

Torquoselective Ring-Opening of Fused Cyclobutenamides: Evidence for a *Cis,Trans*-Cyclooctadienone Intermediate

Xiao-Na Wang,[†] Elizabeth H. Krenske,^{*,‡} Ryne C. Johnston,^{‡,§}
K. N. Houk,^{*,¶} and Richard P. Hsung^{*,†}

[†]Division of Pharmaceutical Sciences and Department of Chemistry, University of Wisconsin, Madison, WI 53705

[‡]School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, QLD 4072, Australia

[¶]Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095

Supporting Information Part 2

Proton NMR and Selected Carbon NMR Spectra

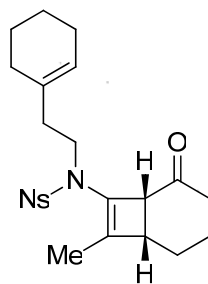
wxn582-2_27Nov2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn582-2_27Nov2013

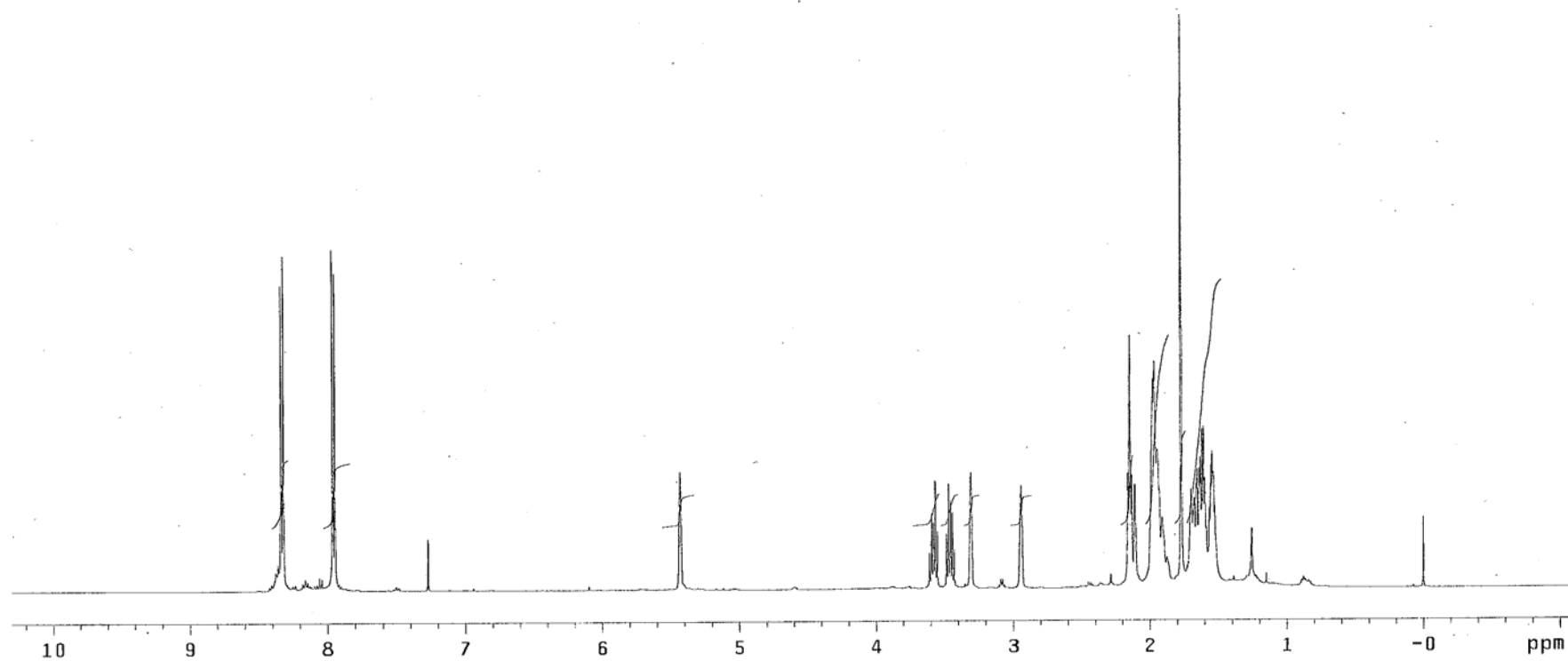
Pulse Sequence: s2pul

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 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288080 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



1f

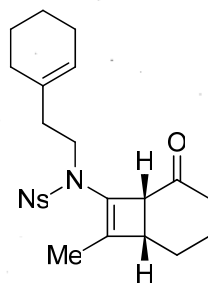


wxn538-3-2_24Sep2013-21:03:35

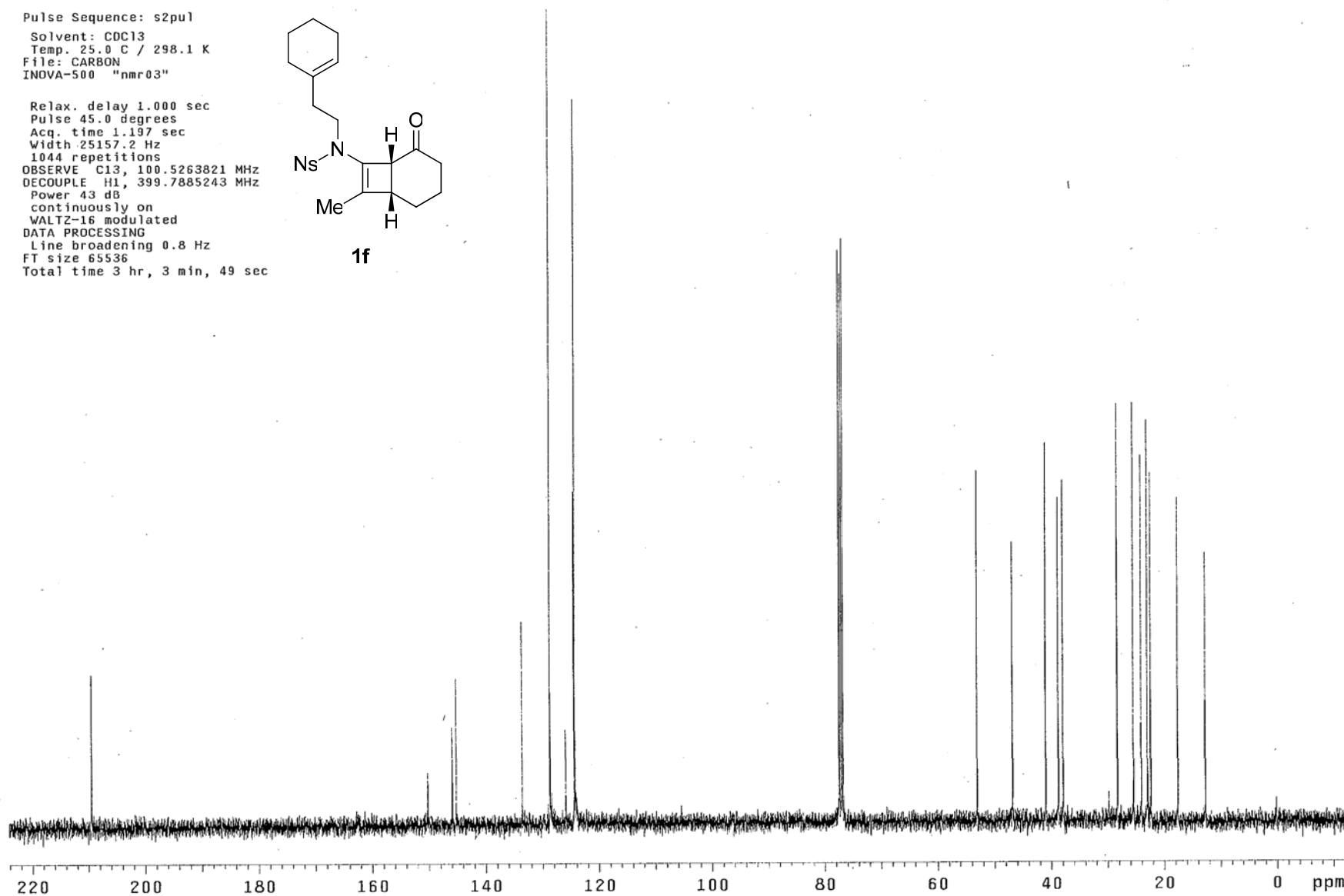
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn538-3-2_24Sep2013-21:03:35

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
1044 repetitions
OBSERVE C13, 100.5263821 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



1f



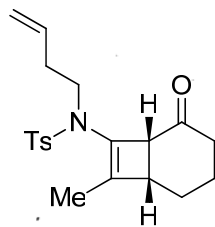
wxn595-1_17Dec2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn595-1_17Dec2013

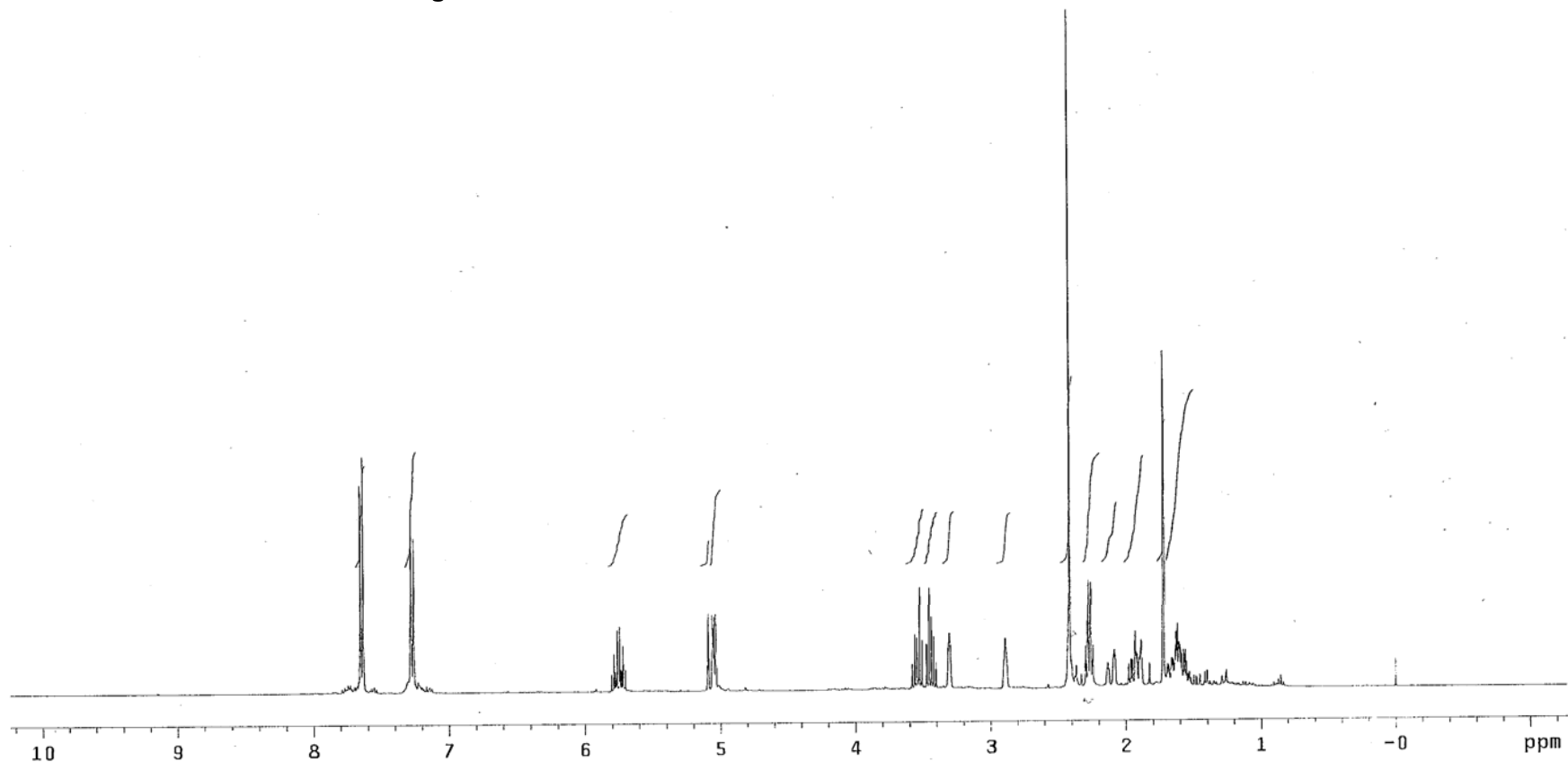
Pulse Sequence: s2pu1

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, 399.7865124 MHz
DATA PROCESSING
F1 size 65536
Total time 0 min, 57 sec



1g



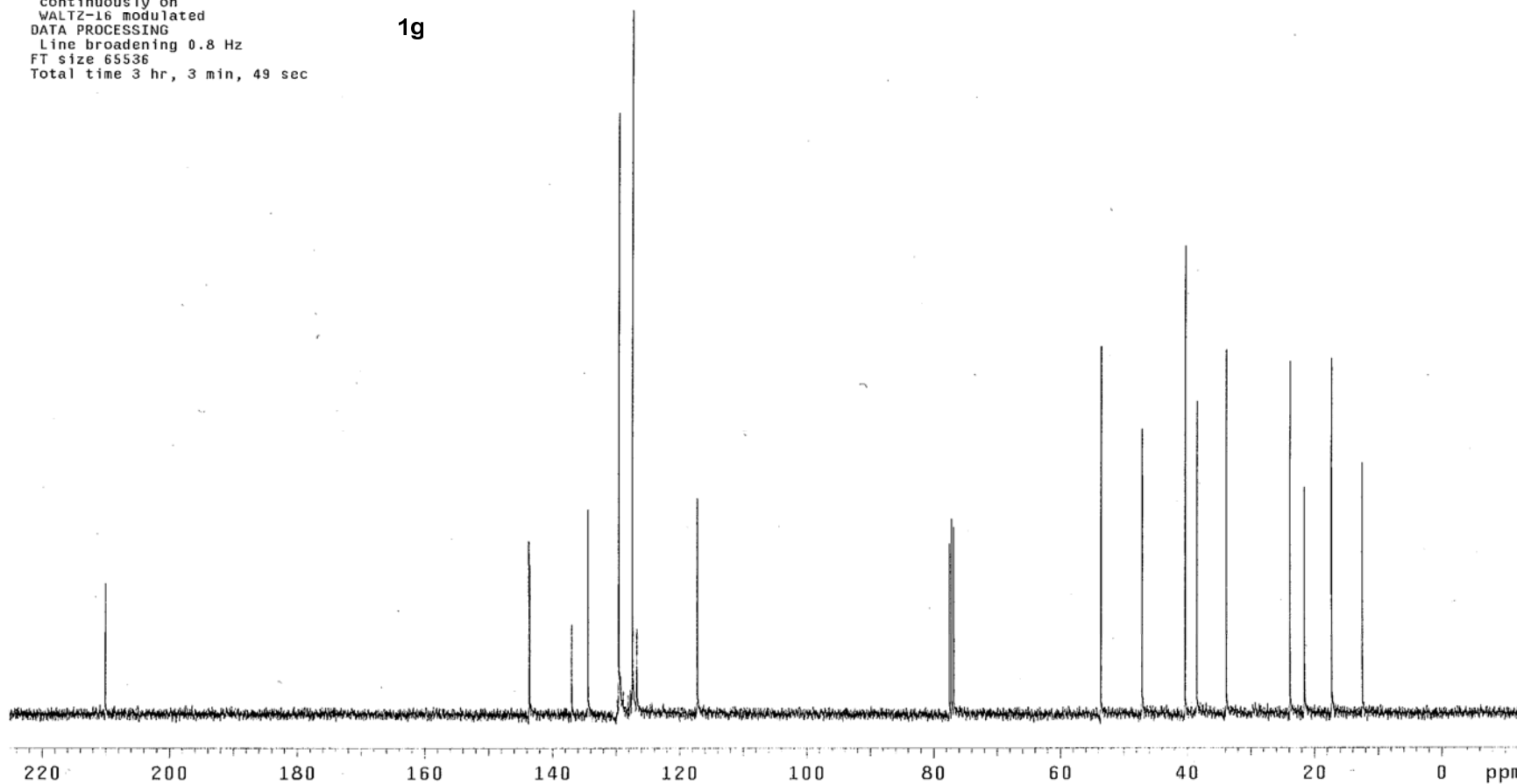
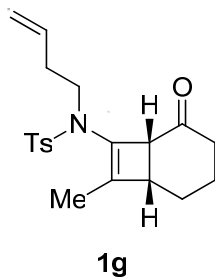
wxn595-1_17Dec2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn595-1_17Dec2013

Pulse Sequence: s2pul

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
212 repetitions
OBSERVE C13, 100.5263913 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec

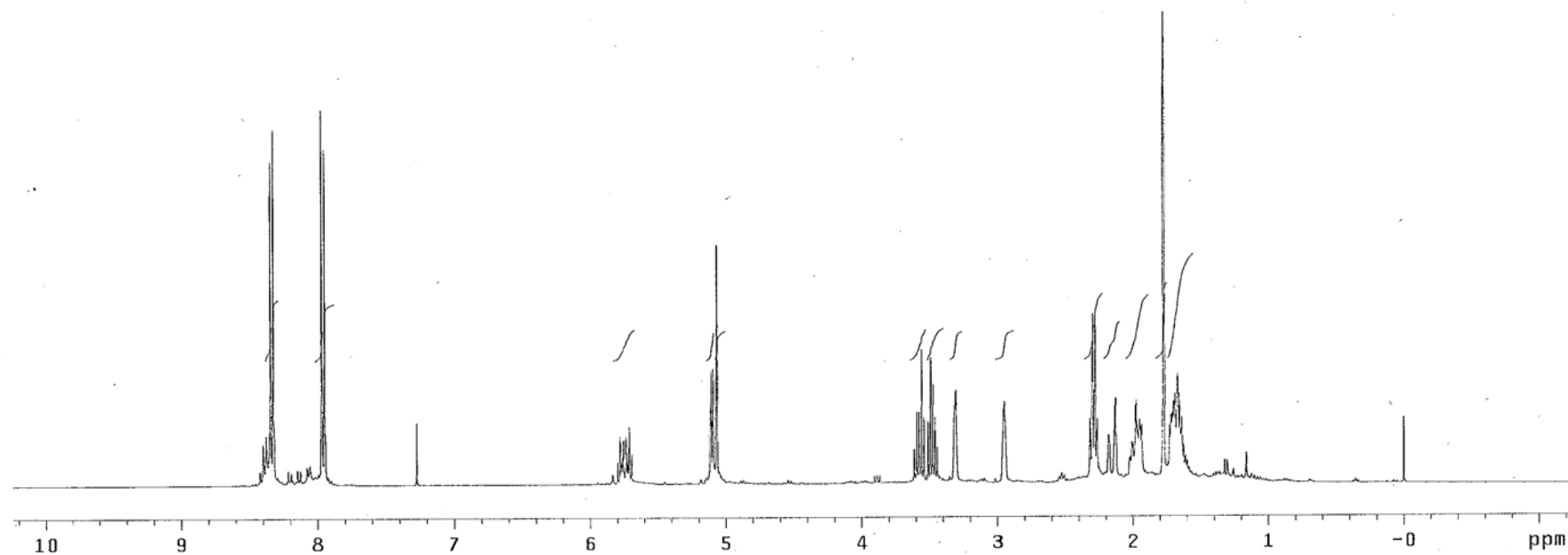
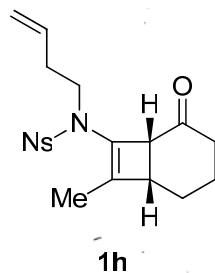


wxn590-1_13Dec2013-14:49:02

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn590-1_13Dec2013-14:49:02

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, 399.7865179 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



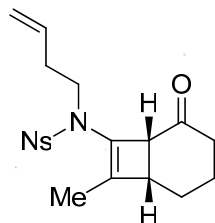
wxn590-1_13Dec2013-13:14:14

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn590-1_13Dec2013-13:14:14

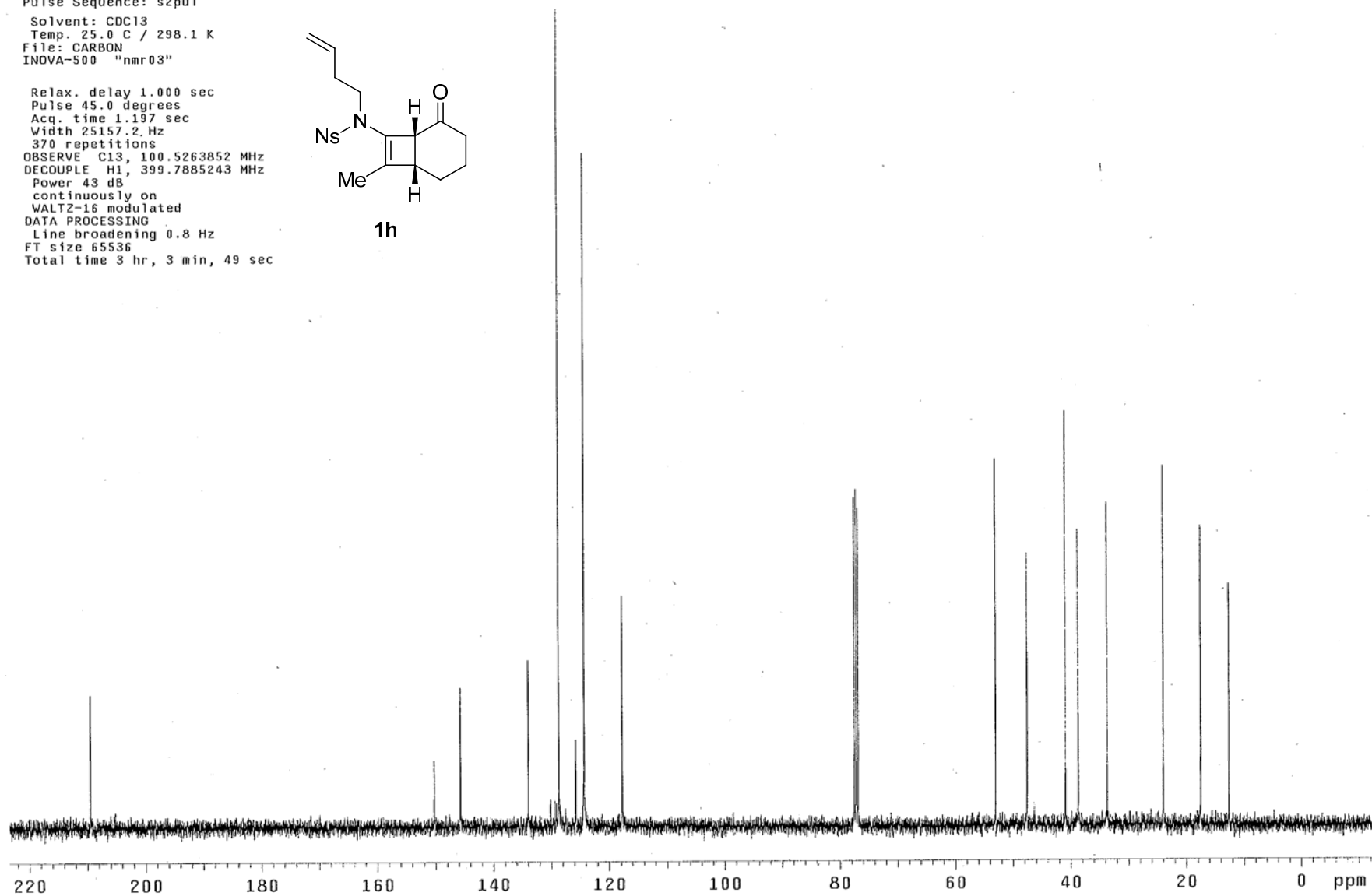
Pulse Sequence: s2pul

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
370 repetitions
OBSERVE C13, 100.5263852 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



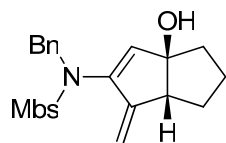
1h



wxn429-2_11Mar2013

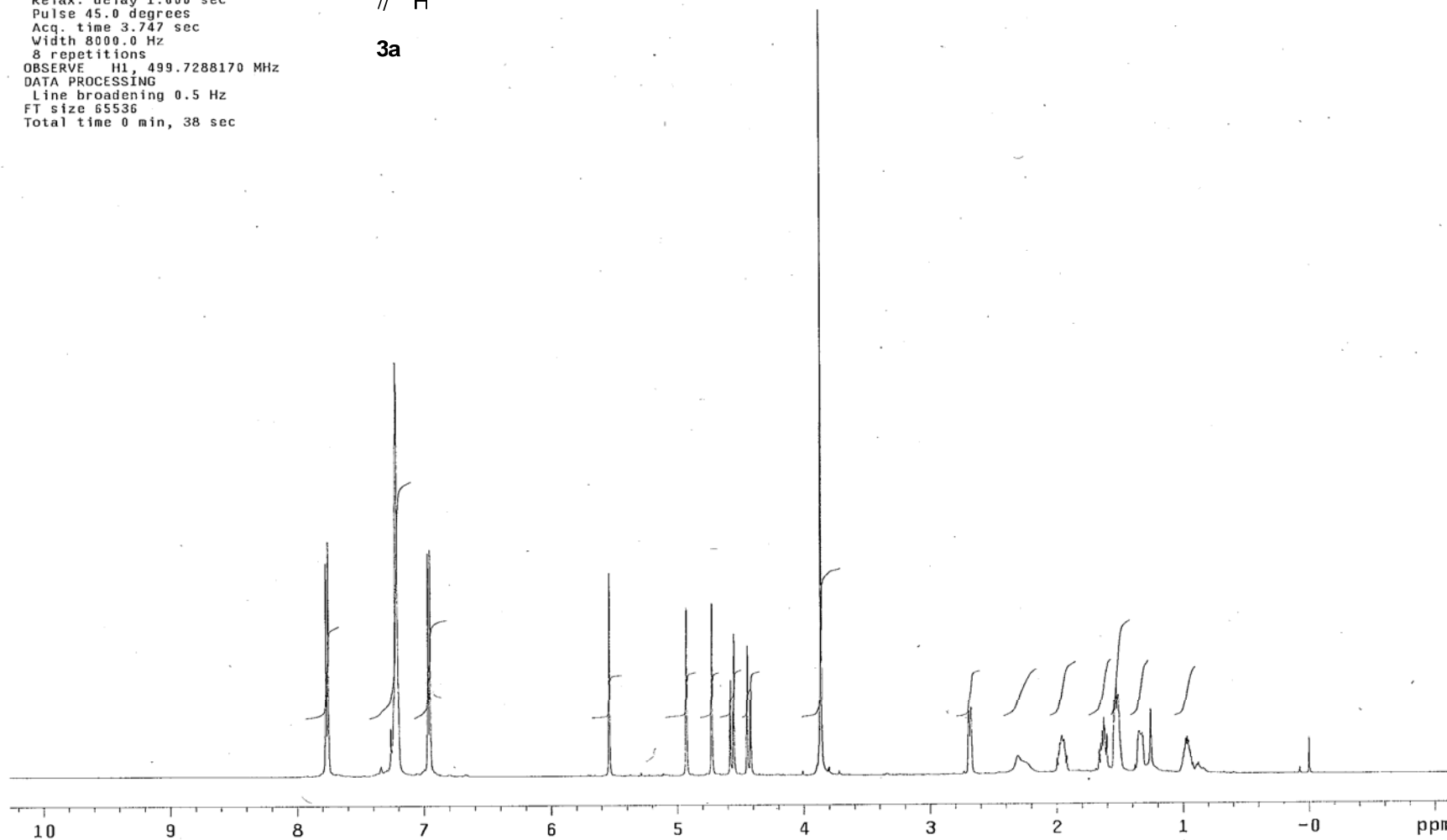
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn429-2_11Mar2013

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"



3a

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288170 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



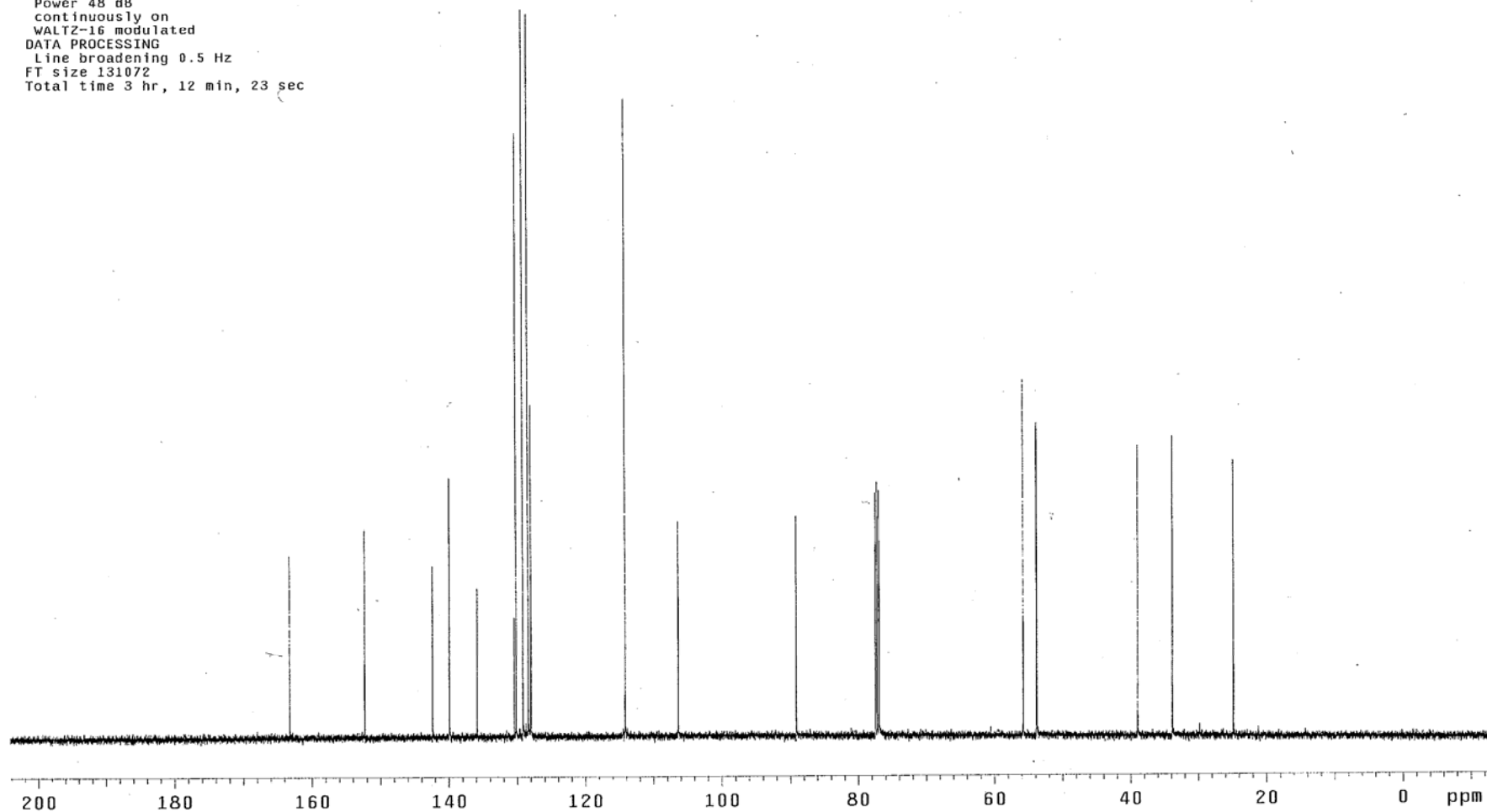
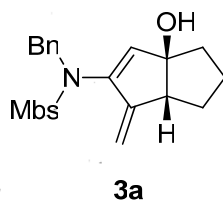
wxn429-2_09Mar2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn429-2_09Mar2013

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.299 sec
Width 31446.5 Hz
267 repetitions
OBSERVE C13, 125.6568915 MHz
DECOUPLE H1, 499.7312897 MHz
Power 48 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 3 hr, 12 min, 23 sec



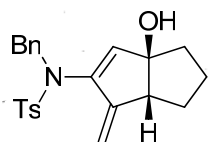
wxn519-1_07Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn519-1_07Sep2013

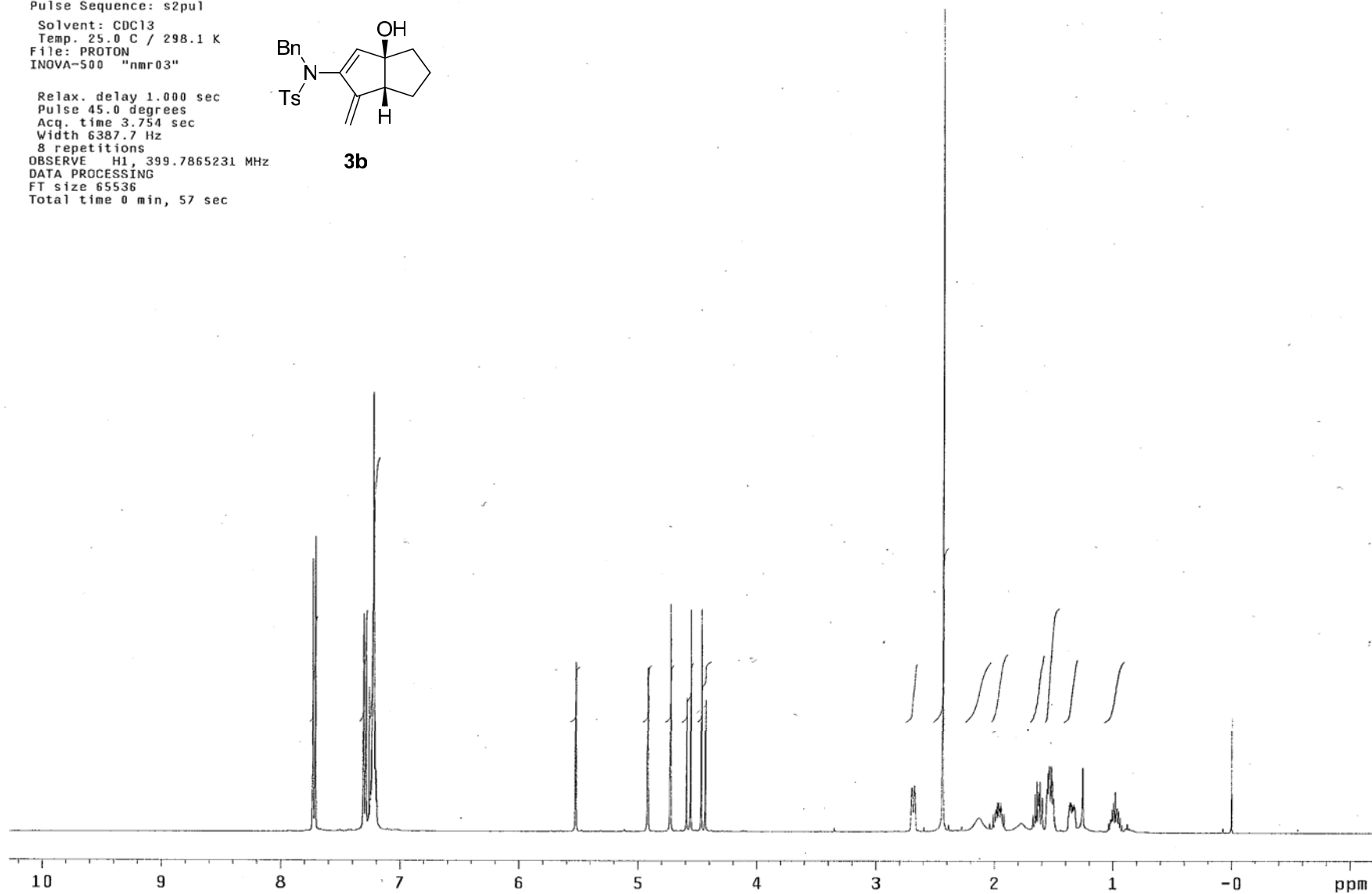
Pulse Sequence: s2pul

Solvent: CDC13
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, 399.7865231 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



3b



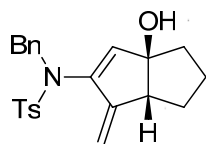
wxn519-1_07Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn519-1_07Sep2013

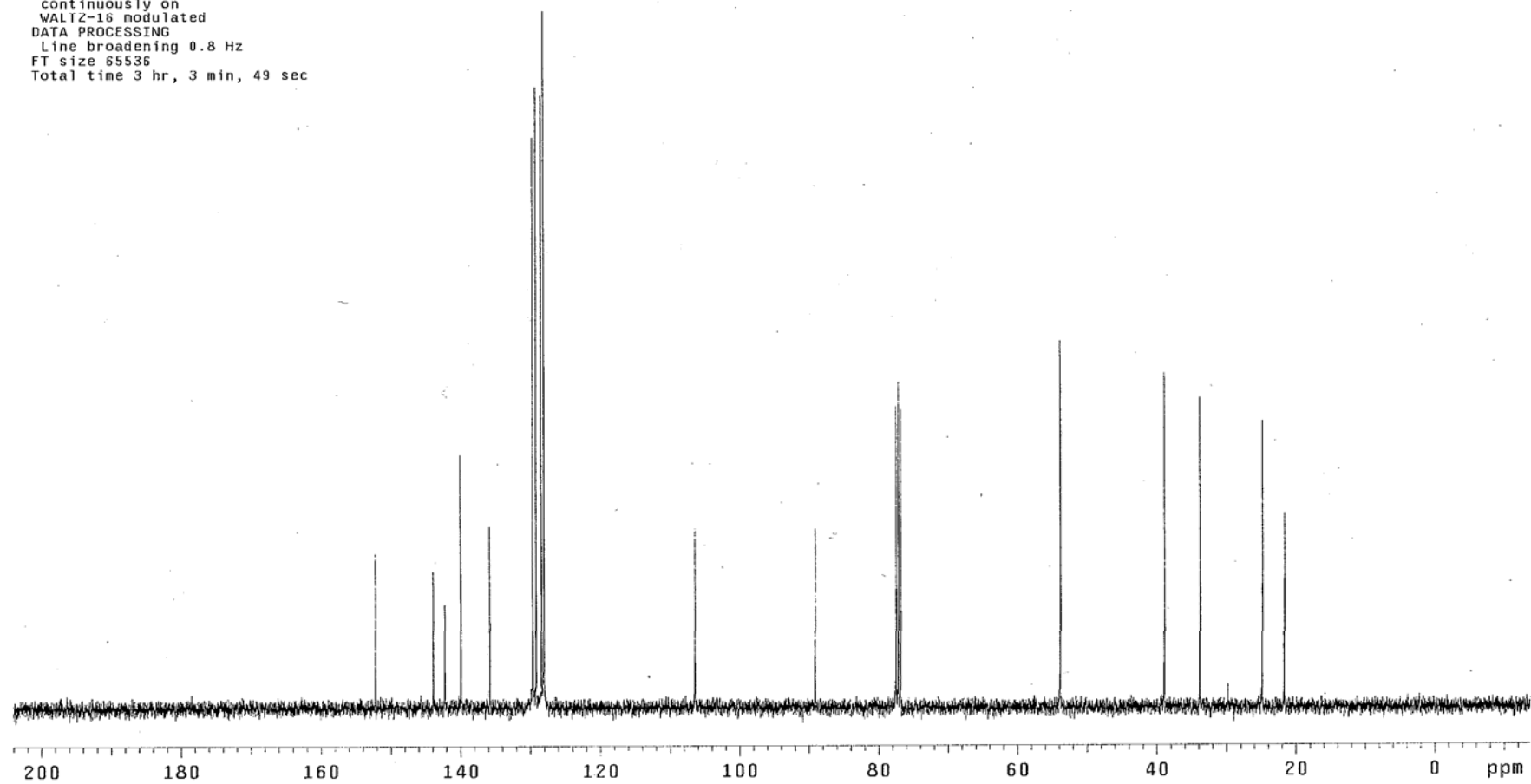
Pulse Sequence: s2pul

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

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
342 repetitions
OBSERVE C13, 100.5263844 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



3b



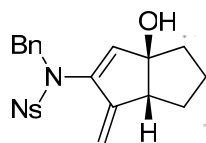
wxn476-1_05Jun2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn476-1_05Jun2013

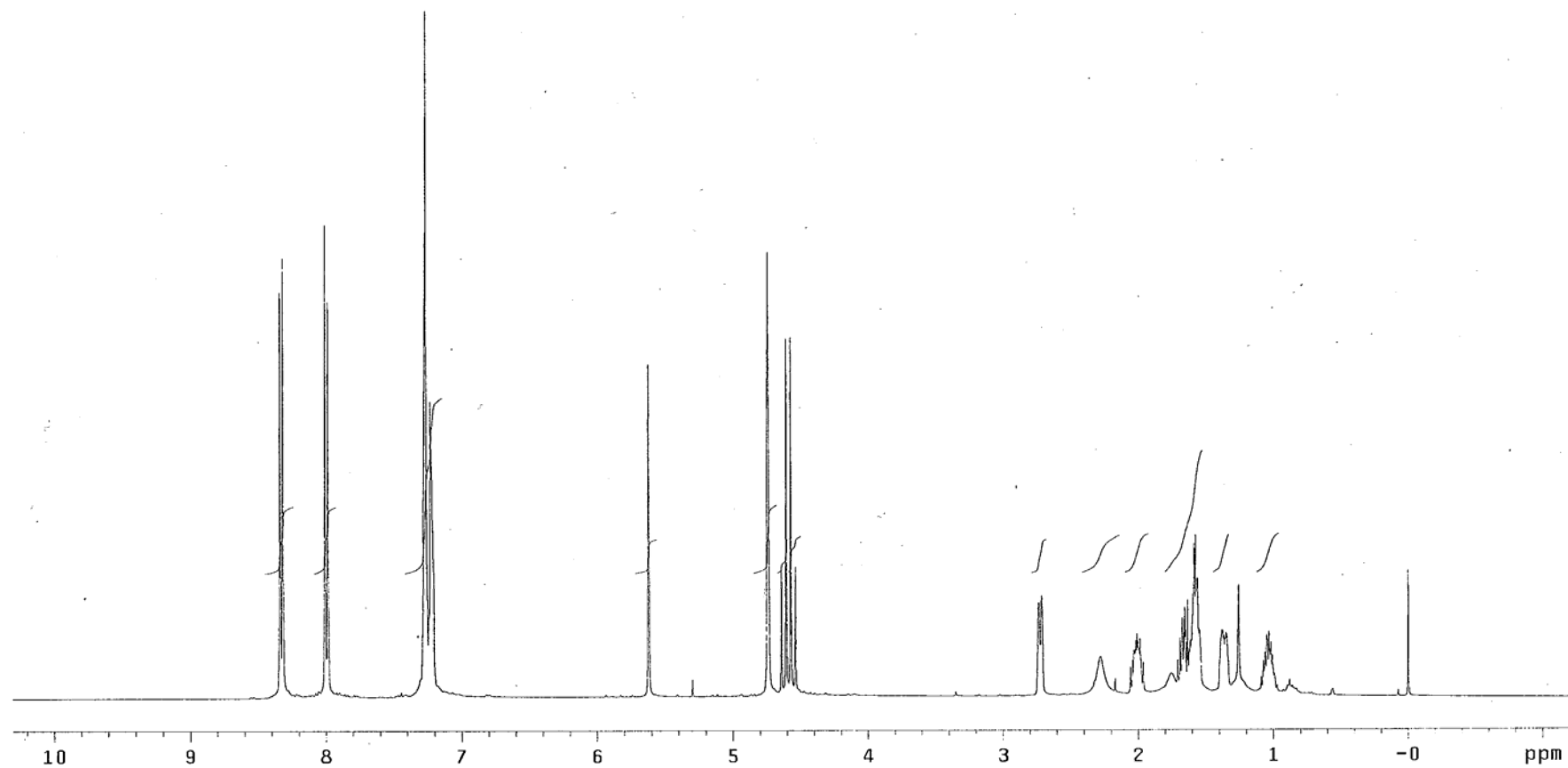
Pulse Sequence: s2pul

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, 399.7865218 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



3c



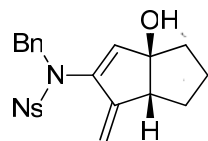
wxn476-1_05Jun2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn476-1_05Jun2013

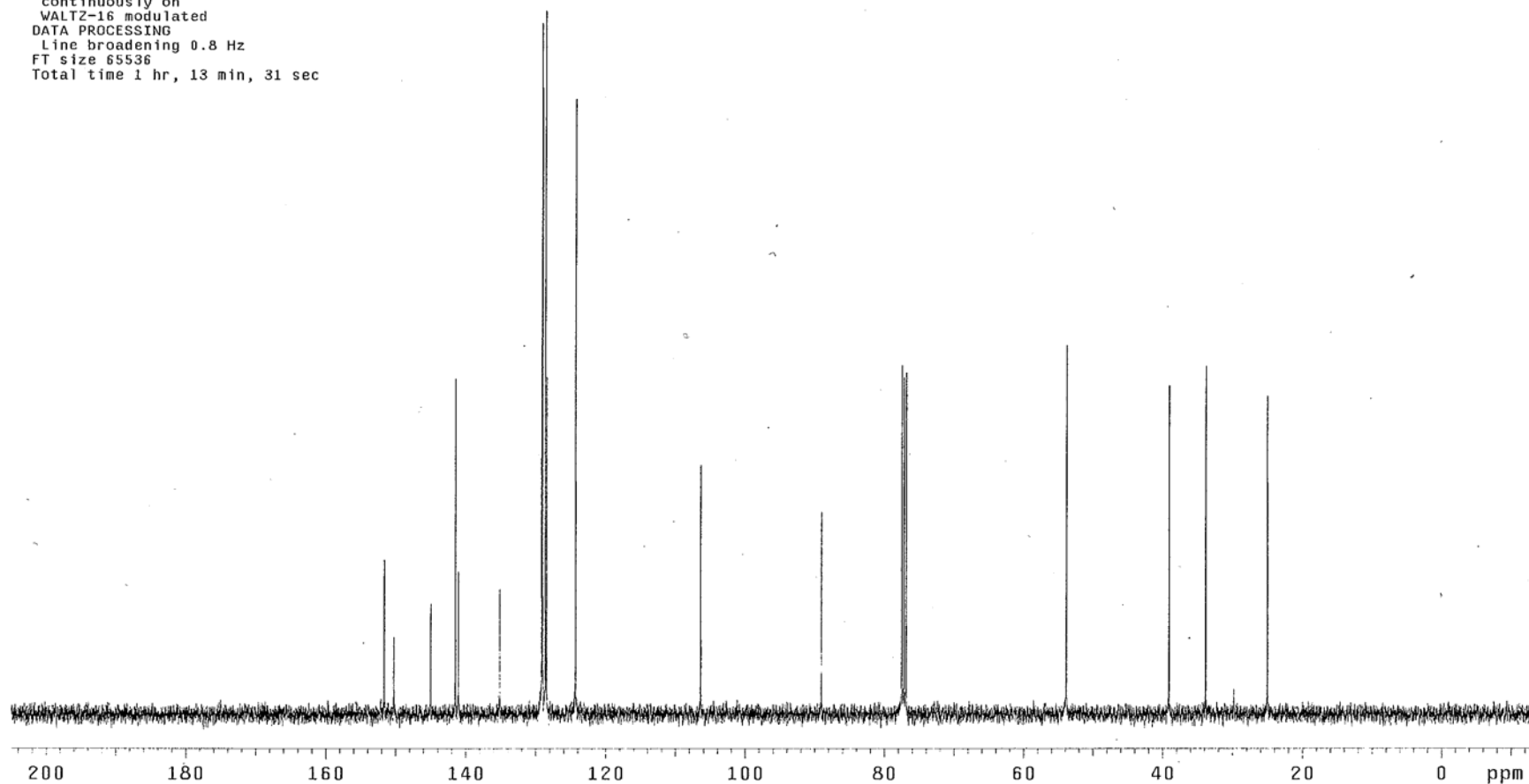
Pulse Sequence: s2pu1

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
306 repetitions
OBSERVE C13, 100.5263844 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 1 hr, 13 min, 31 sec



3c



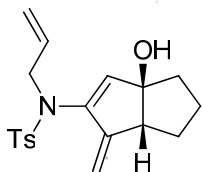
wxn534-2_21Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn534-2_21Sep2013

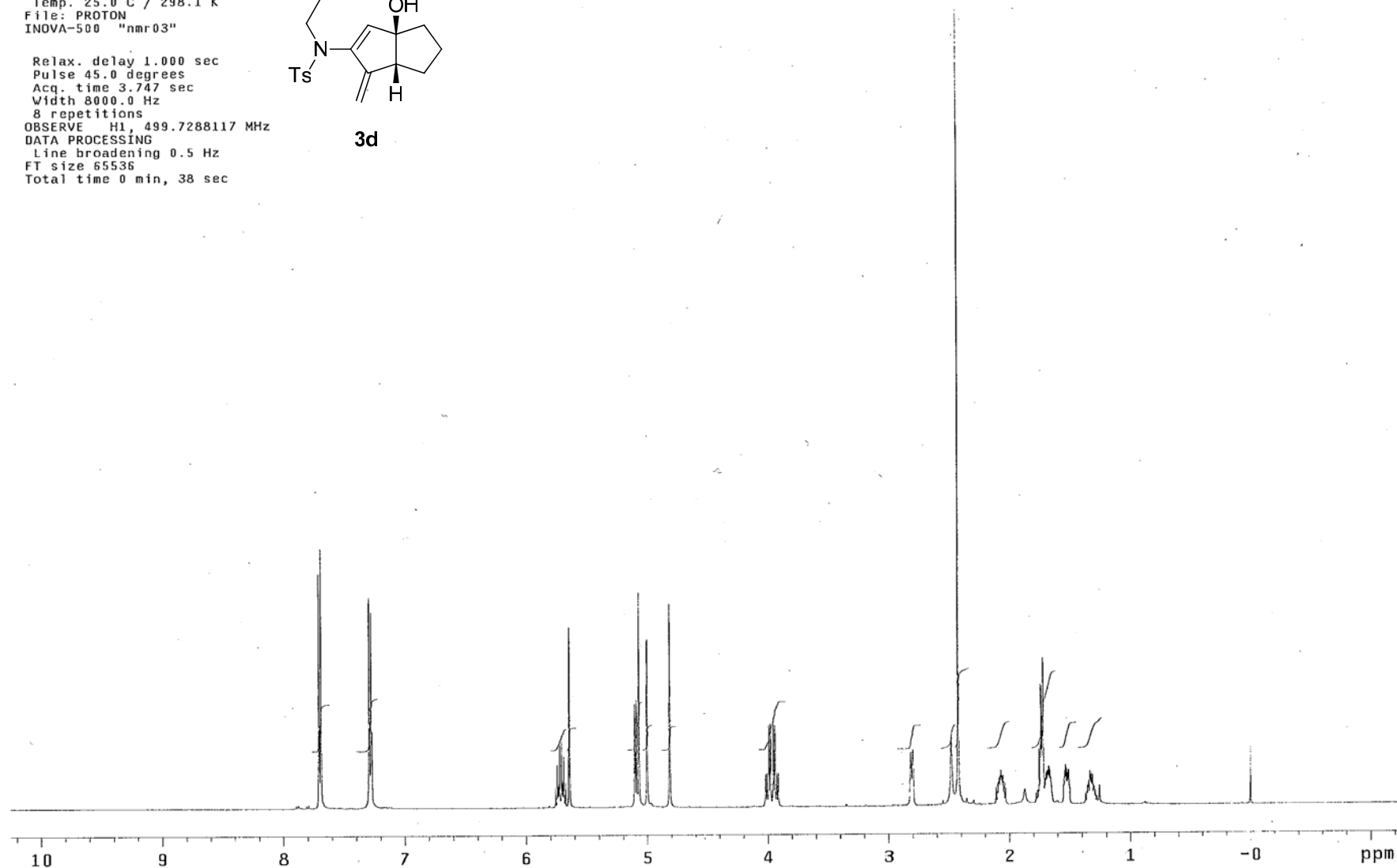
Pulse Sequence: s2pu1

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 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288117 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



3d



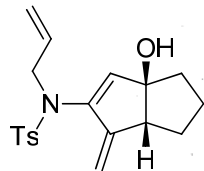
wxn534-2_21Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn534-2_21Sep2013

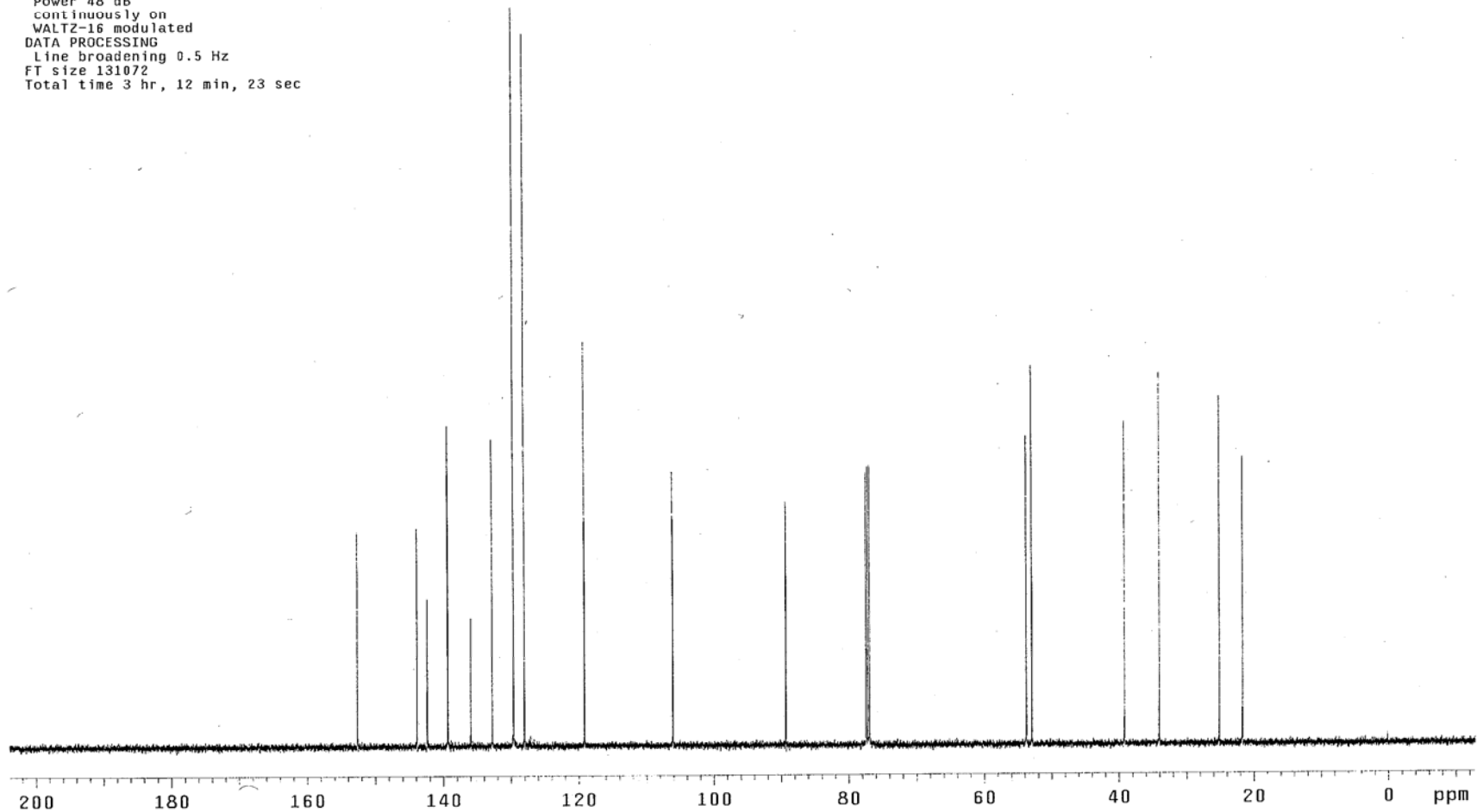
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.299 sec
Width 31446.5 Hz
335 repetitions
OBSERVE C13, 125.6568905 MHz
DECOUPLE H1, 499.7312897 MHz
Power 48 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 3 hr, 12 min, 23 sec



3d

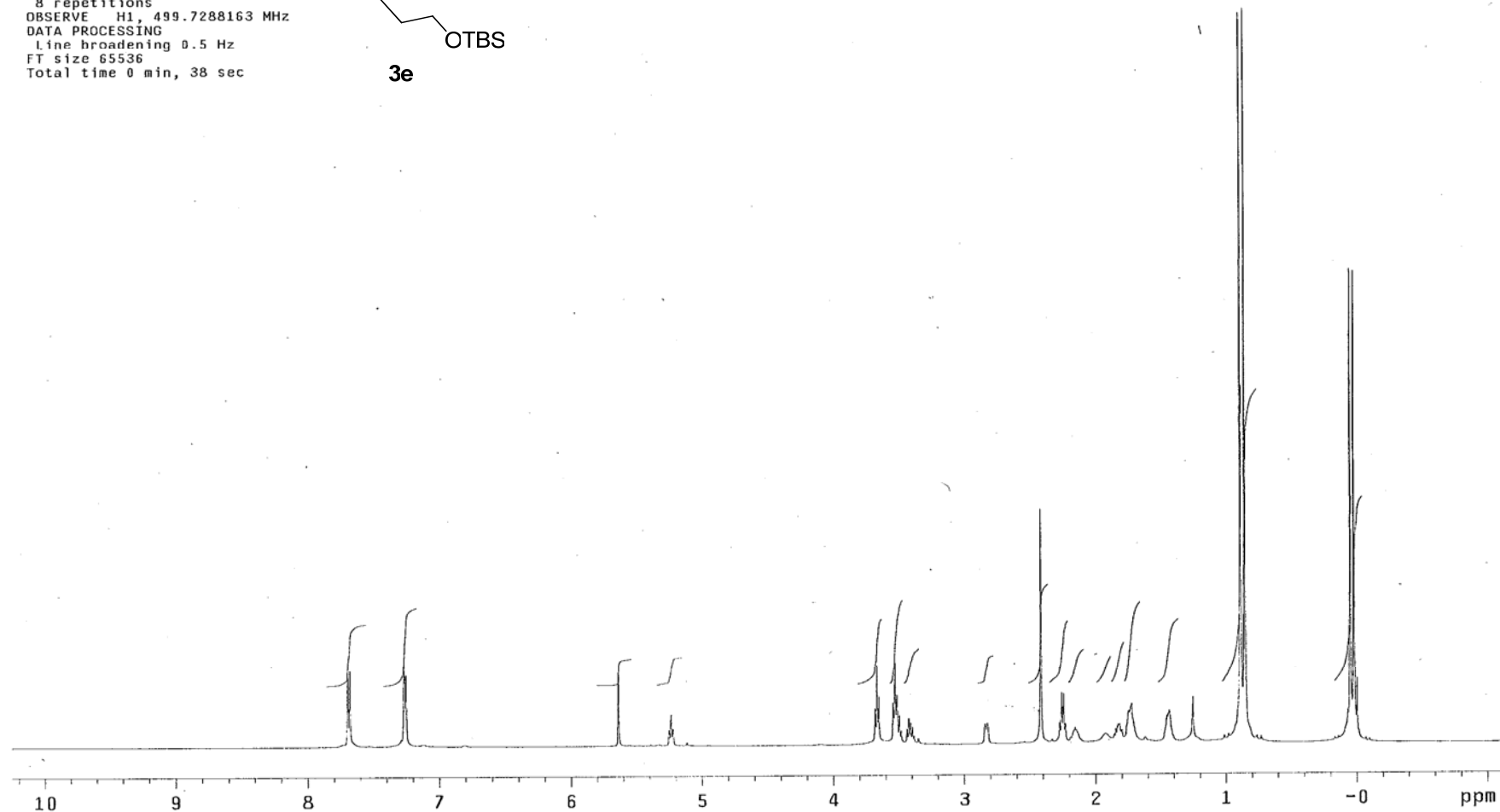
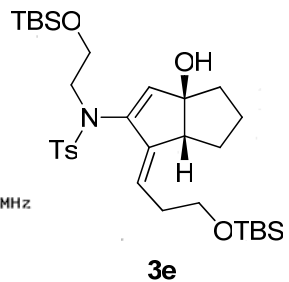


wxn518-3_30Sep2013-14:24:46

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn518-3_30Sep2013-14:24:46

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 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288163 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



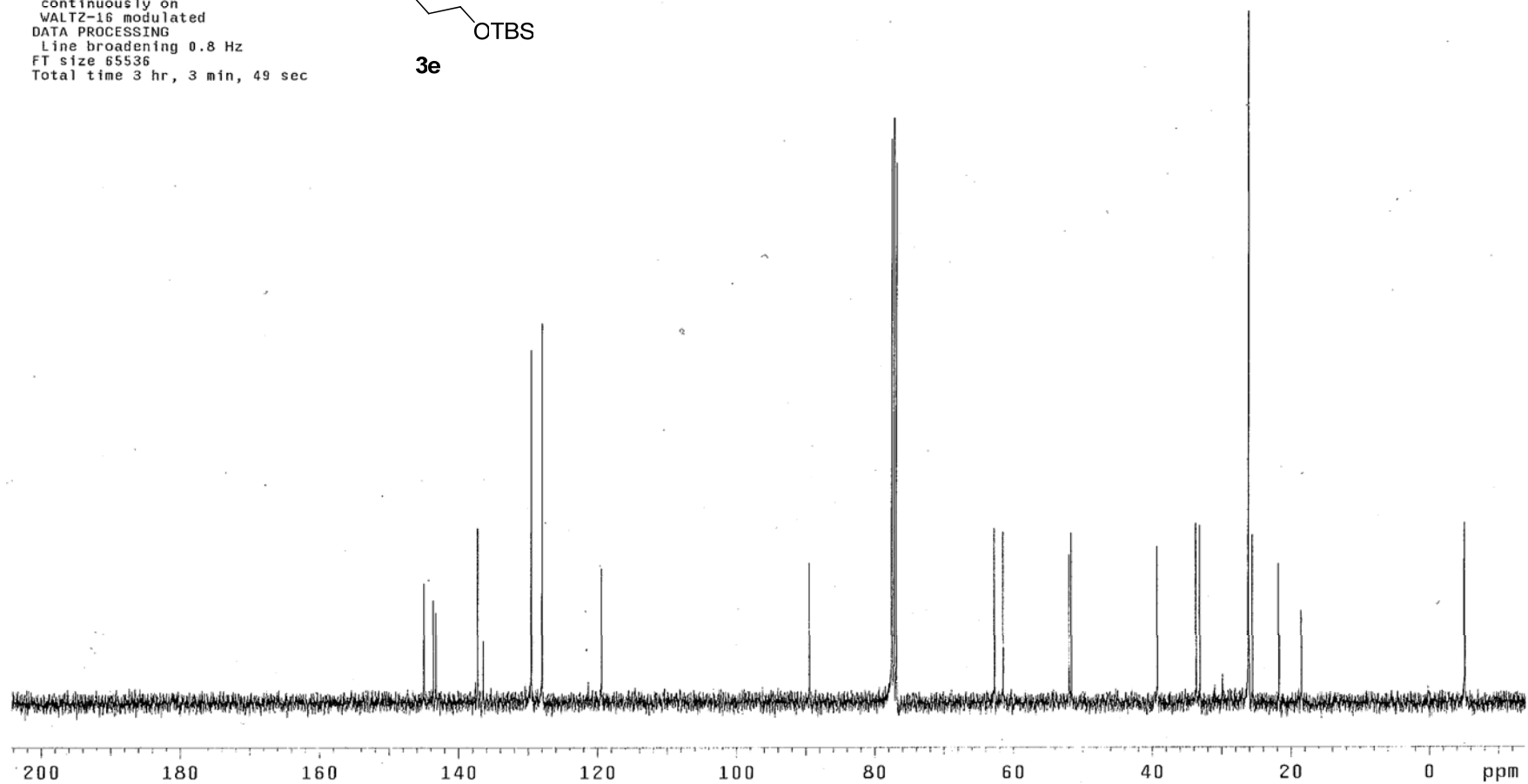
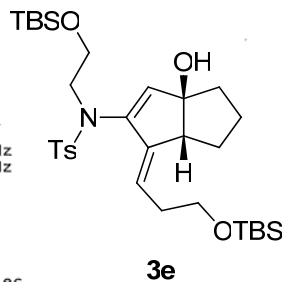
wxn518-3_06Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn518-3_06Sep2013

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
1052 repetitions
OBSERVE C13, 100.5263814 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec

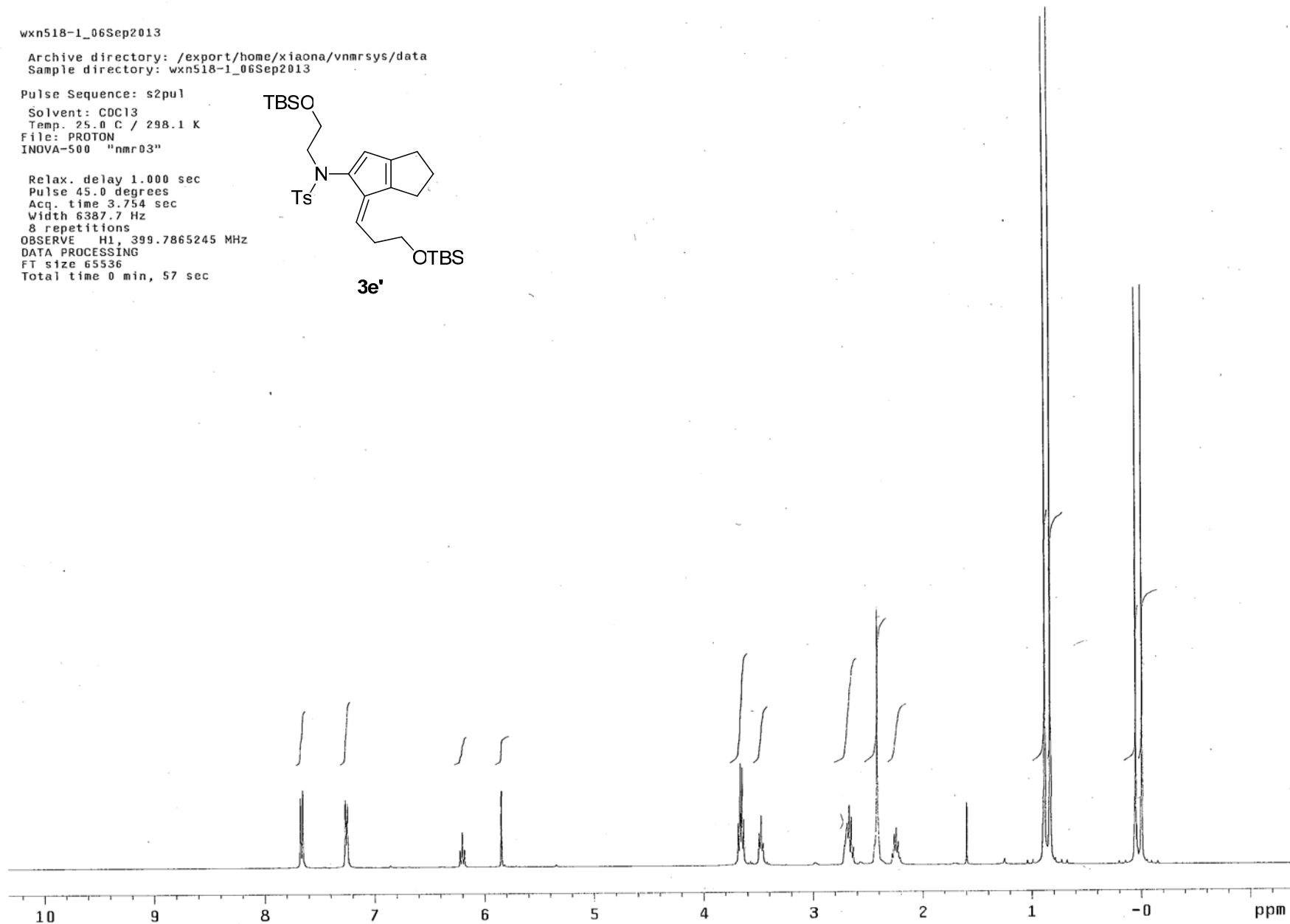
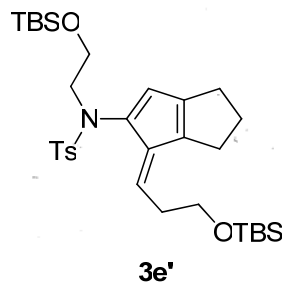


wxn518-1_06Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn518-1_06Sep2013

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.8 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, 399.7865245 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec

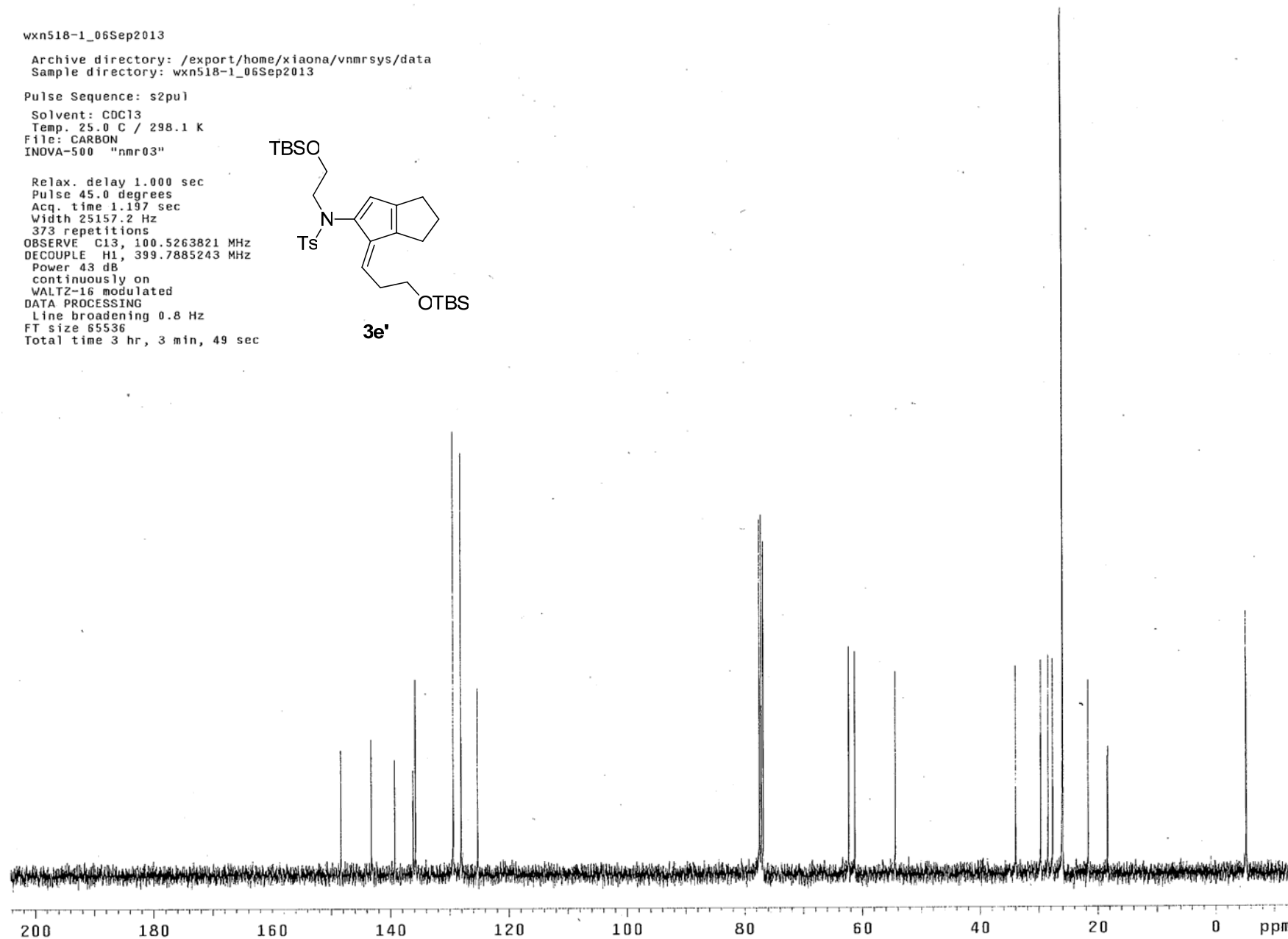
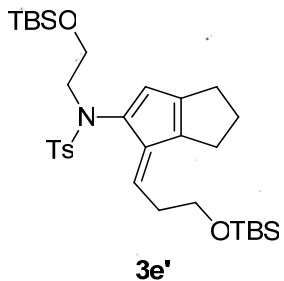


wxn518-1_06Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn518-1_06Sep2013

Pulse Sequence: s2pul
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
373 repetitions
OBSERVE C13, 100.5263821 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec

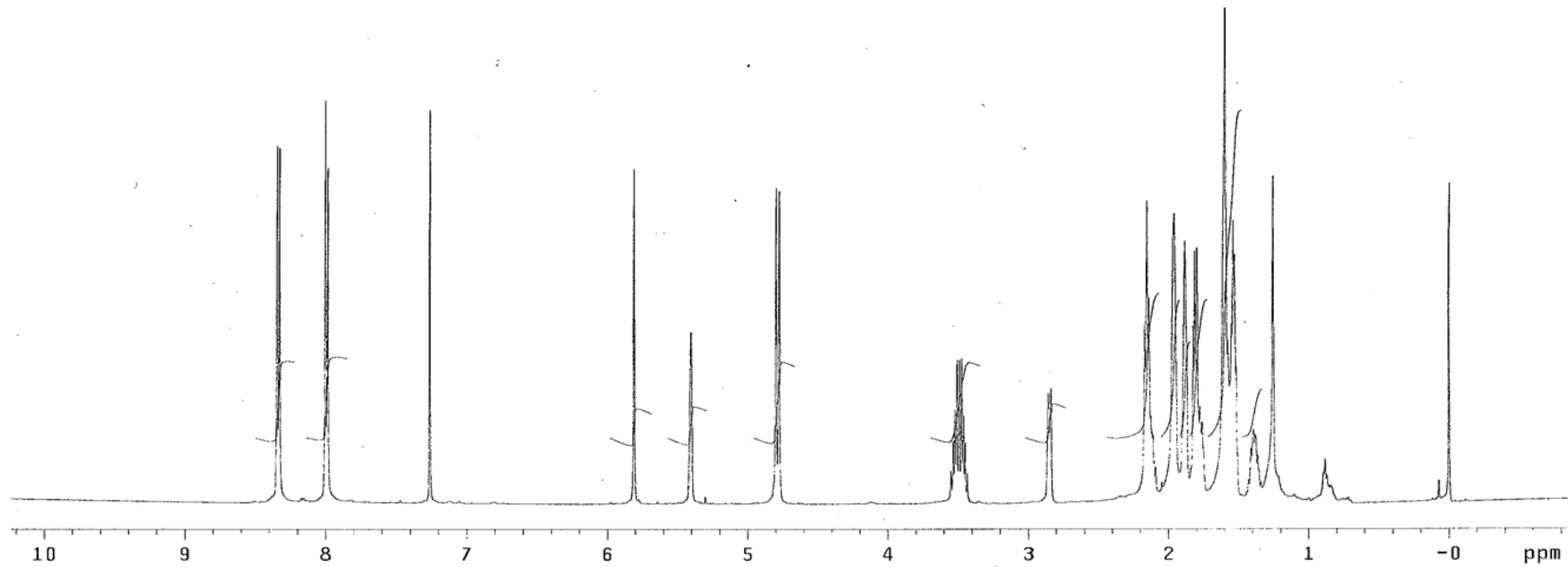
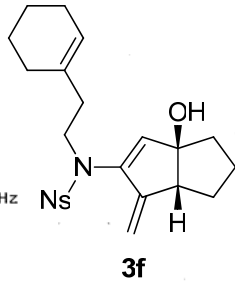


wxn541-3_29Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn541-3_29Sep2013

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INNOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.747 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 499.7288148 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 min, 32 sec



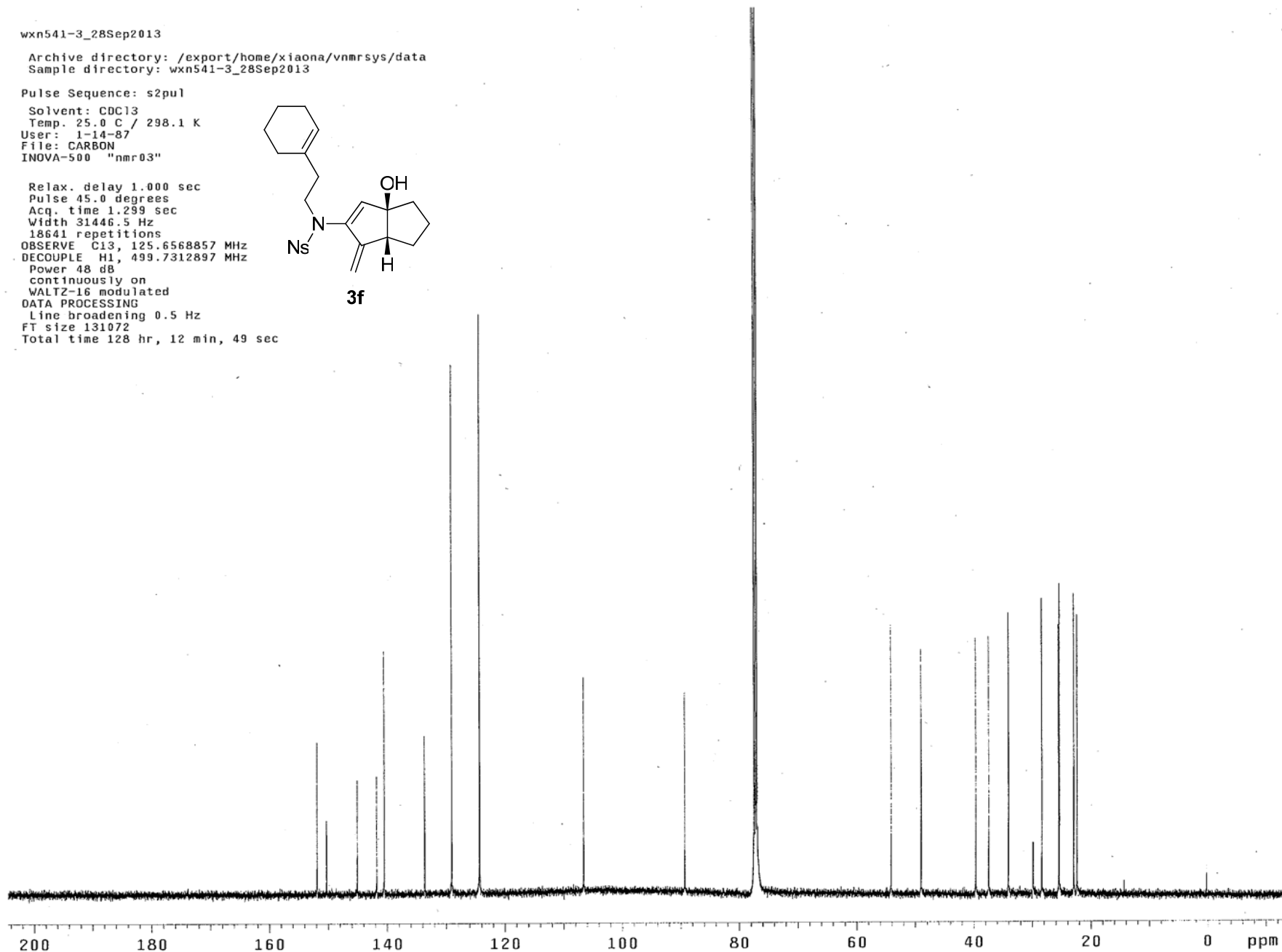
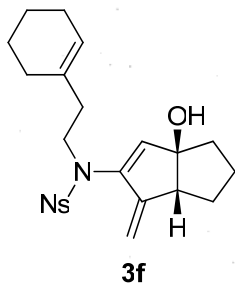
wxn541-3_28Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn541-3_28Sep2013

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.299 sec
Width 31446.5 Hz
18641 repetitions
OBSERVE C13, 125.6568857 MHz
DECOUPLE H1, 499.7312897 MHz
Power 48 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 128 hr, 12 min, 49 sec



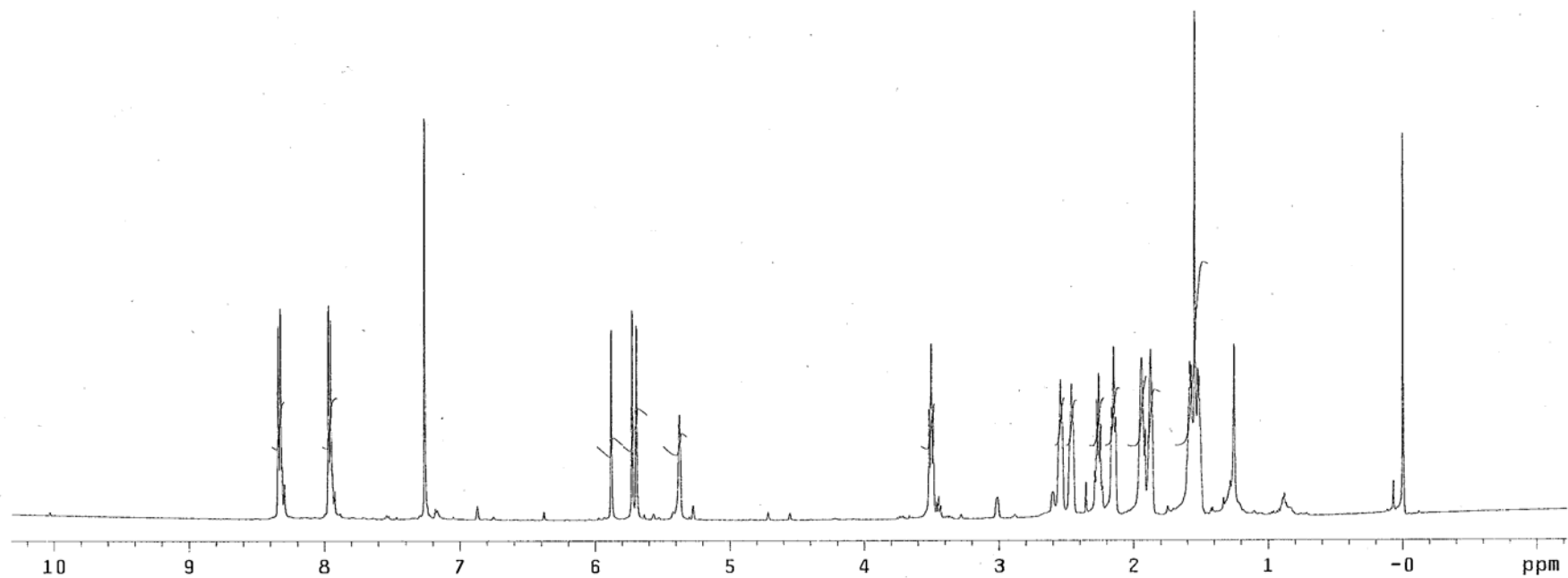
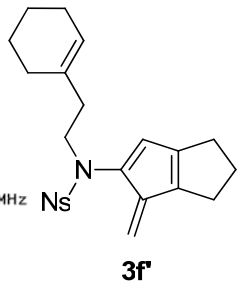
wxn541-1_28Sep2013-22:12:32

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn541-1_28Sep2013-22:12:32

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 3.747 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 499.7288168 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 min, 32 sec



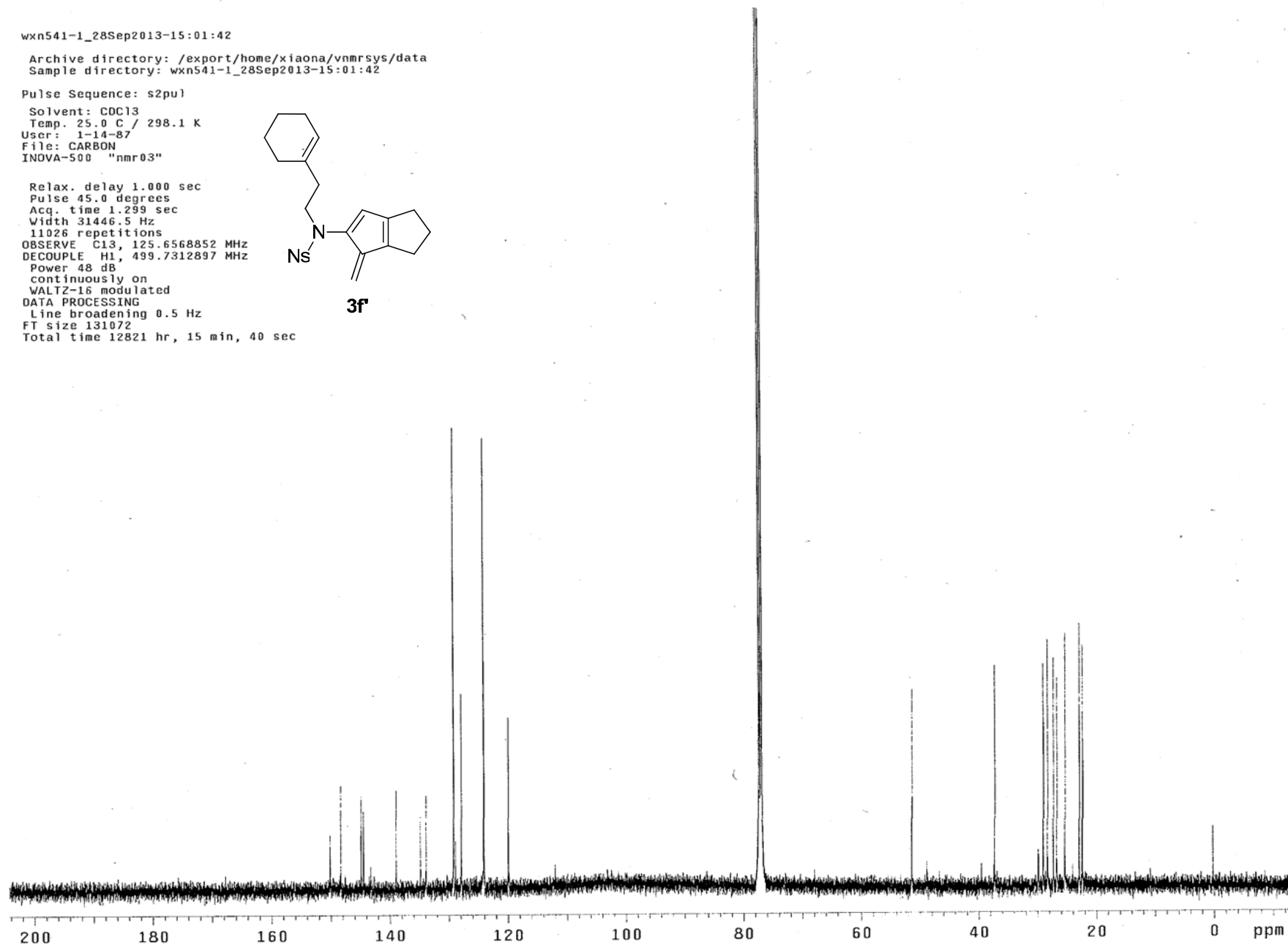
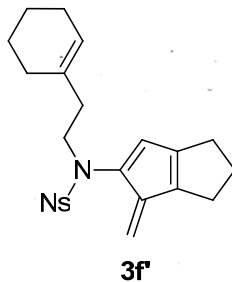
wxn541-1_28Sep2013-15:01:42

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn541-1_28Sep2013-15:01:42

Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.299 sec
Width 31446.5 Hz
11026 repetitions
OBSERVE C13, 125.6568852 MHz
DECOUPLE H1, 499.7312897 MHz
Power 48 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 12821 hr, 15 min, 40 sec



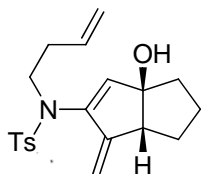
wxn601-2_27Dec2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn601-2_27Dec2013

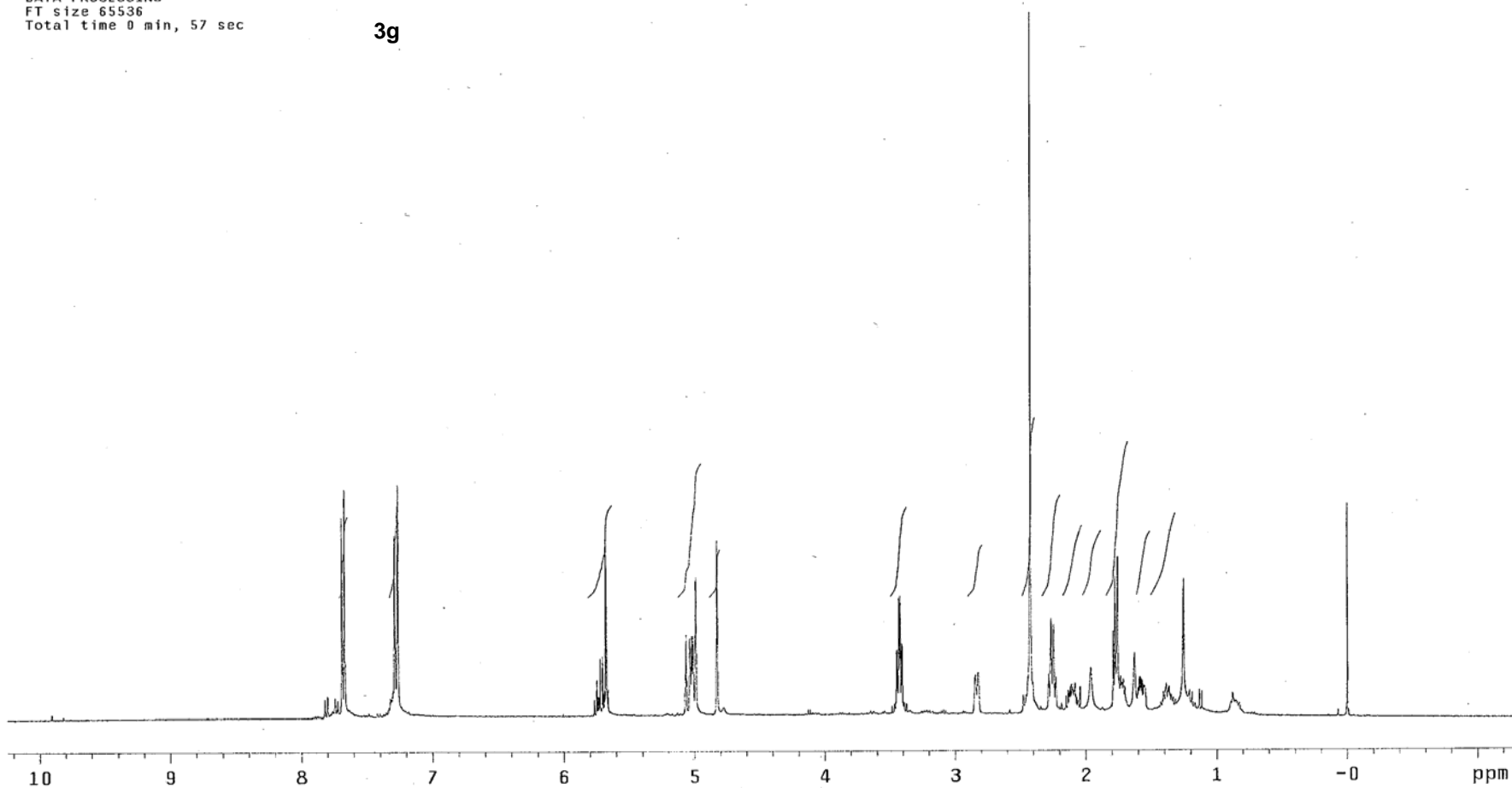
Pulse Sequence: s2pu1

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, 399.7865227 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



3g



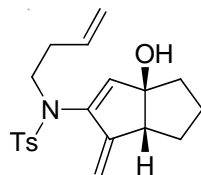
wxn601-2_27Dec2013-10:21:16

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn601-2_27Dec2013-10:21:16

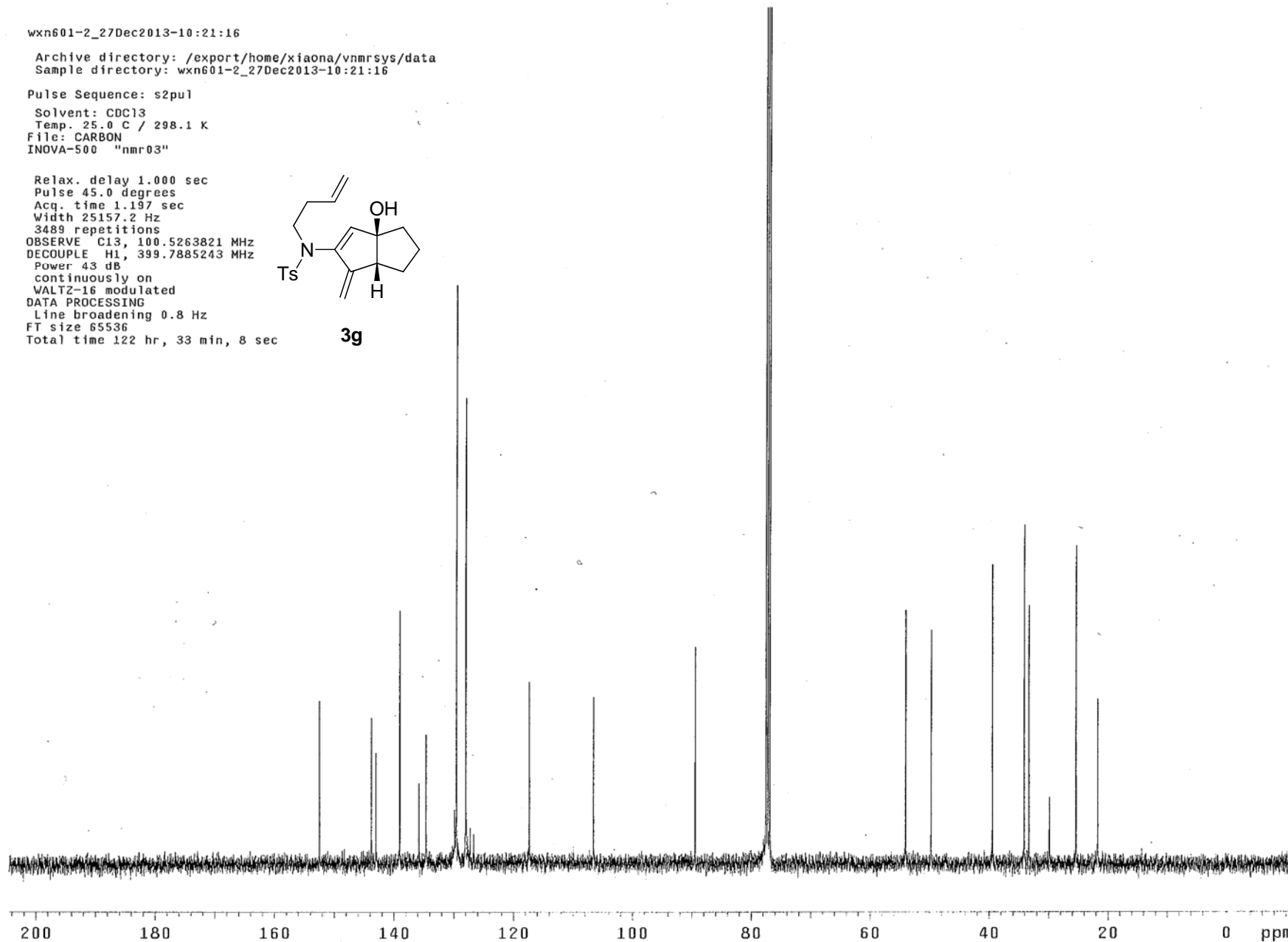
Pulse Sequence: s2pul

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
3489 repetitions
OBSERVE C13, 100.5263821 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 122 hr, 33 min, 8 sec



3g



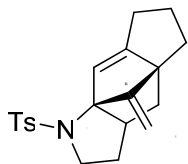
wxn594-601-1_30Dec2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn594-601-1_30Dec2013

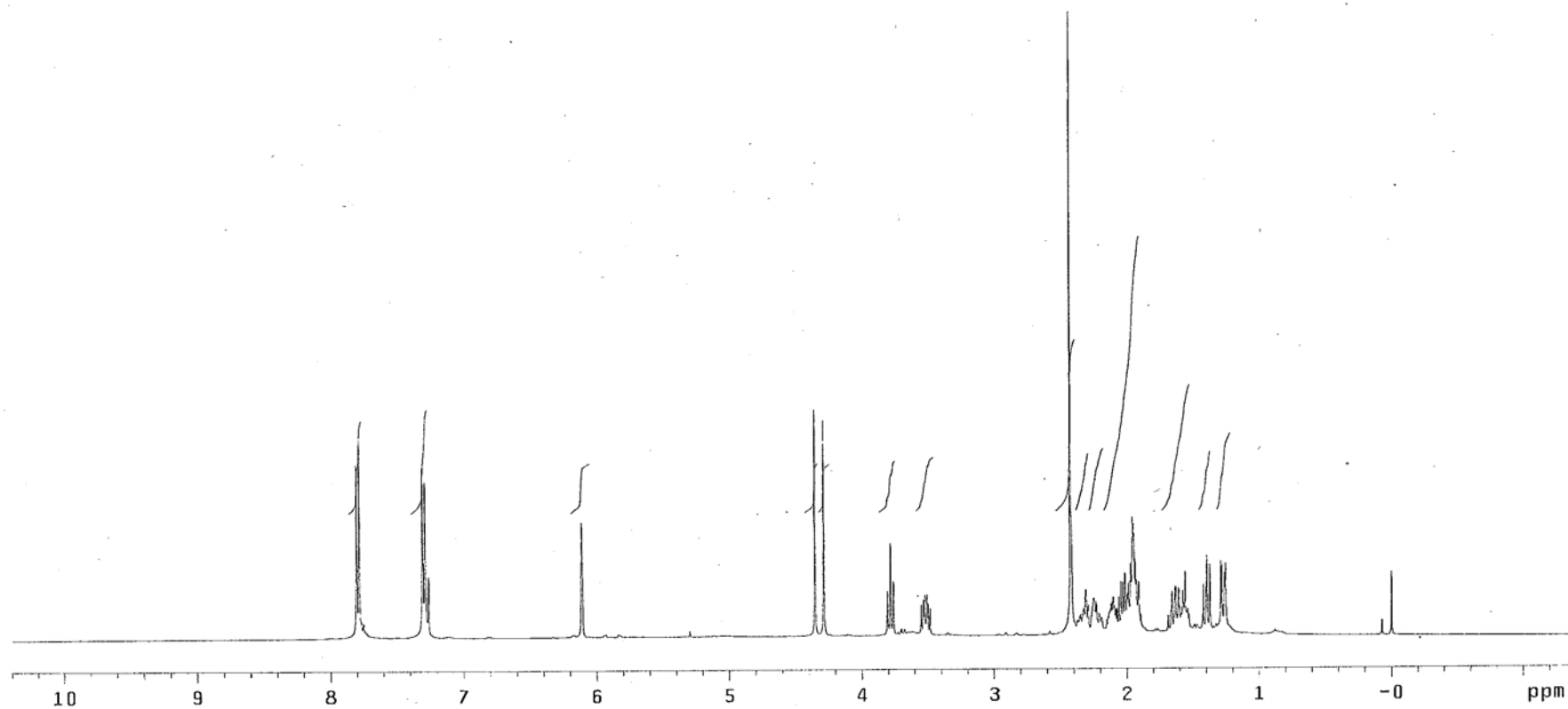
Pulse Sequence: s2pu1

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, 399.7865227 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



3g"

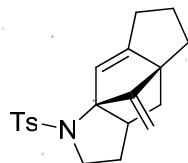


wxn594-601-1_30Dec2013

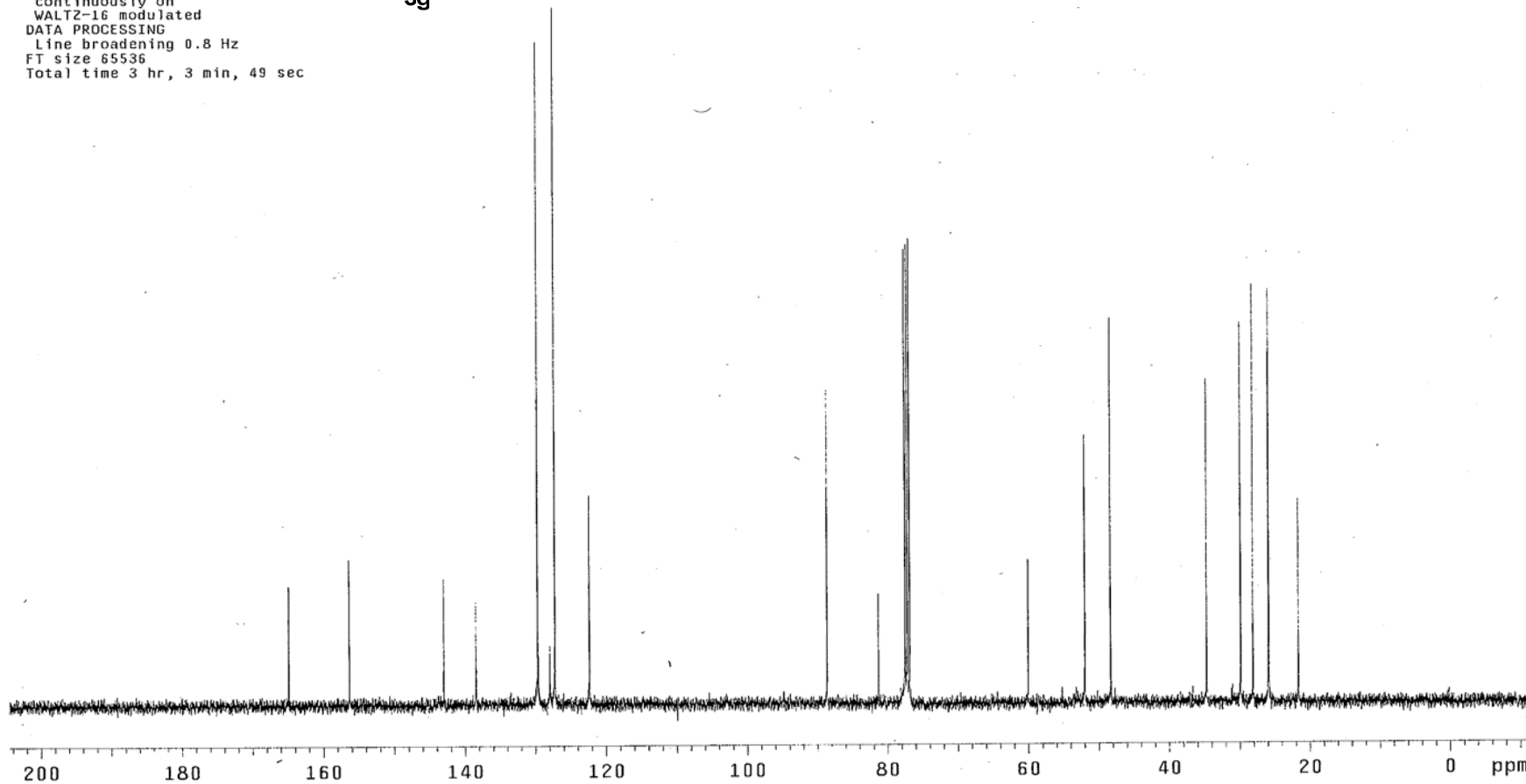
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn594-601-1_30Dec2013

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
1644 repetitions
OBSERVE C13, 100.5263837 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



3g"

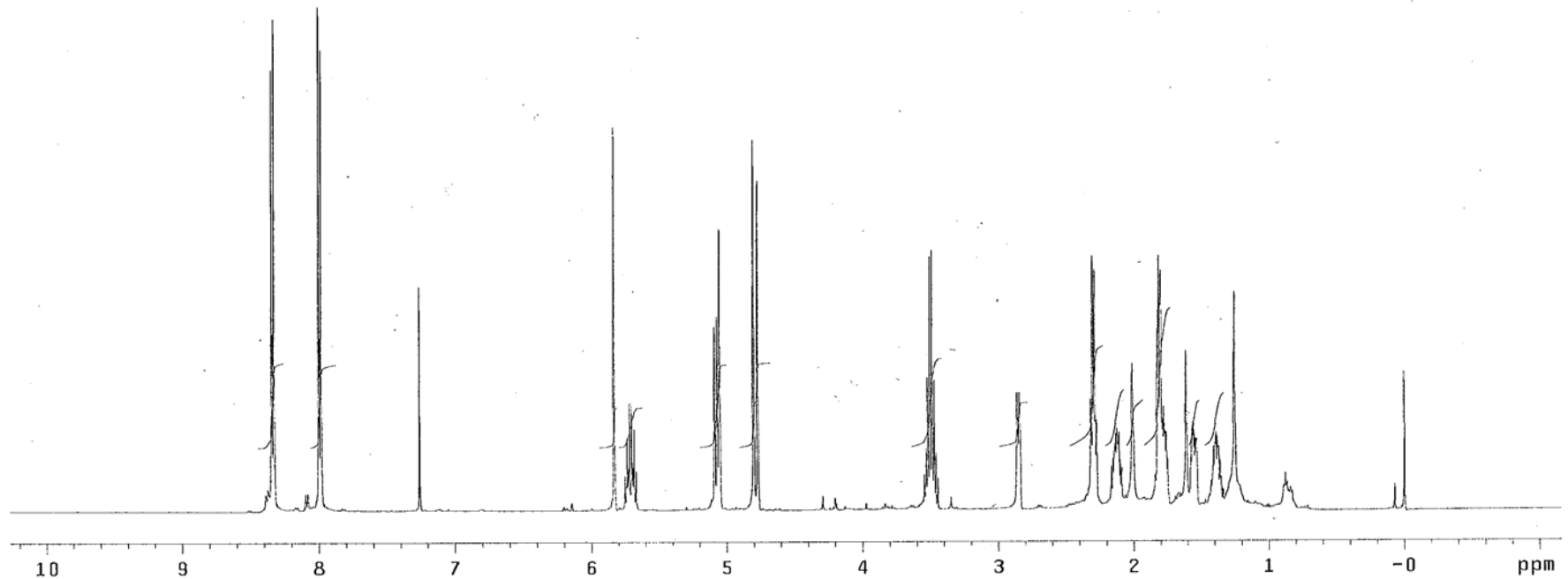
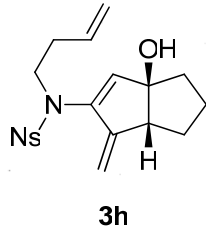


wxn593-4_16Dec2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn593-4_16Dec2013

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INNOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288165 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



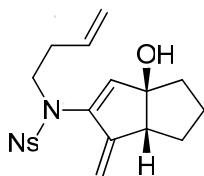
wxn593-4_15Dec2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn593-4_15Dec2013

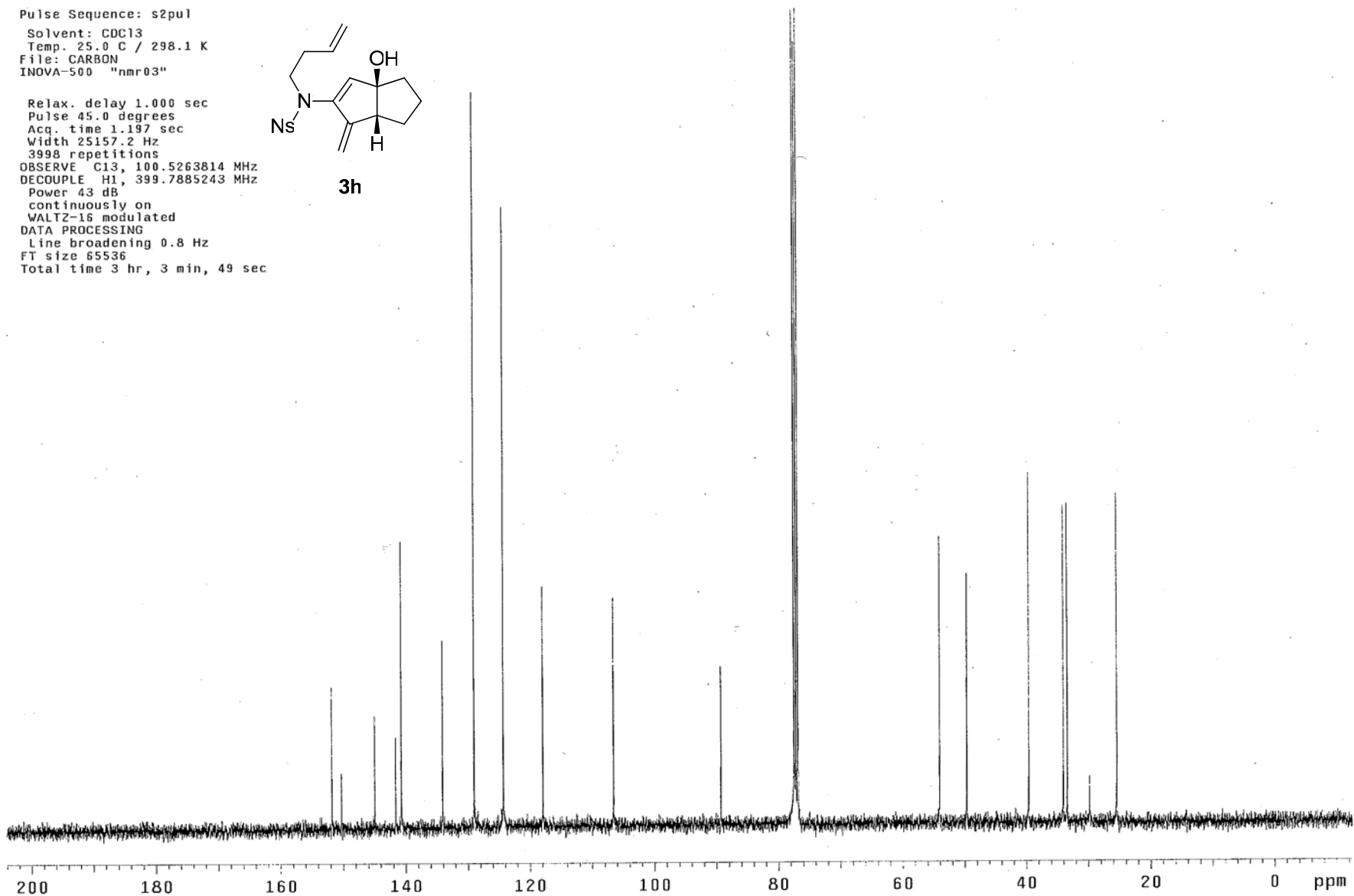
Pulse Sequence: s2pul

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
3998 repetitions
OBSERVE C13, 100.5263814 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



3h



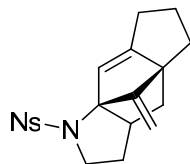
wxn593-1_15Dec2013-19:40:02

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn593-1_15Dec2013-19:40:02

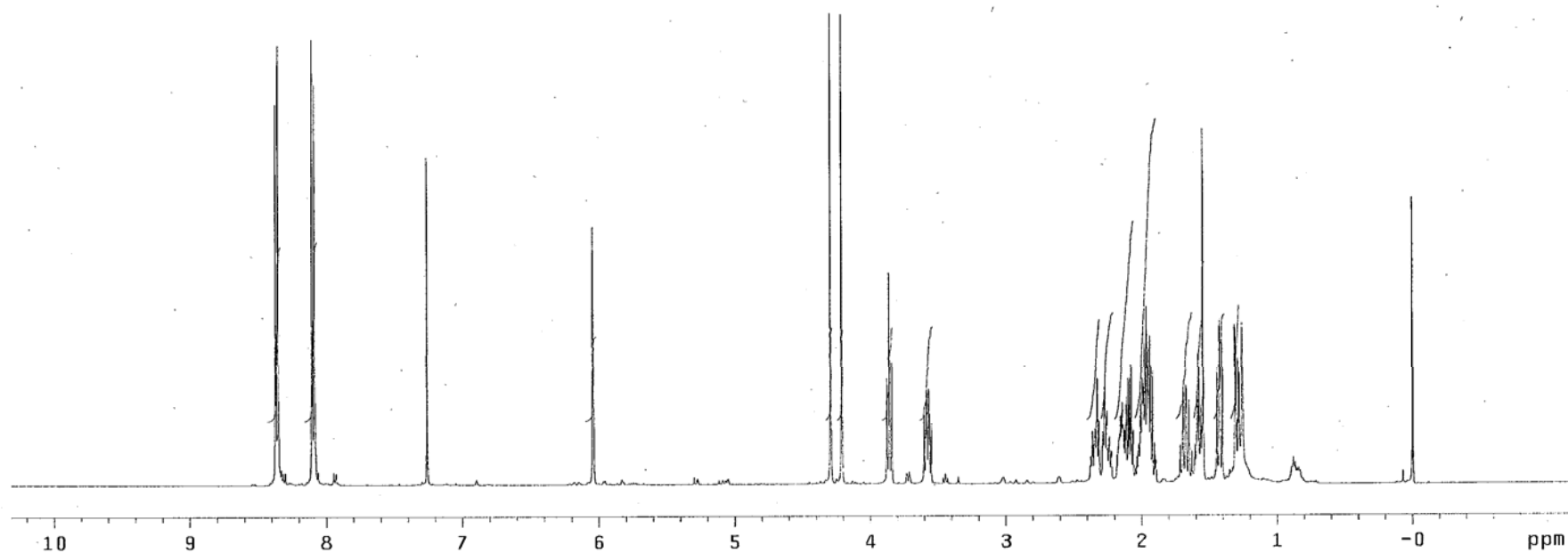
Pulse Sequence: s2pul

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

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.747 sec
Width 8000.0 Hz
& repetitions
OBSERVE H1, 499.7288175 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



3h''



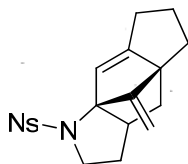
wxn593-1_15Dec2013-21:48:11

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn593-1_15Dec2013-21:48:11

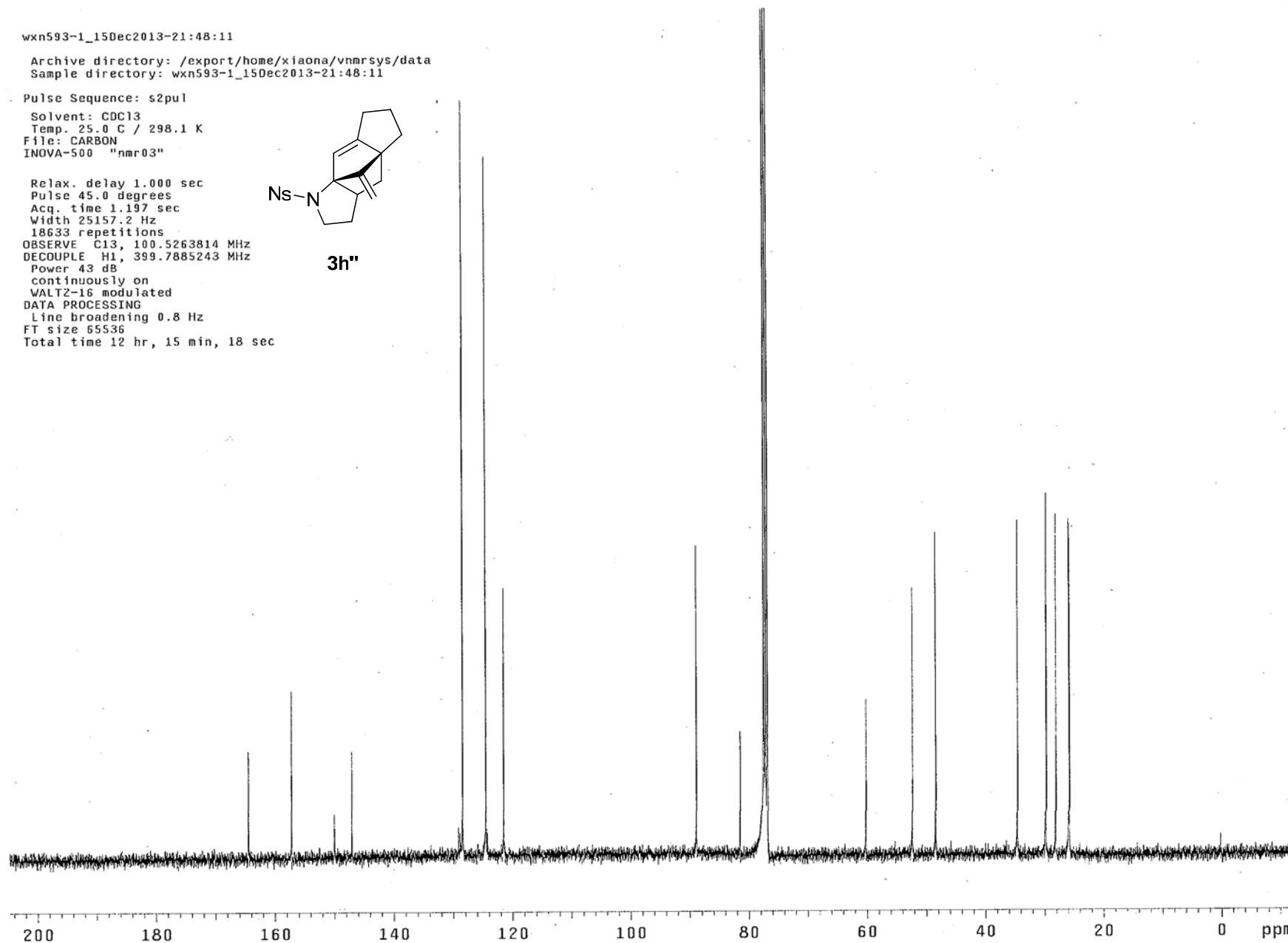
Pulse Sequence: s2pul

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
18633 repetitions
OBSERVE C13, 100.5263814 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 12 hr, 15 min, 18 sec



3h"



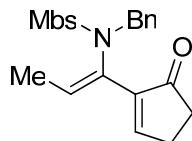
wxn528-4_17Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn528-4_17Sep2013

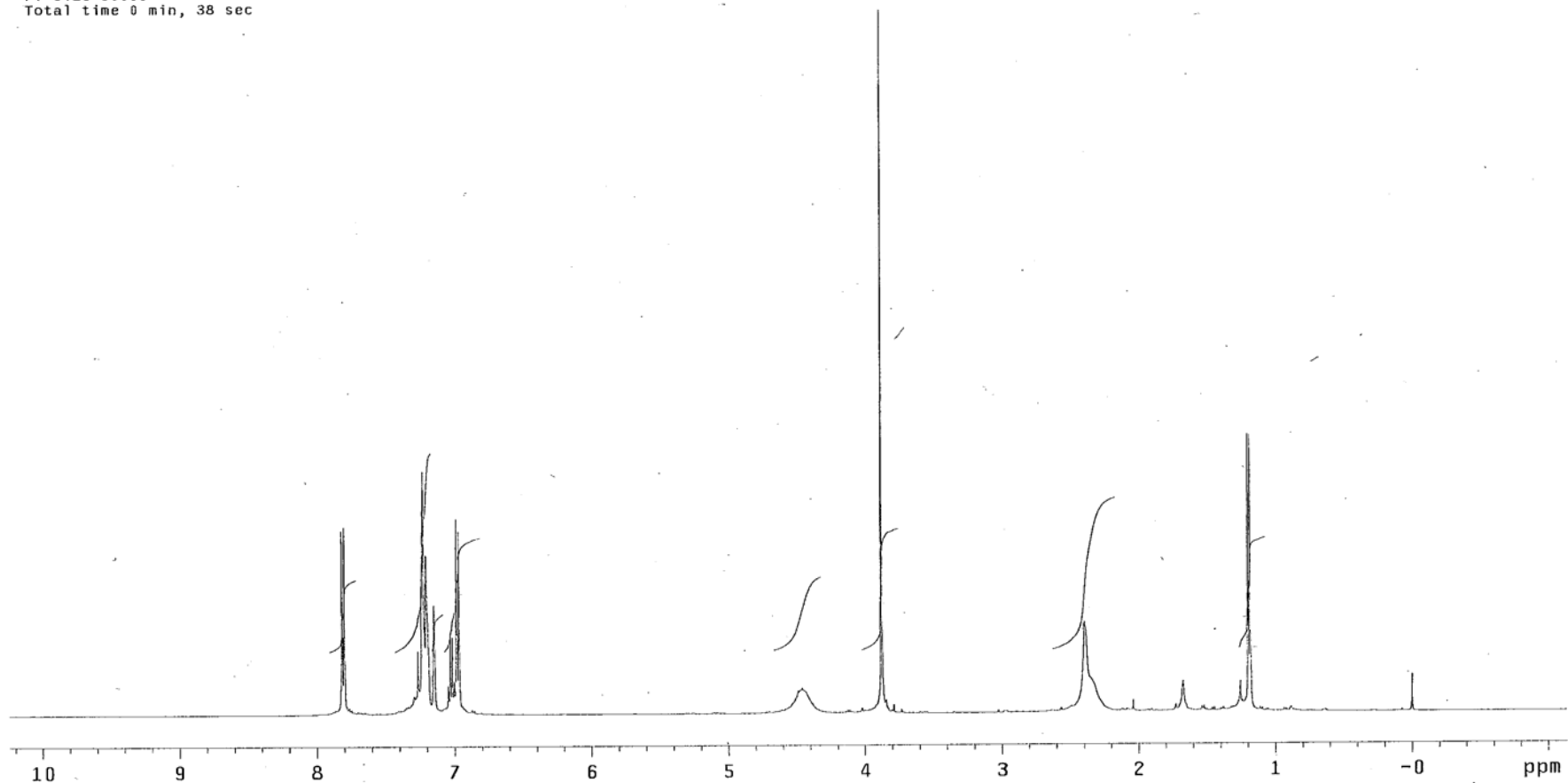
Pulse Sequence: s2pu1

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 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288139 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



12a-cis

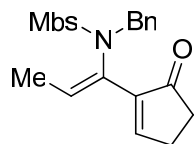


wxn528-4_17Sep2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn528-4_17Sep2013

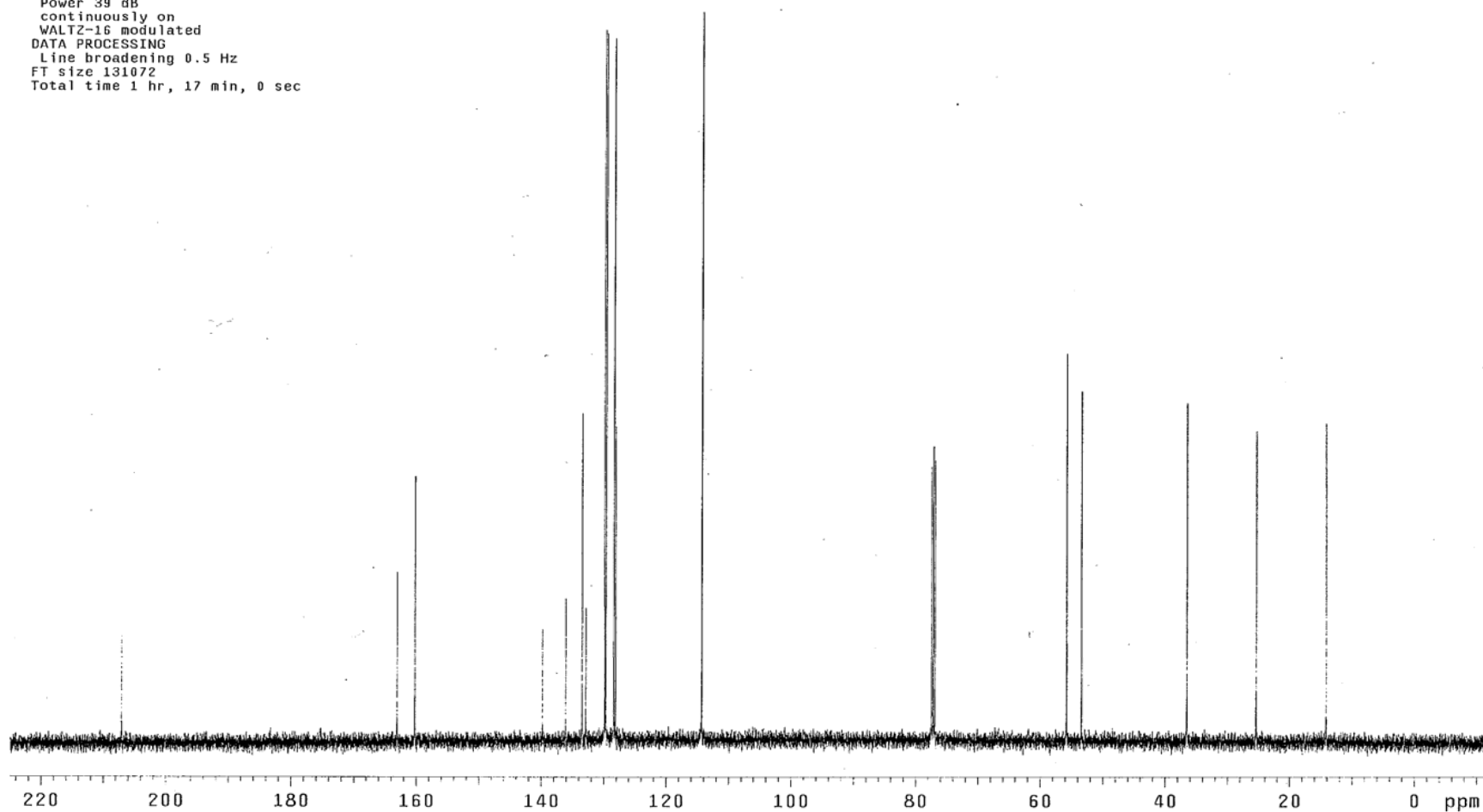
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: CARBON
INNOVA-500 "nmr03"



12a-cis

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.299 sec
Width 31446.5 Hz
579 repetitions
OBSERVE C13, 125.6568910 MHz
DECOUPLE H1, 499.7312897 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 1 hr, 17 min, 0 sec

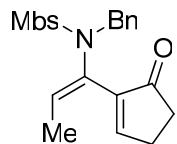


wxn638-1-2-3_01Mar2014-19:32:38

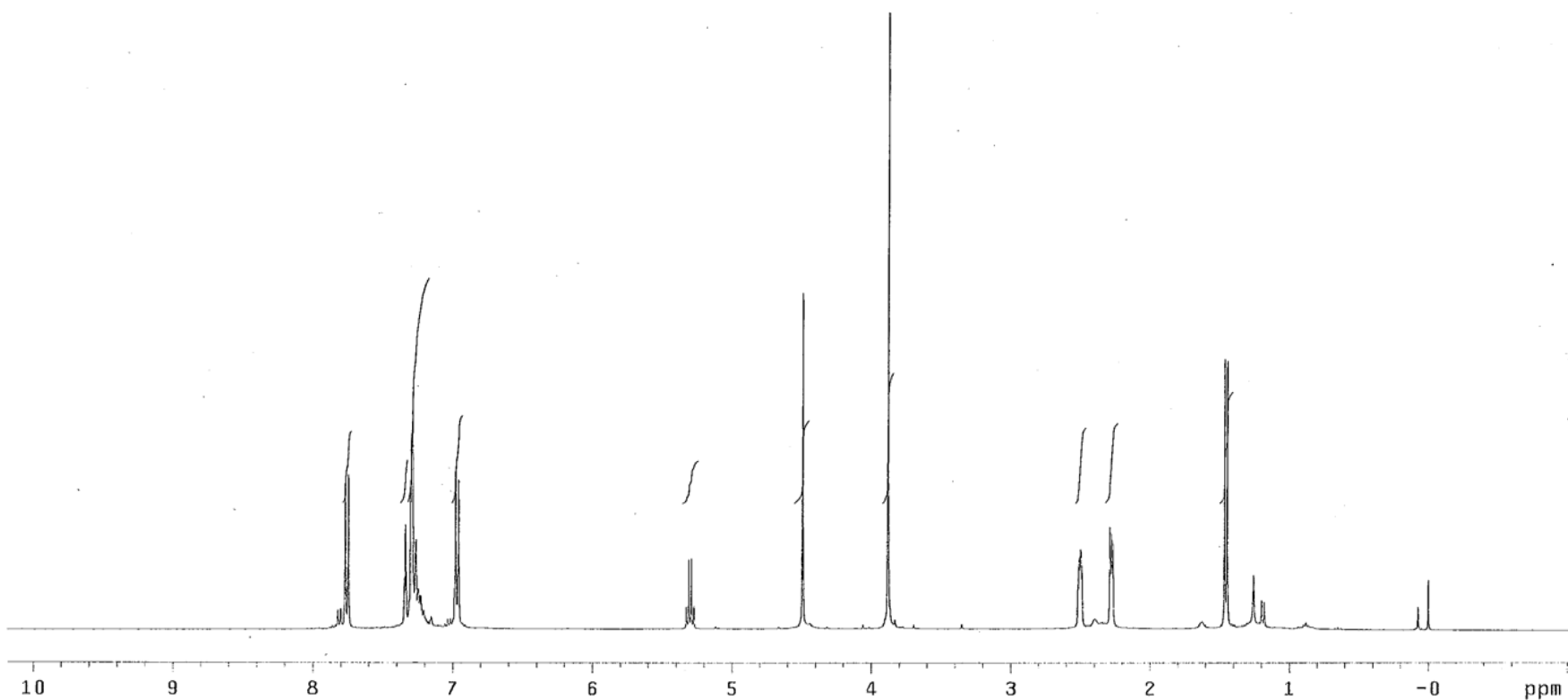
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn638-1-2-3_01Mar2014-19:32:38

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INNOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865224 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



12a-trans

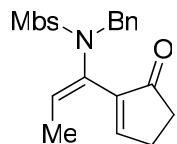


wxn638-1-2-3_01Mar2014-19:32:38

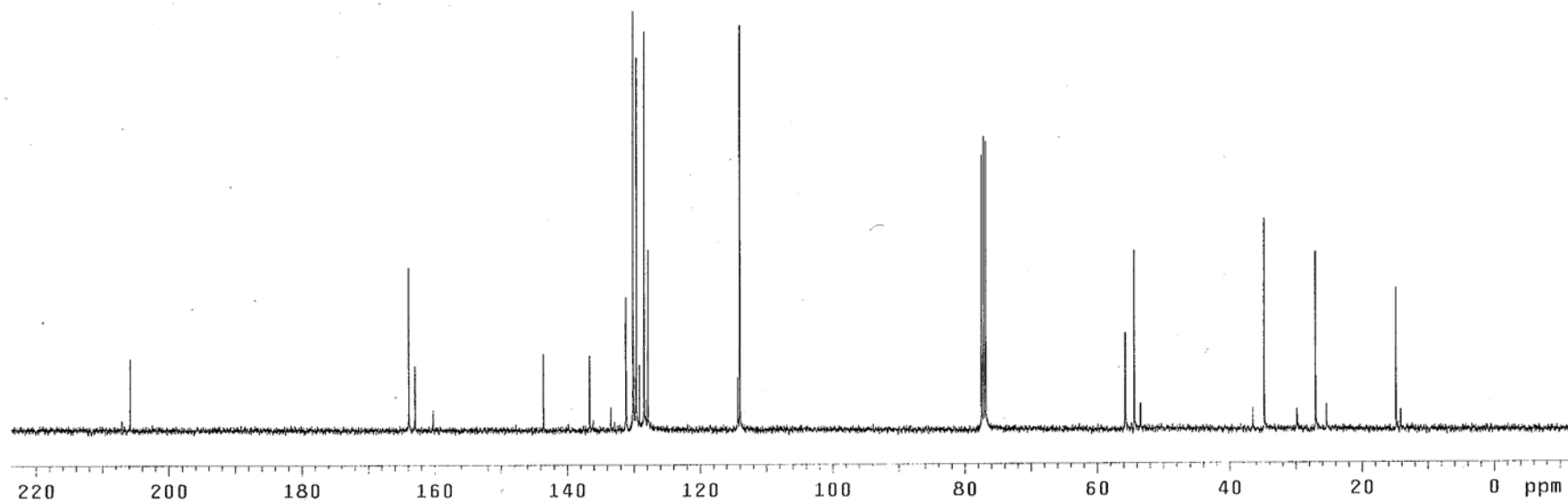
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn638-1-2-3_01Mar2014-19:32:38

Pulse Sequence: s2pul
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
2555 repetitions
OBSERVE C13, 100.5263837 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



12a-trans

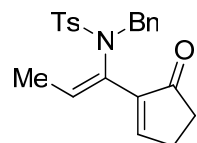


wxn563-1_30Oct2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn563-1_30Oct2013

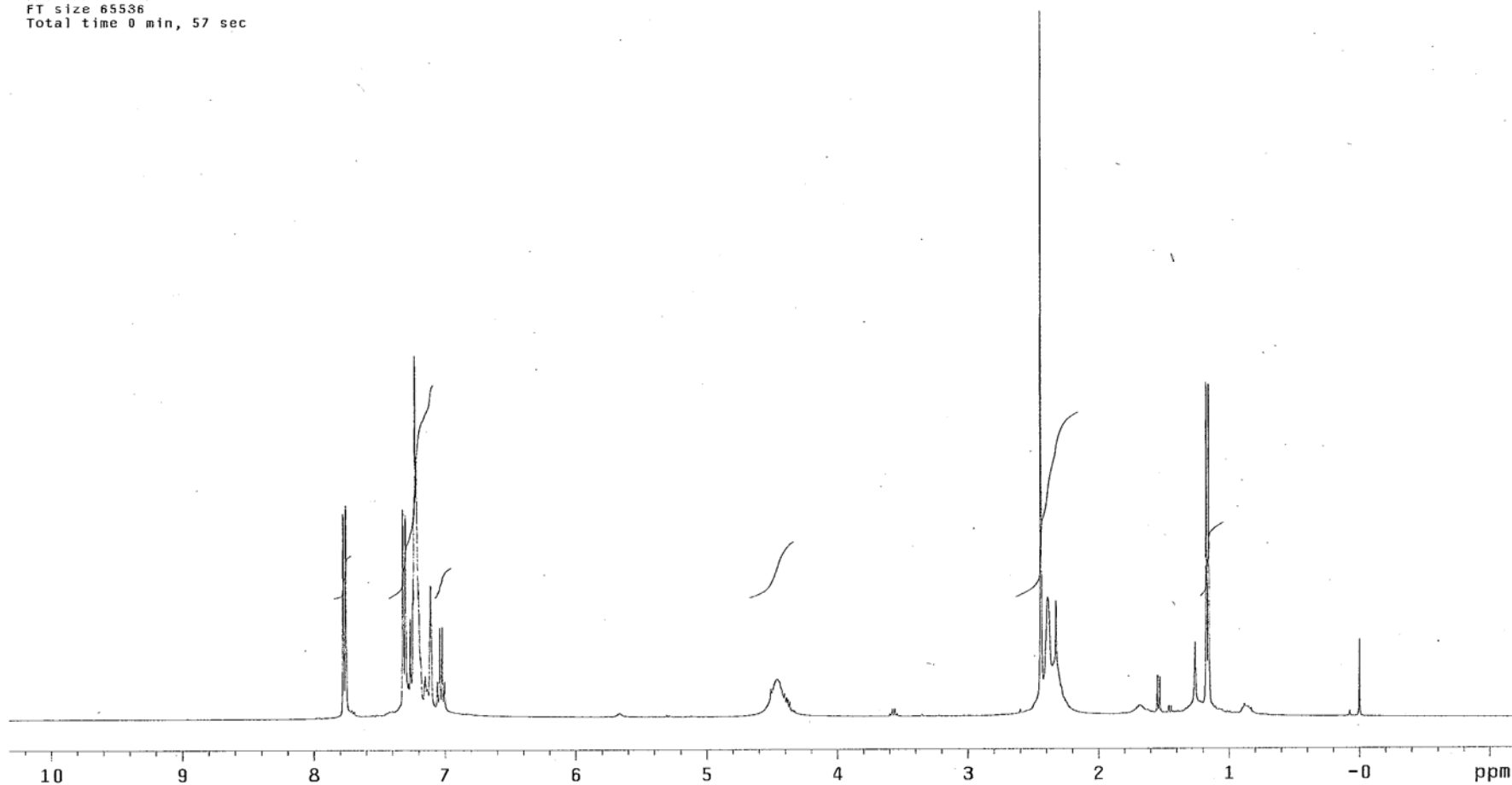
Pulse Sequence: s2pu1

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



12b-cis

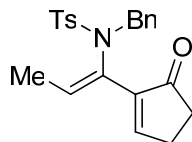
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865220 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



wxn563-1_28Oct2013

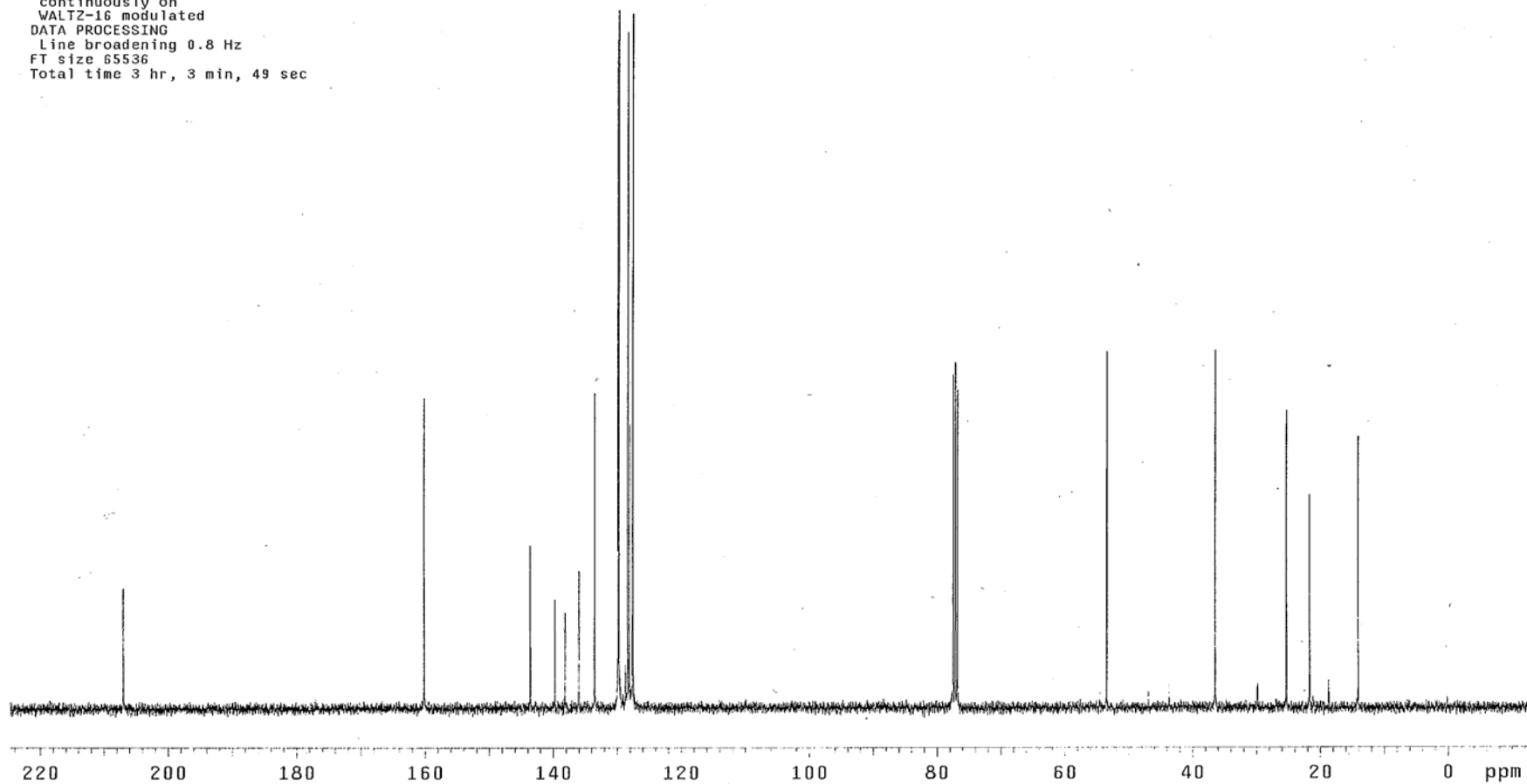
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn563-1_28Oct2013

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INOVA-500 "nmr03"



12b-cis

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
1186 repetitions
OBSERVE C13, 100.5263844 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



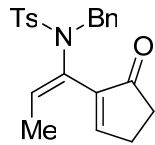
wxn563-2-2_25Nov2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn563-2-2_25Nov2013

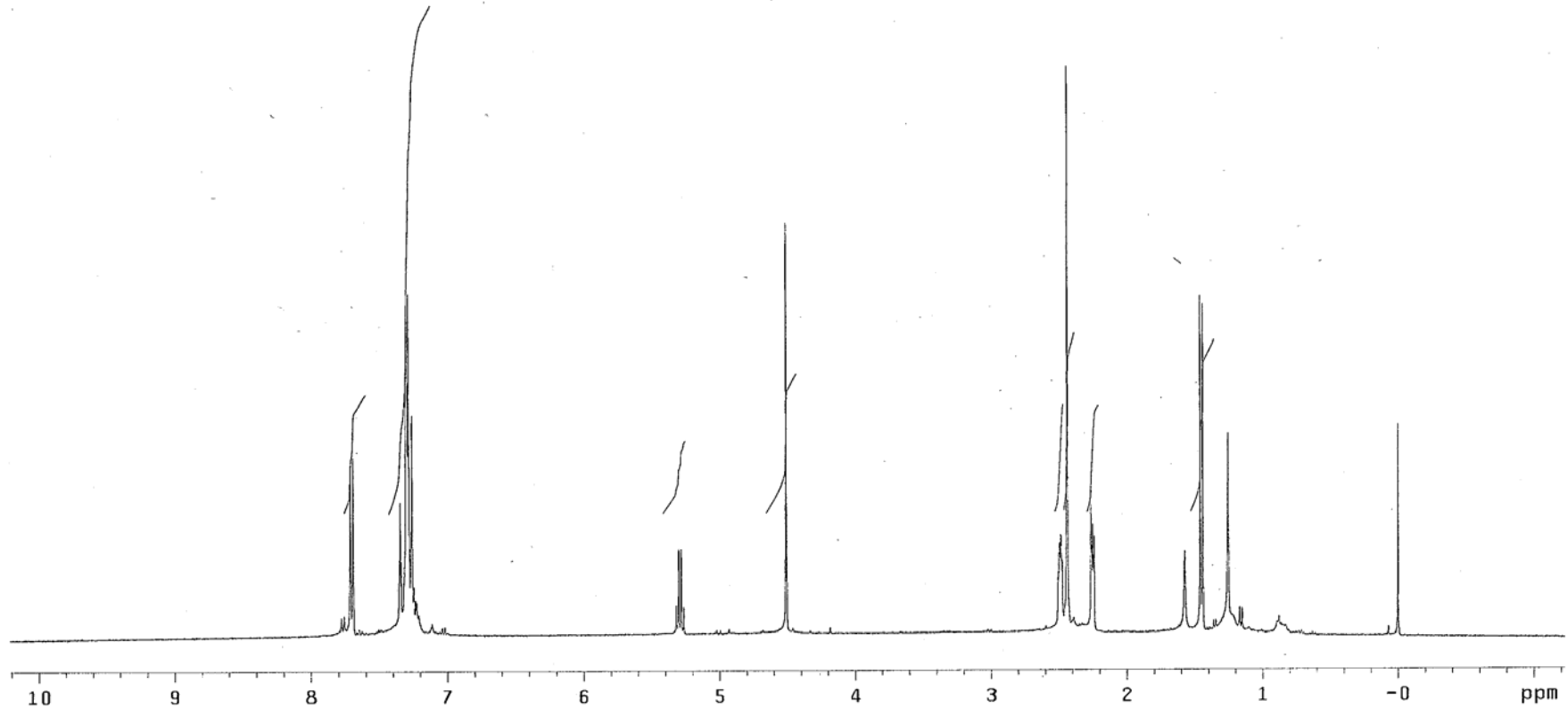
Pulse Sequence: s2pu1

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, 399.7865233 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



12b-trans

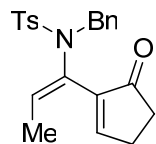


wxn563-2-2_25Nov2013-16:42:23

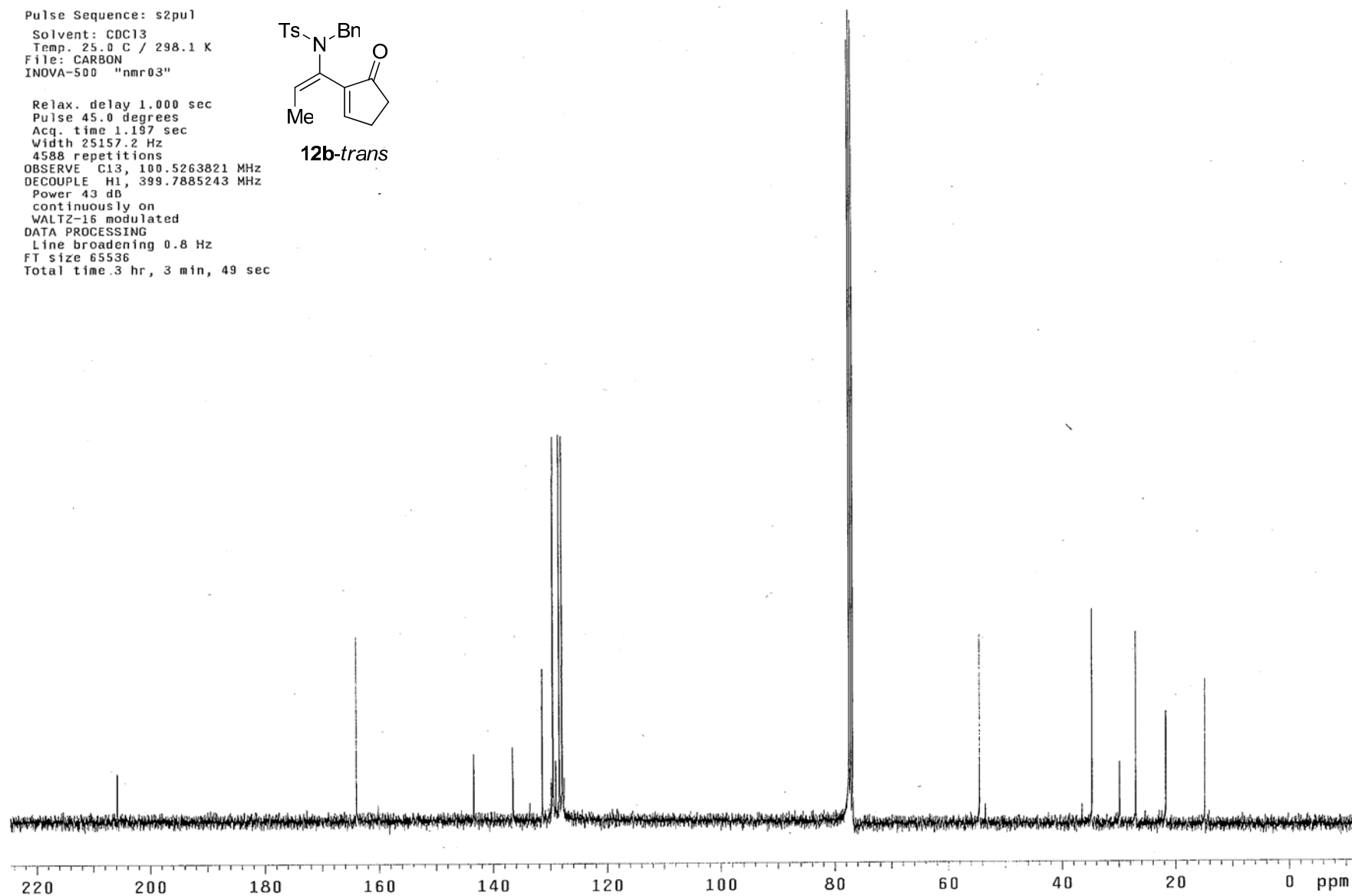
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn563-2-2_25Nov2013-16:42:23

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INDVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
4588 repetitions
OBSERVE C13, 100.5263821 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec



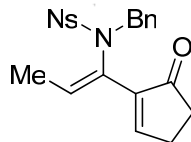
12b-trans



wxn553-2_18Oct2013

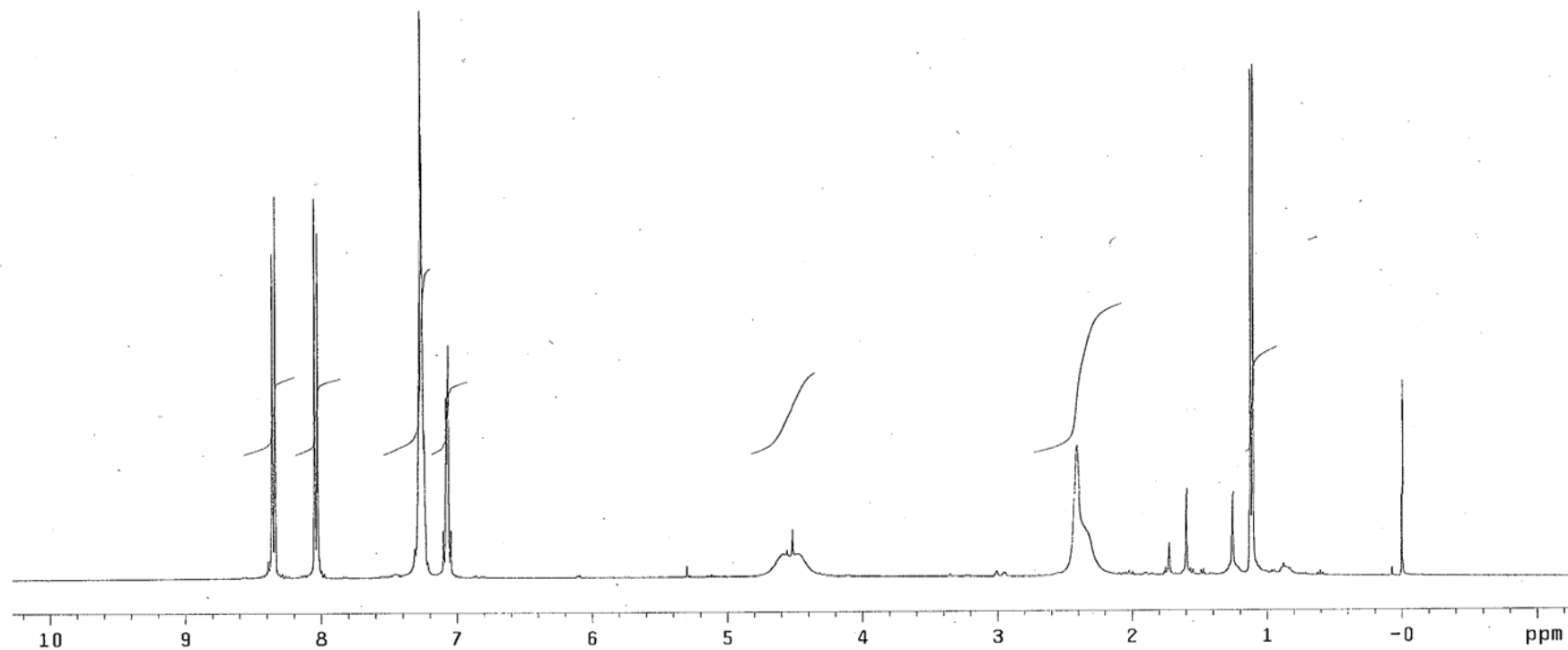
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-2_18Oct2013

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: PROTON
INOVA-500 "nmr03"



12c-cis

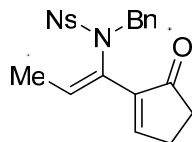
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.754 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7865218 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 57 sec



wxn553-2_18Oct2013-21:59:33

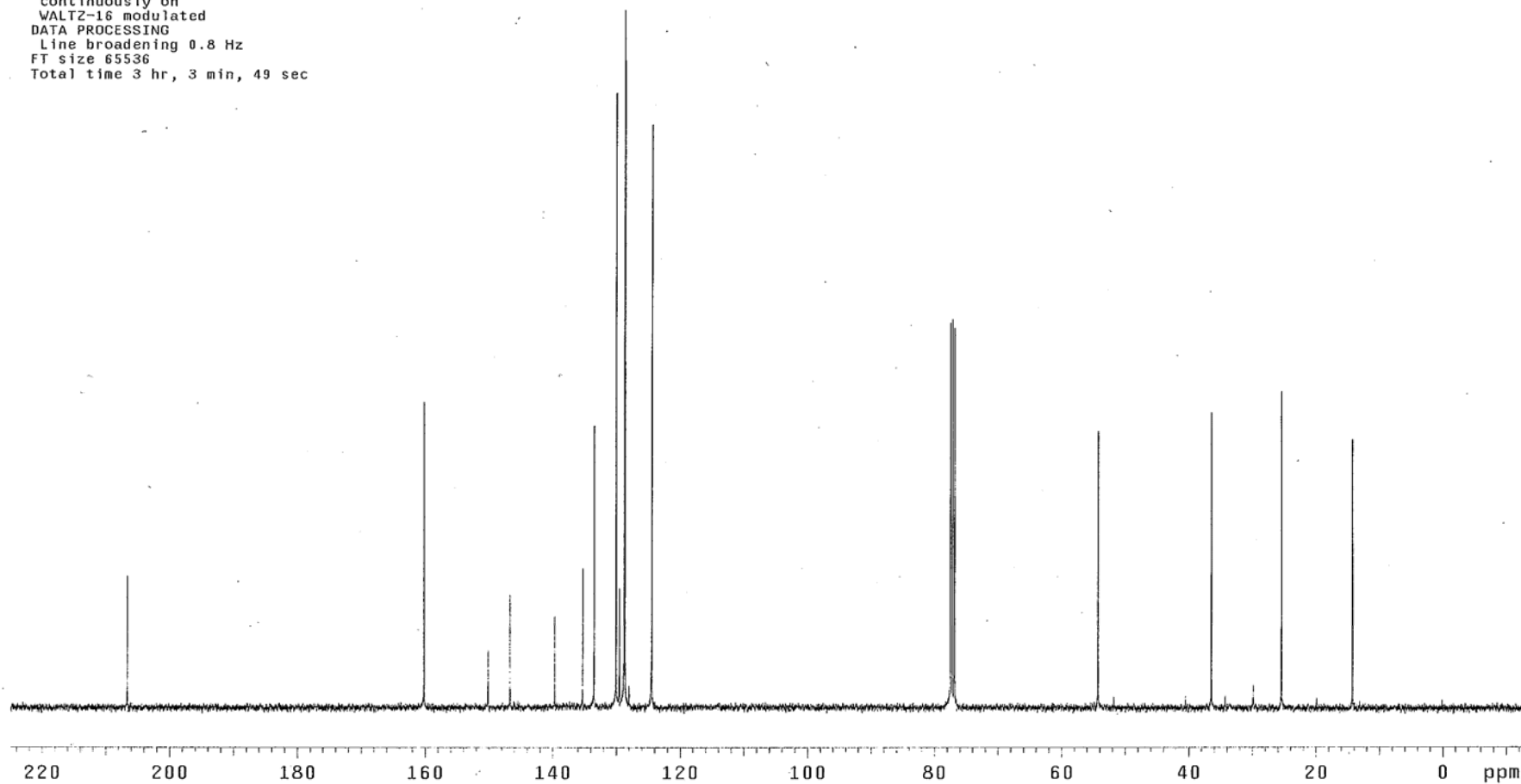
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-2_18Oct2013-21:59:33

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: CARBON
INNOVA-500 "nmr03"



12c-cis

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.197 sec
Width 25157.2 Hz
5000 repetitions
OBSERVE C13, 100.5263829 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 3 hr, 3 min, 49 sec

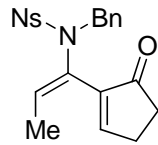


wxn553-3_18Oct2013

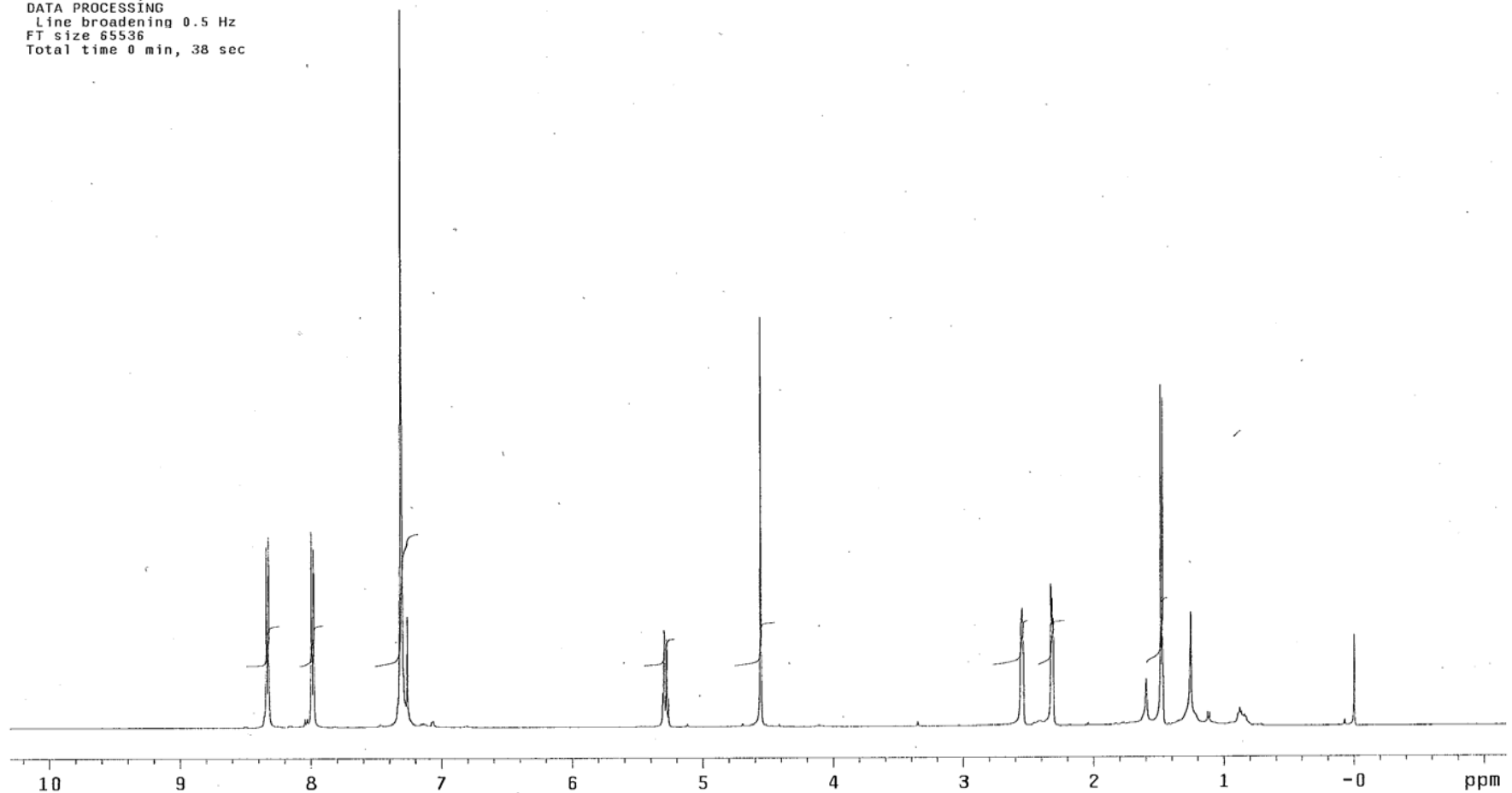
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-3_18Oct2013

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 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288158 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



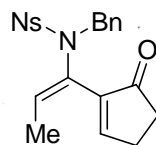
12c-trans



wxn553-3_18Oct2013-22:05:45

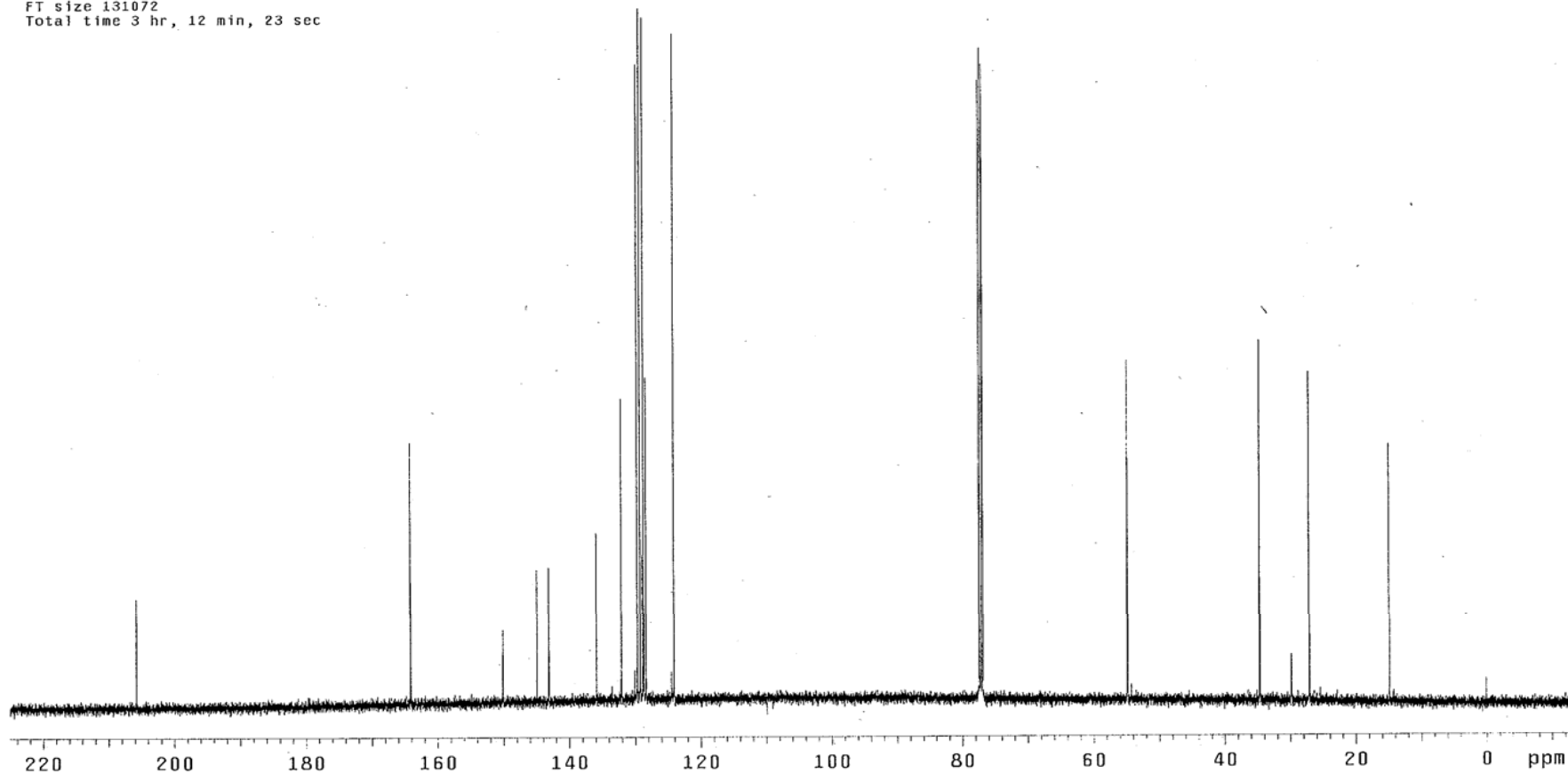
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-3_18Oct2013-22:05:45

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: CARBON
INOVA-500 "nmr03"



12c-trans

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.299 sec
Width 31446.5 Hz
5000 repetitions
OBSERVE C13, 125.6568876 MHz
DECOUPLE H1, 499.7312897 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 3 hr, 12 min, 23 sec



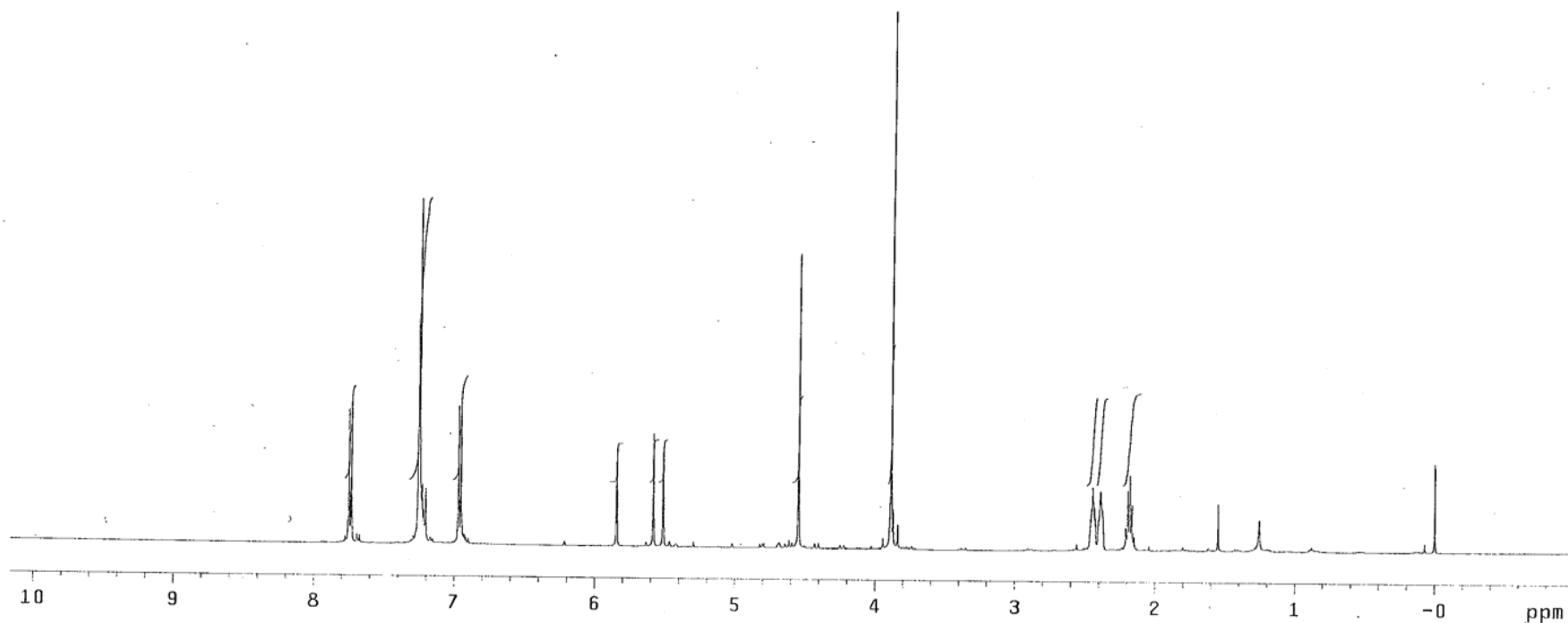
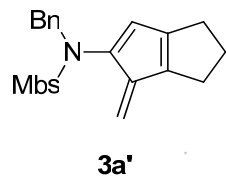
wxn636-641-1_01Mar2014

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn636-641-1_01Mar2014

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 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288183 MHz
DATA PROCESSING
Line broadening 0.5 Hz
ET size 65536
Total time 0 min, 38 sec



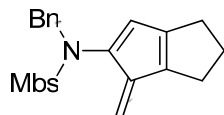
wxn636-641-1_01Mar2014

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn636-641-1_01Mar2014

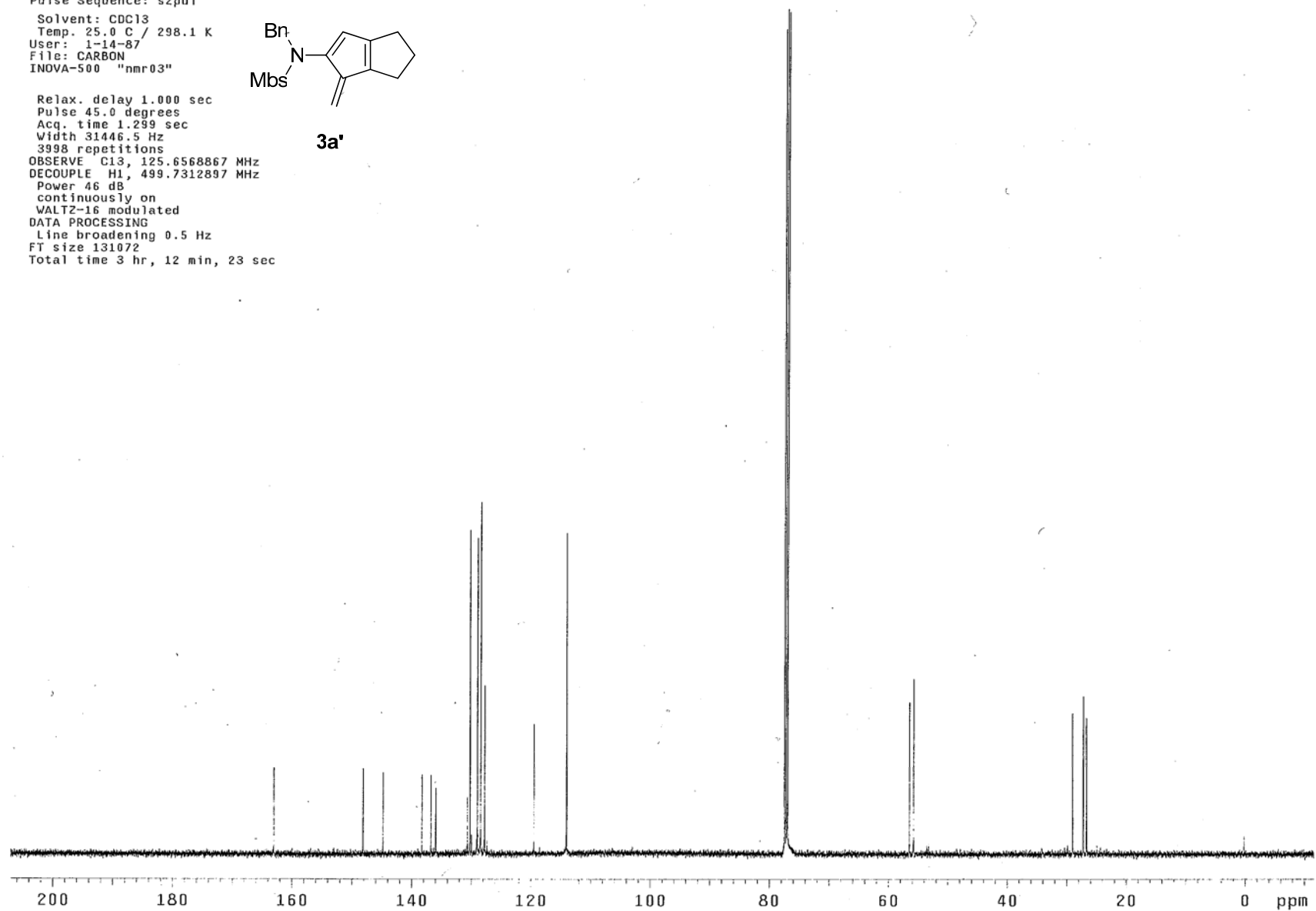
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: CARBON
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.299 sec
Width 31446.5 Hz
3998 repetitions
OBSERVE C13, 125.6568867 MHz
DECOUPLE H1, 499.7312897 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 3 hr, 12 min, 23 sec



3a'



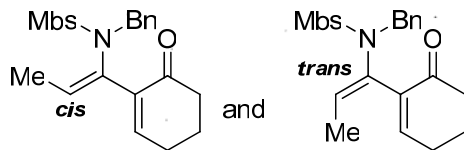
wxn641-636-624-1_01Mar2014

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn641-636-624-1_01Mar2014

Pulse Sequence: s2pul

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

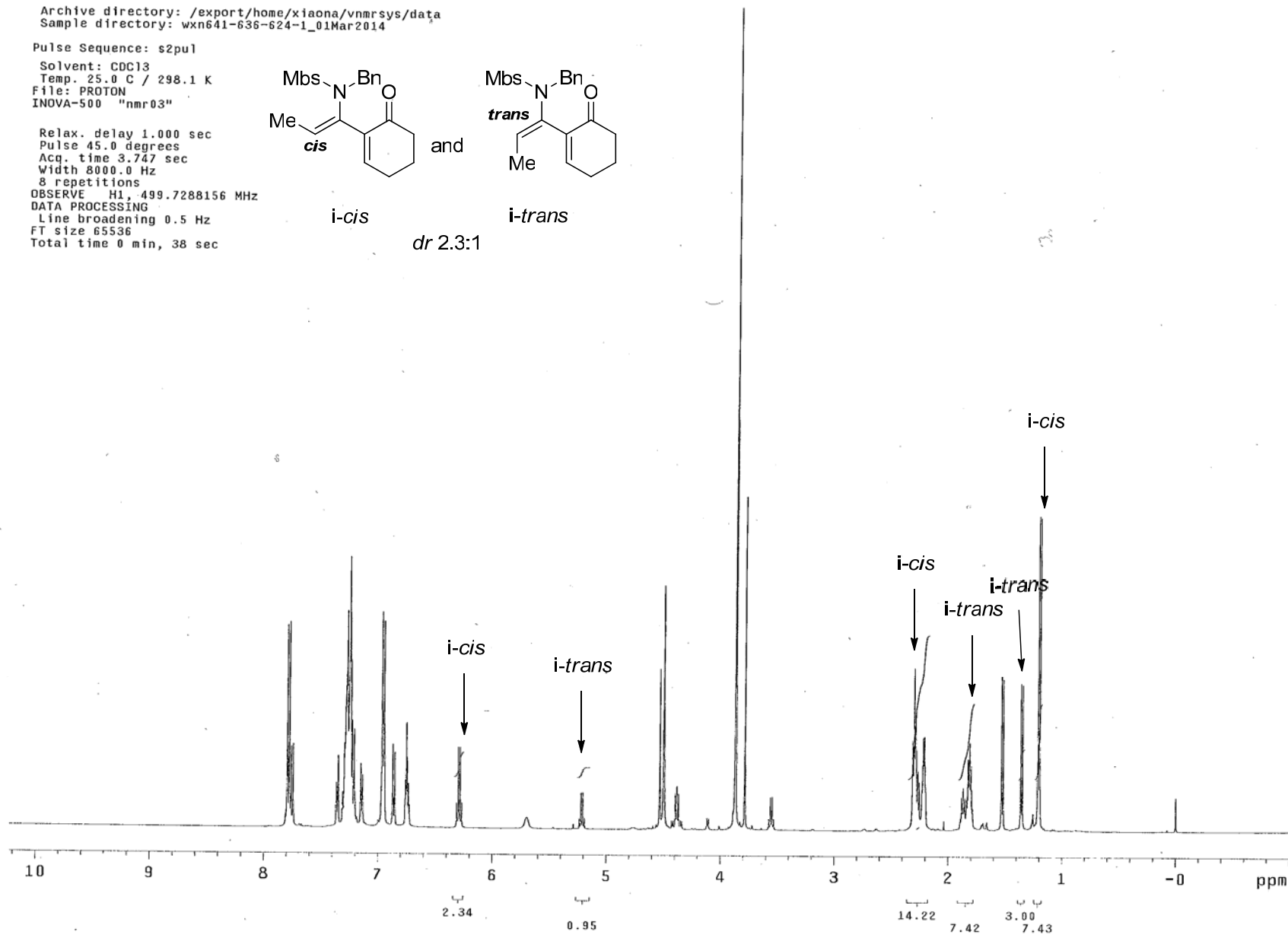
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.747 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7288156 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 38 sec



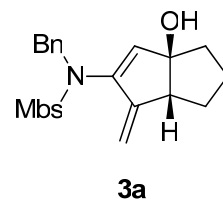
i-cis

i-trans

dr 2.3:1



DEPT, COSY, NOESY, HMQC and HMBC for **3a**



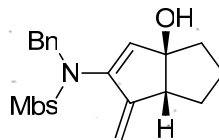
wxn429-2_12Apr2013-10:34:43

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn429-2_12Apr2013-10:34:43

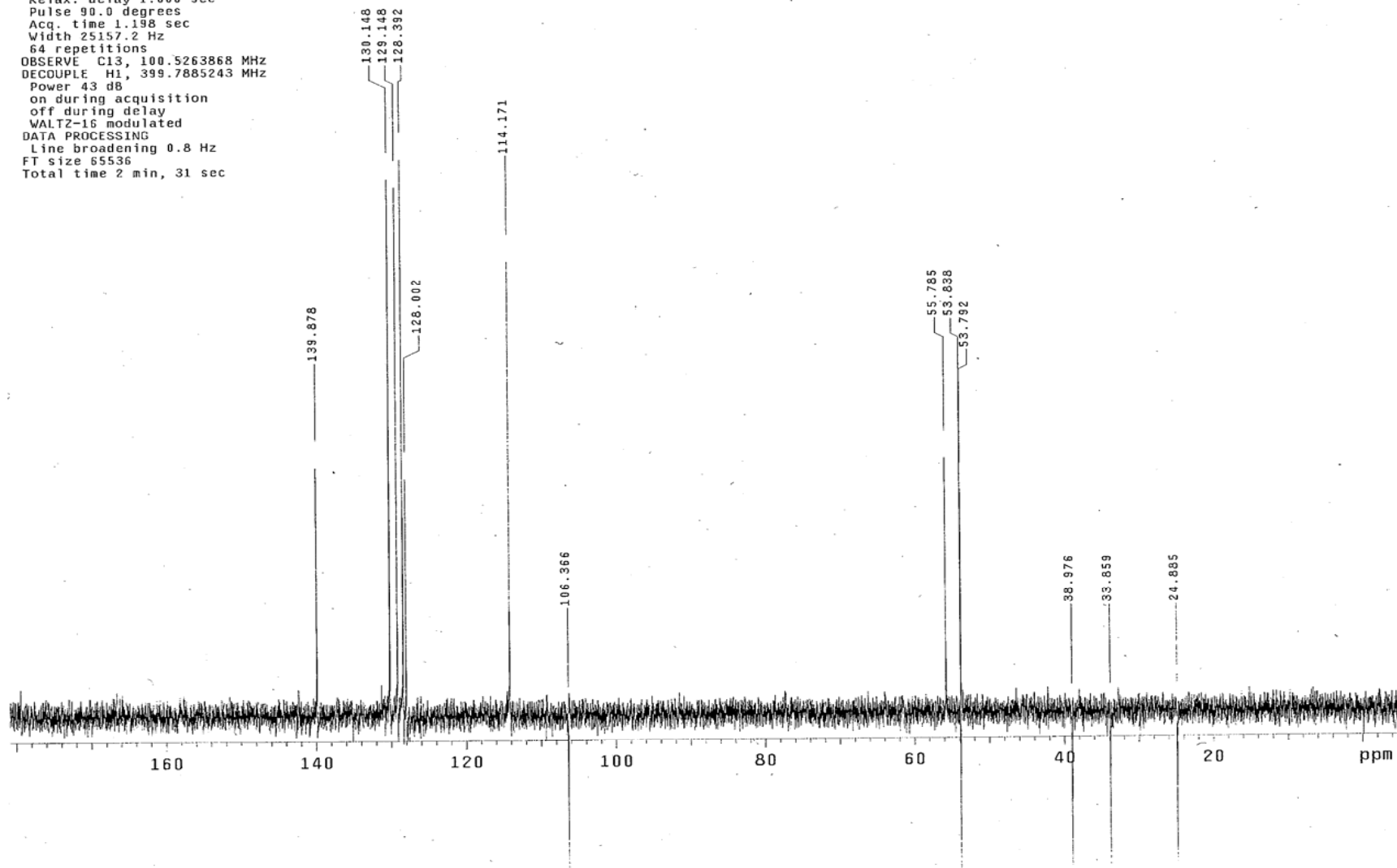
Pulse Sequence: DEPT

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

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.198 sec
Width 25157.2 Hz
64 repetitions
OBSERVE C13, 100.5263868 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 2 min, 31 sec



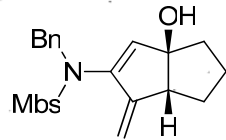
3a



wxn429-2_11Mar2013

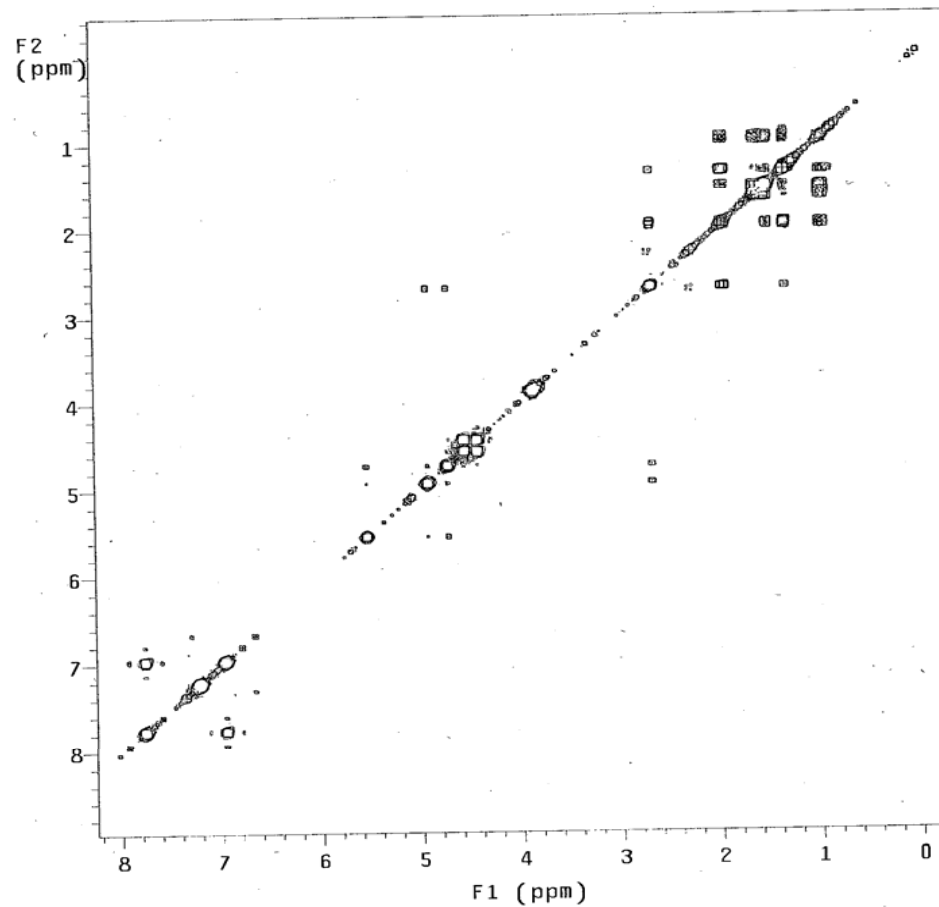
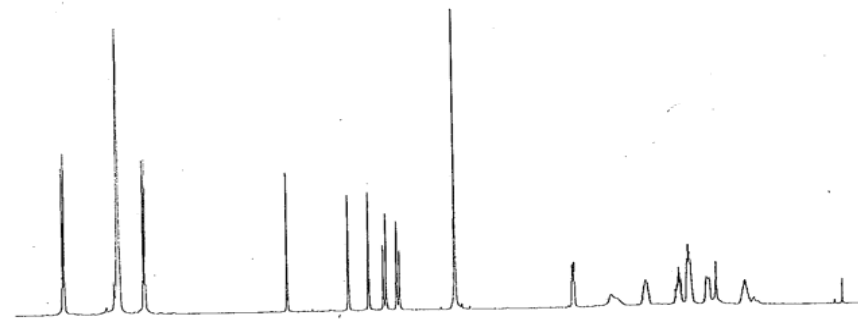
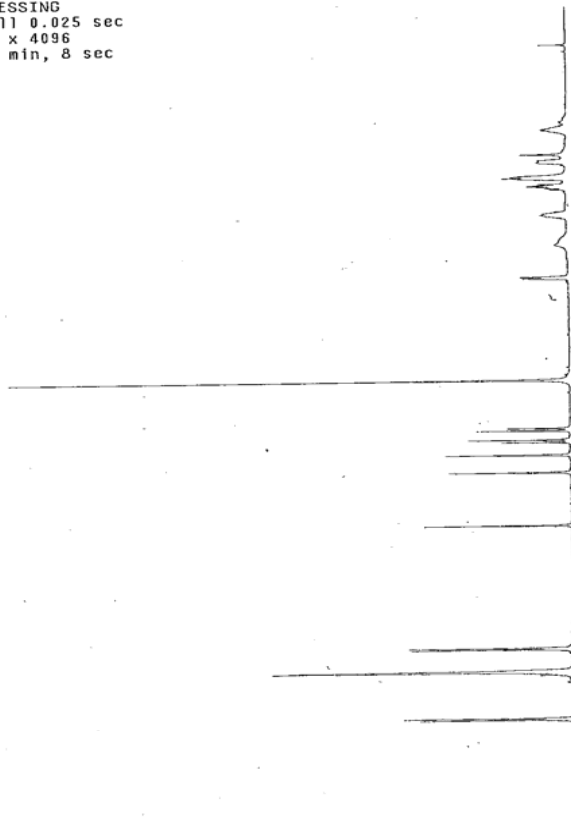
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn429-2_11Mar2013

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



3a

Relax. delay 1.000 sec.
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
Single scan
200 increments
OBSERVE H1, 499.7288170 MHz
DATA PROCESSING
Sq. sine bell 0.064 sec
F1 DATA PROCESSING
Sq. sine bell 0.025 sec
FT size 4096 x 4096
Total time 4 min, 8 sec



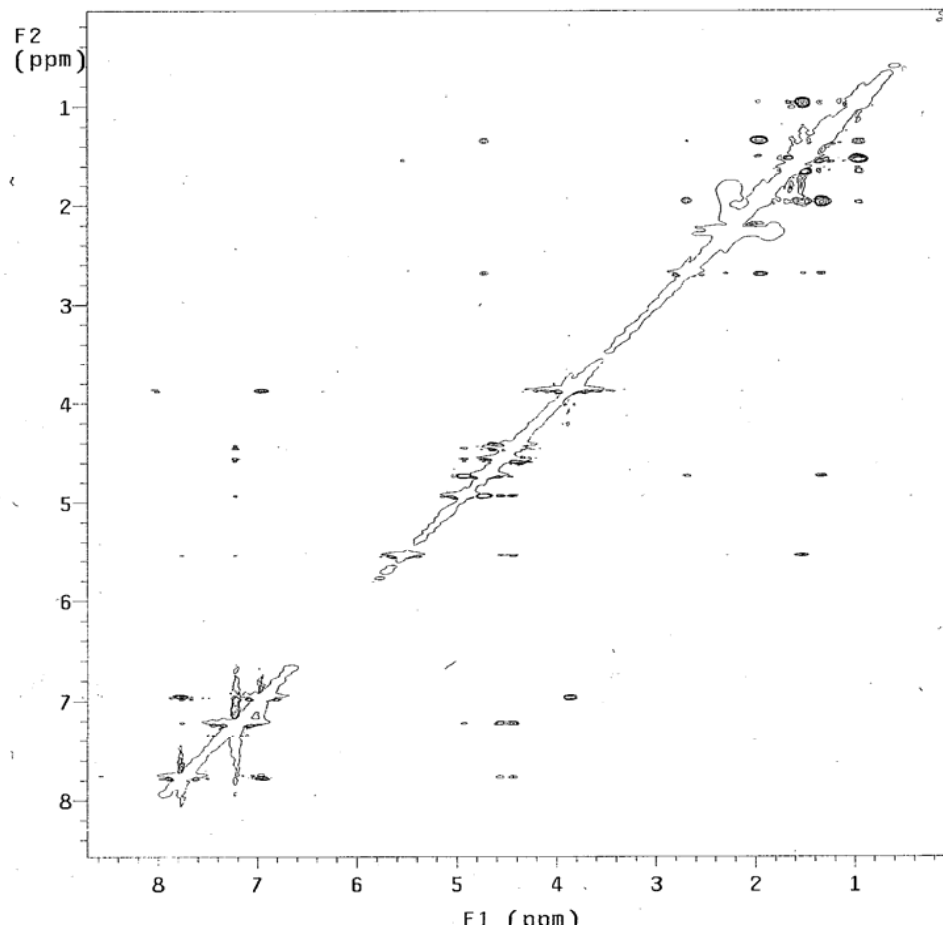
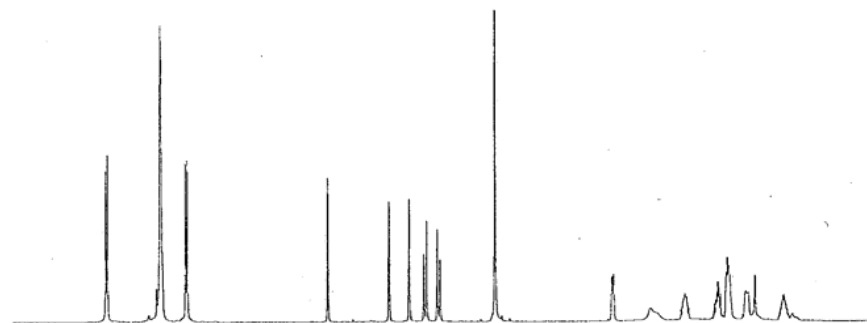
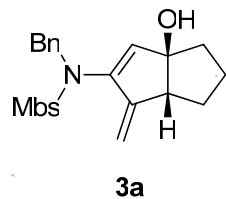
wxn429-2_11Mar2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn429-2_11Mar2013

Pulse Sequence: NOESY

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

Relax. delay 2.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 128 increments
OBSERVE H1, 499.7288170 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.015 sec
FT size 4096 x 4096
Total time 2 hr, 41 min, 39 sec



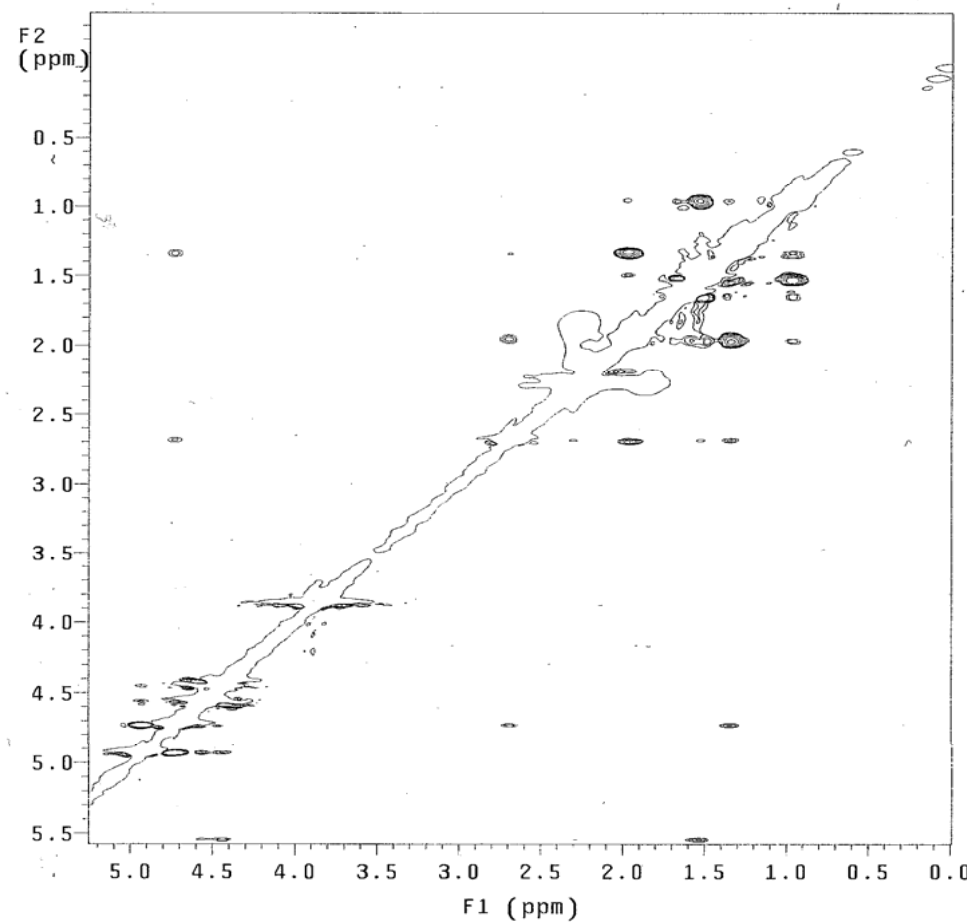
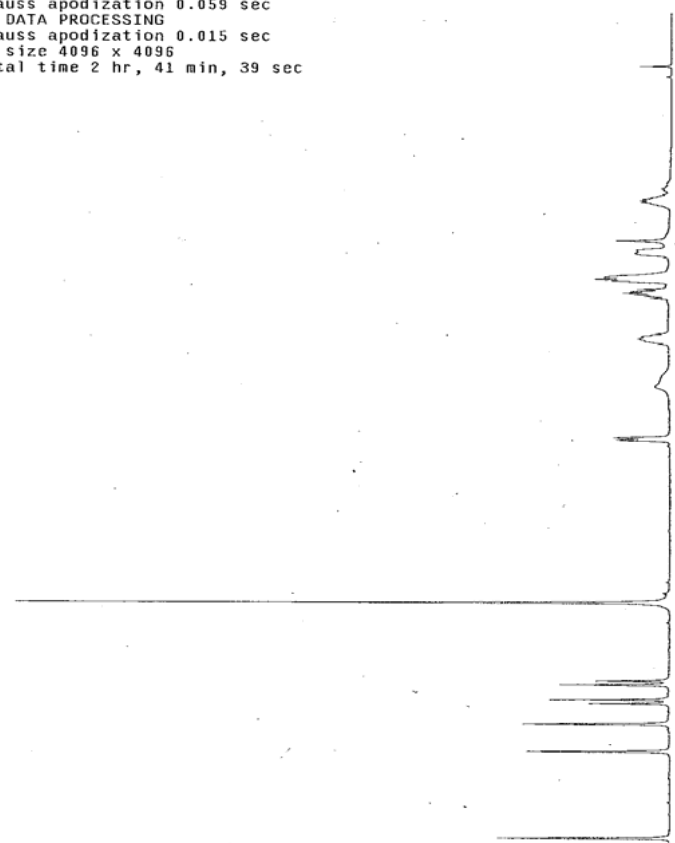
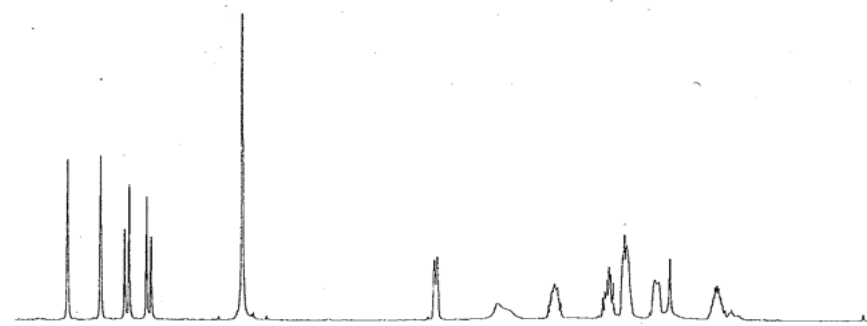
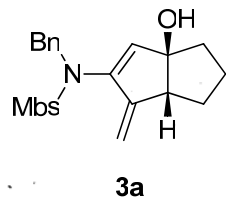
wxn429-2_11Mar2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn429-2_11Mar2013

Pulse Sequence: NOESY

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

Relax. delay 2.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 128 increments
OBSERVE H1, 499.7288170 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.015 sec
FT size 4096 x 4096
Total time 2 hr, 41 min, 39 sec



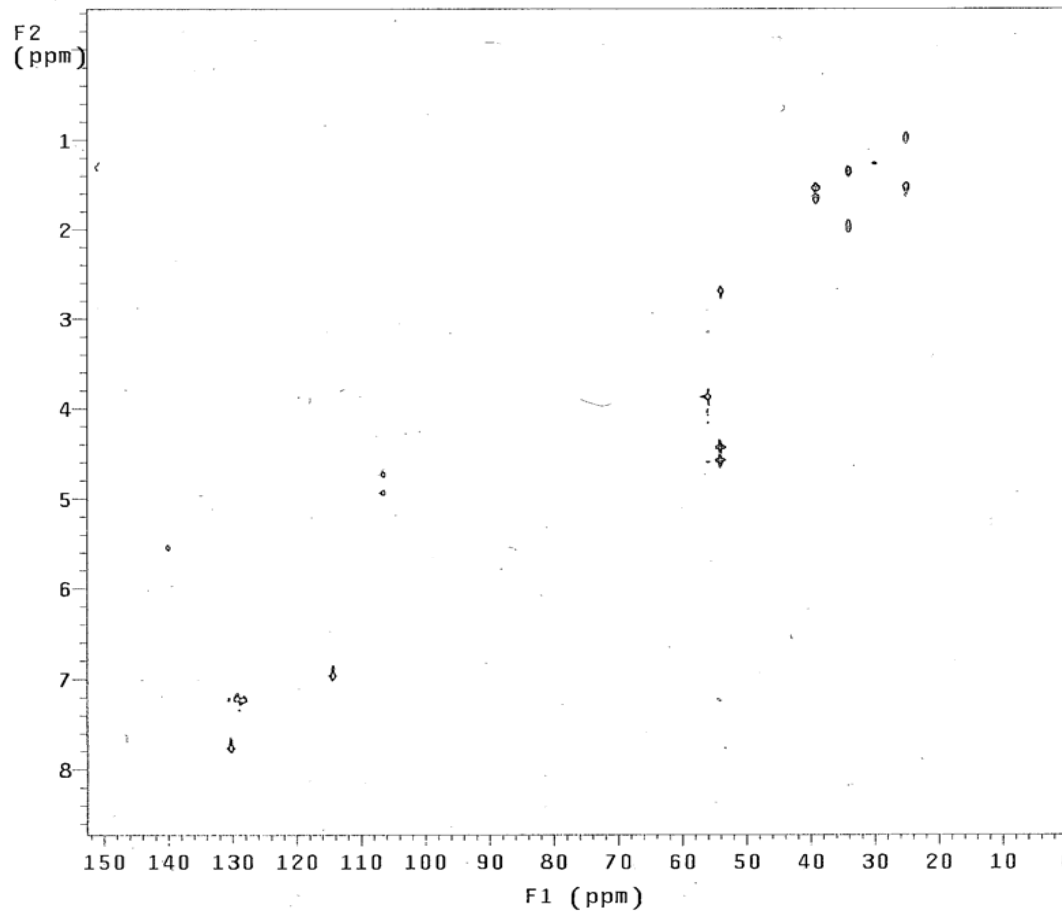
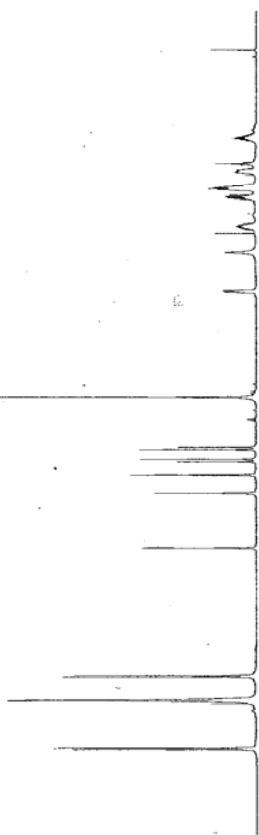
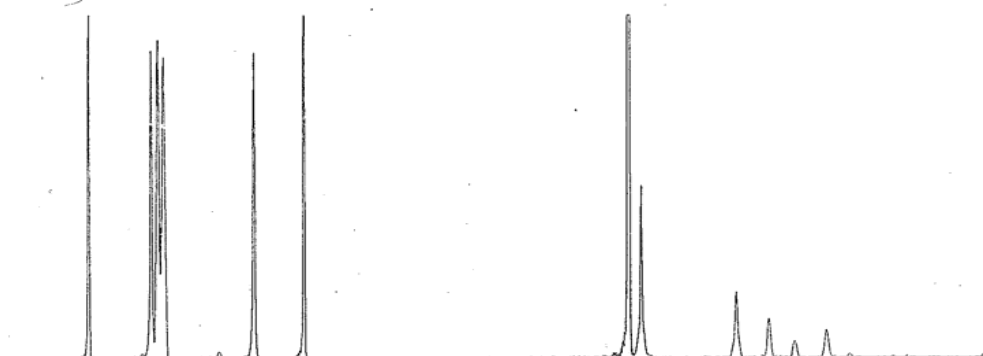
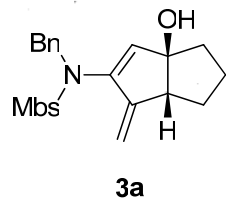
wxn429-2_09Mar2013-22:49:47

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn429-2_09Mar2013-22:49:47

Pulse Sequence: gHMQC

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

Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 25133.5 Hz
4 repetitions
2 x 256 increments
OBSERVE H1, 499.7288153 MHz
DECOUPLE C13, 125.6681836 MHz
Power 37 dB
on during acquisition
off during delay
W40_qn6121 modulated
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.019 sec
FT size 2048 x 4096
Total time 41 min, 3 sec

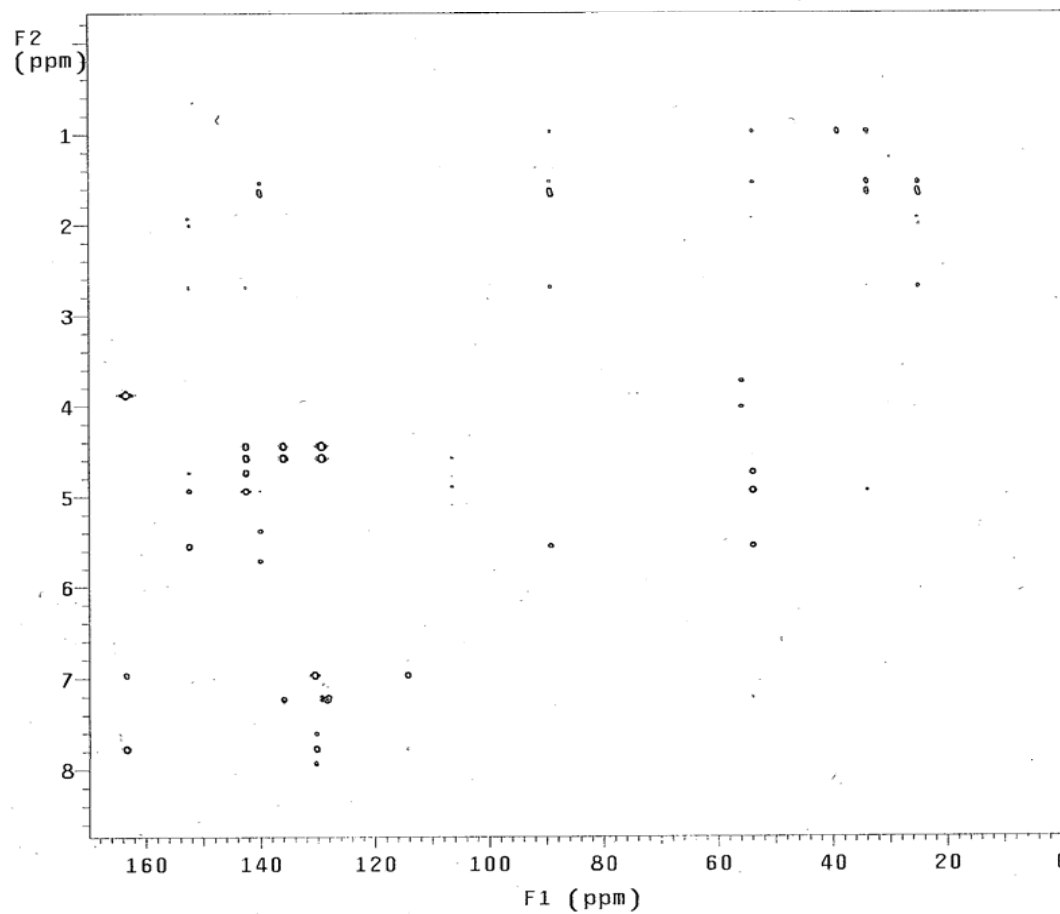
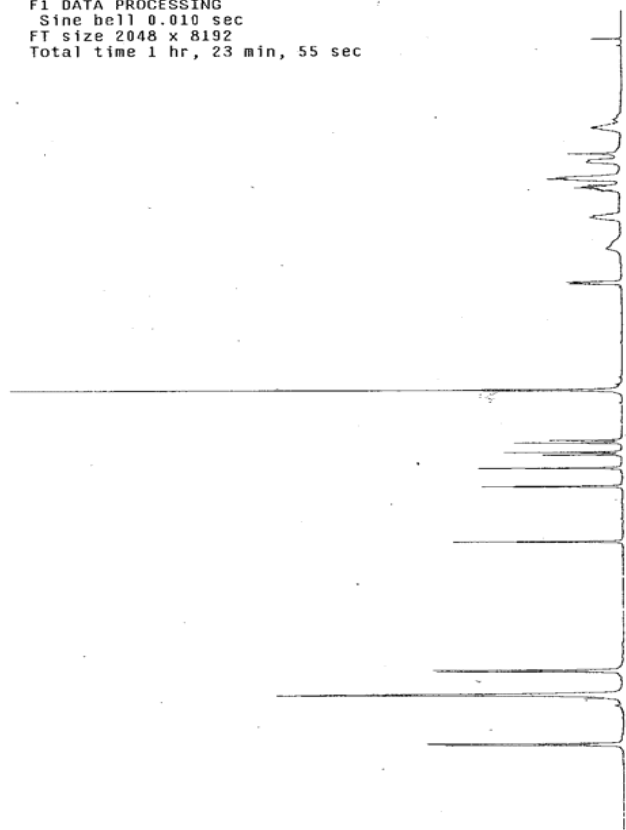
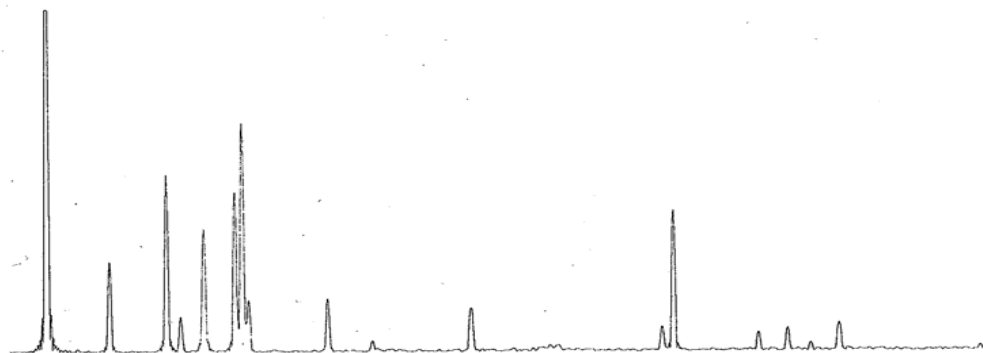
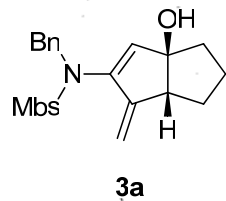


wxn429-2_11Mar2013

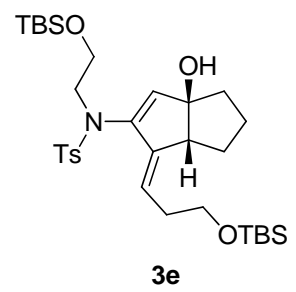
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn429-2_11Mar2013

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

Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 25133.5 Hz
8 repetitions
512 increments
OBSERVE H1, 499.7288170 MHz
DATA PROCESSING
Sine bell 0.064 sec
F1 DATA PROCESSING
Sine bell 0.010 sec
FT size 2048 x 8192
Total time 1 hr, 23 min, 55 sec



NOESY for **3e**



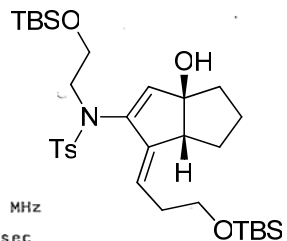
wxn518-3_30Sep2013-14:24:46

Archive directory: /export/home/xiaona/vnarsys/data
Sample directory: wxn518-3_30Sep2013-14:24:46

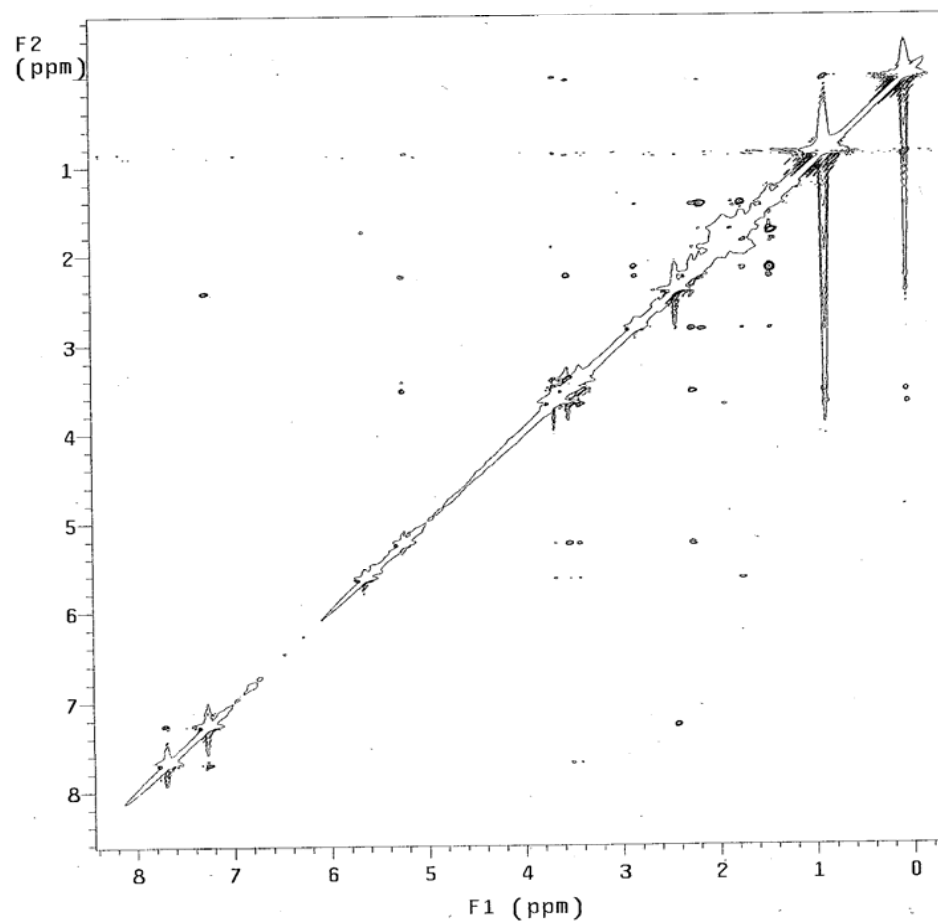
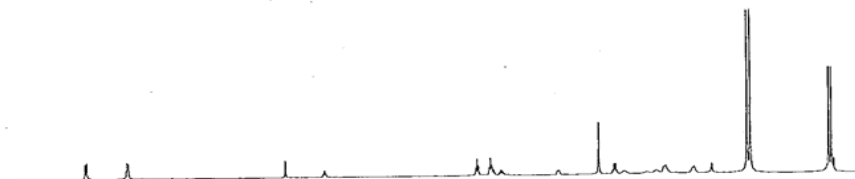
Pulse Sequence: NOESY

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

Relax. delay 2.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 499.7288163 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.030 sec
FT size 4096 x 4096
Total time 5 hr, 23 min, 8 sec



3e



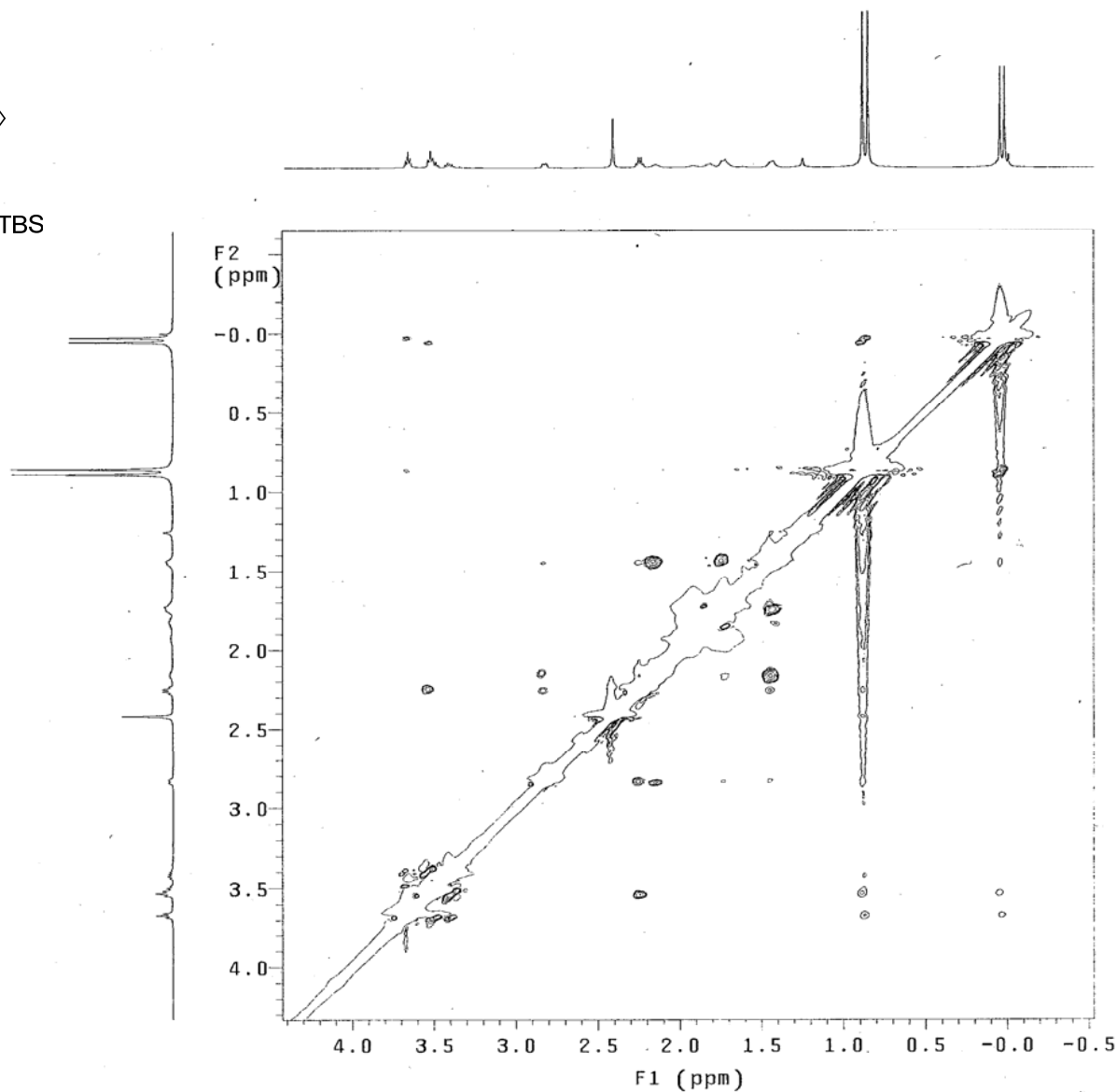
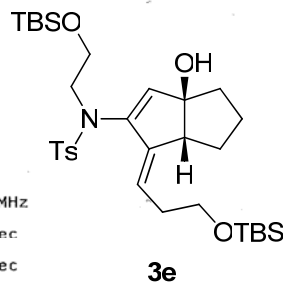
wxn518-3_30Sep2013-14:24:46

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn518-3_30Sep2013-14:24:46

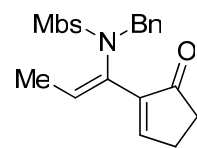
Pulse Sequence: NOESY

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

Relax. delay 2.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 499.7288163 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.030 sec
FT size 4096 x 4096
Total time 5 hr, 23 min, 8 sec



DEPT and NOESY for **12a-cis**

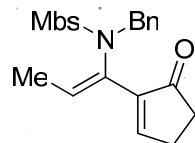


12a-cis

wxn528-4_17Sep2013

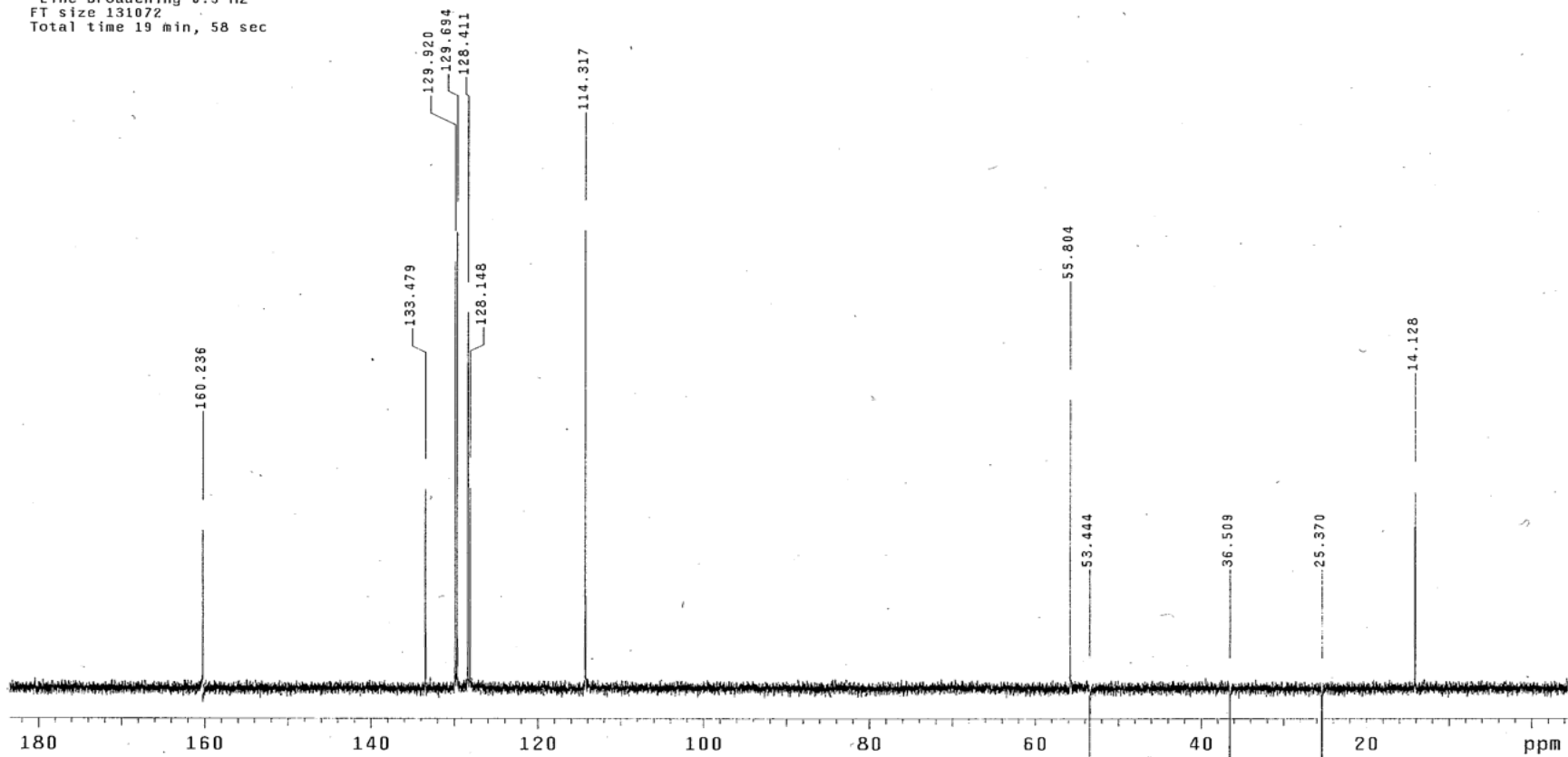
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn528-4_17Sep2013

Pulse Sequence: DEPT
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: DEPT
INOVA-500 "nmr03"



12a-cis

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.299 sec
Width 31446.5 Hz
512 repetitions
OBSERVE C13, 125.6568910 MHz
DECOUPLE H1, 499.7312897 MHz
Power 39 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 19 min, 58 sec



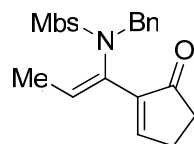
wxn528-4_04Dec2013-17:30:07

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn528-4_04Dec2013-17:30:07

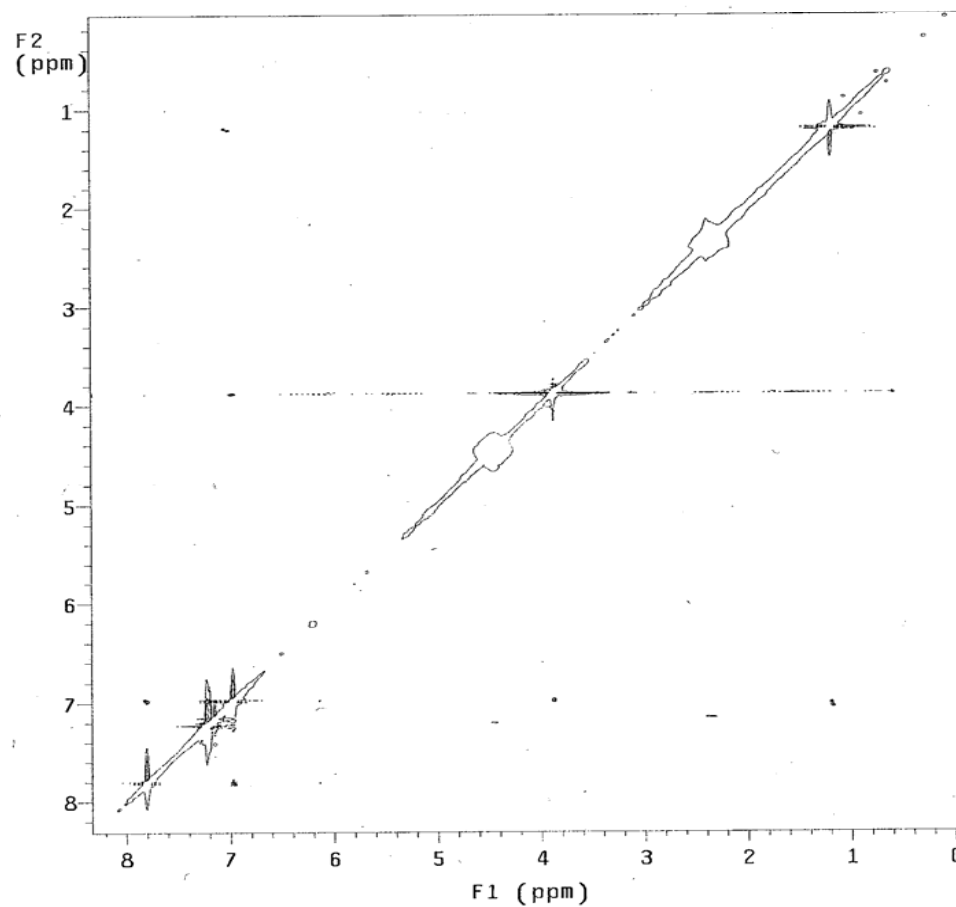
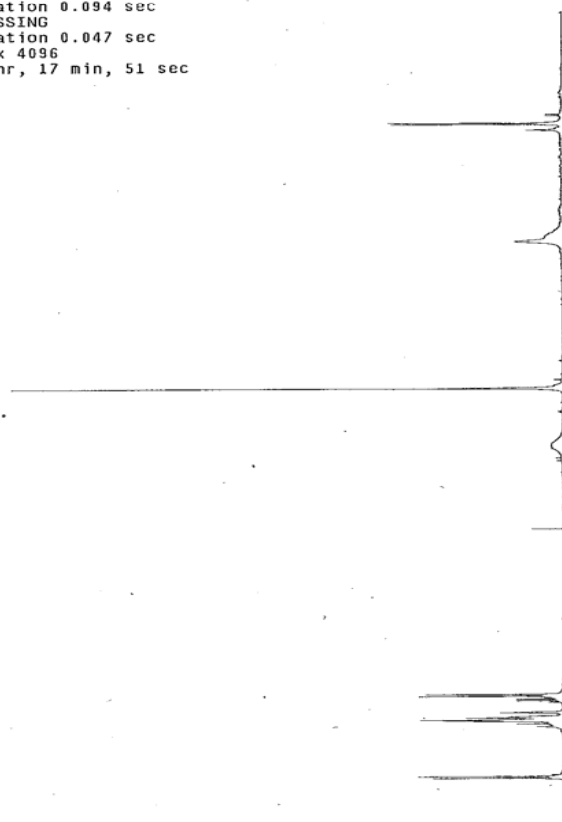
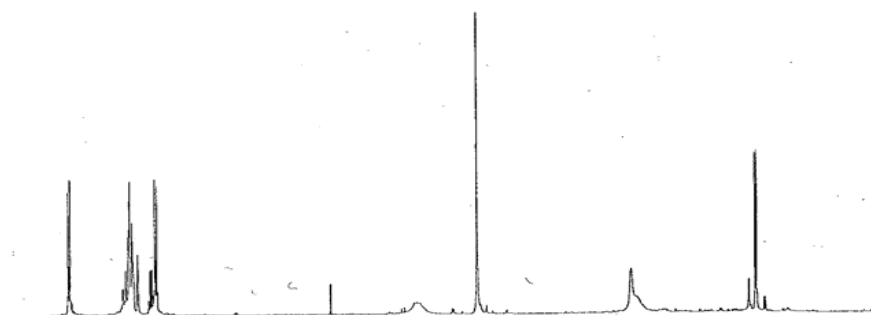
Pulse Sequence: NOESY

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

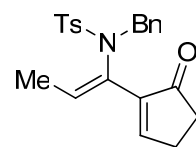
Relax. delay 1.000 sec
Mixing 0.200 sec
Acq. time 0.204 sec
Width 5008.8 Hz
2D Width 5006.3 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 499.7288149 MHz
DATA PROCESSING
Gauss apodization 0.094 sec
F1 DATA PROCESSING
Gauss apodization 0.047 sec
FT size 4096 x 4096
Total time 3 hr, 17 min, 51 sec



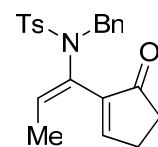
12a-cis



NOESY for **12b-cis** and **12b-trans**



12b-cis



12b-trans

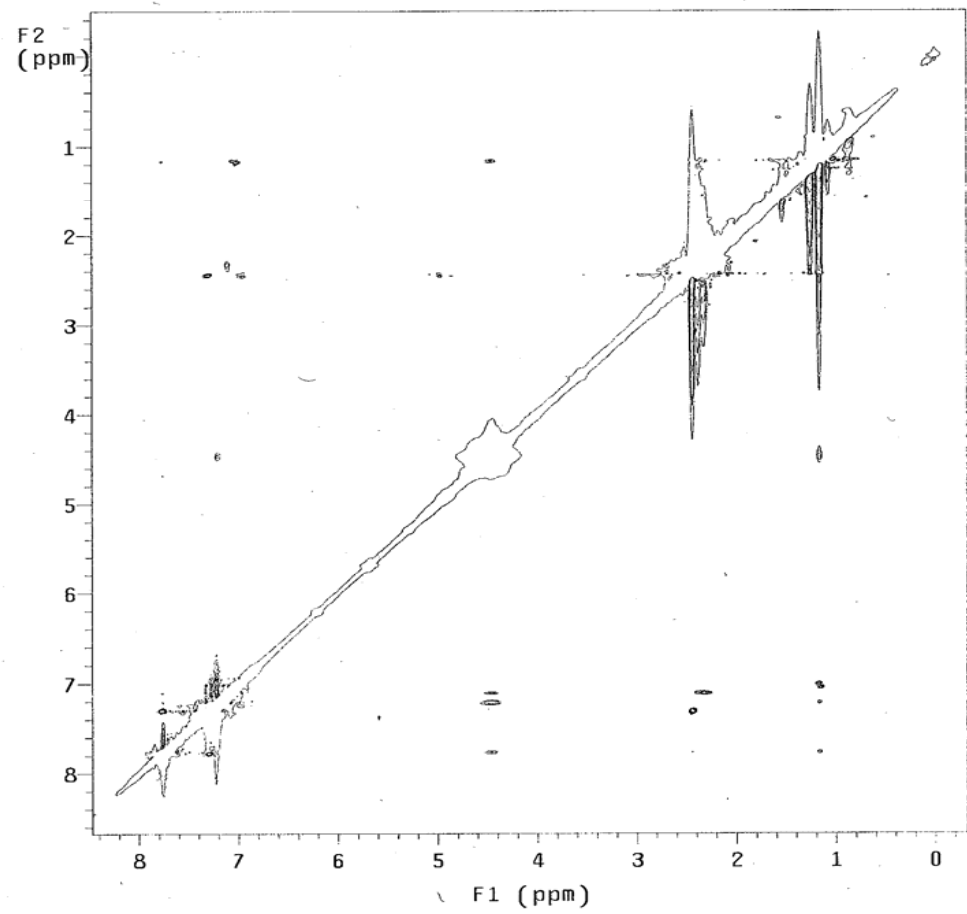
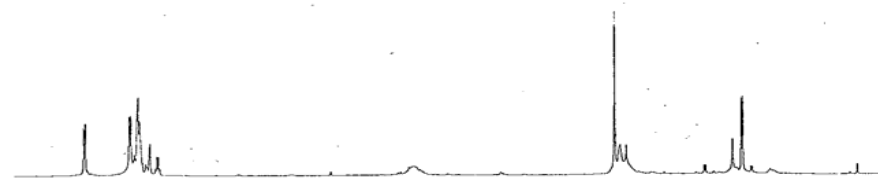
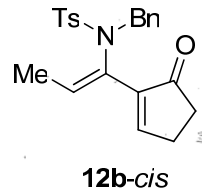
wxn563-1_05Dec2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn563-1_05Dec2013

Pulse Sequence: NOESY

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

Relax. delay 1.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 499.7288161 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.030 sec
FT size 4096 x 4096
Total time 3 hr, 6 min, 4 sec



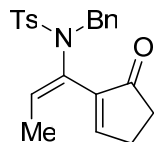
wxn563-2-2_05Dec2013

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn563-2-2_05Dec2013

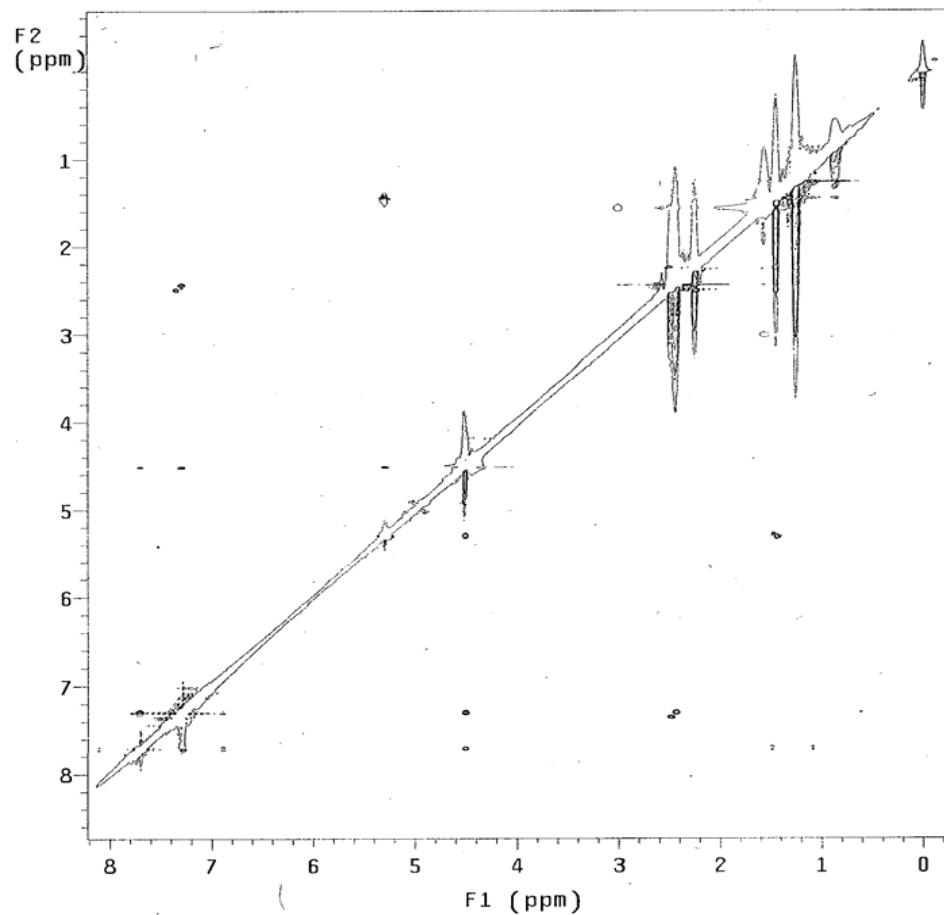
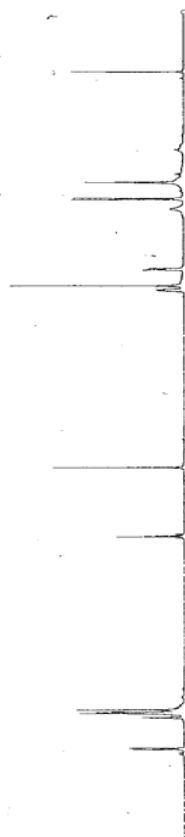
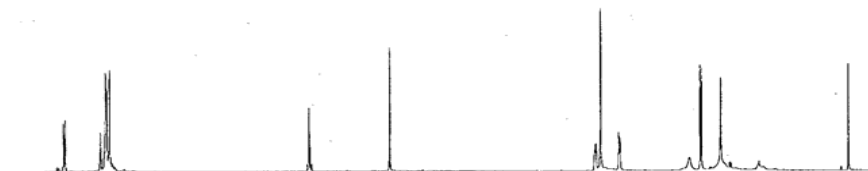
Pulse Sequence: NOESY

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

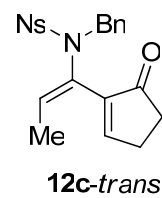
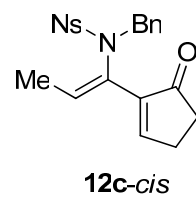
Relax. delay 1.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 499.7288170 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.030 sec
FT size 4096 x 4096
Total time 3 hr, 6 min, 4 sec



12b-trans



DEPT , NOESY and HMQC for **12c-cis** and **12c-trans**

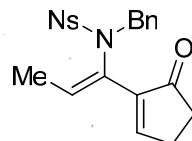


wxn553-2_19Oct2013-13:02:57

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-2_19Oct2013-13:02:57

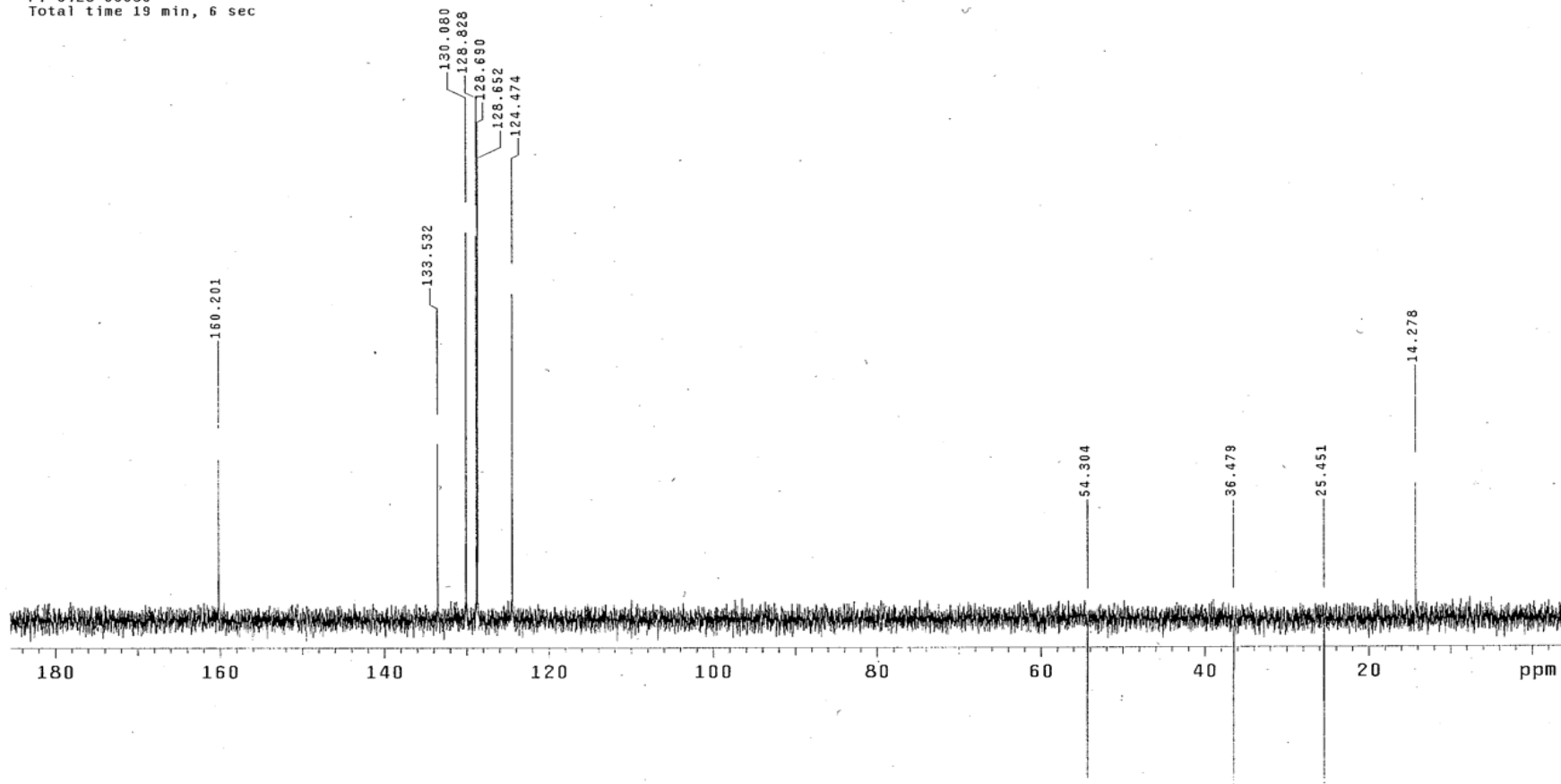
Pulse Sequence: DEPT

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



12c-cis

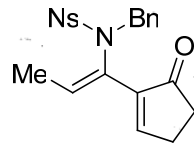
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.198 sec
Width 25157.2 Hz
160 repetitions
OBSERVE C13, 100.5263821 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 19 min, 6 sec



wxn553-2_19oct2013

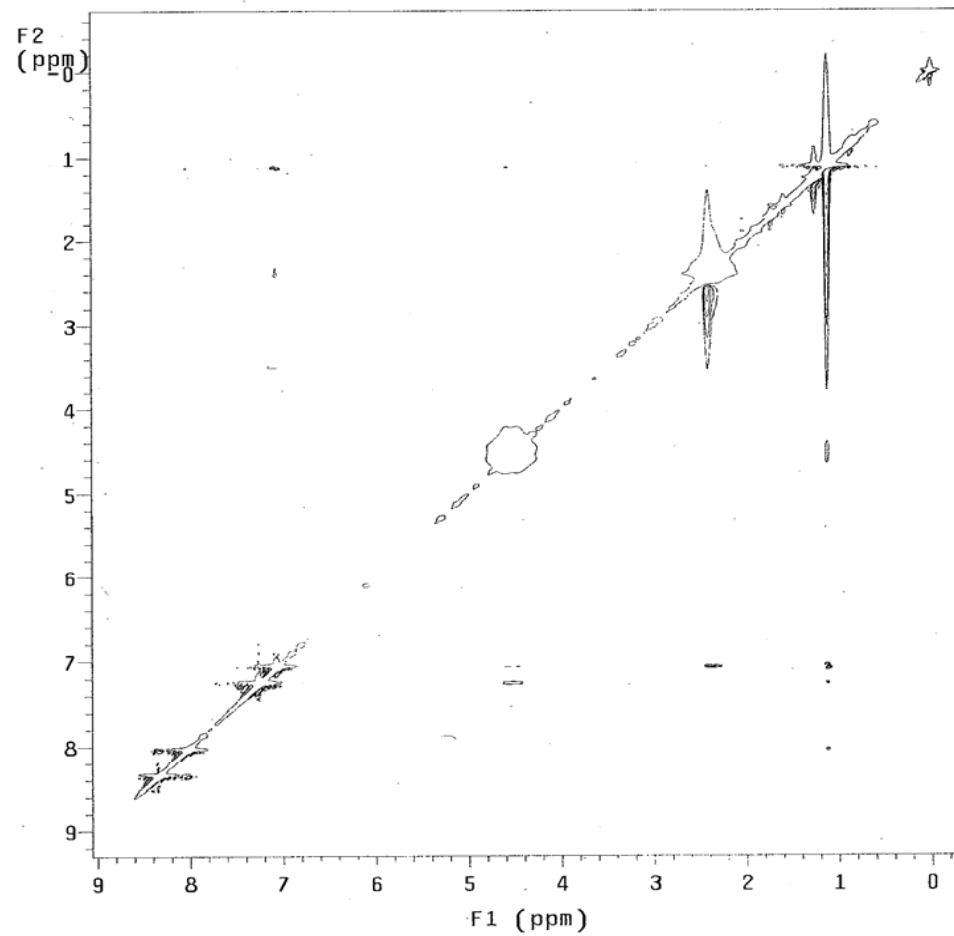
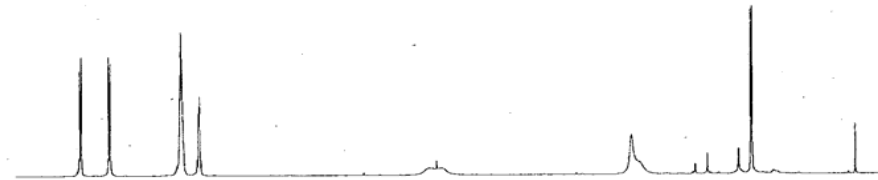
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-2_19oct2013

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



12c-cis

Relax. delay 2.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 499.7288153 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.030 sec
FT size 4096 x 4096
Total time 5 hr, 23 min, 8 sec



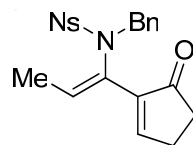
wxn553-2_18Oct2013-21:59:33

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-2_18Oct2013-21:59:33

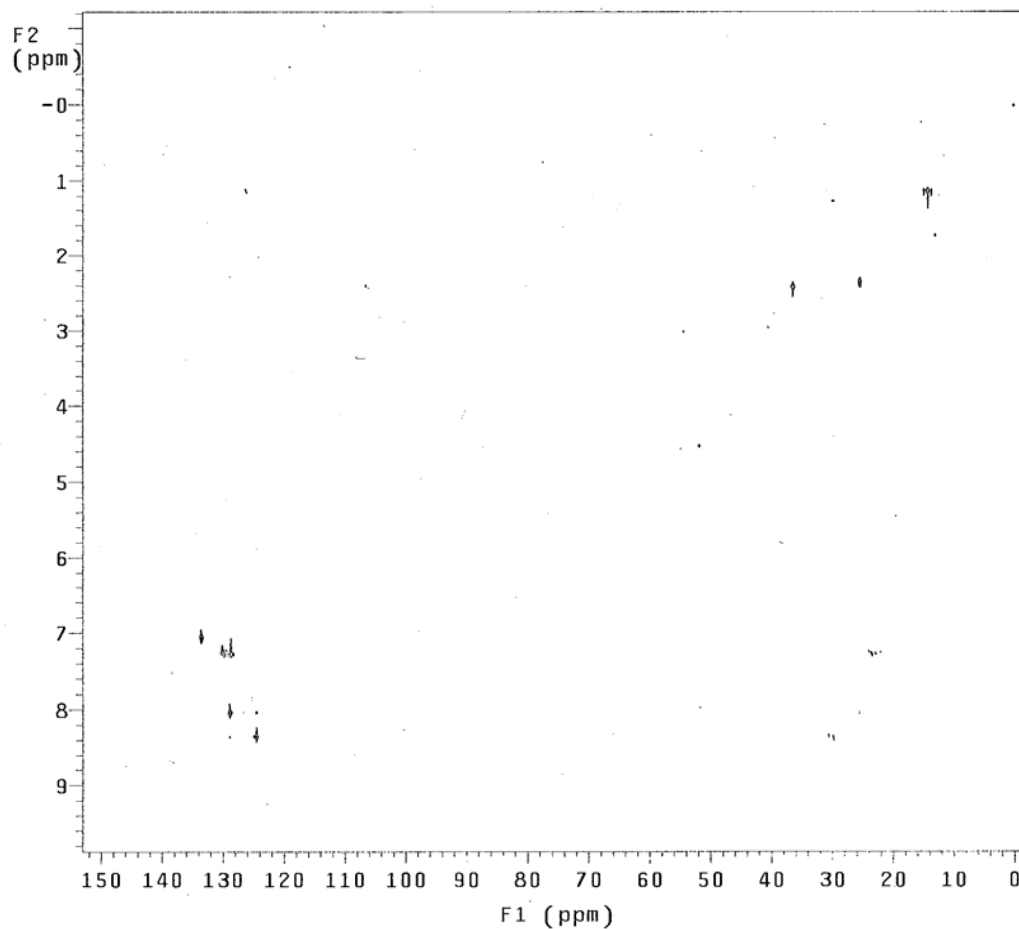
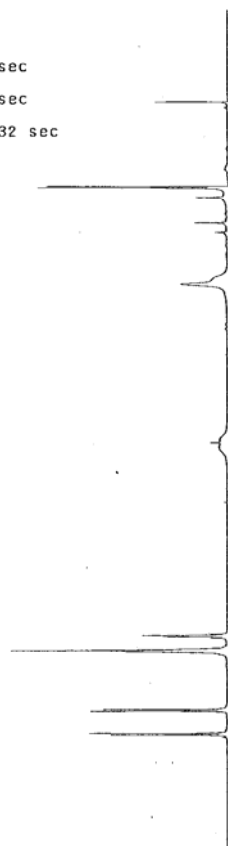
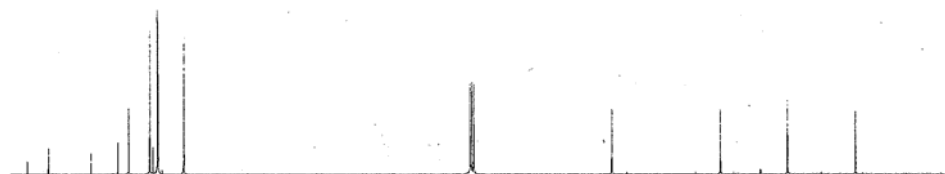
Pulse Sequence: gHMQC

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

Relax. delay 1.000 sec
Acq. time 0.160 sec
Width 6387.7 Hz
2D Width 17090.4 Hz
16 repetitions
2 x 512 increments
OBSERVE H1, 399.7865214 MHz
DECOUPLE C13, 100.5339172 MHz
Power 46 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Gauss apodization 0.074 sec
F1 DATA PROCESSING
Gauss apodization 0.055 sec
FT size 4096 x 8192
Total time 5 hr, 35 min, 32 sec



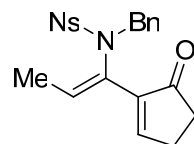
12c-cis



wxn553-2_18Oct2013-21:59:33

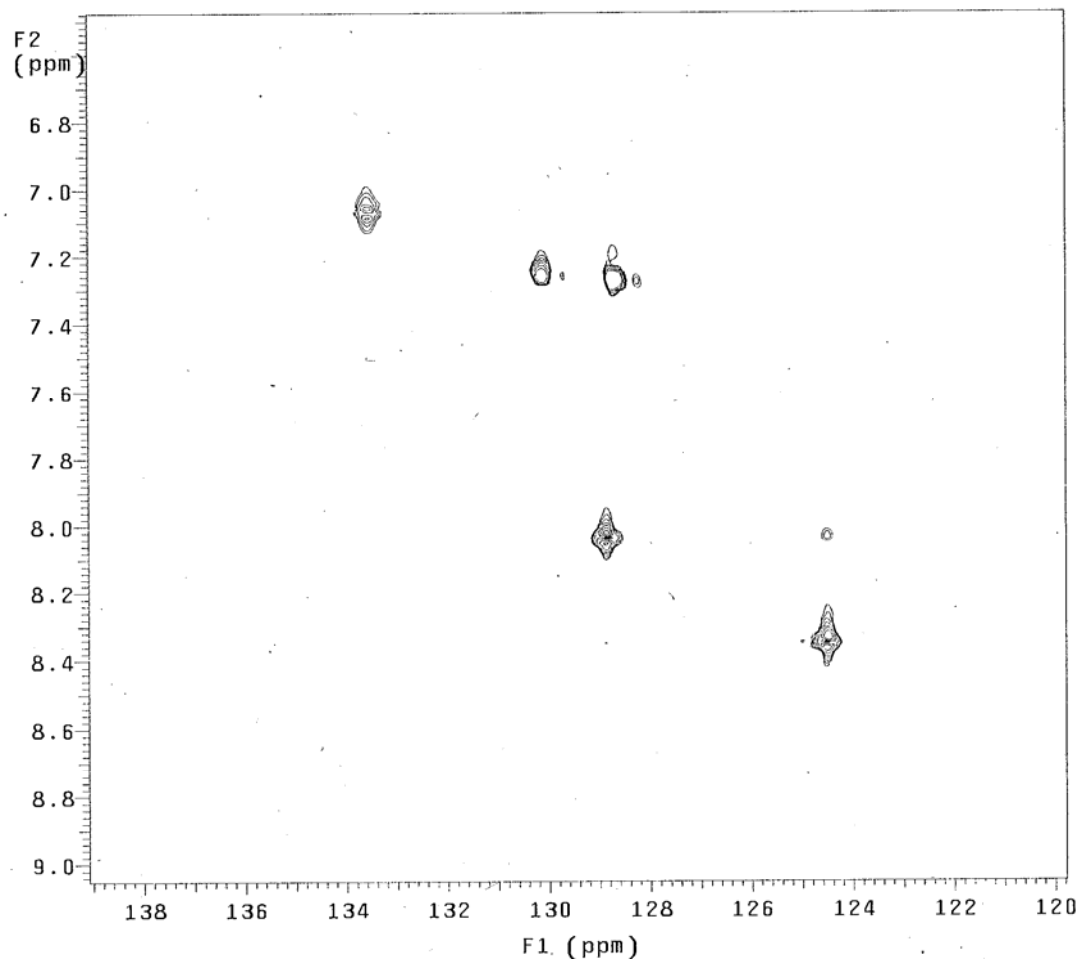
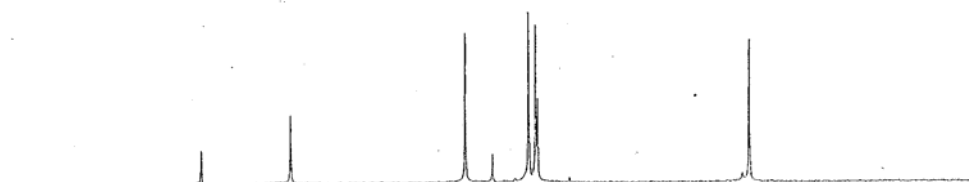
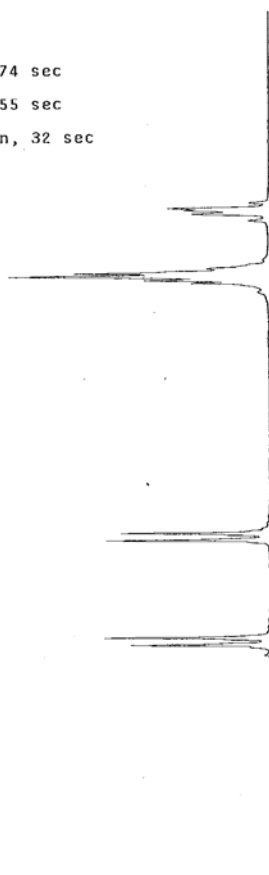
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-2_18Oct2013-21:59:33

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



12c-cis

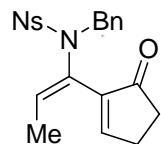
Relax. delay 1.000 sec
Acq. time 0.160 sec
Width 6387.7 Hz
2D Width 17090.4 Hz
16 repetitions
2 x 512 increments
OBSERVE H1, 399.7865214 MHz
DECOUPLE C13, 100.5339172 MHz
Power 46 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Gauss apodization 0.074 sec
F1 DATA PROCESSING
Gauss apodization 0.055 sec
FT size 2048 x 8192
Total time 5 hr, 35 min, 32 sec



wxn553-3_19Oct2013

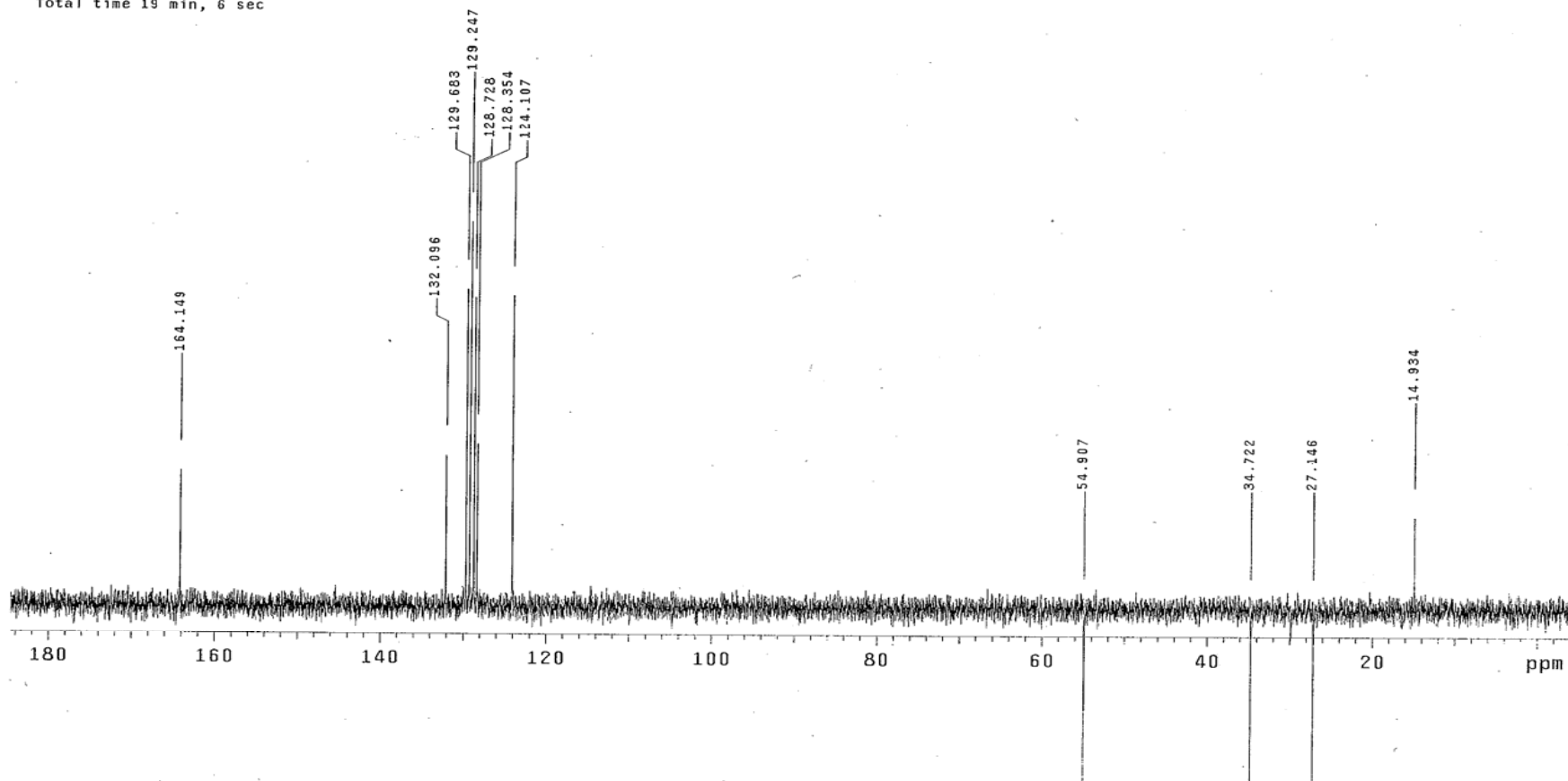
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-3_19Oct2013

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



12c-trans

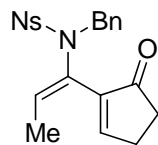
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.198 sec
Width 25157.2 Hz
320 repetitions
OBSERVE C13, 100.5263821 MHz
DECOUPLE H1, 399.7885243 MHz
Power 43 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 19 min, 6 sec



wxn553-3_18Oct2013-22:05:45

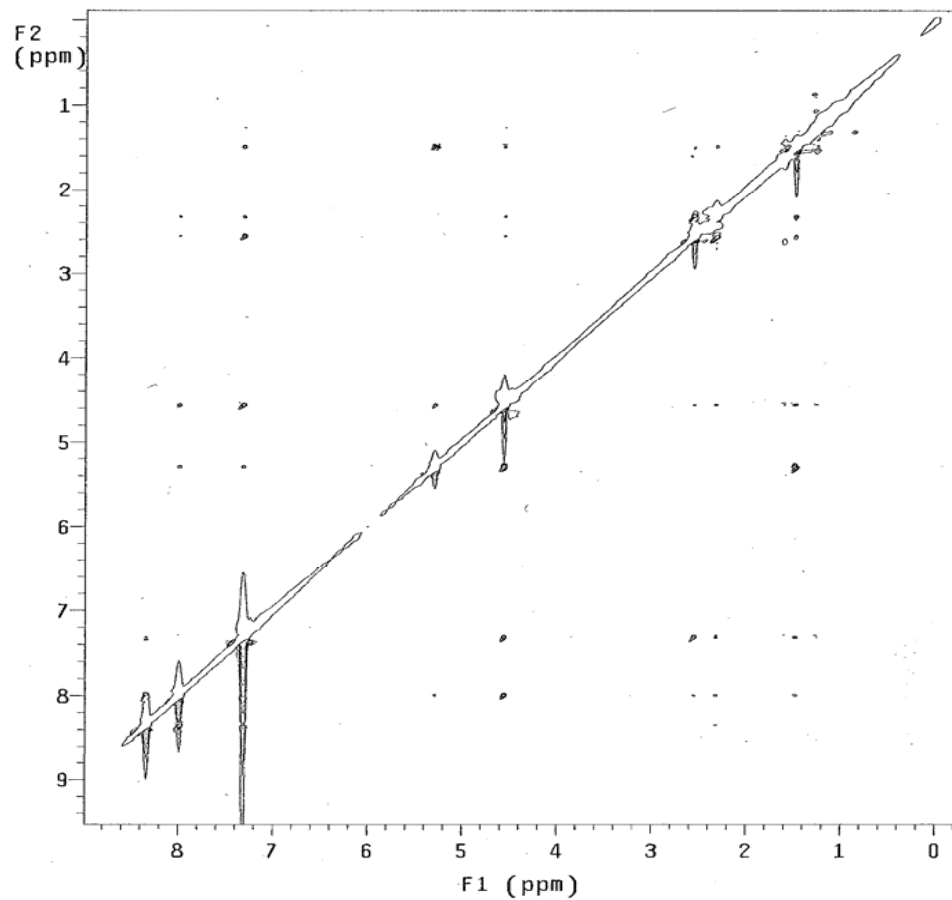
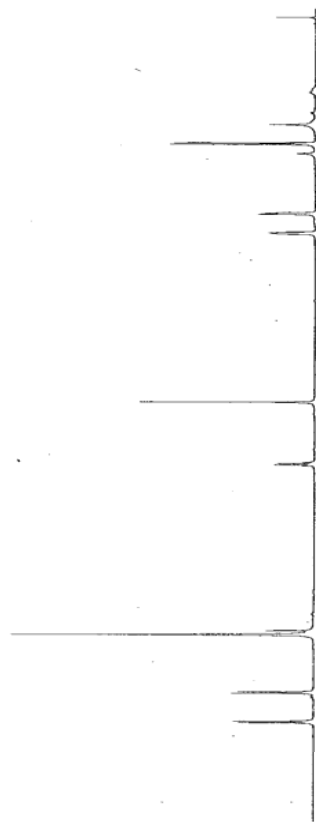
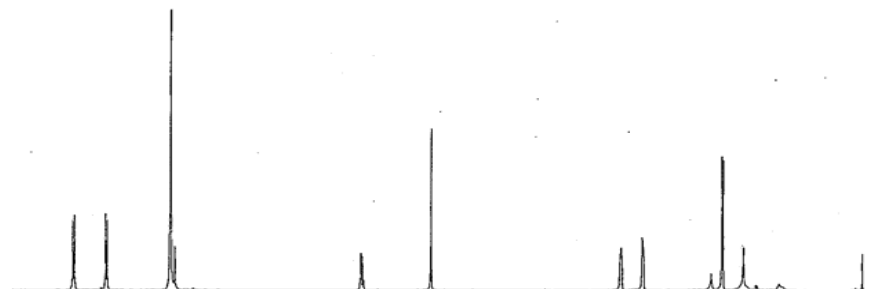
Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-3_18Oct2013-22:05:45

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



12c-trans

Relax. delay 2.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 499.7288158 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.030 sec
FT size 4096 x 4096
Total time 5 hr, 23 min, 8 sec



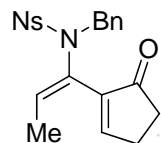
wxn553-3_18Oct2013-22:05:45

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-3_18Oct2013-22:05:45

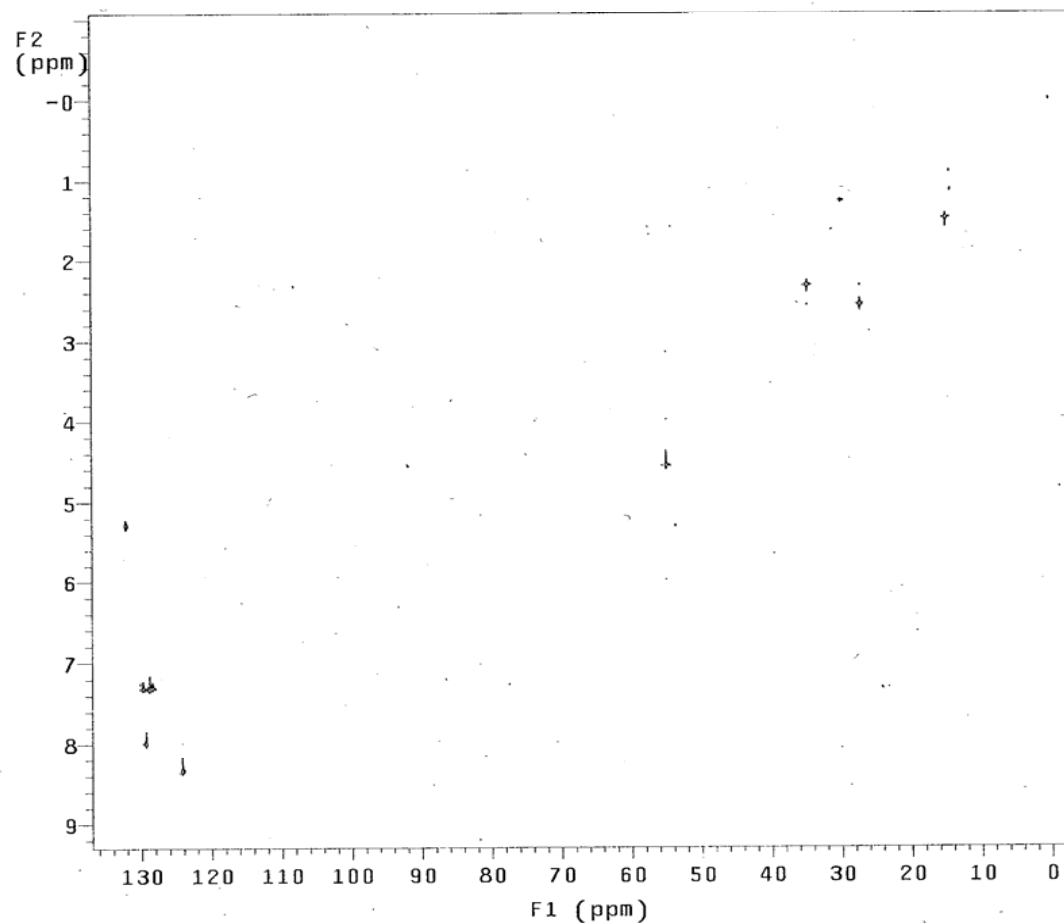
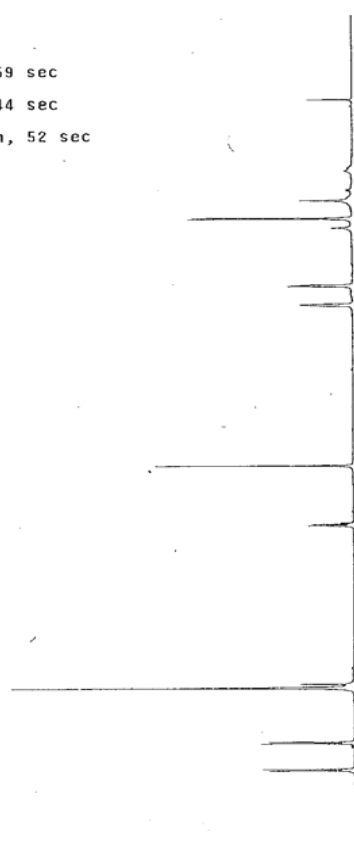
Pulse Sequence: gHMOC

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

Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 21361.8 Hz
16 repetitions
2 x 512 increments
OBSERVE H1, 499.7288158 MHz
DECOUPLE C13, 125.6662987 MHz
Power 44 dB
on during acquisition
off during delay
W40_hcx4765 modulated
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.044 sec
FT size 2048 x 8192
Total time 5 hr, 25 min, 52 sec



12c-trans



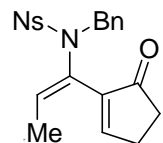
wxn553-3_18Oct2013-22:05:45

Archive directory: /export/home/xiaona/vnmrsys/data
Sample directory: wxn553-3_18Oct2013-22:05:45

Pulse Sequence: gHMQC

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

Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 21361.8 Hz
16 repetitions
2 x 512 increments
OBSERVE H1, 499.7288158 MHz
DECOUPLE C13, 125.6662987 MHz
Power 44 dB
on during acquisition
off during delay
W40_hcx4765 modulated
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.044 sec
FT size 2048 x 8192
Total time 5 hr, 25 min, 52 sec



12c-trans

