

Supporting Information 2
for
Facile synthesis of 1-alkoxy-1*H*-benzo- and 7-azabenzotriazoles
from peptide coupling agents, mechanistic studies, and synthetic
applications

Mahesh K. Lakshman*, Manish K. Singh, Mukesh Kumar, Raghu Ram Chamala, Vijayender R. Yedulla,
Domenick Wagner, Evan Leung, Lijia Yang, Asha Matin, and Sadia Ahmad

Address: Department of Chemistry, The City College and The City University of New York, 160 Convent
Avenue, New York, NY 10031, USA

Email: Mahesh K. Lakshman* - lakshman@sci.ccny.cuny.edu

*Corresponding author

NMR Spectra

Table of Contents

Information	Page
500 MHz ¹ H NMR spectrum of 1a in CDCl ₃	S5
125 MHz ¹³ C NMR spectrum of 1a in CDCl ₃	S6
500 MHz ¹ H NMR spectrum of 1b in CDCl ₃	S7
125 MHz ¹³ C NMR spectrum of 1b in CDCl ₃	S8
500 MHz ¹ H NMR spectrum of 1c in CDCl ₃	S9
125 MHz ¹³ C NMR spectrum of 1c in CDCl ₃	S10
500 MHz ¹ H NMR spectrum of 1d in CDCl ₃	S11
125 MHz ¹³ C NMR spectrum of 1d in CDCl ₃	S12
500 MHz ¹ H NMR spectrum of 1e in CDCl ₃	S13
125 MHz ¹³ C NMR spectrum of 1e in CDCl ₃	S14
500 MHz ¹ H NMR spectrum of 1f in CDCl ₃	S15
125 MHz ¹³ C NMR spectrum of 1f in CDCl ₃	S16
500 MHz ¹ H NMR spectrum of 1g in CDCl ₃	S17
125 MHz ¹³ C NMR spectrum of 1g in CDCl ₃	S18
500 MHz ¹ H NMR spectrum of 1h in CDCl ₃	S19

125 MHz ^{13}C NMR spectrum of 1h in CDCl_3	S20
500 MHz ^1H NMR spectrum of 1i in CDCl_3	S21
125 MHz ^{13}C NMR spectrum of 1i in CDCl_3	S22
500 MHz ^1H NMR spectrum of 1j in CDCl_3	S23
125 MHz ^{13}C NMR spectrum of 1j in CDCl_3	S24
500 MHz ^1H NMR spectrum of 1k in CDCl_3	S25
125 MHz ^{13}C NMR spectrum of 1k in CDCl_3	S26
500 MHz ^1H NMR spectrum of 1l in CDCl_3	S27
125 MHz ^{13}C NMR spectrum of 1l in CDCl_3	S28
500 MHz ^1H NMR spectrum of 1m in CDCl_3	S29
Expanded 500 MHz ^1H NMR spectrum of 1m in CDCl_3	S30
125 MHz ^{13}C NMR spectrum of 1m in CDCl_3	S31
500 MHz ^1H NMR spectrum of 1n in CDCl_3	S32
125 MHz ^{13}C NMR spectrum of 1n in CDCl_3	S33
500 MHz ^1H NMR spectrum of 1o in CDCl_3	S34
125 MHz ^{13}C NMR spectrum of 1o in CDCl_3	S35
500 MHz ^1H NMR spectrum of 1p in CDCl_3	S36
500 MHz ^1H NMR spectrum of 2a in CDCl_3	S37
125 MHz ^{13}C NMR spectrum of 2a in CDCl_3	S38
500 MHz ^1H NMR spectrum of 2b in CDCl_3	S39
125 MHz ^{13}C NMR spectrum of 2b in CDCl_3	S40
500 MHz ^1H NMR spectrum of 2c in CDCl_3	S41
125 MHz ^{13}C NMR spectrum of 2c in CDCl_3	S42
500 MHz ^1H NMR spectrum of 2d in CDCl_3	S43
125 MHz ^{13}C NMR spectrum of 2d in CDCl_3	S44
500 MHz ^1H NMR spectrum of 2e in CDCl_3	S45
125 MHz ^{13}C NMR spectrum of 2e in CDCl_3	S46
500 MHz ^1H NMR spectrum of 2f in CDCl_3	S47
125 MHz ^{13}C NMR spectrum of 2f in CDCl_3	S48
500 MHz ^1H NMR spectrum of 2g in CDCl_3	S49
125 MHz ^{13}C NMR spectrum of 2g in CDCl_3	S50
500 MHz ^1H NMR spectrum of 2h in CDCl_3	S51
Expanded 500 MHz ^1H NMR spectrum of 2h in CDCl_3	S52
125 MHz ^{13}C NMR spectrum of 2h in CDCl_3	S53
500 MHz ^1H NMR spectrum of 2i in CDCl_3	S54
Expanded 500 MHz ^1H NMR spectrum of 2i in CDCl_3	S55
125 MHz ^{13}C NMR spectrum of 2i in CDCl_3	S56
500 MHz ^1H NMR spectrum of 2j in CDCl_3	S57

125 MHz ^{13}C NMR spectrum of 2j in CDCl_3	S58
500 MHz ^1H NMR spectrum of 3a in CDCl_3	S59
Expanded 500 MHz ^1H NMR spectrum of 3a in CDCl_3	S60
125 MHz ^{13}C NMR spectrum of 3a in CDCl_3	S61
500 MHz ^1H NMR spectrum of 3a' in CDCl_3	S62
125 MHz ^{13}C NMR spectrum of 3a' in CDCl_3	S63
500 MHz ^1H NMR spectrum of 3b in CDCl_3	S64
125 MHz ^{13}C NMR spectrum of 3b in CDCl_3	S65
500 MHz ^1H NMR spectrum of 4a in CDCl_3	S66
125 MHz ^{13}C NMR spectrum of 4a in CDCl_3	S67
500 MHz ^1H NMR spectrum of 4b in CDCl_3	S68
Expanded 500 MHz ^1H NMR spectrum of 4b in CDCl_3	S69
125 MHz ^{13}C NMR spectrum of 4b in CDCl_3	S70
500 MHz ^1H NMR spectrum of 5a in CDCl_3	S71
125 MHz ^{13}C NMR spectrum of 5a in CDCl_3	S72
500 MHz ^1H NMR spectrum of 5b in CDCl_3	S73
Expanded 500 MHz ^1H NMR spectrum of 5b in CDCl_3	S74
125 MHz ^{13}C NMR spectrum of 5b in CDCl_3	S75
500 MHz ^1H NMR spectrum of 6 in CDCl_3	S76
125 MHz ^{13}C NMR spectrum of 6 in CDCl_3	S77
500 MHz ^1H NMR spectrum of 7 in CDCl_3	S78
125 MHz ^{13}C NMR spectrum of 7 in CDCl_3	S79
500 MHz ^1H NMR spectrum of 8 in CDCl_3	S80
125 MHz ^{13}C NMR spectrum of 8 in CDCl_3	S81
500 MHz ^1H NMR spectrum of 9a in CDCl_3	S82
125 MHz ^{13}C NMR spectrum of 9a in CDCl_3	S83
500 MHz ^1H NMR spectrum of 9b in CDCl_3	S84
125 MHz ^{13}C NMR spectrum of 9b in CDCl_3	S85
500 MHz ^1H NMR spectrum of 10 in CDCl_3	S86
125 MHz ^{13}C NMR spectrum of 10 in CDCl_3	S87
500 MHz ^1H NMR spectrum of a pure sample of 2-(azidomethyl)furan in $\text{DMSO}-d_6$	S88
500 MHz ^1H NMR spectrum in $\text{DMSO}-d_6$ of the reaction mixture containing 11	S89
500 MHz ^1H NMR spectrum of 12 in CDCl_3	S90
125 MHz ^{13}C NMR spectrum of 12 in CDCl_3	S91
500 MHz ^1H NMR spectrum of 13a in CDCl_3	S92
125 MHz ^{13}C NMR spectrum of 13a in CDCl_3	S93
500 MHz ^1H NMR spectrum of 13b in CDCl_3	S94

500 MHz ^1H NMR spectrum of 14 in CDCl_3	S95
125 MHz ^{13}C NMR spectrum of 14 in CDCl_3	S96
500 MHz ^1H NMR spectrum of 15 in CDCl_3	S97
125 MHz ^{13}C NMR spectrum of 15 in CDCl_3	S98
500 MHz ^1H NMR spectrum of 16 in CDCl_3	S99
125 MHz ^{13}C NMR spectrum of 16 in CDCl_3	S100
500 MHz ^1H NMR spectrum of 17a in CDCl_3	S101
125 MHz ^{13}C NMR spectrum of 17a in CDCl_3	S102
500 MHz ^1H NMR spectrum of 17b in CDCl_3	S103
125 MHz ^{13}C NMR spectrum of 17b in CDCl_3	S104
500 MHz ^1H NMR spectrum in CDCl_3 of the mixture containing a 7.3:1 ratio of 2-(azidoethyl)benzene/benzotriazolyl ether 1f	S105
500 MHz ^1H NMR spectrum of 18 in CDCl_3	S106
Expanded 500 MHz ^1H NMR spectrum of 18 in CDCl_3	S107
125 MHz ^{13}C NMR spectrum of 18 in CDCl_3	S108
500 MHz ^1H NMR spectrum of 19 in CDCl_3	S109
Expanded 500 MHz ^1H NMR spectrum of 19 in CDCl_3	S110
125 MHz ^{13}C NMR spectrum of 19 in CDCl_3	S111
500 MHz ^1H NMR spectrum of 20a,b in CDCl_3	S112
Expanded 500 MHz ^1H NMR spectrum of 20a,b in CDCl_3	S113
500 MHz ^1H NMR spectrum of 20a in CDCl_3	S114
Expanded 500 MHz ^1H NMR spectrum of 20a in CDCl_3	S115
125 MHz ^{13}C NMR spectrum of 20a in CDCl_3	S116
500 MHz ^1H NMR spectrum of 20b in CDCl_3	S117
Expanded 500 MHz ^1H NMR spectrum of 20b in CDCl_3	S118
125 MHz ^{13}C NMR spectrum of 20b in CDCl_3	S119
500 MHz gCOSY spectrum of 20a in CDCl_3	S120
500 MHz NOESY spectrum of 20a in CDCl_3	S121
500 MHz gHMQC spectrum of 20a in CDCl_3	S122

DW-1205-1-HNMR-CDCl3-10-methoxy

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: 1205-DW-01-CDCl3-HNMR-0010-methoxy
INOVA-500 "riga"

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

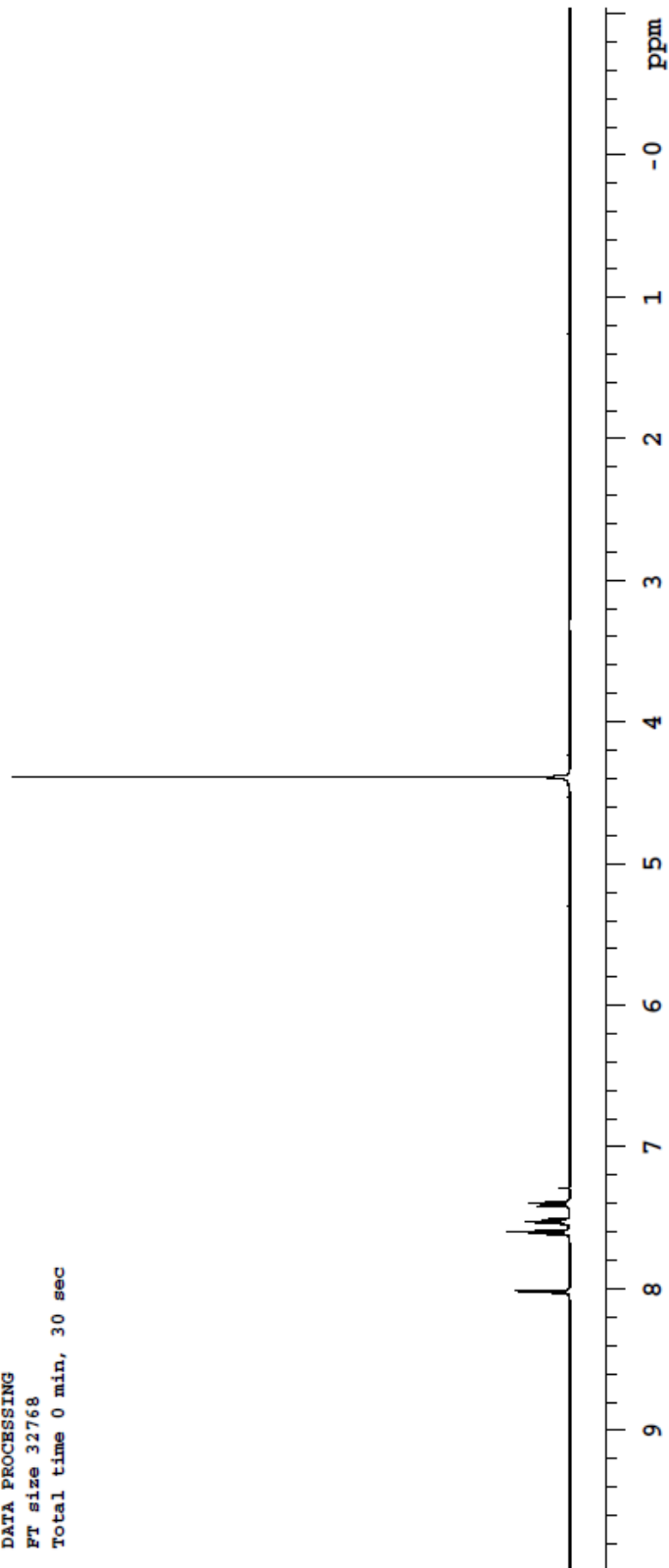
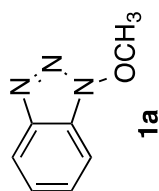
16 repetitions

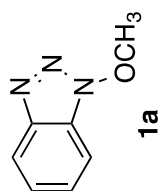
OBSERVE H1, 499.7707095 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 30 sec





DW-1205-I-CNMR-CDCl3-10-methoxybt

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: 1205-DW-01-CDCl3-CNMR-0001-methoxybt

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

384 repetitions

OBSERVE C13, 125.5674149 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

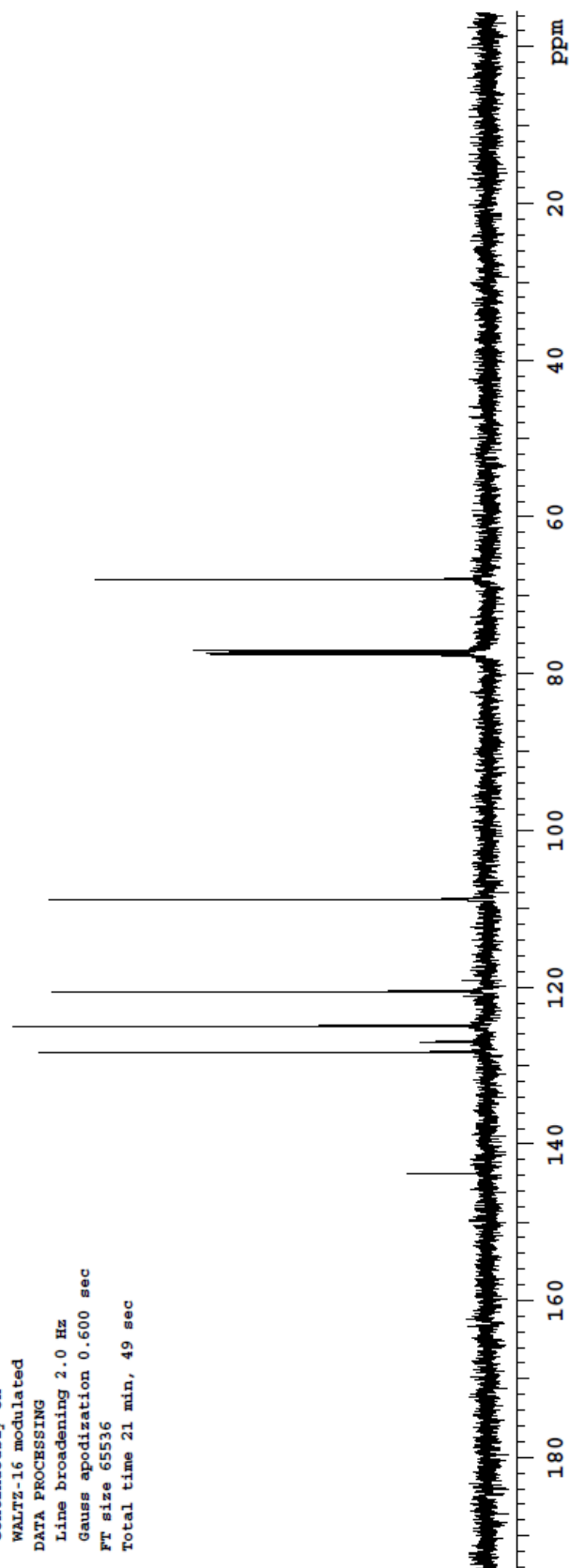
DATA PROCESSING

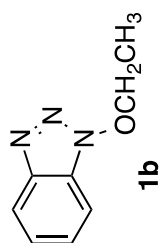
Line broadening 2.0 Hz

Gauss apodization 0.600 sec

FT size 65536

Total time 21 min, 49 sec





MKS-1205-08-53-CDCl3-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-08-53-CDCl3-CC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

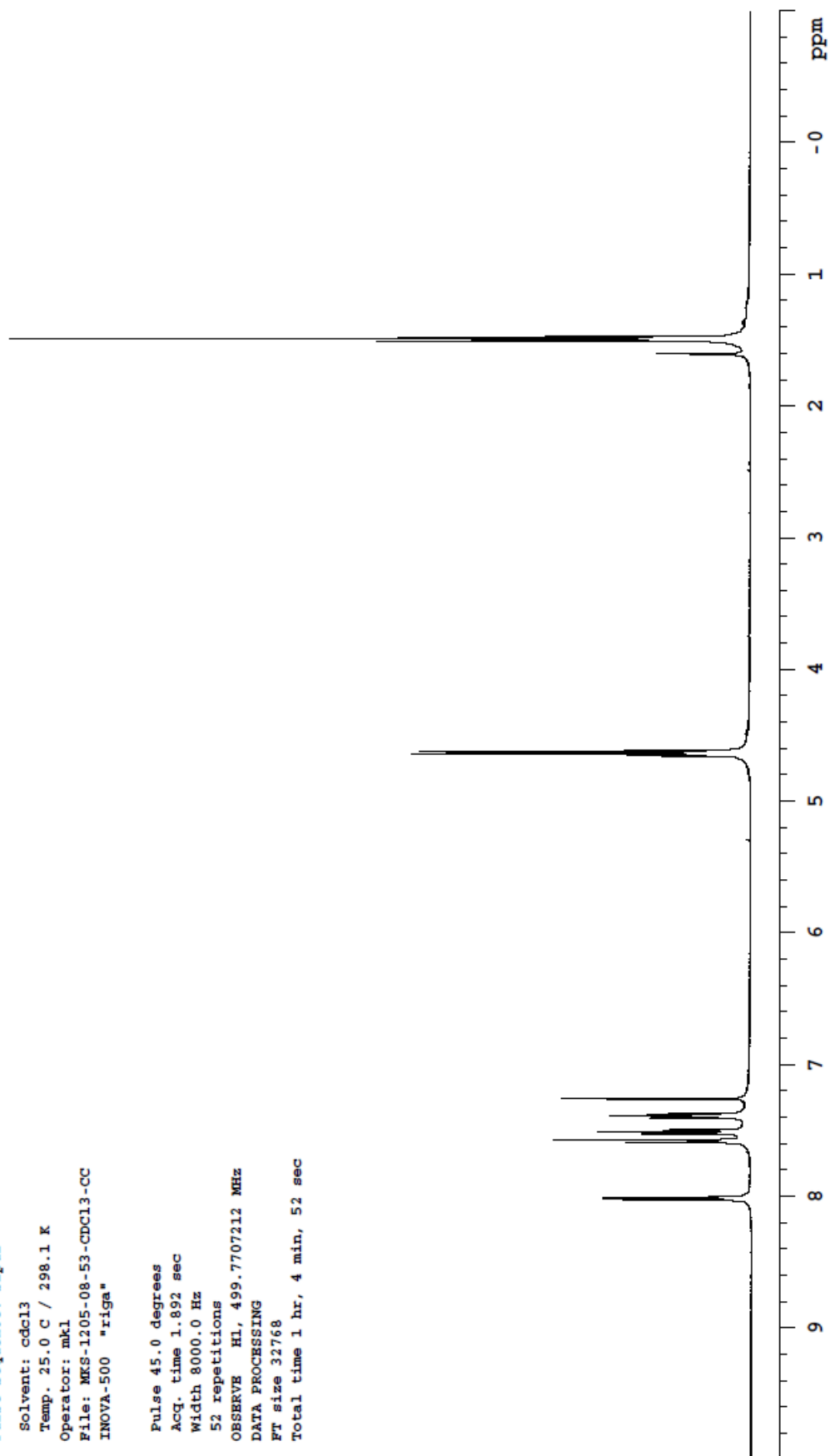
52 repetitions

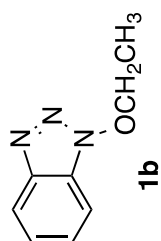
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

FT size 32768

Total time 1 hr, 4 min, 52 sec





MKS-1205-08-53-CDCl3-13C-CC

Pulse Sequence: s2pul1

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-08-53-CDCl3-13C-CC

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

52 repetitions

OBSERVE C13, 125.6674382 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

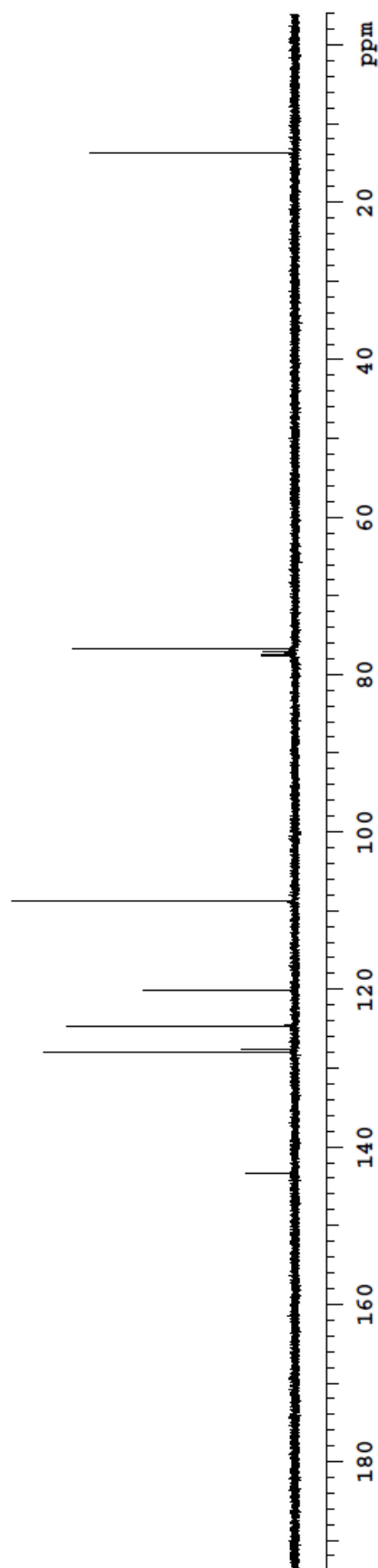
WALTZ-16 modulated

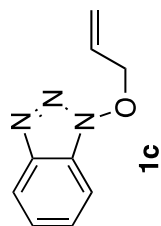
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





MKS-1205-13-AllylEtEtther-CDCl3-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-13-AllylEtEtther-CDCl3-CC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

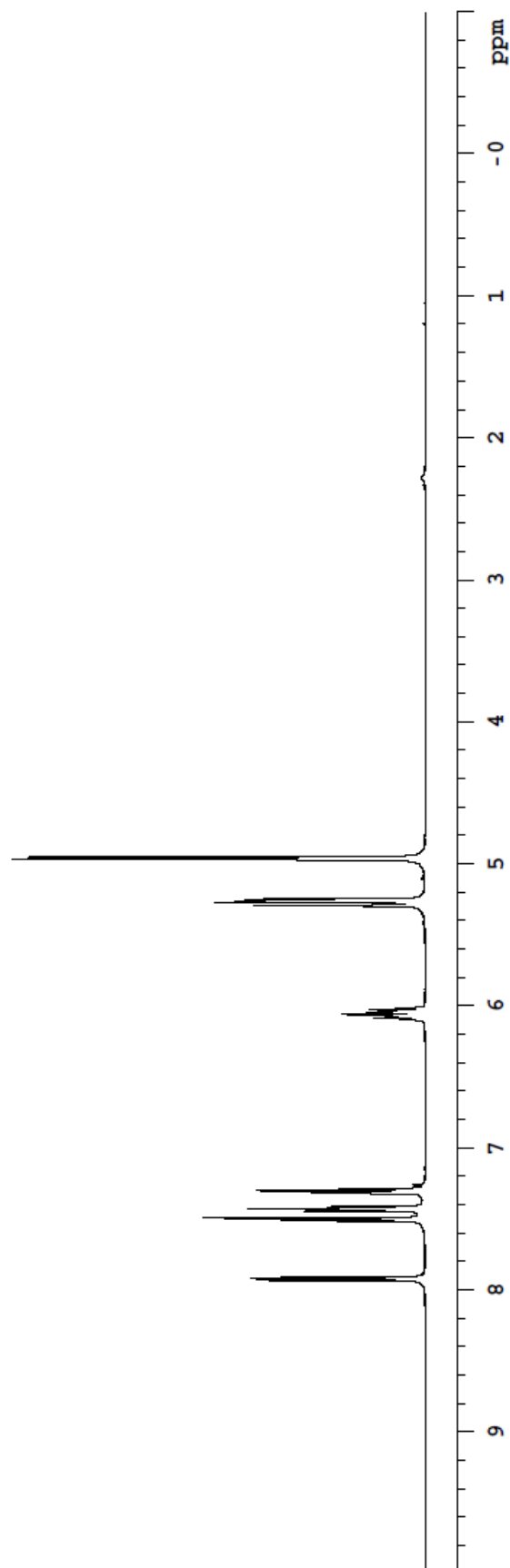
OBSERVE H1, 499.7707217 MHz

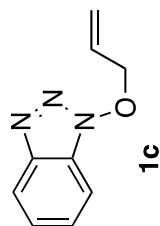
DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 hr, 3 min, 21 sec





MKS-1205-13-AllylBtEtHer-13C-CDCl3-CC

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-13-AllylBtEtHer-13C-CDCl3-CC

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

64 repetitions

OBSERVE C13, 125.6674385 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

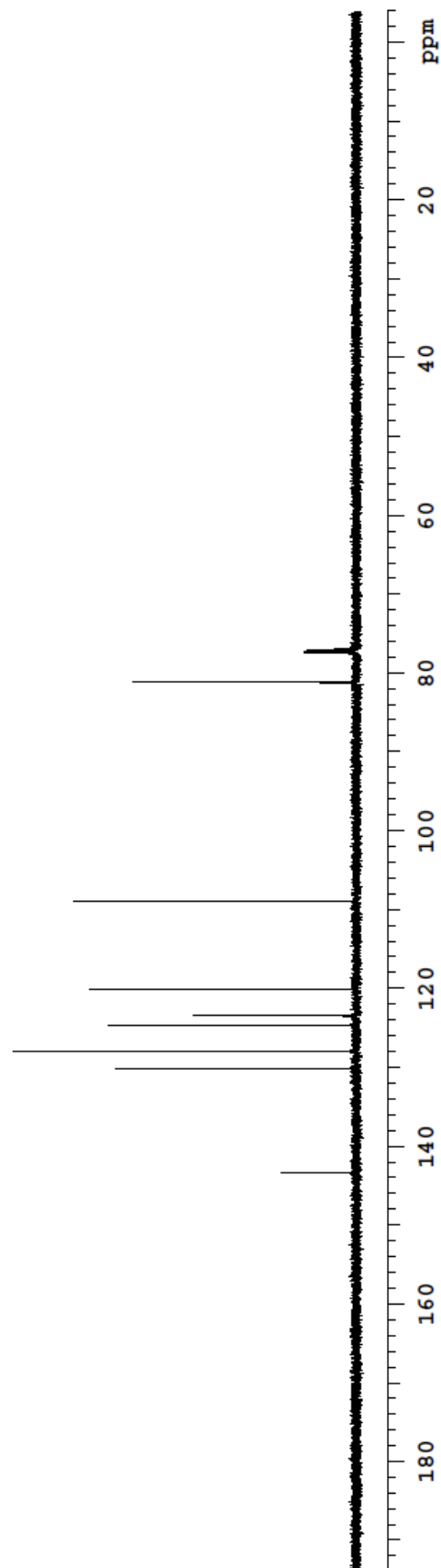
WALTZ-16 modulated

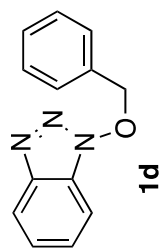
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





MKS-1205-12-73-CDCl3-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: mkl

File: MKS-1205-12-73-CDCl3-CC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

112 repetitions

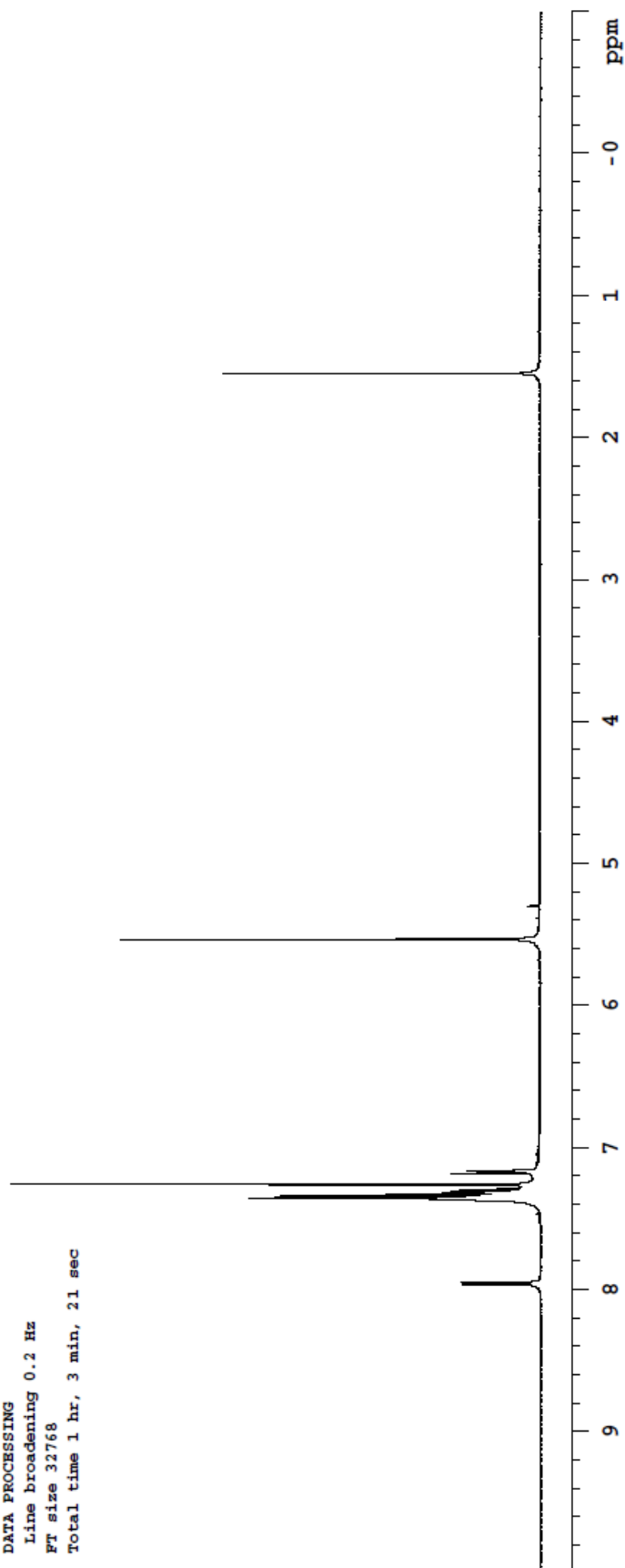
OBSERVE H1, 499.7707217 MHz

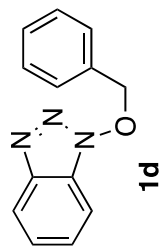
DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 hr, 3 min, 21 sec





MKS-1205-12-73-13C-repeat-CDCl3-CC

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-73-13C-repeat-CDCl3-CC

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

10028 repetitions

OBSERVE C13, 125.6674197 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

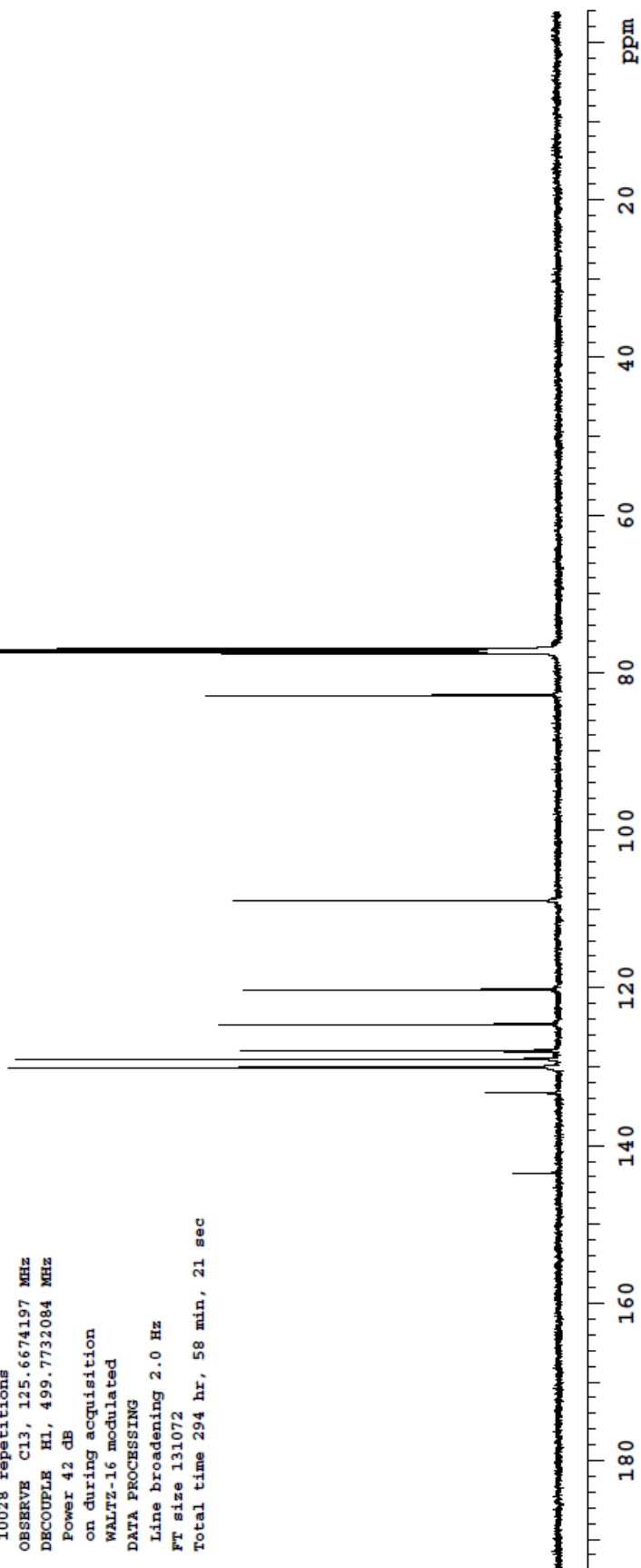
WALTZ-16 modulated

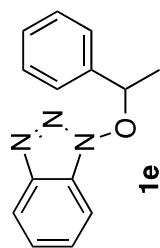
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 294 hr, 58 min, 21 sec





RRC-1205-III-243-HNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-III-243-HNMR-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

24 repetitions

OBSERVE H1, 499.7707212 MHz

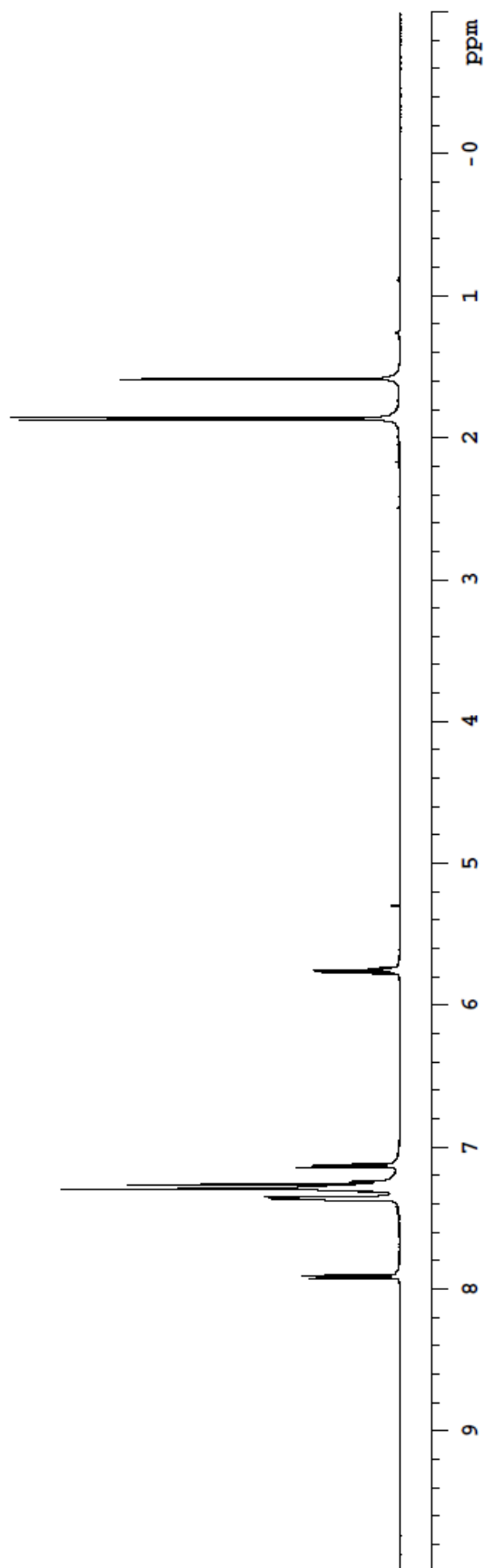
DATA PROCESSING

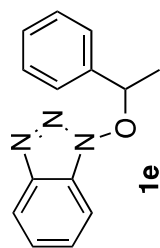
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 2 min, 45 sec





MKS-1205-11-05-CDC13-13C-2ndCC-repeat

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 24.0 C / 297.1 K

Operator: mkl

File: MKS-1205-11-05-CDC13-13C-2ndCC-repeat

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

24 repetitions

OBSERVE C13, 125.667484 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

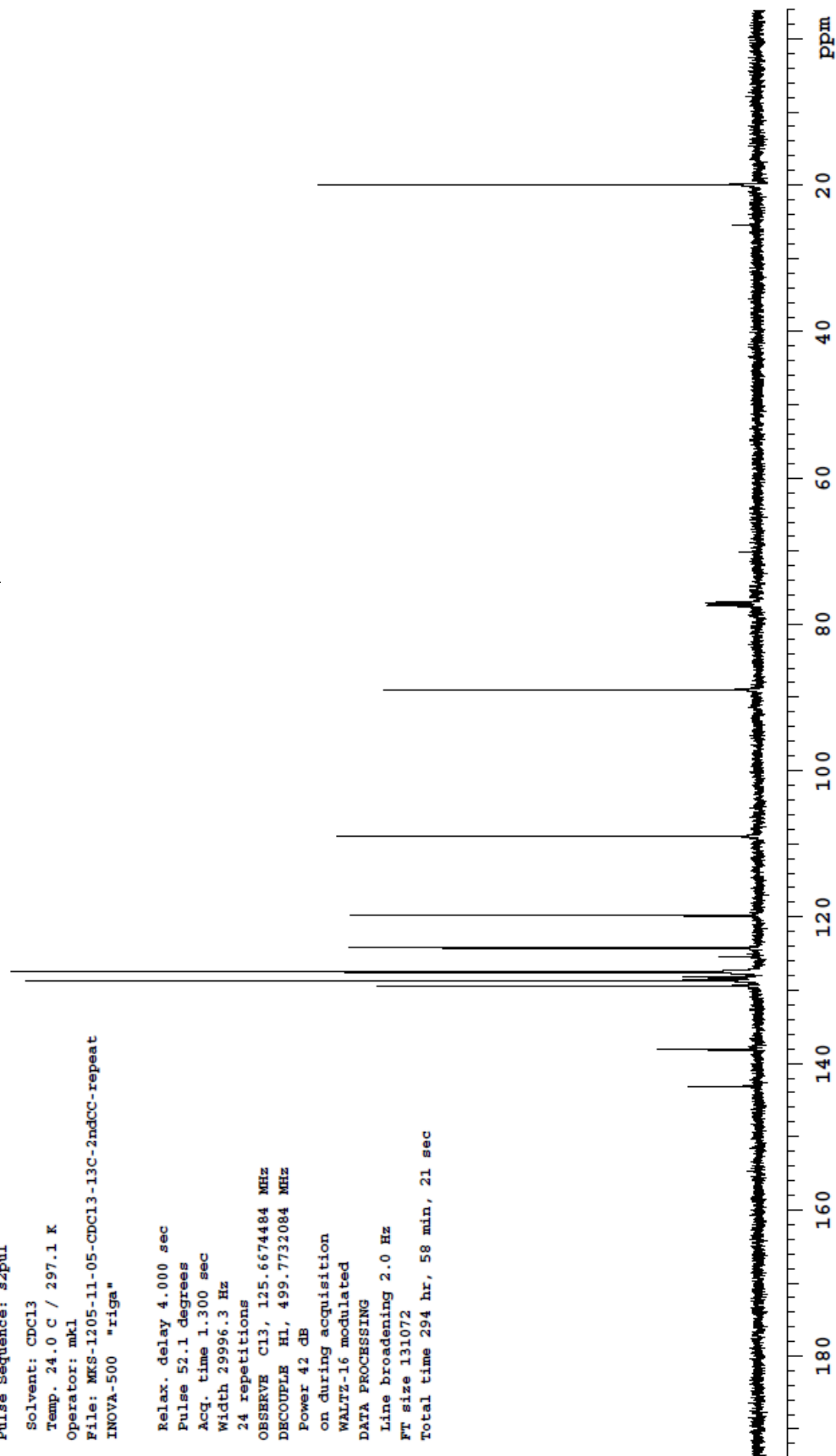
WALTZ-16 modulated

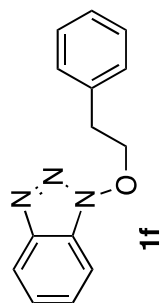
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 294 hr, 58 min, 21 sec





MKS-1205-08-51-CDCl3-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-08-51-CDCl3-CC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

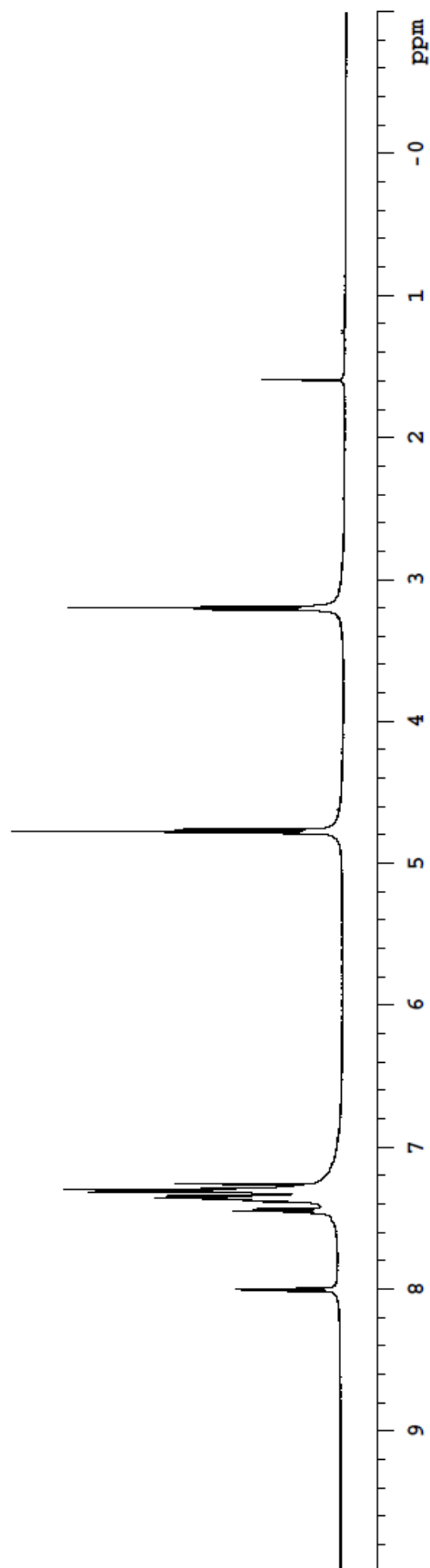
48 repetitions

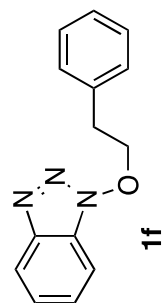
OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

FT size 32768

Total time 1 hr, 4 min, 52 sec





MKS-1205-08-51-CDC13-13C-CC

Pulse Sequence: s2pul

Solvent: CDC13

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-08-51-CDC13-13C-CC
INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

96 repetitions

OBSERVE C13, 125.6674382 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

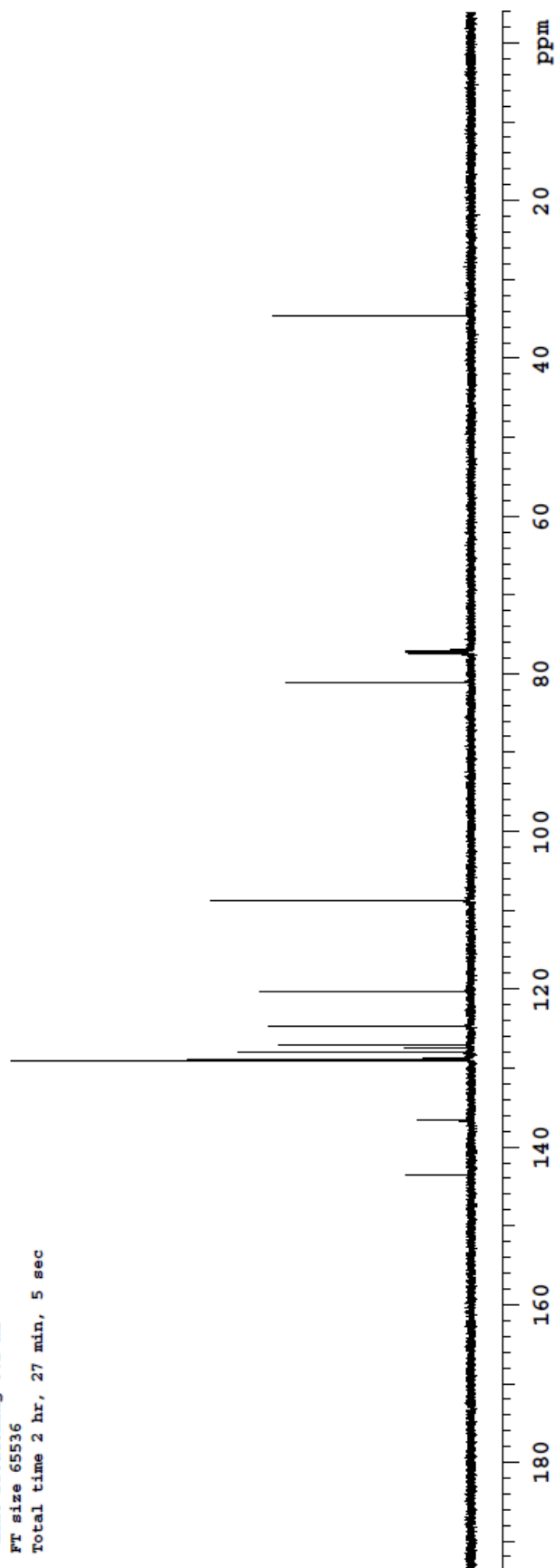
WALTZ-16 modulated

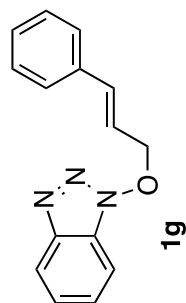
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





RRC-1205-IV-276-HNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-IV-276-HNMR-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

32 repetitions

OBSERVE H1, 499.7707212 MHz

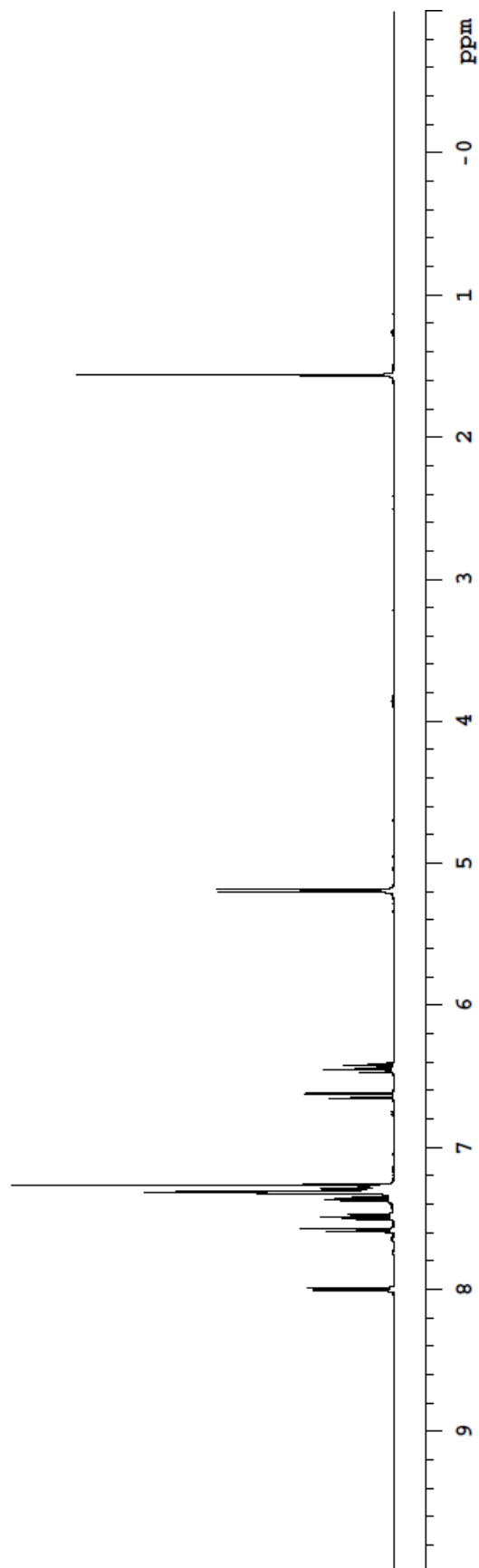
DATA PROCESSING

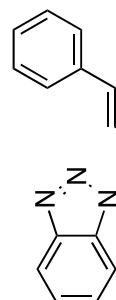
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec





1g

REC-1205-IV-276-CNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-IV-276-CNMR-CDCl3

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30499.4 Hz

12910 repetitions

OBSERVE C13, 125.6674203 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

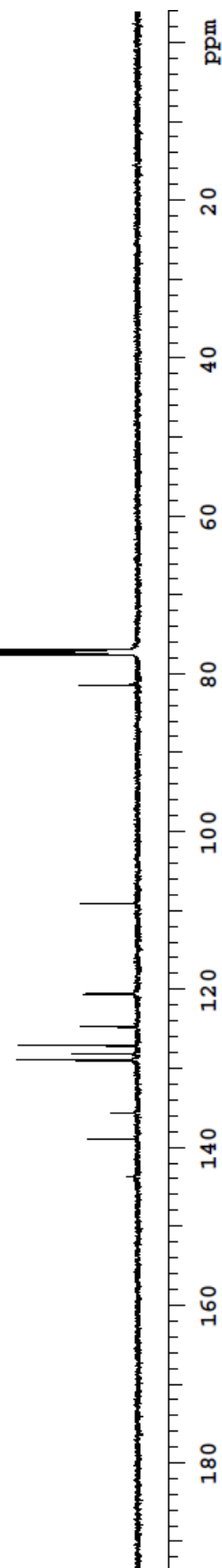
WALTZ-16 modulated

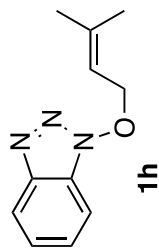
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 23 hr, 56 min, 27 sec





1205-Evan-isoprenyltether-1H-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: 1205-Evan-isoprenyltether-1H-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

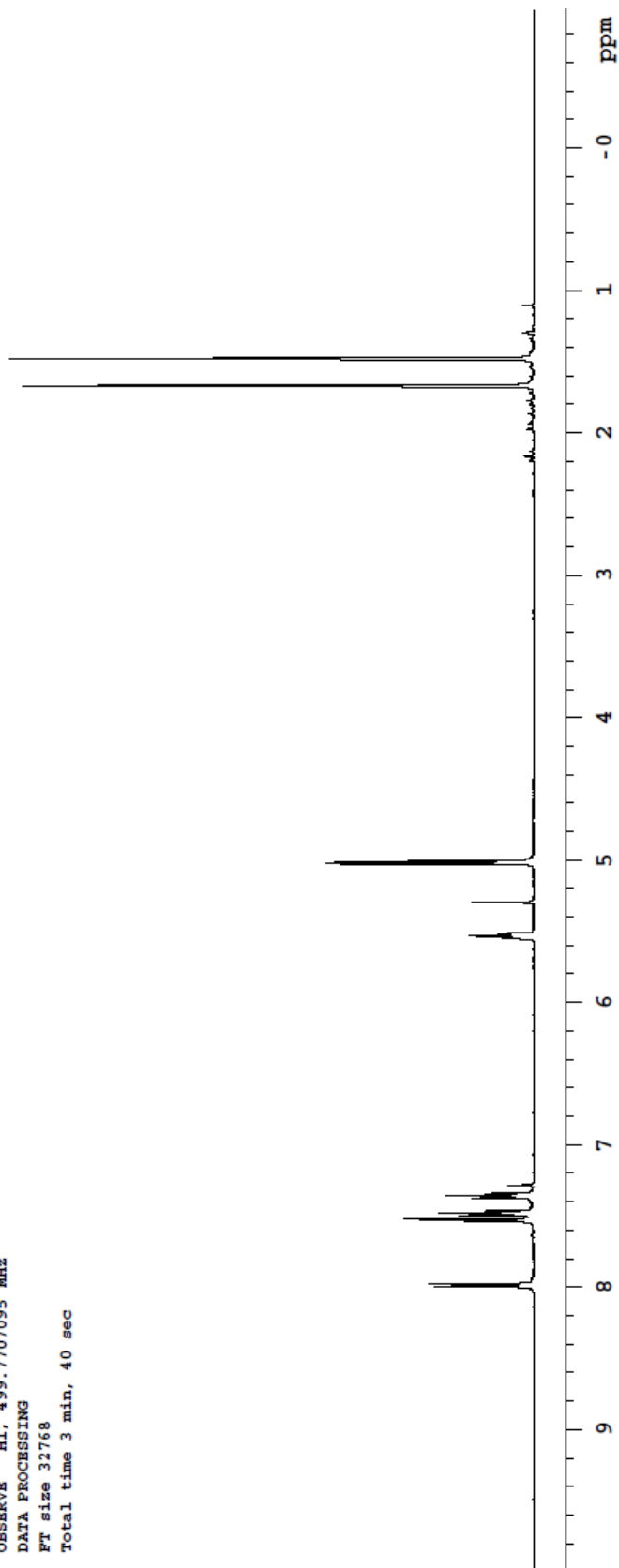
8 repetitions

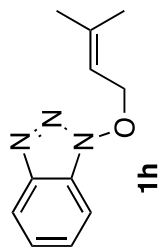
OBSERVE H1, 499.7707095 MHz

DATA PROCESSING

FT size 32768

Total time 3 min, 40 sec





1205-Evans-isoprenylEtether-13C-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: 1205-Evans-isoprenylEtether-13C-CDCl3

INOVA-500 "riga"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

1752 repetitions

OBSERVE C13, 125.6674264 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

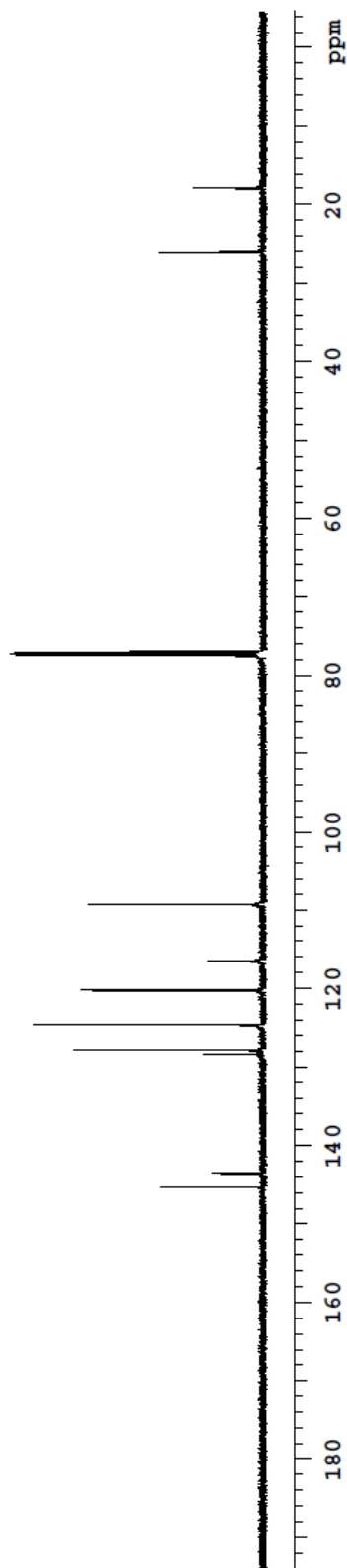
WALTZ-16 modulated

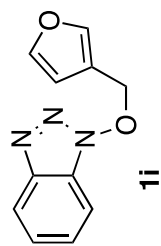
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 18 hr, 23 min, 8 sec





MKS-1205-12-13-CDCl3-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-13-CDCl3-CC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

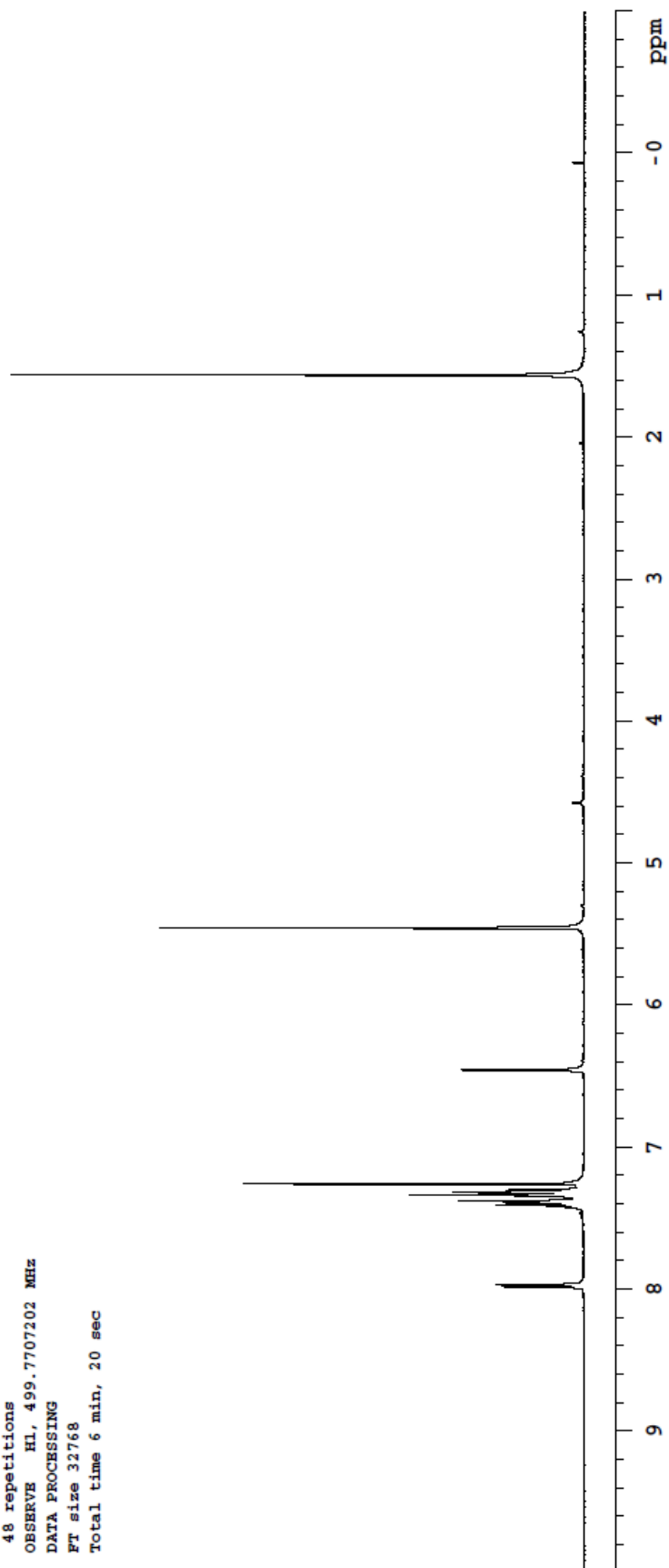
48 repetitions

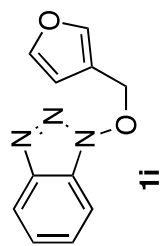
OBSERVE H1, 499.7707202 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 20 sec





MKS-1205-09-47-CDCl3-13C-CC

Pulse Sequence: *s2pul*

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-09-47-CDCl3-13C-CC

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

368 repetitions

OBSERVE C13, 125.6674240 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

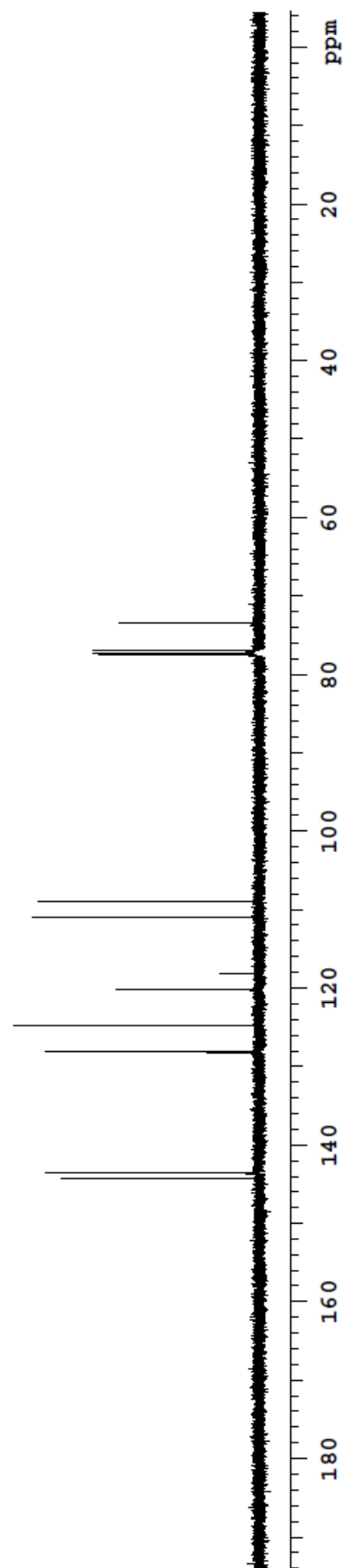
WALTZ-16 modulated

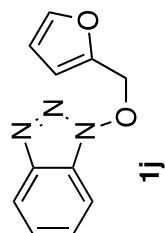
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





1205-Vijay-03-34-1H-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

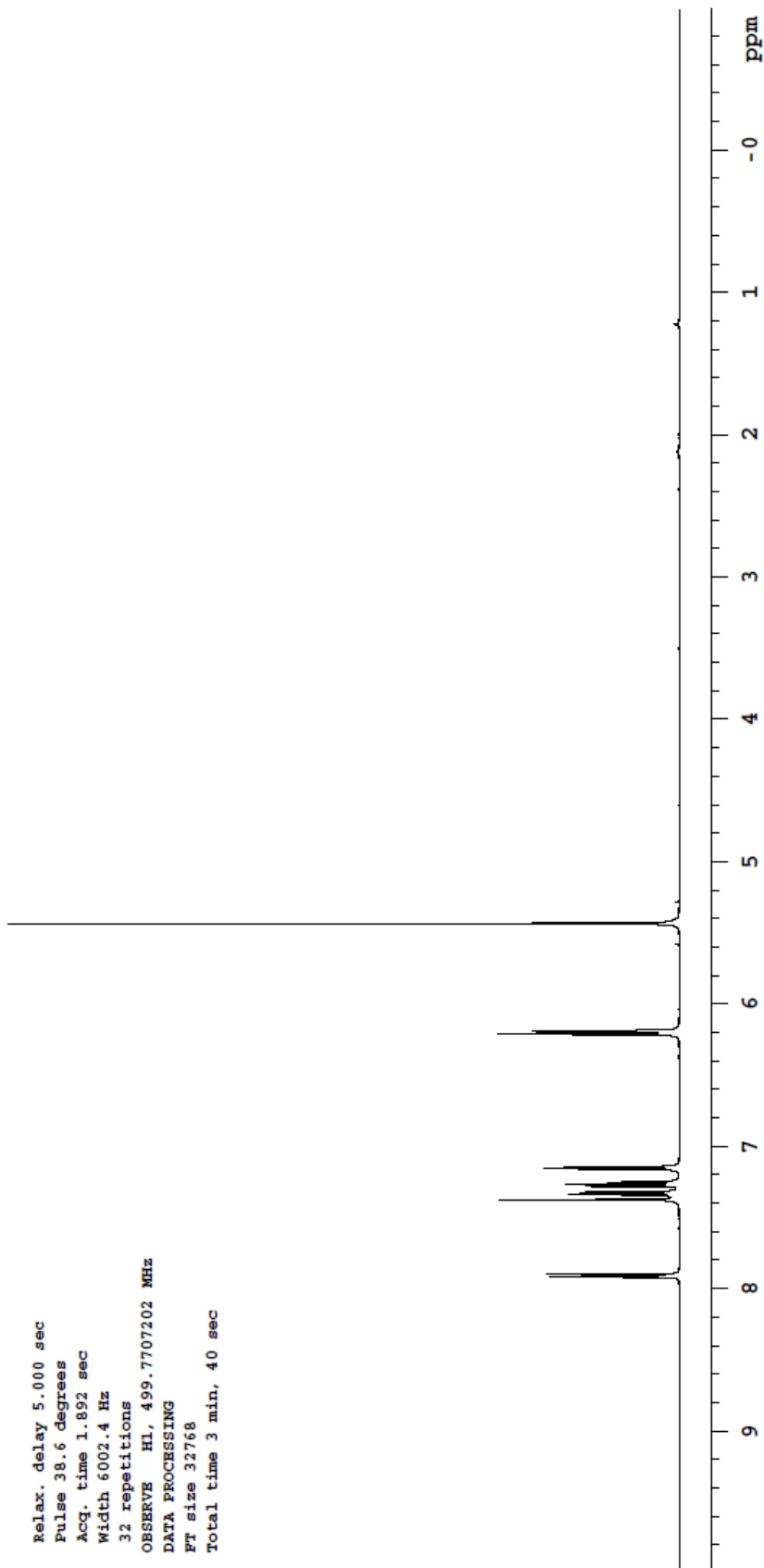
32 repetitions

OBSERVE HL, 499.7707202 MHz

DATA PROCESSING

FT size 32768

Total time 3 min, 40 sec



1205-Vijay-03-34-13C-CDC13

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

Operator: mk1

File:

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

204 repetitions

OBSERVE C13, 125.6674263 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

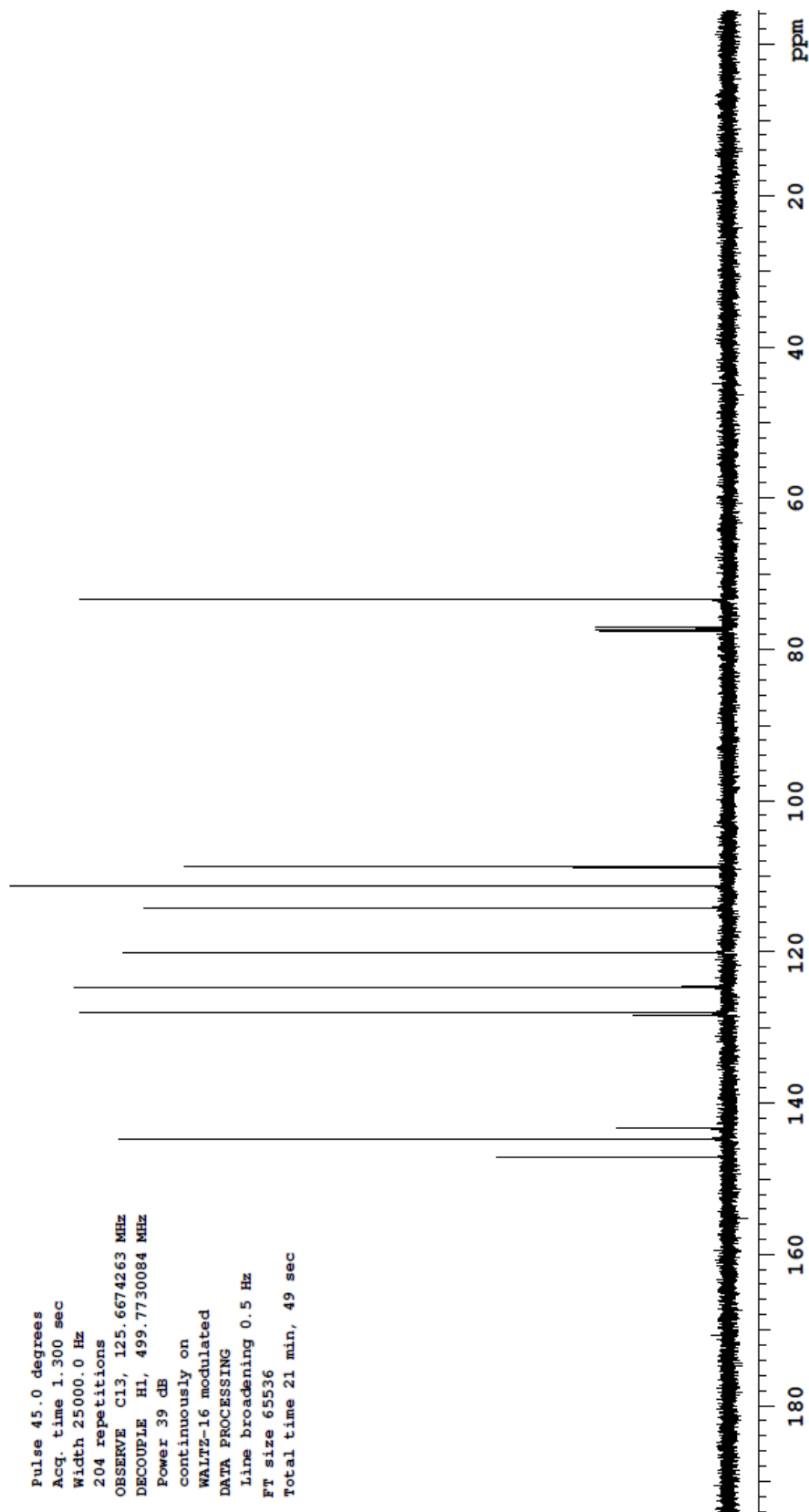
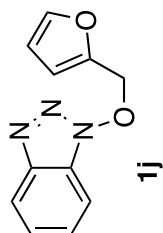
WALTZ-16 modulated

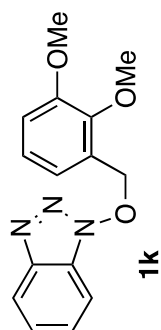
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 21 min, 49 sec





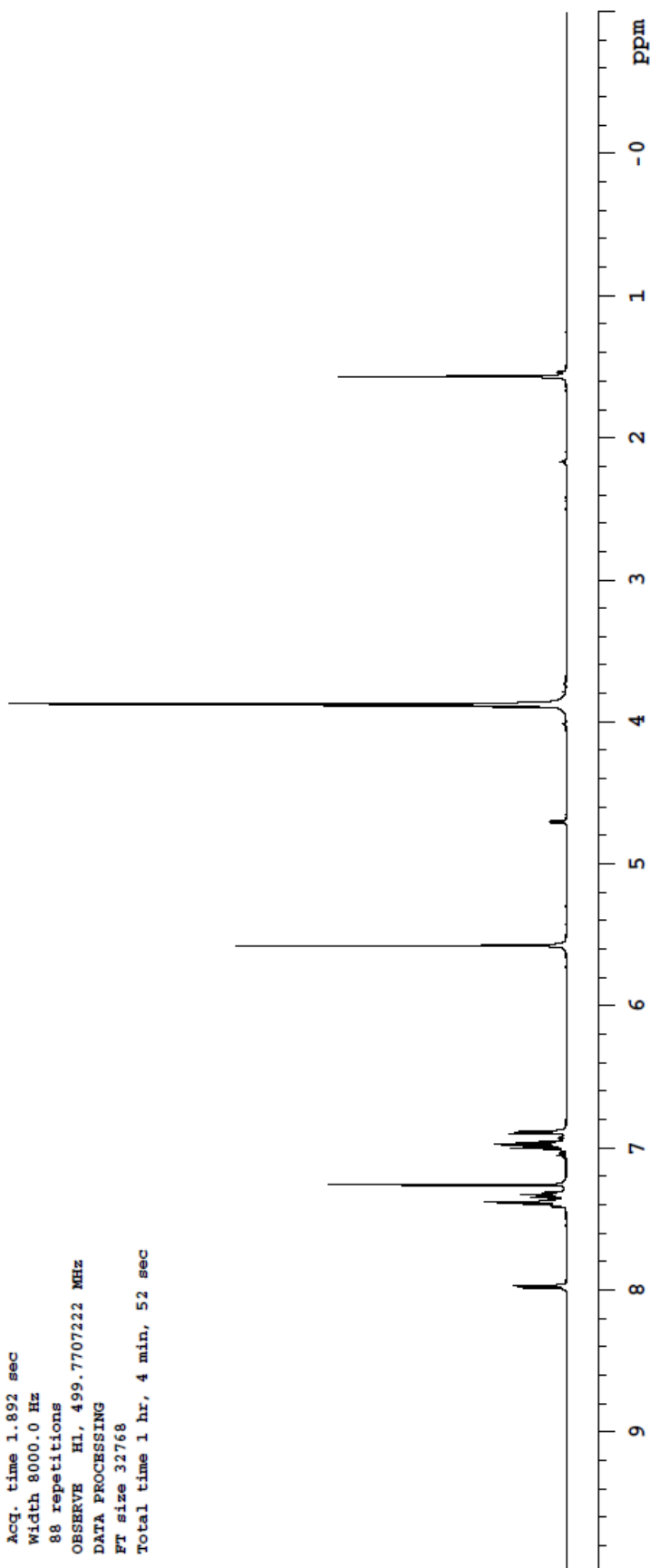
MKS-1205-08-02-CDCl3-CC

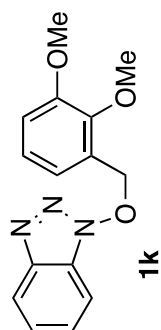
Archive directory: /export/home/mkl/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: mkl
File: MKS-1205-08-02-CDCl3-CC
INOVA-500 "r1ga"

Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
88 repetitions
OBSERVE H1, 499.770722 MHz
DATA PROCESSING
FT size 32768
Total time 1 hr, 4 min, 52 sec





MKS-1205-08-02-CDC13-13C-1st

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-08-02-CDC13-13C-1st

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

640 repetitions

OBSERVE C13, 125.6674232 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

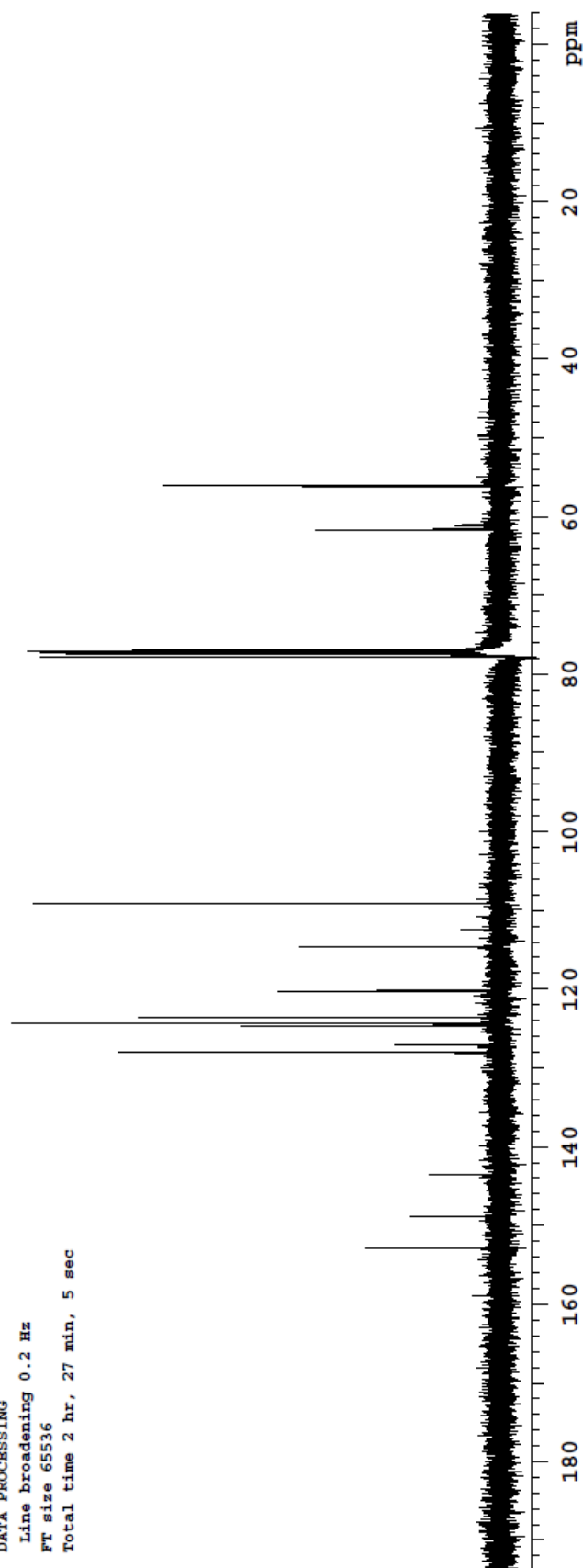
WALTZ-16 modulated

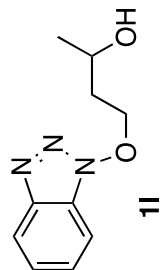
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





MKS-1205-11-61-CDCl3-3rdFrac-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-11-61-CDCl3-3rdFrac-CC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

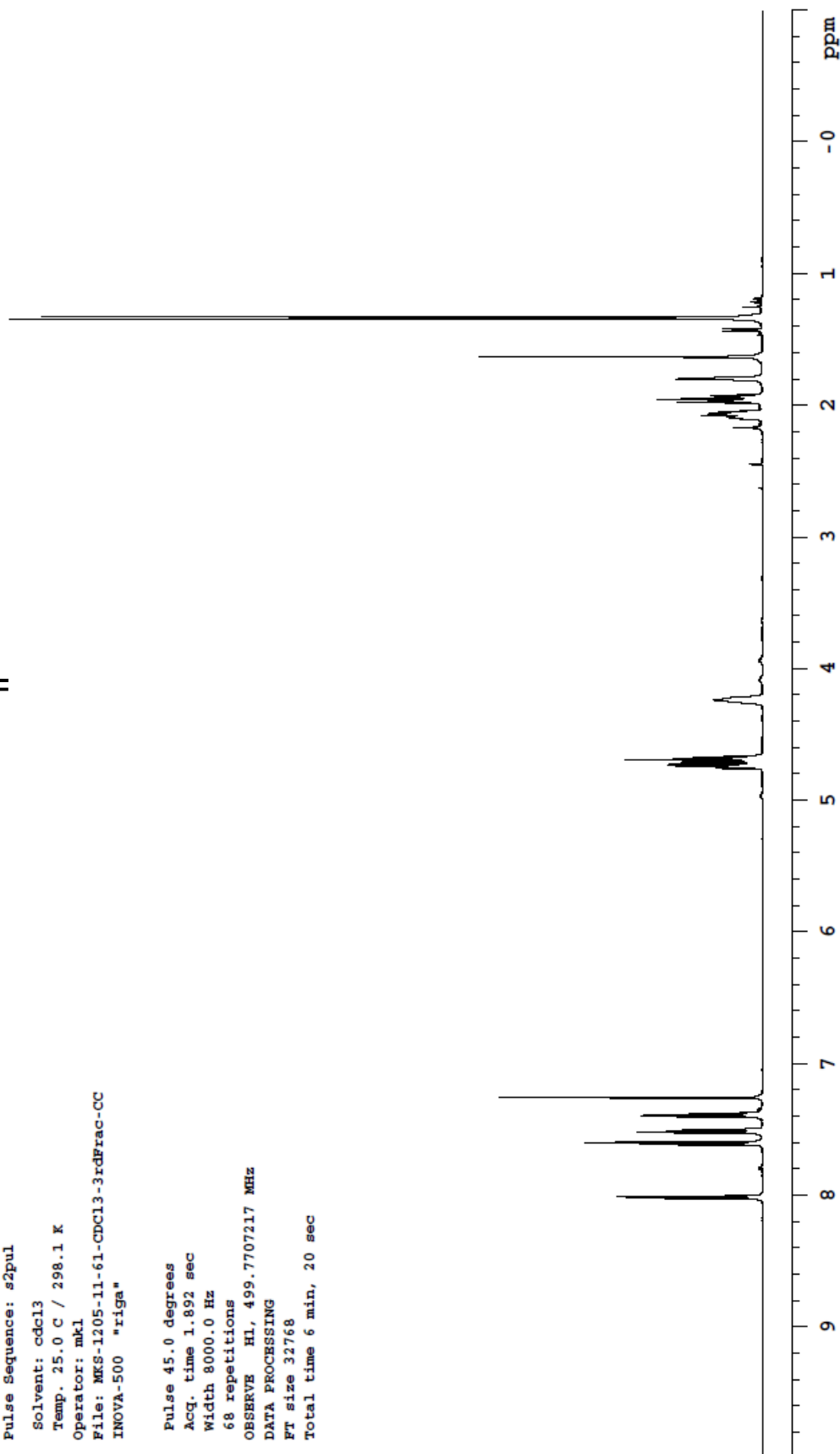
68 repetitions

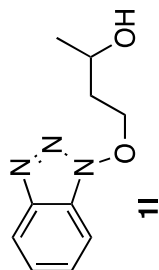
OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 20 sec





MKS-1205-11-61-CDCl3-13C-2ndFrac-CC

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 24.0 C / 297.1 K

Operator: mkl

File: MKS-1205-11-61-CDCl3-13C-2ndFrac-CC

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

34224 repetitions

OBSERVE C13, 125.6674271 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

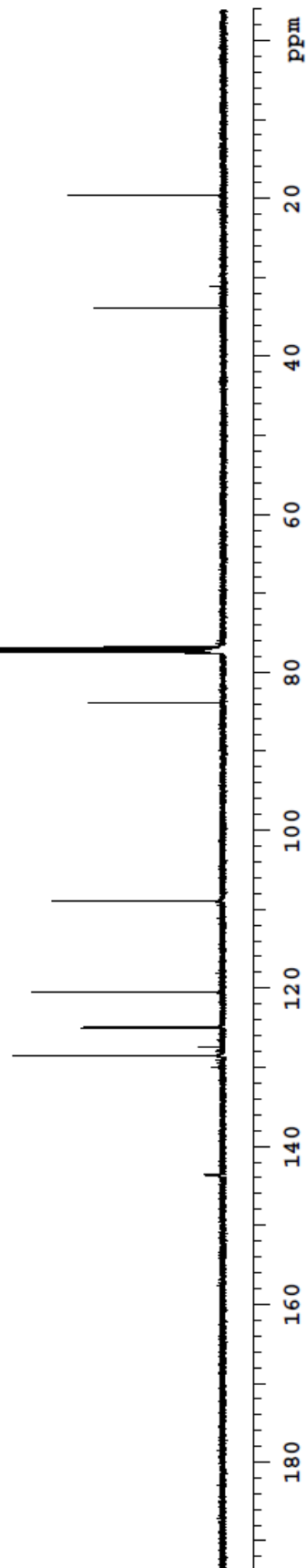
WALTZ-16 modulated

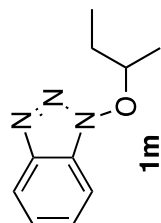
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 47 hr, 52 min, 55 sec





RRC-1205-III-249-HNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-III-249-HNMR-CDCl3

INOVA-500 "r1ga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

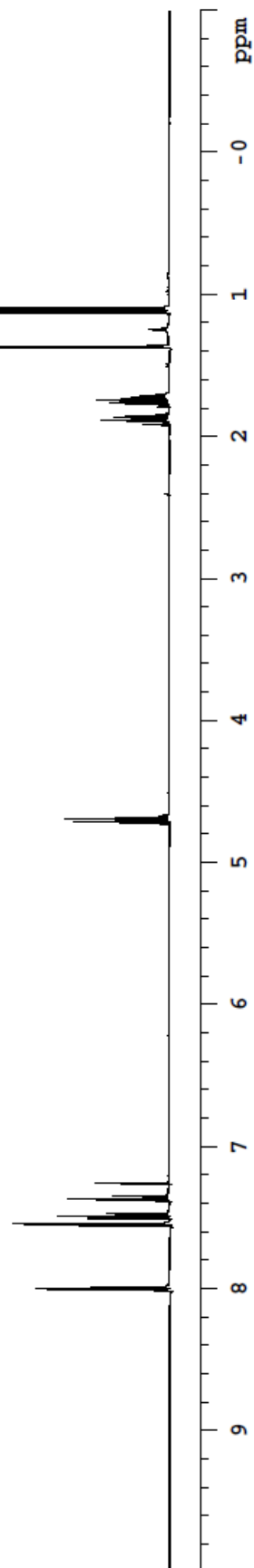
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec



RRC-1205-111-249-¹H-NMR-CDCl₃

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-111-249-¹H-NMR-CDCl₃

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

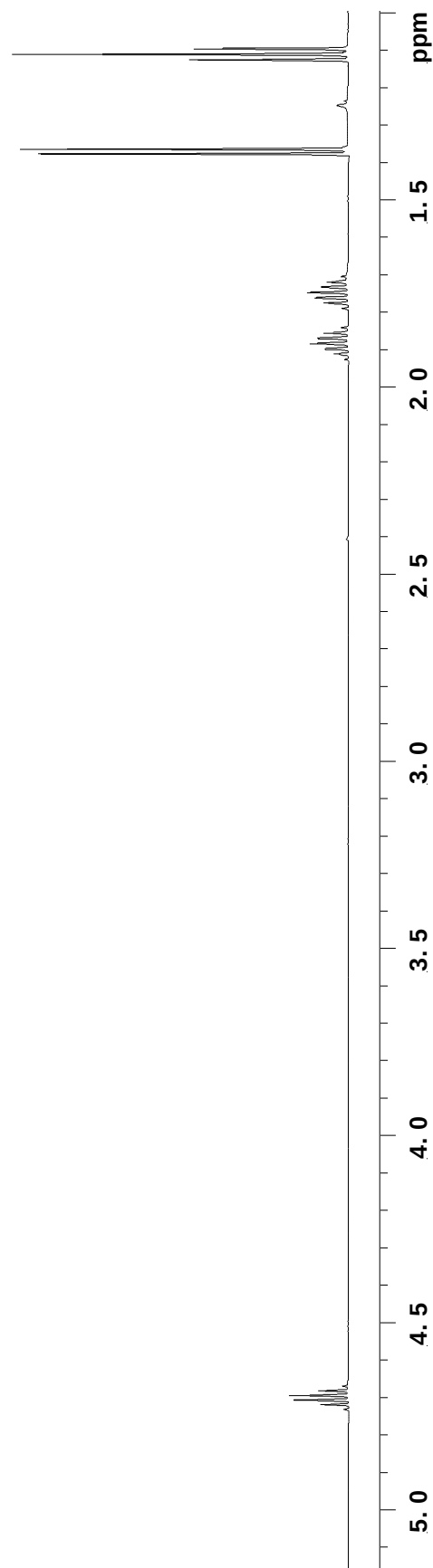
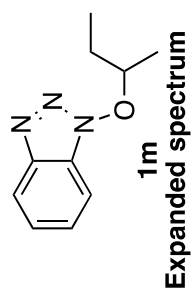
DATA PROCESSING

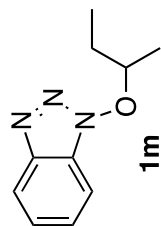
Resol. enhancement 0.5 Hz

Gaussian apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec





REC-1205-249-CNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-249-CNMR-CDCl3

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

13310 repetitions

OBSERVE C13, 125.6674209 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

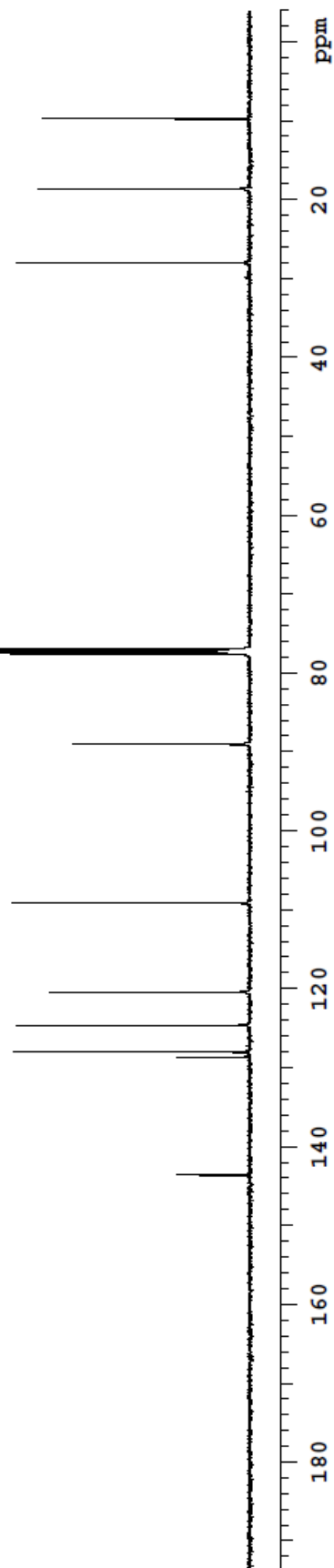
WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 29 hr, 55 min, 35 sec



RRC-1205-I-59-HNMR-CDCl3-pure

Solvent: CDCl3

Ambient temperature

Operator: Raghu

File: RRC-1205-I-59-HNMR-CDCl3-pure

INOVA-500 "rīga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707317 MHz

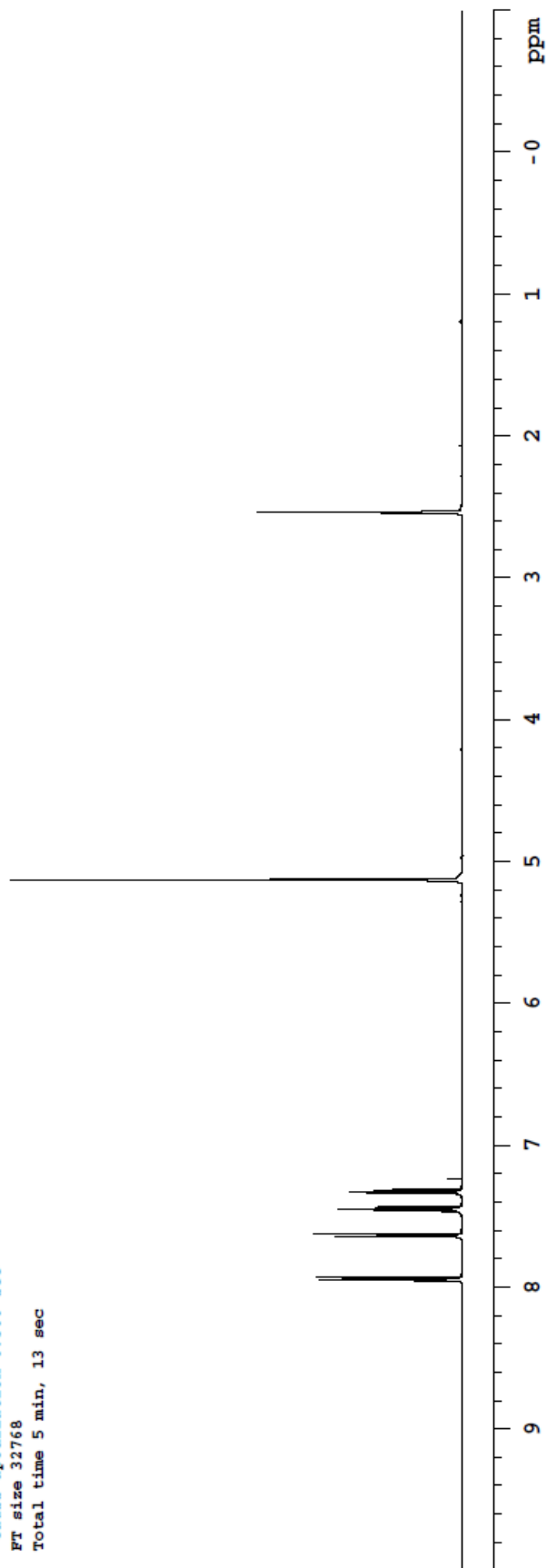
DATA PROCESSING

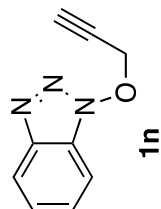
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 5 min, 13 sec





REC-1205-I-59-CNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-I-59-CNMR-CDCl3

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

11860 repetitions

OBSERVE C13, 125.6674191 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

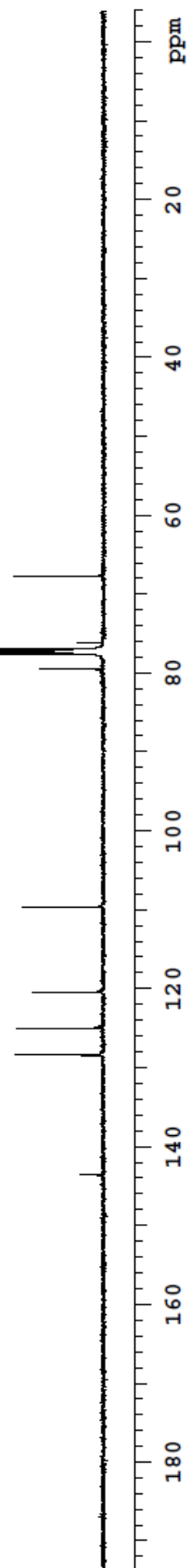
WALTZ-16 modulated

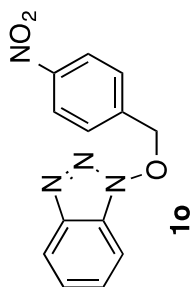
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 23 hr, 56 min, 28 sec





MKS-1205-12-17-CDCl3-pureFrac-2ndCC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-17-CDCl3-pureFrac-2ndCC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

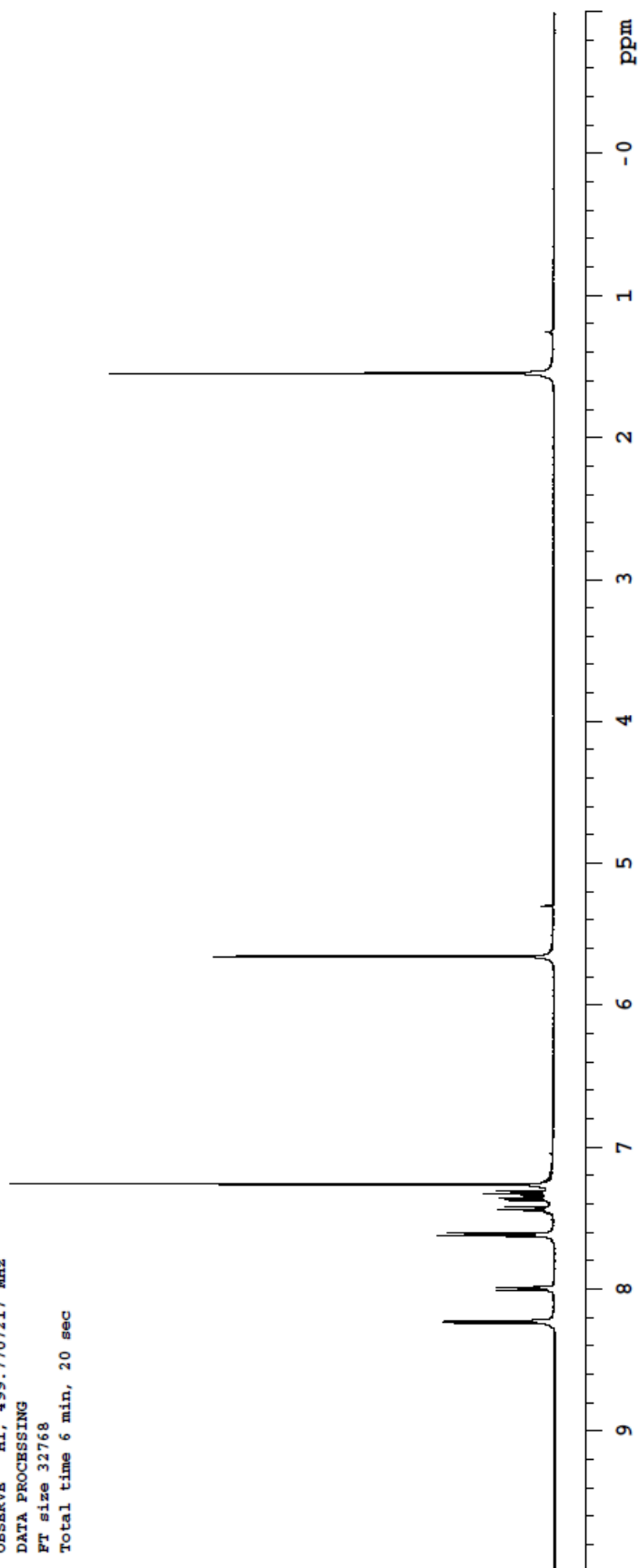
60 repetitions

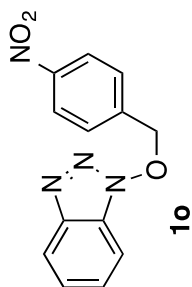
OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 20 sec





MKS-1205-12-17-CDC13-13C-CC-pure

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-17-CDC13-13C-CC-pure

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

10632 repetitions

OBSERVE C13, 125.6674200 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

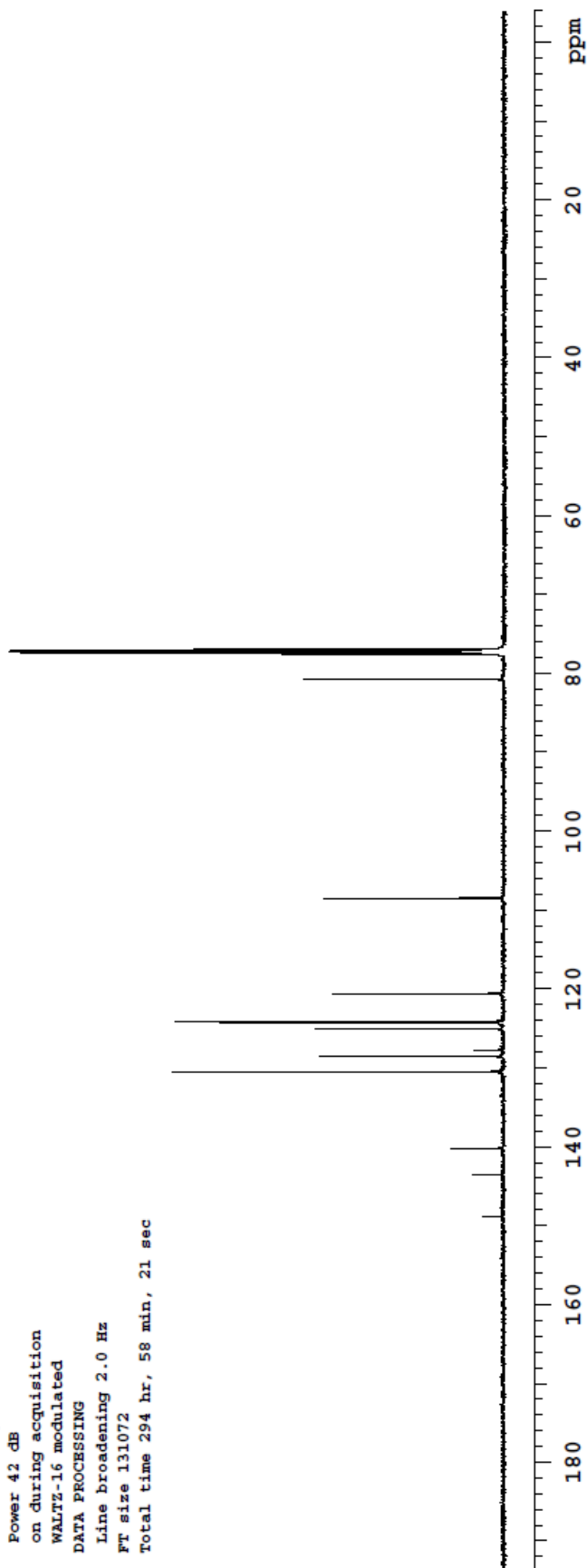
WALTZ-16 modulated

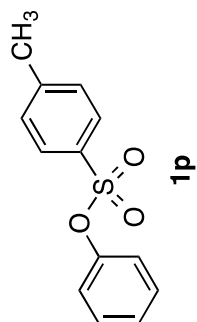
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 294 hr, 58 min, 21 sec





MKS-1205-13-54-CDCl3-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 24.0 C / 297.1 K

Operator: mkl

File: MKS-1205-13-54-CDCl3-CC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

56 repetitions

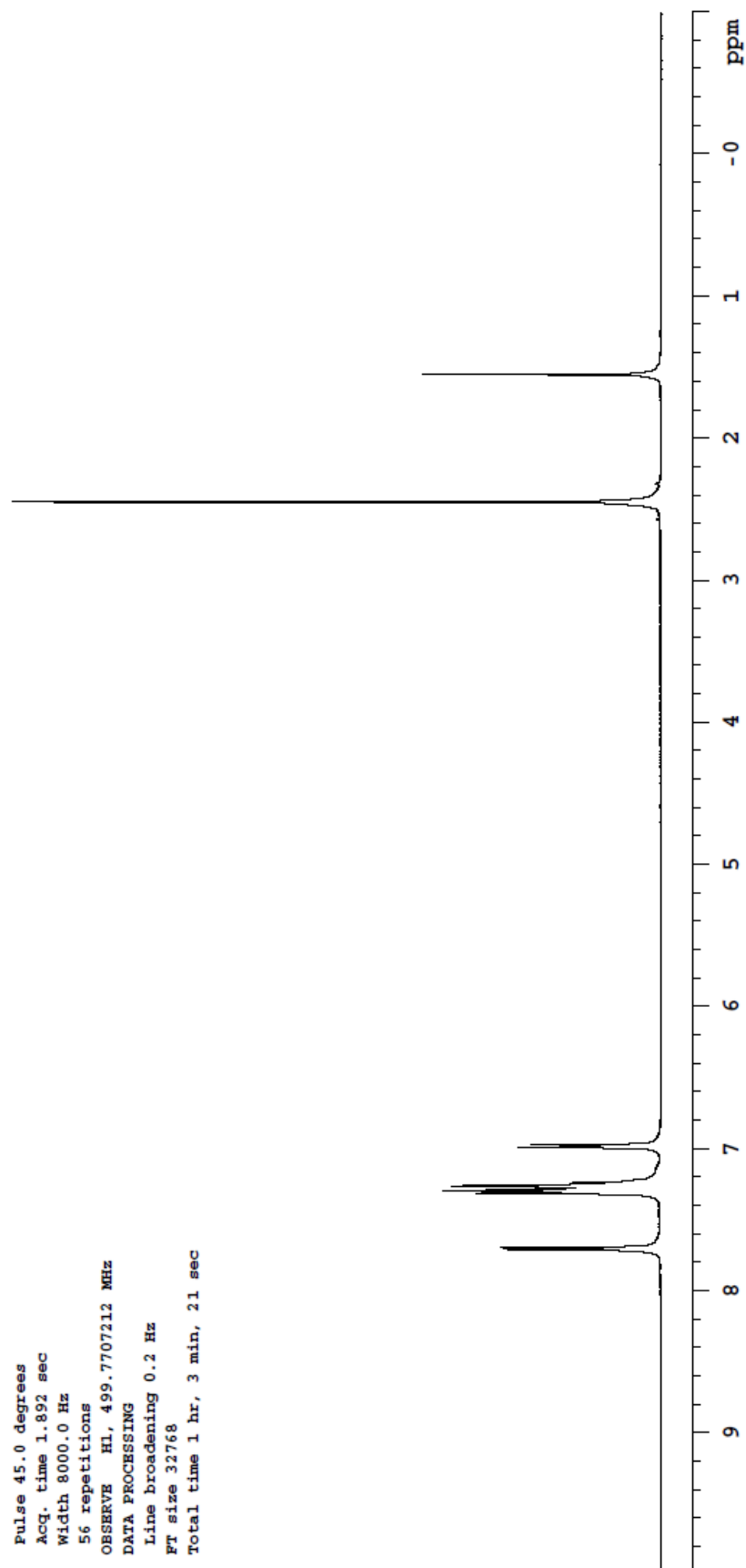
OBSERVE H1, 499.7707212 MHz

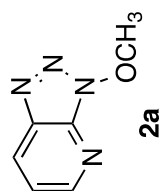
DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 hr, 3 min, 21 sec





MKS-1205-13-58-CDCl3-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 24.0 C / 297.1 K

Operator: mkl

File: MKS-1205-13-58-CDCl3-CC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

76 repetitions

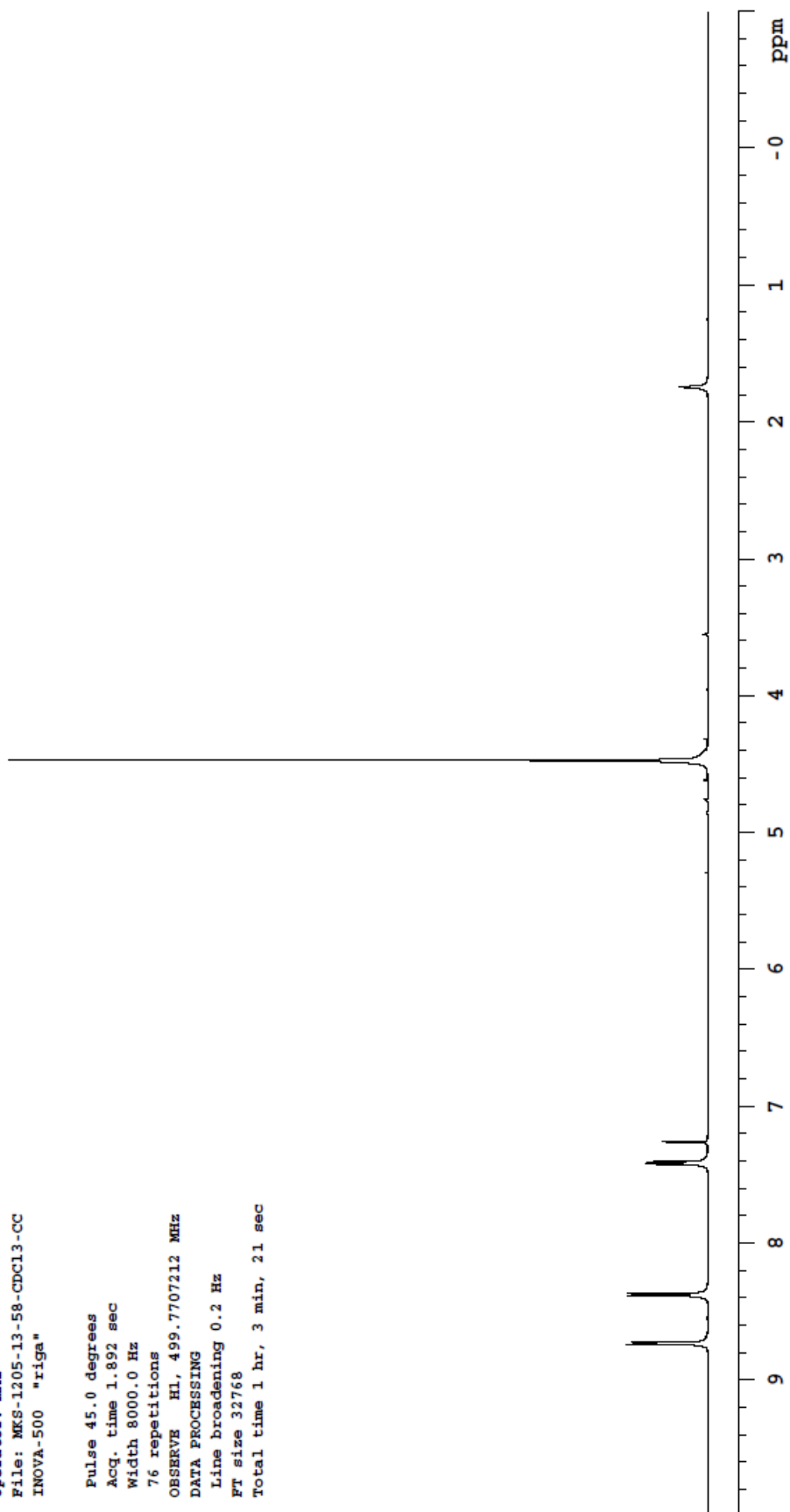
OBSERVE H1, 499.7707212 MHz

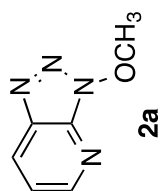
DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 hr, 3 min, 21 sec





MKS-1205-13-58-CDCl3-13C-CC-rep

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 24.0 C / 297.1 K

Operator: mkl

File: MKS-1205-13-58-CDCl3-13C-CC-rep

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

2048 repetitions

OBSERVE C13, 125.6674202 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

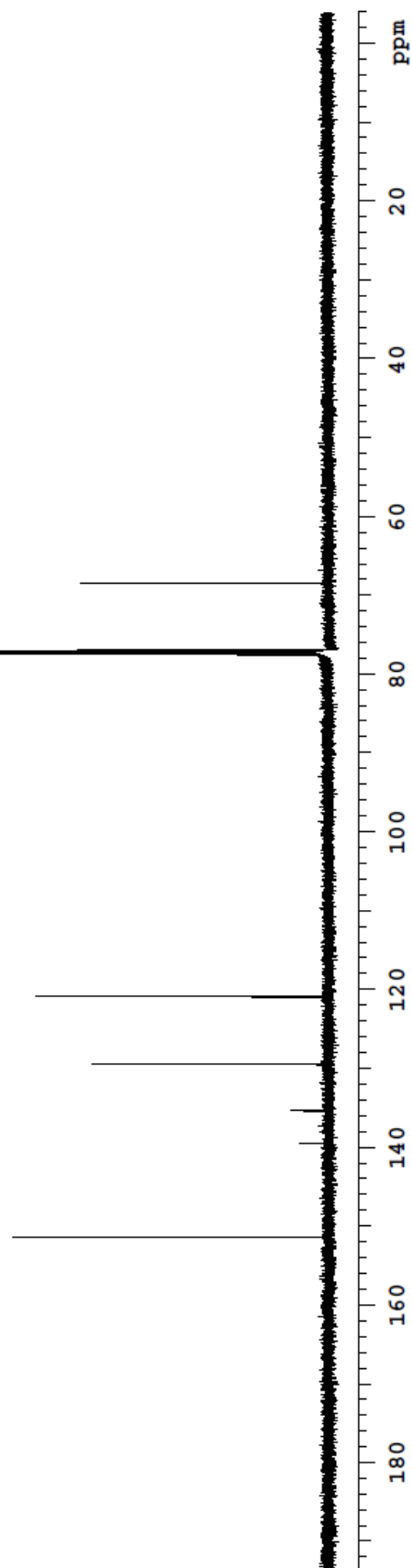
WALTZ-16 modulated

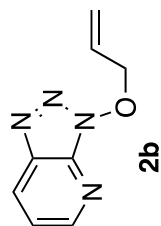
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





mk-1205-I-HNMR-CDCL3-28-allyl

Pulse Sequence: s2pul

Solvent: CDCL3

Ambient temperature

Operator: mkl

File: mk-1205-I-HNMR-CDCL3-28-allyl

INOVA-500 "riga"

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

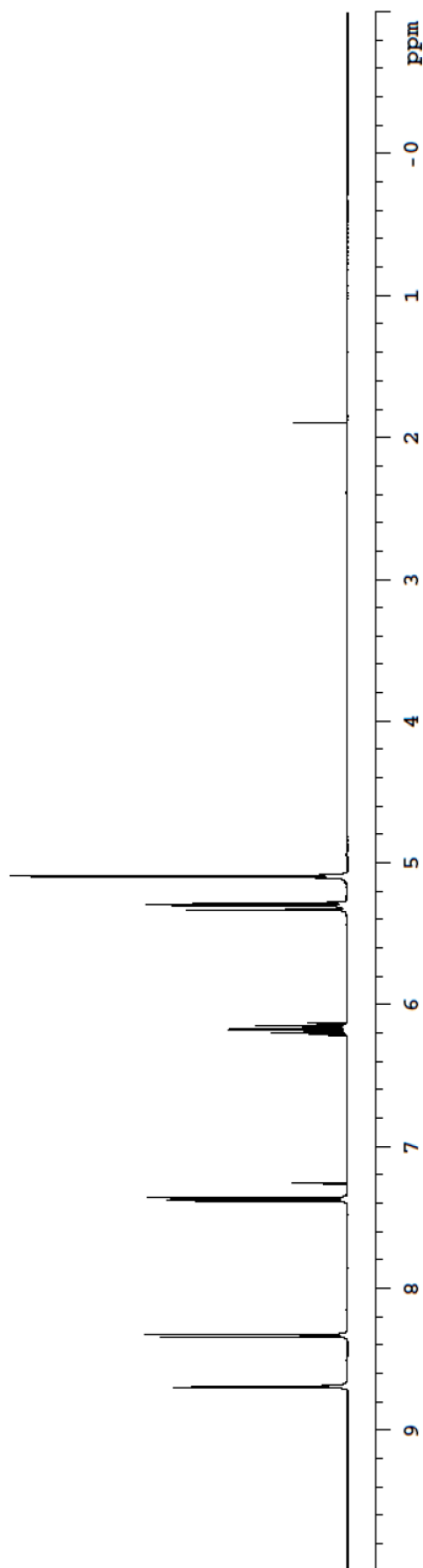
16 repetitions

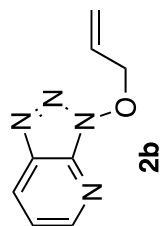
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 30 sec





mk-1205-I-C13-CDCl3-28-allyl

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-I-C13-CDCl3-28-allyl

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

500 repetitions

OBSERVE C13, 125.6674355 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

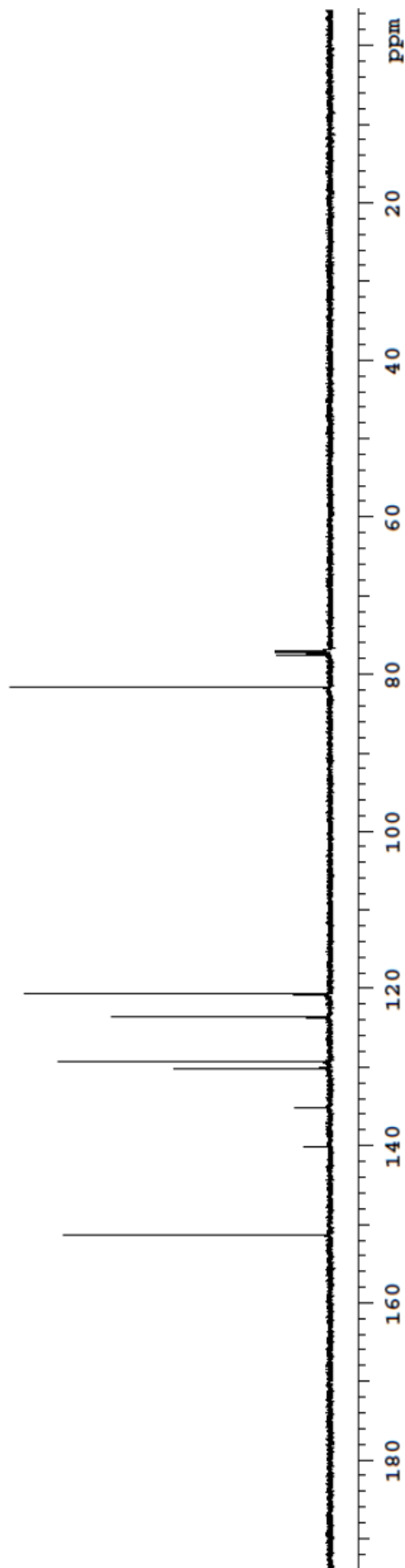
WALTZ-16 modulated

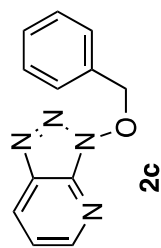
DATA PROCESSING

Line broadening 0.5 Hz

Ft size 65536

Total time 7 hr, 16 min, 27 sec





mk-1205-1-HNMR-CDCL3-120-benzylazabt

Pulse Sequence: s2pul

Solvent: CDCL3

Ambient temperature

Operator: mkl

File: mk-1205-1-HNMR-CDCL3-120-benzylazabt

INOVA-500 "riga"

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

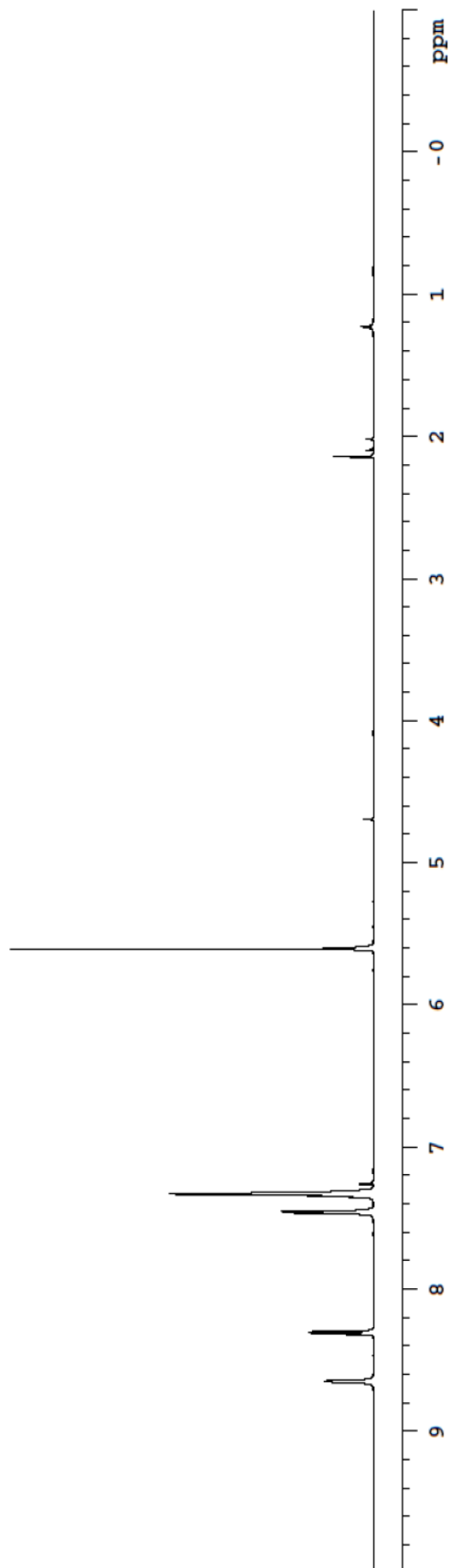
64 repetitions

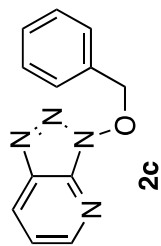
OBSERVE H1, 499.7707207 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec





mk-1205-I-C13-CDCL3-120-benzylaza

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-I-C13-CDCL3-120-benzylaza

INOVA-500 "rfga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

2064 repetitions

OBSERVE C13, 125.6674332 MHz

DECOUPLE H1, 499.7730084 MHz

power 39 dB

continuously on

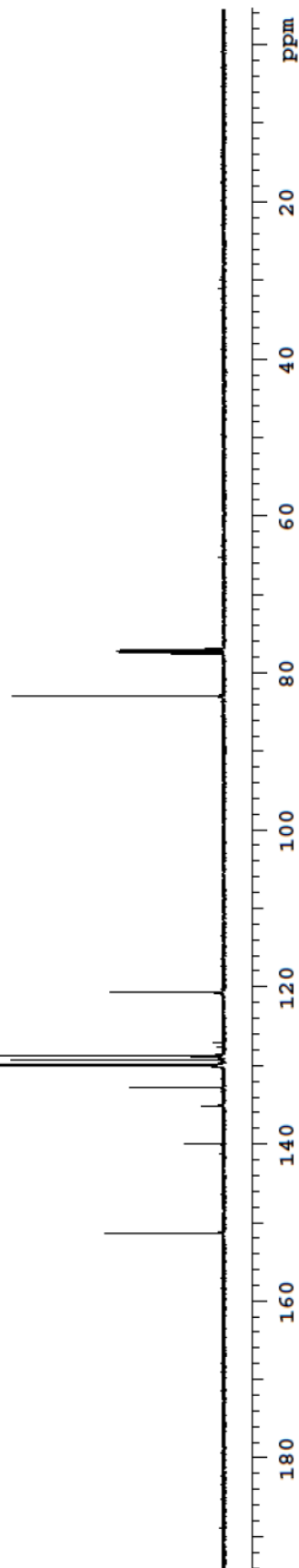
WALTZ-16 modulated

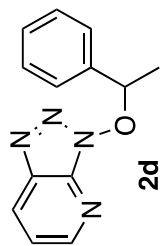
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 49 min, 6 sec





mk-1205-I-HNMR-CDCL3-26-secphenyl

Pulse Sequence: s2pul

Solvent: CDCL3

Ambient temperature

Operator: mkl

File: mk-1205-I-HNMR-CDCL3-26-secphenyl

INOVA-500 "riga"

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

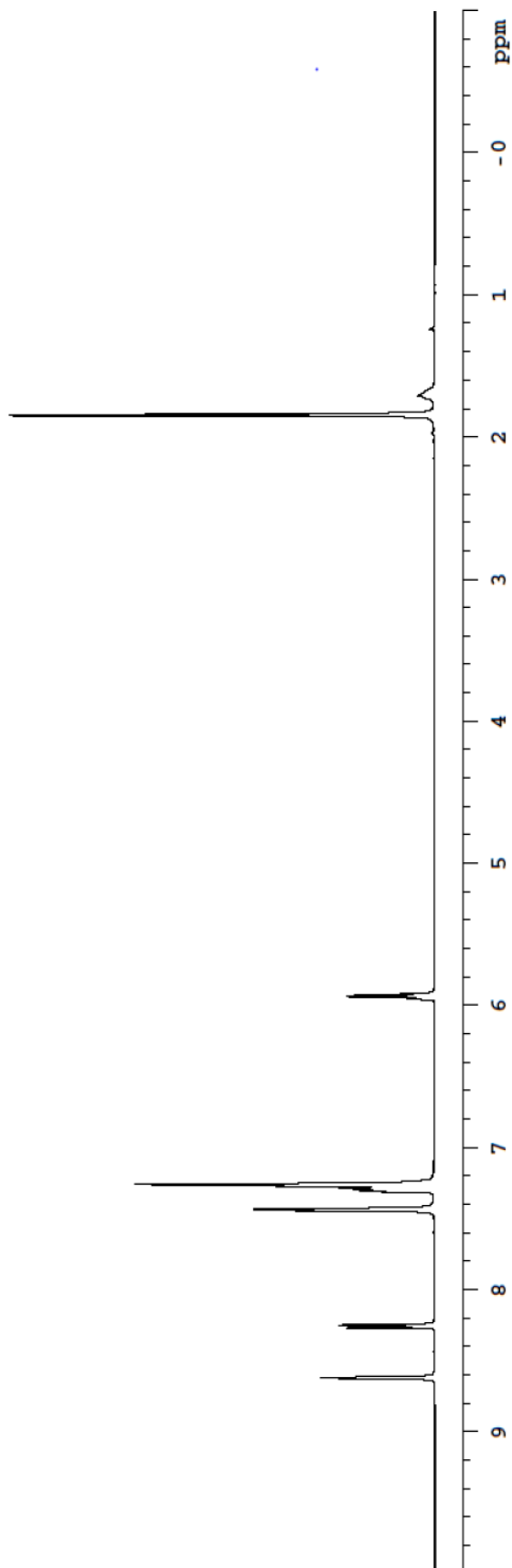
64 repetitions

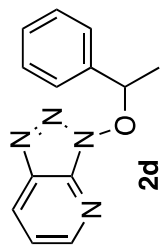
OBSERVE H1, 499.7707246 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec





mk-1205-I-C13-CDCl3-26-secphenyl

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-I-C13-CDCl3-26-secphenyl

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

2020 repetitions

OBSERVE C13, 125.6674263 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

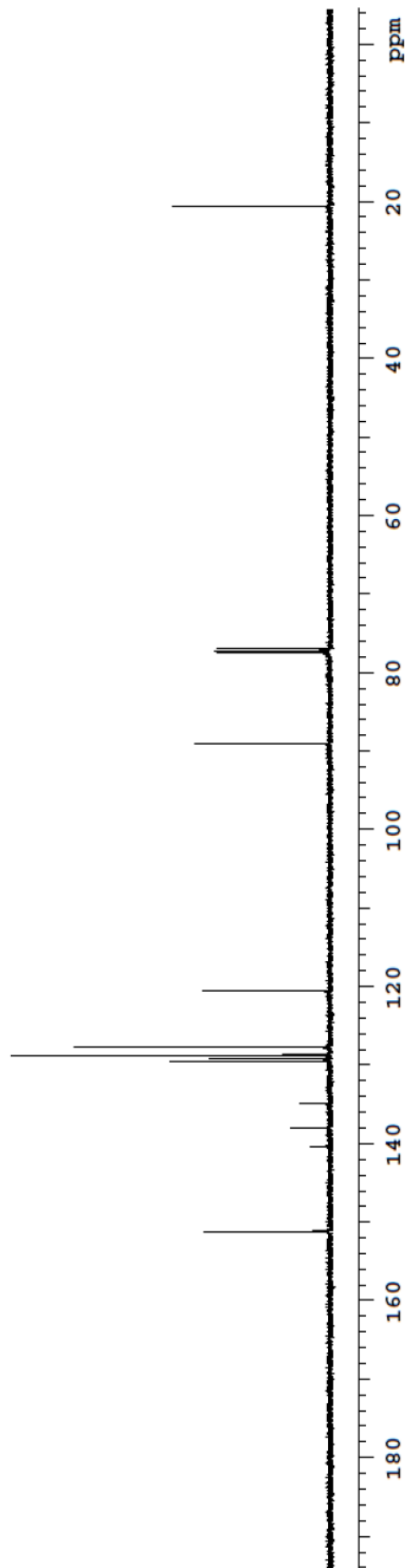
WALTZ-16 modulated

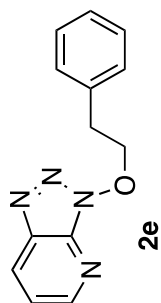
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 7 hr, 16 min, 27 sec





mk-1205-I-HNMR-CDCl3-29-nphenyl

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-I-HNMR-CDCl3-29-nphenyl

INOVA-500 "riga"

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

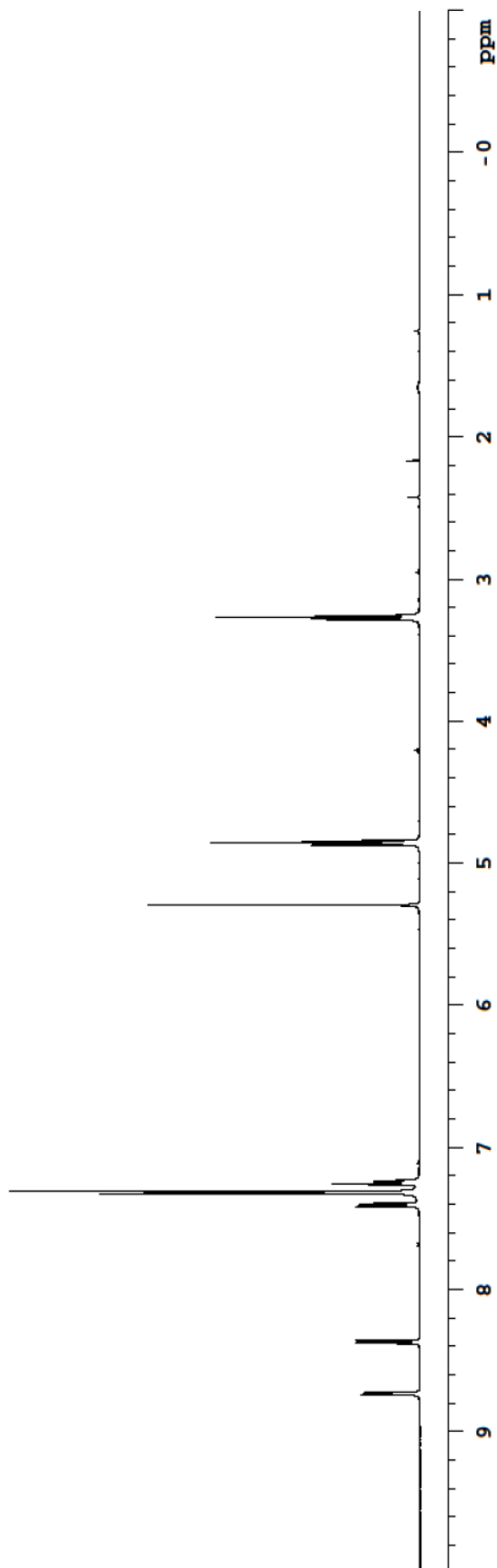
64 repetitions

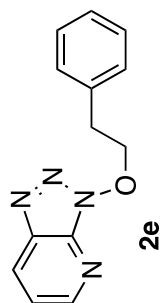
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec





mk-1205-I-C13-CDCl3-29-nphenyl

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mk1

File: mk-1205-I-C13-CDCl3-29-nphenyl

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

2050 repetitions

OBSERVE C13, 125.6674271 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

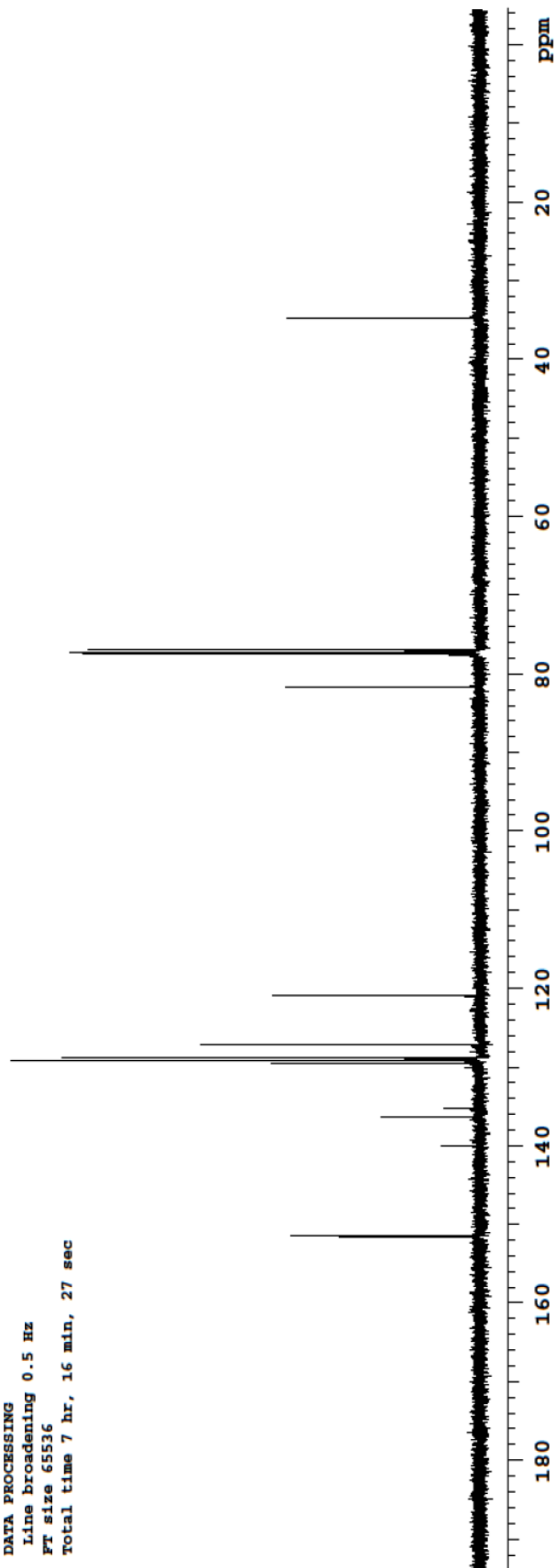
WALTZ-16 modulated

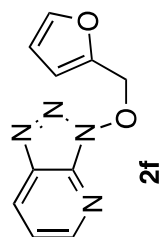
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 7 hr, 16 min, 27 sec





mk-1205-1-HNMR-CDCL3-121-furfurylaza

Pulse Sequence: s2pul

Solvent: CDCL3

Ambient temperature

Operator: mkl

File: mk-1205-1-HNMR-CDCL3-121-furfurylaza
INOVA-500 "r1ga"

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

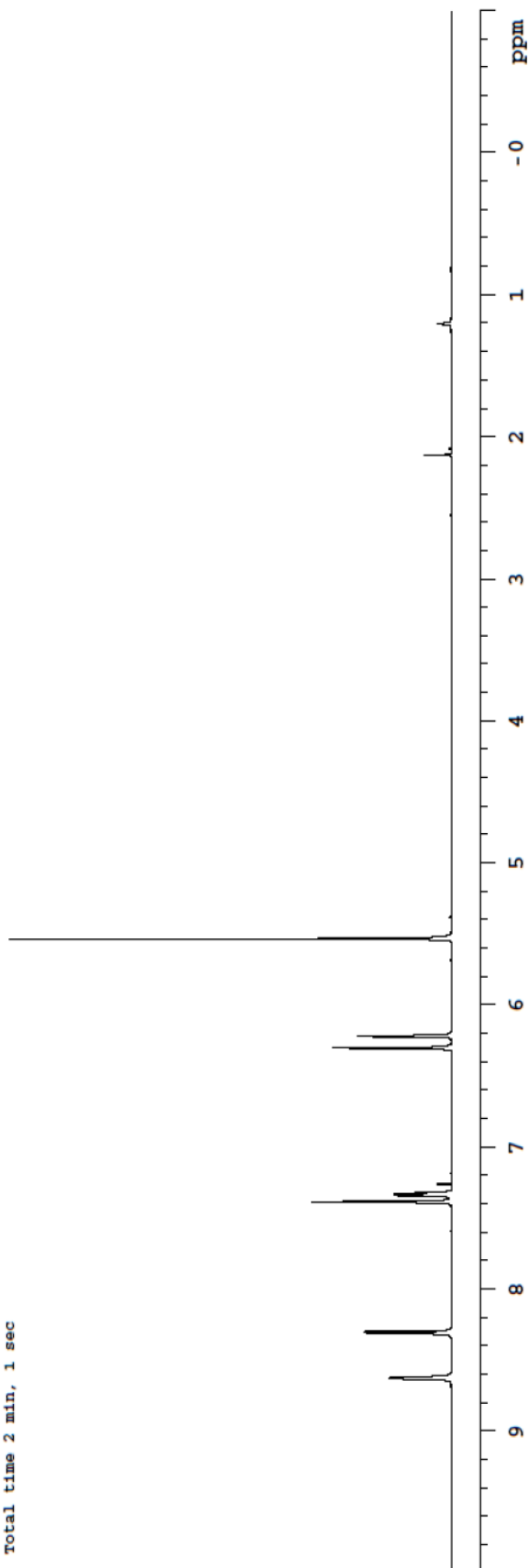
64 repetitions

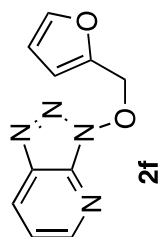
OBSERVE H1, 499.7707202 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec





mk-1205-I-C13-CDCL3-121-furfurylaza

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-I-C13-CDCL3-121-furfurylaza

INOVA-500 "r1ga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

355 repetitions

OBSERVE C13, 125.6674339 MHz

DECOUPLE H1, 499.7730084 MHz

power 39 dB

continuously on

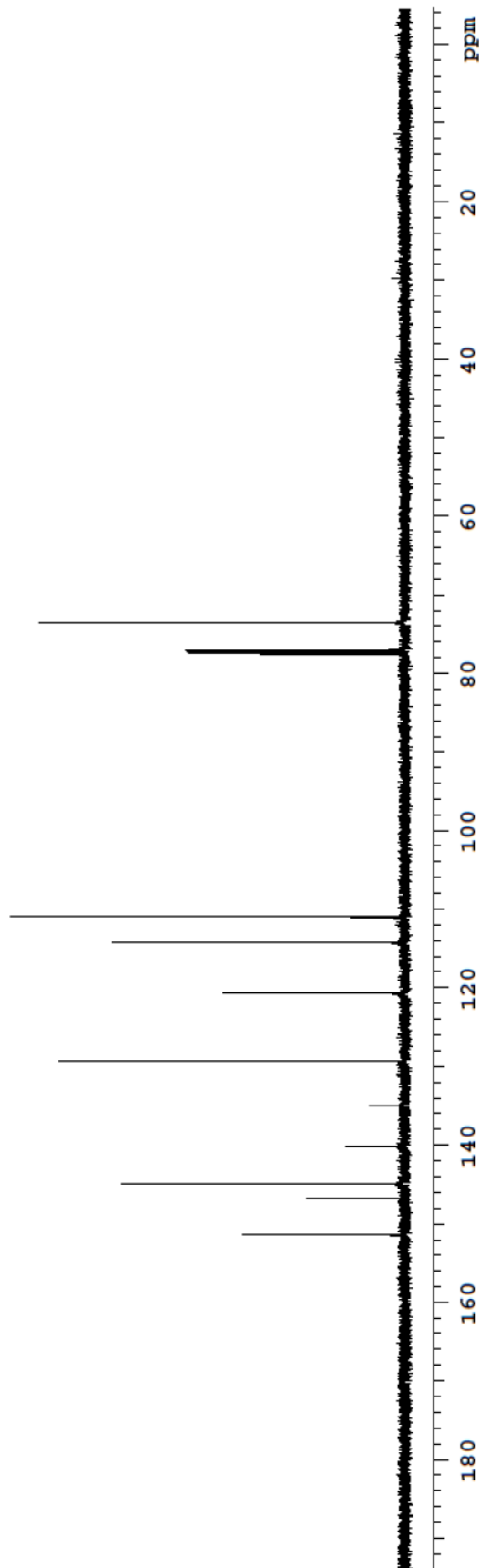
WALTZ-16 modulated

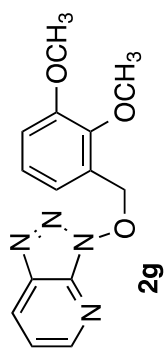
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 49 min, 6 sec





mk-1205-I-HNMR-CDCL3-27-diether

Pulse Sequence: s2pul

Solvent: CDCL3

Ambient temperature

Operator: mk1

File: mk-1205-I-HNMR-CDCL3-27-diether

INOVA-500 "riga"

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

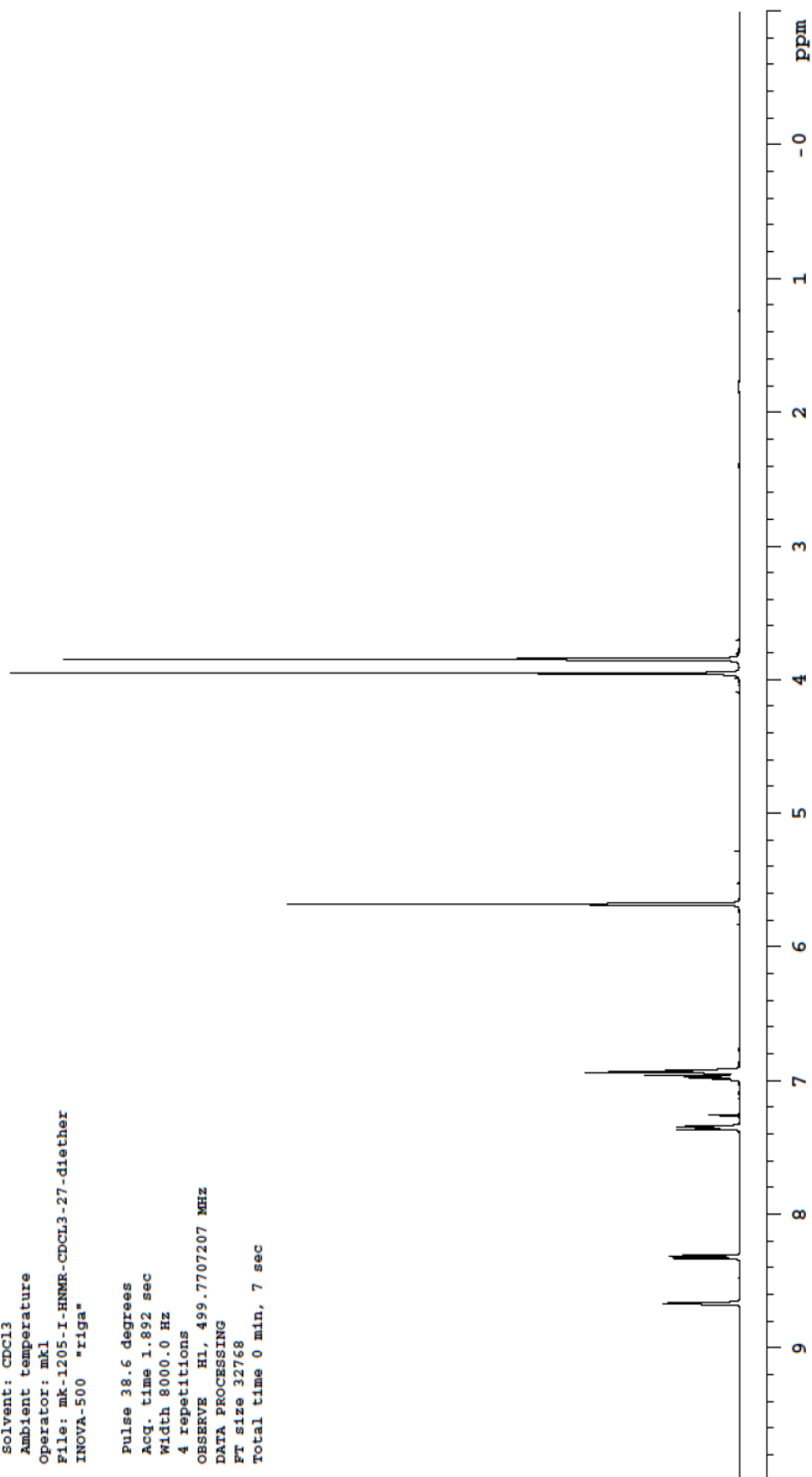
4 repetitions

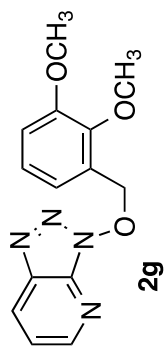
OBSERVE H1, 499.7707207 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 7 sec





mk-1205-I-C13-CDCL3-39-diether

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mk1

File: mk-1205-I-C13-CDCL3-39-diether

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

1280 repetitions

OBSERVE C13, 125.6674255 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

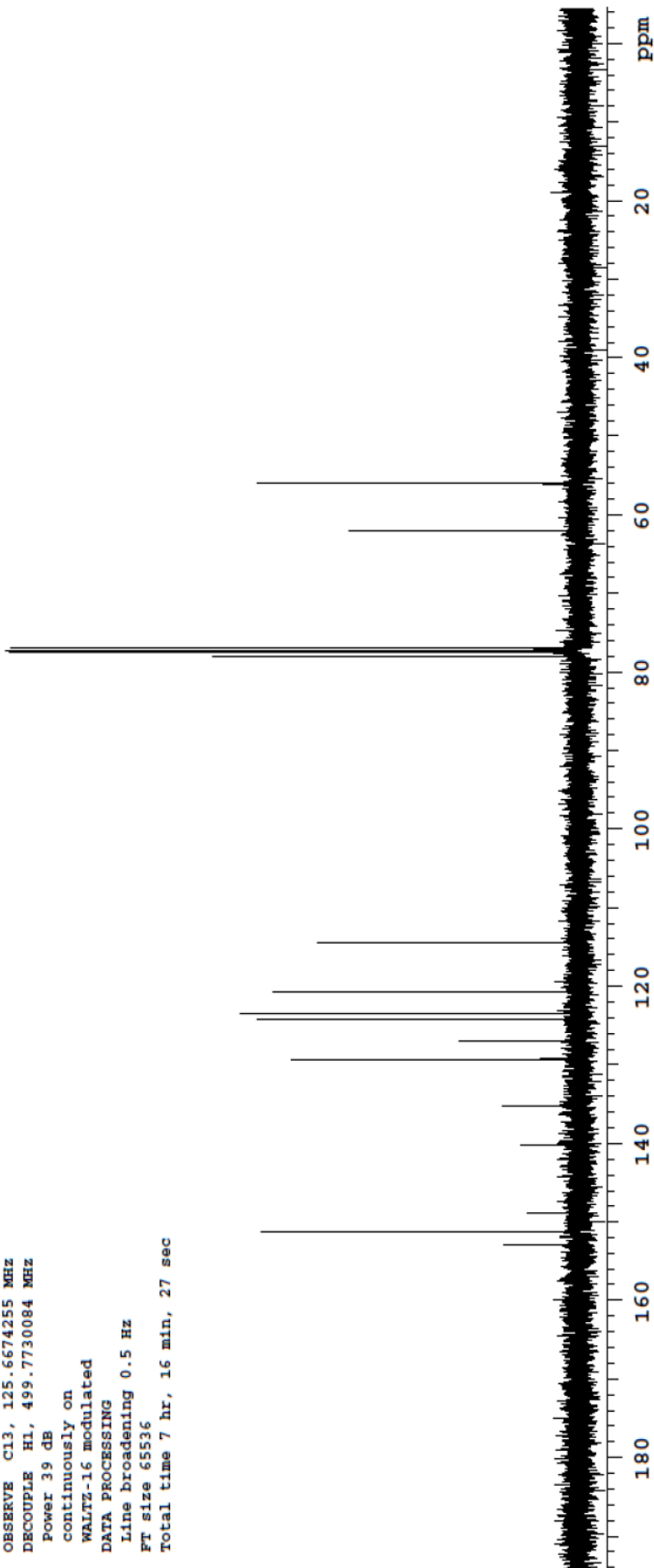
WALTZ-16 modulated

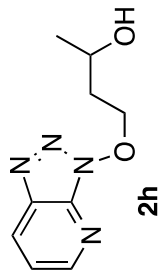
DATA PROCESSING

Line broadening 0.5 Hz

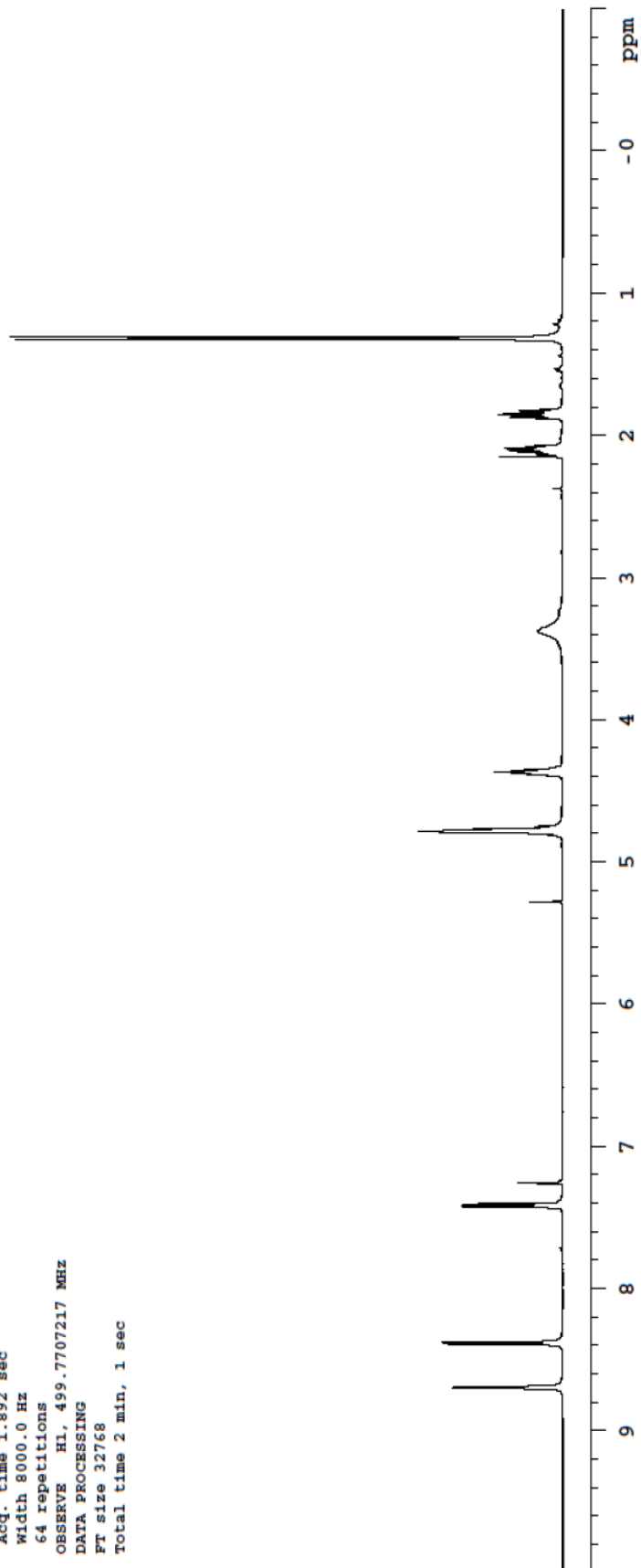
FT size 65536

Total time 7 hr, 16 min, 27 sec





mk-1205-1-HNMR-CDCL3-36-1.3butanediol
Pulse Sequence: s2pul
Solvent: CDCL3
Ambient temperature
Operator: mkl
File: mk-1205-1-HNMR-CDCL3-36-1.3butanediol
INOVA-500 "riga"
Pulse 34.7 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
64 repetitions
OBSERVE H1, 499.7707217 MHz
DATA PROCESSING
FT size 32768
Total time 2 min, 1 sec



STANDARD PROTON PARAMETERS

Pul se Sequence: s2pul

Sol vent : CDCl 3

Am bi ent tem per a ture

Oper a tor : mkl

File : mk-1205-1 - HMR- CDCl3- 36- 1. 3but anedi ol - re t aken08152012

1 NOVA- 500 "ri ga"

2h

Expanded spectrum

Pul se 34. 7 degrees

Acq. time 1. 892 sec

Wd th 8000. 0 Hz

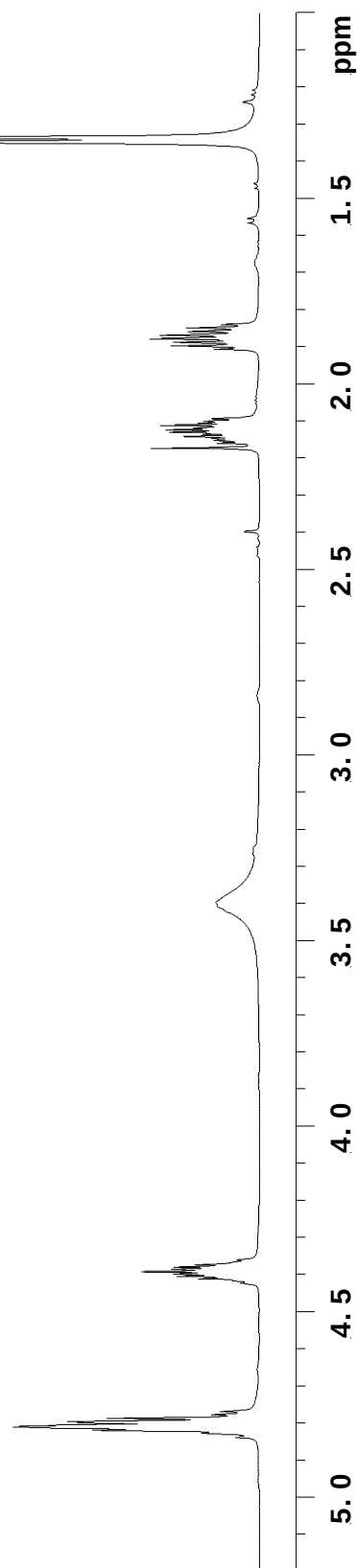
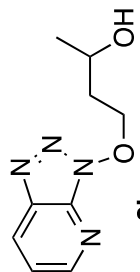
64 repetitions

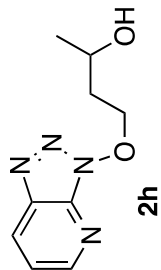
OBSERVE H1, 499. 7707095 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec





mk-1205-I-C13-CDCL3-36-1.3butanediol

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-I-C13-CDCL3-36-1.3butanediol

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

1390 repetitions

OBSERVE C13, 125.6674286 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

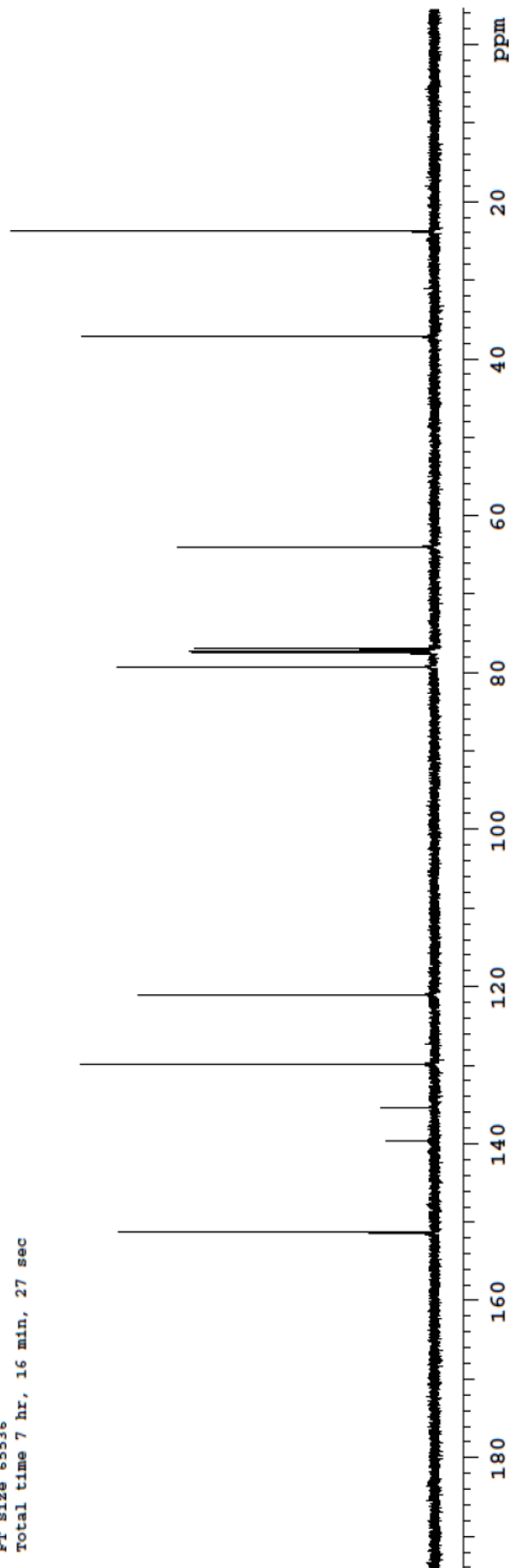
WALTZ-16 modulated

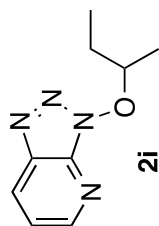
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 7 hr, 16 min, 27 sec





mk-1205-1-HNMR-CDCL3-122-aza2butanol

Pulse Sequence: s2pul

Solvent: CDCL3

Ambient temperature

Operator: mkl

File: mk-1205-1-HNMR-CDCL3-122-aza2butanol
INOVA-500 "riga"

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

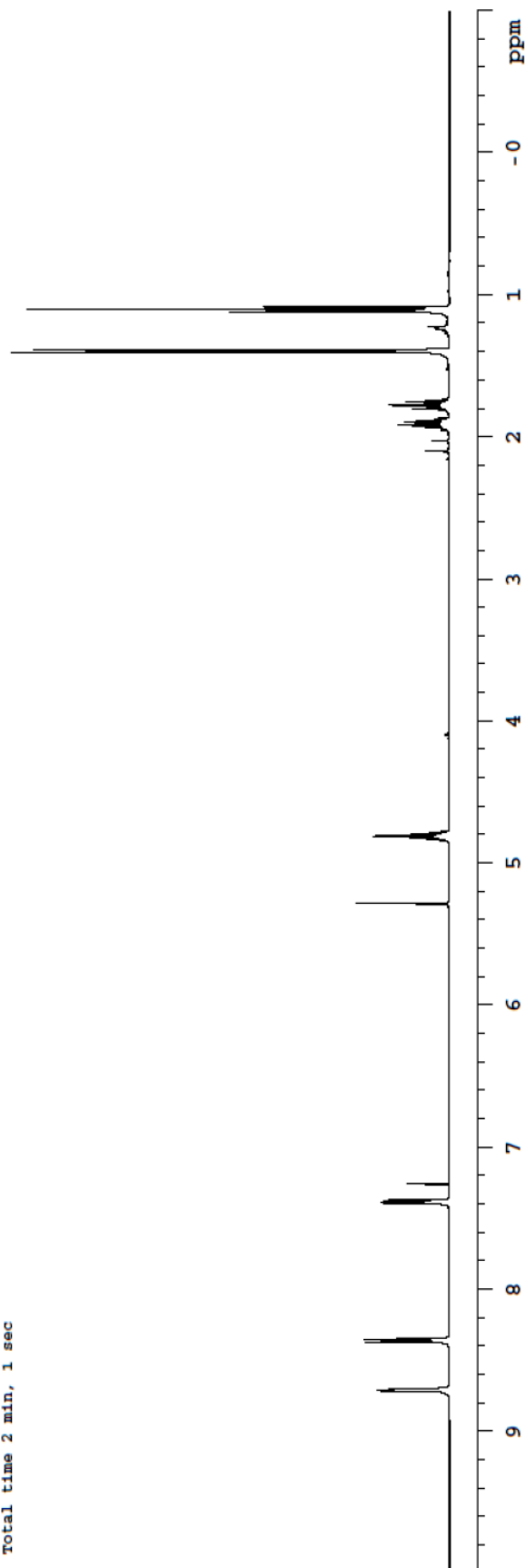
64 repetitions

OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec



nk-1205-1 - HMR- CDCL3- 122- aza2but anol

Pul se Sequence: s2pul

Sol vent : CDCl 3

Am bi ent tem per a ture

Oper a tor : nkl

File: nk-1205-1 - HMR- CDCL3- 122- aza2but anol

1 NOVA- 500 "ri ga"

Pul se 34.7 degrees

Acq. time 1.892 sec

Wdth 8000.0 Hz

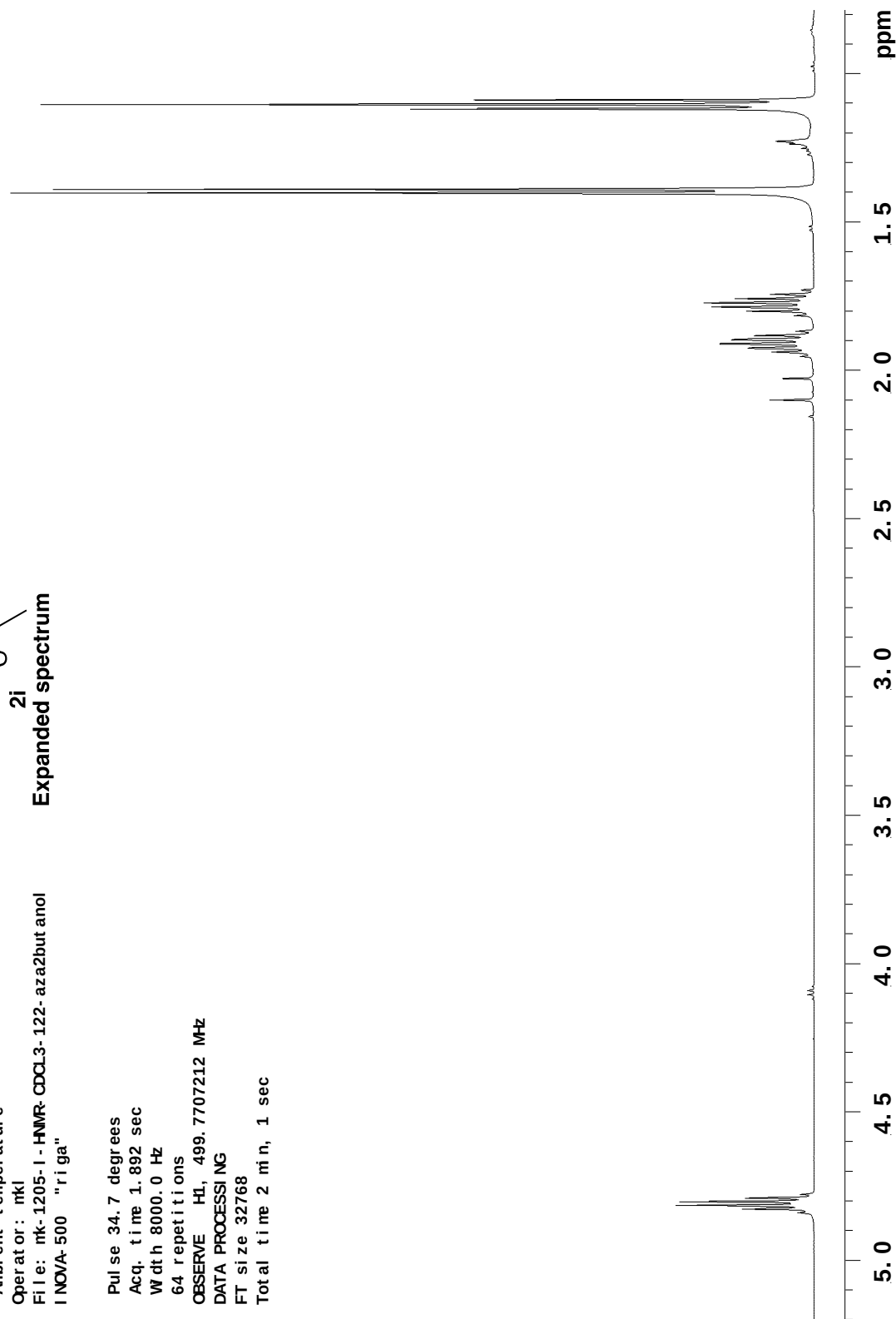
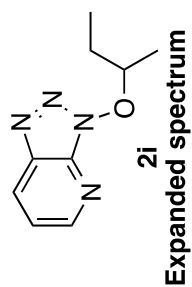
64 repetitions

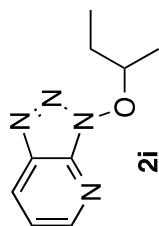
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec





mk-1205-I-C13-CDCL3-122-aza2butanol

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-I-C13-CDCL3-122-aza2butanol

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

3455 repetitions

OBSERVE C13, 125.6674255 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

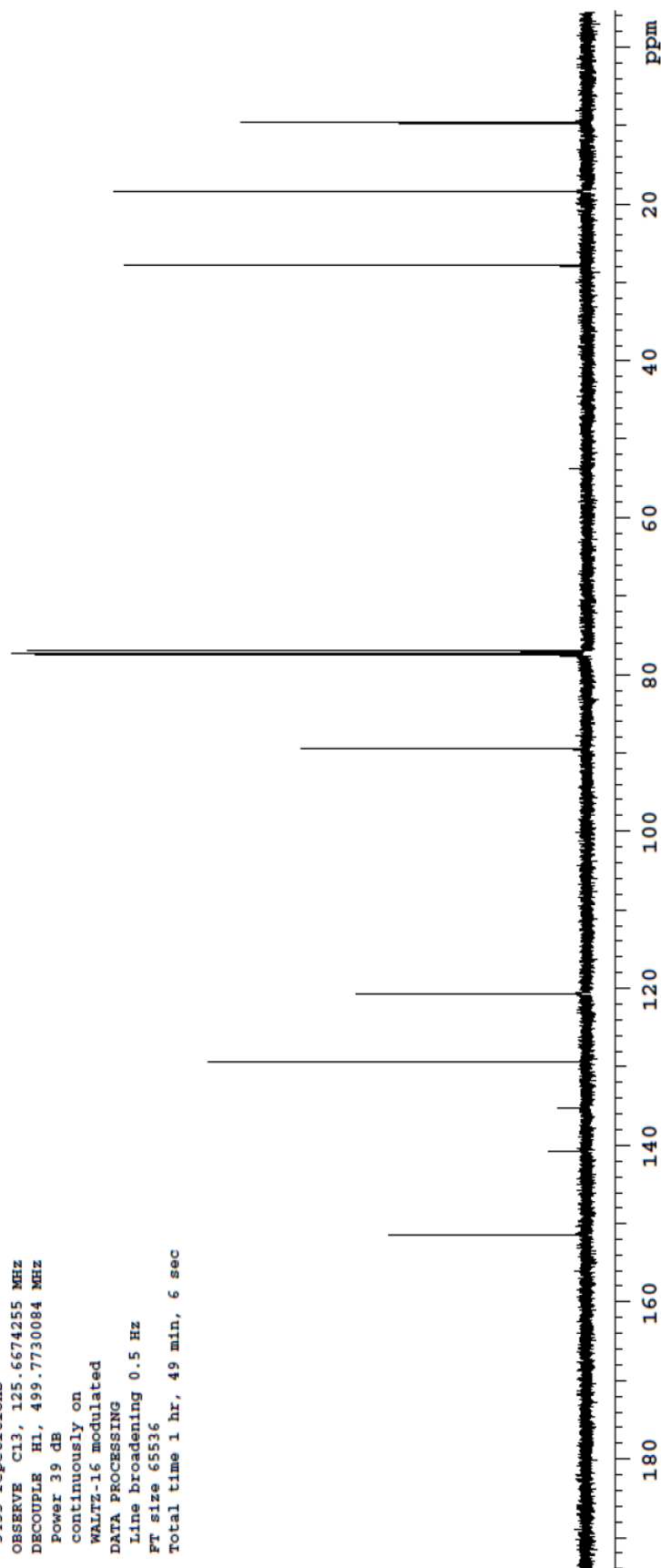
WALTZ-16 modulated

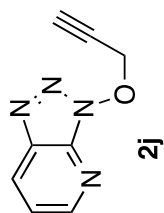
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 49 min, 6 sec





1205-Vijay-03-87-1H-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

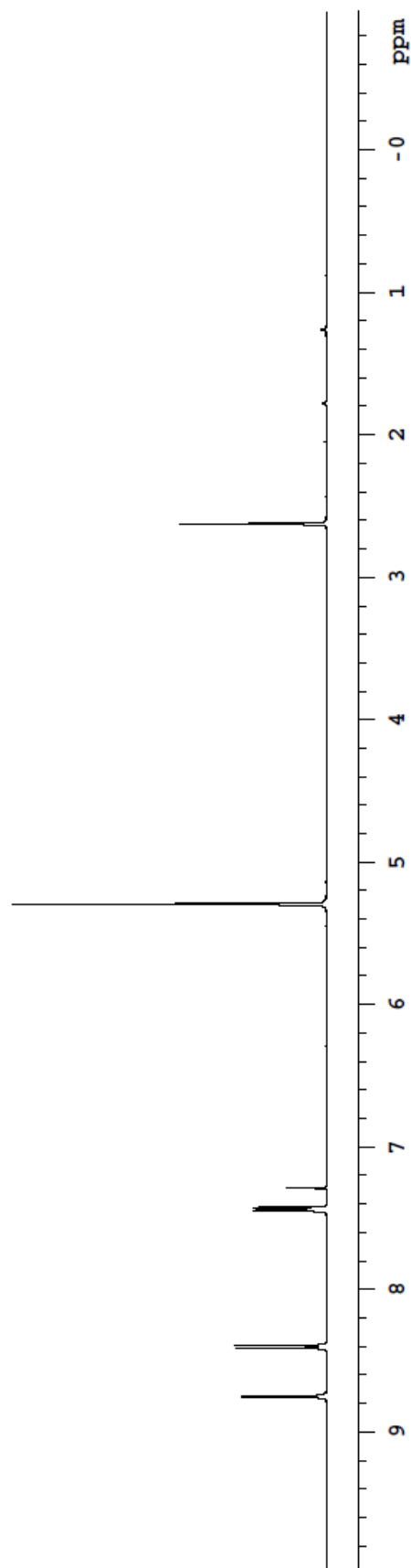
32 repetitions

OBSERVE H1, 499.7707095 MHz

DATA PROCESSING

FT size 32768

Total time 3 min, 40 sec



1205-Vijay-03-87-13C-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mk1

File:

INOVA-500 "riga"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

588 repetitions

OBSERVE C13, 125.6674286 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

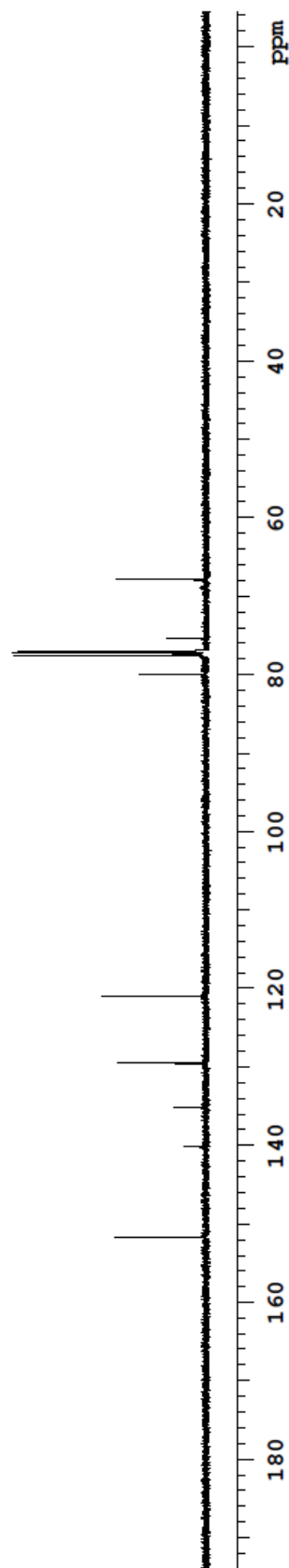
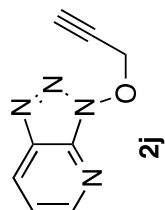
WALTZ-16 modulated

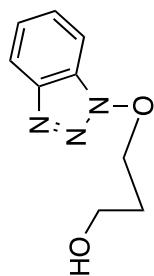
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 55 min, 9 sec





3a

RRC-1205-II-124-HNMR-CDCl3-monoether

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-II-124-HNMR-CDCl3-monoether

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707217 MHz

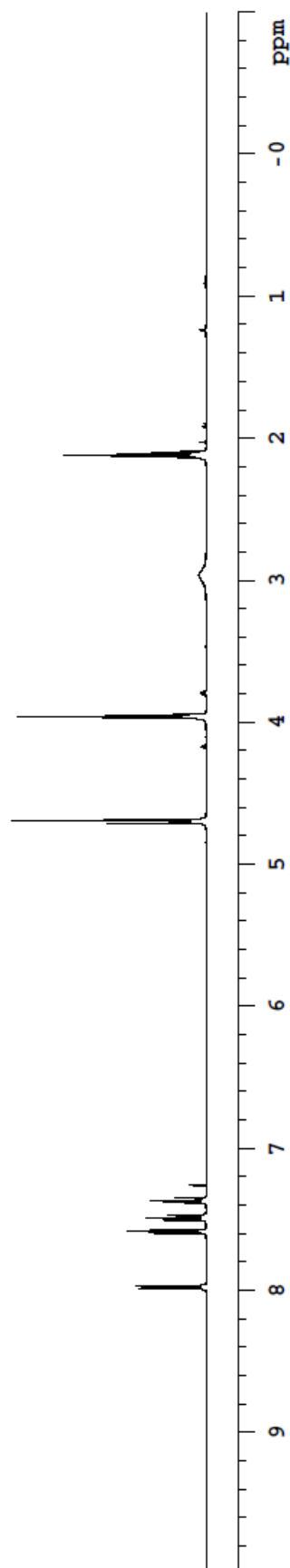
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 5 min, 13 sec



RRC-1205-11 - 124-HNMR-CDCl₃-monoether

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-11 - 124-HNMR-CDCl₃-monoether

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707217 MHz

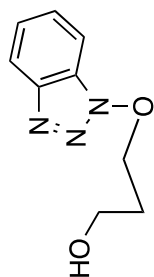
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

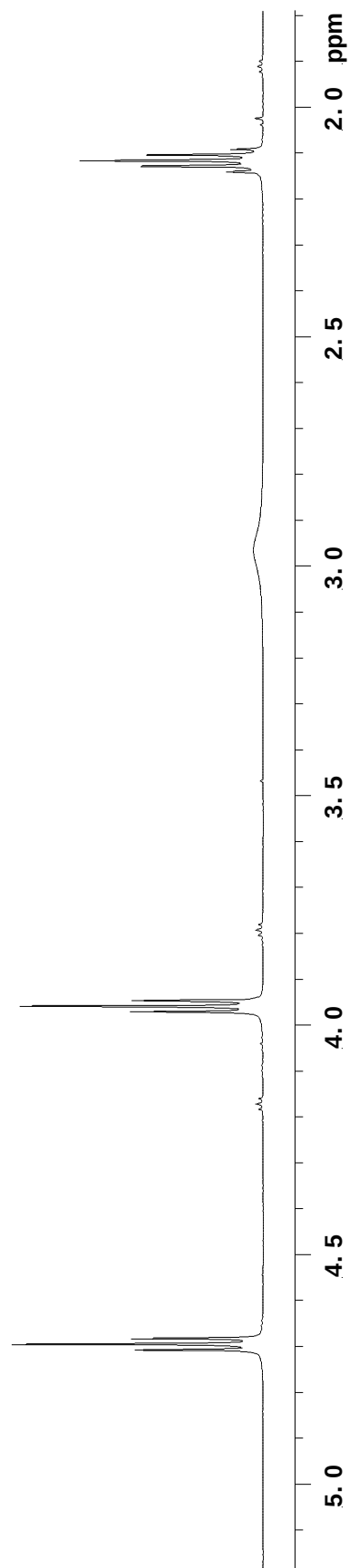
FT size 32768

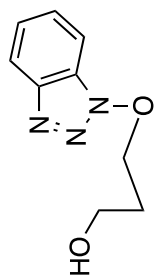
Total time 5 min, 13 sec



3a

Expanded spectrum





3a

REC-1205-II-124-CNMR-CDCl3-monoether

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-II-124-CNMR-CDCl3-monoether

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

12210 repetitions

OBSERVE C13, 125.6674273 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

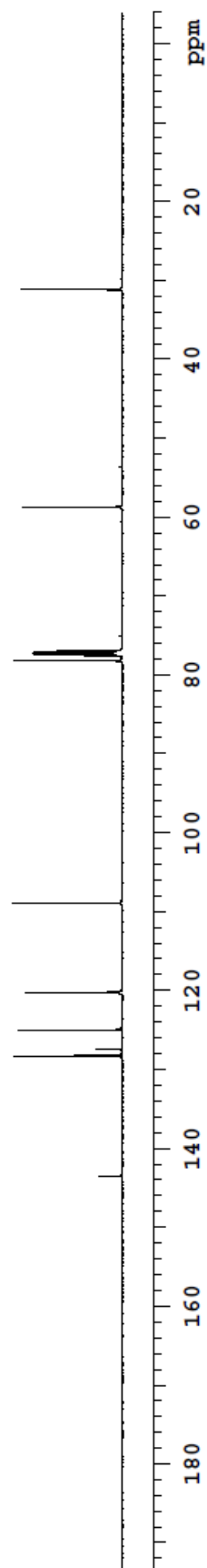
WALTZ-16 modulated

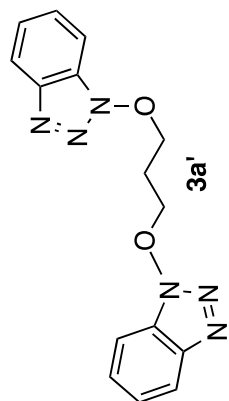
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 29 hr, 55 min, 35 sec





RRC-1205-II-124-HNMR-CDCl3-bisether

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-II-124-HNMR-CDCl3-bisether

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

44 repetitions

OBSERVE H1, 499.7707217 MHz

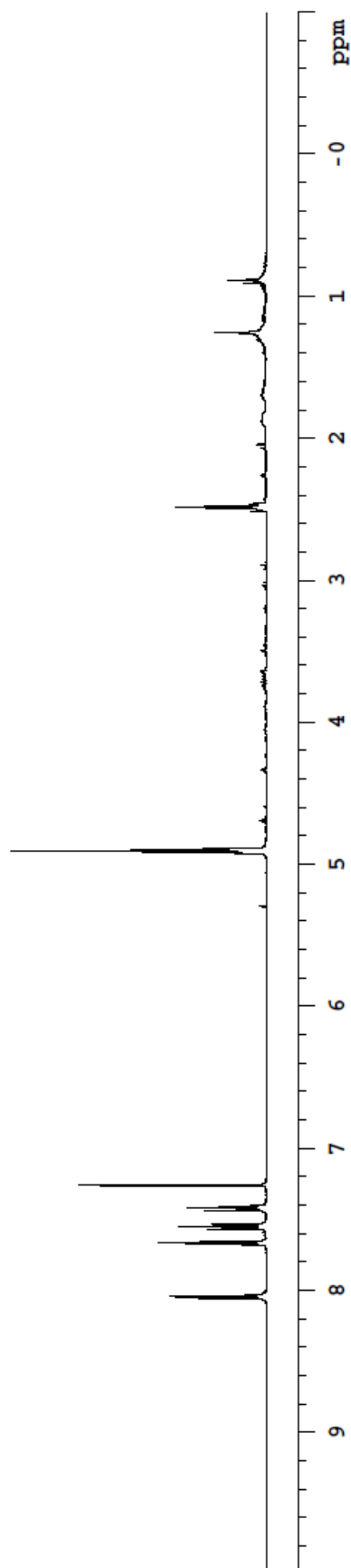
DATA PROCESSING

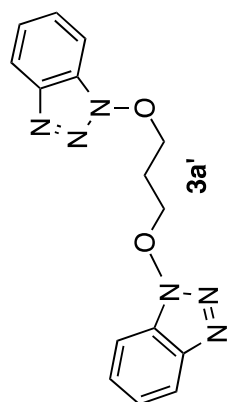
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 5 min, 13 sec





REC-1205-II-124-CNMR-CDCl3-bisether

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-II-124-CNMR-CDCl3-bisether

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

14490 repetitions

OBSERVE C13, 125.6674182 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

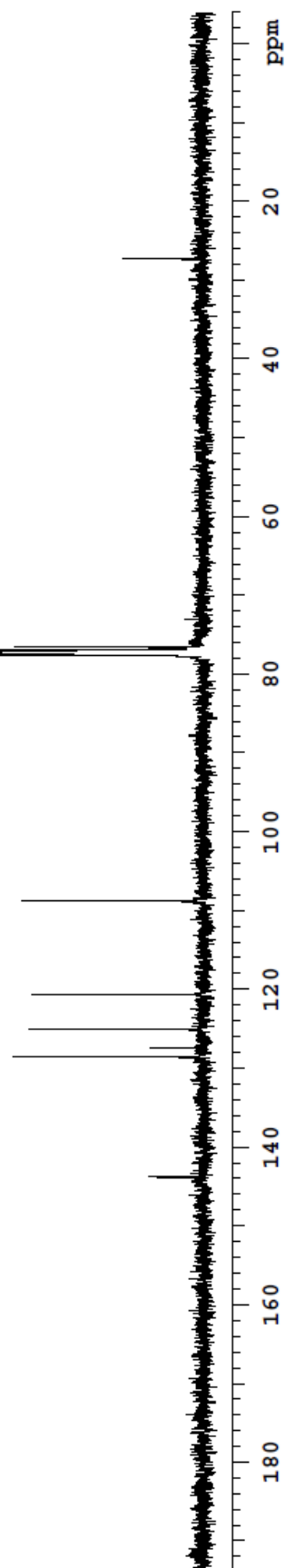
WALTZ-16 modulated

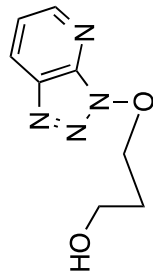
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 29 hr, 55 min, 35 sec





3b

mk-1205-1-HNMR-CDCL3-propanediol-12122012

Pulse Sequence: s2pul

Solvent: CDCL3

Temp. 25.0 C / 298.1 K

Operator: mk1

File: mk-1205-1-HNMR-CDCL3-propanediol-12122012

INOVA-500 "riga"

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

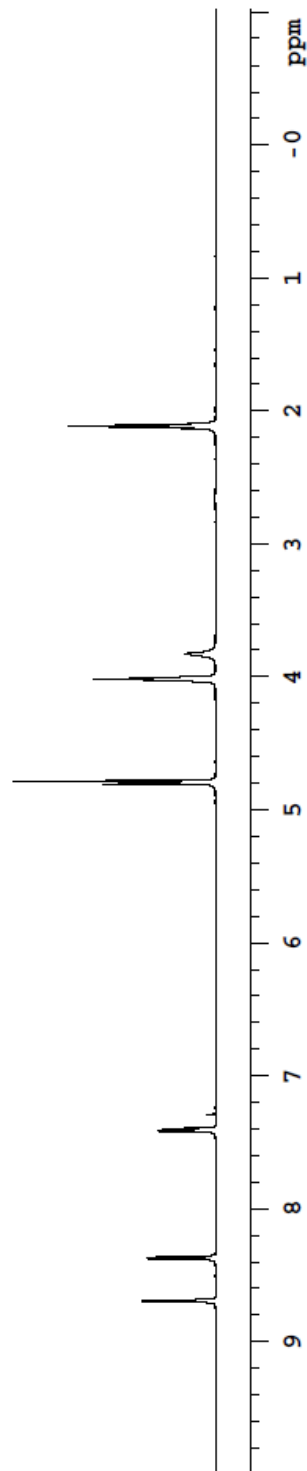
64 repetitions

OBSERVE H1, 499.777095 MHz

DATA PROCESSING

FT size 32768

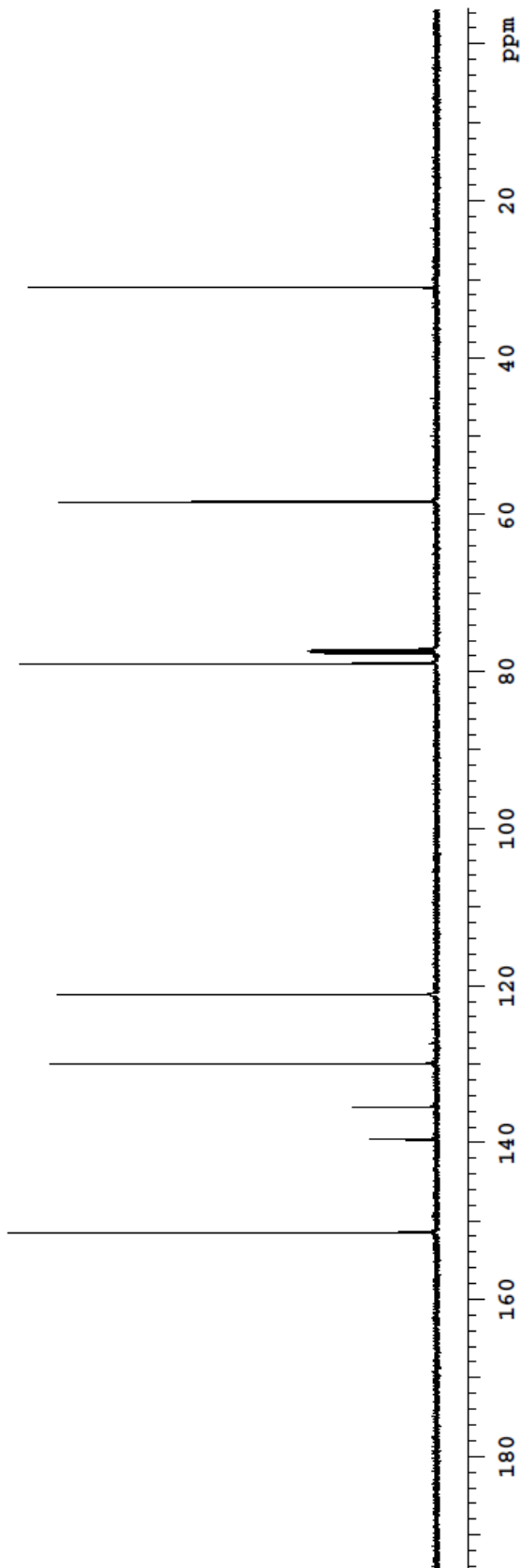
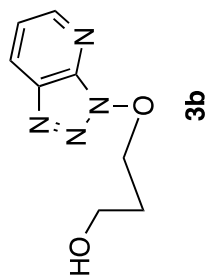
Total time 2 min, 1 sec

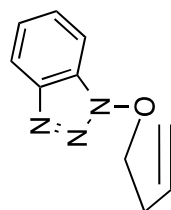


STANDARD CARBON PARAMETERS

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 Operator: mkl
 File: mk-1205-I-CDCl3-propanediolazanucleosidemimic-cl3-8042012
 INOVA-500 "riga"

Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 25000.0 Hz
 2290 repetitions
 OBSERVE C13, 125.6674149 MHz
 DECOUPLE H1, 499.7730084 MHz
 Power 39 dB
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 7 hr, 16 min, 27 sec





4a

1205-Vijay-03-89-1H-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

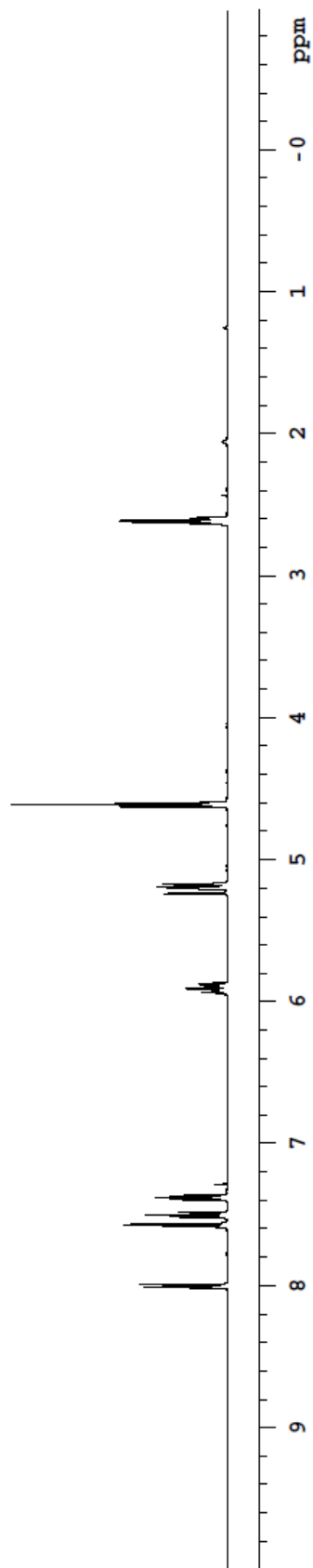
32 repetitions

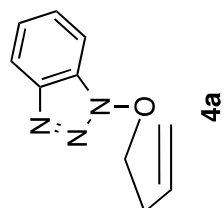
OBSERVE HL, 499.7707095 MHz

DATA PROCESSING

FT size 32768

Total time 3 min, 40 sec





1205-Vijay-03-89-13C-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

104 repetitions

OBSERVE C13, 125.6674149 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

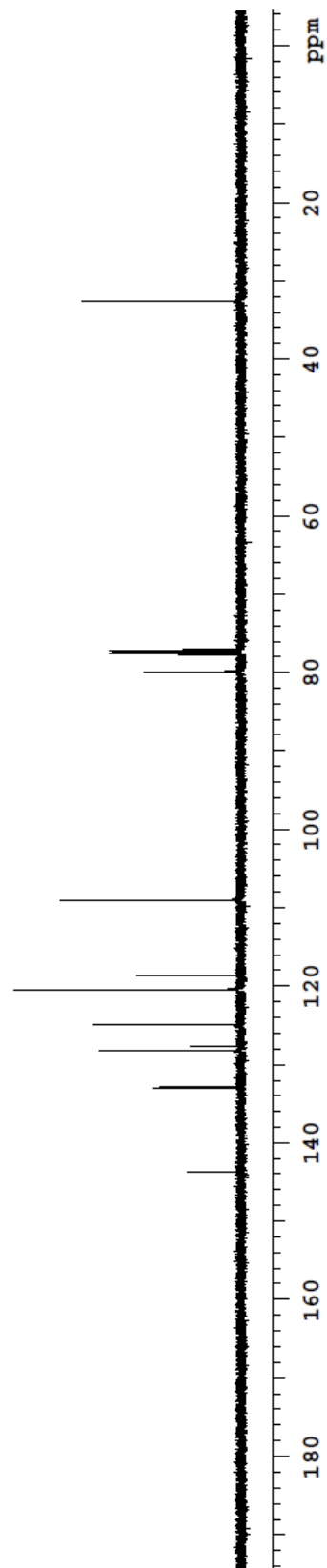
WALTZ-16 modulated

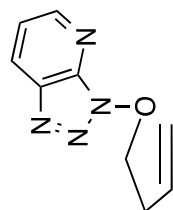
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 55 min, 9 sec





4b

mk-1205-1-HNMR-CDCL3-59-nucleoside-butEnol

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-1-HNMR-CDCL3-59-nucleoside-butEnol
INOVA-500 "riga"

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

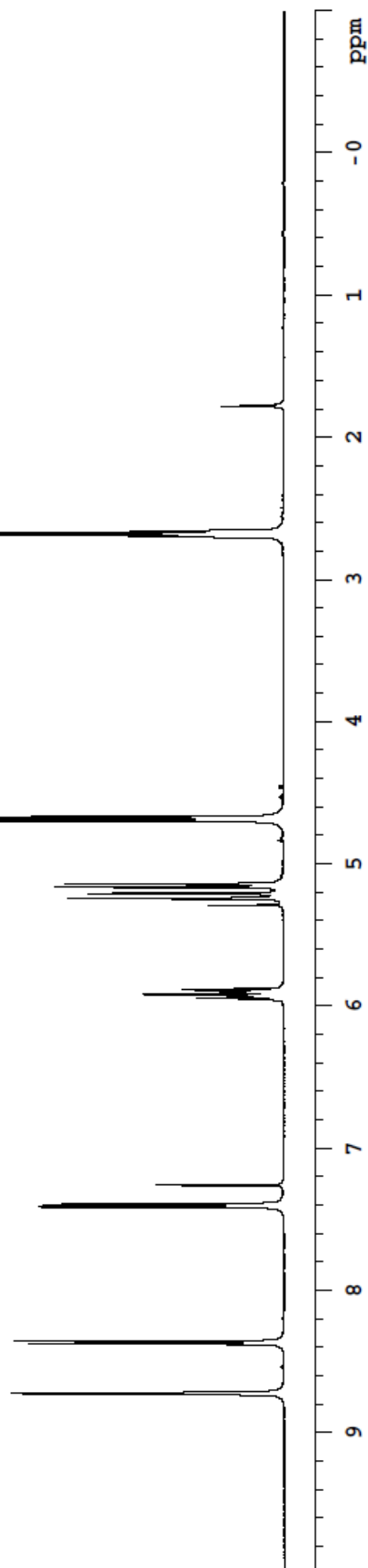
64 repetitions

OBSERVE H1, 499.7707202 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec



mk-1205-1 - HMR- CDCL3- 60- nuclei eosi de- but Enol

Pul se Sequence: s2pul

Sol vent : CDCl 3

Ambi ent temperat ure

Oper at or: mkl

File: mk-1205-1 - HMR- CDCL3- 59- nuclei eosi de- but Enol

INOV A- 500 "ri ga"

Pul se 34.7 degrees

Acq. time 1.892 sec

Wdth 8000.0 Hz

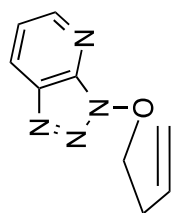
64 repetitions

OBSERVE H1, 499.7707202 MHz

DATA PROCESSING

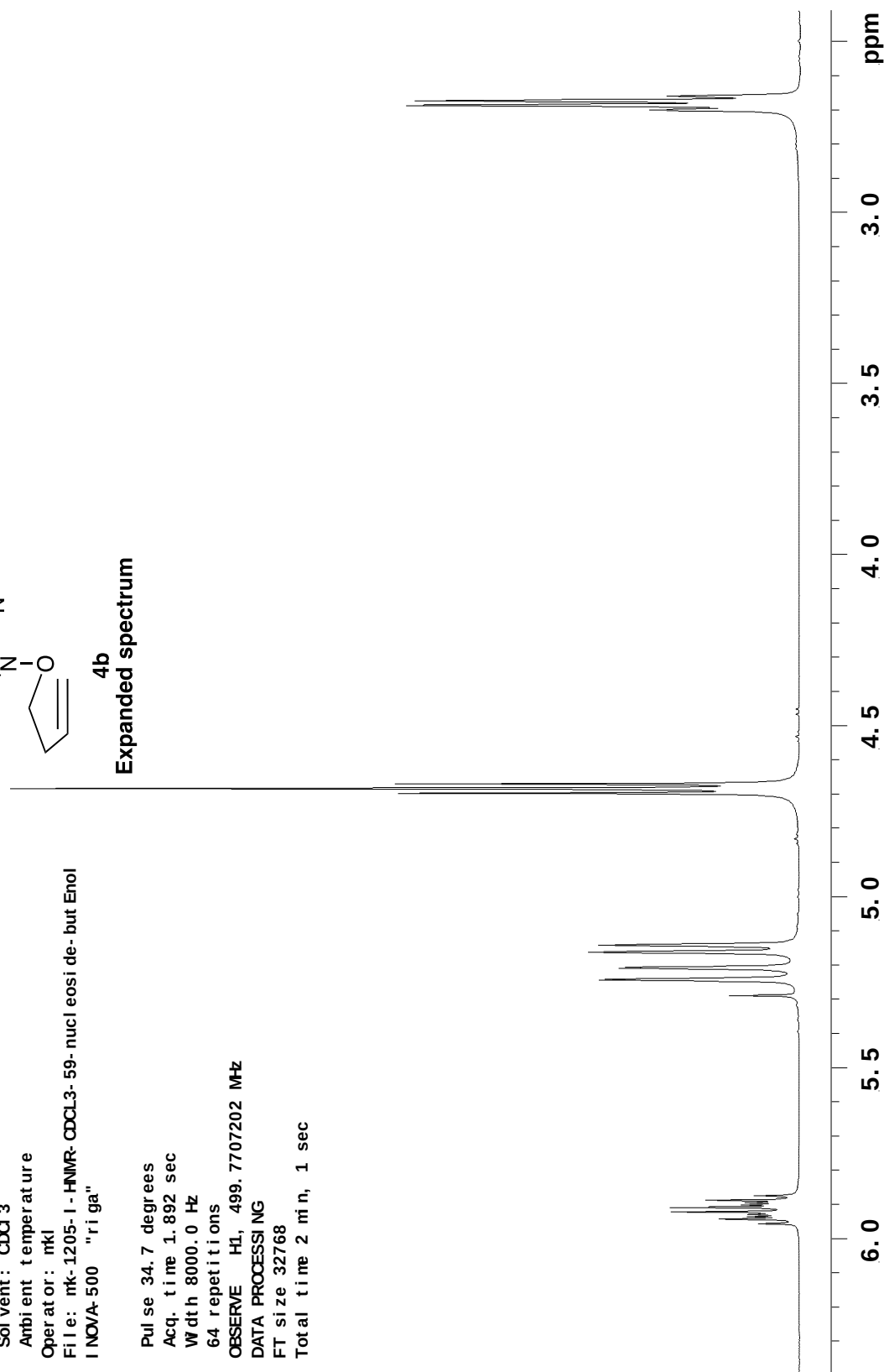
FT size 32768

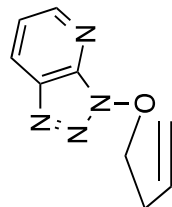
Total time 2 min, 1 sec



4b

Expanded spectrum





4b

mk-1205-I-C13-CDCL3-59-nucleoside-butEnol

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-I-C13-CDCL3-60-nucleoside-butEnol
INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

3110 repetitions

OBSERVE C13, 125.6674248 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

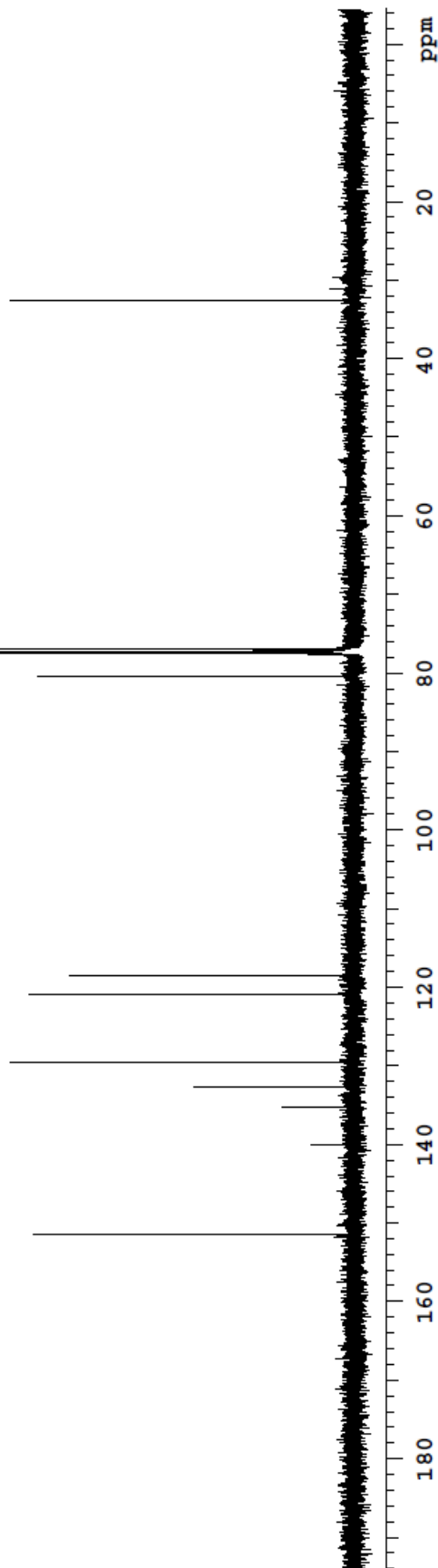
WALTZ-16 modulated

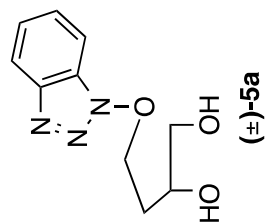
DATA PROCESSING

Line broadening 0.5 Hz

Ft size 65536

Total time 7 hr, 16 min, 27 sec





1205-Vijay-01-42-pure-1H-CDC13

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File:

INOVA-500 "riga"

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

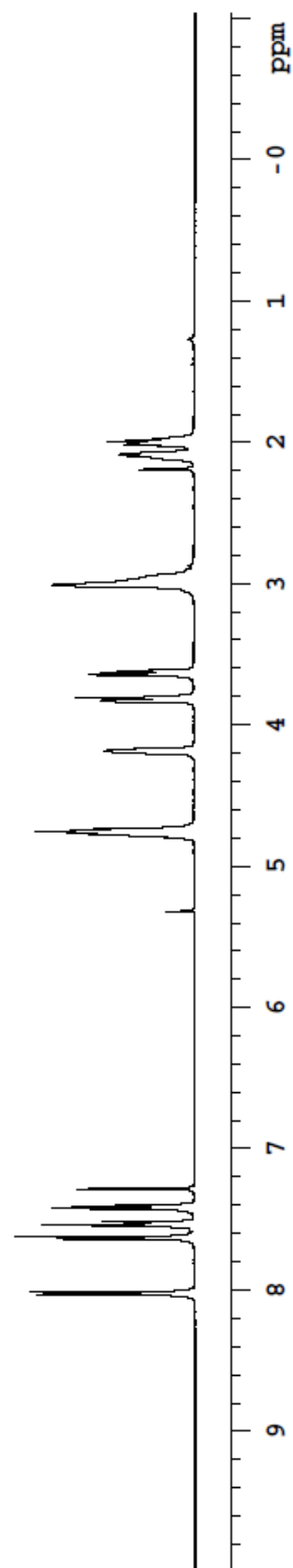
42 repetitions

OBSERVE H1, 499.7707095 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 20 sec



1205-vijay-01-42-13C-cdcl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mk1

File:

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

2831 repetitions

OBSERVE C13, 125.6674210 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

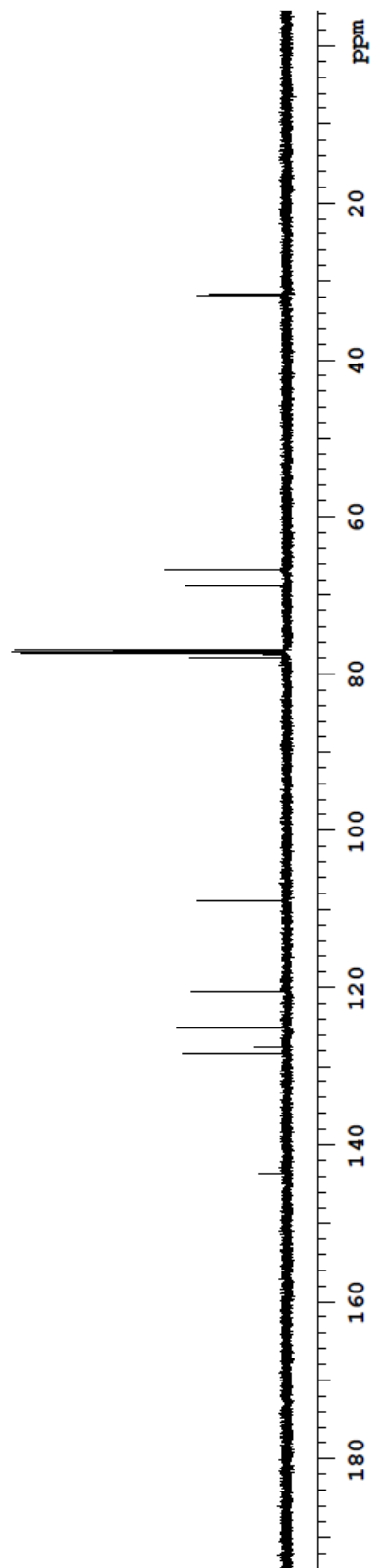
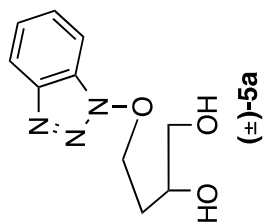
WALTZ-16 modulated

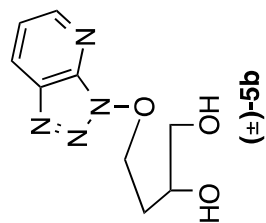
DATA PROCESSING

Line broadening 0.5 Hz

Ft size 65536

Total time 3 hr, 38 min, 13 sec





mk-1205-1-HNMR-CDCL3-62-dihydroxybutenol

Pulse Sequence: s2pul

Solvent: CDCL3

Ambient temperature

Operator: mkl

File: mk-1205-1-HNMR-CDCL3-62-dihydroxybutenol
INOVA-500 "riga"

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

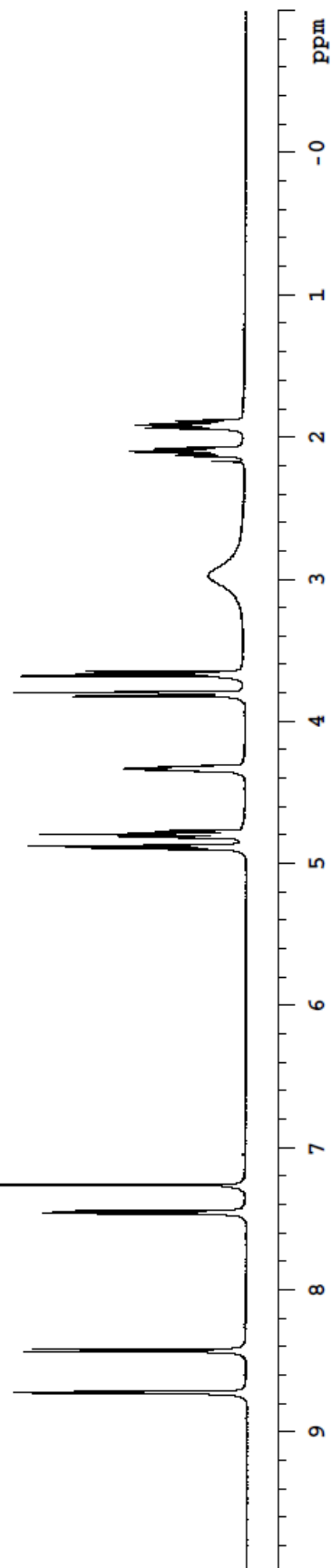
64 repetitions

OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 1 sec



mk-1205-1 - HMR- CDCL3- 62- al nyar oxybut enol

Pul se Sequence: s2pul

Sol vent: CDCl 3

Ambi ent t emper at ure

Oper ator: nkl

Fi le: mk-1205-1 - HMR- CDCL3- 62- di hydr oxybut enol

INOVA-500 "riga"

Pul se 34.7 degrees

Acq. time 1.892 sec

Wdth 8000.0 Hz

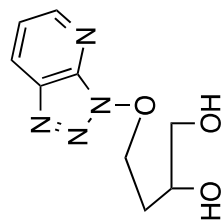
64 repetitions

OBSERVE HL, 499.7707217 MHz

DATA PROCESSING

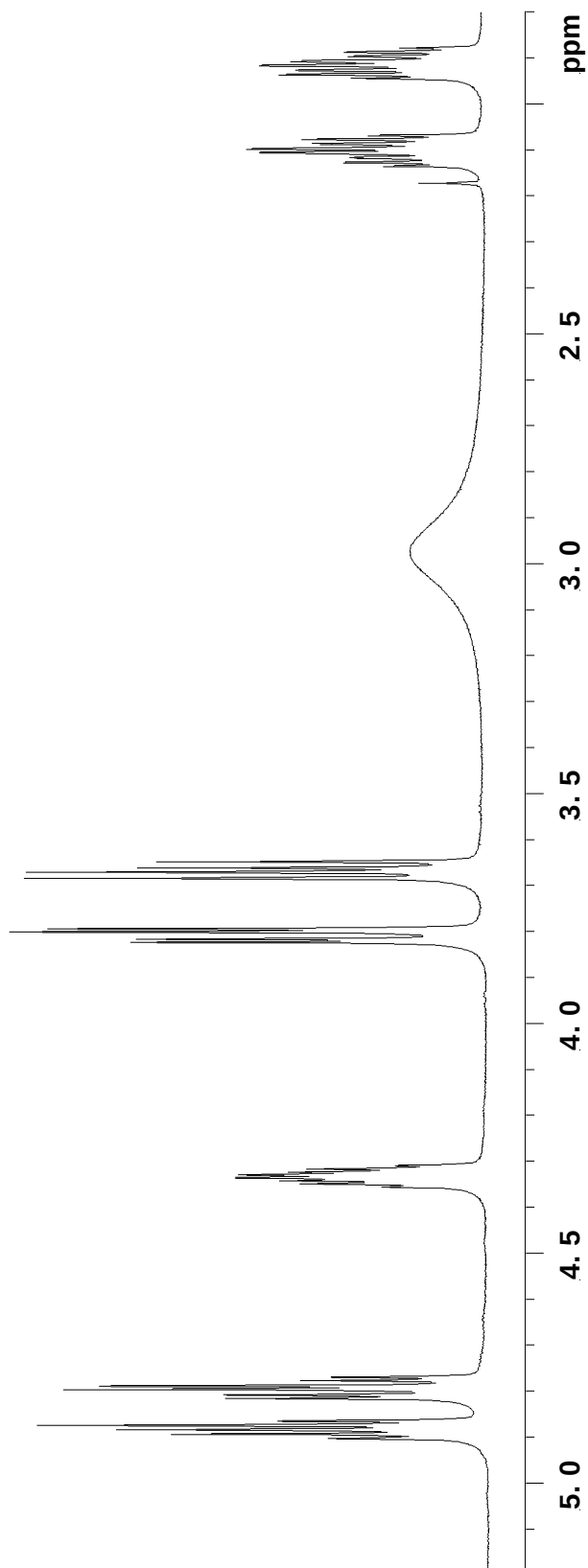
FT size 32768

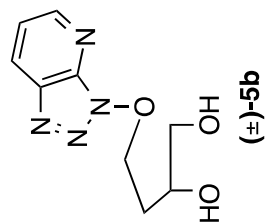
Total time 2 min, 1 sec



(±)-5b

Expanded spectrum





dihydroxybutenol-cl3

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File: mk-1205-1-cl3-CDCl3-62-dihydroxybutenol
INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

2240 repetitions

OBSERVE Cl3, 125.6674263 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

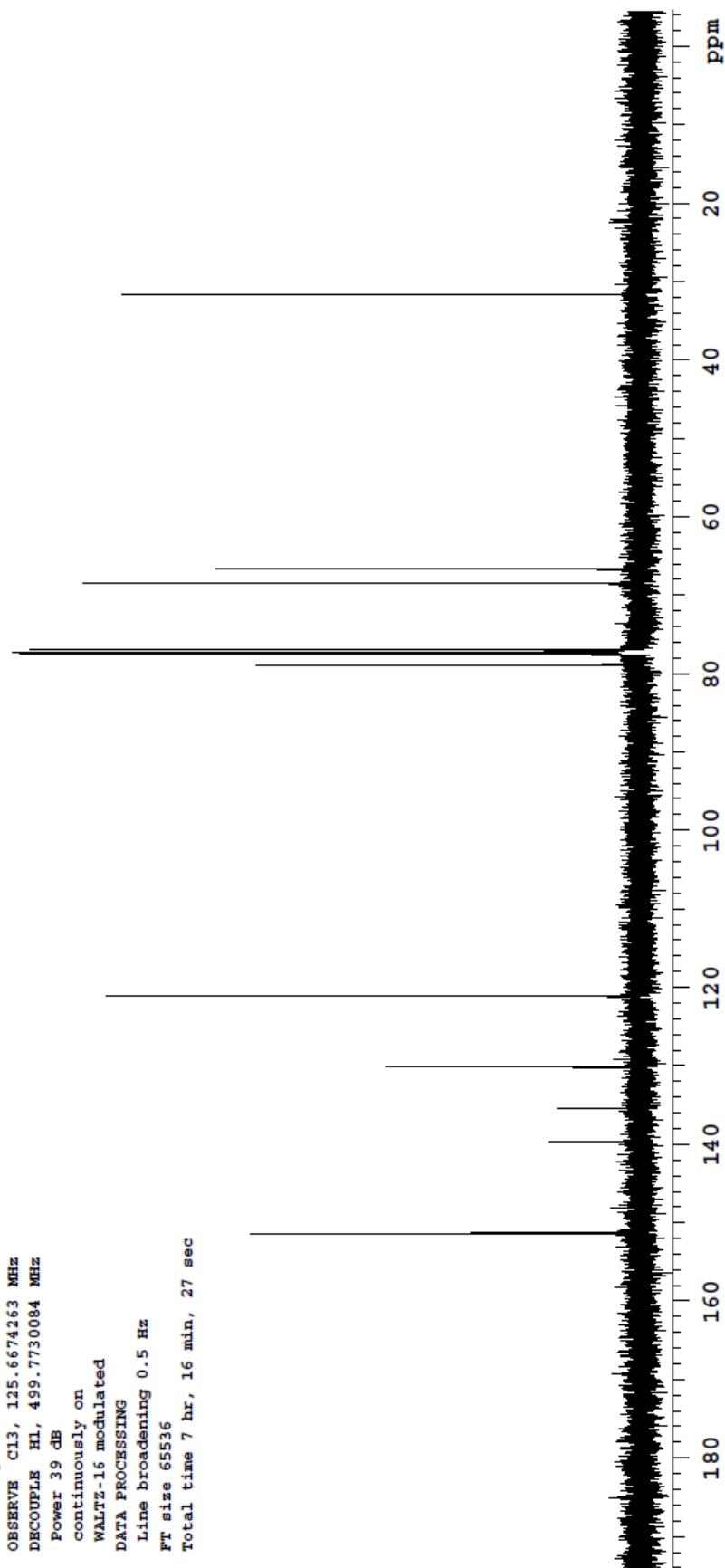
WALTZ-16 modulated

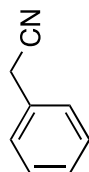
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 7 hr, 16 min, 27 sec





6

REC-1205-III-273-HNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-III-273-HNMR-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

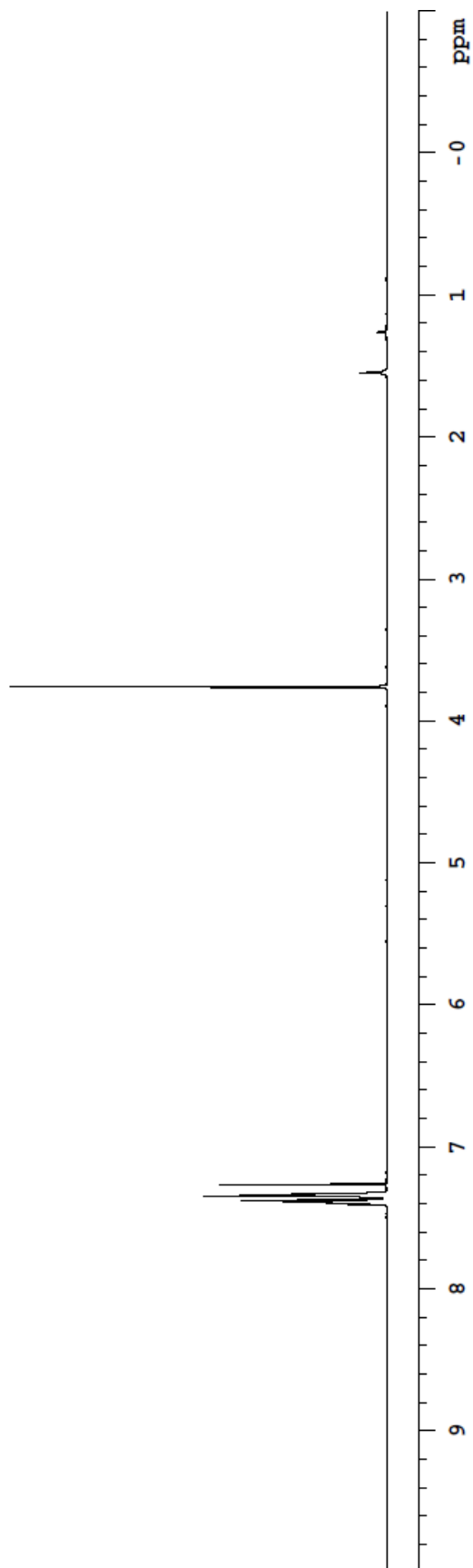
DATA PROCESSING

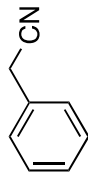
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec





6

RRC-1205-III-273-CNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-III-273-CNMR-CDCl3

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

12150 repetitions

OBSERVE C13, 125.6674191 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

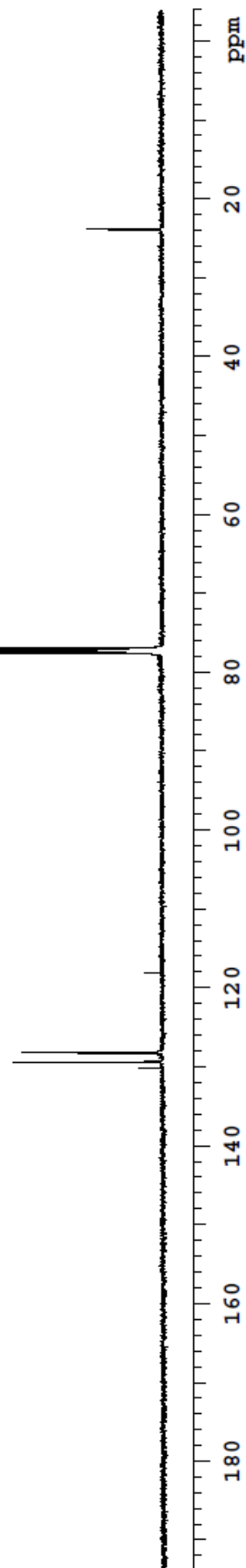
WALTZ-16 modulated

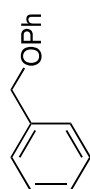
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 23 hr, 56 min, 28 sec





7

REC-1205-III-272-HNMR-CDCl3-topspot

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-III-272-HNMR-CDCl3-topspot

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

32 repetitions

OBSERVE HL, 499.7707212 MHz

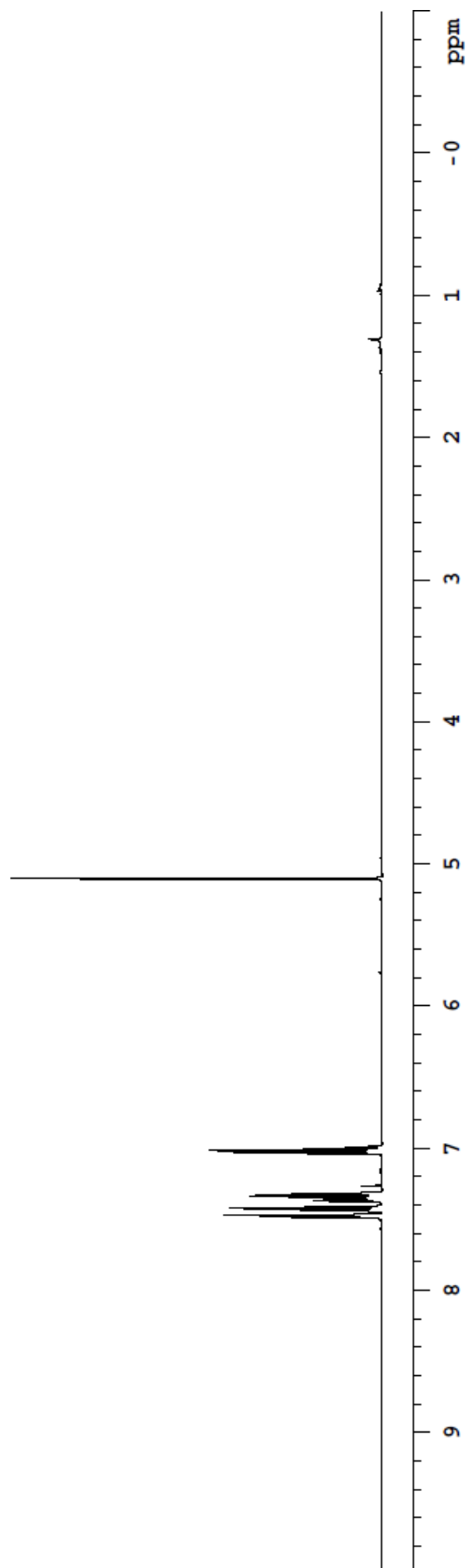
DATA PROCESSING

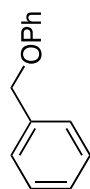
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

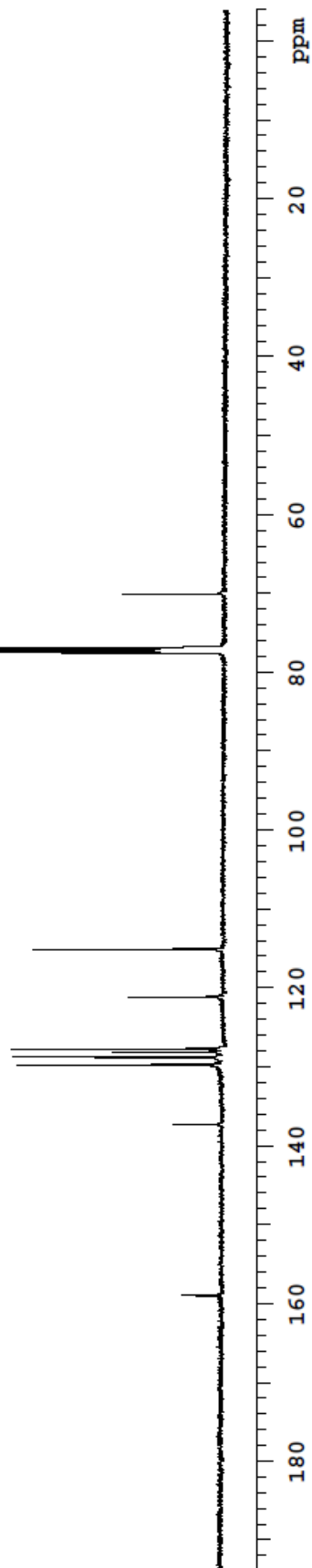
Total time 7 min, 21 sec

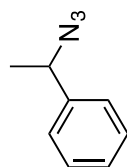




7

REC-1205-III-272-CNMR-CDCl3
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: Raghu
File: REC-1205-III-272-CNMR-CDCl3
INOVA-500 "riga"
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30499.4 Hz
12570 repetitions
OBSERVE C13, 125.6674212 MHz
DECOUPLE H1, 499.7730084 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
Ft size 131072
Total time 23 hr, 56 min, 27 sec





8

REC-1205-III-252-HNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-III-252-HNMR-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

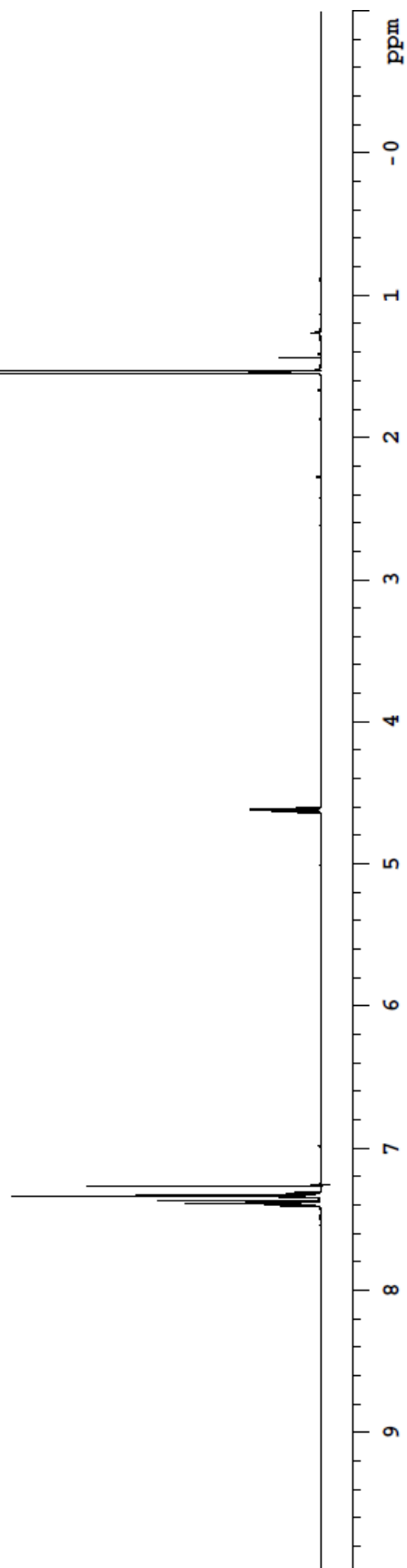
DATA PROCESSING

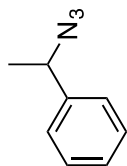
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec





8

REC-1205-III-252-CNMN-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-III-252-CNMN-CDCl3

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

12220 repetitions

OBSERVE C13, 125.6674186 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

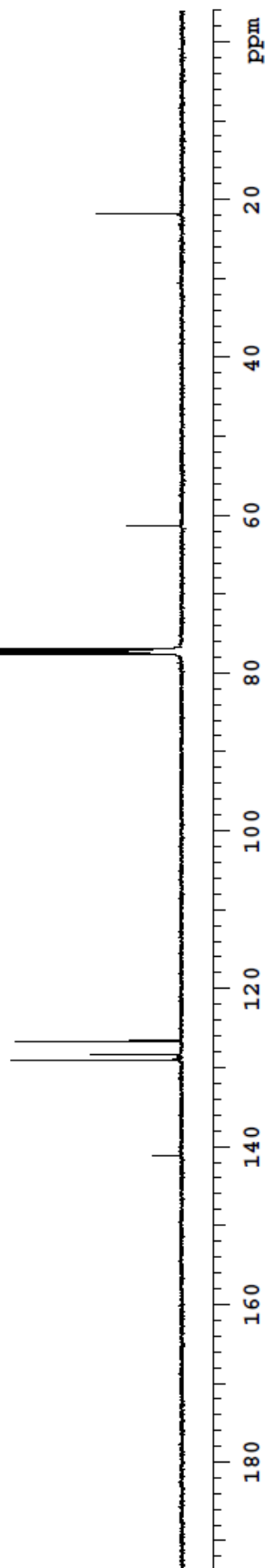
WALTZ-16 modulated

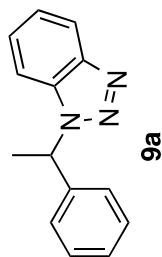
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 29 hr, 55 min, 35 sec





REC-1205-III-thirdspot-HNMR-CDCl3-Bt

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-III-256-HNMR-CDCl3-thirdspot

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

32 repetitions

OBSERVE H1, 499.7707212 MHz

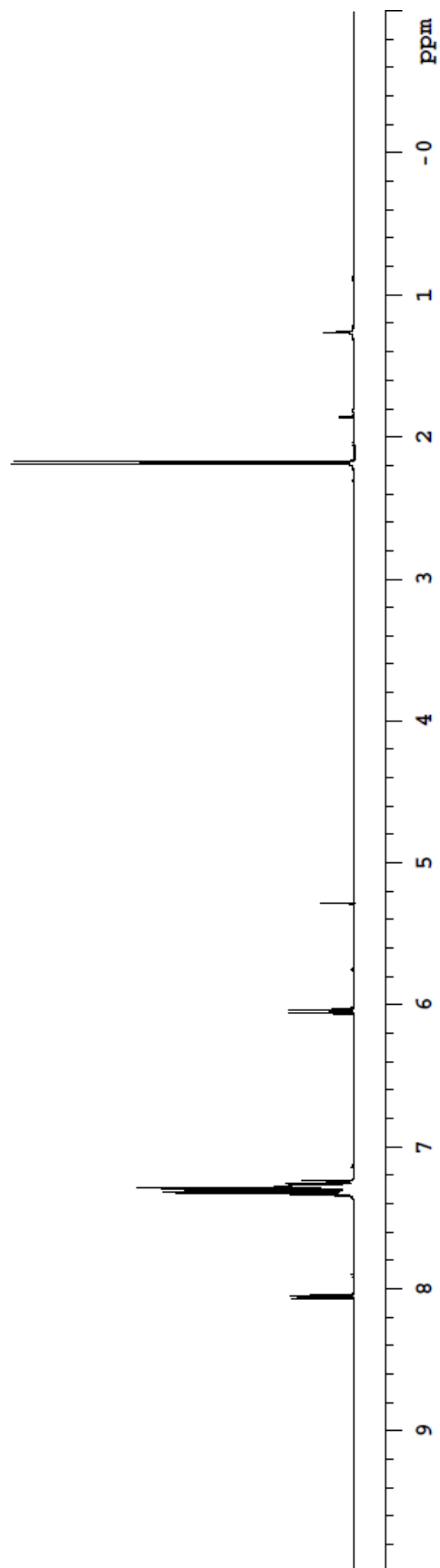
DATA PROCESSING

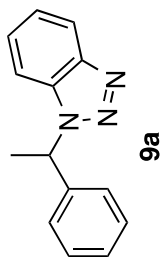
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 3 min, 40 sec





REC-1205-III-256-CNMR-CDCl3-thirdspot

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-III-256-CNMR-CDCl3-thirdspot

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

13760 repetitions

OBSERVE C13, 125.6674283 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

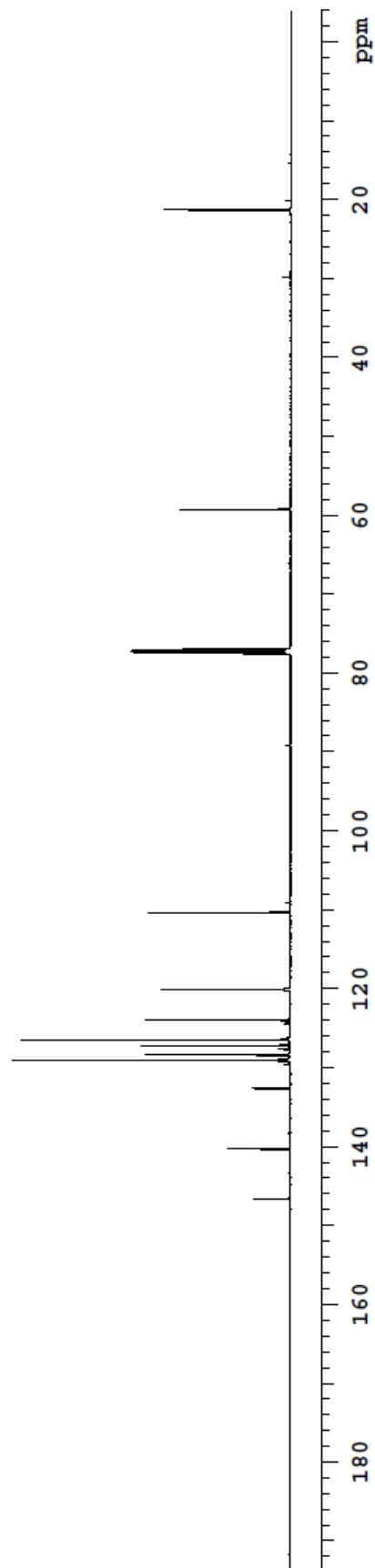
WALTZ-16 modulated

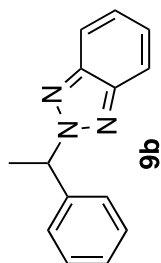
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 29 hr, 55 min, 35 sec





REC-1205-III-firstspot-HNMR-CDCl3-Bt

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-III-256-HNMR-CDCl3-firstspot

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

32 repetitions

OBSERVE H1, 499.7707212 MHz

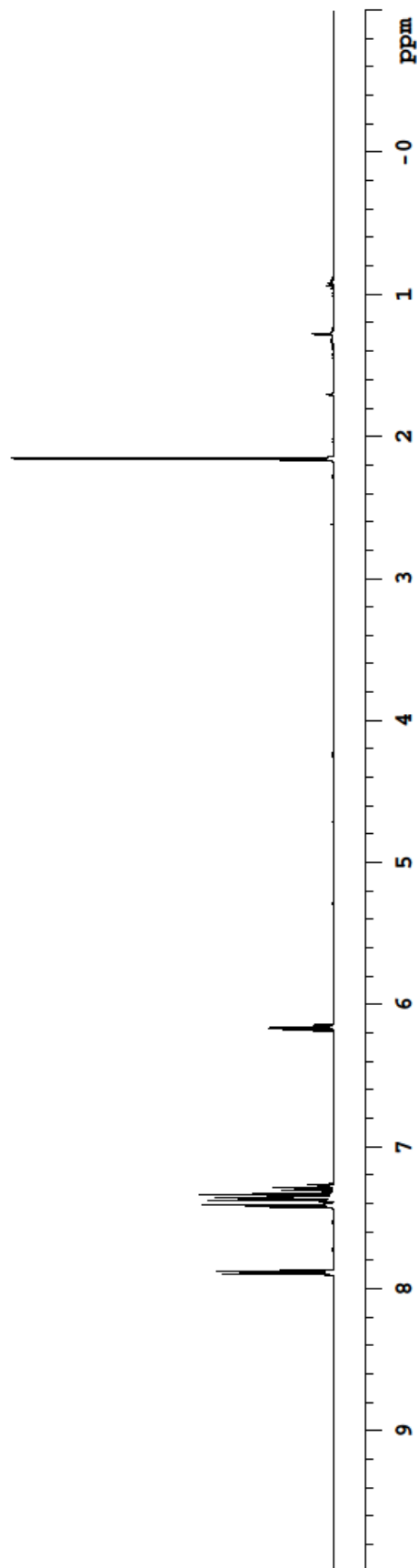
DATA PROCESSING

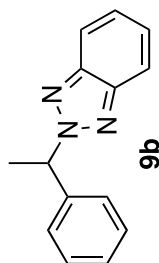
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 3 min, 40 sec





RRC-1205-III-256-CNMR-CDCl3-firstspot

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-III-256-CNMR-CDCl3-firstspot

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

12700 repetitions

OBSERVE C13, 125.6674246 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

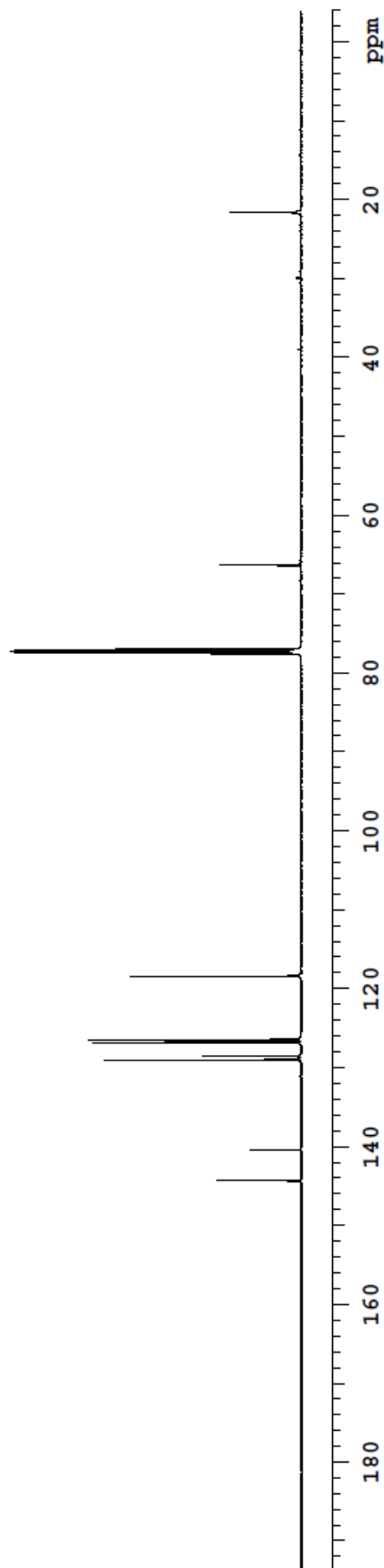
WALTZ-16 modulated

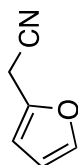
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 29 hr, 55 min, 35 sec





10

1205-Vijay-03-54-1H-Pure-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

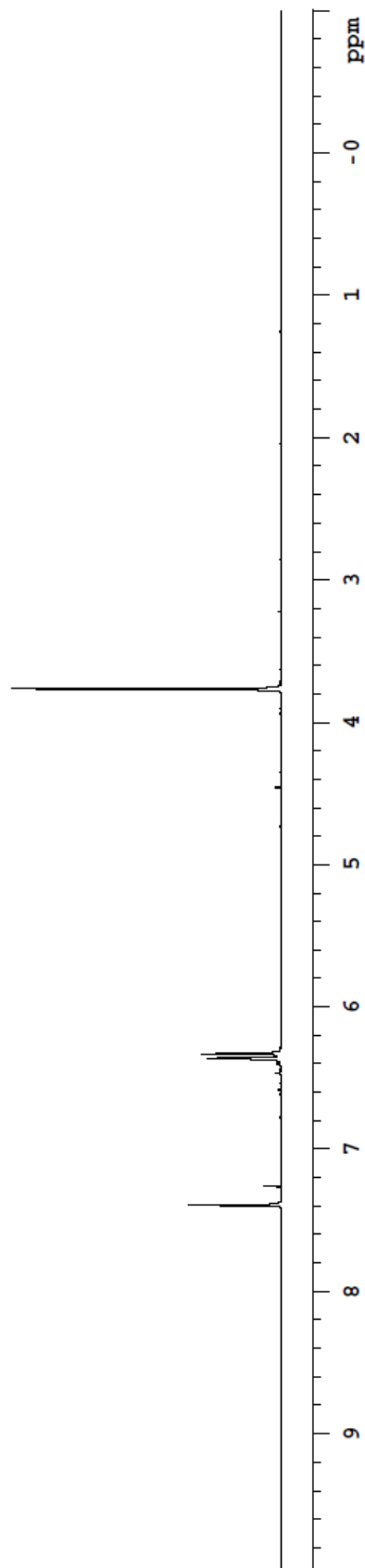
8 repetitions

OBSERVE H1, 499.7707207 MHz

DATA PROCESSING

FT size 32768

Total time 3 min, 40 sec



1205-Vijay-03-44-13C-CDCl3

Pulse Sequence: *s2pul*

Solvent: CDCl3

Ambient temperature

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

200 repetitions

OBSERVE C13, 125.6674149 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

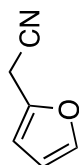
WALTZ-16 modulated

DATA PROCESSING

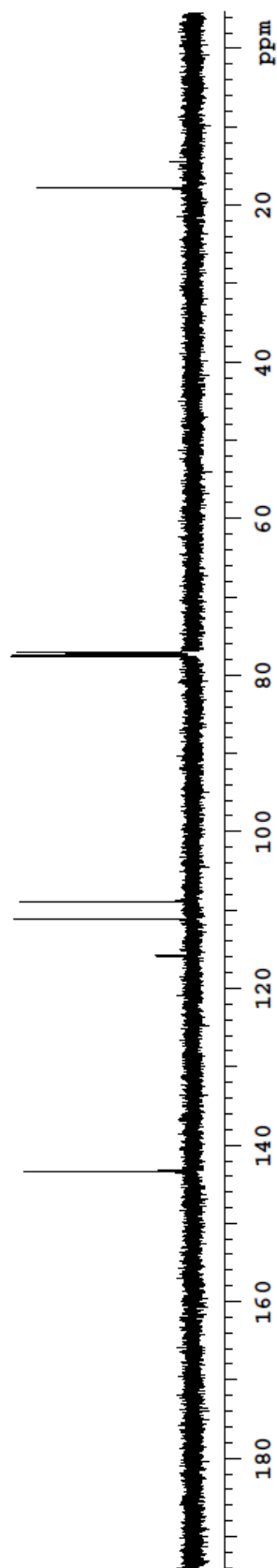
Line broadening 0.5 Hz

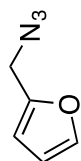
FT size 131072

Total time 55 min, 9 sec



10





Pure standard

1205-Vijay-furfurylazide-1H-DMSO-D6

Pulse Sequence: s2pul

Solvent: dmsc

Temp. 25.0 C / 298.1 K

Operator: mkl

File: 1205-Vijay-2furfurylazide-1H-DMSO-D6

INOVA-500 "riga"

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

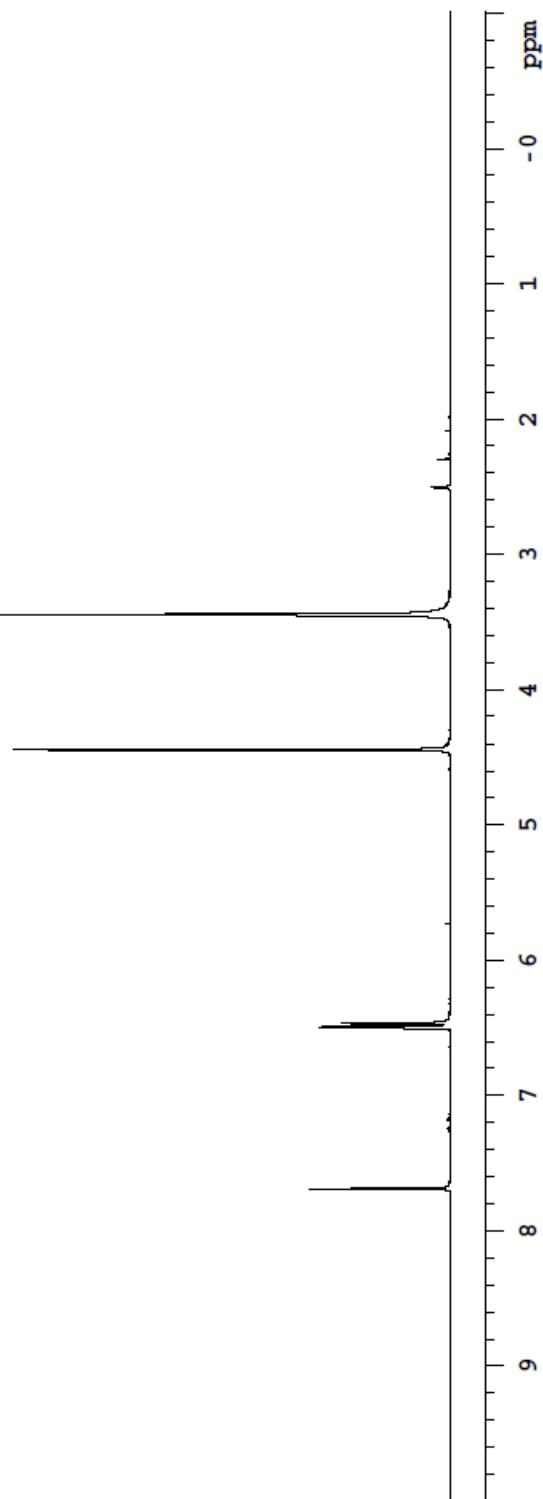
32 repetitions

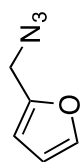
OBSERVE H1, 499.7730834 MHz

DATA PROCESSING

FT size 32768

Total time 1 min, 0 sec





Reaction mixture containing 11

1205-Vijay-03-72-1H-DMSO-D6

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

Operator: mkl

File: 1205-Vijay-03-72-1H-DMSO-D6

INOVA-500 "riga"

Relax. delay 2.000 sec

Pulse 34.7 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

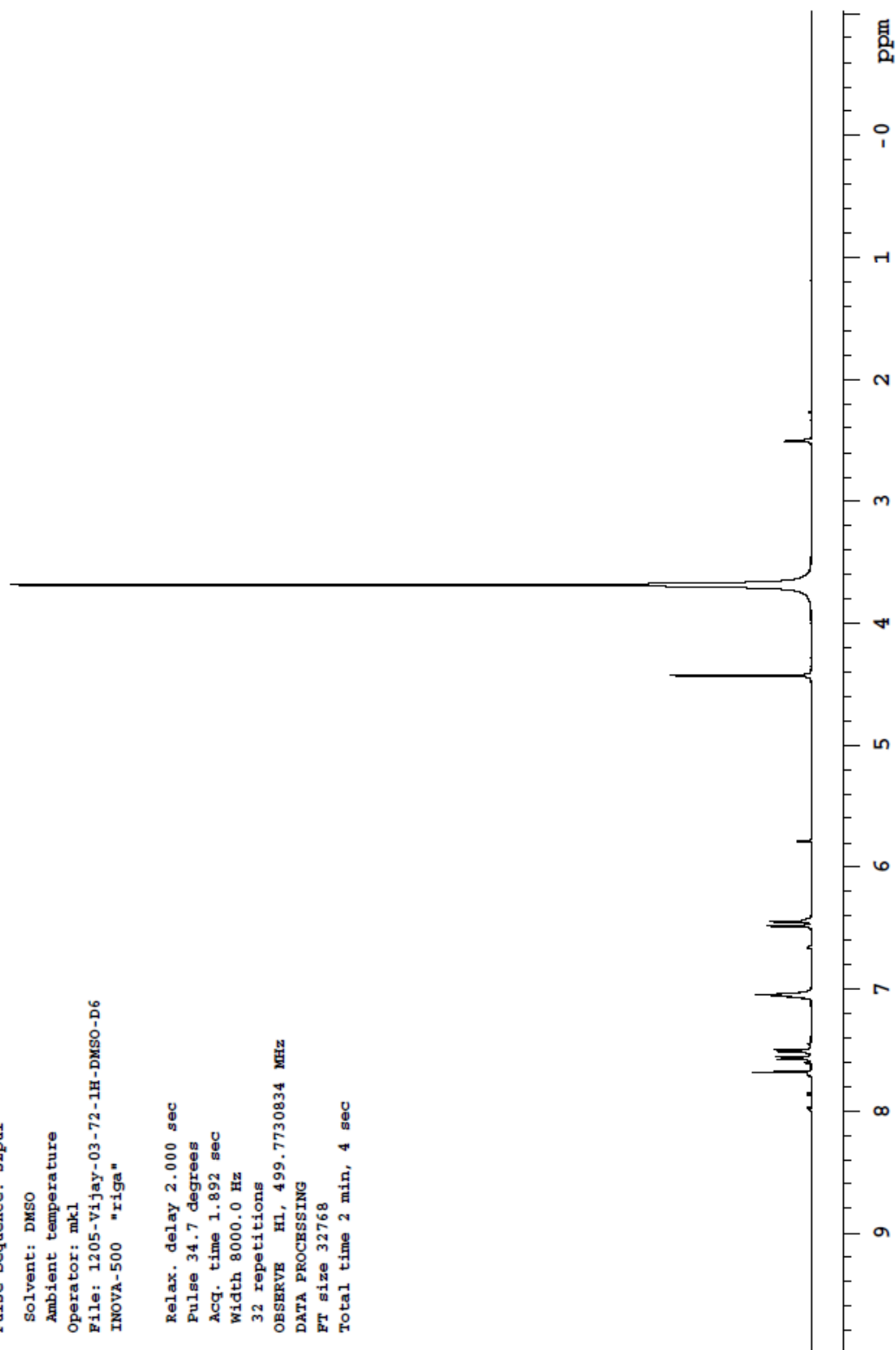
32 repetitions

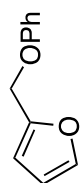
OBSERVE H1, 499.7730834 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 4 sec





12

1205-Vijay-03-40-1H-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

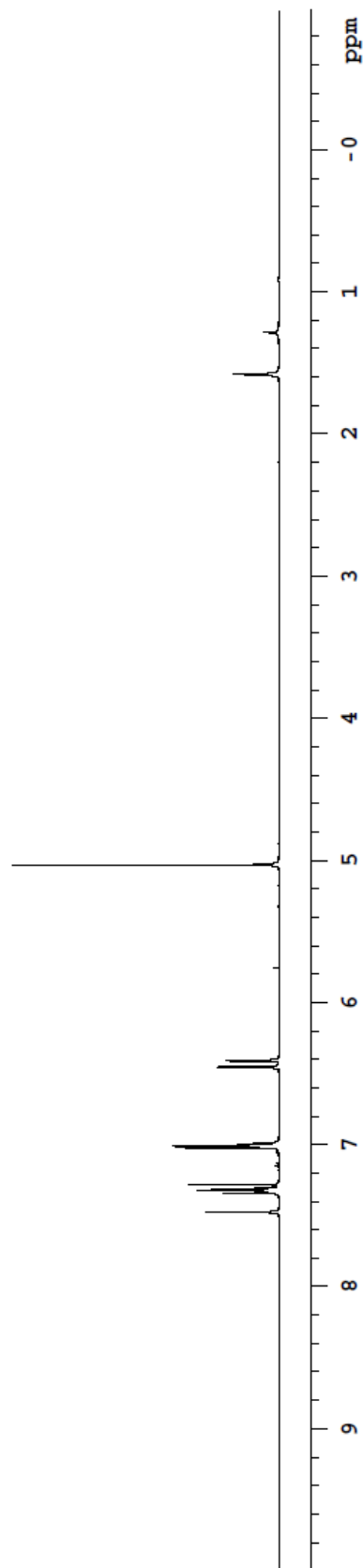
32 repetitions

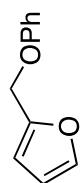
OBSERVE H1, 499.7707095 MHz

DATA PROCESSING

FT size 32768

Total time 3 min, 40 sec





12

1205-Vijay-03-40-13C-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

1200 repetitions

OBSERVE C13, 125.6674149 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

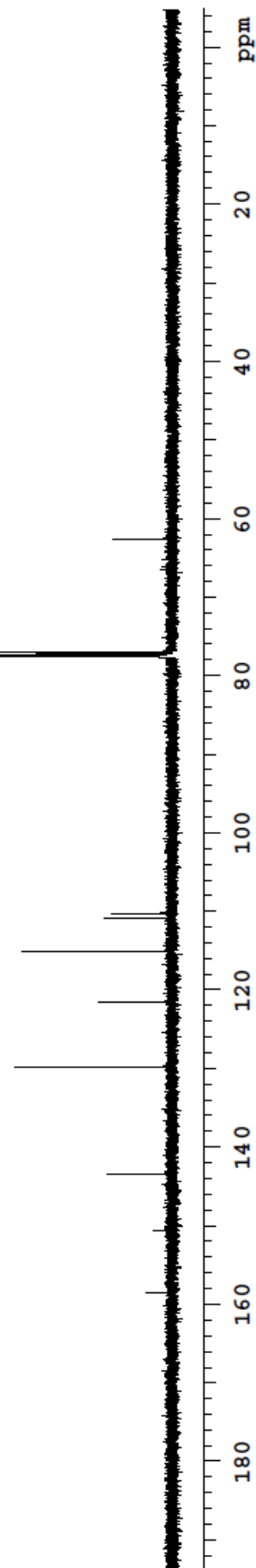
WALTZ-16 modulated

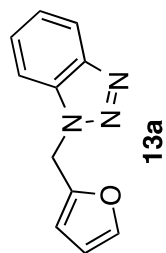
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 1 hr, 6 min, 11 sec





1205-Vijay-03-42-21H-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

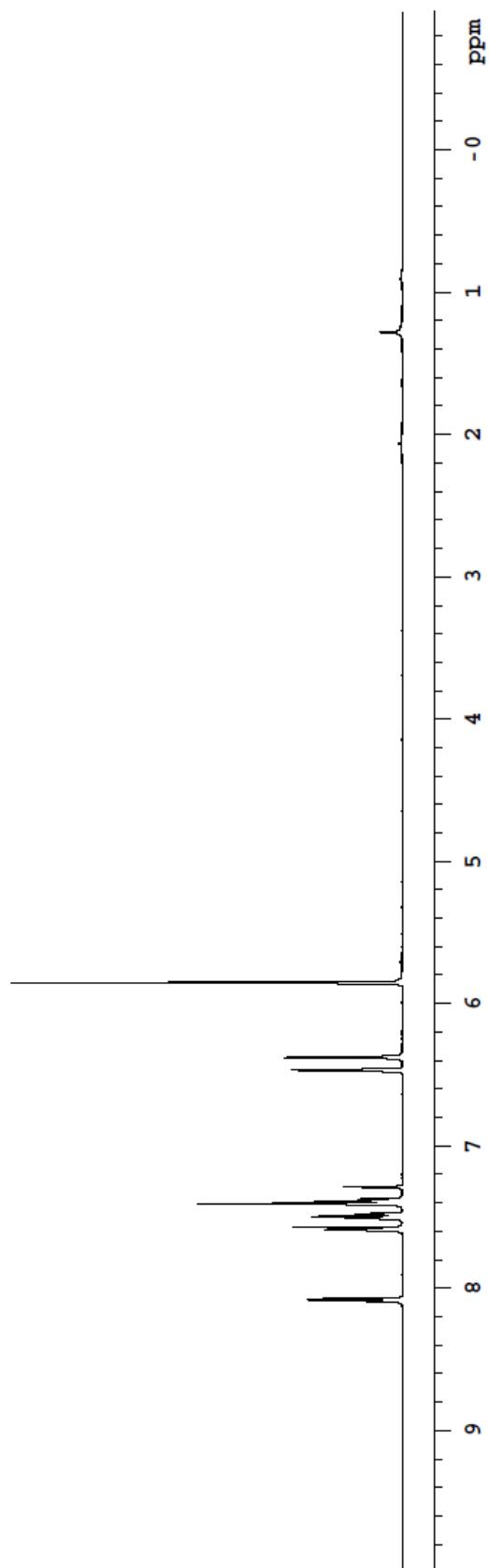
32 repetitions

OBSERVE H1, 499.7707095 MHz

DATA PROCESSING

FT size 32768

Total time 3 min, 40 sec



1205-Vijay-03-68-2-13C-CDCl3

Pulse Sequence: *s2pul*

Solvent: CDCl3

Ambient temperature

Operator: mkl

File:

INOVA-500 "riga"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

316 repetitions

OBSERVE C13, 125.6674309 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

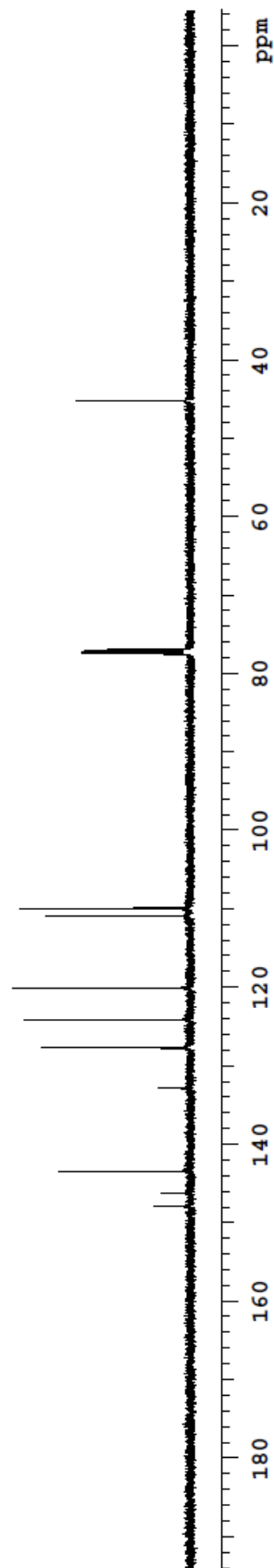
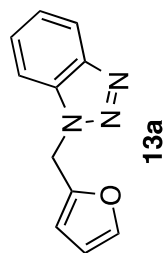
WALTZ-16 modulated

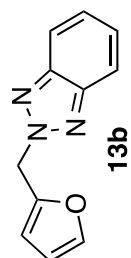
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 2 hr, 45 min, 28 sec





1205-Vijay-03-68-1-1H-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: 1205-Vijay-03-68-1-1H-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

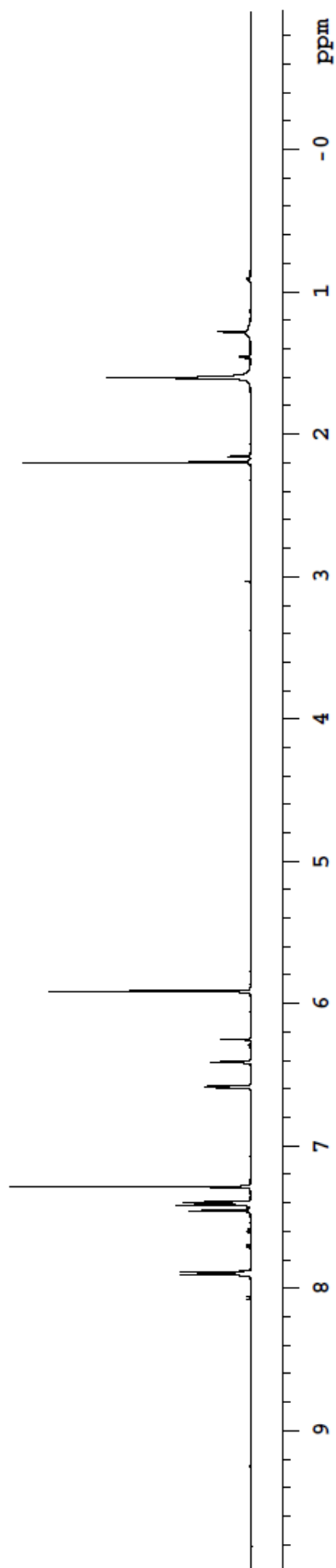
32 repetitions

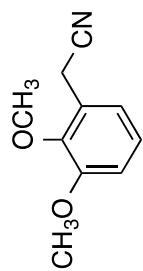
OBSERVE HL, 499.7707095 MHz

DATA PROCESSING

FT size 32768

Total time 14 min, 43 sec





MKS-1205-11-74-CDCl3-2ndCC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-11-74-CDCl3-2ndCC

INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

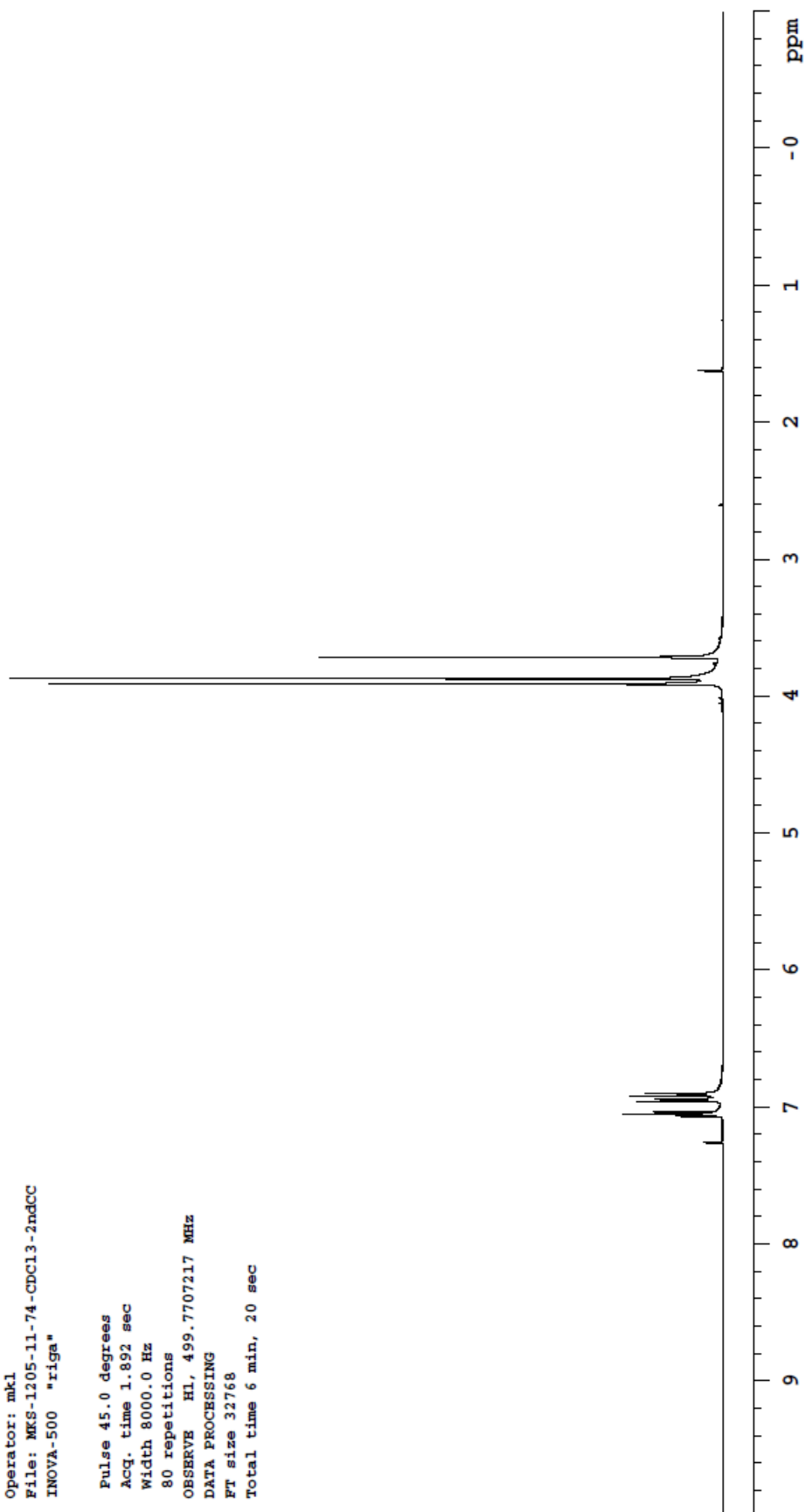
80 repetitions

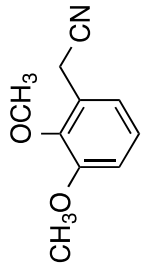
OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 20 sec





14

MKS-1205-11-74-CDCl3-13C-CC

Pulse Sequence: *s2pul*

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-11-74-CDCl3-13C-CC

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

780 repetitions

OBSERVE C13, 125.6674271 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

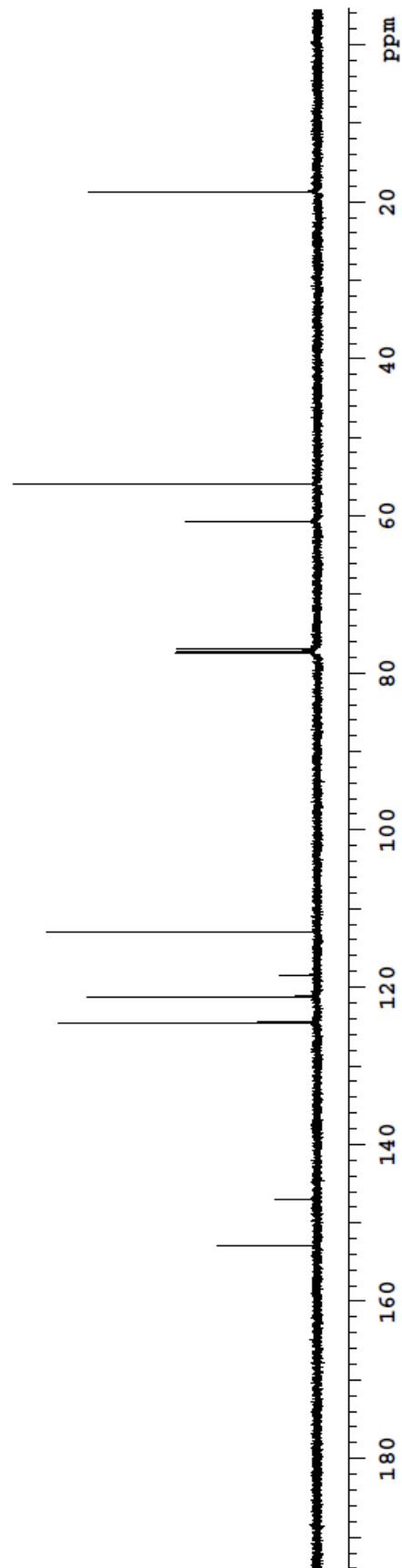
WALTZ-16 modulated

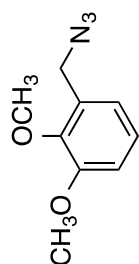
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





15

MKS-1205-12-36-CDCl3-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-36-CDCl3-CC

INOVA-500 "r1ga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

44 repetitions

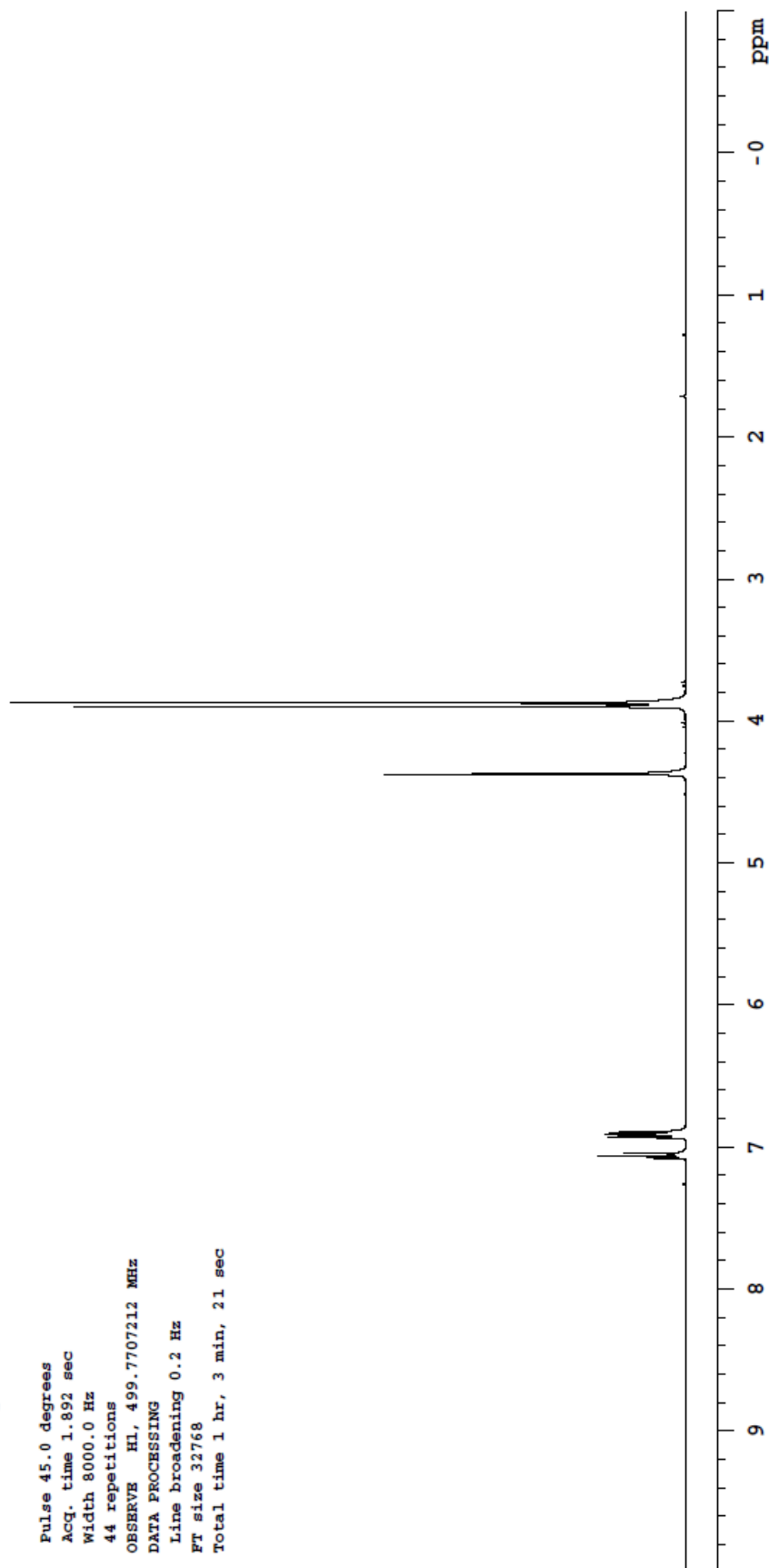
OBSERVE H1, 499.7707212 MHz

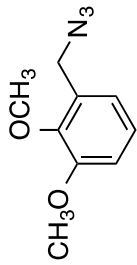
DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 hr, 3 min, 21 sec





15

MKS-1205-12-36-13C-CDCl3-CC

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-36-13C-CDCl3-CC

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

268 repetitions

OBSERVE C13, 125.6674360 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

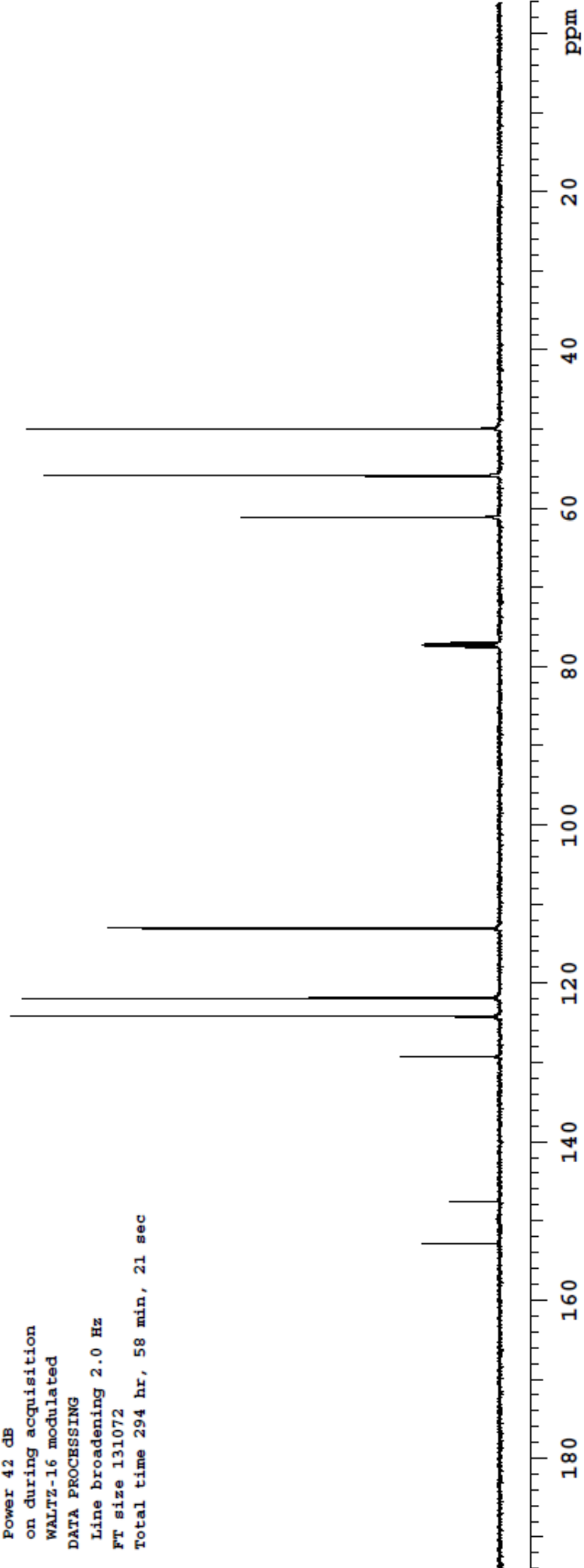
WALTZ-16 modulated

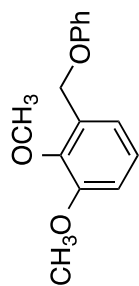
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 294 hr, 58 min, 21 sec





16

MKS-1205-12-32-CDCl3-1stFrac-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-32-CDCl3-1stFrac-CC

INOVA-500 "r1ga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

60 repetitions

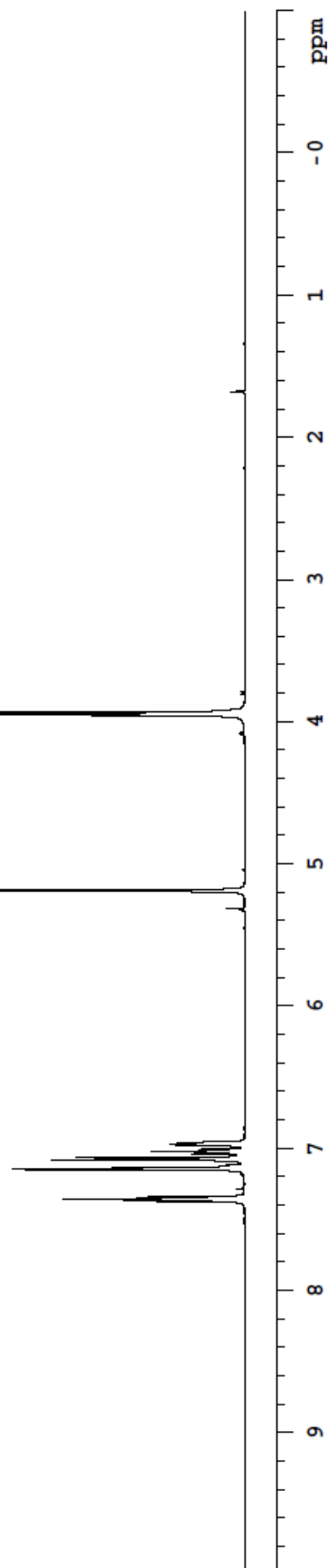
OBSERVE H1, 499.7707095 MHz

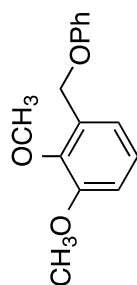
DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 hr, 3 min, 21 sec





16

MKS-1205-12-32-CDCl3-13C-1st-Frac-CC

Pulse Sequence: *s2pul*

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-32-CDCl3-13C-1st-Frac-CC

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

560 repetitions

OBSERVE C13, 125.6674324 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

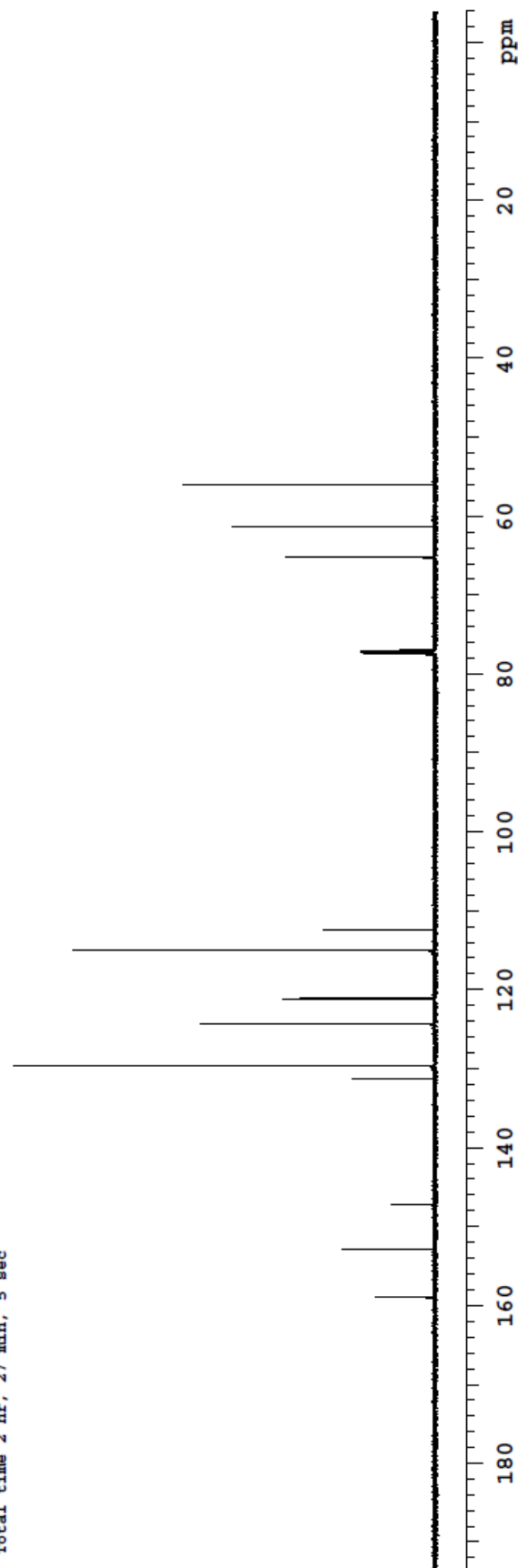
WALTZ-16 modulated

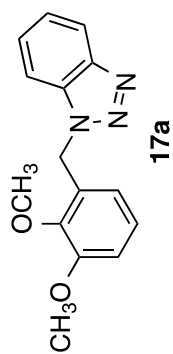
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





MKS-1205-12-30-CDCl3-2ndFrac-CC-Repeat

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 24.0 C / 297.1 K

Operator: mkl

File: MKS-1205-12-30-CDCl3-2ndFrac-CC-Repeat
INOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

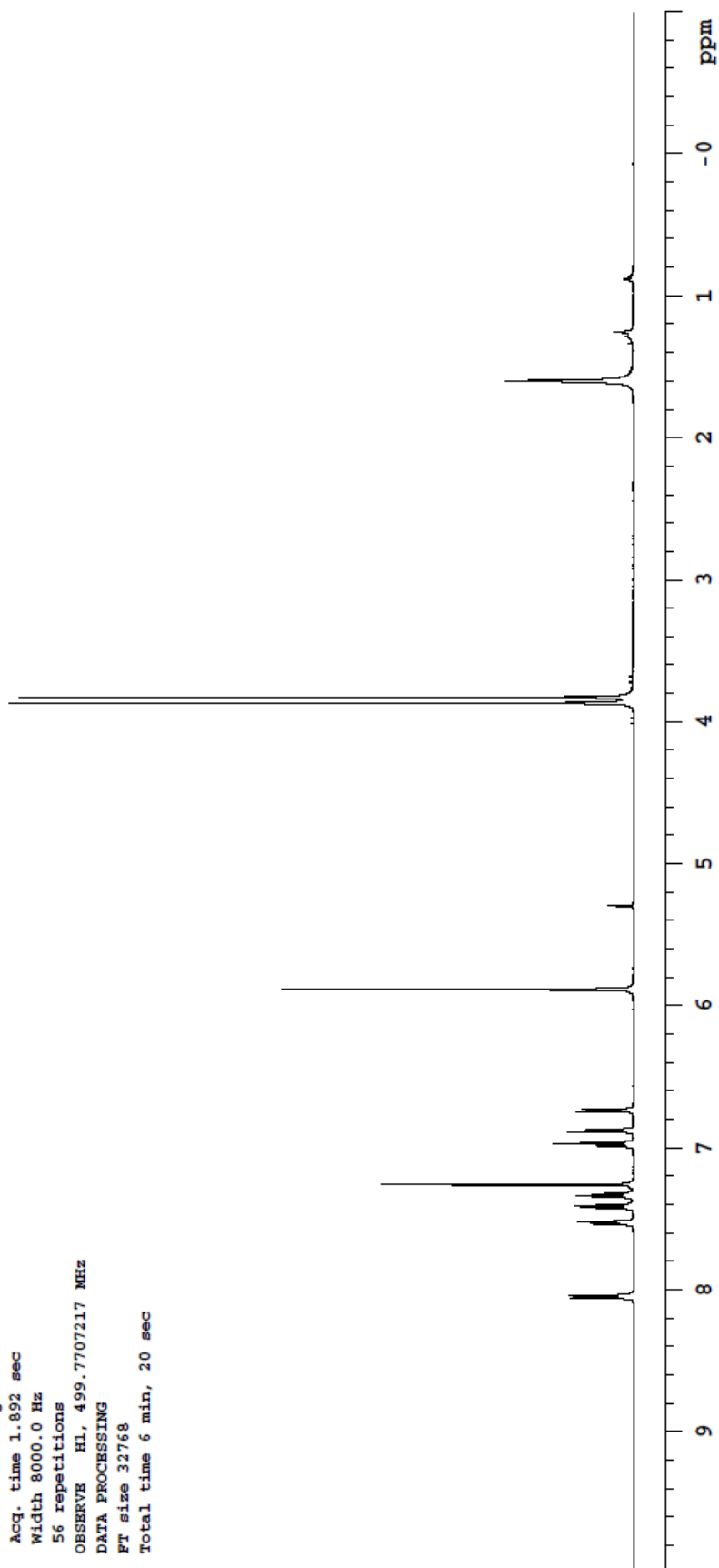
56 repetitions

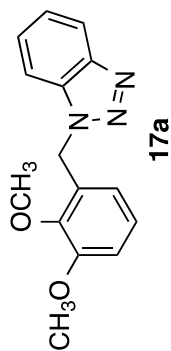
OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 20 sec





MKS-1205-12-30-CDC13-13C-2nd-Frac-CC-repeat

Pulse Sequence: s2pul

Solvent: CDC13

Temp. 24.0 C / 297.1 K

Operator: mkl

File: MKS-1205-12-30-CDC13-13C-2nd-Frac-CC-repeat
INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

2048 repetitions

OBSERVE C13, 125.6674194 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

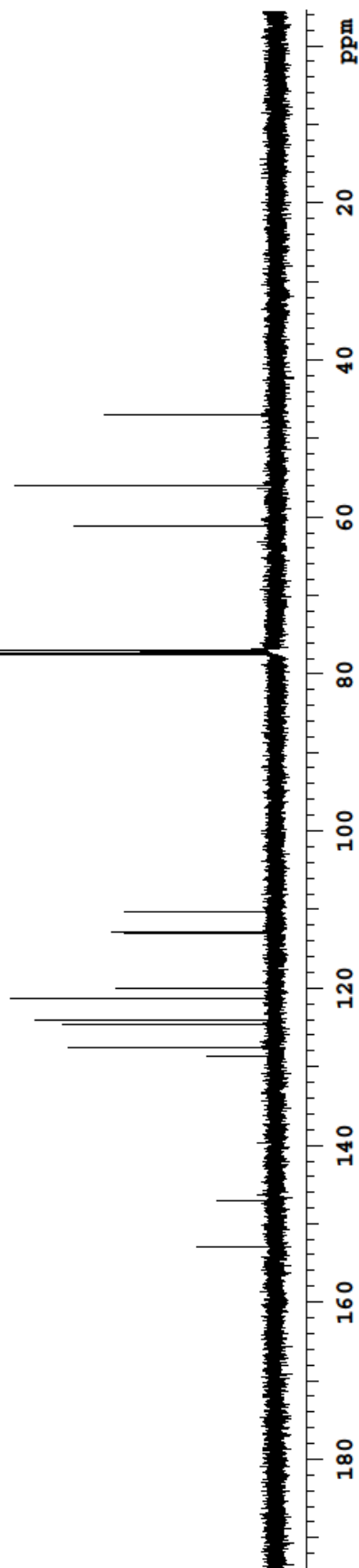
WALTZ-16 modulated

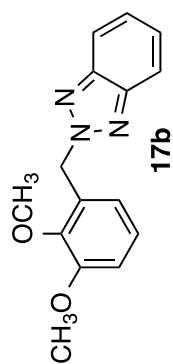
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





MKS-1205-12-30-CDCl3-1stFrac-CC

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-30-CDCl3-1stFrac-CC

INNOVA-500 "riga"

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

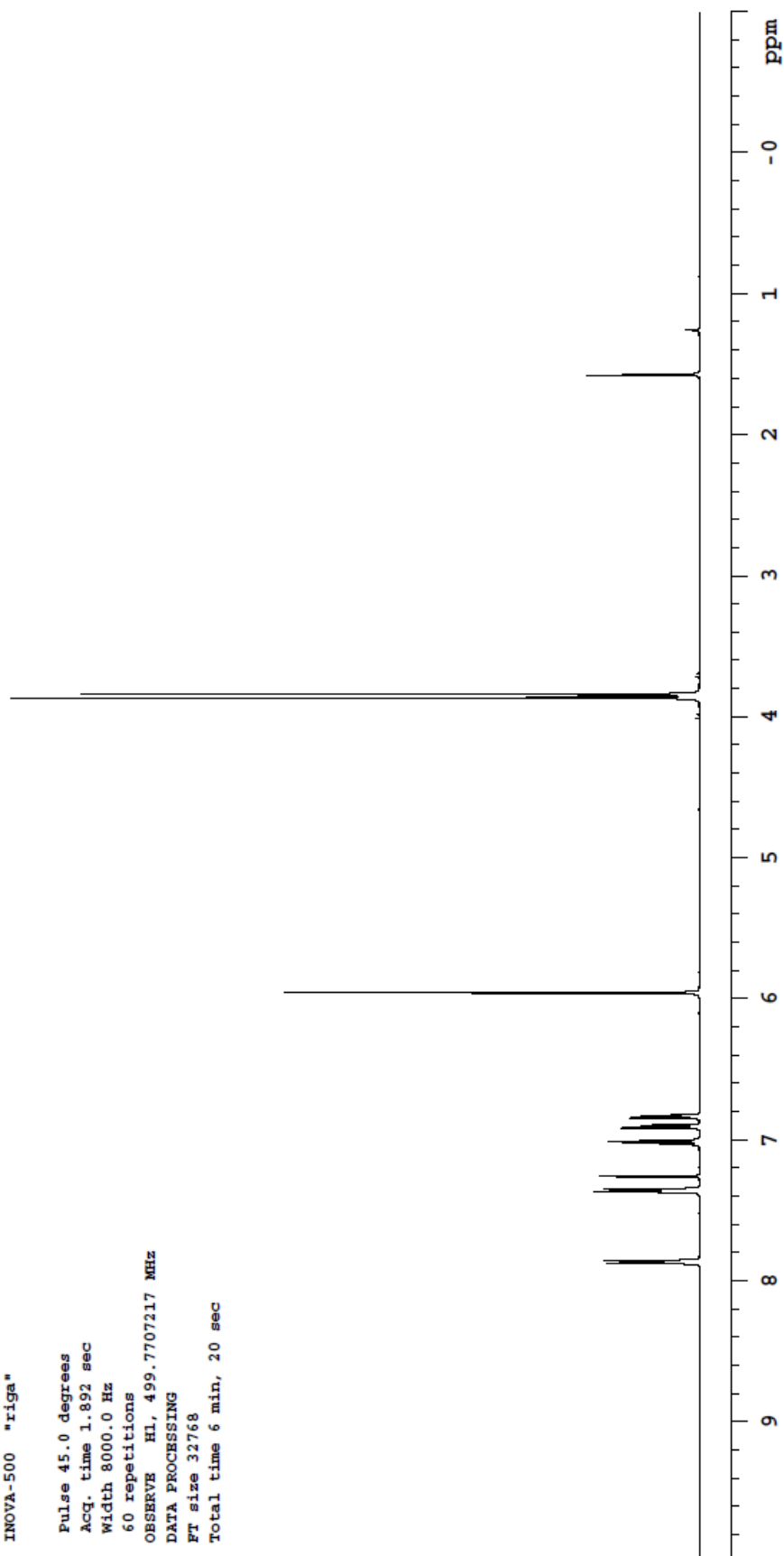
60 repetitions

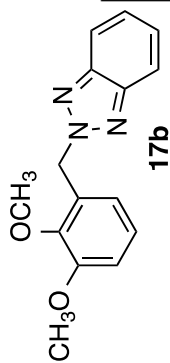
OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 20 sec





MKS-1205-12-30-CDCl3-13C-1st-Frac-CC

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: MKS-1205-12-30-CDCl3-13C-1st-Frac-CC
INOVA-500 "r1ga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

2048 repetitions

OBSERVE C13, 125.6674232 MHz

DECOUPLE H1, 499.7730084 MHz

Power 39 dB

continuously on

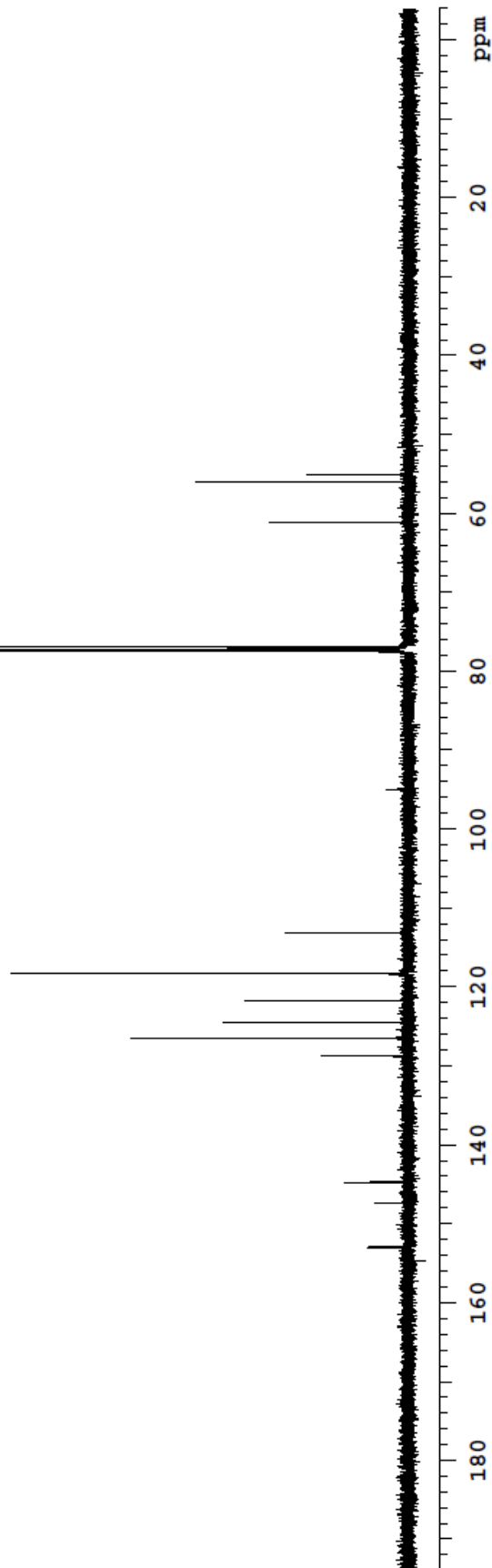
WALTZ-16 modulated

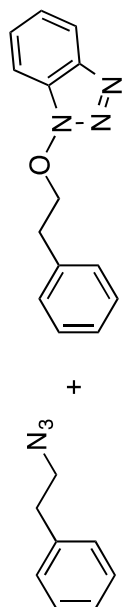
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 hr, 27 min, 5 sec





Ratio = 7.3:1

1205-Vijay-04-25-1H-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: 1205-Vijay-04-25-completedry-1H-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 38.6 degrees

Acq. time 1.892 sec

Width 6002.4 Hz

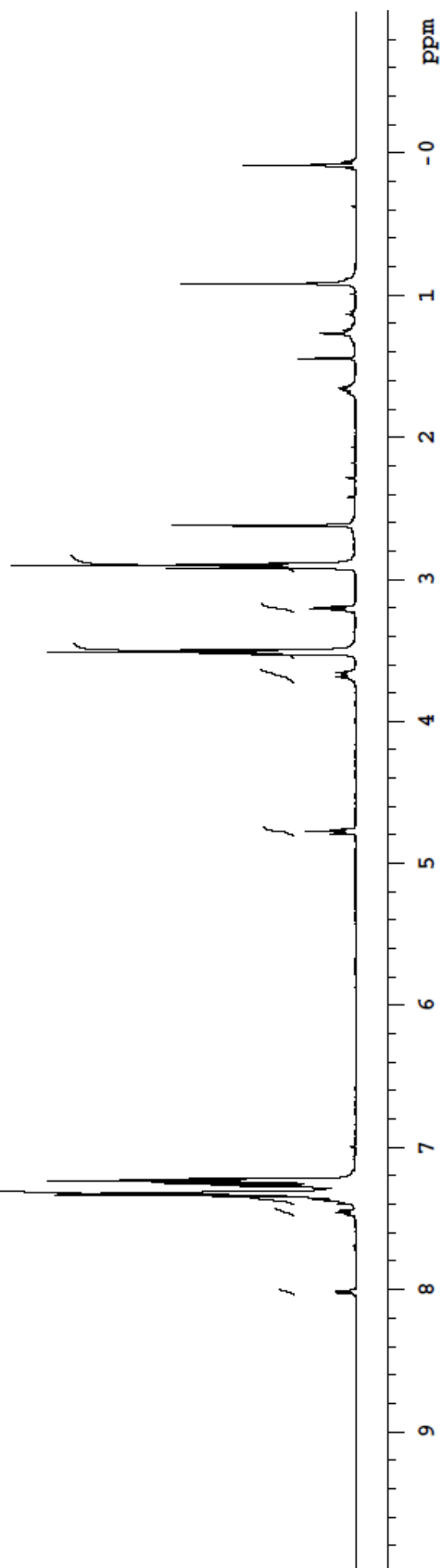
20 repetitions

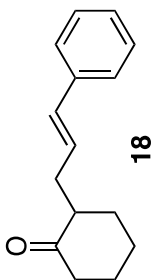
OBSERVE H1, 499.7707215 MHz

DATA PROCESSING

FT size 32768

Total time 3 min, 40 sec





REC-1205-IV-300-HNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-IV-300-HNMR-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE HL, 499.7707212 MHz

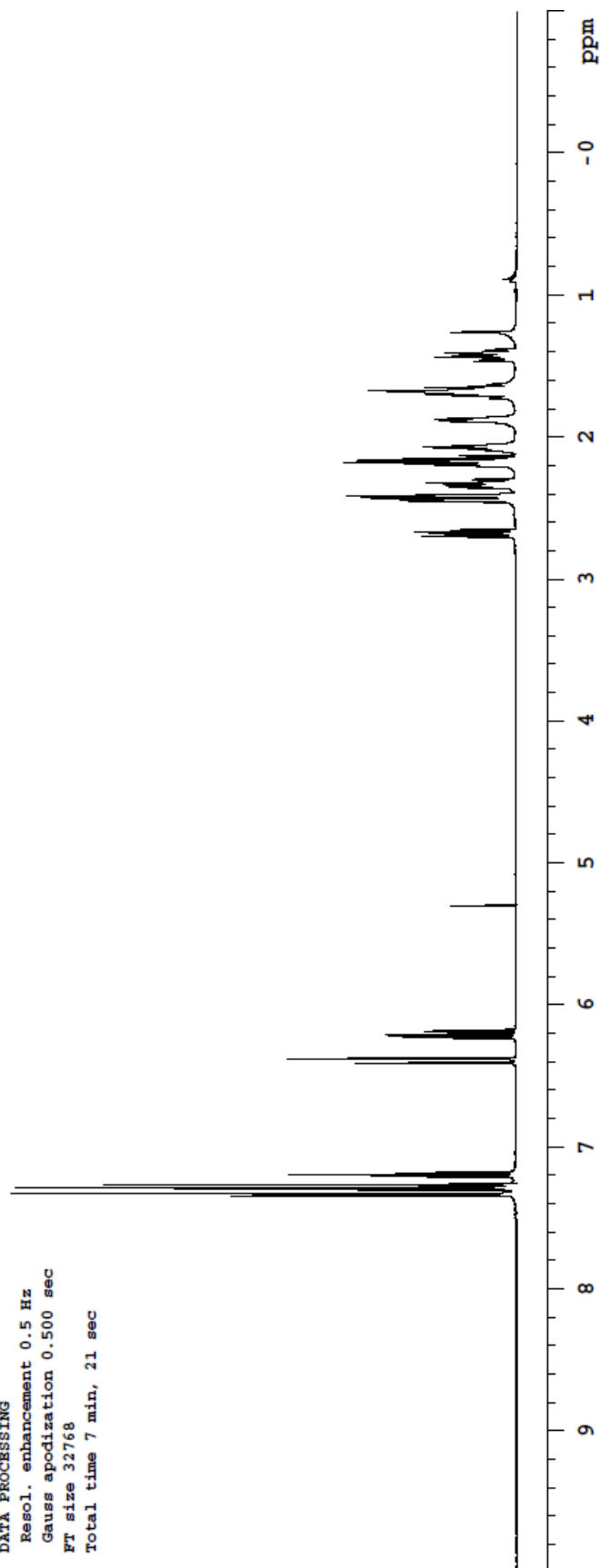
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec



RRC-1205-1V-300-HMR-CDCl₃

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-1V-300-HMR-CDCl₃

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

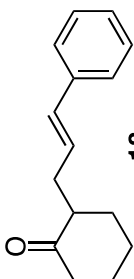
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

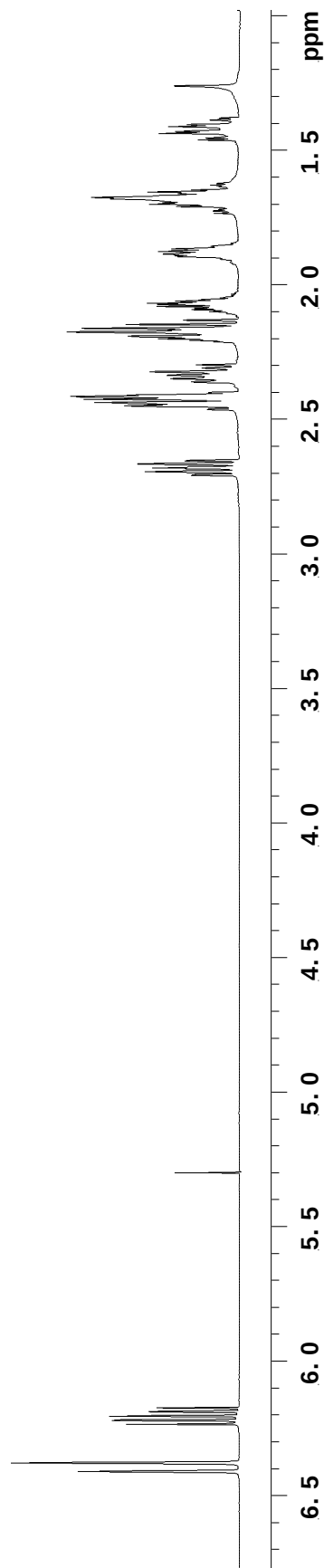
FT size 32768

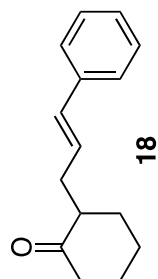
Total time 7 min, 21 sec



18

Expanded spectrum





REC-1205-IV-300-CNMN-CDCl3

Pulse Sequence: *s2pul*

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-IV-300-CNMN-CDCl3

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

12810 repetitions

OBSERVE C13, 125.6674200 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

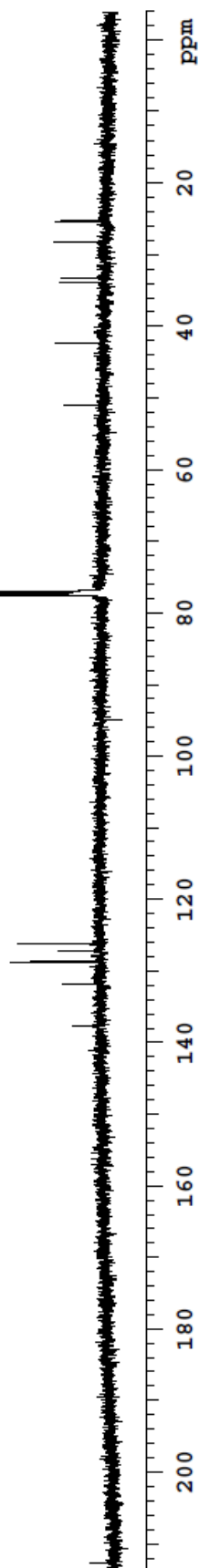
WALTZ-16 modulated

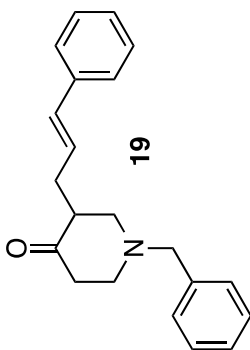
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 23 hr, 56 min, 28 sec





REC-1205-IV-301-HNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-IV-301-HNMR-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

48 repetitions

OBSERVE HL, 499.7707212 MHz

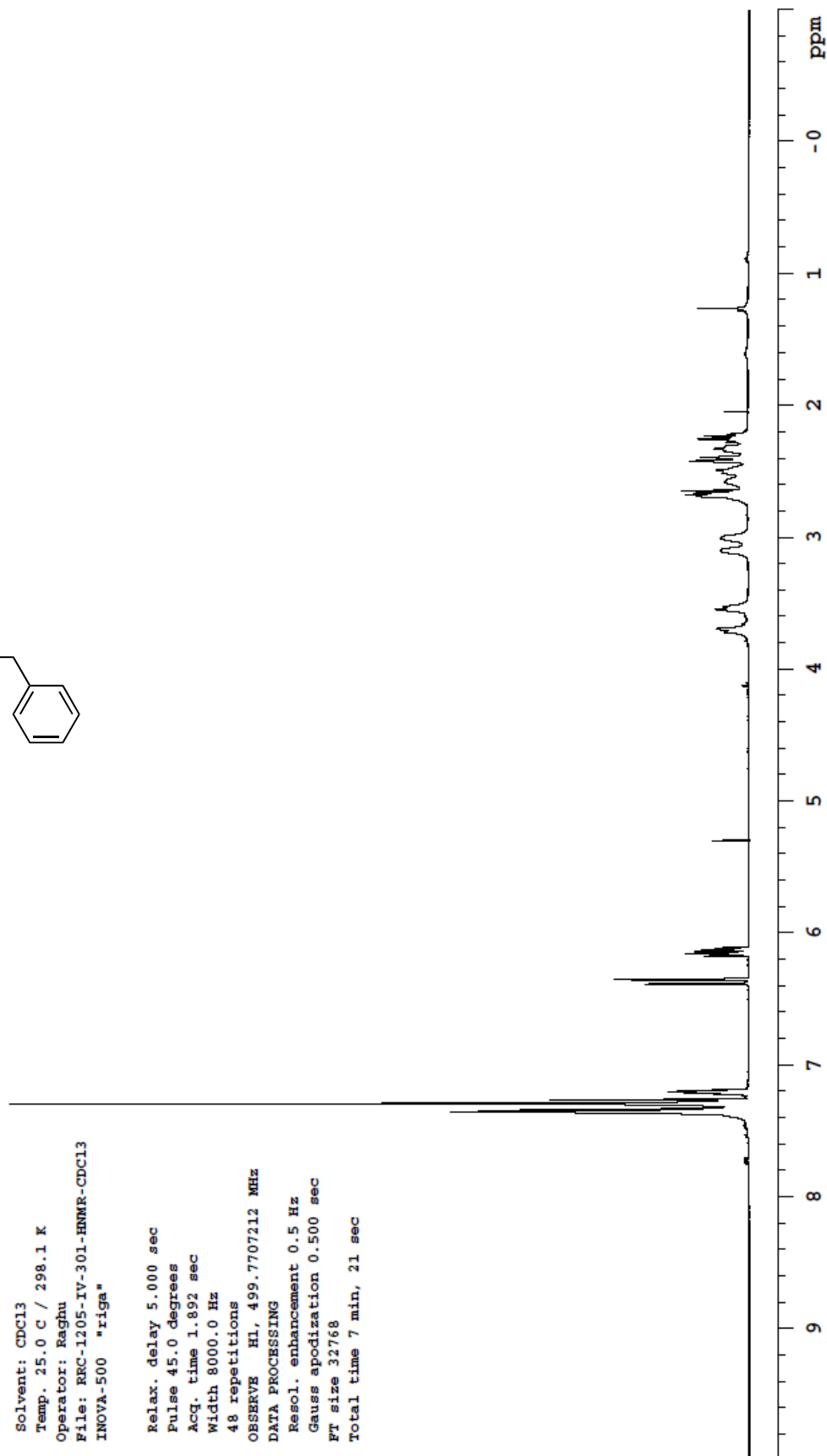
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec



RRC-1205-IV-301-HNMR-CDCl 3

Pul se Sequence: s2pul

Sol vent : CDCl 3

Temp. 25.0 C / 298.1 K

Operator : Raghu

File: RRC-1205-IV-301-HNMR-CDCl 3

NOVA-500 "riga"

Rel ax. delay 5.000 sec

Pul se 45.0 degrees

Acq. time 1.892 sec

Wdth 8000.0 Hz

48 repetitions

OBSERVE H1, 499.7707212 MHz

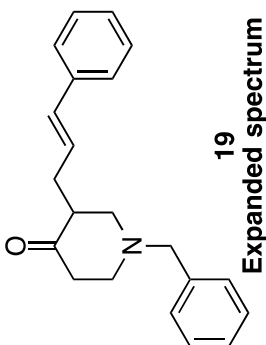
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

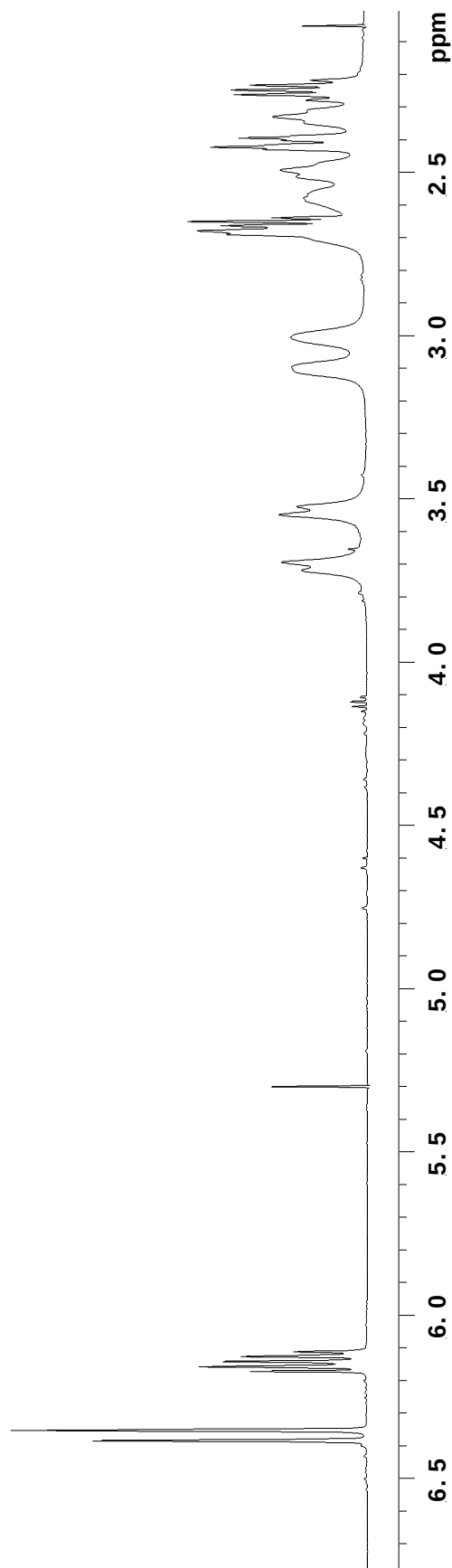
FT size 32768

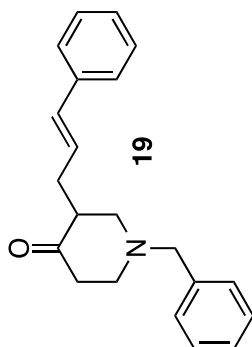
Total time 7 min, 21 sec



19

Expanded spectrum





REC-1205-IV-301-CNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-IV-301-CNMR-CDCl3

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

12700 repetitions

OBSERVE C13, 125.6674214 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

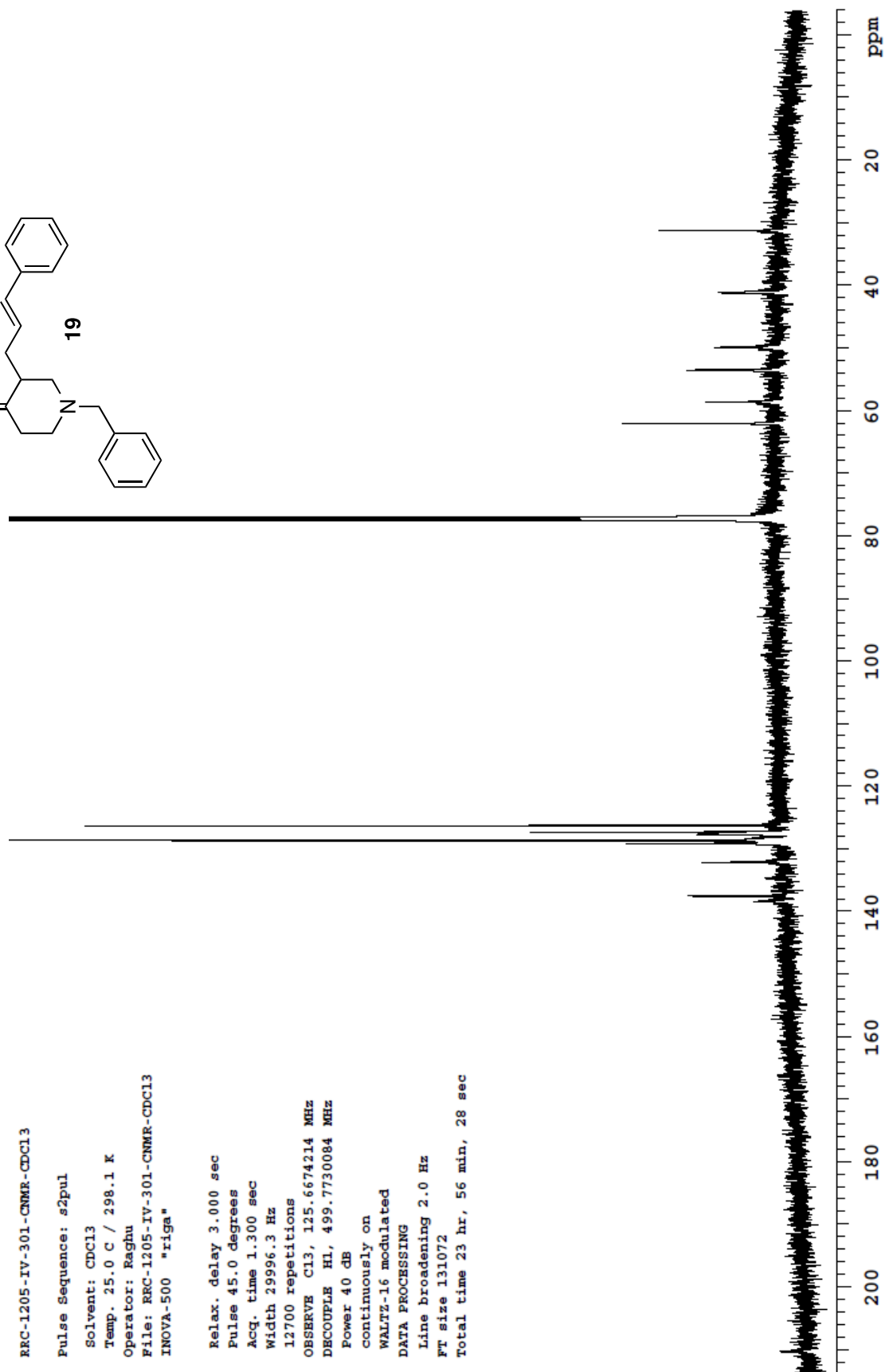
WALTZ-16 modulated

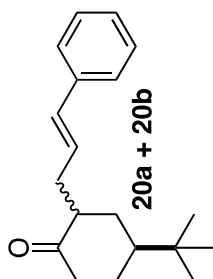
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 23 hr, 56 min, 28 sec





REC-1205-IV-298-HNMR-CDCl3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: REC-1205-IV-298-HNMR-CDCl3

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

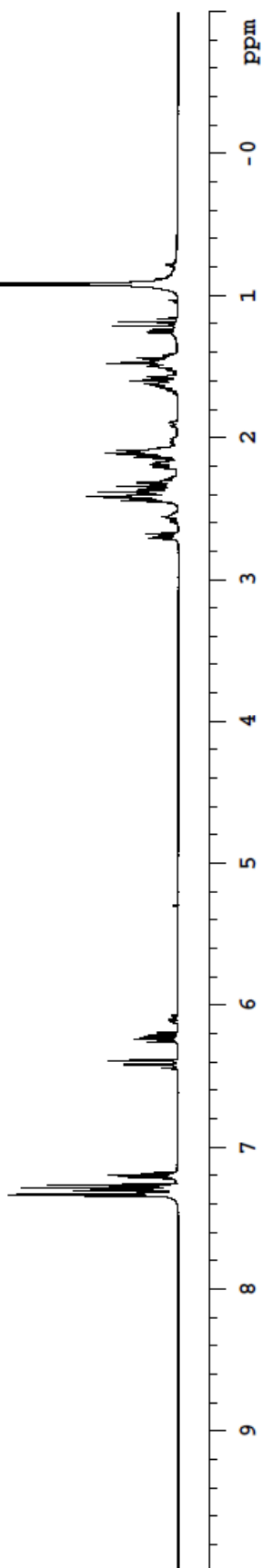
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec



RRC-1205-1V-298-¹H-NMR-CDCl₃

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 °C / 298.1 K

Operator: Raghu

File: RRC-1205-1V-298-¹H-NMR-CDCl₃

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

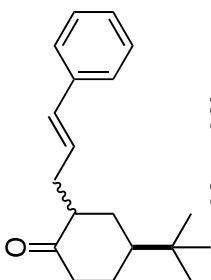
DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

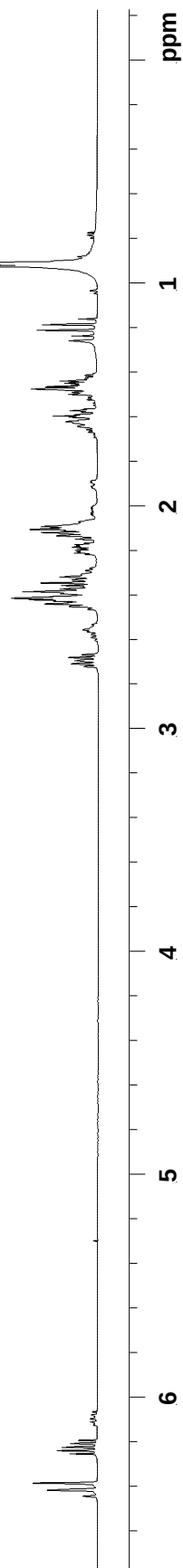
FT size 32768

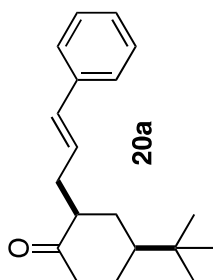
Total time 7 min, 21 sec



20a + 20b

Expanded spectrum





RRC-1205-IV-302-HNMR-CDCl3-major diastereomer

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-IV-302-HNMR-CDCl3-major diastereomer

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

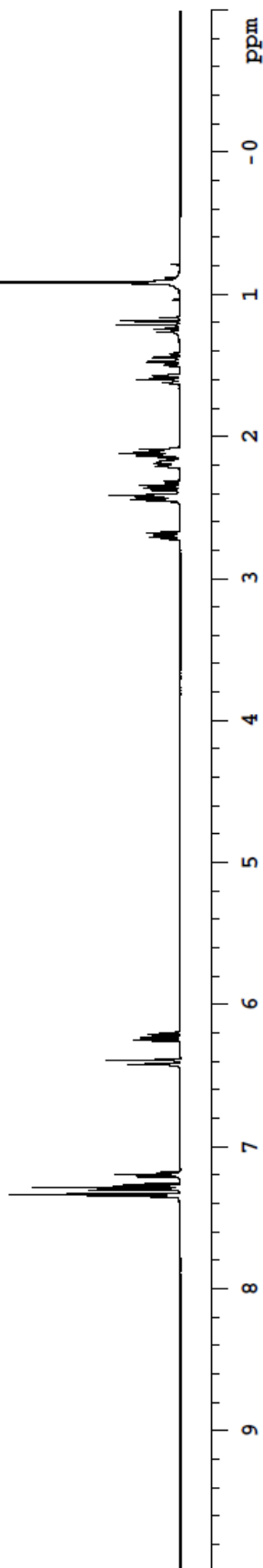
DATA PROCESSING

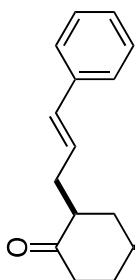
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec





20a

Expanded spectrum

RRC-1205-1V-302-HNMR-CDCl₃-major diastereomer

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-1V-302-HNMR-CDCl₃-major diastereomer

NOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

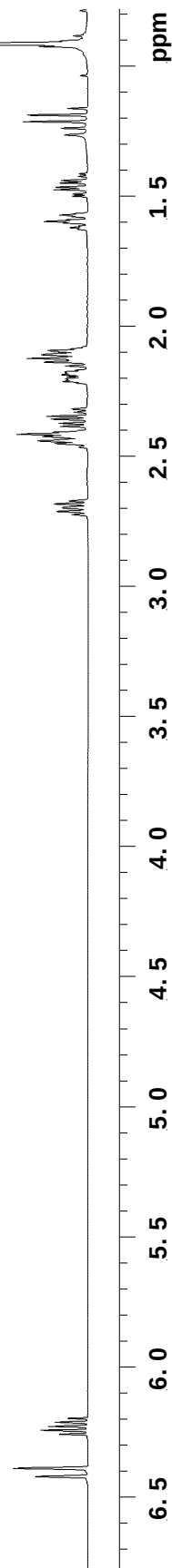
DATA PROCESSING

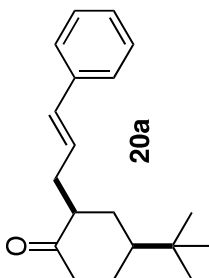
Resolution enhancement 0.5 Hz

Gaussian apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec





RRC-1205-IV-302-CNMR-CDCl₃-majordiastereomer

Pulse Sequence: *s2pul*

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-IV-302-CNMR-CDCl₃-majordiastereomer

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30499.4 Hz

13270 repetitions

OBSERVE C13, 125.6674231 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

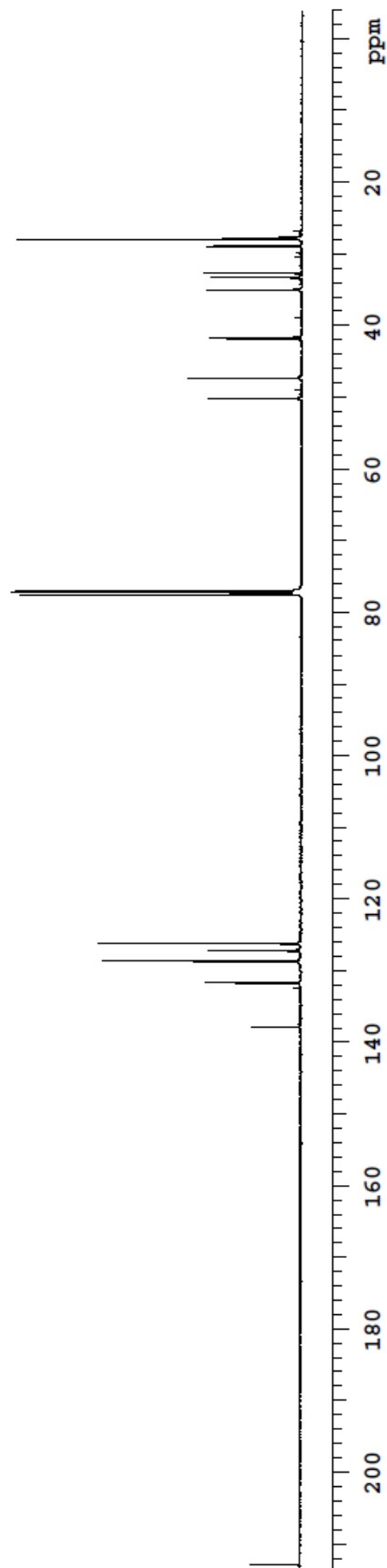
WALTZ-16 modulated

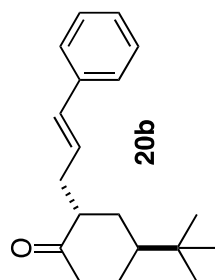
DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 23 hr, 56 min, 27 sec





RRC-1205-IV-302-HNMR-CDCl3-minordiastereomer

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-IV-302-HNMR-CDCl3-minordiastereomer

INOVA-500 "riga"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

64 repetitions

OBSERVE H1, 499.7707212 MHz

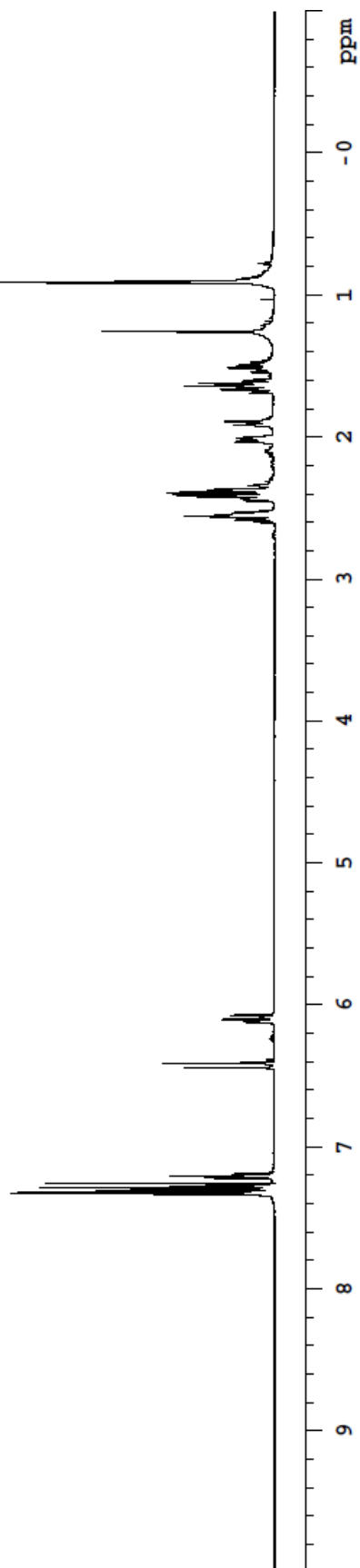
DATA PROCESSING

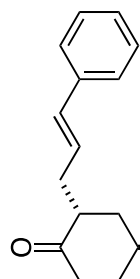
Resol. enhancement 0.5 Hz

Gauss apodization 0.500 sec

FT size 32768

Total time 7 min, 21 sec





20b

Expanded spectrum

RRC-1205-1 V-302- HMR- CDCl₃- m i n o r d i a s t e r e o m e r

Pul se Sequence: s2pul

Sol vent : CDCl₃

Temp. 25. 0 C / 298. 1 K

Operator: Raghu

File: RRC-1205-1 V-302- HMR- CDCl₃- m i n o r d i a s t e r e o m e r

INOVA- 500 "r i g a"

Rel ax. delay 5. 000 sec

Pul se 45. 0 degrees

Acq. time 1. 892 sec

Wdth 8000. 0 Hz

64 repetitions

OBSERVE H1, 499. 7707212 MHz

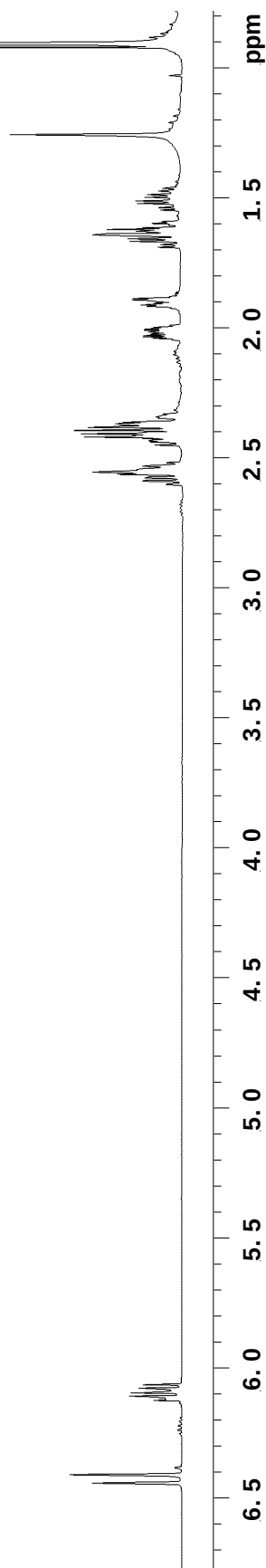
DATA PROCESSING

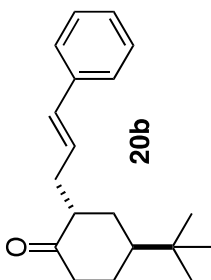
Resol . enhancement 0. 5 Hz

Gauss apodization 0. 500 sec

FT size 32768

Total time 7 m i n, 21 sec





RRC-1205-IV-302-CNMR-minordiastereomer

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Raghu

File: RRC-1205-IV-302-CNMR-minordiastereomer

INOVA-500 "riga"

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30499.4 Hz

3330 repetitions

OBSERVE C13, 125.6674198 MHz

DECOUPLE H1, 499.7730084 MHz

Power 40 dB

continuously on

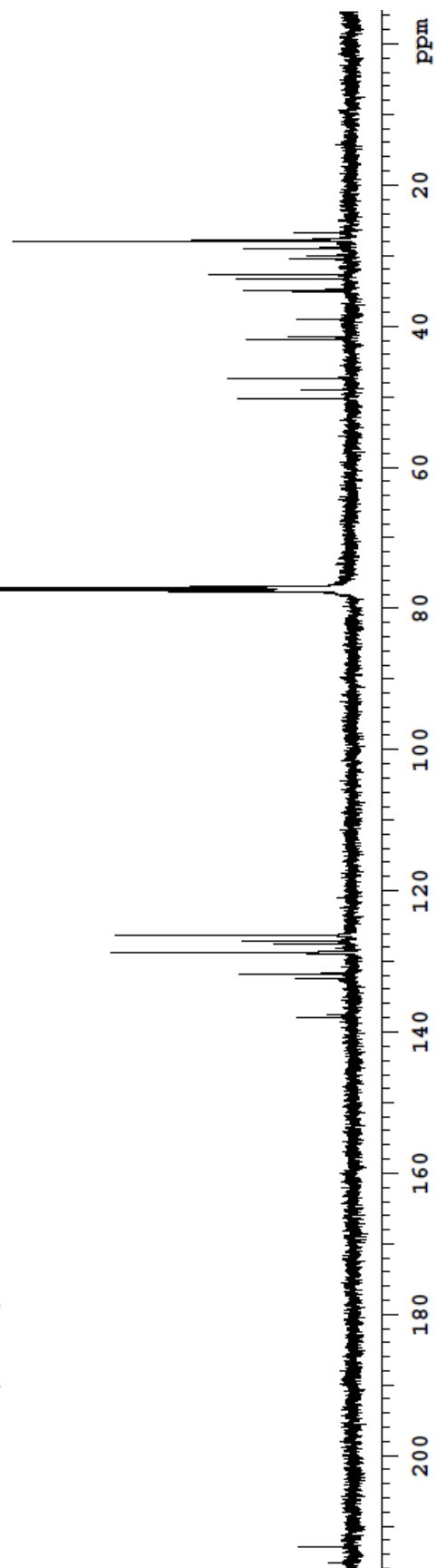
WALTZ-16 modulated

DATA PROCESSING

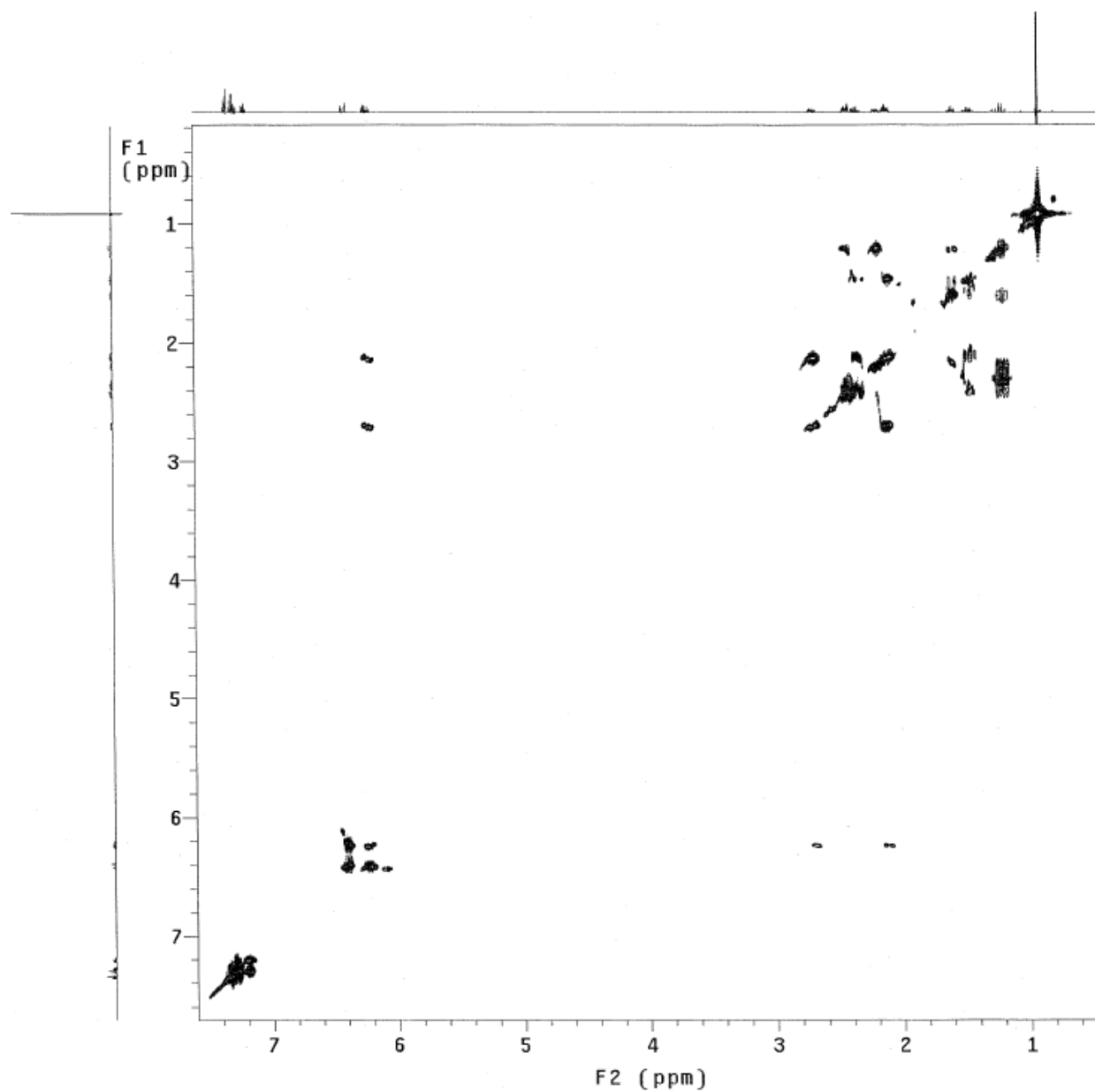
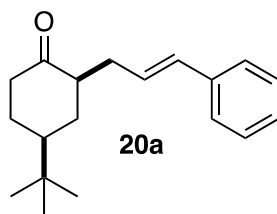
Line broadening 2.0 Hz

FT size 131072

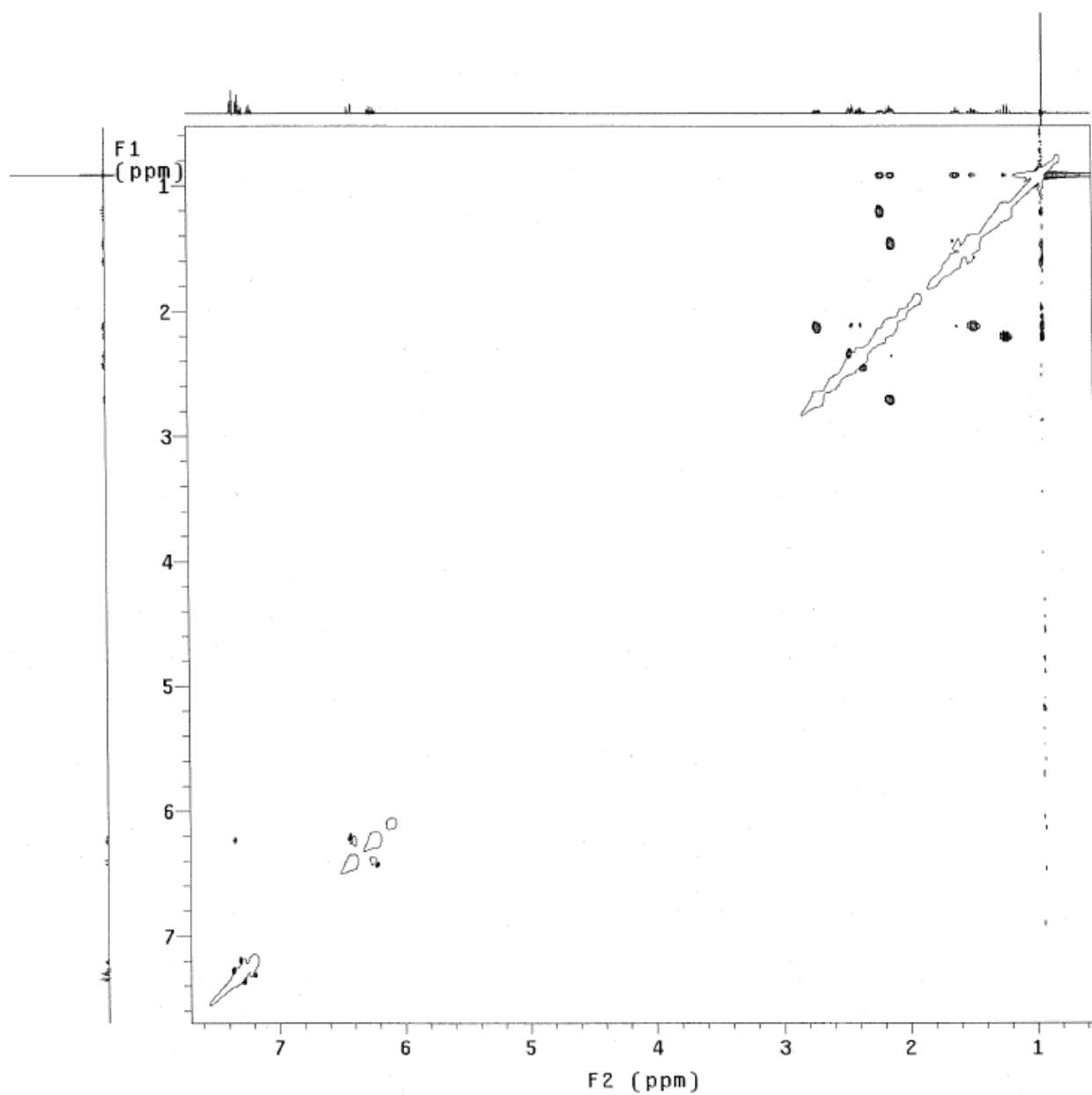
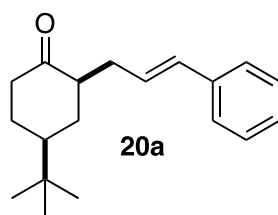
Total time 23 hr, 56 min, 27 sec



500 MHz gCOSY NMR spectrum of **20a**



500 MHz NOESY NMR spectrum of **20a**



500 MHz gHMQC NMR spectrum of **20a**

