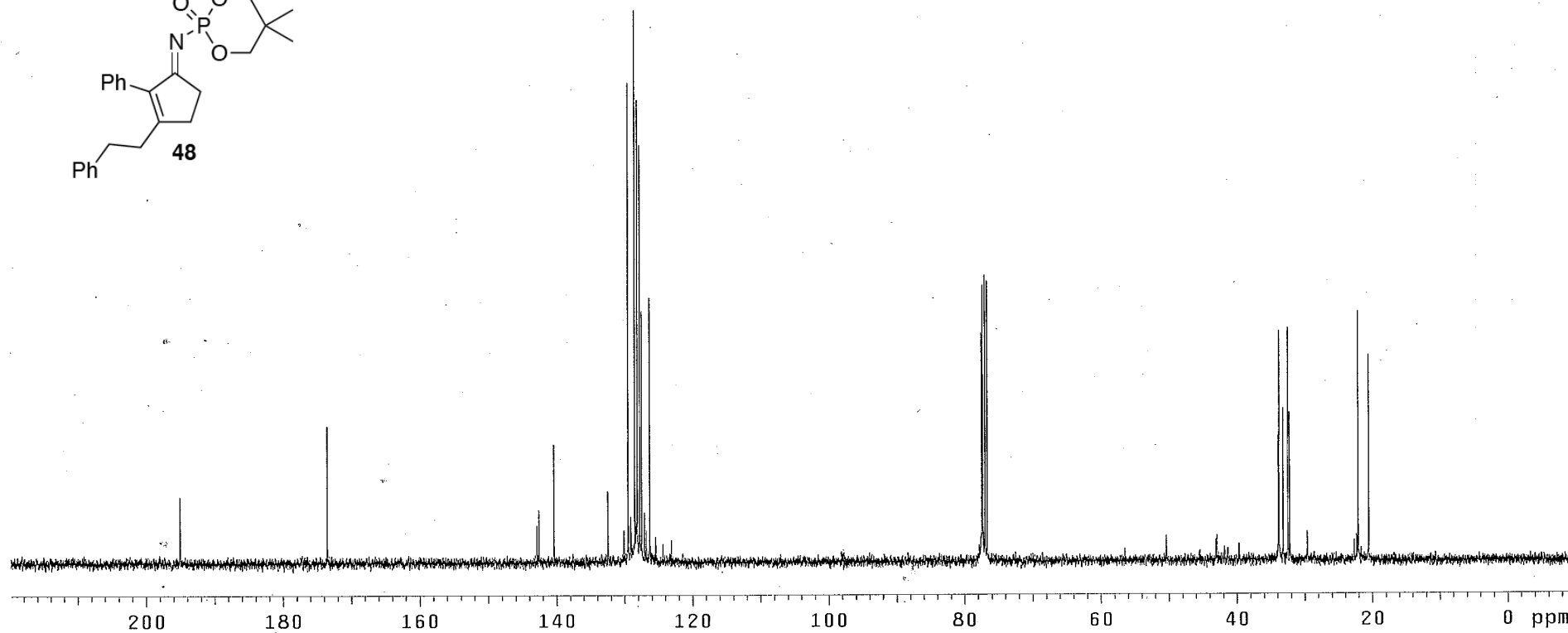
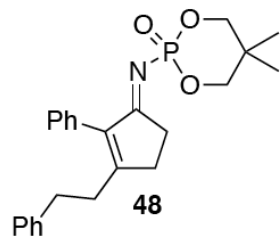
wxn80-a-1_07Dec2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn80-a-1_07Dec2011

Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
599 repetitions
OBSERVE C13, 100.5264099 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 36 min, 45 sec



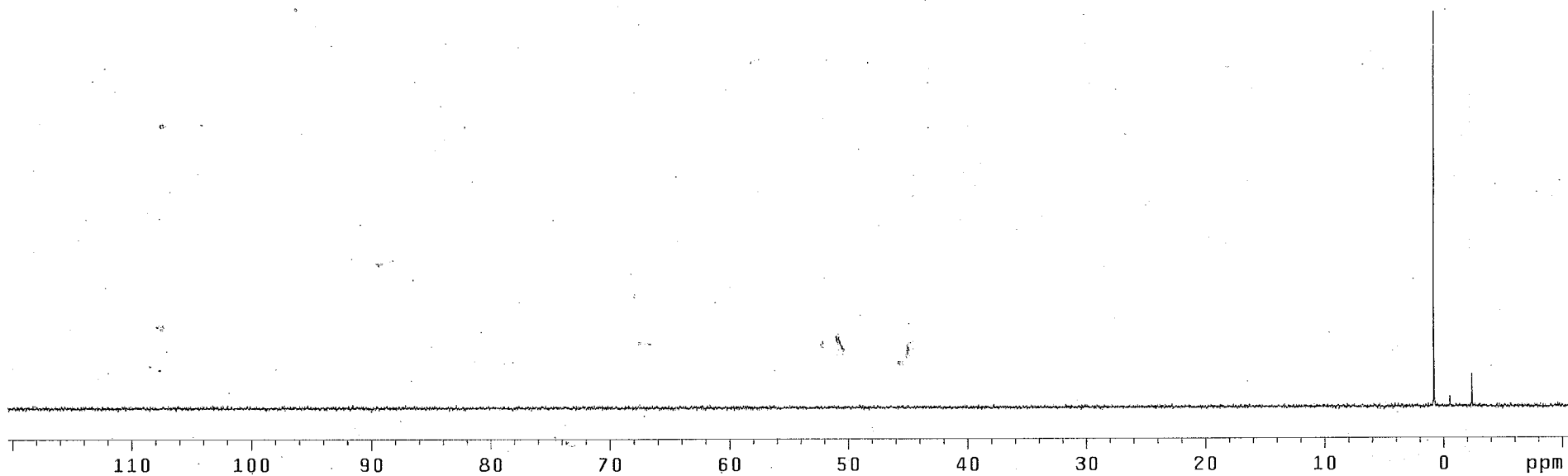
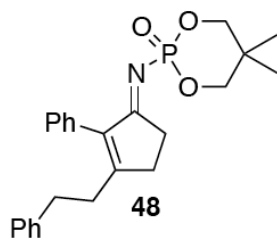
wxn80-a-1_07Dec2011

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn80-a-1_07Dec2011

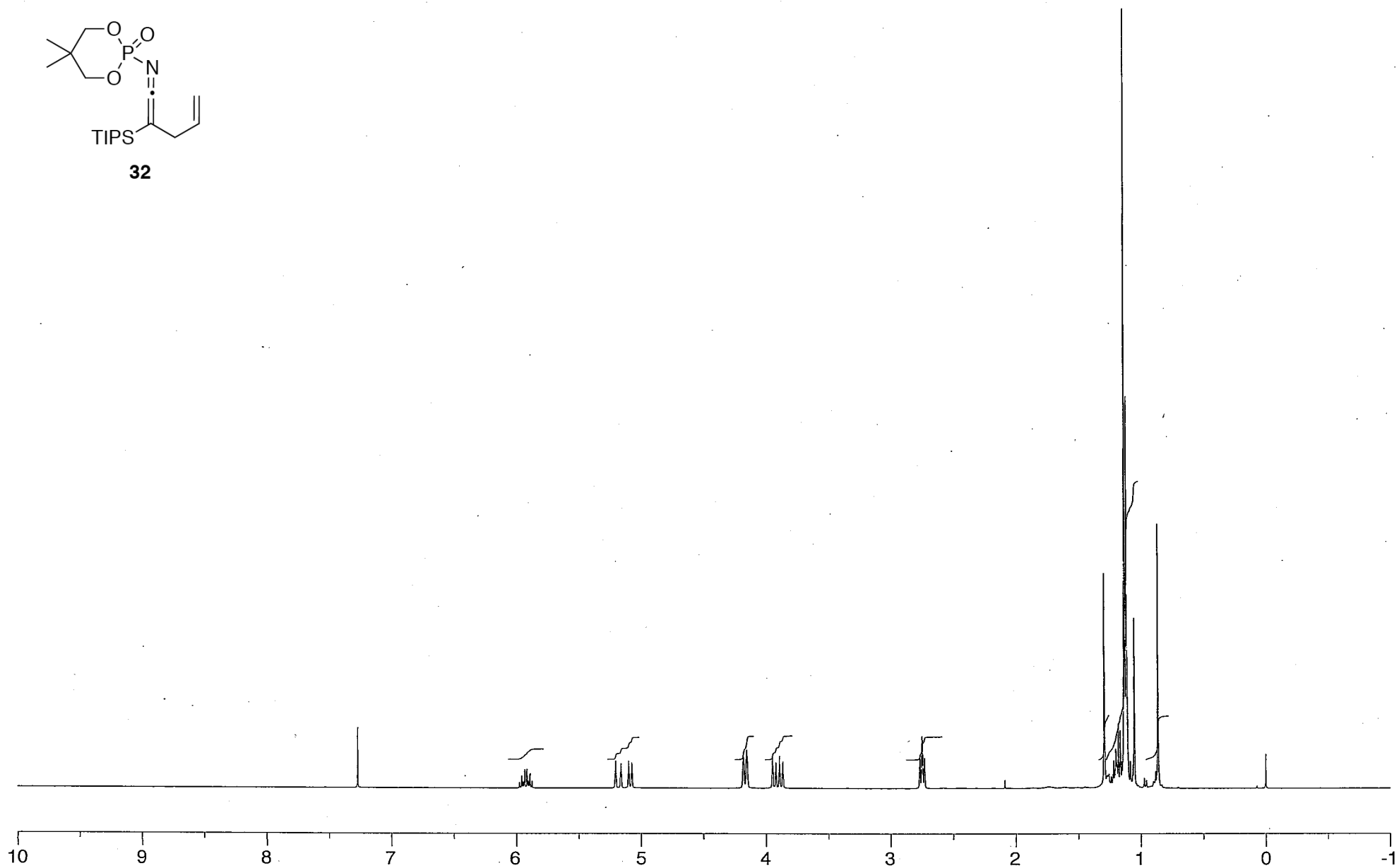
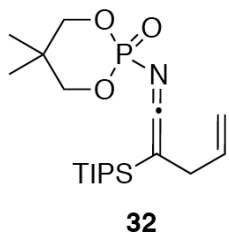
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PHOSPHORUS
INNOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 0.799 sec
Width 35650.6 Hz
64 repetitions
OBSERVE P31, 161.8363711 MHz
DECOUPLE H1, 399.7885243 MHz
Power 41 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 min, 2 sec

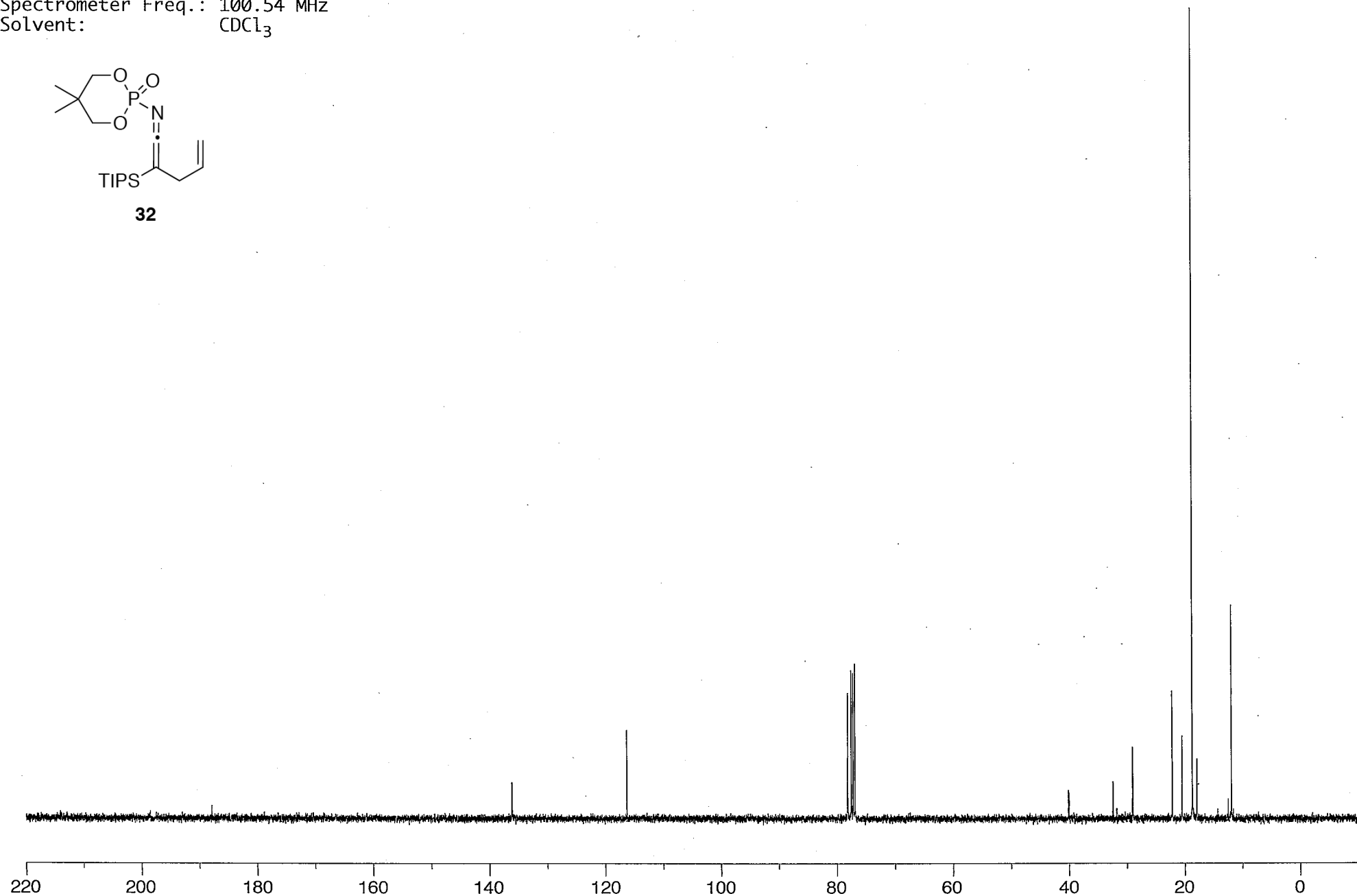
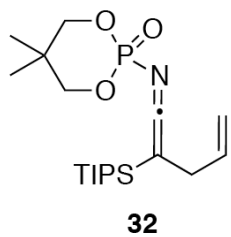


Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



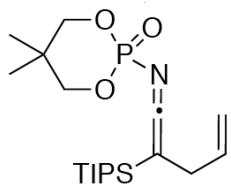
MW-1-137_01Nov2011

Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃



MW-1-137_01Nov2011

Pulse Sequence: s2pul
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃

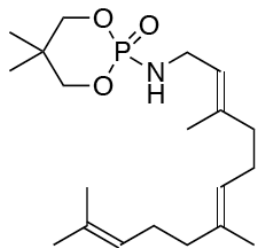


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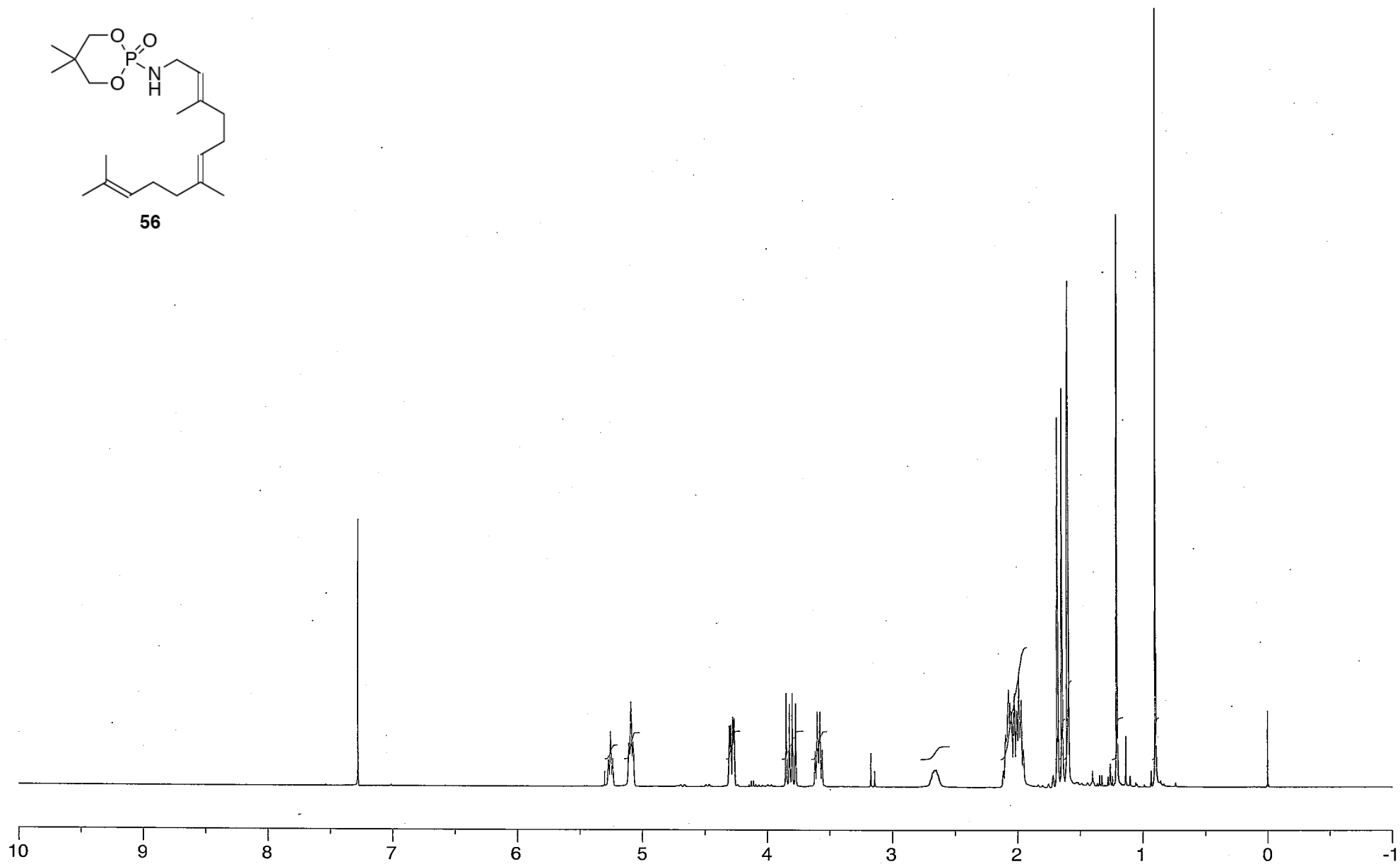
100 90 80 70 60 50 40 30 20 10 0 -10

KAD-03-229_22Dec2011

Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

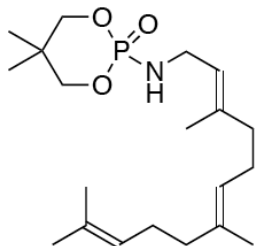


56

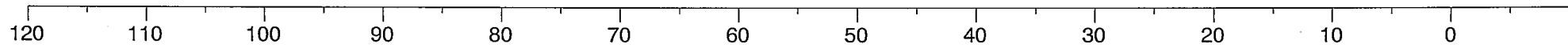


KAD-03-229PC_22Dec2011

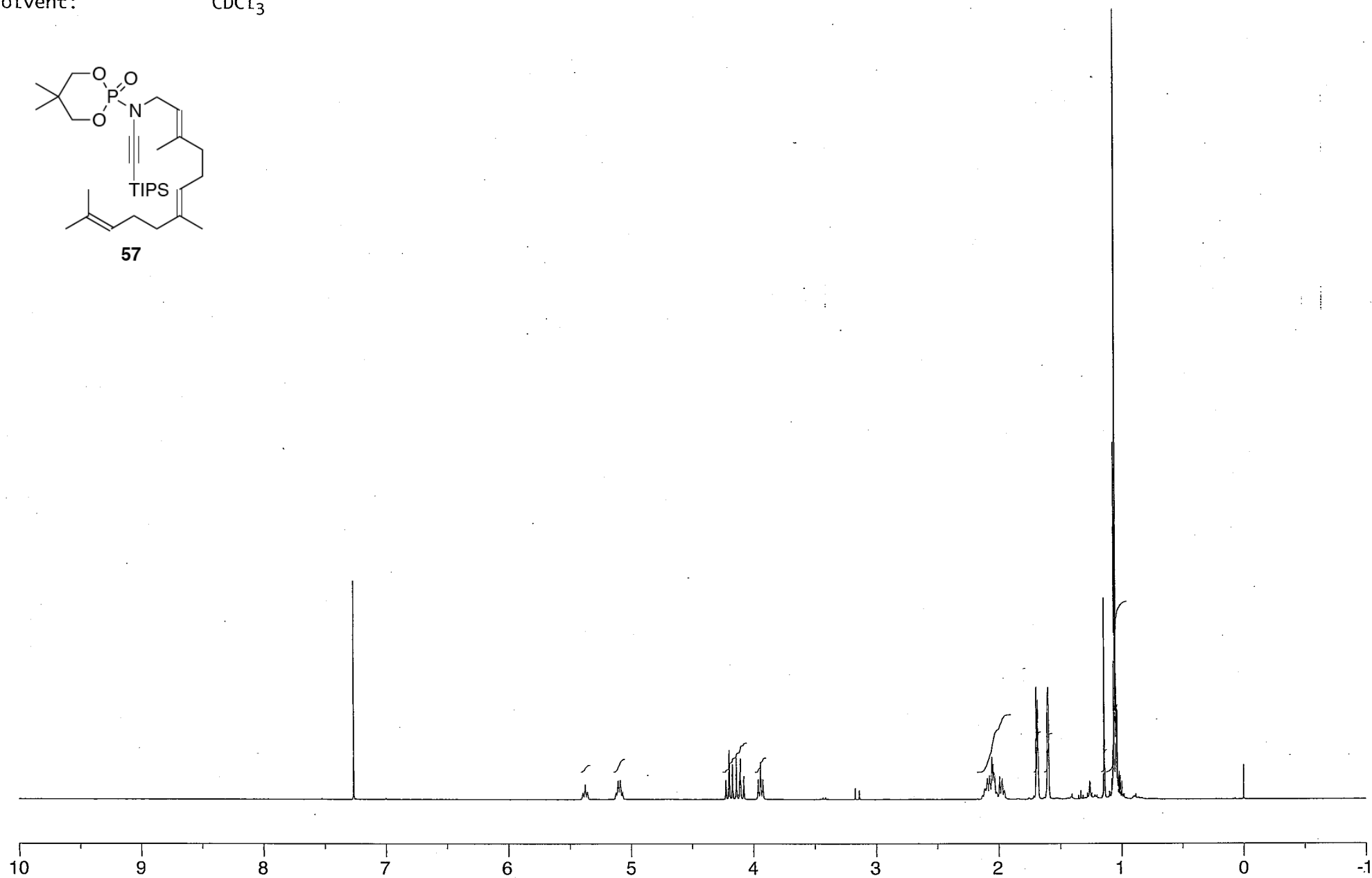
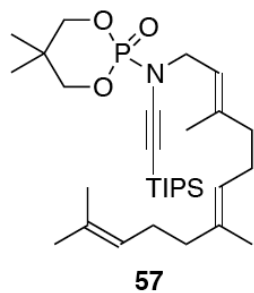
Pulse Sequence: s2pu1
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



56

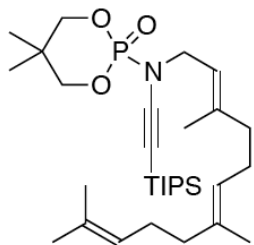


Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

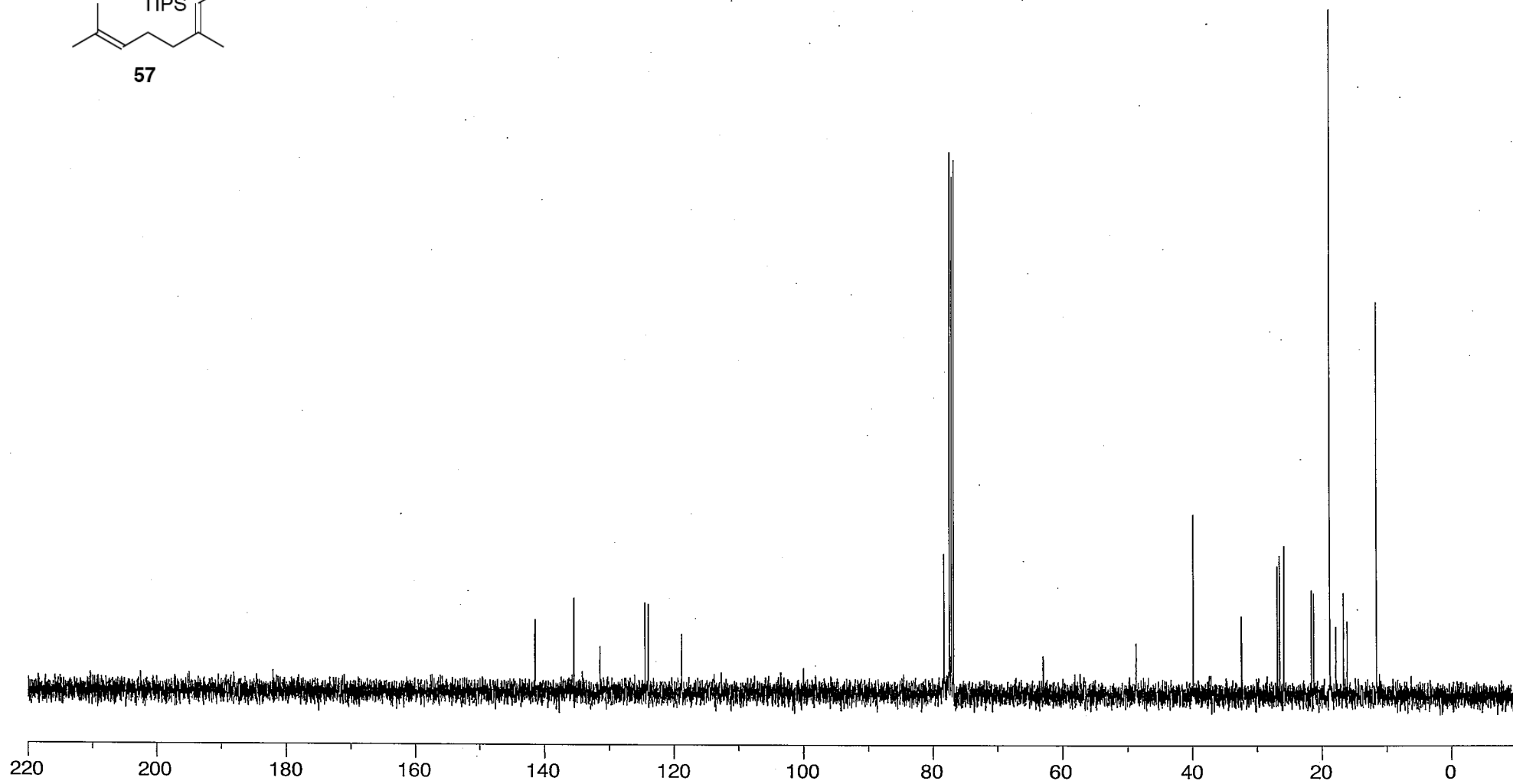


KAD-03-230_31Dec2011

Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

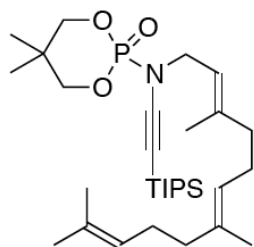


57

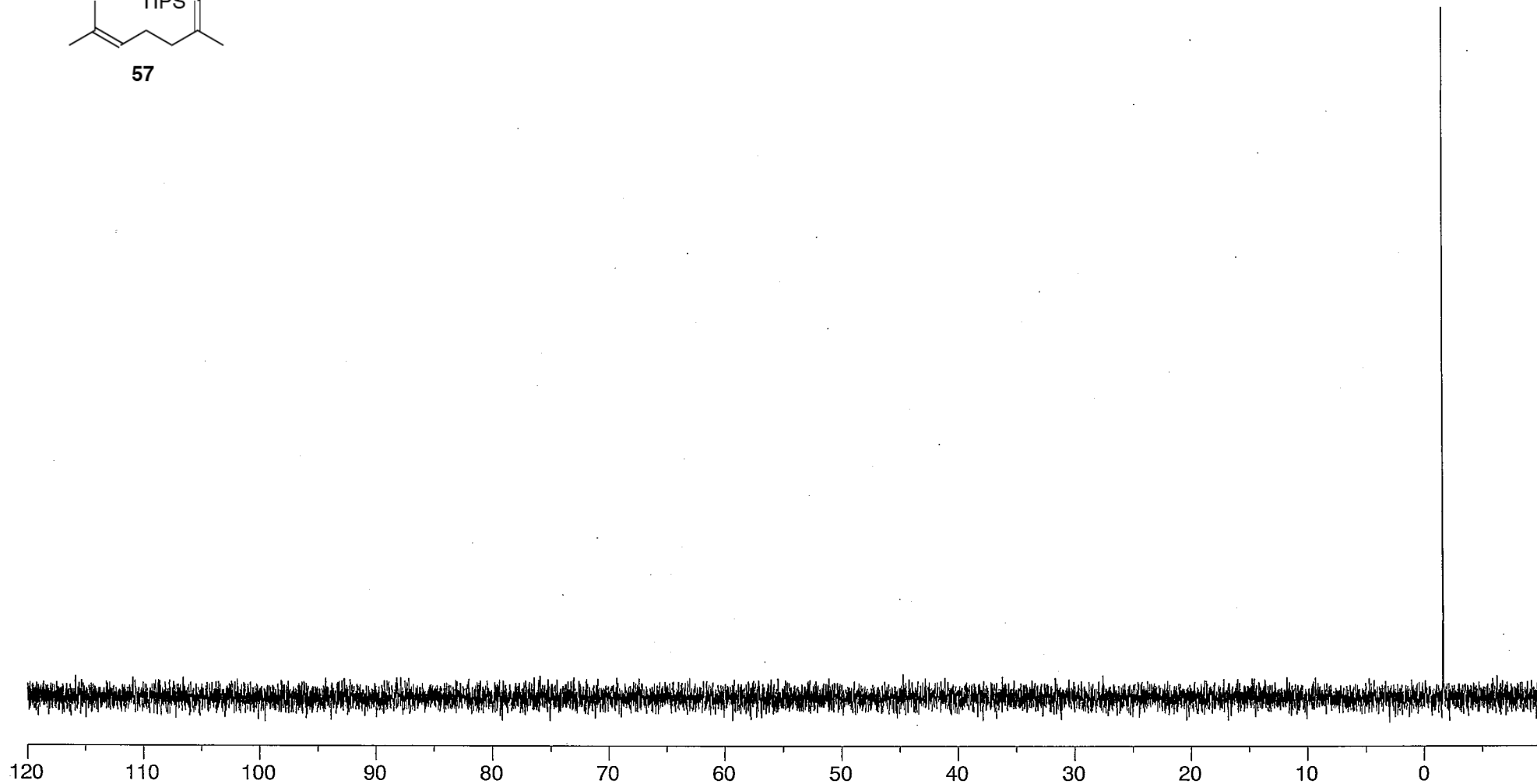


KAD-03-230_31Dec2011

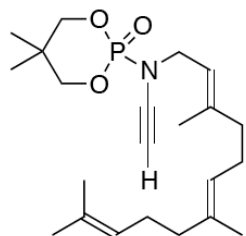
Pulse Sequence: s2pul
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



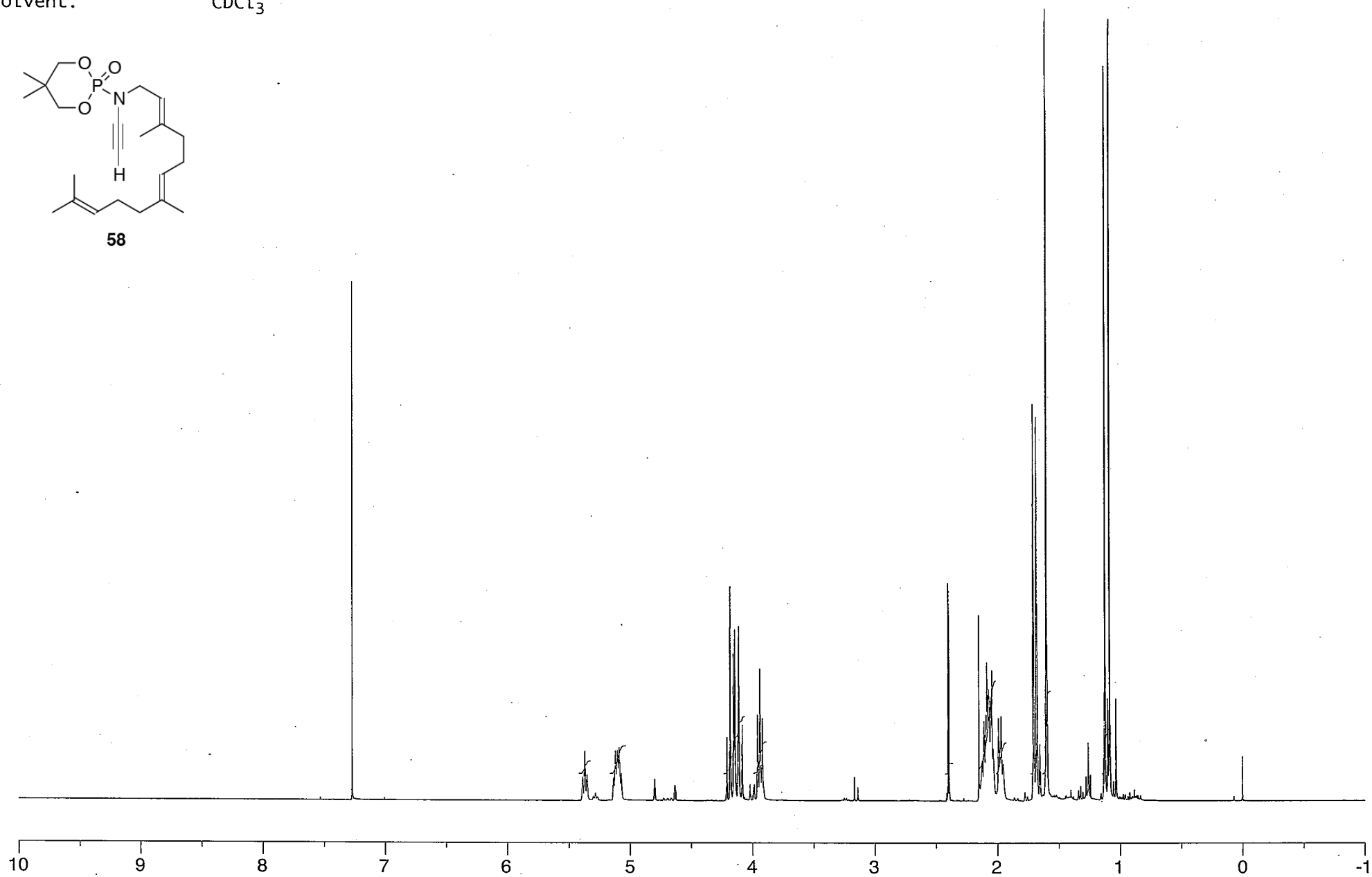
57



Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃

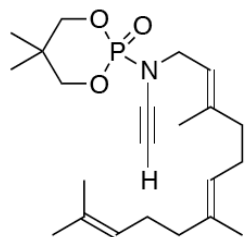


58

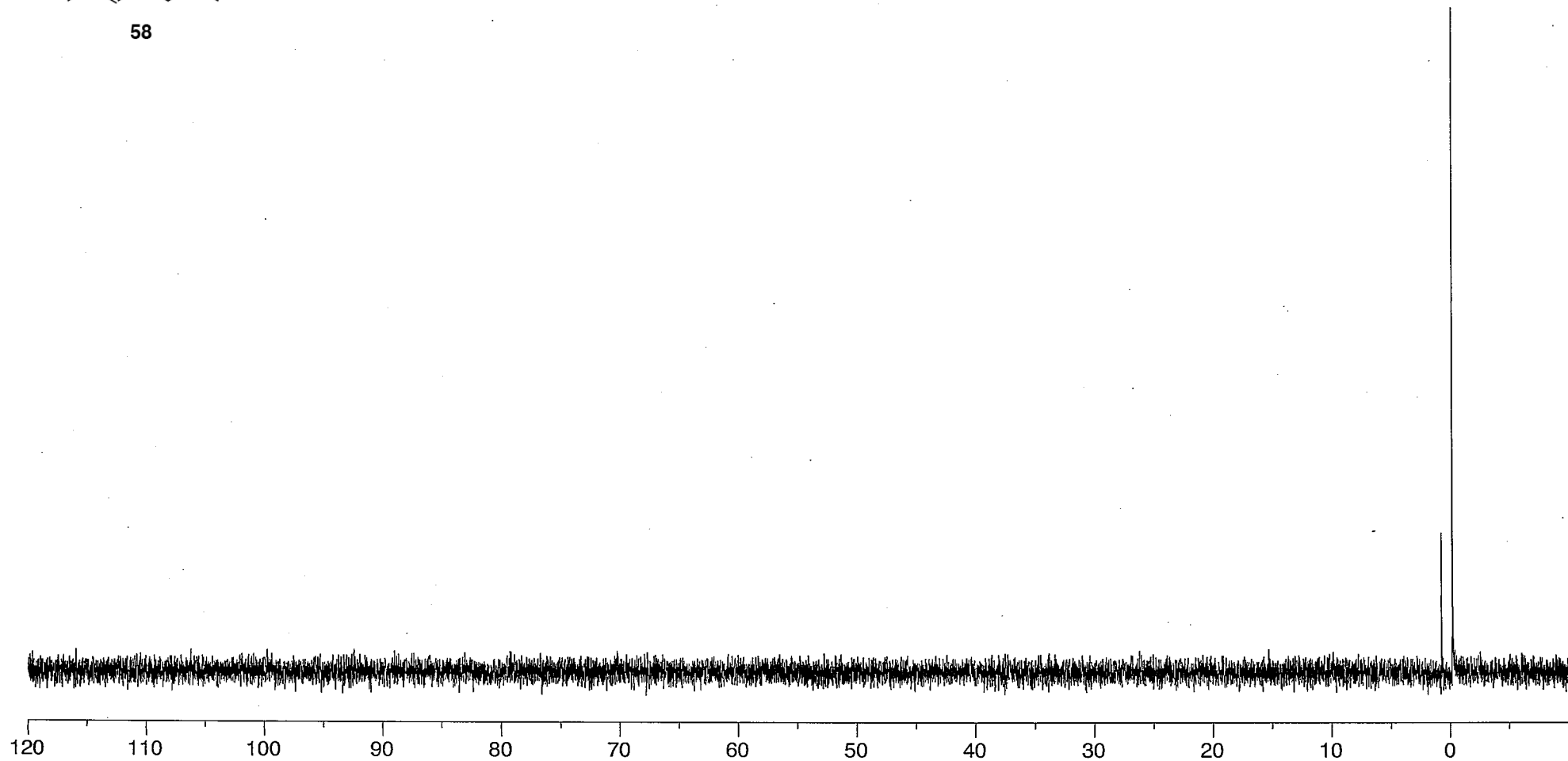


KAD-03-232_02Jan2012

Pulse Sequence: s2pu1
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃

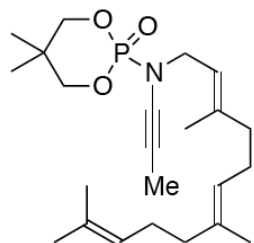


58

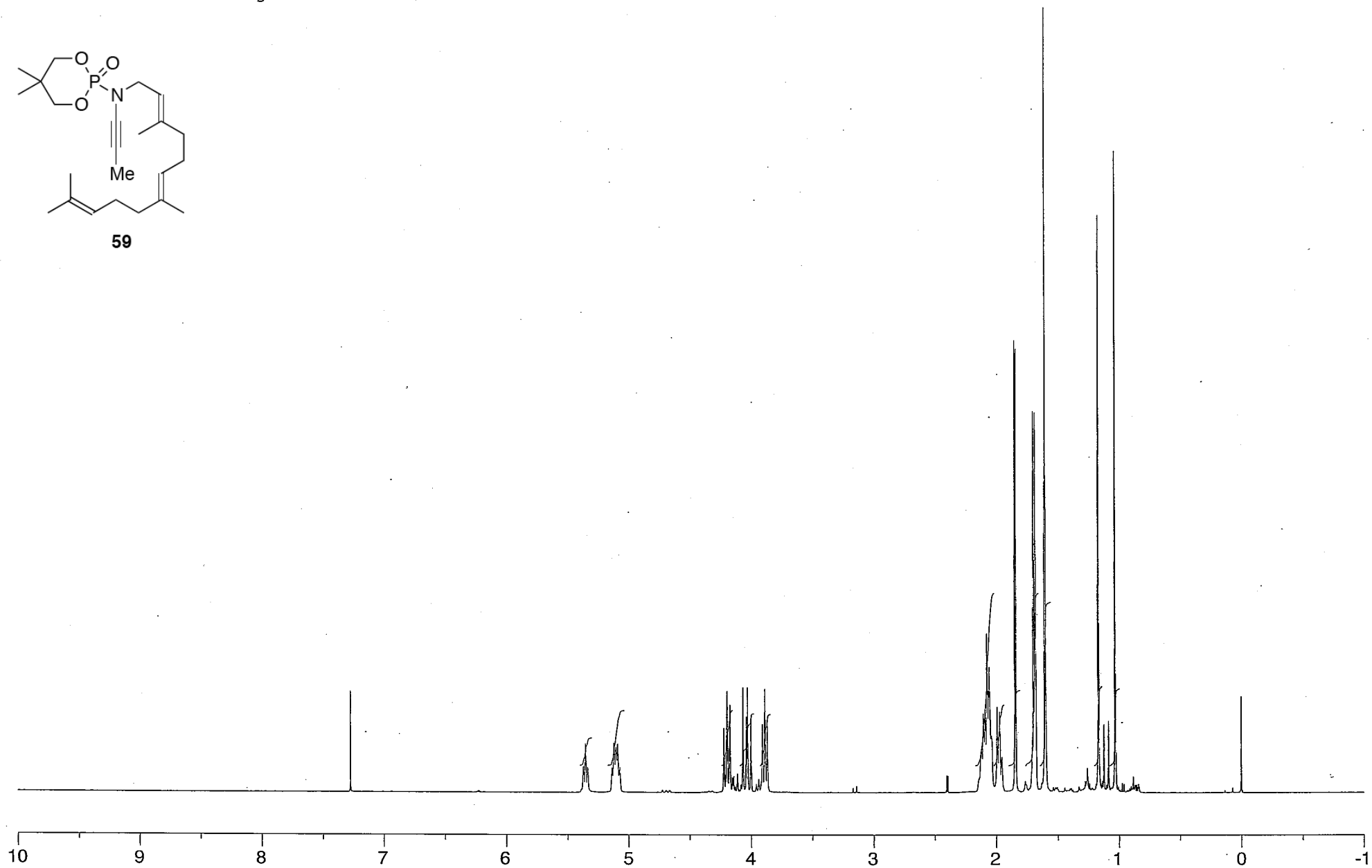


KAD-03-259_30Jan2012

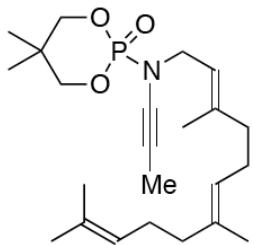
Pulse Sequence: s2pul
Spectrometer Freq.: 399.79 MHz
Solvent: CDCl₃



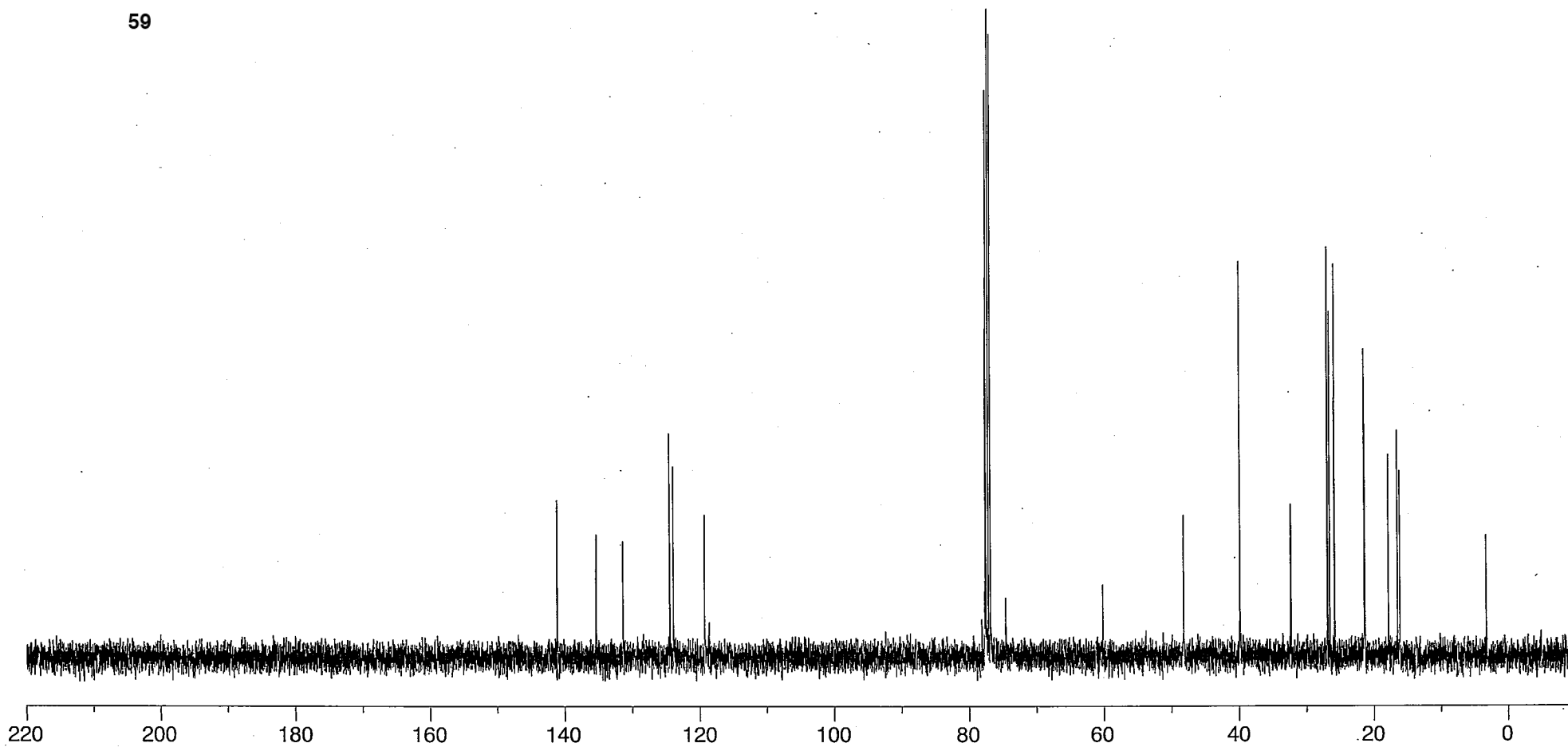
59



Pulse Sequence: s2pul
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

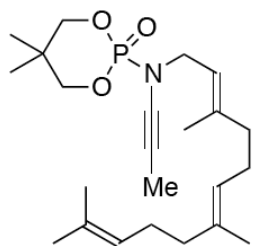


59

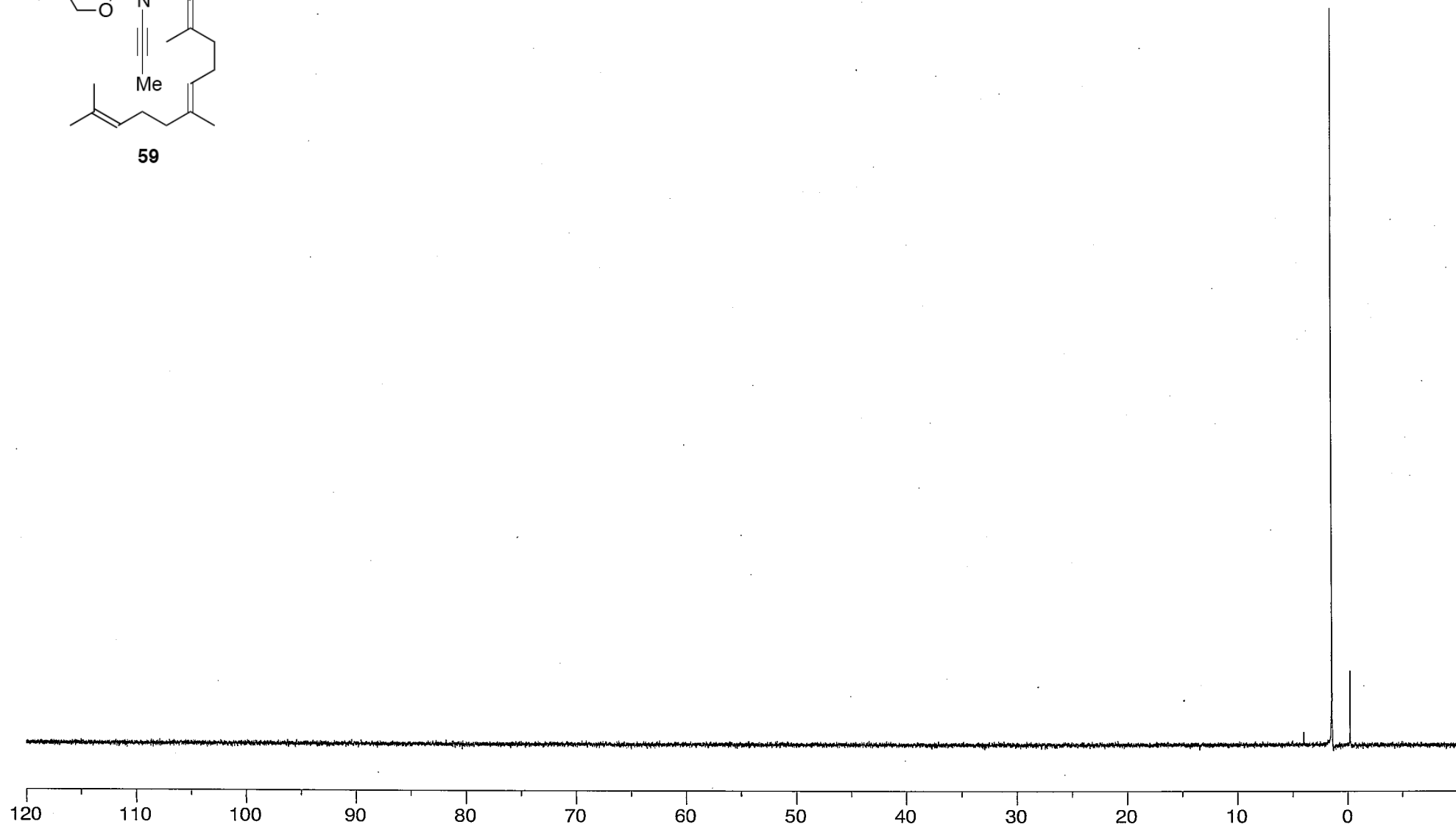


KAD-03-259_30Jan2012

Pulse Sequence: s2pul
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



59

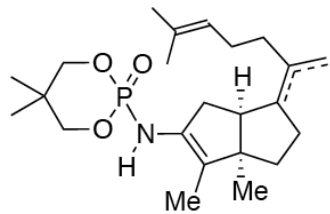


KAD-03-260Elim2_02Feb2012

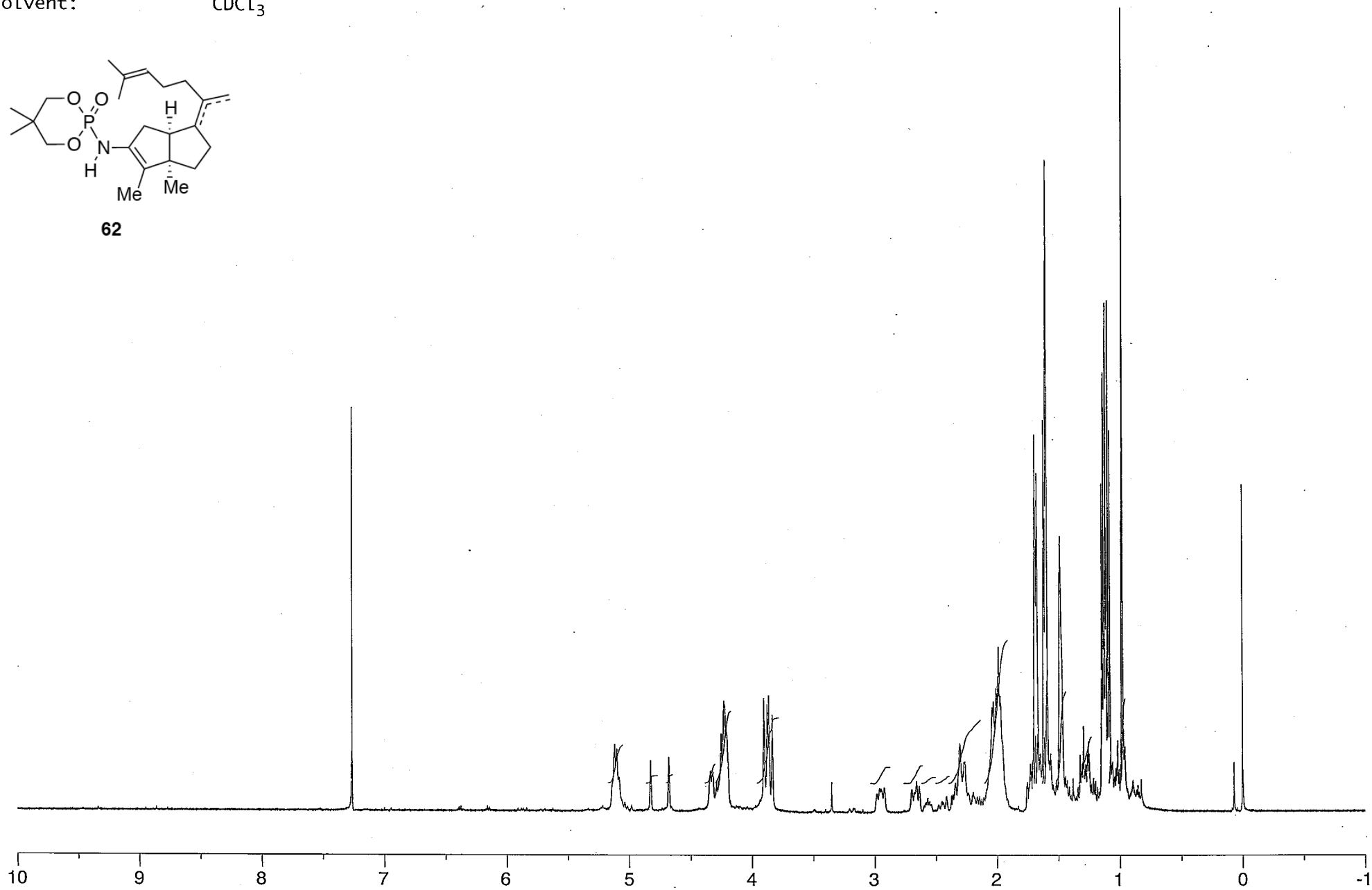
Pulse Sequence: s2pul

Spectrometer Freq.: 399.79 MHz

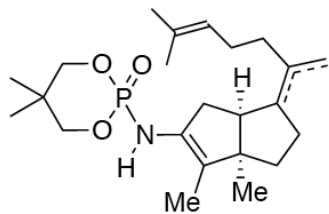
Solvent: CDCl₃



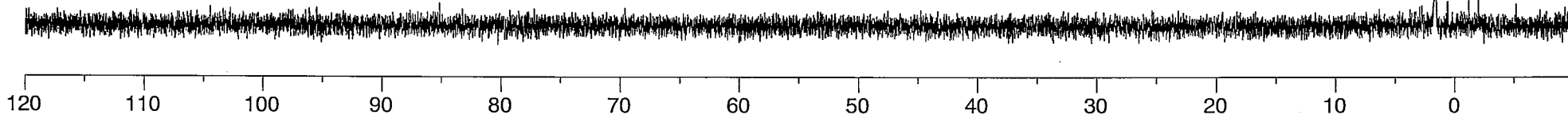
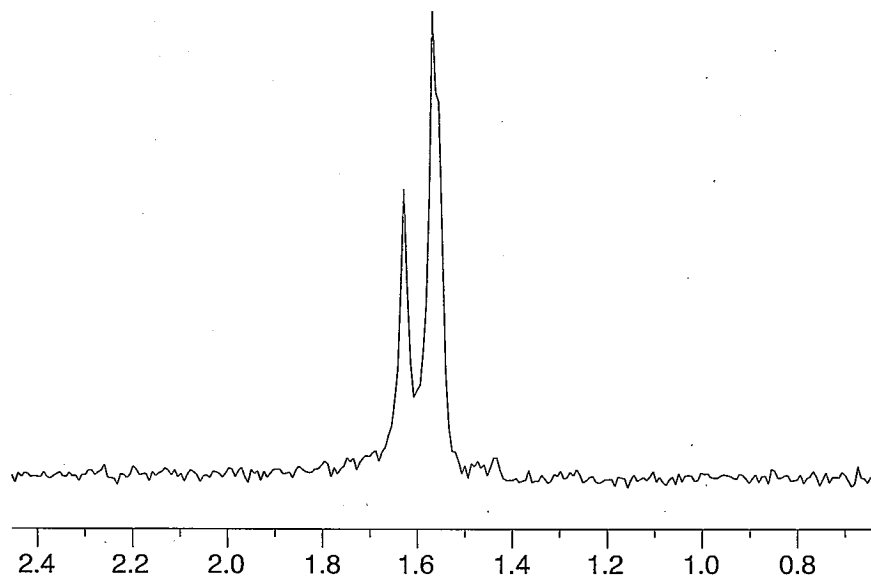
62



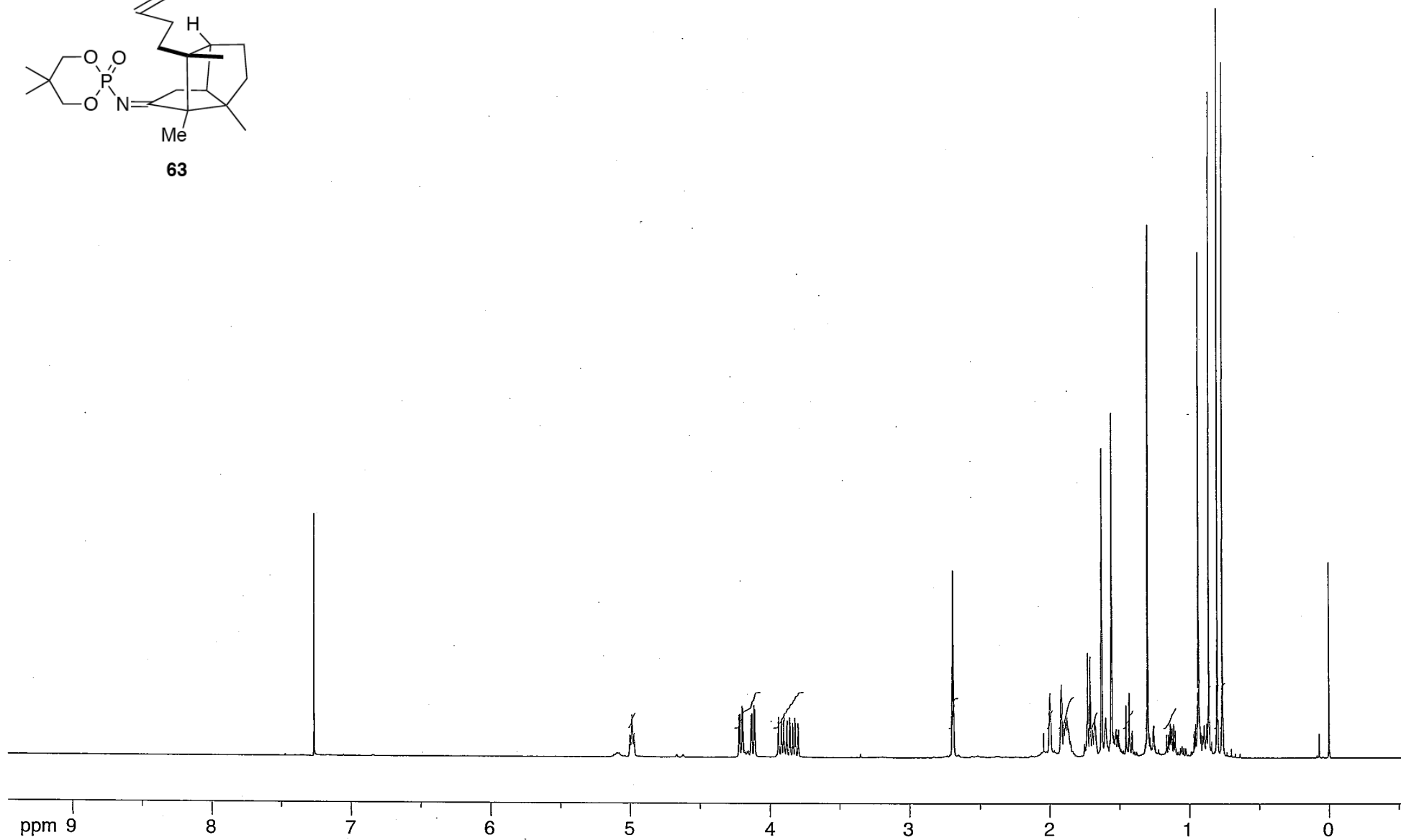
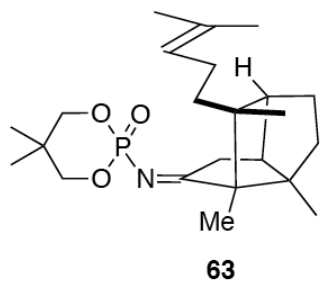
Pulse Sequence: s2pul
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



62

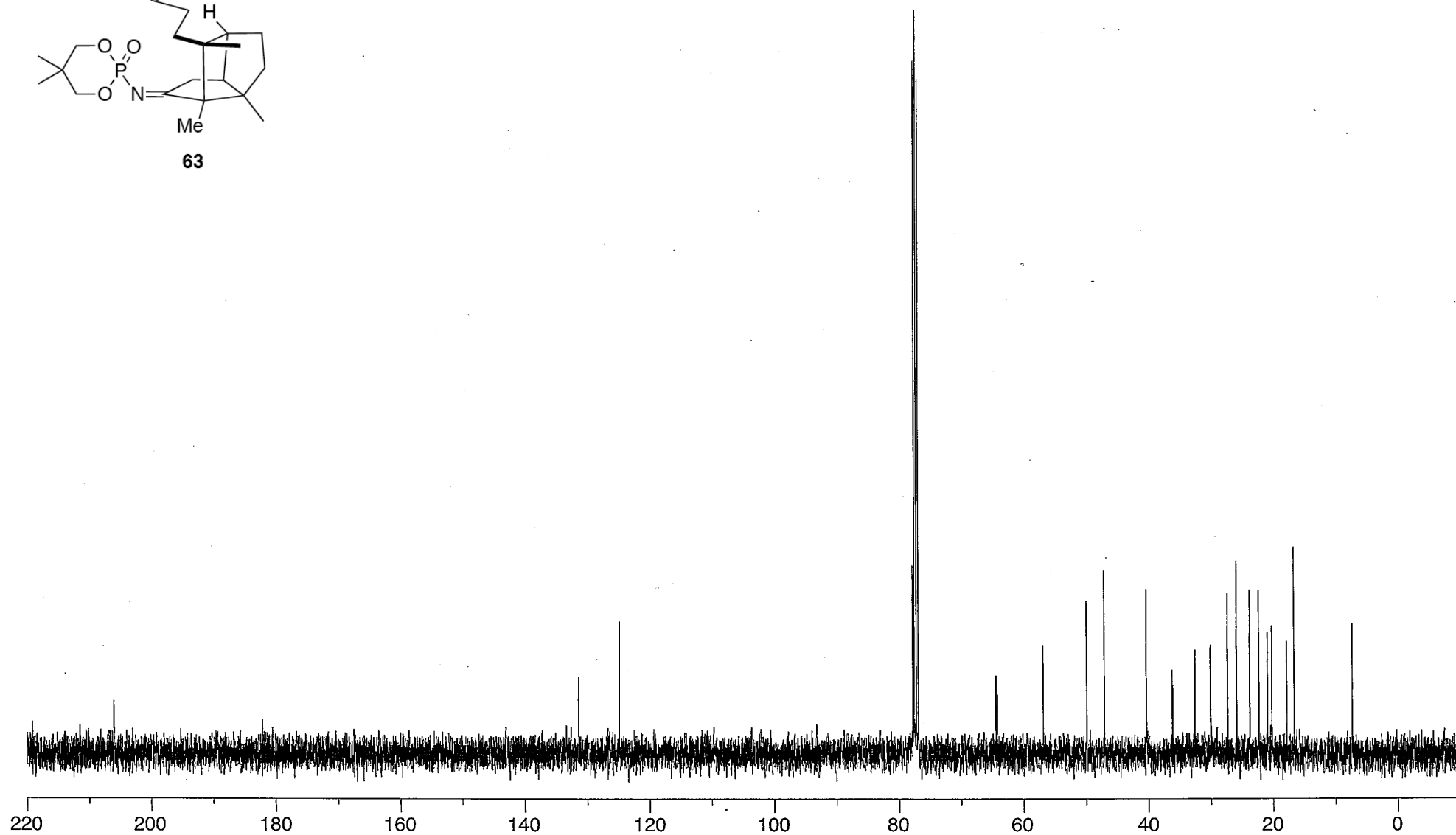
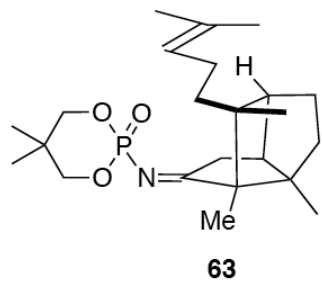


Pulse Sequence: s2pul
Spectrometer Freq.: 499.73 MHz
Solvent: CDCl₃



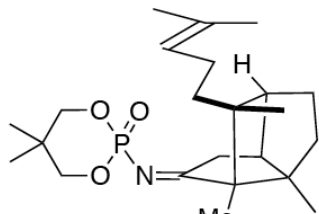
KAD-03-260FR8-9C__01Feb2012

Pulse Sequence: s2pu1
Spectrometer Freq.: 100.54 MHz
Solvent: CDCl₃

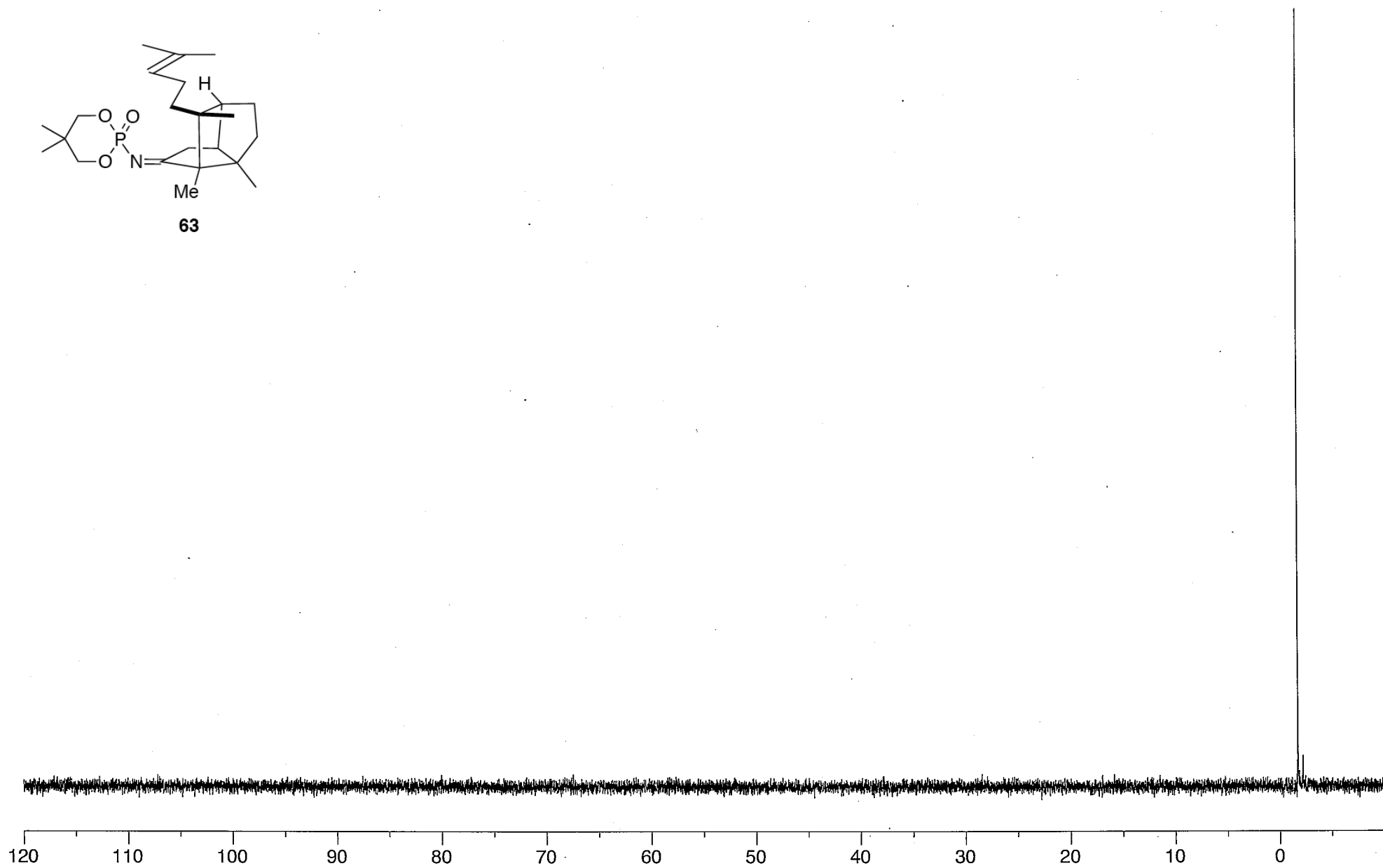


KAD-03-260FR8-9_01Feb2012

Pulse Sequence: s2pul
Spectrometer Freq.: 161.85 MHz
Solvent: CDCl₃



63



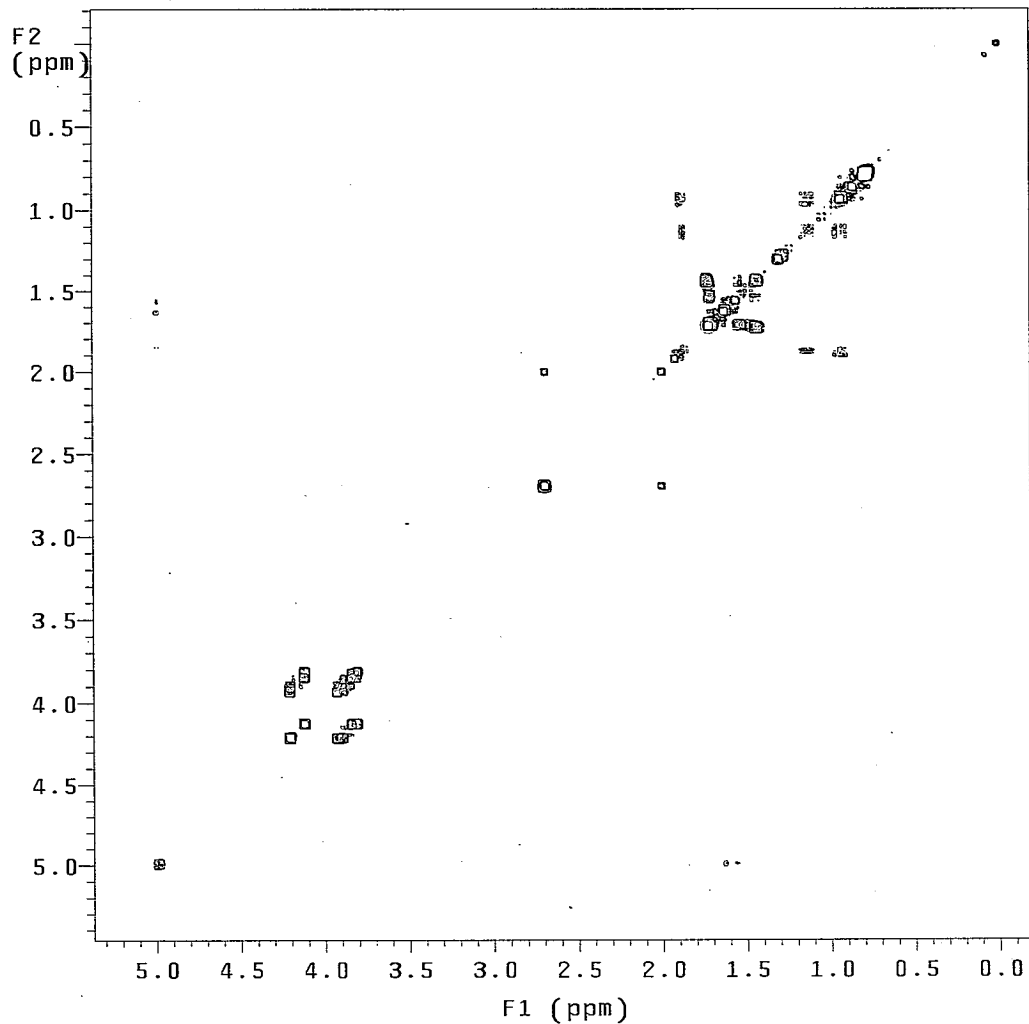
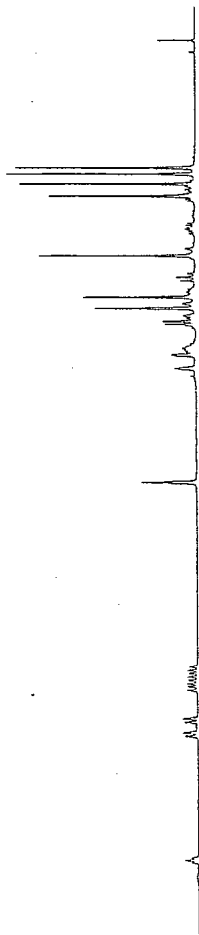
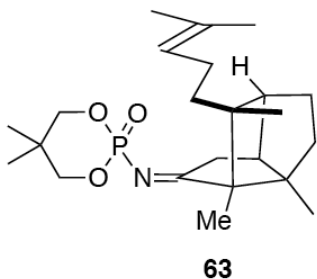
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012

Pulse Sequence: gCOSY

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: gCOSY
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Acq. time 0.204 sec
Width 5008.8 Hz
2D Width 5006.3 Hz
Single scan
128 increments
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Sq. sine bell 0.102 sec
F1 DATA PROCESSING
Sq. sine bell 0.026 sec
FT size 2048 x 2048
Total time 2 min, 56 sec



S113

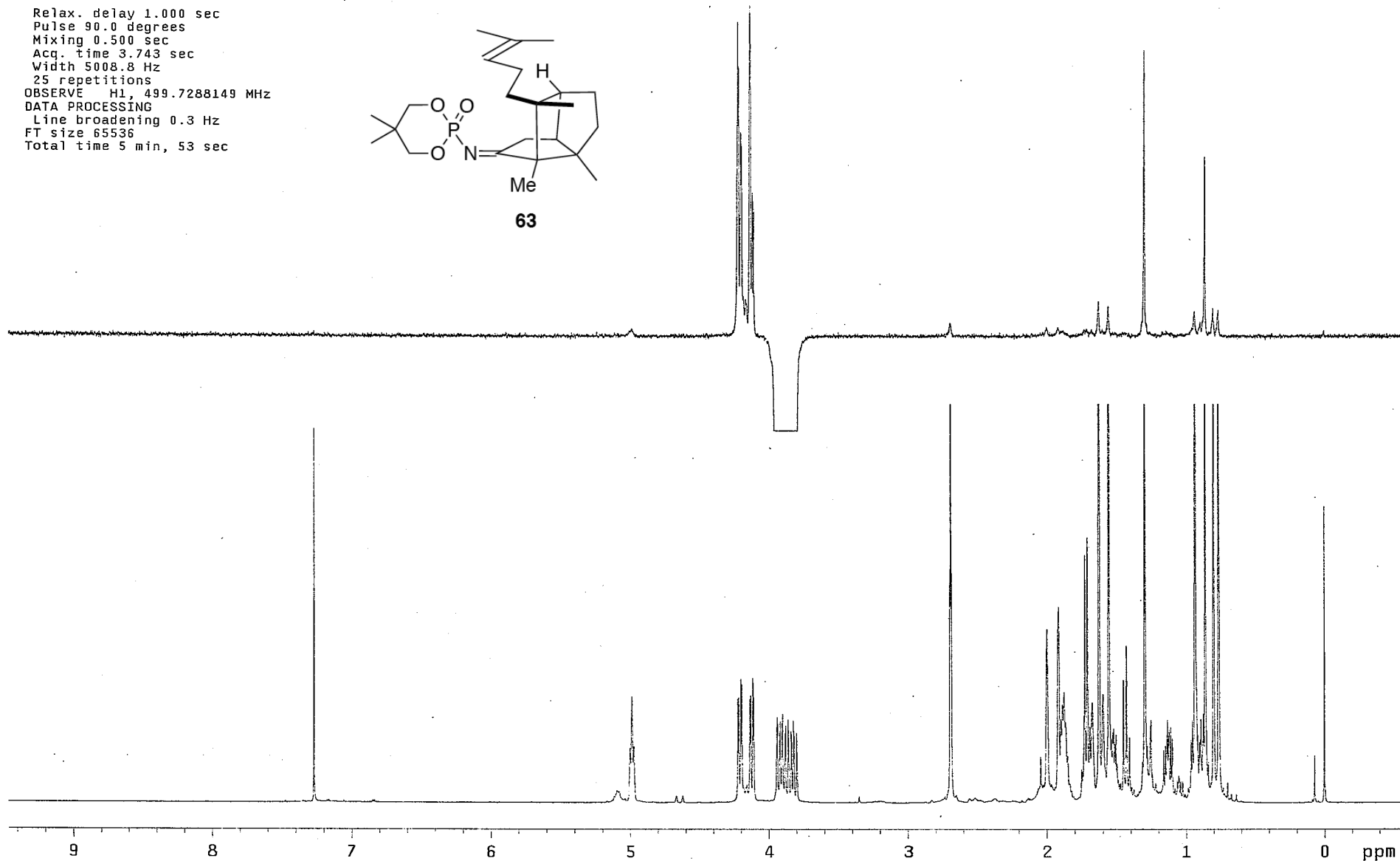
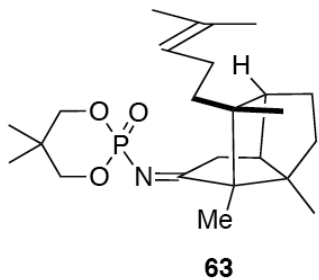
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012
File: NOESY1D_3_87p

Pulse Sequence: NOESY1D

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "ui500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
25 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 5 min, 53 sec



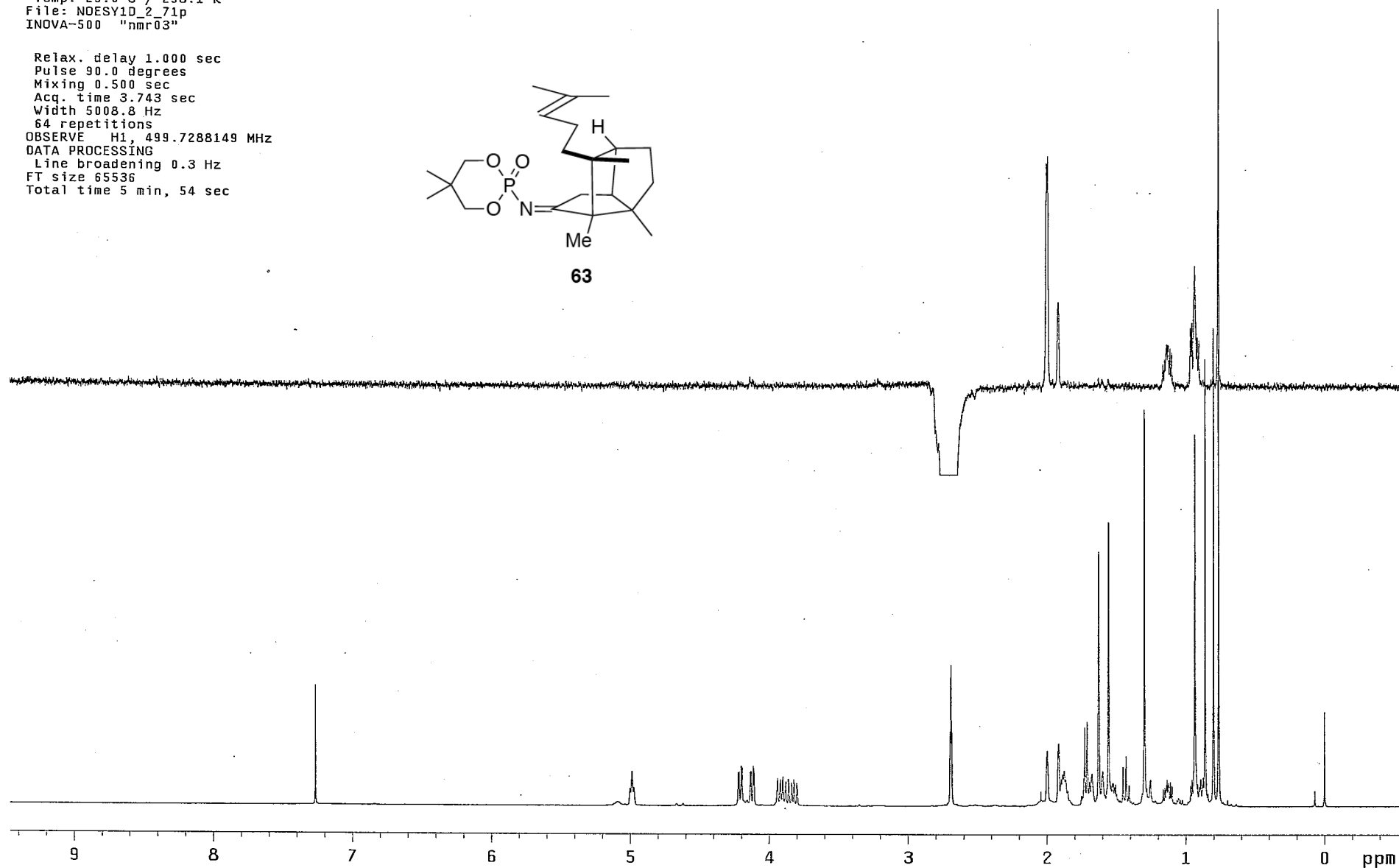
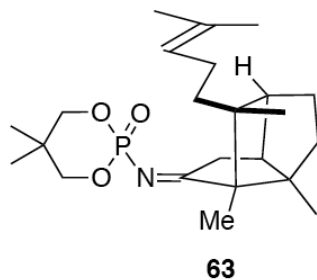
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012

Pulse Sequence: NOESY1D

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: NOESY1D_2_71p
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
64 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 5 min, 54 sec



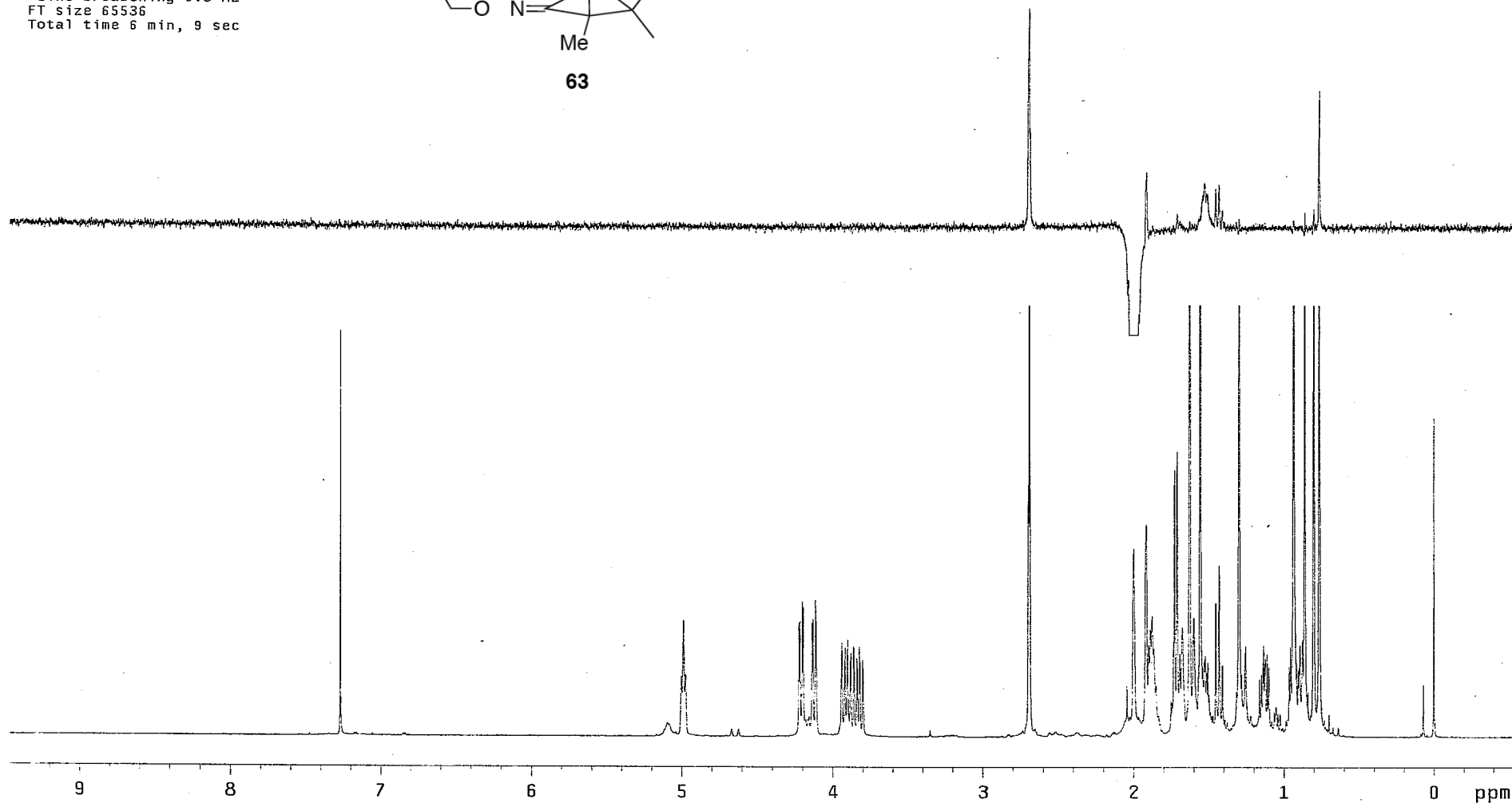
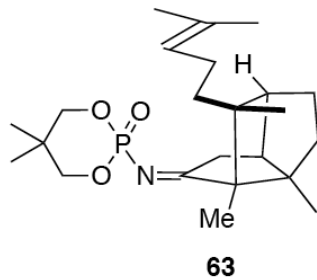
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012
File: NOESY1D_2_00p

Pulse Sequence: NOESY1D

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "ui500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
64 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 6 min, 9 sec



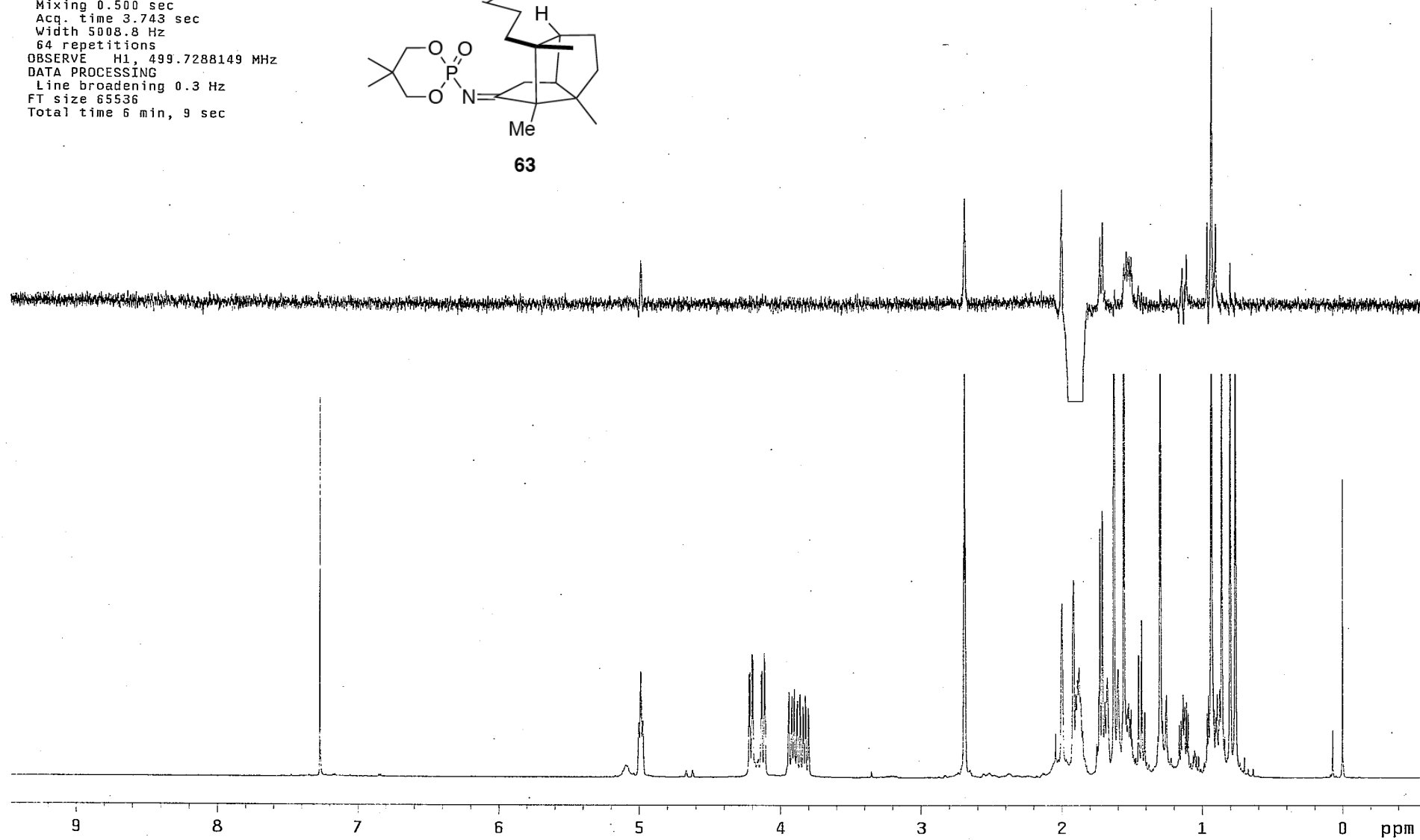
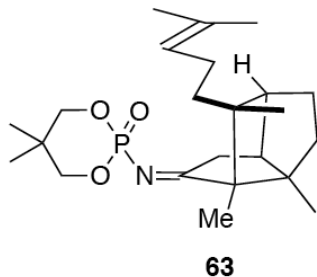
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012
File: NOESY1D_1_92p

Pulse Sequence: NOESY1D

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "ui500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
64 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 6 min, 9 sec



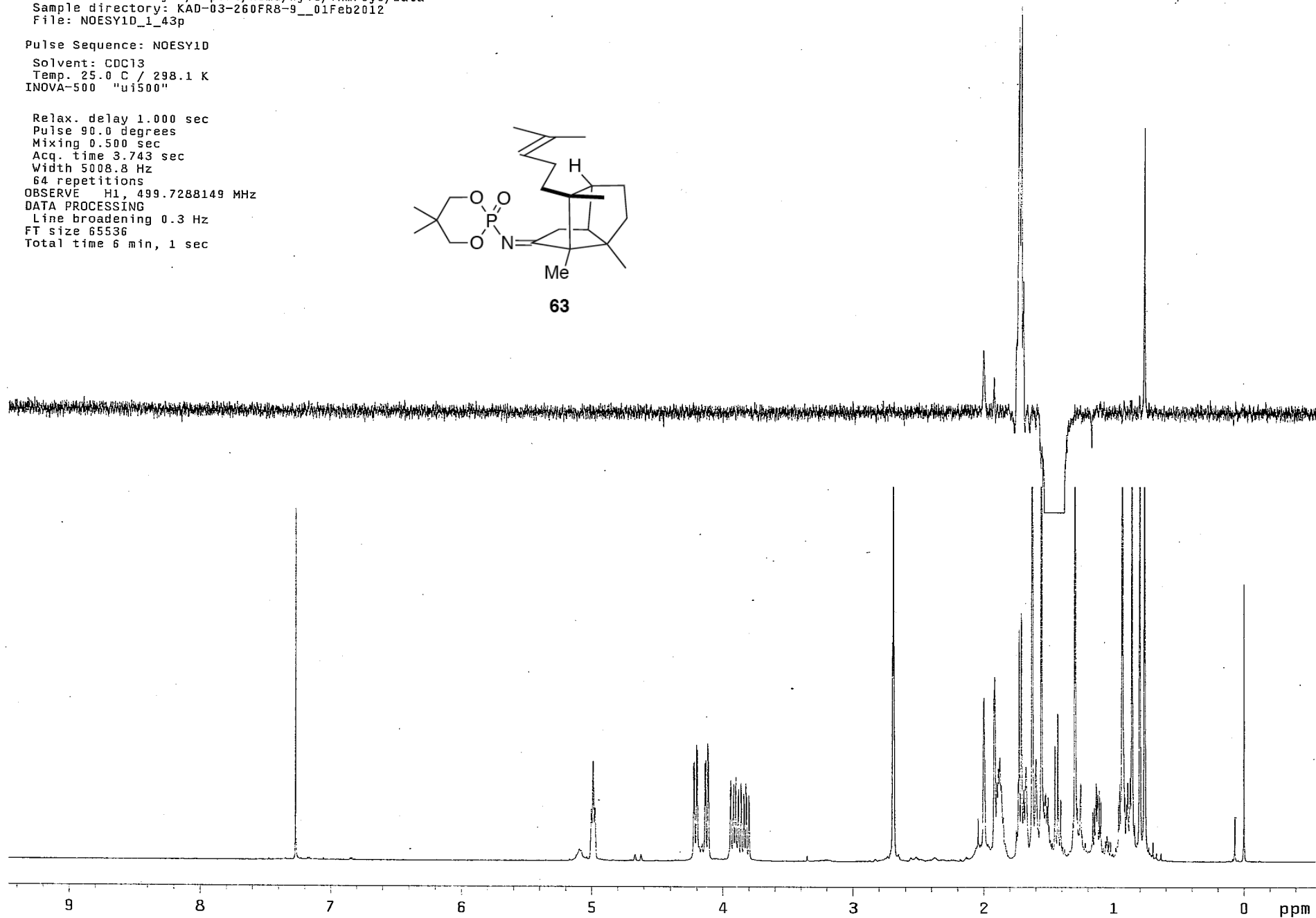
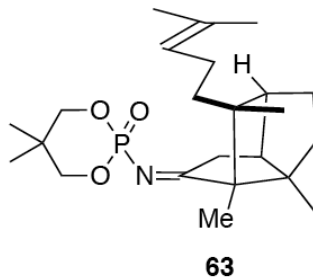
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012
File: NOESY1D_1_43p

Pulse Sequence: NOESY1D

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "ui500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
64 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 6 min, 1 sec



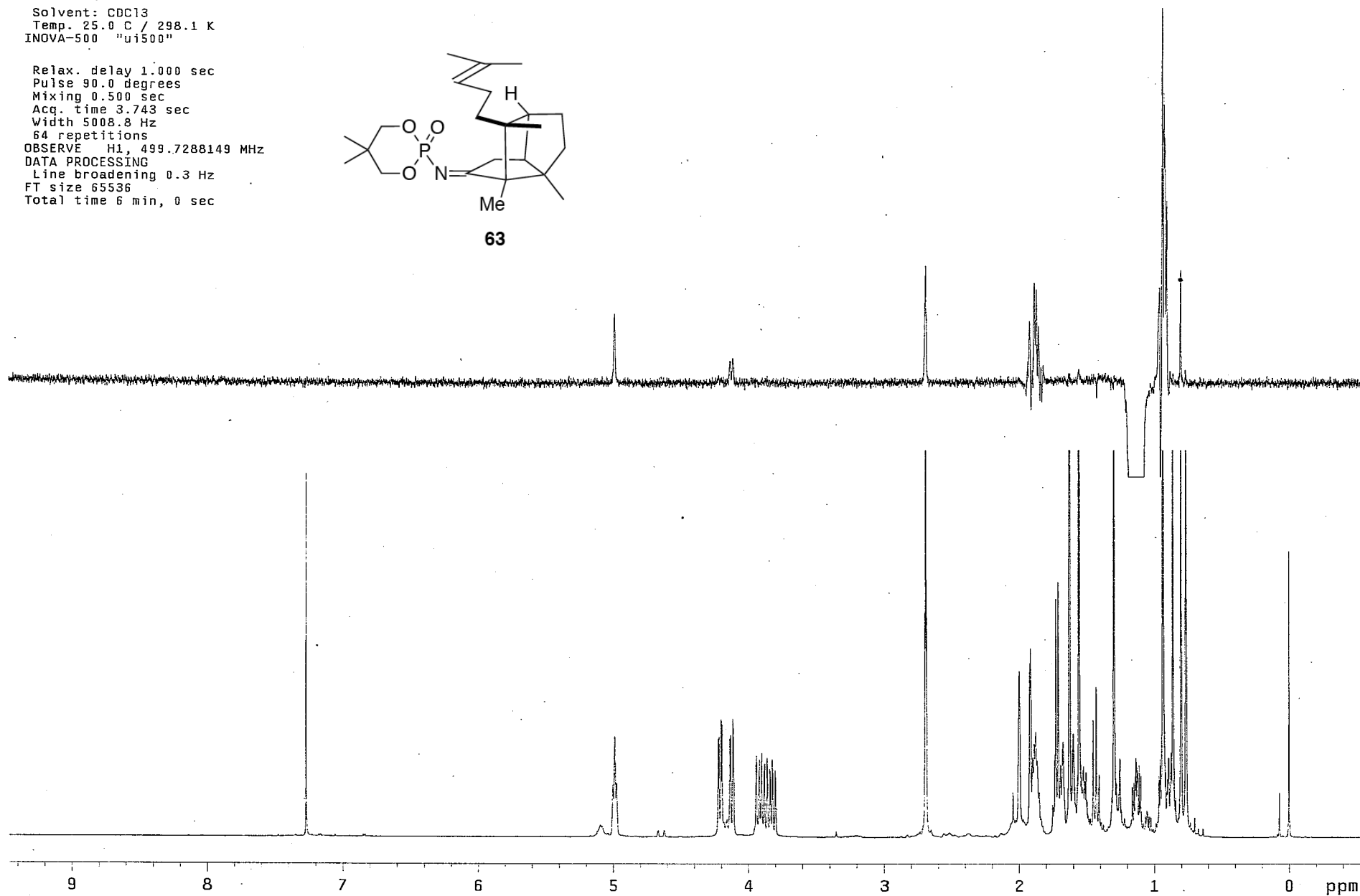
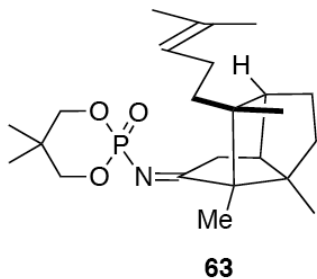
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012
File: NOESY1D_1_14p

Pulse Sequence: NOESY1D

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "ui500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
64 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 6 min, 0 sec



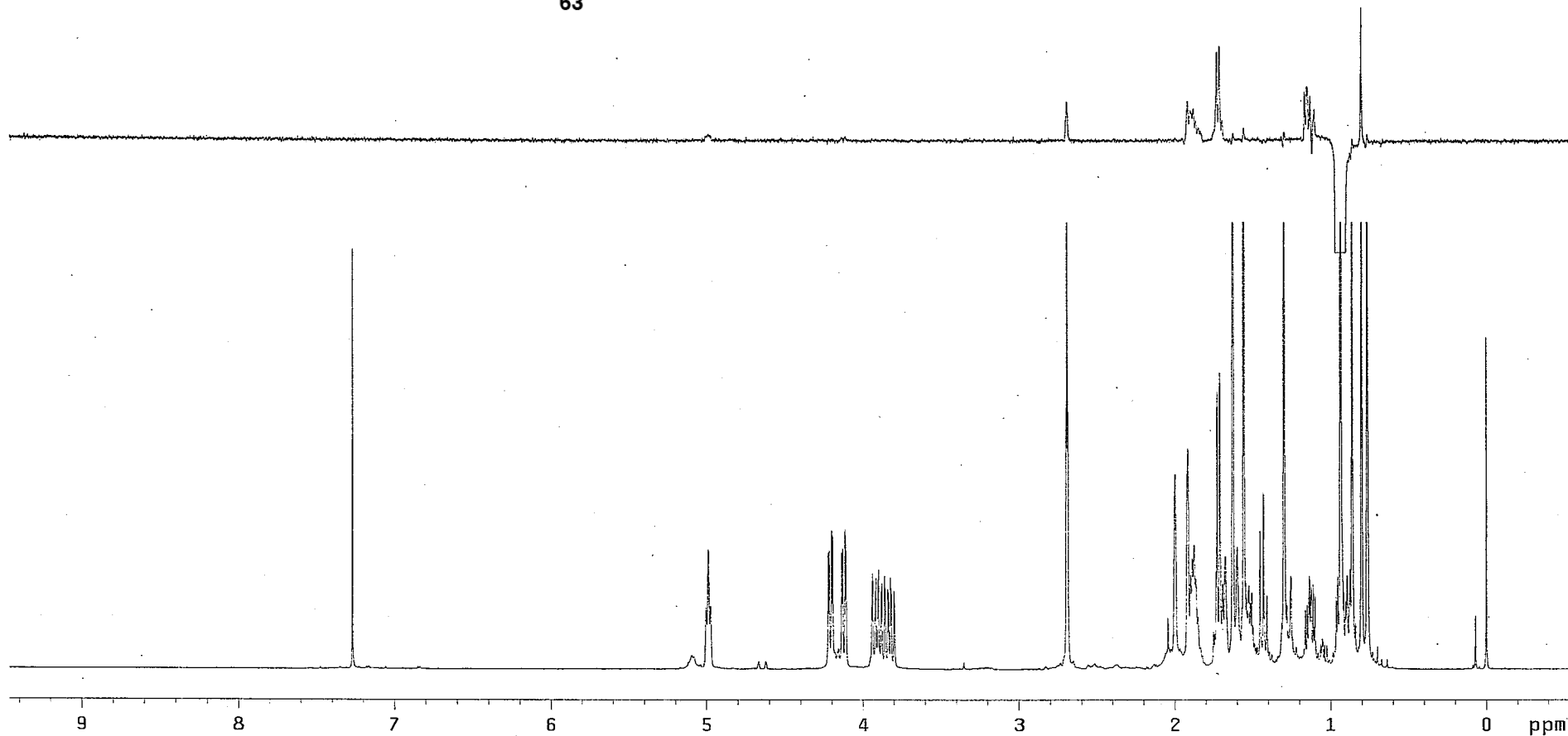
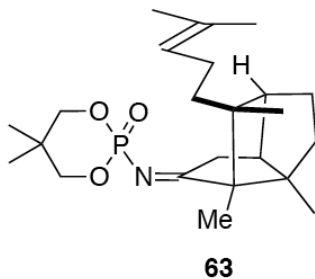
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012
File: NOESY1D_0_94p

Pulse Sequence: NOESY1D

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "ui500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
64 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 6 min, 15 sec



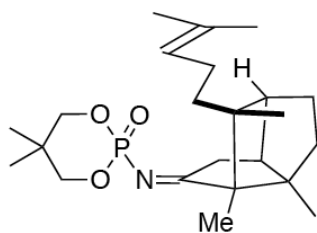
KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012
File: NOESY1D_0_86p

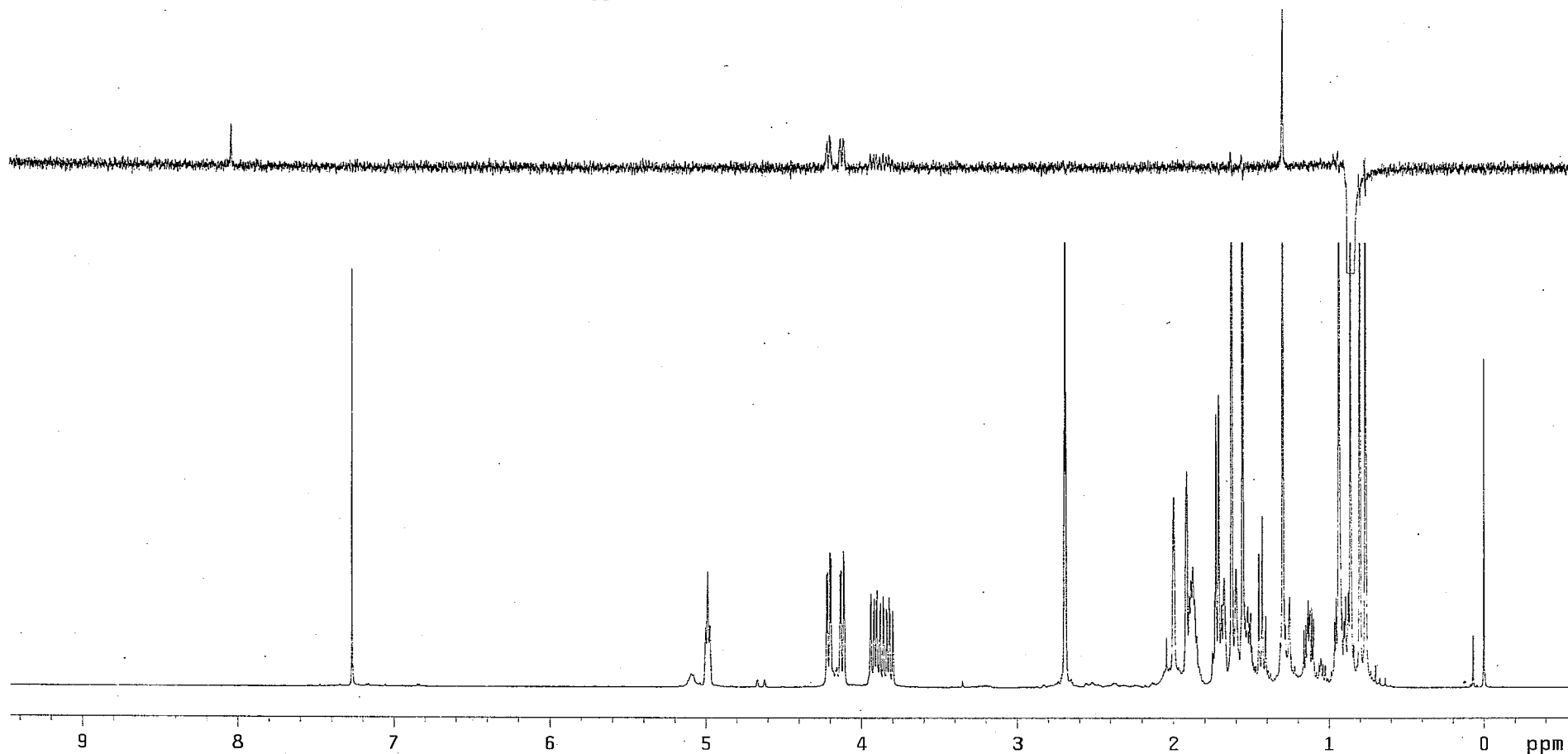
Pulse Sequence: NOESY1D

Solvent: CDC13
Temp. 25.0 C / 298.1 K
INOVA-500 "u1500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
12 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 6 min, 15 sec



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KAD-03-260FR8-9__01Feb2012

Archive directory: /export/home/kyle/vnmrsys/data
Sample directory: KAD-03-260FR8-9__01Feb2012
File: NOESY1D_0_81p

Pulse Sequence: NOESY1D

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "ui500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 3.743 sec
Width 5008.8 Hz
64 repetitions
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 6 min, 15 sec

