

Synthesis and Reactivity of Unique Heterocyclic Structures en route to Substituted Diamines

Spectral Data

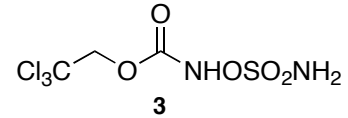
(41 pages)

David E. Olson, Autumn Maruniak, Sushant Malhotra, Barry M. Trost, and J. Du Bois *

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Stanford University

Stanford, CA 94305-5080



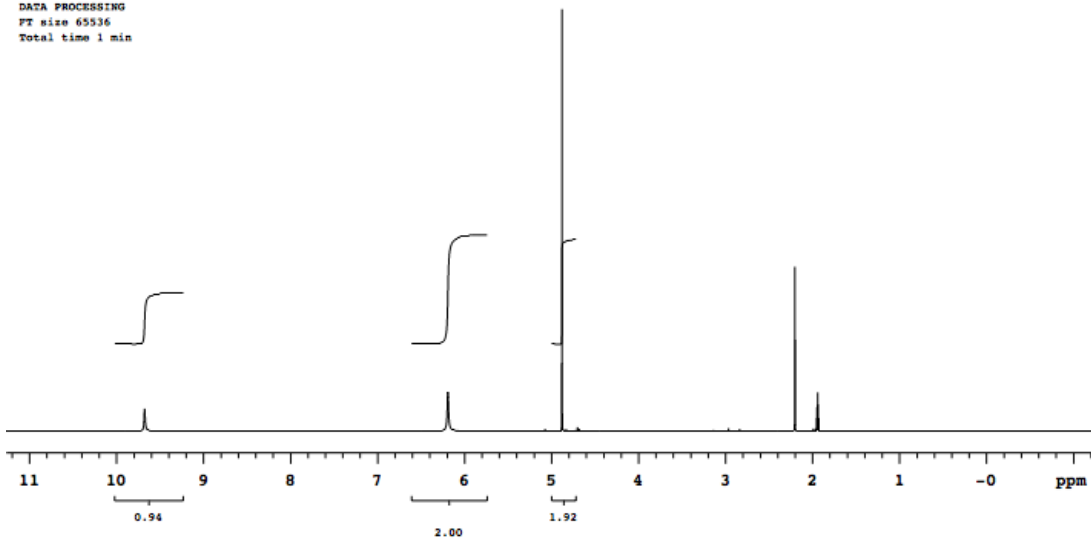
STANDARD 1H OBSERVE

Archive directory:
/export/home/deolson/vnmrsws/data
Sample directory:

File: DDE97-1

Pulse Sequence: s2pul
Solvent: CD3CN

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1136633 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



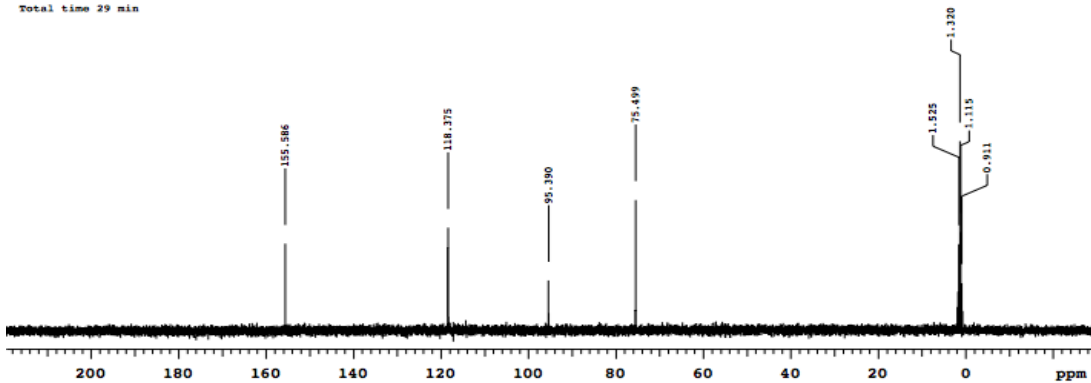
13C OBSERVE

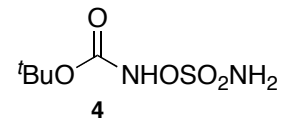
Archive directory:
/export/home/deolson/vnmrsws/data
Sample directory:

File: DDE97-2

Pulse Sequence: s2pul
Solvent: CD3CN

Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
32 repetitions
OBSERVE C13, 100.6085835 MHz
DECOUPLE H1, 400.1156728 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min





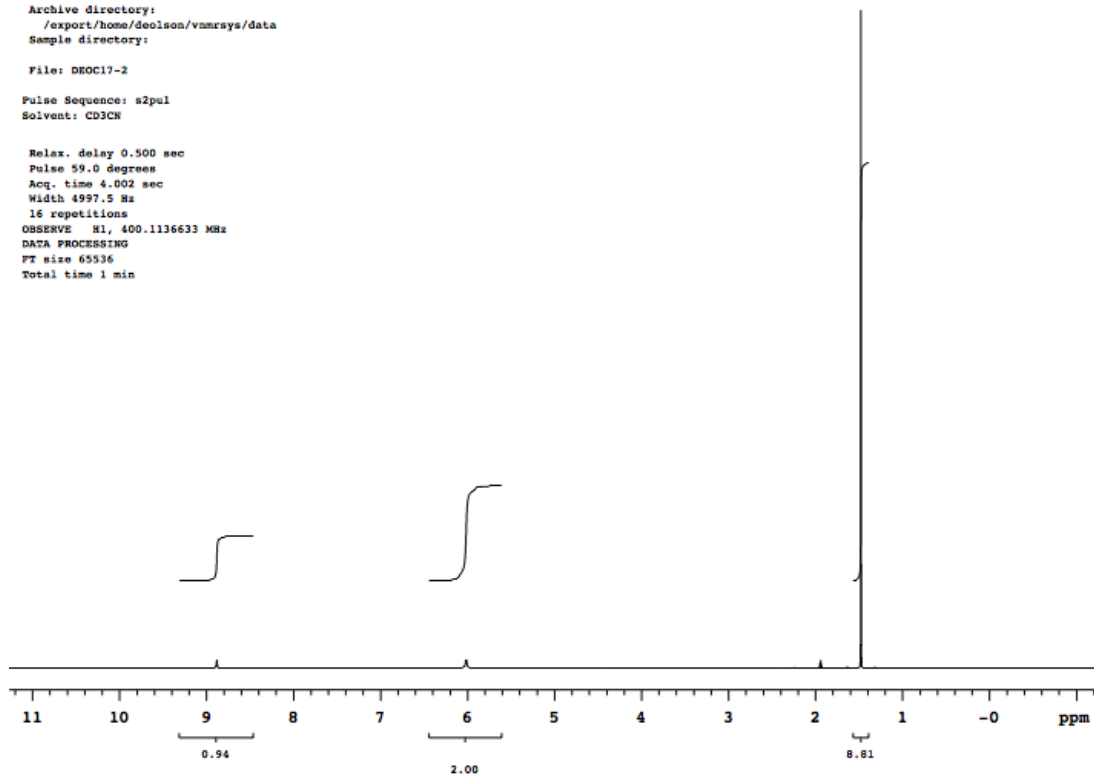
STANDARD IN OBSERVE

Archive directory:
/export/home/deolson/vnmrsvs/data
Sample directory:

File: DEOC17-2

Pulse Sequence: s2pul
Solvent: CD3CN

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.113633 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



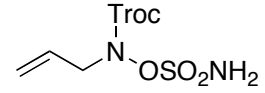
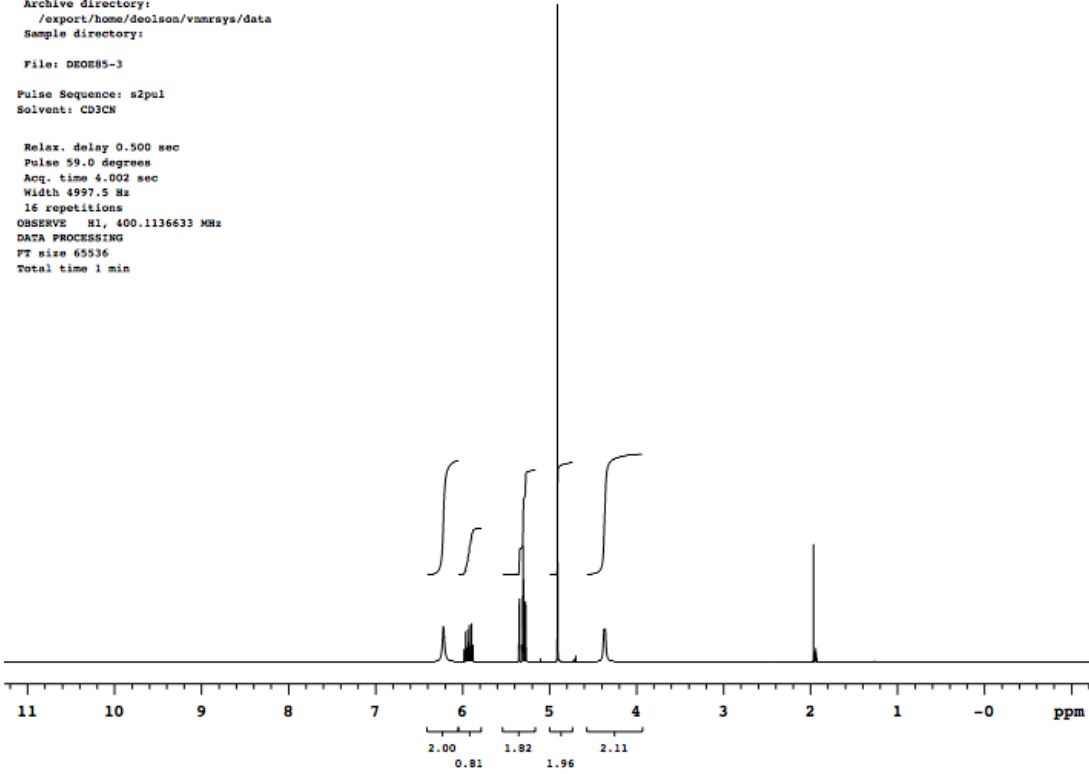


Table 1, entry 1 substrate

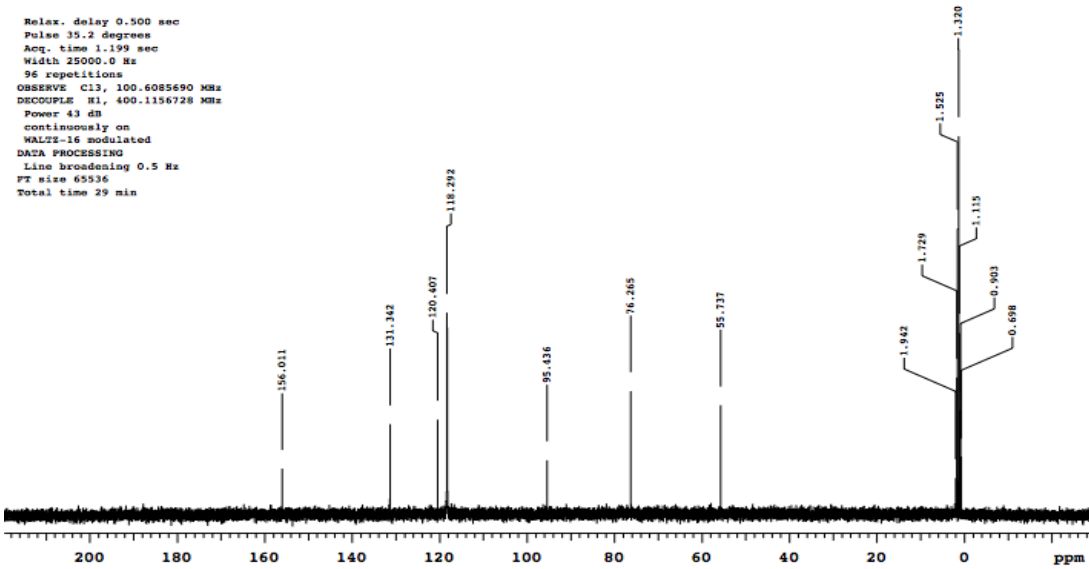
STANDARD IN OBSERVE

Archive directory:
 /export/home/geolson/vmrays/data
 Sample directory:
 File: DQ085-3
 Pulse Sequence: s2pul
 Solvent: CD3CN
 Relax. delay 0.500 sec
 Pulse 59.0 degrees
 Acq. time 4.002 sec
 Width 4997.5 Hz
 16 repetitions
 OBSERVE H1, 400.113633 MHz
 DATA PROCESSING
 FT size 65536
 Total time 1 min



13C OBSERVE

Archive directory:
 /export/home/geolson/vmrays/data
 Sample directory:
 File: DQ085-4
 Pulse Sequence: s2pul
 Solvent: CD3CN
 Relax. delay 0.500 sec
 Pulse 35.2 degrees
 Acq. time 1.199 sec
 Width 25000.0 Hz
 96 repetitions
 OBSERVE C13, 100.6085690 MHz
 DECOUPLE H1, 400.1156728 MHz
 Power 43 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 29 min



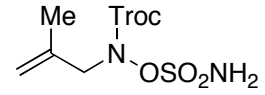


Table 1, entry 3 substrate

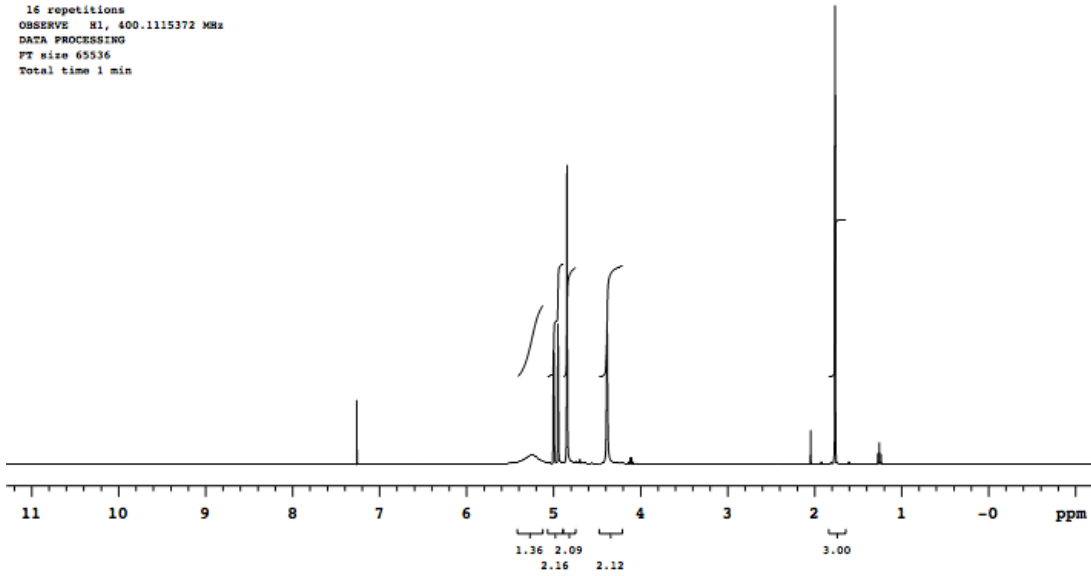
STANDARD IN OBSERVE

Archive directory:
/export/home/deolson/vnmrsys/data
Sample directory:

File: DQOE101-1

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115372 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



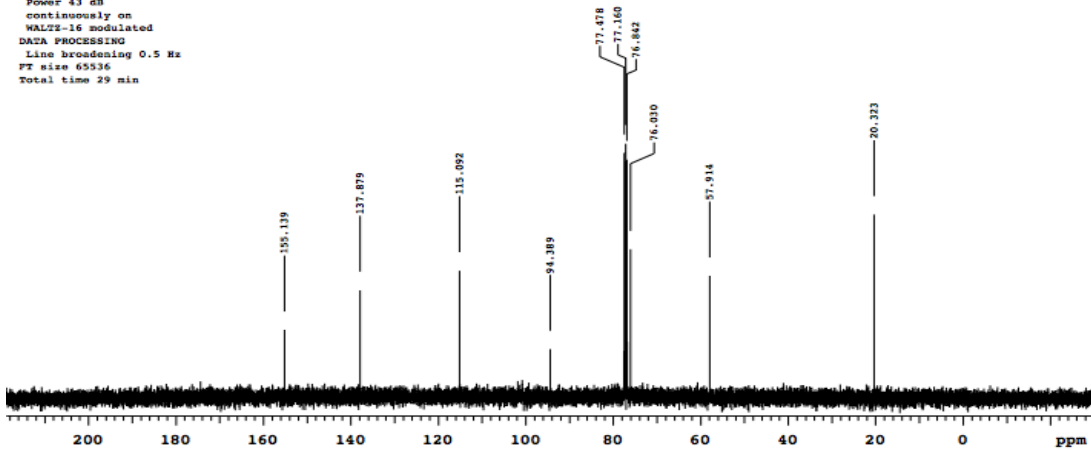
13C OBSERVE

Archive directory:
/export/home/deolson/vnmrsys/data
Sample directory:

File: DQOE101-2

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
128 repetitions
OBSERVE C13, 100.6081131 MHz
DECOUPLE H1, 400.1135562 MHz
Power: 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min



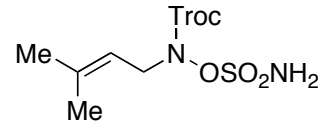


Table 1, entry 5 substrate

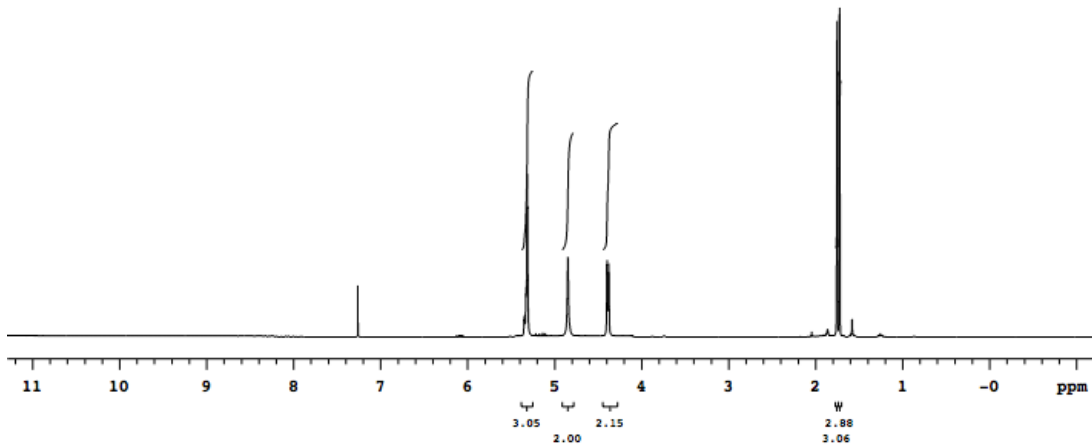
STANDARD IN OBSERVE

Archive directory:
/export/home/deolson/vnmrsys/data
Sample directory:

File: DEOE105-1

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115371 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



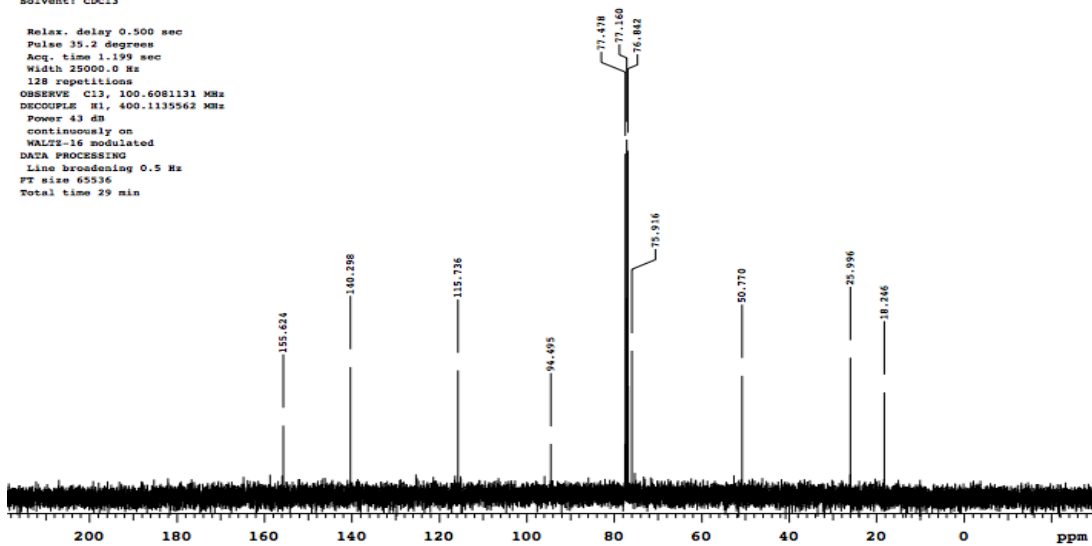
13C OBSERVE

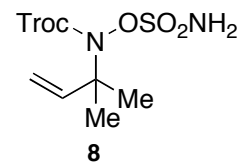
Archive directory:
/export/home/deolson/vnmrsys/data
Sample directory:

File: DEOE105-2

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
128 repetitions
OBSERVE C13, 100.6081131 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min





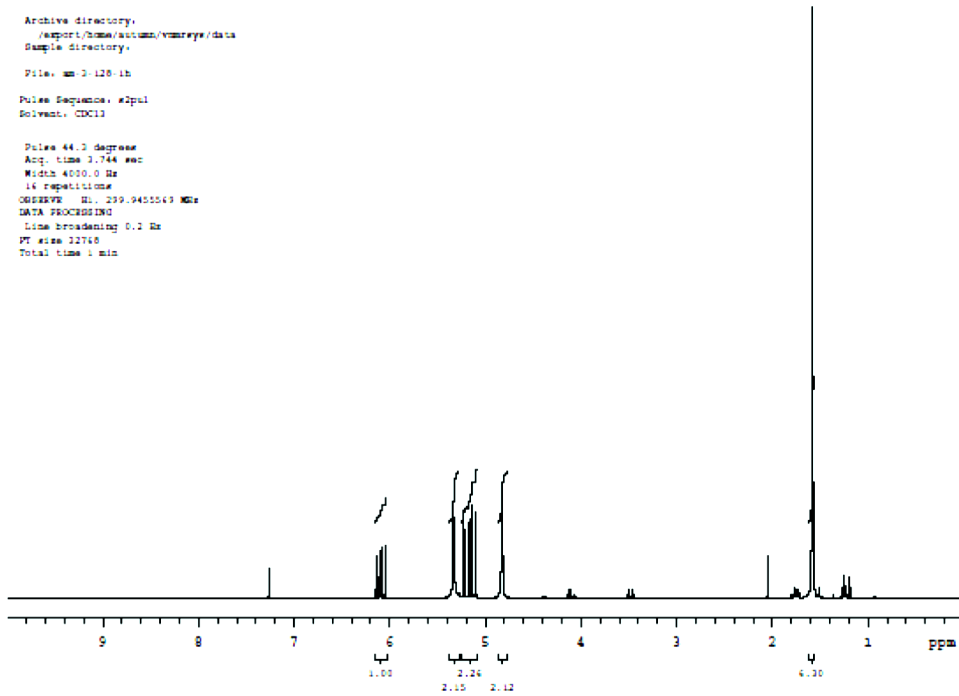
STANDARD 1H OBSERVE

Archive directory:
/export/home/acomm/vmreyes/data
Sample directory:

File: sm-2-128-1h

Pulse Sequence: #spul
Solvent: CDCl₃

Pulse 44.3 degree
Acq. time 3.744 sec
Width 4000.0 Hz
14 repetitions
OBSERVE F1: 299.9455043 MHz
DATA PROCESSING
Line broadening 0.3 Hz
PT size 12710
Total time 1 min



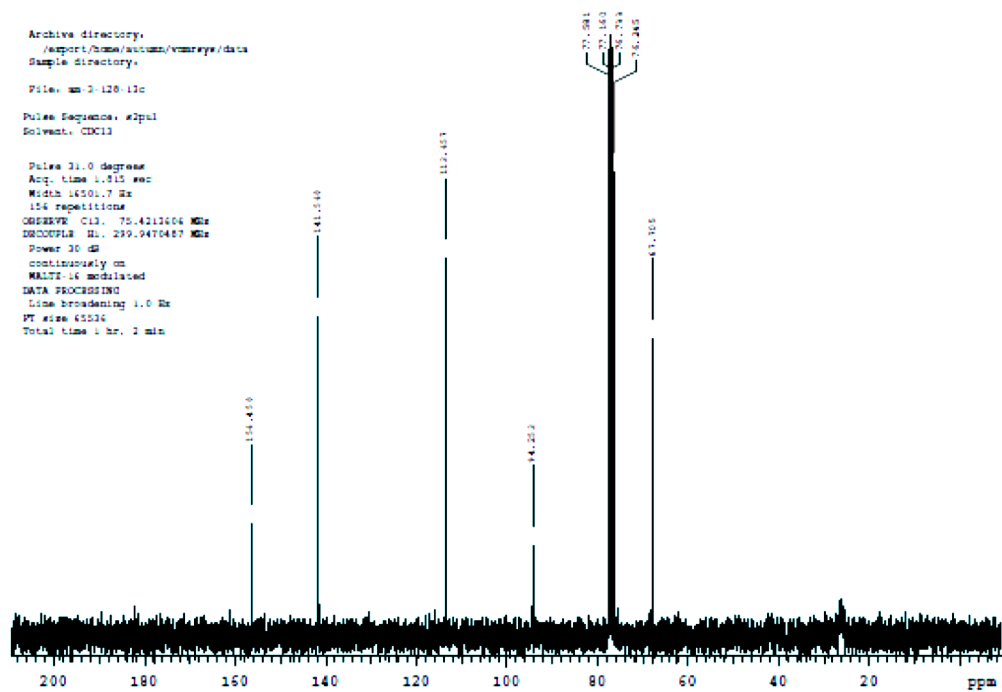
13C OBSERVE

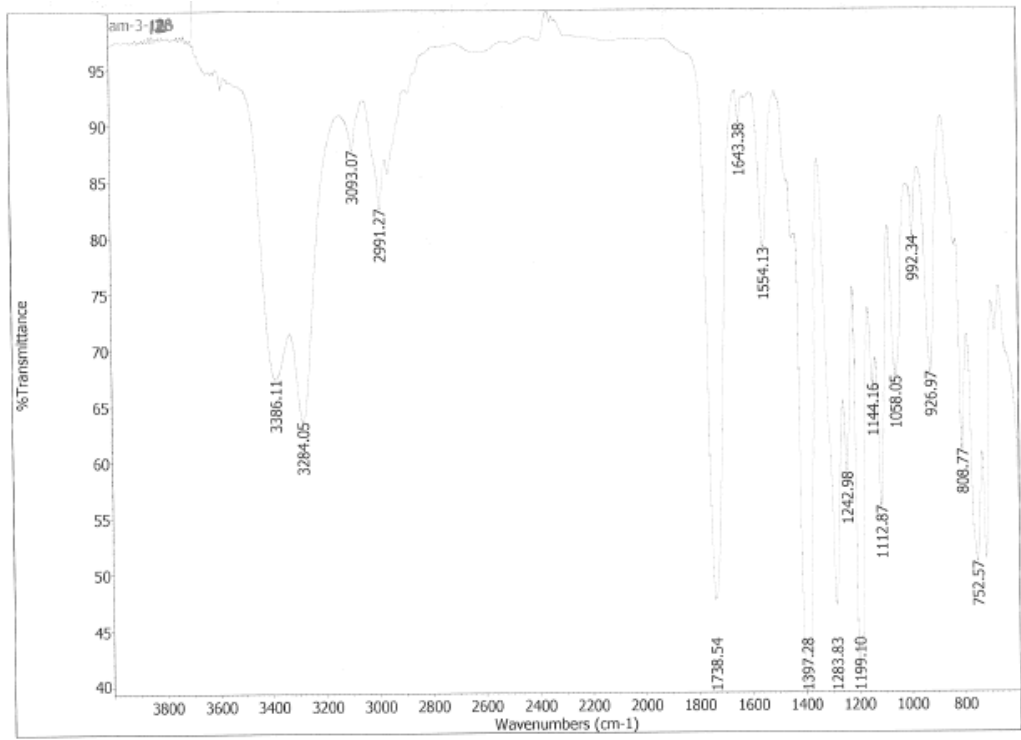
Archive directory:
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Sample directory:

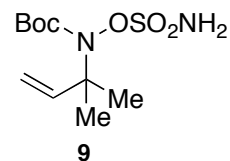
File: sm-2-128-13c

Pulse Sequence: #spul
Solvent: CDCl₃

Pulse 31.0 degree
Acq. time 1.515 sec
Width 14501.7 Hz
154 repetitions
OBSERVE C13: 75.4213004 MHz
DECOUPLE H1: 299.9470487 MHz
Power 30 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
PT size 65534
Total time 1 hr. 2 min







Std proton

Archive directory:

Sample directory:

File: sm-4-148-1h

Pulse Sequence: s2pul

Solvent: cdcl3

Relax. delay 0.500 sec

Pulse 45.0 degree

Acq. time 4.000 sec

Width 5605.4 Hz

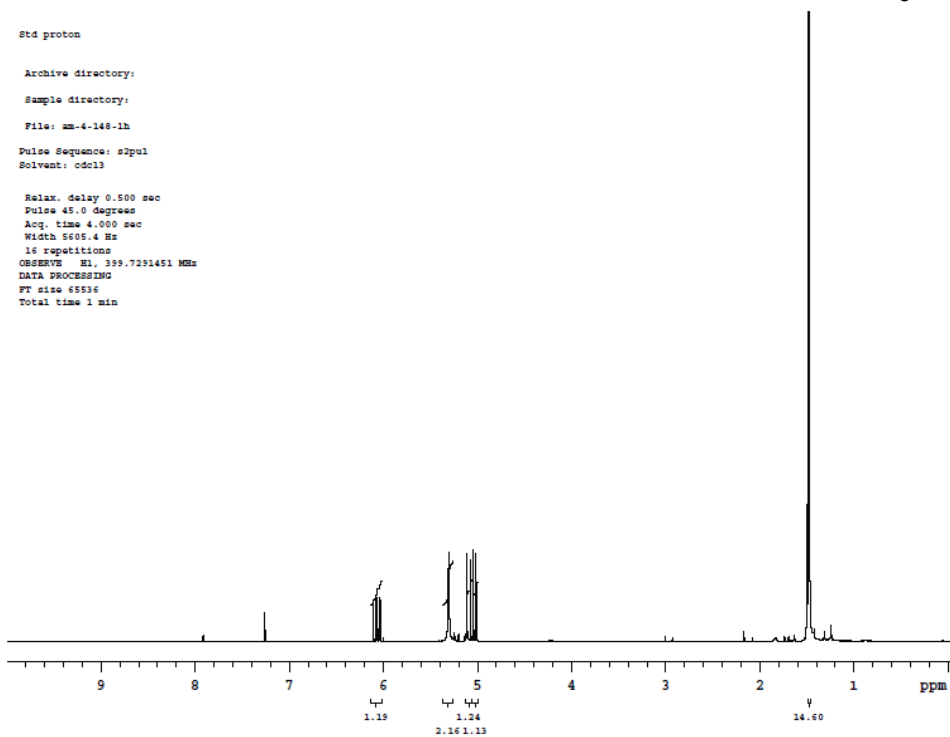
16 repetitions

OBSERVE F1: 399.7291451 MHz

DATA PROCESSING

PT size 65536

Total time 1 min



Std proton

Archive directory:

Sample directory:

File: sm-4-148-13c

Pulse Sequence: #2pul

Solvent: cdcl3

Acq. 1-14-07

Relax. delay 1.000 sec

Pulse 40.0 degree

Acq. time 1.300 sec

Width 24509.8 Hz

100 repetitions

OBSERVE C13: 100.5119407 MHz

INOCOPPLA H1: 399.7311429 MHz

Power 43 dB

continuously on

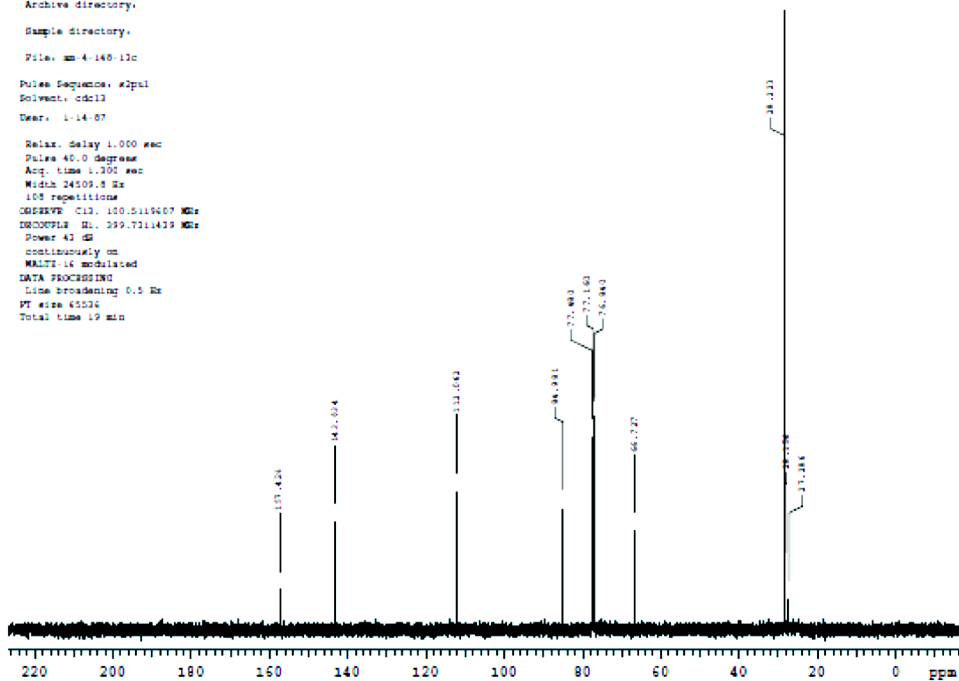
MULTI-16 modulated

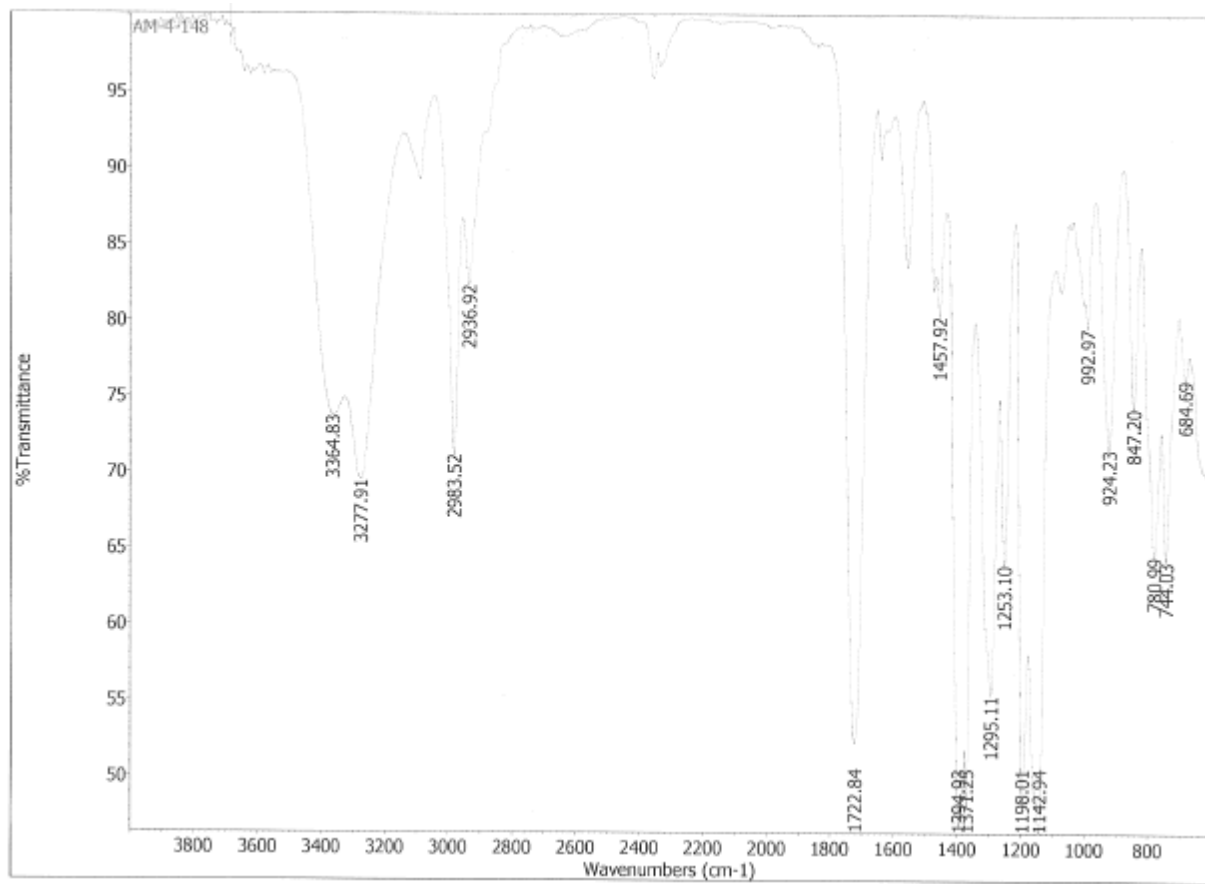
DATA PROCESSING

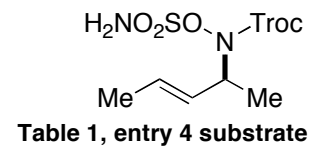
Line broadening 0.5 Hz

PT size 65536

Total time 19 min







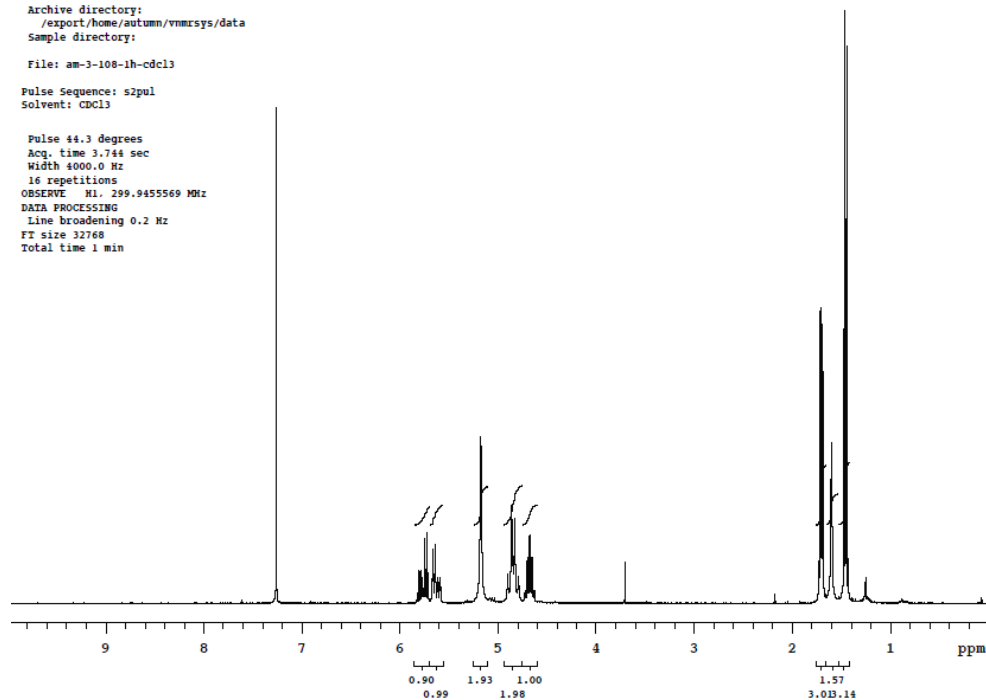
STANDARD 1H OBSERVE

Archive directory:
/export/home/autumn/vnmrsys/data
Sample directory:

File: am-3-108-1h-cdcl3

Pulse Sequence: s2pul
Solvent: CDCl3

Pulse 44.3 degrees
Acq. time 3.744 sec
Width 4000.0 Hz
16 repetitions
OBSERVE H1. 299.945569 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 1 min



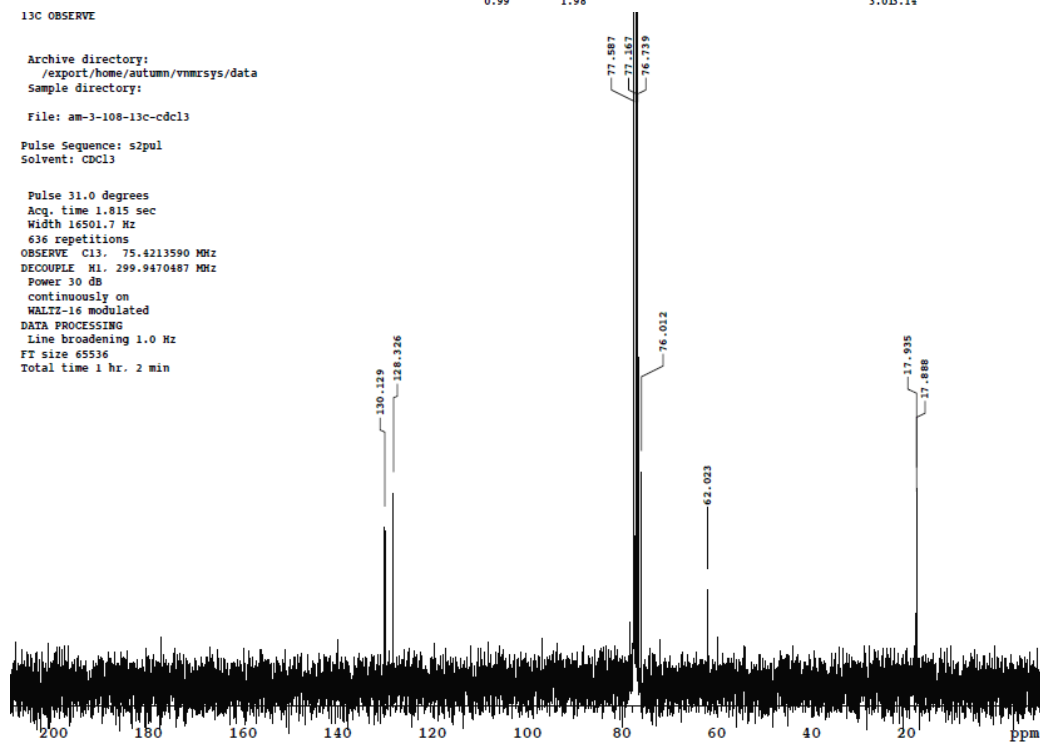
13C OBSERVE

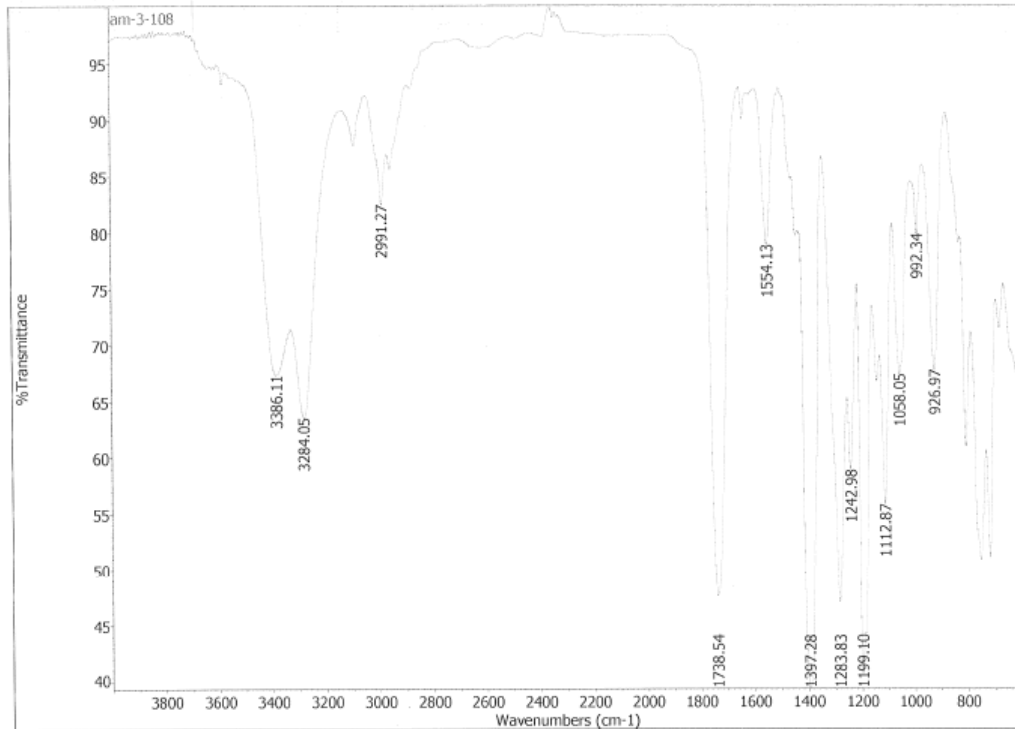
Archive directory:
/export/home/autumn/vnmrsys/data
Sample directory:

File: am-3-108-13c-cdcl3

Pulse Sequence: s2pul
Solvent: CDCl3

Pulse 31.0 degrees
Acq. time 1.815 sec
Width 16501.7 Hz
636 repetitions
OBSERVE C13. 75.4213590 MHz
DECOUPLE H1. 299.9470487 MHz
Power 30 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr. 2 min

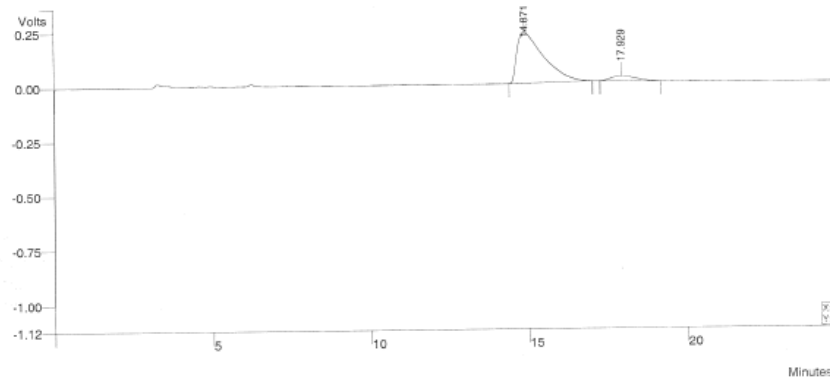




**Stanford University Chemistry Department
Trost Lab HPLC Report**

Data File: c:\star\data\autumn\am-3-108-oi-90.10-
 Injection Date: 11/26/2008 02:19:59
 Injection Method: c:\star\data\dauid\chiral right method
 Run Time (min): 24.562
 Instrument (Inj): Chiral LC Right

Sample Prep Info
Manual injection



Peak No	Ret. Time (min)	Peak Area	Width 1/2 (sec)	Percent Area
1	14.871	13577906	63.1	92.29
2	17.929	1134630	45.9	7.71
		14712536		100.00

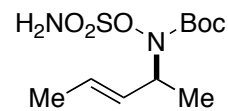
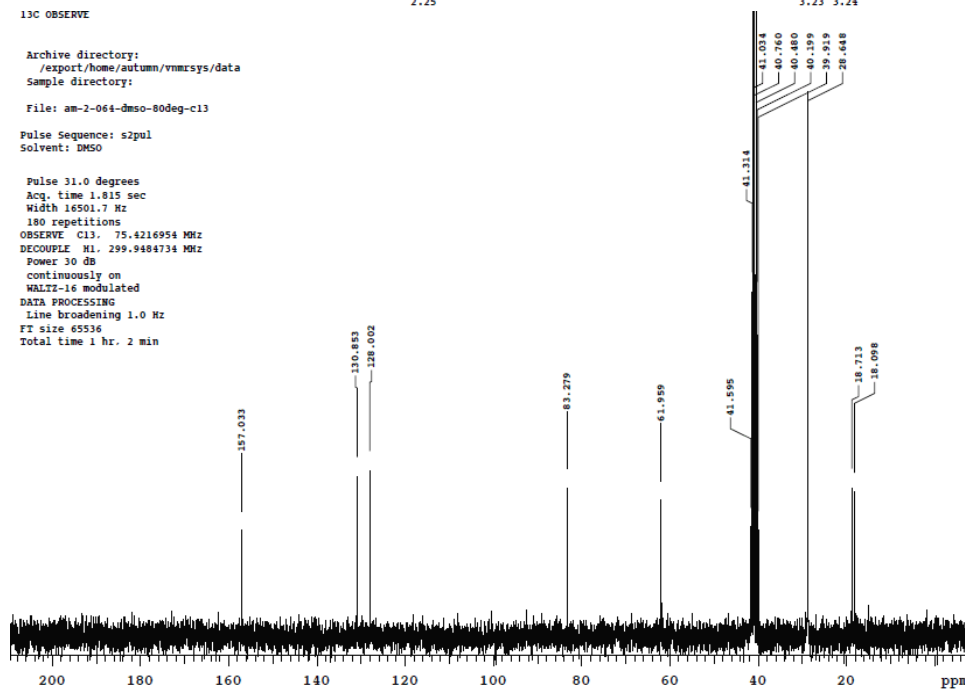
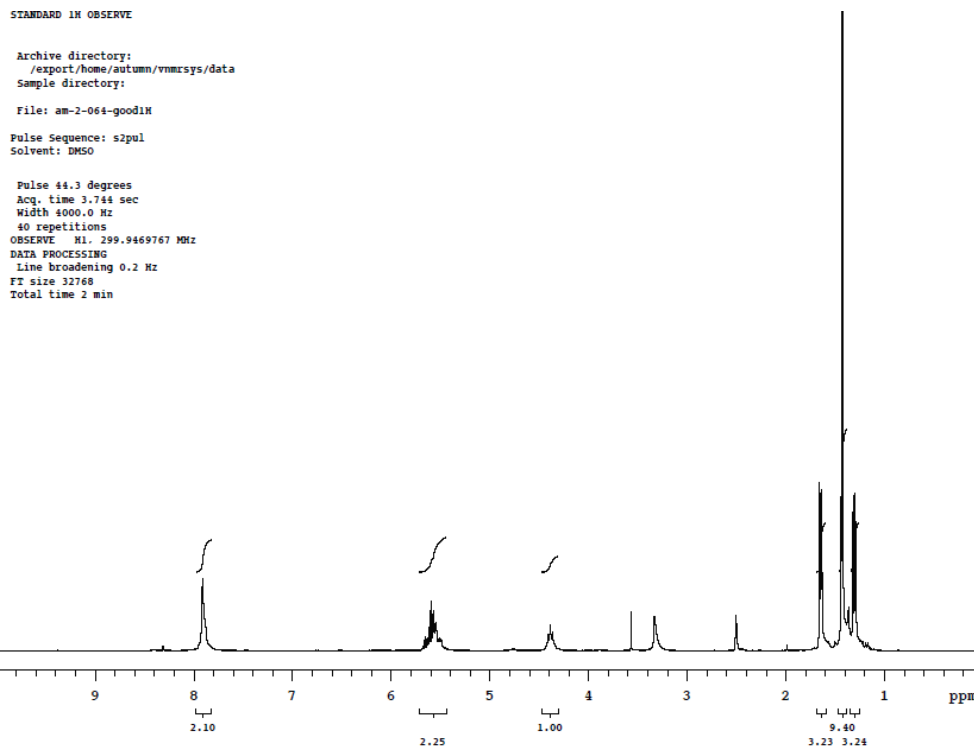
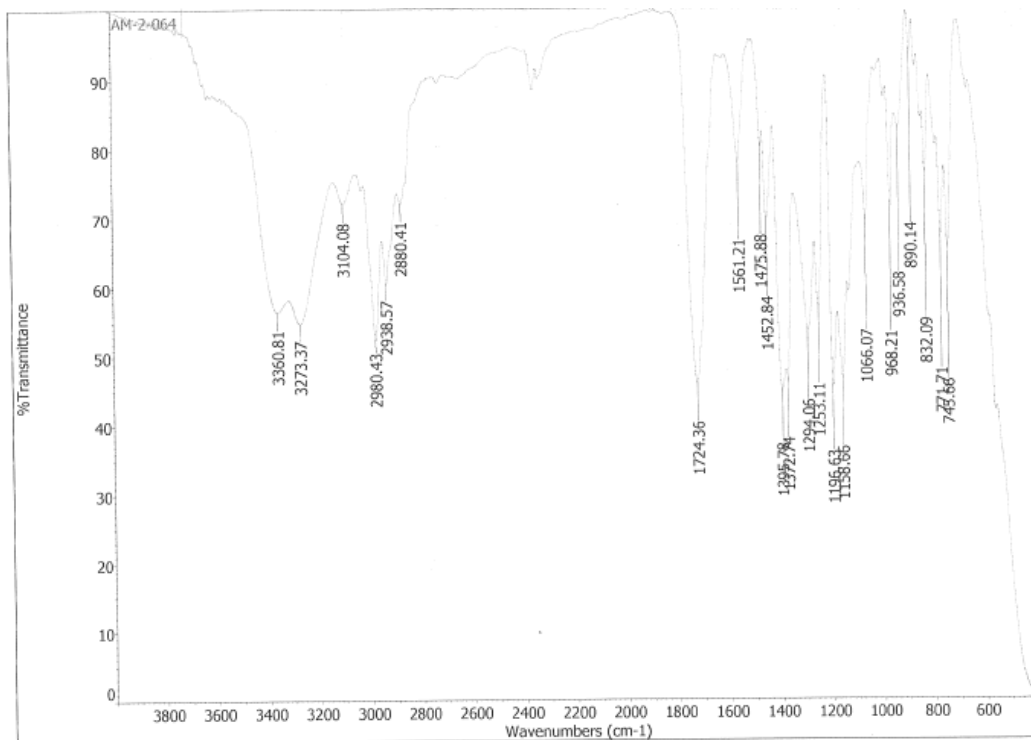


Table 1, entry 4 substrate

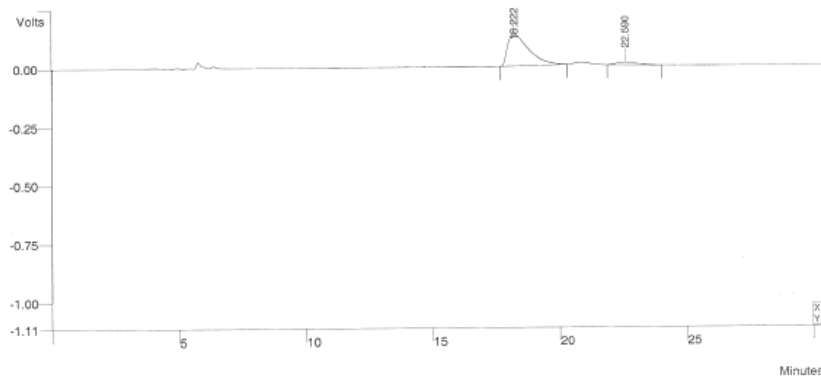




**Stanford University Chemistry Department
Trost Lab HPLC Report**

Data File: c:\star\data\autumn\am-2-64-oi-95-5-9
 Injection Date: 07/28/2008 06:27:10
 Injection Method: c:\star\data\dauid\chiral right method
 Run Time (min): 30.377
 Instrument (Inj): Chiral LC Right

Sample Prep Info
 Manual injection



Peak No	Ret. Time (min)	Peak Area	Width 1/2 (sec)	Percent Area
1	18.222	7653673	64.0	93.03
2	22.590	573245	46.4	6.97
		8226918		100.00

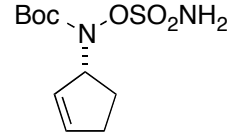
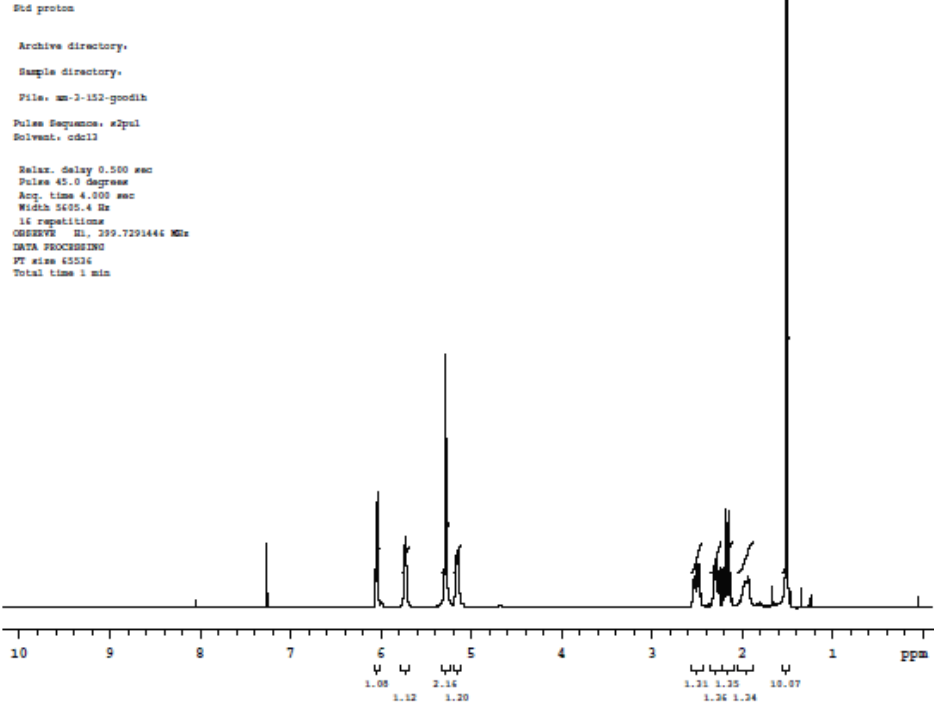
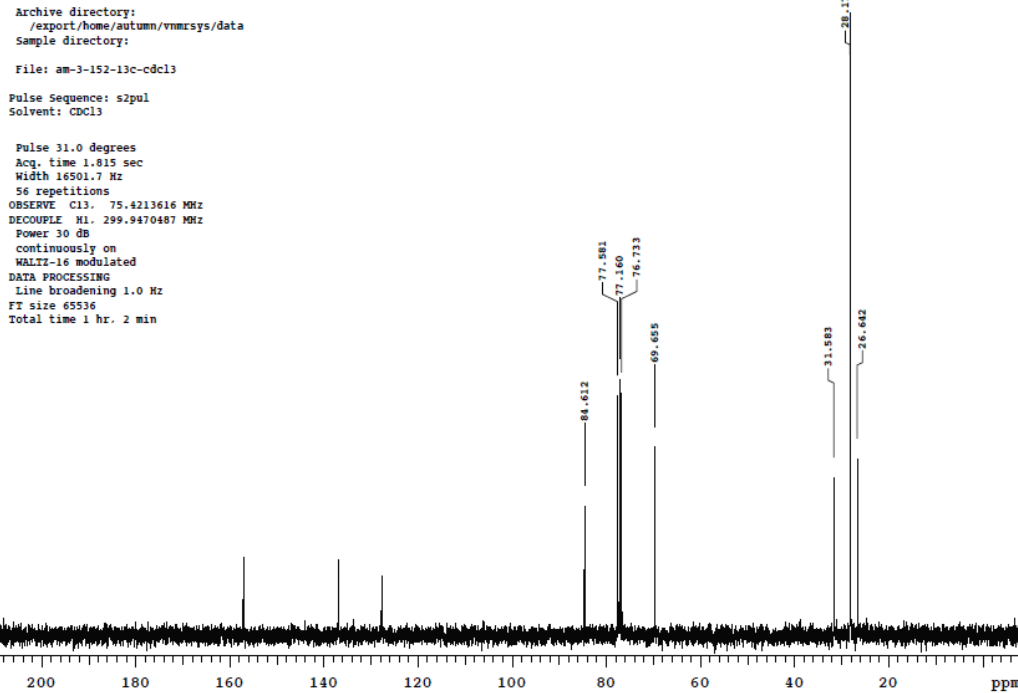
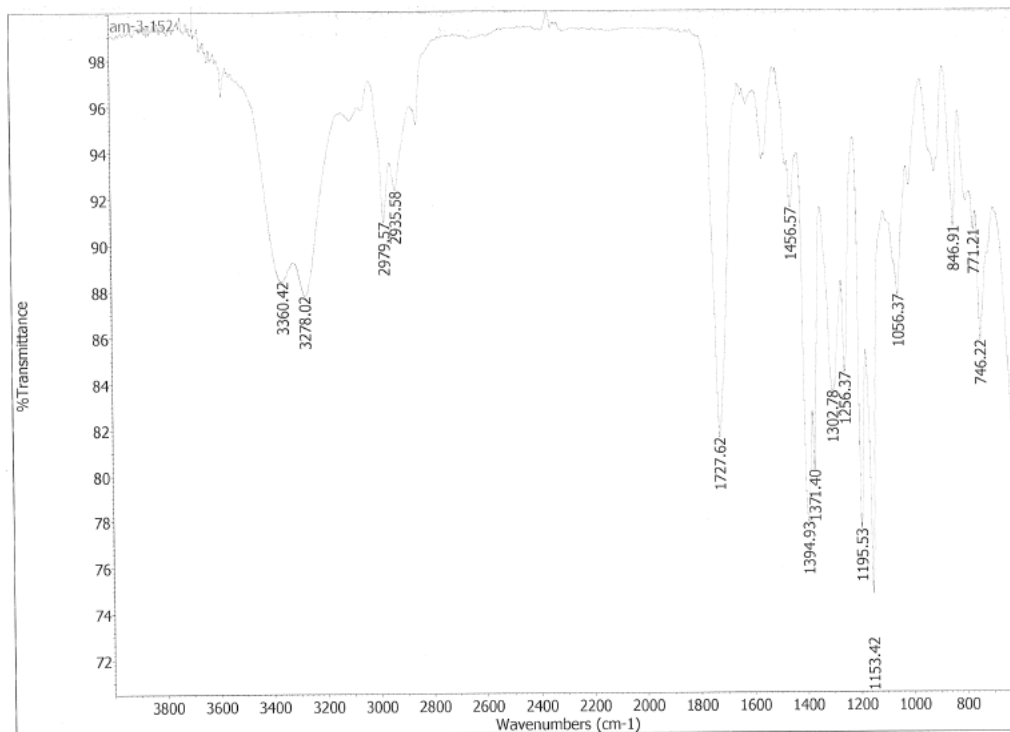


Table 1, entry 6 substrate



13C OBSERVE

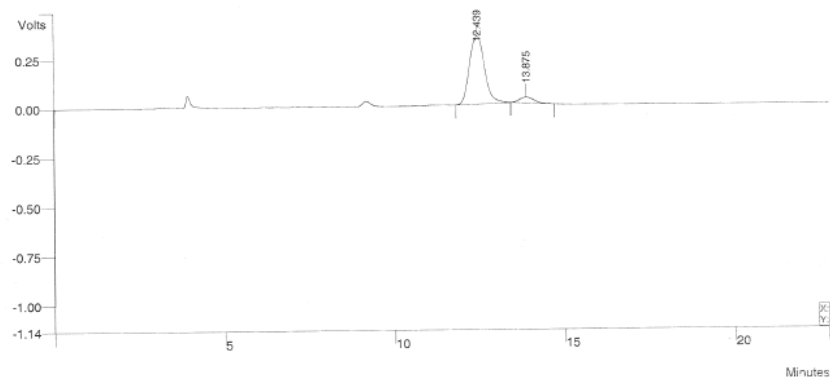




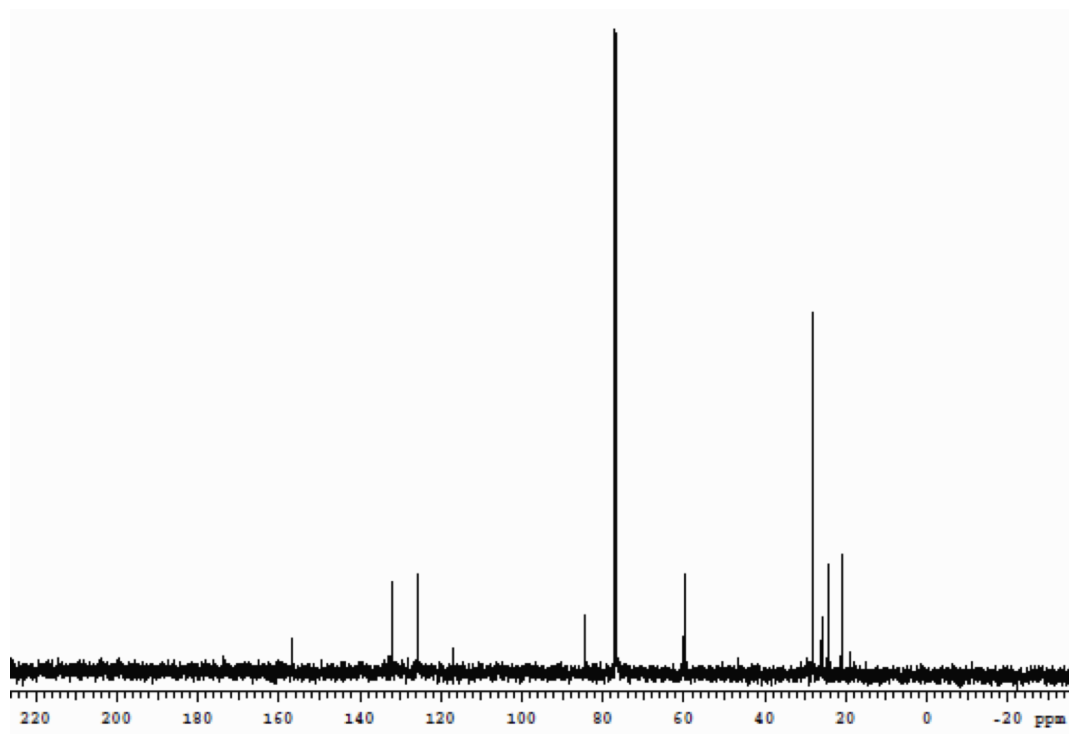
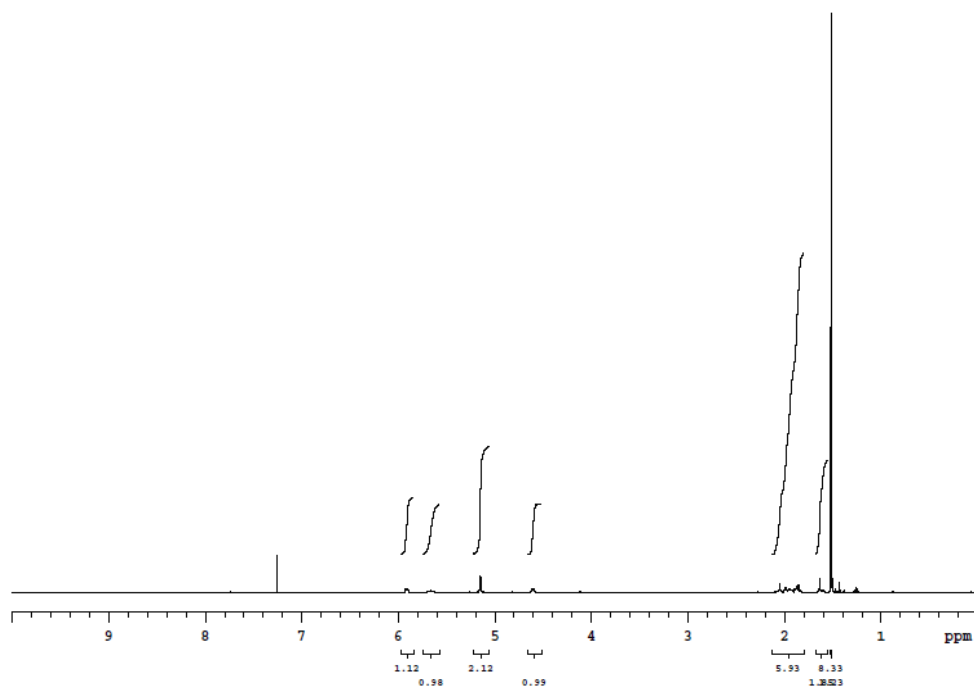
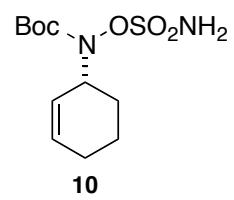
**Stanford University Chemistry Department
Trost Lab HPLC Report**

Data File: c:\star\data\autumn\am-3-152b-ad-90.1
Injection Date: 12/08/2008 07:26:30
Injection Method: c:\star\data\dauid\chiral right method
Run Time (min): 22.758
Instrument (Inj): Chiral LC Right

Sample Prep Info
Manual injection



Peak No	Ret. Time (min)	Peak Area	Width 1/2 (sec)	Percent Area
1	12.439	10715629	29.3	92.76
2	13.875	835919	24.2	7.24
		11551548		100.00



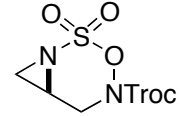
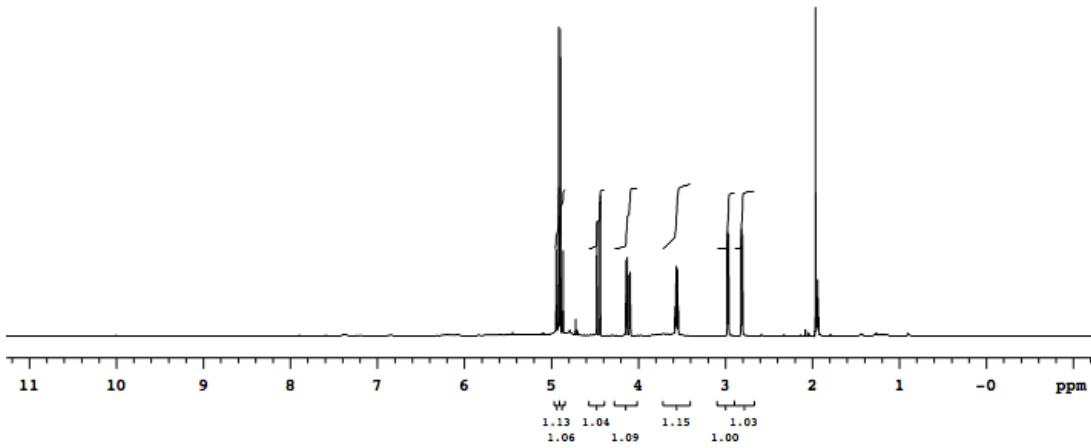


Table 1, entry 1 product

STANDARD 1H OBSERVE

Archive directory:
 /export/home/deolson/vnmrsys/data
 Sample directory:
 File: DEOE145-1
 Pulse Sequence: s2pul
 Solvent: CD3CN

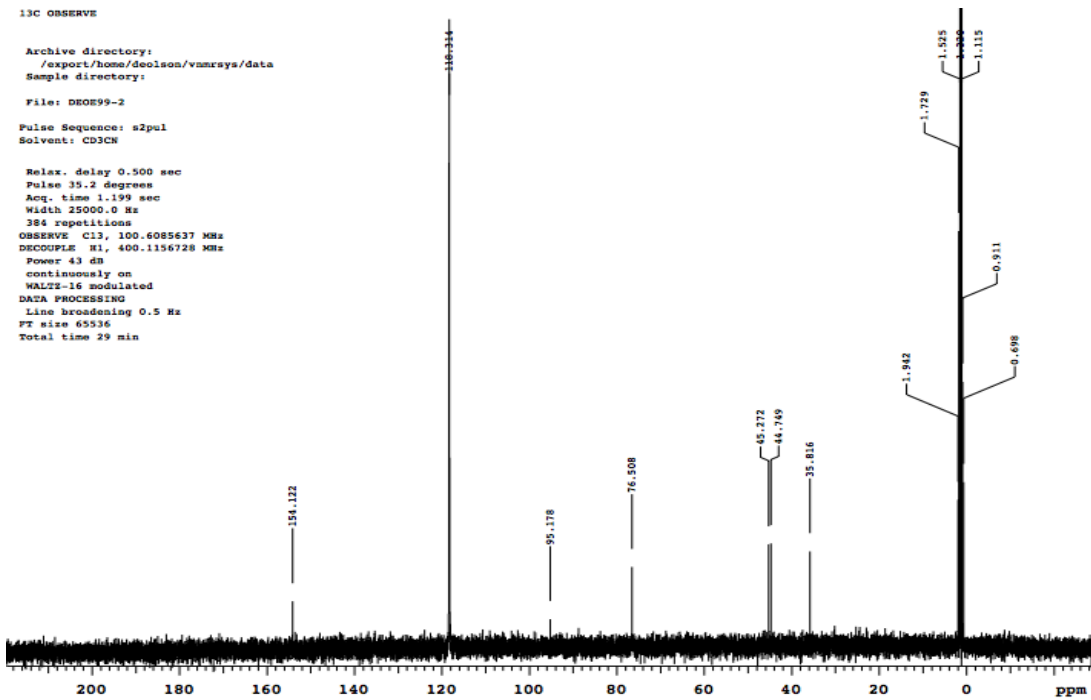
Relax. delay 0.500 sec
 Pulse 59.0 degrees
 Acq. time 4.002 sec
 Width 4997.5 Hz
 12 repetitions
 OBSERVE H1, 400.1136637 MHz
 DATA PROCESSING
 FT size 65536
 Total time 1 min

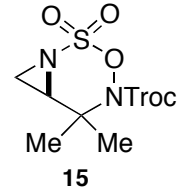


¹³C OBSERVE

Archive directory:
 /export/home/deolson/vnmrsys/data
 Sample directory:
 File: DEOE99-2
 Pulse Sequence: s2pul
 Solvent: CD3CN

Relax. delay 0.500 sec
 Pulse 35.2 degrees
 Acq. time 1.199 sec
 Width 25000.0 Hz
 384 repetitions
 OBSERVE C13, 100.6085637 MHz
 DECOUPLE H1, 400.1156728 MHz
 Power 43 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 29 min





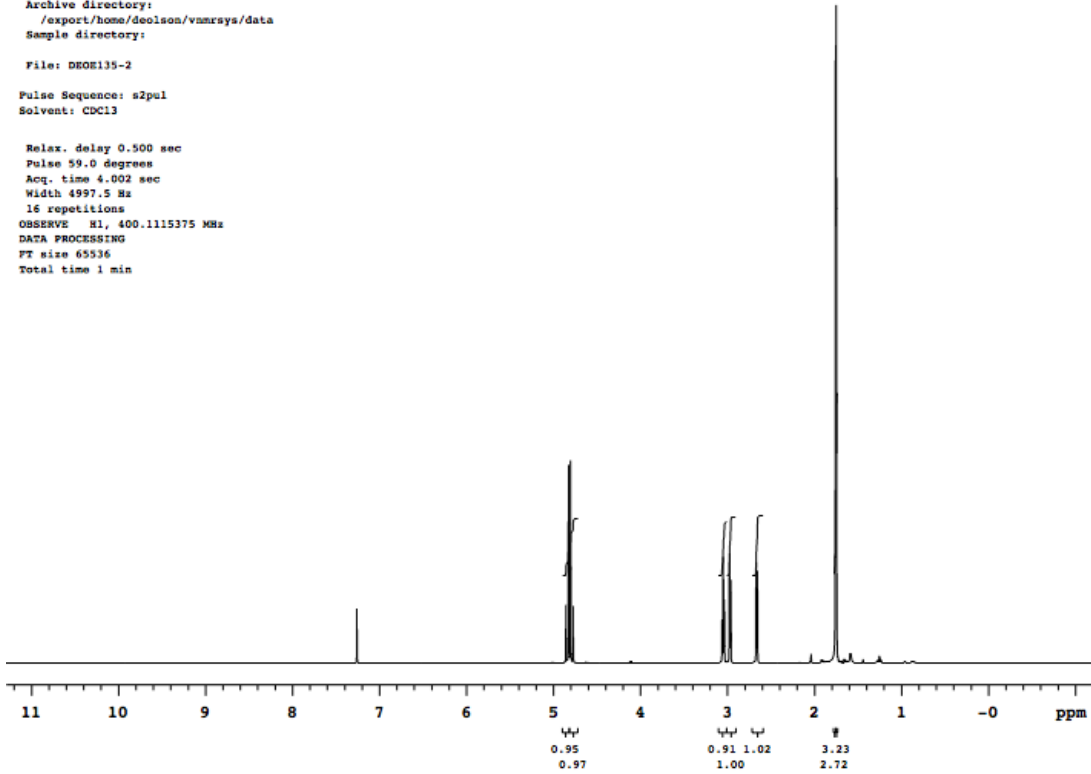
STANDARD IN OBSERVE

Archive directory:
/export/home/geolson/vmrsys/data
Sample directory:

File: DEOE135-2

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115375 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



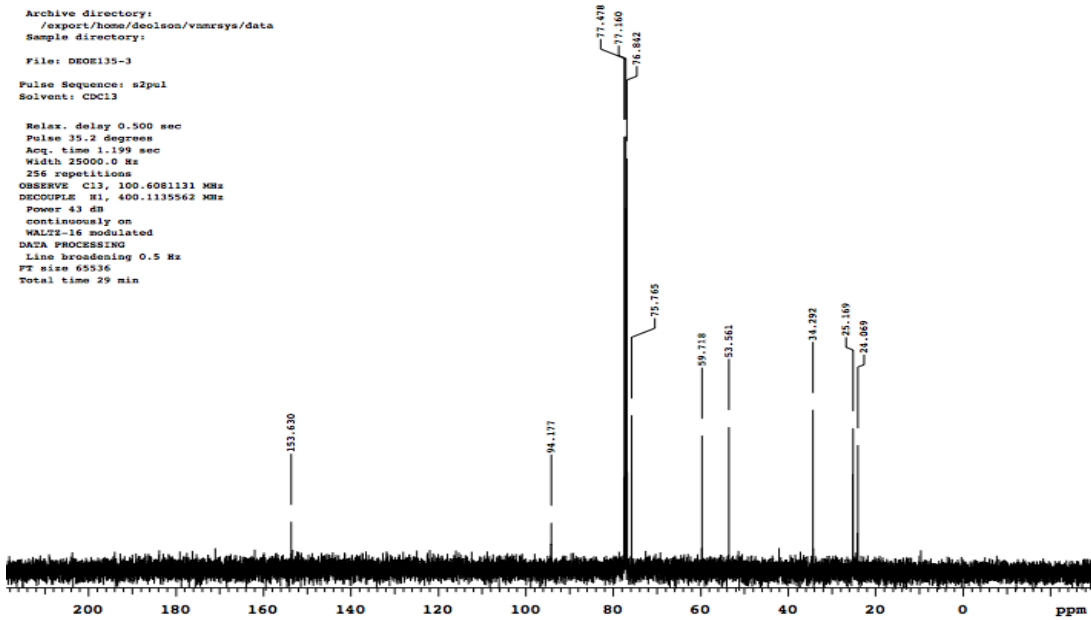
13C OBSERVE

Archive directory:
/export/home/geolson/vmrsys/data
Sample directory:

File: DEOE135-3

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
256 repetitions
OBSERVE C13, 100.6081131 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min



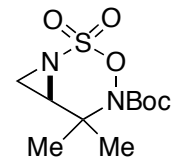


Table 1, entry 2 product

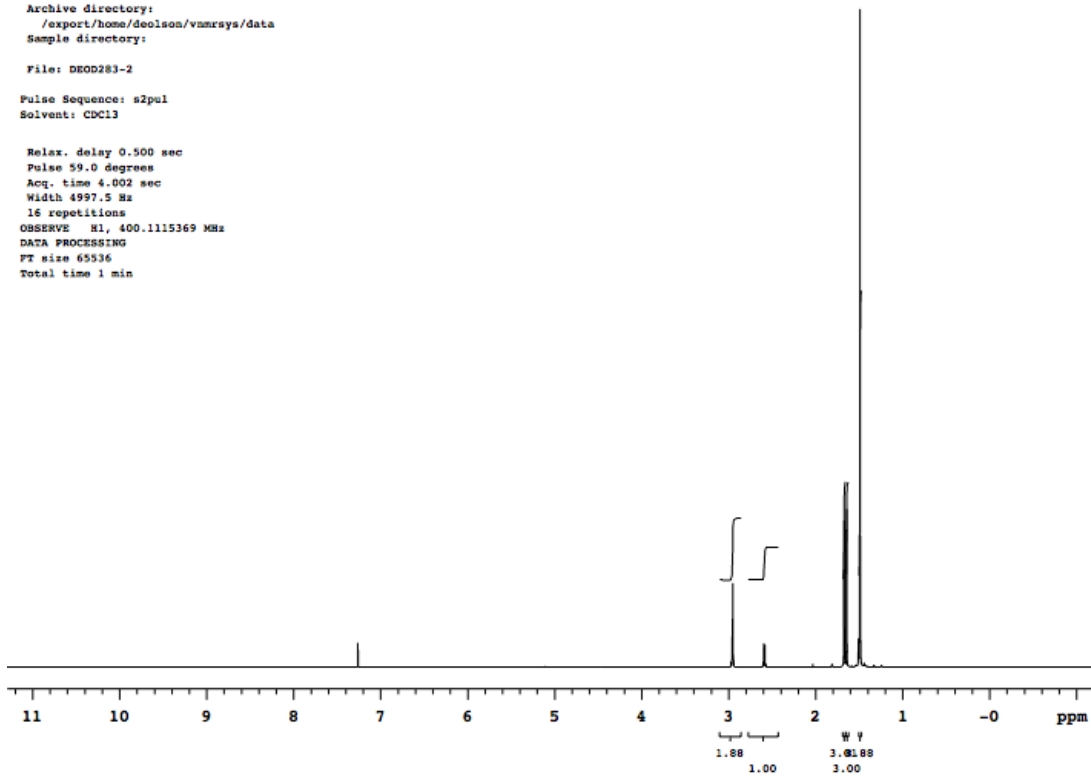
STANDARD IN OBSERVE

Archive directory:
/export/home/deolson/vmrrsys/data
Sample directory:

File: DEOD283-2

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115369 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



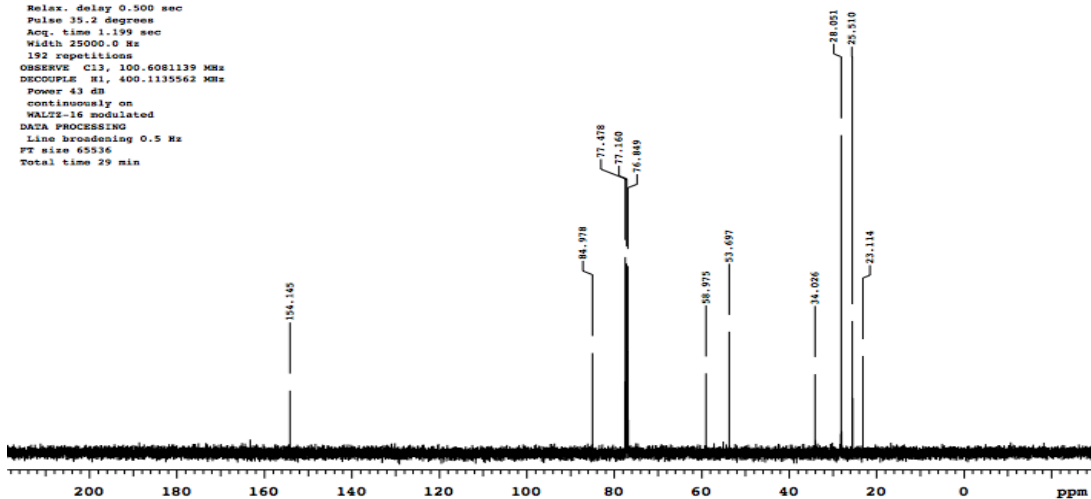
13C OBSERVE

Archive directory:
/export/home/deolson/vmrrsys/data
Sample directory:

File: DEOD283-3

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
192 repetitions
OBSERVE C13, 100.6081139 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min



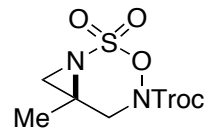


Table 1, entry 3 product

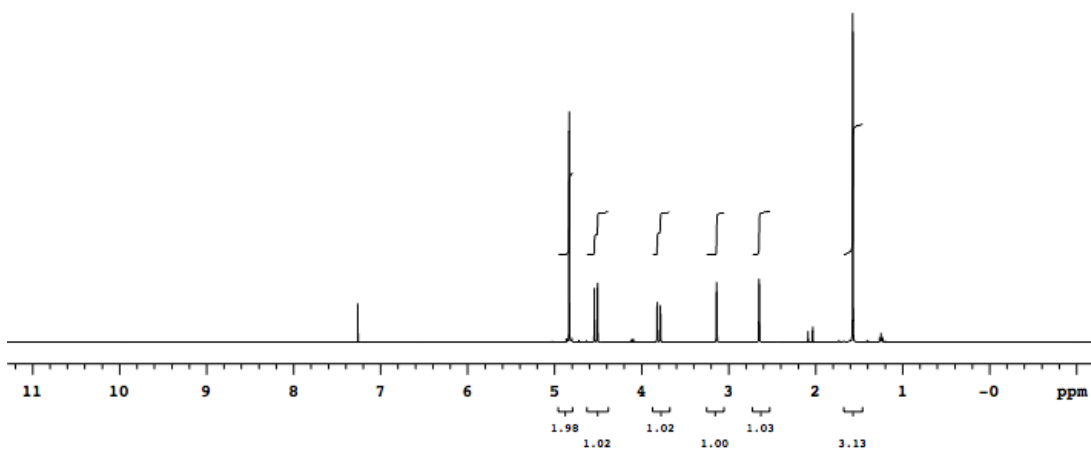
STANDARD 1H OBSERVE

Archive directory:
/export/home/deolson/vnmrsys/data
Sample directory:

File: DEOE107-2

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115372 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



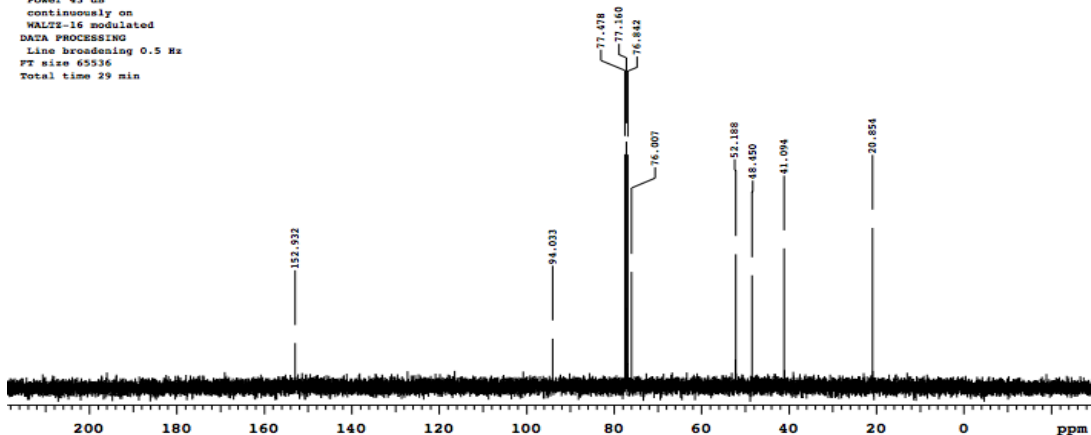
13C OBSERVE

Archive directory:
/export/home/deolson/vnmrsys/data
Sample directory:

File: DEOE107-3

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
112 repetitions
OBSERVE C13, 100.6081162 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min



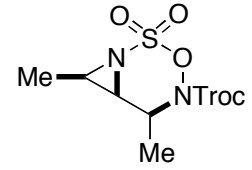


Table 1, entry 4 product (major diastereomer)

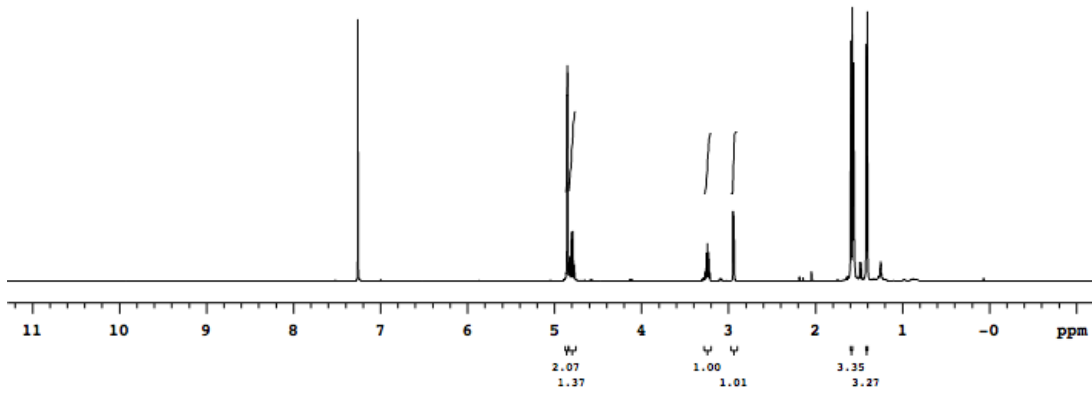
STANDARD IN OBSERVE

Archive directory:
/export/home/deolson/vnmrsws/data
Sample directory:

File: DEOE131-1

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
64 repetitions
OBSERVE H1, 400.115375 MHz
DATA PROCESSING
FT size 65536
Total time 4 min



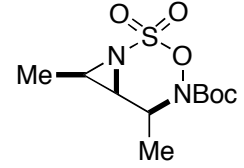


Table 1, entry 4 product (major diastereomer)

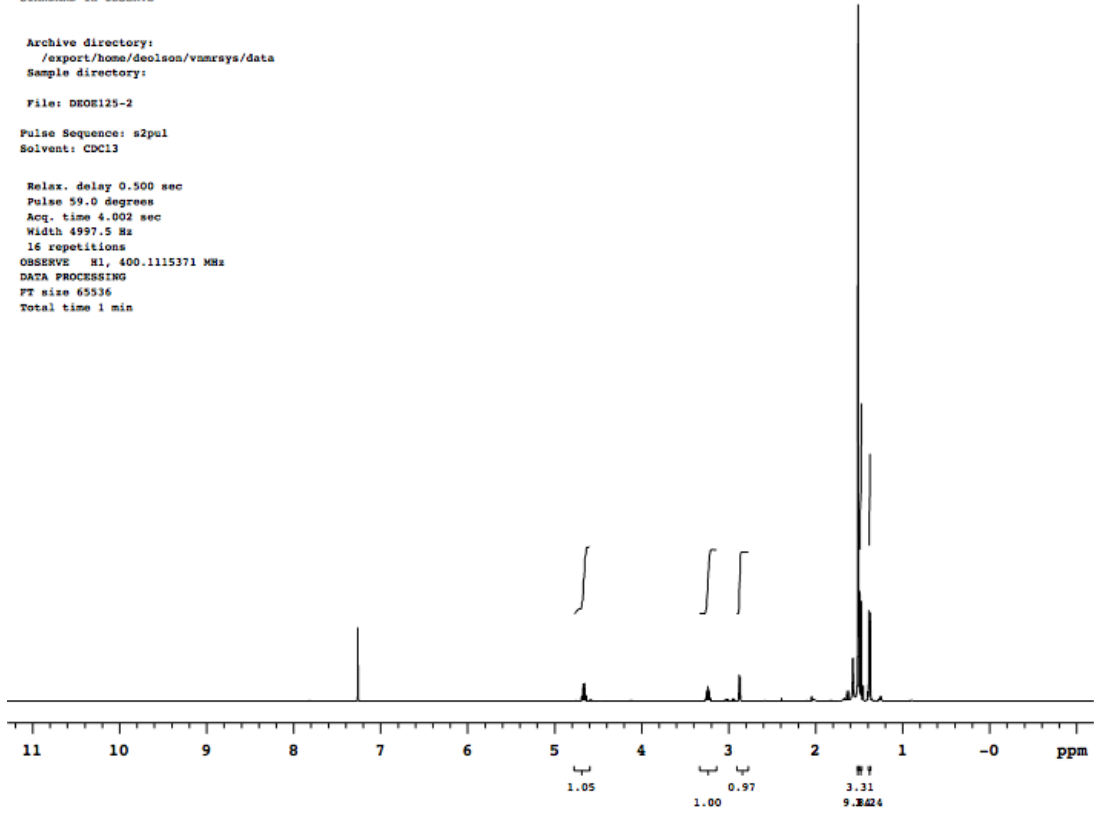
STANDARD IN OBSERVE

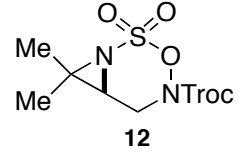
Archive directory:
/export/home/deolson/vnmrsvs/data
Sample directory:

File: DEOE125-2

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115371 MHz
DATA PROCESSING
FT size 65536
Total time 1 min

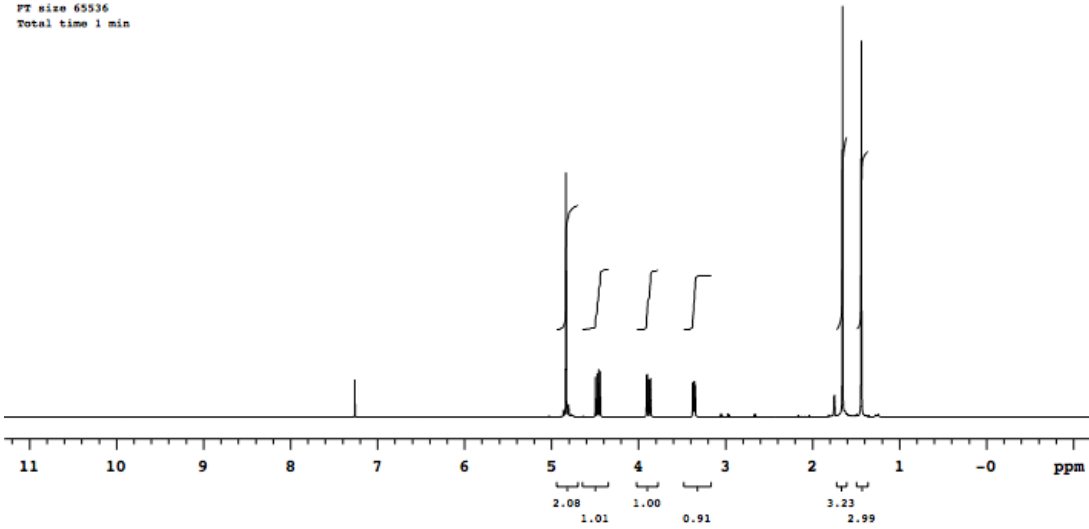




STANDARD IN OBSERVE

Archive directory:
 /export/home/deolson/vmrsys/data
 Sample directory:
 File: DEOE109-2
 Pulse Sequence: s2pul
 Solvent: CDCl3

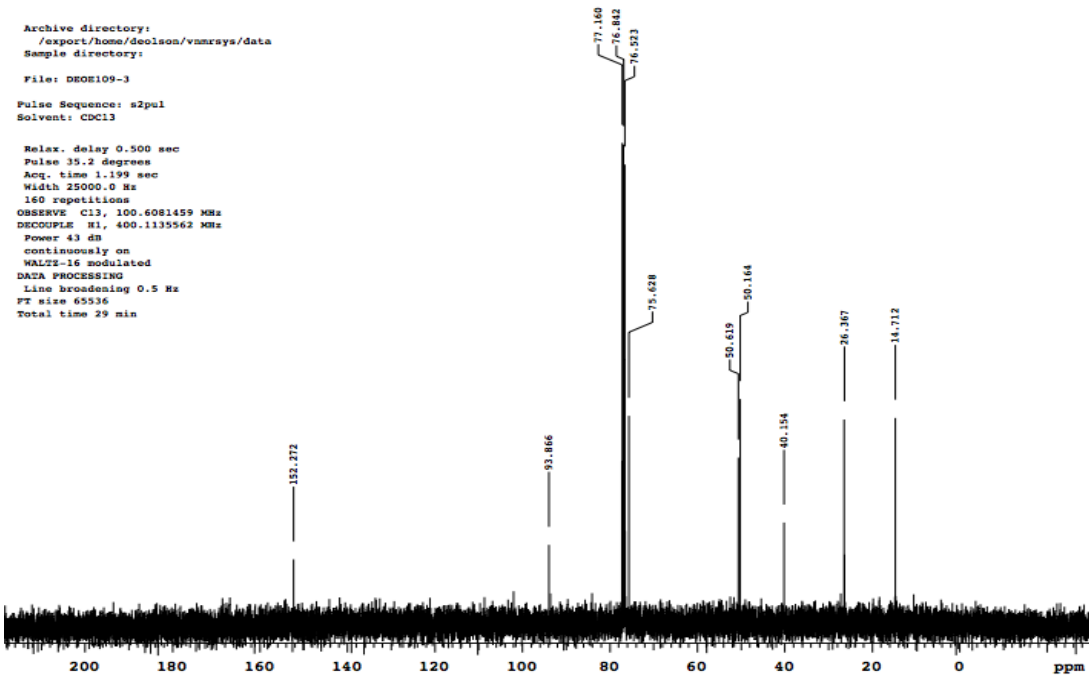
Relax. delay 0.500 sec
 Pulse 59.0 degrees
 Acq. time 4.002 sec
 Width 4997.5 Hz
 16 repetitions
 OBSERVE H1, 400.115374 MHz
 DATA PROCESSING
 FT size 65536
 Total time 1 min



13C OBSERVE

Archive directory:
 /export/home/deolson/vmrsys/data
 Sample directory:
 File: DEOE109-3
 Pulse Sequence: s2pul
 Solvent: CDCl3

Relax. delay 0.500 sec
 Pulse 35.2 degrees
 Acq. time 1.199 sec
 Width 25000.0 Hz
 150 repetitions
 OBSERVE C13, 100.6081459 MHz
 DECOUPLE H1, 400.115562 MHz
 Power 43 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 29 min



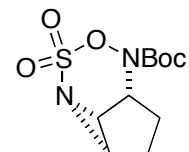


Table 1, entry 6 product

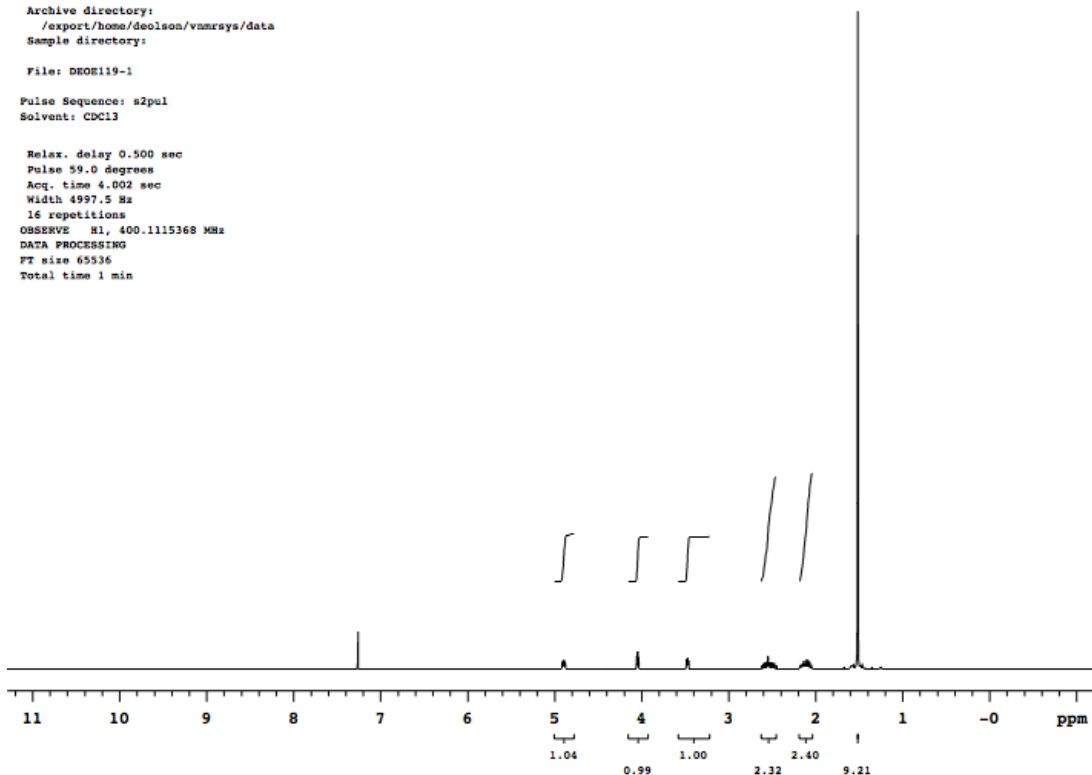
STANDARD IN OBSERVE

Archive directory:
/export/home/deolson/vmrsys/data
Sample directory:

File: DEOE119-1

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115368 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



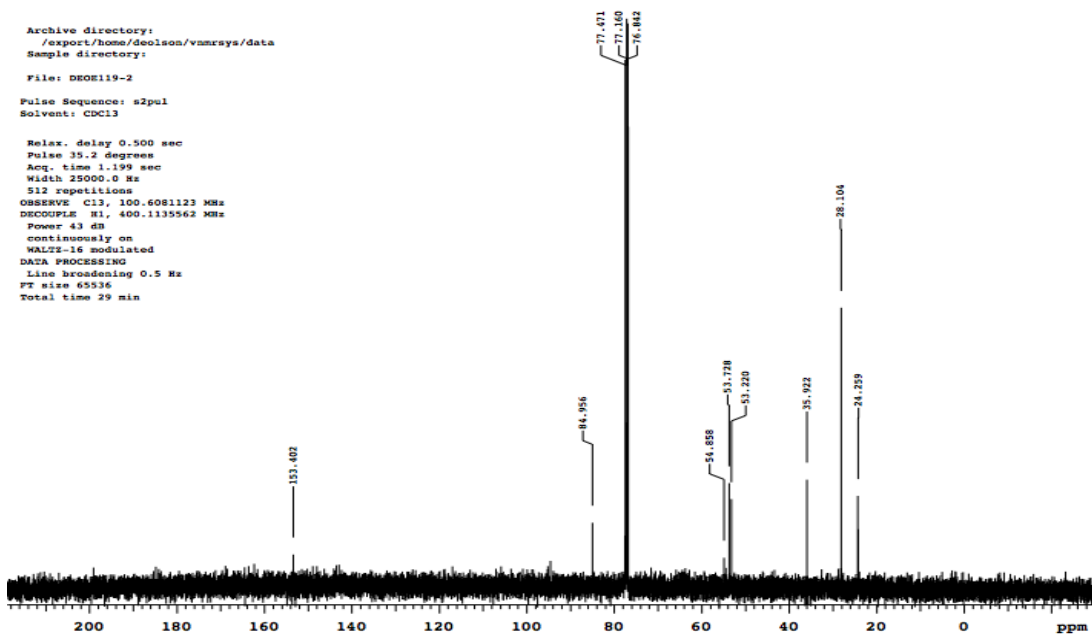
13C OBSERVE

Archive directory:
/export/home/deolson/vmrsys/data
Sample directory:

File: DEOE119-2

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
512 repetitions
OBSERVE C13, 100.6081123 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min



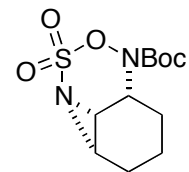


Table 1, entry 7 product

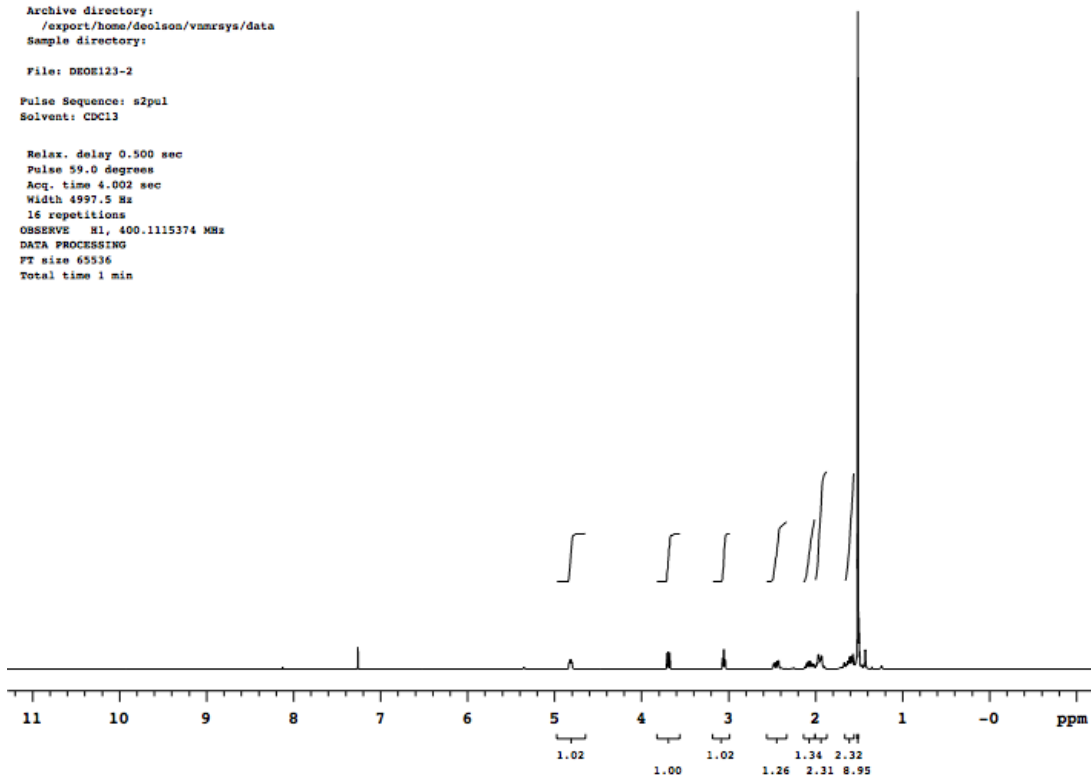
STANDARD IN OBSERVE

Archive directory:
/export/home/deolson/vnmrsvs/data
Sample directory:

File: DEOE123-2

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115374 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



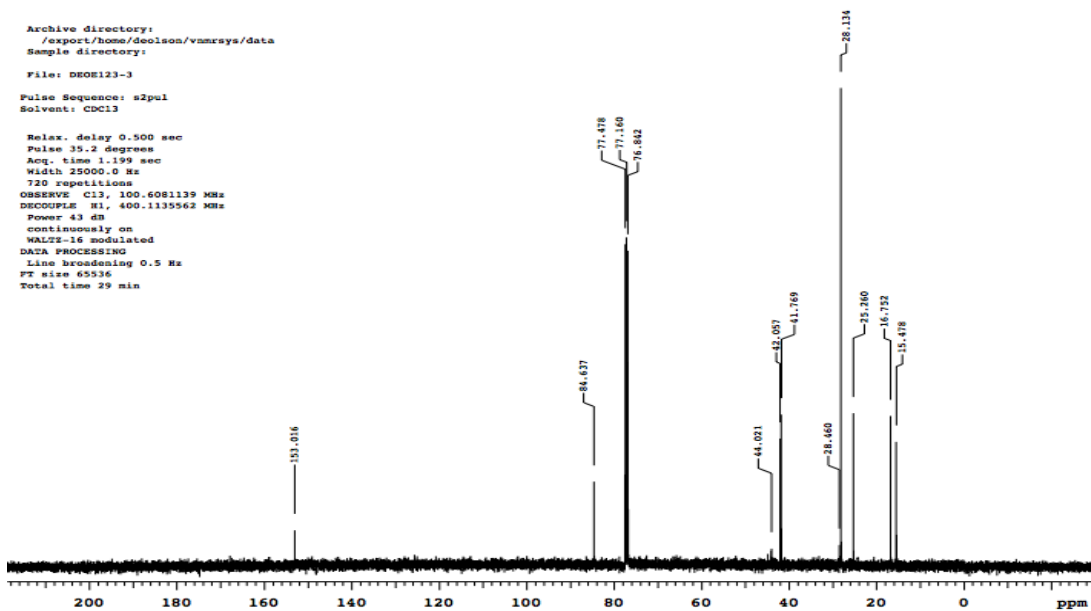
13C OBSERVE

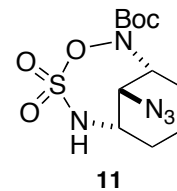
Archive directory:
/export/home/deolson/vnmrsvs/data
Sample directory:

File: DEOE123-3

Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
720 repetitions
OBSERVE C13, 100.6081139 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min





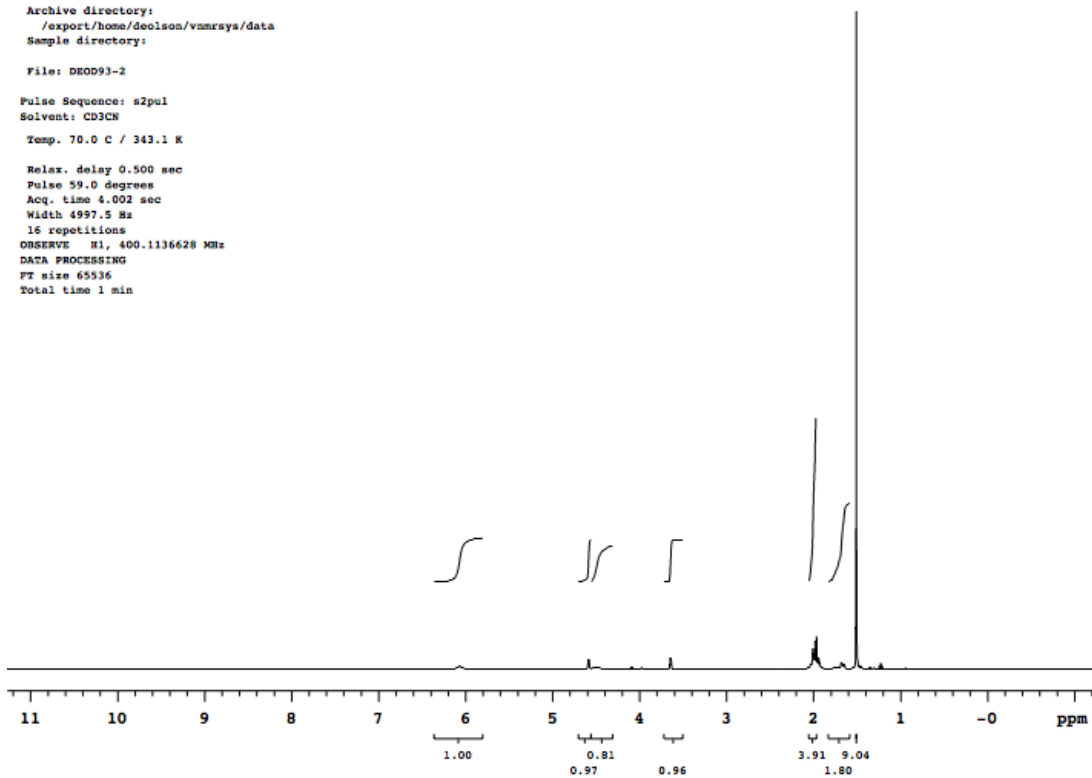
STANDARD IN OBSERVE

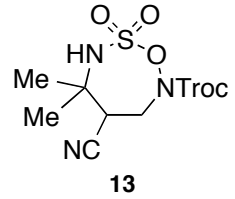
Archive directory:
 /export/home/deolson/vmmsys/data
 Sample directory:

File: DEOD93-2

Pulse Sequence: s2pul
 Solvent: CD3CN
 Temp. 70.0 C / 343.1 K

Relax. delay 0.500 sec
 Pulse 59.0 degrees
 Acq. time 4.002 sec
 Width 4997.5 Hz
 16 repetitions
 OBSERVE M1, 400.113628 MHz
 DATA PROCESSING
 FT size 65536
 Total time 1 min





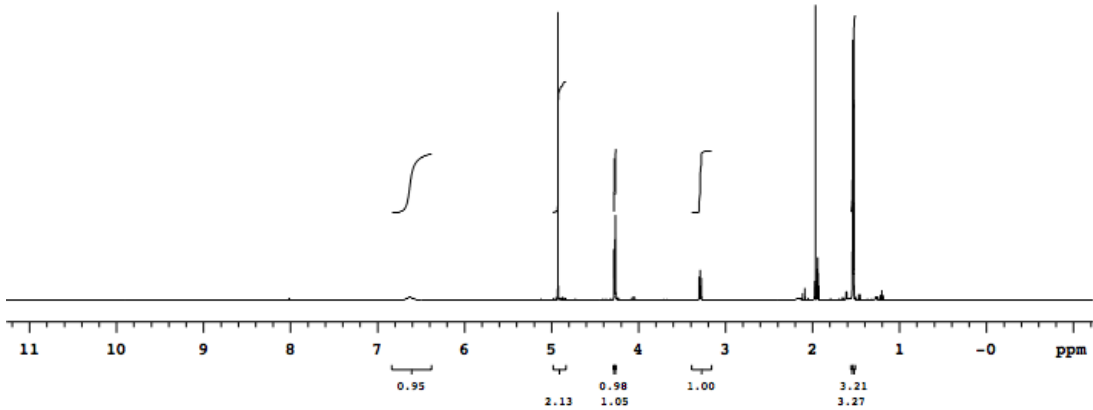
STANDARD 1H OBSERVE

Archive directory:
/export/home/deolson/vnmrsws/data
Sample directory:

File: DEOE161-4

Pulse Sequence: s2pul
Solvent: CD3CN

Relax. delay 0.500 sec
Pulse 60.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1136634 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



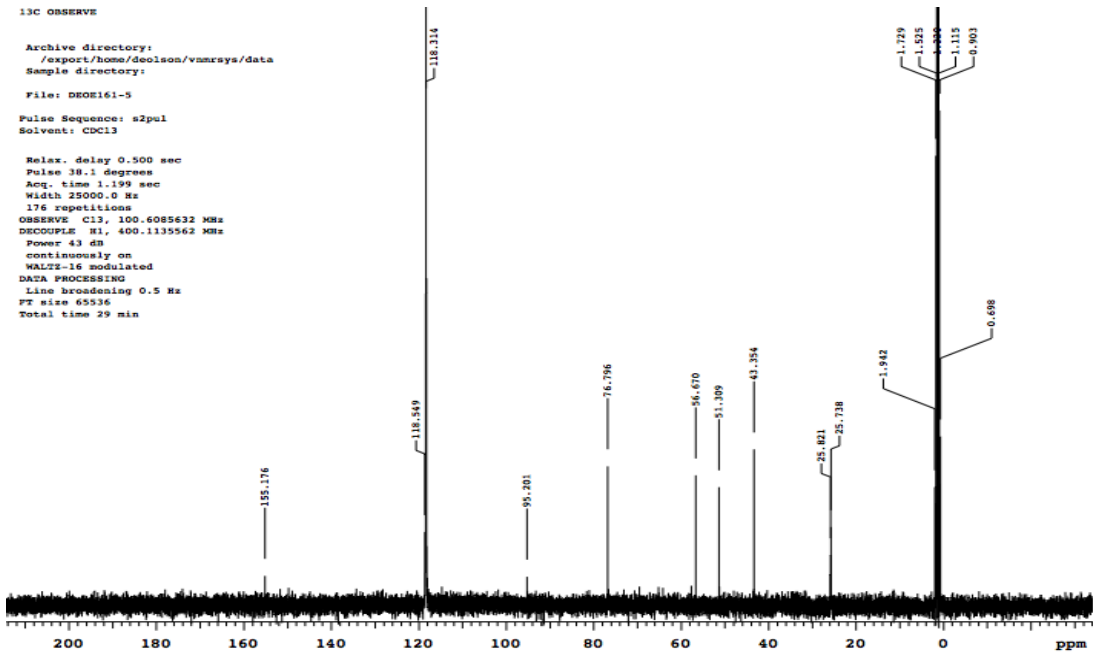
13C OBSERVE

Archive directory:
/export/home/deolson/vnmrsws/data
Sample directory:

File: DEOE161-5

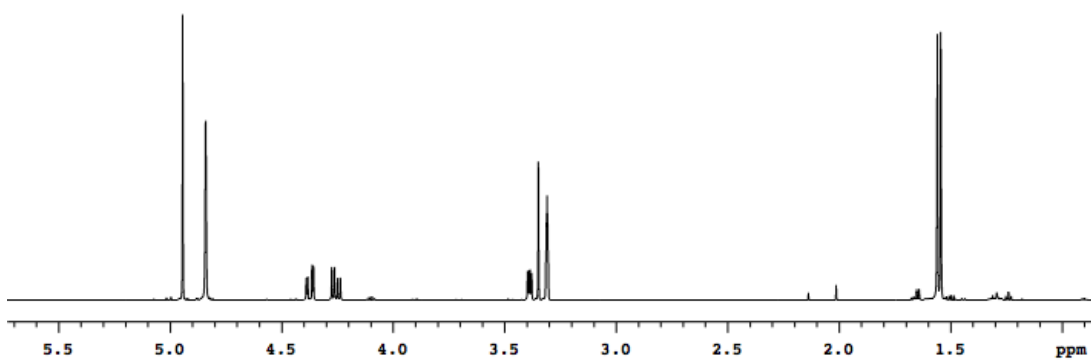
Pulse Sequence: s2pul
Solvent: CDCl3

Relax. delay 0.500 sec
Pulse 38.1 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
176 repetitions
OBSERVE C13, 100.6085632 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 29 min

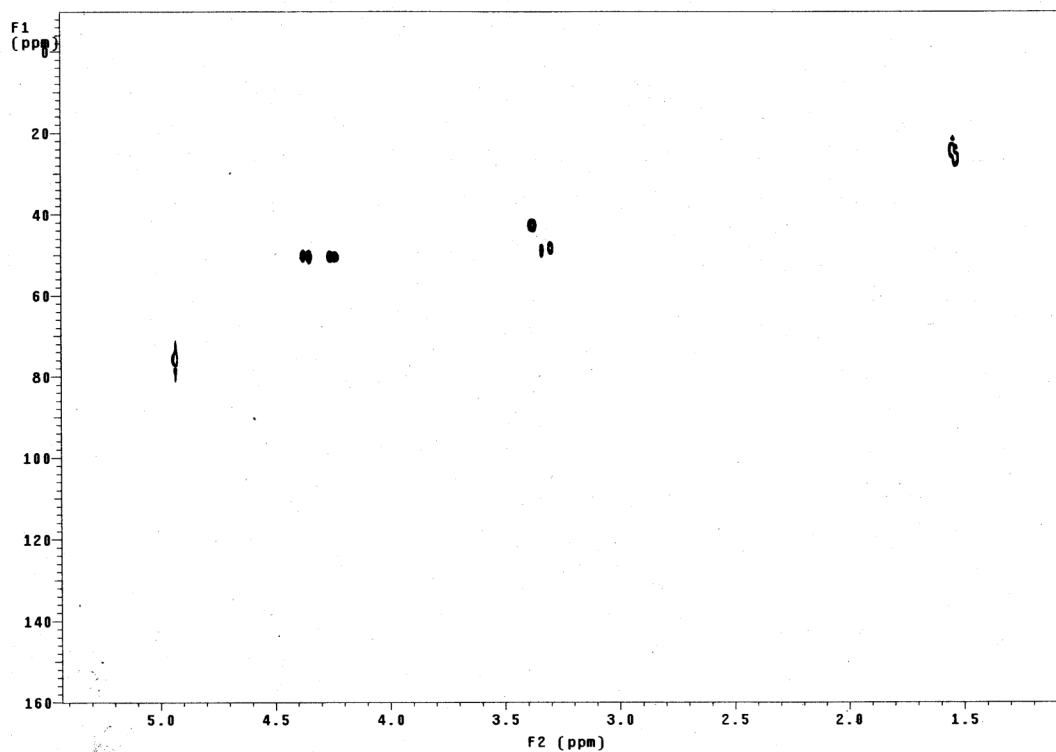


Std proton

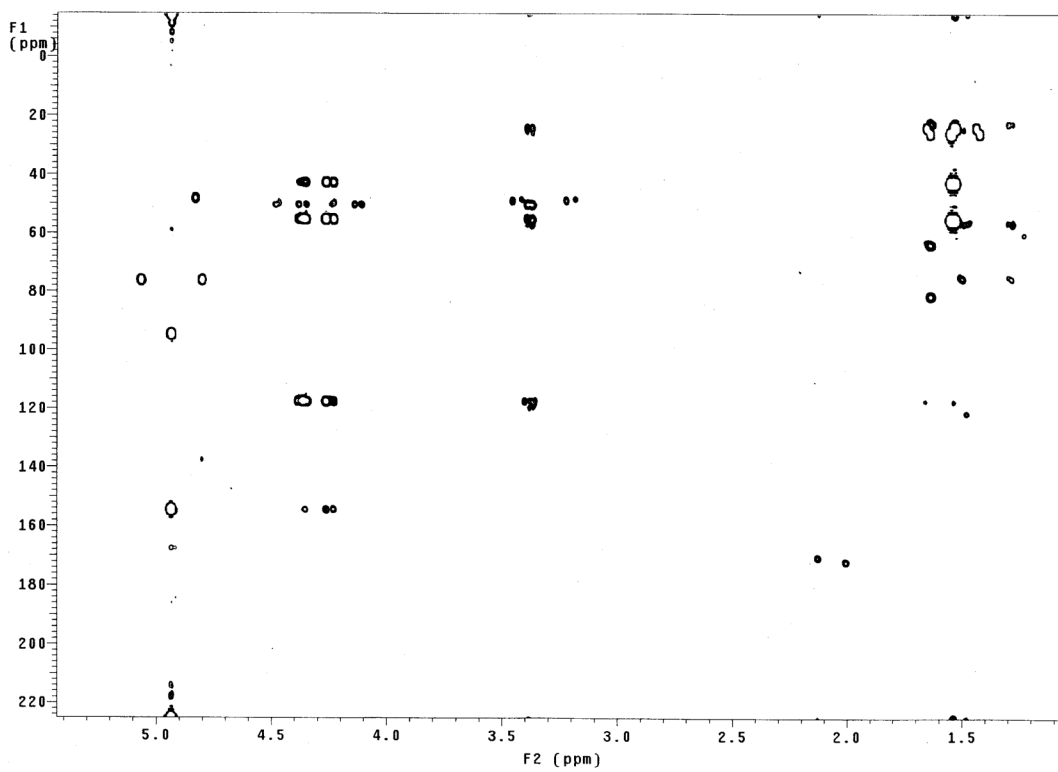
Archive directory:
Sample directory:
File: DEOE161-7
Pulse Sequence: s2pul
Solvent: cd3od
Temp. 25.0 C / 298.1 K
Relax. delay 0.200 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 9611.9 Hz
16 repetitions
OBSERVE H1, 599.7996482 MHz
DATA PROCESSING
FT size 131072
Total time 1 min

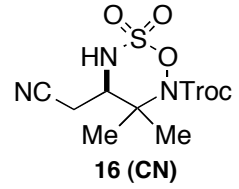


HSQC



HMBC





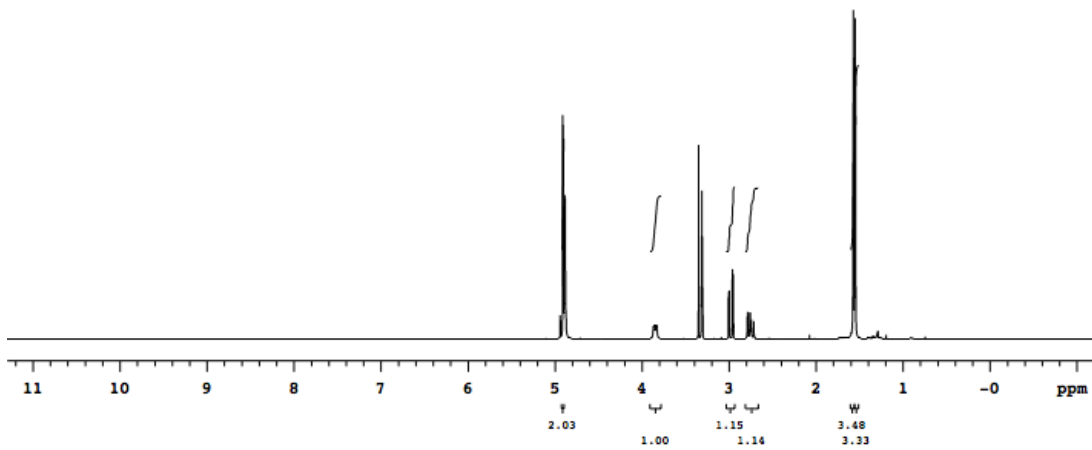
STANDARD IN OBSERVE

Archive directory:
/export/home/deolson/vnmrsvs/data
Sample directory:

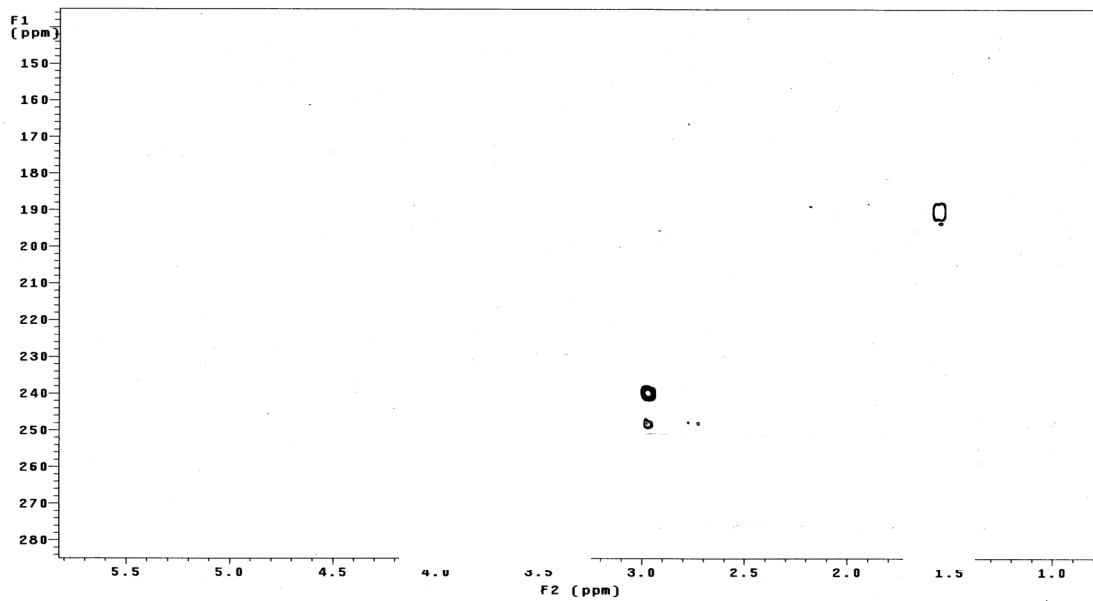
File: DEOE193-1

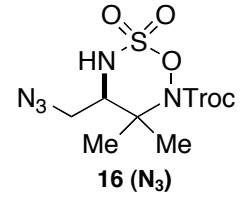
Pulse Sequence: s2pul
Solvent: CD3OD

Relax. delay 0.500 sec
Pulse 60.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1131115 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



15N HMBC





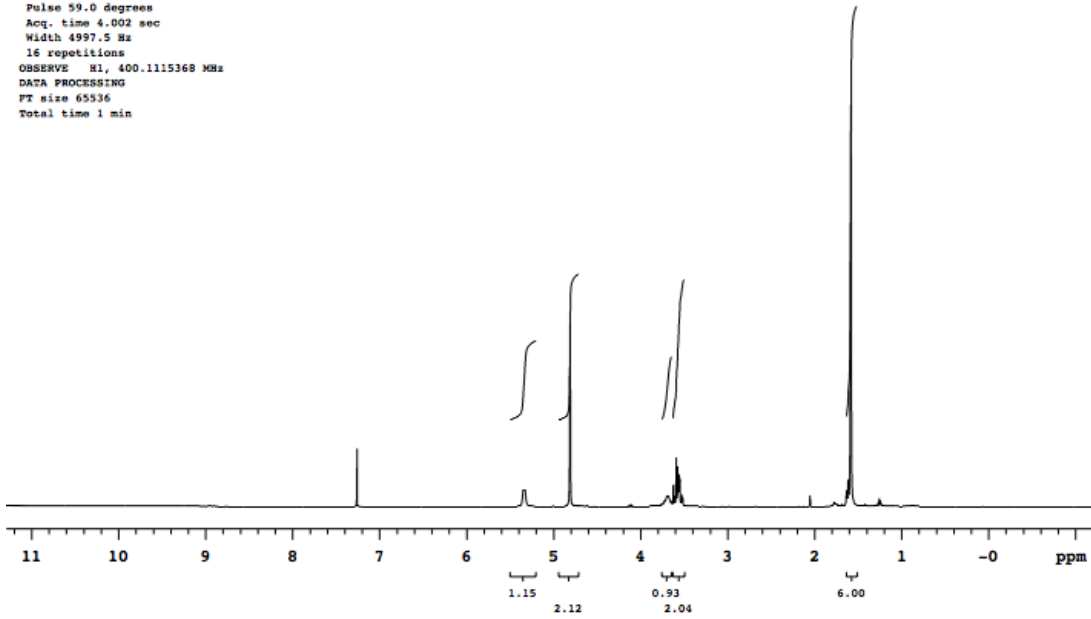
STANDARD 1H OBSERVE

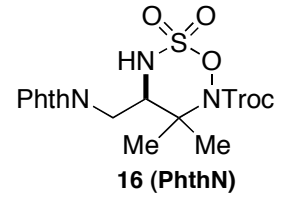
Archive directory:
/export/home/deolson/vnmrsvs/data
Sample directory:

File: DEOE139-7

Pulse Sequence: s2pul
Solvent: CDCl3

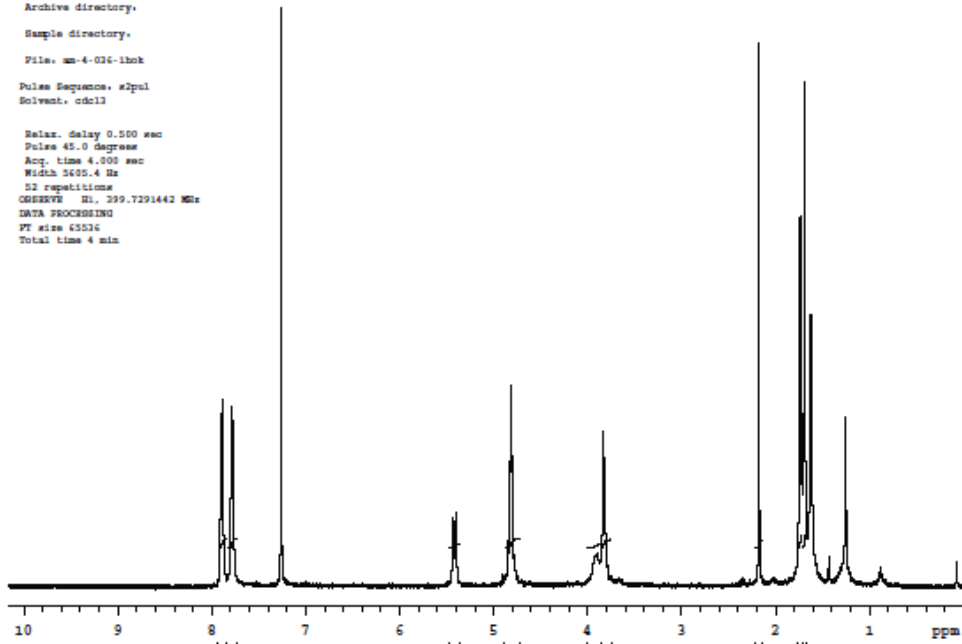
Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115368 MHz
DATA PROCESSING
FT size 65536
Total time 1 min



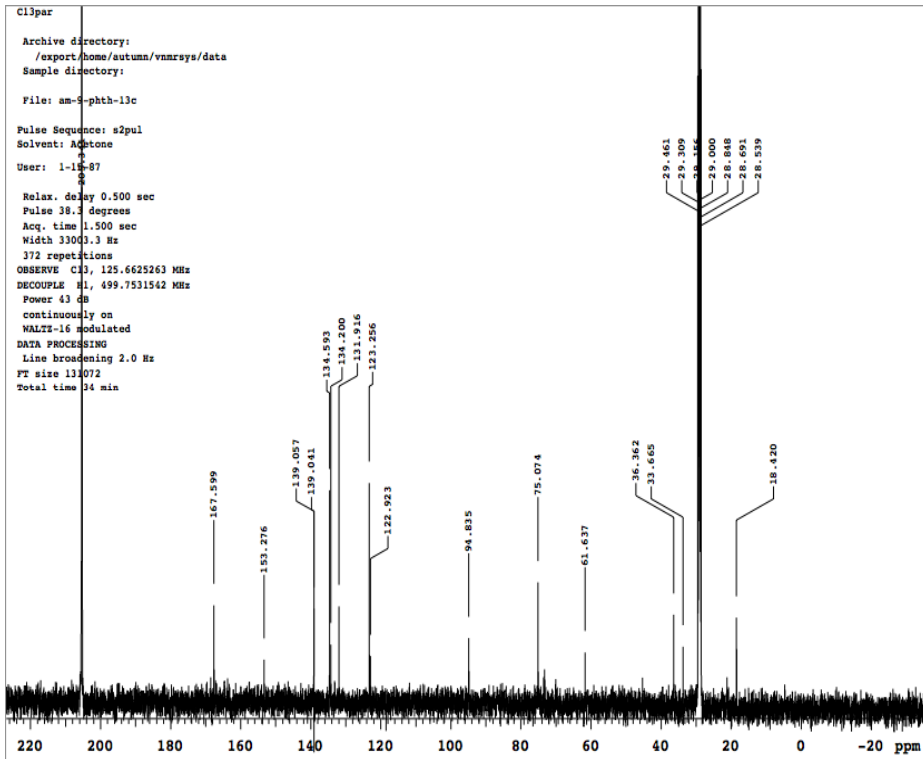


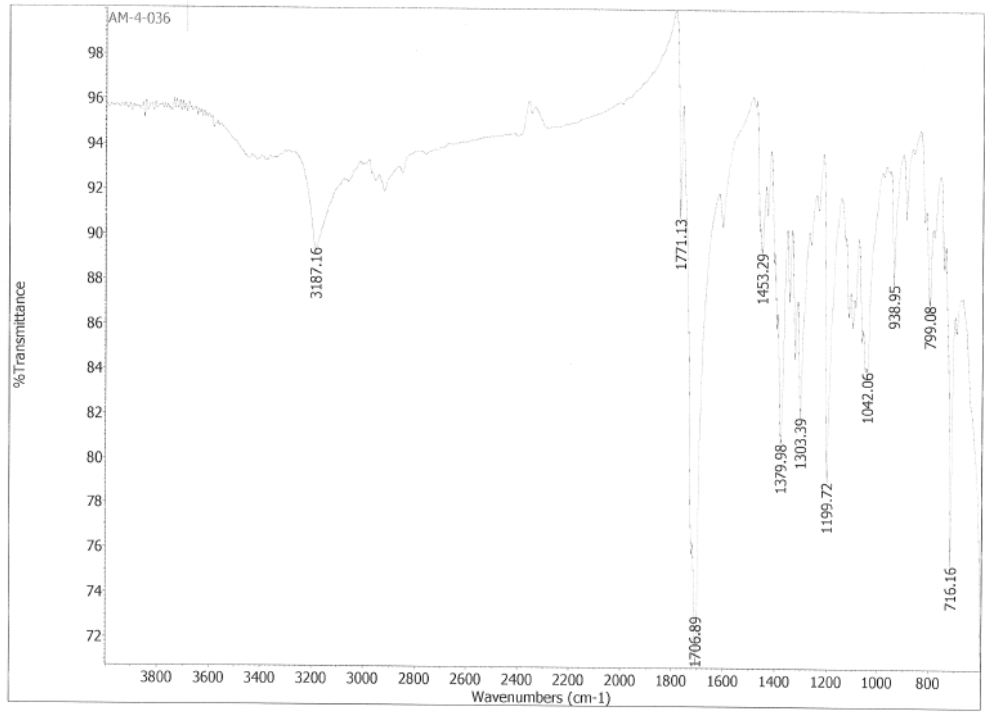
8H6 proton

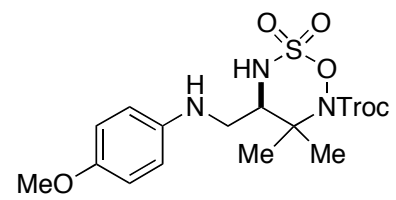
Archive directory.
 Sample directory.
 File: nm-4-036-1hok
 Pulse Sequence: s2pul
 Solvent: cdcl3
 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 4.000 sec
 Width 5605.4 Hz
 S2 repetition
 OBSERVE H1, 299.7291442 MHz
 DATA PROCESSING
 FT size 65536
 Total time 4 min



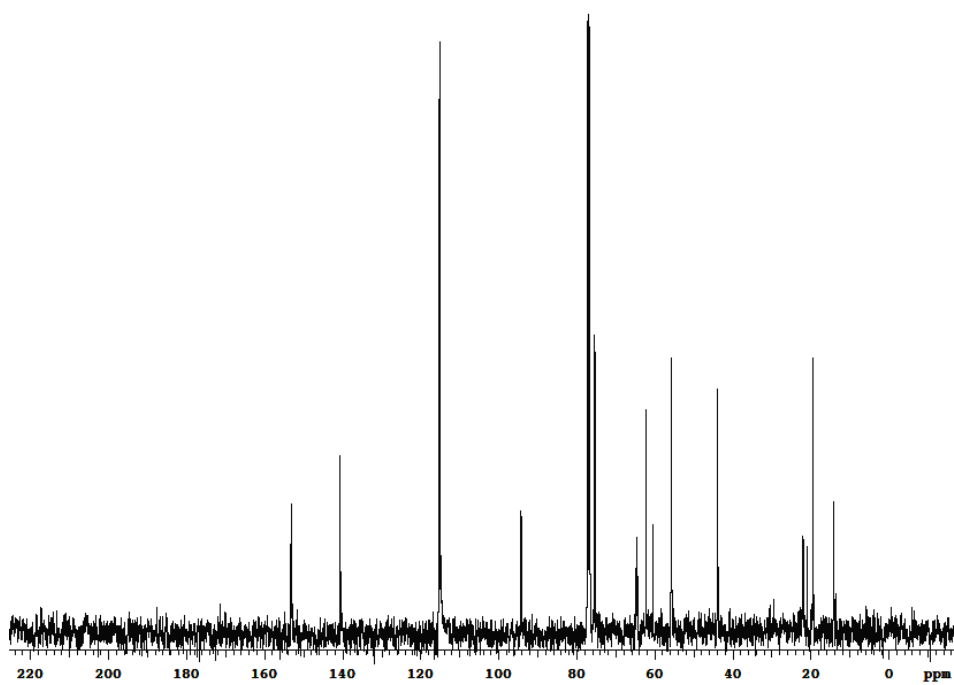
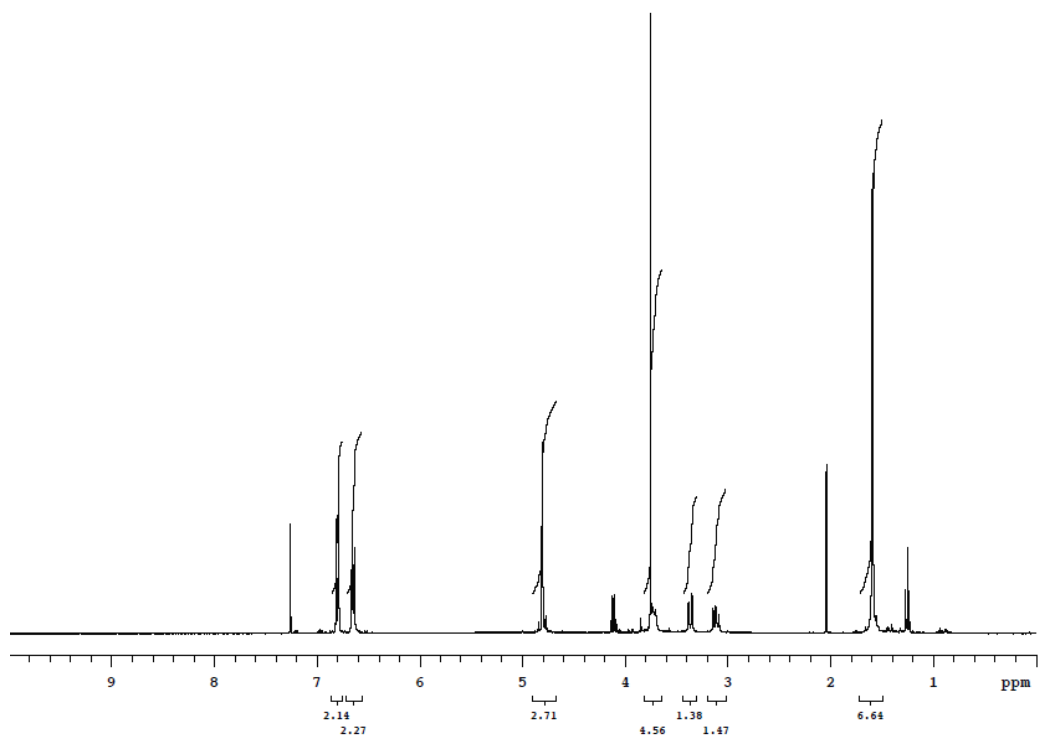
C13par
 Archive directory:
 /export/home/autumn/vmrsvs/data
 Sample directory:
 File: nm-6-phth-13c
 Pulse Sequence: s2pul
 Solvent: Acetone
 User: 1-18-87
 Relax. delay 0.500 sec
 Pulse 38.2 degrees
 Acq. time 1.500 sec
 Width 33003.3 Hz
 372 repetitions
 OBSERVE C13, 125.6625263 MHz
 DECOUPLE H1, 499.7531542 MHz
 Power 43 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 2.0 Hz
 FT size 131072
 Total time 34 min

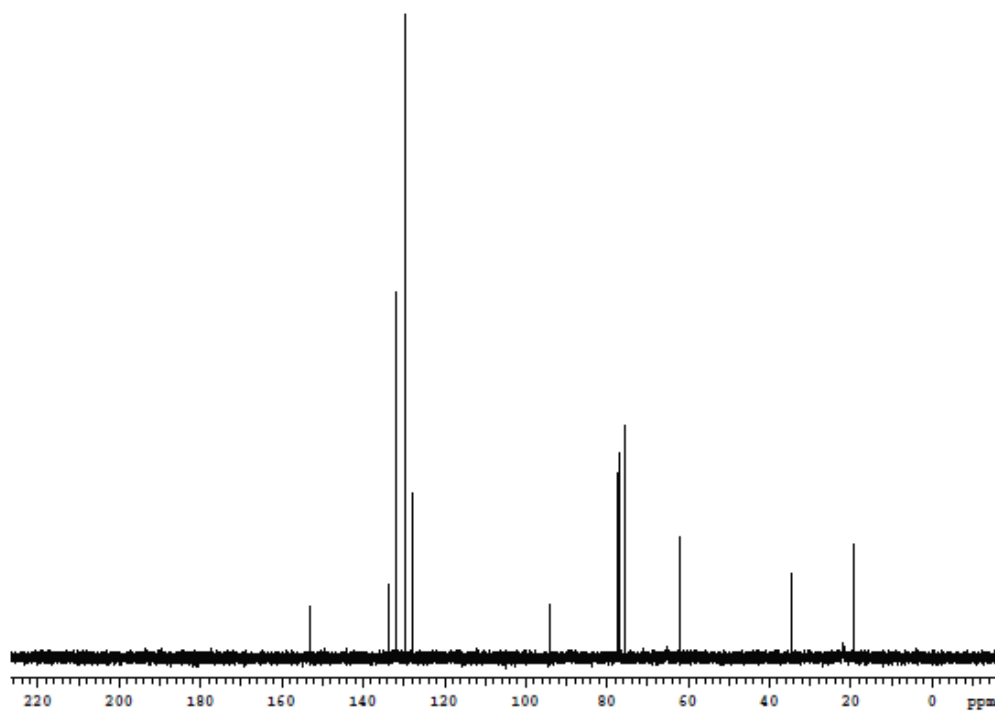
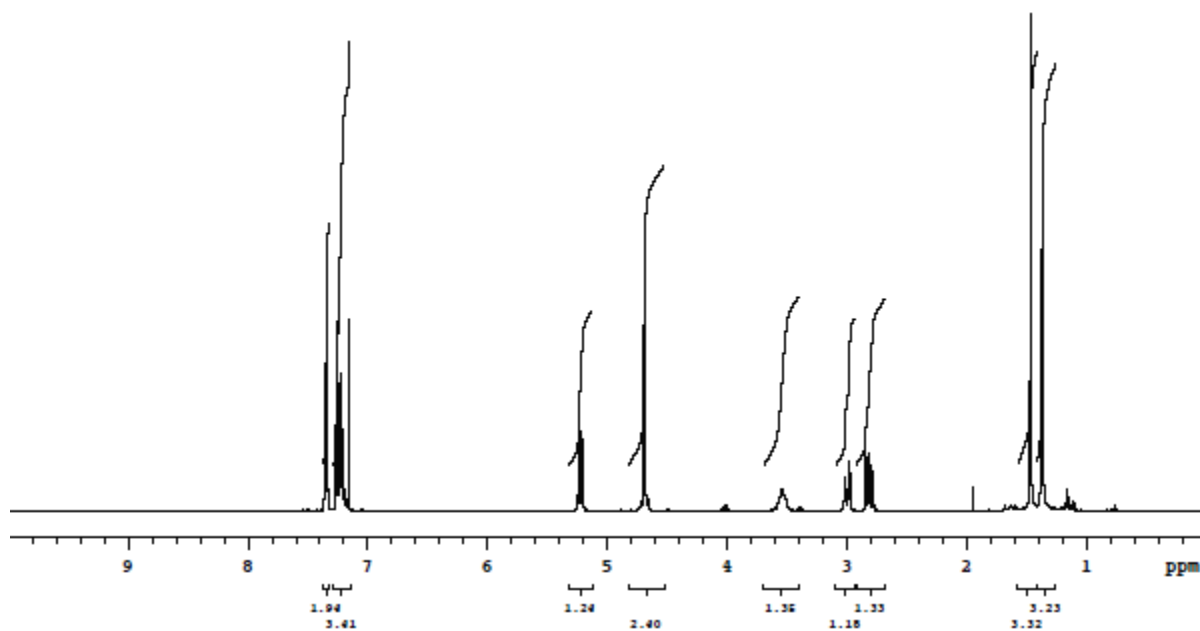
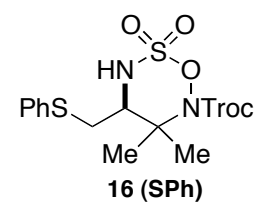


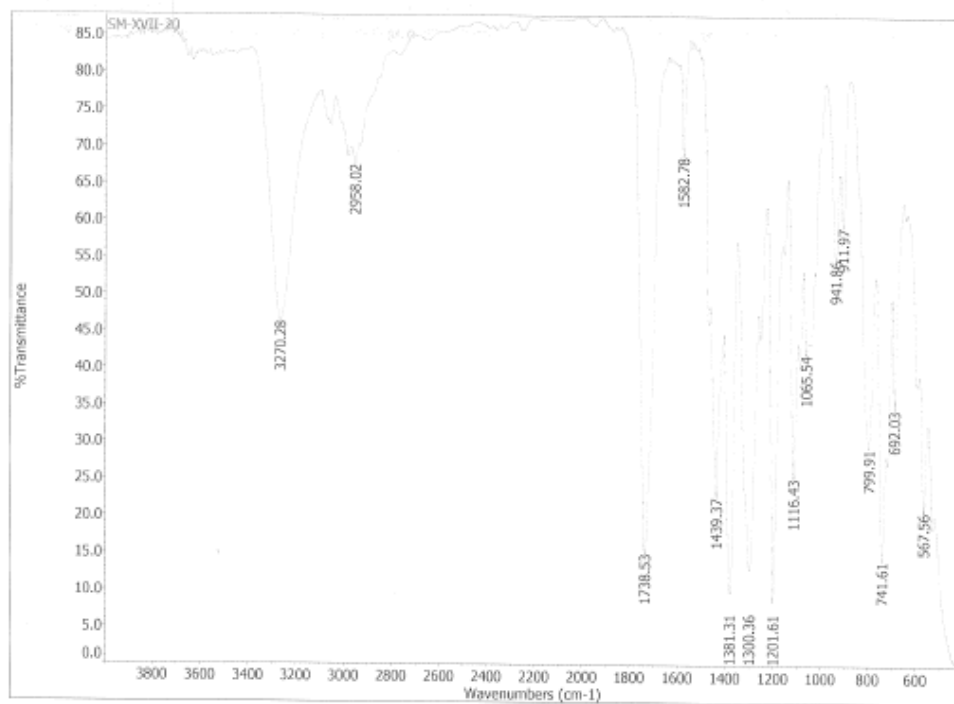


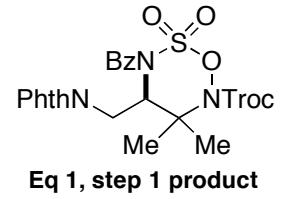


16 (NHC₆H₄OMe)





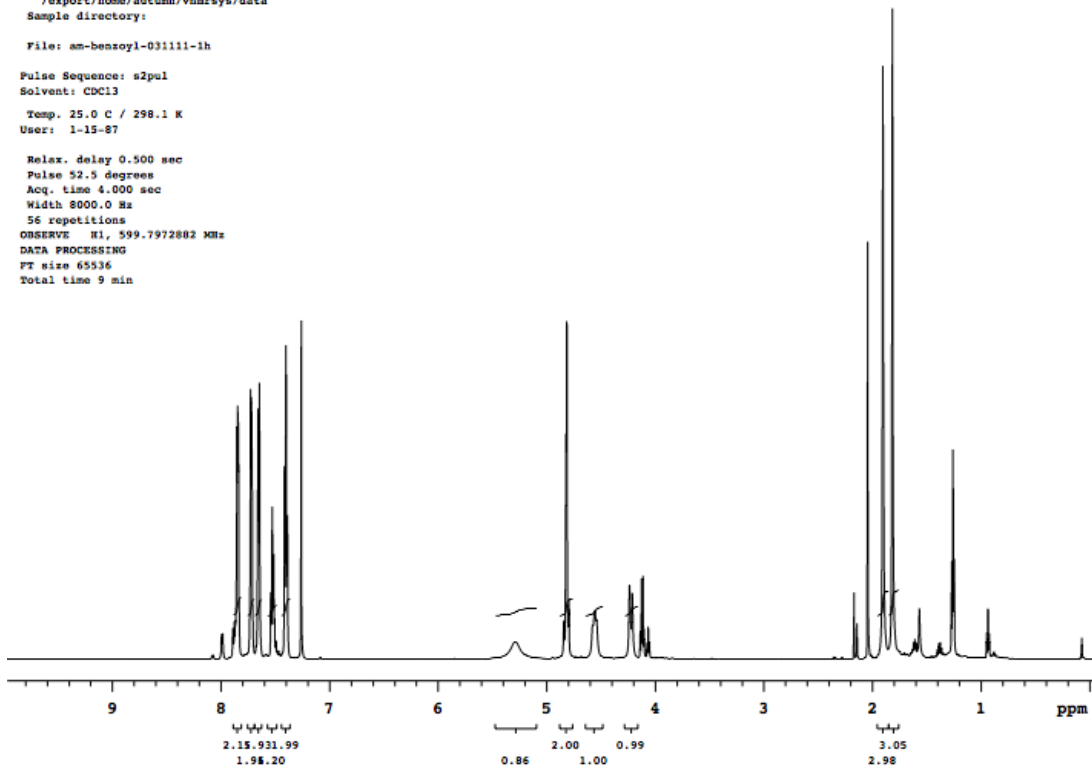




STANDARD PROTON PARAMETERS

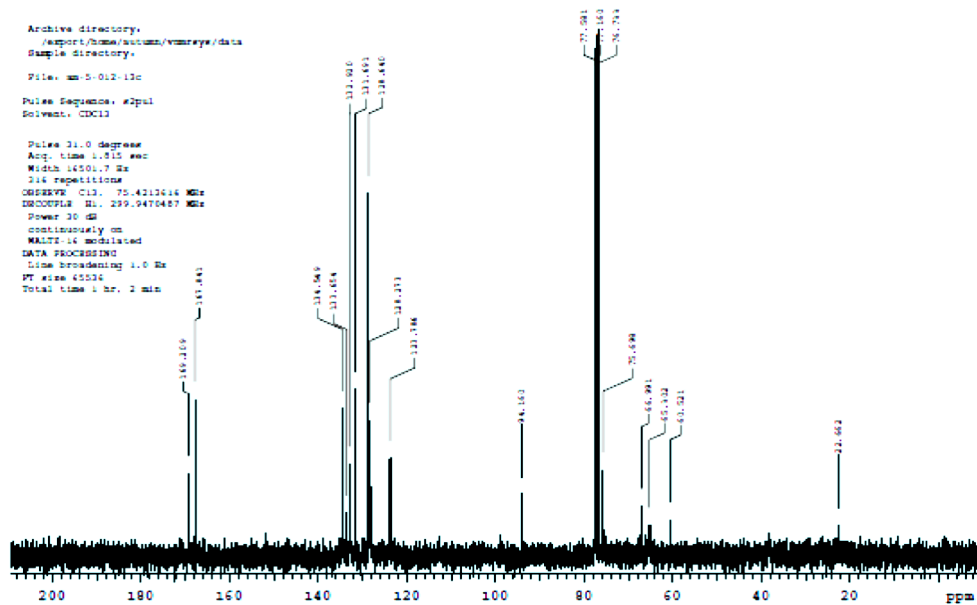
Archive directory:
 /export/home/autumn/vmrsys/data
 Sample directory:
 File: am-benzoyl-031111-1h
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
 User: 1-15-87

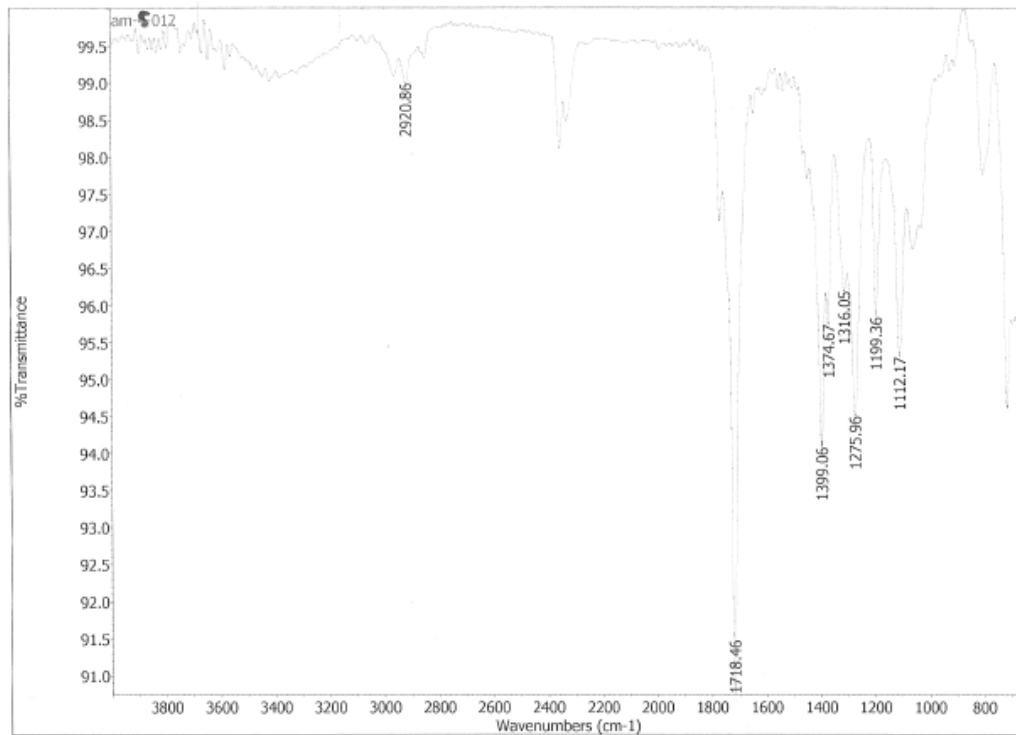
Relax. delay 0.500 sec
 Pulse 52.5 degrees
 Acq. time 4.000 sec
 Width 8000.0 Hz
 56 repetitions
 OBSERVE H1, 599.7972882 MHz
 DATA PROCESSING
 FT size 65536
 Total time 9 min

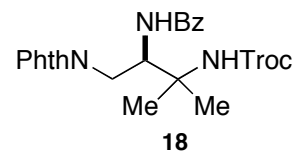


13C NMR

Archive directory:
 /export/home/autumn/vmrsys/data
 Sample directory:
 File: am-0-012-13c
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Pulse 31.0 degree
 Acq. time 1.915 sec
 Width 14501.7 Hz
 214 repetitions
 OBSERVE C13, 75.4213614 MHz
 DECOUPLE H1, 299.0470487 MHz
 Power 30 dB
 Continuously on
 MALTZ-14 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 1 hr, 2 min







STANDARD PROTON PARAMETERS

Archive directory:
 /export/home/autumn/vmrays/data
 Sample directory:

File: an-reducedbenz

Pulse Sequence: s2pul
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
 User: 1-15-87

Relax. delay 0.500 sec
 Pulse 52.5 degrees
 Acq. time 4.000 sec
 Width 8000.0 Hz
 32 repetitions
 OBSERVE H1, 599.7972879 MHz
 DATA PROCESSING
 FT size 65536
 Total time 9 min

