

**Supporting Information for:**  
**Insights into Directing Group Ability in Palladium-Catalyzed C-H Bond**  
**Functionalization**

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<sup>1</sup>HNMR and <sup>13</sup>CNMR for compounds **1 – 15, 17**

pMeSM-proton

File: 11lvdpMeproton

Pulse Sequence: s2pul

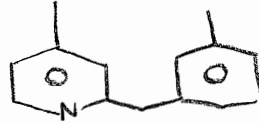
Solvent: cdcl3

Ambient temperature

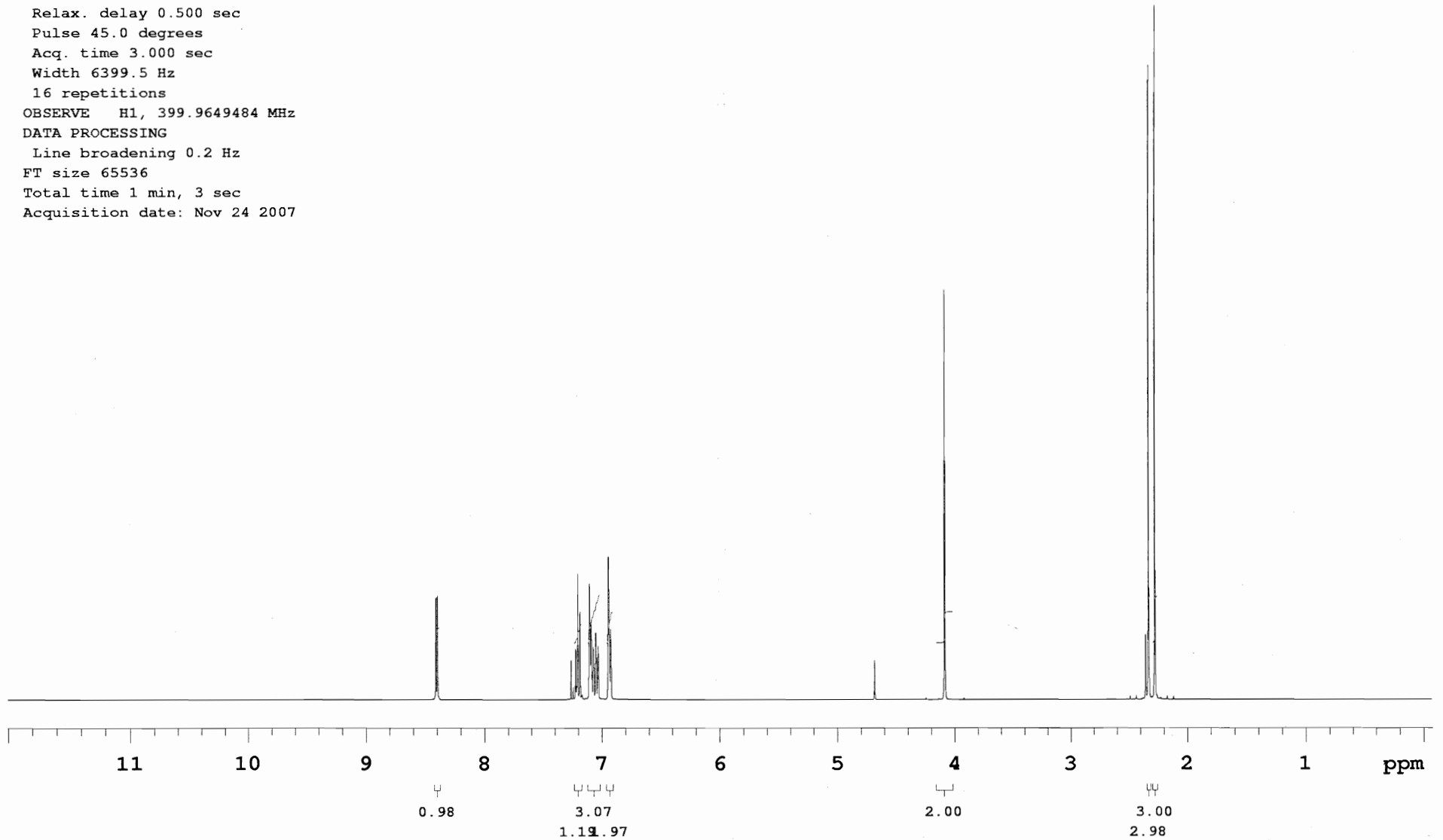
Operator: lopa

File: 11lvdpMeproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 6399.5 Hz  
 16 repetitions  
 OBSERVE H1, 399.9649484 MHz  
 DATA PROCESSING  
 Line broadening 0.2 Hz  
 FT size 65536  
 Total time 1 min, 3 sec  
 Acquisition date: Nov 24 2007



pMeSM-carbon

File: 111vdpMecarbon

Pulse Sequence: s2pul

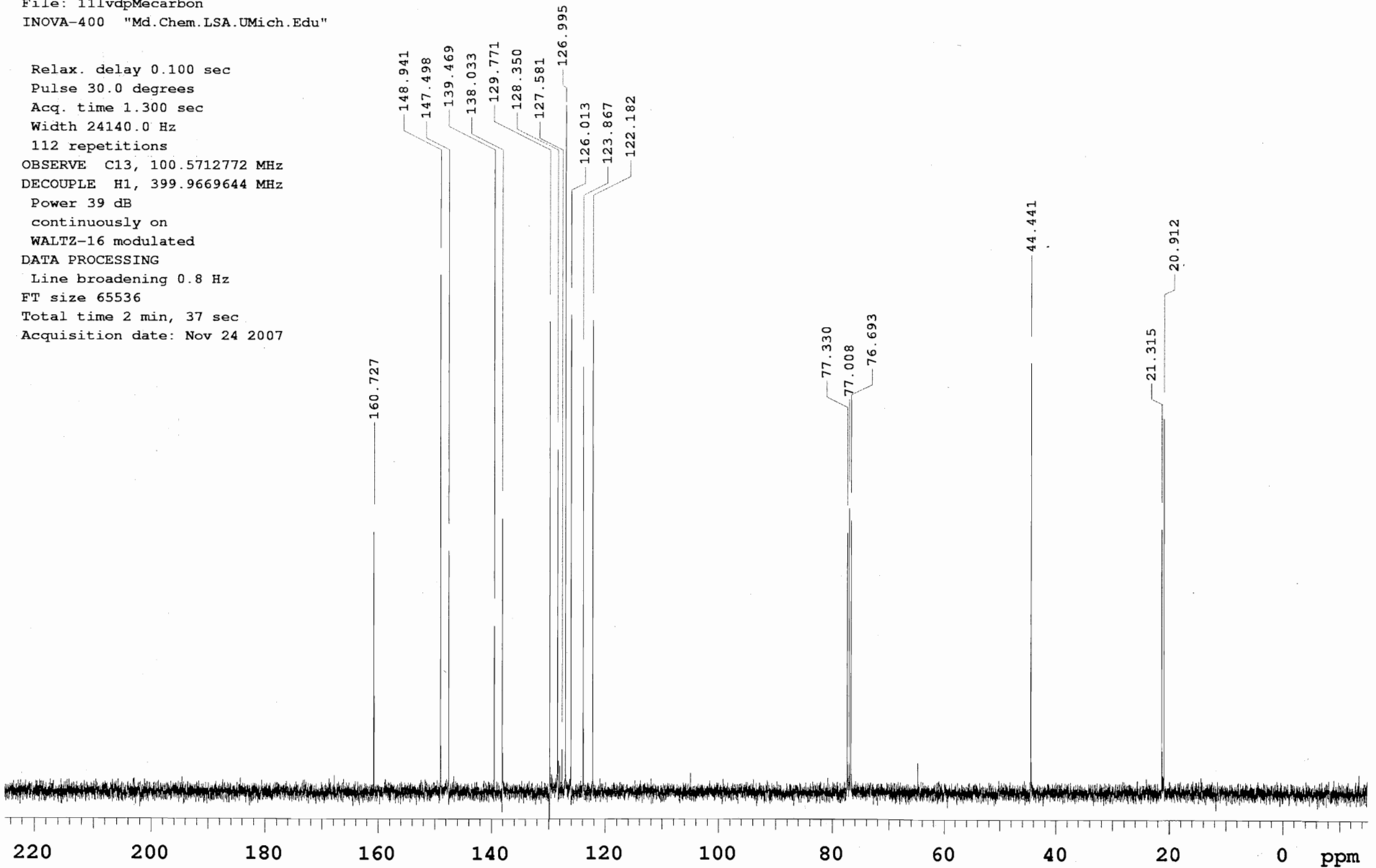
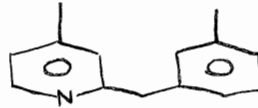
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdpMecarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



pOMeSM-proton

File: 111vdpOMeproton

Pulse Sequence: s2pul

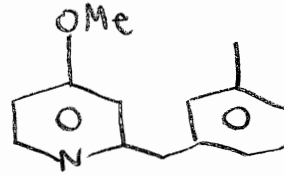
Solvent: cdcl3

Ambient temperature

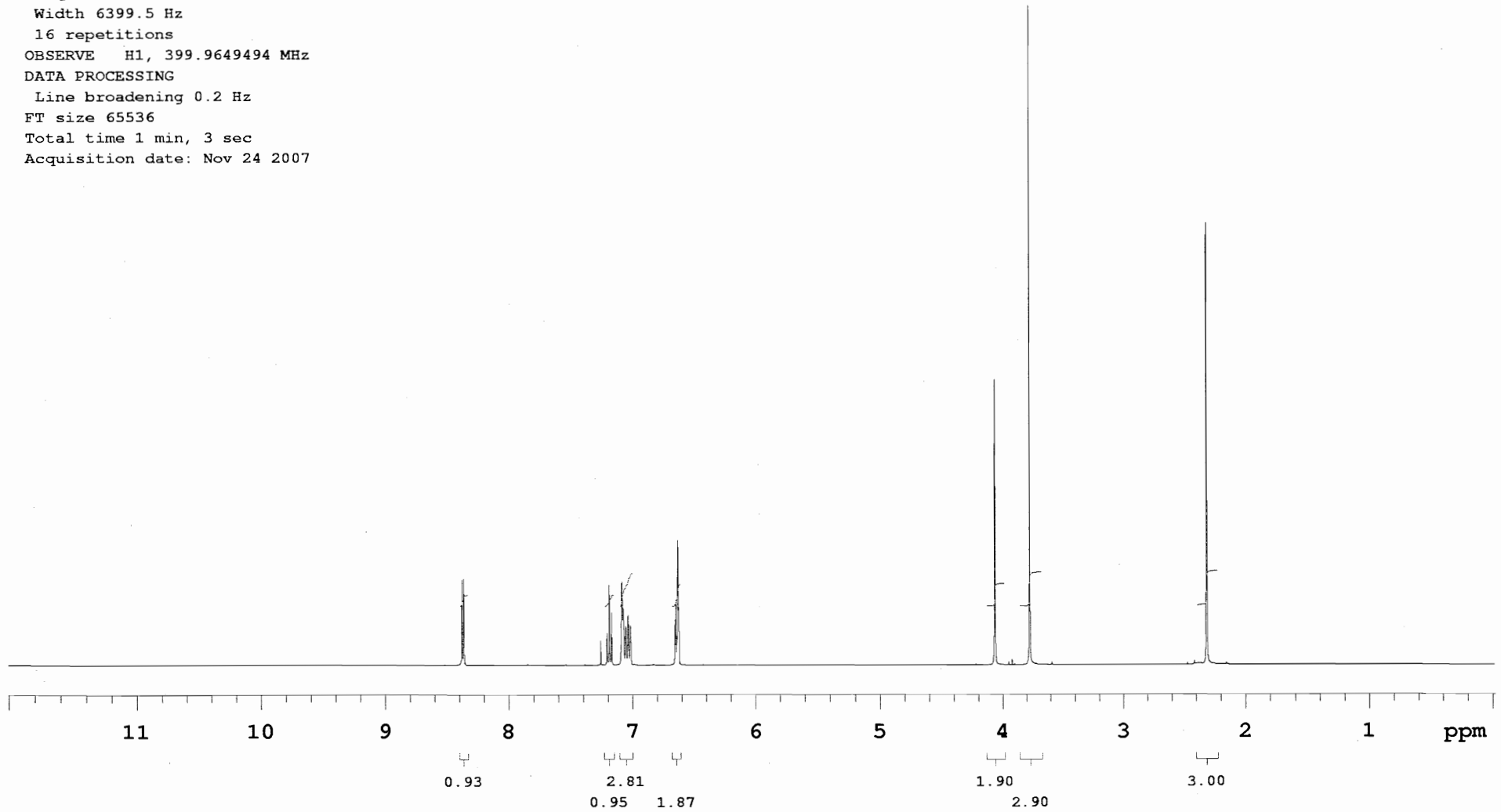
Operator: lopa

File: 111vdpOMeproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649494 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007



pOMeSM-carbon

File: 111vdpOMecarbon

Pulse Sequence: s2pul

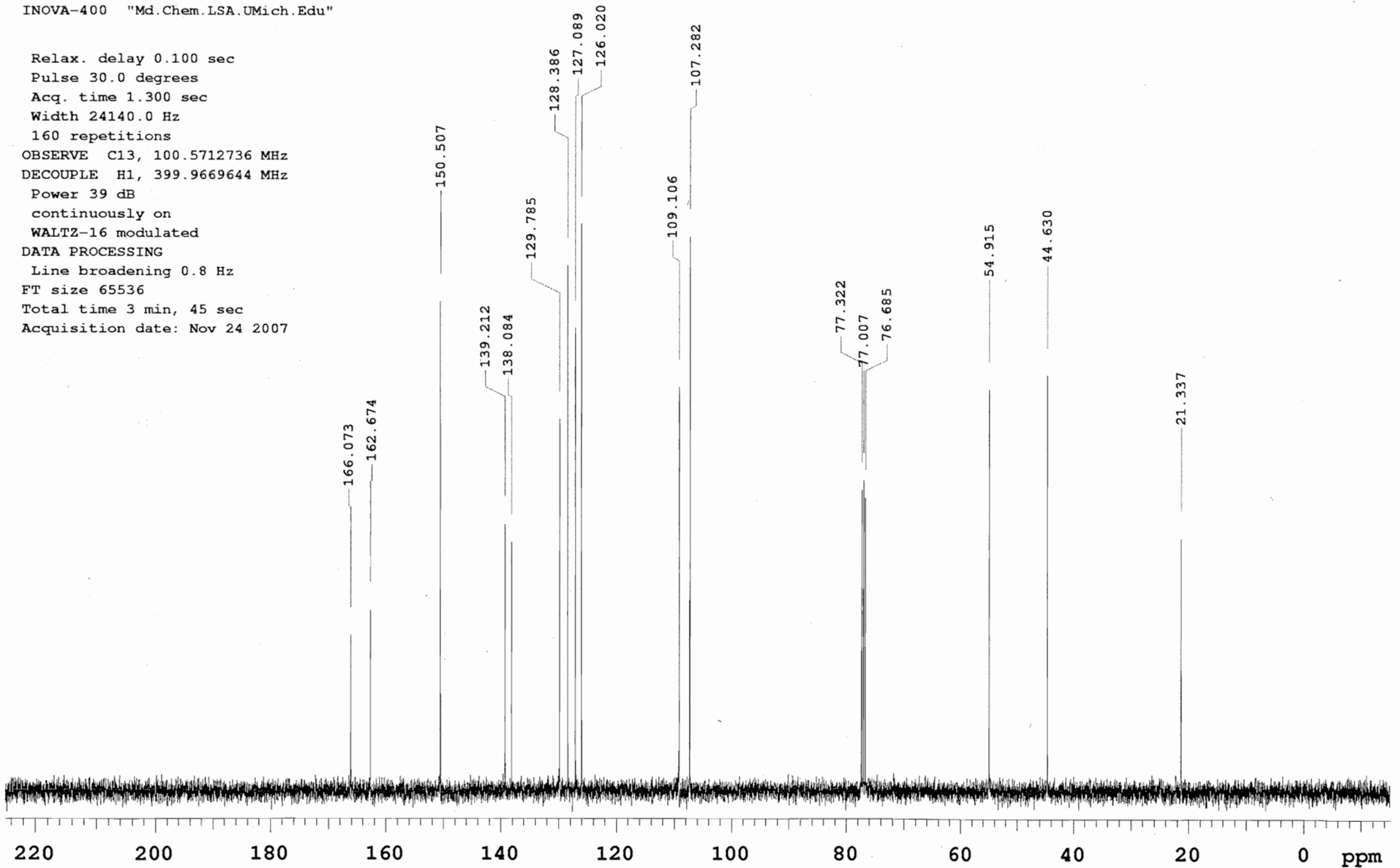
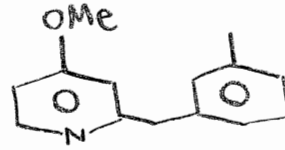
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdpOMecarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



pCF3SM-proton

File: 111vdpCF3proton

Pulse Sequence: s2pul

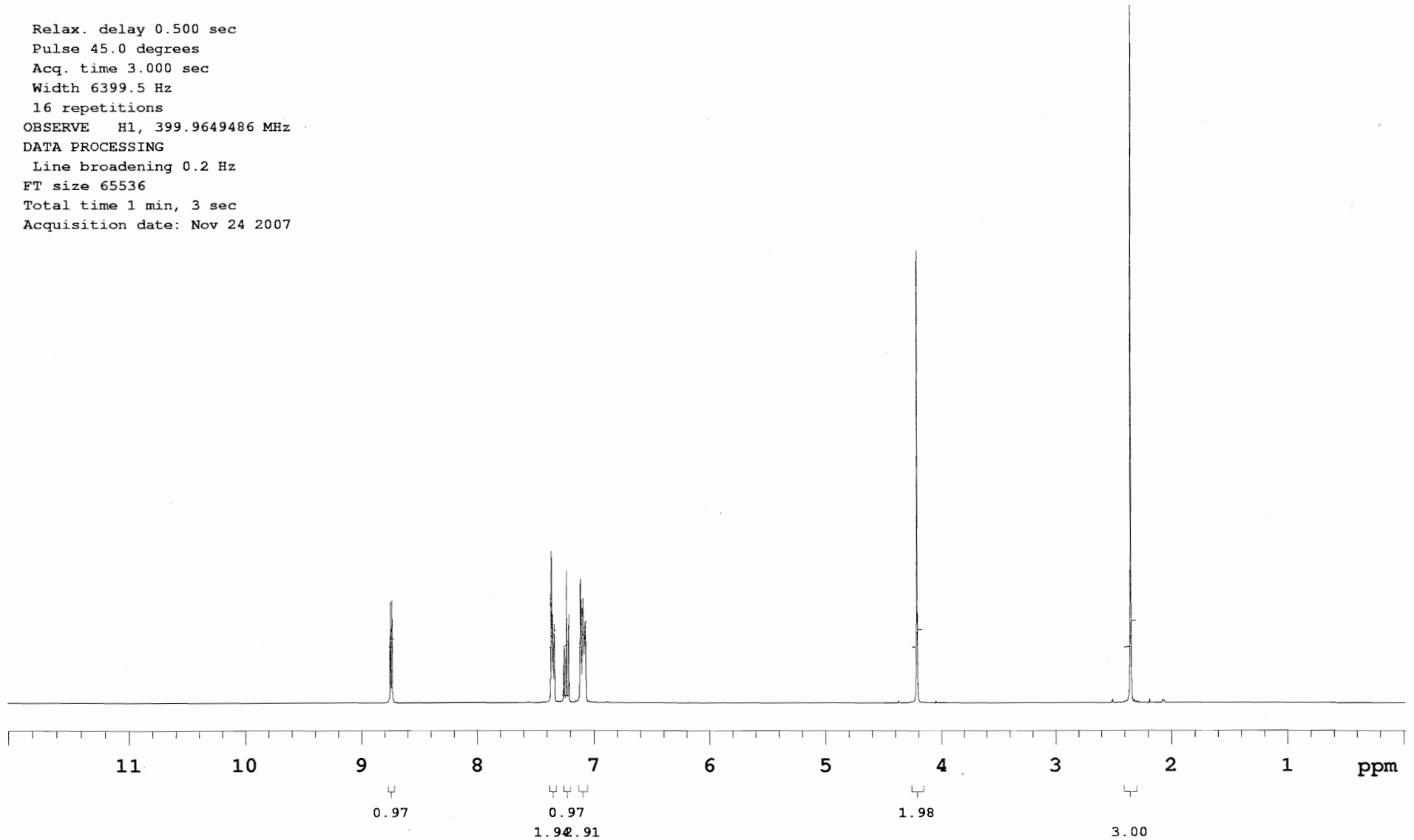
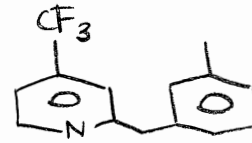
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdpCF3proton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



pCF3SM-carbon

File: 11lvdpCF3carbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 11lvdpCF3carbon

INOVA-400 "Md.Chem.LSA.UMich

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

480 repetitions

OBSERVE C13, 100.5712721 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

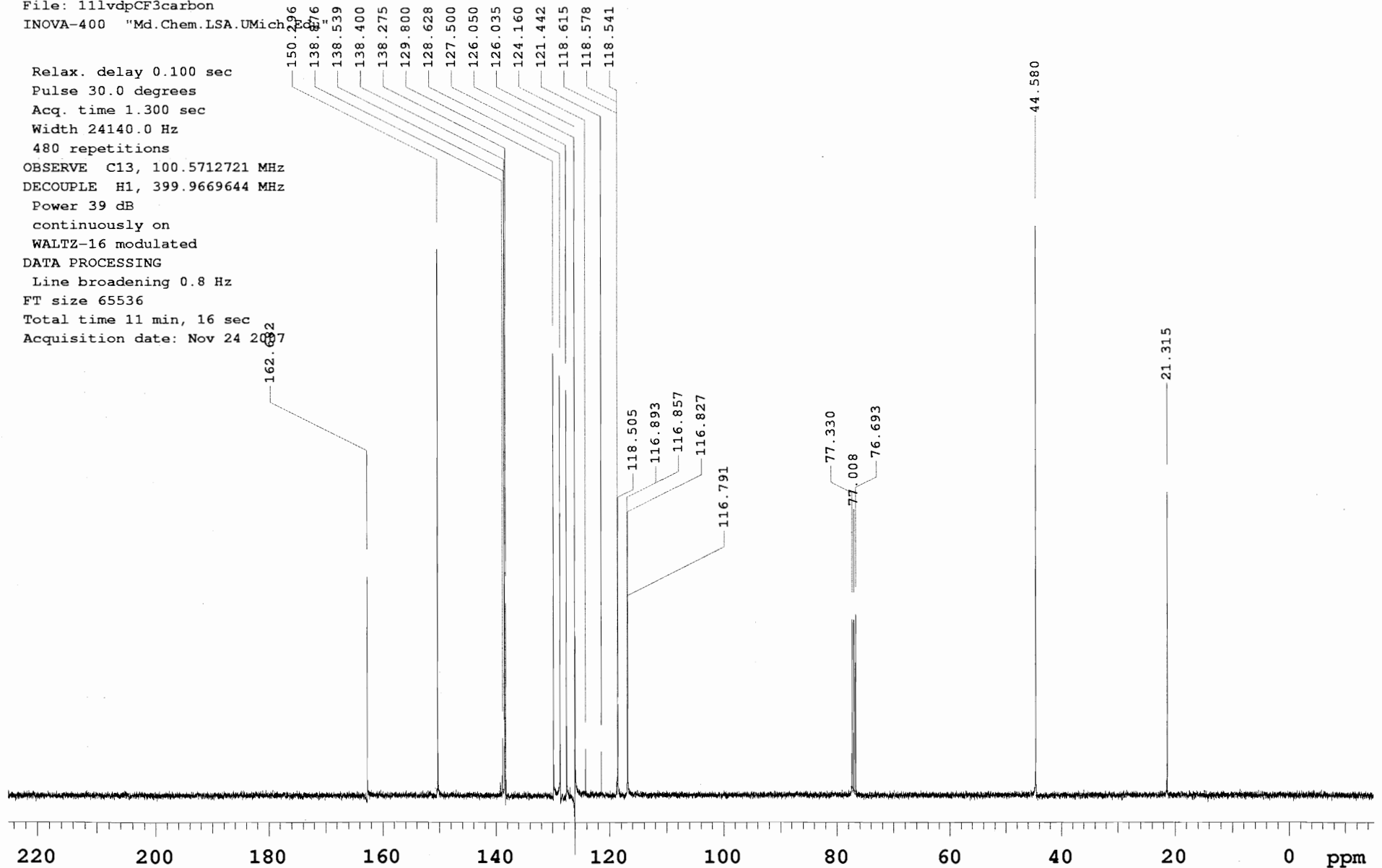
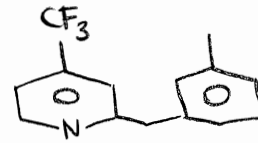
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 11 min, 16 sec

Acquisition date: Nov 24 2007



pClSM-proton

File: 11lvdpClproton

Pulse Sequence: s2pul

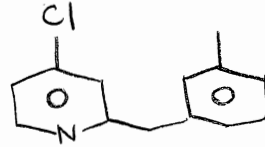
Solvent: cdcl3

Ambient temperature

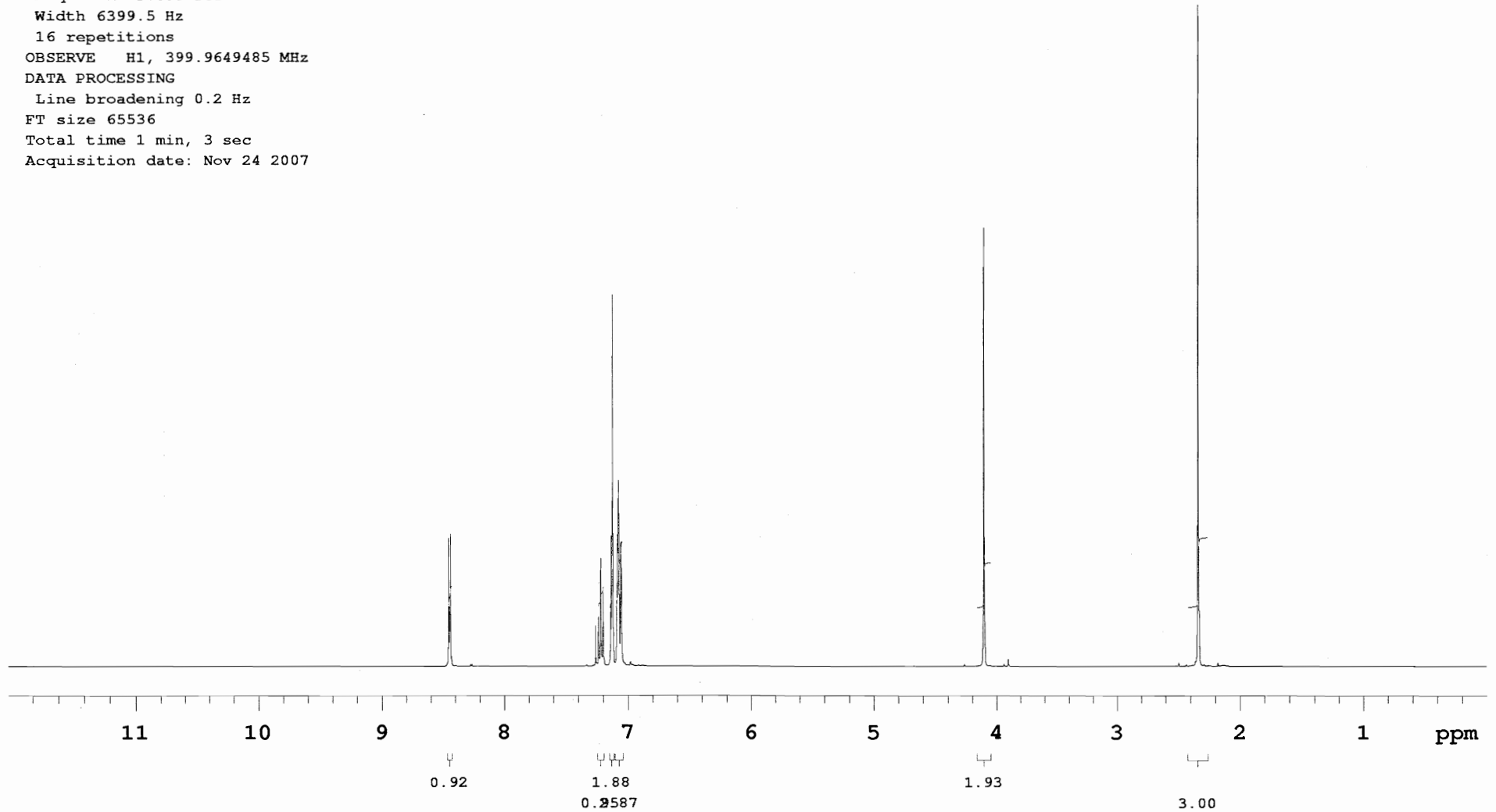
Operator: lopa

File: 11lvdpClproton

INNOVA-400 "Md.Chem.LSA.UMich.Edu"

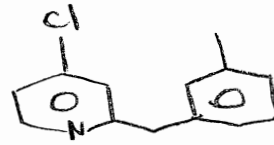


Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649485 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007





pClSM-carbon



File: 111vdpClcarbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdpClcarbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

80 repetitions

OBSERVE C13, 100.5712735 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

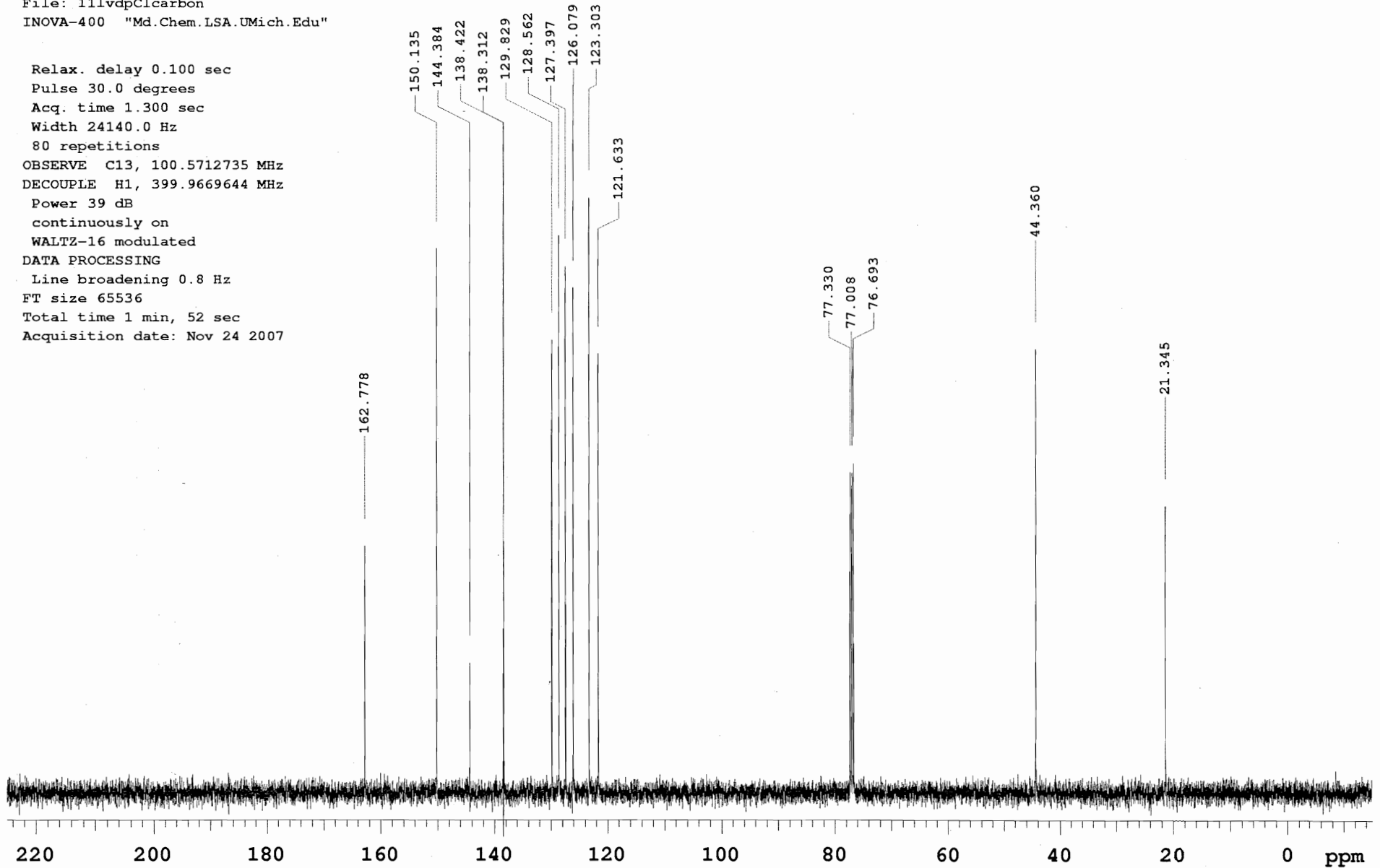
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 1 min, 52 sec

Acquisition date: Nov 24 2007



mMeSM-proton

File: 111vdmMeproton

Pulse Sequence: s2pul

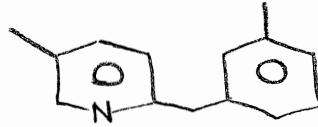
Solvent: cdcl3

Ambient temperature

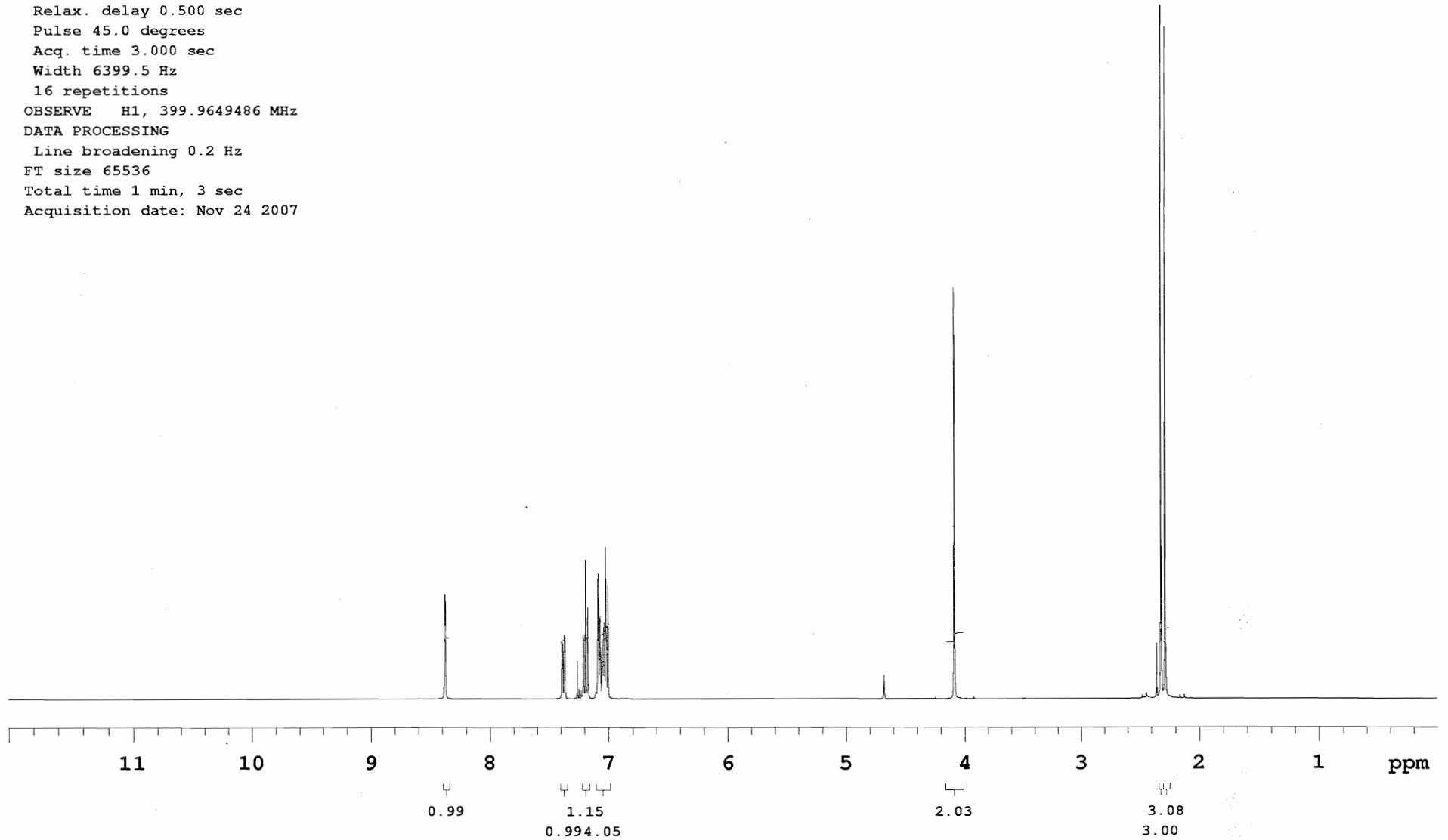
Operator: lopa

File: 111vdmMeproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649486 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007



mMeSM-carbon

File: 111vdmMecarbon

Pulse Sequence: s2pul

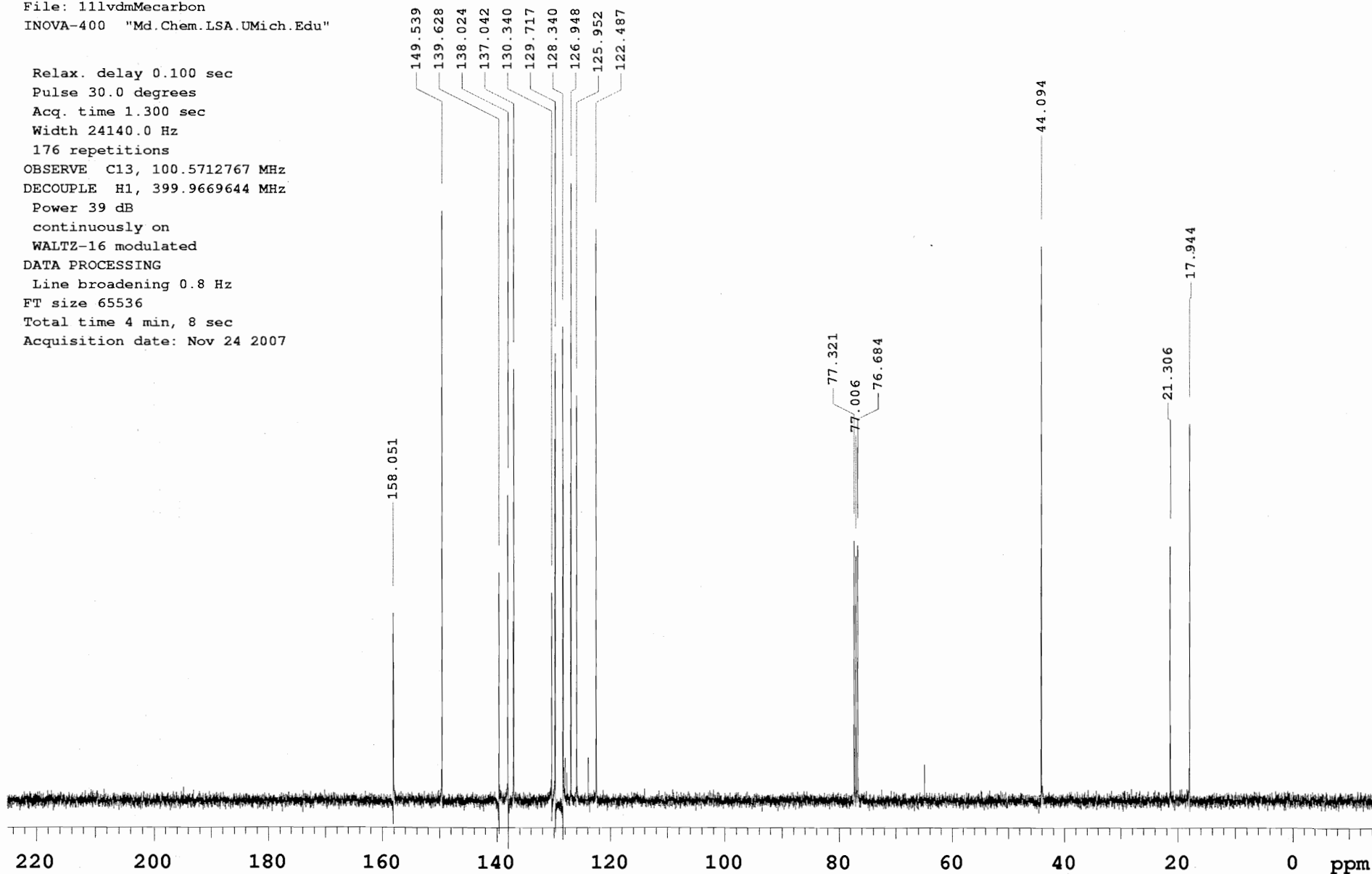
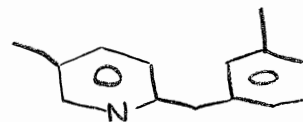
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdmMecarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



PyridineSM-proton

File: 111vdpyridineproton

Pulse Sequence: s2pul

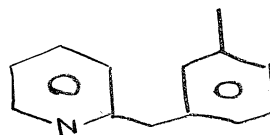
Solvent: cdcl3

Ambient temperature

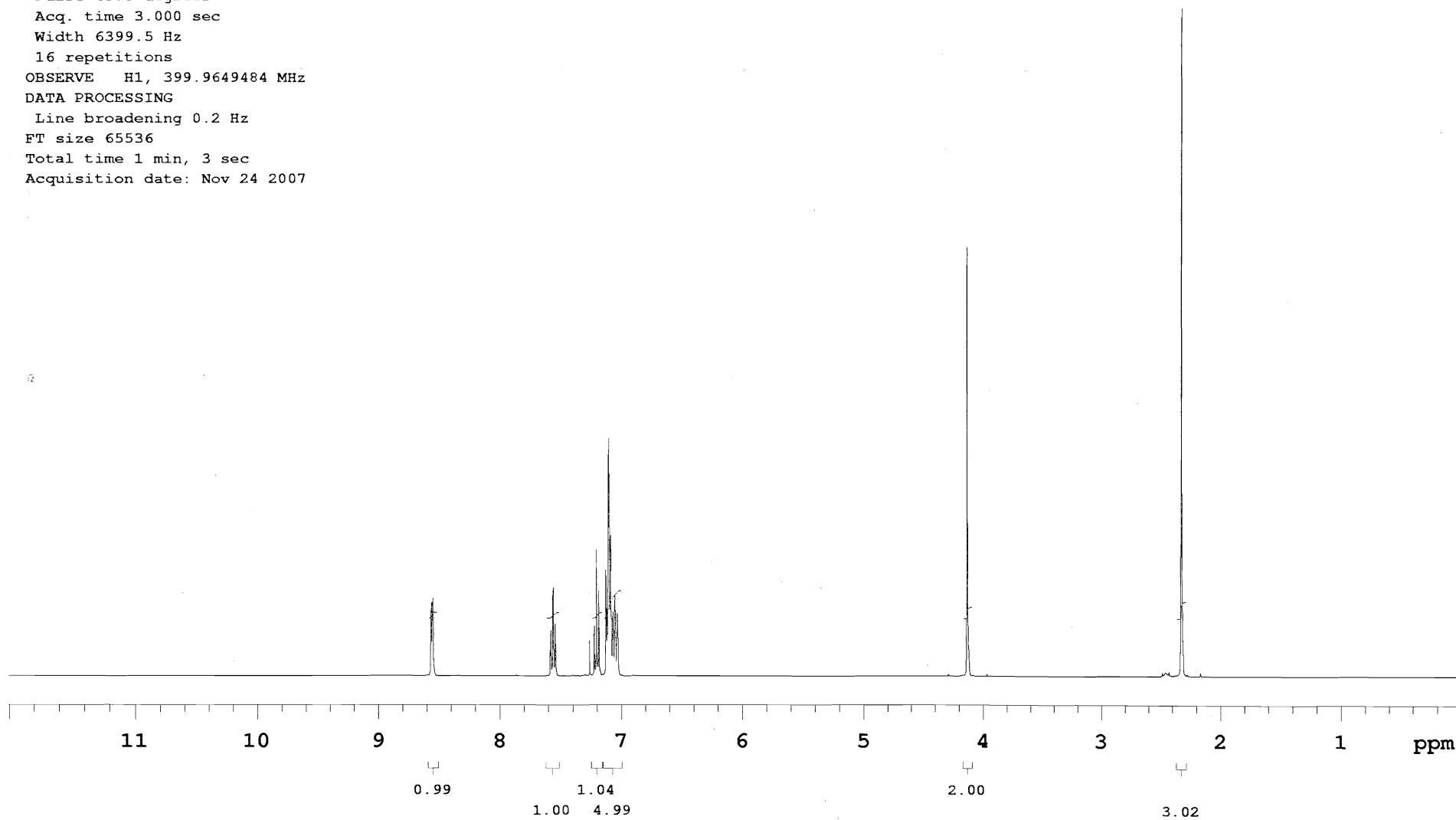
Operator: lopa

File: 111vdpyridineproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649484 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007



PyridineSM-carbon

File: 111vdpyridinecarbon

Pulse Sequence: s2pul

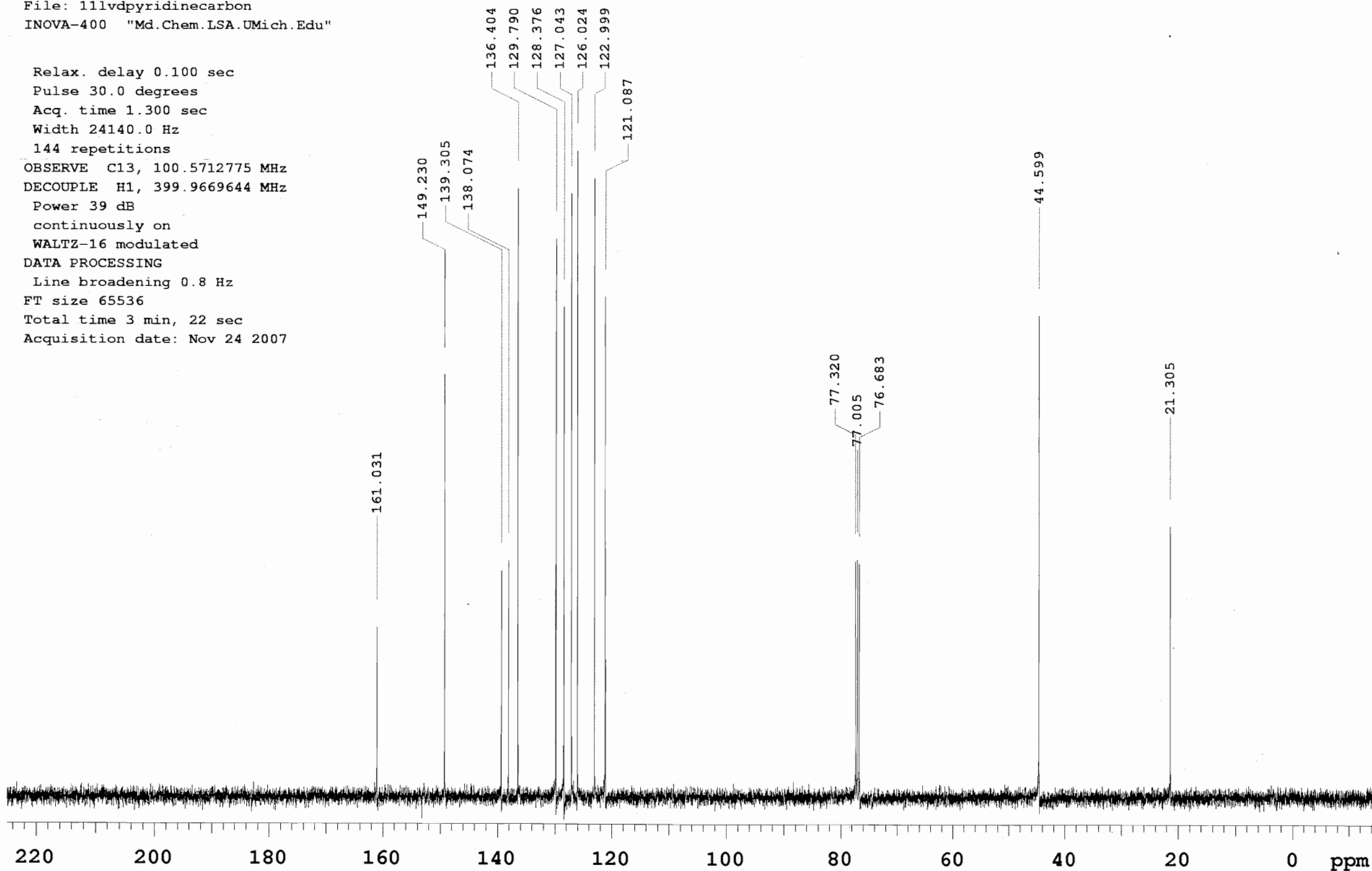
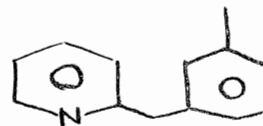
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdpyridinecarbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



mFSM-proton

File: 11lvdmFproton

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

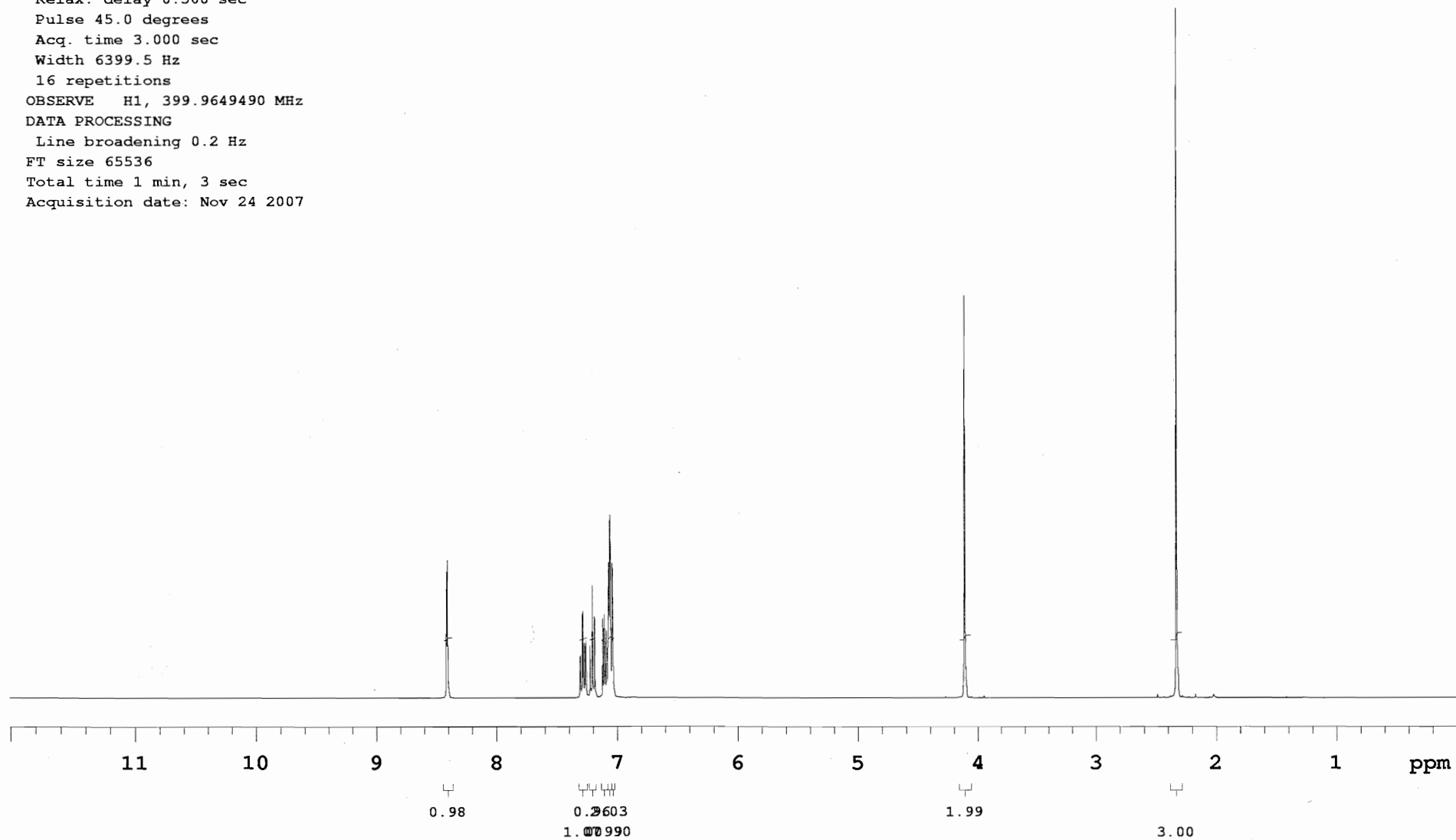
Operator: lopa

File: 11lvdmFproton

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649490 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007



mFSM-carbon

File: 111vdmFcarbon

Pulse Sequence: s2pul

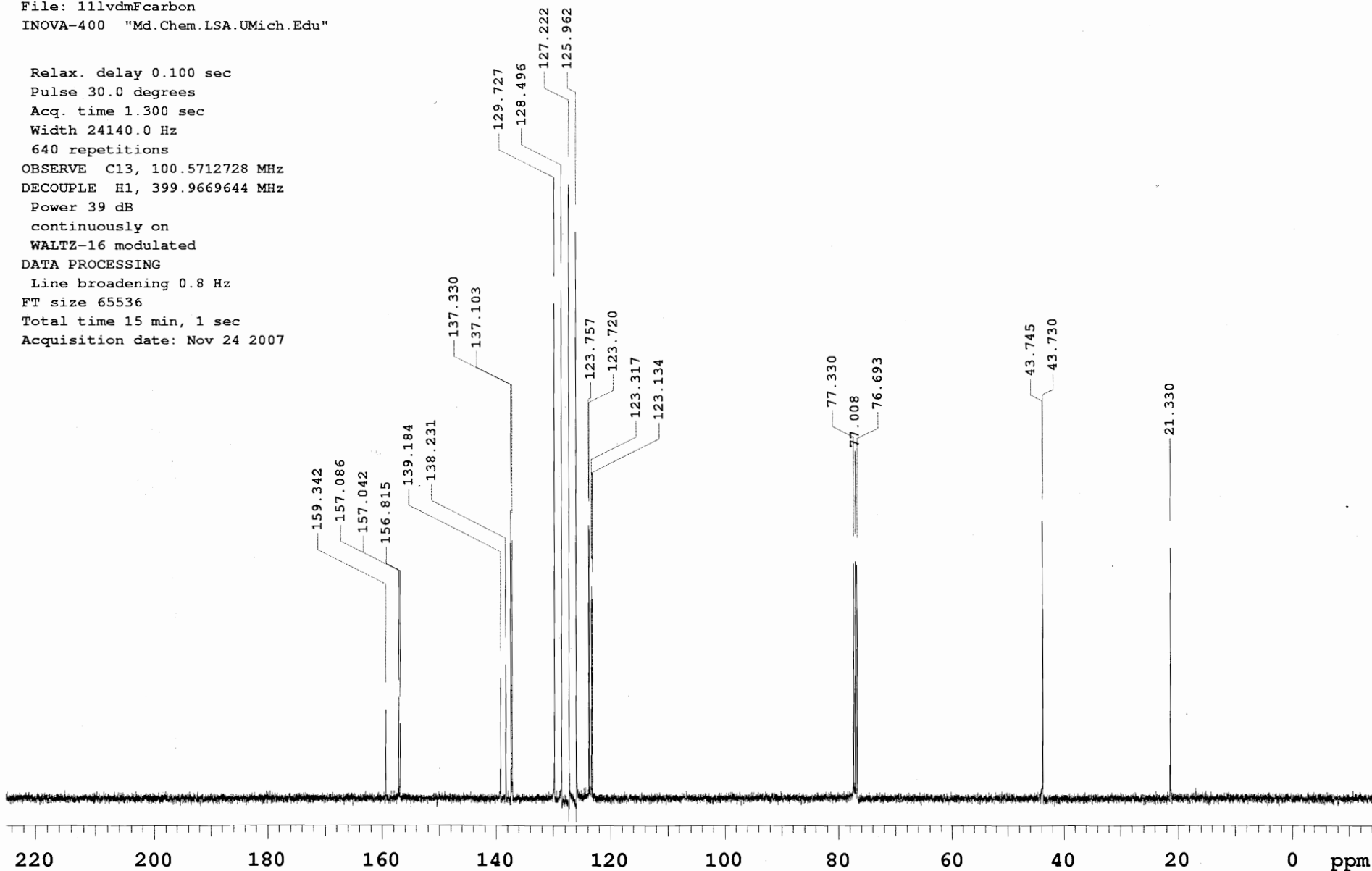
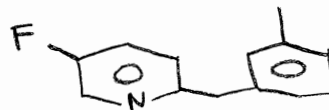
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdmFcarbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



PyrimidineSM-proton

File: 11lvdpyrimidineproton

Pulse Sequence: s2pul

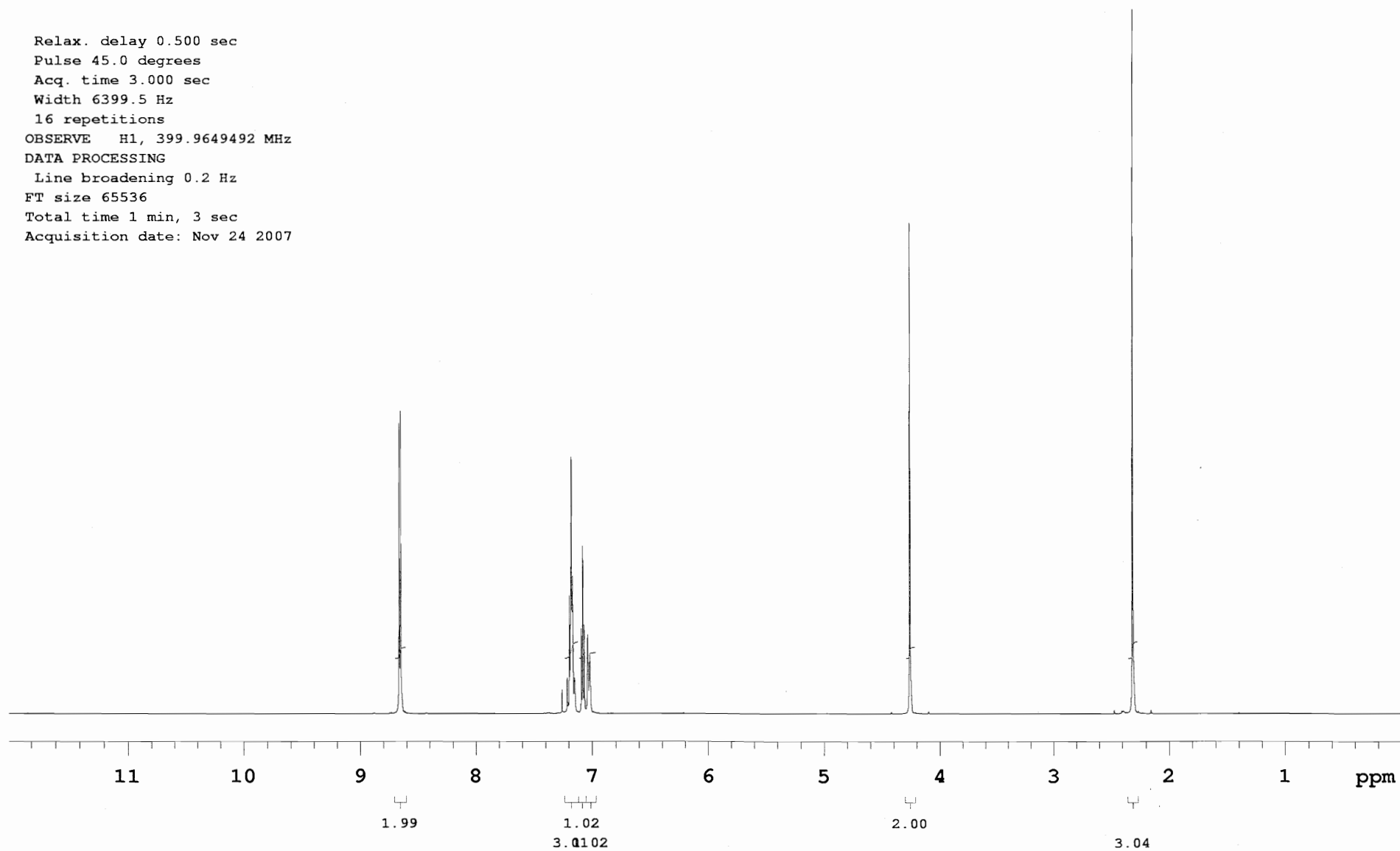
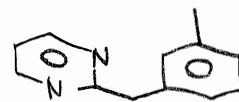
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 11lvdpyrimidineproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"





PyrimidineSM-carbon

File: 111vdpyrimidinecarbon

Pulse Sequence: s2pul

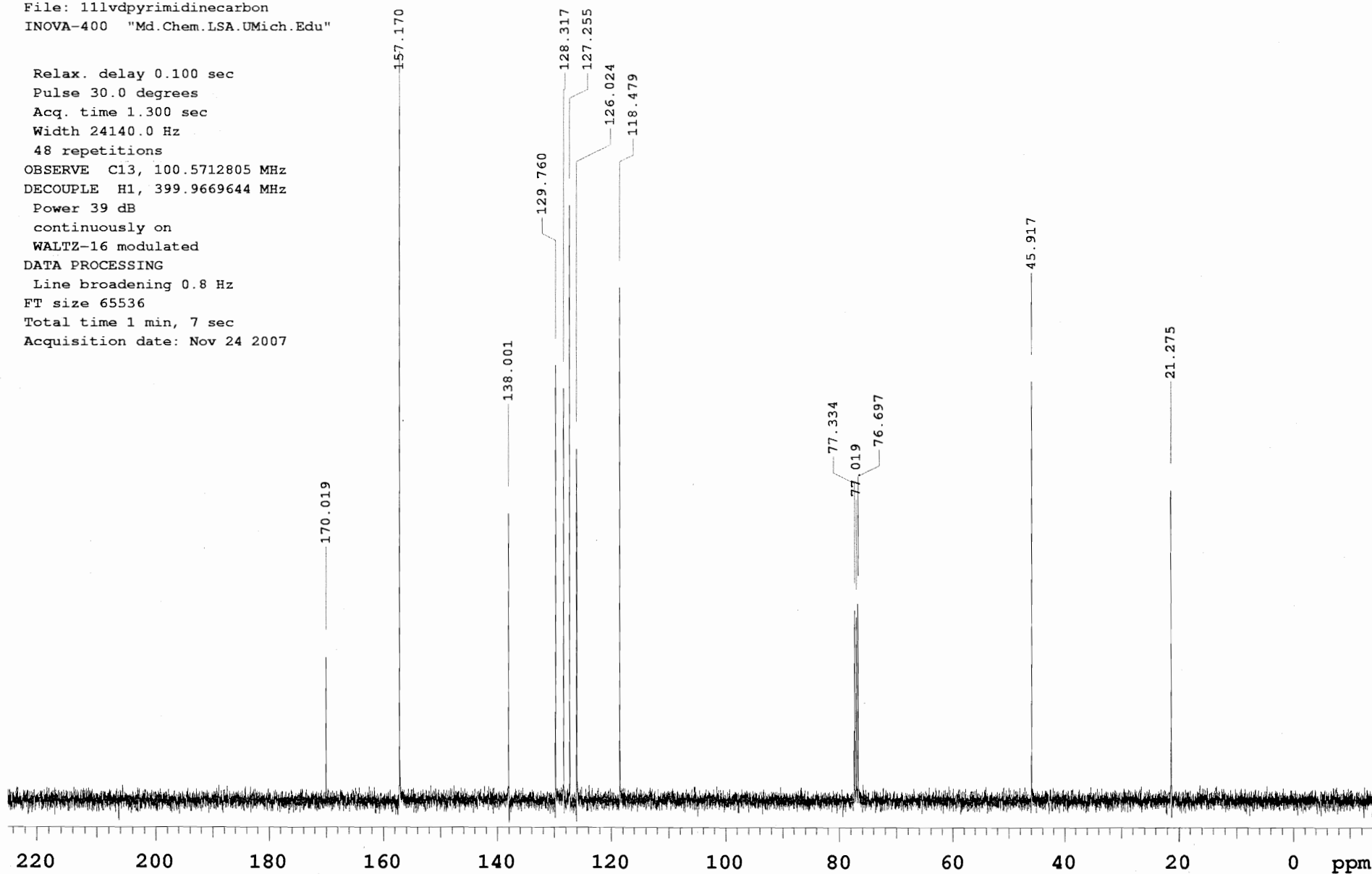
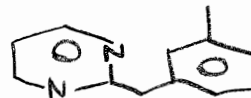
Solvent: cdcl3

Ambient temperature

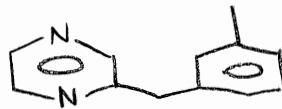
Operator: lopa

File: 111vdpyrimidinecarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



PyrazineSM-proton



File: 111vdpyrazineproton

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdpyrazineproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

16 repetitions

OBSERVE H1, 399.9649484 MHz

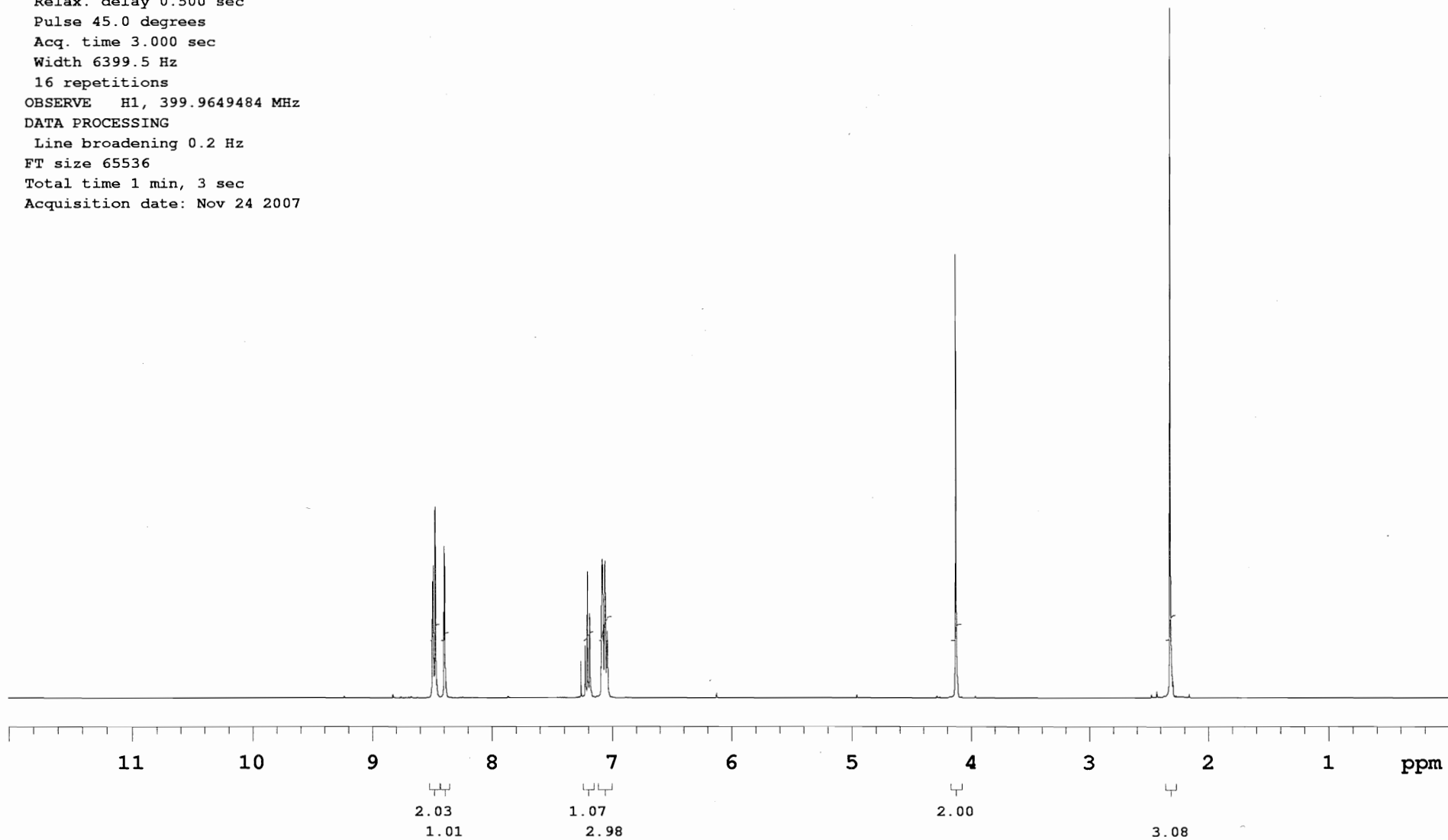
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 3 sec

Acquisition date: Nov 24 2007



PyrazineSM-carbon

File: 111vdpyrazinecarbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdpyrazinecarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

96 repetitions

OBSERVE C13, 100.5712777 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

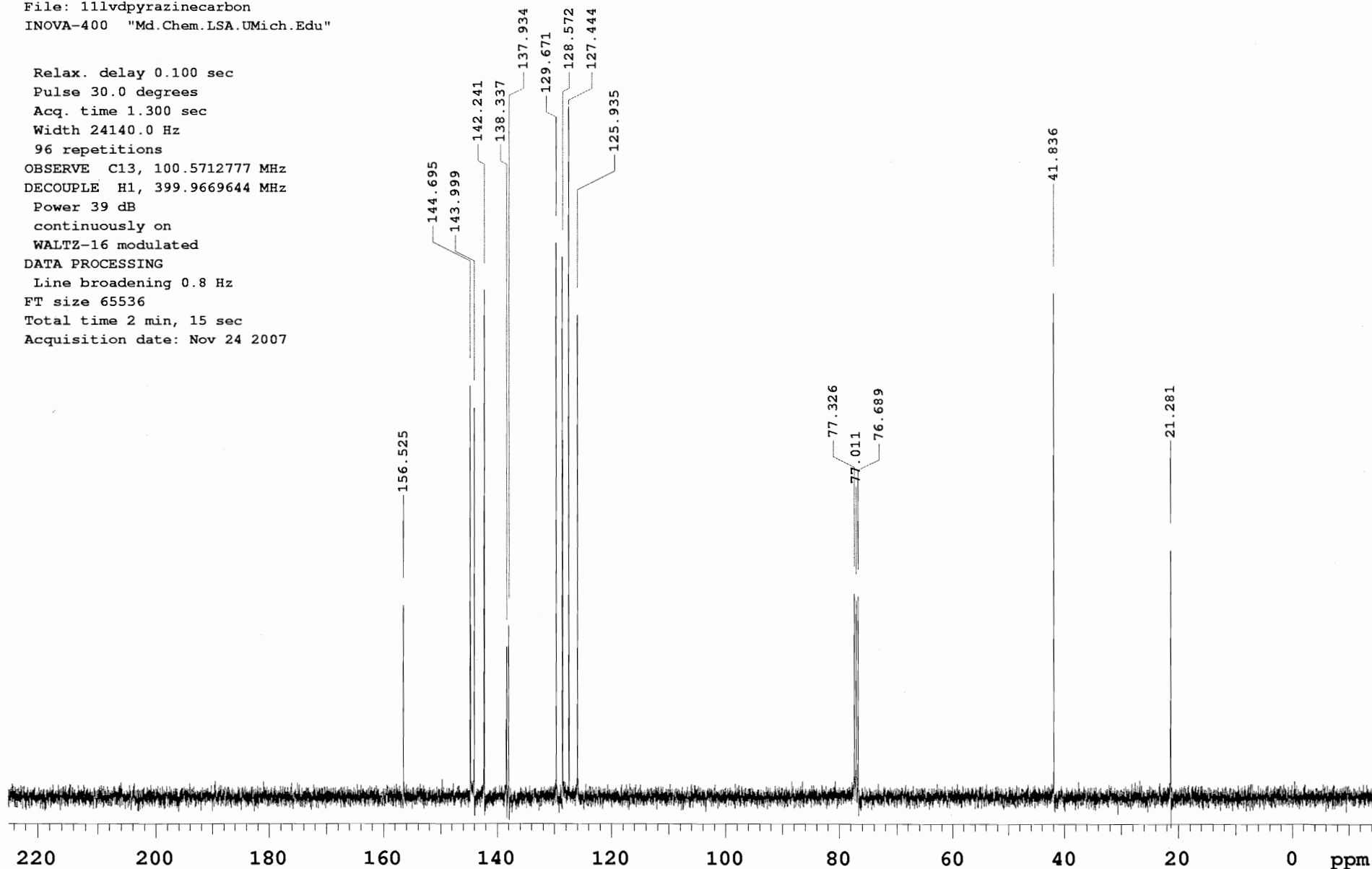
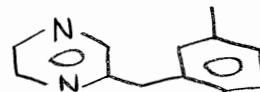
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 2 min, 15 sec

Acquisition date: Nov 24 2007



IsoxazolineSM-proton

File: 11lvdisoxazolineproton

Pulse Sequence: s2pul

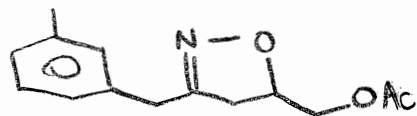
Solvent: cdcl3

Ambient temperature

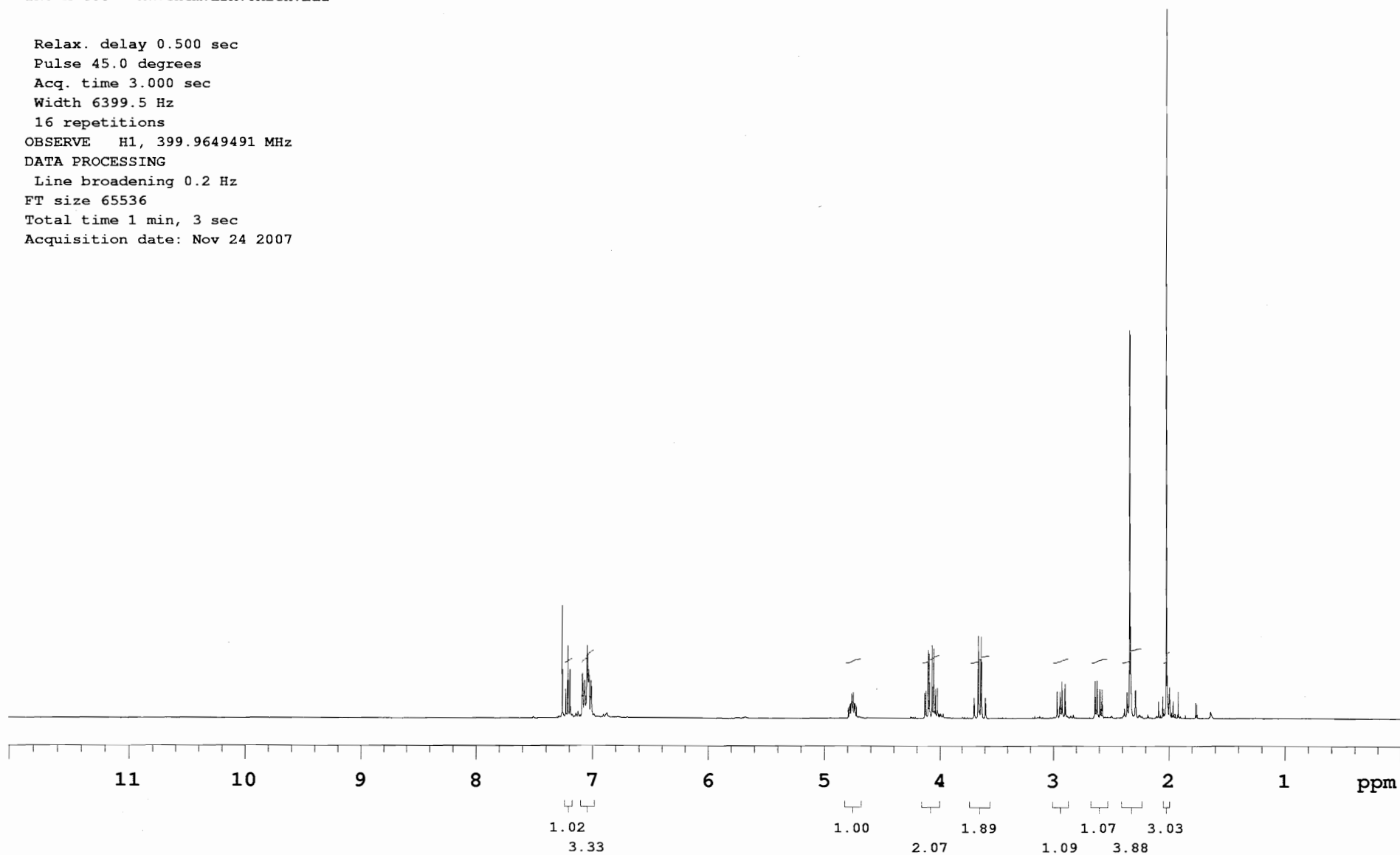
Operator: lopa

File: 11lvdisoxazolineproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649491 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007



IsoxazolineSM-carbon

File: 11lvdisoxazolinecarbon



Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 11lvdisoxazolinecarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

272 repetitions

OBSERVE C13, 100.5712701 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

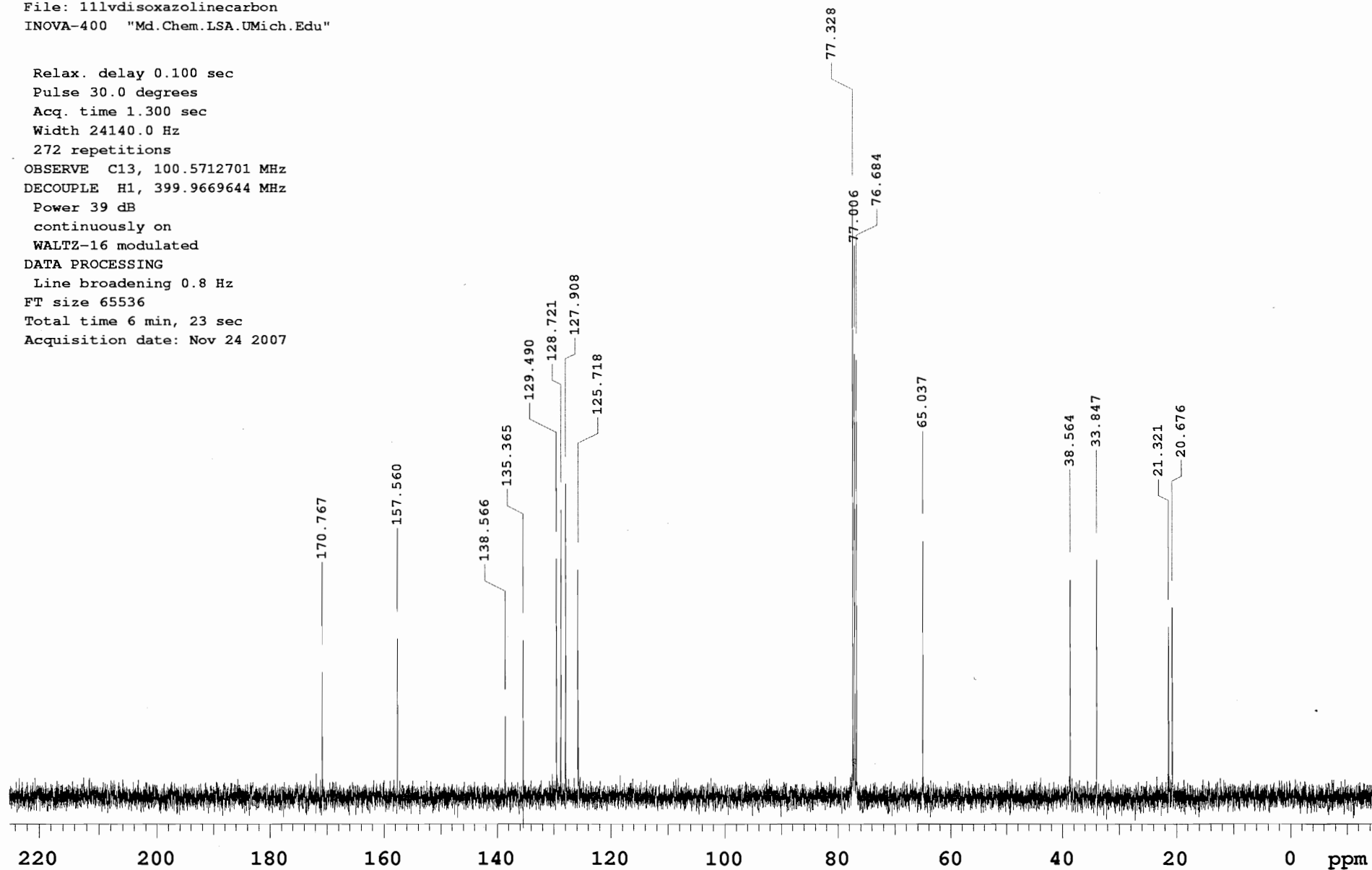
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 6 min, 23 sec

Acquisition date: Nov 24 2007



PyrazoleSM-proton

File: 111vdpyrazoleproton

Pulse Sequence: s2pul

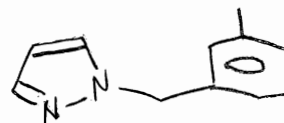
Solvent: cdcl3

Ambient temperature

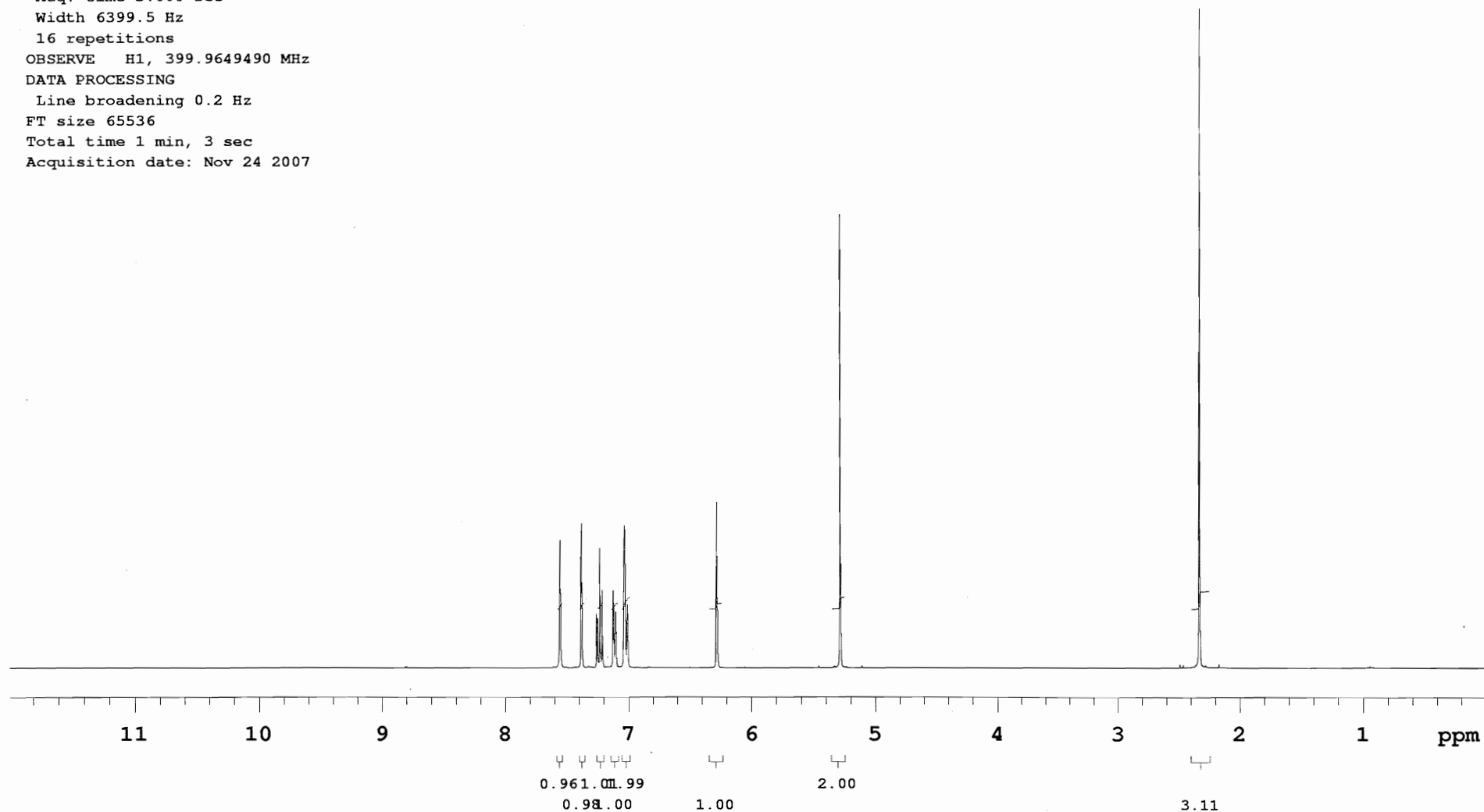
Operator: lopa

File: 111vdpyrazoleproton

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649490 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007



PyrazoleSM-carbon

File: 111vdpyrazolecarbon

Pulse Sequence: s2pul

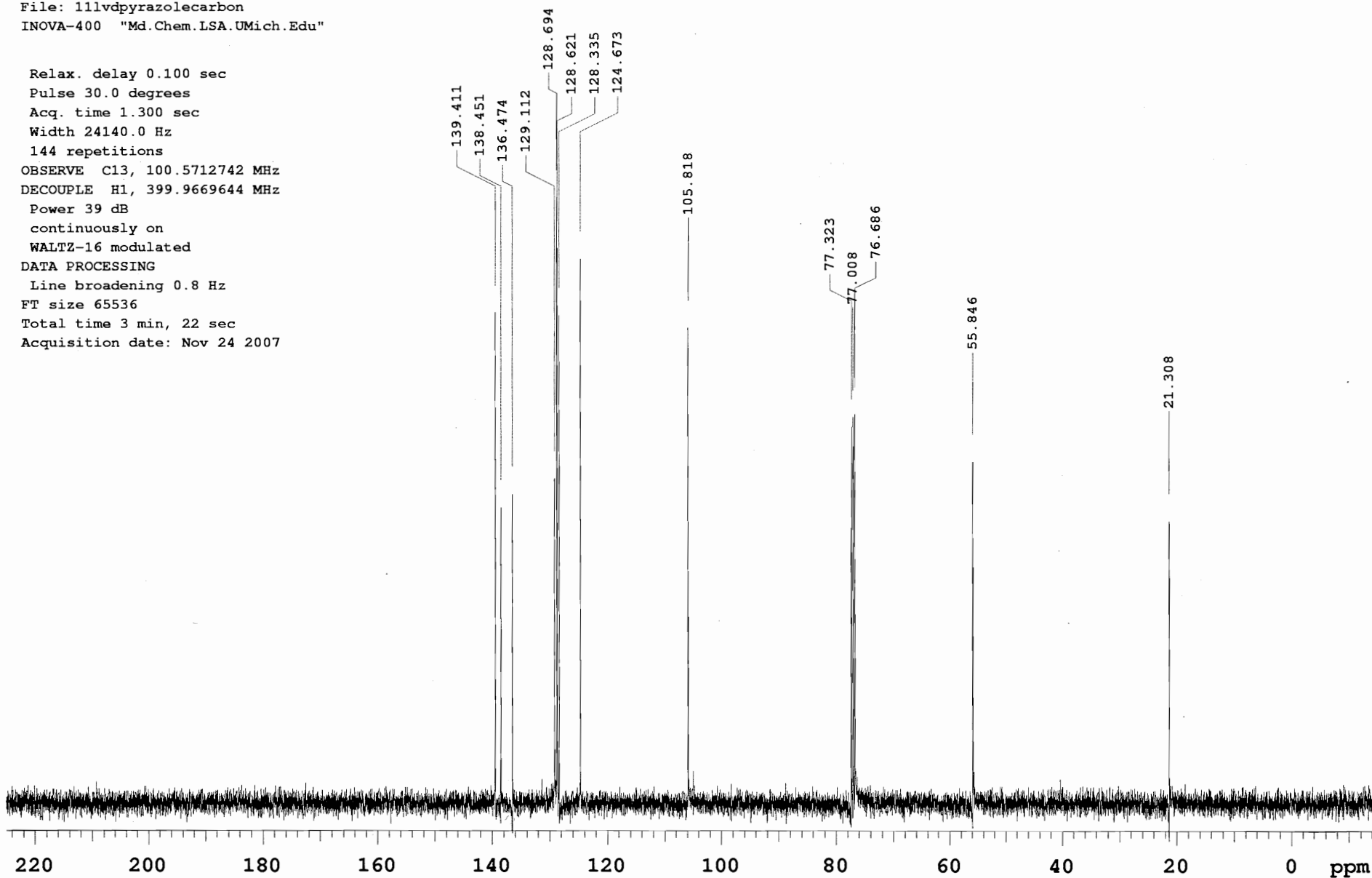
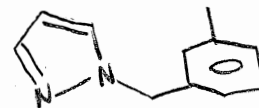
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdpyrazolecarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Methyloximeether-proton

File: 111vdmethyloximeetherproton

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vdmethyloximeetherproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

16 repetitions

OBSERVE H1, 399.9649487 MHz

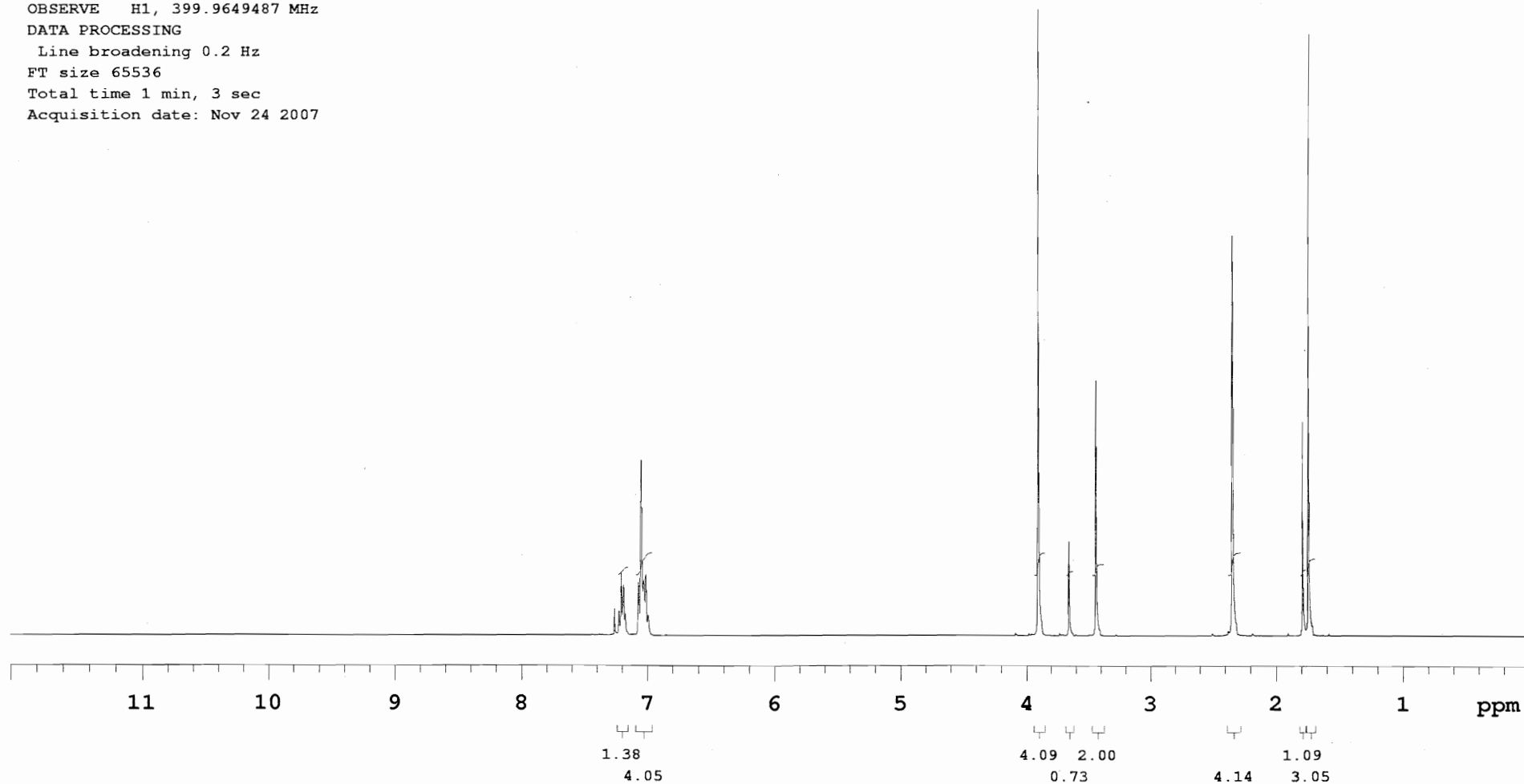
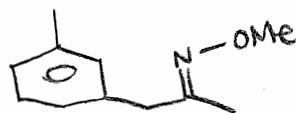
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 3 sec

Acquisition date: Nov 24 2007





Methyloximeether-carbon

File: 111vdmethyloximeethercarbon

Pulse Sequence: s2pul

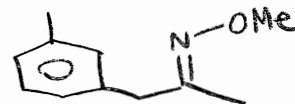
Solvent: cdcl3

Ambient temperature

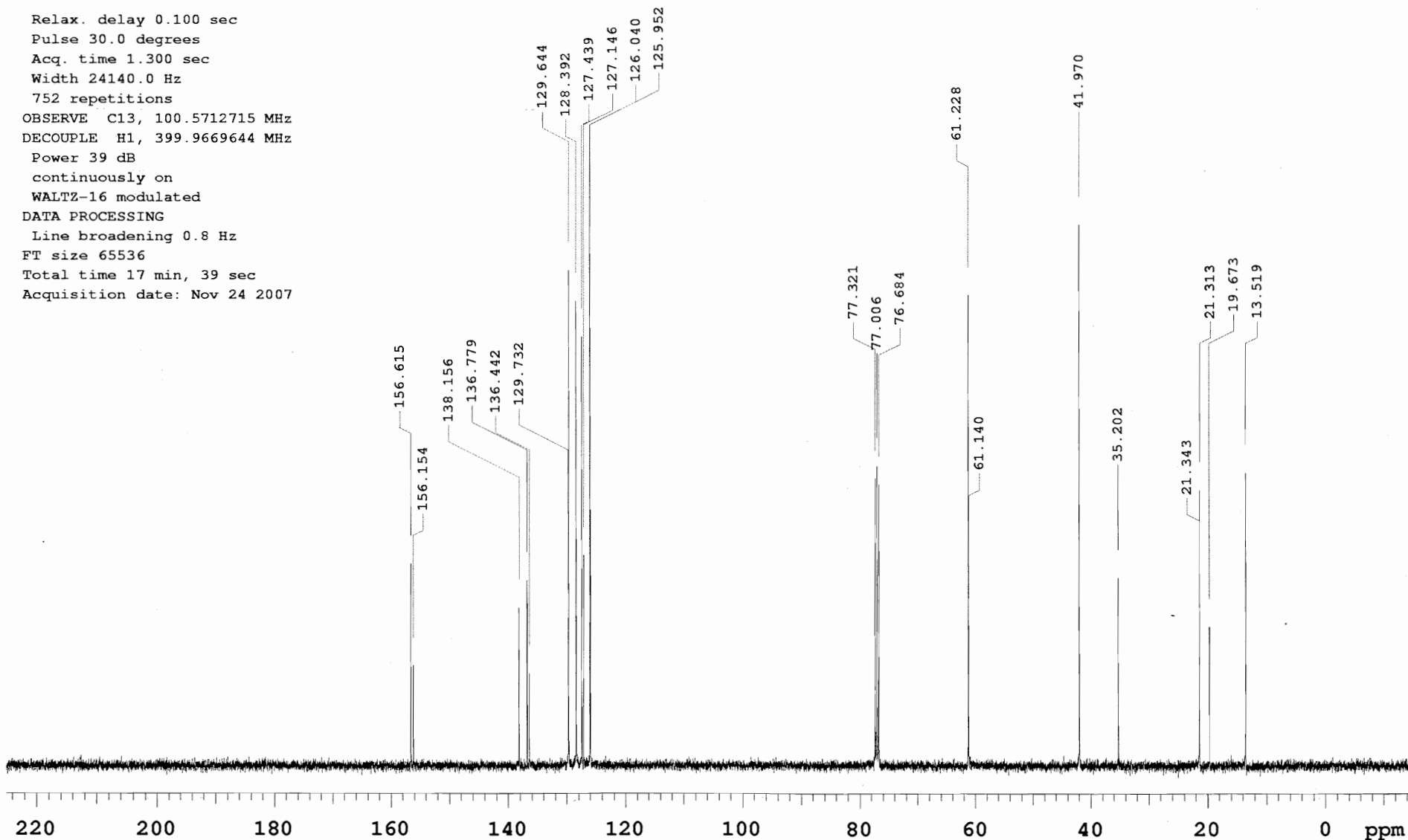
Operator: lopa

File: 111vdmethyloximeethercarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
Pulse 30.0 degrees  
Acq. time 1.300 sec  
Width 24140.0 Hz  
752 repetitions  
OBSERVE C13, 100.5712715 MHz  
DECOUPLE H1, 399.9669644 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.8 Hz  
FT size 65536  
Total time 17 min, 39 sec  
Acquisition date: Nov 24 2007



BenzyloximeSM-proton

File: 11lvdbenzyloximeproton

Pulse Sequence: s2pul

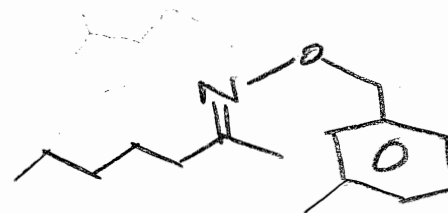
Solvent: cdcl3

Ambient temperature

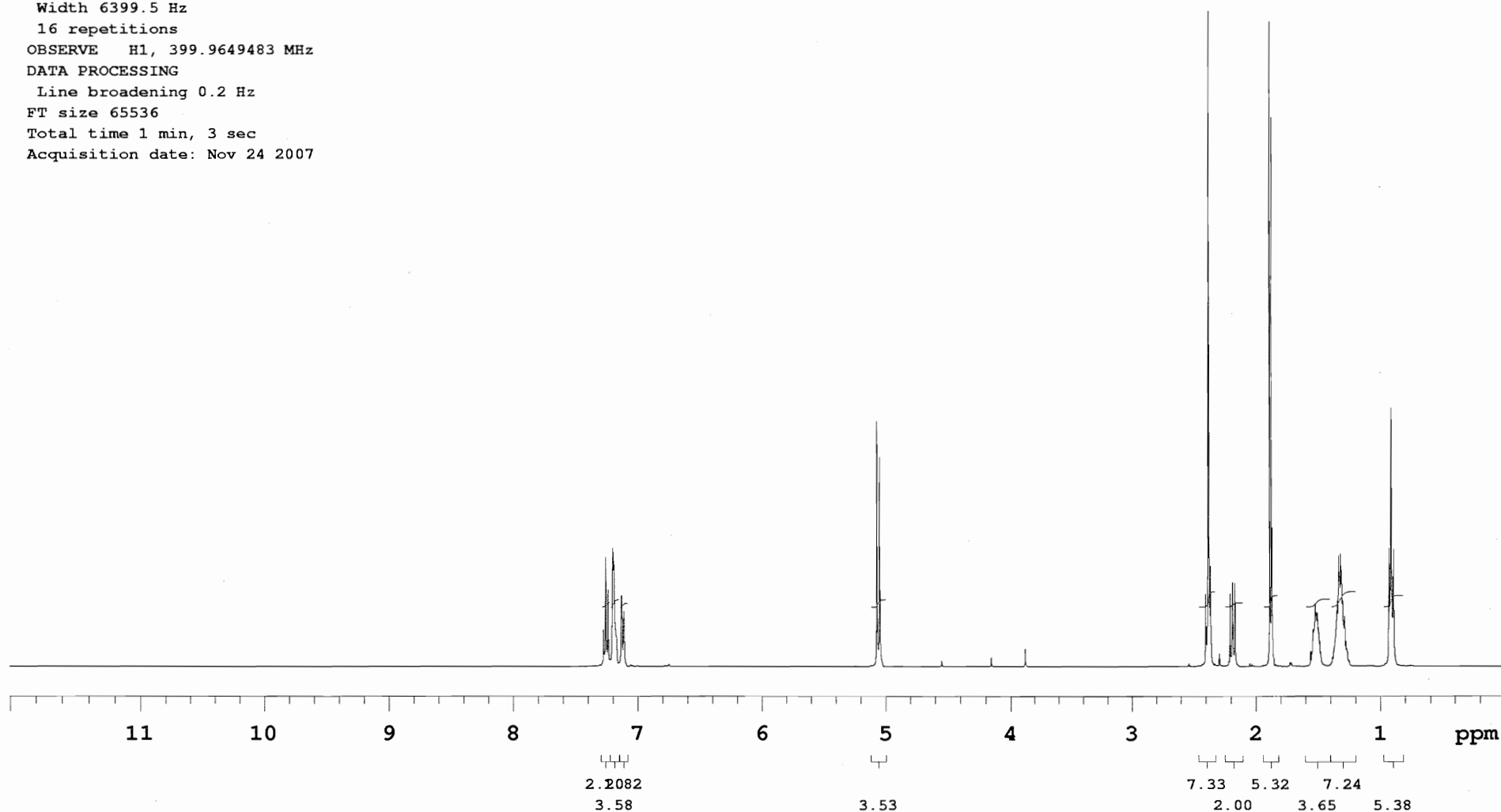
Operator: lopa

File: 11lvdbenzyloximeproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649483 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007



BenzyloximeSM-carbon

File: 111vdbenzyloximecarbon

Pulse Sequence: s2pul

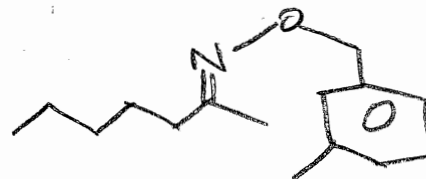
Solvent: cdcl3

Ambient temperature

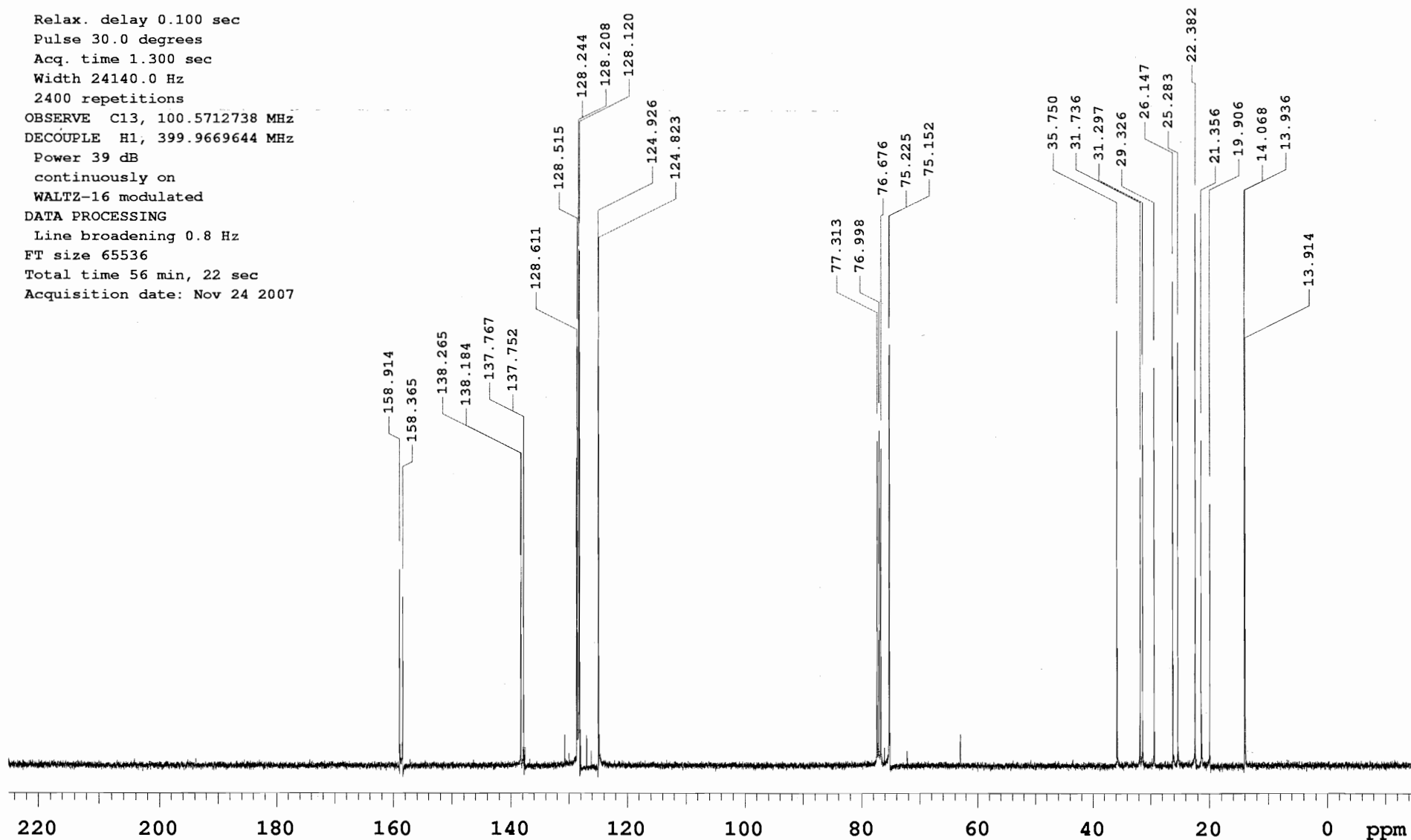
Operator: lopa

File: 111vdbenzyloximecarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
 Pulse 30.0 degrees  
 Acq. time 1.300 sec  
 Width 24140.0 Hz  
 2400 repetitions  
 OBSERVE C13, 100.5712738 MHz  
 DECOUPLE H1, 399.9669644 MHz  
 Power 39 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.8 Hz  
 FT size 65536  
 Total time 56 min, 22 sec  
 Acquisition date: Nov 24 2007



BiphenylKetone-proton

File: 111vd212proton

Pulse Sequence: s2pul

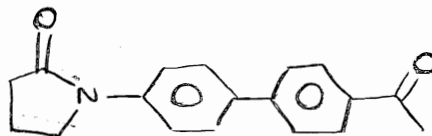
Solvent: cdcl3

Ambient temperature

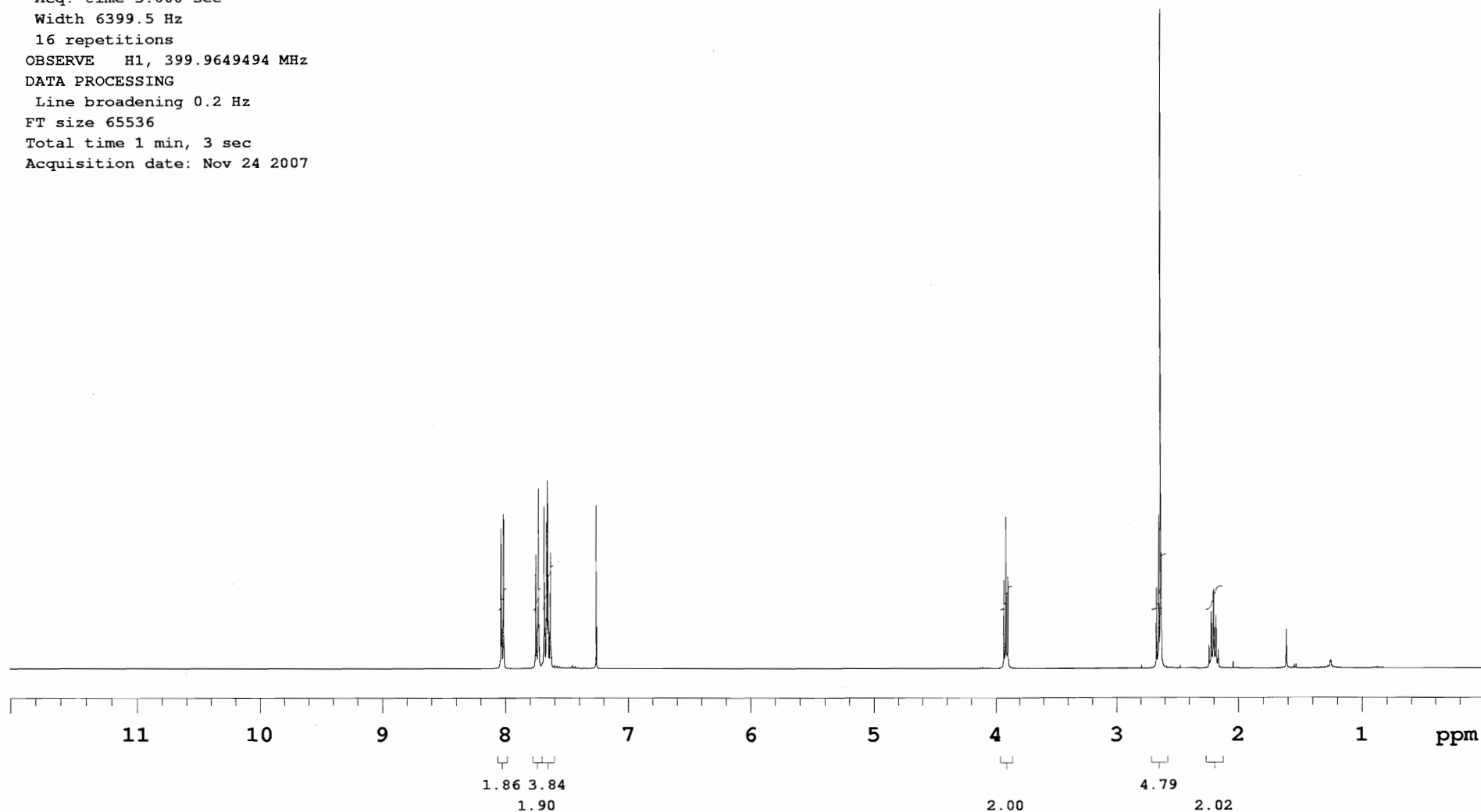
Operator: lopa

File: 111vd212proton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649494 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 24 2007



BiphenylKetone-carbon

File: 111vd212carbon

Pulse Sequence: s2pul

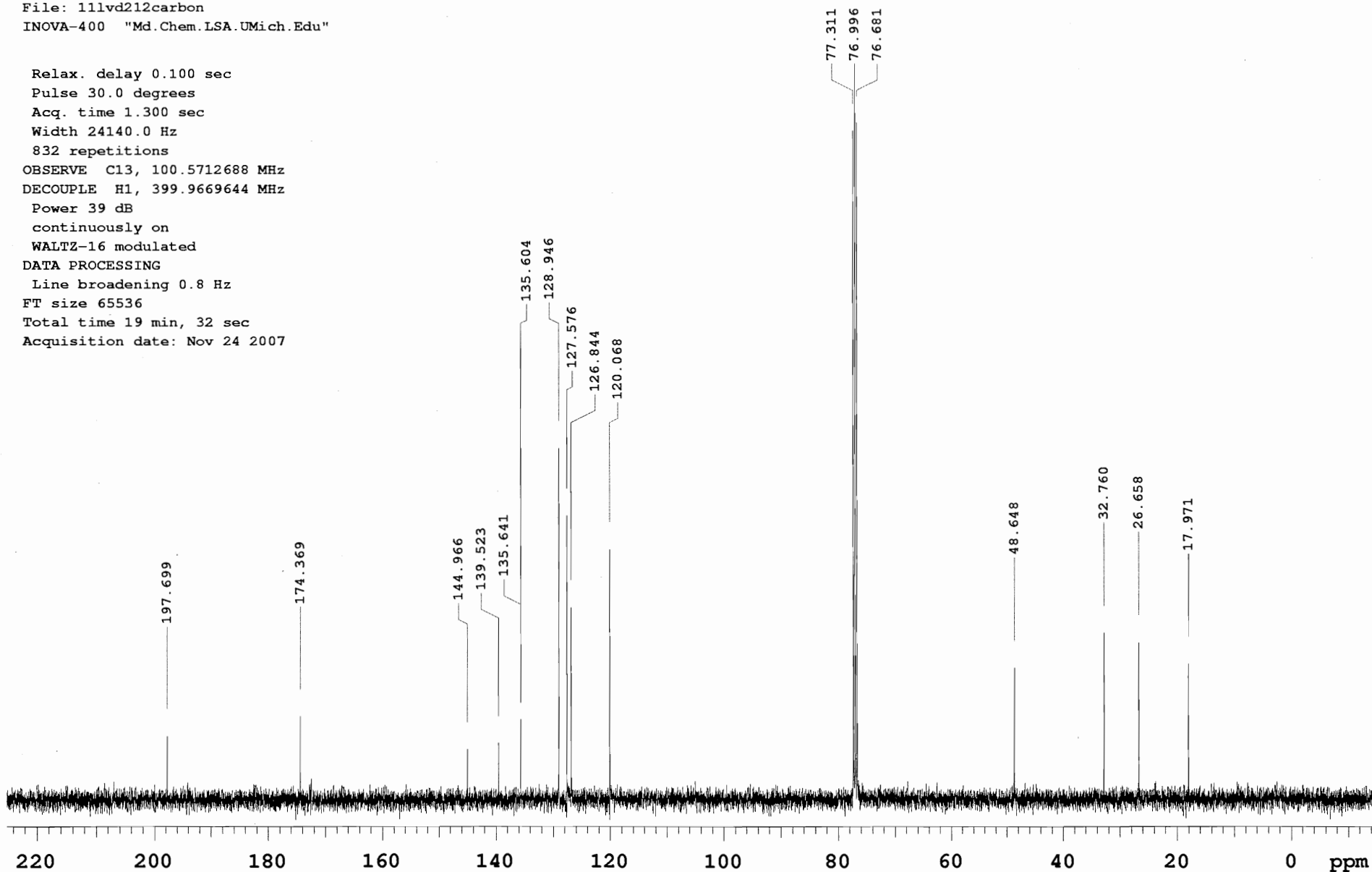
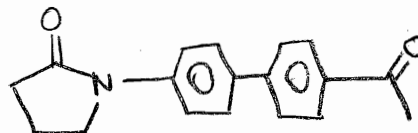
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vd212carbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



BiphenylOxime-proton

File: 111vd215proton

Pulse Sequence: s2pul

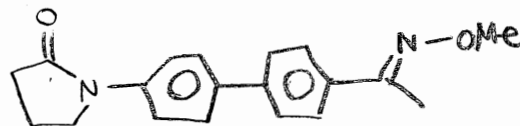
Solvent: cdcl3

Ambient temperature

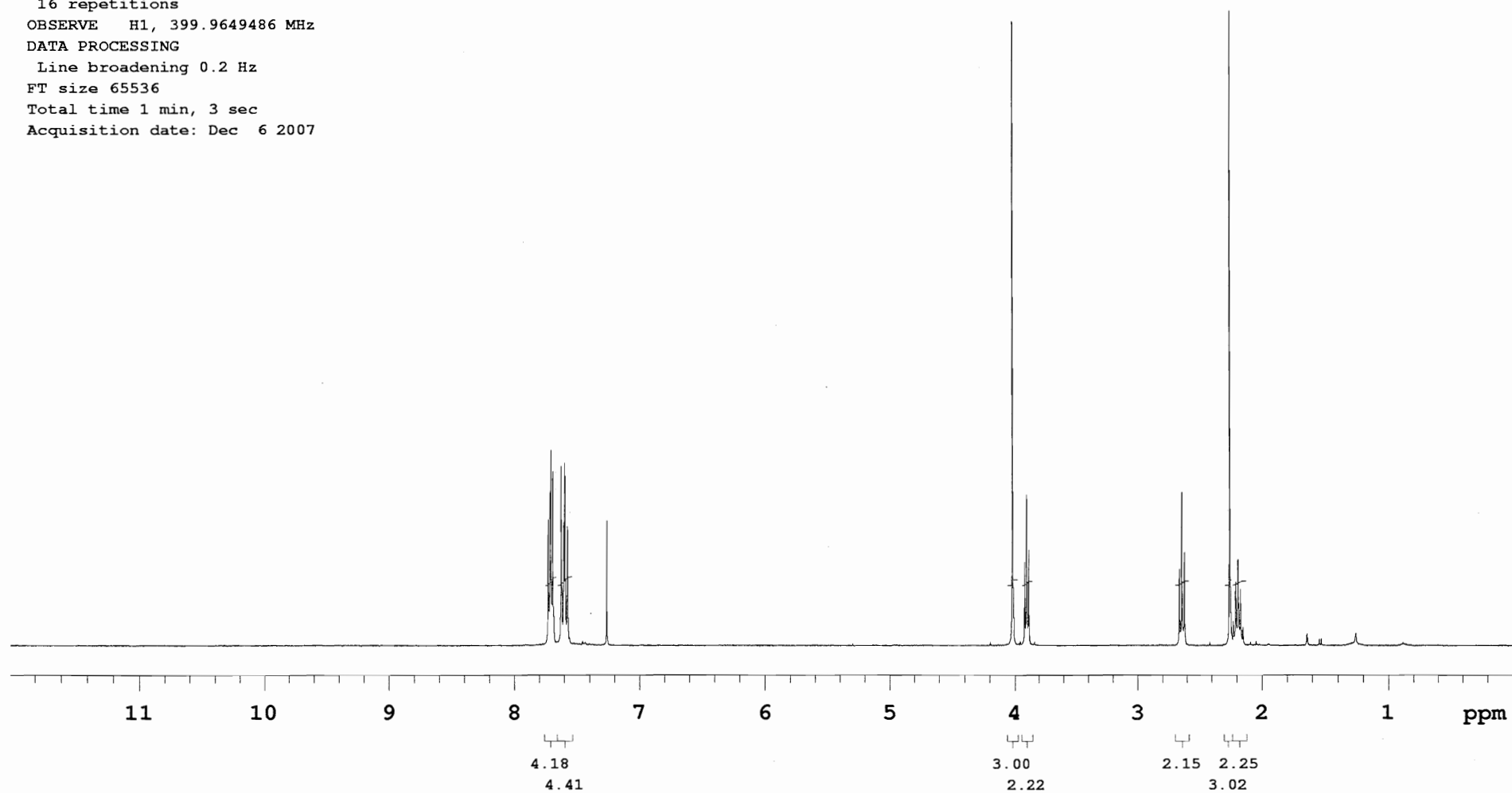
Operator: lopa

File: 111vd215proton

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649486 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Dec 6 2007



BiphenylOxime-carbon

File: 111vd215carbon

Pulse Sequence: s2pul

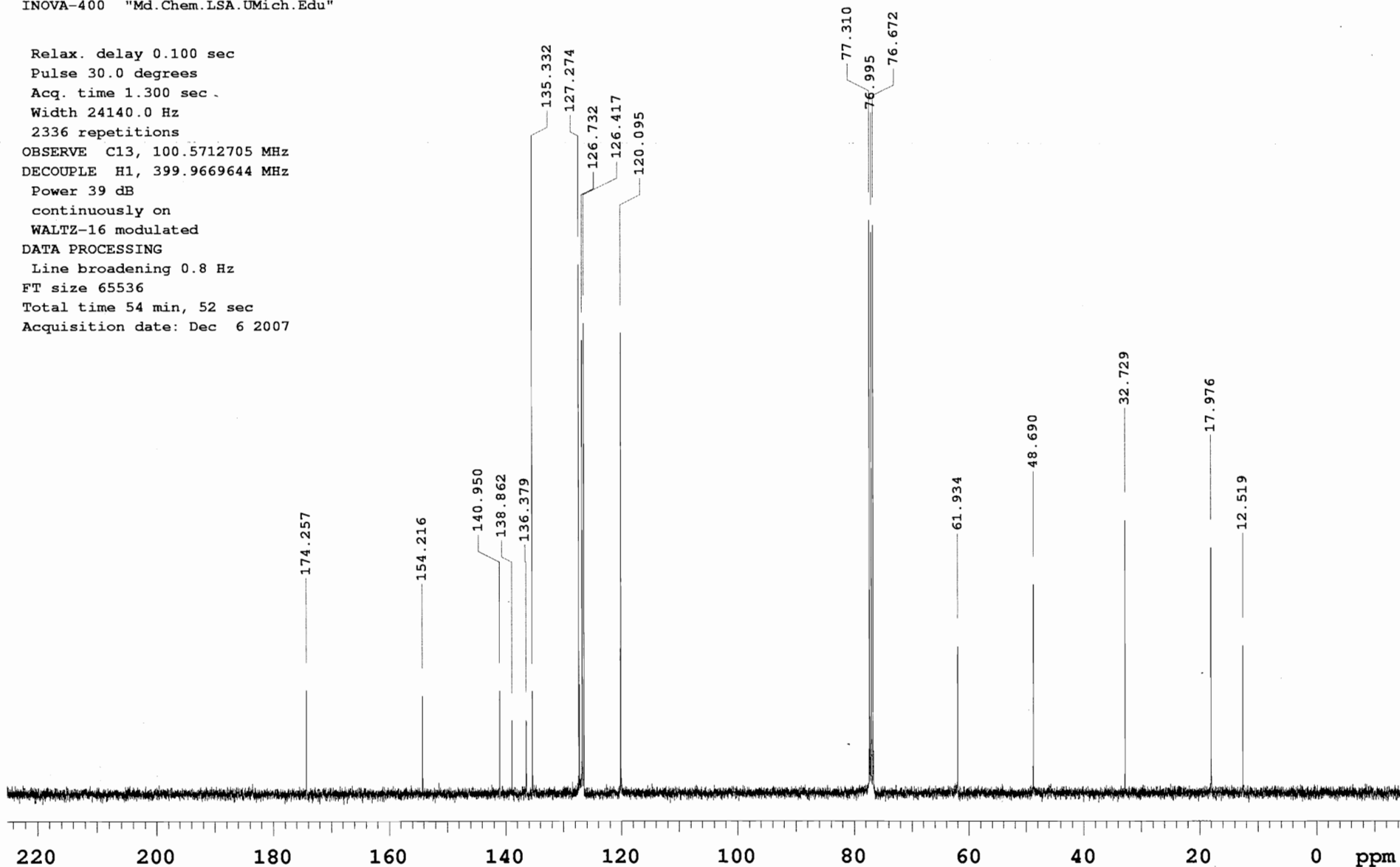
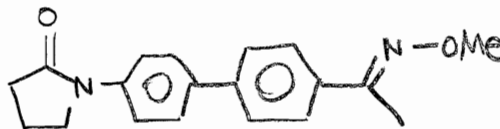
Solvent: cdcl3

Ambient temperature

Operator: lopa

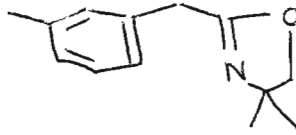
File: 111vd215carbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"

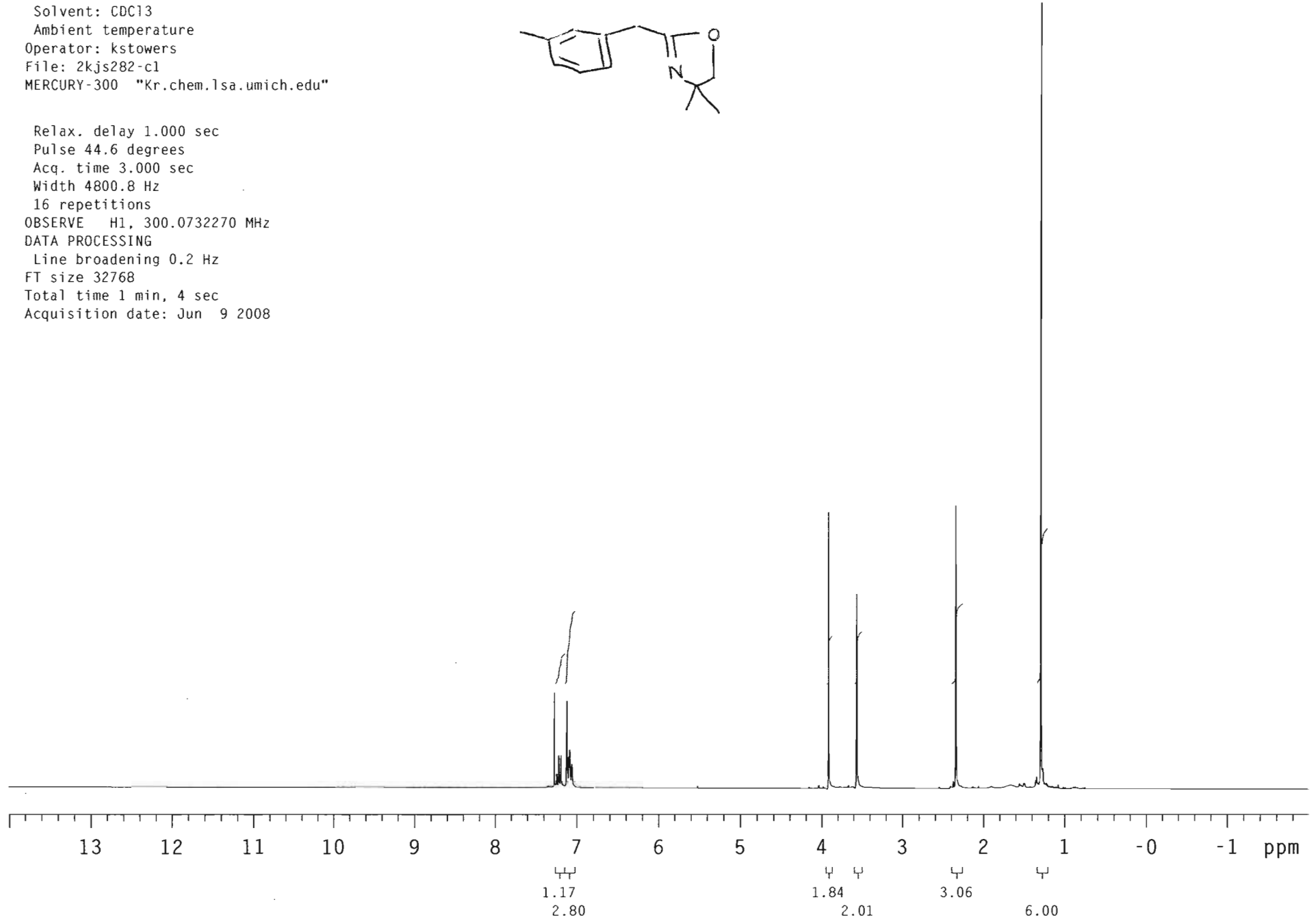


Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Operator: kstowers  
File: 2kjs282-c1  
MERCURY-300 "Kr.chem.lsa.umich.edu"



Relax. delay 1.000 sec  
Pulse 44.6 degrees  
Acq. time 3.000 sec  
Width 4800.8 Hz  
16 repetitions  
OBSERVE H1, 300.0732270 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 32768  
Total time 1 min, 4 sec  
Acquisition date: Jun 9 2008





2kjs289-smC

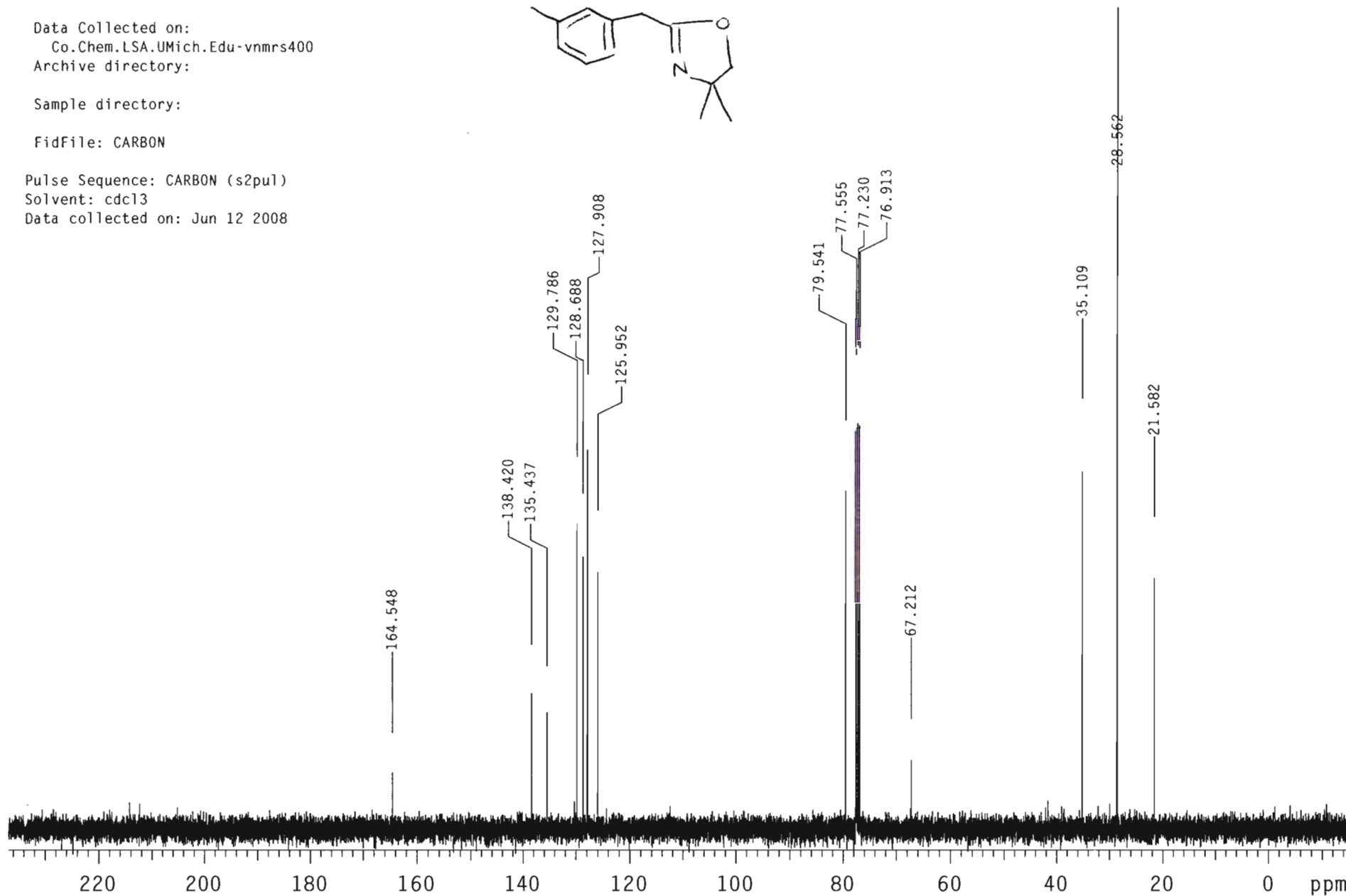
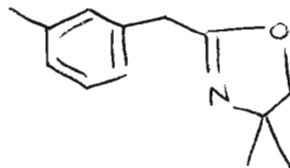
Sample Name:

Data Collected on:  
Co.Chem.LSA.UMich.Edu-vnmrs400  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)  
Solvent: cdcl3  
Data collected on: Jun 12 2008



pMe-proton

File: 111vd205-2proton

Pulse Sequence: s2pul

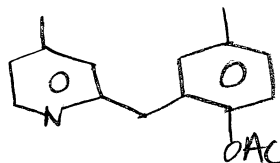
Solvent: cdcl3

Ambient temperature

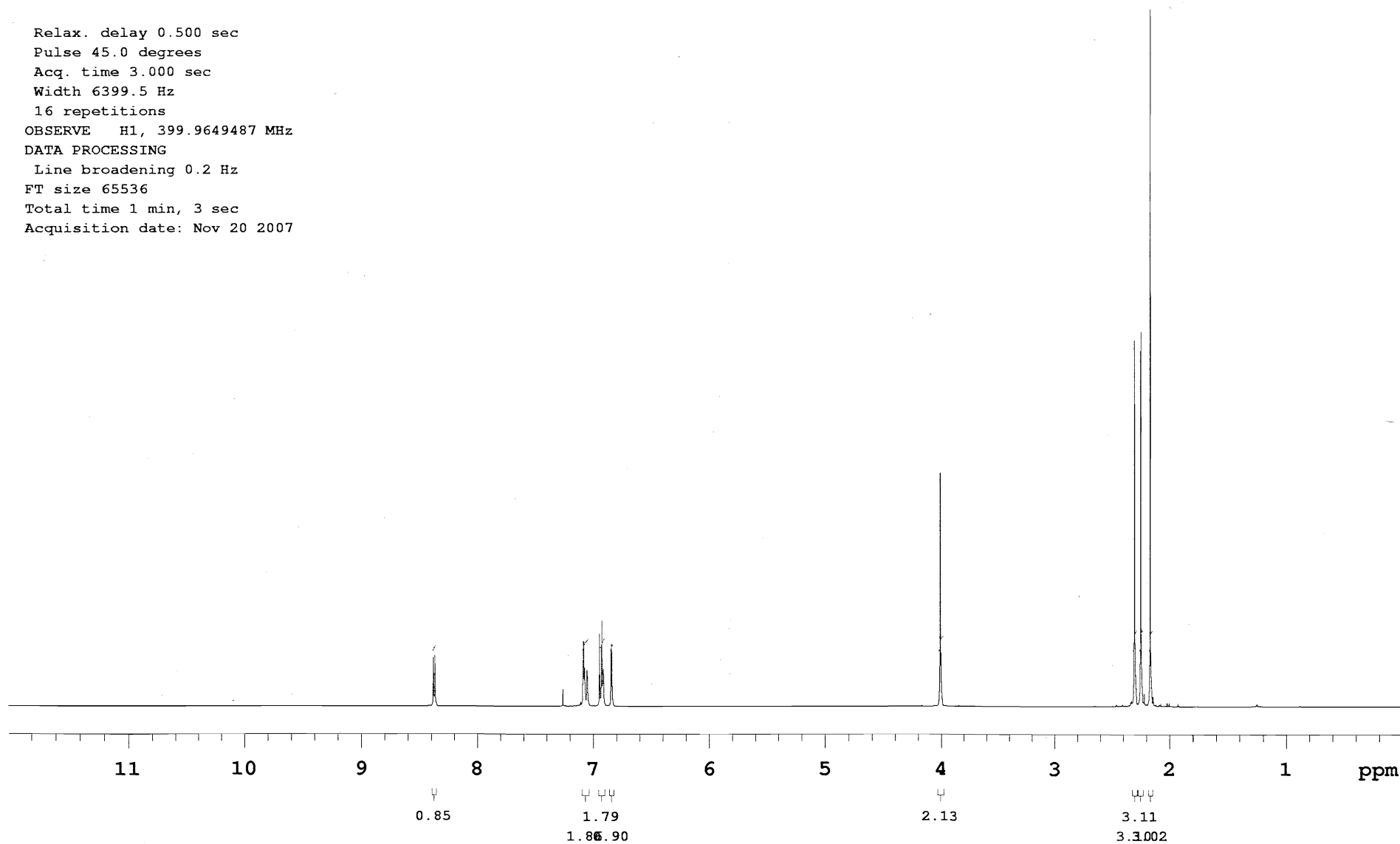
Operator: lopa

File: 111vd205-2proton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649487 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 20 2007



pMe-carbon

File: 111vd205-2carbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vd205-2carbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

400 repetitions

OBSERVE C13, 100.5712757 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

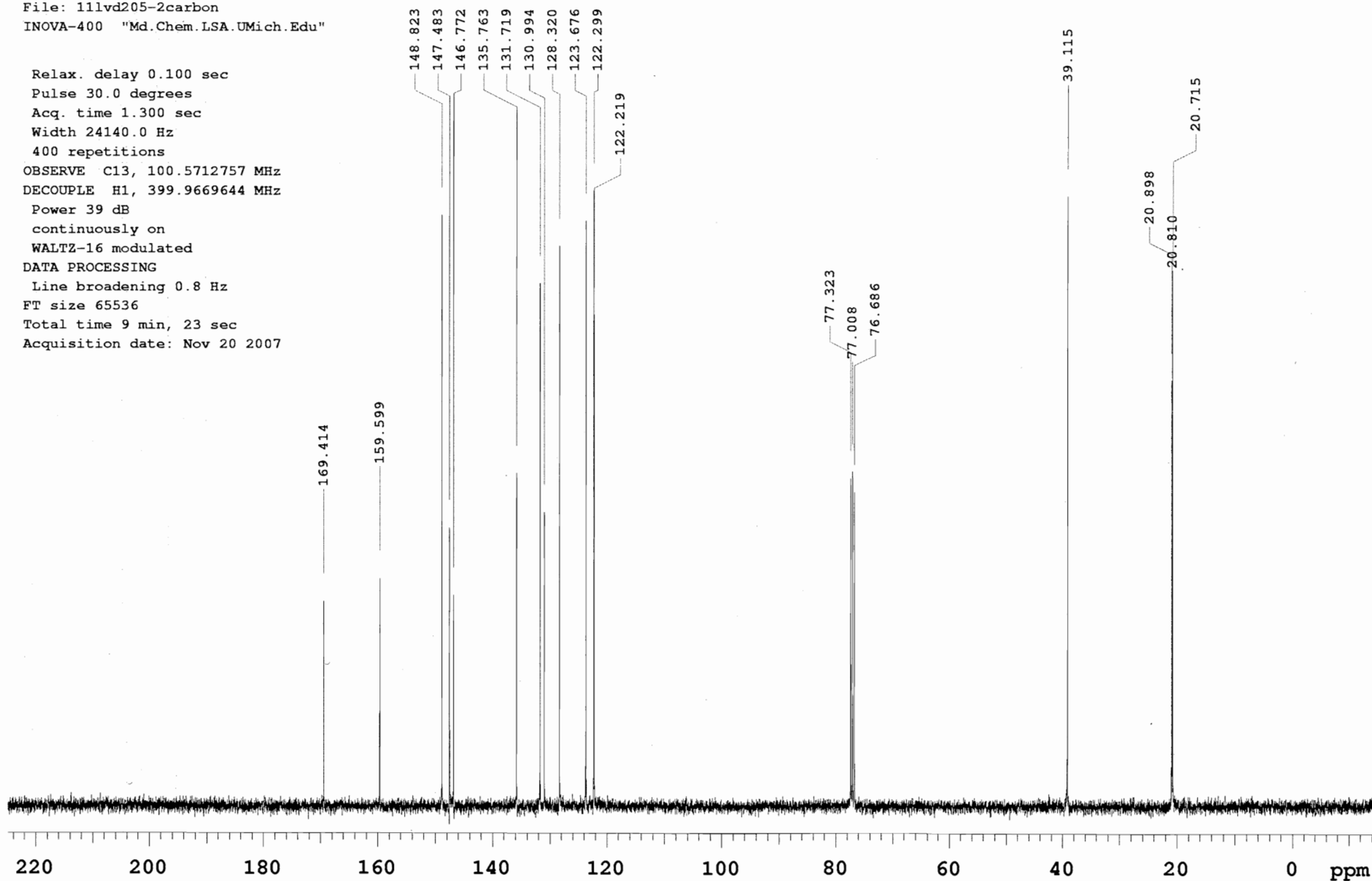
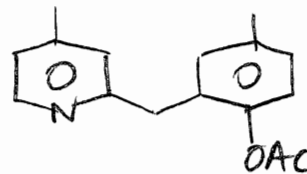
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 9 min, 23 sec

Acquisition date: Nov 20 2007



pOMe-proton

File: 111vd205-3proton

Pulse Sequence: s2pul

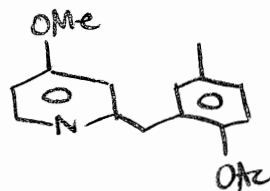
Solvent: cdcl3

Ambient temperature

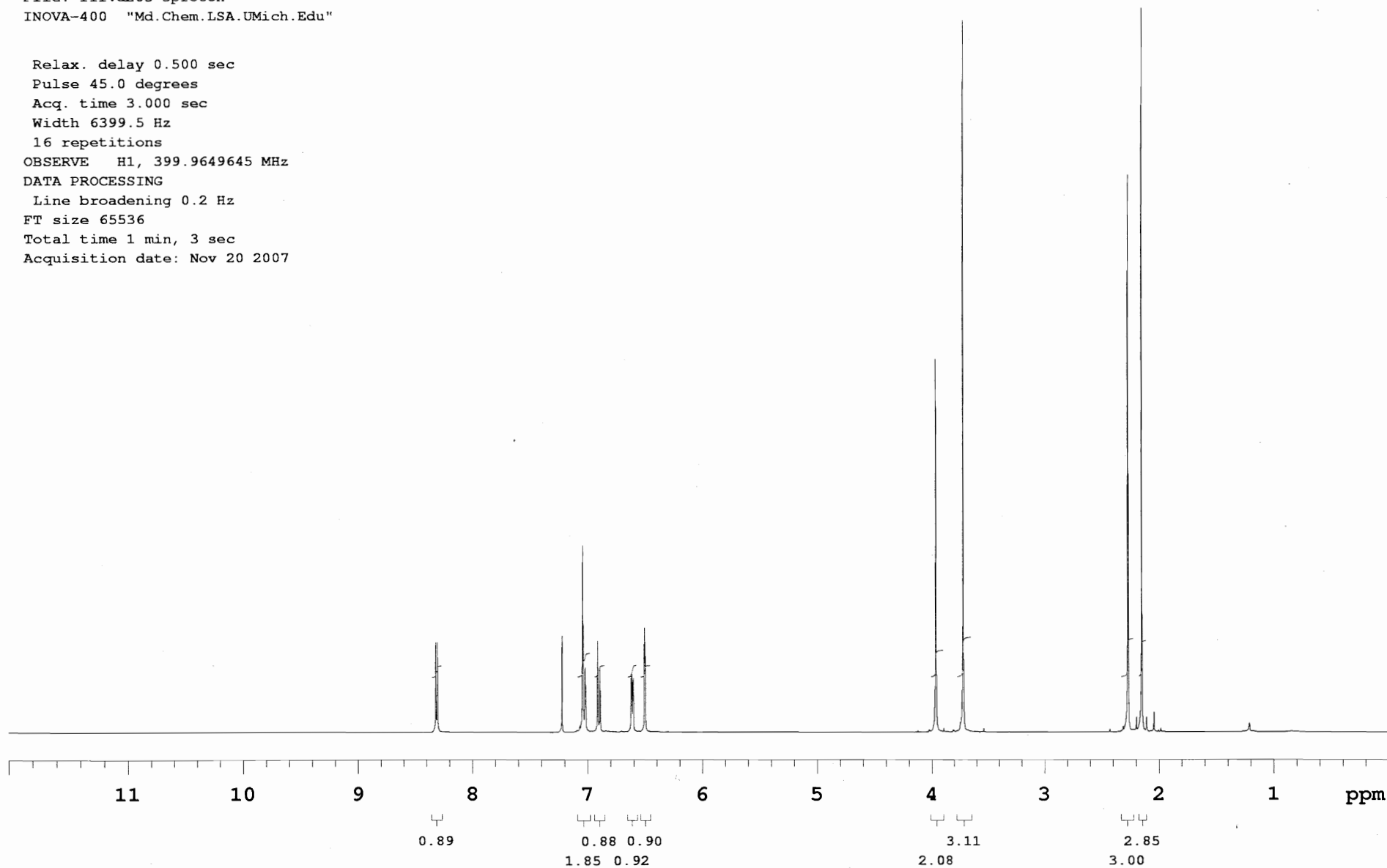
Operator: lopa

File: 111vd205-3proton

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649645 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Nov 20 2007



pOMe-carbon

File: 1-kjs-113-CNMR

Pulse Sequence: s2pul

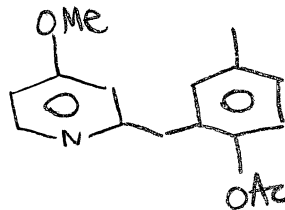
Solvent: cdcl3

Ambient temperature

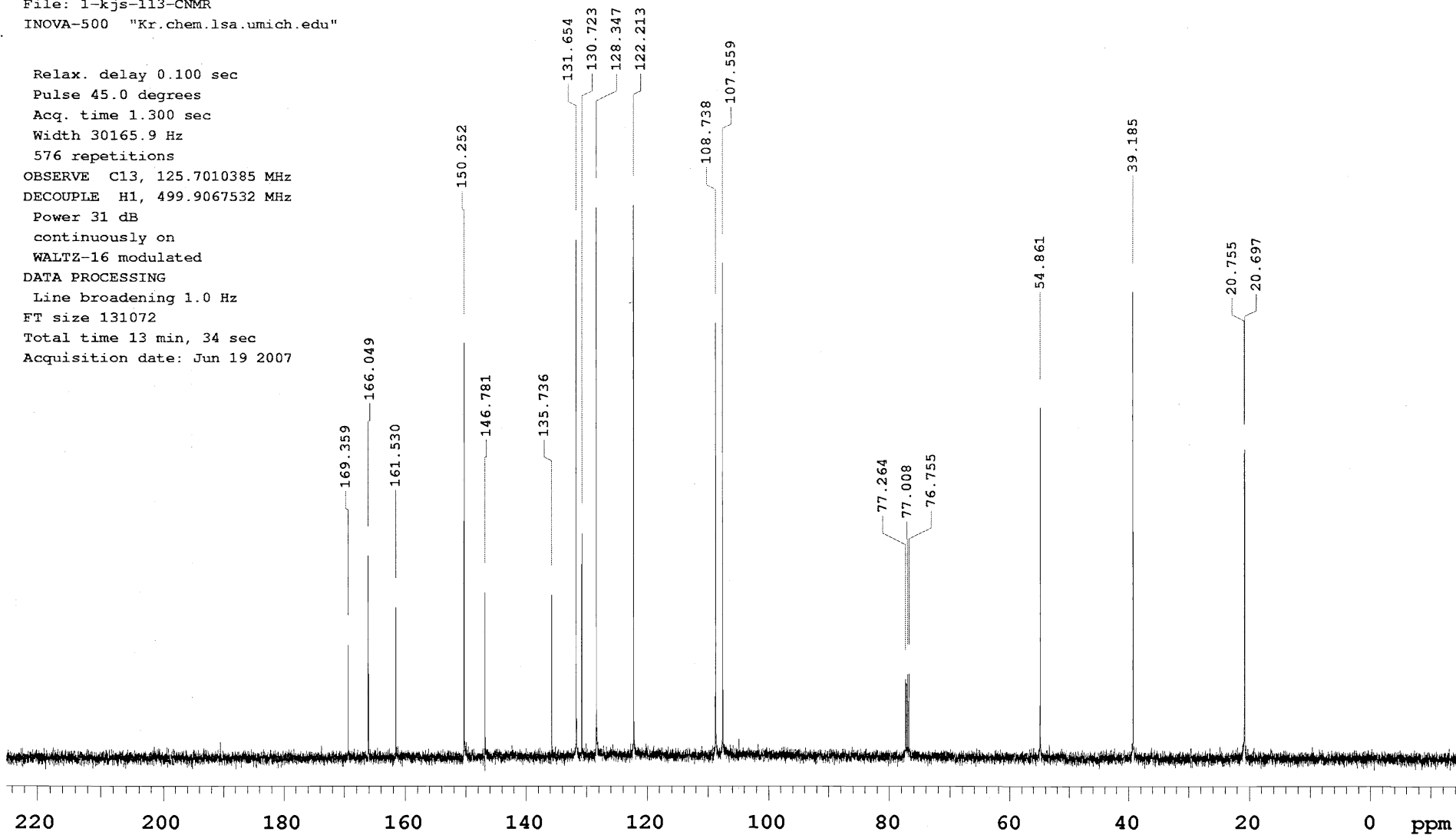
Operator: kstowers

File: 1-kjs-113-CNMR

INNOVA-500 "Kr.chem.lsa.umich.edu"



Relax. delay 0.100 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 30165.9 Hz  
576 repetitions  
OBSERVE C13, 125.7010385 MHz  
DECOUPLE H1, 499.9067532 MHz  
Power 31 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 131072  
Total time 13 min, 34 sec  
Acquisition date: Jun 19 2007



pCF3-proton

File: 1-kjs-83-CF3-pure

Pulse Sequence: s2pul

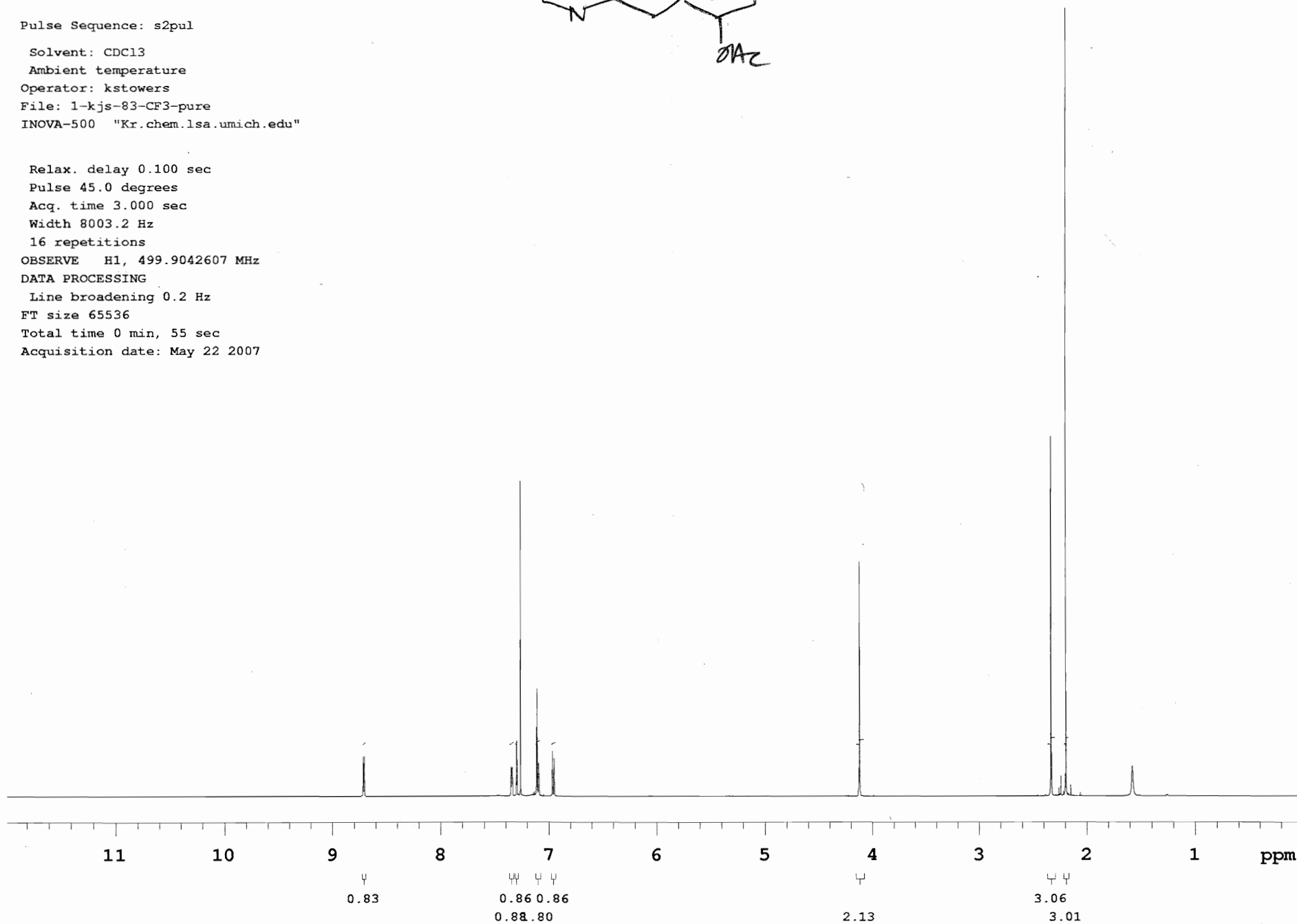
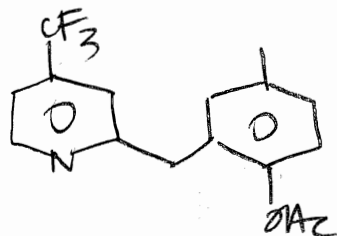
Solvent: CDCl3

Ambient temperature

Operator: kstowers

File: 1-kjs-83-CF3-pure

INOVA-500 "Kr.chem.lsa.umich.edu"



pCF3-carbon

File: 1-kjs-83-CNMR

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: kstowers

File: 1-kjs-83-CNMR

INNOVA-400 "Kr.chem.lsa.umich

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

656 repetitions

OBSERVE C13, 100.5712706 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

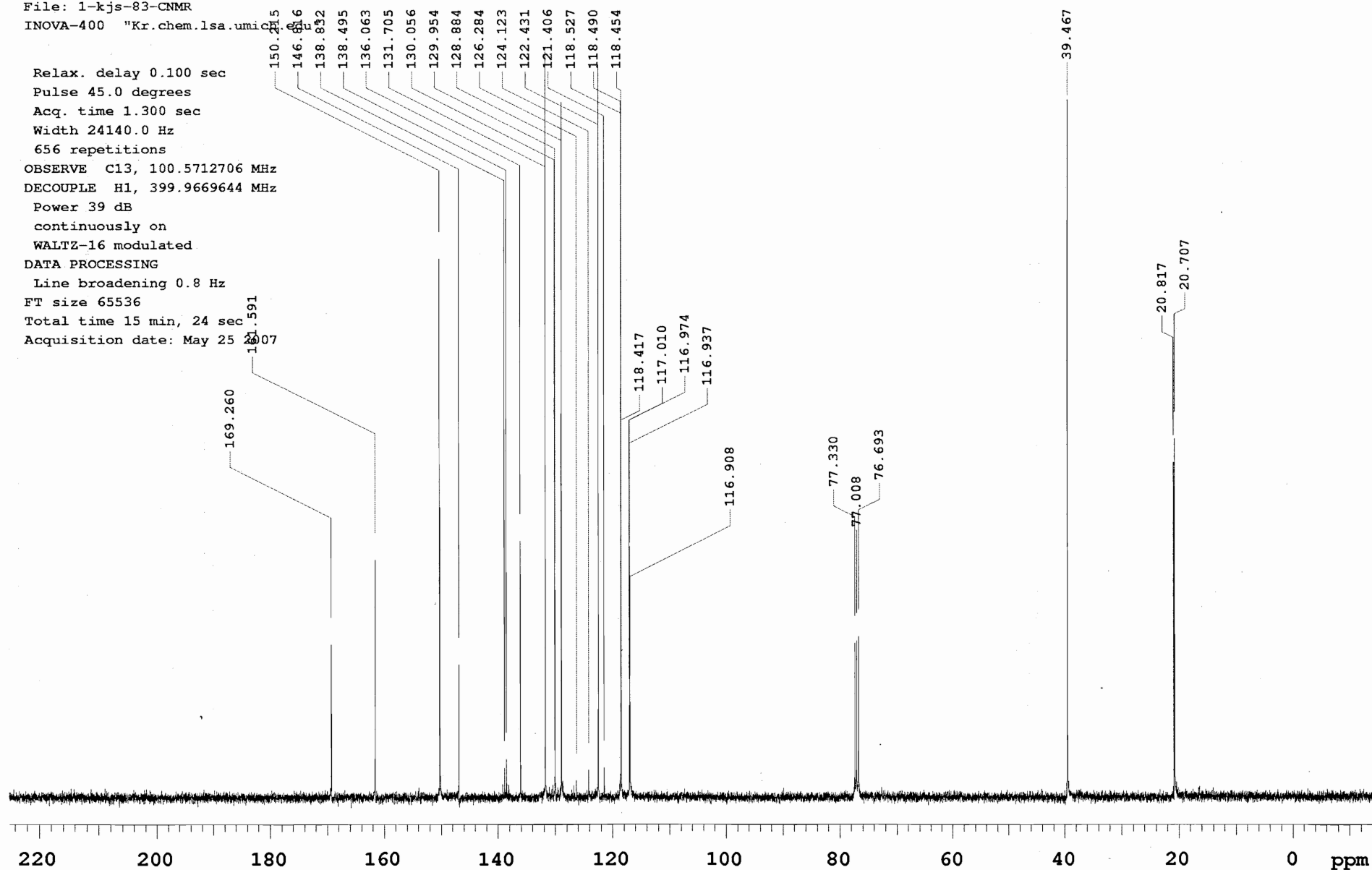
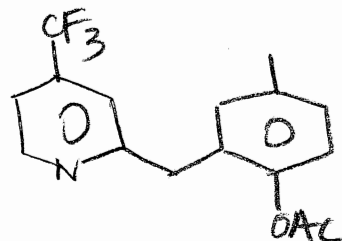
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 15 min, 24 sec

Acquisition date: May 25 1987



pCl-proton

File: 111vd189-8proton

Pulse Sequence: s2pul

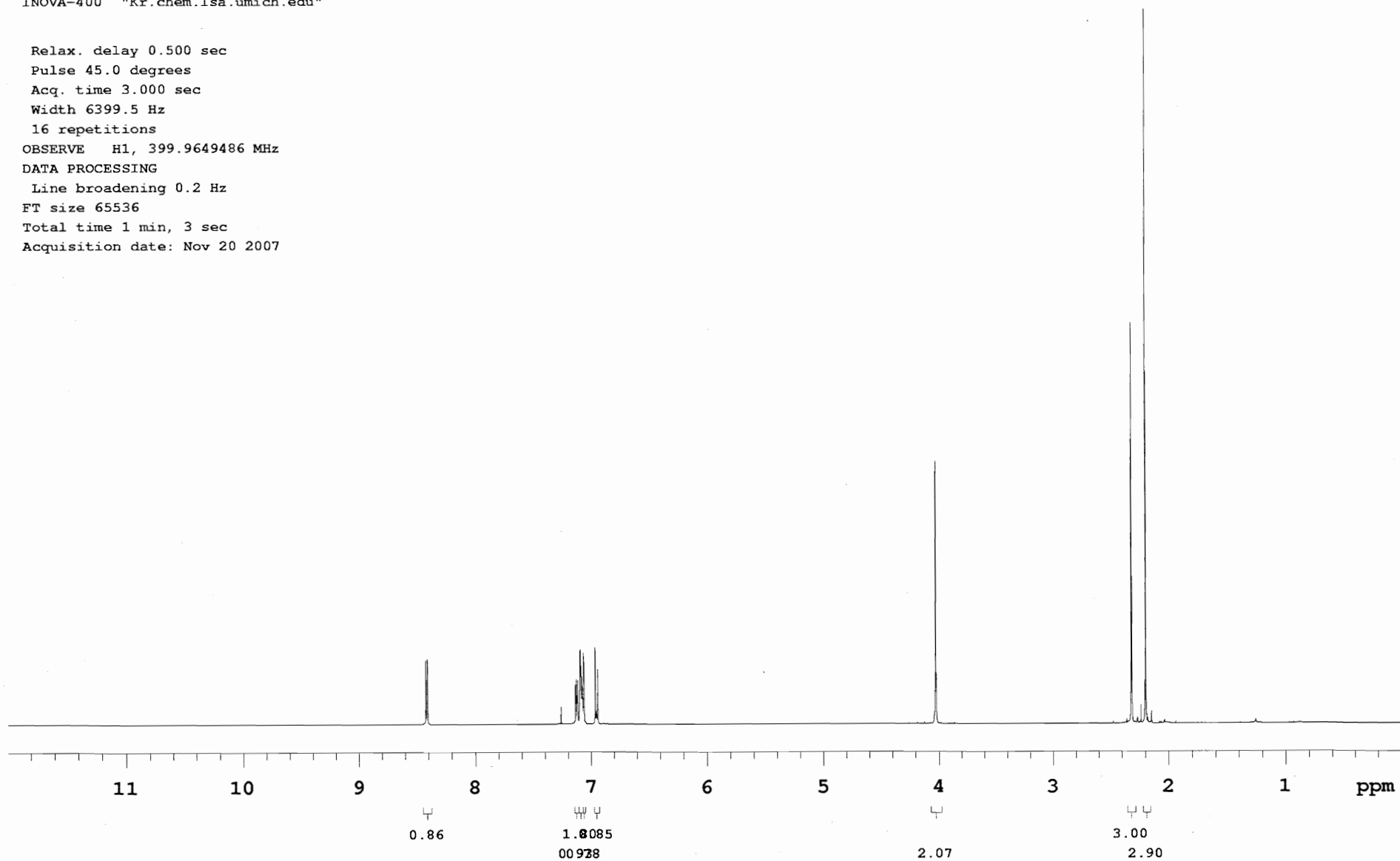
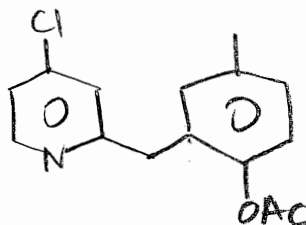
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vd189-8proton

INOVA-400 "Kr.chem.lsa.umich.edu"





pCl-carbon

File: 111vd189-8carbon

Pulse Sequence: s2pul

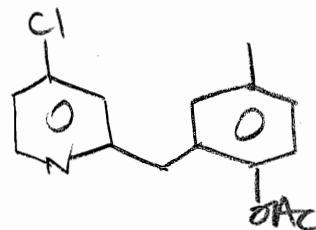
Solvent: cdcl3

Ambient temperature

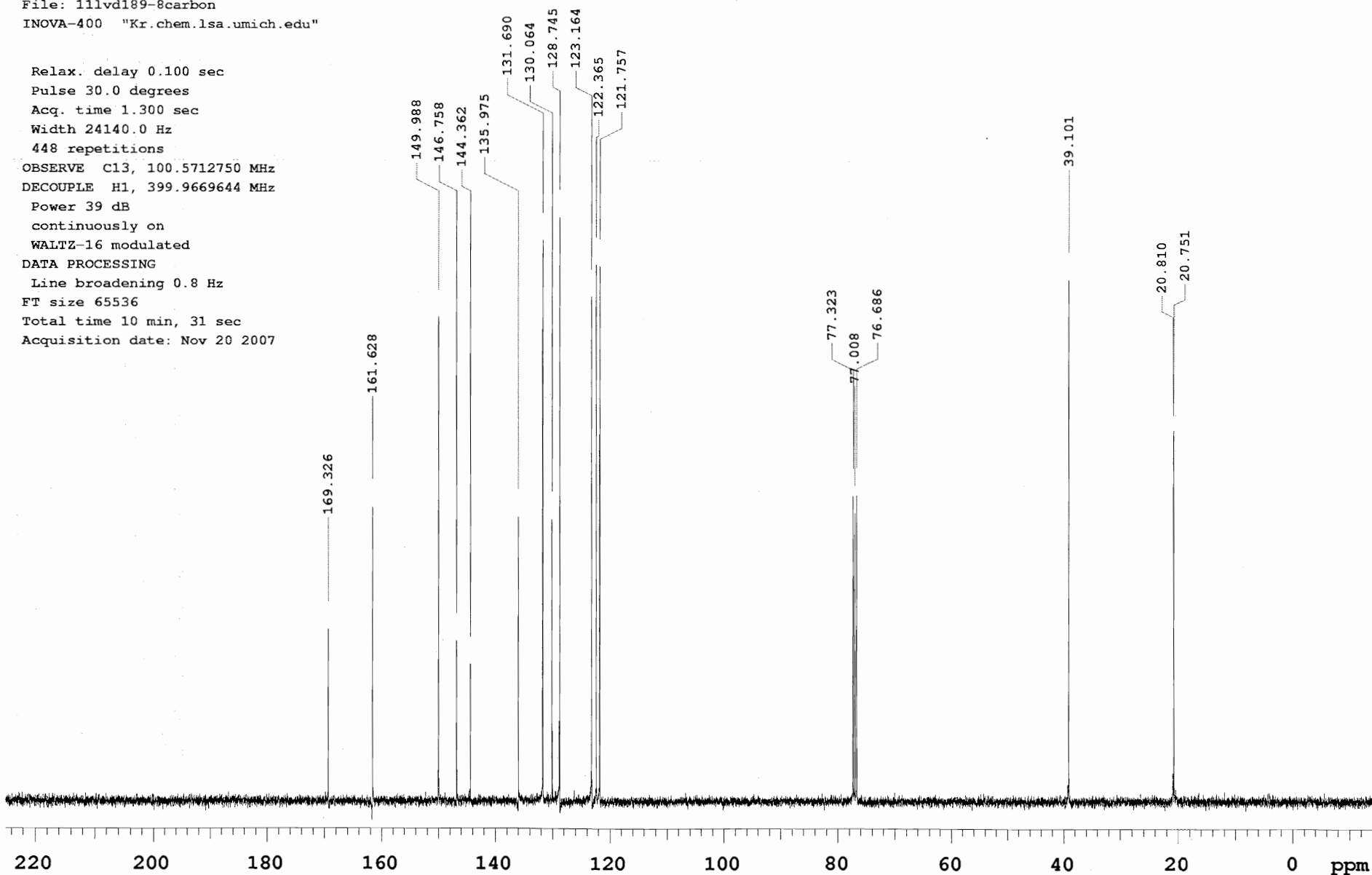
Operator: lopa

File: 111vd189-8carbon

INOVA-400 "Kr.chem.lsa.umich.edu"



Relax. delay 0.100 sec  
 Pulse 30.0 degrees  
 Acq. time 1.300 sec  
 Width 24140.0 Hz  
 448 repetitions  
 OBSERVE C13, 100.5712750 MHz  
 DECOUPLE H1, 399.9669644 MHz  
 Power 39 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.8 Hz  
 FT size 65536  
 Total time 10 min, 31 sec  
 Acquisition date: Nov 20 2007



mMe-proton

File: 111vd205-1proton

Pulse Sequence: s2pul

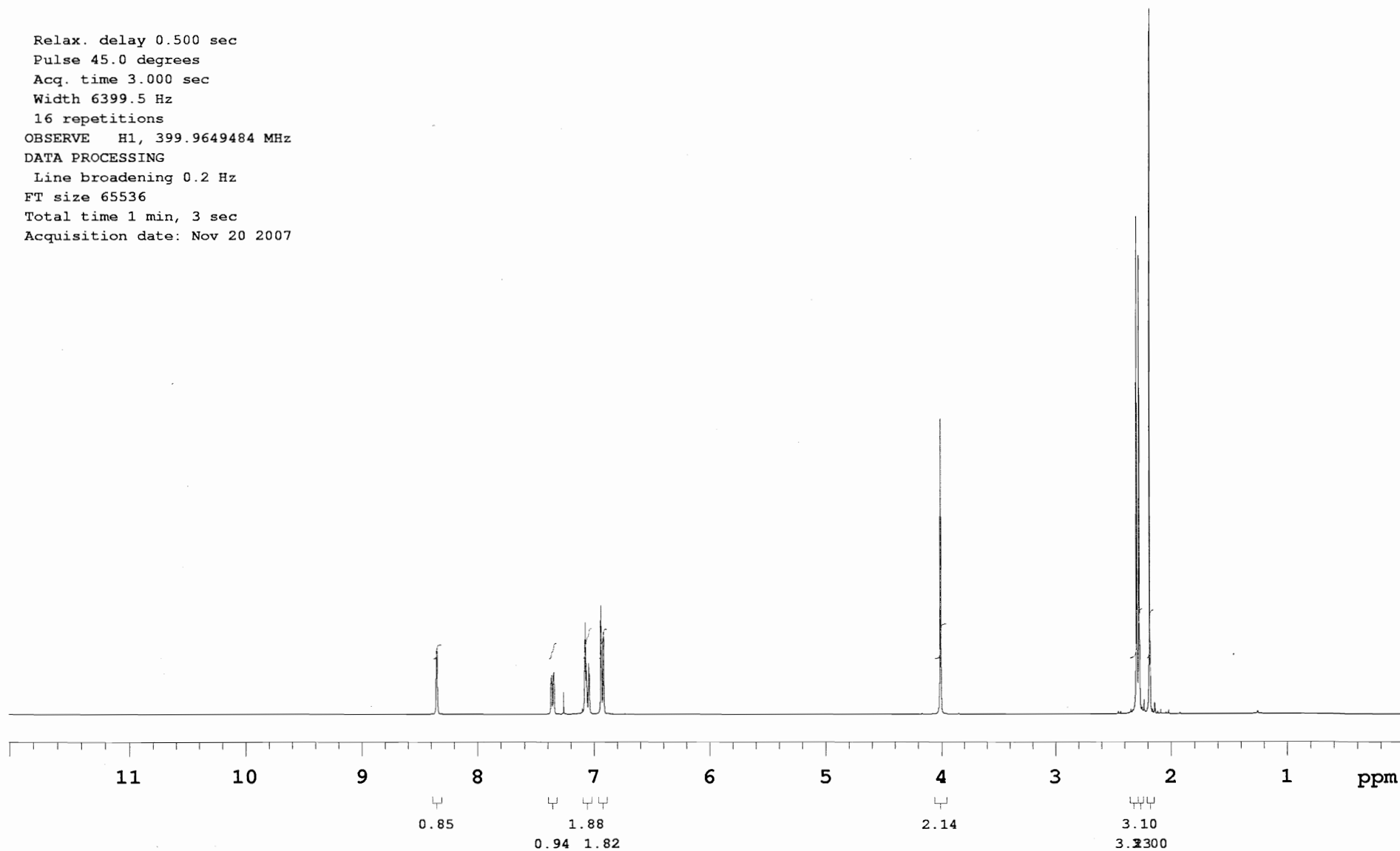
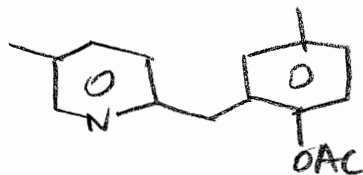
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vd205-1proton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



mMe-carbon

File: 111vd205-1carbon

Pulse Sequence: s2pul

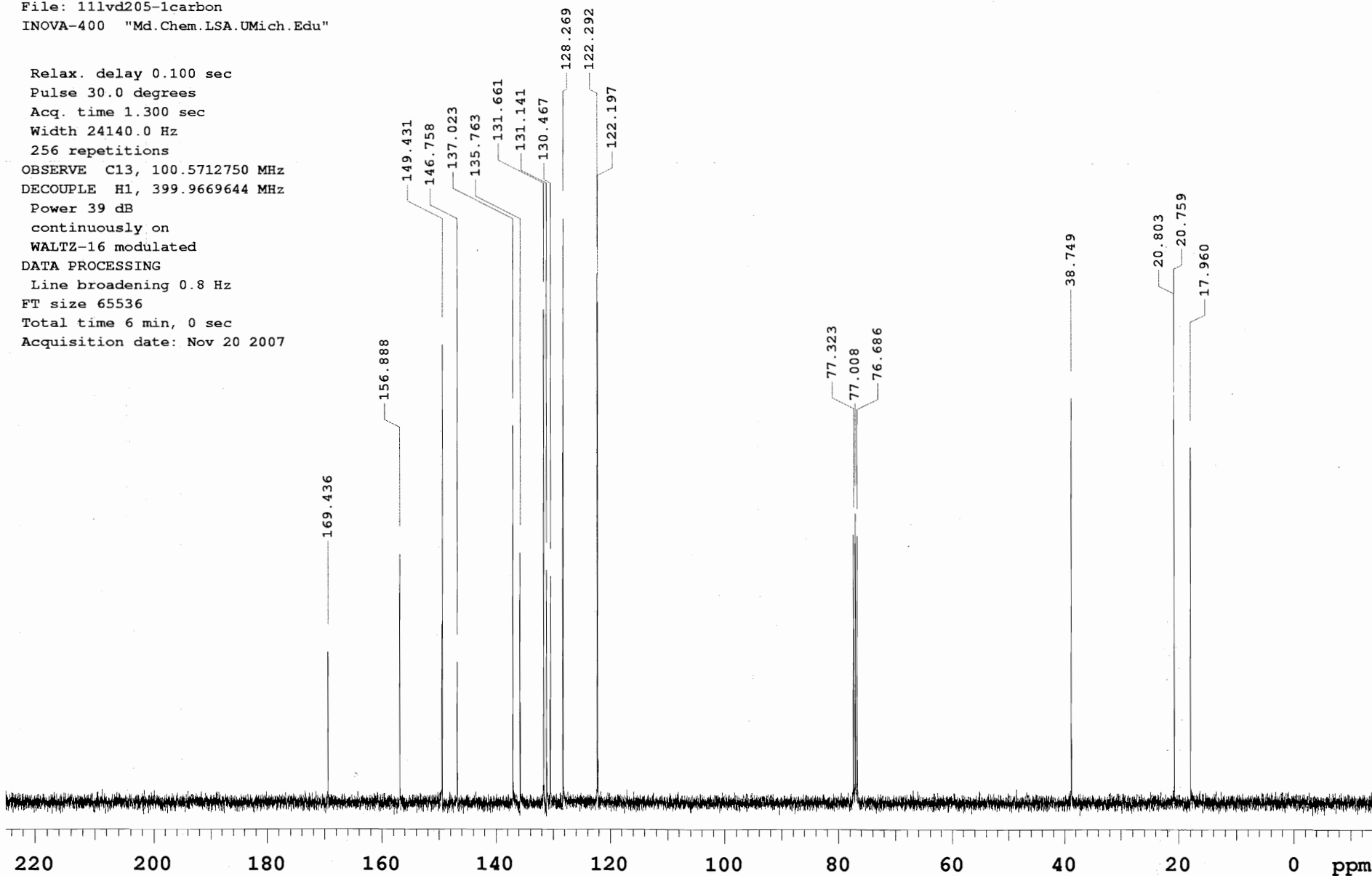
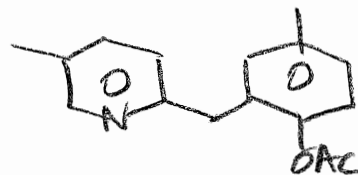
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vd205-1carbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Pyridine-proton

File: 11lvd143proton

Pulse Sequence: s2pul

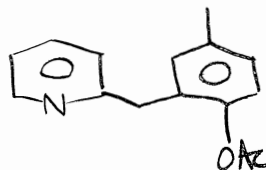
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 11lvd143proton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

16 repetitions

OBSERVE H1, 399.9649488 MHz

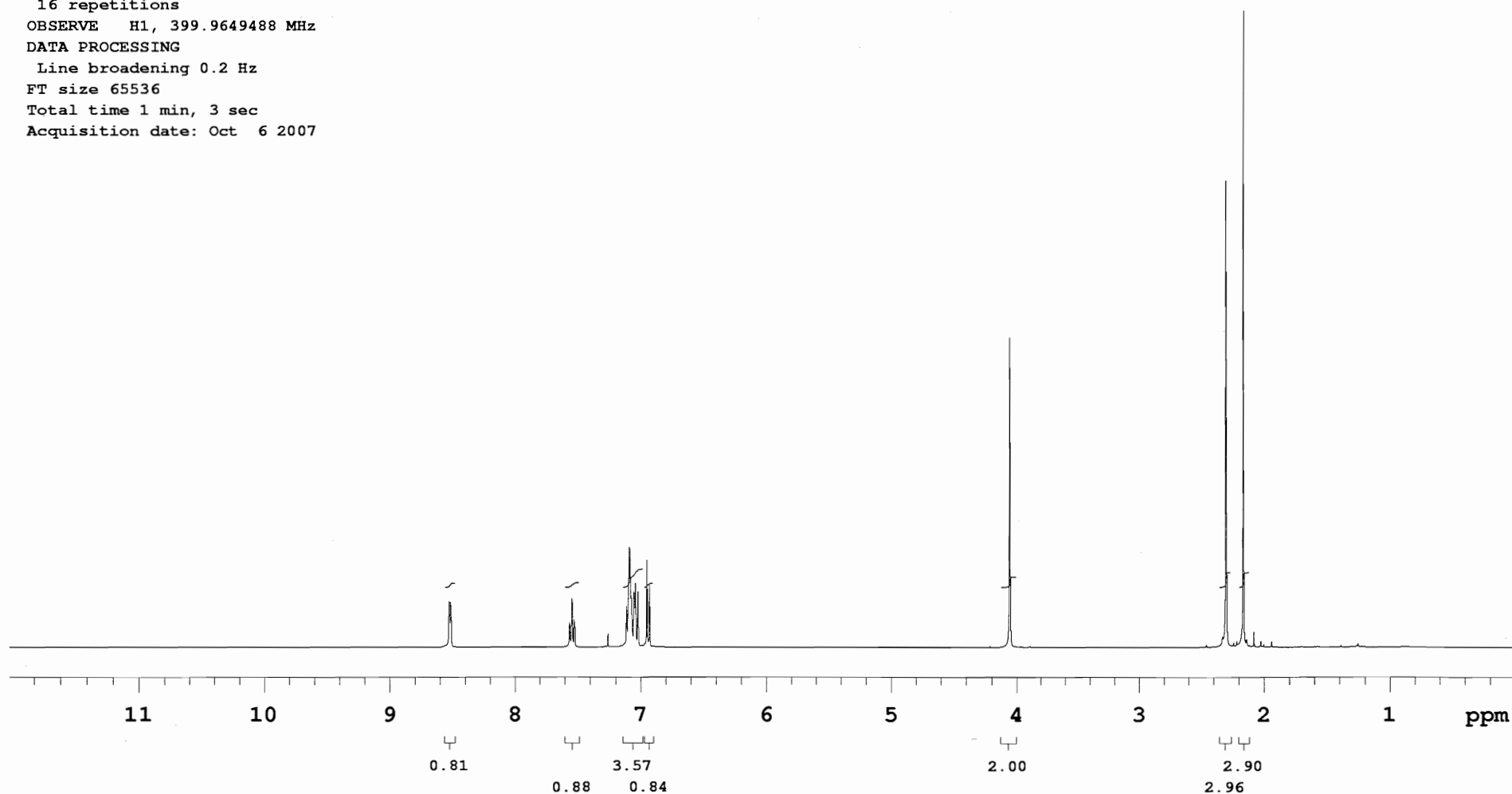
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 3 sec

Acquisition date: Oct 6 2007



Pyridine-Carbon

File: 111vd143carbon

Pulse Sequence: s2pul

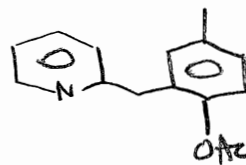
Solvent: cdcl3

Ambient temperature

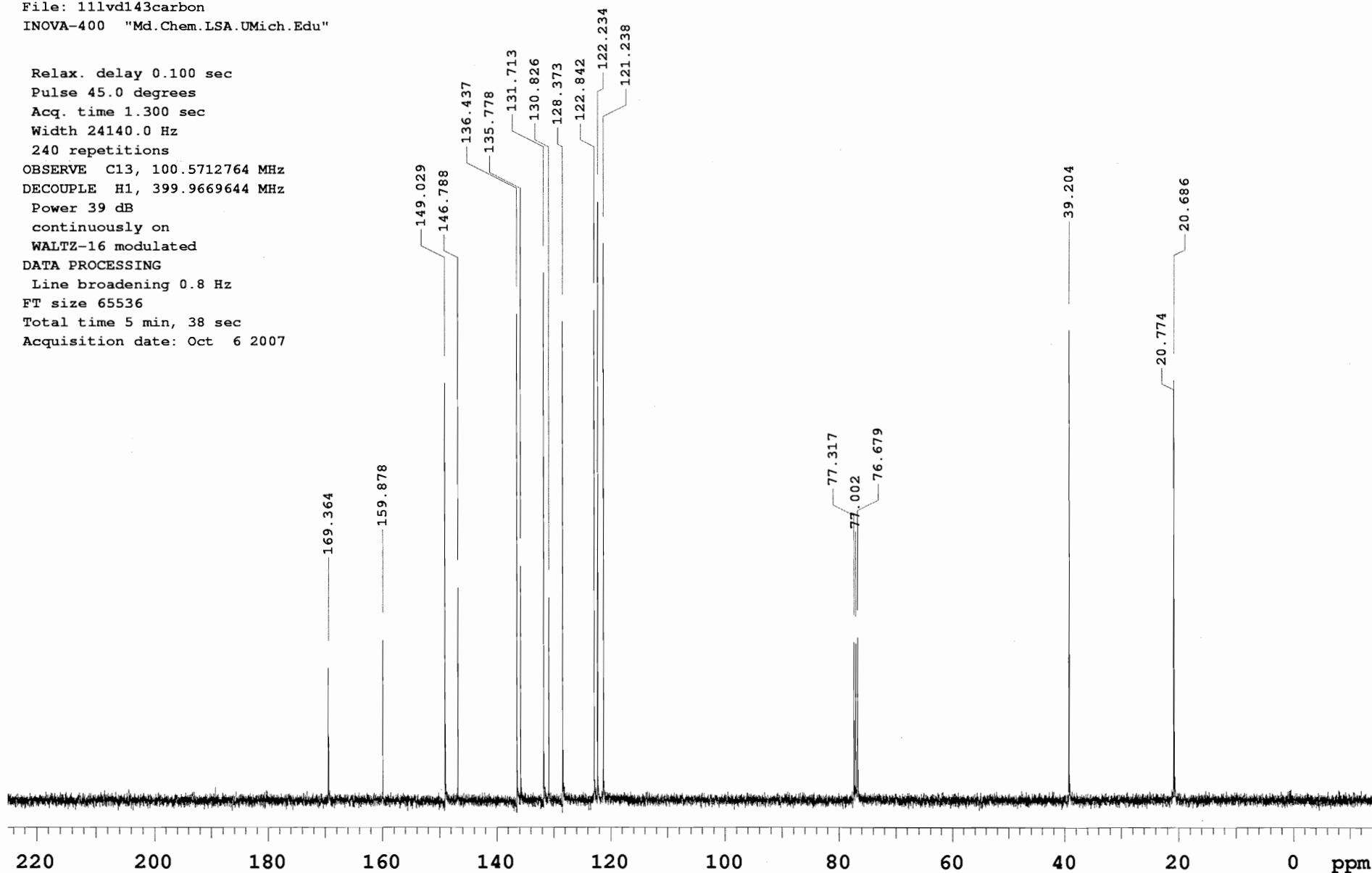
Operator: lopa

File: 111vd143carbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24140.0 Hz  
240 repetitions  
OBSERVE C13, 100.5712764 MHz  
DECOUPLE H1, 399.9669644 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.8 Hz  
FT size 65536  
Total time 5 min, 38 sec  
Acquisition date: Oct 6 2007



mF-proton

File: kjs-2-59-1-mF-H

Pulse Sequence: s2pul

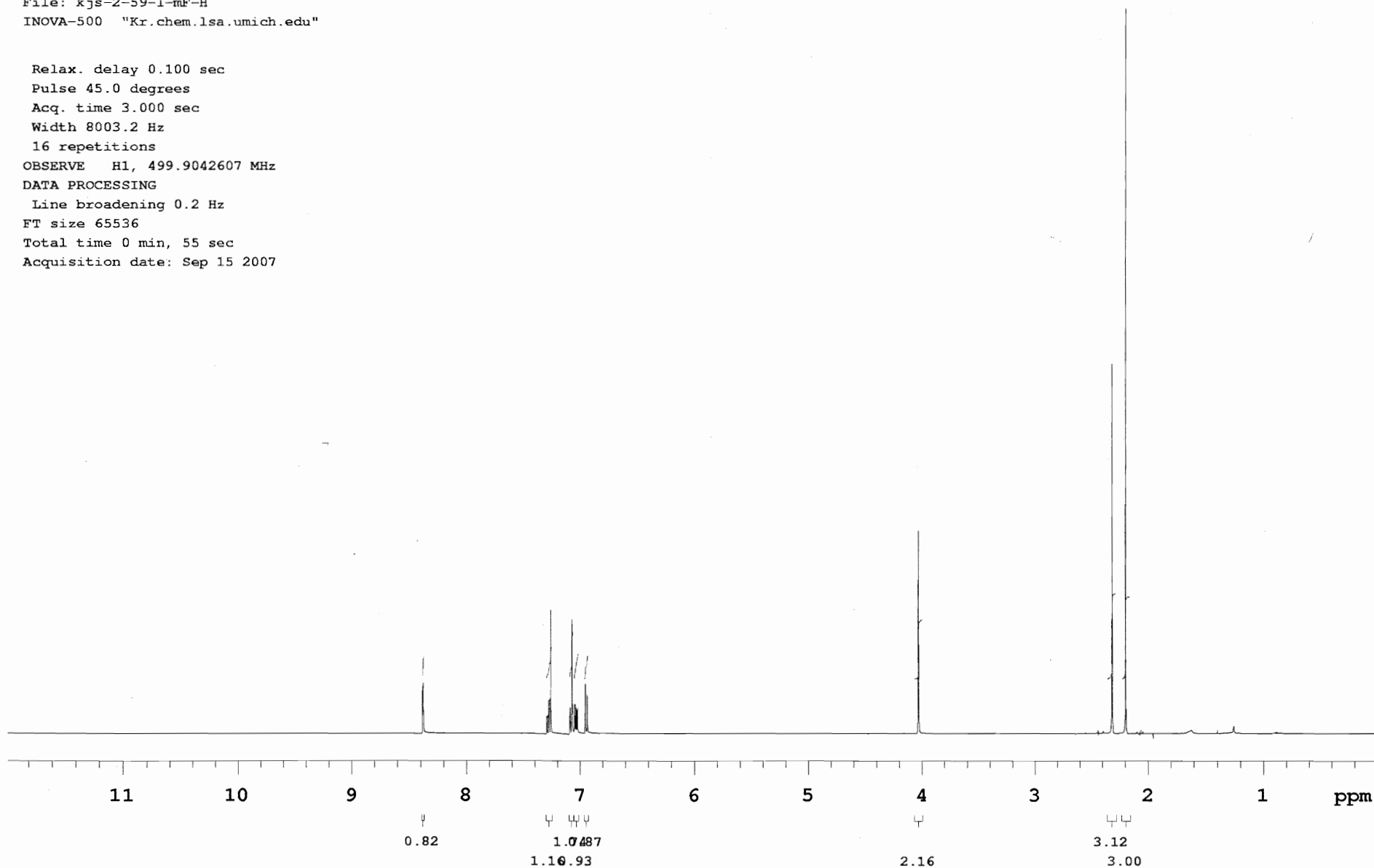
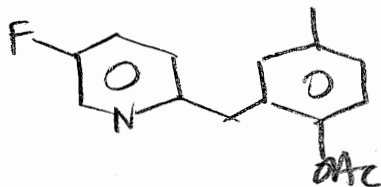
Solvent: cdcl3

Ambient temperature

Operator: kstowers

File: kjs-2-59-1-mF-H

INOVA-500 "Kr.chem.lsa.umich.edu"



mF-carbon

File: kjs-2-69-2-mF-C

Pulse Sequence: s2pul

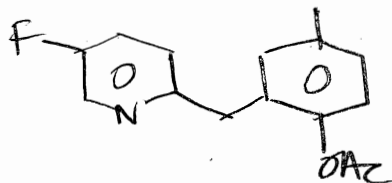
Solvent: cdcl3

Ambient temperature

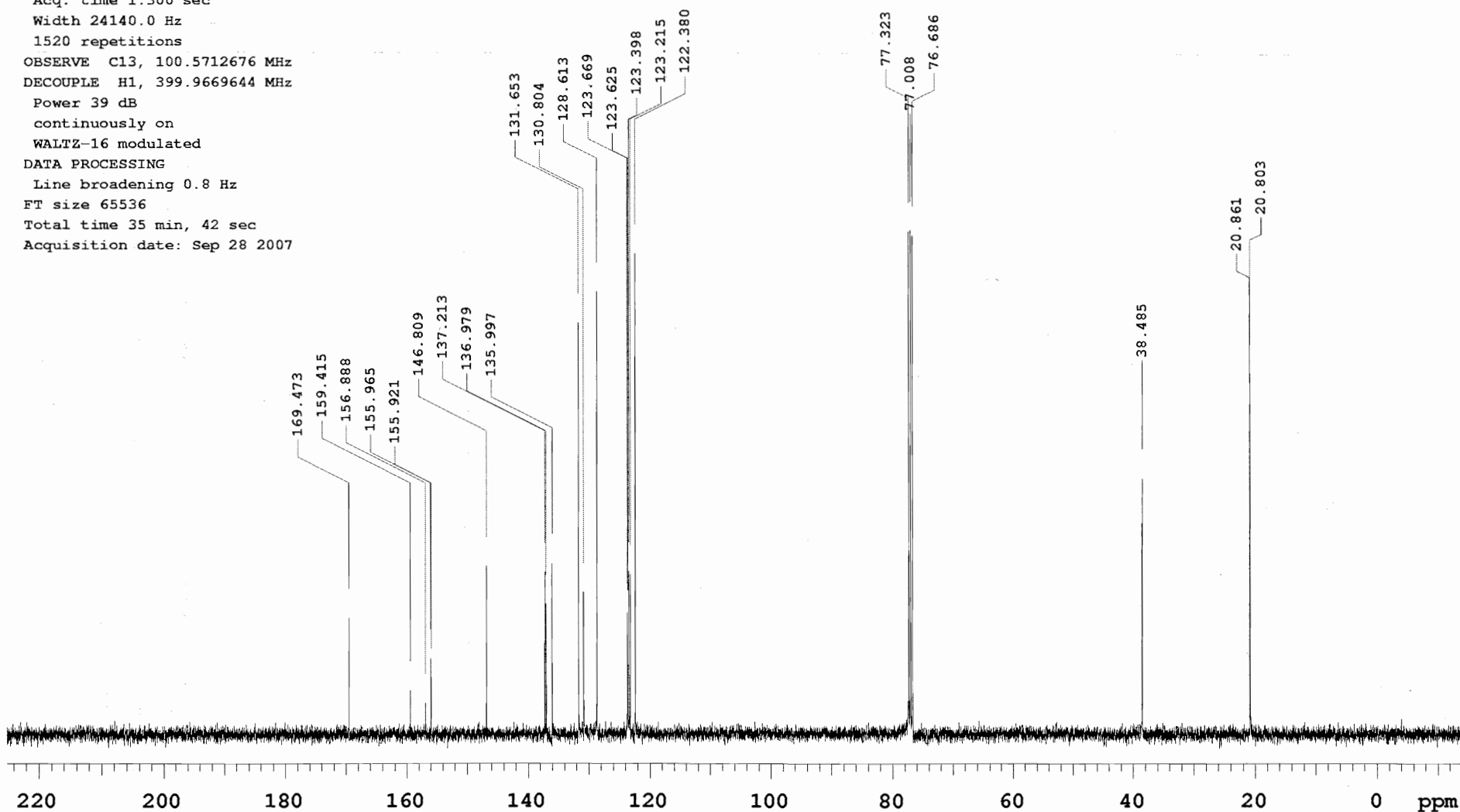
Operator: kstowers

File: kjs-2-69-2-mF-C

INNOVA-400 "Kr.chem.lsa.umich.edu"



Relax. delay 0.100 sec  
 Pulse 45.0 degrees  
 Acq. time 1.300 sec  
 Width 24140.0 Hz  
 1520 repetitions  
 OBSERVE C13, 100.5712676 MHz  
 DECOUPLE H1, 399.9669644 MHz  
 Power 39 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.8 Hz  
 FT size 65536  
 Total time 35 min, 42 sec  
 Acquisition date: Sep 28 2007



## Pyrimidine-proton

File: 101vd201fr60-75proton

Pulse Sequence: s2pul

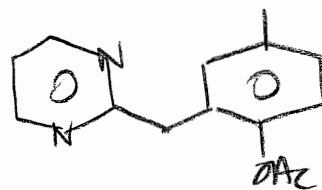
Solvent: cdcl3

Ambient temperature

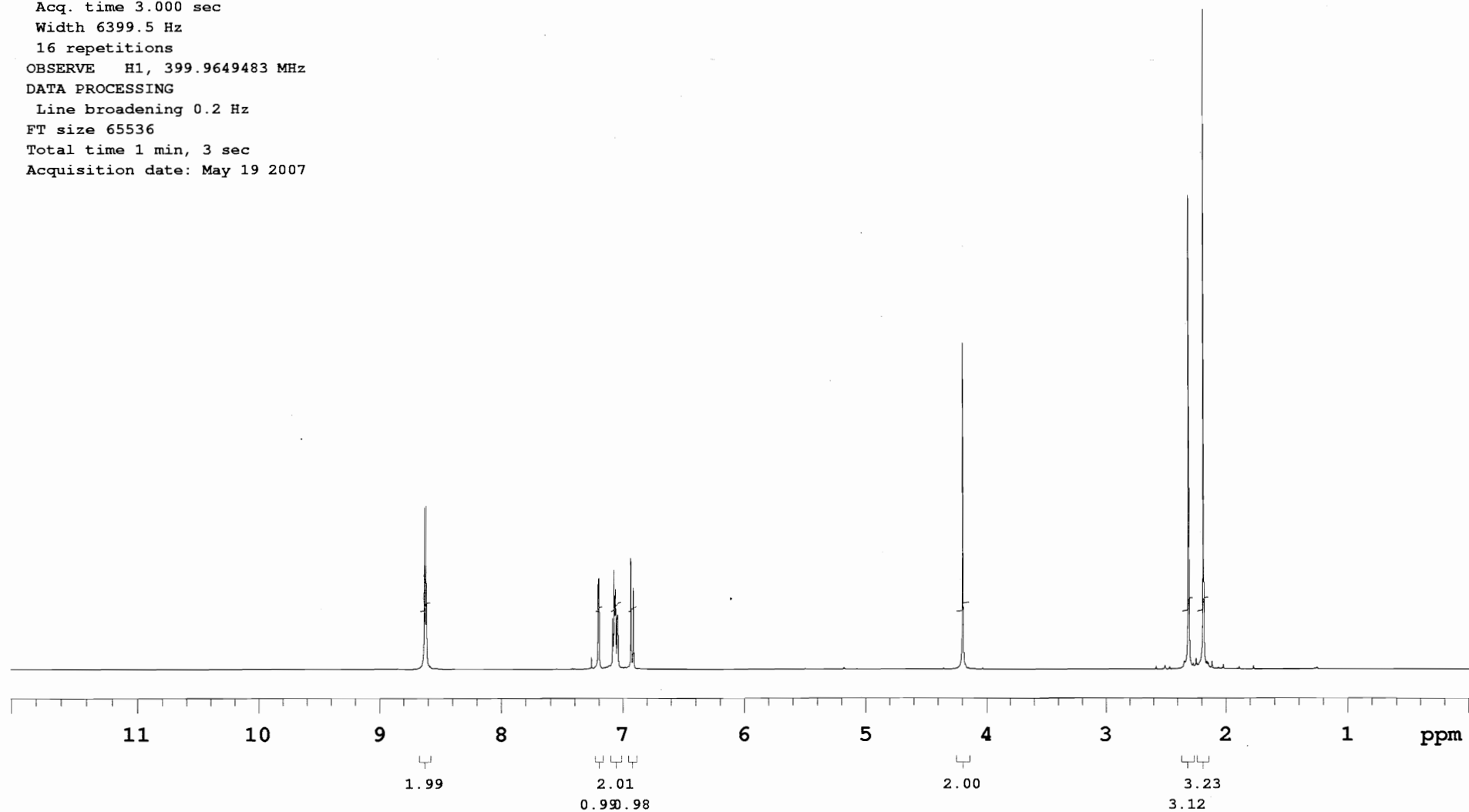
Operator: lopa

File: 101vd201fr60-75proton

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649483 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: May 19 2007





Pyrimidine-carbon

File: 101vd201fr60-75carbon

Pulse Sequence: s2pul

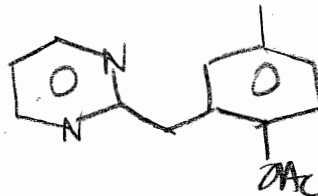
Solvent: cdcl3

Ambient temperature

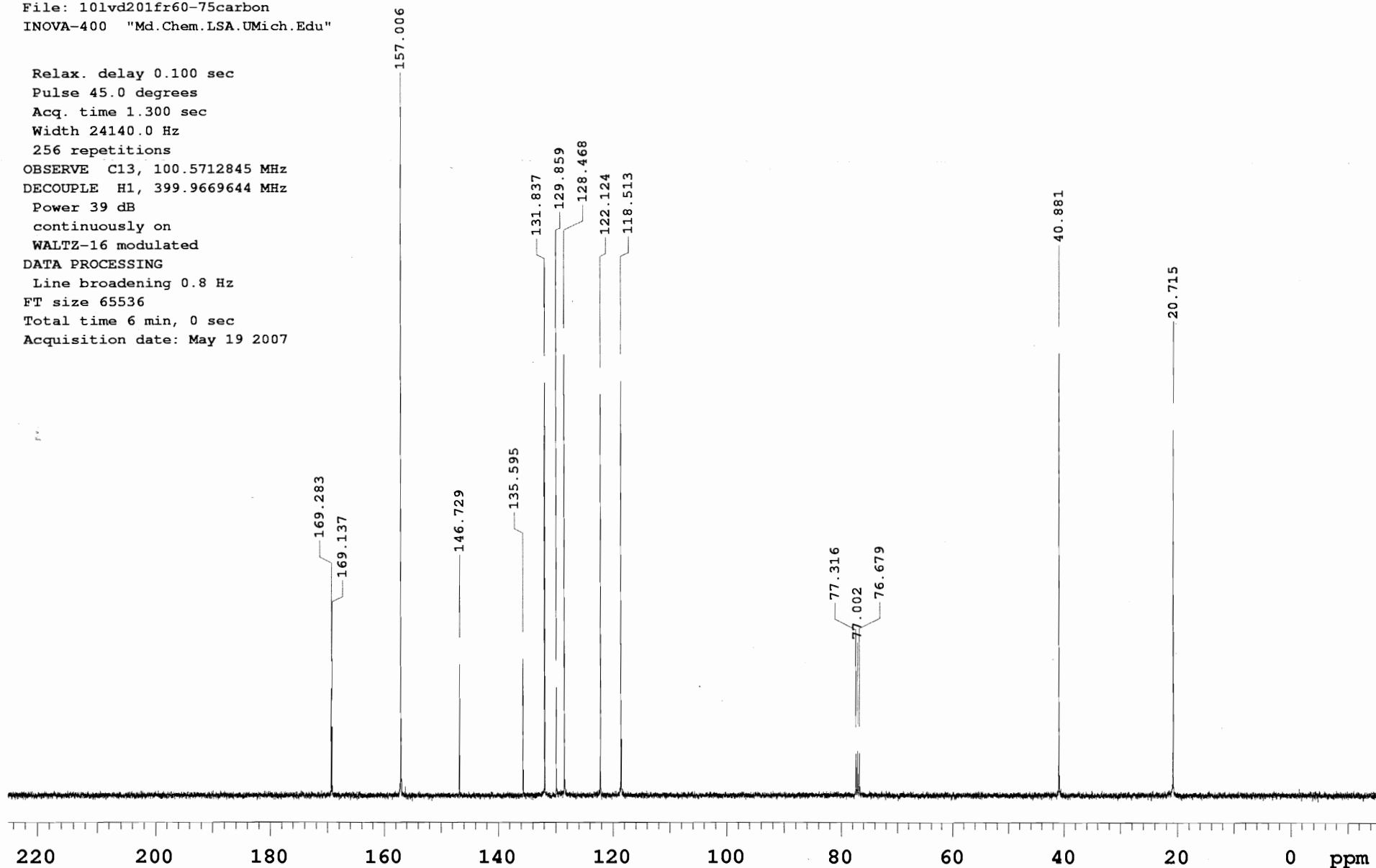
Operator: lopa

File: 101vd201fr60-75carbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24140.0 Hz  
256 repetitions  
OBSERVE C13, 100.5712845 MHz  
DECOUPLE H1, 399.9669644 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.8 Hz  
FT size 65536  
Total time 6 min, 0 sec  
Acquisition date: May 19 2007



Isloxazoline-proton

File: 101vd261proton

Pulse Sequence: s2pul

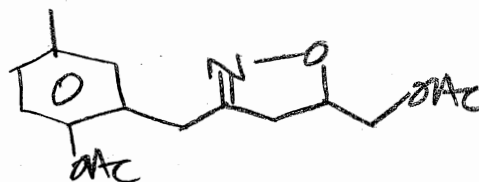
Solvent: cdcl3

Ambient temperature

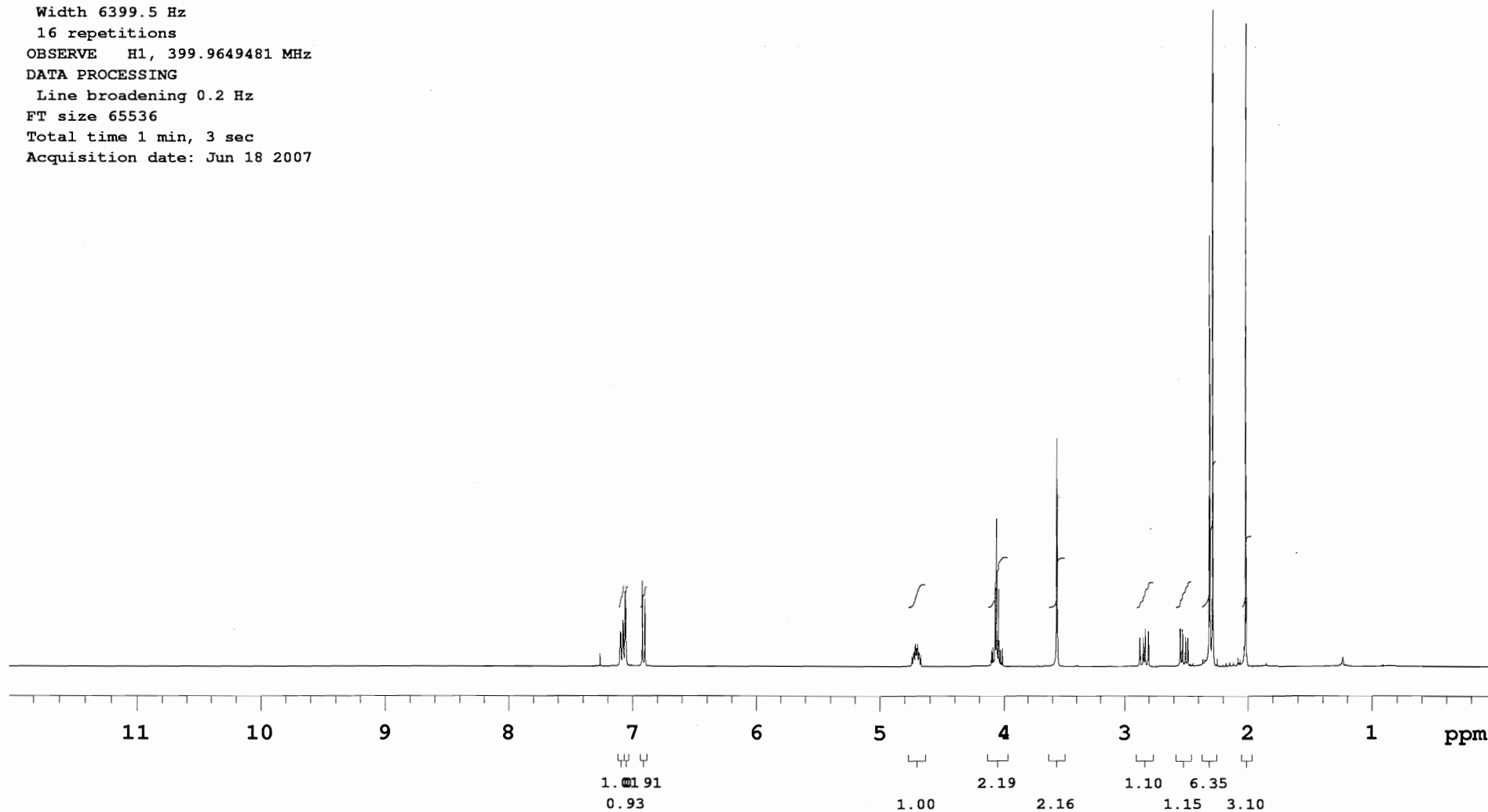
Operator: lopa

File: 101vd261proton

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 6399.5 Hz  
 16 repetitions  
 OBSERVE H1, 399.9649481 MHz  
 DATA PROCESSING  
 Line broadening 0.2 Hz  
 FT size 65536  
 Total time 1 min, 3 sec  
 Acquisition date: Jun 18 2007



Isoxazoline-carbon

File: 101vd261carbon

Pulse Sequence: s2pul

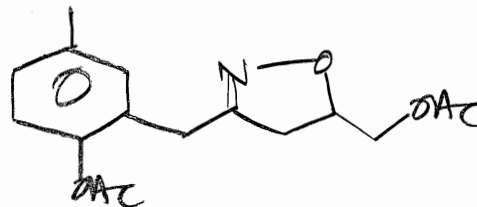
Solvent: cdcl3

Ambient temperature

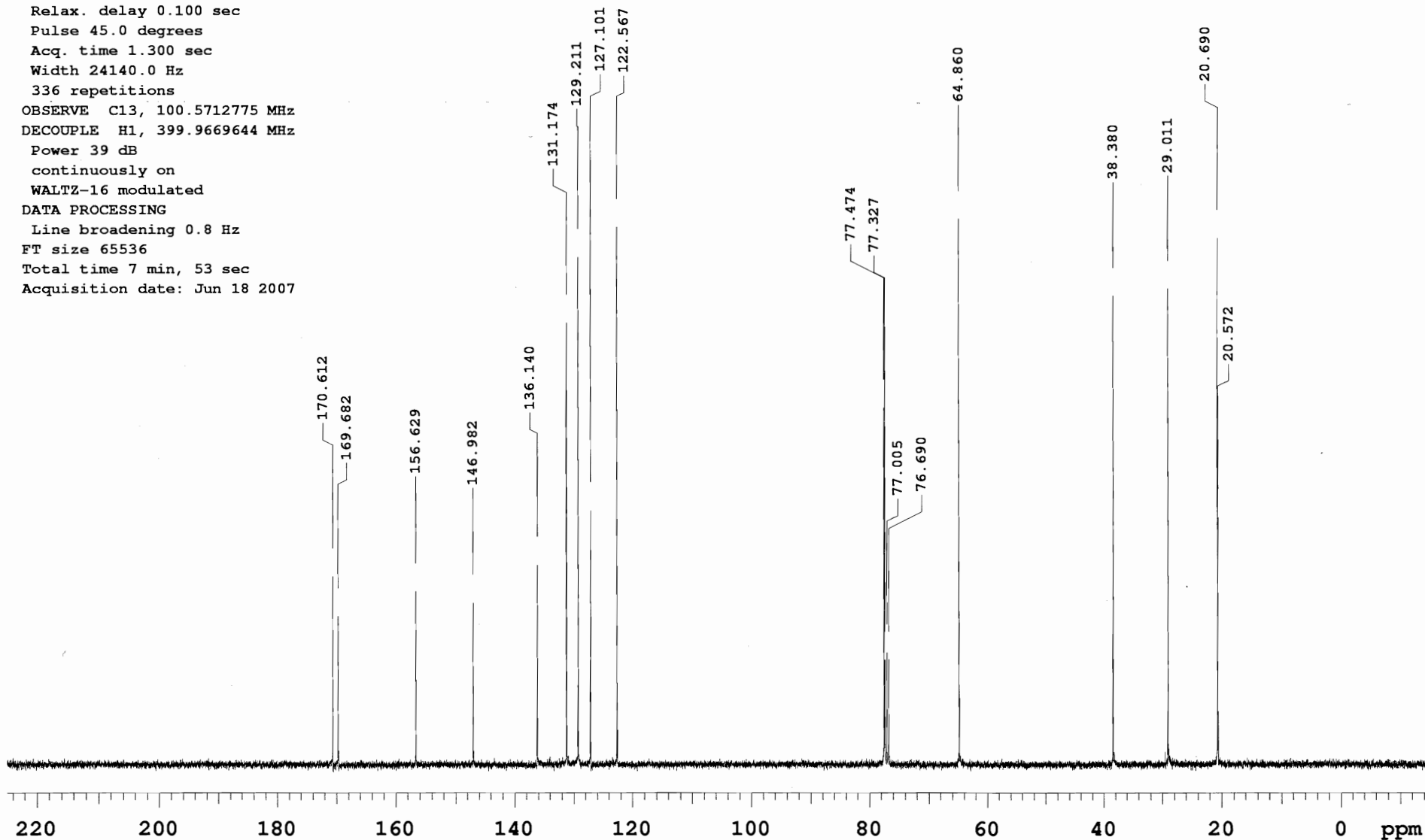
Operator: lopa

File: 101vd261carbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
 Pulse 45.0 degrees  
 Acq. time 1.300 sec  
 Width 24140.0 Hz  
 336 repetitions  
 OBSERVE C13, 100.5712775 MHz  
 DECOUPLE H1, 399.9669644 MHz  
 Power 39 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.8 Hz  
 FT size 65536  
 Total time 7 min, 53 sec  
 Acquisition date: Jun 18 2007



Pyrazole-proton

File: 101vd189isolated

Pulse Sequence: s2pul

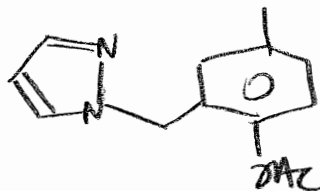
Solvent: cdcl3

Ambient temperature

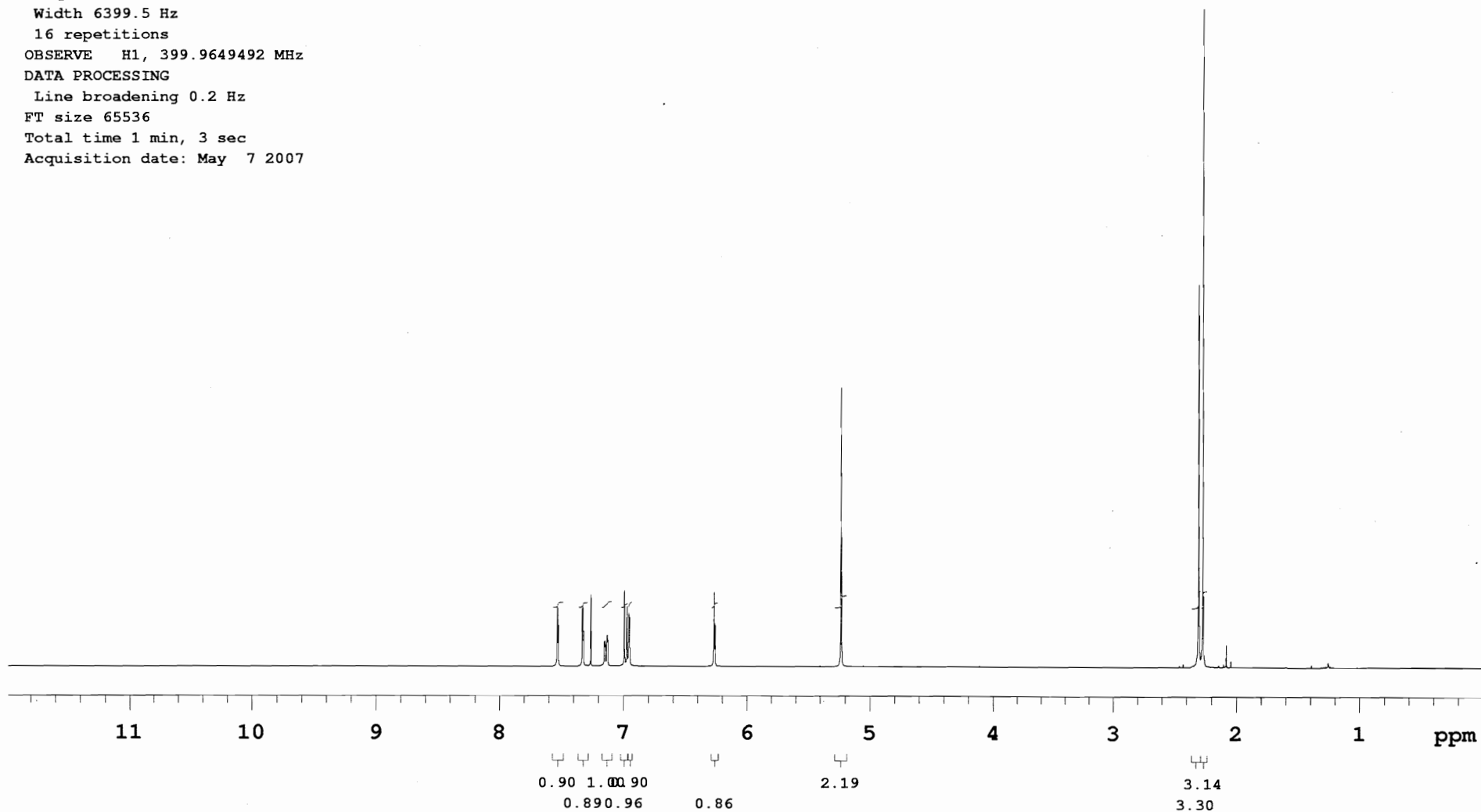
Operator: lopa

File: 101vd189isolated

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649492 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: May 7 2007



Pyrazole-carbon

File: 101vd189carbon

Pulse Sequence: s2pul

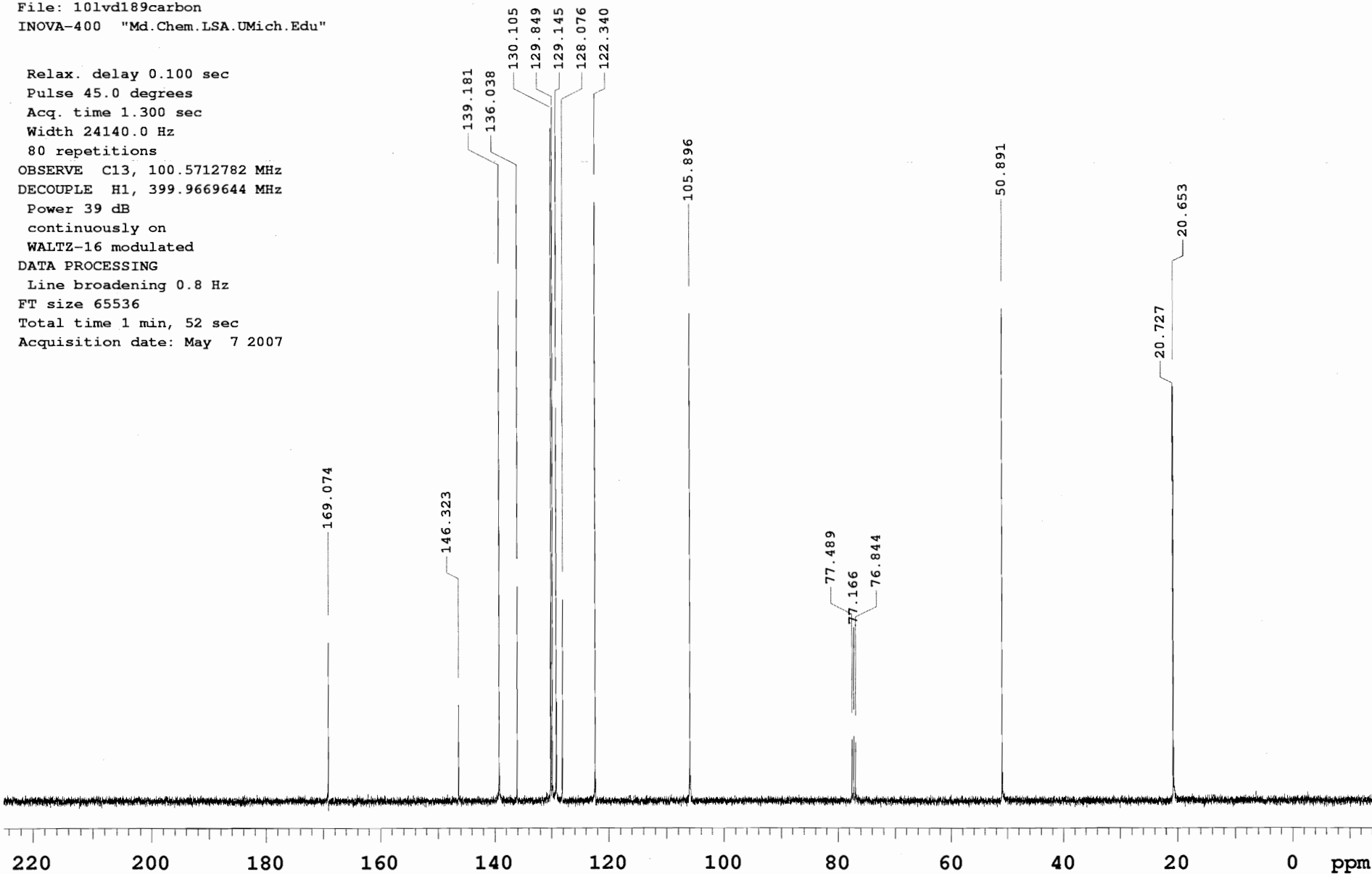
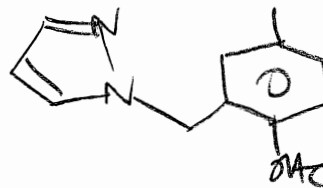
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 101vd189carbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Oximemajor-proton

File: 101vd176fr56-59

Pulse Sequence: s2pul

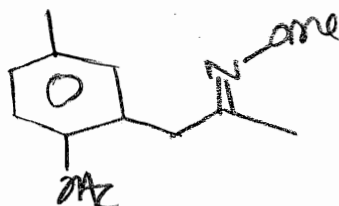
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 101vd176fr56-59

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

8 repetitions

OBSERVE H1, 399.9649485 MHz

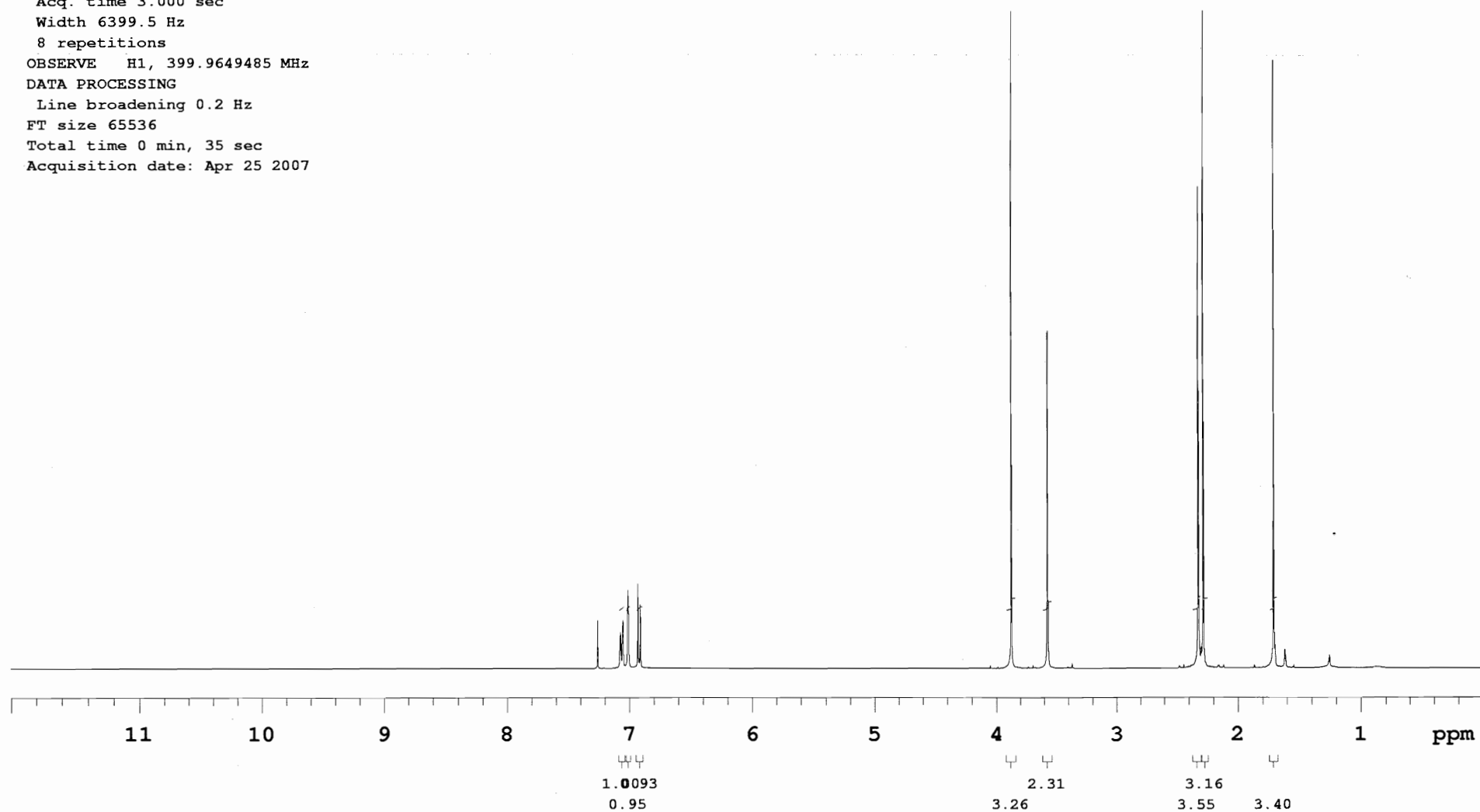
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 35 sec

Acquisition date: Apr 25 2007



Oximemajor-carbon

File: 101vdl76fr56-59carbon

Pulse Sequence: s2pul

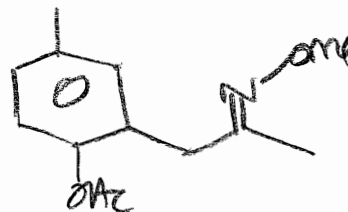
Solvent: cdcl3

Ambient temperature

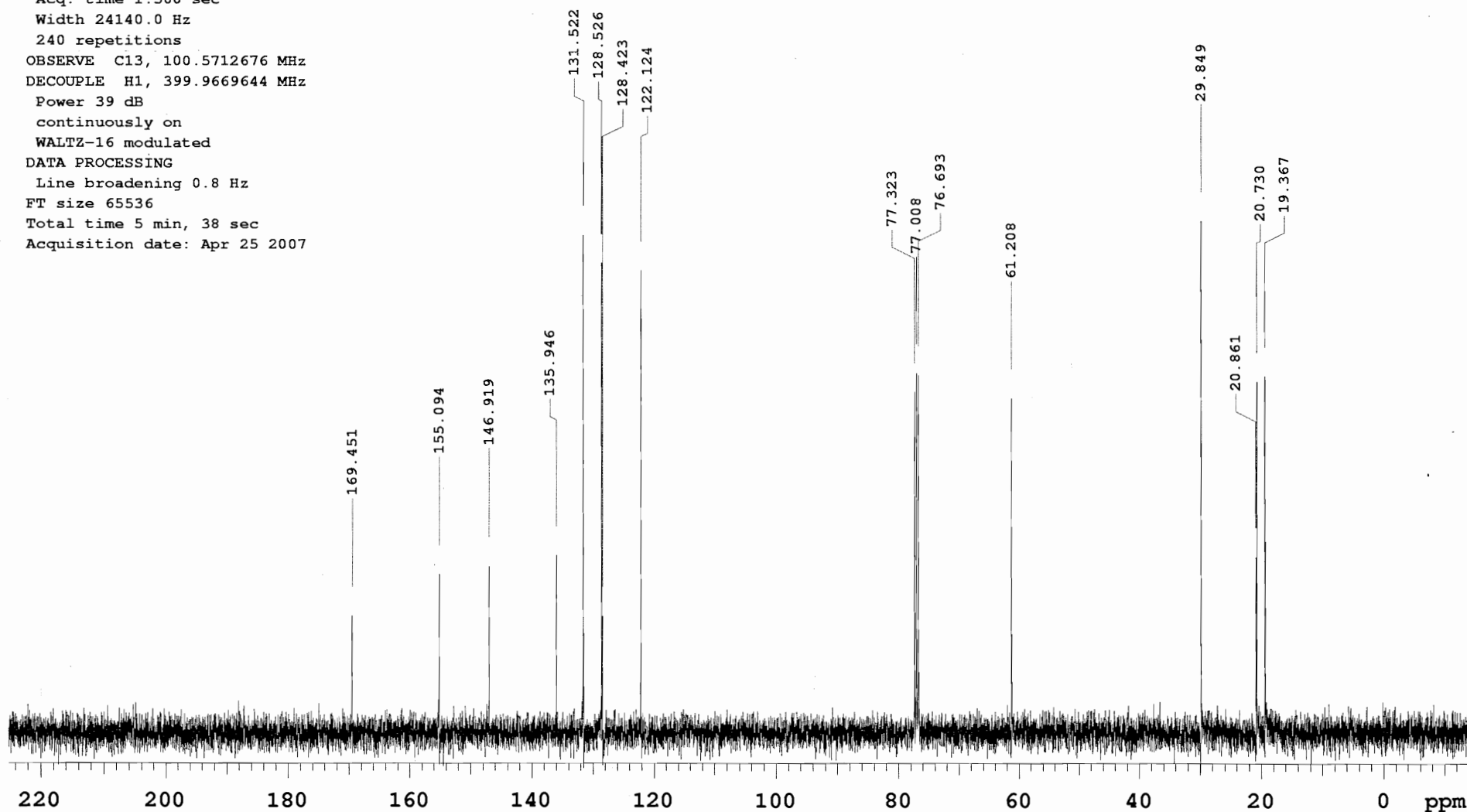
Operator: lopa

File: 101vdl76fr56-59carbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24140.0 Hz  
240 repetitions  
OBSERVE C13, 100.5712676 MHz  
DECOUPLE H1, 399.9669644 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.8 Hz  
FT size 65536  
Total time 5 min, 38 sec  
Acquisition date: Apr 25 2007



Oximeminor-proton

File: 101vd176fr39-41

Pulse Sequence: s2pul

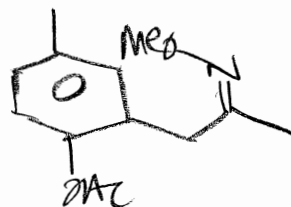
Solvent: cdcl3

Ambient temperature

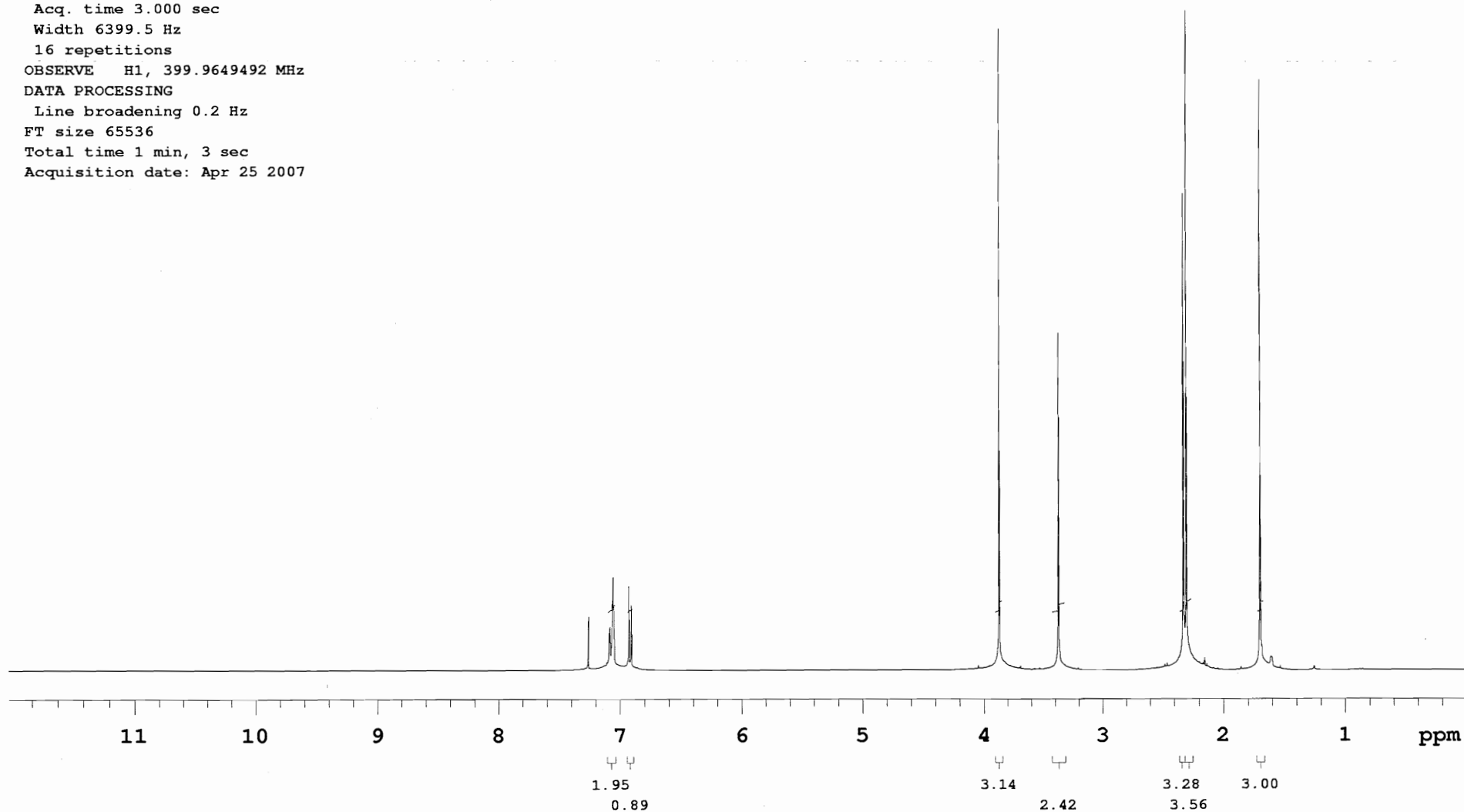
Operator: lopa

File: 101vd176fr39-41

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649492 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: Apr 25 2007





Oximeminor-carbon

File: 101vd176fr39-41carbon

Pulse Sequence: s2pul

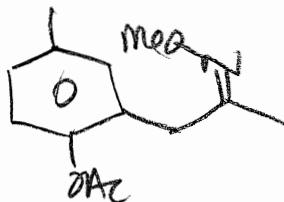
Solvent: cdcl3

Ambient temperature

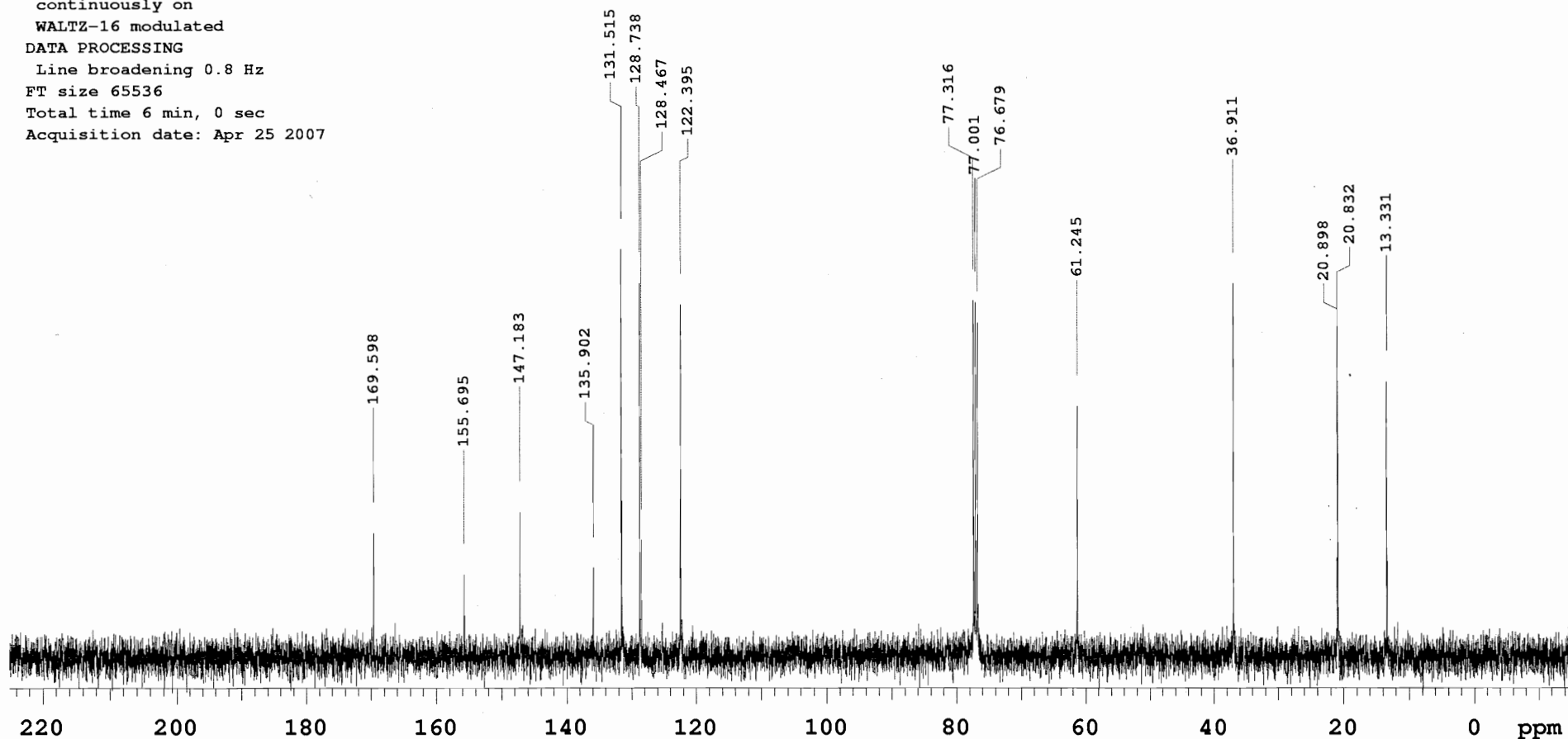
Operator: lopa

File: 101vd176fr39-41carbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24140.0 Hz  
256 repetitions  
OBSERVE C13, 100.5712683 MHz  
DECOUPLE H1, 399.9669644 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.8 Hz  
FT size 65536  
Total time 6 min, 0 sec  
Acquisition date: Apr 25 2007



Benzyloximemajor-proton

File: 101vd177fr19-21

Pulse Sequence: s2pul

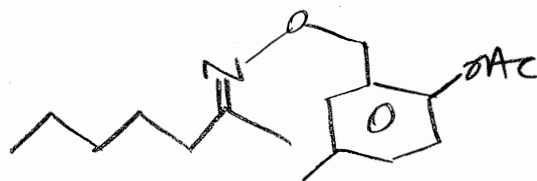
Solvent: cdcl3

Ambient temperature

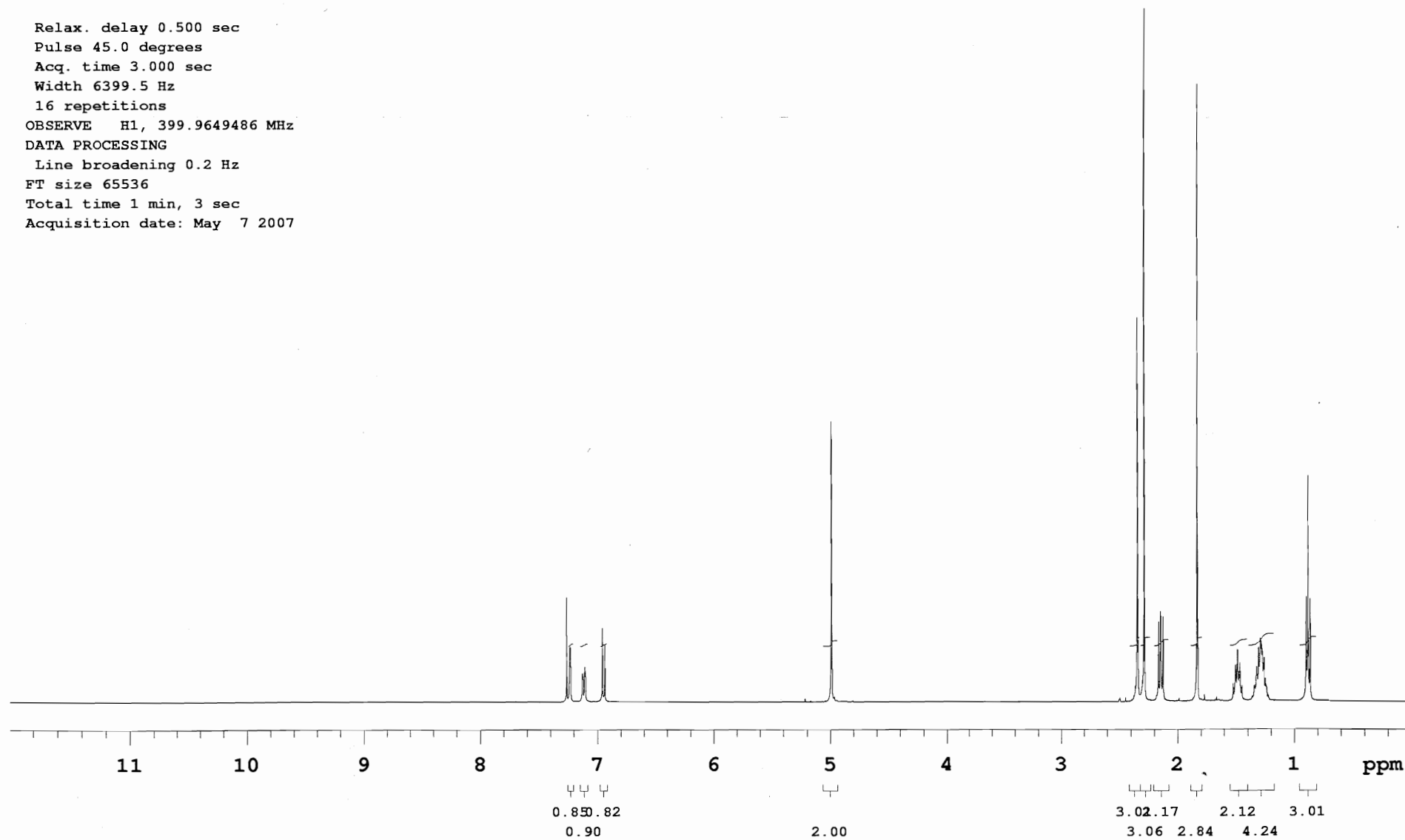
Operator: lopa

File: 101vd177fr19-21

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 6399.5 Hz  
 16 repetitions  
 OBSERVE H1, 399.9649486 MHz  
 DATA PROCESSING  
 Line broadening 0.2 Hz  
 FT size 65536  
 Total time 1 min, 3 sec  
 Acquisition date: May 7 2007



Benzyloximemajor-carbon

File: 101vd177fr19-21carbon

Pulse Sequence: s2pul

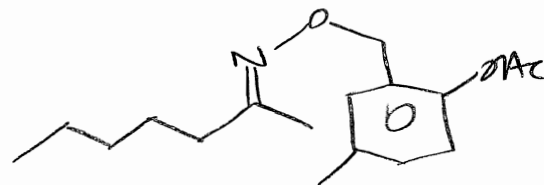
Solvent: cdcl3

Ambient temperature

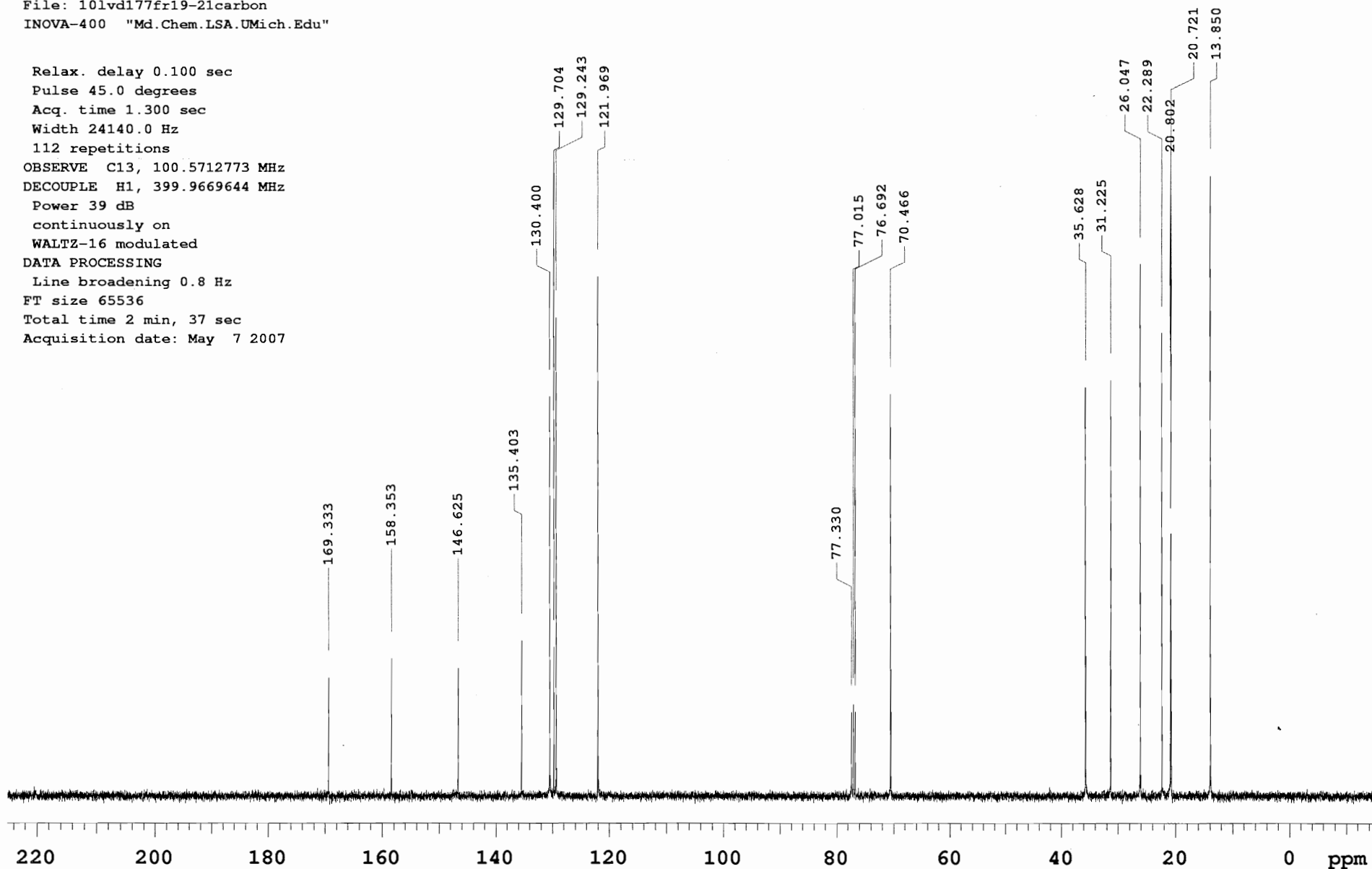
Operator: lopa

File: 101vd177fr19-21carbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
 Pulse 45.0 degrees  
 Acq. time 1.300 sec  
 Width 24140.0 Hz  
 112 repetitions  
 OBSERVE C13, 100.5712773 MHz  
 DECOUPLE H1, 399.9669644 MHz  
 Power 39 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.8 Hz  
 FT size 65536  
 Total time 2 min, 37 sec  
 Acquisition date: May 7 2007



Benzyloximeminor-proton

File: 101vd177fr26-30

Pulse Sequence: s2pul

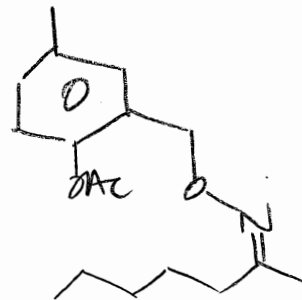
Solvent: cdcl3

Ambient temperature

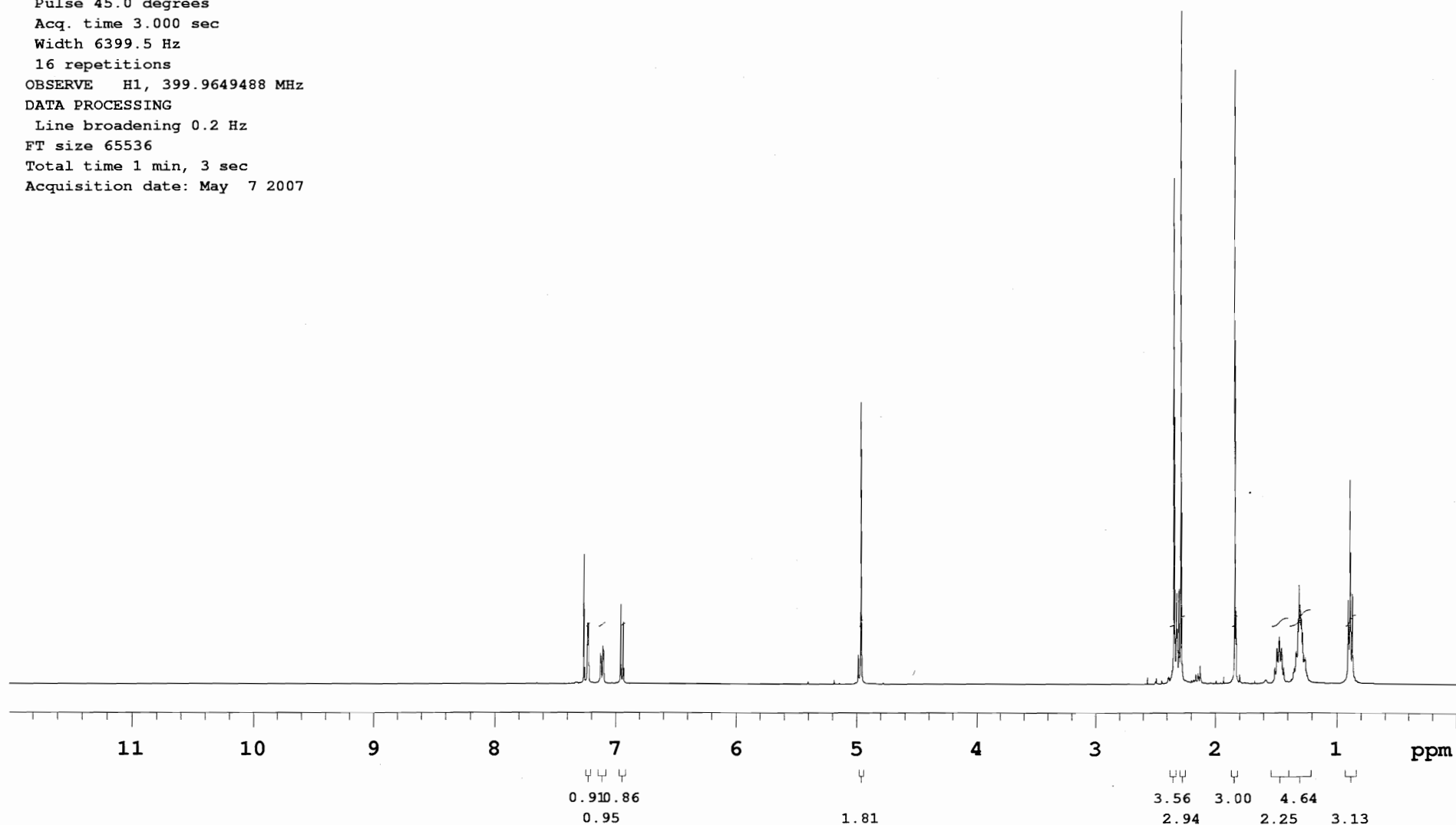
Operator: lopa

File: 101vd177fr26-30

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 6399.5 Hz  
 16 repetitions  
 OBSERVE H1, 399.9649488 MHz  
 DATA PROCESSING  
 Line broadening 0.2 Hz  
 FT size 65536  
 Total time 1 min, 3 sec  
 Acquisition date: May 7 2007



Amide-proton

File: 111vd243fr21-28

Pulse Sequence: s2pul

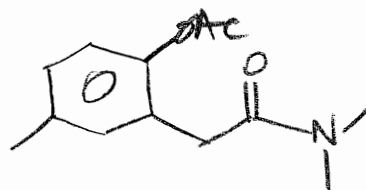
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vd243fr21-28

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

16 repetitions

OBSERVE H1, 399.9649482 MHz

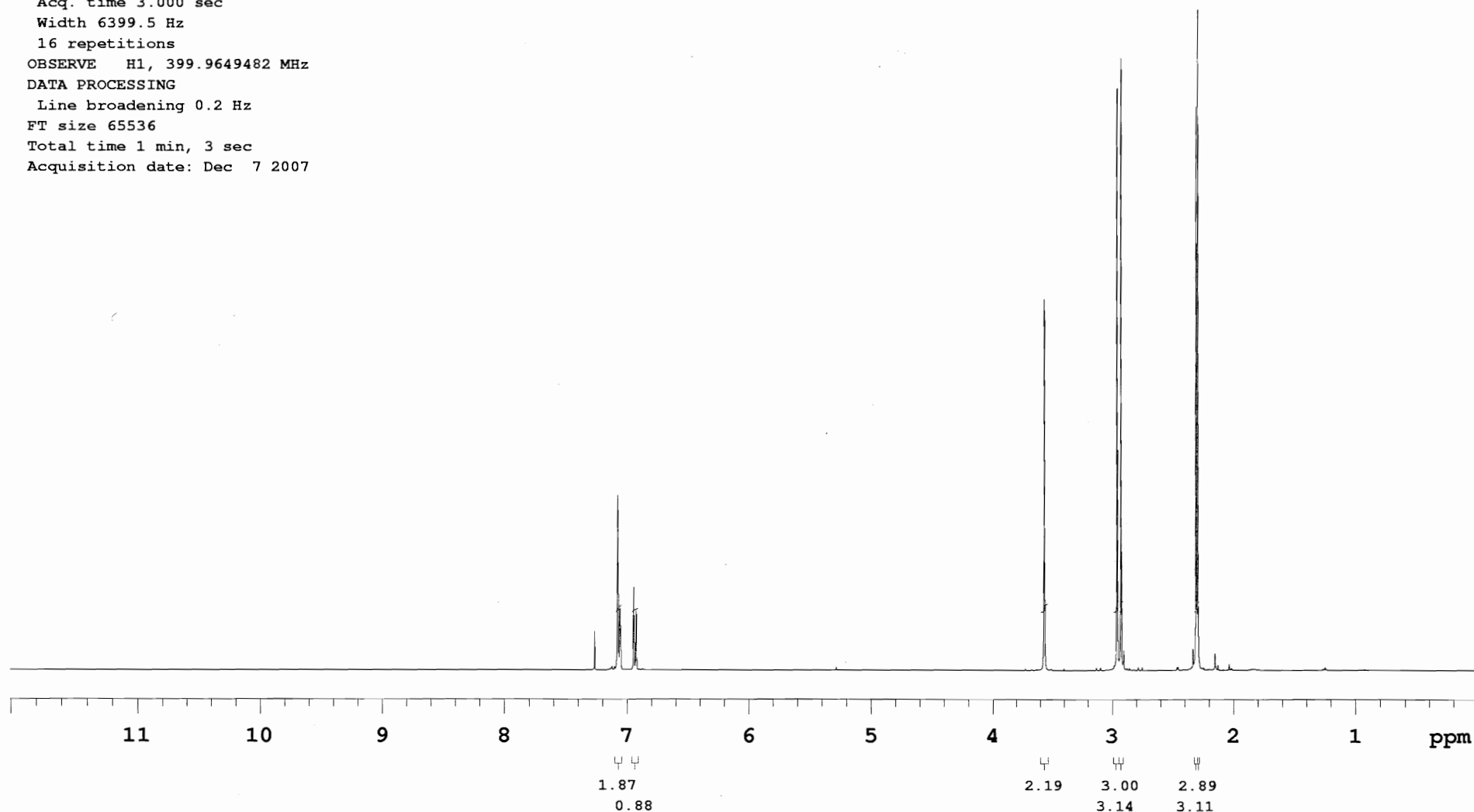
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 3 sec

Acquisition date: Dec 7 2007



Amide-carbon

File: 111vd243fr21-28carbon

Pulse Sequence: s2pul

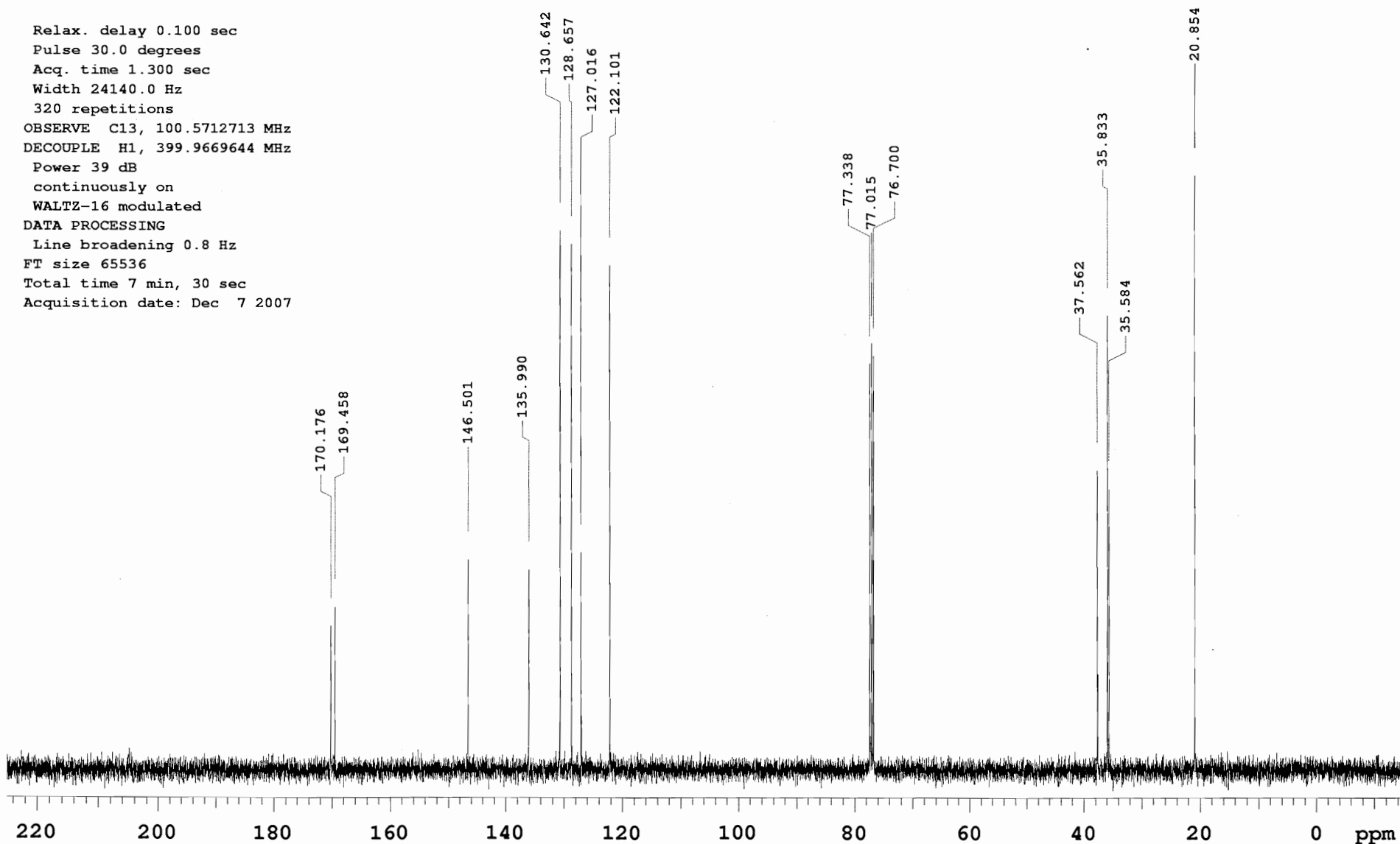
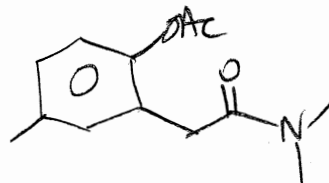
Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vd243fr21-28carbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Pyrazine-proton

File: 101vd202fr30-45

Pulse Sequence: s2pul

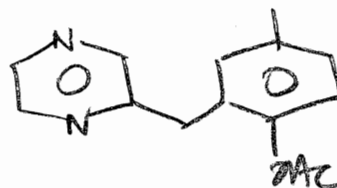
Solvent: cdcl3

Ambient temperature

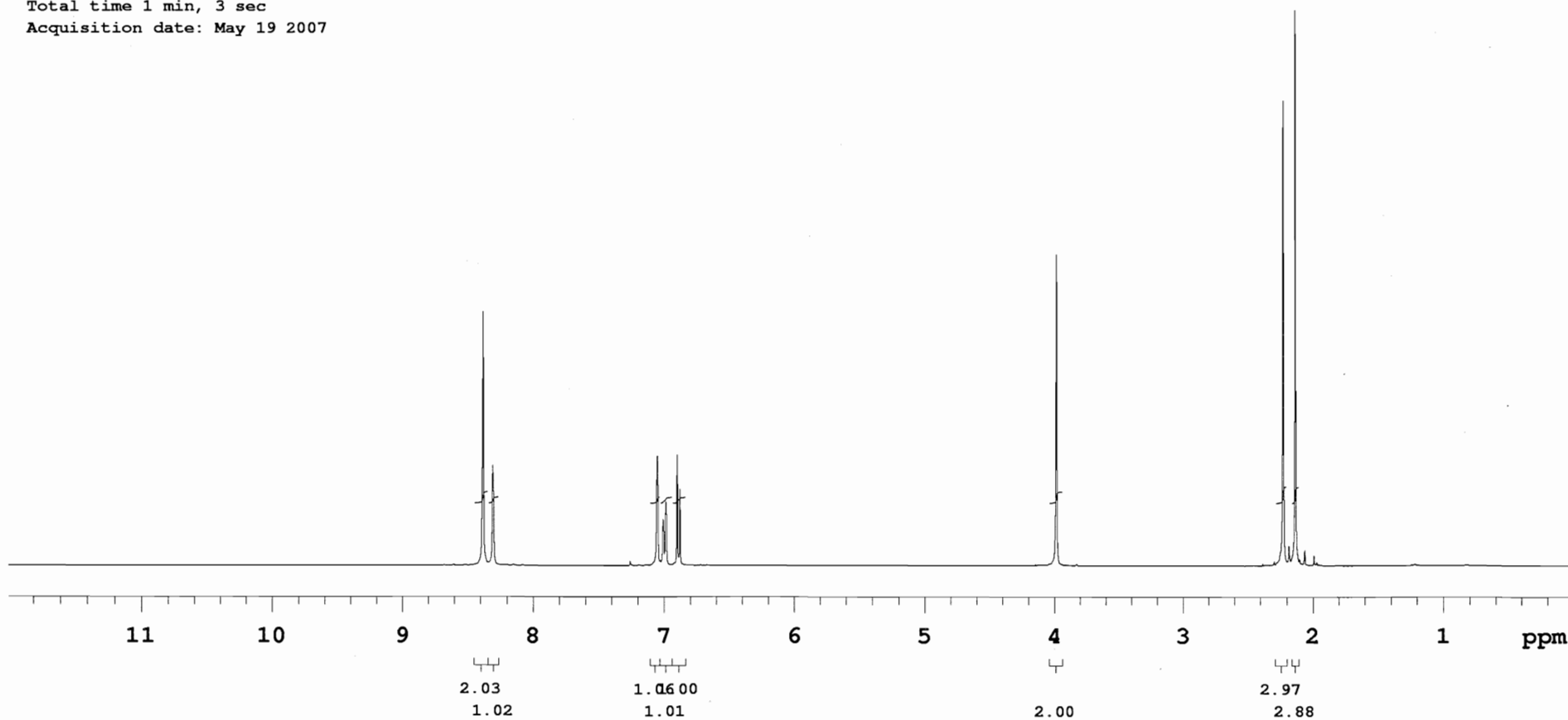
Operator: lopa

File: 101vd202fr30-45

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 6399.5 Hz  
16 repetitions  
OBSERVE H1, 399.9649493 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 1 min, 3 sec  
Acquisition date: May 19 2007



Pyrazine-carbon

File: 101vd202fr30-45carbon

Pulse Sequence: s2pul

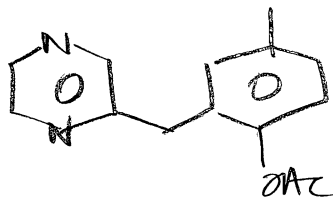
Solvent: cdcl3

Ambient temperature

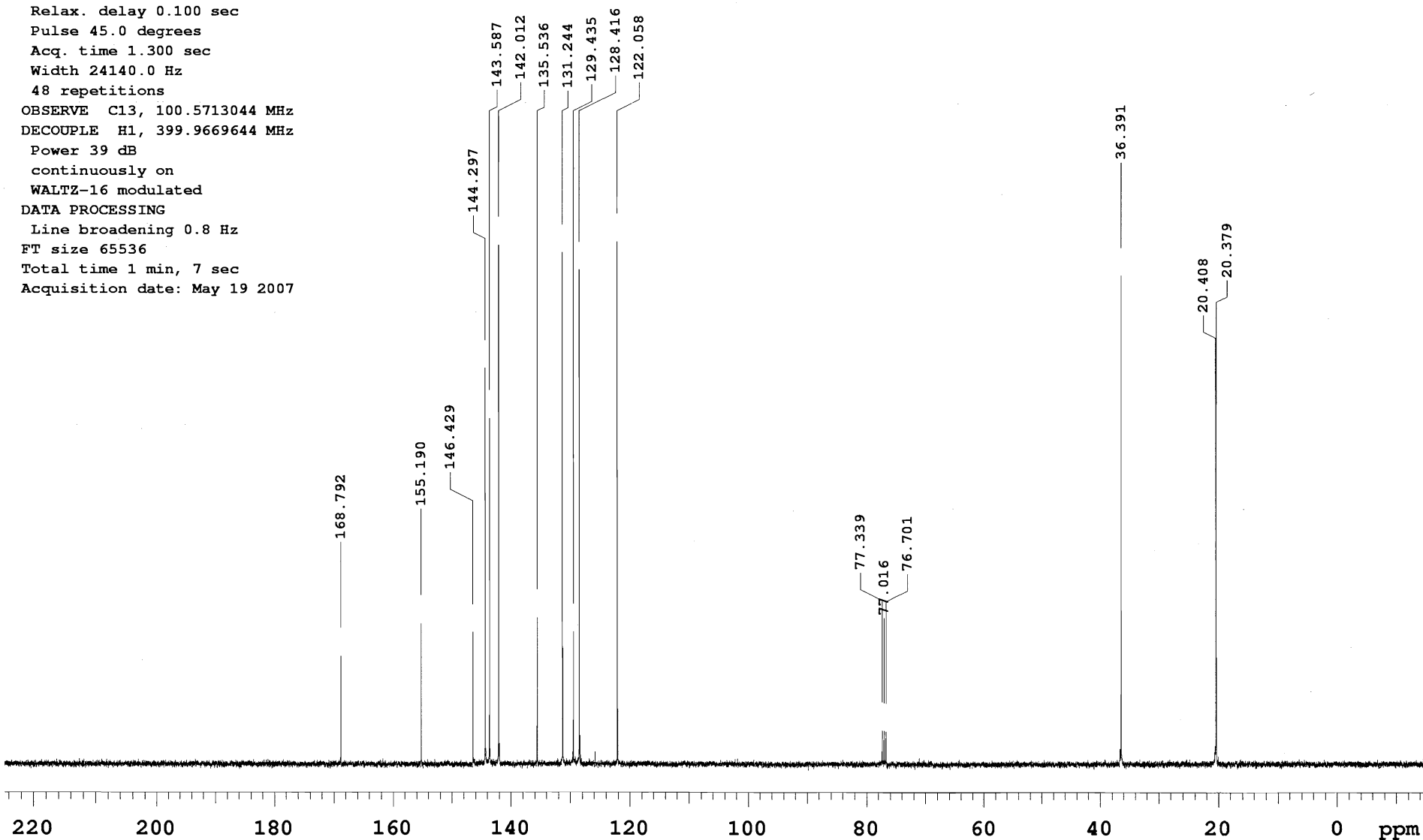
Operator: lopa

File: 101vd202fr30-45carbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
 Pulse 45.0 degrees  
 Acq. time 1.300 sec  
 Width 24140.0 Hz  
 48 repetitions  
 OBSERVE C13, 100.5713044 MHz  
 DECOUPLE H1, 399.9669644 MHz  
 Power 39 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.8 Hz  
 FT size 65536  
 Total time 1 min, 7 sec  
 Acquisition date: May 19 2007





Diacetoxy-proton

File: 111vd230diacetoxyproton

Pulse Sequence: s2pul

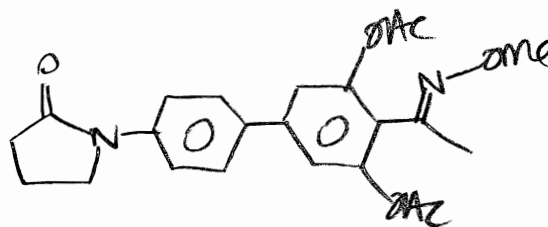
Solvent: cdcl3

Ambient temperature

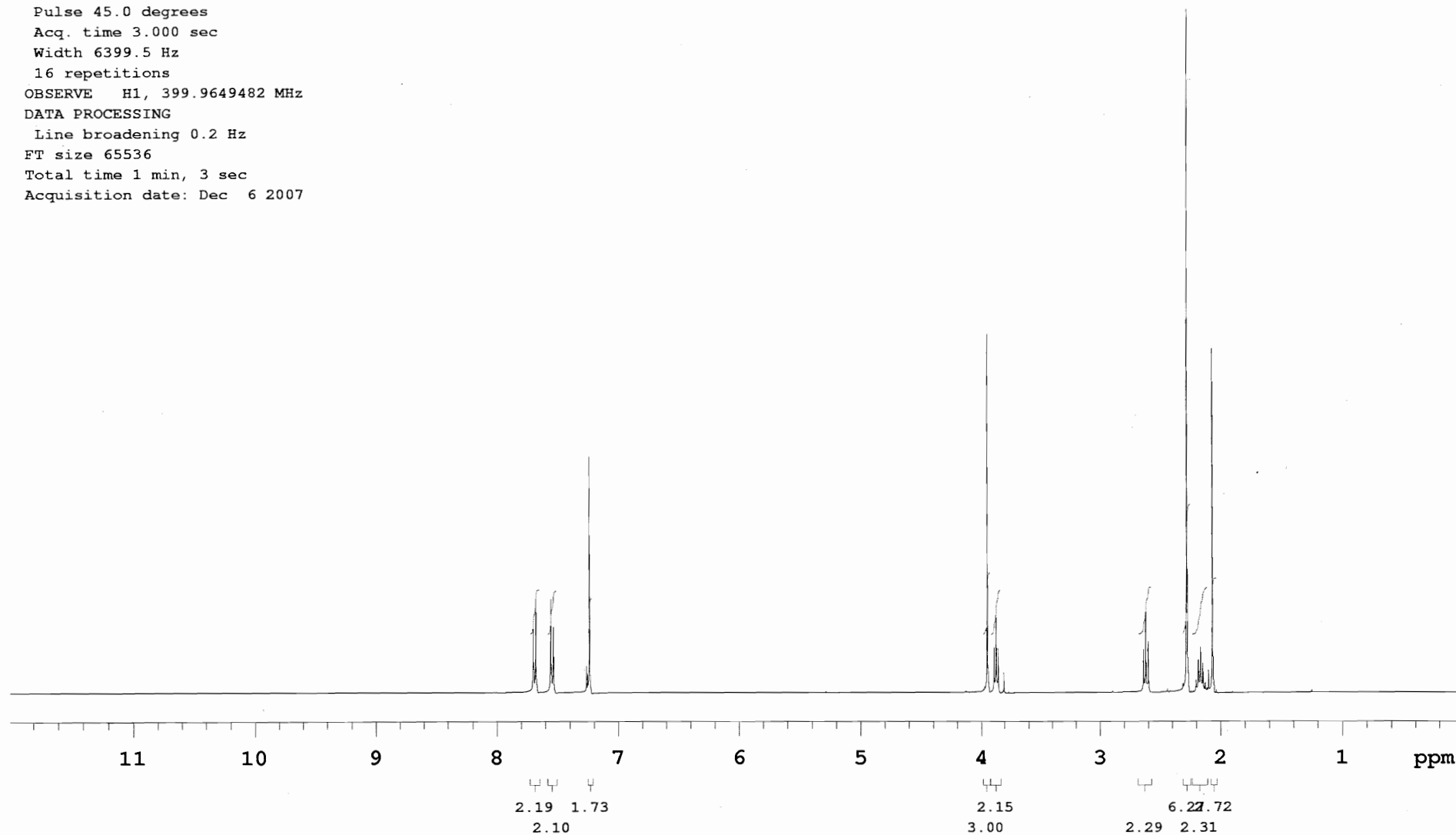
Operator: lopa

File: 111vd230diacetoxyproton

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 6399.5 Hz  
 16 repetitions  
 OBSERVE H1, 399.9649482 MHz  
 DATA PROCESSING  
 Line broadening 0.2 Hz  
 FT size 65536  
 Total time 1 min, 3 sec  
 Acquisition date: Dec 6 2007



Diacetoxy-carbon

File: 111vd230diacetoxycarbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: lopa

File: 111vd230diacetoxycarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

400 repetitions

OBSERVE C13, 100.5712728 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

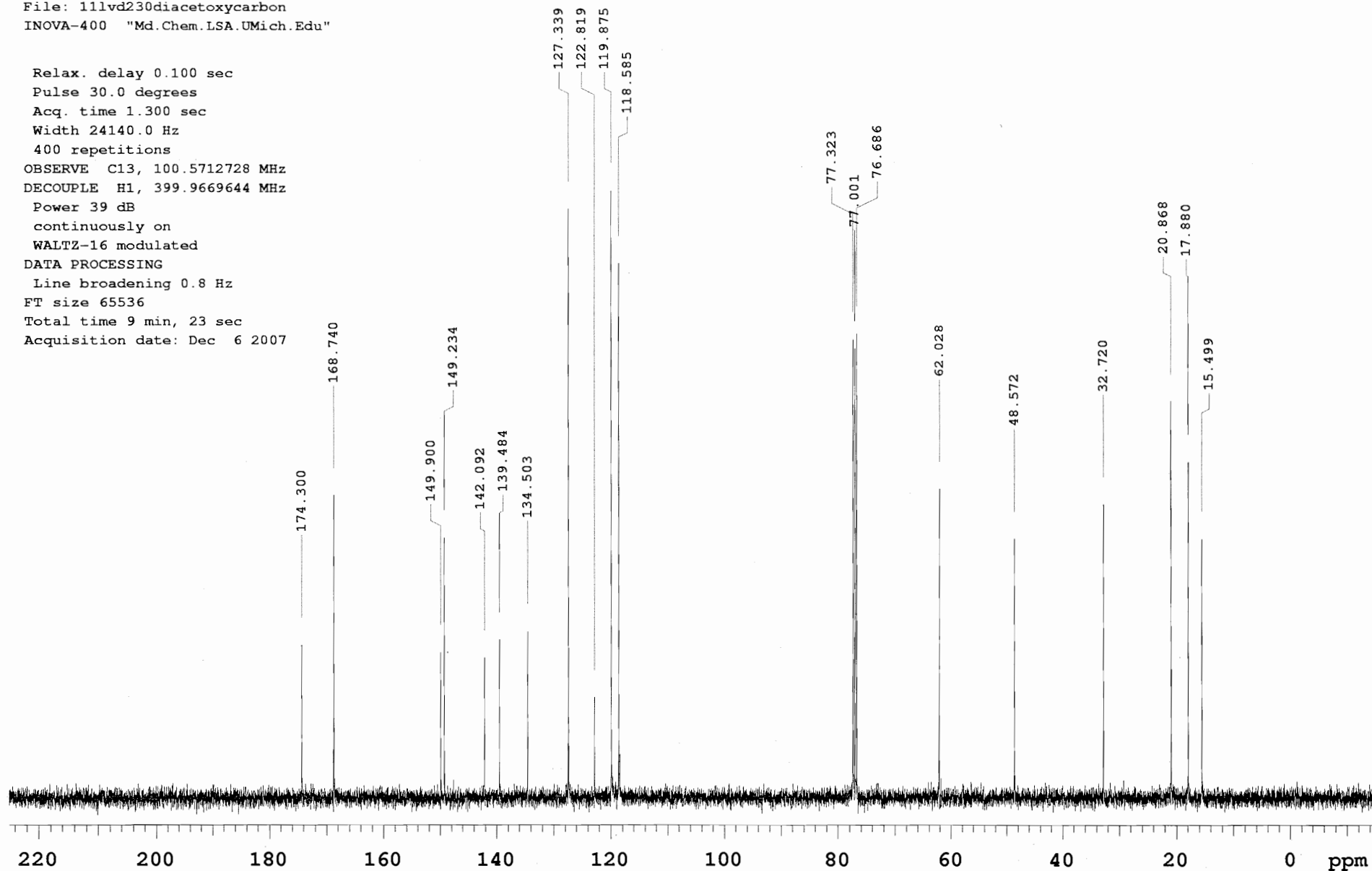
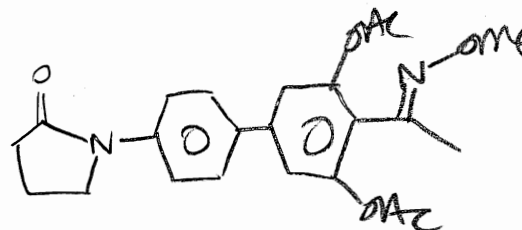
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 9 min, 23 sec

Acquisition date: Dec 6 2007



BiphenylDiacetoxyOAc-proton

File: F10vtd035-20Acproton2

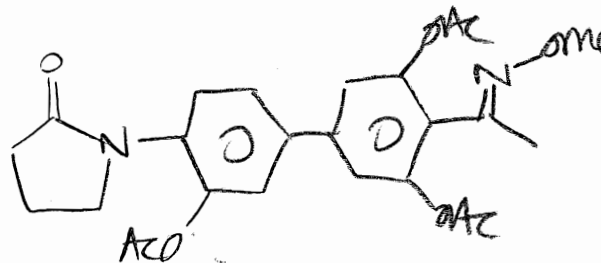
Pulse Sequence: s2pul

Solvent: cdcl3

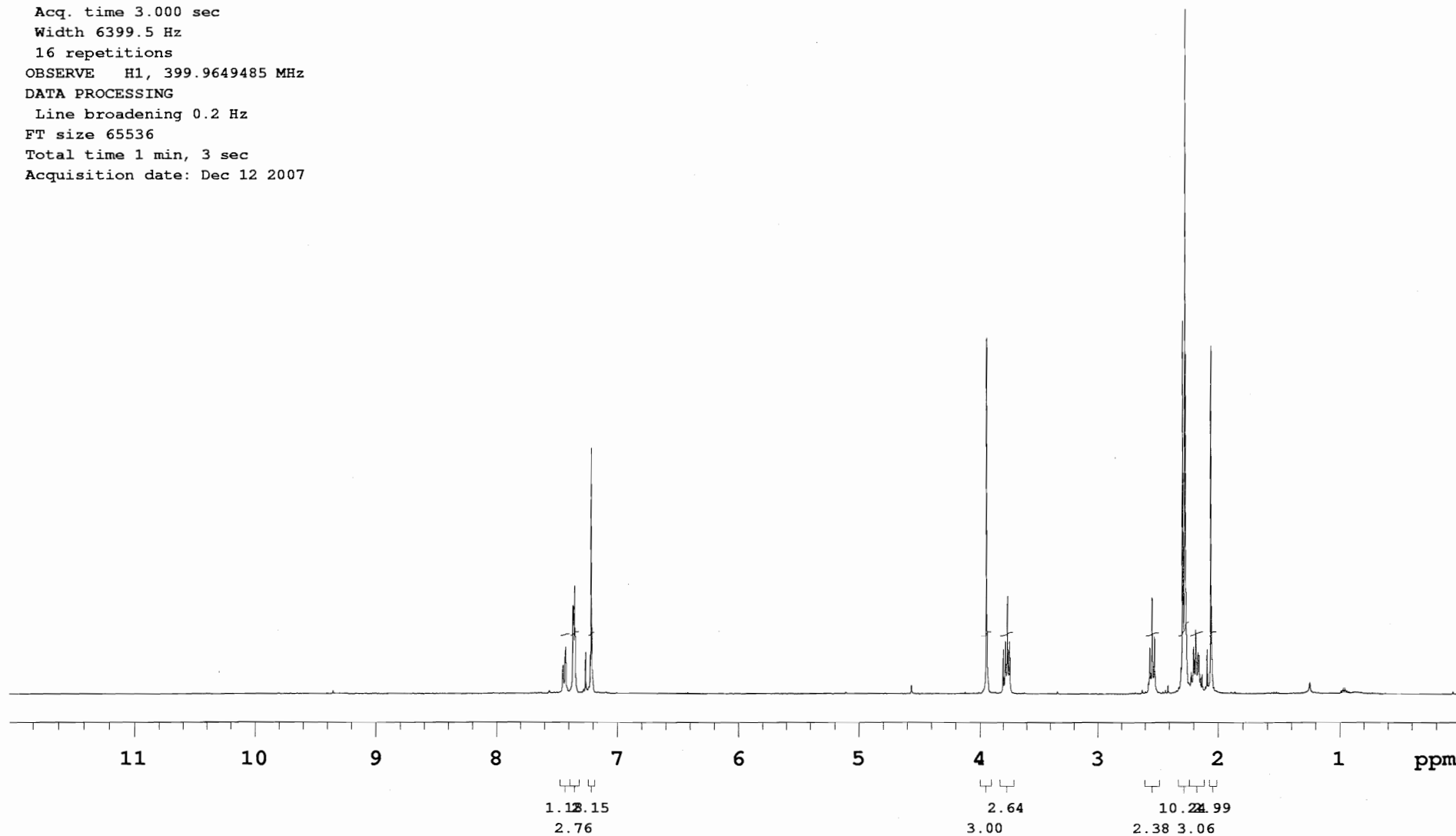
Ambient temperature

Operator: lopa

INOVA-400 "Zr.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 6399.5 Hz  
 16 repetitions  
 OBSERVE H1, 399.9649485 MHz  
 DATA PROCESSING  
 Line broadening 0.2 Hz  
 FT size 65536  
 Total time 1 min, 3 sec  
 Acquisition date: Dec 12 2007



BiphenylDiacetoxyOAc-carbon

File: 111vd235-20Accarbon2

Pulse Sequence: s2pul

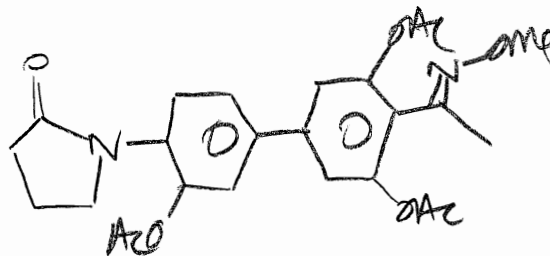
Solvent: cdcl3

Ambient temperature

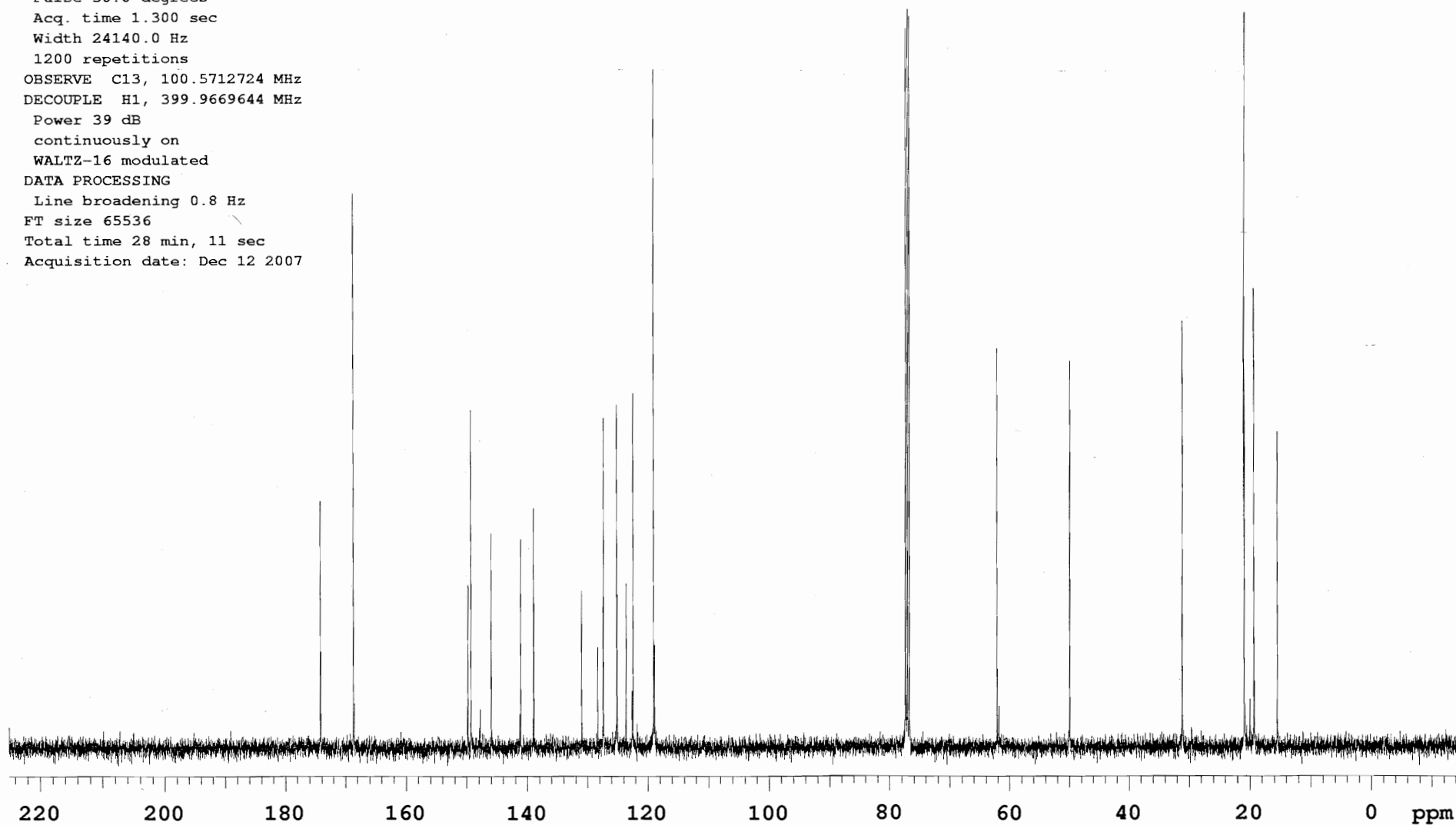
Operator: lopa

File: 111vd235-20Accarbon2

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
Pulse 30.0 degrees  
Acq. time 1.300 sec  
Width 24140.0 Hz  
1200 repetitions  
OBSERVE C13, 100.5712724 MHz  
DECOUPLE H1, 399.9669644 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.8 Hz  
FT size 65536  
Total time 28 min, 11 sec  
Acquisition date: Dec 12 2007



BiphenylDiacetoxyCl-proton

File: #147d235-3Clproton

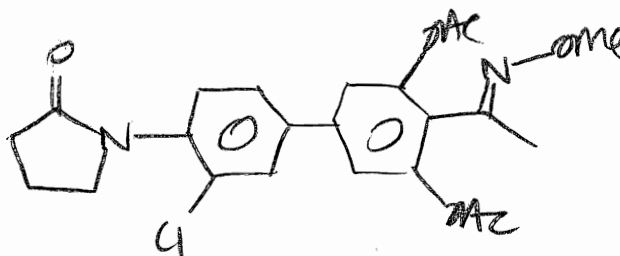
Pulse Sequence: s2pul

Solvent: cdcl3

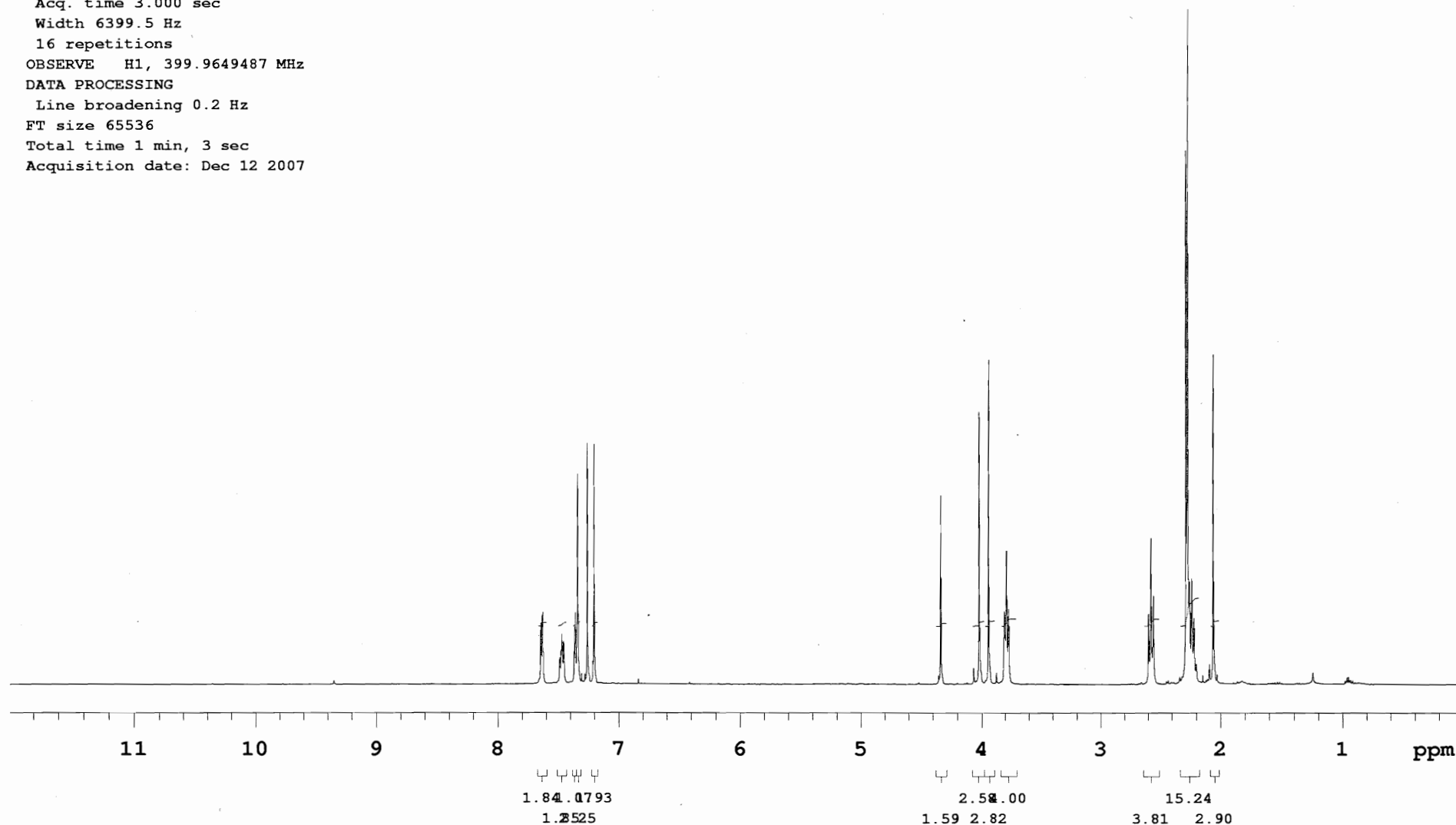
Ambient temperature

Operator: lopa

INOVA-400 "Zr.Chem.LSA.UMich.Edu"



Relax. delay 0.500 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 6399.5 Hz  
 16 repetitions  
 OBSERVE H1, 399.9649487 MHz  
 DATA PROCESSING  
 Line broadening 0.2 Hz  
 FT size 65536  
 Total time 1 min, 3 sec  
 Acquisition date: Dec 12 2007



BiphenylDiaceoxyCl-carbon

File: 111vd235-3Clcarbon

Pulse Sequence: s2pul

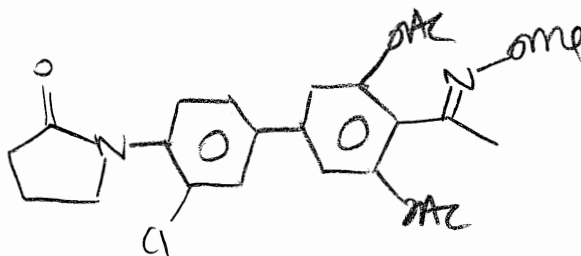
Solvent: cdcl3

Ambient temperature

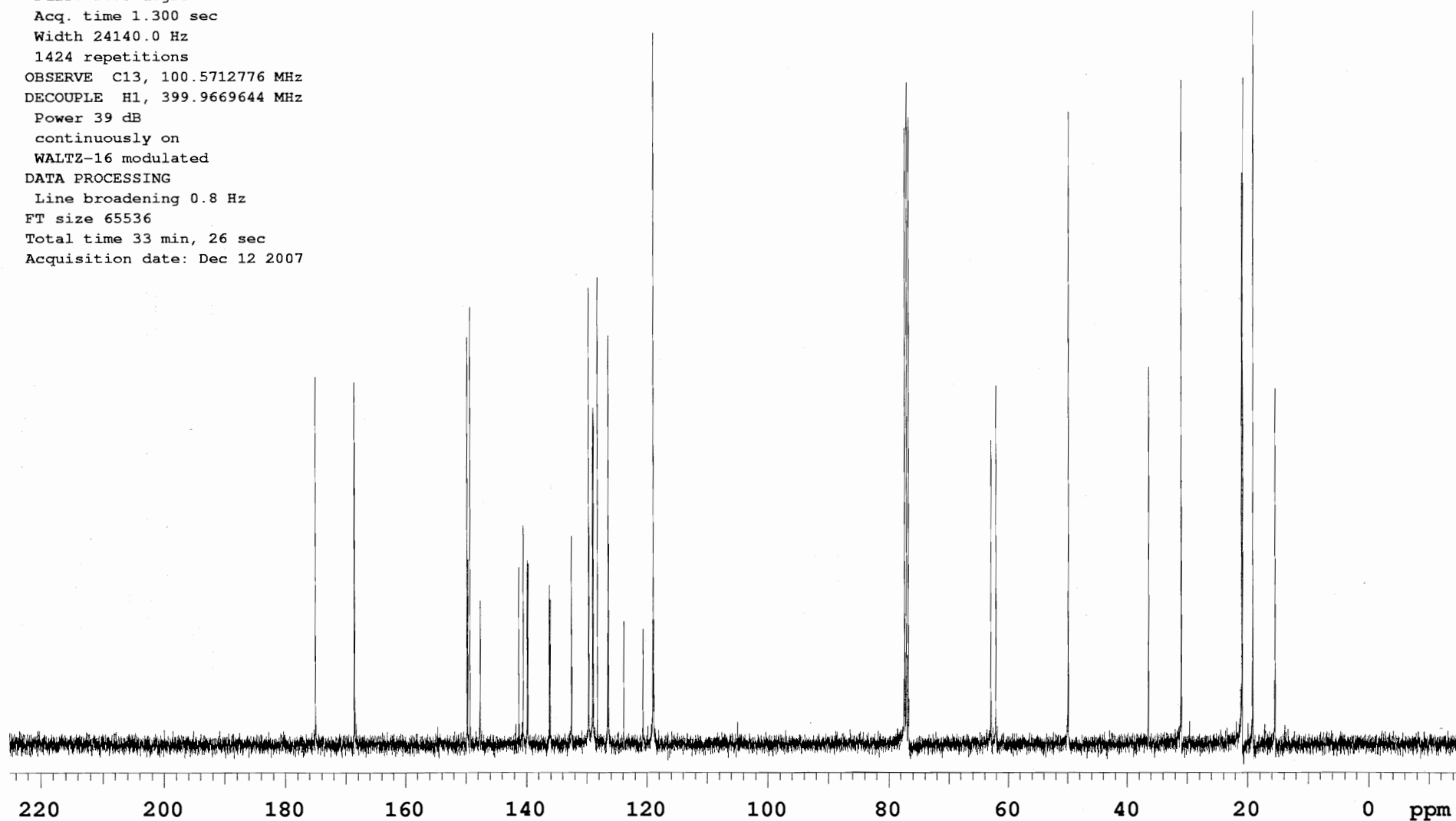
Operator: lopa

File: 111vd235-3Clcarbon

INNOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
Pulse 30.0 degrees  
Acq. time 1.300 sec  
Width 24140.0 Hz  
1424 repetitions  
OBSERVE C13, 100.5712776 MHz  
DECOUPLE H1, 399.9669644 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.8 Hz  
FT size 65536  
Total time 33 min, 26 sec  
Acquisition date: Dec 12 2007



DiacetoxyPh-proton

File: 111vd235-1Phproton

Pulse Sequence: s2pul

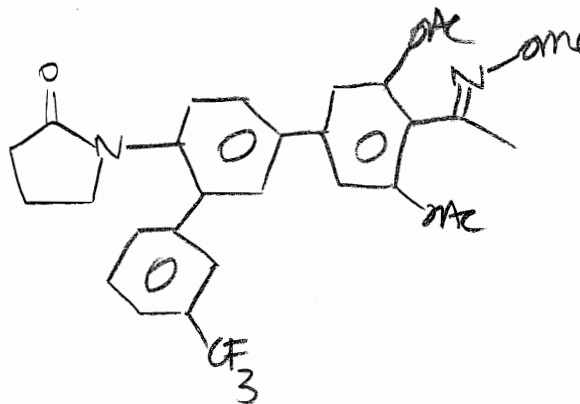
Solvent: cdc13

Ambient temperature

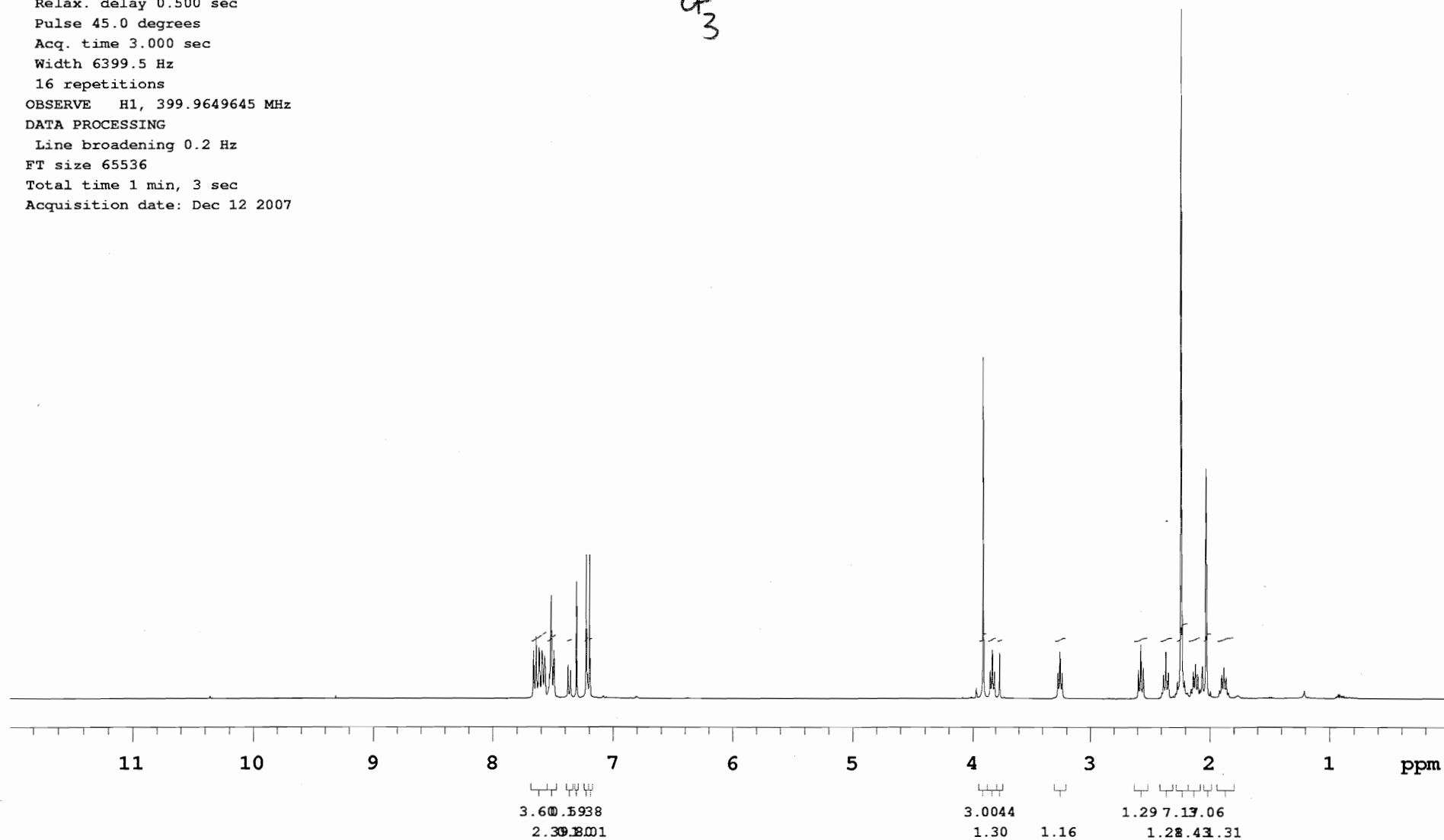
Operator: lopa

File: 111vd235-1Phproton

INOVA-400 "Kr.chem.lsa.umich.edu"



Relax. delay 0.500 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 6399.5 Hz  
 16 repetitions  
 OBSERVE H1, 399.9649645 MHz  
 DATA PROCESSING  
 Line broadening 0.2 Hz  
 FT size 65536  
 Total time 1 min, 3 sec  
 Acquisition date: Dec 12 2007



DiacetoxyPh-carbon

File: 111vd235-1Phcarbon

Pulse Sequence: s2pul

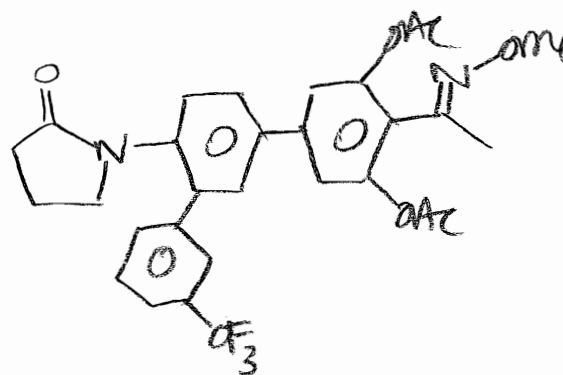
Solvent: cdcl3

Ambient temperature

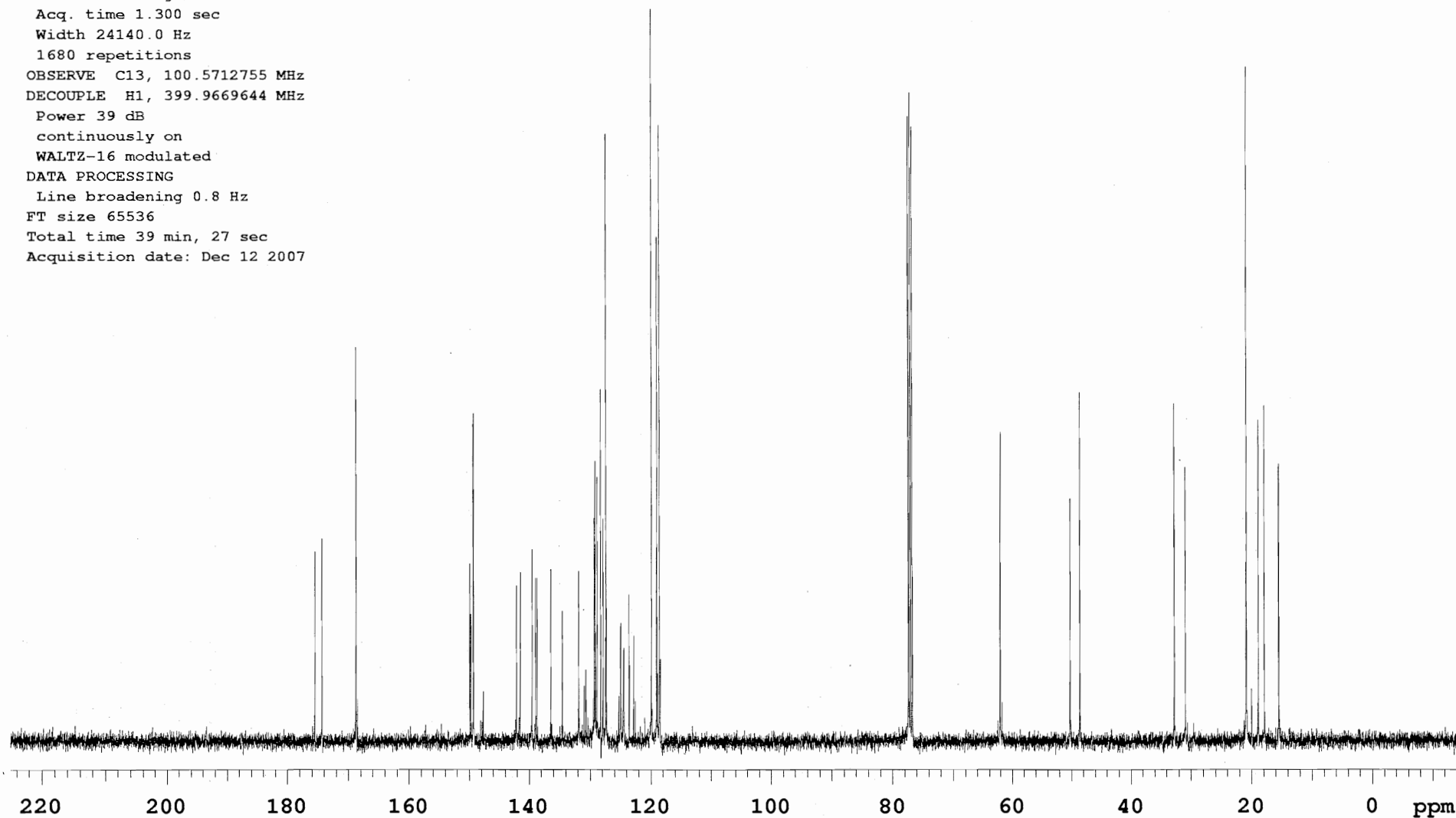
Operator: lopa

File: 111vd235-1Phcarbon

INOVA-400 "Md.Chem.LSA.UMich.Edu"



Relax. delay 0.100 sec  
Pulse 30.0 degrees  
Acq. time 1.300 sec  
Width 24140.0 Hz  
1680 repetitions  
OBSERVE C13, 100.5712755 MHz  
DECOUPLE H1, 399.9669644 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.8 Hz  
FT size 65536  
Total time 39 min, 27 sec  
Acquisition date: Dec 12 2007





Std proton

File: 2kjs258-E

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: kstowers

File: 2kjs258-E

INOVA-400 "Kr.chem.lsa.umich.edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

16 repetitions

OBSERVE H1, 399.9649778 MHz

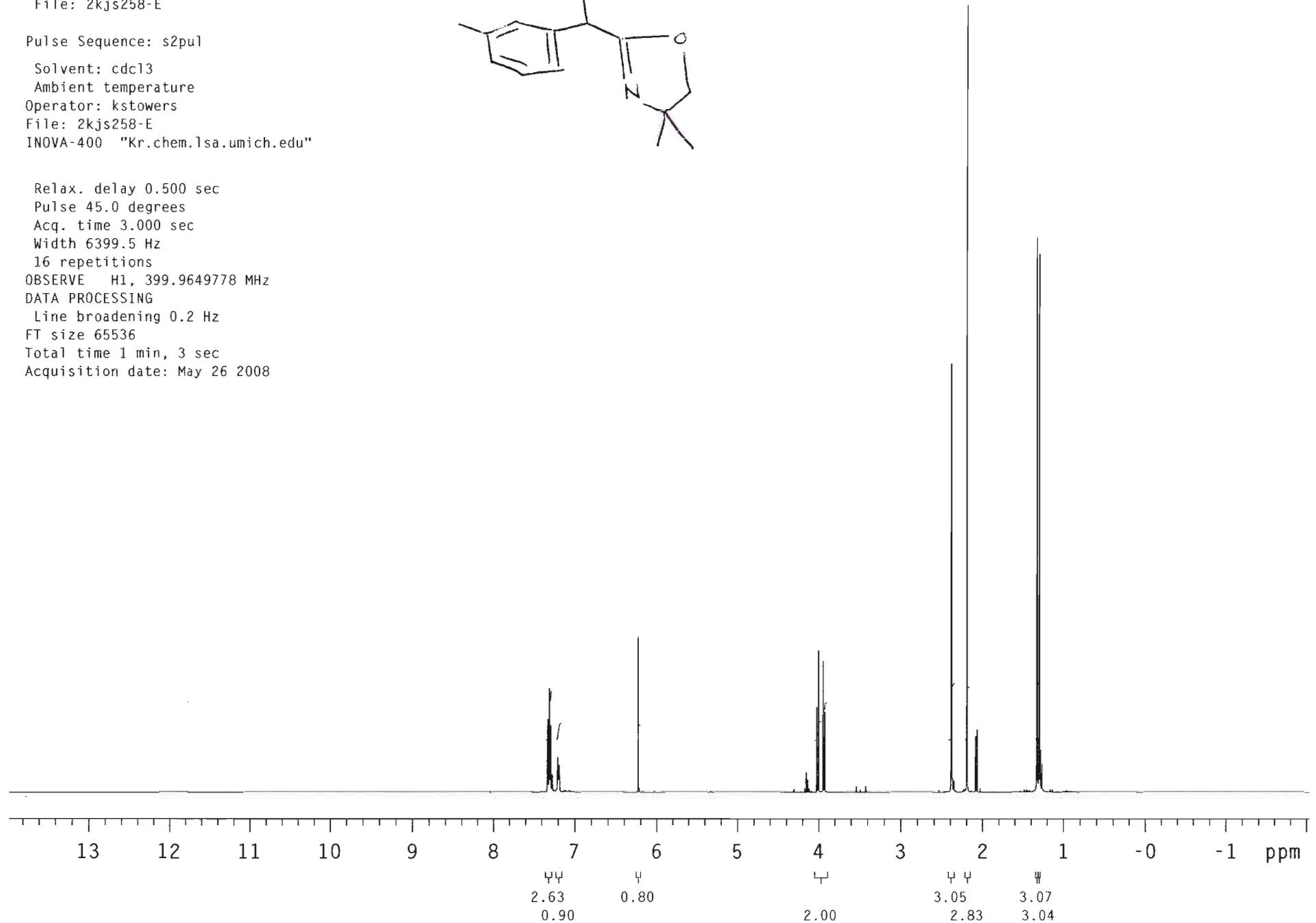
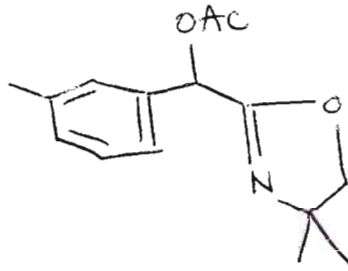
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 3 sec

Acquisition date: May 26 2008



## STANDARD CARBON PARAMETERS

File: 2kjs289-5C

Pulse Sequence: s2pul

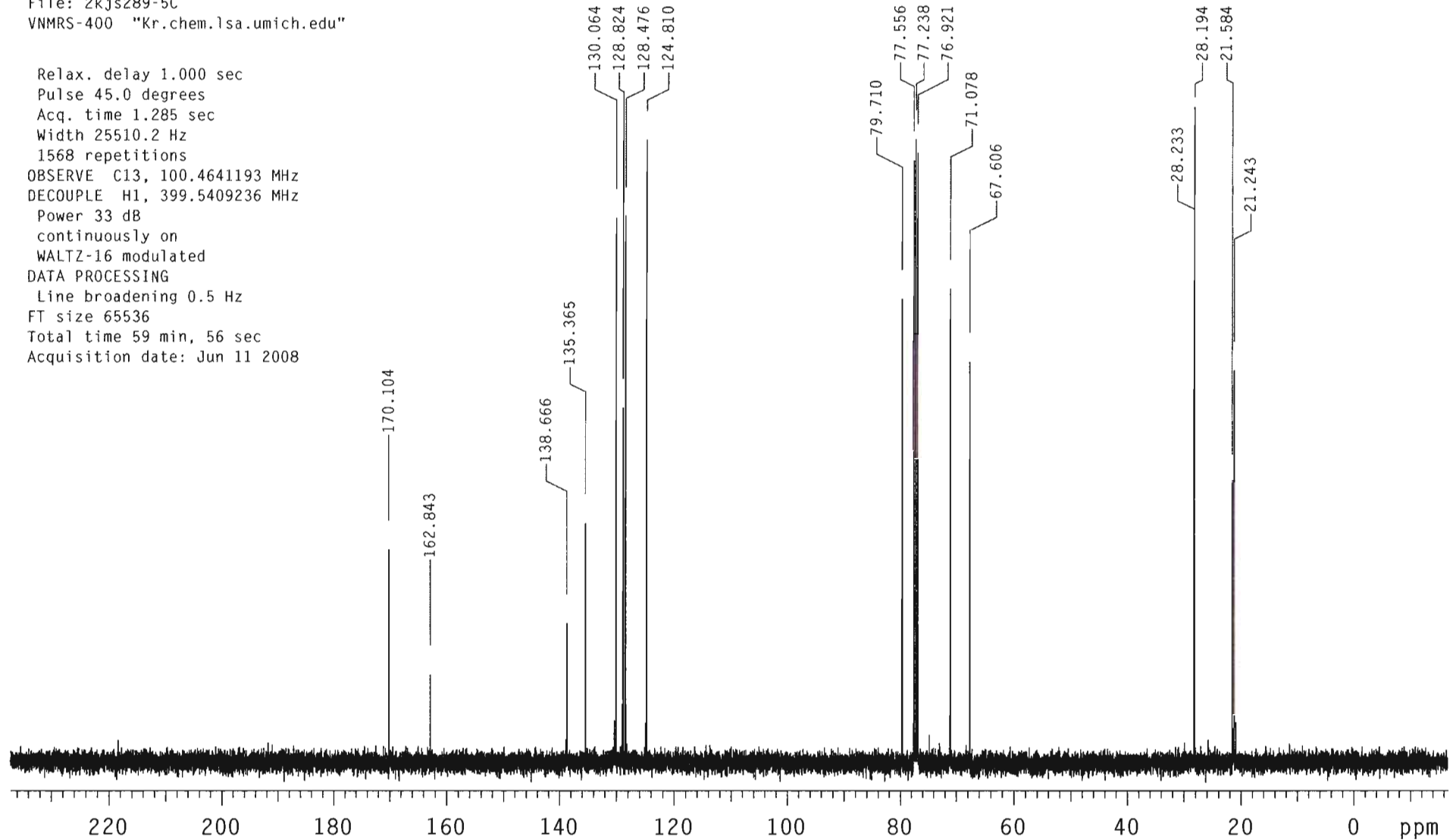
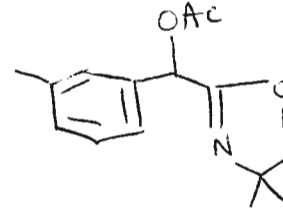
Solvent: cdcl3

Ambient temperature

Operator: kstowers

File: 2kjs289-5C

VNMRS-400 "Kr.chem.lsa.umich.edu"



## STANDARD PROTON PARAMETERS

File: 2kjs245-proton

Pulse Sequence: s2pu1

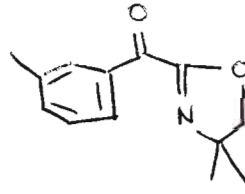
Solvent: cdcl3

Ambient temperature

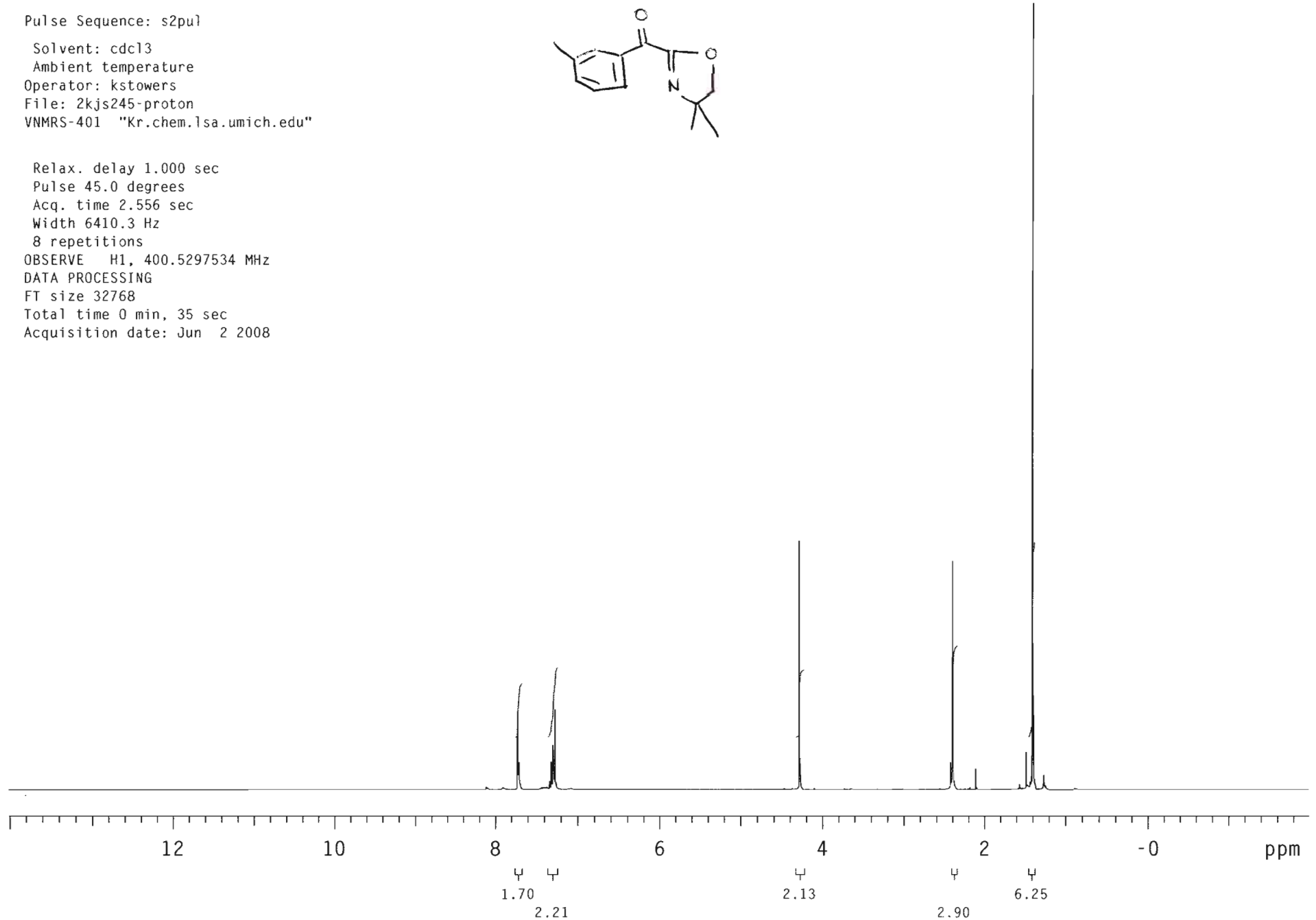
Operator: kstowers

File: 2kjs245-proton

VNMR5-401 "Kr.chem.lsa.umich.edu"



Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
8 repetitions  
OBSERVE H1, 400.5297534 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min, 35 sec  
Acquisition date: Jun 2 2008



## STANDARD CARBON PARAMETERS

File: 2kjs289-2C

Pulse Sequence: s2pul

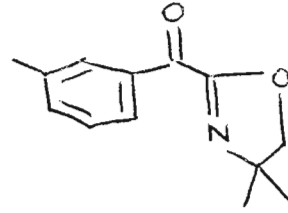
Solvent: cdcl3

Ambient temperature

Operator: kstowers

File: 2kjs289-2C

VNMRS-401 "Kr.chem.lsa.umich.edu"



Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
4416 repetitions  
OBSERVE C13, 100.7132632 MHz  
DECOUPLE H1, 400.5317616 MHz  
Power 45 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 2 hr, 48 min, 47 sec  
Acquisition date: Jun 11 2008

