

Supporting information

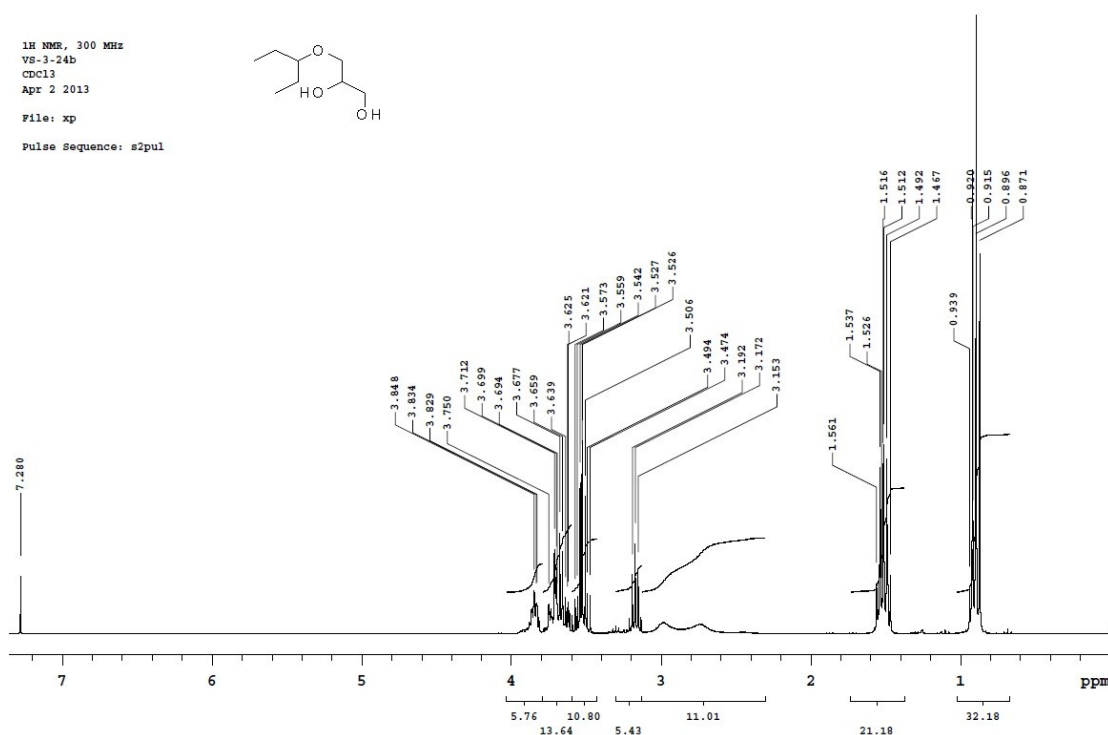
Stereoisomers of oseltamivir – synthesis, in silico prediction and biological evaluation

V. Hajzer, R. Fišera, A. Latika, J. Durmis, J. Kollár, V. Frečer, Z. Tučková, S. Miertuš, F. Kostolanský, E. Varečková, R. Šebesta

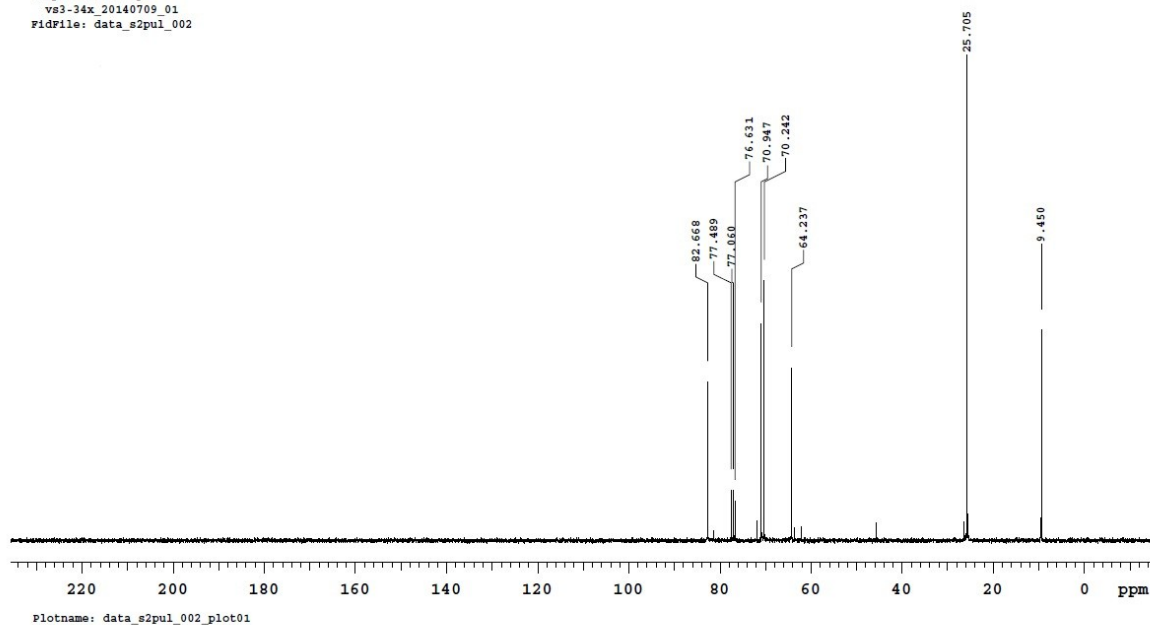
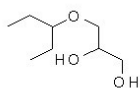
Table of Contents

Pictures of ^1H and ^{13}C NMR spectra.....	1
Pictures of 2D NMR spectra	29
Pictures of ^1H and ^{13}C NMR spectra for derivatized samples for HPLC analyses.....	40
Pictures of HPLC chromatograms	42

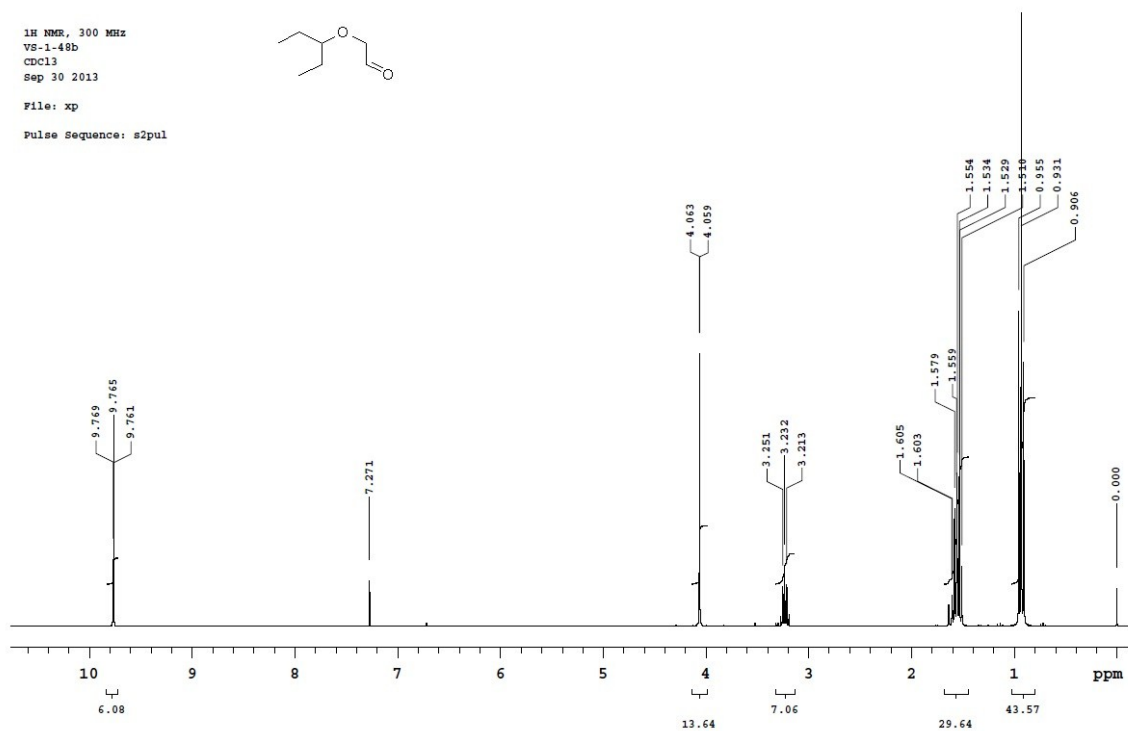
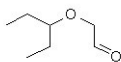
Pictures of ^1H and ^{13}C NMR spectra

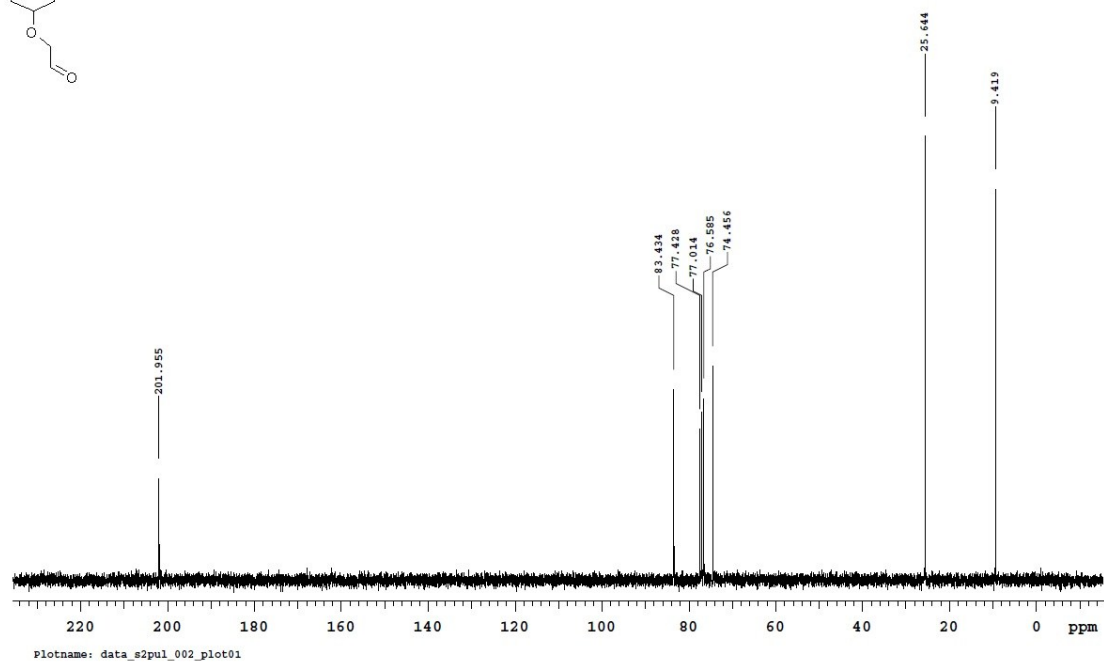
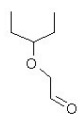


Sample Name:
vs3-34x
Data Collected on:
VNMRS300-VNMR300
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
vs3-34x_20140709_01
Fidfile: data_s2pul_002

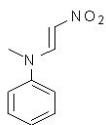


1H NMR, 300 MHz
VS-1-48b
CDCl3
Sep 30 2013
File: xp
Pulse Sequence: s2pul

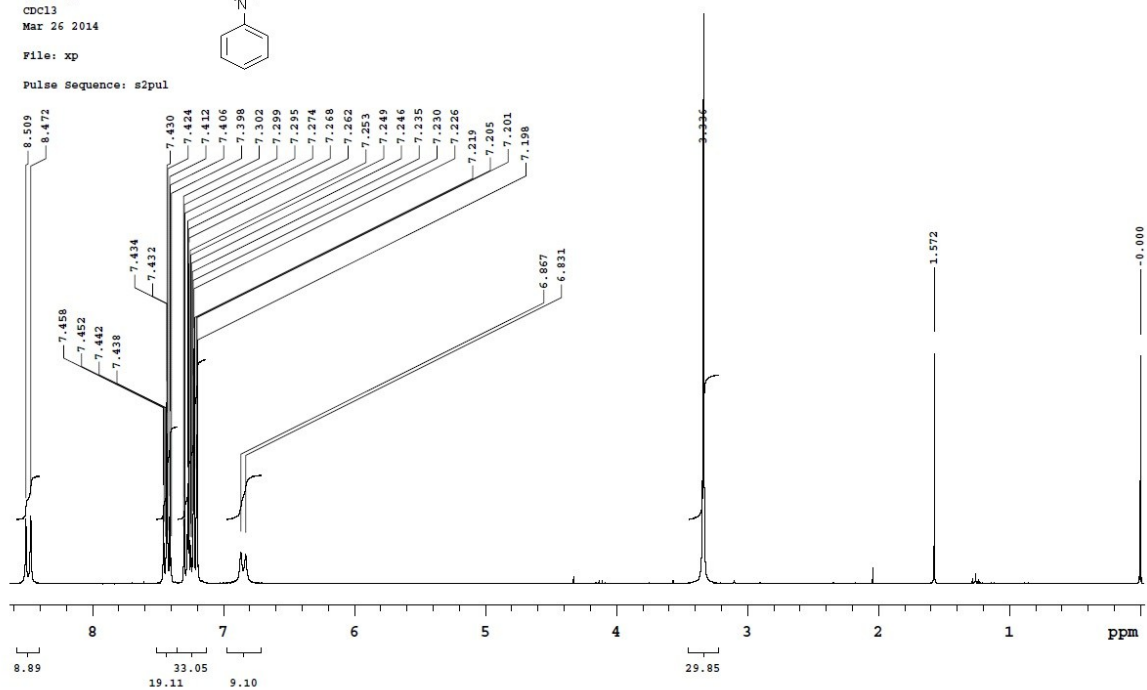




¹H NMR, 300 MHz
 VS-13-7a
 CDCl₃
 Mar 26 2014
 File: xp

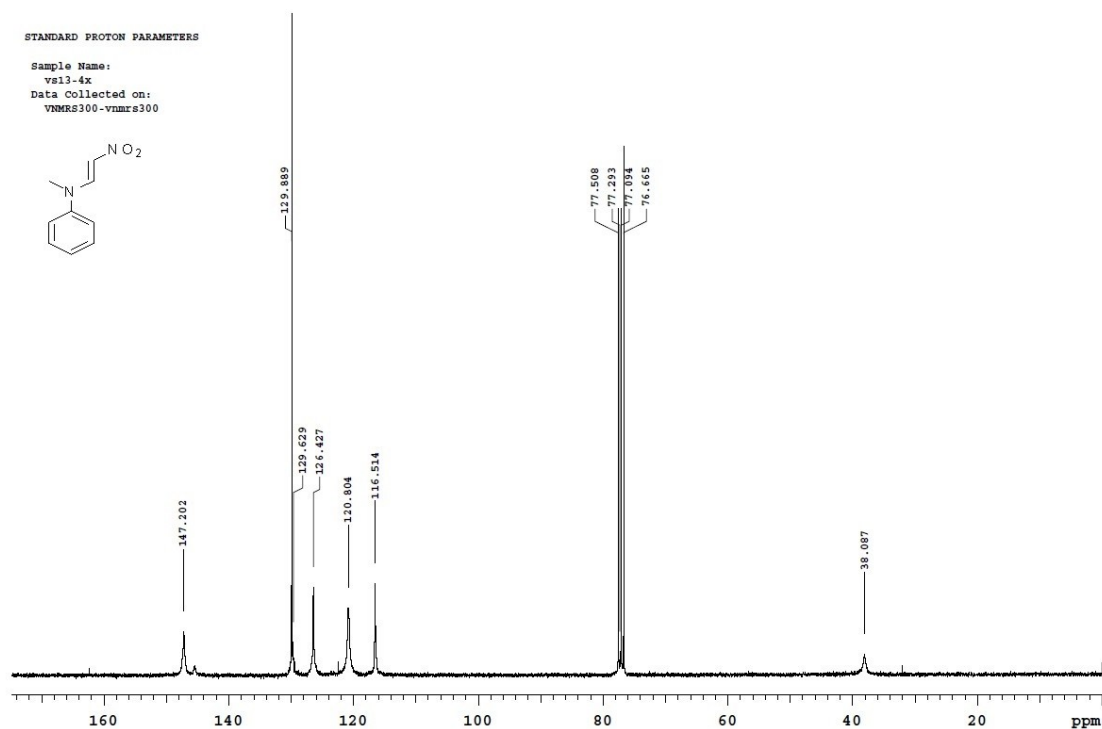
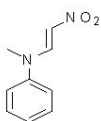


Pulse Sequence: s2pul



STANDARD PROTON PARAMETERS

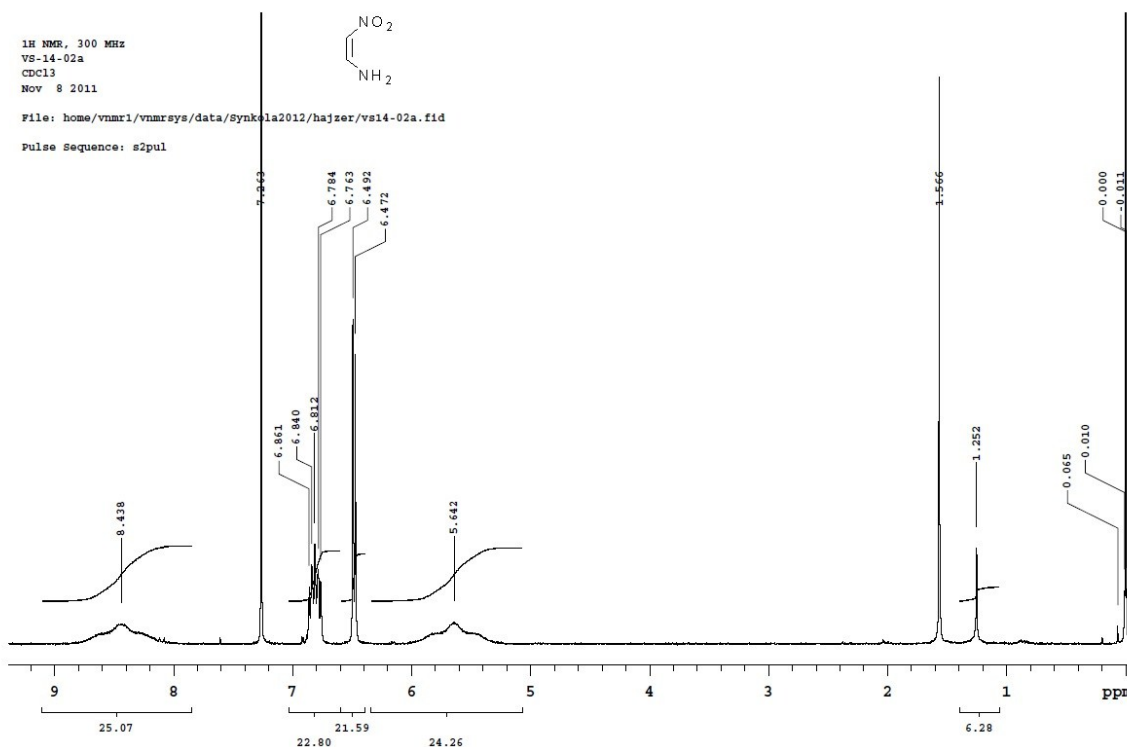
Sample Name:
vs13-4x
Data Collected on:
VNMR300-VNMR300



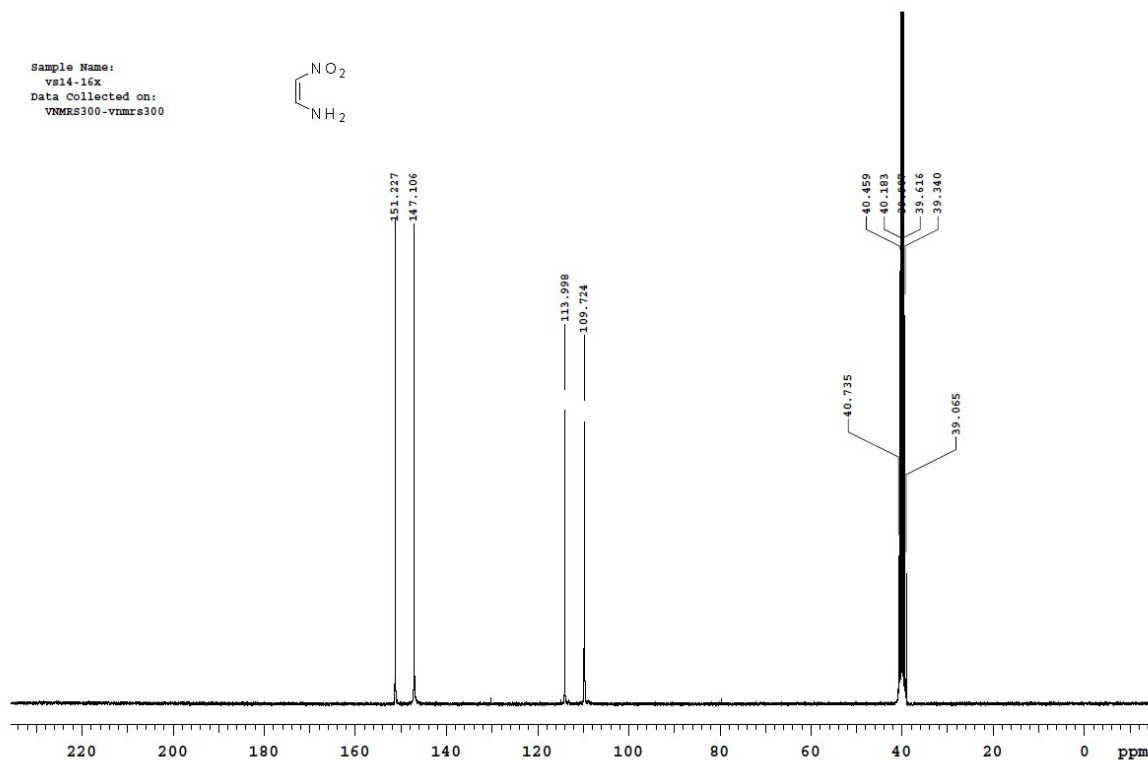
1H NMR, 300 MHz
VS-14-02a
CDCl3
Nov 8 2011



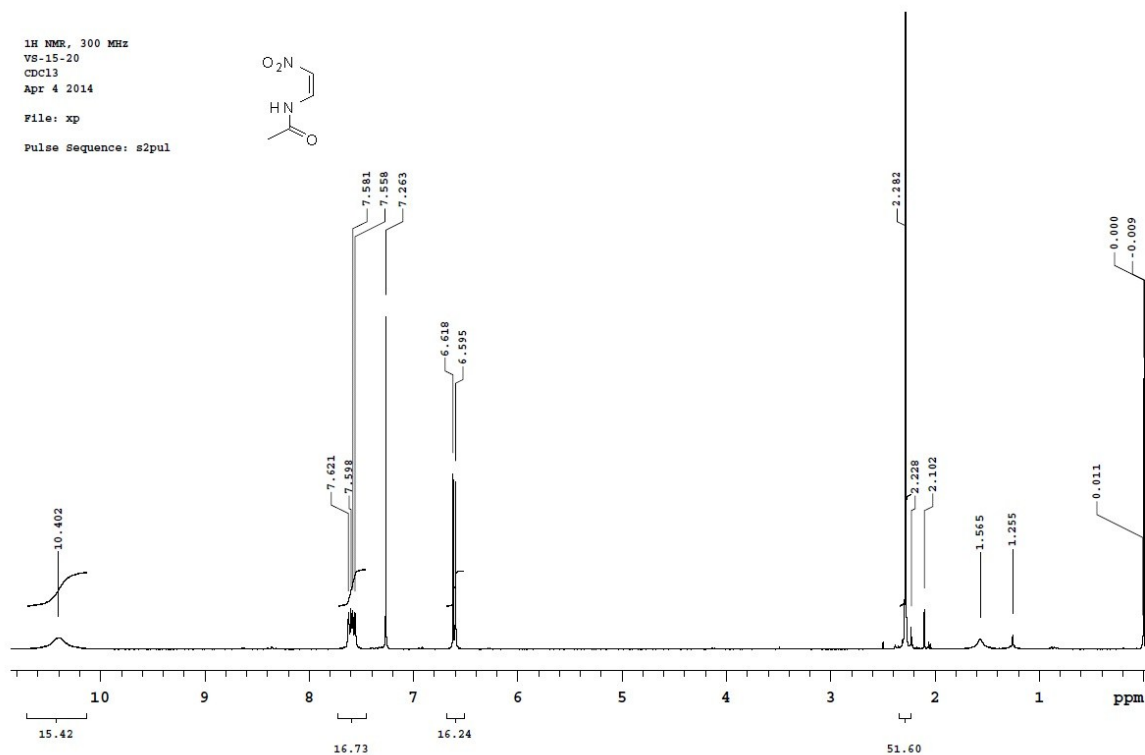
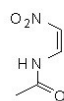
File: home/vnmr1/vnmrsys/data/synkola2012/hajzer/vs14-02a.fid
Pulse Sequence: s2pul



Sample Name:
vs14-16x
Data Collected on:
VNMR300-VNMR300

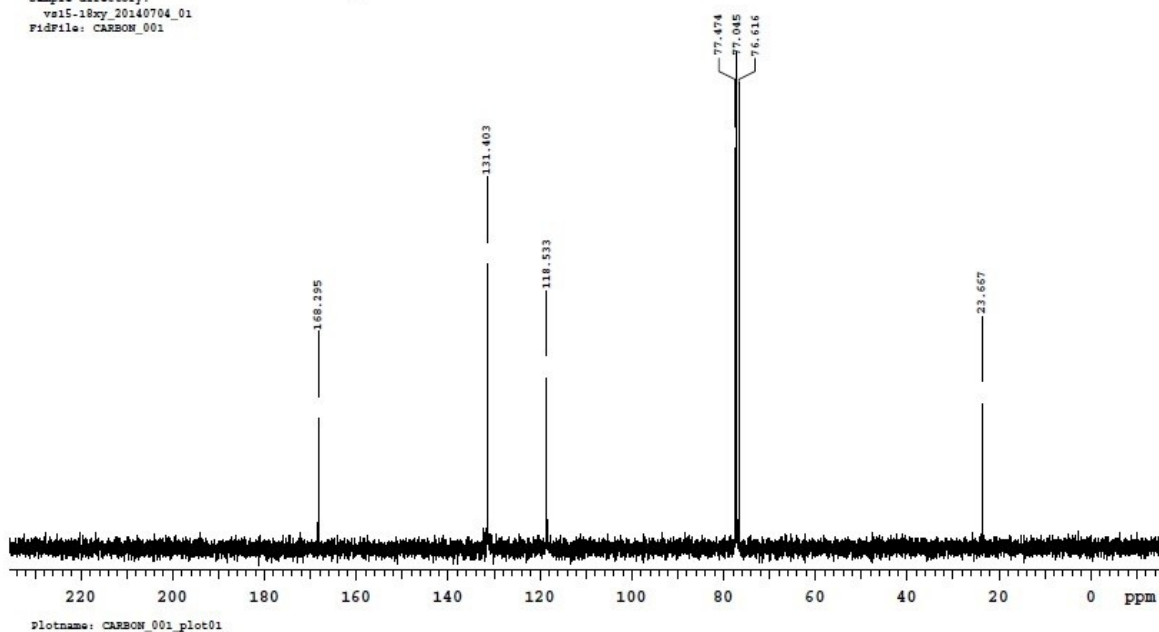
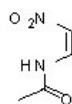


1H NMR, 300 MHz
VS-15-20
CDCl3
Apr 4 2014
File: xp
Pulse Sequence: s2pul

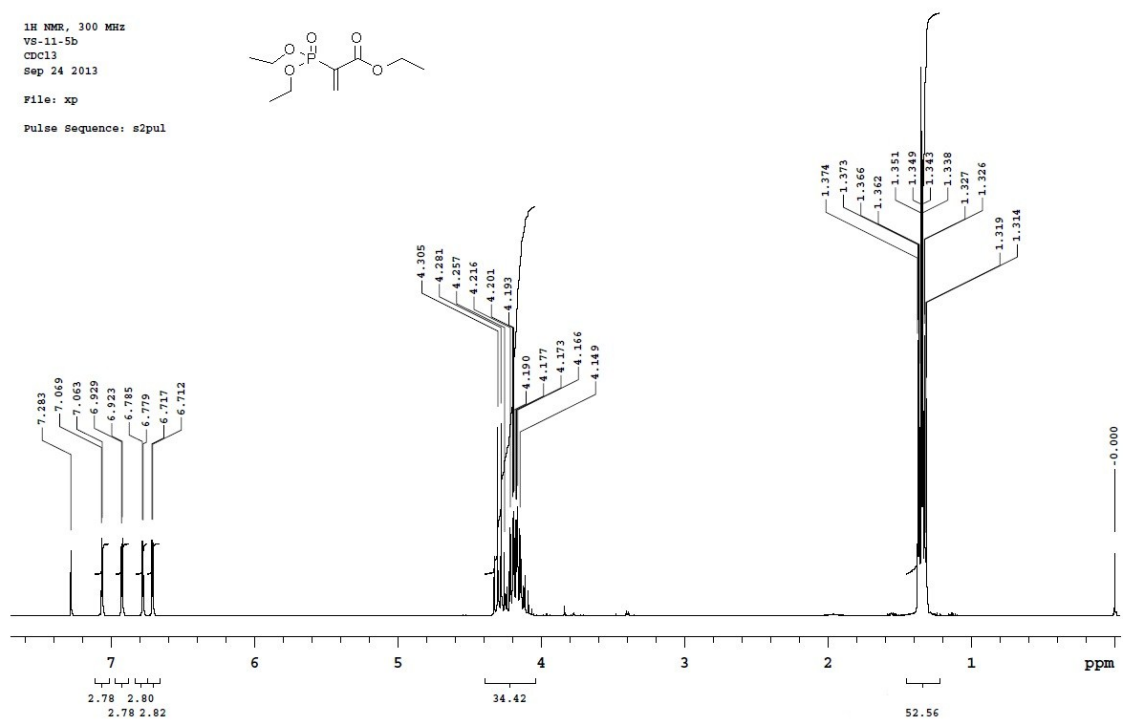
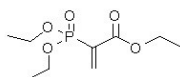


STANDARD PROTON PARAMETERS

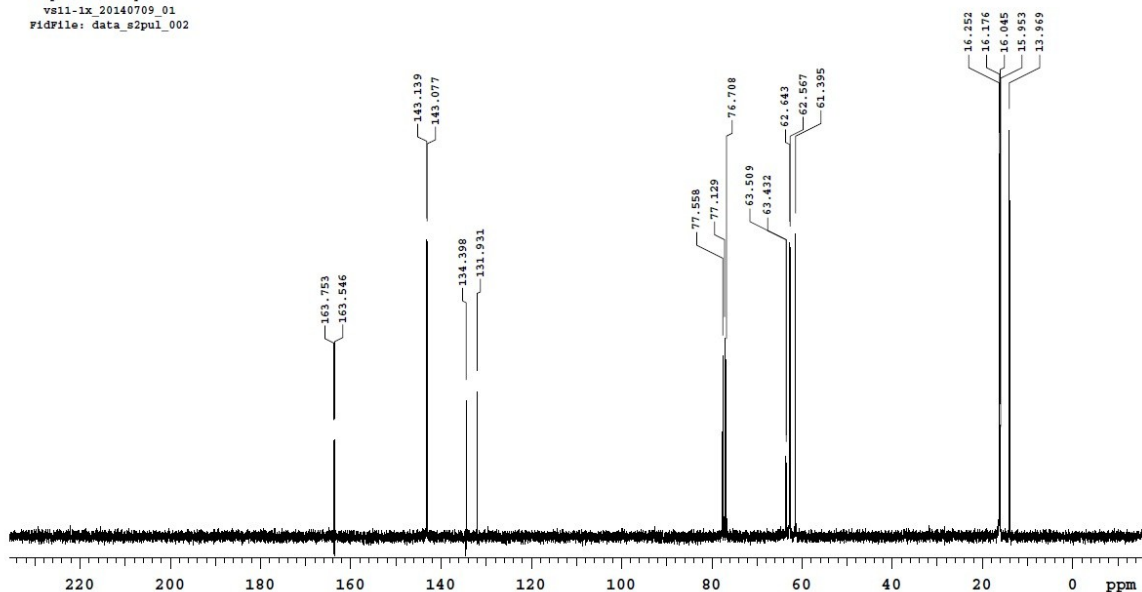
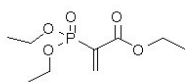
Sample Name:
vs15-18xy
Data Collected on:
VNMRS300-vnmrs300
Archive directory:
/home/chempack/vnmrsys/data
Sample directory:
vs15-18xy_20140704_01
FidFile: CARBON_001



1H NMR, 300 MHz
VS-11-5b
CDCl3
Sep 24 2013
File: xp
Pulse Sequence: s2pul

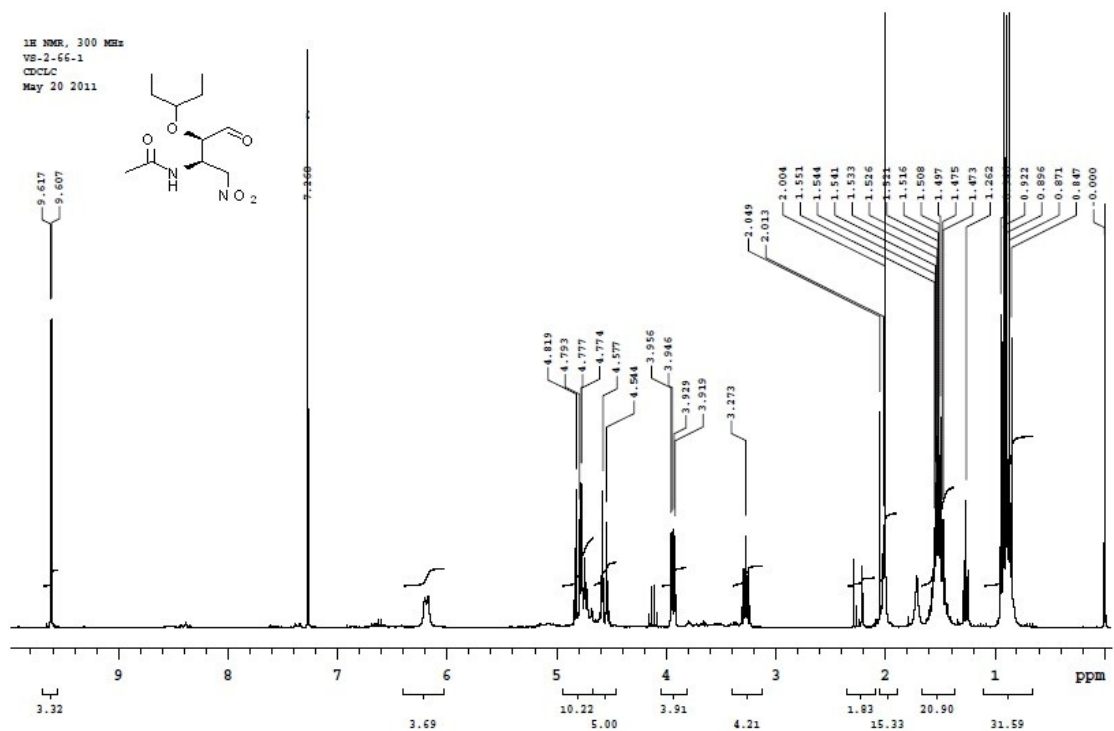
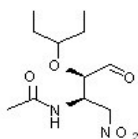


Sample Name:
vs11-1x
Data Collected on:
VNMRS300-vnmrs300
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
vs11-1x 20140709_01
Fidfile: data_s2pul_002



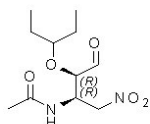
Plotname: data_s2pul_002_plot01

1H NMR, 300 MHz
VS-2-55-1
CDCl3
May 20 2011



STANDARD PROTON PARAMETERS

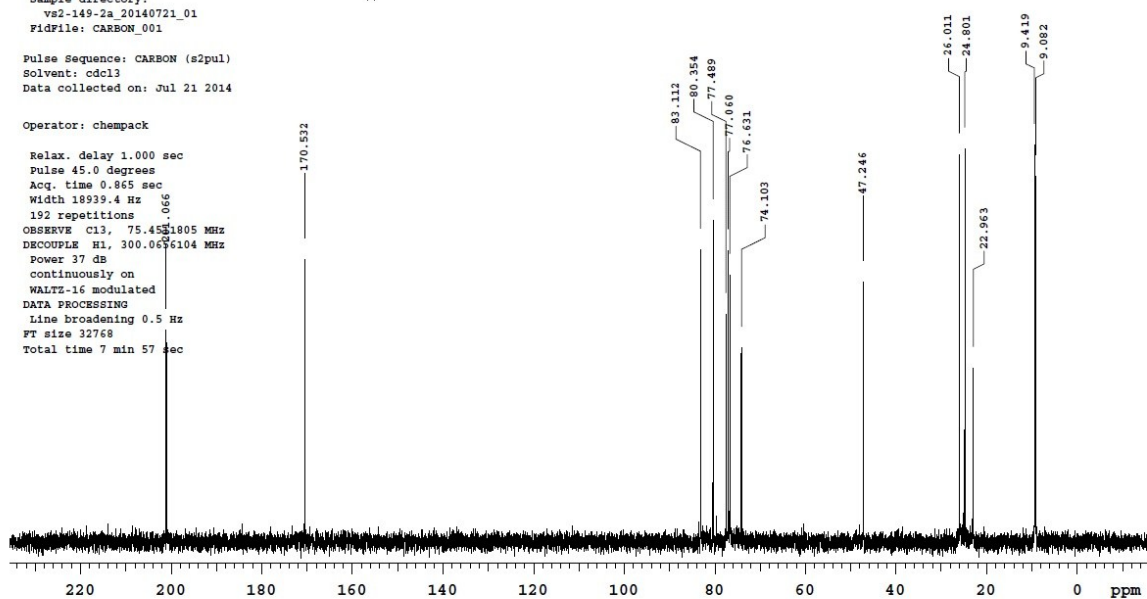
Sample Name:
vs2-149-2a
Data Collected on:
VNMRS300-vnmrs300
Archive directory:
/home/chempack/vnmrsys/data
Sample directory:
vs2-149-2a 20140721_01
FidFile: CARBON_001



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 21 2014

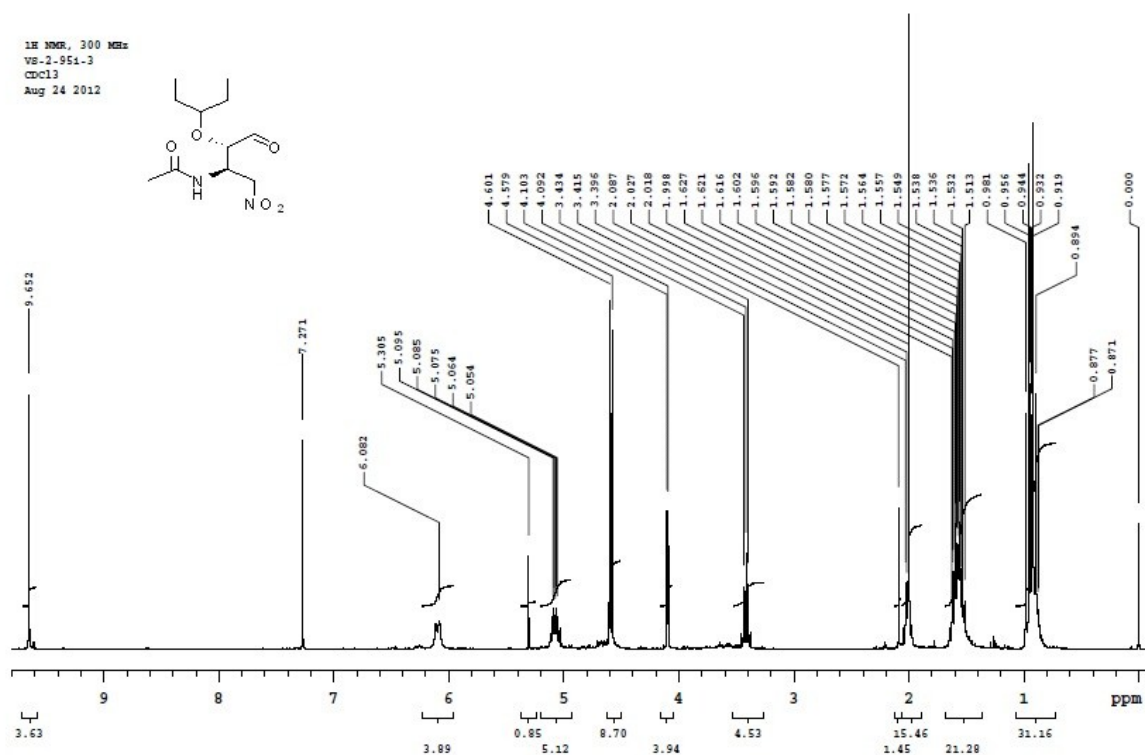
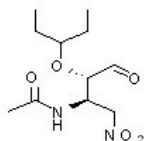
Operator: chempack

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 18939.4 Hz
192 repetitions
OBSERVE C13, 75.451805 MHz
DECOUPLE H1, 300.06104 MHz
Power 37 db
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 7 min 57 sec



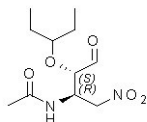
Plotname: CARBON_001_plot01

1H NMR, 300 MHz
vs-2-951-3
CDCl3
Aug 24 2012



STANDARD PROTON PARAMETERS

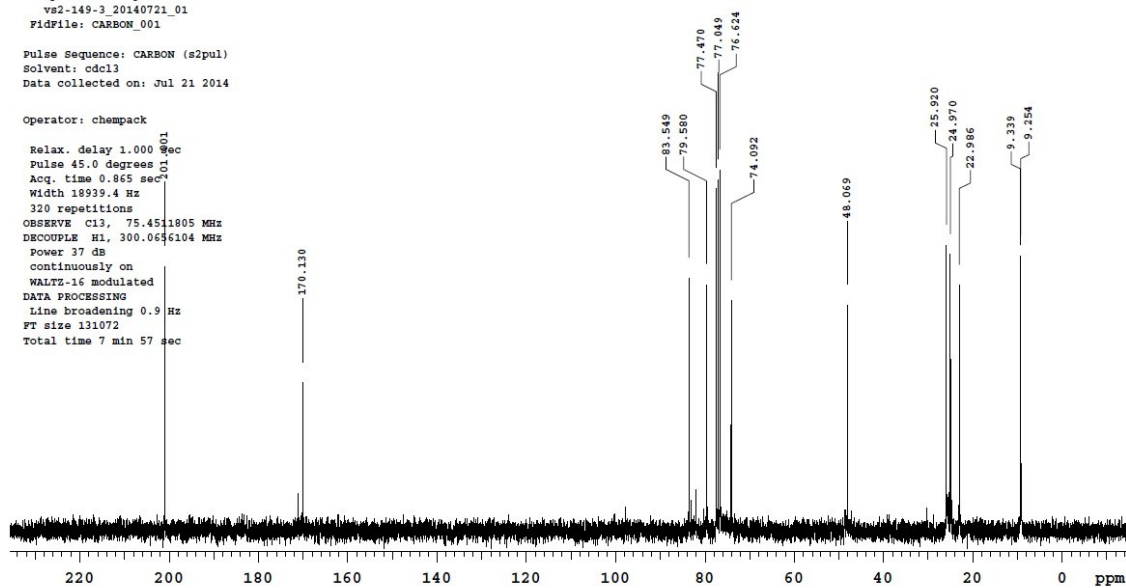
Sample Name:
vs2-149-3
Data Collected on:
VNMR300-vnmrs300
Archive directory:
/home/chempack/vnmrsys/data
Sample directory:
vs2-149-3 20140721_01
FidFile: CARBON_001



Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Jul 21 2014

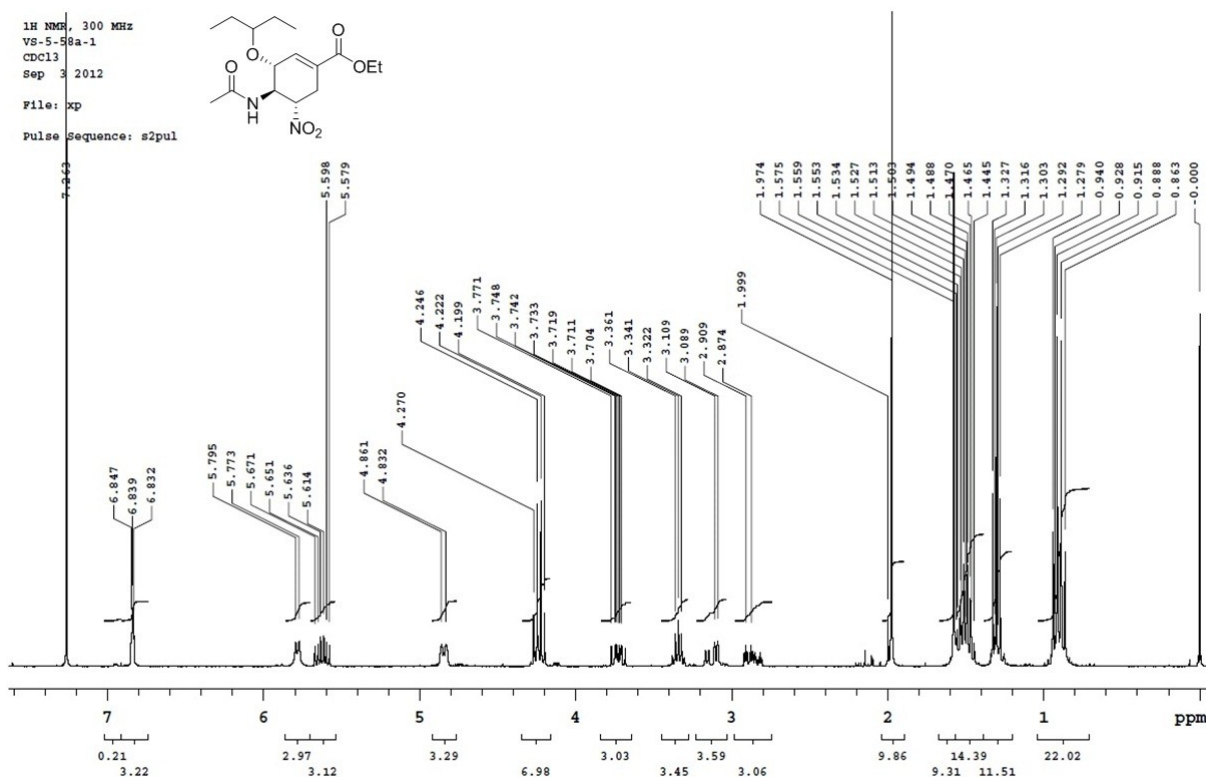
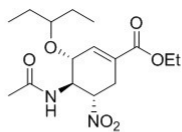
Operator: chempack

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 18939.4 Hz
320 repetitions
OBSERVE C13, 75.4511805 MHz
DECOUPLE H1, 300.0636104 MHz
Power 37 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.9 Hz
FT size 131072
Total time 7 min 57 sec

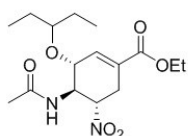
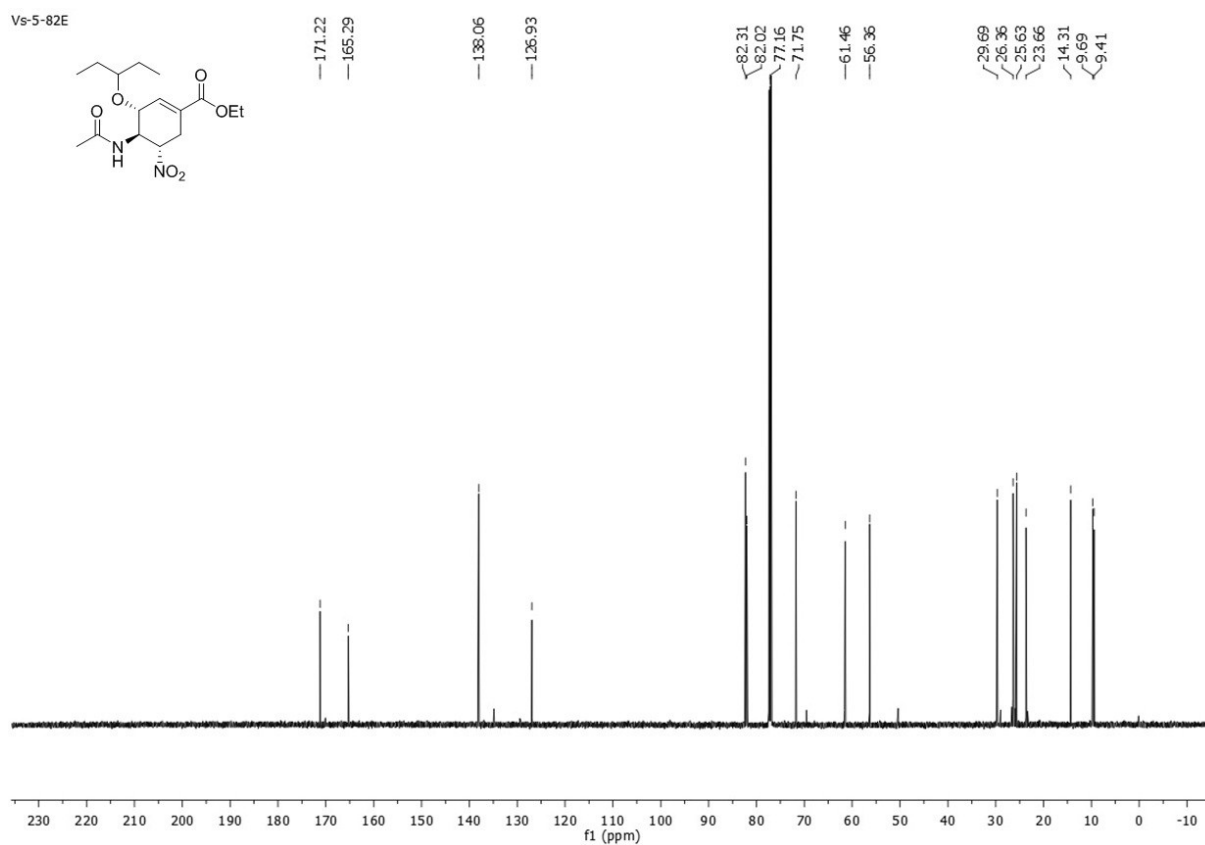
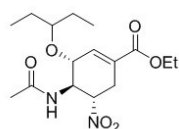


Plotname: CARBON_001_plot01

1H NMR, 300 MHz
VS-5-58a-1
CDCl3
Sep 3 2012
File: xp
Pulse Sequence: s2pul



Vs-5-82E



vs5-82E

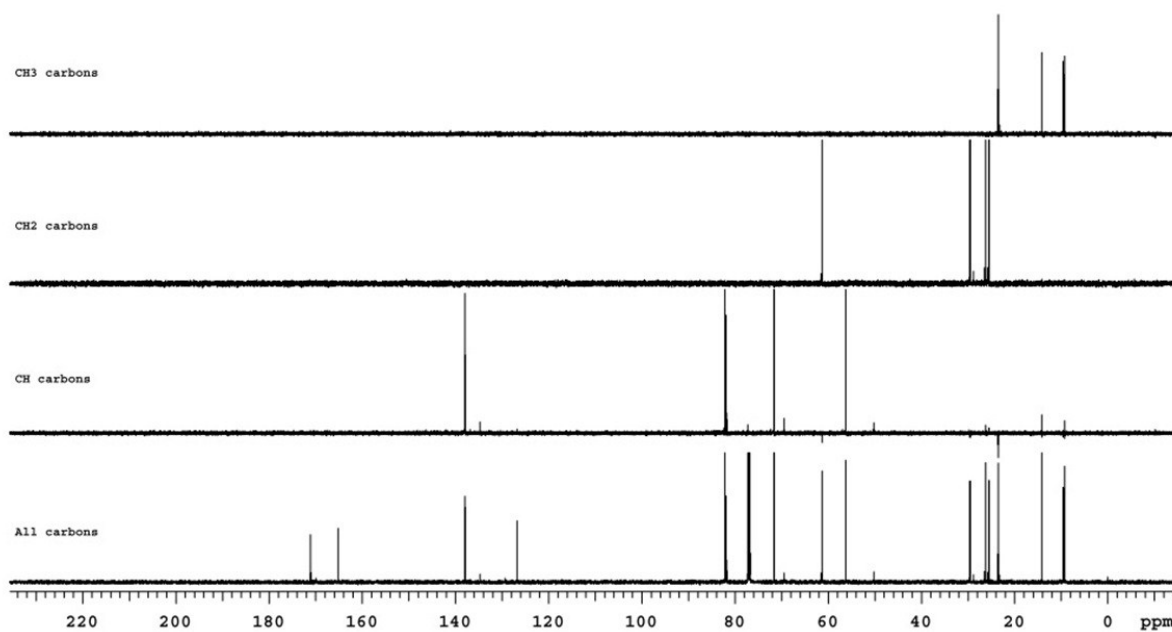
Sample Name	vs5-82E	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr1
Date collected	2015-02-27	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs600	Operator	vnmr1

CH3 carbons

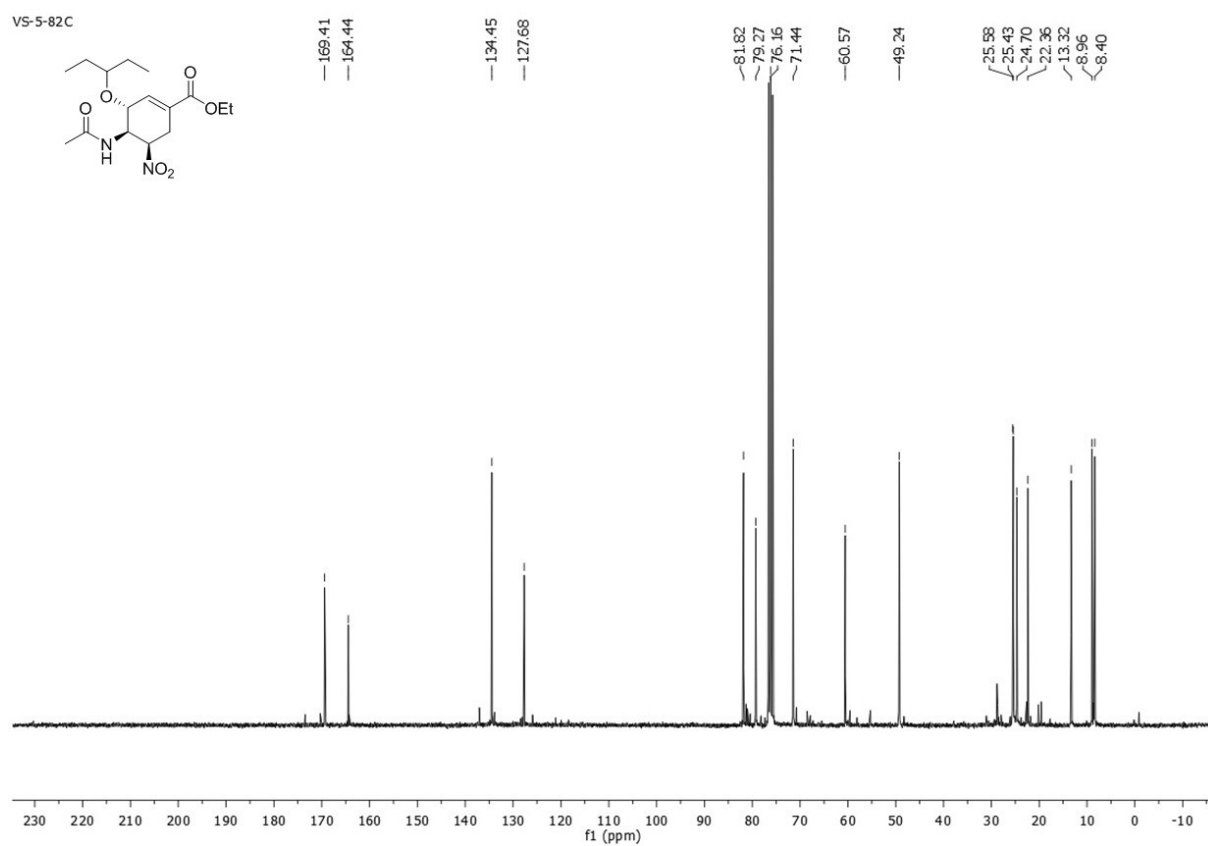
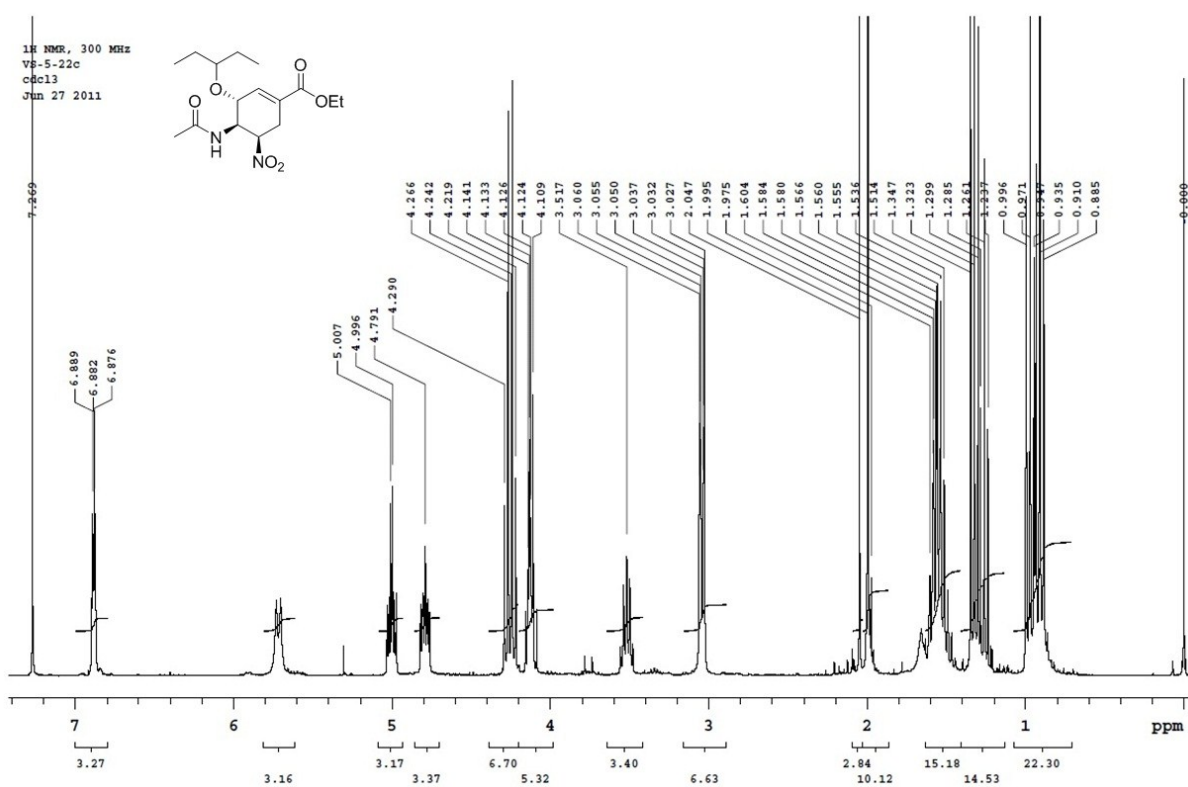
CH2 carbons

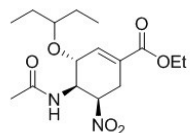
CH carbons

All carbons

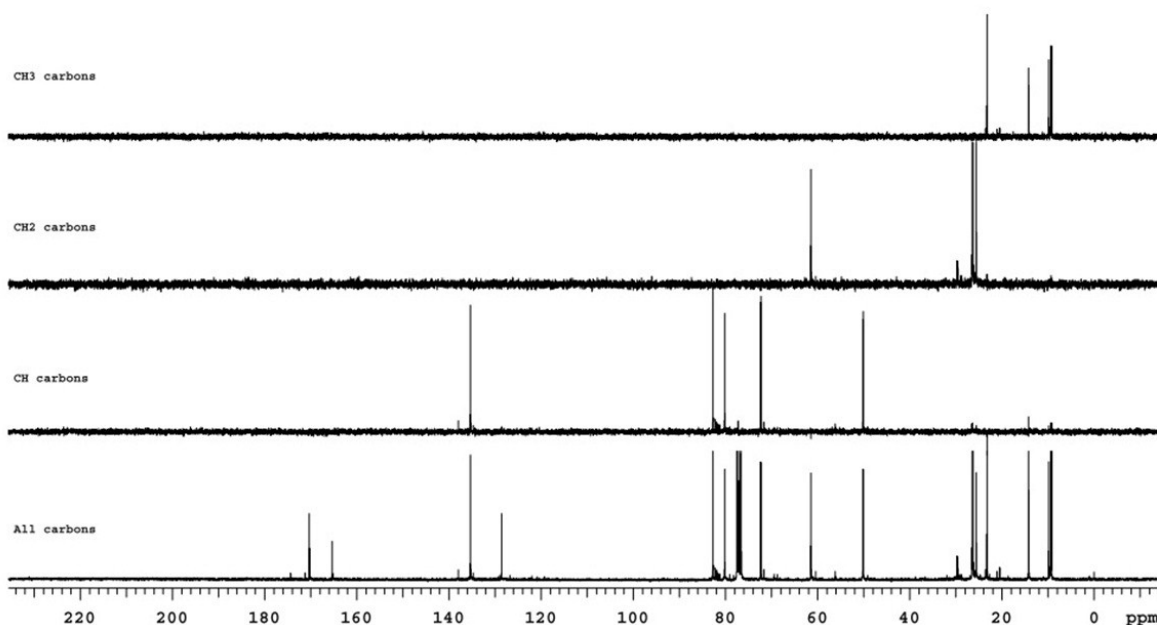


Plotname: DEPT_01_plot01

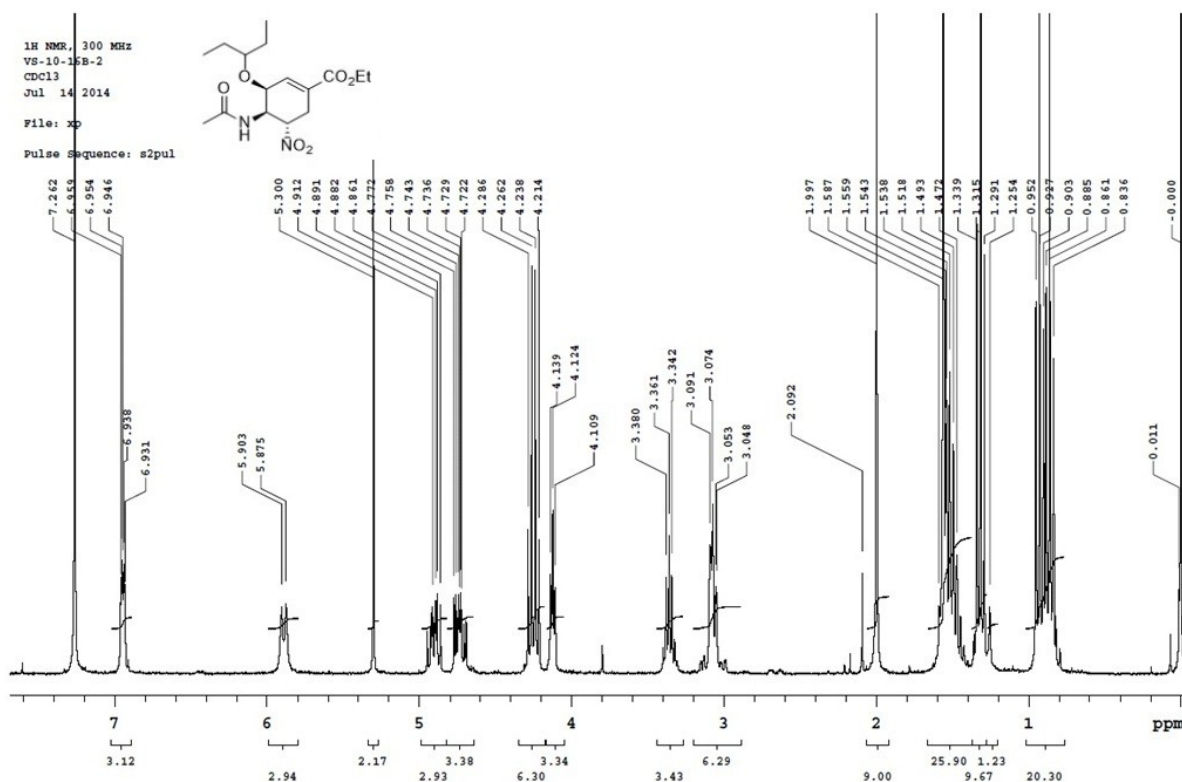




Vs-5-82c							
Sample Name	Vs-5-82c	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr1
Date collected	2015-05-14	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1

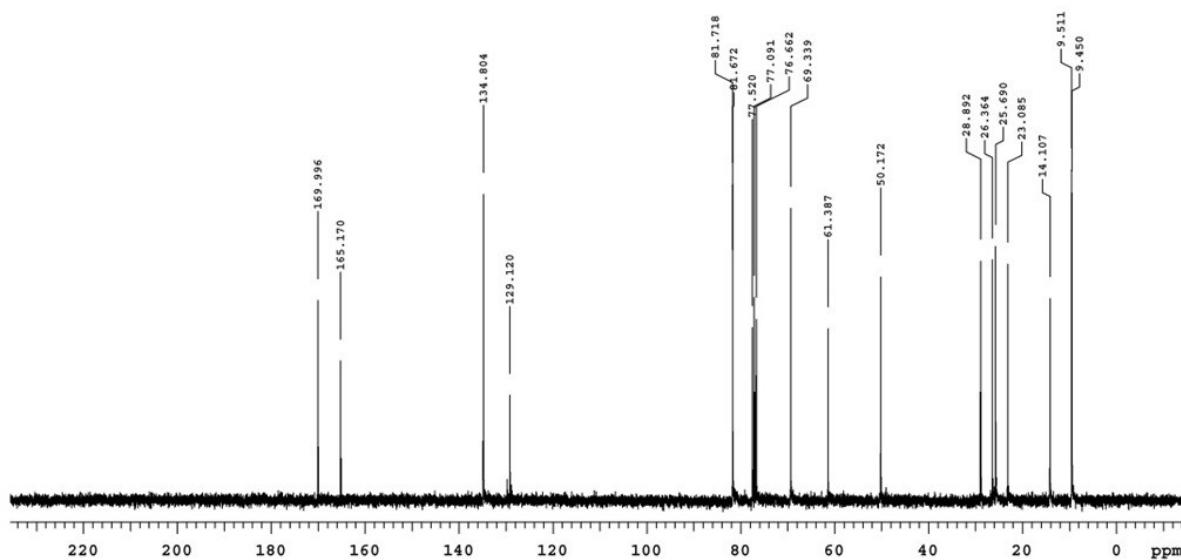
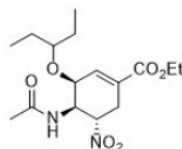


Plotname: DEPT_01_plot01



STANDARD PROTON PARAMETERS

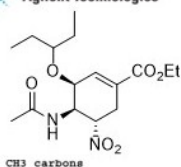
Sample Name:
vs10-16B-2
Data Collected on:



Plotname: CARBON_001_plot01

Vs-10-31A

Agilent Technologies

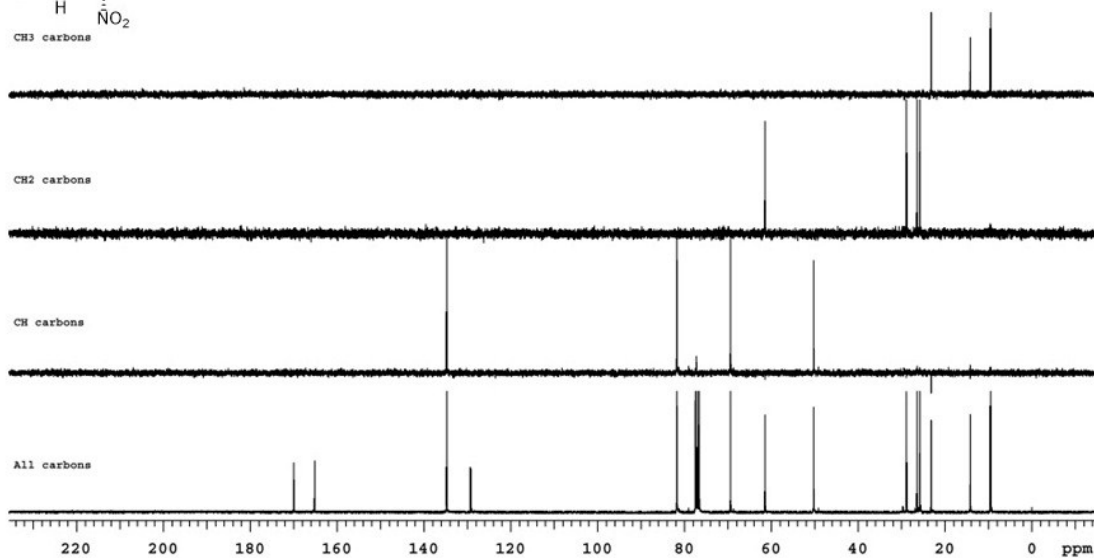


CH3 carbons

CH2 carbons

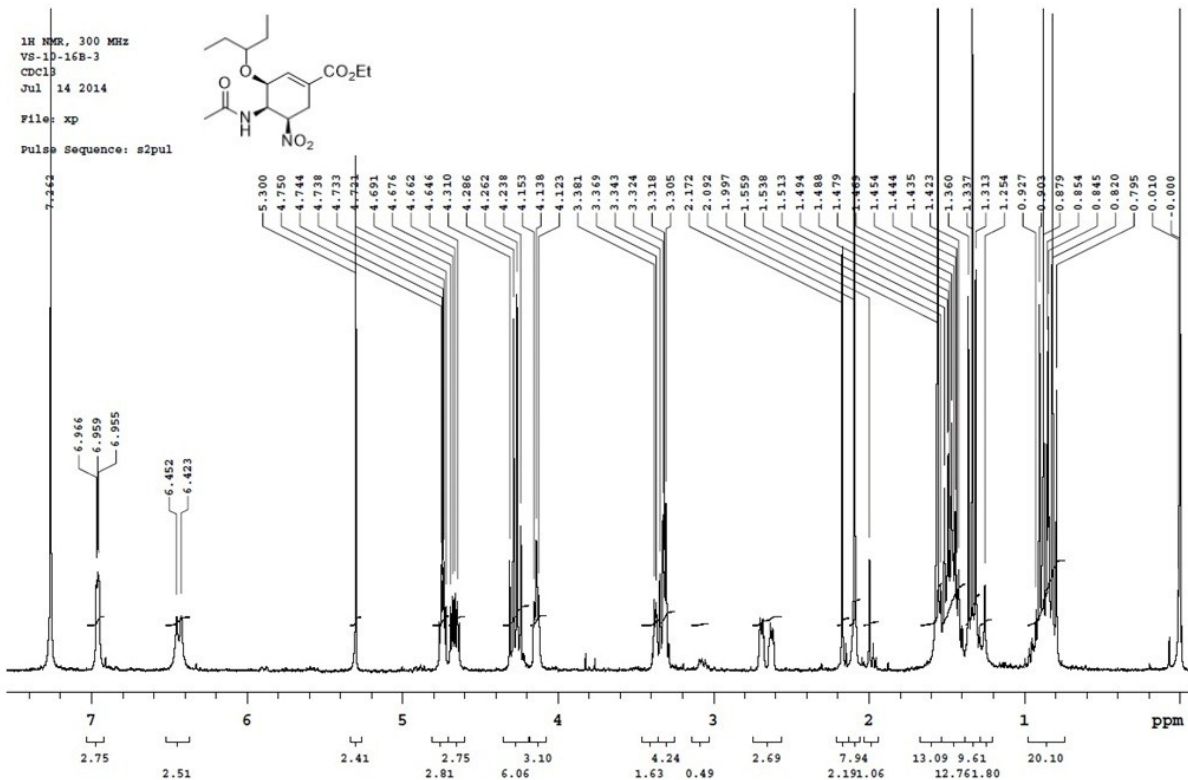
CH carbons

All carbons



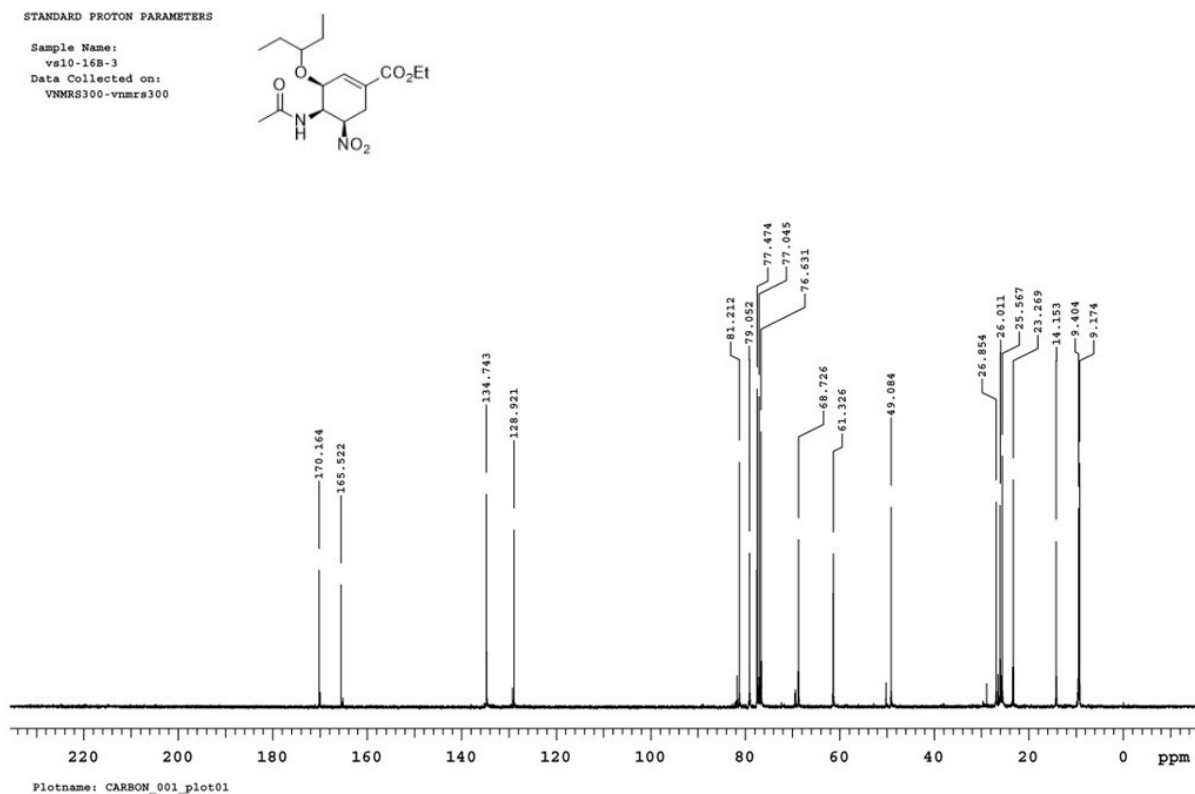
Data file: /home/vnmr1/vnmrsys/data/vs-62C_20150210_02/DEPT_01.fid

Plot date: 2015-02-11



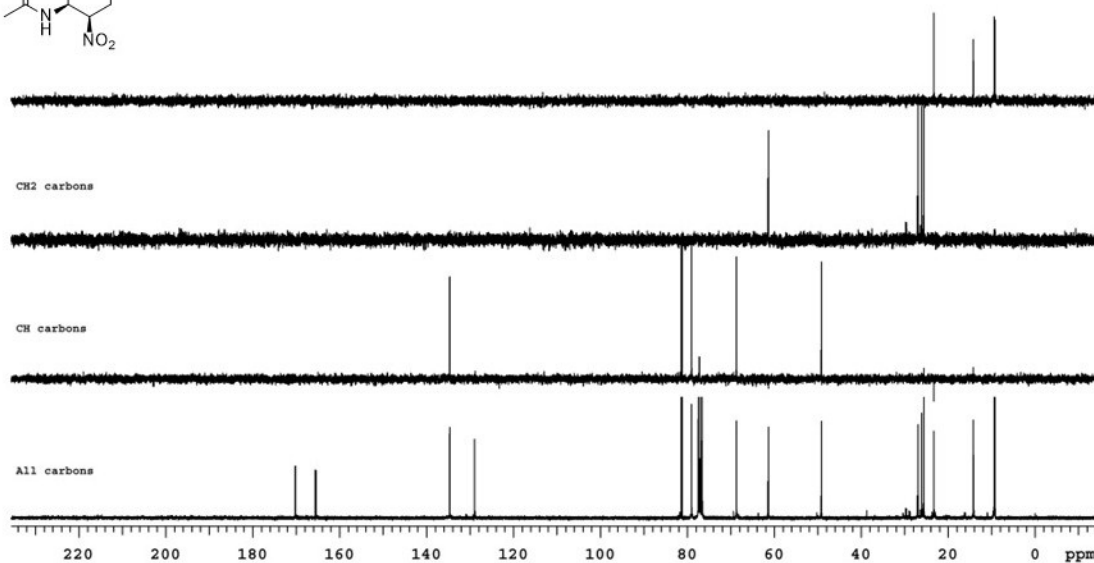
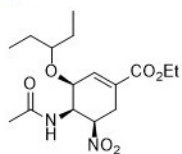
STANDARD PROTON PARAMETERS

Sample Name:
 vs10-16B-3
 Data Collected on:
 VNMR300-vnmrs300



vs10-31B

Sample Name	vs10-31B	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr1
Date collected	2015-02-18	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1



Plotname: DEPT_01_plot01

Data file: /home/vnmr1/vnmrsys/data/vs10-31B_20150217_01/DEPT_01.fid

Plot date: 2015-02-18

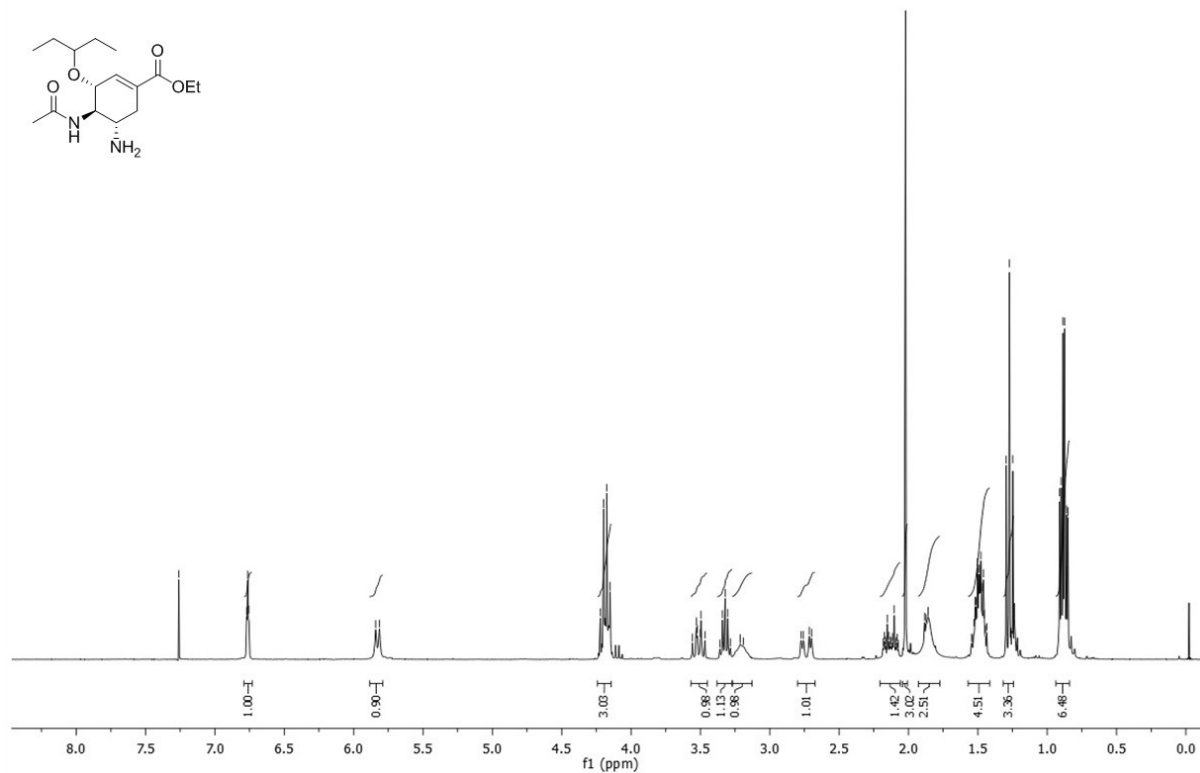
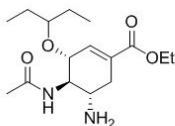
vs-63-5b

7.26

6.77
6.76
6.76

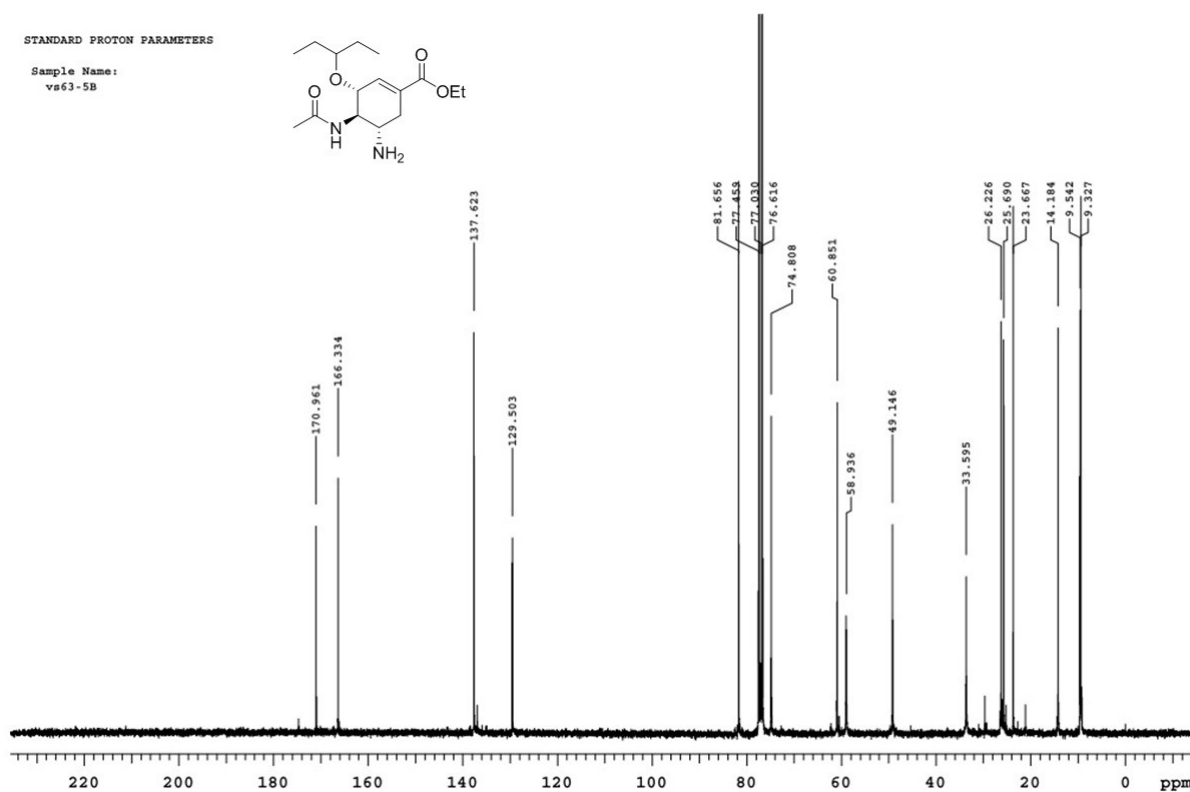
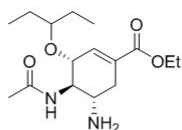
5.84
5.81

4.22
4.20
4.17
4.15
3.56
3.53
3.52
3.50
3.49
3.47
3.34
3.32
3.30
3.27
3.26
3.22
3.20
2.17
2.15
2.13
2.10
2.02
1.88
1.87
1.86
1.50
1.49
1.48
1.35
1.27
1.25
0.90
0.89
0.87
0.86
0.85



STANDARD PROTON PARAMETERS

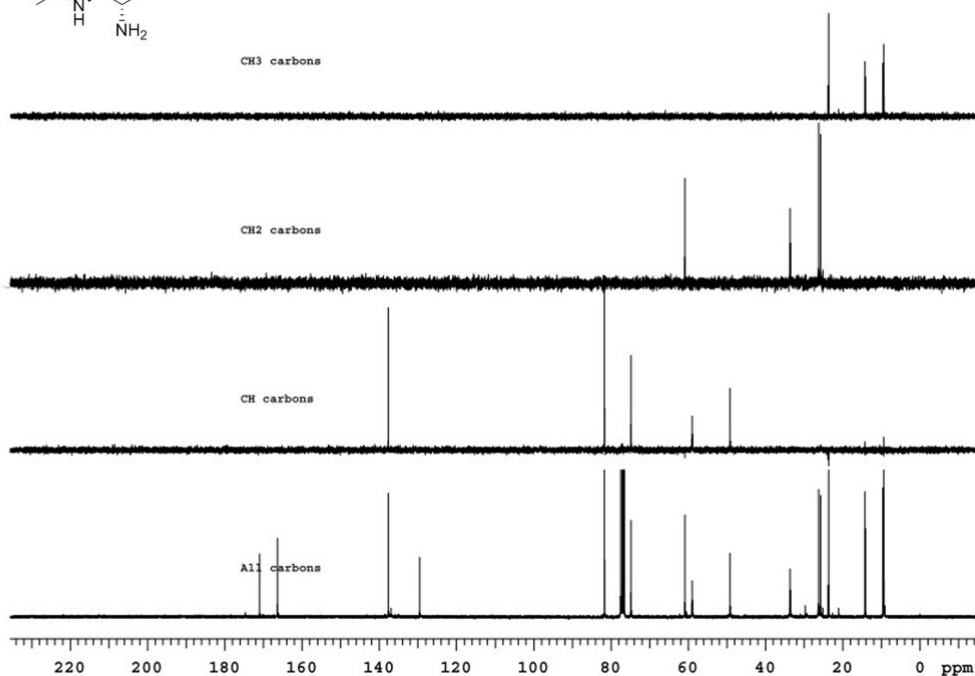
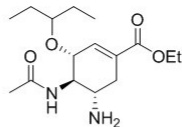
Sample Name:
vs63-5B



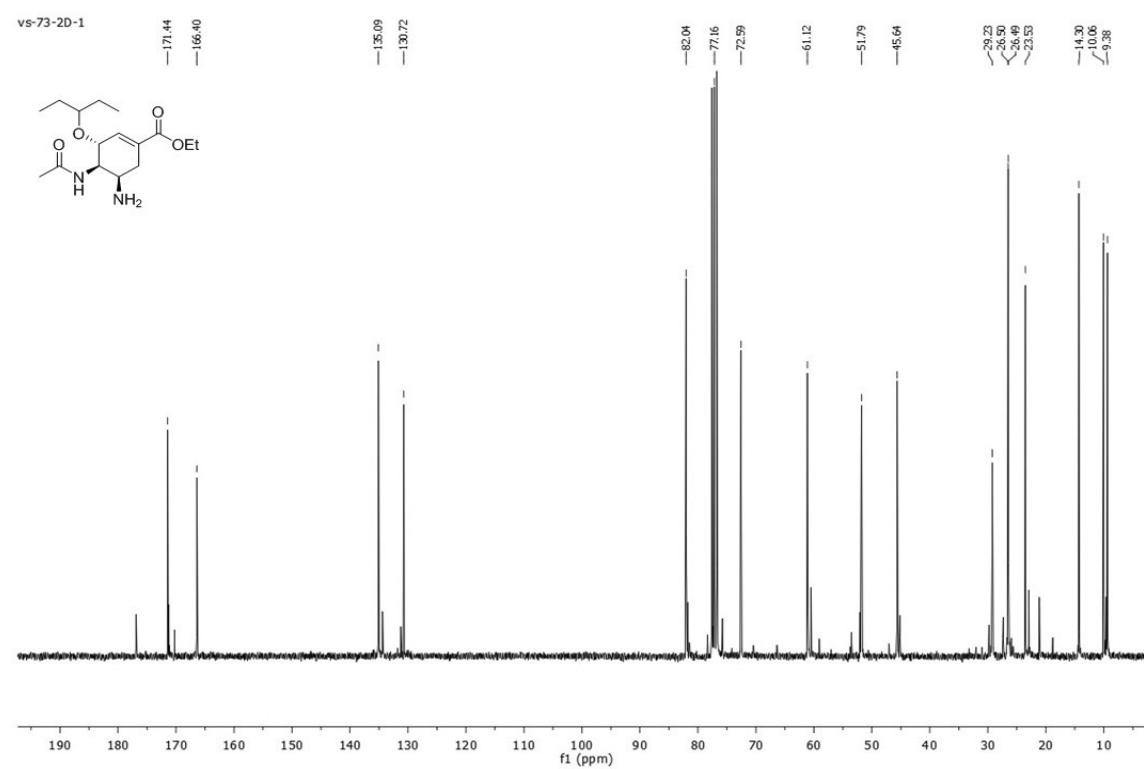
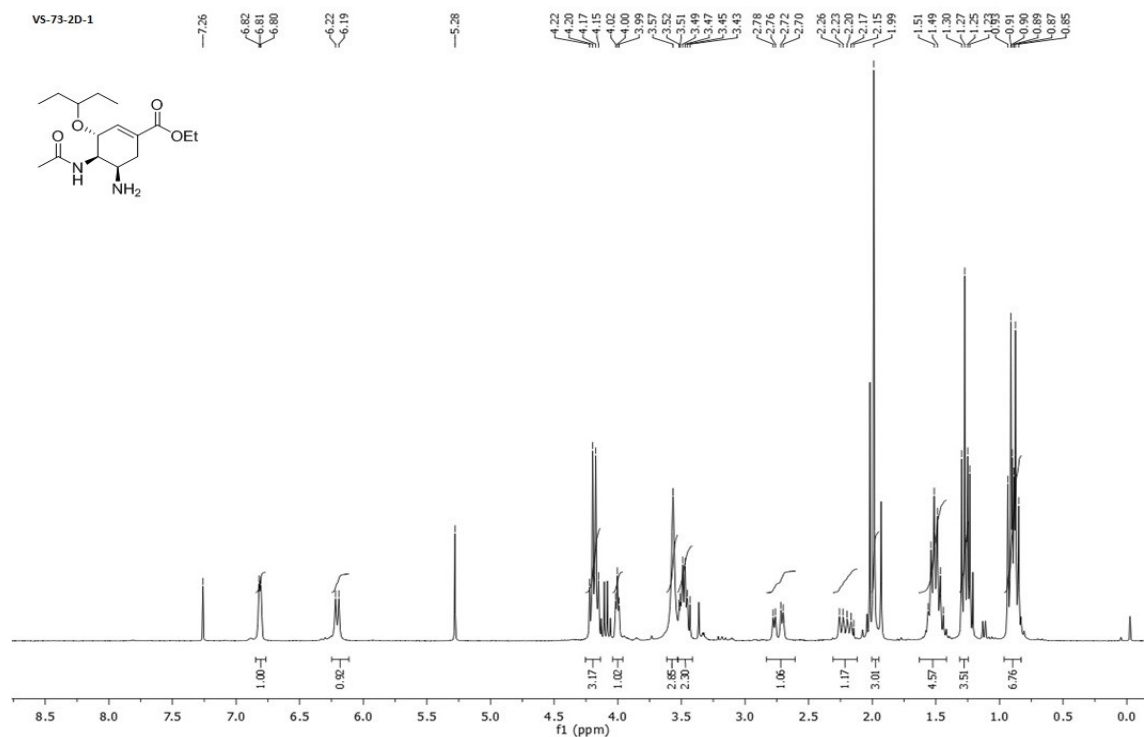
Plotname: CARBON_001_plot01

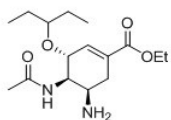
STANDARD PROTON PARAMETERS

Sample Name:
vs63-5B
Data Collected on:
VNMRS300-vnmrs300



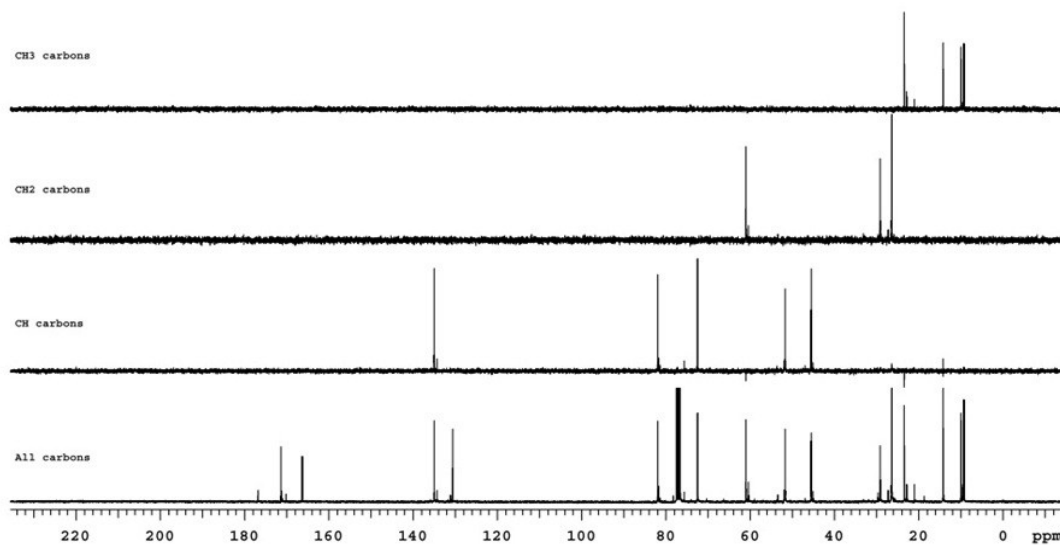
Plotname: DEPT_001_plot01





vs73-2D1

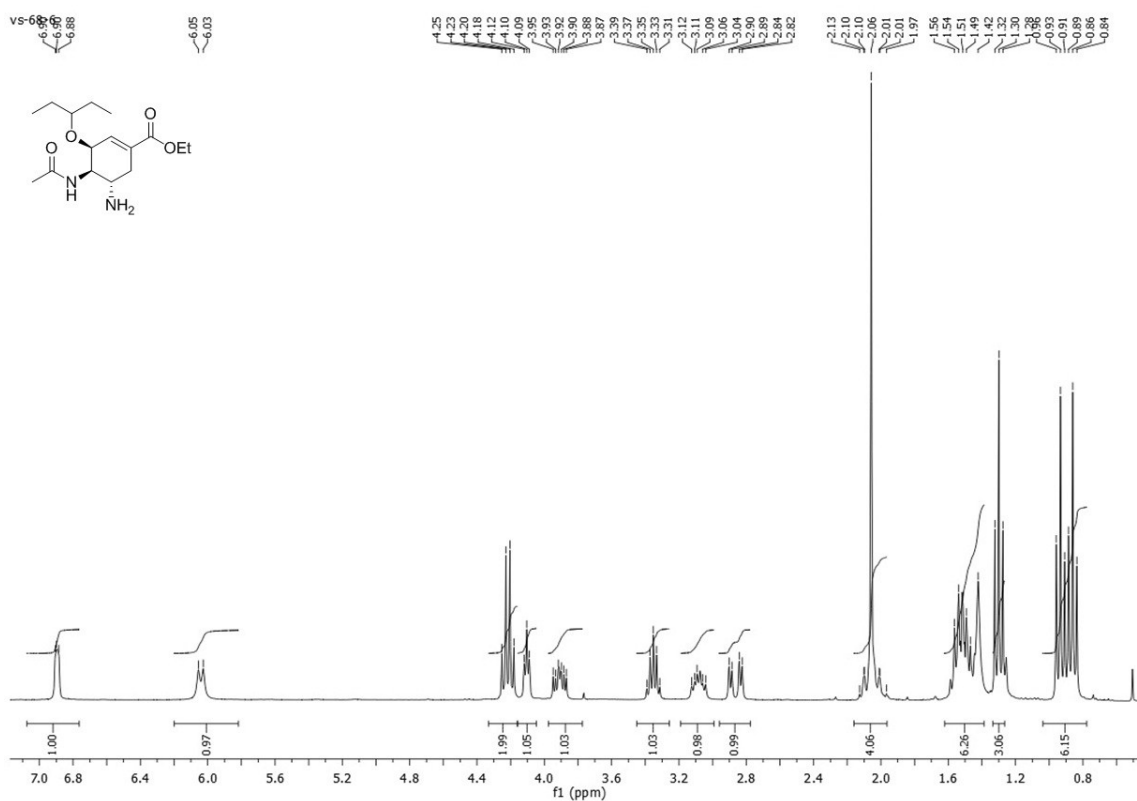
Sample Name	vs73-2D1	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr1
Date collected	2015-02-20	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1

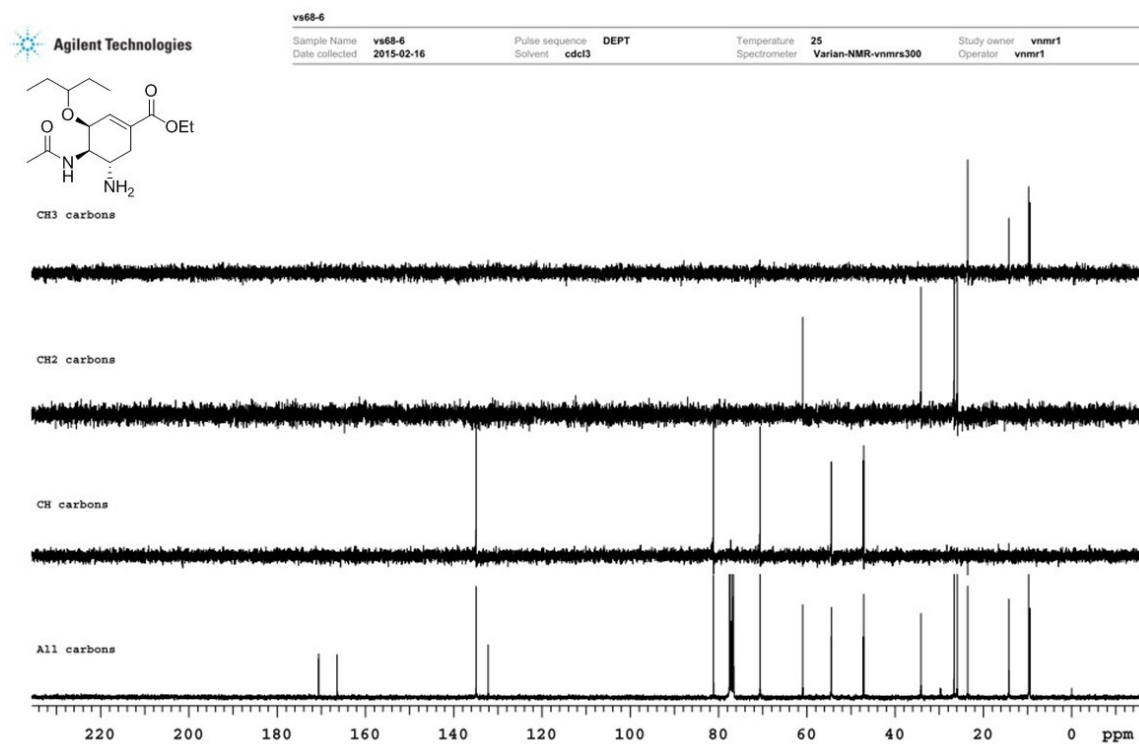
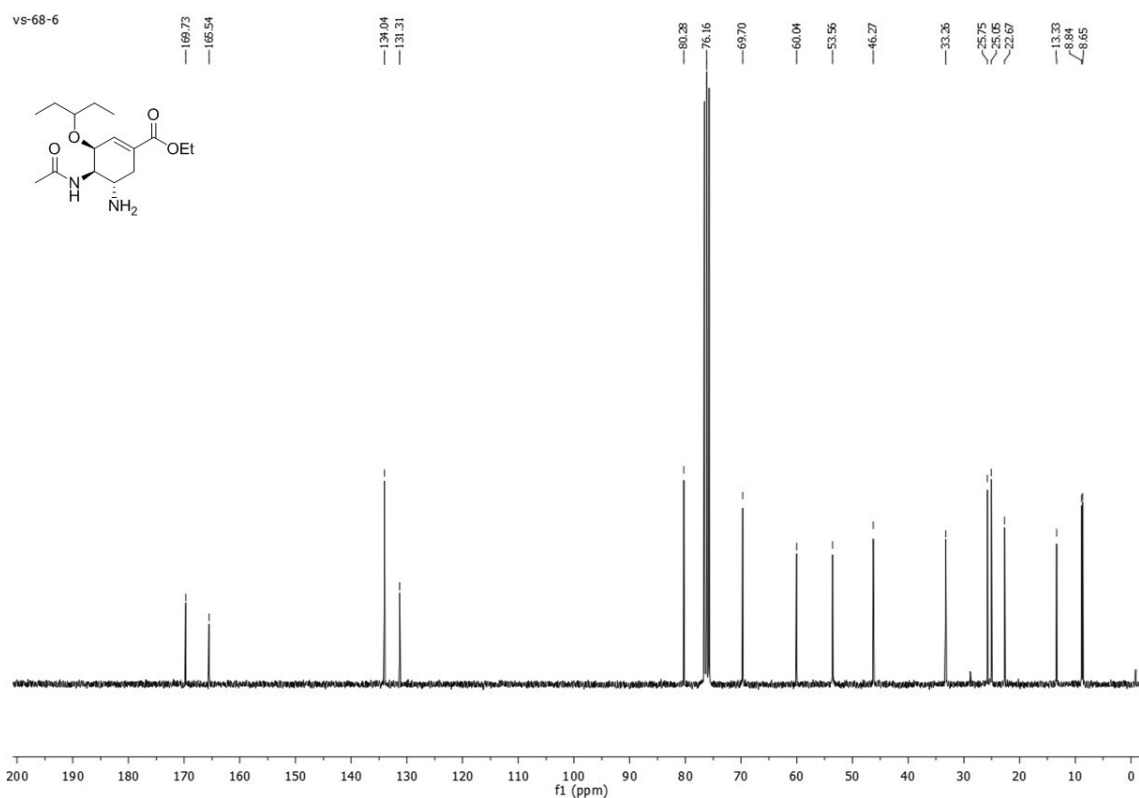


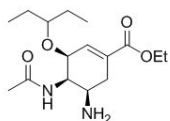
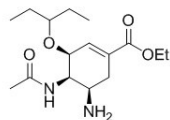
Plotname: DEPT_01_plot01

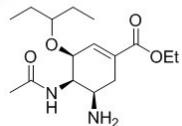
Data file: /home/vnmr1/vnmrsys/data/vs73-2D1_20150219_01/DEPT_01.f2

Plot date: 2015-02-20









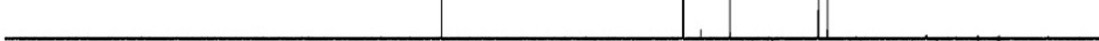
CH3 carbons



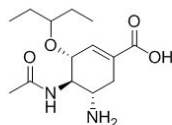
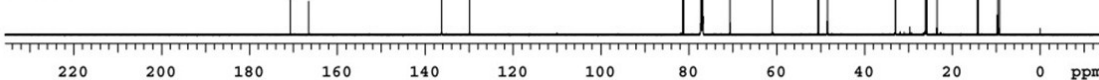
CH2 carbons



CH carbons

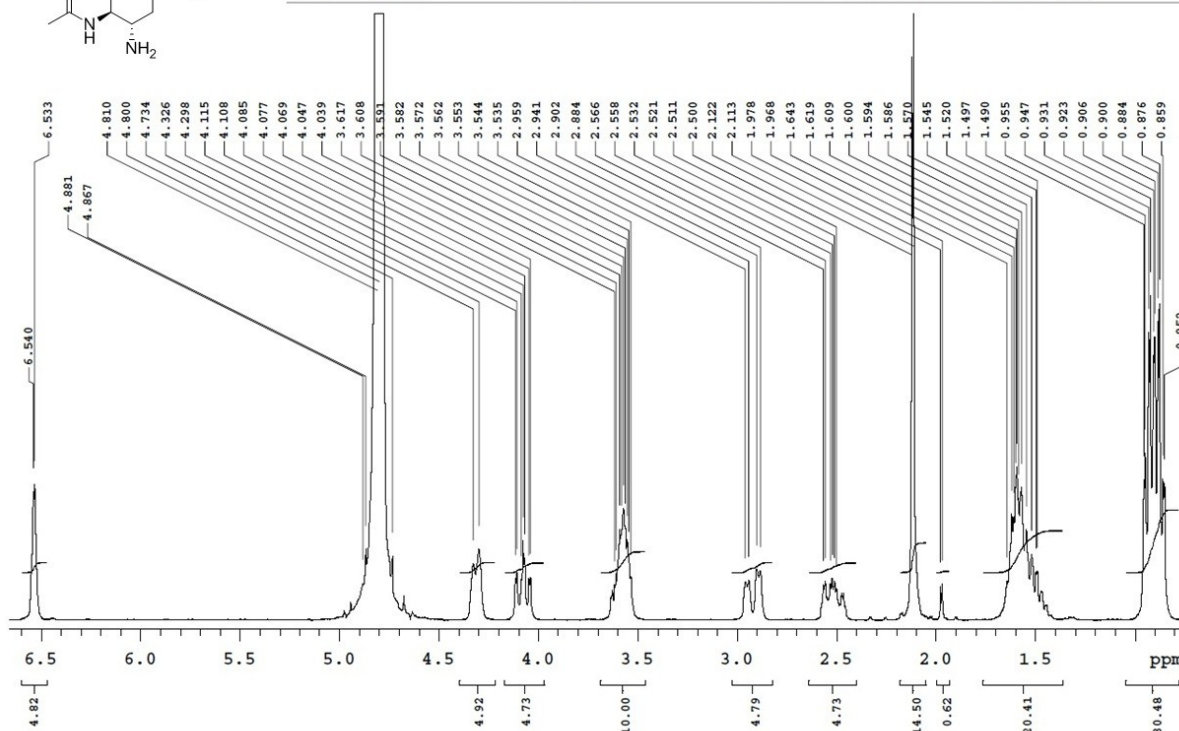


All carbons

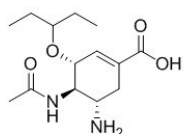
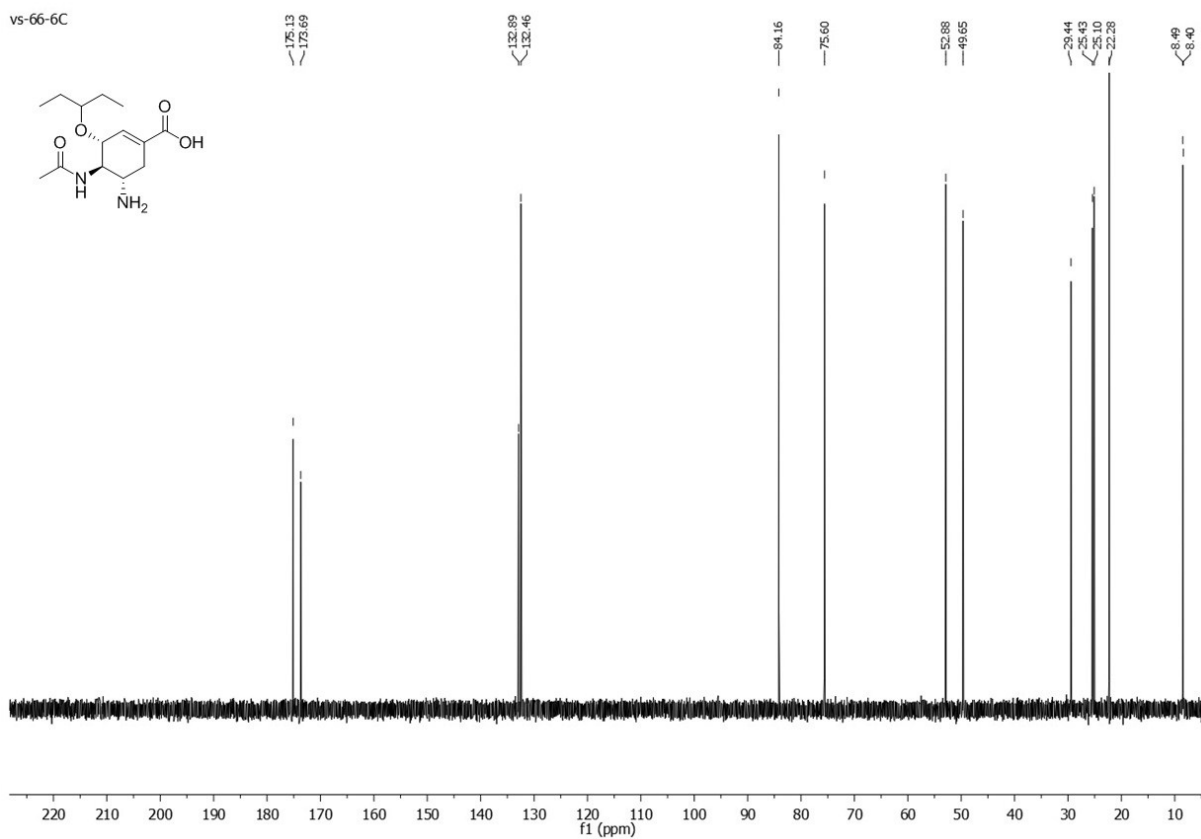
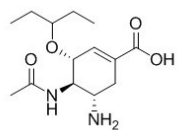


vs66-6C

Sample Name	vs66-6C	Pulse sequence	PROTON	Temperature	25	Study owner	vnmr1
Date collected	2015-03-03	Solvent	d2o	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1

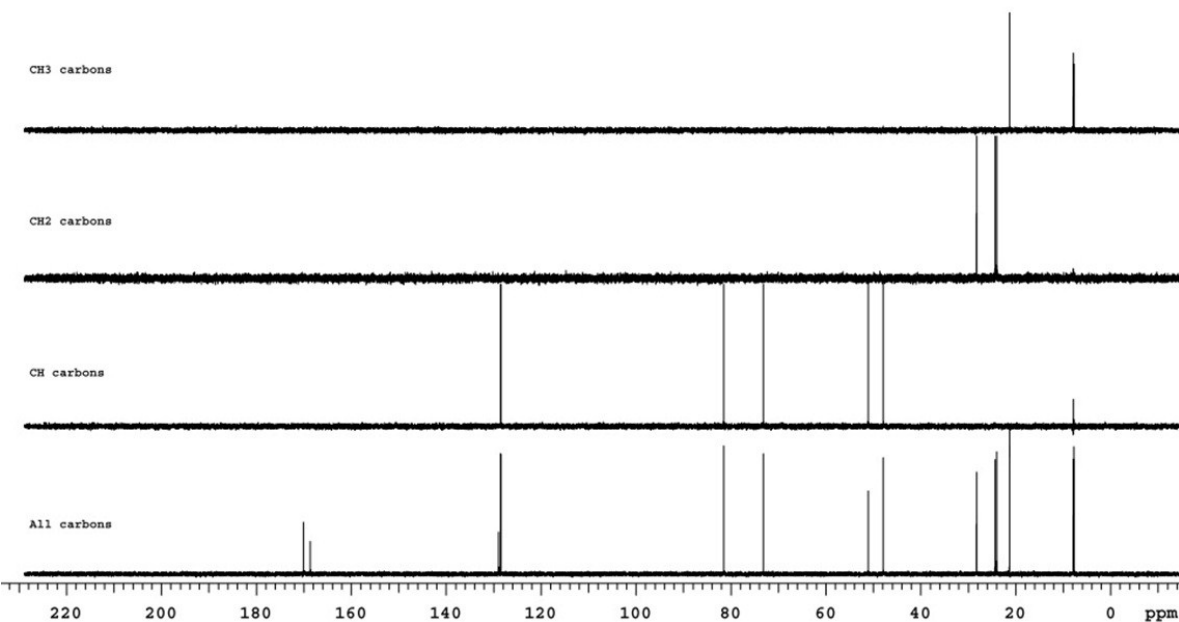


vs-66-6C

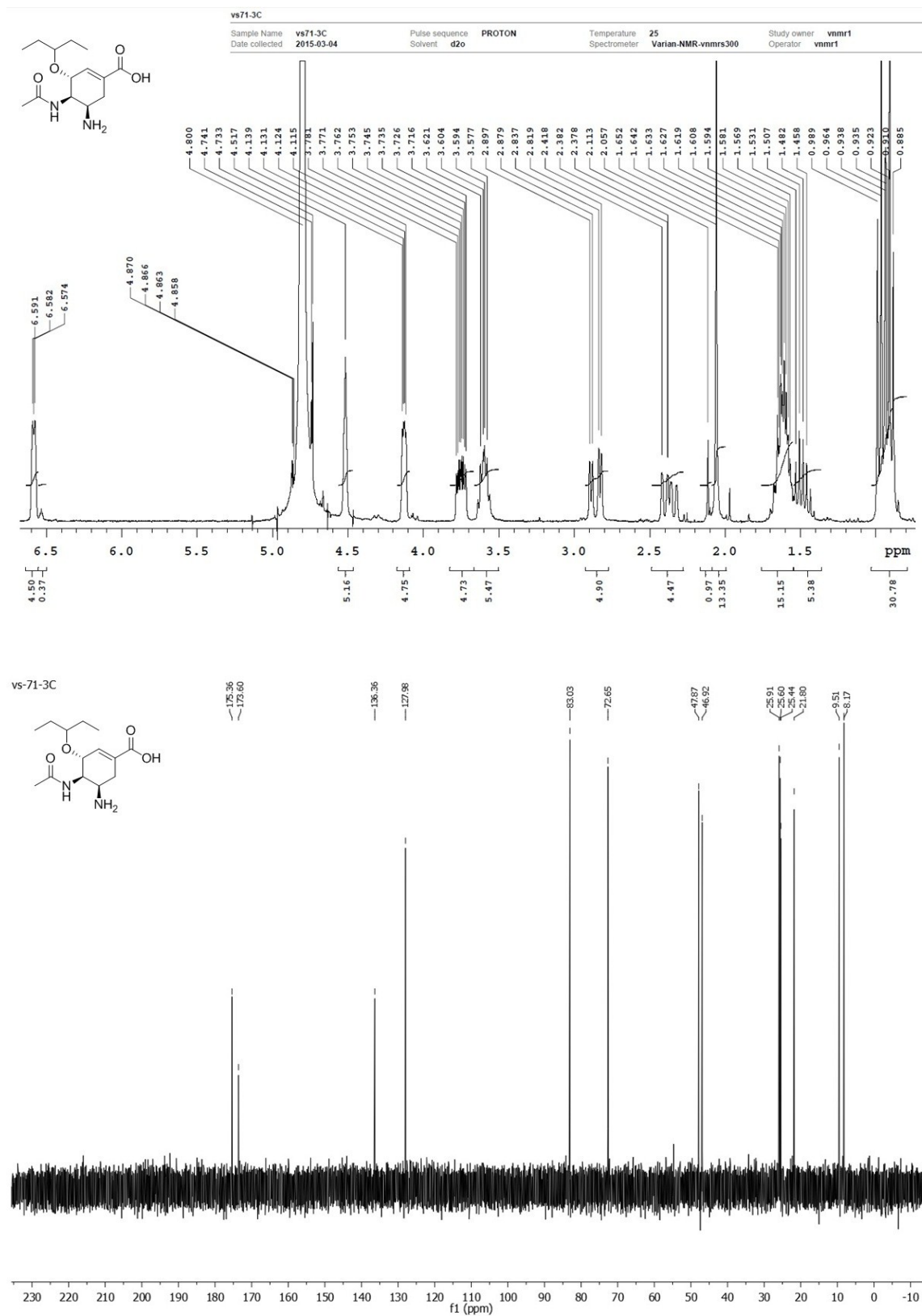


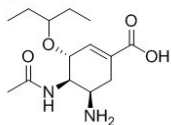
vs66-6c

Sample Name	vs66-6c	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr1
Date collected	2015-03-04	Solvent	d2o	Spectrometer	Varian-NMR-vnmrs600	Operator	vnmr1



Plotname: DEPT_01_plot01



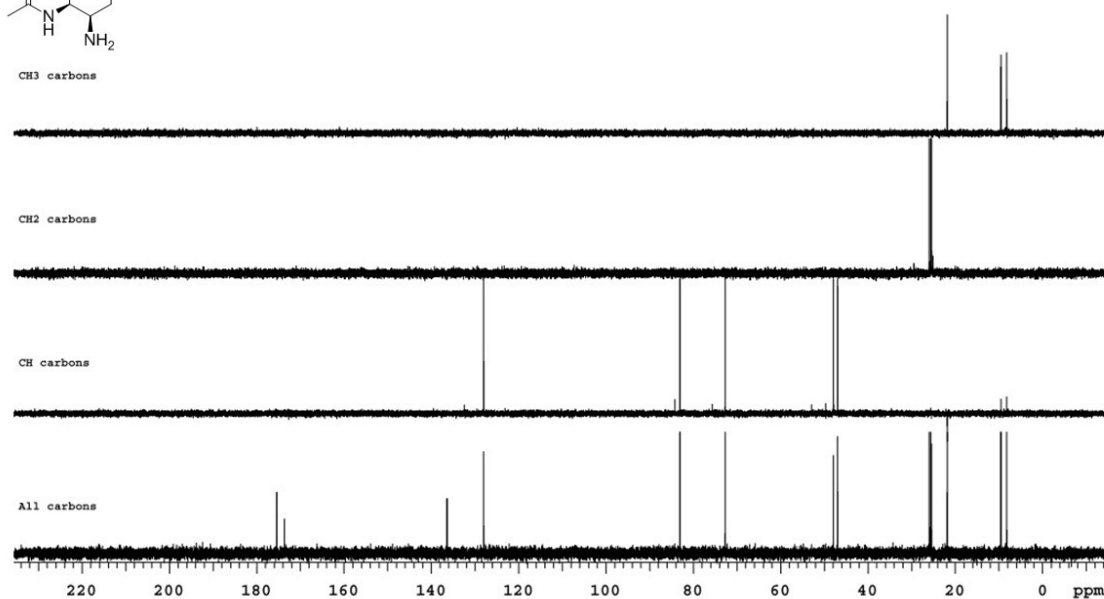


CH3 carbons

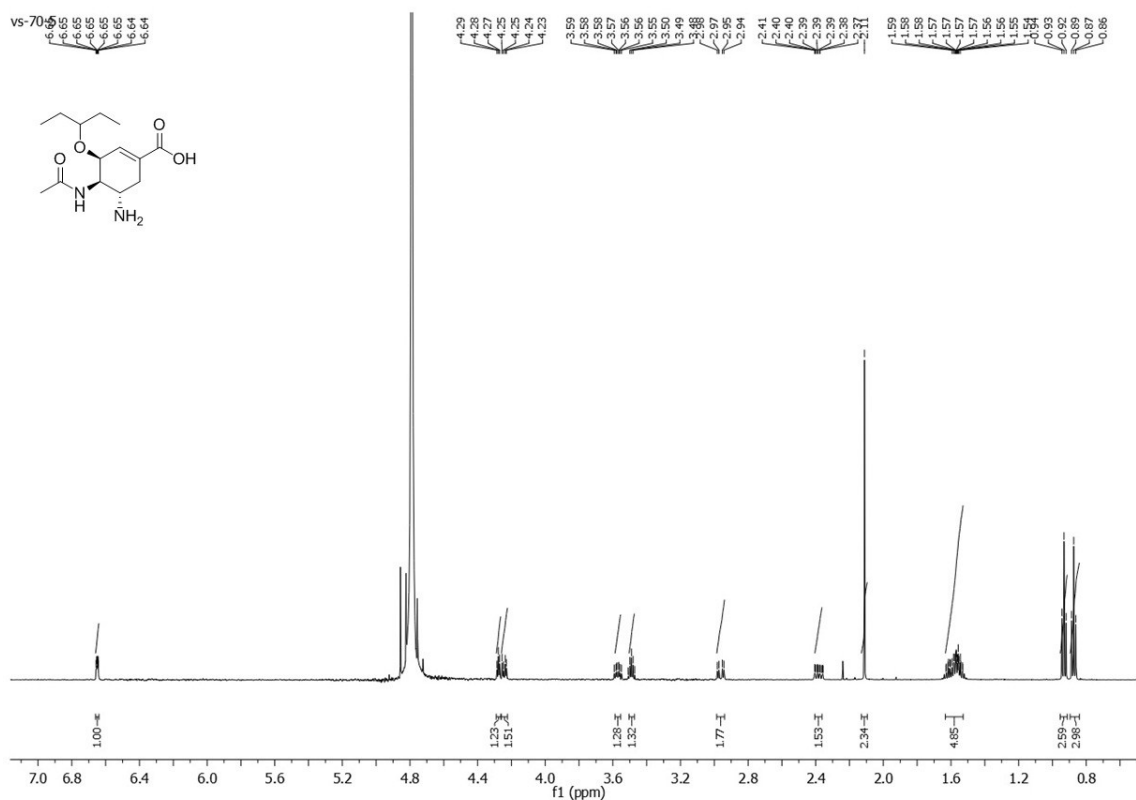
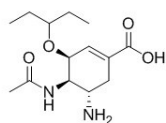
CH2 carbons

CH carbons

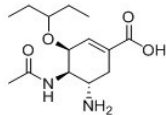
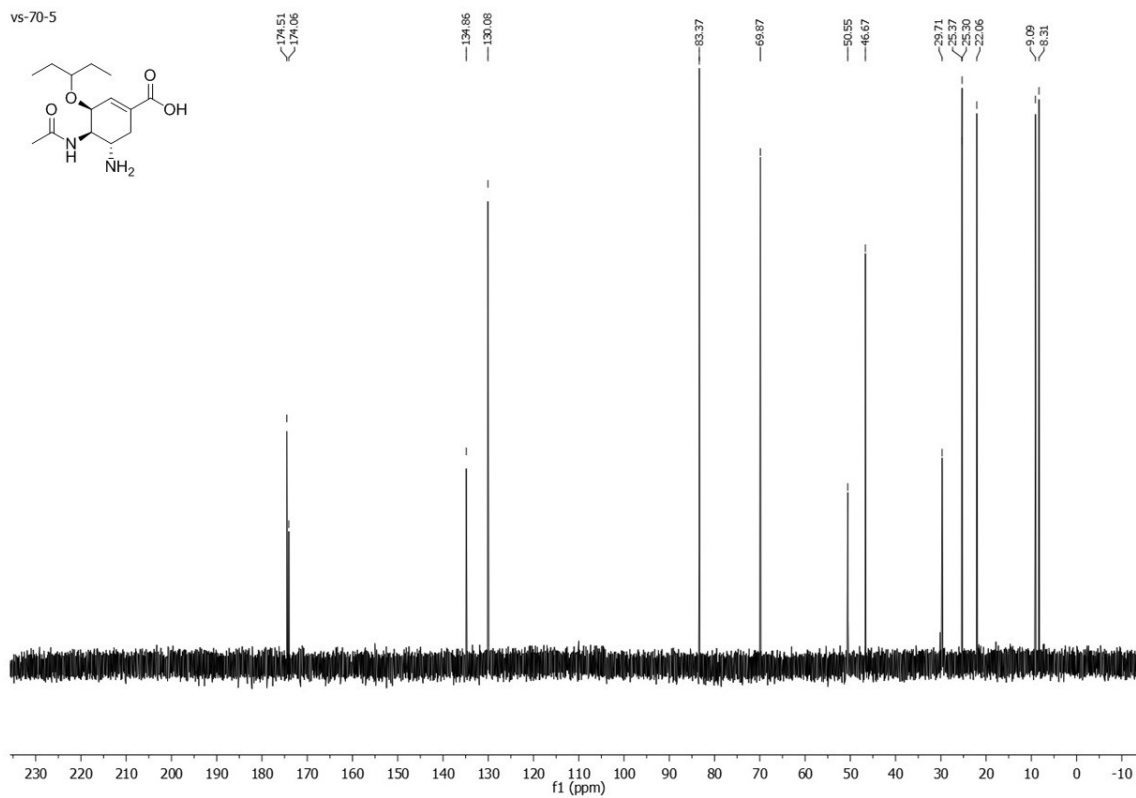
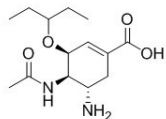
All carbons



VS-70-6



vs-70-5



vs70-5

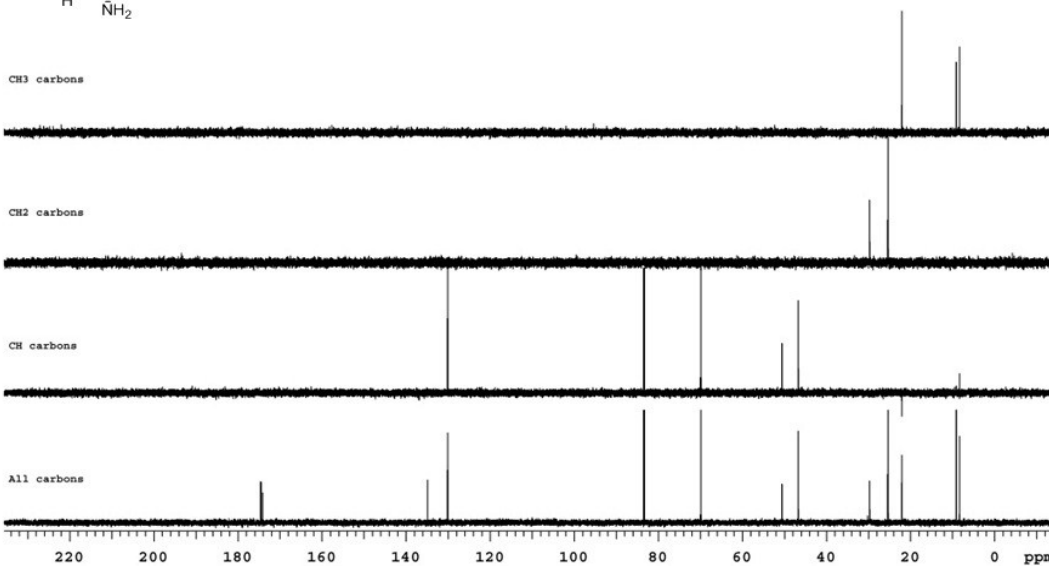
Sample Name	vs70-5	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr1
Date collected	2015-02-22	Solvent	d2o	Spectrometer	Varian-NMR-vnmrs600	Operator	vnmr1

CH3 carbons

CH2 carbons

CH carbons

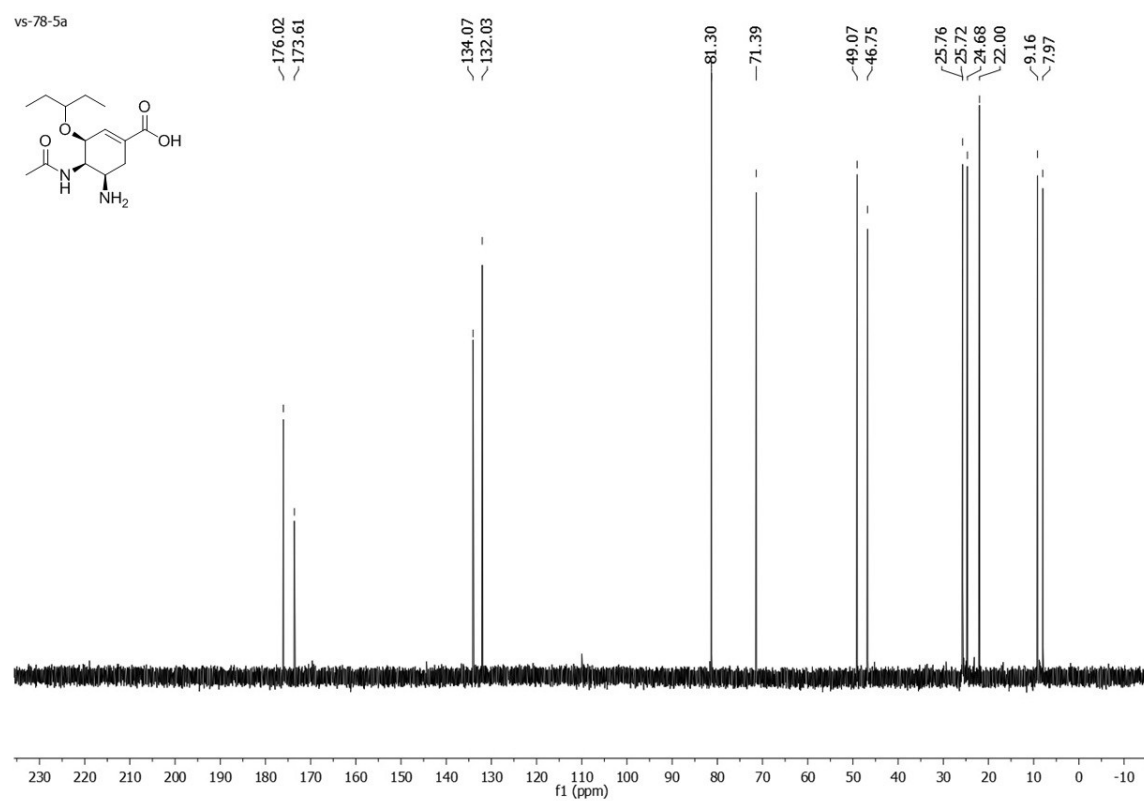
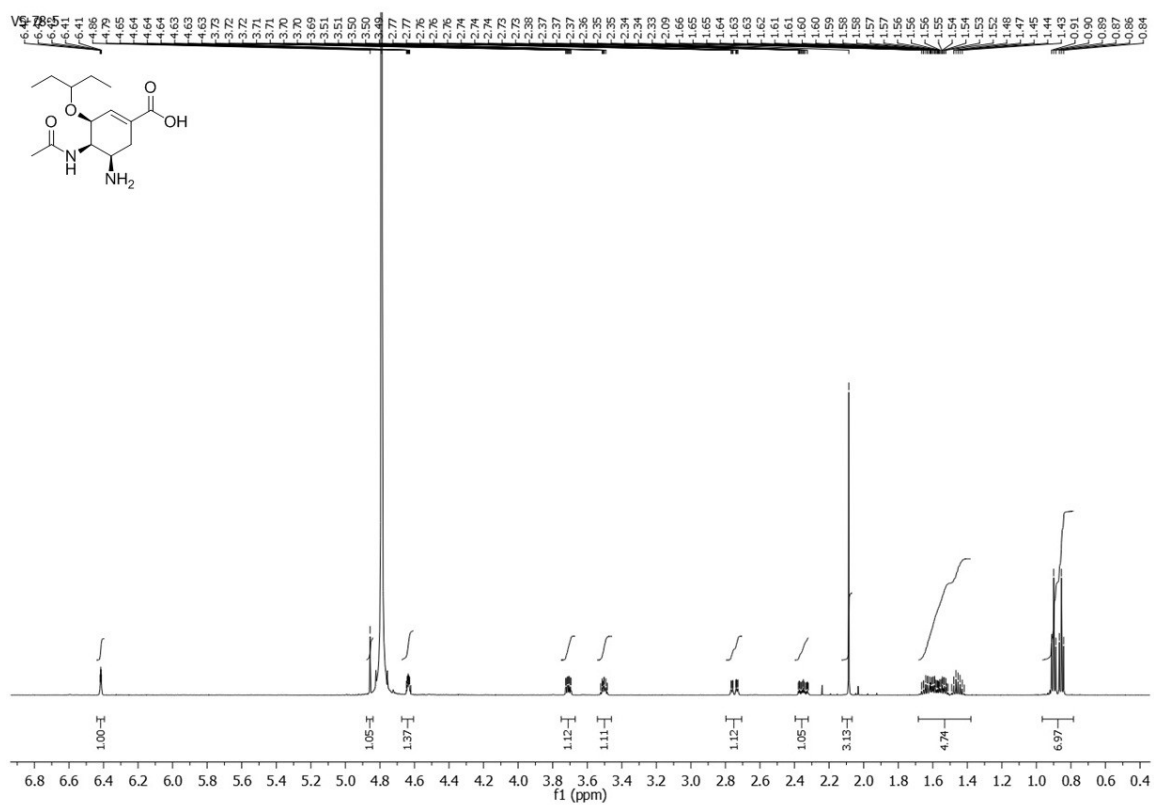
All carbons

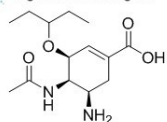


Plotname: DEPT_01_plot01

Data file /home/vnmr1/vnmrsys/data/vs70-5_20150220_01/DEPT_01.fid

Plot date 2015-02-23





vs78-5a

Sample Name	vs78-5a	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr1
Date collected	2015-03-25	Solvent	d2o	Spectrometer	Varian-NMR-vnmrs600	Operator	vnmr1

CH3 carbons



CH2 carbons



CH carbons

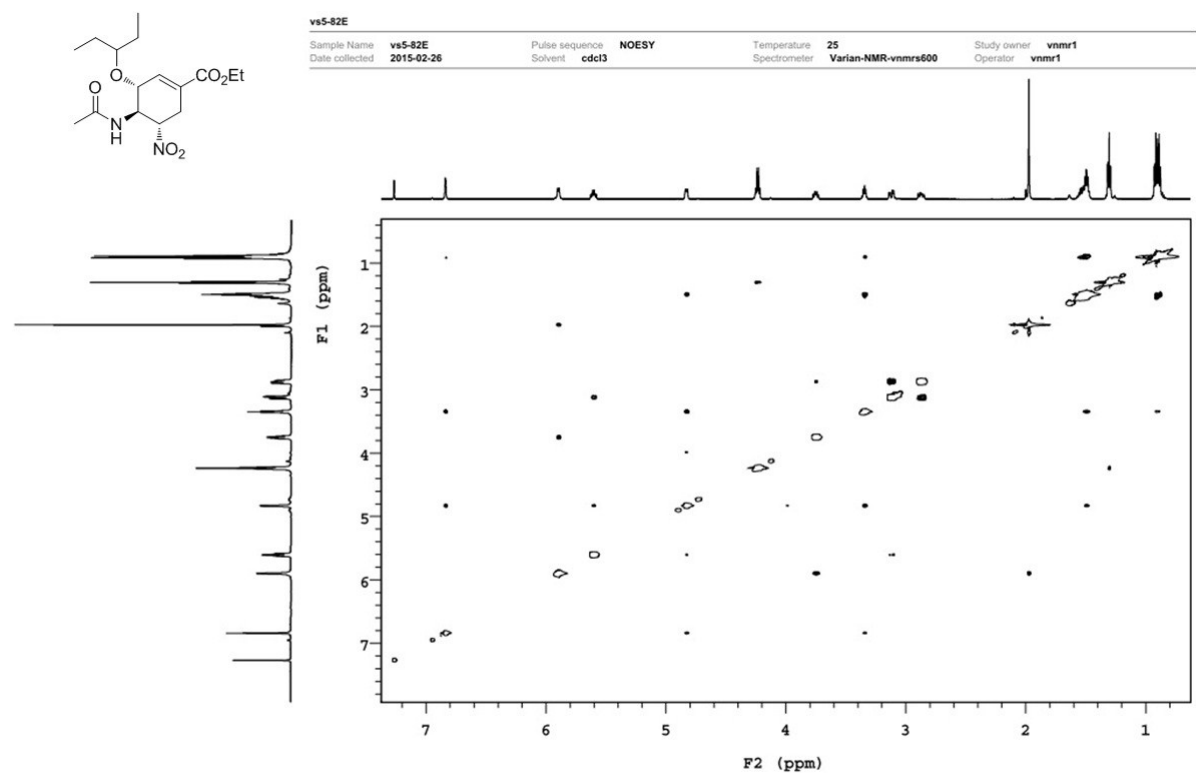
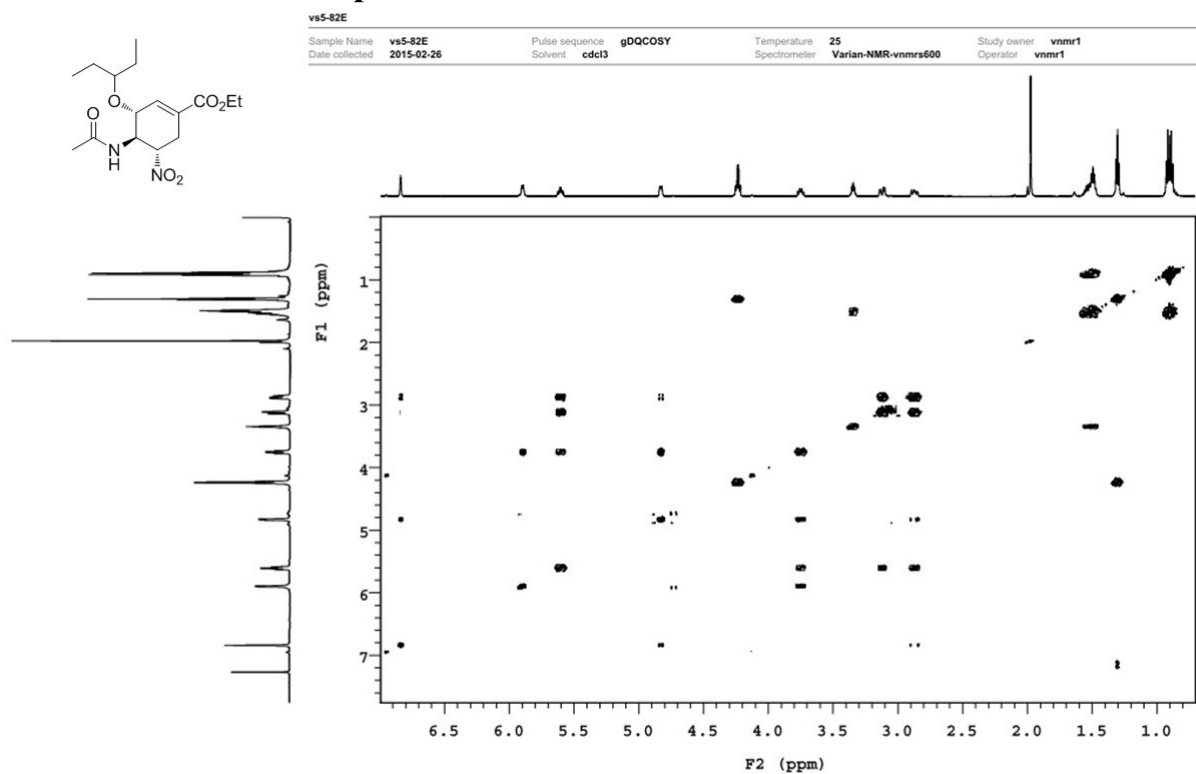


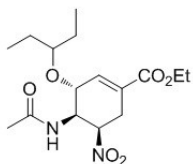
All carbons



220 200 180 160 140 120 100 80 60 40 20 0 ppm

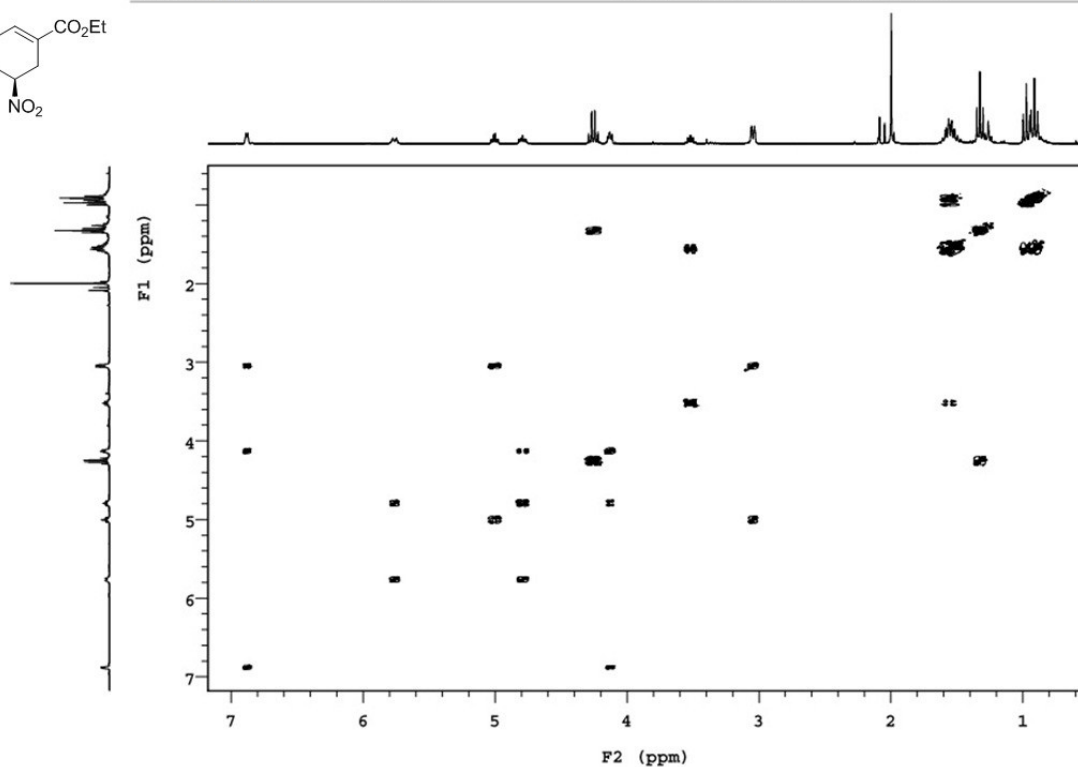
Pictures of 2D NMR spectra





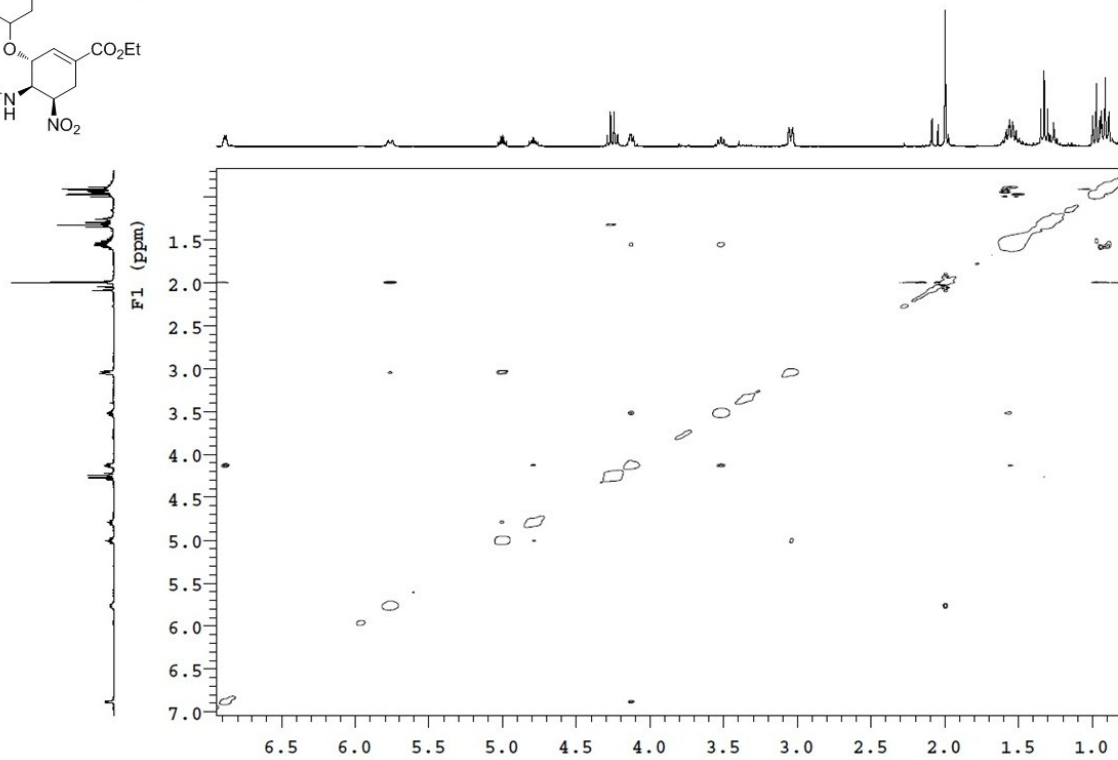
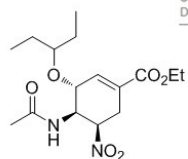
Vs-5-82c

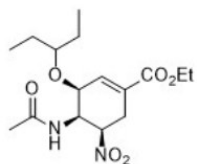
Sample Name	Vs-5-82c	Pulse sequence	gDQCOSY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-13	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1



Vs-5-82c

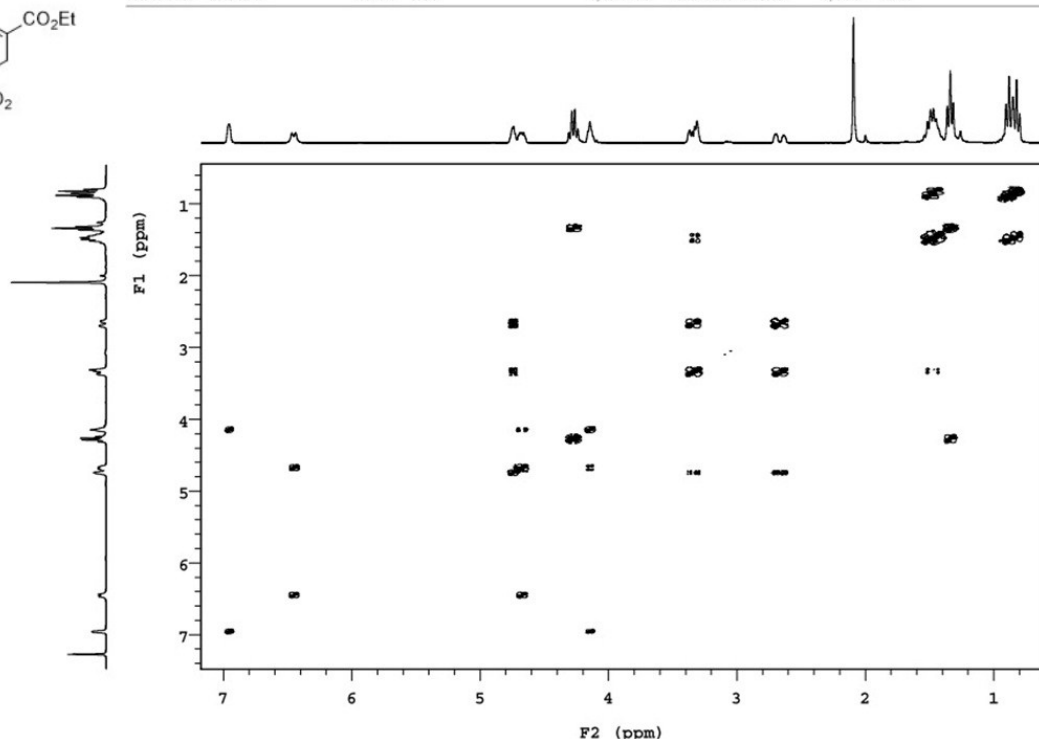
Sample Name	Vs-5-82c	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-13	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1



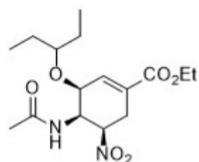


vs10-31B

Sample Name	vs10-31B	Pulse sequence	gDQCOSY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-17	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1

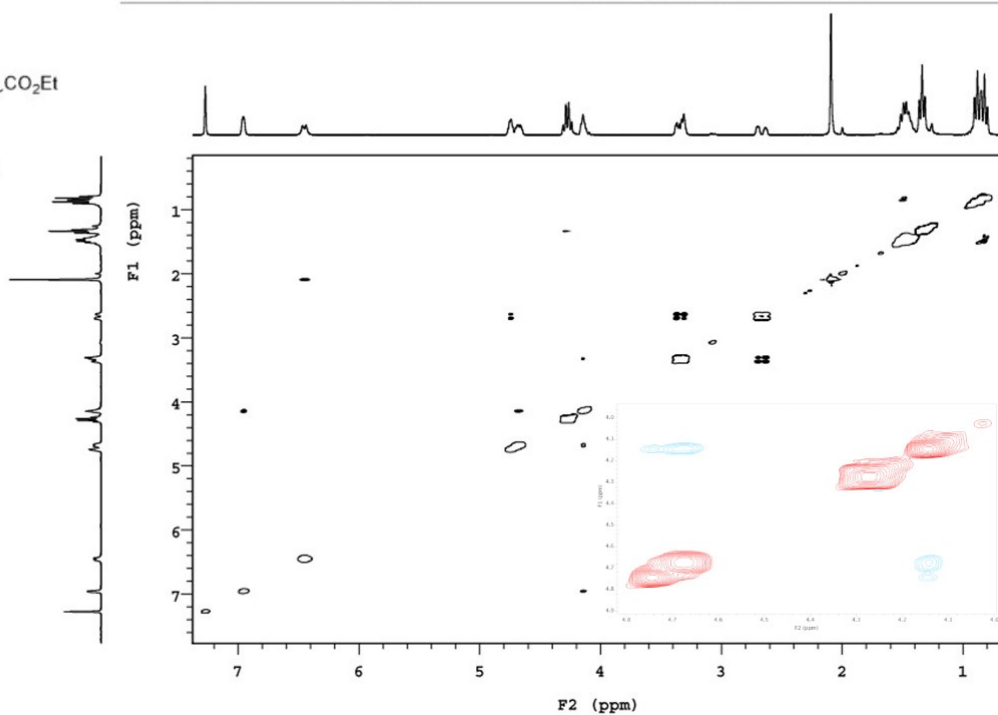


Agilent Technologies

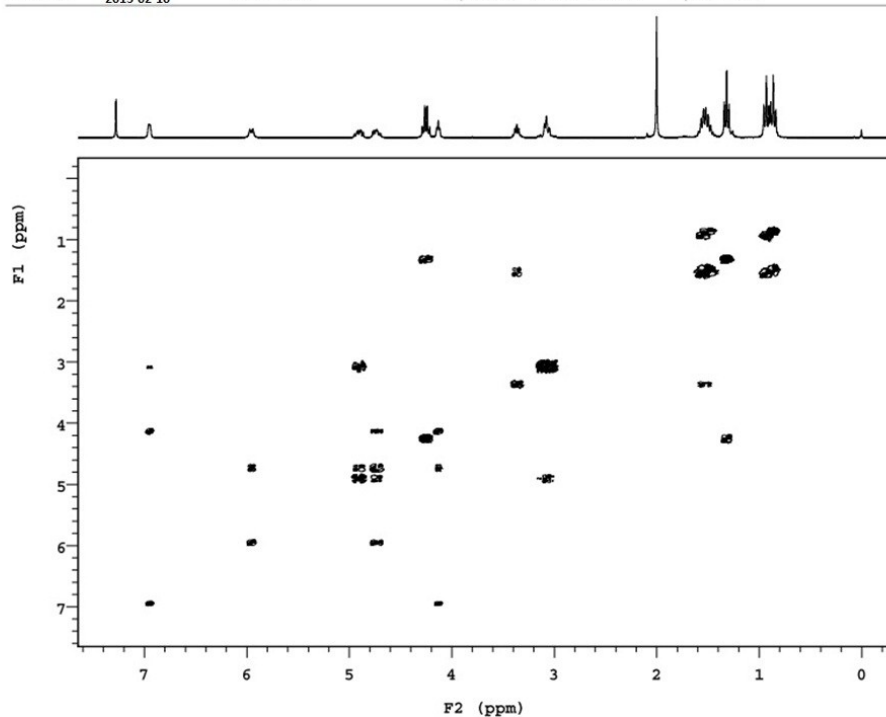
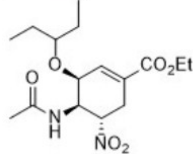


vs10-31B

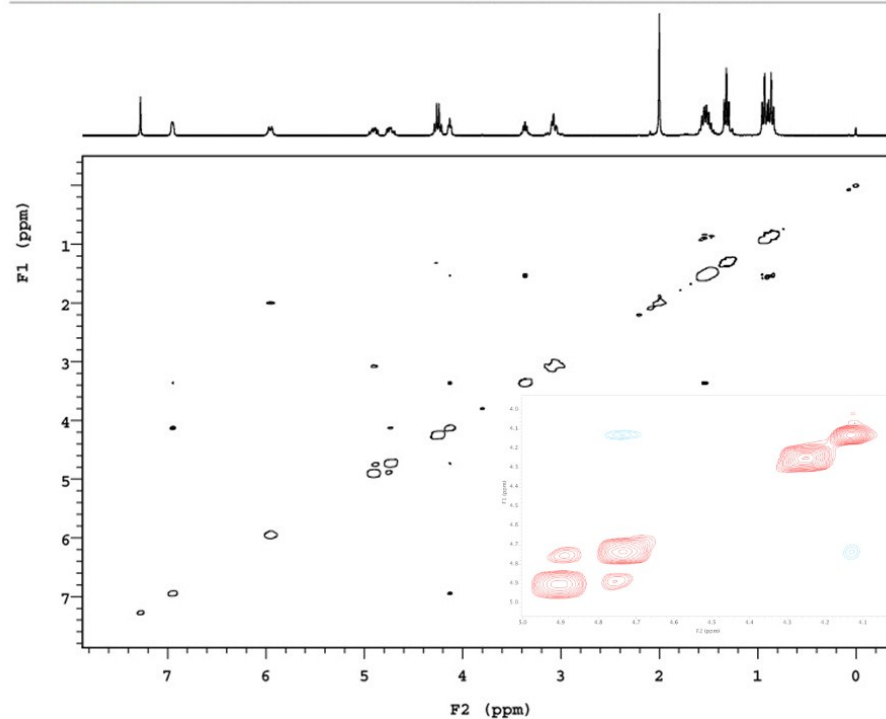
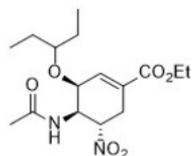
Sample Name	vs10-31B	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-17	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1



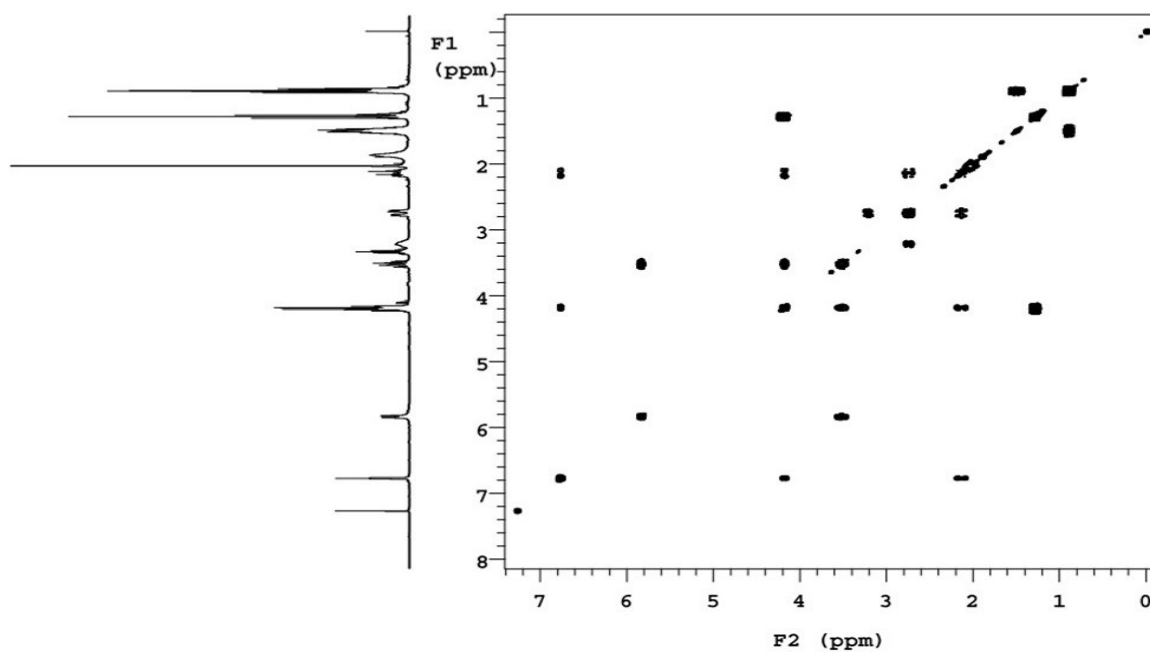
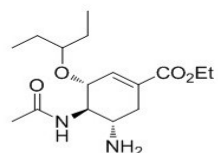
Sample Name	Vs-10-31A	Pulse sequence	gDQCOSY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-10	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1



Sample Name	Vs-10-31A	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-10	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1

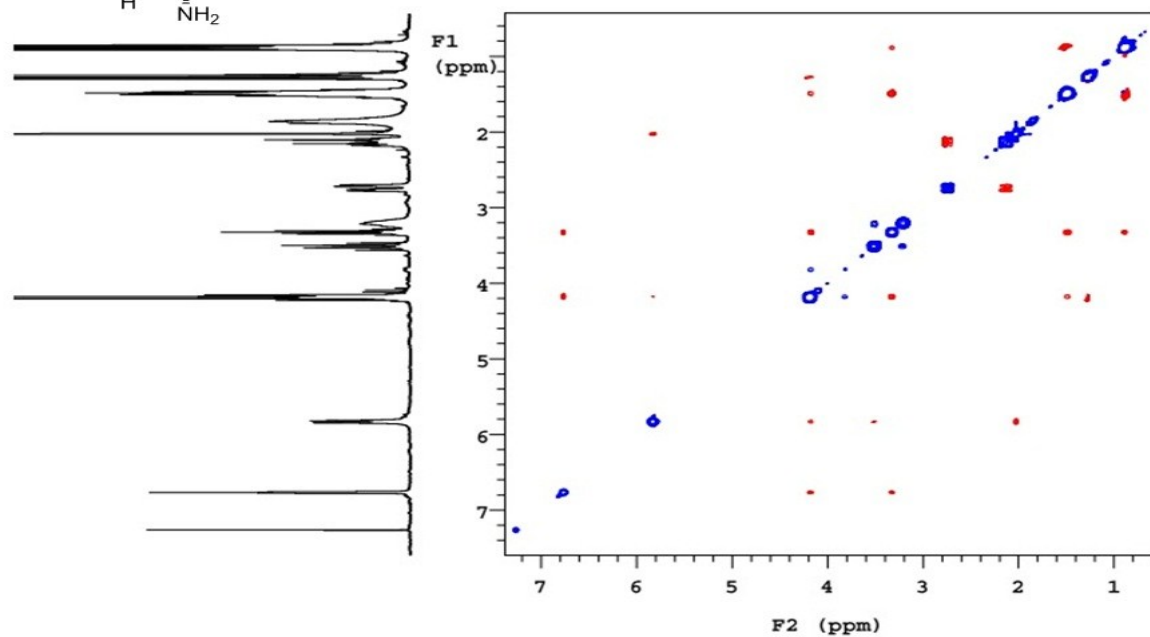
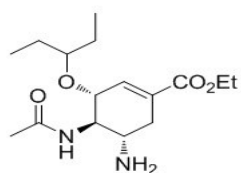


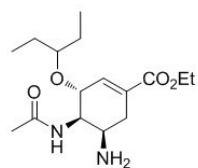
Sample Name:
vs63-5B
Data Collected on:
VNMR300-vnmrs300



STANDARD PROTON PARAMETERS

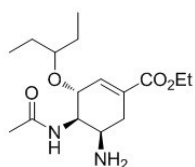
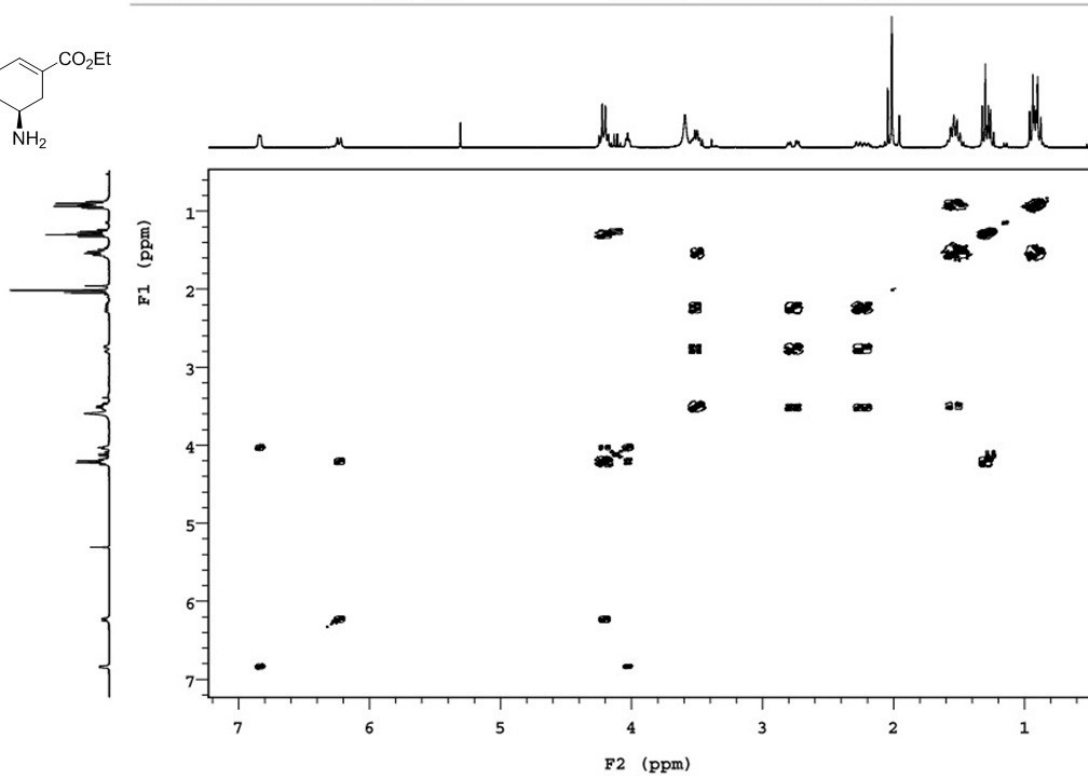
Sample Name:
vs63-5B
Data Collected on:
VNMR300-vnmrs300





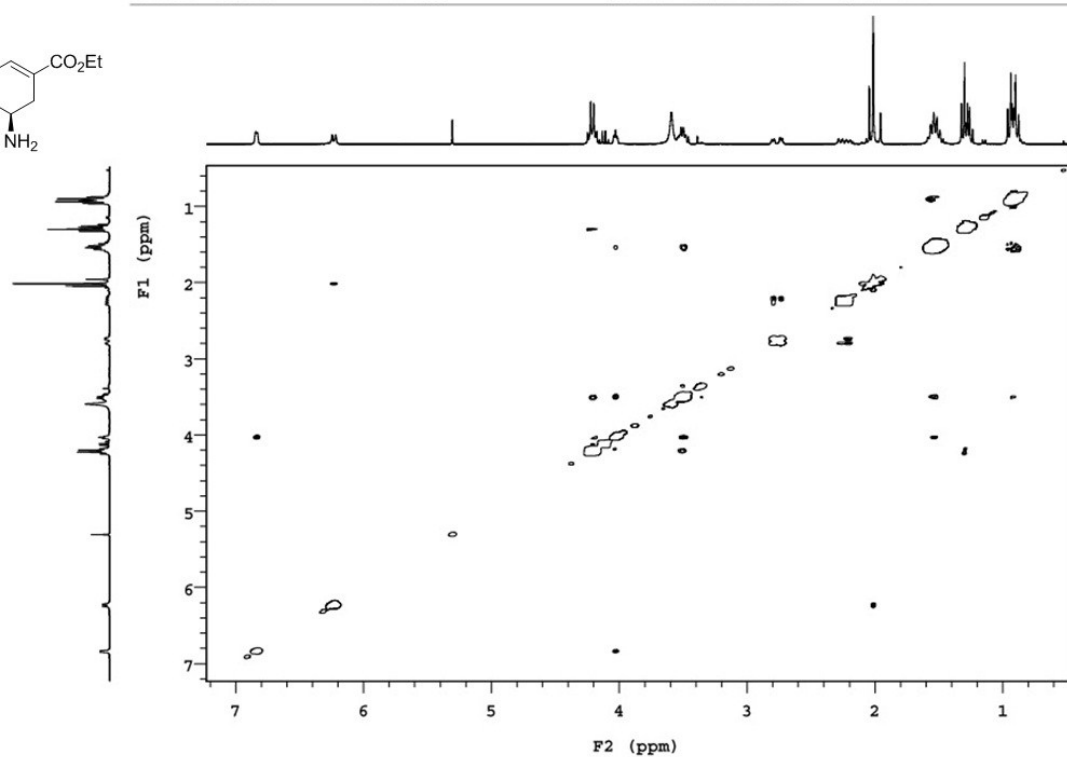
vs73-2D1

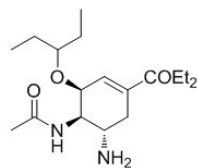
Sample Name	vs73-2D1	Pulse sequence	gDQCOSY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-19	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1



vs73-2D1

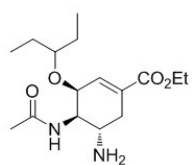
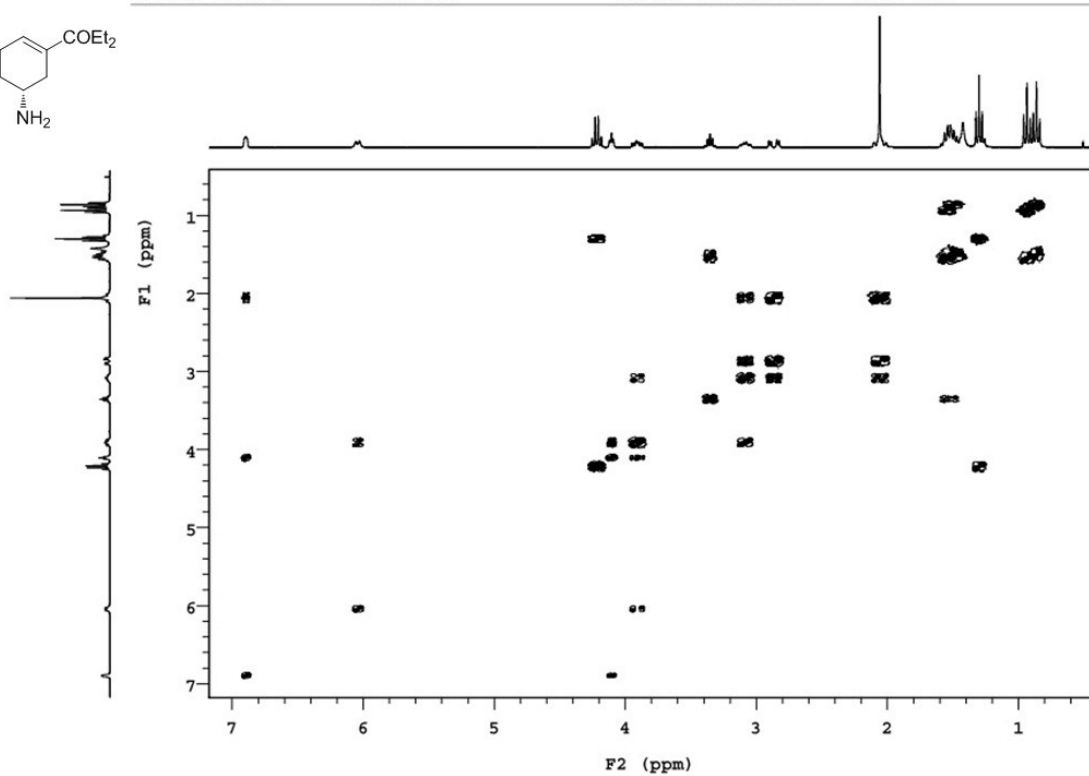
Sample Name	vs73-2D1	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-19	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1





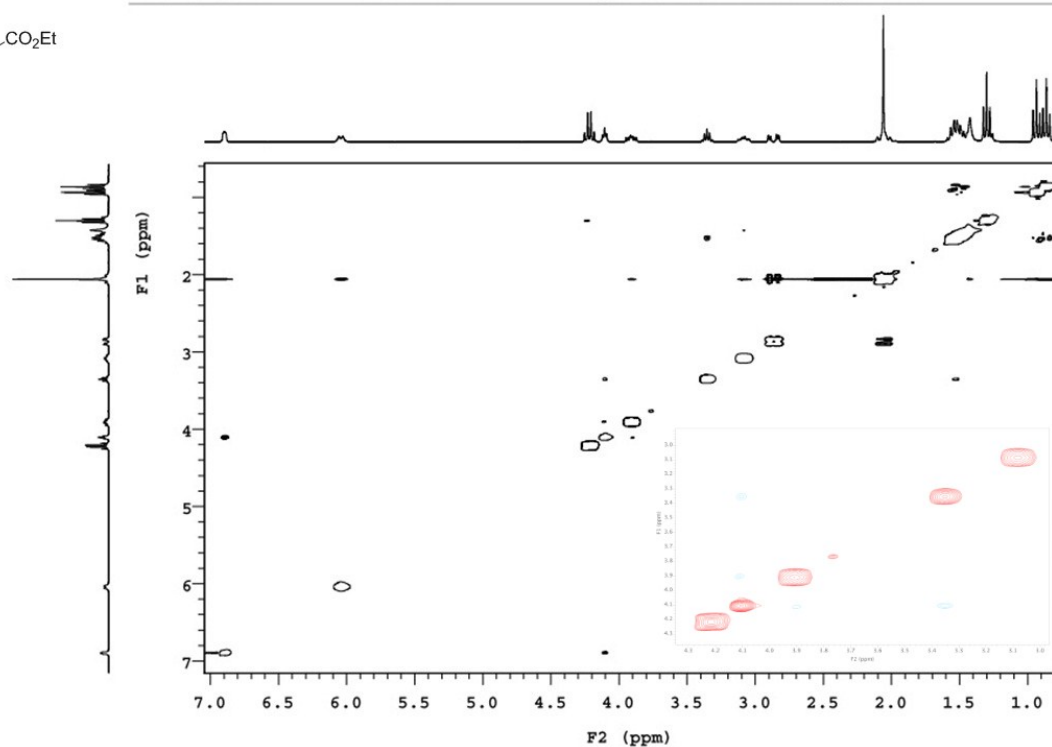
vs68-6

Sample Name	vs68-6	Pulse sequence	gDQCOSY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-16	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1



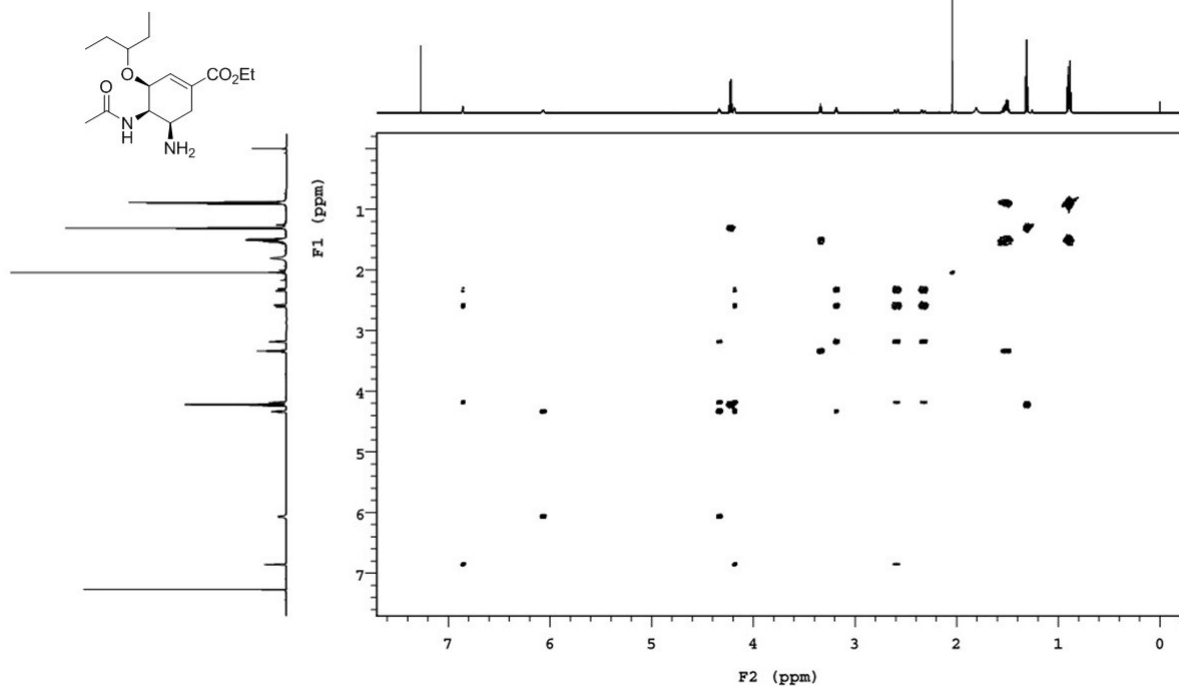
vs68-6

Sample Name	vs68-6	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-16	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs300	Operator	vnmr1



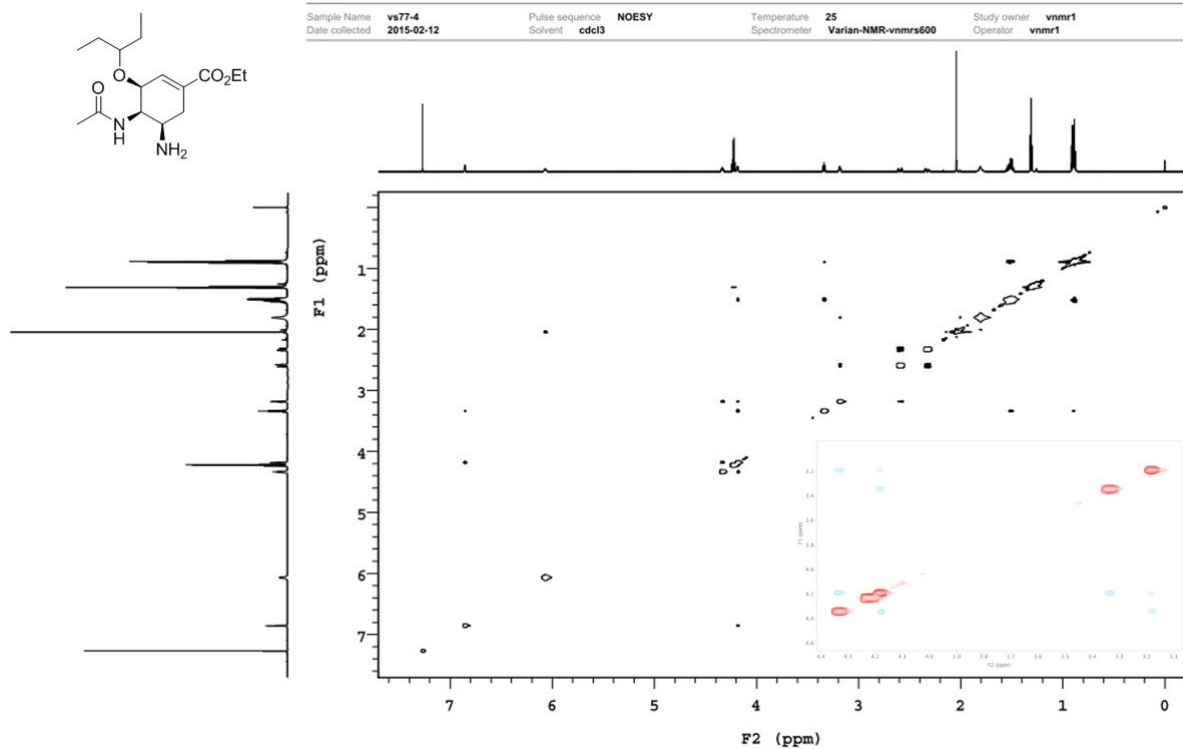
vs77-4

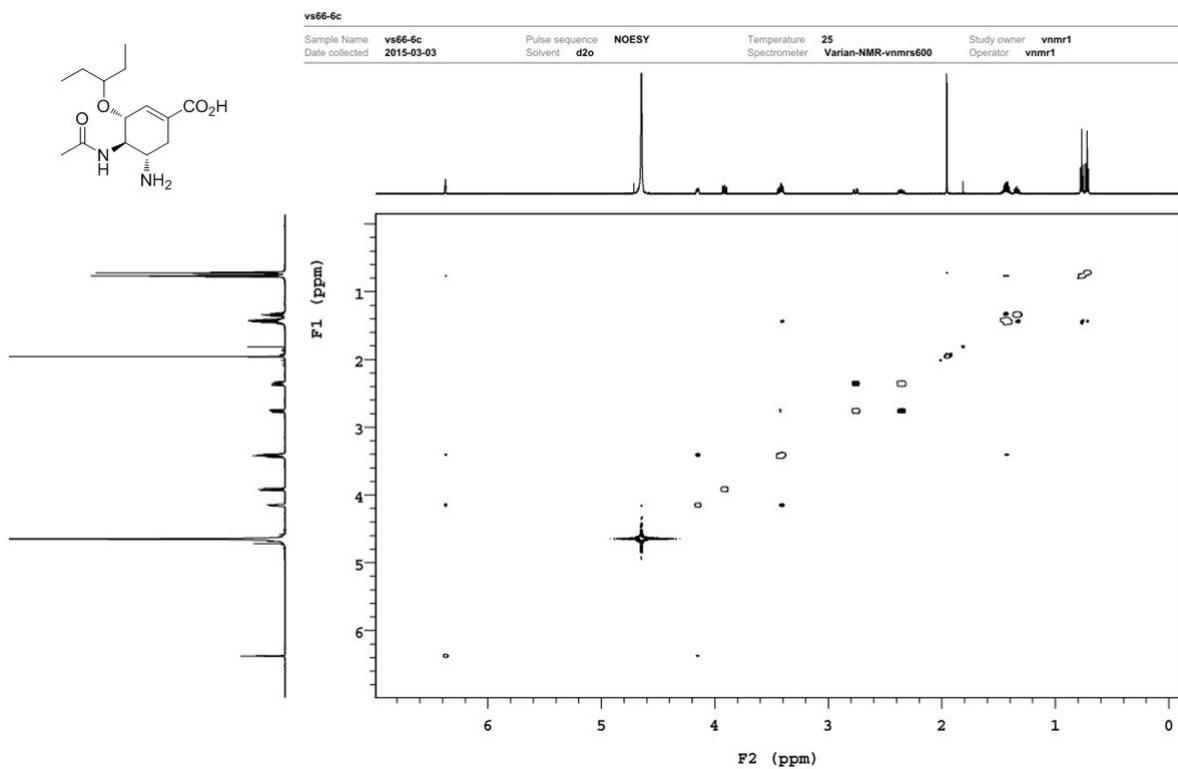
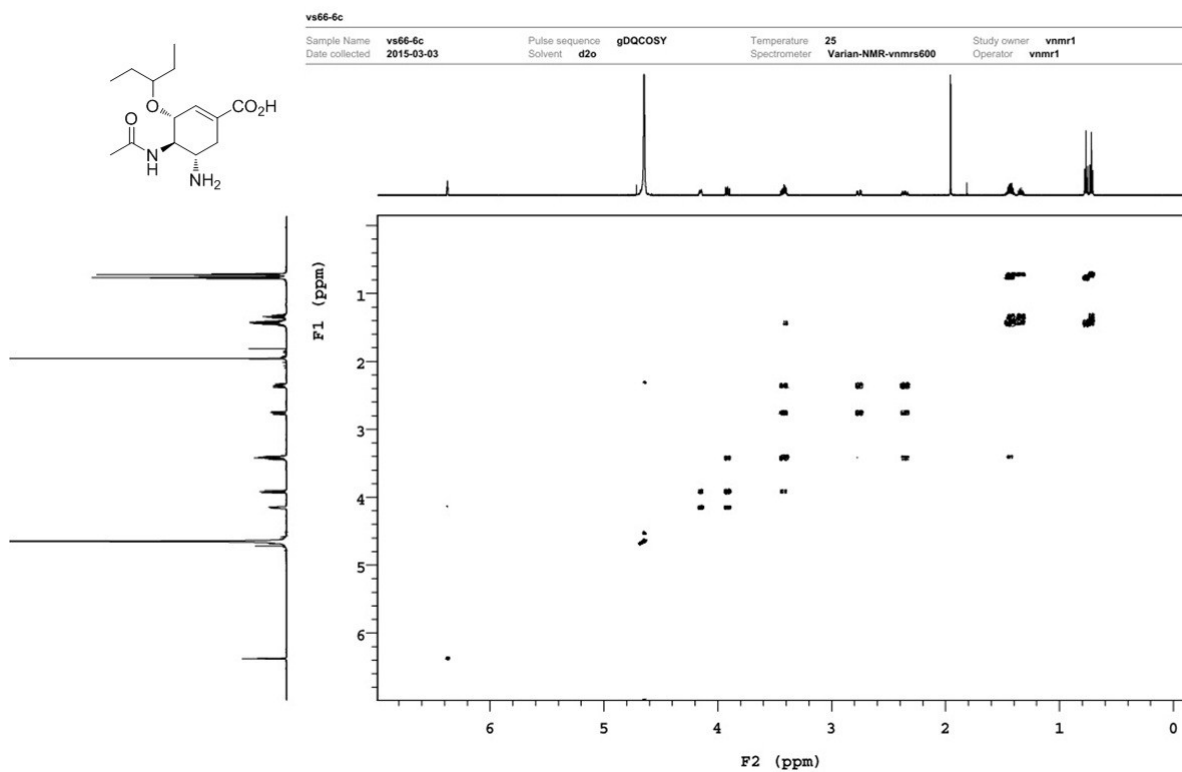
Sample Name	vs77-4	Pulse sequence	gDQCOSY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-12	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs600	Operator	vnmr1

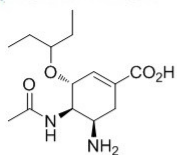


vs77-4

Sample Name	vs77-4	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr1
Date collected	2015-02-12	Solvent	cdcl3	Spectrometer	Varian-NMR-vnmrs600	Operator	vnmr1

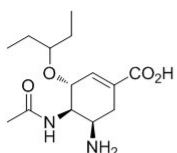
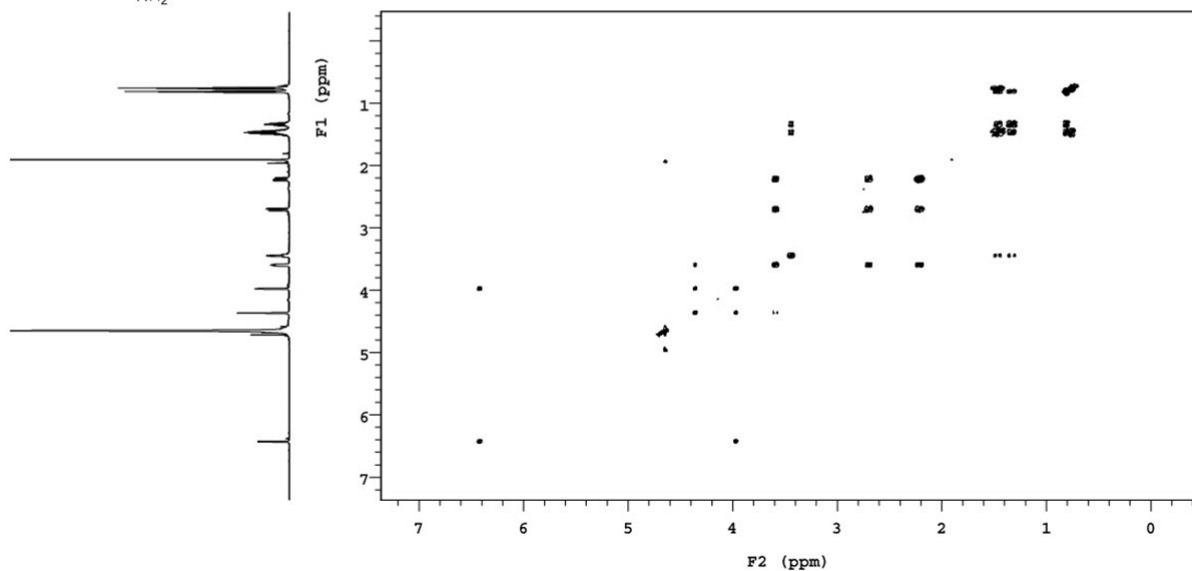






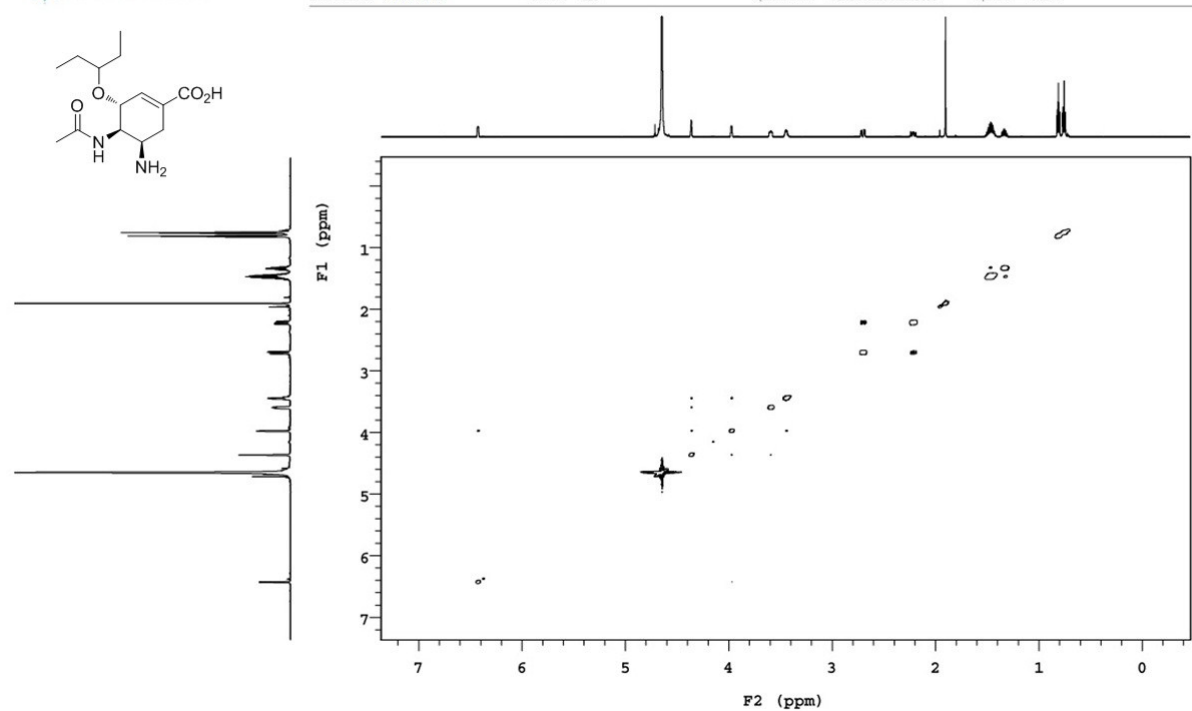
Vs-71-3C

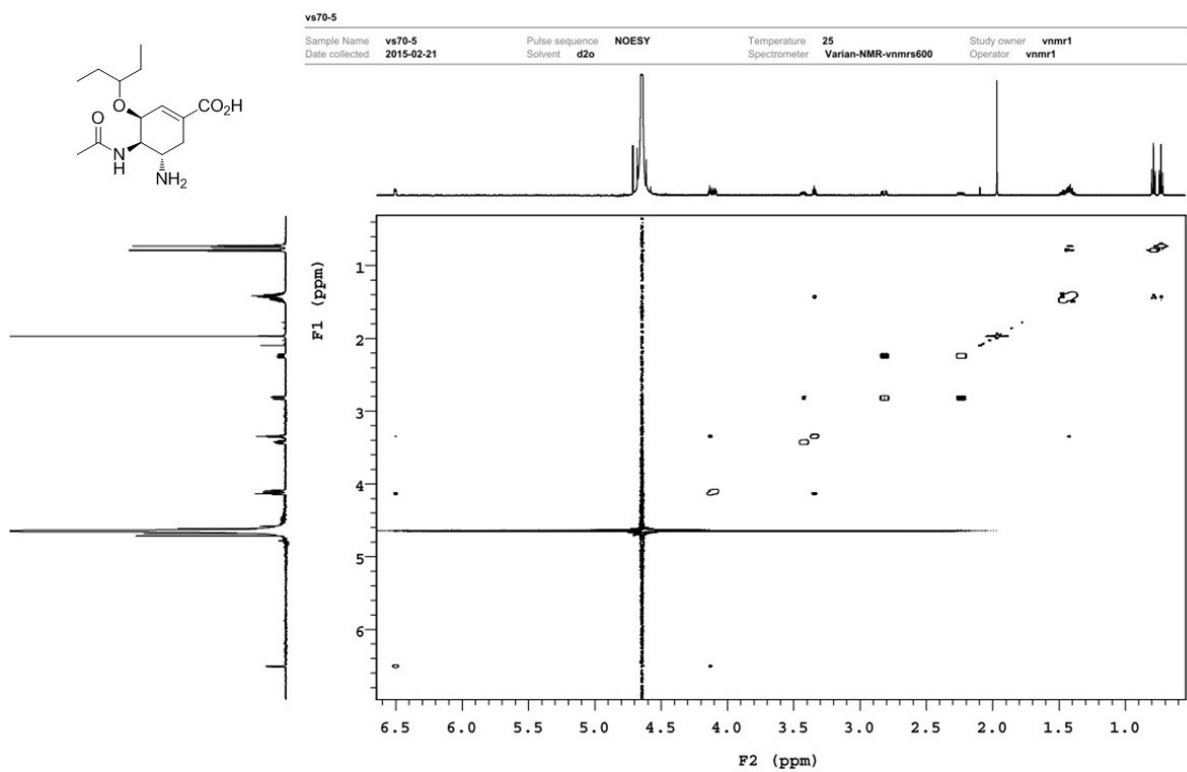
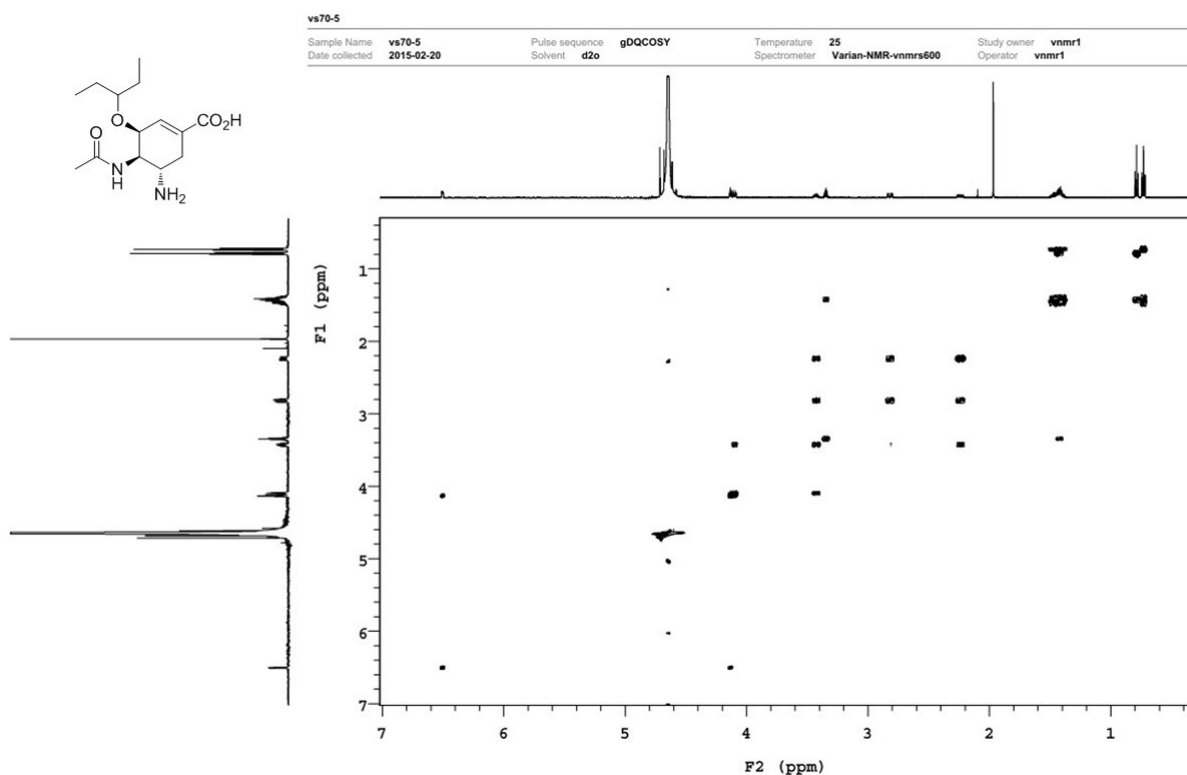
Sample Name	Vs-71-3C	Pulse sequence	gDQCOSY	Temperature	25	Study owner	vnmr1
Date collected	2015-03-05	Solvent	d2o	Spectrometer	Varian-NMR-vnmrs600	Operator	vnmr1

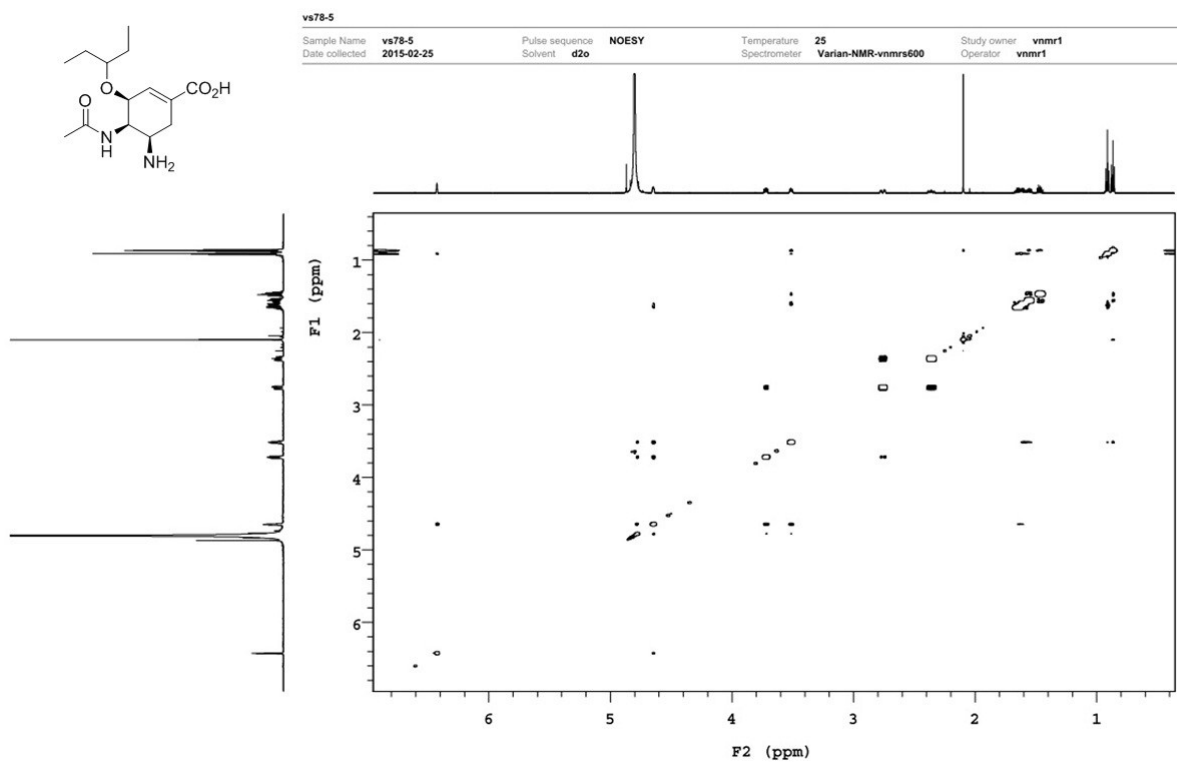
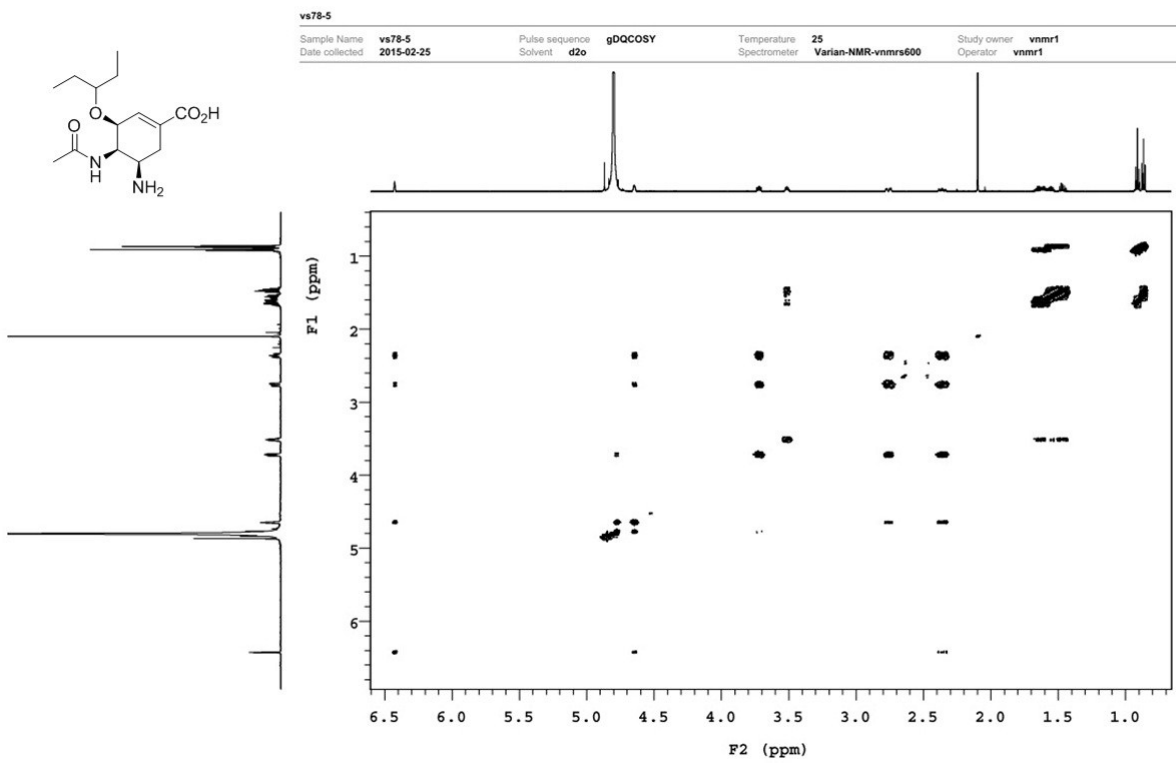


Vs-71-3C

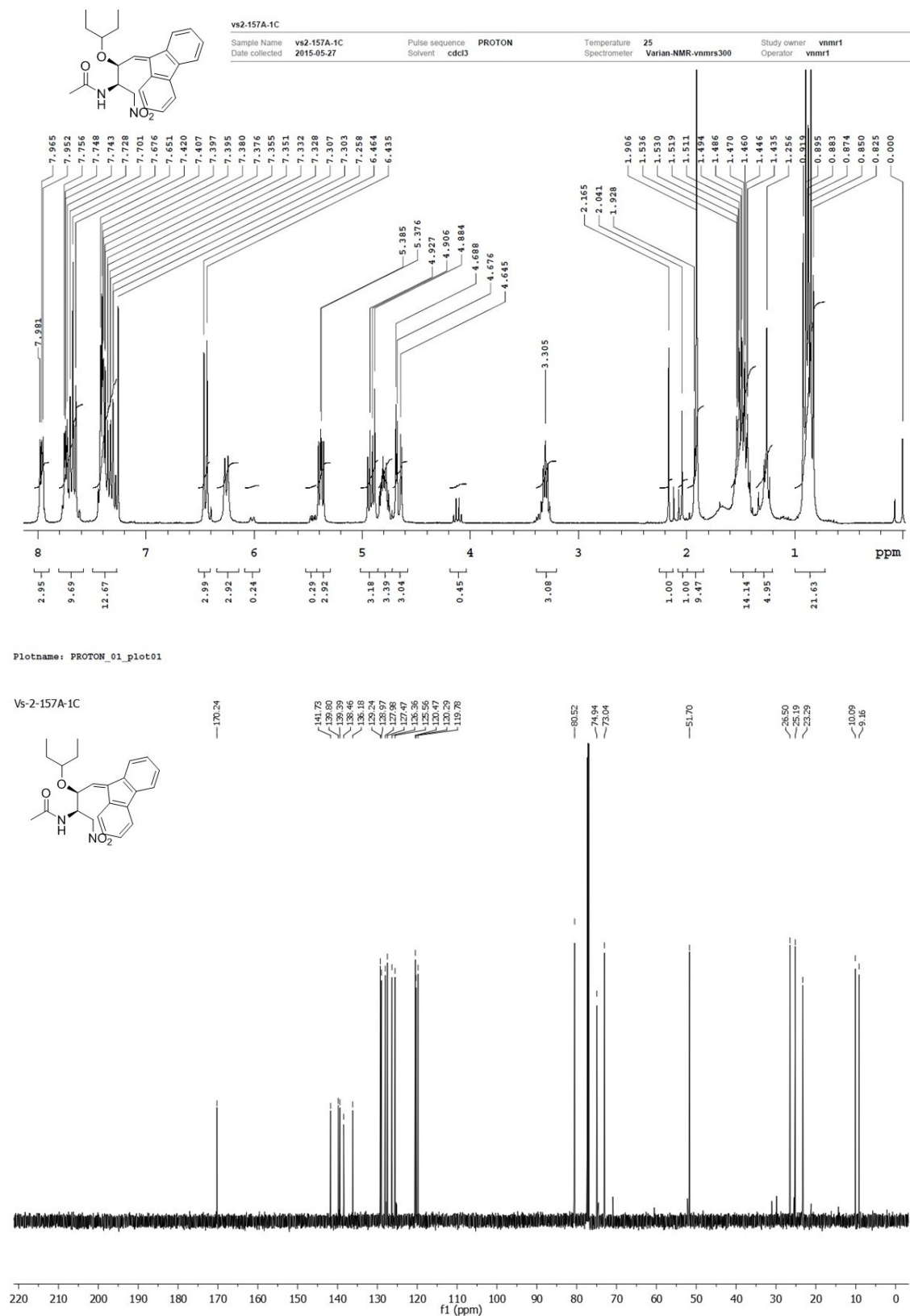
Sample Name	Vs-71-3C	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr1
Date collected	2015-03-05	Solvent	d2o	Spectrometer	Varian-NMR-vnmrs600	Operator	vnmr1



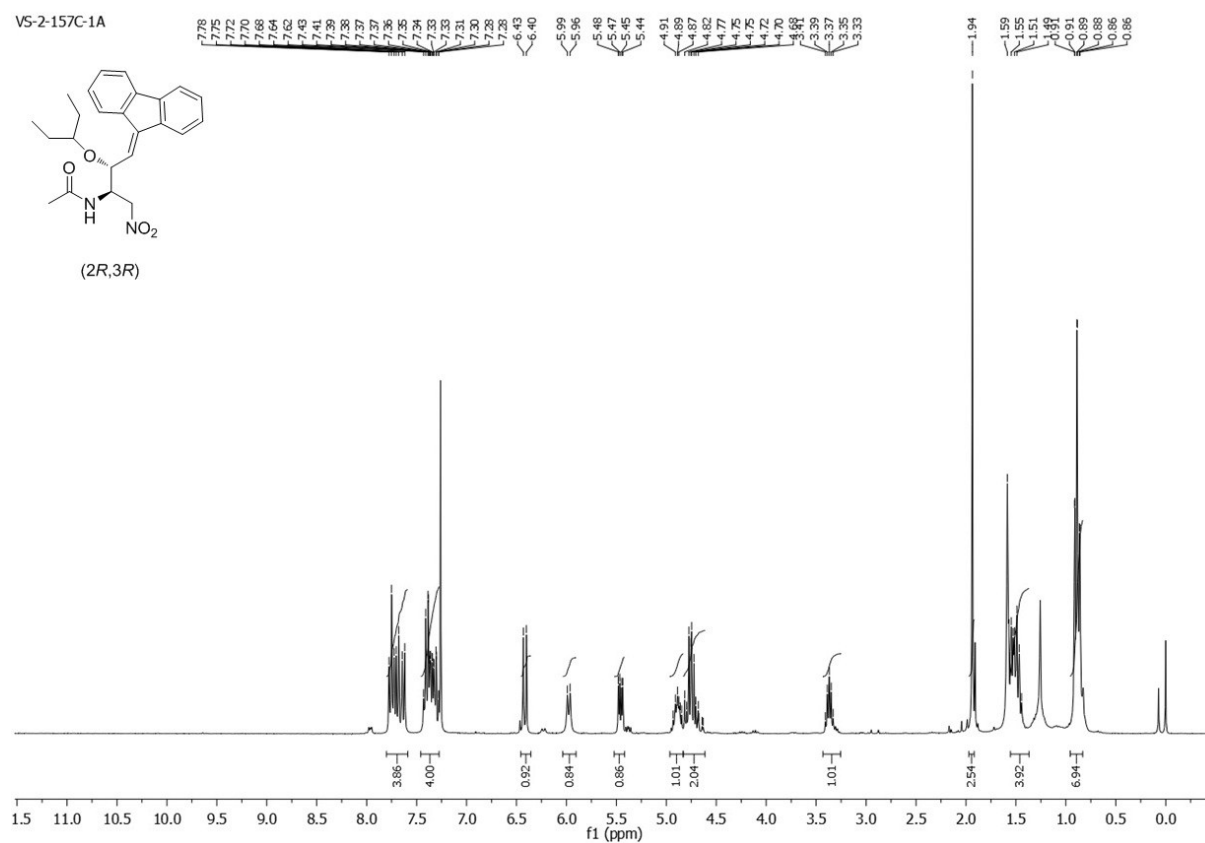
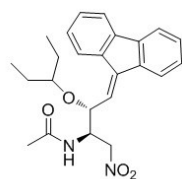




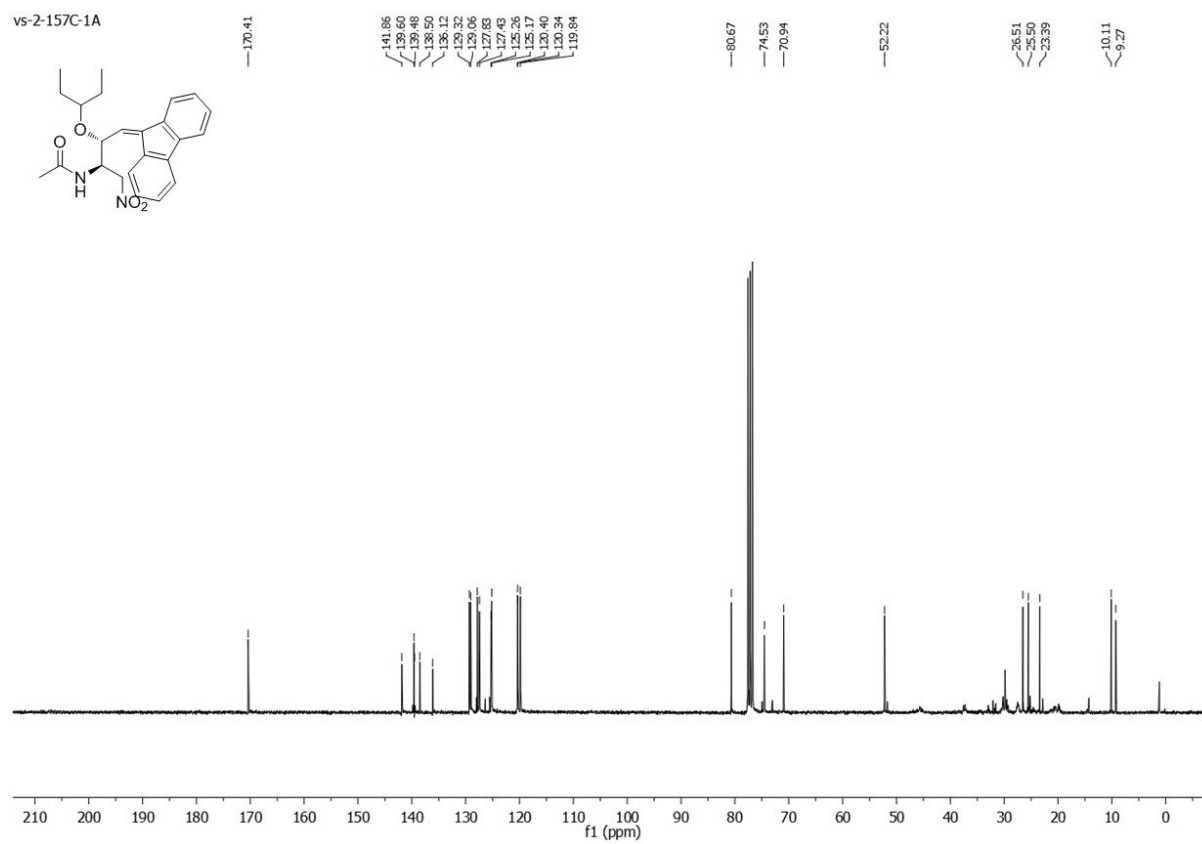
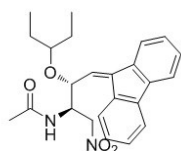
Pictures of ^1H and ^{13}C NMR spectra for darivatized samples for HPLC analyses



VS-2-157C-1A



vs-2-157C-1A



Pictures of HPLC chromatograms

