

**Cascade Intramolecular *N*-Arylation/Intermolecular Carboamination
Reactions for the Construction of Tricyclic Heterocycles.**

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Supporting Information (continued)

NMR data for products in Table 2

gsl-IV-34-2

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gsl-IV-34-2rerun

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 31 2009

Operator: geolemen

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 7998.4 Hz

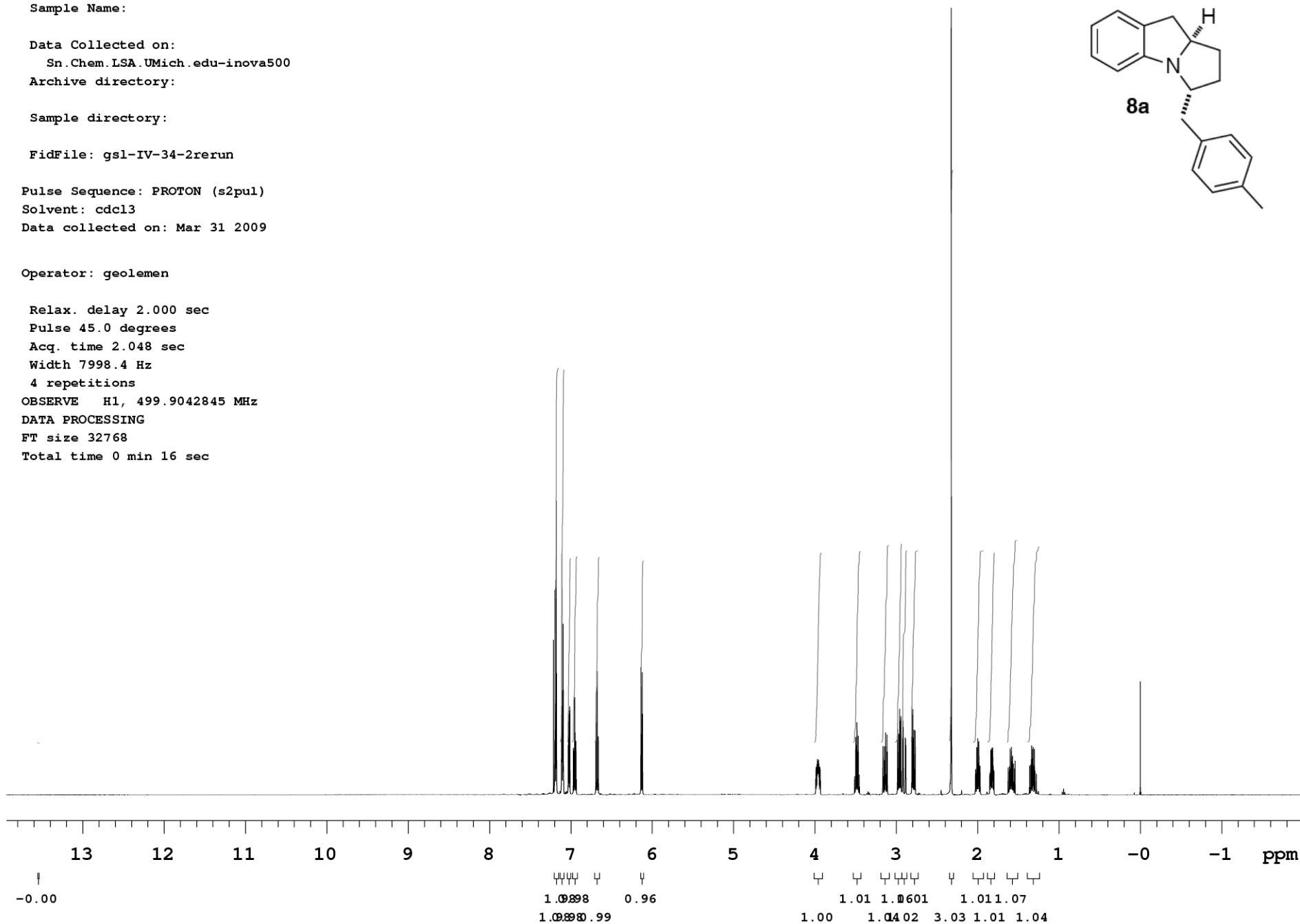
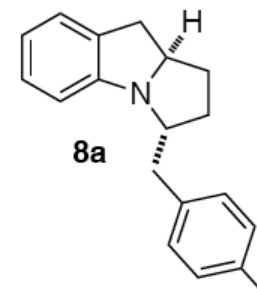
4 repetitions

OBSERVE H1, 499.9042845 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 16 sec

VARIAN 


gs1-IV-34-2 carbon

Sample Name:

Data Collected on:

Zr-inova400

Archive directory:

Sample directory:

FidFile: gs1-IV-34-2carbon

Pulse Sequence: Carbon (s2pul)

Solvent: cdcl3

Data collected on: Mar 31 2009

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

160 repetitions

OBSERVE C13, 100.5712729 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

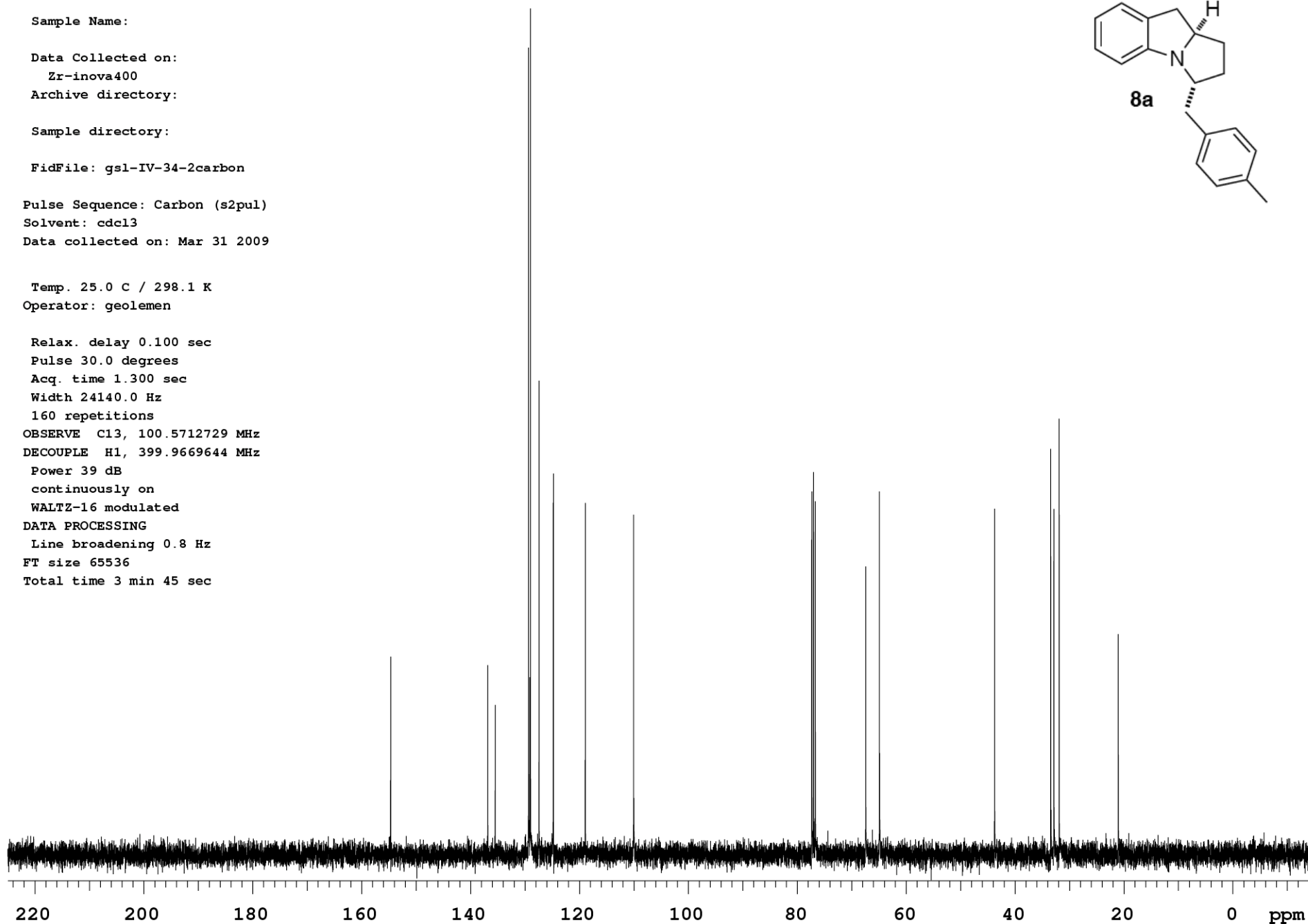
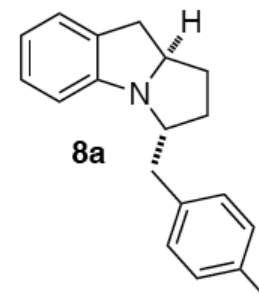
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 3 min 45 sec

VARIAN 

gsl-IV-34-2 cosy

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gsl-IV-34-2cosy

Pulse Sequence: gCOSY

Solvent: CDC13

Data collected on: Mar 31 2009

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 7998.4 Hz

2D Width 7998.4 Hz

2 repetitions

200 increments

OBSERVE H1, 499.9042816 MHz

DATA PROCESSING

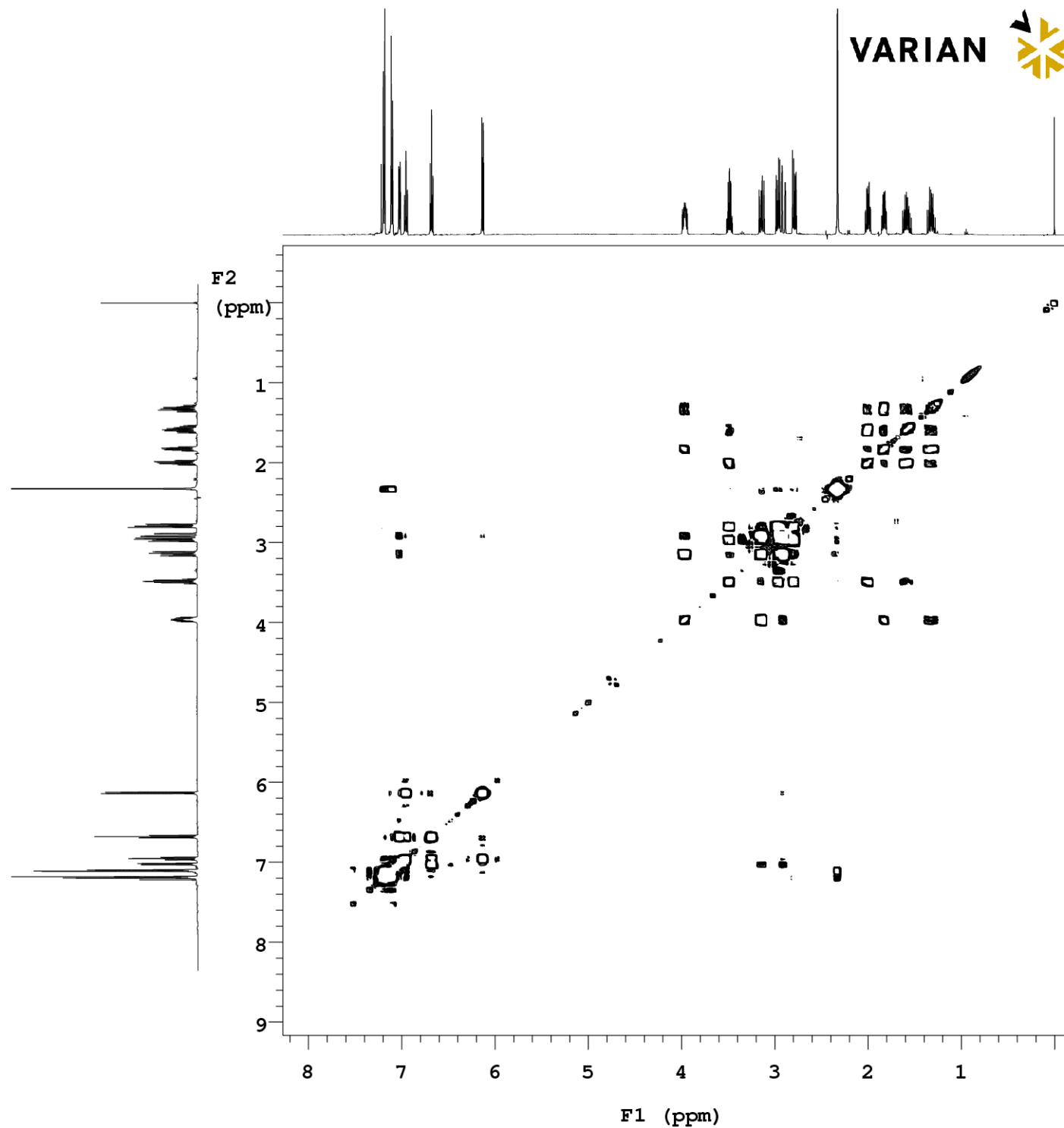
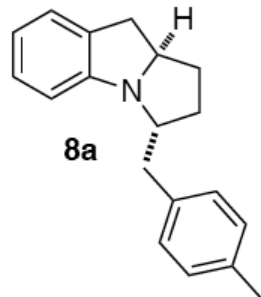
Sq. sine bell 0.064 sec

F1 DATA PROCESSING

Sq. sine bell 0.025 sec

FT size 2048 x 2048

Total time 8 min 38 sec



gsl-IV-34-2

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gsl-IV-34-2noesy

Pulse Sequence: NOESY

Solvent: cdcl3

Data collected on: Apr 4 2009

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4294.4 Hz

2D Width 4294.4 Hz

4 repetitions

2 x 256 increments

OBSERVE H1, 499.9042615 MHz

DATA PROCESSING

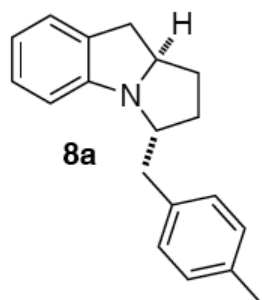
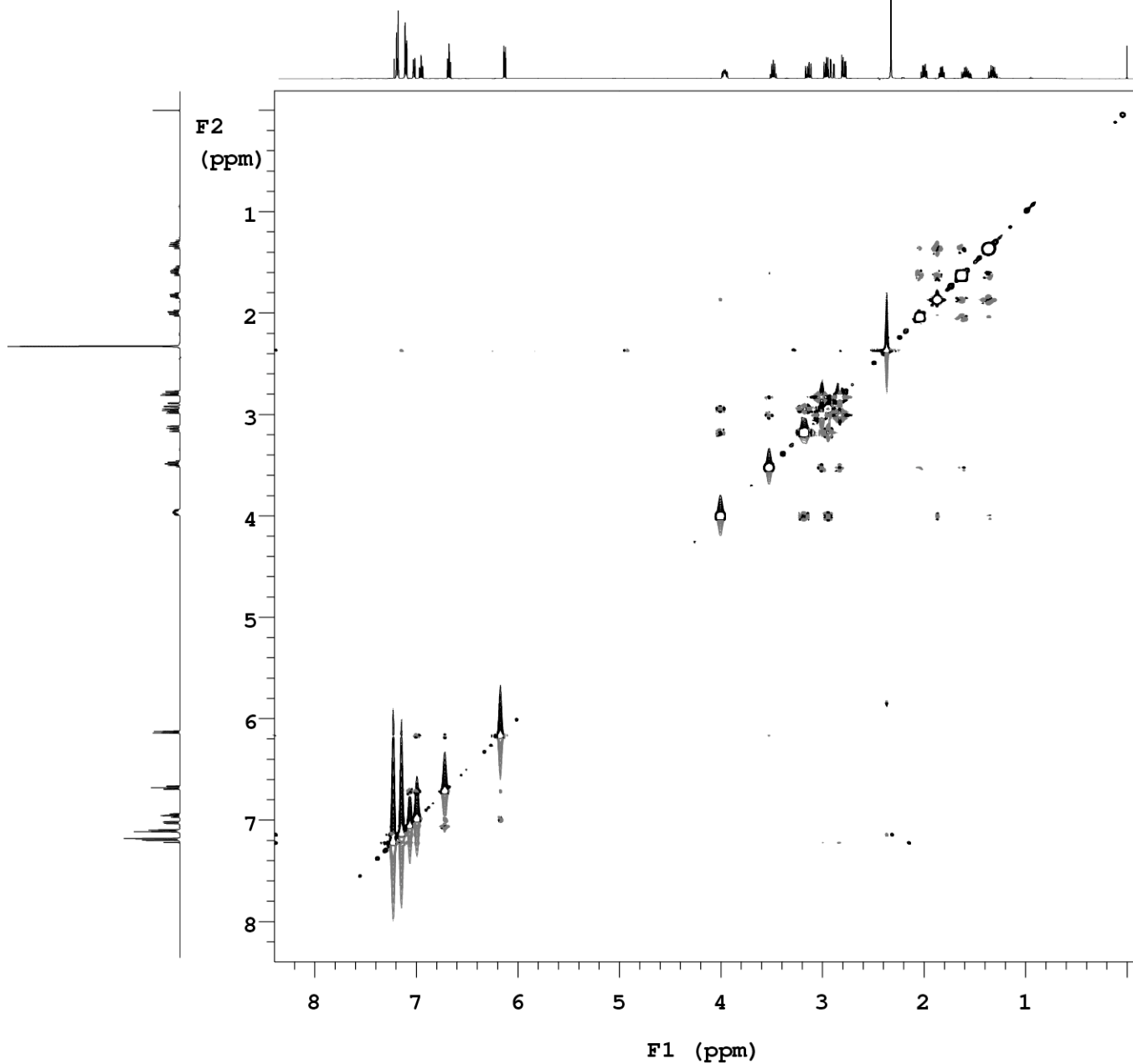
Gauss apodization 0.069 sec

F1 DATA PROCESSING

Gauss apodization 0.055 sec

FT size 2048 x 2048

Total time 1 hr, 37 min

VARIAN 

gs1-IV-59-2

Sample Name:

Data Collected on:

Ga.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-IV-59-2

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Apr 20 2009

Operator: geolemen

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

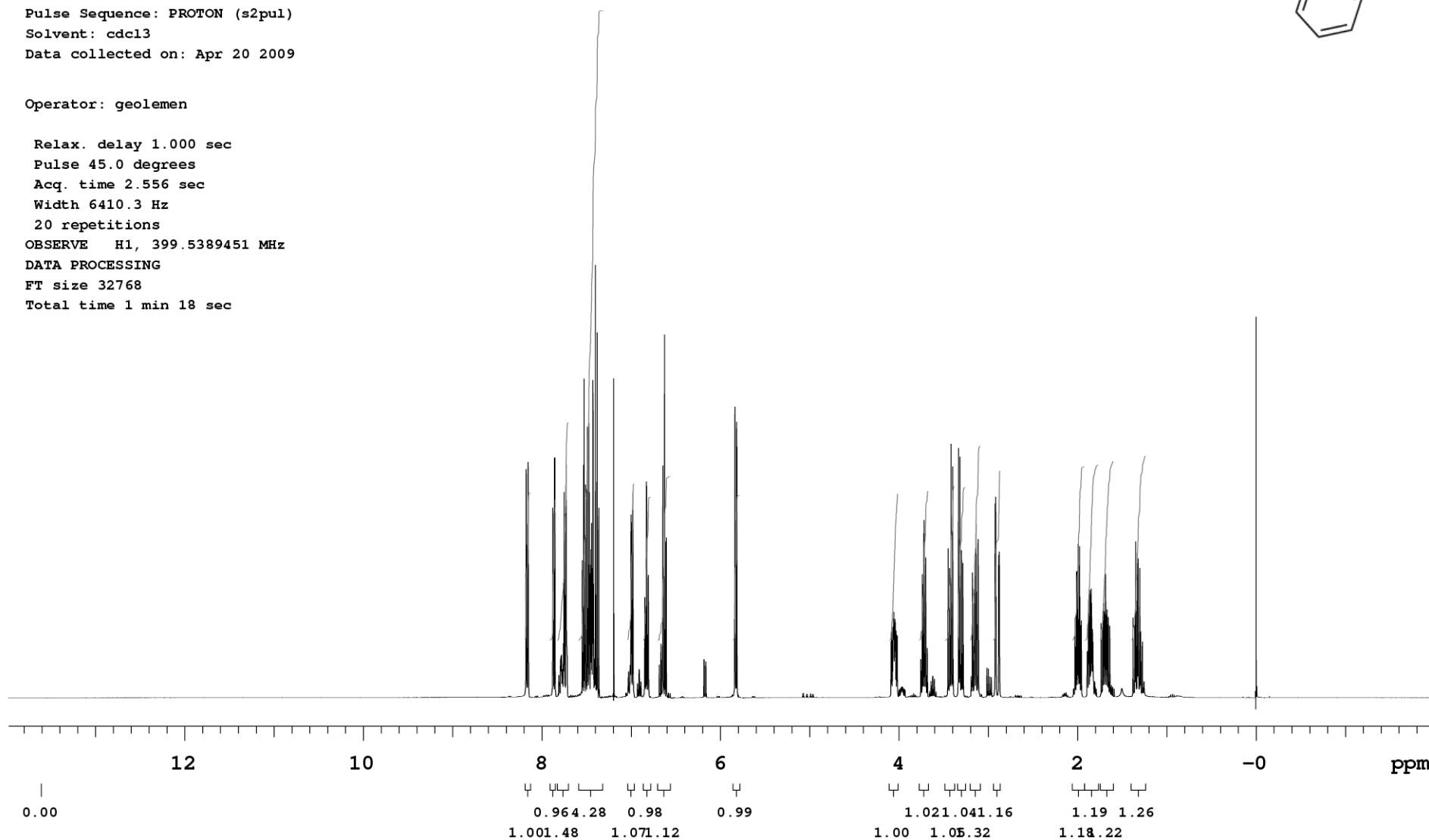
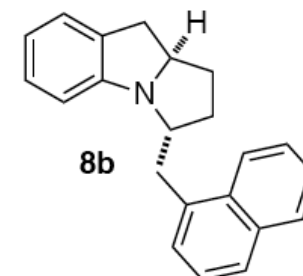
20 repetitions

OBSERVE H1, 399.5389451 MHz

DATA PROCESSING

FT size 32768

Total time 1 min 18 sec

VARIAN 


gs1-IV-59-2 carbon

Sample Name:

Data Collected on:

Ga.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-IV-59-2carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Apr 20 2009

Operator: geolemen

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

48 repetitions

OBSERVE C13, 100.4641487 MHz

DECOUPLE H1, 399.5409236 MHz

Power 33 dB

continuously on

WALTZ-16 modulated

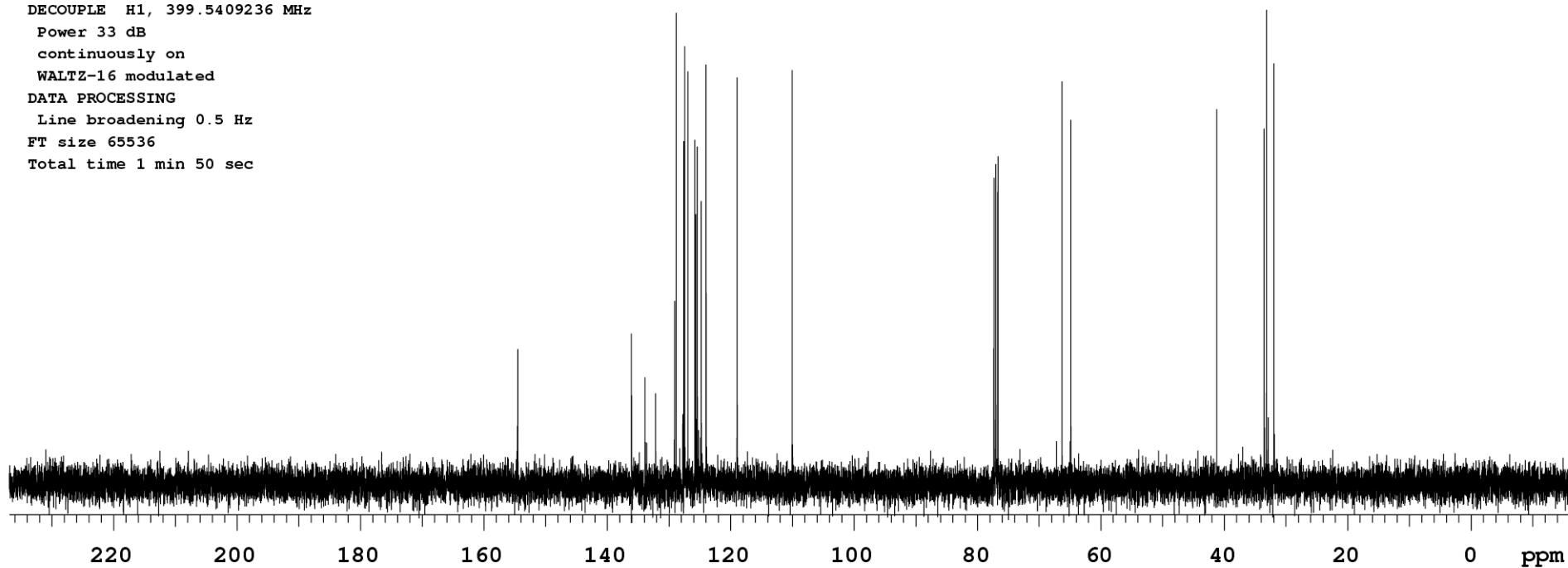
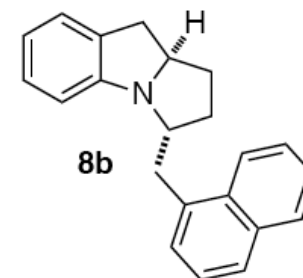
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 min 50 sec

VARIAN 



gsl-VIII-126-3

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gsl-VIII-126-3

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 26 2011

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.500 sec

Width 7998.4 Hz

16 repetitions

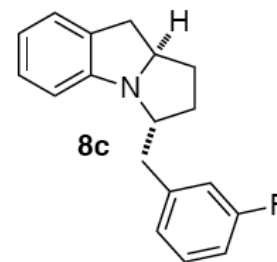
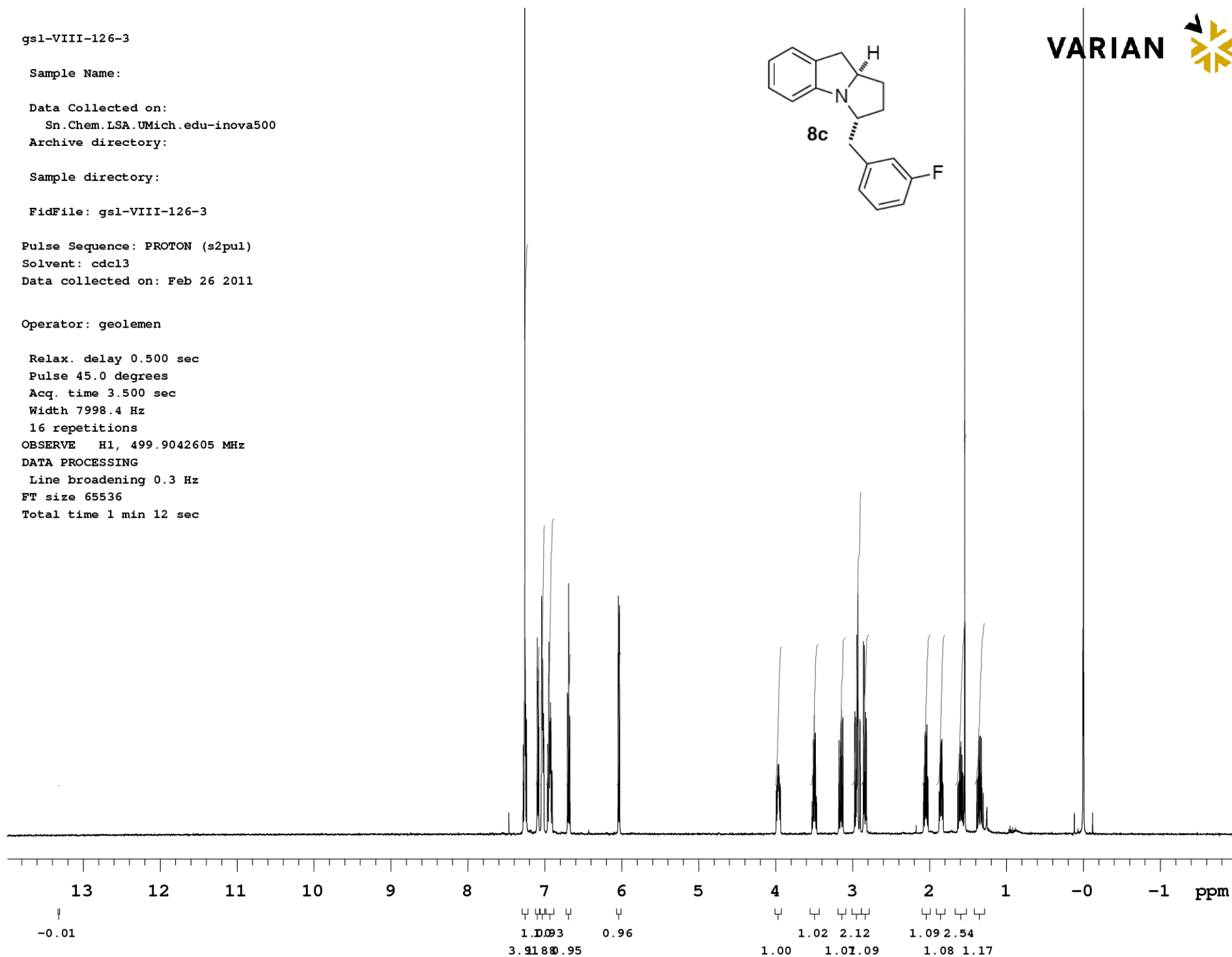
OBSERVE H1, 499.9042605 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min 12 sec


VARIAN 


gs1-VIII-126-2 carbon

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gs1-VIII-126-3carbon

Pulse Sequence: CARBON (s2pul)

Solvent: CDCl3

Data collected on: Mar 1 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 2.045 sec

Width 32051.3 Hz

1072 repetitions

OBSERVE C13, 125.7485305 MHz

DECOUPLE H1, 500.0956704 MHz

Power 42 dB

continuously on

WALTZ-16 modulated

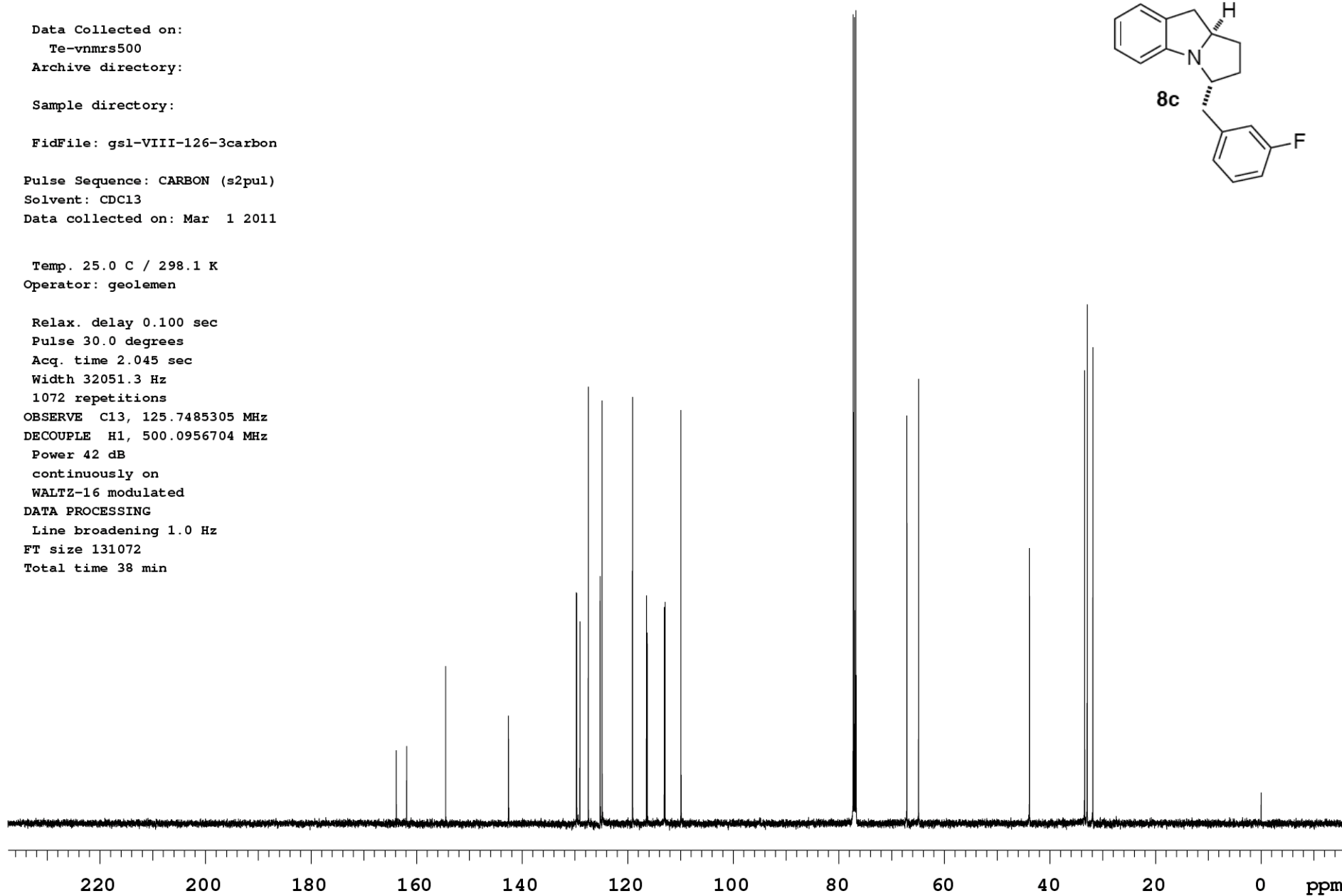
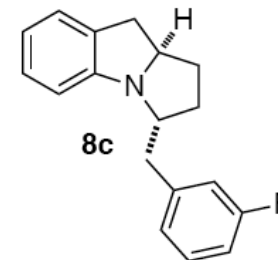
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 38 min

VARIAN



gsl-VIII-126-3

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-126-3cosy

Pulse Sequence: gCOSY

Solvent: CDCl₃

Data collected on: Mar 1 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4310.3 Hz

2D Width 4310.3 Hz

Single scan

128 increments

OBSERVE H1, 500.0931768 MHz

DATA PROCESSING

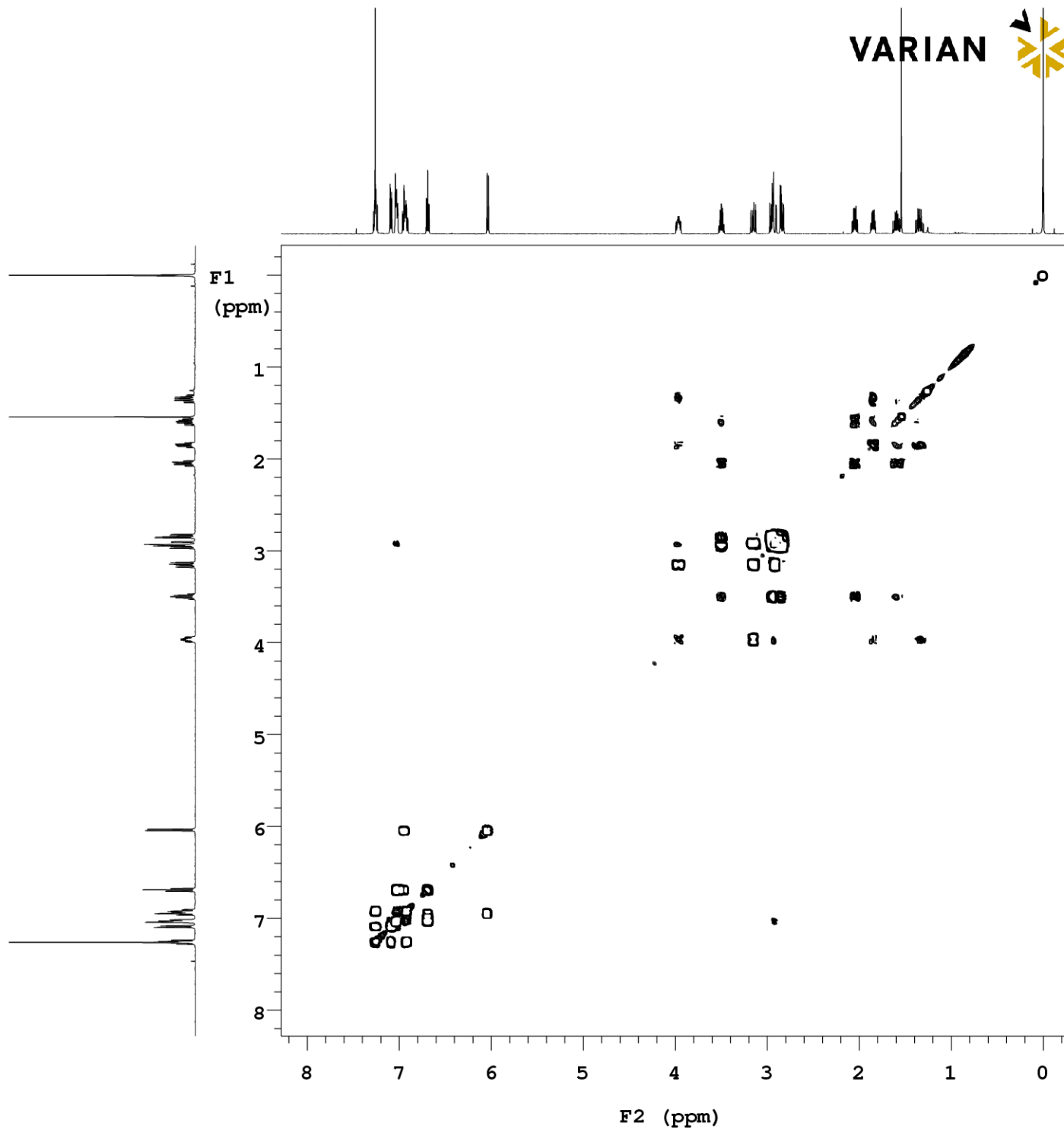
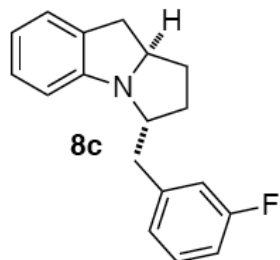
Sq. sine bell 0.059 sec

F1 DATA PROCESSING

Sq. sine bell 0.030 sec

FT size 1024 x 1024

Total time 3 min 12 sec



STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-126-2fluorine

Pulse Sequence: FLUORINE (s2pul)

Solvent: CDC13

Data collected on: Feb 25 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 1.000 sec

Pulse 30.0 degrees

Acq. time 0.603 sec

Width 108.7 kHz

16 repetitions

OBSERVE F19, 470.5577288 MHz

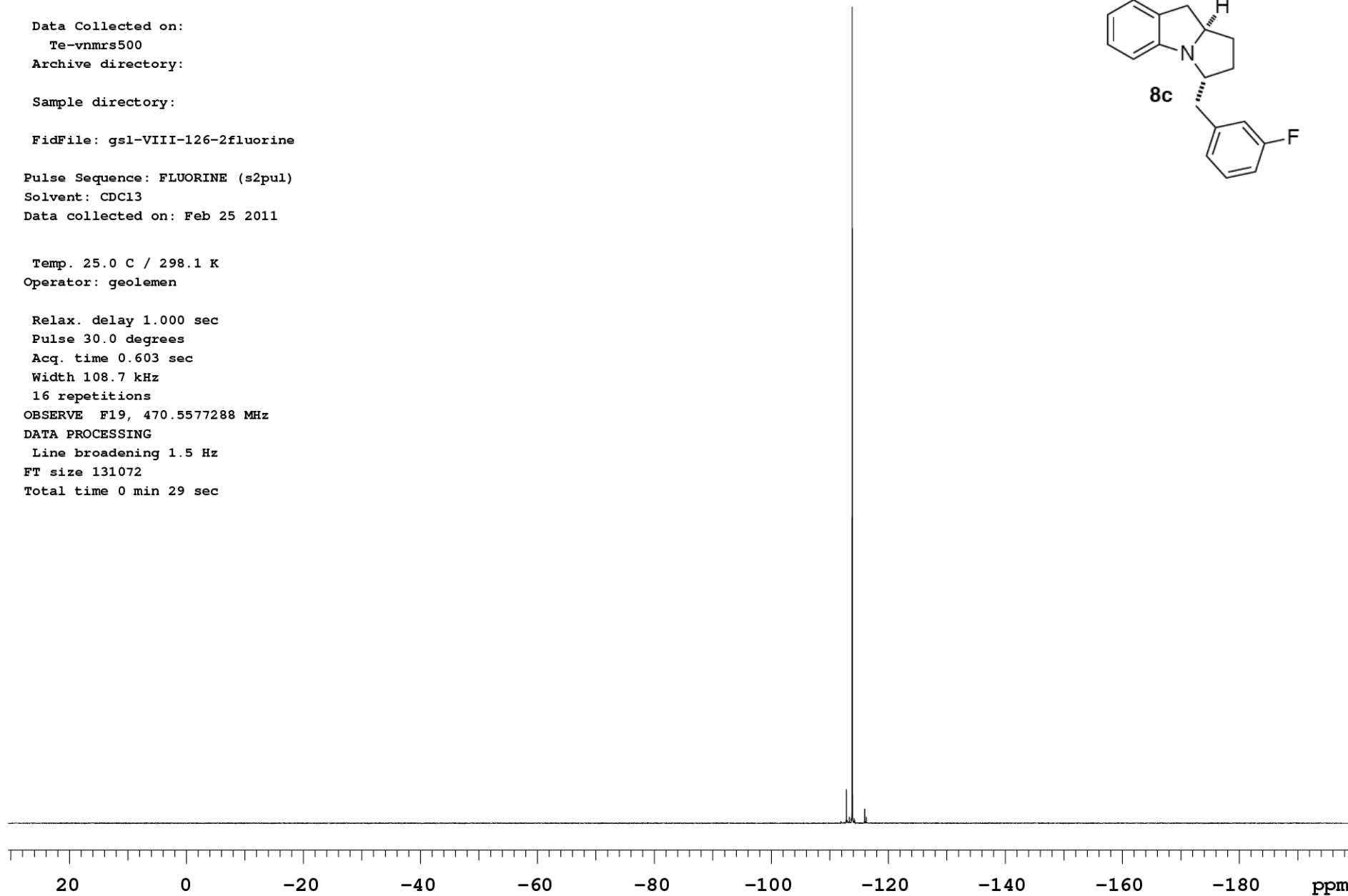
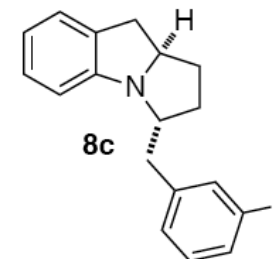
DATA PROCESSING

Line broadening 1.5 Hz

FT size 131072

Total time 0 min 29 sec

VARIAN



gs1-VII-113-2

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gs1-VII-113-2

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Sep 29 2010

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.500 sec

Width 7998.4 Hz

24 repetitions

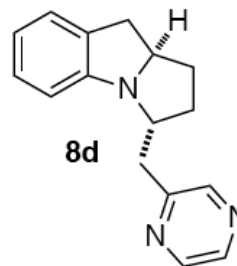
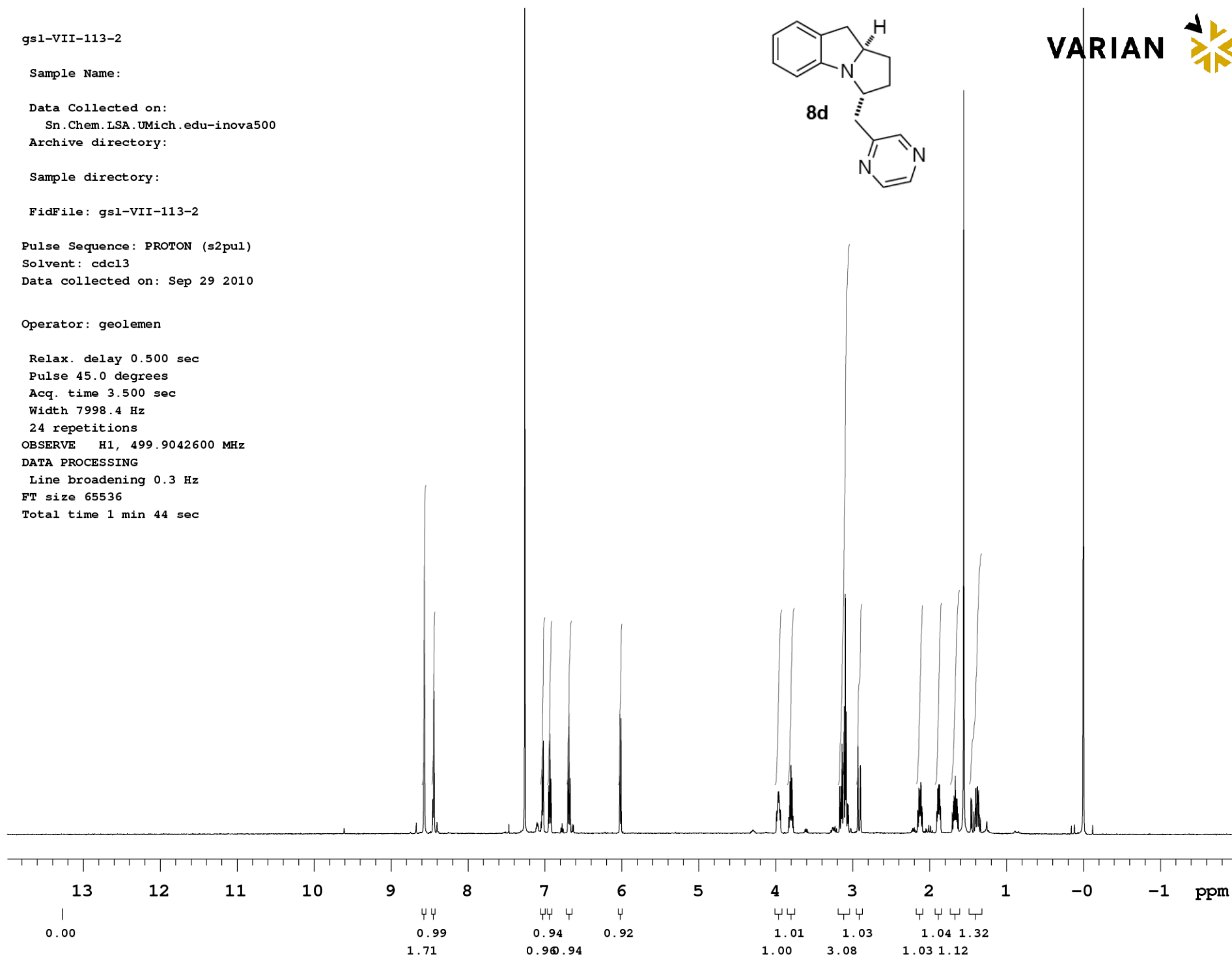
OBSERVE H1, 499.9042600 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min 44 sec


VARIAN 


gs1-VII-113-2 carbon

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-113-2carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 30 2010

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 2.569 sec

Width 25510.2 Hz

88 repetitions

OBSERVE C13, 100.7109978 MHz

DECOUPLE H1, 400.5226414 MHz

Power 41 dB

continuously on

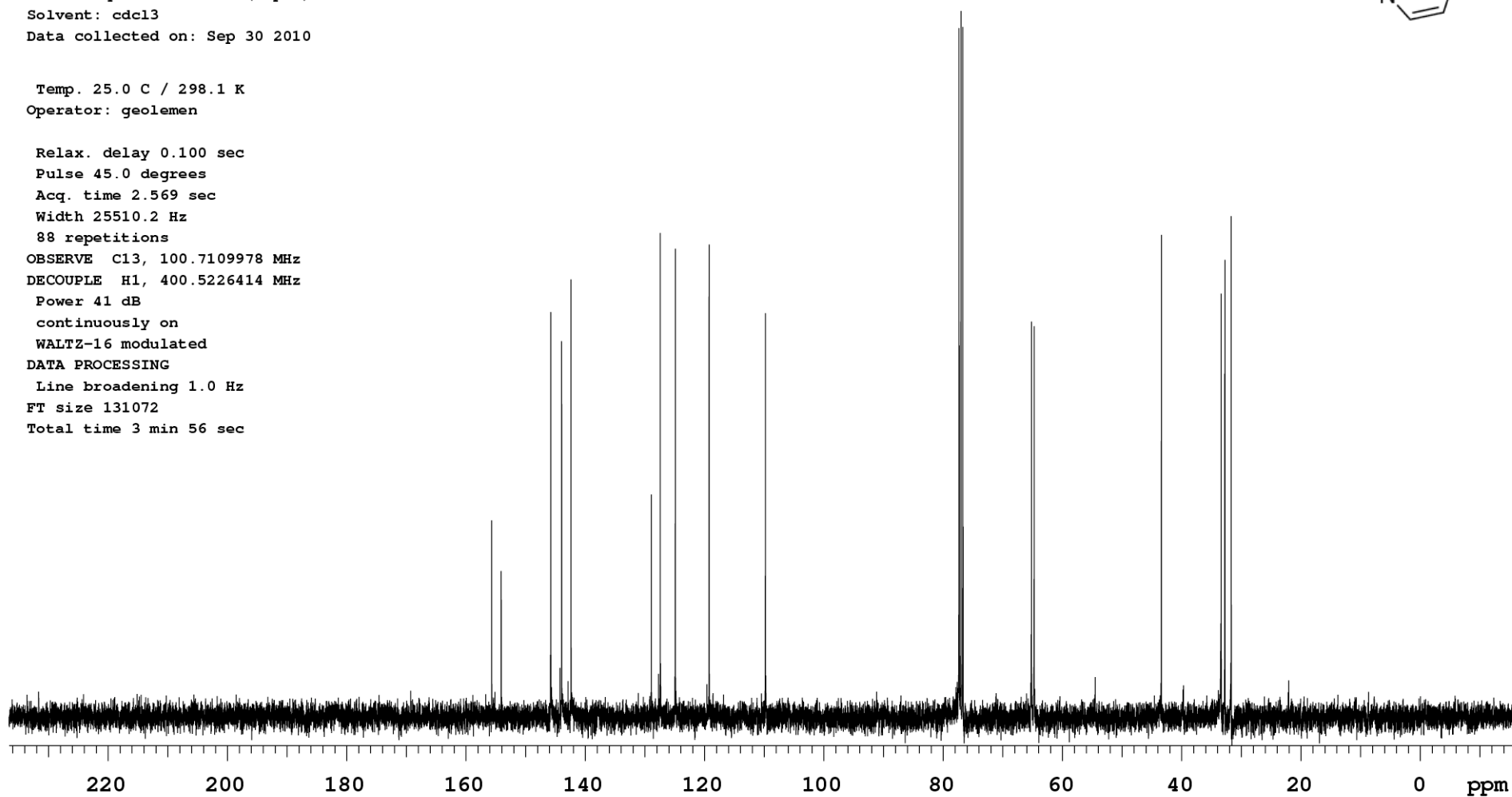
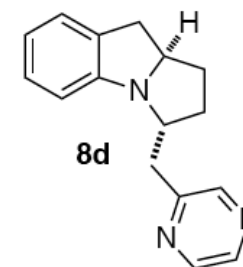
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 3 min 56 sec

VARIAN 

gs1-VII-113-2

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-113-2cosy

Pulse Sequence: gCOSY

Solvent: cdcl3

Data collected on: Sep 30 2010

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4280.8 Hz

2D Width 4280.8 Hz

Single scan

128 increments

OBSERVE H1, 400.5206328 MHz

DATA PROCESSING

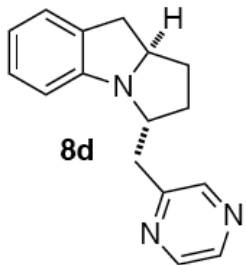
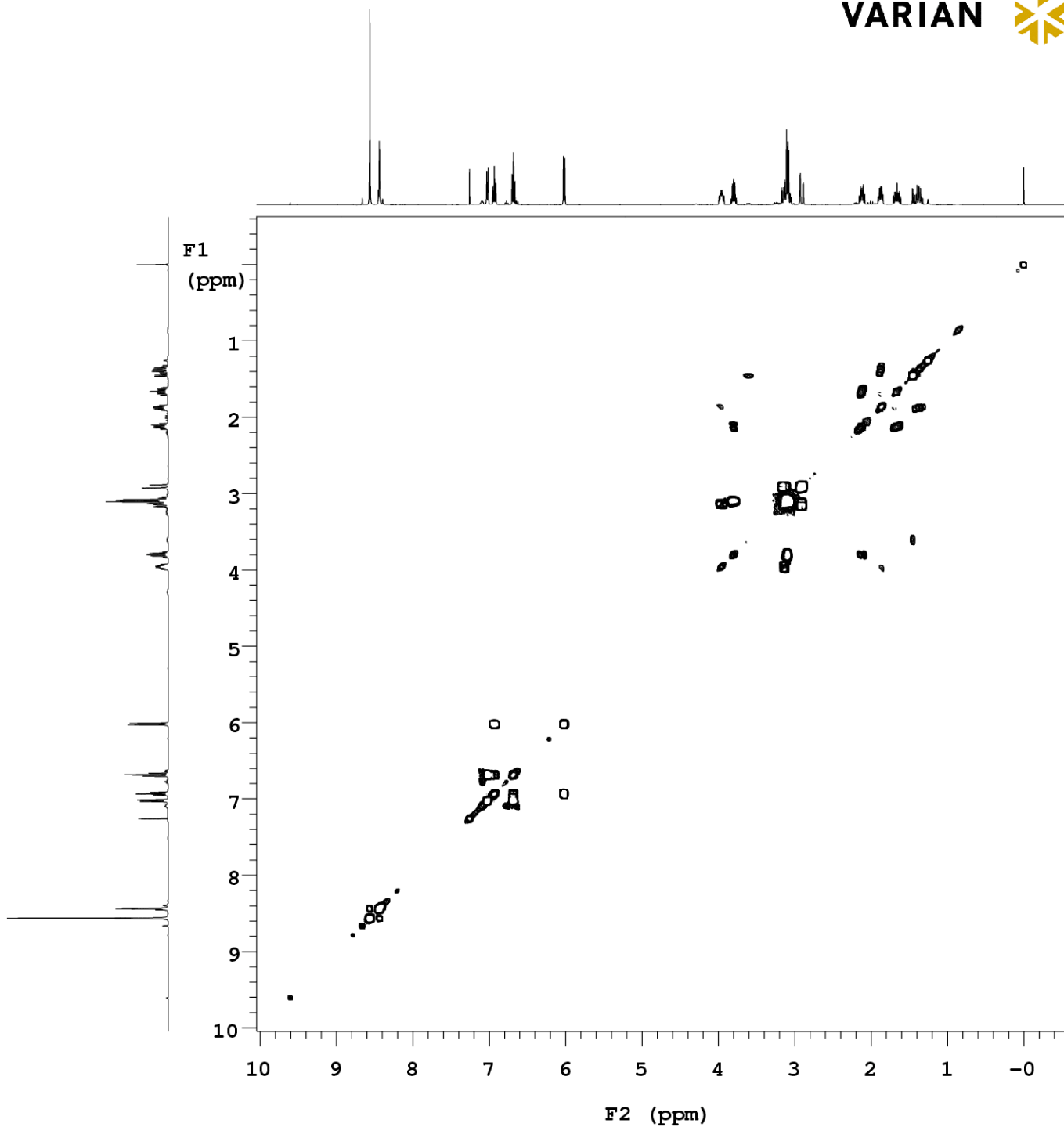
Sq. sine bell 0.060 sec

F1 DATA PROCESSING

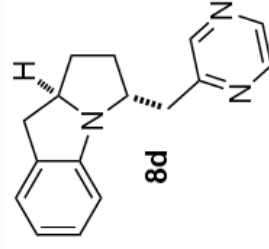
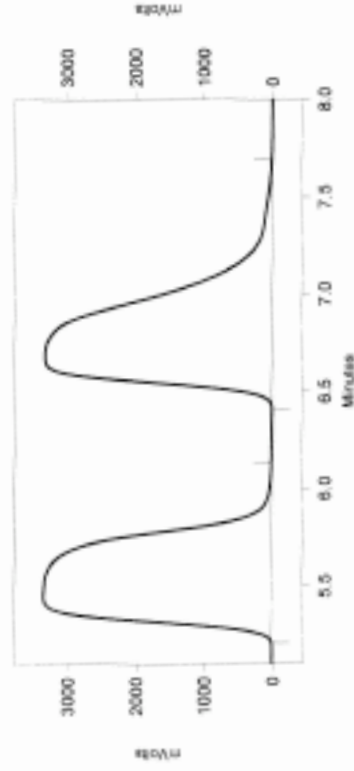
Sq. sine bell 0.030 sec

FT size 1024 x 1024

Total time 3 min 12 sec

VARIAN 

C:\CLASS-VP\Enterprise\Projects\Default\Data\Lemen\gs1-VII-115-2RAC_OD-H_8\IP
A_1mL-minrerun.dat

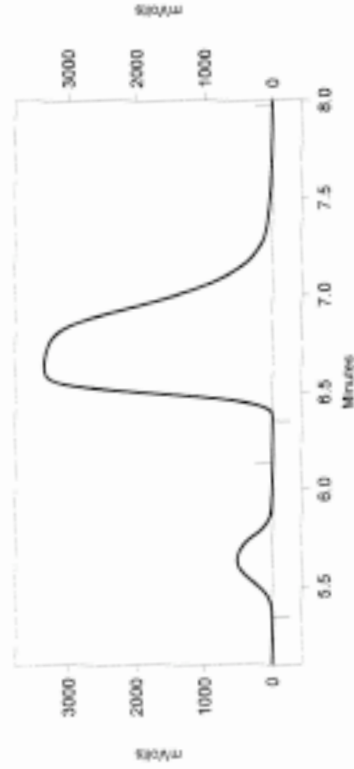


SPD-10Avp Ch2-254nm

Results

Retention Time	Area	Area Percent
5.450	91401883	49.188
6.675	94418553	50.812
Totals		185820436
		100.000

C:\CLASS-VP\Enterprise\Projects\Default\Data\Lemen\gs1-VIII-86-2chiral_OD-H_8
%IPA_1mL-min.dat



SPD-10Avp Ch2-254nm

Results

Retention Time	Area	Area Percent
5.633	7981896	7.290
6.633	101504627	92.710
Totals		109486523
		100.000

gsl-VIII-118-2

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gsl-VIII-118-2

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 22 2011

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.500 sec

Width 7998.4 Hz

18 repetitions

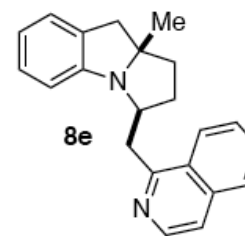
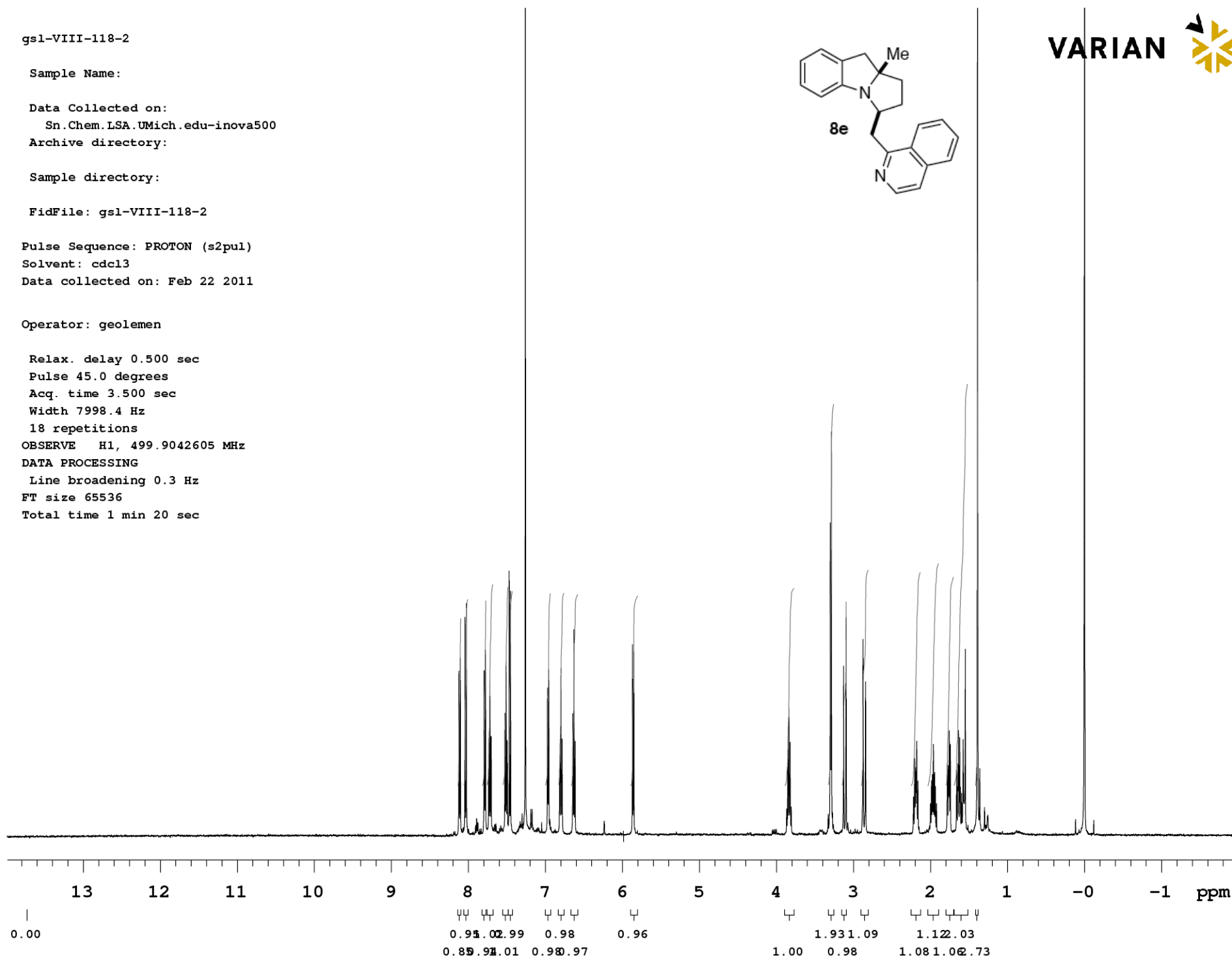
OBSERVE H1, 499.9042605 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min 20 sec


VARIAN 


gs1-VIII-118-2 carbon

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gs1-VIII-118-2carbon

Pulse Sequence: CARBON (s2pul)

Solvent: CDCl3

Data collected on: Feb 23 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 2.045 sec

Width 32051.3 Hz

192 repetitions

OBSERVE C13, 125.7485300 MHz

DECOUPLE H1, 500.0956704 MHz

Power 42 dB

continuously on

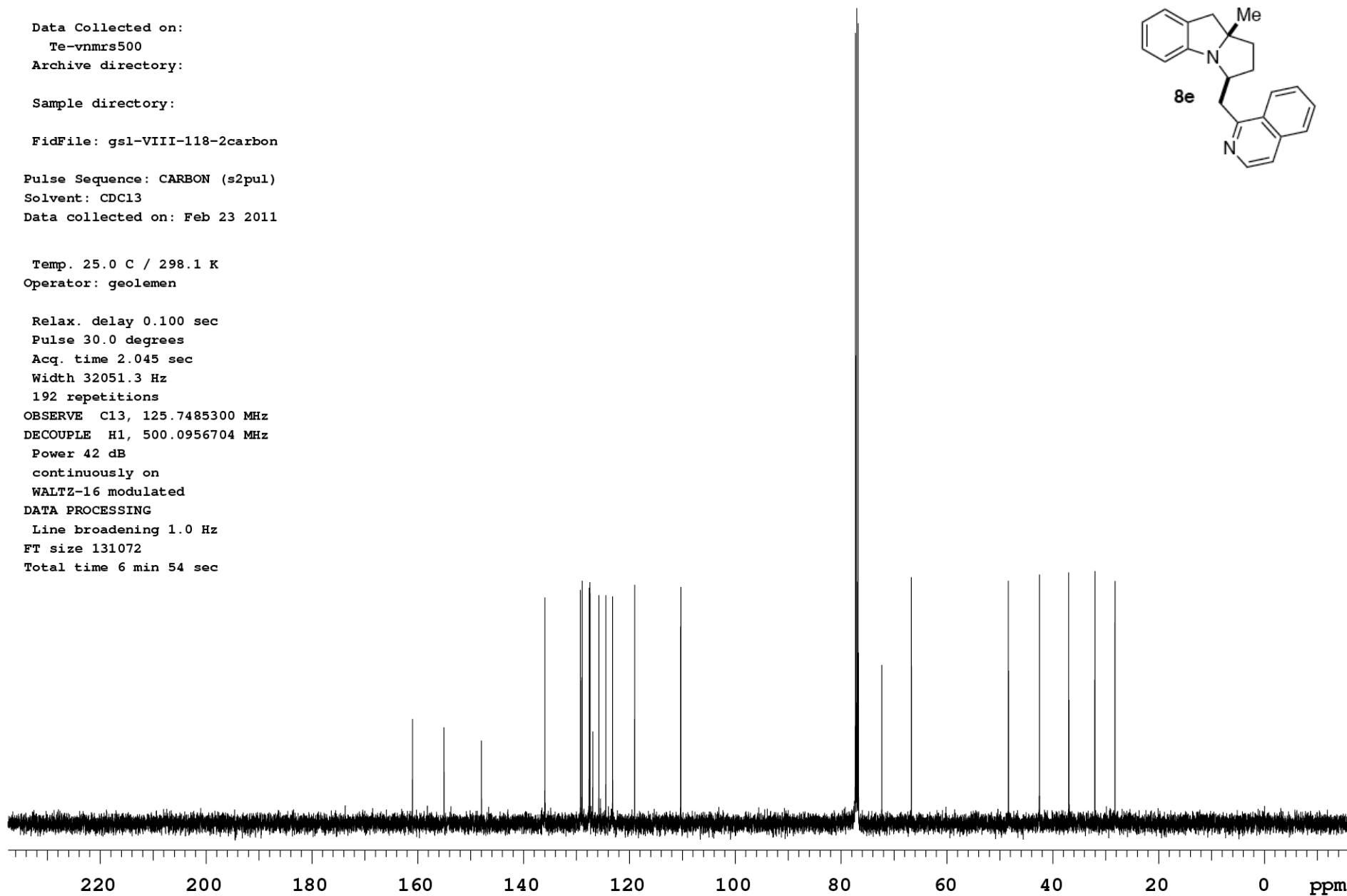
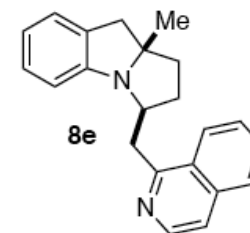
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 6 min 54 sec

VARIAN 

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-118-2cosy

Pulse Sequence: gCOSY

Solvent: CDC13

Data collected on: Feb 23 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4960.3 Hz

2D Width 4960.3 Hz

Single scan

128 increments

OBSERVE H1, 500.0931741 MHz

DATA PROCESSING

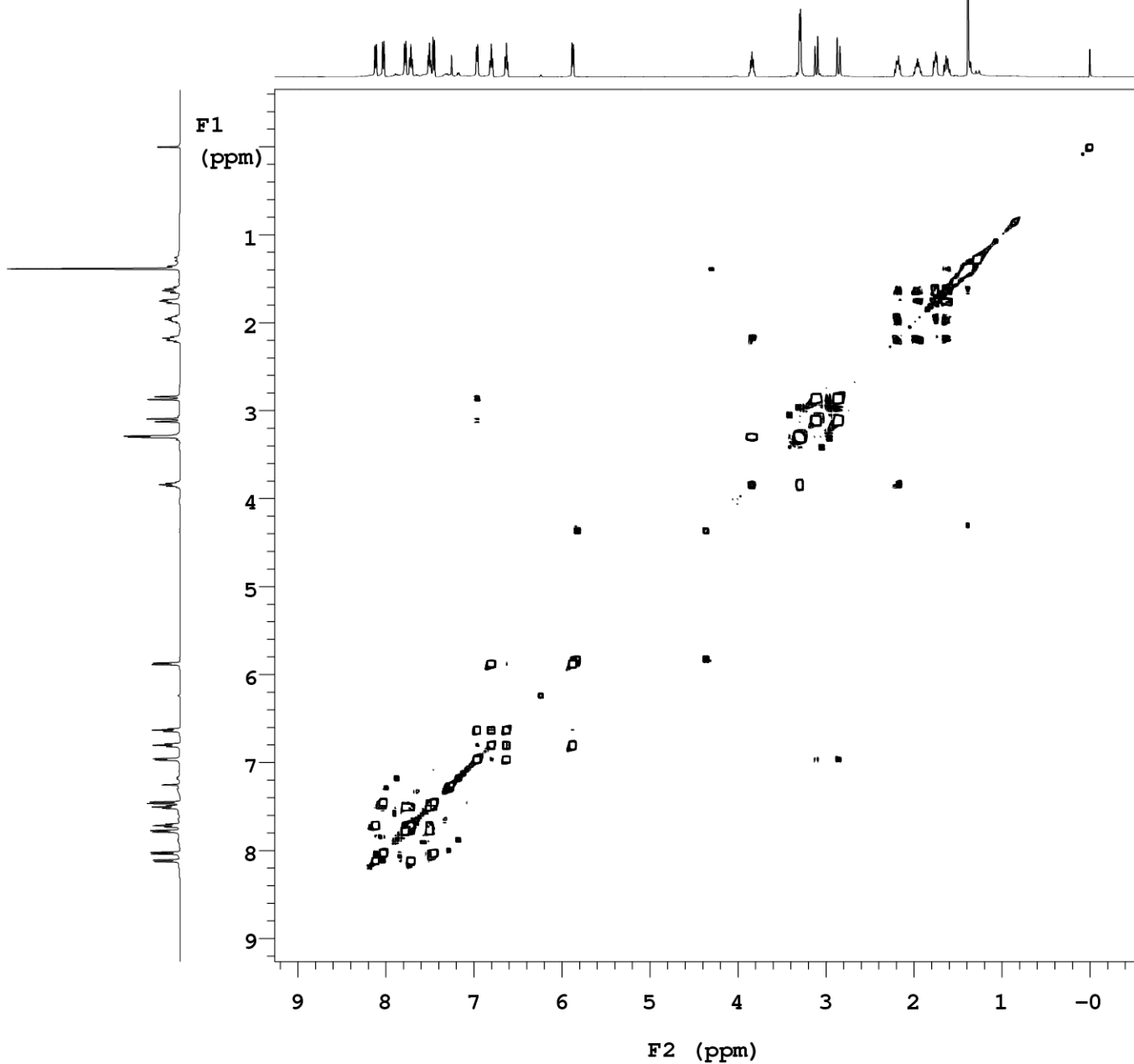
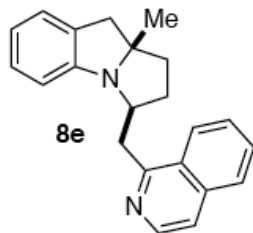
Sq. sine bell 0.075 sec

F1 DATA PROCESSING

Sq. sine bell 0.026 sec

FT size 2048 x 2048

Total time 3 min 12 sec



gs1-VII-139-1

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-139-2

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Oct 22 2010

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 10.224 sec

Width 6410.3 Hz

2 repetitions

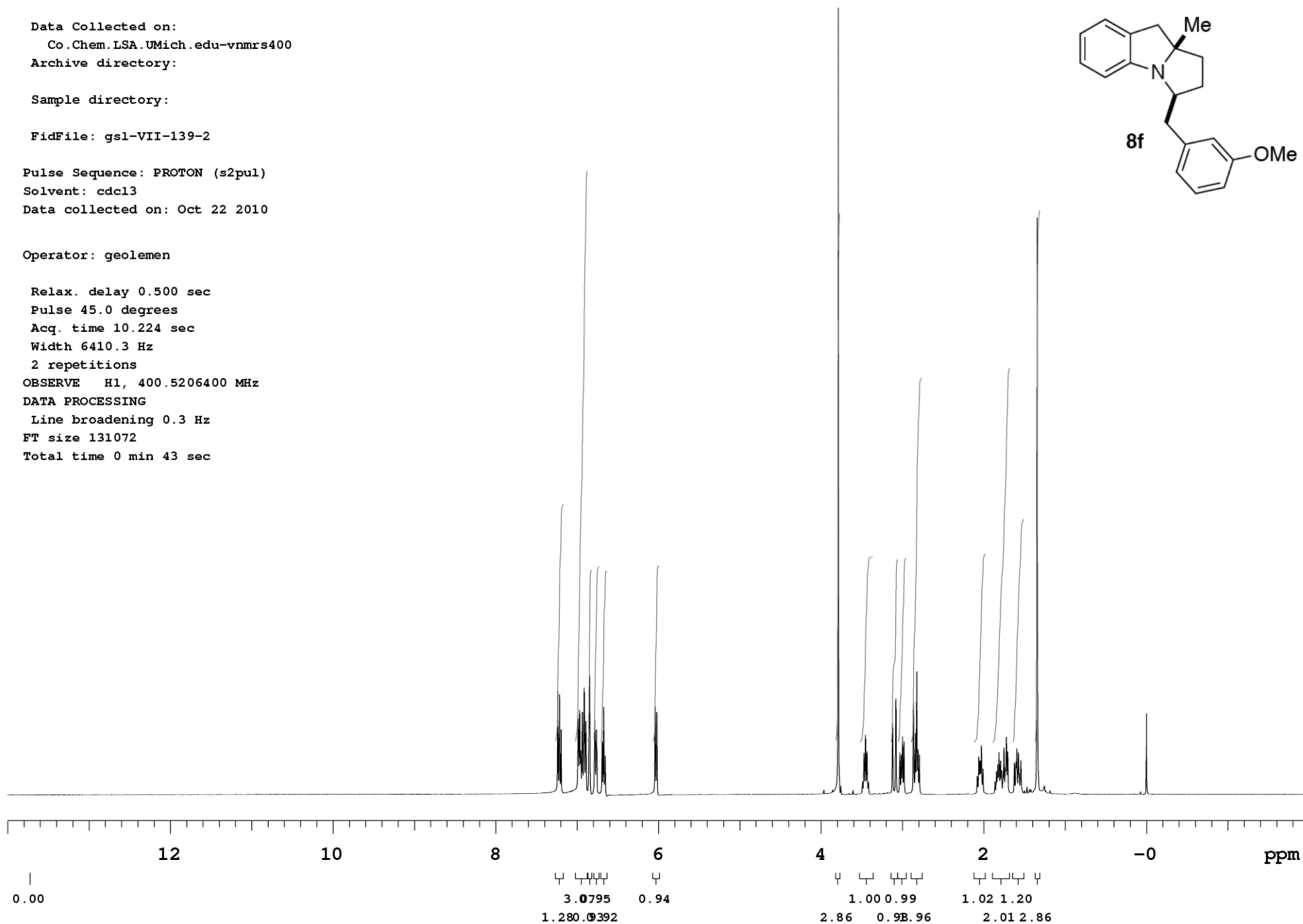
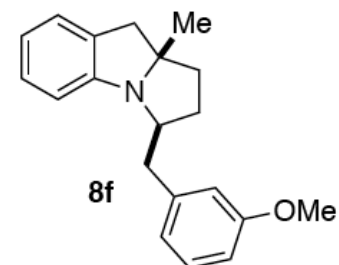
OBSERVE H1, 400.5206400 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 131072

Total time 0 min 43 sec

VARIAN 


gs1-VII-139-2 carbon

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-139-2carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Oct 22 2010

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 2.569 sec

Width 25510.2 Hz

88 repetitions

OBSERVE C13, 100.7109963 MHz

DECOUPLE H1, 400.5226414 MHz

Power 41 dB

continuously on

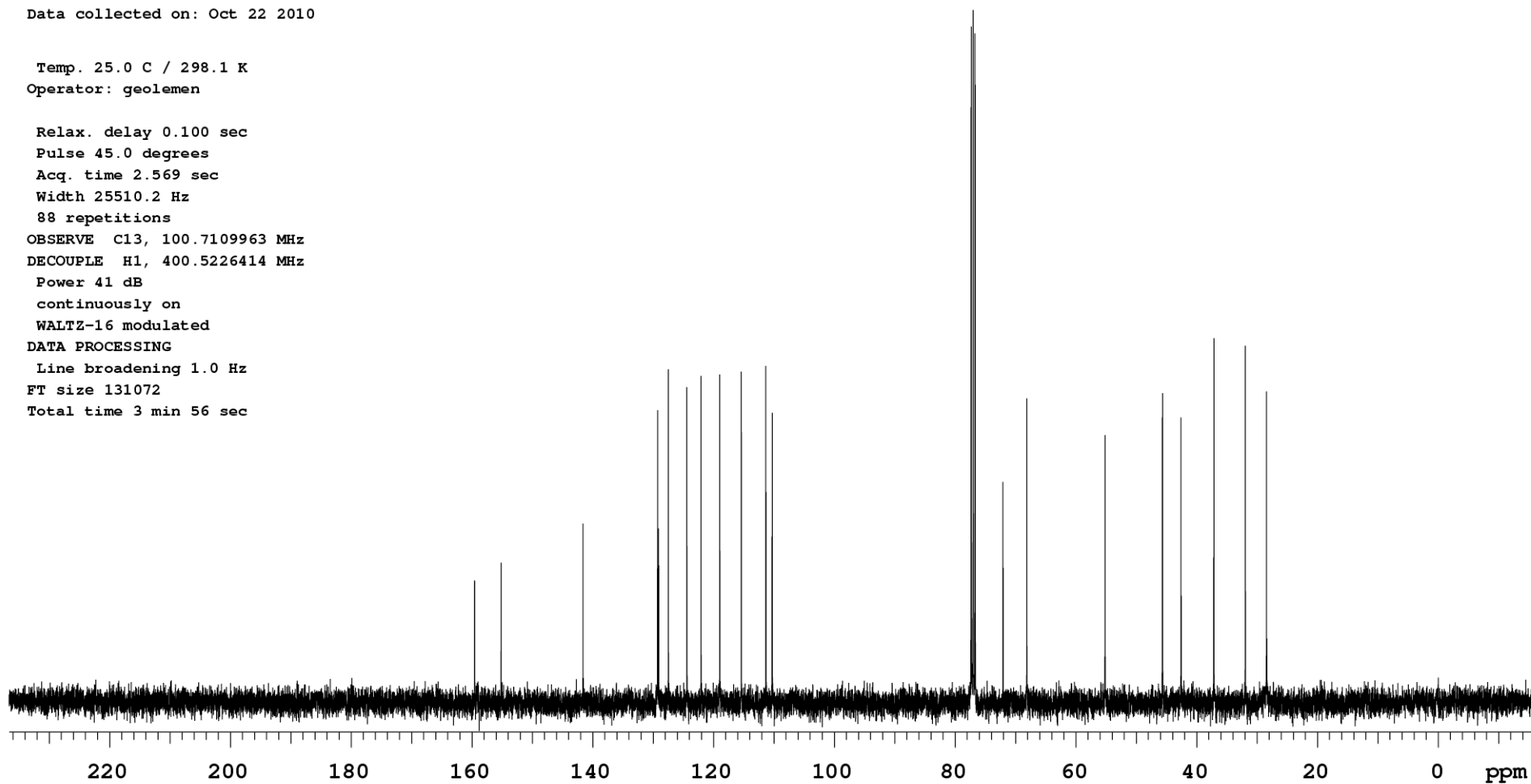
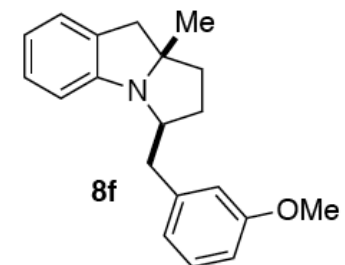
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 3 min 56 sec

VARIAN 

gs1-VII-139-2

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-139-2noesy

Pulse Sequence: NOESY

Solvent: cdc13

Data collected on: Oct 22 2010

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 3453.0 Hz

2D Width 3453.0 Hz

4 repetitions

2 x 200 increments

OBSERVE H1, 400.5206401 MHz

DATA PROCESSING

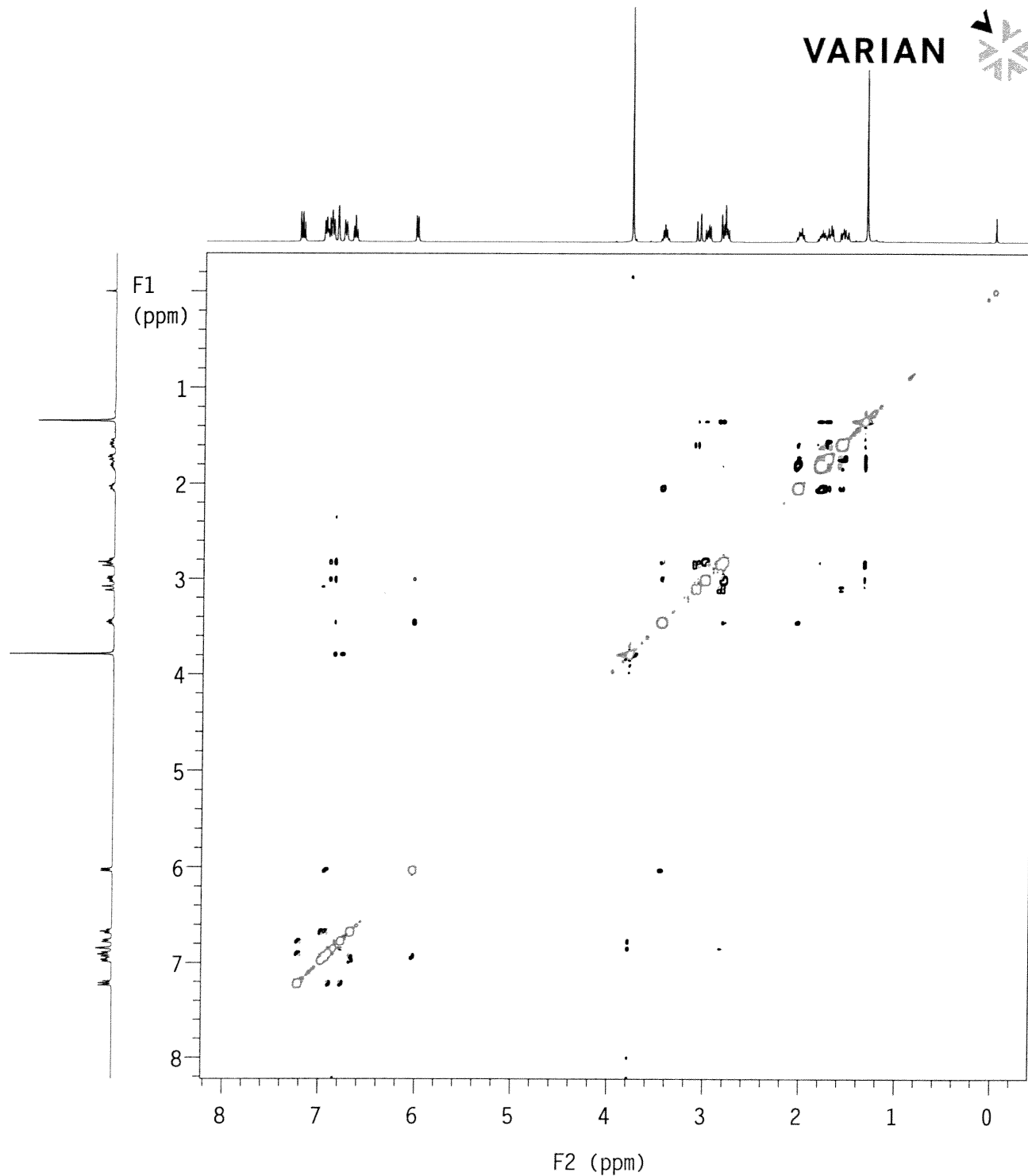
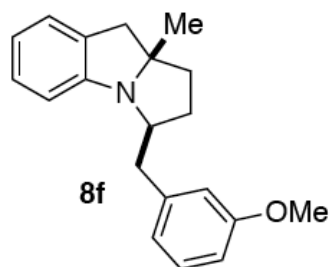
Gauss apodization 0.069 sec

F1 DATA PROCESSING

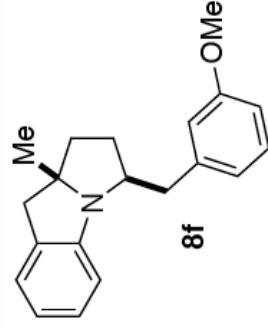
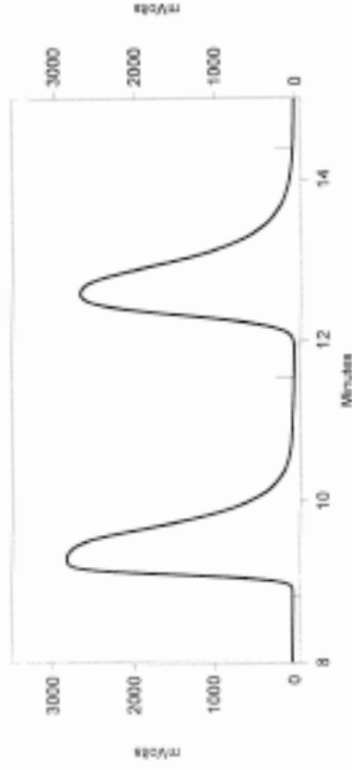
Gauss apodization 0.053 sec

FT size 2048 x 2048

Total time 1 hr. 48 min



C:\CLASS-VP\Enterprise\Projects\Default\Data\Lemen\gsl-VIII-116-2-RAC-0-1&IPA_0-8mlmin_OJ-H-sol-5%IPAdilute.dat



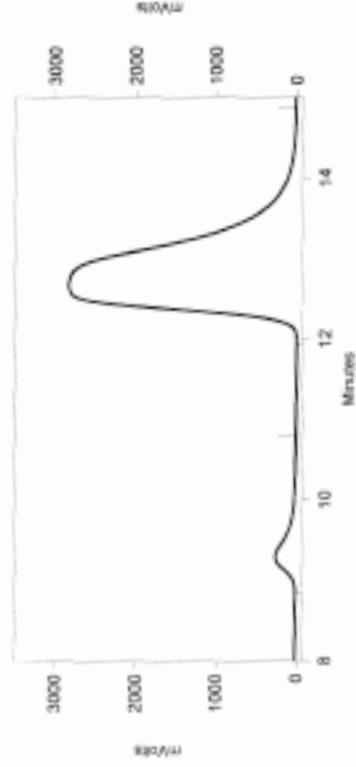
SPD-10Avp Ch2-254nm

Results

Retention Time	Area	Area Percent
9.283	120853116	49.005
12.583	125759222	50.995

Totals	246612338	100.000
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C:\CLASS-VP\Enterprise\Projects\Default\Data\Lemen\gsl-VII-200-2-chiral-0-1&IPA_0-8mlmin_OJ-H-sol-1&IPA.dat



SPD-10Avp Ch2-254nm

Results

Retention Time	Area	Area Percent
9.292	7123927	4.324
12.667	157622399	95.676

Totals	164746326	100.000
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gsl-VIII-161-2frac18-24

Sample Name:

Data Collected on:

Te.Chem.LSA.UMich.edu-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-164-2benzene

Pulse Sequence: PROTON (s2pul)

Solvent: c6d6

Data collected on: Apr 14 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 4.089 sec

Width 8012.8 Hz

10 repetitions

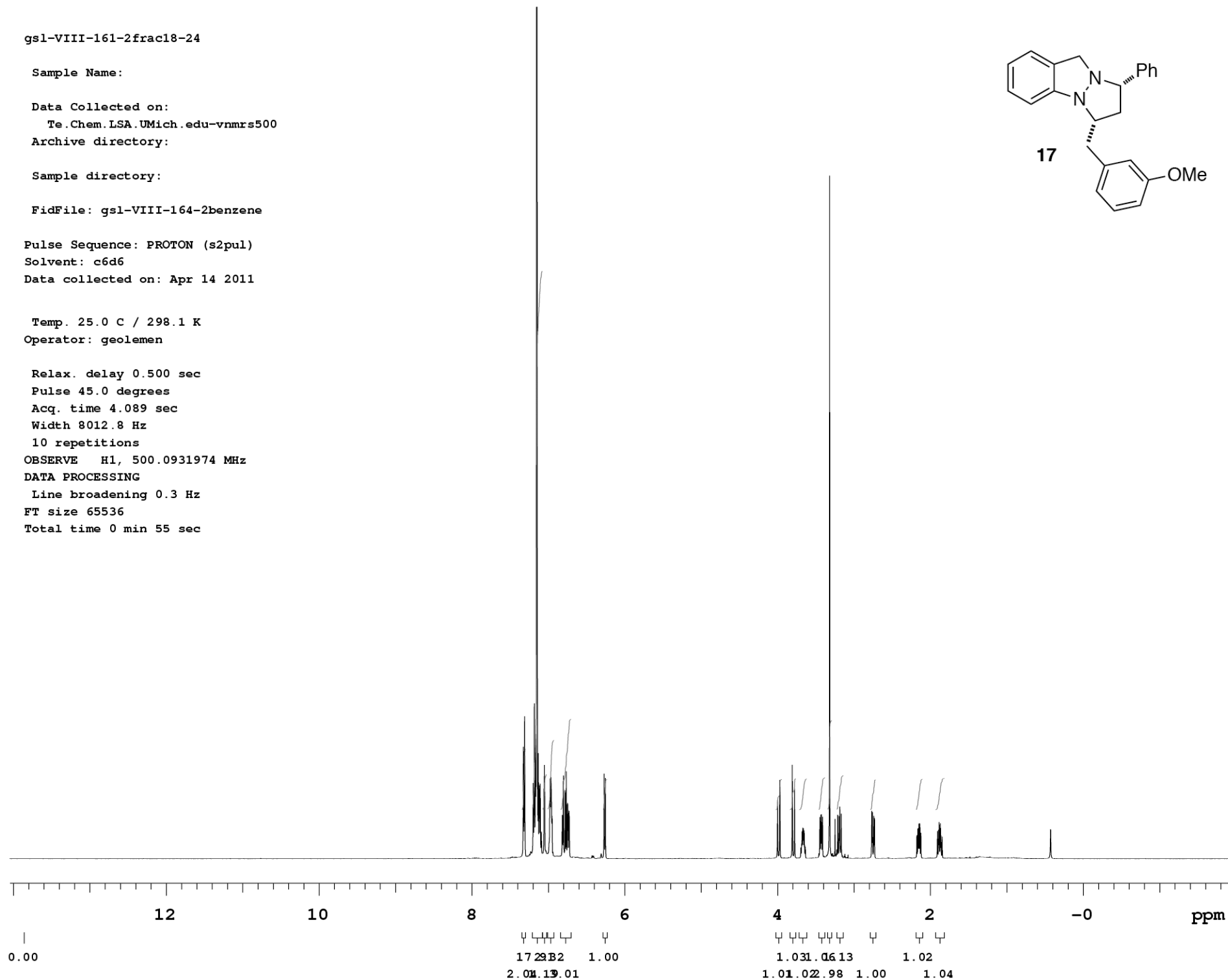
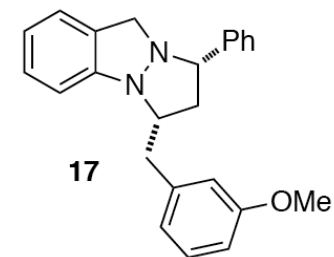
OBSERVE H1, 500.0931974 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 0 min 55 sec



gsl-VIII-161-2frac18-24

Sample Name:

Data Collected on:

Te.Chem.LSA.UMich.edu-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-161-2frac18-24carbon

Pulse Sequence: CARBON (s2pul)

Solvent: CDCl3

Data collected on: Apr 12 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 2.045 sec

Width 32051.3 Hz

184 repetitions

OBSERVE C13, 125.7485285 MHz

DECOUPLE H1, 500.0956704 MHz

Power 42 dB

continuously on

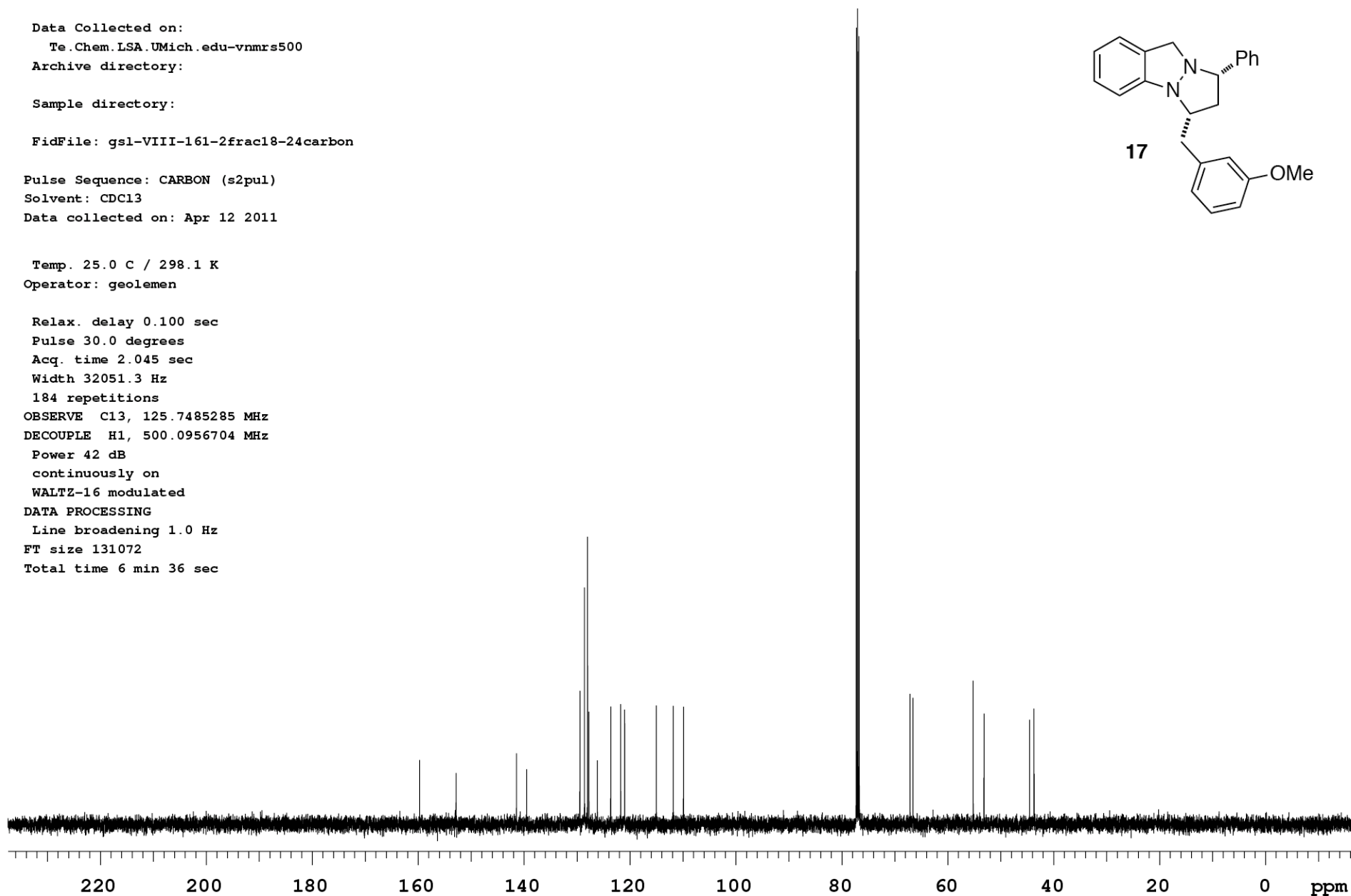
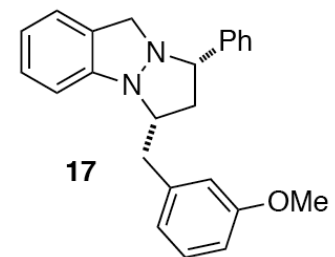
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 6 min 36 sec

VARIAN 

gsl-VIII-164-2

Sample Name:

Data Collected on:

Te.Chem.LSA.UMich.edu-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-164-2benzenecosy

Pulse Sequence: gCOSY

Solvent: c6d6

Data collected on: Apr 14 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4006.4 Hz

2D Width 4006.4 Hz

Single scan

128 increments

OBSERVE H1, 500.0931974 MHz

DATA PROCESSING

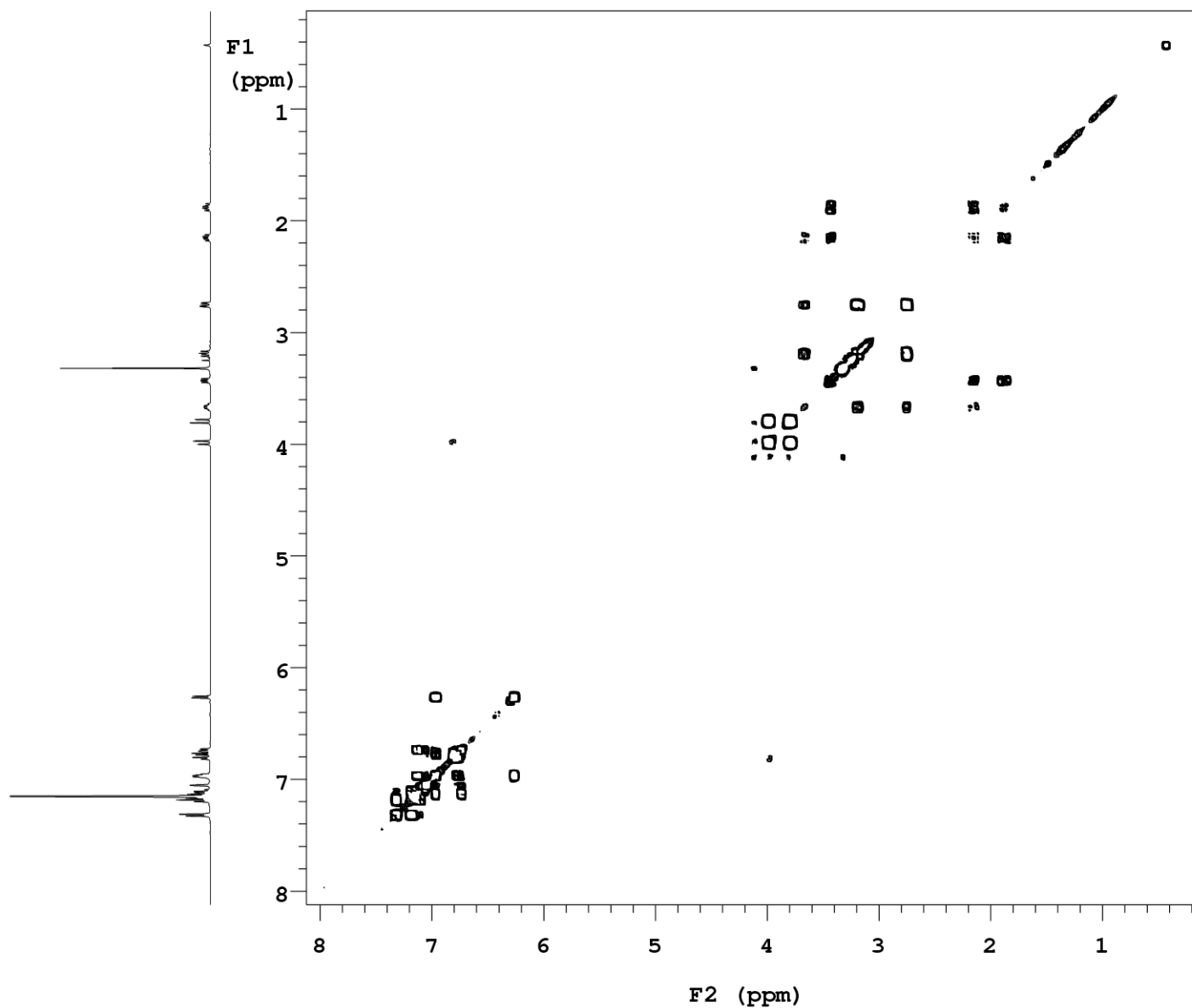
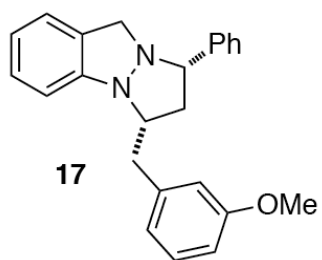
Sq. sine bell 0.064 sec

F1 DATA PROCESSING

Sq. sine bell 0.032 sec

FT size 1024 x 1024

Total time 3 min 10 sec



gsl-VIII-164-2

Sample Name:

Data Collected on:

Te.Chem.LSA.UMich.edu-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-164-2benzenoesy

Pulse Sequence: NOESY

Solvent: c6d6

Data collected on: Apr 14 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4006.4 Hz

2D Width 4006.4 Hz

4 repetitions

2 x 128 increments

OBSERVE H1, 500.0931974 MHz

DATA PROCESSING

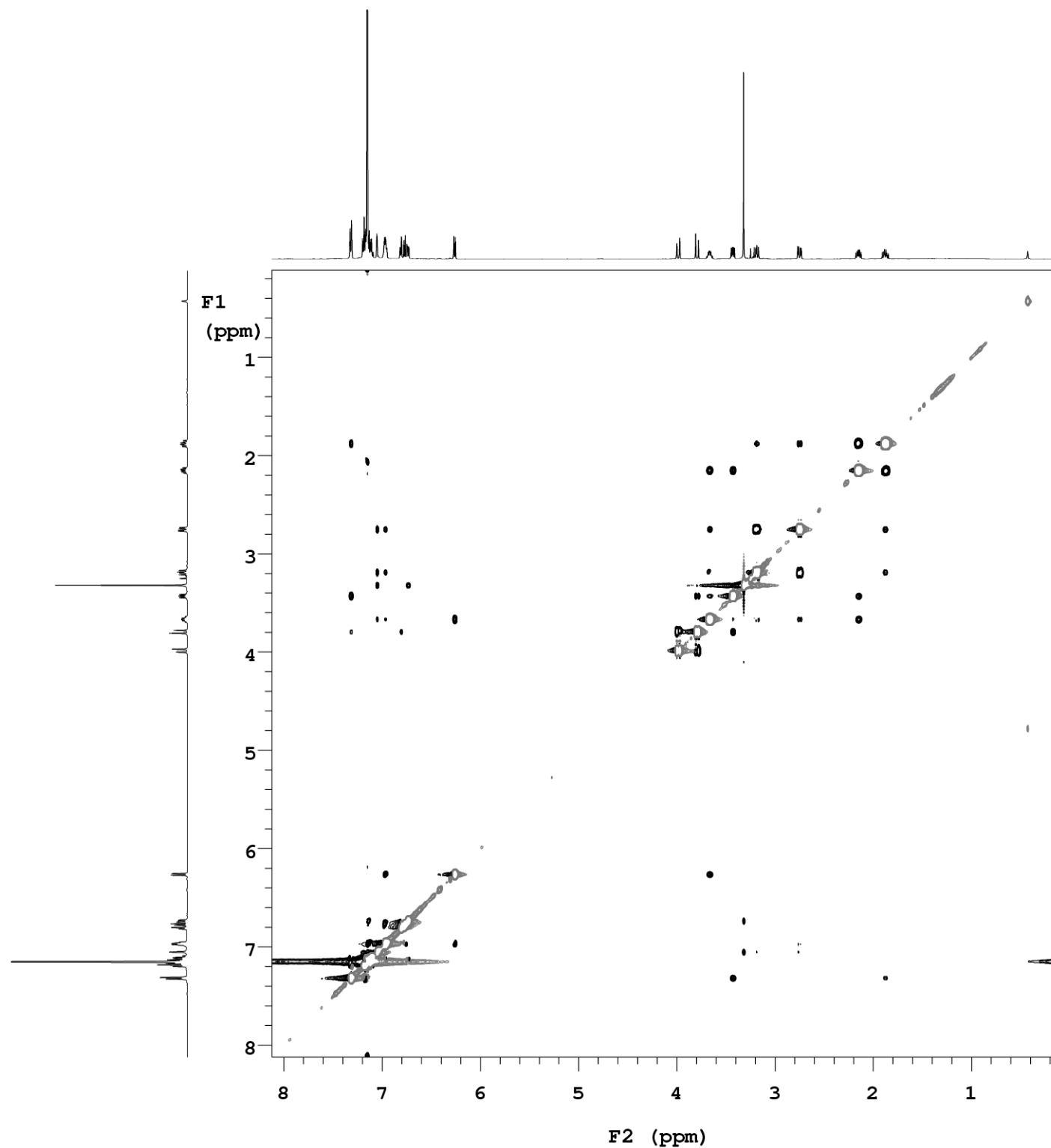
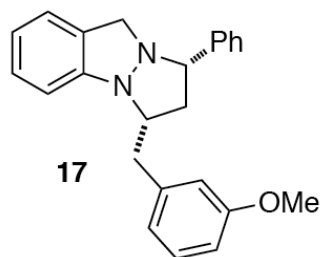
Gauss apodization 0.069 sec

F1 DATA PROCESSING

Gauss apodization 0.029 sec

FT size 2048 x 2048

Total time 1 hr, 8 min



gs1-IV-25-2

Sample Name:

Data Collected on:

Sn-inova500

Archive directory:

Sample directory:

FidFile: gs1-IV-25-2

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 27 2009

Operator: geolemen

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 7998.4 Hz

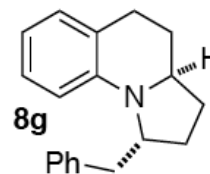
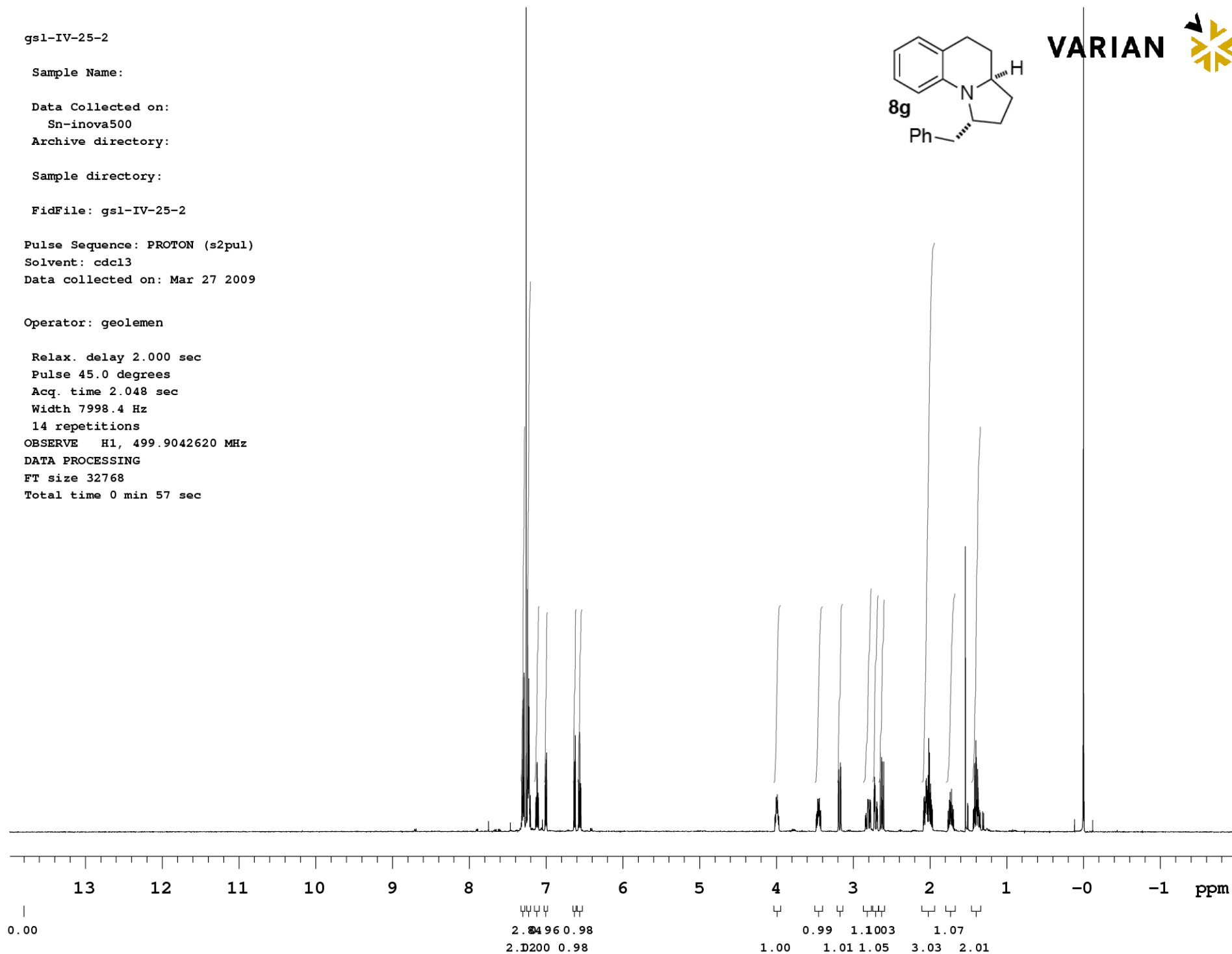
14 repetitions

OBSERVE H1, 499.9042620 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 57 sec


VARIAN 


gs1-III-141-2carbon

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.Edu-vnmrs400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)

Solvent: cdc13

Data collected on: Dec 19 2008

Operator: geolemen

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

128 repetitions

OBSERVE C13, 100.7132896 MHz

DECOUPLE H1, 400.5317616 MHz

Power 40 dB

continuously on

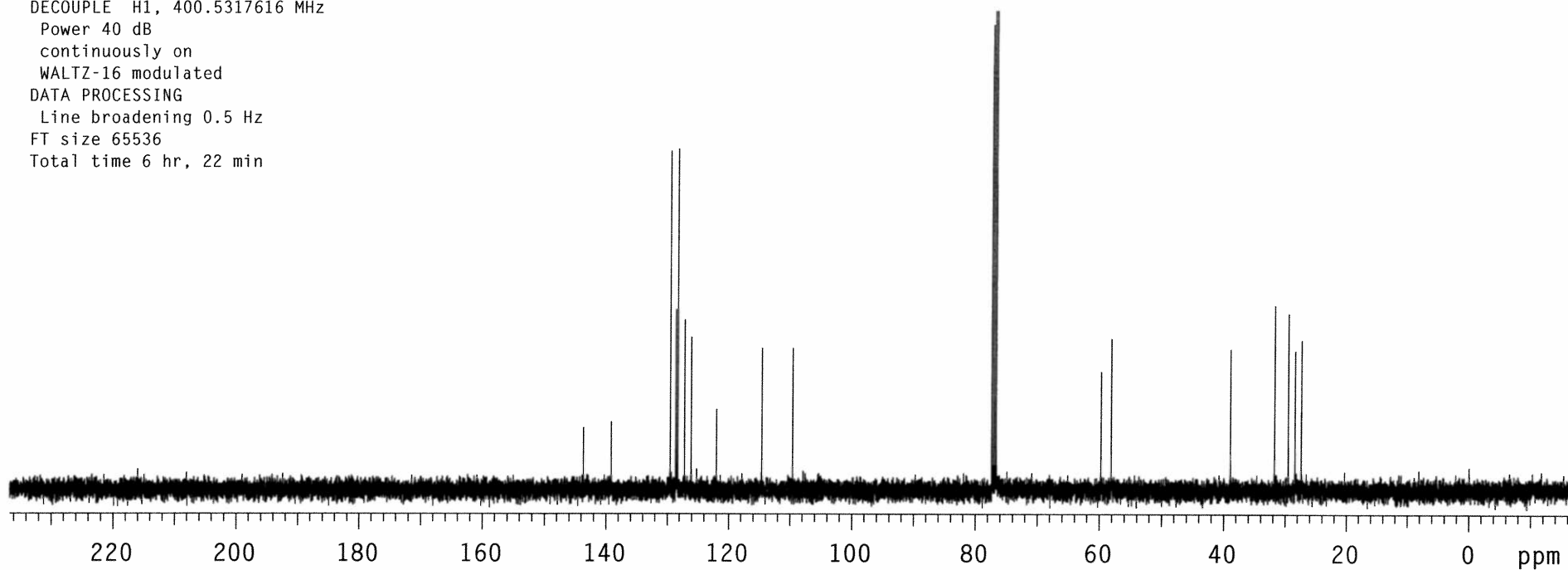
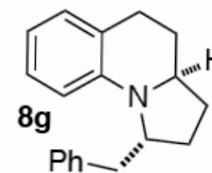
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 6 hr, 22 min

VARIAN 

gsl-III-141-2cosy

File: Gcosy

Pulse Sequence: gCOSY

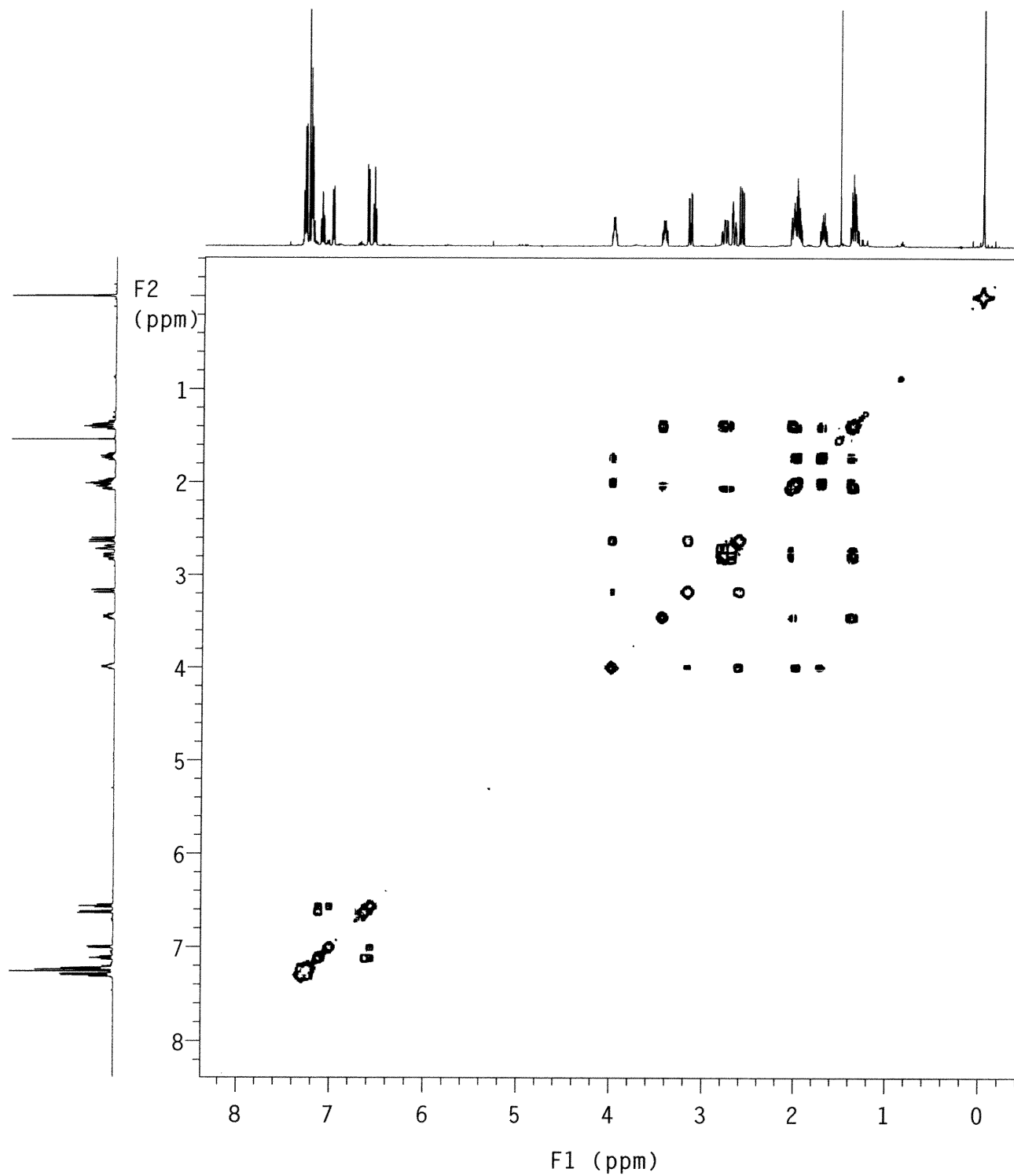
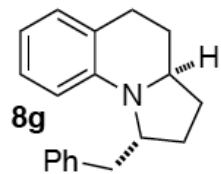
Solvent: cdc13

Ambient temperature

Operator: geolemen

INOVA-500 "Sn.Chem.LSA.UMich.Edu"

Relax. delay 1.301 sec
Acq. time 0.128 sec
Width 4399.2 Hz
2D Width 4399.2 Hz
Single scan
128 increments
OBSERVE H1, 499.9042616 MHz
DATA PROCESSING
Sine bell 0.064 sec
F1 DATA PROCESSING
Sine bell 0.058 sec
FT size 2048 x 2048
Total time 3 min, 29 sec
Acquisition date: Dec 19 2008



gs1-IV-30-2

Sample Name:

Data Collected on:

Sn-inova500

Archive directory:

Sample directory:

FidFile: gs1-IV-30-2

Pulse Sequence: PROTON (s2pul)

Solvent: CDC13

Data collected on: Mar 28 2009

Operator: geolemen

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 7998.4 Hz

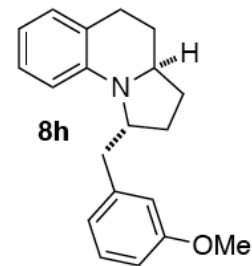
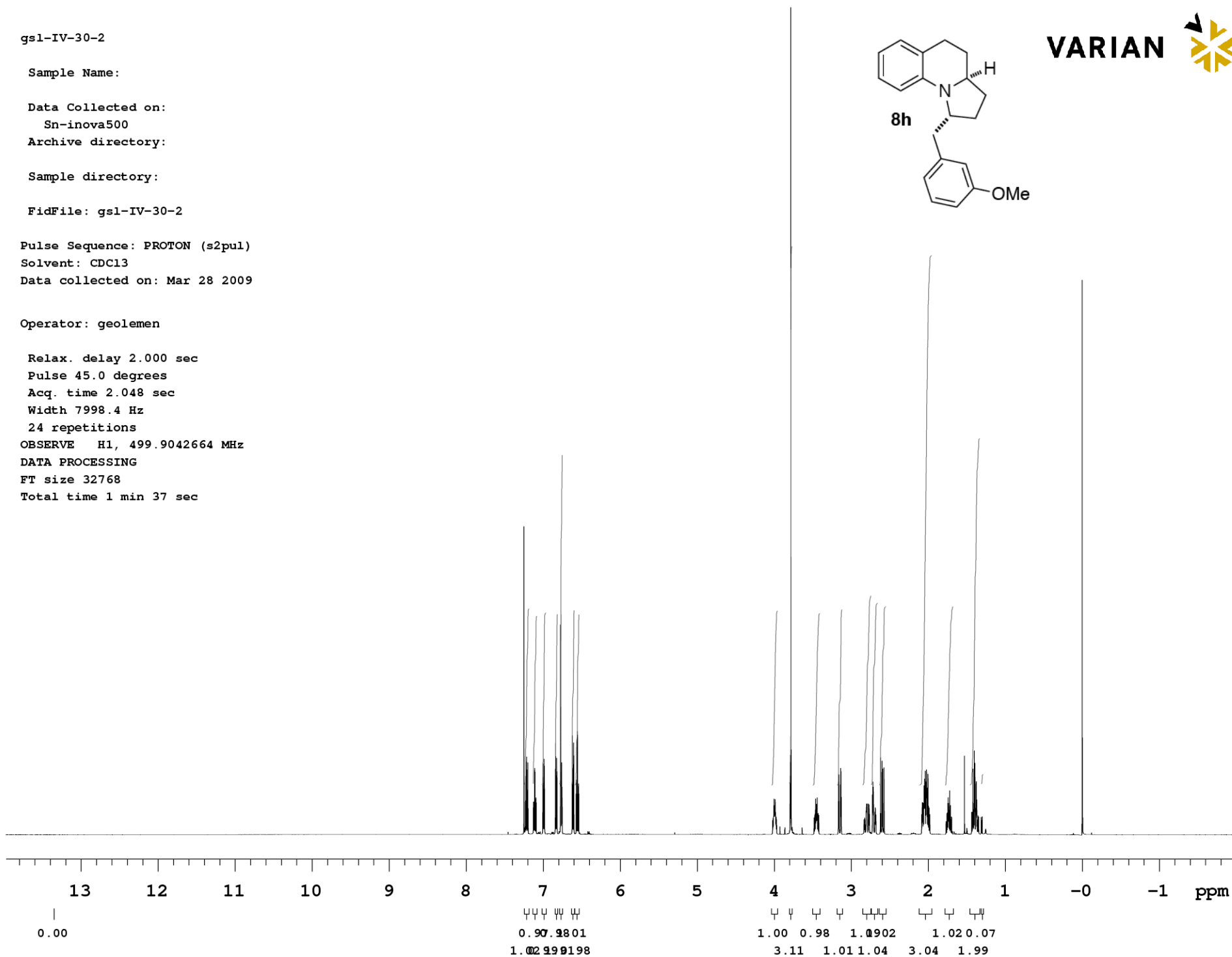
24 repetitions

OBSERVE H1, 499.9042664 MHz

DATA PROCESSING

FT size 32768

Total time 1 min 37 sec


VARIAN 


gs1-IV-30-2 carbon

Sample Name:

Data Collected on:

Ga.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-IV-30-2carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Mar 28 2009

Operator: geolemen

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

640 repetitions

OBSERVE C13, 100.4641417 MHz

DECOUPLE H1, 399.5409236 MHz

Power 33 dB

continuously on

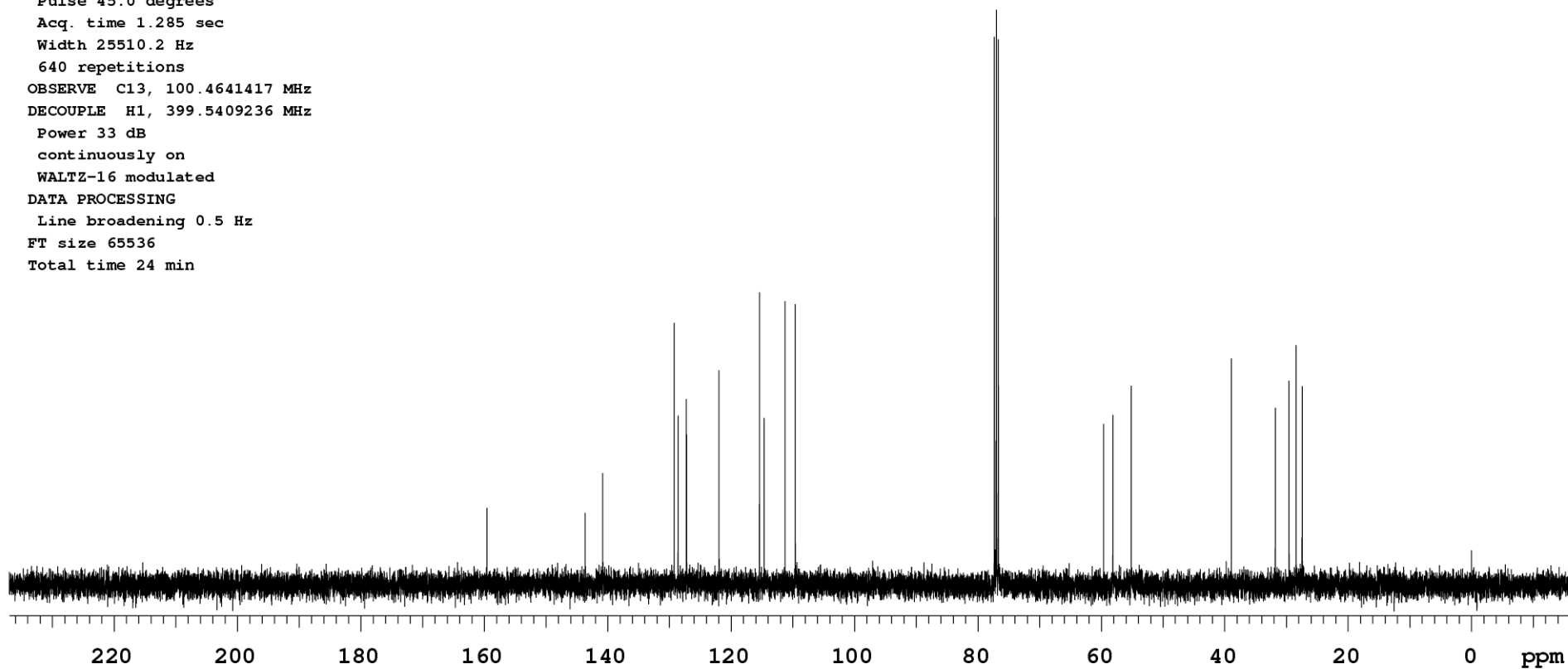
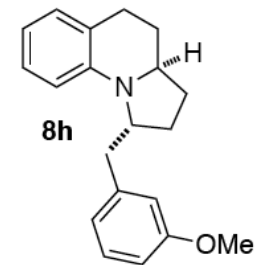
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 24 min

VARIAN 

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:

Sn-inova500

Archive directory:

Sample directory:

FidFile: gsl-IV-30-2cosy

Pulse Sequence: gCOSY

Solvent: CDCl3

Data collected on: Mar 28 2009

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 7998.4 Hz

2D Width 7998.4 Hz

2 repetitions

200 increments

OBSERVE H1, 499.9042771 MHz

DATA PROCESSING

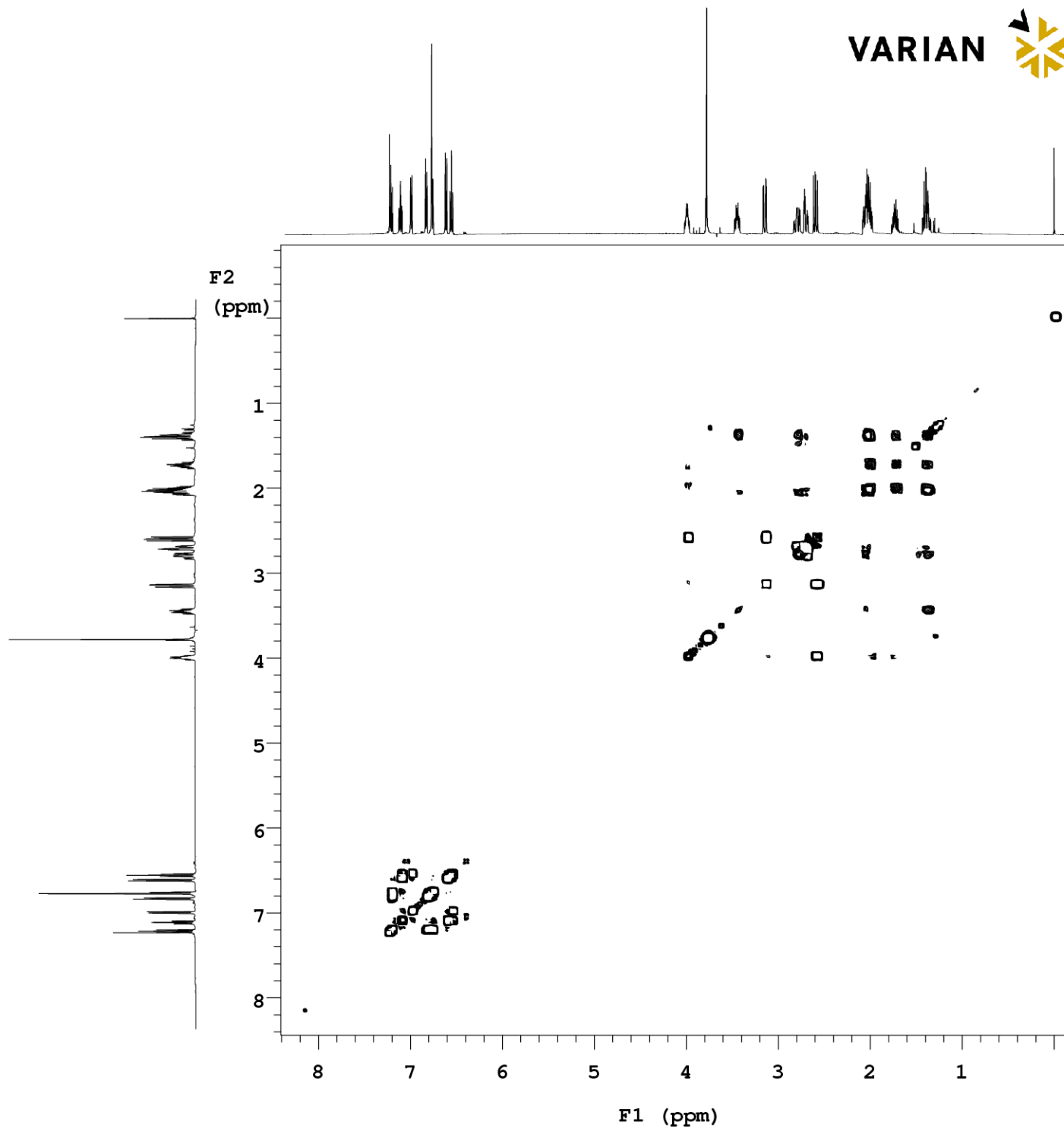
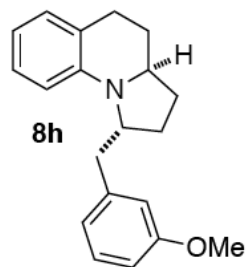
Sq. sine bell 0.064 sec

F1 DATA PROCESSING

Sq. sine bell 0.025 sec

FT size 2048 x 2048

Total time 8 min 38 sec



Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gsl-IV-30-2noesy

Pulse Sequence: NOESY

Solvent: CDCl3

Data collected on: Apr 4 2009

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 7998.4 Hz

2D Width 7998.4 Hz

4 repetitions

2 x 256 increments

OBSERVE H1, 499.9042663 MHz

DATA PROCESSING

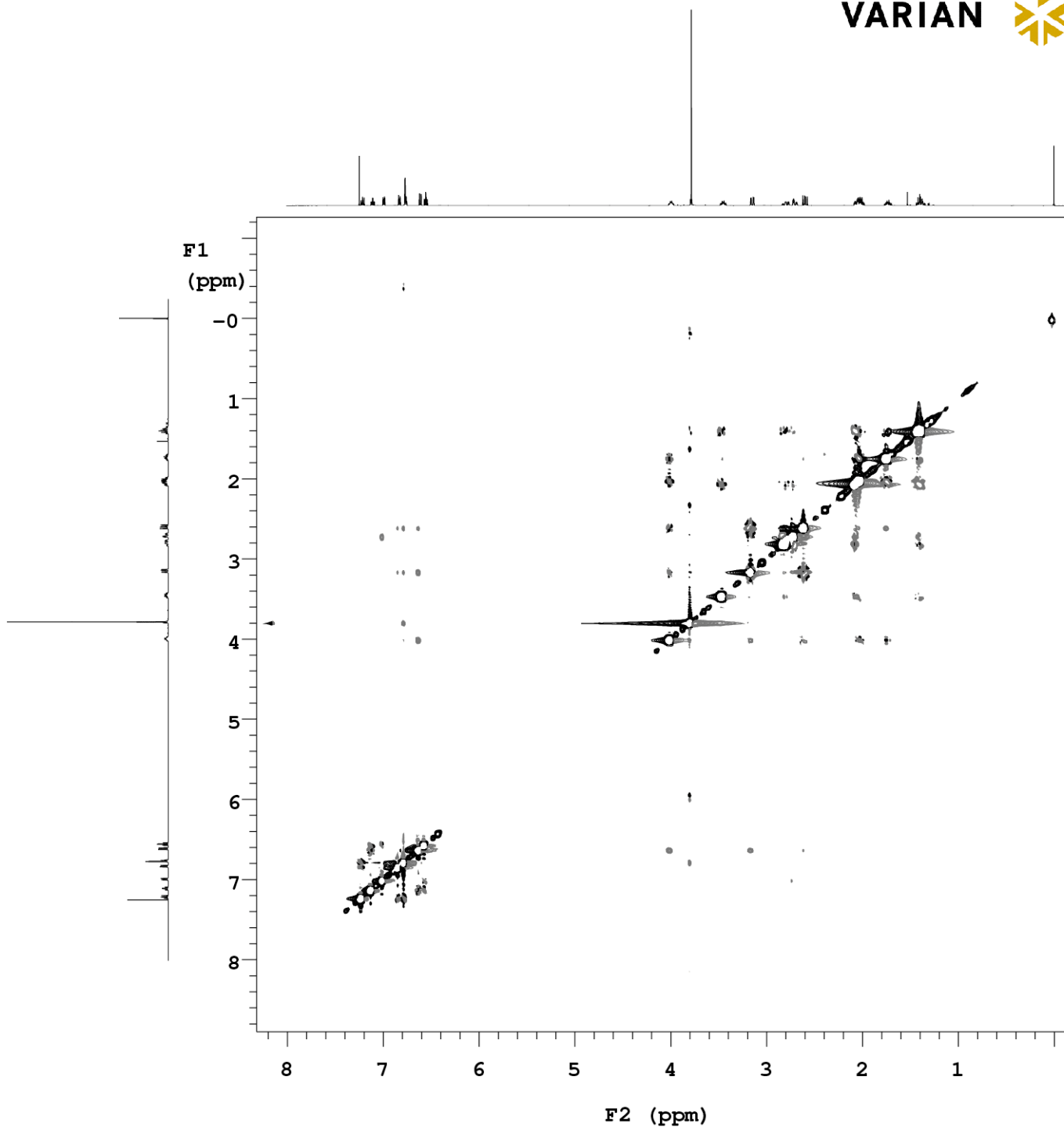
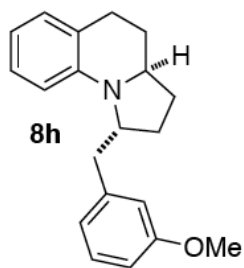
Gauss apodization 0.059 sec

F1 DATA PROCESSING

Gauss apodization 0.030 sec

FT size 2048 x 2048

Total time 1 hr, 36 min



S119

gs1-IV-30-2 hsgc

VARIAN 

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gHSQC

Pulse Sequence: gHSQC

Solvent: cdc13

Data collected on: Apr 4 2009

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 7998.4 Hz

2D Width 21367.5 Hz

4 repetitions

2 x 128 increments

OBSERVE H1, 499.9042771 MHz

DECOUPLE C13, 125.7104522 MHz

Power 40 dB

on during acquisition

off during delay

W40_id modulated

DATA PROCESSING

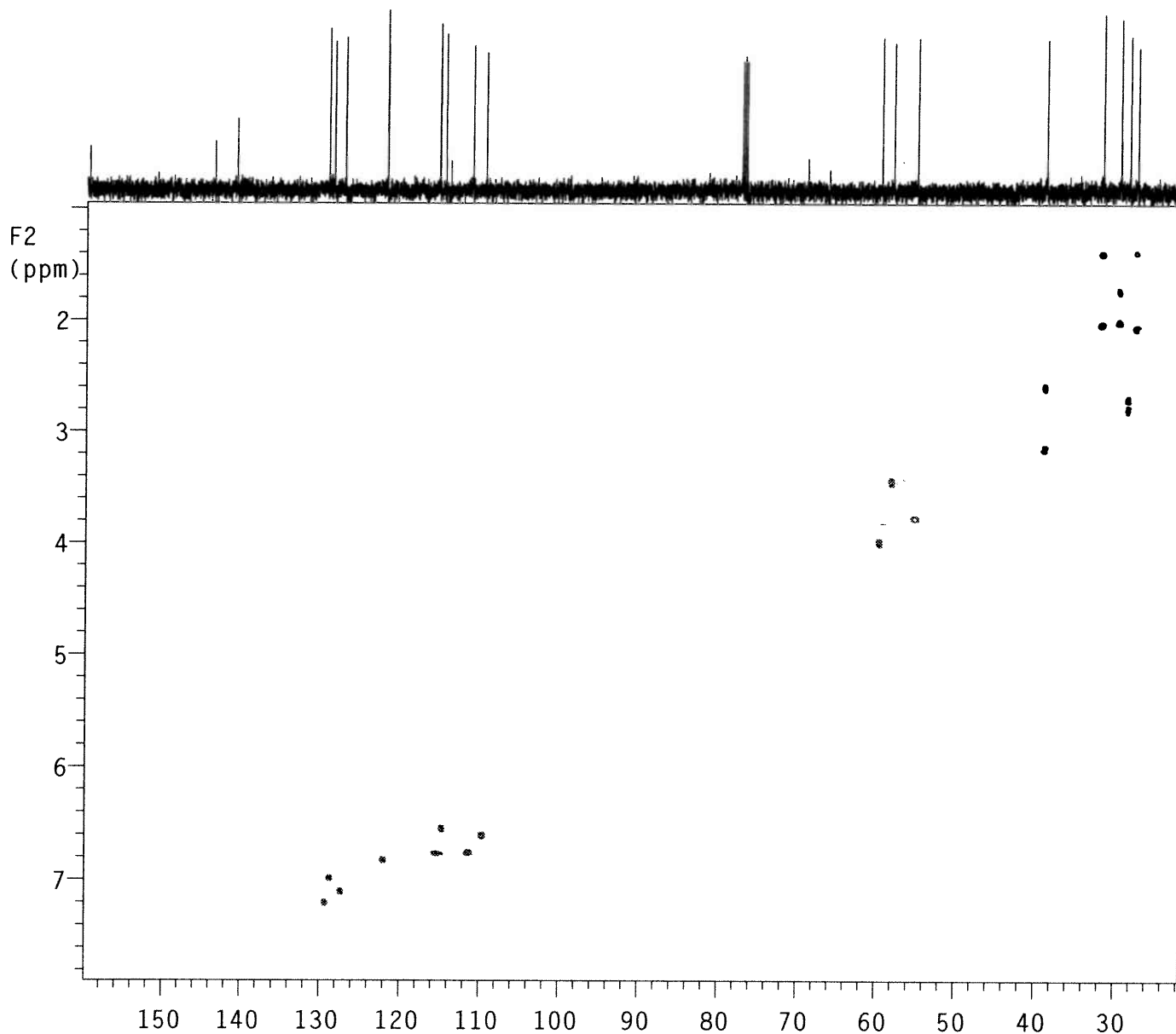
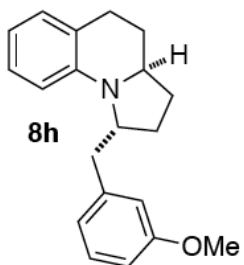
Gauss apodization 0.059 sec

F1 DATA PROCESSING

Gauss apodization 0.011 sec

FT size 2048 x 2048

Total time 21 min



gs1-IV-30-2hmbc

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gHMBC

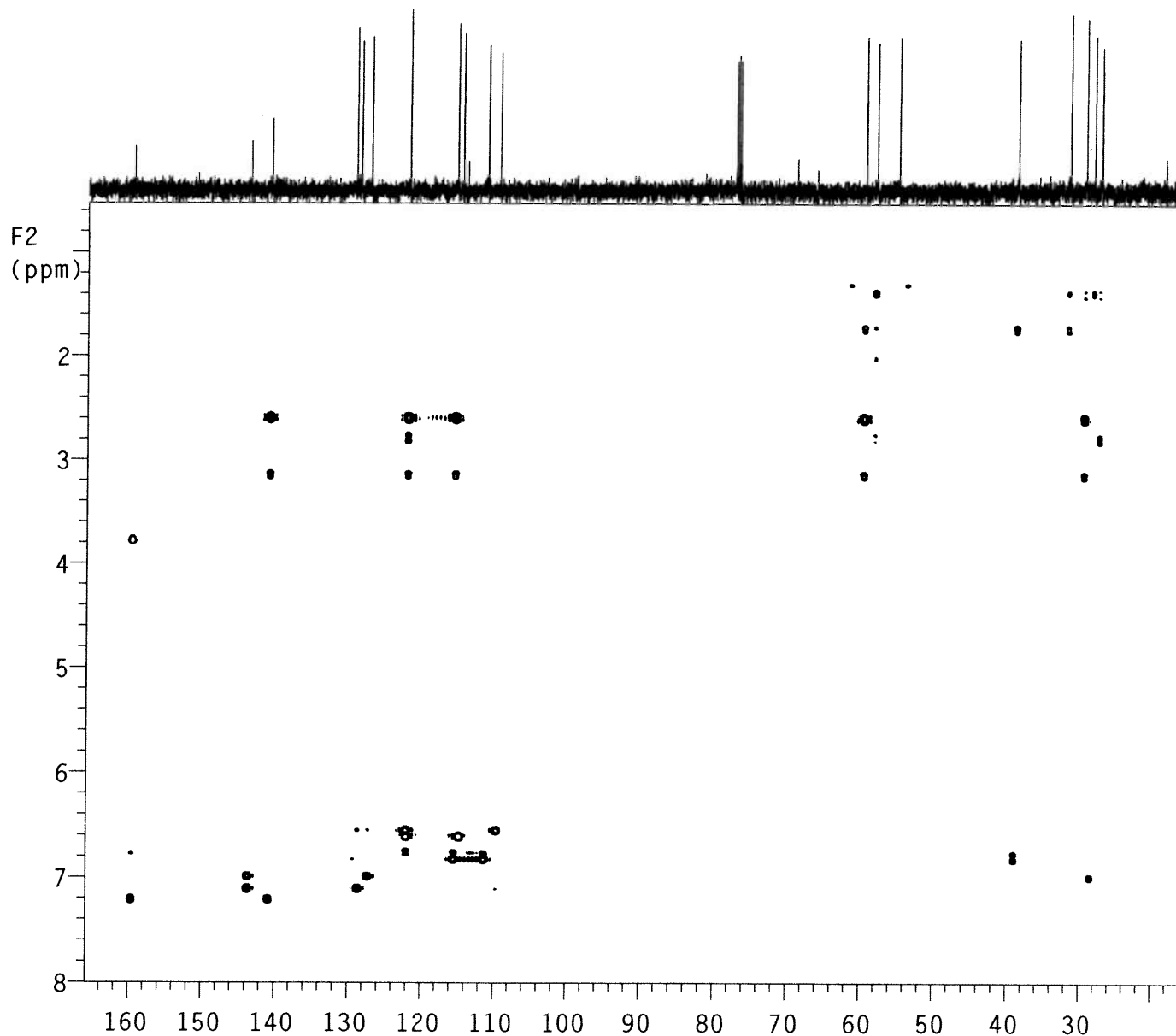
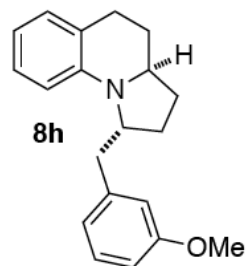
Pulse Sequence: gHMBC

Solvent: cdc13

Data collected on: Apr 4 2009

Operator: geolemen

Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 7998.4 Hz
2D Width 30165.9 Hz
4 repetitions
2 x 200 increments
OBSERVE H1, 499.9042771 MHz
DATA PROCESSING
Sq. sine bell 0.064 sec
F1 DATA PROCESSING
Gauss apodization 0.012 sec
FT size 2048 x 4096
Total time 33 min



gs1-VII-151-3

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-151-3

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Oct 30 2010

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 10.224 sec

Width 6410.3 Hz

4 repetitions

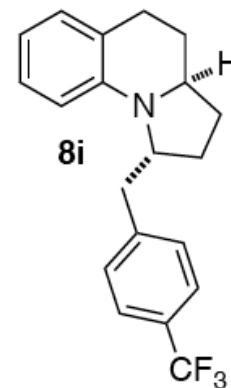
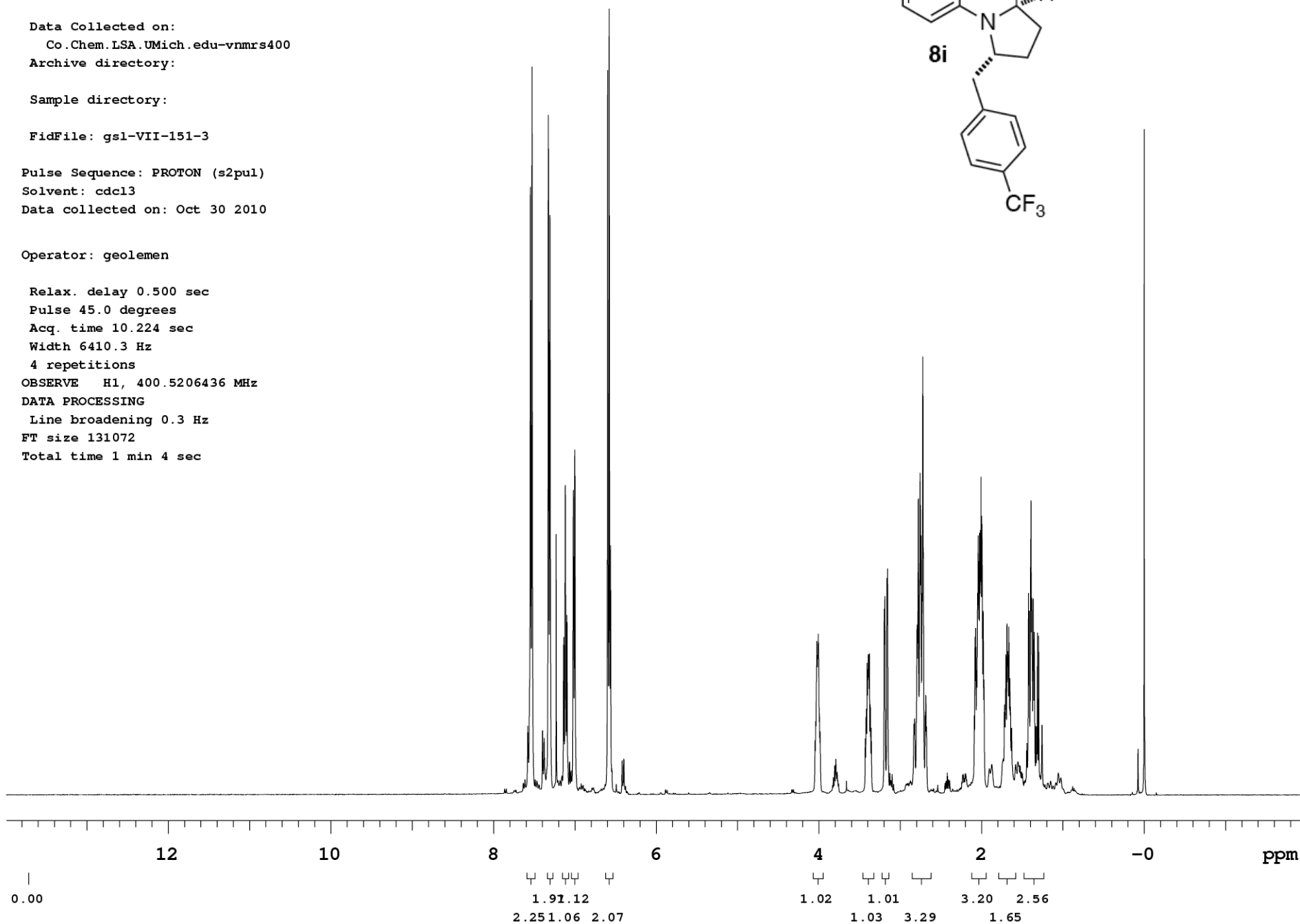
OBSERVE H1, 400.5206436 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 131072

Total time 1 min 4 sec


VARIAN 


gs1-VII-151-3 carbon

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-151-3carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Oct 30 2010

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 2.569 sec

Width 25510.2 Hz

1256 repetitions

OBSERVE C13, 100.7109959 MHz

DECOUPLE H1, 400.5226414 MHz

Power 41 dB

continuously on

WALTZ-16 modulated

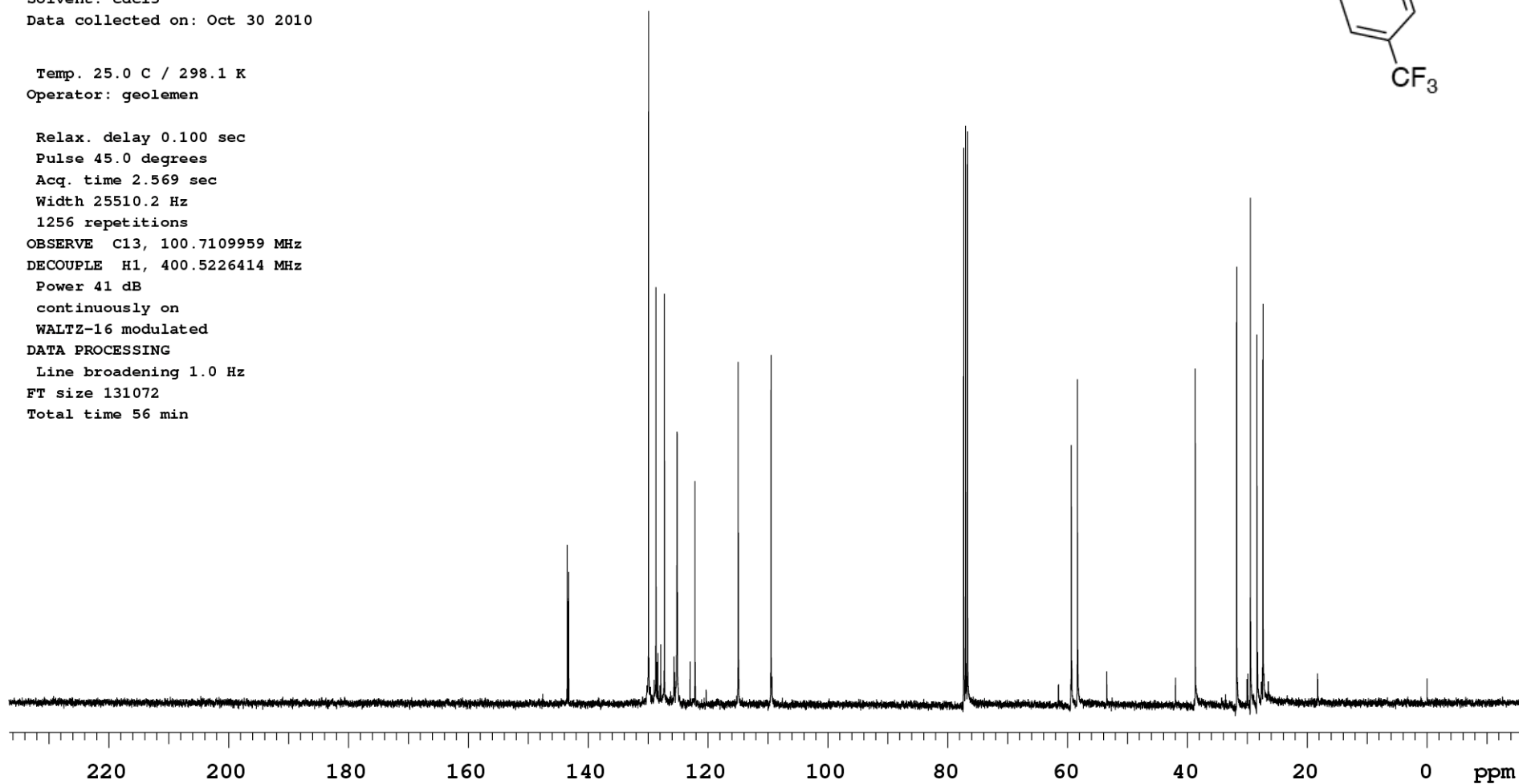
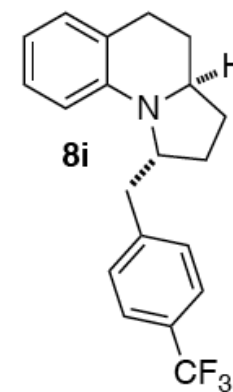
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 56 min

VARIAN



gs1-VII-151-3

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-151-3cosy

Pulse Sequence: gCOSY

Solvent: cdcl3

Data collected on: Oct 30 2010

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 6410.3 Hz

2D Width 6410.3 Hz

Single scan

128 increments

OBSERVE H1, 400.5206436 MHz

DATA PROCESSING

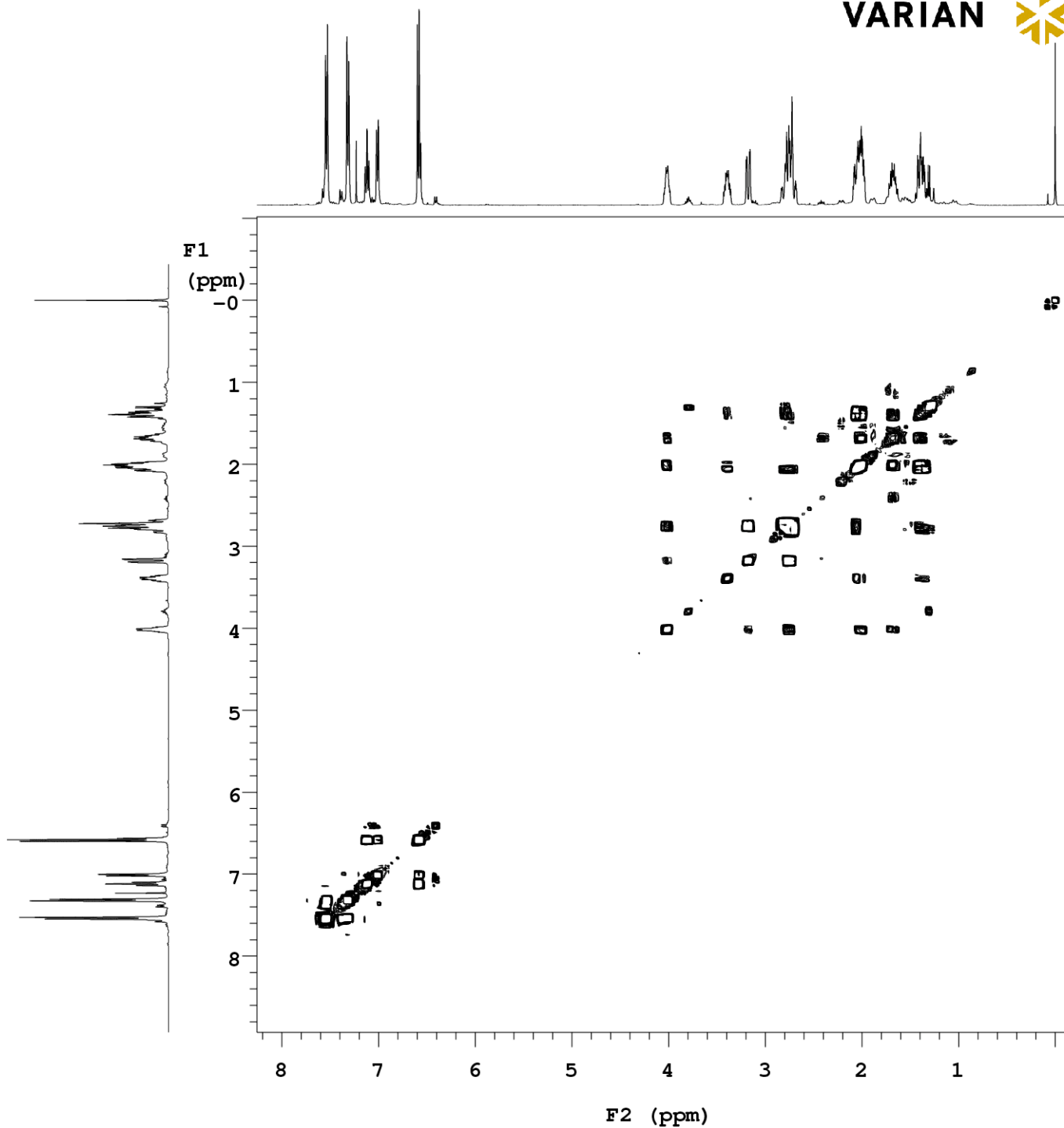
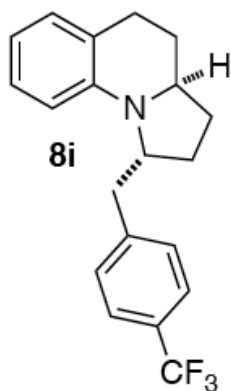
Sq. sine bell 0.075 sec

F1 DATA PROCESSING

Sq. sine bell 0.020 sec

FT size 2048 x 2048

Total time 3 min 11 sec



STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gsl-VII-151-3fluorine

Pulse Sequence: FLUORINE (s2pul)

Solvent: cdcl3

Data collected on: Oct 30 2010

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 1.000 sec

Pulse 30.0 degrees

Acq. time 0.734 sec

Width 89285.7 Hz

16 repetitions

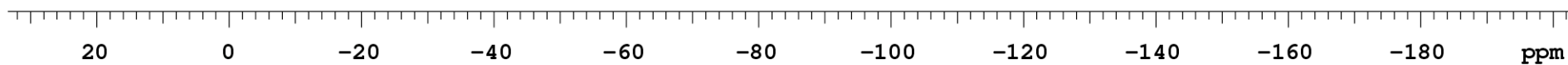
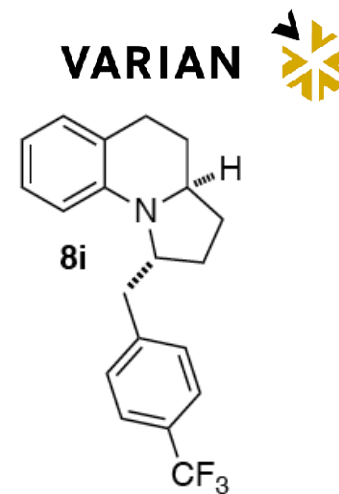
OBSERVE F19, 376.8659384 MHz

DATA PROCESSING

Line broadening 1.5 Hz

FT size 131072

Total time 0 min 31 sec



gs1-VII-144-2

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-144-2

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Oct 23 2010

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 10.224 sec

Width 6410.3 Hz

2 repetitions

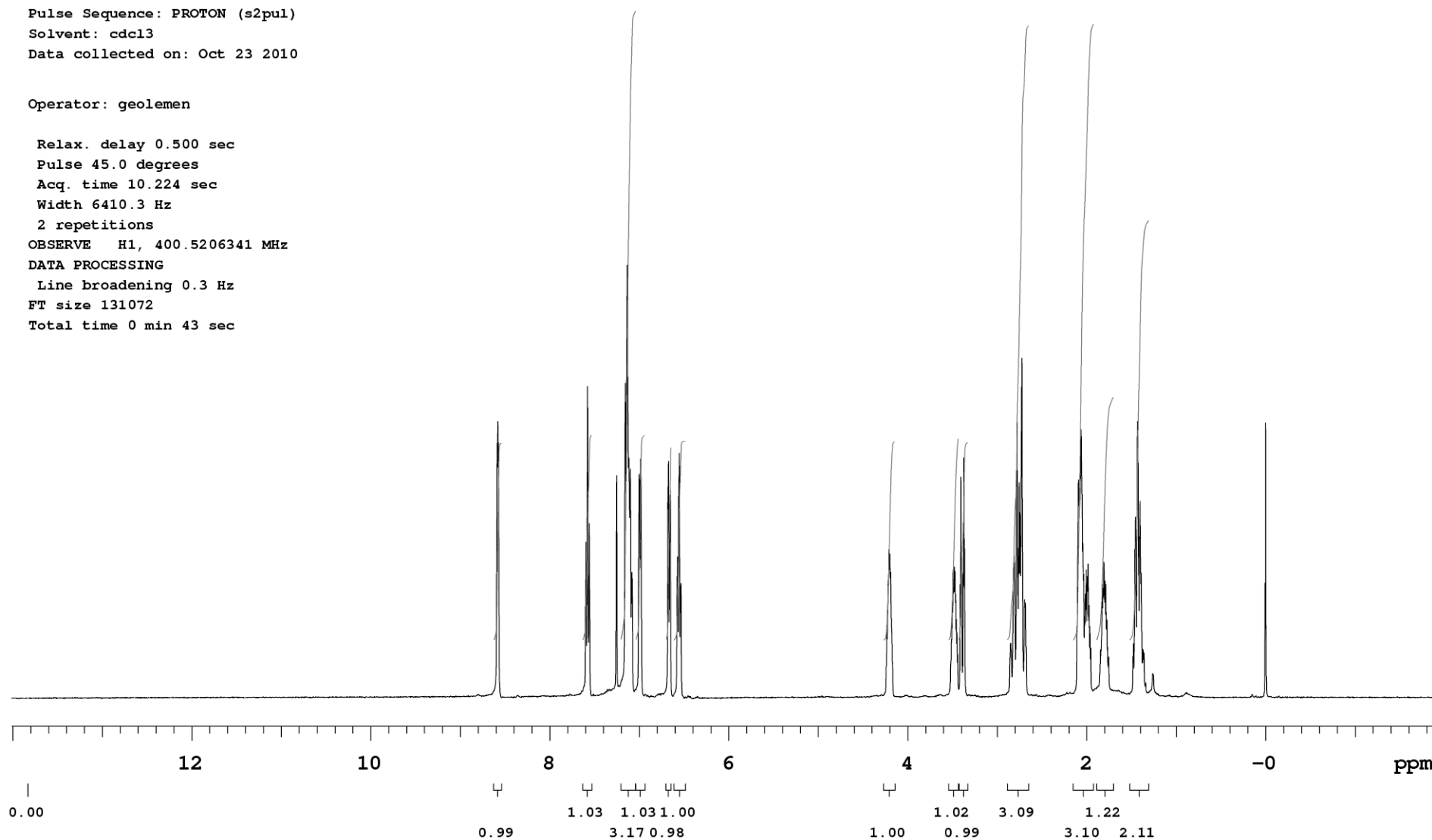
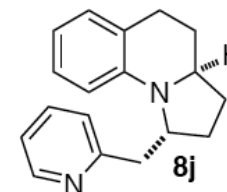
OBSERVE H1, 400.5206341 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 131072

Total time 0 min 43 sec

VARIAN 

gs1-VII-144-2 carbon

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-144-2carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Oct 23 2010

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 2.569 sec

Width 25510.2 Hz

272 repetitions

OBSERVE C13, 100.7109951 MHz

DECOUPLE H1, 400.5226414 MHz

Power 41 dB

continuously on

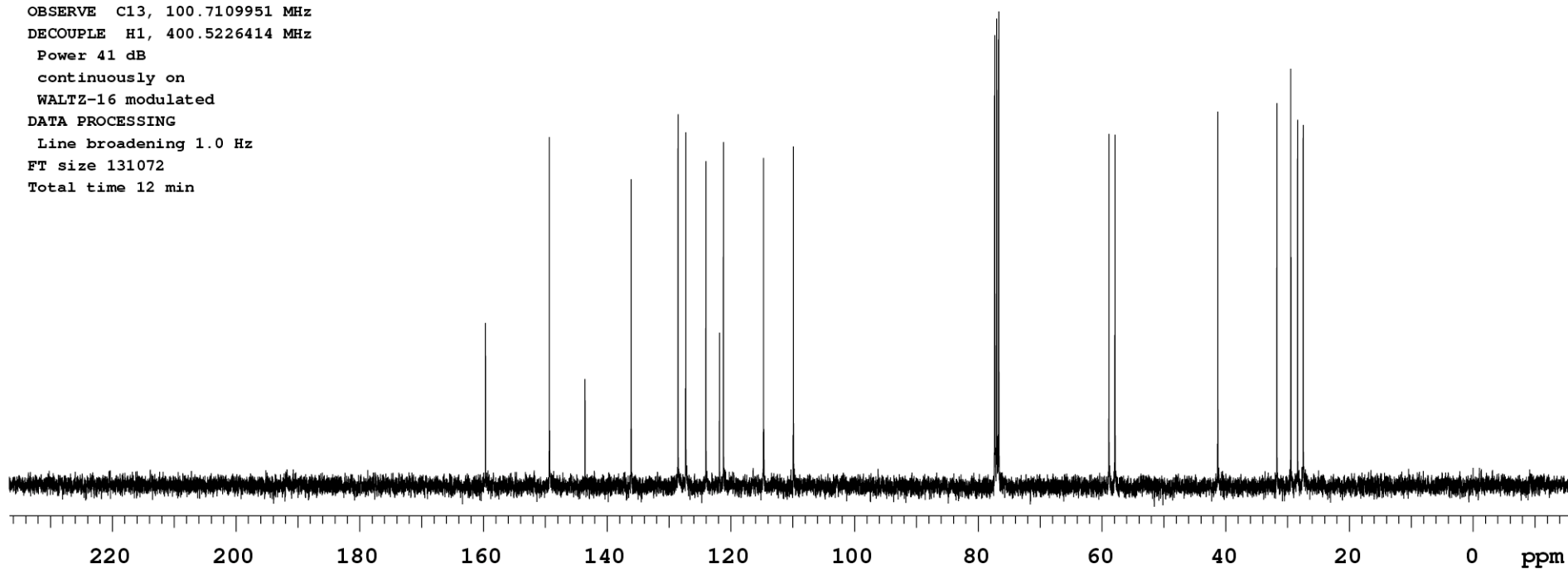
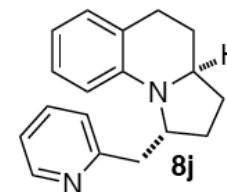
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 12 min

VARIAN 

gs1-VII-144-2 cosy

Sample Name:

Data Collected on:

Co.Chem.LSA.UMich.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: gs1-VII-144-2cosy

Pulse Sequence: gCOSY

Solvent: cdcl3

Data collected on: Oct 23 2010

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4111.8 Hz

2D Width 4111.8 Hz

Single scan

128 increments

OBSERVE H1, 400.5206341 MHz

DATA PROCESSING

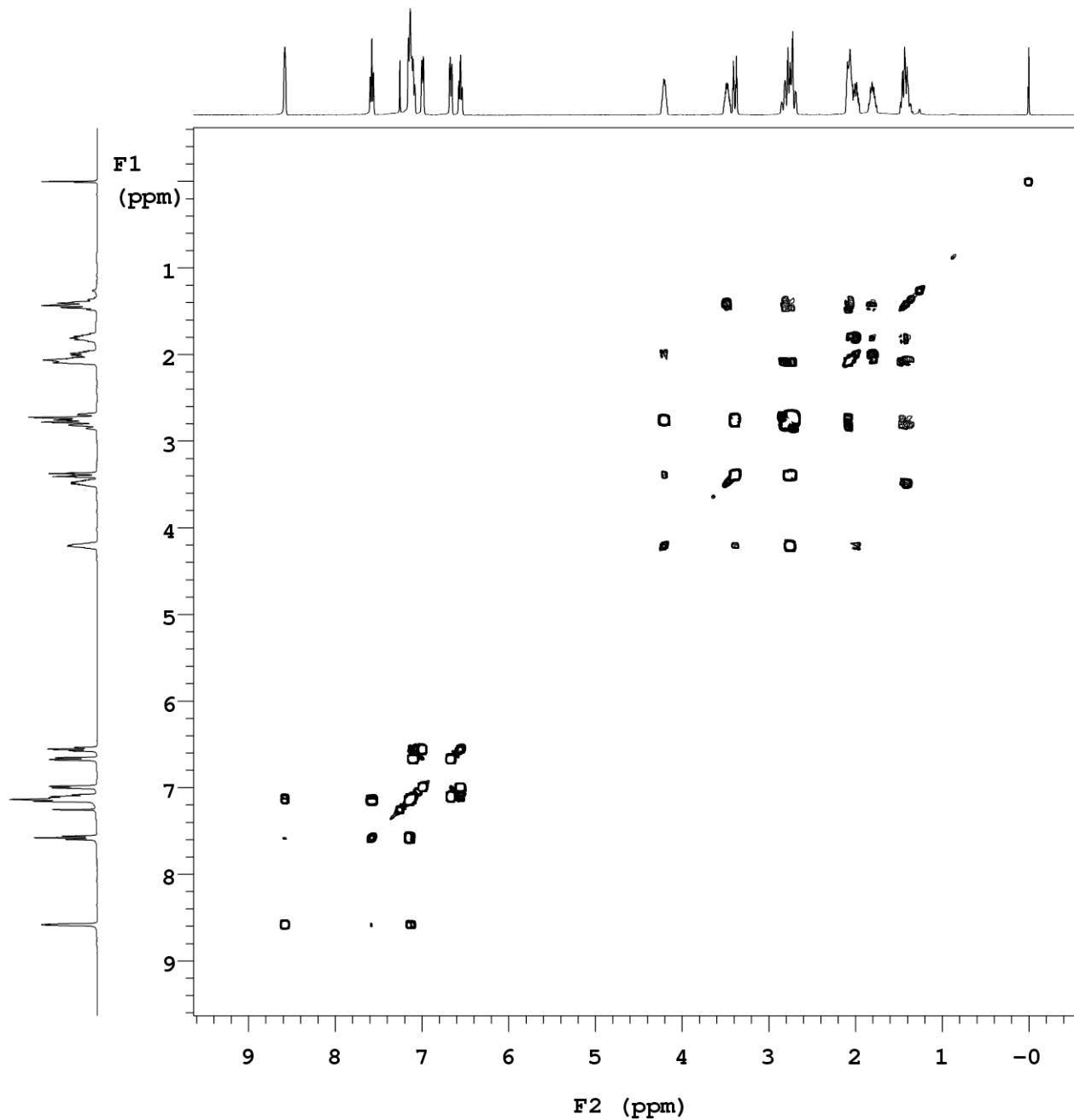
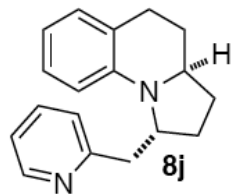
Sq. sine bell 0.062 sec

F1 DATA PROCESSING

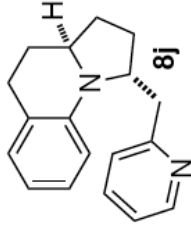
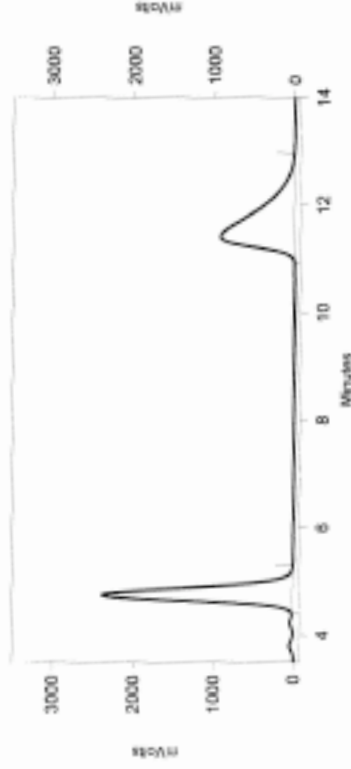
Sq. sine bell 0.031 sec

FT size 1024 x 1024

Total time 3 min 12 sec



C:\CLASS-VP\Enterprise\Projects\Default\Data\Lemen\HPLC.10015 11-20-2010
11-13-58 AM.dat

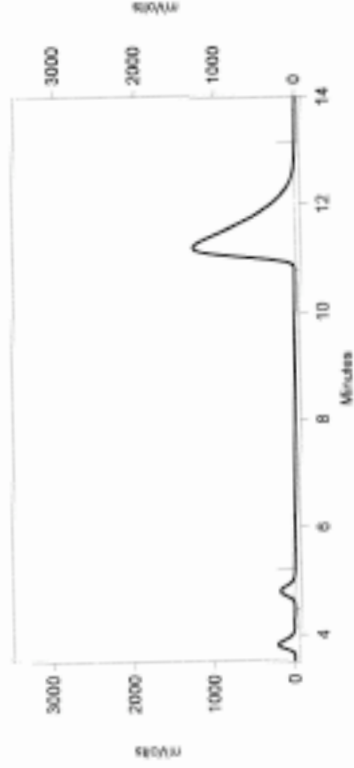


SPD-10Avp Ch2-254nm

Results

Retention Time	Area	Area Percent
4.750	40328719	49.119
11.417	41775901	50.881
Totals		82104620
		100.000

C:\CLASS-VP\Enterprise\Projects\Default\Data\Lemen\gsl-VII-189-2morediluteCHI
RAL_00-H_0.5%IPA_2-0min.dat



SPD-10Avp Ch2-254nm

Results

Retention Time	Area	Area Percent
4.808	2429469	4.182
11.200	55659077	95.818
Totals		58088546
		100.000

gsl-VIII-93-2

Sample Name:

Data Collected on:

Sn.Chem.LSA.UMich.edu-inova500

Archive directory:

Sample directory:

FidFile: gsl-VIII-93-2

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jan 20 2011

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.500 sec

Width 7998.4 Hz

20 repetitions

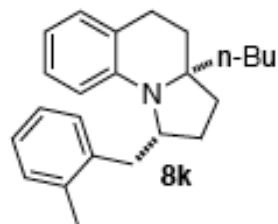
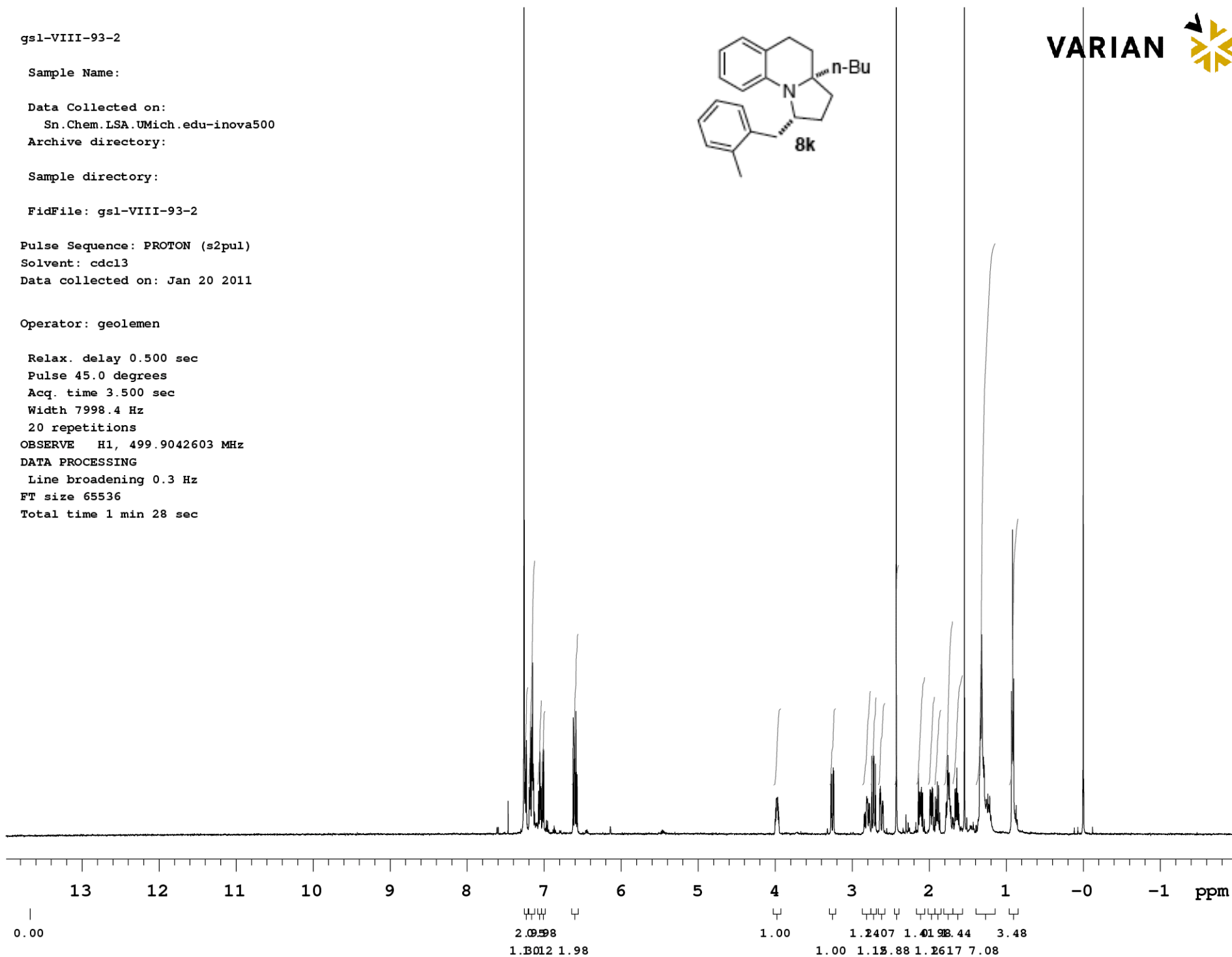
OBSERVE H1, 499.9042603 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min 28 sec


VARIAN 


gs1-VIII-93-2 carbon

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gs1-VIII-93-2carbon

Pulse Sequence: CARBON (s2pul)

Solvent: CDCl3

Data collected on: Jan 21 2011

Operator: geolemen

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 2.045 sec

Width 32051.3 Hz

128 repetitions

OBSERVE C13, 125.7485300 MHz

DECOUPLE H1, 500.0956704 MHz

Power 42 dB

continuously on

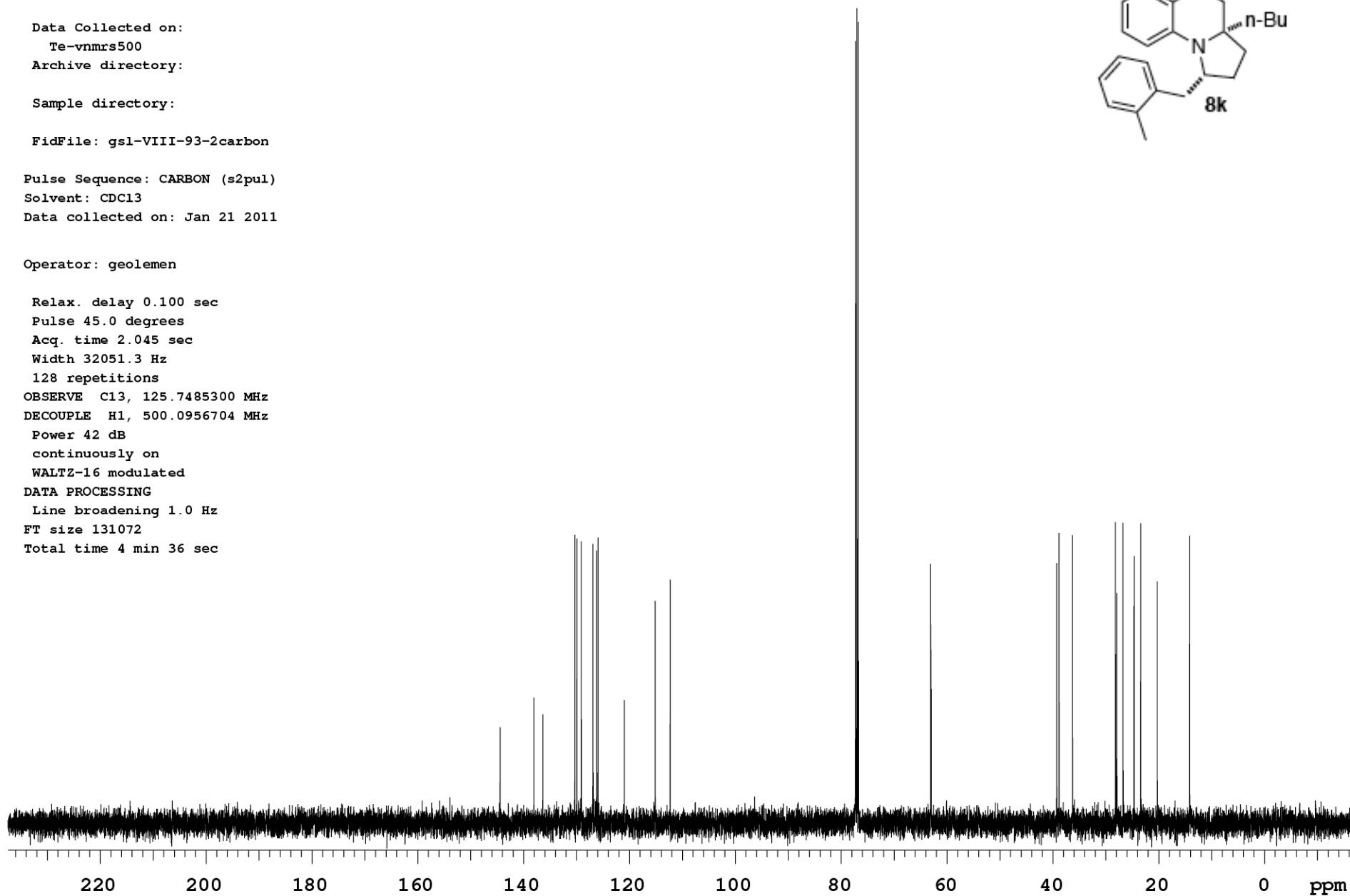
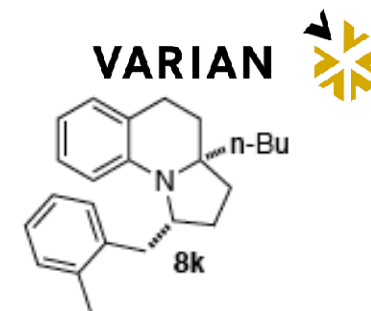
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 4 min 36 sec



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-93-2cosy

Pulse Sequence: gCOSY

Solvent: CDC13

Data collected on: Jan 21 2011

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4496.4 Hz

2D Width 4496.4 Hz

Single scan

128 increments

OBSERVE H1, 500.0931771 MHz

DATA PROCESSING

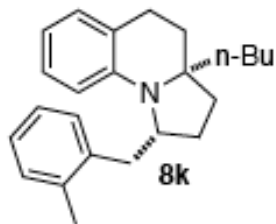
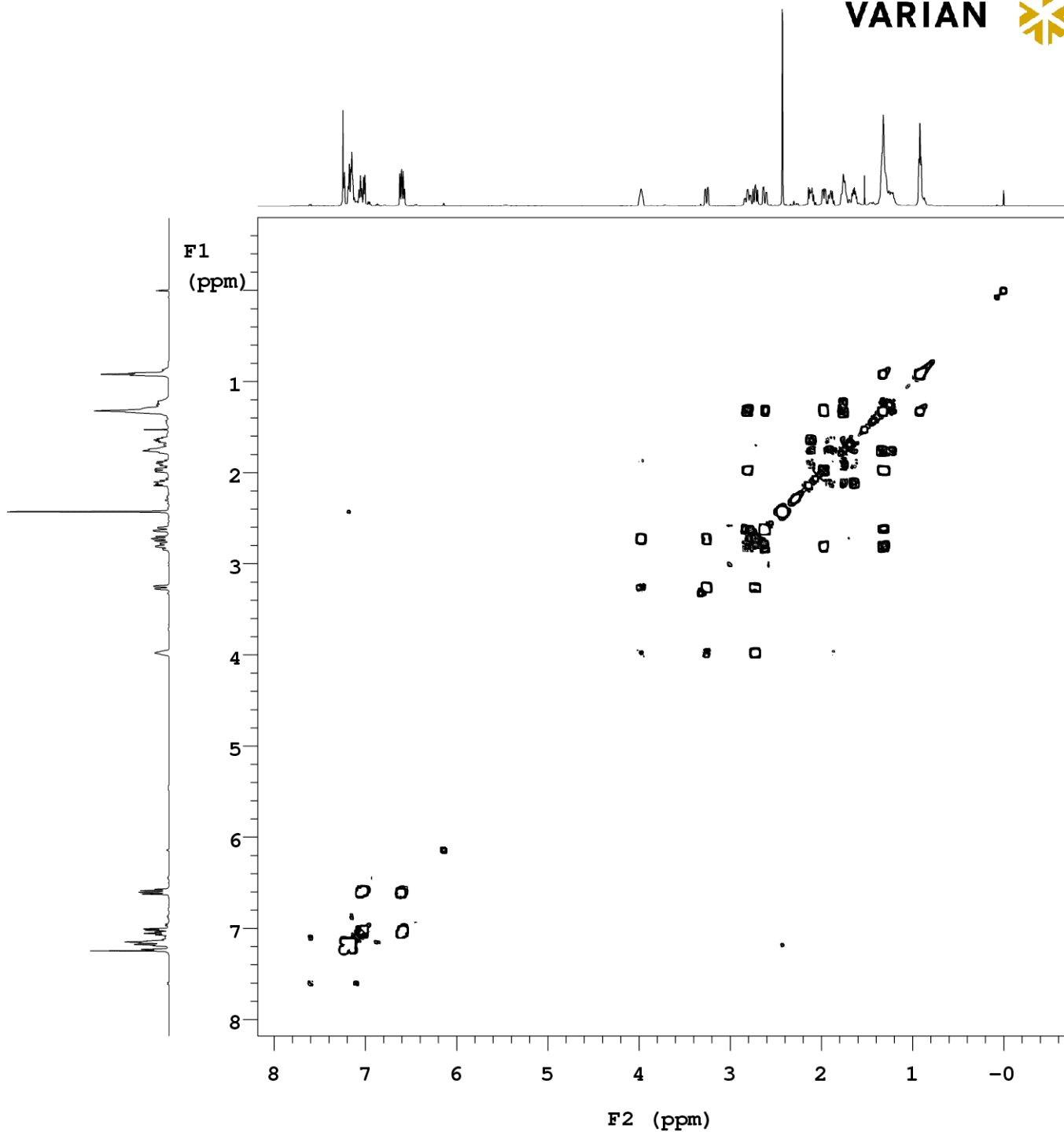
Sq. sine bell 0.057 sec

F1 DATA PROCESSING

Sq. sine bell 0.028 sec

FT size 1024 x 1024

Total time 3 min 12 sec

VARIAN 

gsl-VIII-93-2 hsqc

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-93-2hsqc

Pulse Sequence: gHSQC

Solvent: CDC13

Data collected on: Jan 21 2011

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4496.4 Hz

2D Width 21378.9 Hz

4 repetitions

2 x 128 increments

OBSERVE H1, 500.0931771 MHz

DECOUPLE C13, 125.7579587 MHz

Power 39 dB

on during acquisition

off during delay

W40_OneNMR_W010 modulated

DATA PROCESSING

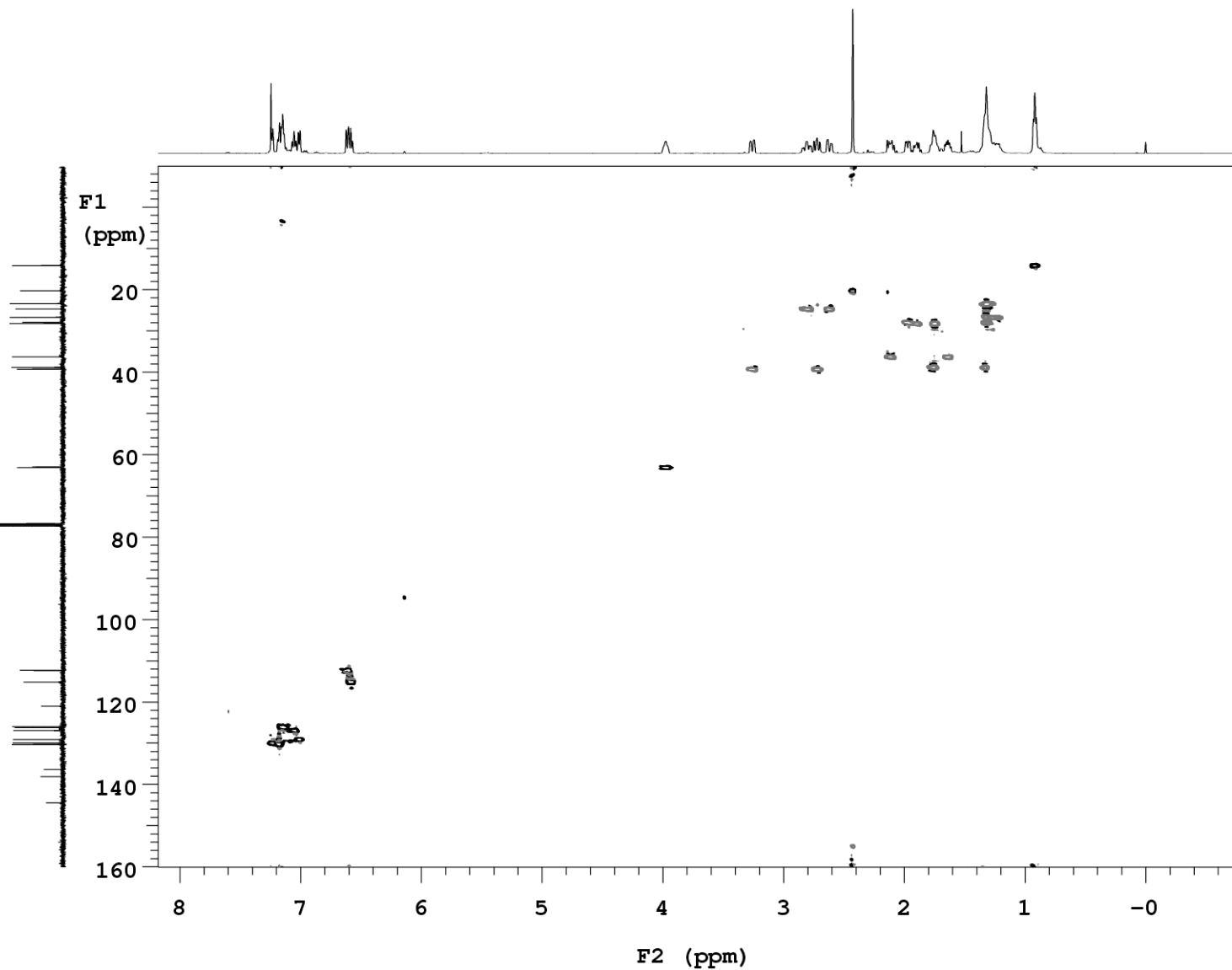
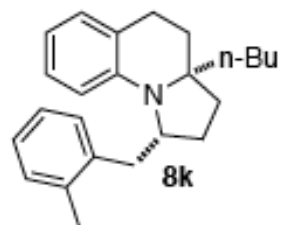
Gauss apodization 0.053 sec

F1 DATA PROCESSING

Gauss apodization 0.011 sec

FT size 1024 x 2048

Total time 41 min



gs1-VIII-93-2

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gs1-VIII-93-2noesy

Pulse Sequence: NOESY

Solvent: CDC13

Data collected on: Jan 21 2011

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4496.4 Hz

2D Width 4496.4 Hz

4 repetitions

2 x 200 increments

OBSERVE H1, 500.0931771 MHz

DATA PROCESSING

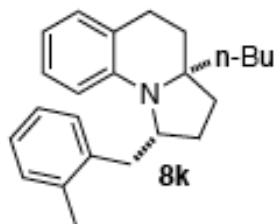
Gauss apodization 0.069 sec

F1 DATA PROCESSING

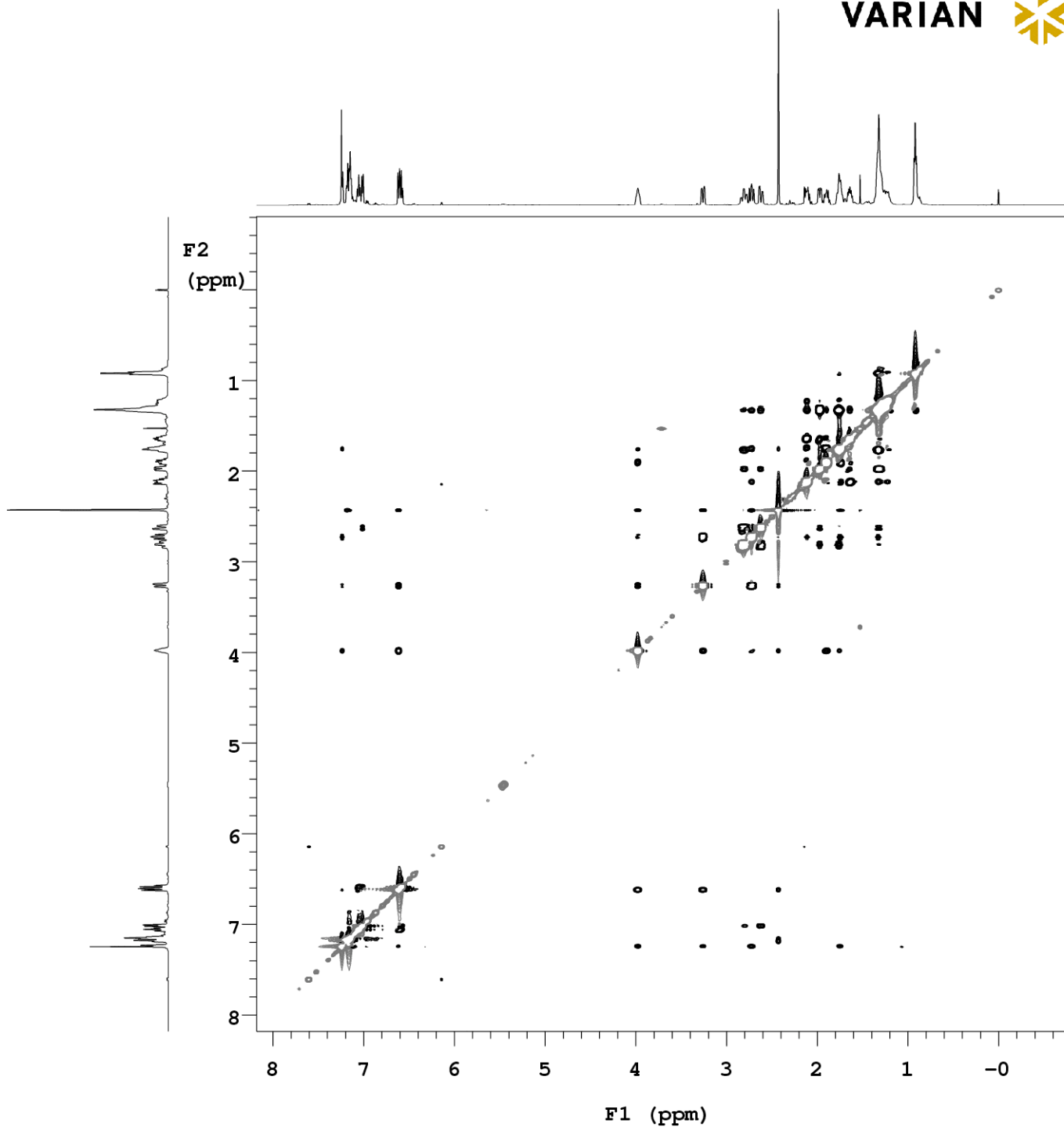
Gauss apodization 0.041 sec

FT size 2048 x 2048

Total time 1 hr, 48 min



VARIAN



gs1-VIII-92-2

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gs1-VIII-92-2

Pulse Sequence: PROTON (s2pul)

Solvent: CDC13

Data collected on: Jan 21 2011

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 5.453 sec

Width 6009.6 Hz

4 repetitions

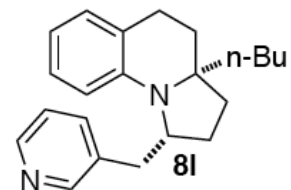
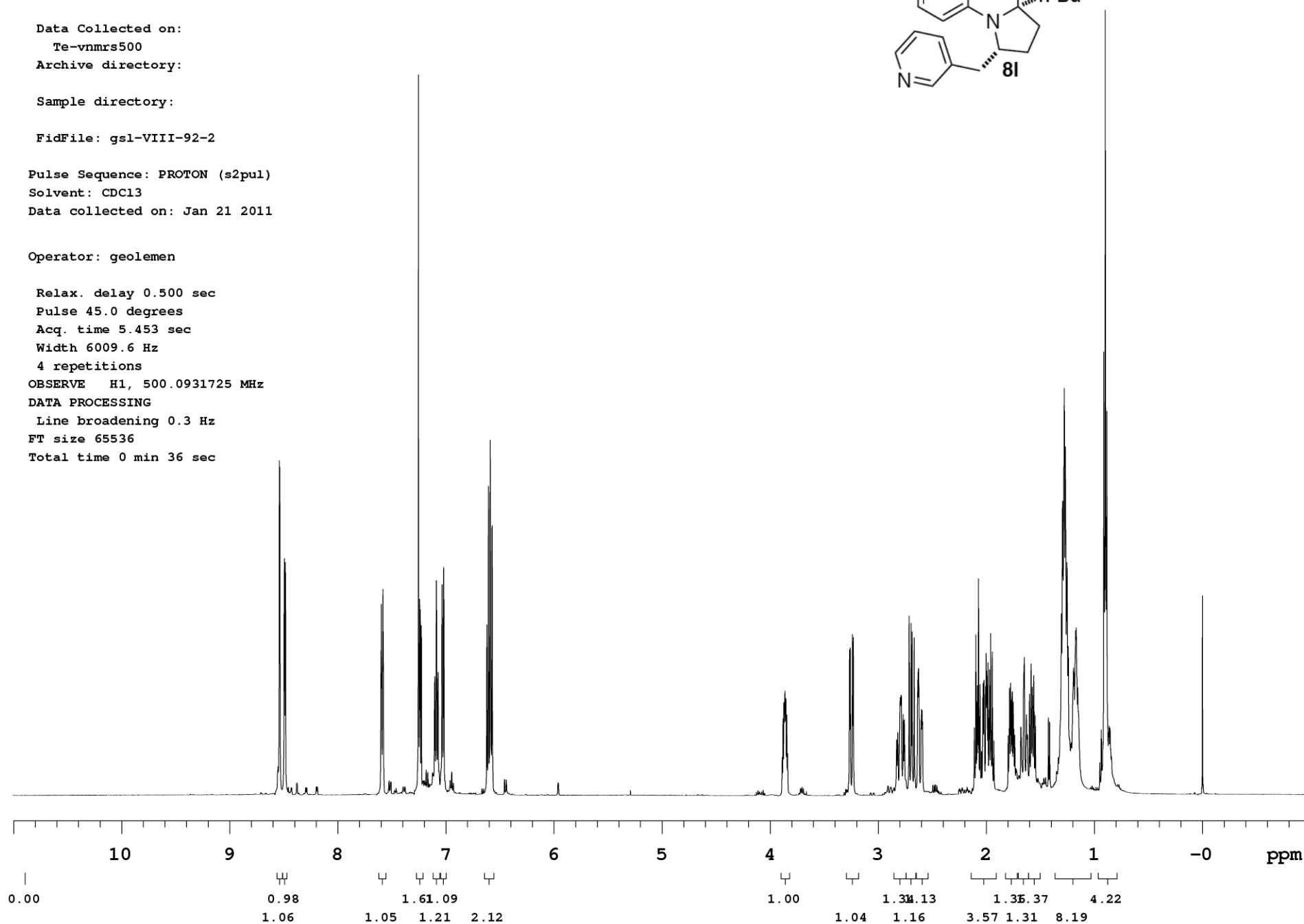
OBSERVE H1, 500.0931725 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 0 min 36 sec


VARIAN 


gs1-VIII-92-2 carbon

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gs1-VIII-92-2carbon

Pulse Sequence: CARBON (s2pul)

Solvent: CDC13

Data collected on: Jan 21 2011

Operator: geolemen

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 2.045 sec

Width 32051.3 Hz

136 repetitions

OBSERVE C13, 125.7485305 MHz

DECOUPLE H1, 500.0956704 MHz

Power 42 dB

continuously on

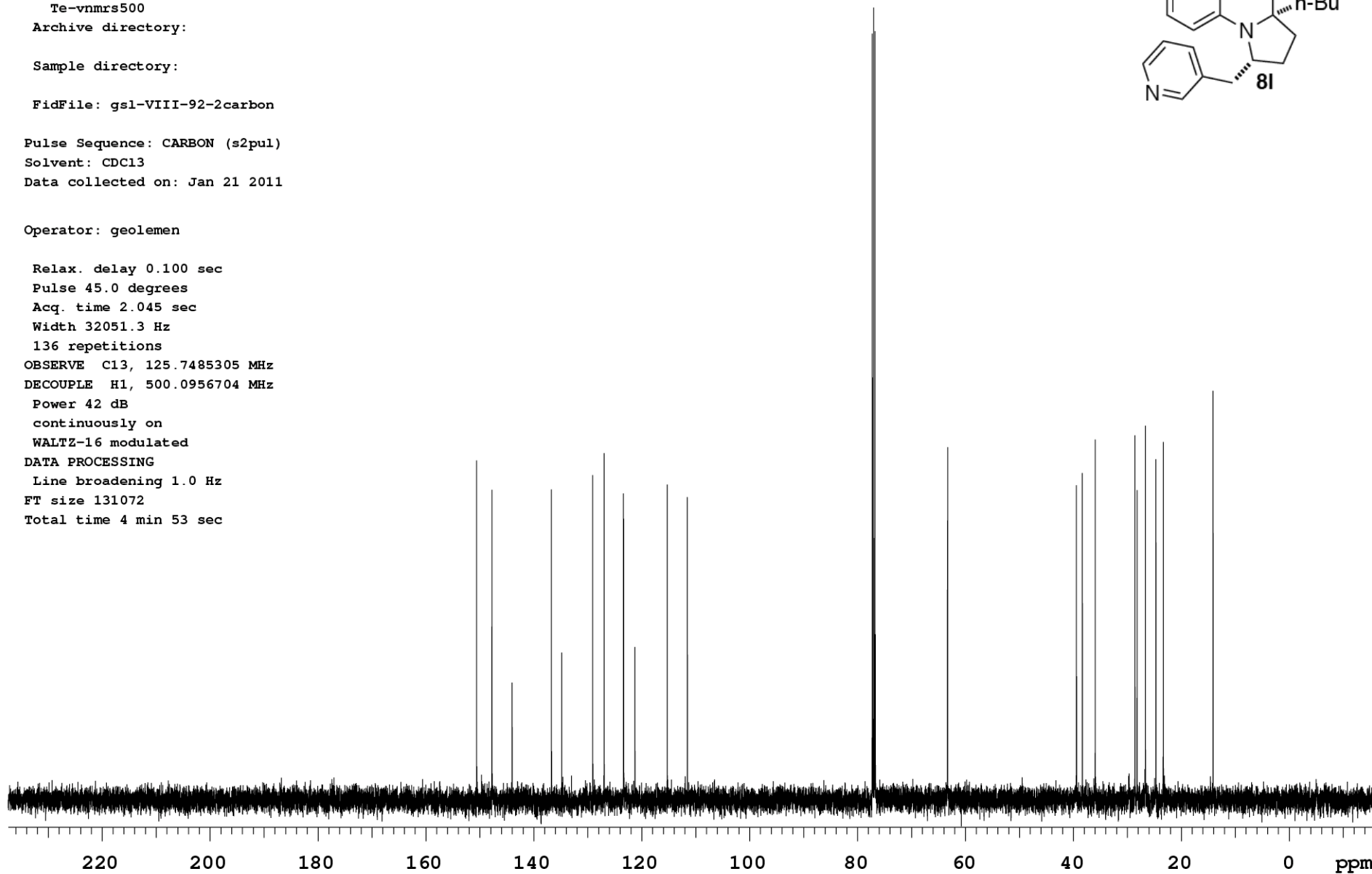
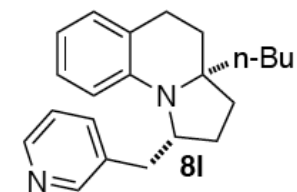
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 4 min 53 sec

VARIAN 

gs1-VIII-92-2 cosy

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gs1-VIII-92-2cosy

Pulse Sequence: gCOSY

Solvent: CDC13

Data collected on: Jan 21 2011

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 5506.6 Hz

2D Width 5506.6 Hz

Single scan

128 increments

OBSERVE H1, 500.0931725 MHz

DATA PROCESSING

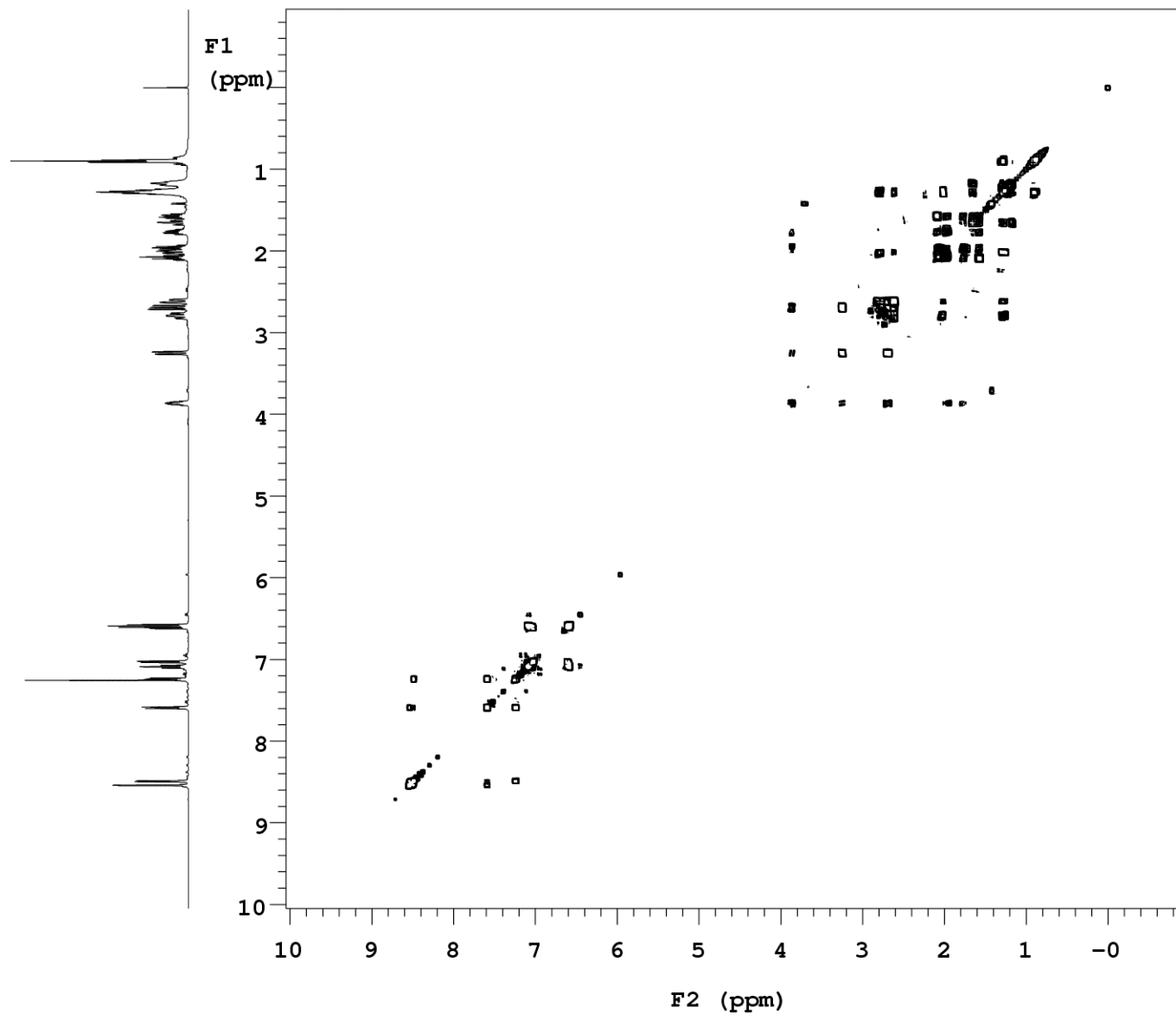
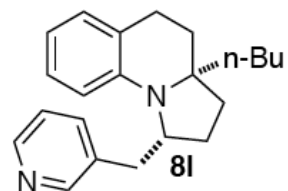
Sq. sine bell 0.075 sec

F1 DATA PROCESSING

Sq. sine bell 0.023 sec

FT size 2048 x 2048

Total time 3 min 12 sec



gsl-VII-120-2frac28-32

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-120-2frac28-32

Pulse Sequence: PROTON (s2pul)

Solvent: CDCl3

Data collected on: Feb 23 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.303 sec

Width 4960.3 Hz

8 repetitions

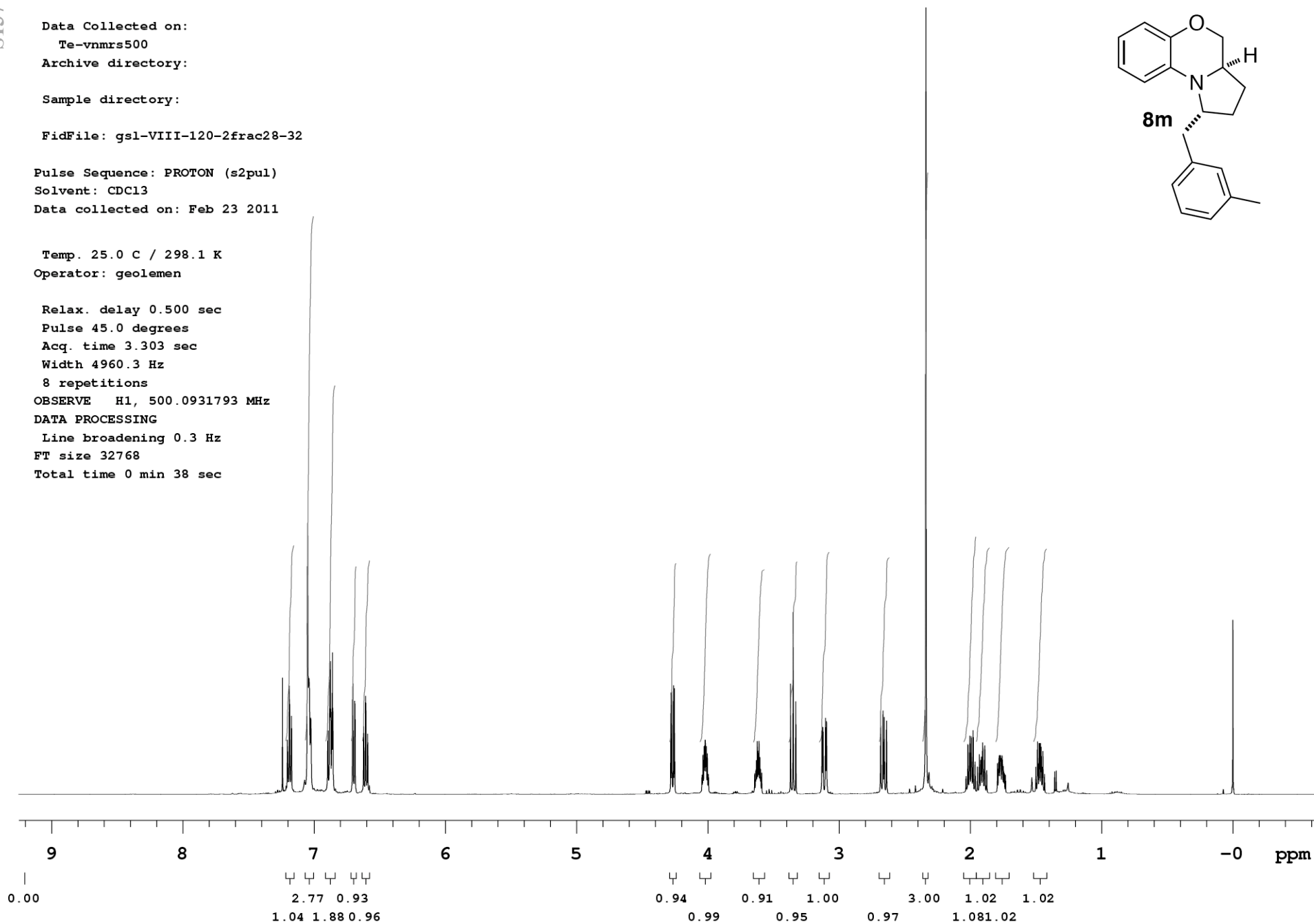
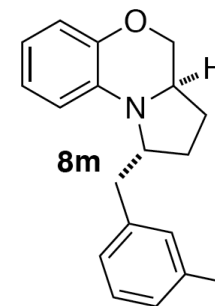
OBSERVE H1, 500.0931793 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 32768

Total time 0 min 38 sec

VARIAN 


gsl-VIII-118-2 carbon

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-120-2frac28-32carbon

Pulse Sequence: CARBON (s2pul)

Solvent: CDCl3

Data collected on: Feb 23 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 0.100 sec

Pulse 30.0 degrees

Acq. time 2.045 sec

Width 32051.3 Hz

424 repetitions

OBSERVE C13, 125.7485305 MHz

DECOUPLE H1, 500.0956704 MHz

Power 42 dB

continuously on

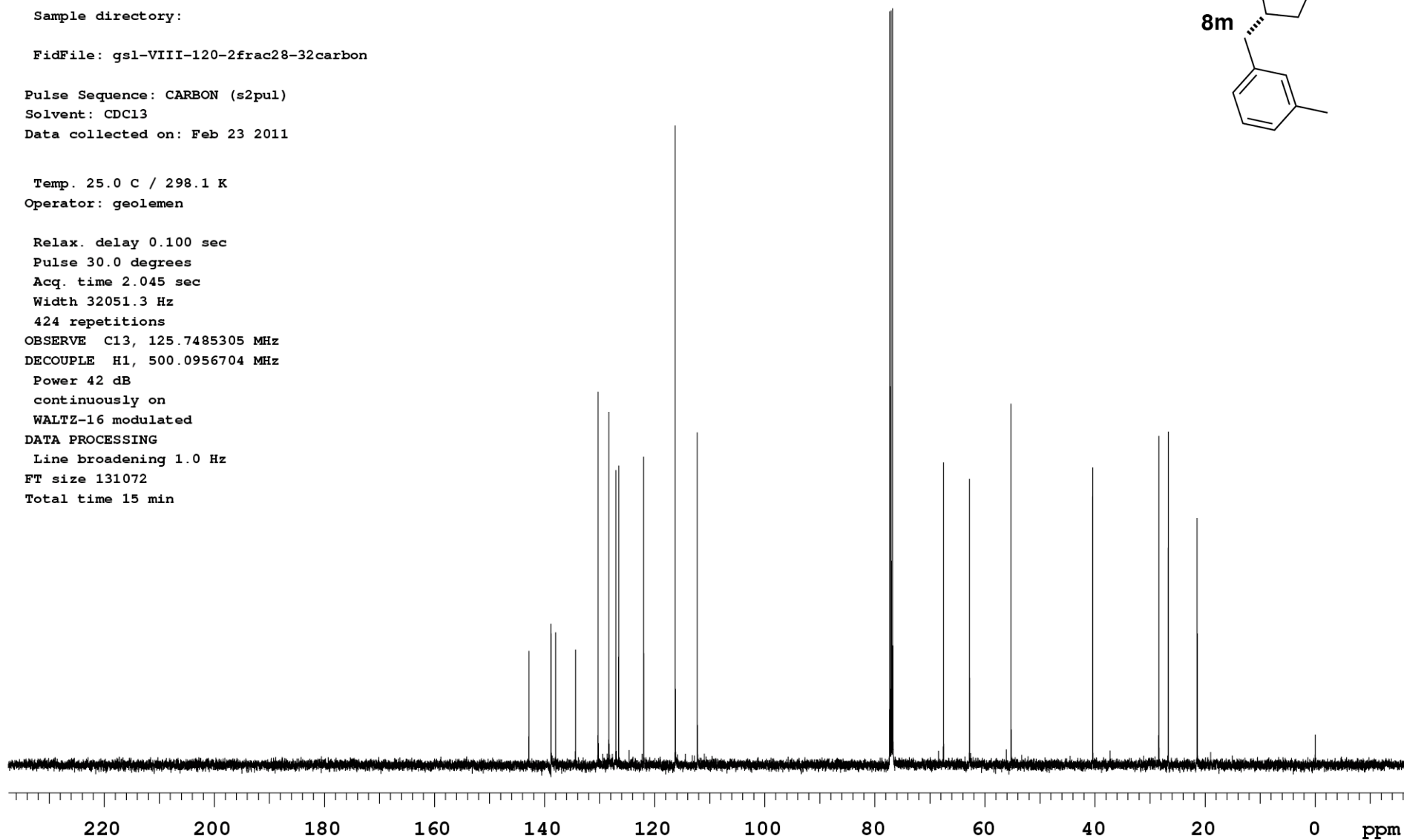
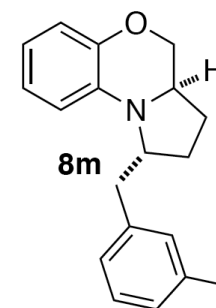
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 15 min

VARIAN 

gsl-VII-120-2frac28-32

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-120-2frac28-32cosy

Pulse Sequence: gCOSY

Solvent: CDCl3

Data collected on: Feb 23 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4251.7 Hz

2D Width 4251.7 Hz

Single scan

128 increments

OBSERVE H1, 500.0931790 MHz

DATA PROCESSING

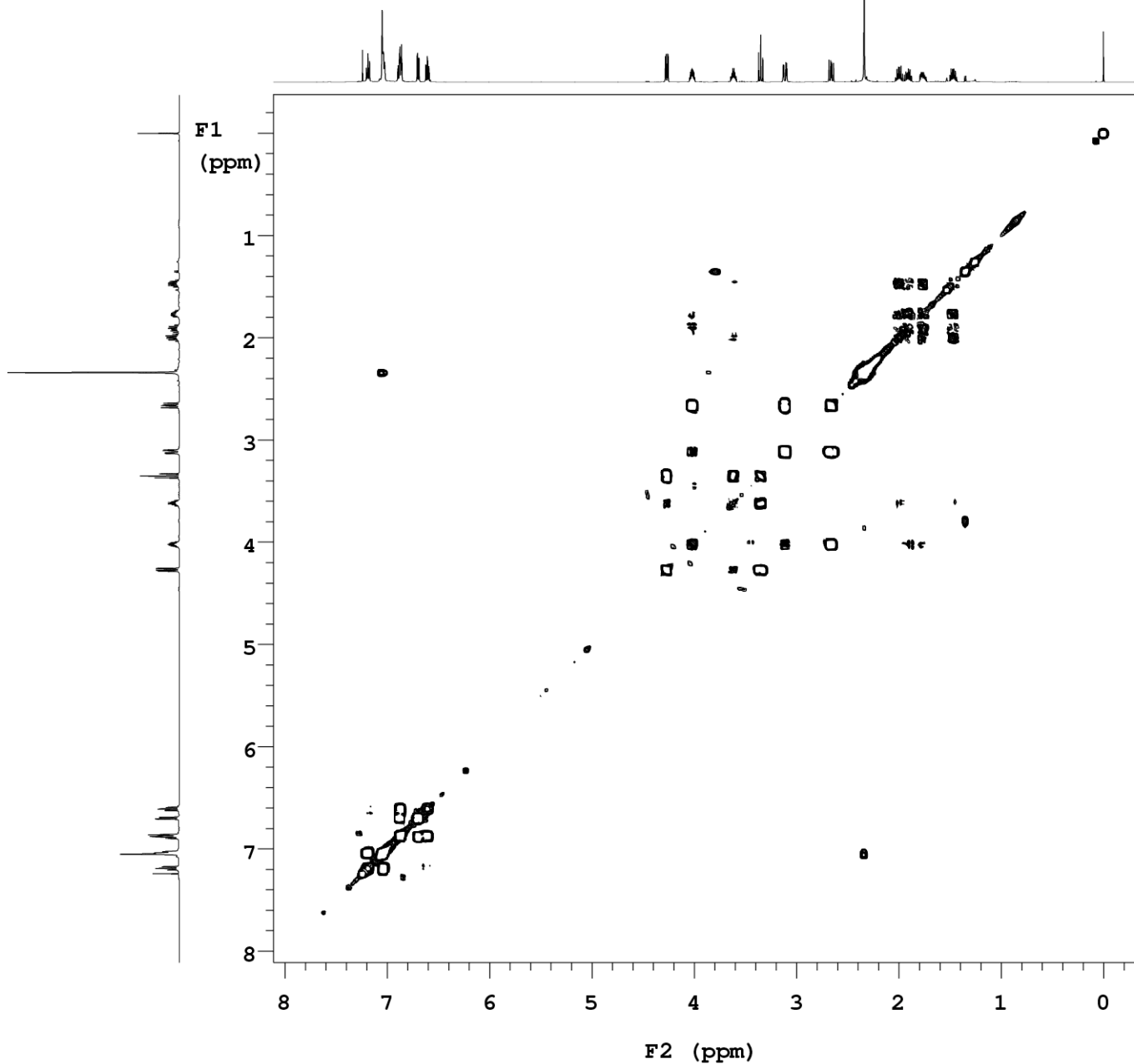
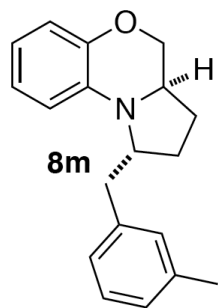
Sq. sine bell 0.060 sec

F1 DATA PROCESSING

Sq. sine bell 0.030 sec

FT size 1024 x 1024

Total time 3 min 12 sec



gsl-VII-120-2frac28-32

Sample Name:

Data Collected on:

Te-vnmrs500

Archive directory:

Sample directory:

FidFile: gsl-VIII-120-2frac28-32noesy

Pulse Sequence: NOESY

Solvent: CDCl3

Data collected on: Feb 23 2011

Temp. 25.0 C / 298.1 K

Operator: geolemen

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 4251.7 Hz

2D Width 4251.7 Hz

4 repetitions

2 x 200 increments

OBSERVE H1, 500.0931790 MHz

DATA PROCESSING

Gauss apodization 0.069 sec

F1 DATA PROCESSING

Gauss apodization 0.043 sec

FT size 2048 x 2048

Total time 1 hr, 48 min

