

SUPPORTING INFORMATION

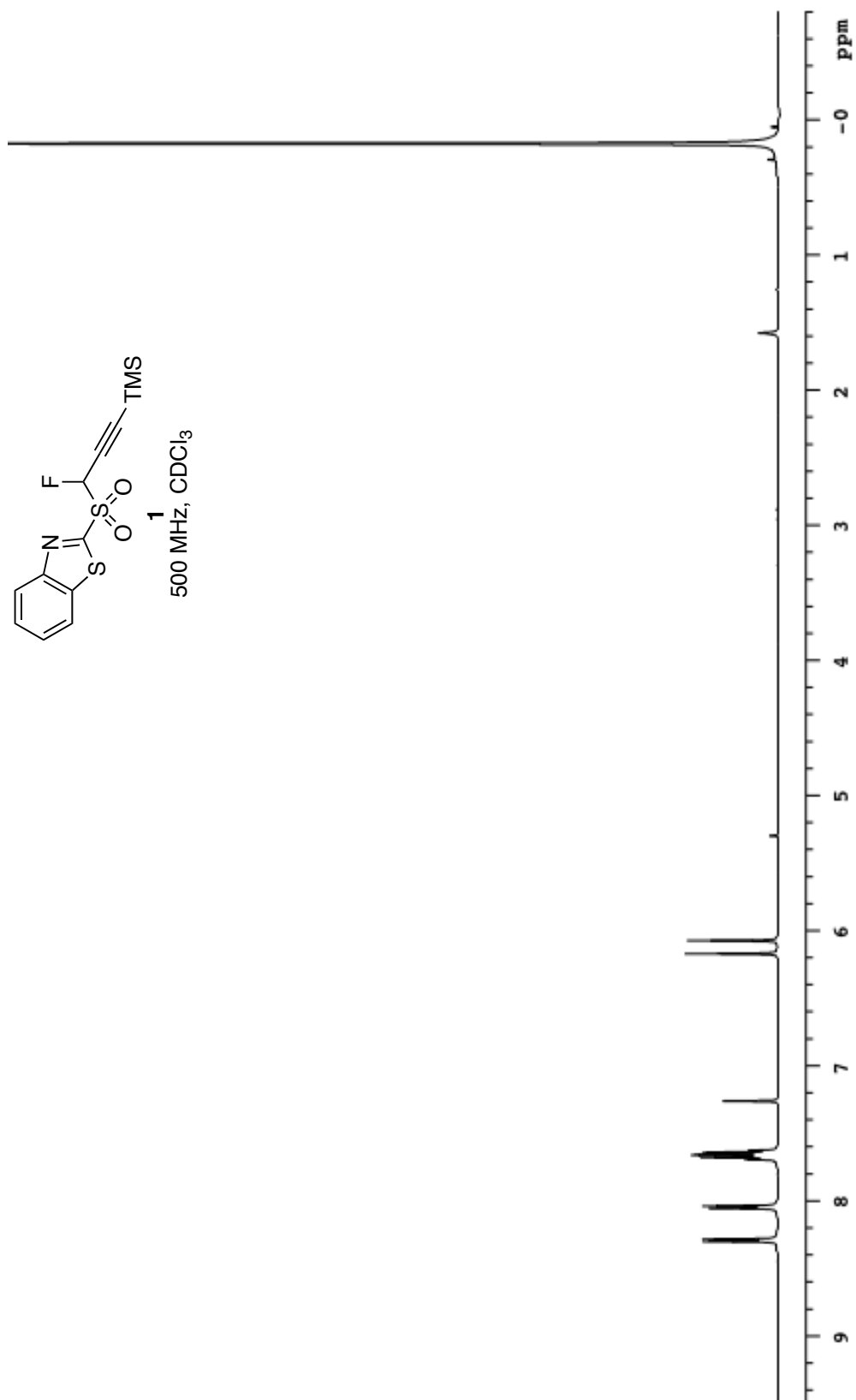
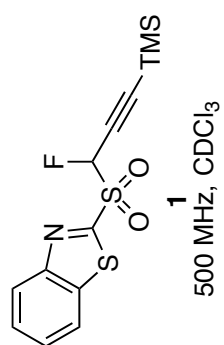
E- or *Z*-Selective synthesis of 4-fluorovinyl-1,2,3-triazoles with fluorinated *second-generation* Julia-Kocienski reagents

Rakesh Kumar,^a Govindra Singh,^a Louis J. Todaro,^b Lijia Yang,^a and Barbara Zajc^{*a}

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1222-RK-02-144-13C

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-02-144-13C

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

100 repetitions

ONSERVE C13, 125.6674411 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

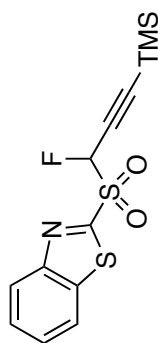
WALTZ-16 modulated

DATA PROCESSING

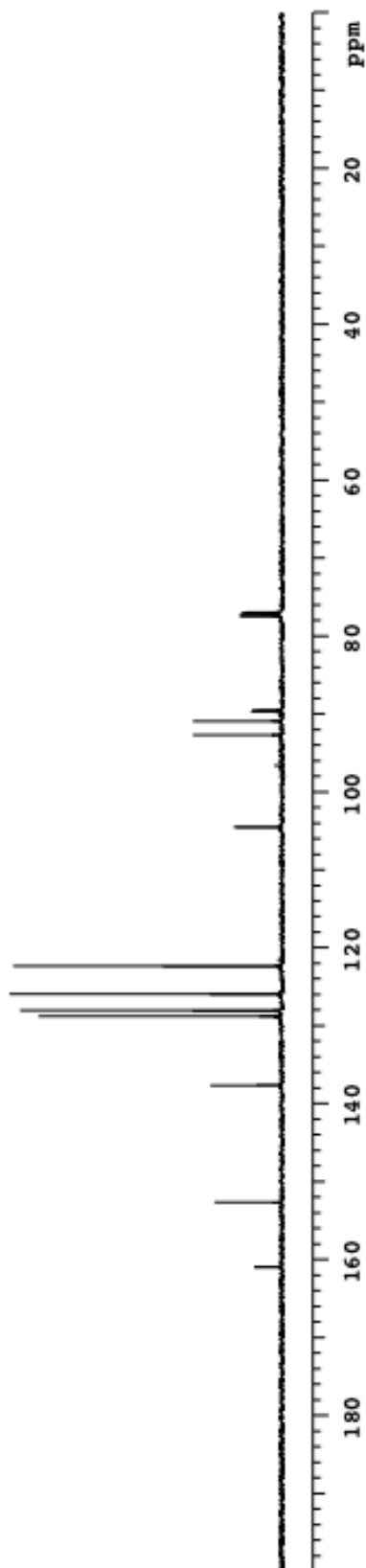
Line broadening 1.0 Hz

FT size 131072

Total time 9 min, 12 sec



1
125 MHz, CDCl₃



1222-RK-04-259-pure

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

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-259-pure

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

20 repetitions

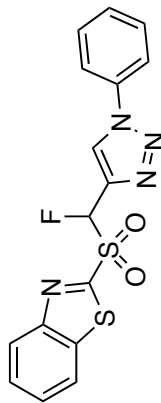
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

Line broadening 0.1 Hz

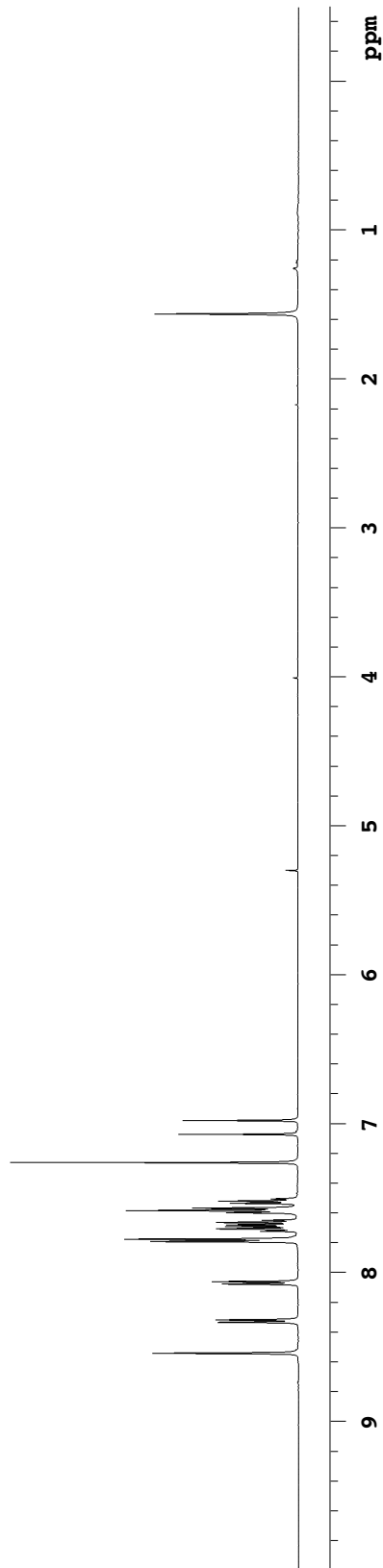
FT size 32768

Total time 1 min, 32 sec



2

500 MHz, CDCl₃



1222-RK-04-259-13C-1

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

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-259-13C-1

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

1892 repetitions

OBSERVE C13, 125.6674182 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

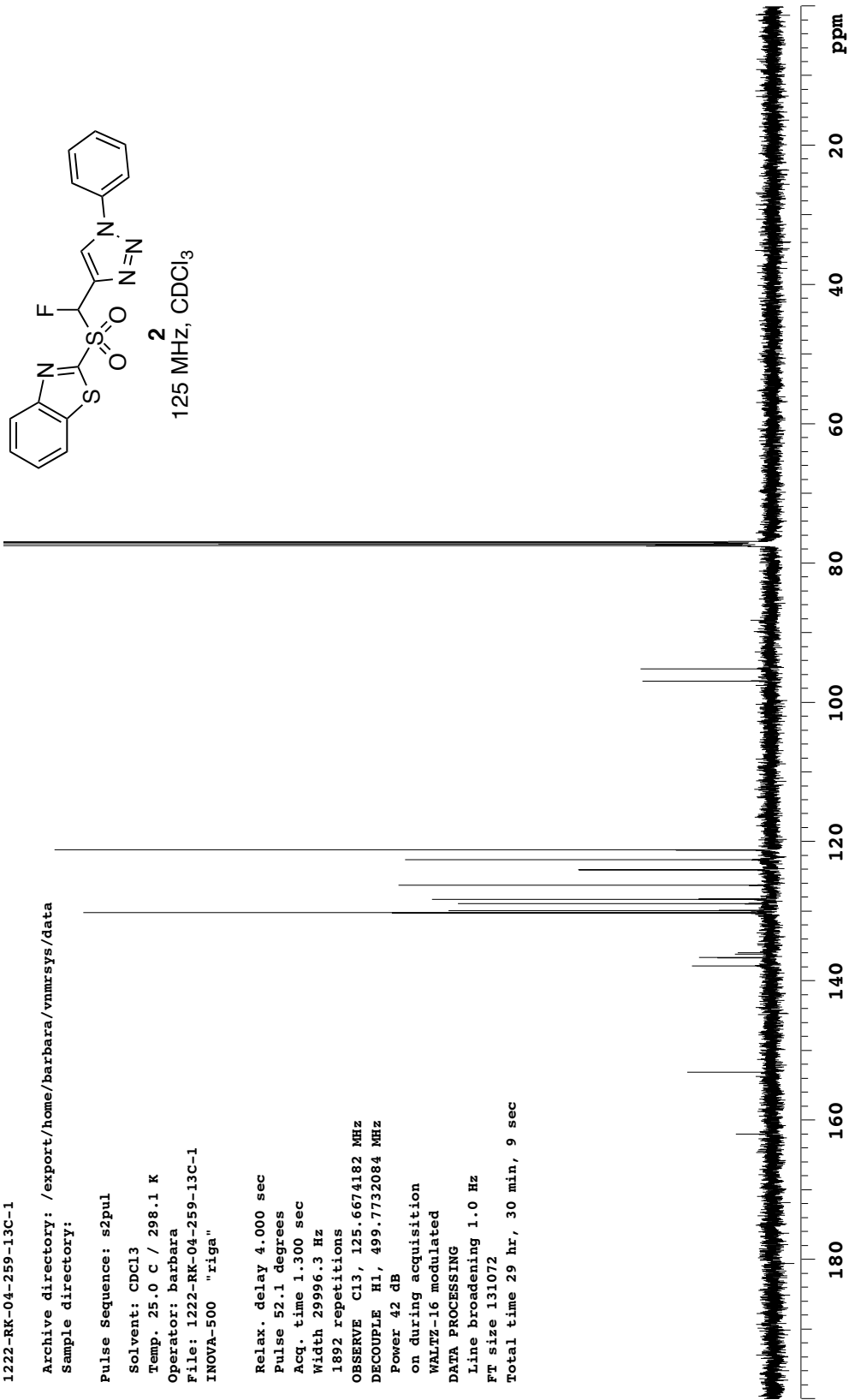
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 29 hr, 30 min, 9 sec



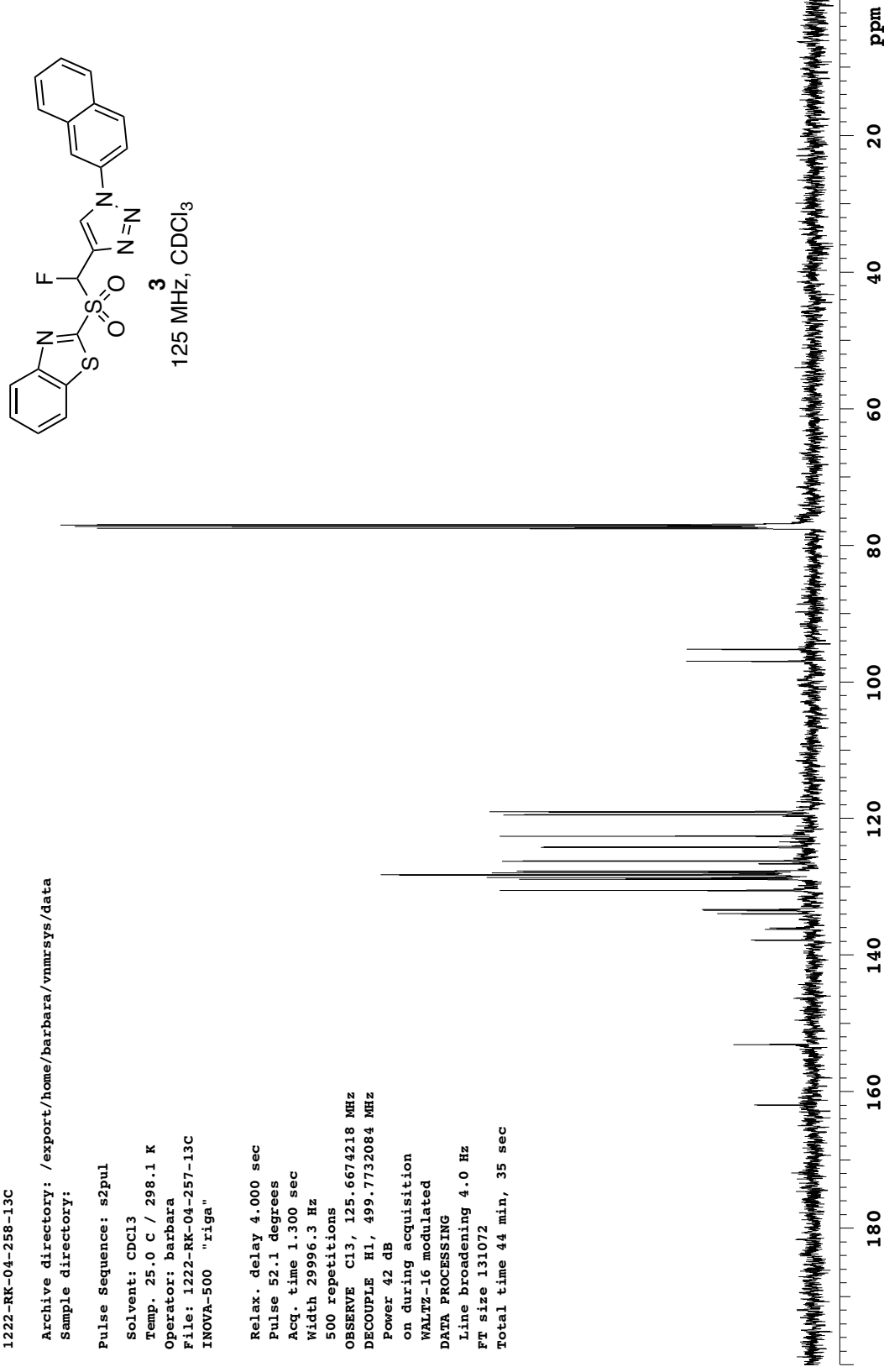
1222-RK-04-258-13C

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

Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
Operator: Barbara
File: 1222-RK-04-257-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
500 repetitions
OBSERVE C13, 125.6674218 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 4.0 Hz
FT size 131072
Total time 44 min, 35 sec



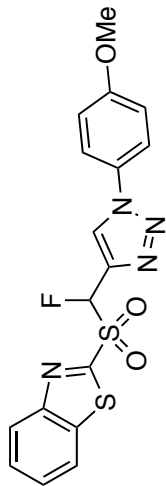
1222-RK-04-246-pure-1H

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

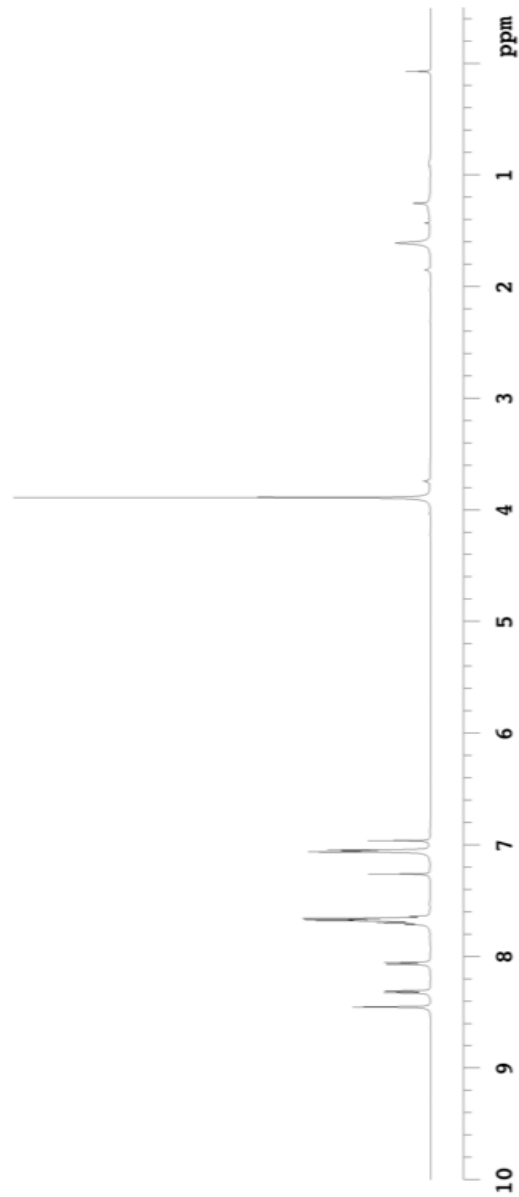
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-246-pure-1H
INOVA-500 "r1ga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
52 repetitions
OBSERVE H1, 499.7707216 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 9 min, 40 sec



4

500 MHz, CDCl₃



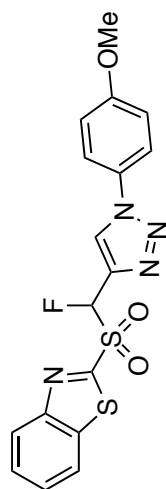
1222-RK-04-246-pure

Archive directory: /export/home/barbara/vnarsys/data
Sample directory: 1222-RK-04-246-pure_24Mar2008

Pulse Sequence: s2pul

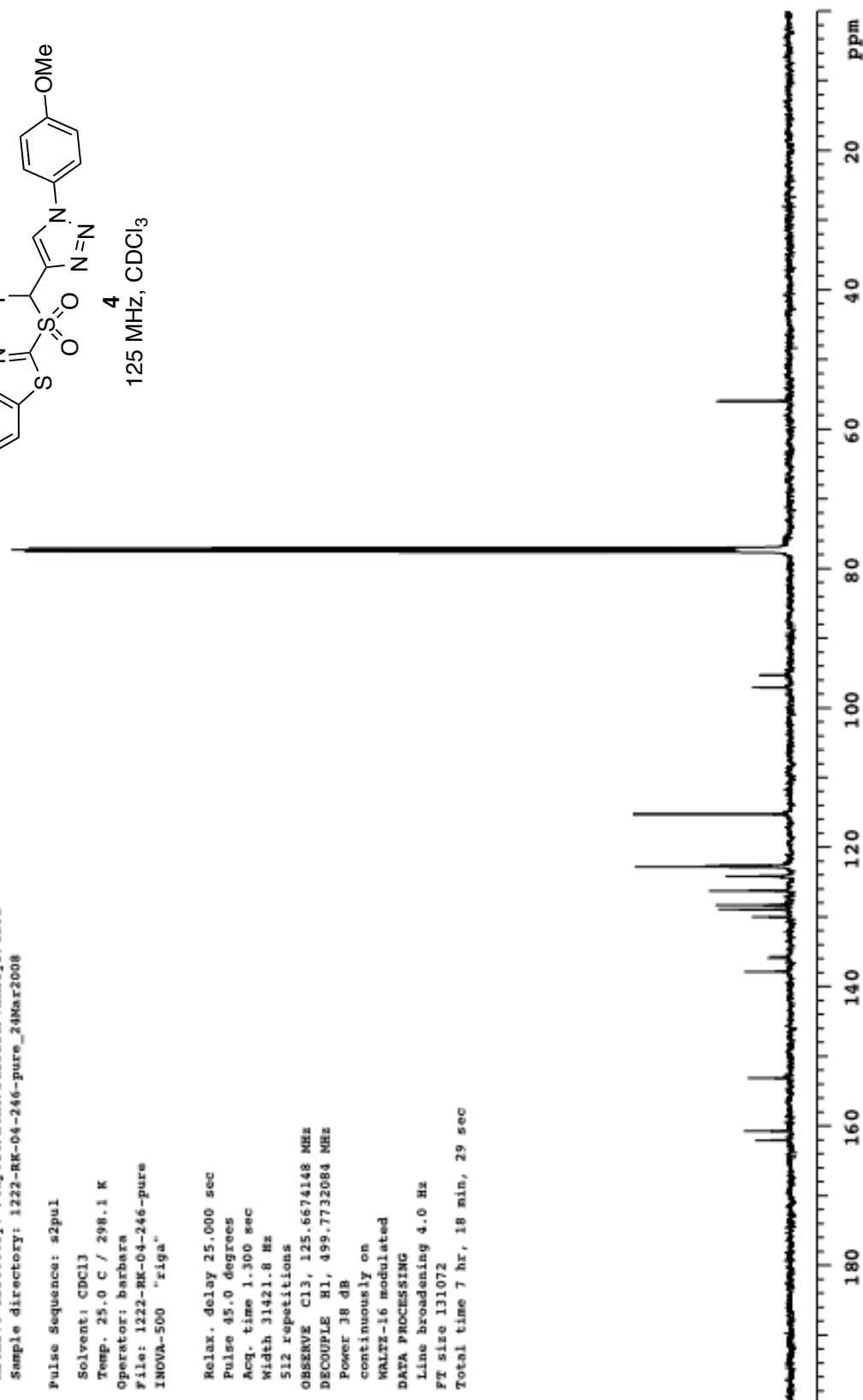
Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-246-pure
INOVA-500 "ziga"

Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
512 repetitions
OBSERVE C13, 125.6674148 MHz
DECOUPLE H1, 499.7732084 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 4.0 Hz
FT size 131072
Total time 7 hr, 18 min, 29 sec



4

125 MHz, CDCl₃



1222-RK-04-242-2ndfraction

Archive directory: /export/home/mkl/vmrsys/data

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-242-2ndfraction

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

24 repetitions

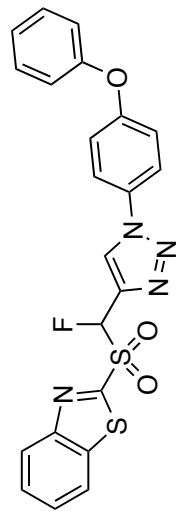
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

Line broadening 0.1 Hz

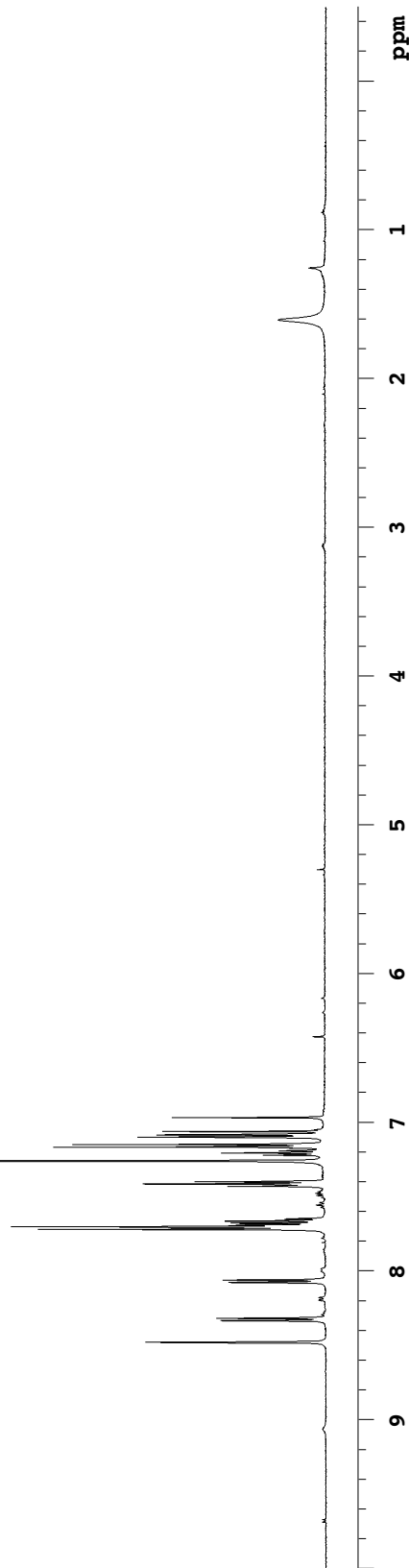
FT size 32768

Total time 1 min, 32 sec



5

500 MHz, CDCl₃



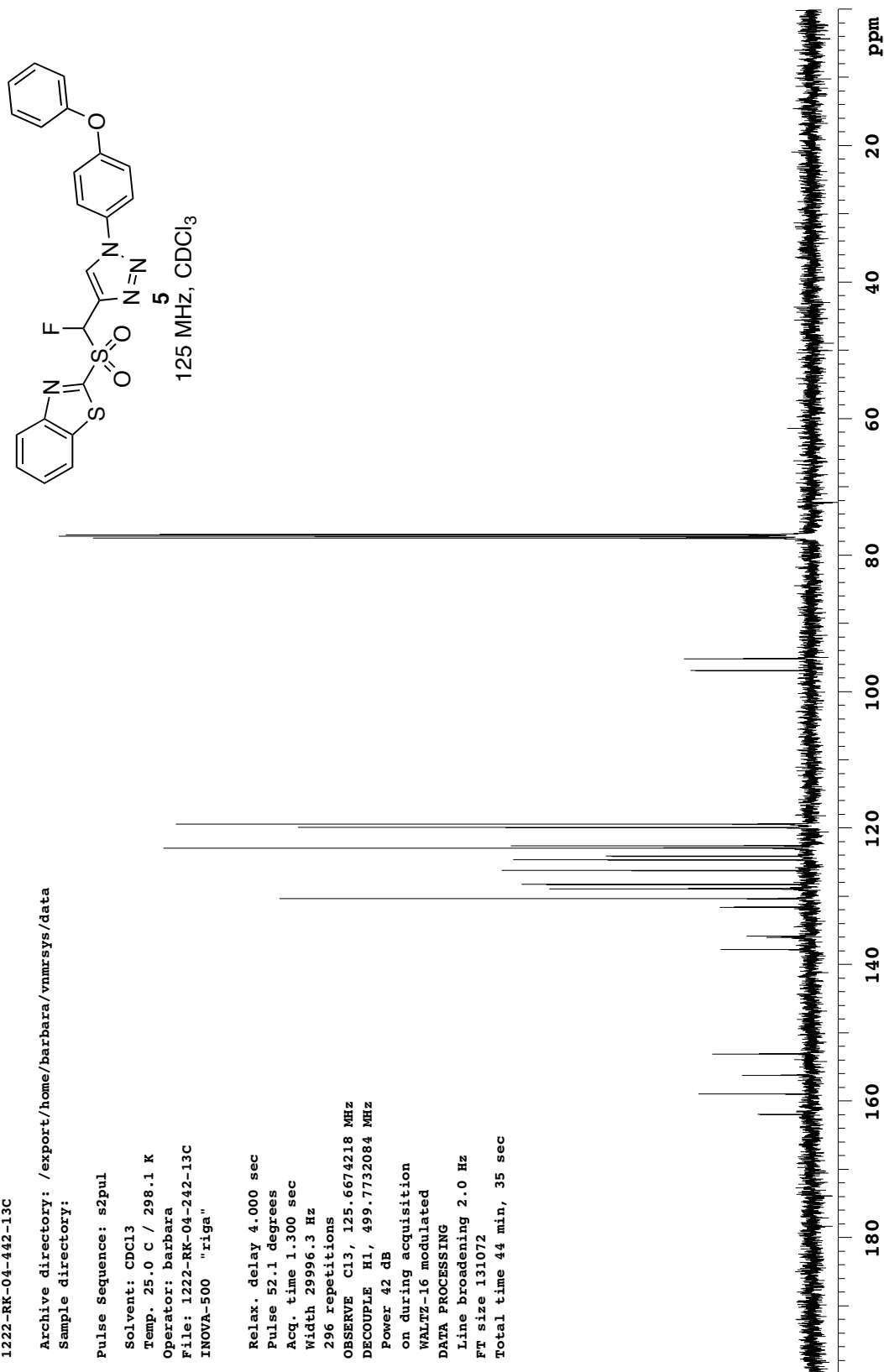
1222-RK-04-442-13C

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

Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
Operator: Barbara
File: 1222-RK-04-242-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
296 repetitions
OBSERVE C13, 125.6674218 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 44 min, 35 sec



1222-RK-04-304-2-pure-DMSO

Archive directory: /export/home/mkl/vmrsys/data

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: dmsd

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-304-2-pure-DMSO

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

28 repetitions

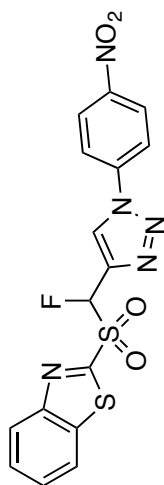
OBSERVE H1, 499.7730861 MHz

DATA PROCESSING

Line broadening 0.0 Hz

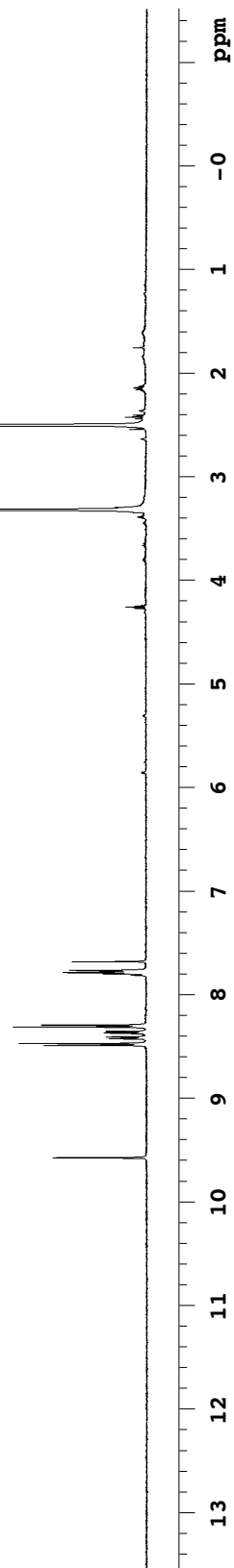
FT size 32768

Total time 1 min, 32 sec



6

500 MHz, DMSO-*d*₆



1222-RK-04-304-13C-DMSO

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

Pulse Sequence: s2pul

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-304-13C-DMSO

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

388 repetitions

OBSERVE C13, 125.6674526 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

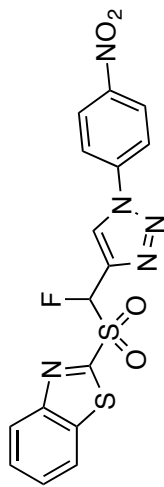
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

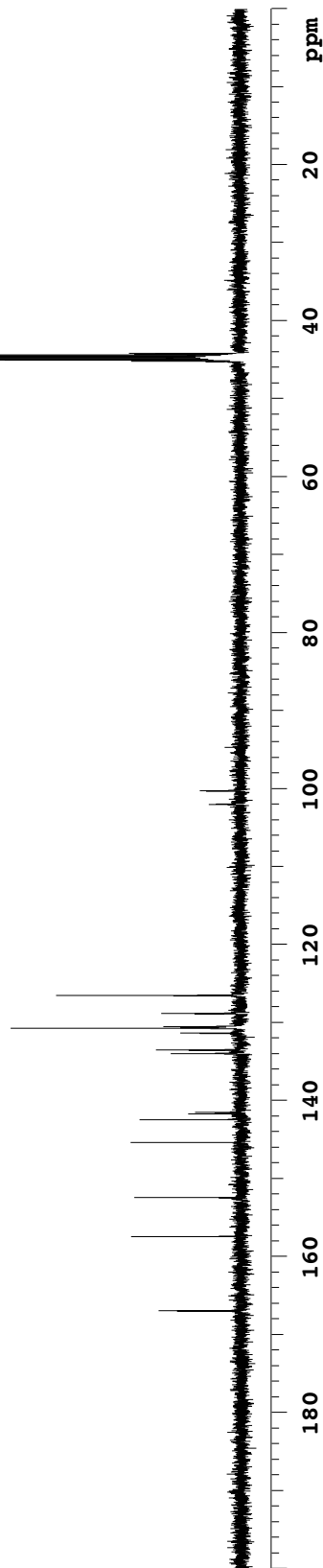
FT size 131072

Total time 53 min, 26 sec



6

125 MHz, DMSO-*d*₆



1222-RK-04-247-pure

Archive directory: /export/home/mkl/vmrsys/data

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-247-pure

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

20 repetitions

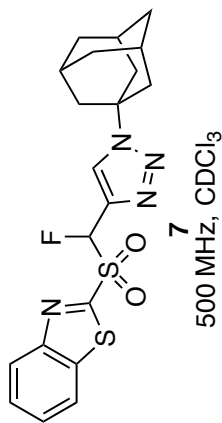
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

Line broadening 0.1 Hz

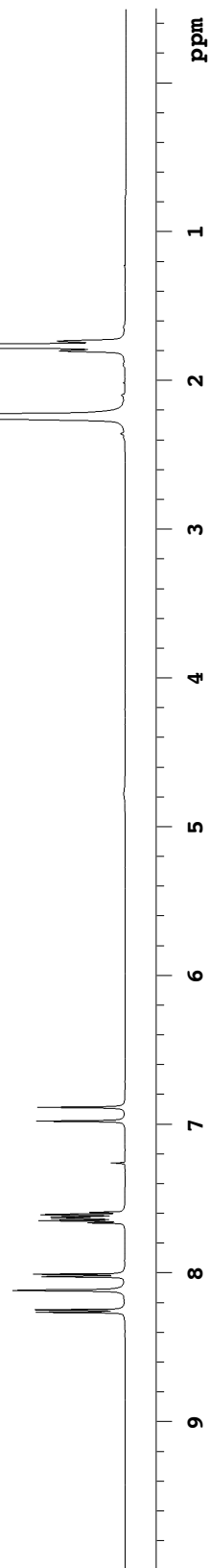
FT size 32768

Total time 1 min, 32 sec



7

500 MHz, CDCl₃



1222-RK-04-247-13C

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-247-13C

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

84 repetitions

OBSERVE C13, 125.6674273 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

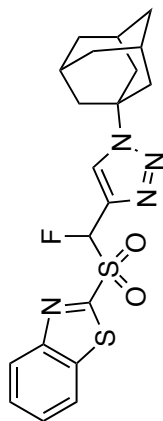
WALTZ-16 modulated

DATA PROCESSING

Line broadening 3.0 Hz

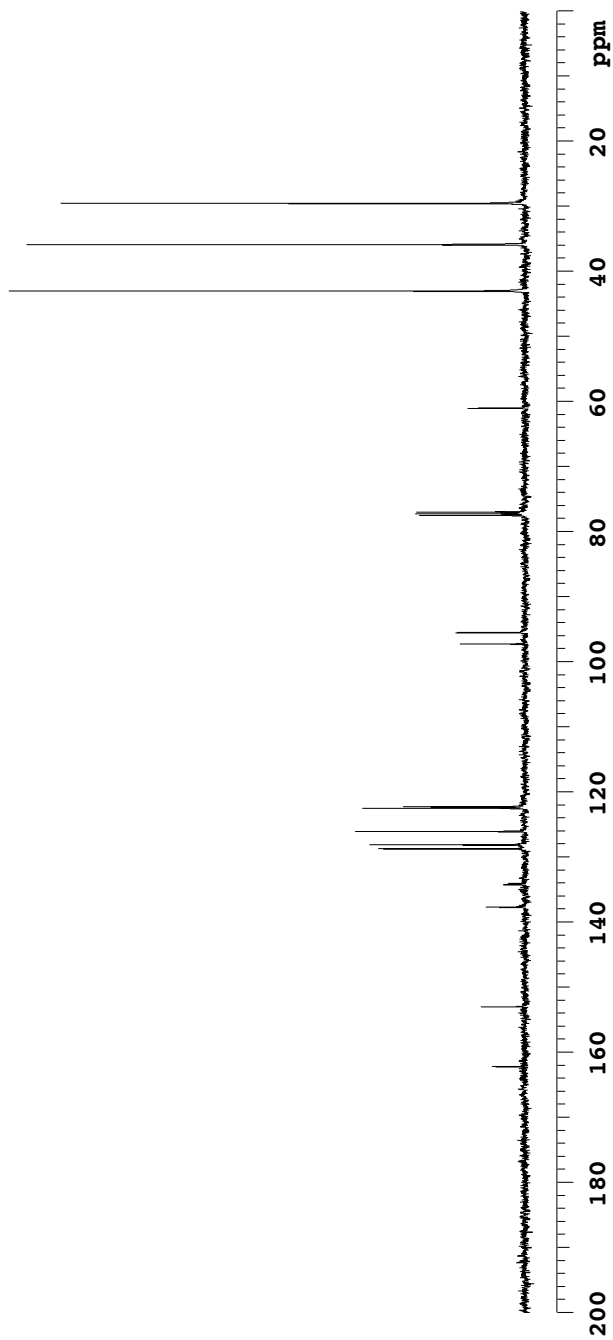
FT size 131072

Total time 18 min, 3 sec



7

125 MHz, CDCl₃



1222-RK-04-270-pure

Archive directory: /export/home/mkl/vmrsys/data

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-270-pure

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

16 repetitions

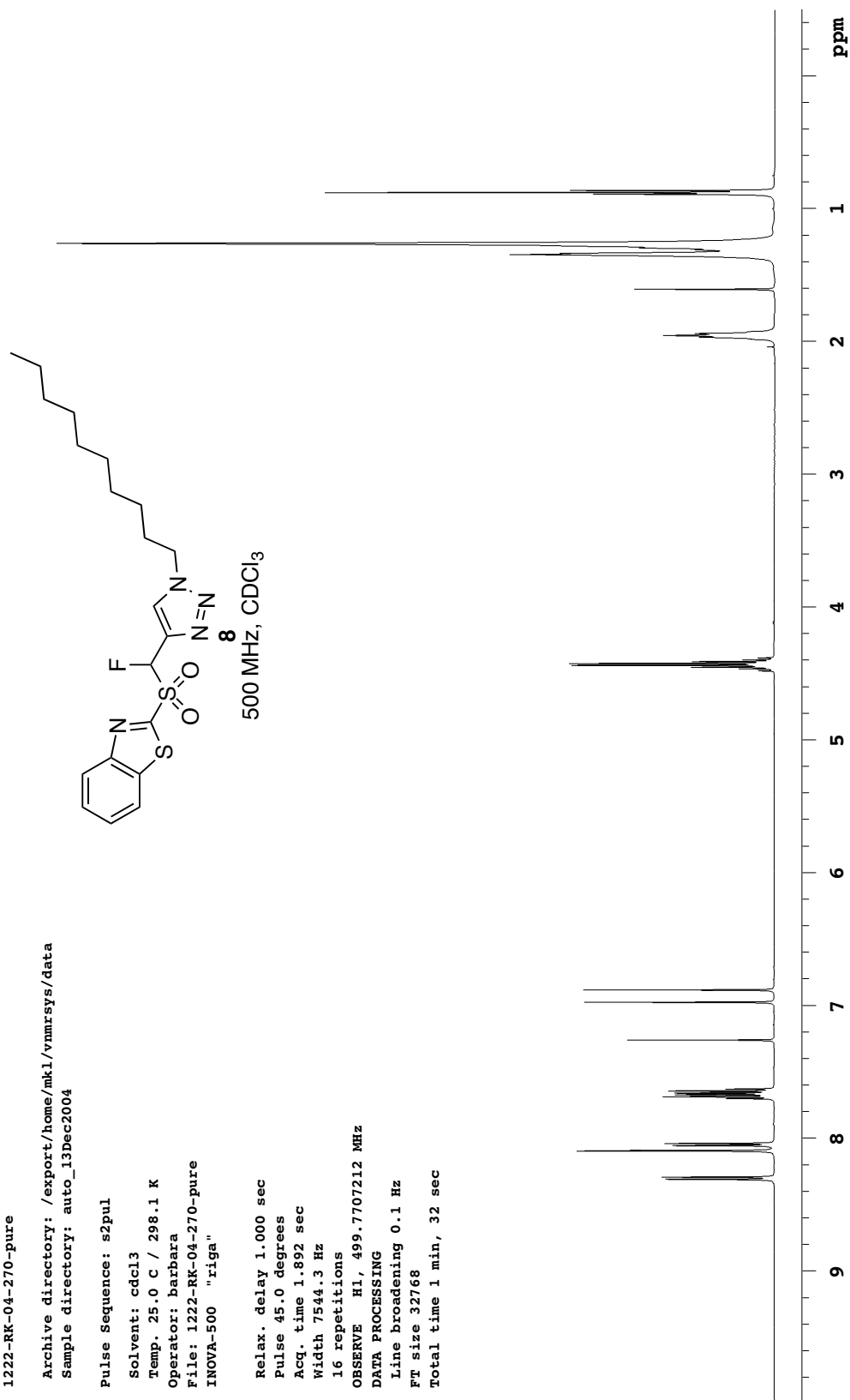
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 1 min, 32 sec



1222-RK-04-270-13C

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-270-13C

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

64 repetitions

OBSERVE C13, 125.6674571 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

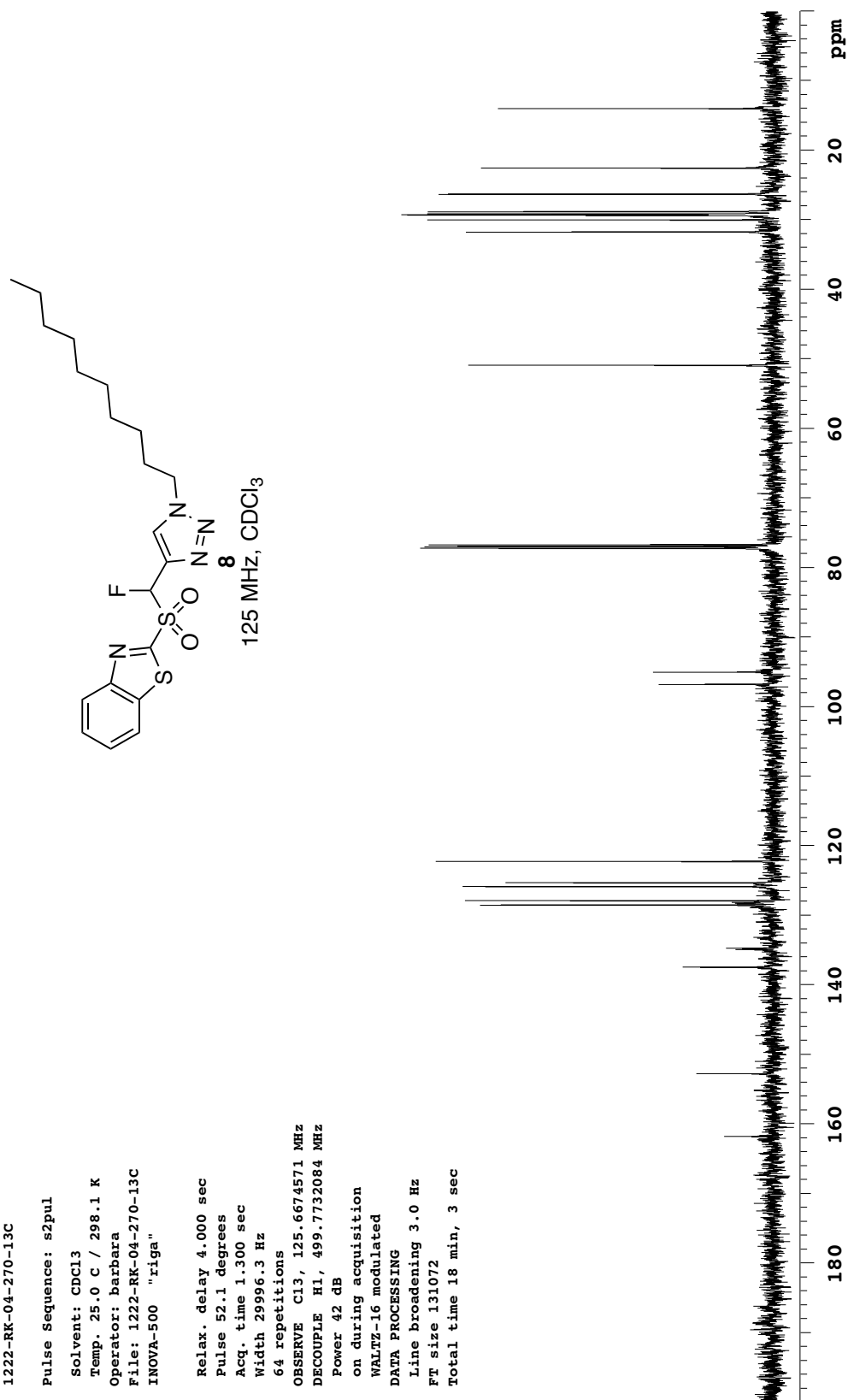
WALTZ-16 modulated

DATA PROCESSING

Line broadening 3.0 Hz

FT size 131072

Total time 18 min, 3 sec



1222-RK-04-258-pure

Archive directory: /export/home/mkl/vnmrsws/data

Sample directory: auto_1jDec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-258-pure

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

32 repetitions

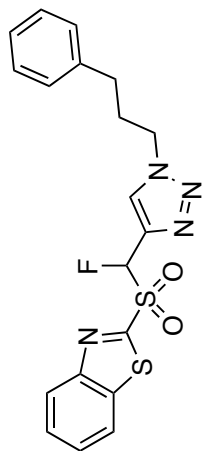
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

Line broadening 0.1 Hz

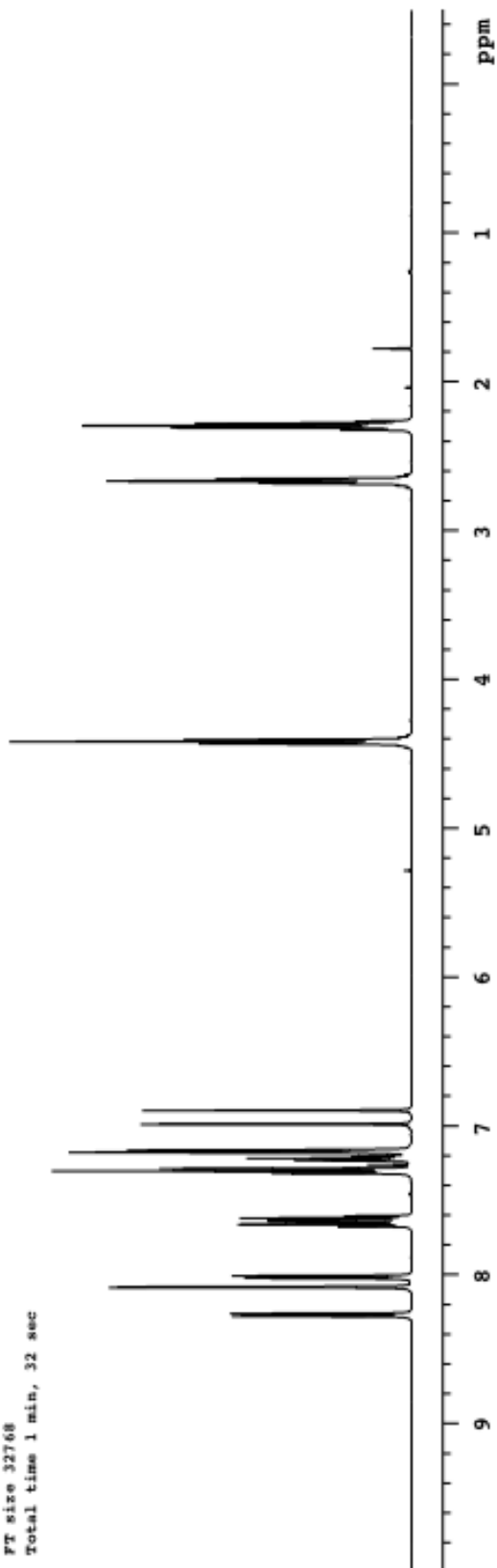
FT size 32768

Total time 1 min, 32 sec



9

500 MHz, CDCl₃



1222-RK-04-258-pure-13C

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-258-pure-13C

INOVA-500 "ziga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

52 repetitions

OBSERVE C13, 125.6674273 MHz

DECOUPLE H1, 499.732084 MHz

Power 42 dB

on during acquisition

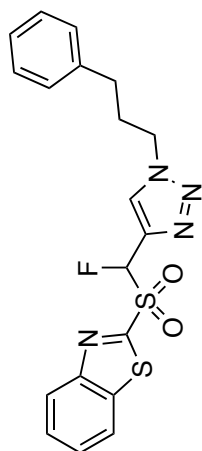
WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

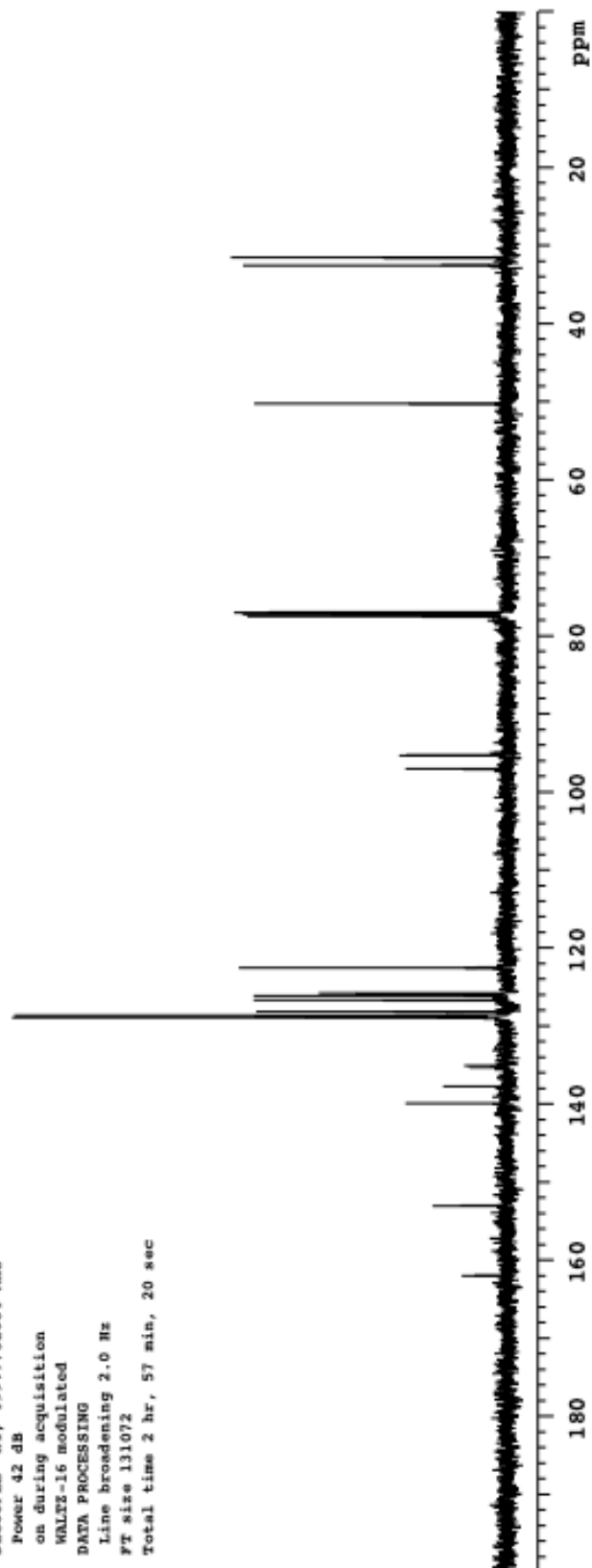
FT size 131072

Total time 2 hr, 57 min, 20 sec



9

125 MHz, CDCl₃



1222-RK-04-254-1stfraction

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

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-254-1stfraction

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

12 repetitions

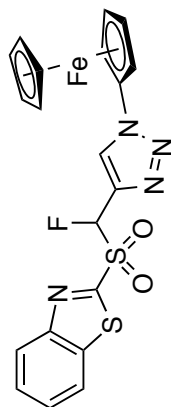
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

Line broadening 0.1 Hz

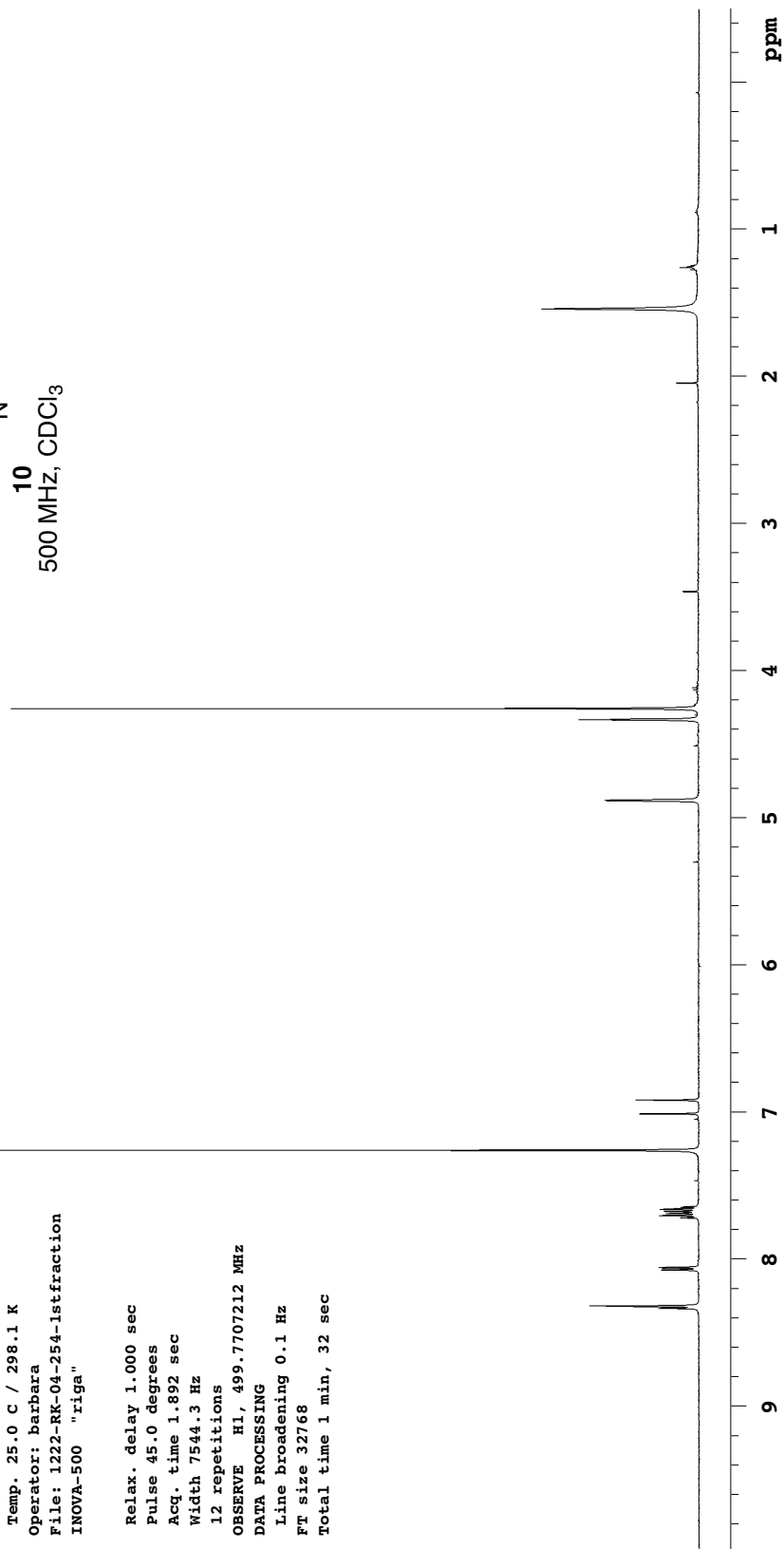
FT size 32768

Total time 1 min, 32 sec



10

500 MHz, CDCl₃



1222-RK-04-254-13C

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

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-254-pure-13C

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

856 repetitions

OBSERVE C13, 125.6674205 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

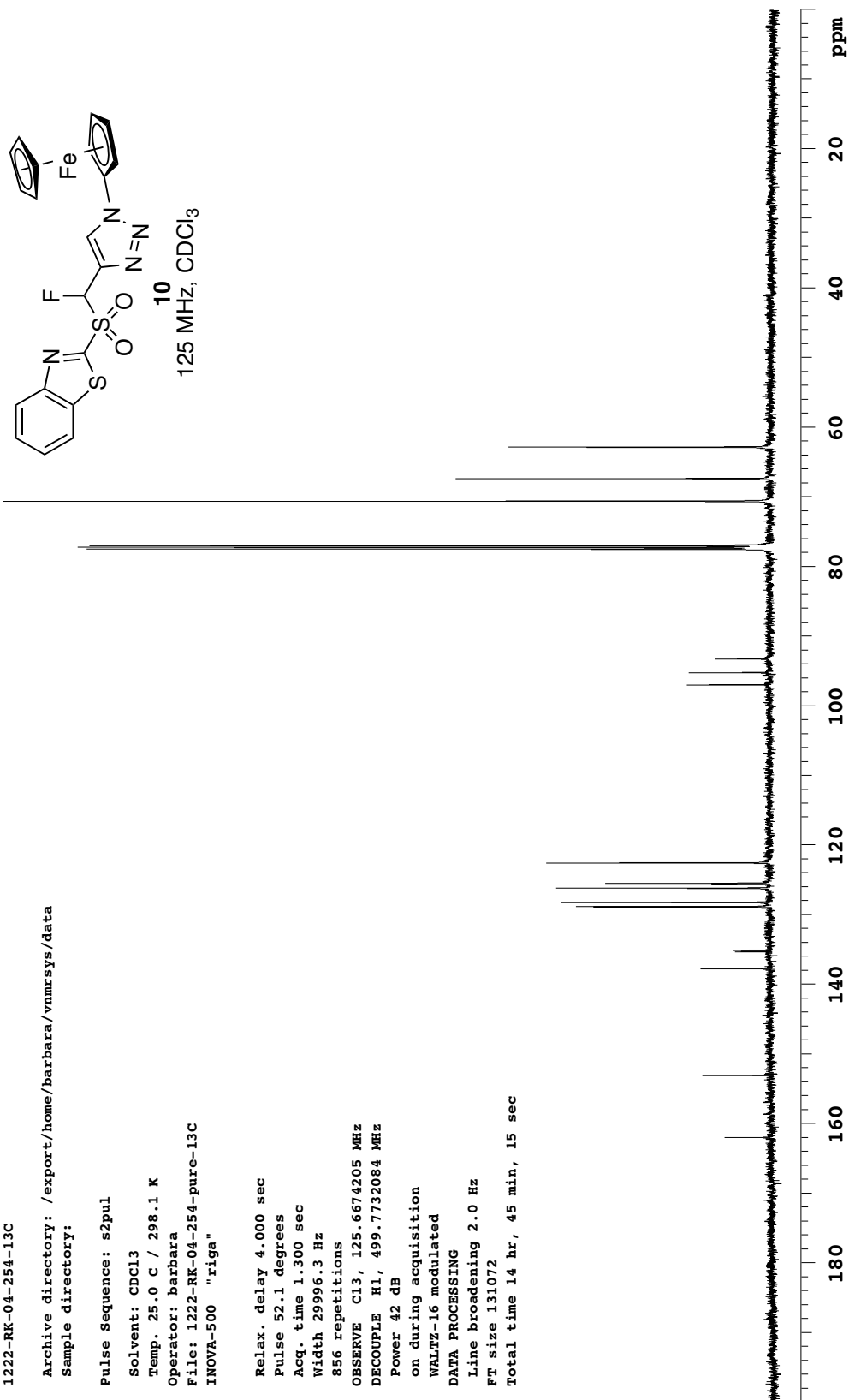
WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 14 hr, 45 min, 15 sec



1222-RK-05-365-pure

Archive directory: /export/home/mkl/vmrsys/data

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: dmsd

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-05-365-pure

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

32 repetitions

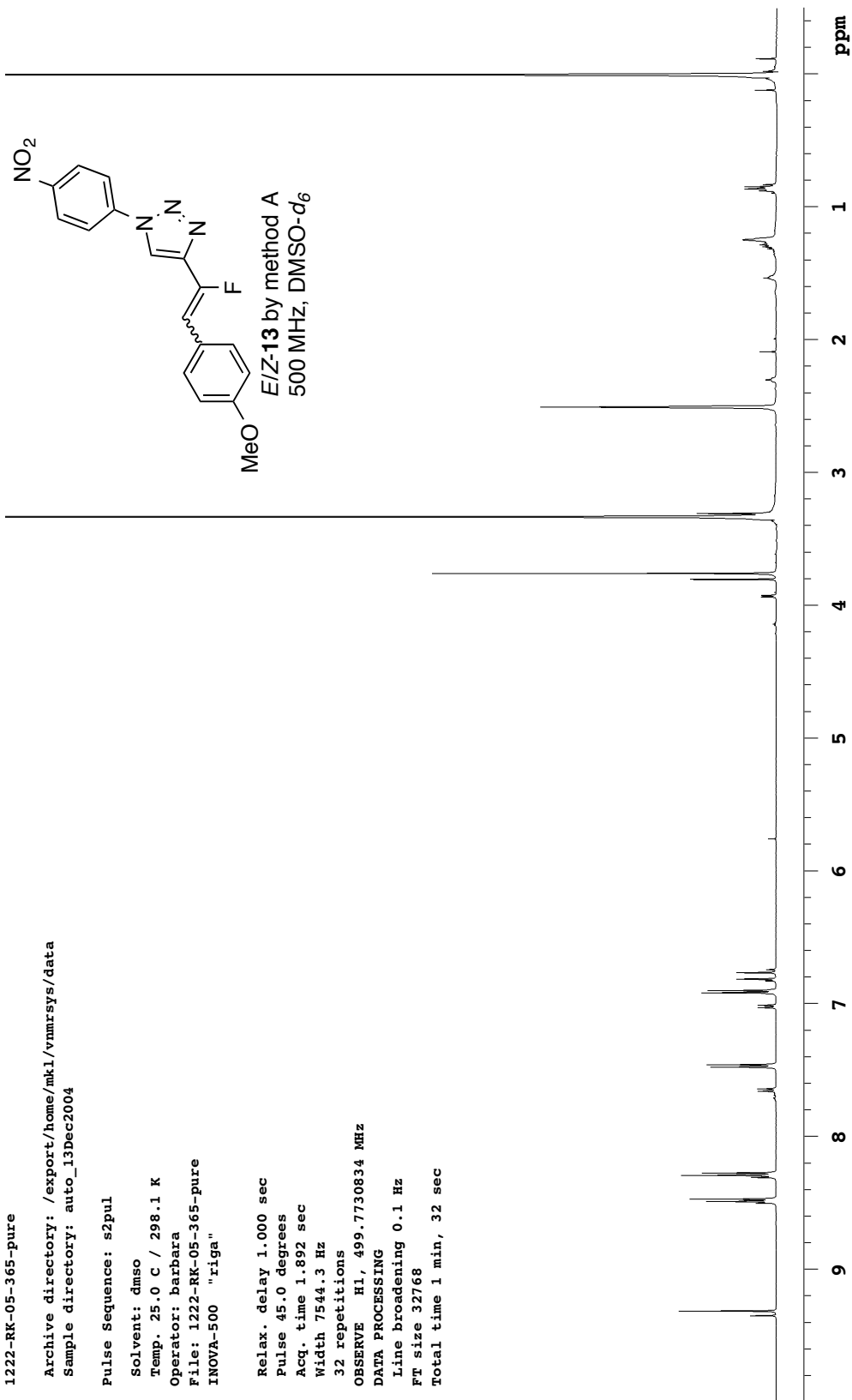
OBSERVE H1, 499.7730834 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 1 min, 32 sec



1222-RK-04-308-pure

Archive directory: /export/home/mkl/vmrsys/data

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-308-pure

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

48 repetitions

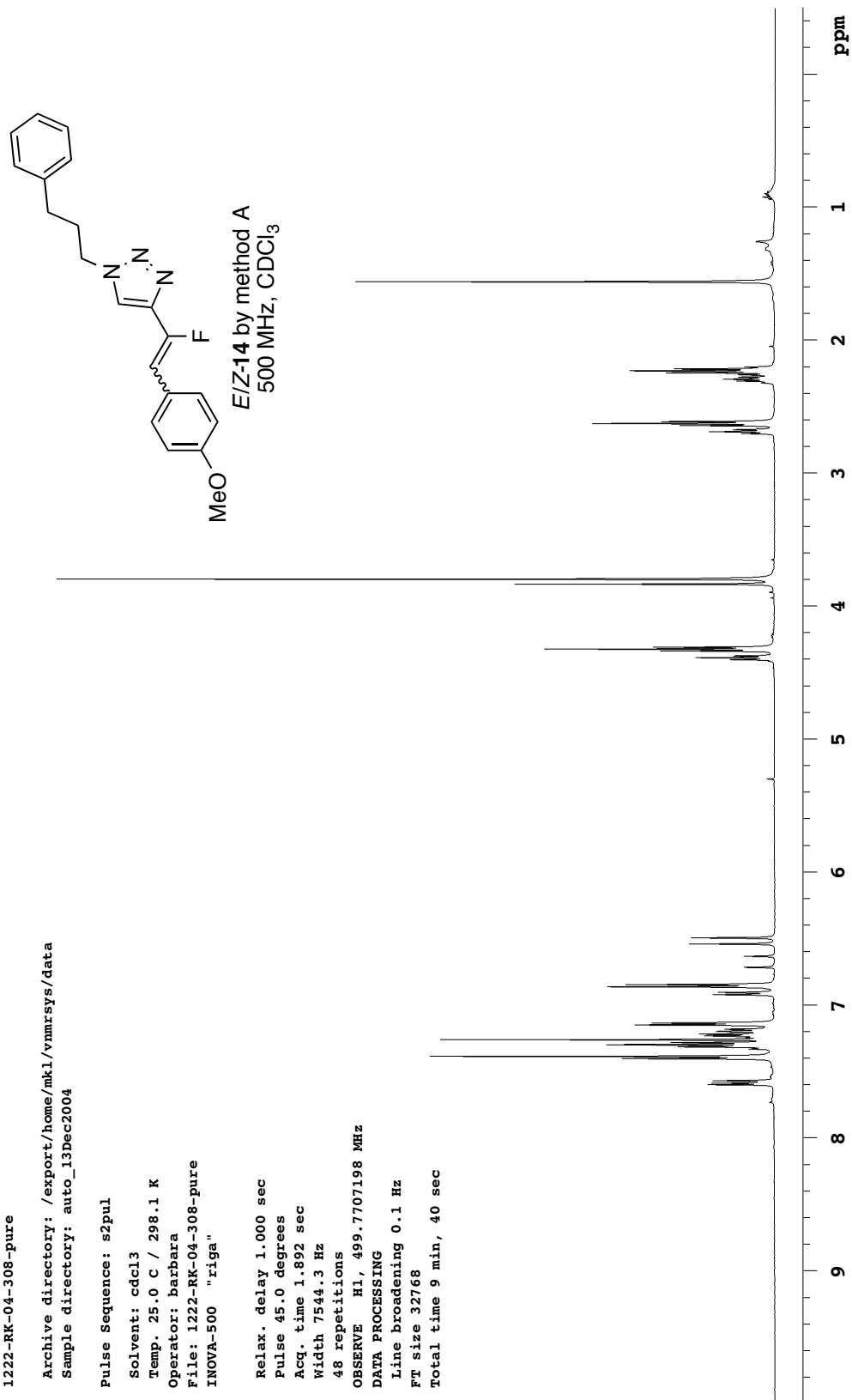
OBSERVE H1, 499.7707198 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 9 min, 40 sec



1222-RK-11-851-pure

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: barbara

File: 1222-RK-11-851-pure

INOVA-500 "riga"

Pulse 48.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

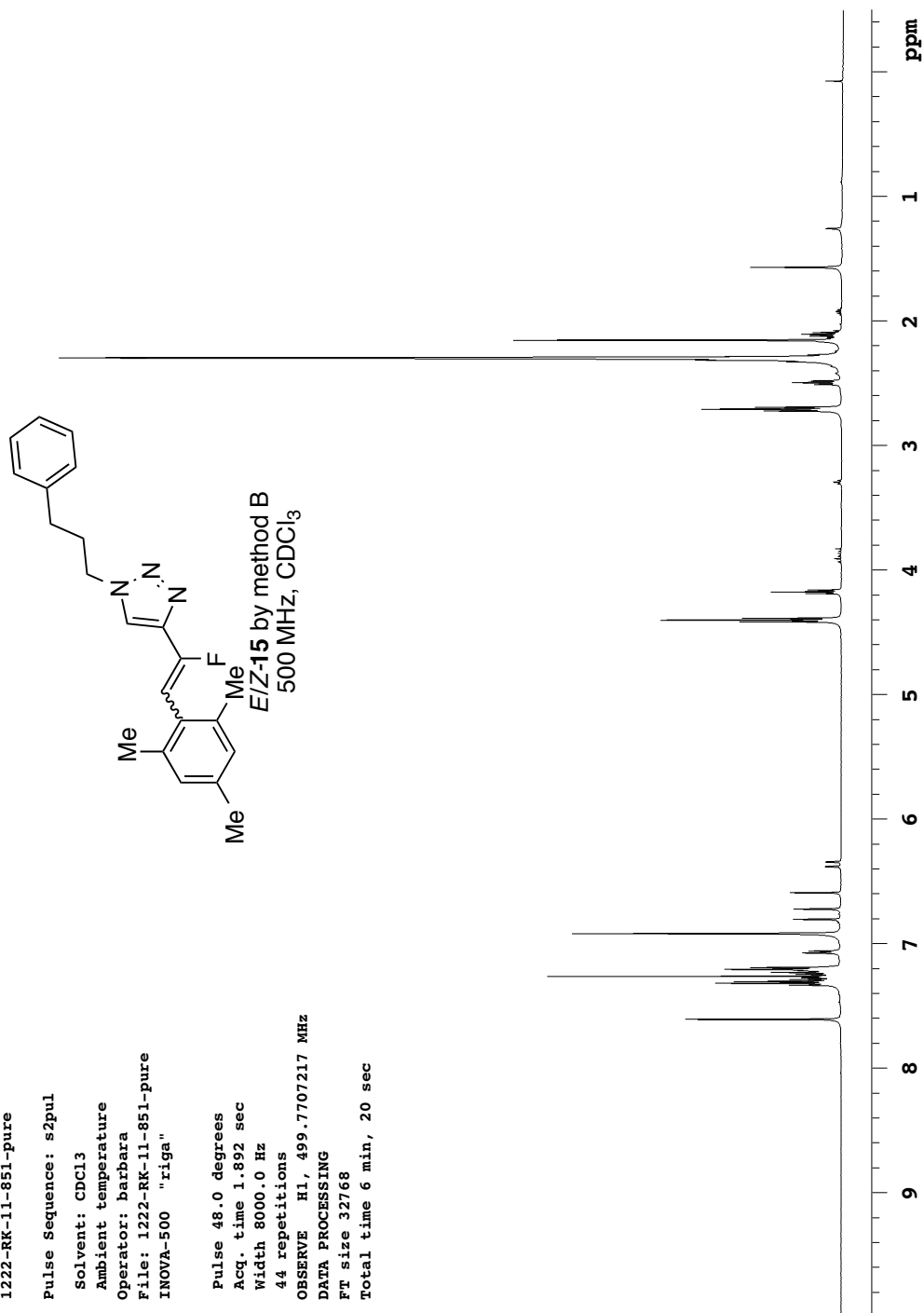
44 repetitions

OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 20 sec



1231-RK-15-09-pure

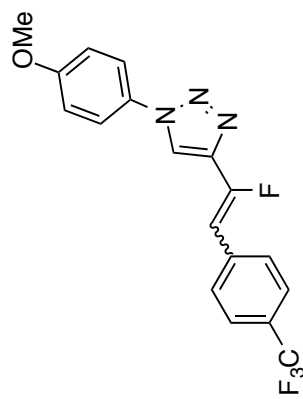
Archive directory: /export/home/mkl/vmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

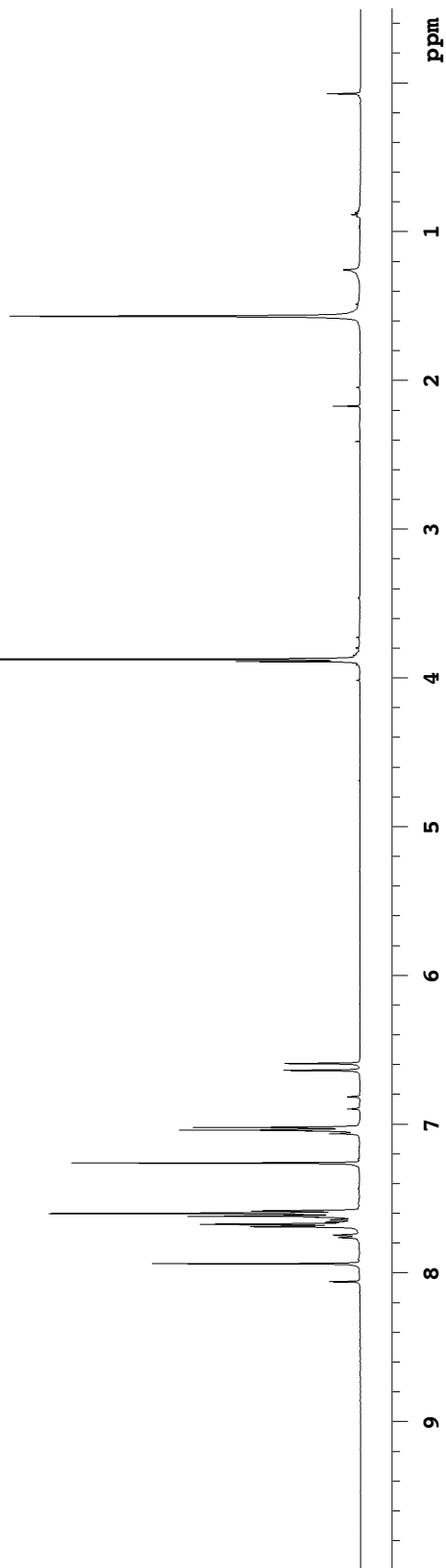
Solvent: cdcl3
Temp. 24.0 C / 297.1 K
Operator: Barbara
File: 1231-RK-15-09-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
28 repetitions

OBSERVE H1, 499.7707216 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec



E/Z-16 by method A
500 MHz, CDCl₃



1231-RK-14-85-pure

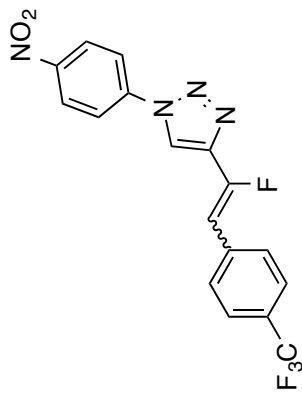
Archive directory: /export/home/mkl/vmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

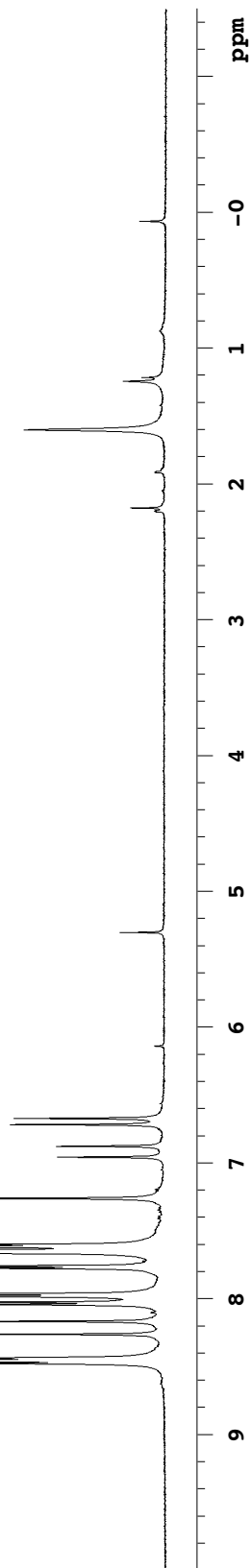
Solvent: cdcl3
Ambient temperature
Operator: Barbara
File: 1231-RK-14-85-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
12 repetitions

OBSERVE H1, 499.7707221 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec



E/Z-17 by method A
500 MHz, CDCl₃



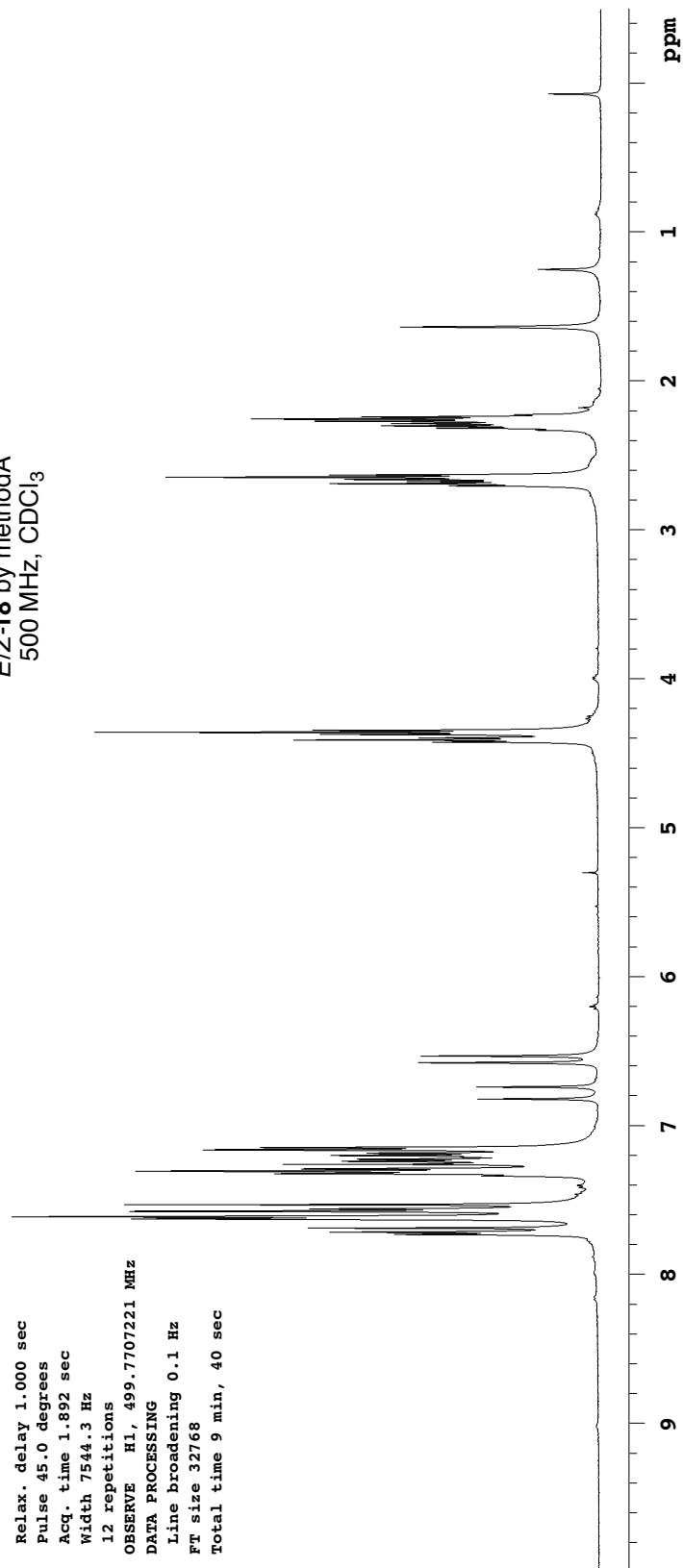
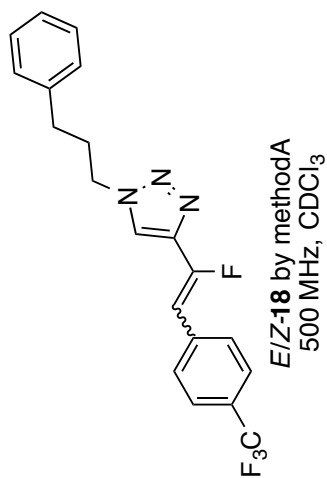
1231-RK-14-86-pure

Archive directory: /export/home/mkl/vmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
Operator: Barbara
File: 1231-RK-14-86-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
12 repetitions
OBSERVE H1, 499.7707221 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec



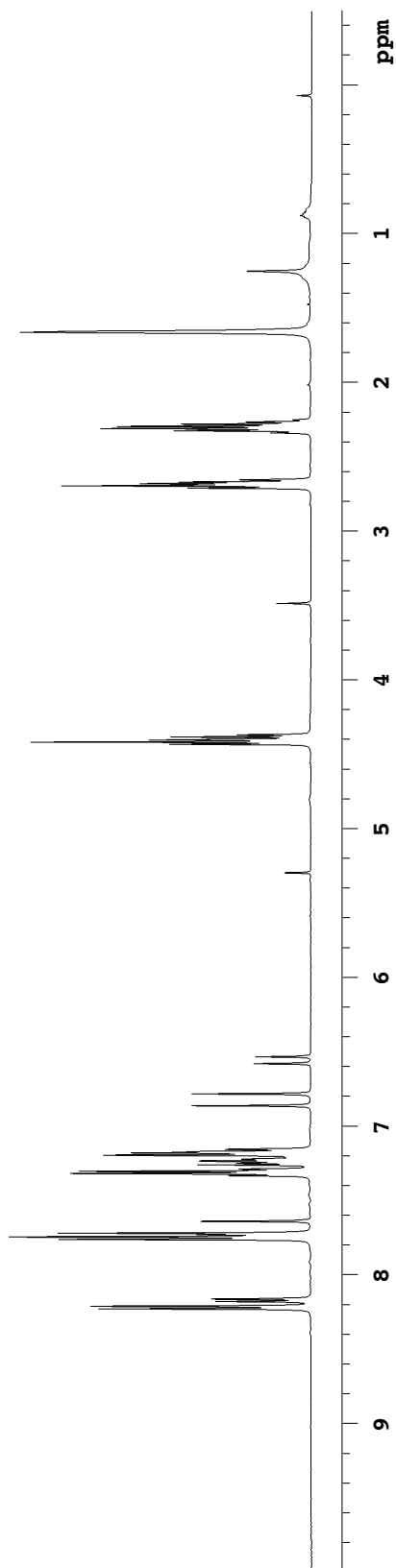
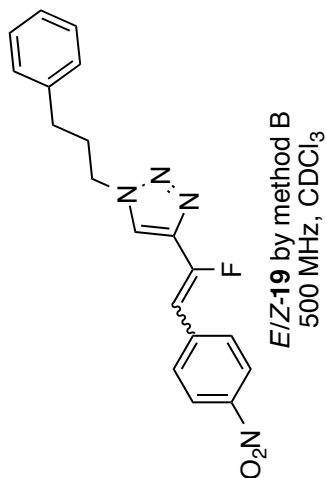
1222-RK-04-314-pure

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

Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-314-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
64 repetitions
OBSERVE H1, 499.7707189 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec



1222-RK-04-328-1stfraction

Archive directory: /export/home/mkl/vmrsys/data

Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-328-1stfraction

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

20 repetitions

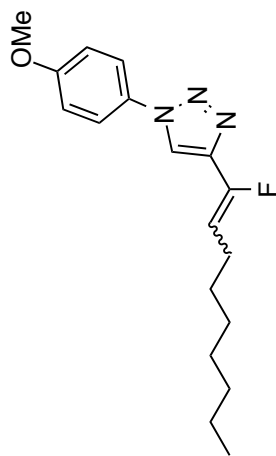
OBSERVE H1, 499.7707189 MHz

DATA PROCESSING

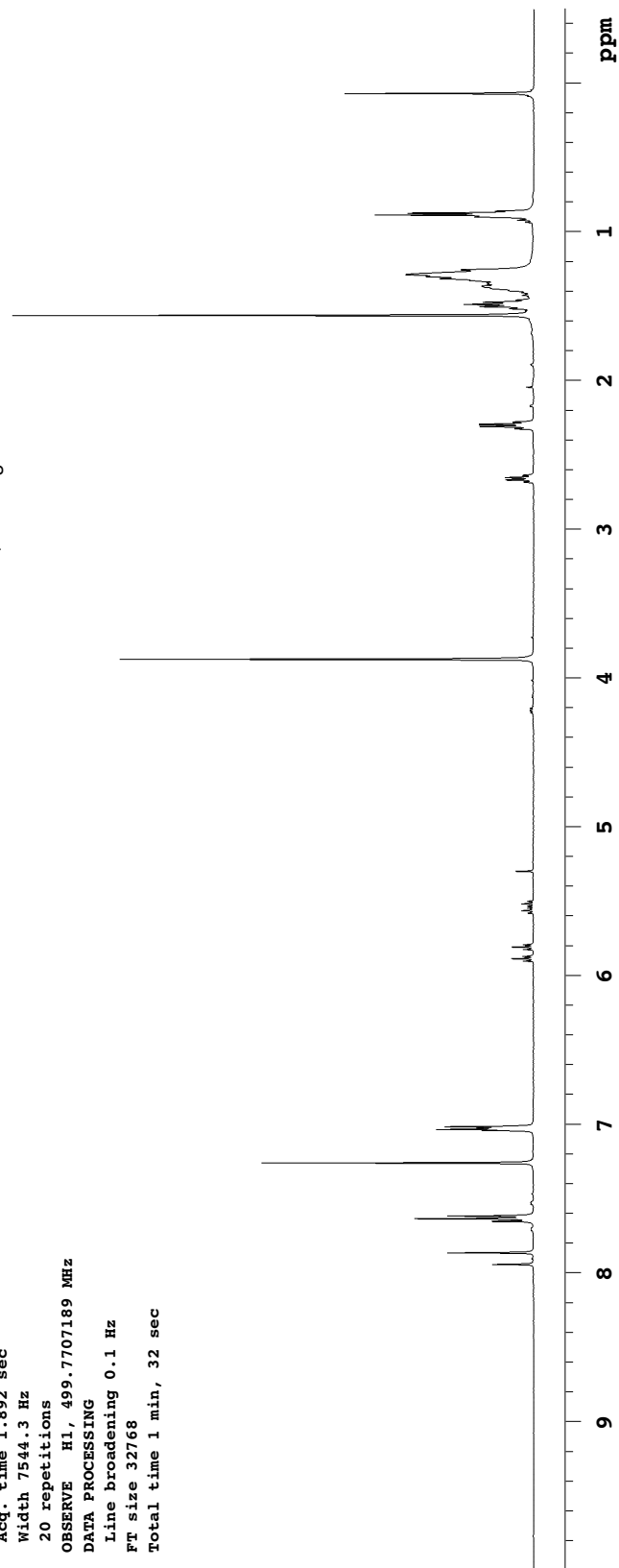
Line broadening 0.1 Hz

FT size 32768

Total time 1 min, 32 sec



E/Z-20 by method B
500 MHz, CDCl₃



1222-RK-04-312-pure-2

Archive directory: /export/home/barbara/vnmrsys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-04-312-pure-2

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

36 repetitions

OBSERVE H1, 499.7707193 MHz

DATA PROCESSING

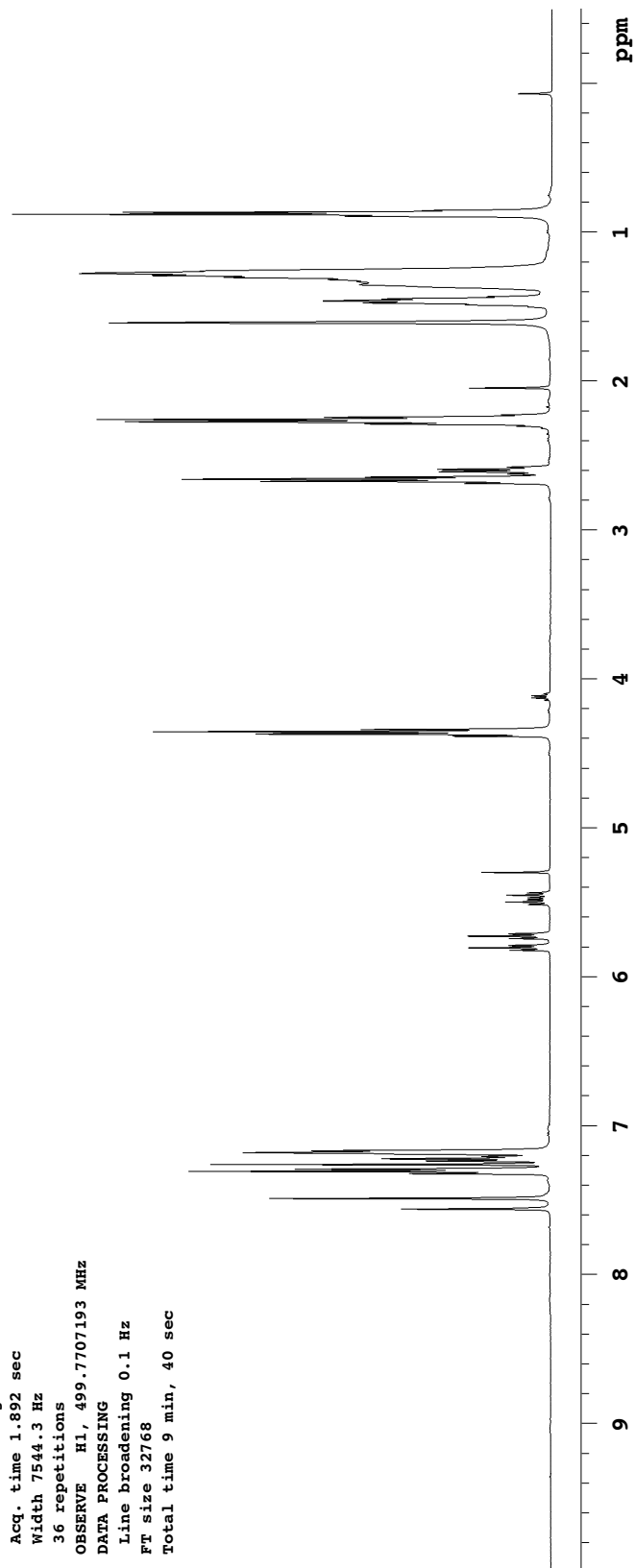
Line broadening 0.1 Hz

FT size 32768

Total time 9 min, 40 sec



E/Z-22 by method B
500 MHz, CDCl₃



1222-RK-05-352

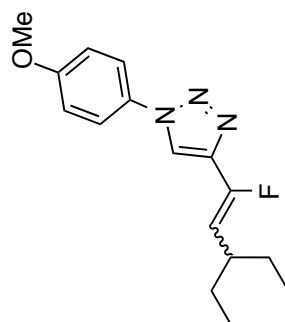
Archive directory: /export/home/mkl/vmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

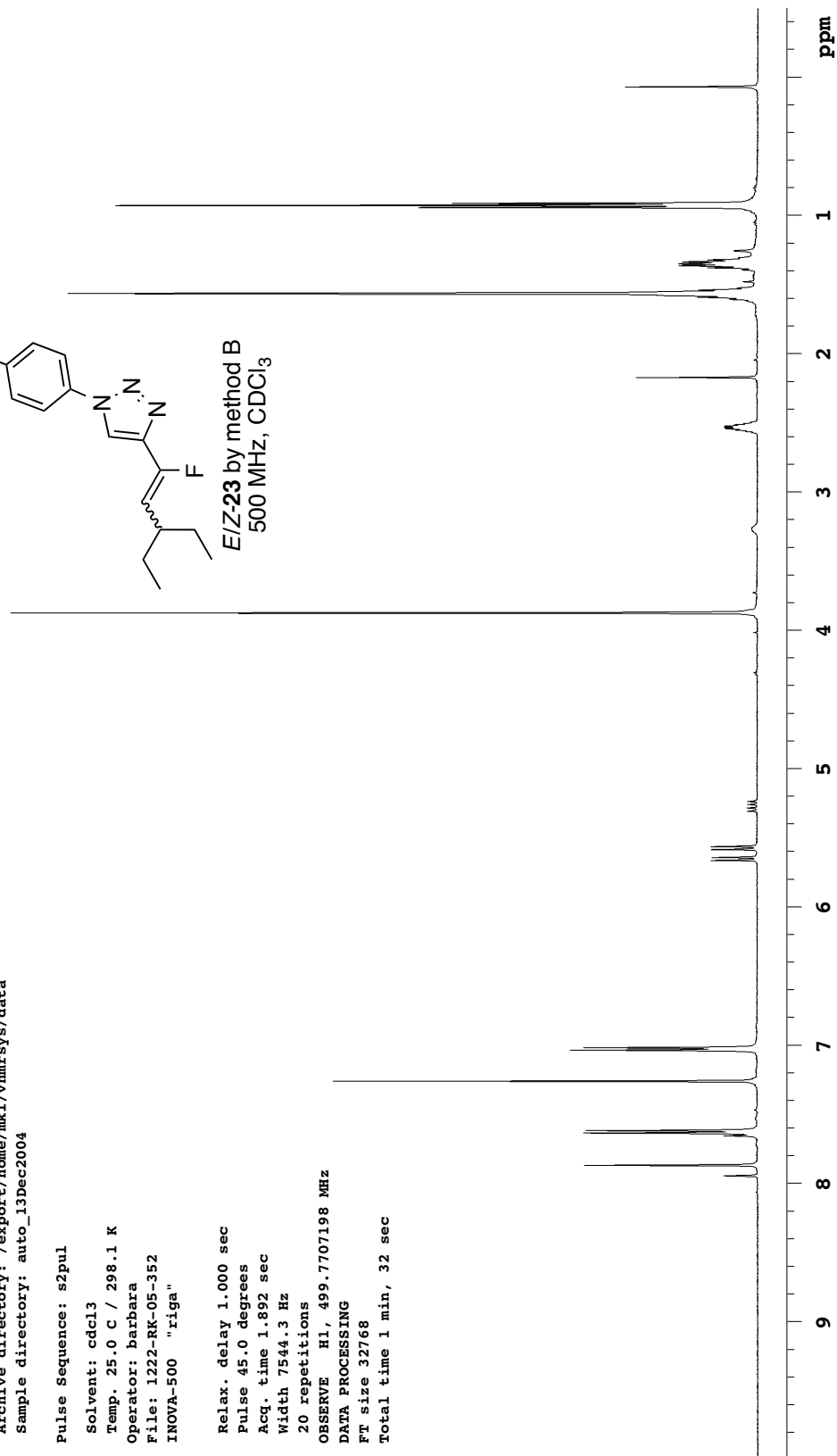
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: Barbara
File: 1222-RK-05-352
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
20 repetitions

OBSERVE H1, 499.7707198 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 32 sec



E/Z-**23** by method B
500 MHz, CDCl₃



1222-RK-05-349

Archive directory: /export/home/mkl/vmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: Barbara
File: 1222-RK-05-349
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10000.0 Hz
48 repetitions

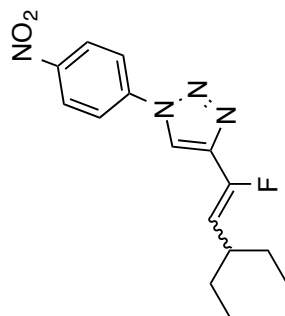
OBSERVE H1, 499.7707203 MHz

DATA PROCESSING

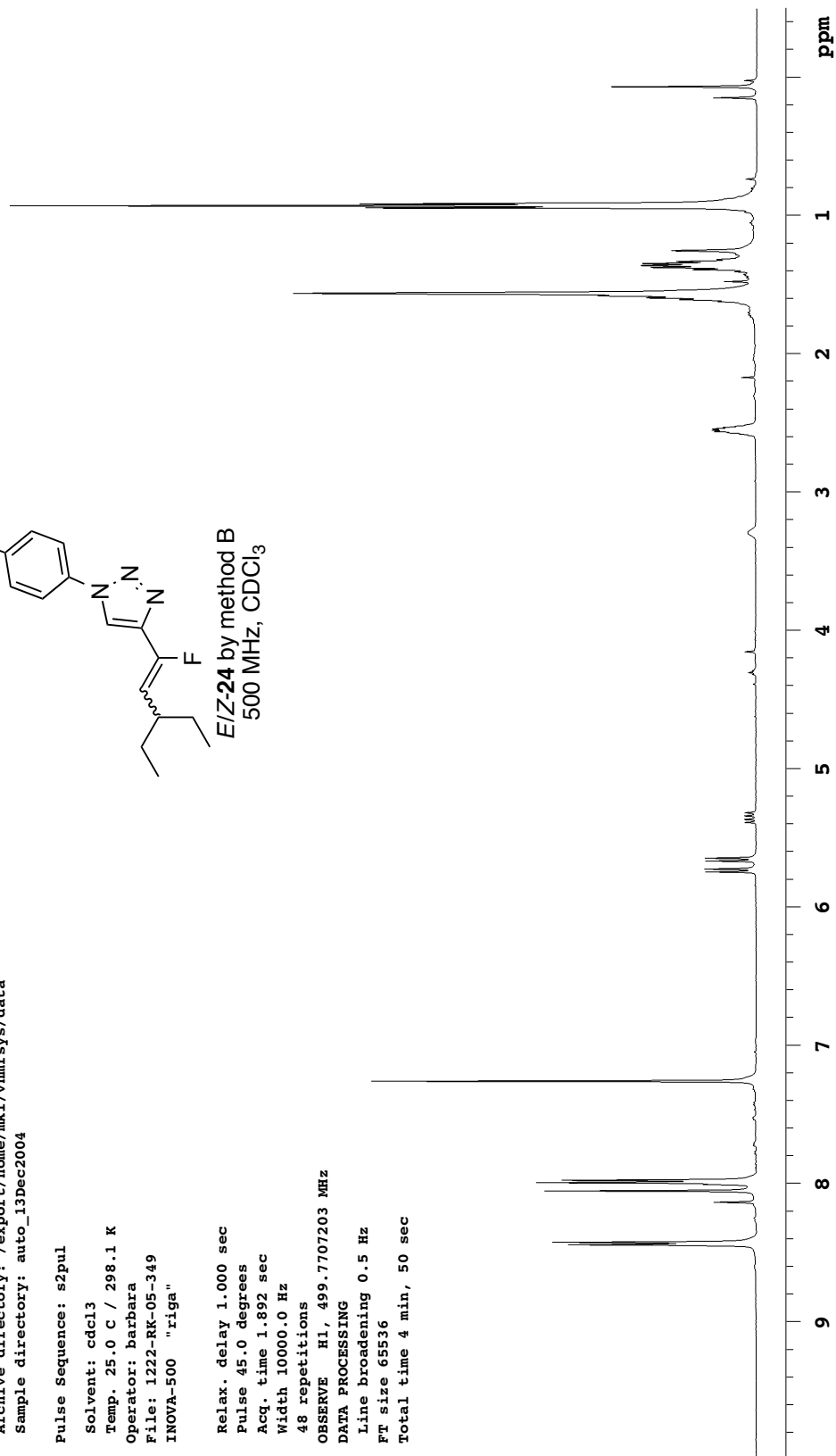
Line broadening 0.5 Hz

FT size 65536

Total time 4 min, 50 sec



E/Z-24 by method B
500 MHz, CDCl₃



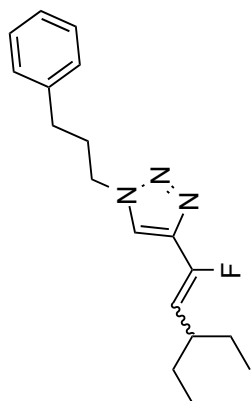
1222-RK-05-336

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13dec2004
File: 1222-RK-05-336

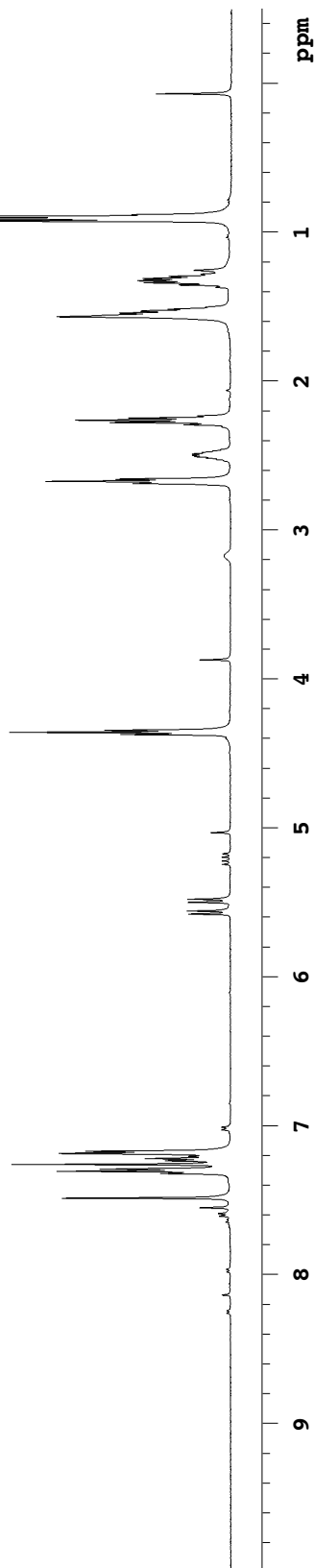
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-336
INOVIA-500 "capella500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
16 repetitions
OBSERVE H1, 499.7707226 MHz
DATA PROCESSING
Line broadening 0.1 Hz
Ft size 32768
Total time 9 min, 40 sec



E/Z-25 by method B
500 MHz, CDCl₃



1222-RK-05-392-pure

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

Sample directory: auto_13dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-05-392-pure

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 10000.0 Hz

16 repetitions

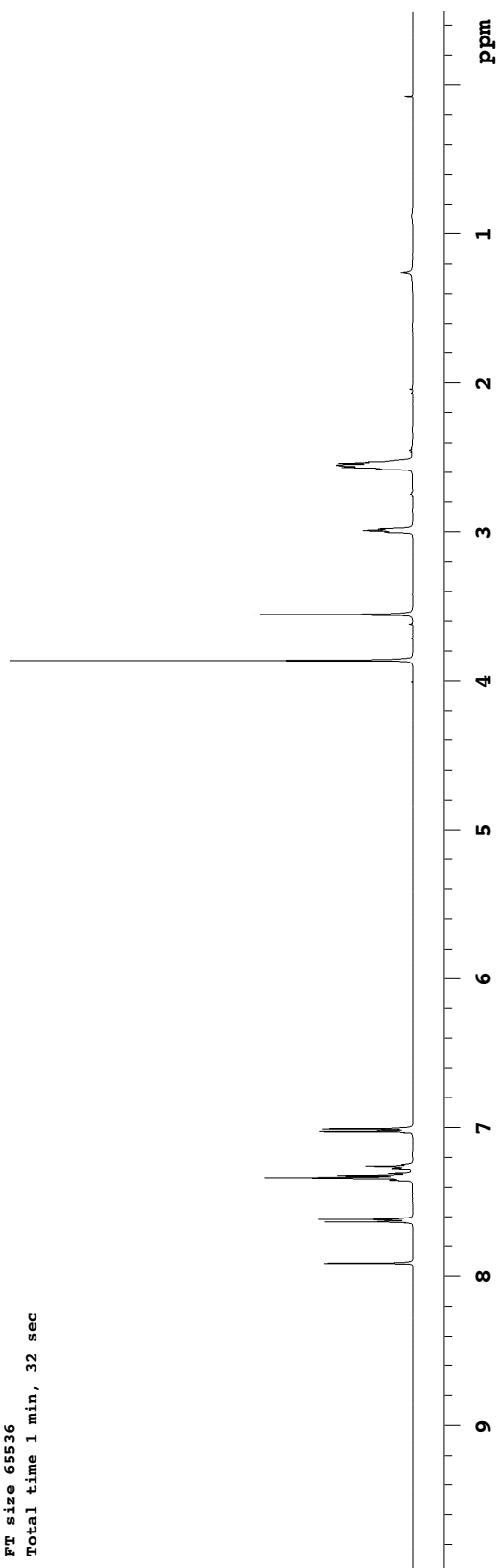
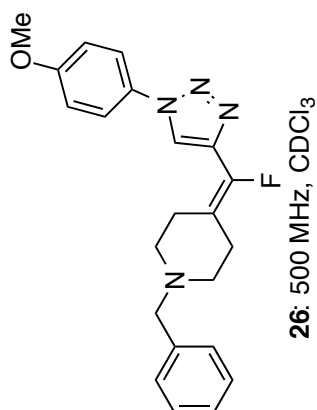
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 1 min, 32 sec



1222-RK-05-392-p-13C

Archive directory: /export/home/barbara/vnmrsys/data

File: 1222-RK-05-392-p-13C

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-05-392-p-13C

INOVA-500 "capella500"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

320 repetitions

OBSERVE C13, 125.6674218 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

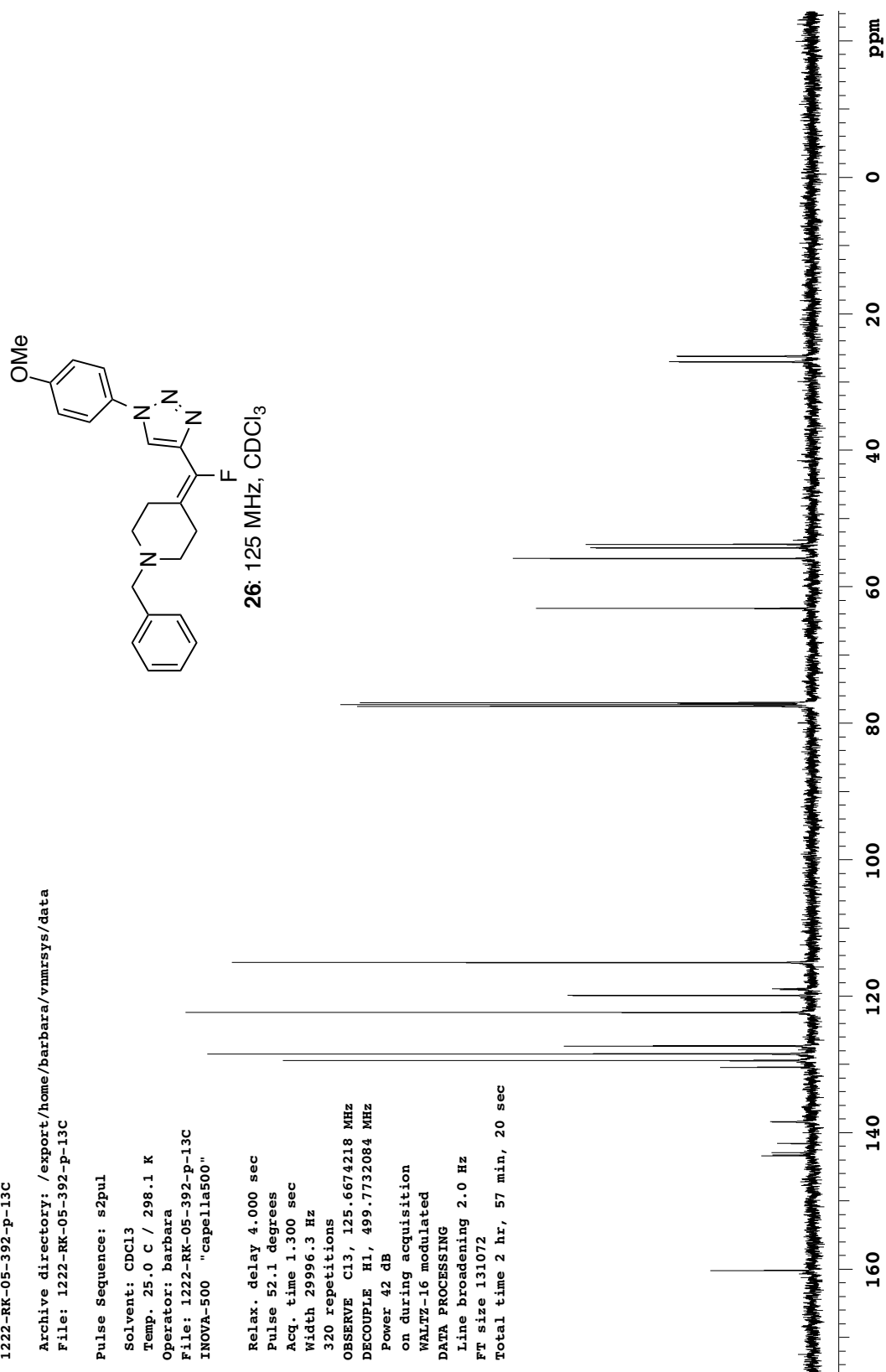
WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

FT size 131072

Total time 2 hr, 57 min, 20 sec



1231-RK-15-30-pure

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

Sample directory: auto_13dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1231-RK-15-30-pure

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

20 repetitions

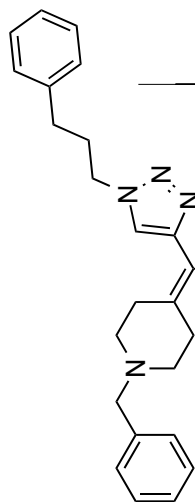
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

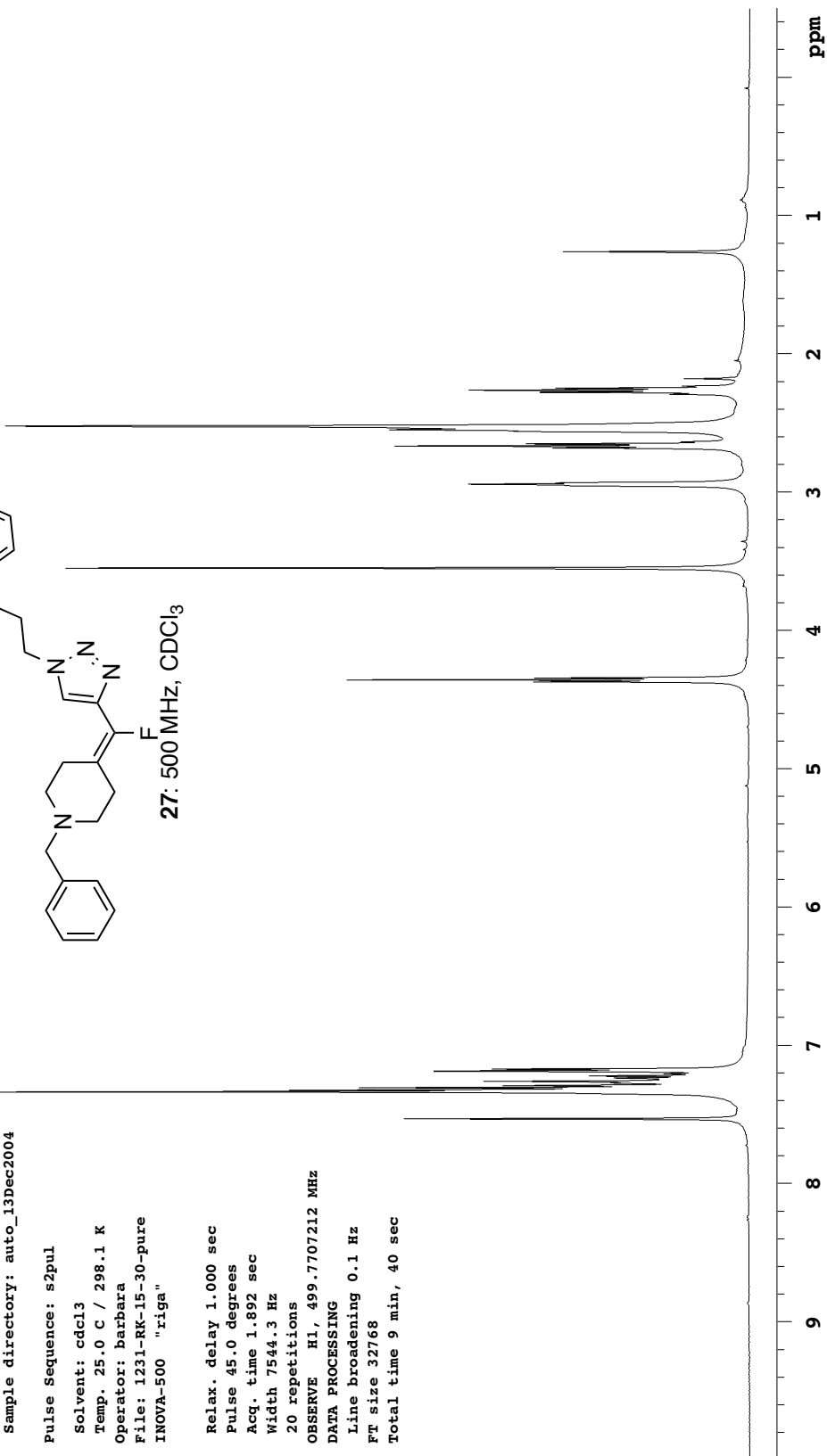
Line broadening 0.1 Hz

FT size 32768

Total time 9 min, 40 sec



27: 500 MHz, CDCl₃



1231-Rk-15-30-13C

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: barbara

File: 1231-Rk-15-30-13C

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

8472 repetitions

OBSERVE C13, 125.6674095 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

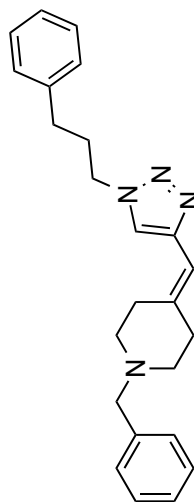
WALTZ-16 modulated

DATA PROCESSING

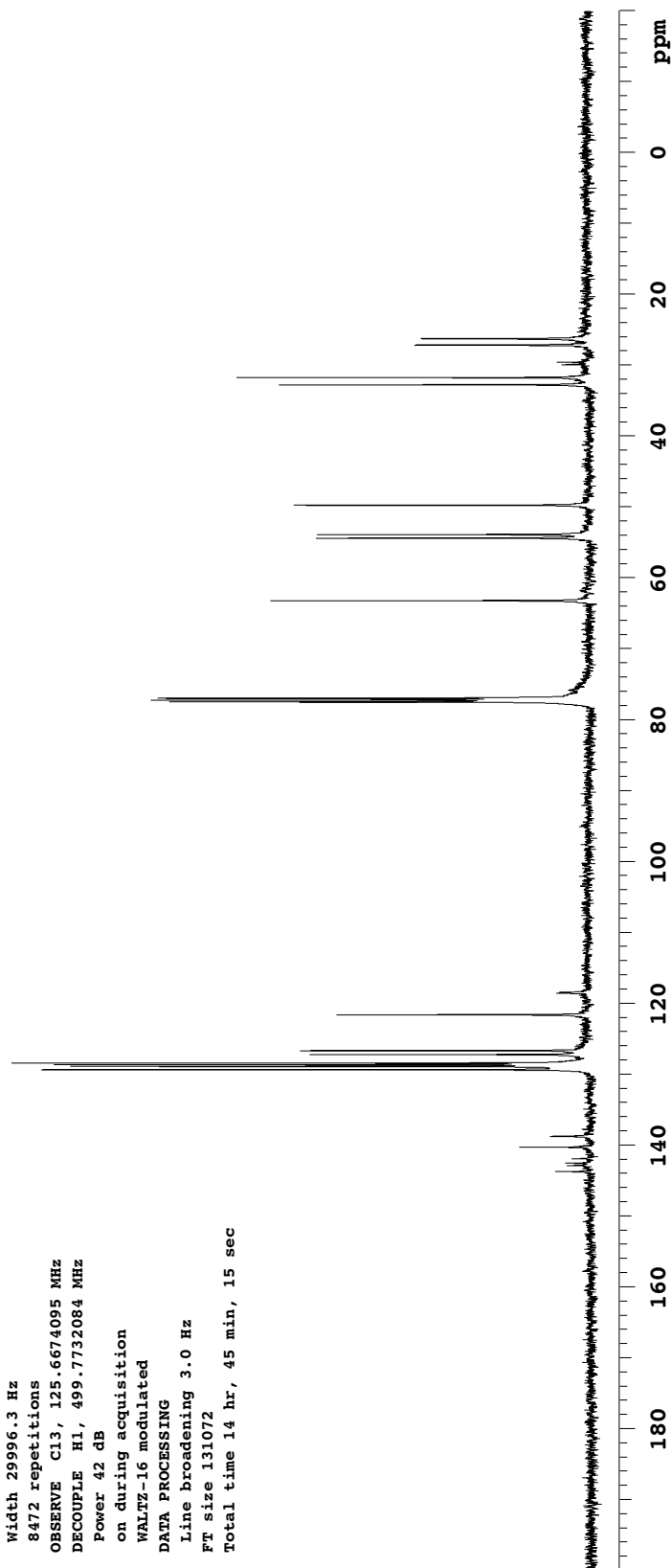
Line broadening 3.0 Hz

FT size 131072

Total time 14 hr, 45 min, 15 sec



27: 125 MHz, CDCl₃



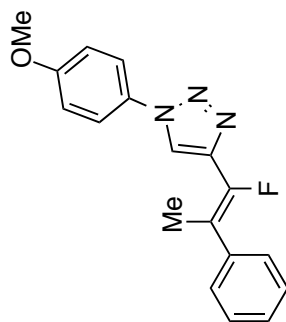
1222-RK-05-381-1

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13dec2004

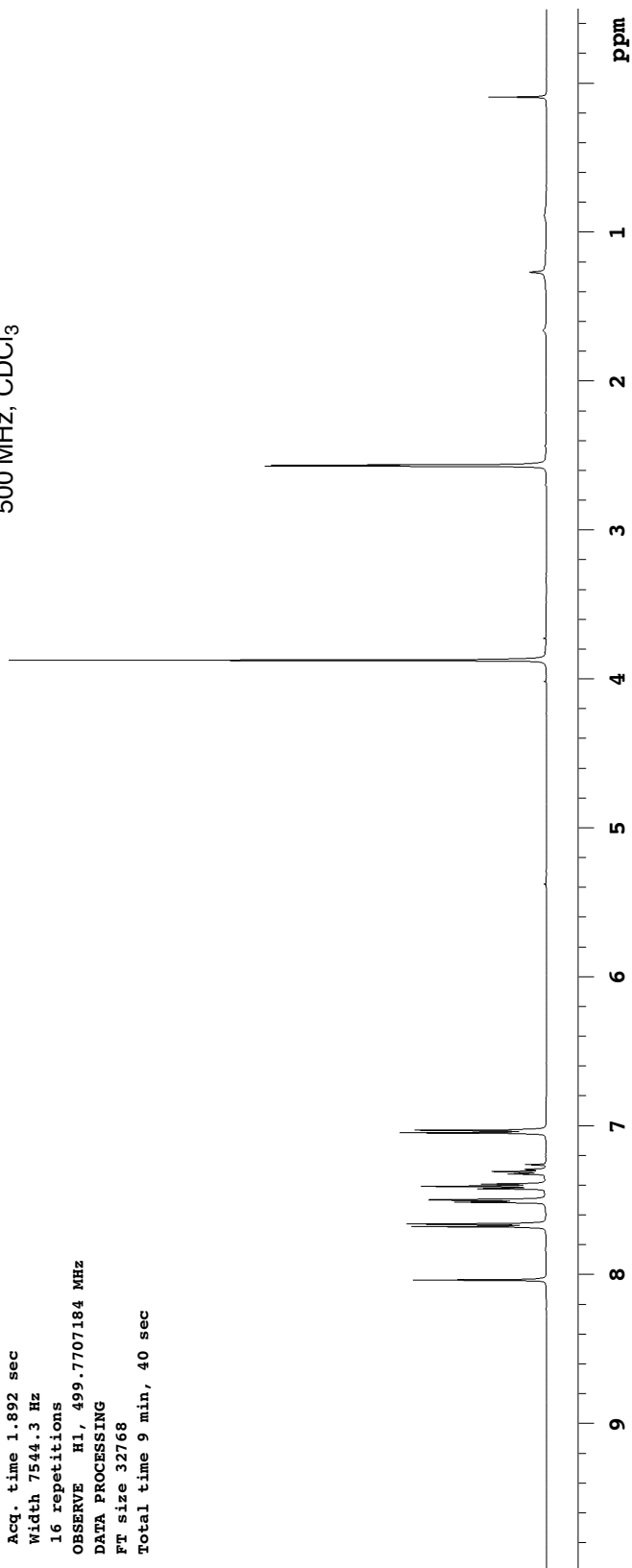
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: Barbara
File: 1222-RK-05-381-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
16 repetitions
OBSERVE H1, 499.7707184 MHz
DATA PROCESSING
Ft size 32768
Total time 9 min, 40 sec



28: Major isomer
500 MHz, CDCl₃



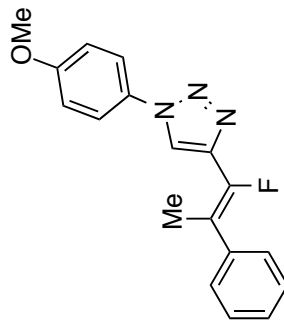
1222-RK-05-381-13C

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

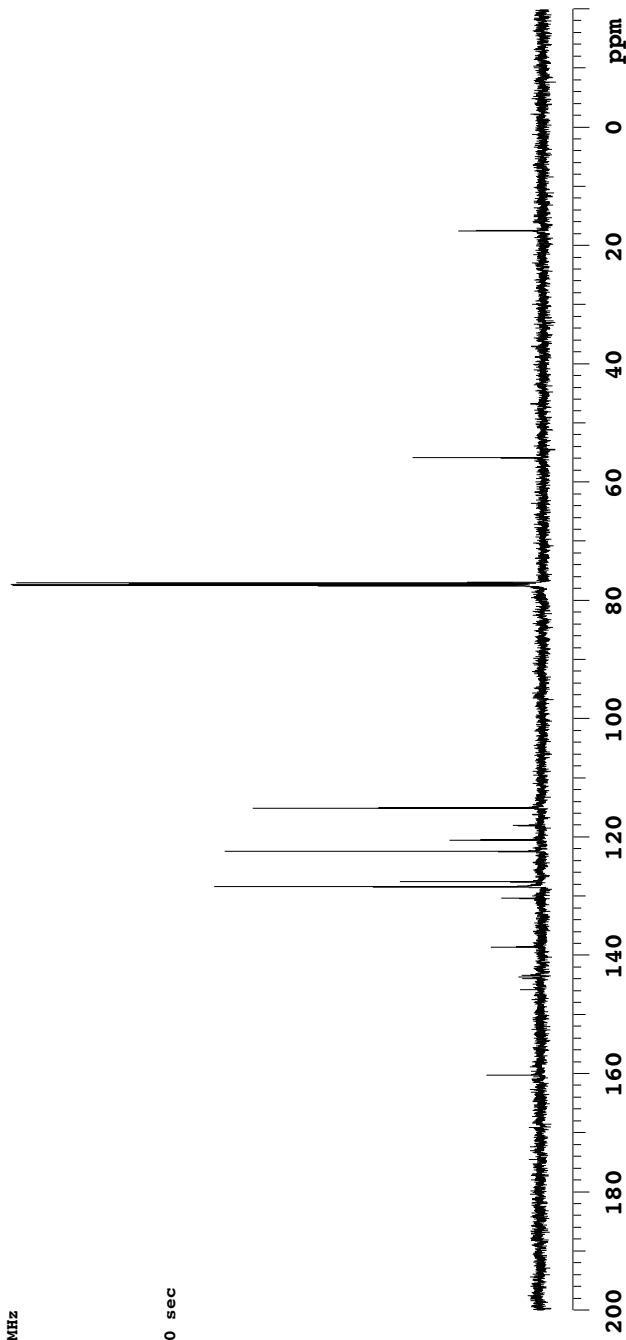
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
Operator: Barbara
File: 1222-RK-05-381-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
176 repetitions
OBSERVE C13, 125.6674214 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 2 hr, 57 min, 20 sec



28: Major isomer
125 MHz, CDCl₃



1222-RK-05-fraction2

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

Sample directory: auto_13dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1222-RK-05-381-fraction2

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 10000.0 Hz

20 repetitions

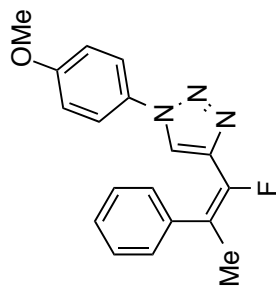
OBSERVE H1, 499.7707212 MHz

DATA PROCESSING

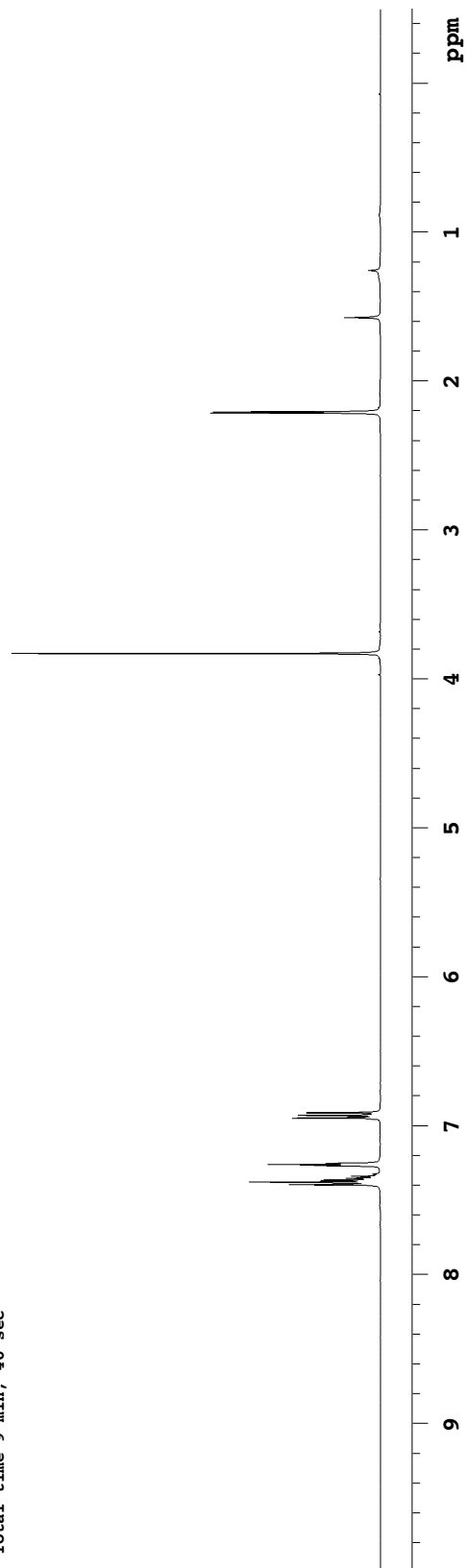
Line broadening 0.1 Hz

FT size 65536

Total time 9 min, 40 sec



28: Minor isomer
500 MHz, CDCl₃



1231-RK-05-381-fraction2-13C

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1231-RK-05-381-fraction2-13C

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

10228 repetitions

OBSERVE C13, 125.6674191 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

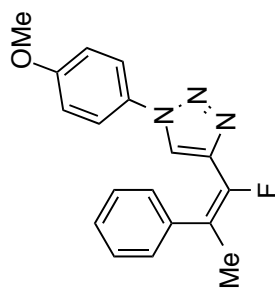
WALTZ-16 modulated

DATA PROCESSING

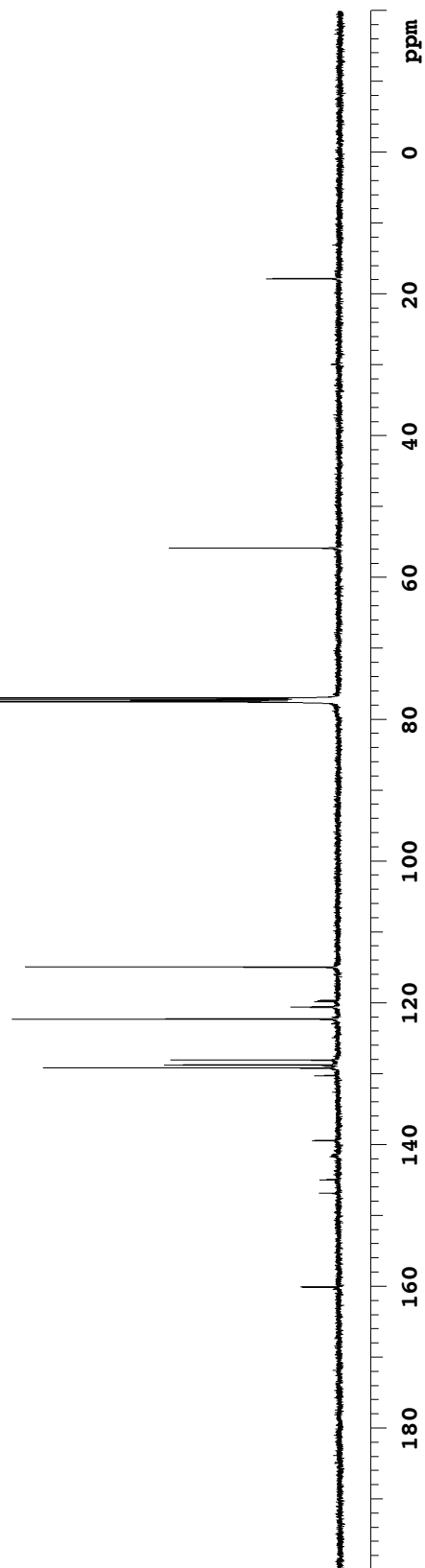
Line broadening 1.0 Hz

FT size 131072

Total time 29 hr, 30 min, 9 sec



28: Minor isomer
125 MHz, CDCl₃



1231-RK-15-31-fraction1

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

Sample directory: auto_13dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1231-RK-15-31-fraction1

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

32 repetitions

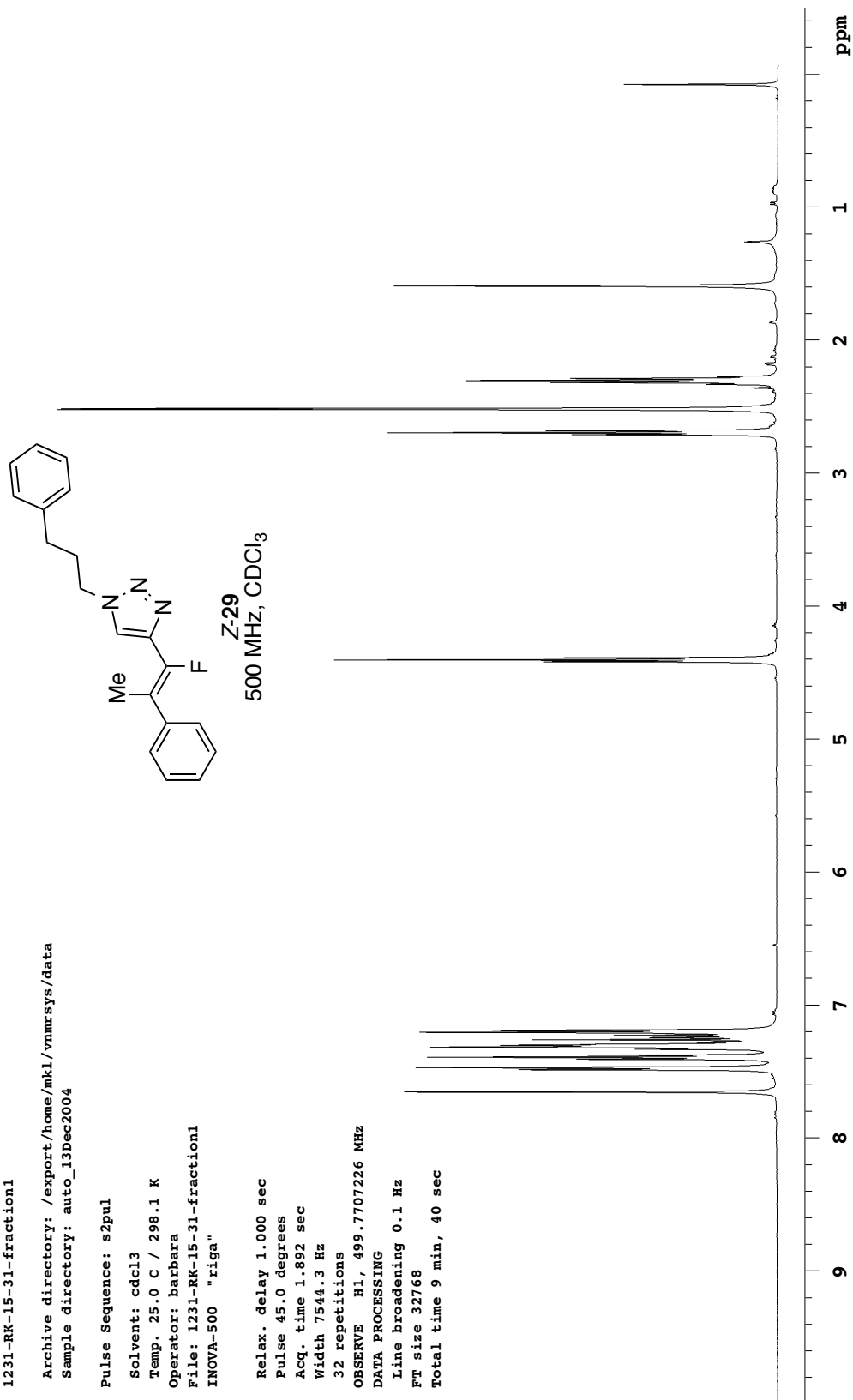
OBSERVE H1, 499.7707226 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 9 min, 40 sec



1231-RK-15-31-fraction1-13C

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

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1231-RK-15-31-fraction1-13C

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

320 repetitions

OBSERVE C13, 125.6674246 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

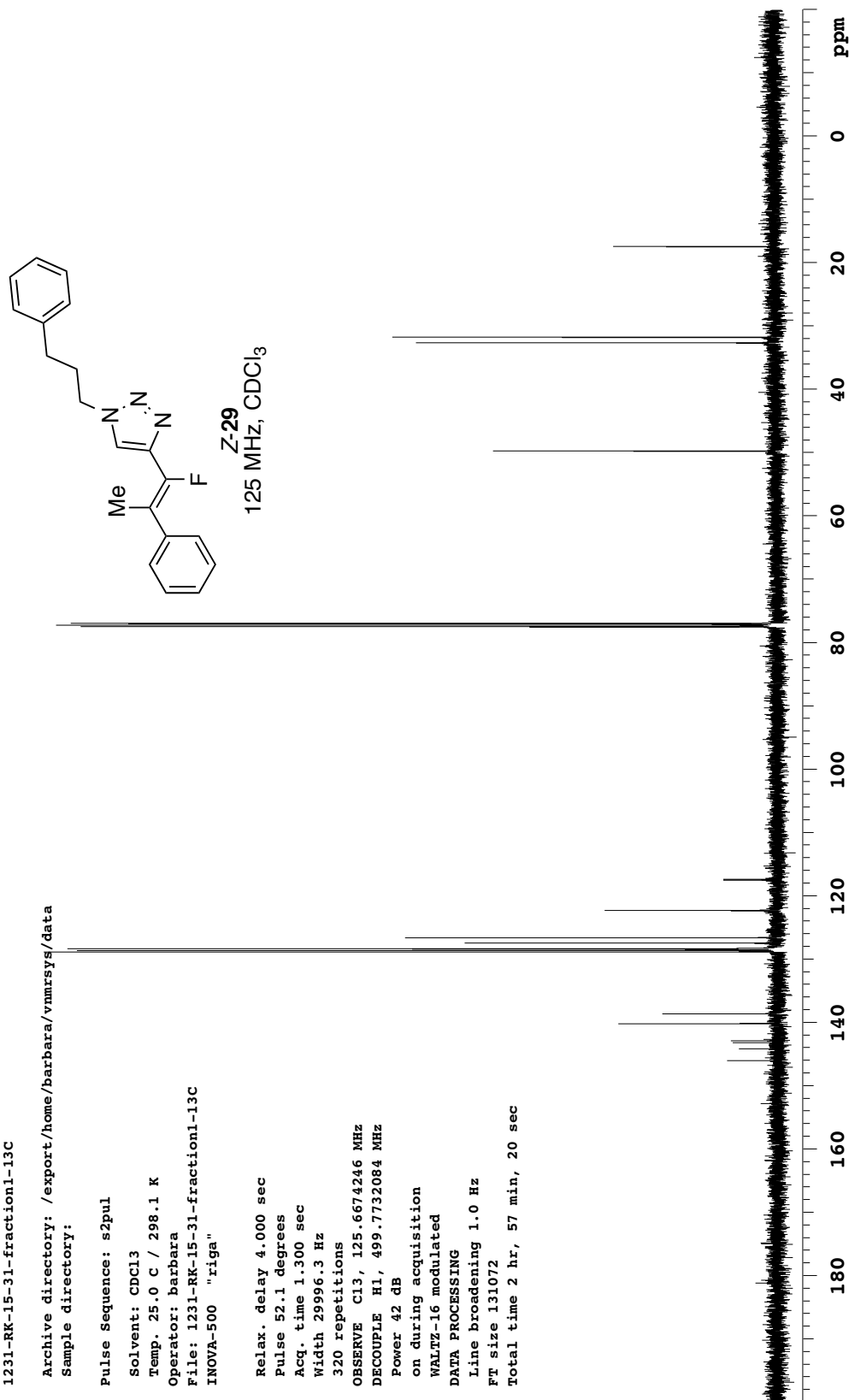
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 2 hr, 57 min, 20 sec



1231-RK-15-31-fraction2

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

Sample directory: auto_13dec2004

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: 1231-RK-15-31-fraction2

INOVA-500 "riga"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 7544.3 Hz

76 repetitions

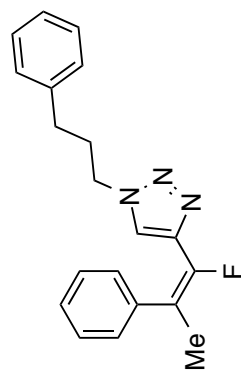
OBSERVE H1, 499.7707221 MHz

DATA PROCESSING

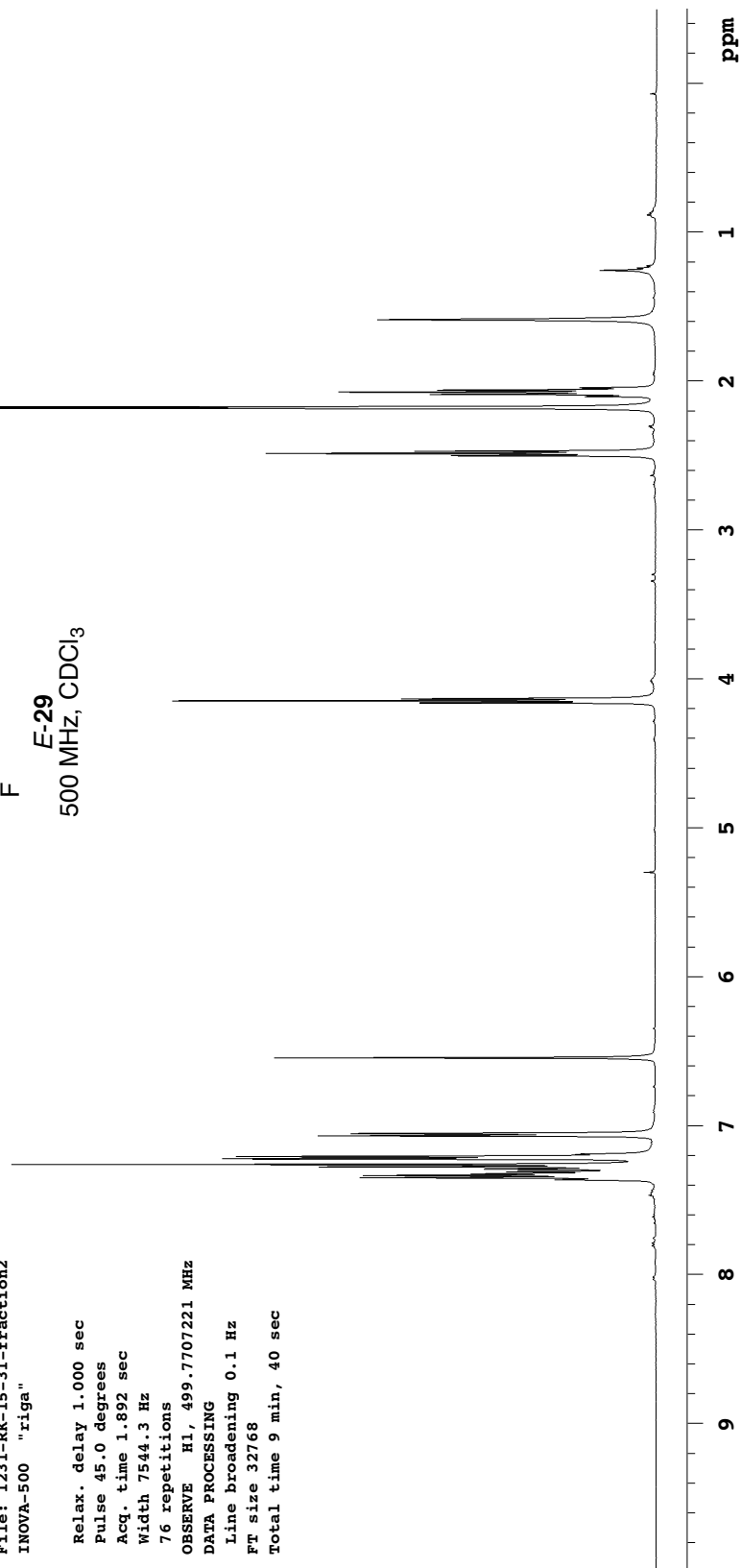
Line broadening 0.1 Hz

FT size 32768

Total time 9 min, 40 sec



E-29
500 MHz, CDCl₃



1231-RK-15-31-fraction2-13C

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: barbara

File: 1231-RK-15-31-fraction2-13C

INOVA-500 "riga"

Relax. delay 4.000 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

10000 repetitions

OBSERVE C13, 125.6674177 MHz

DECOUPLE H1, 499.7732084 MHz

Power 42 dB

on during acquisition

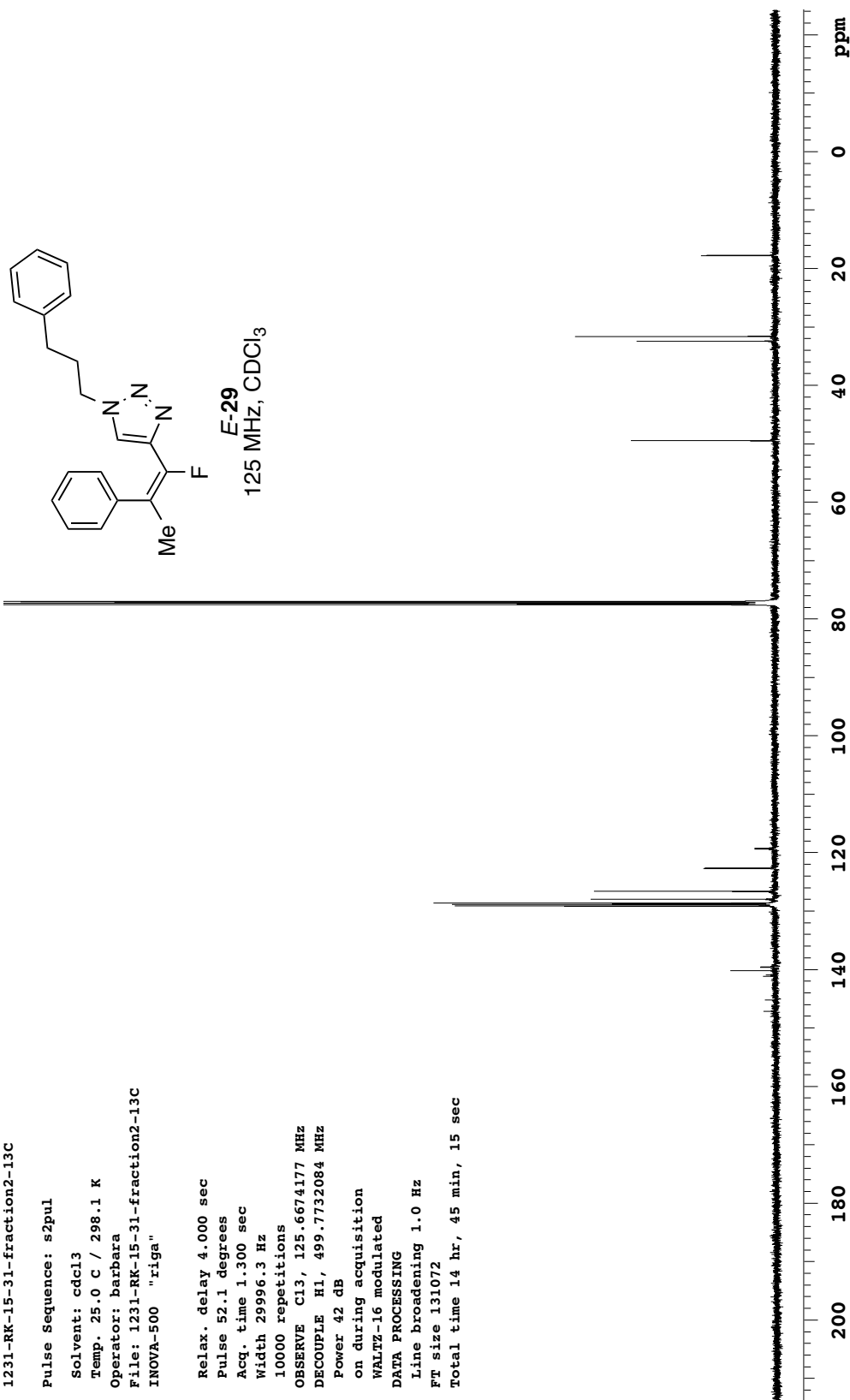
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 14 hr, 45 min, 15 sec



GS-1231-03-209-pure1

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: barbara

File: GS-1231-03-209-pure1

INOVA-500 "r1ga"

Pulse 57.9 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

60 repetitions

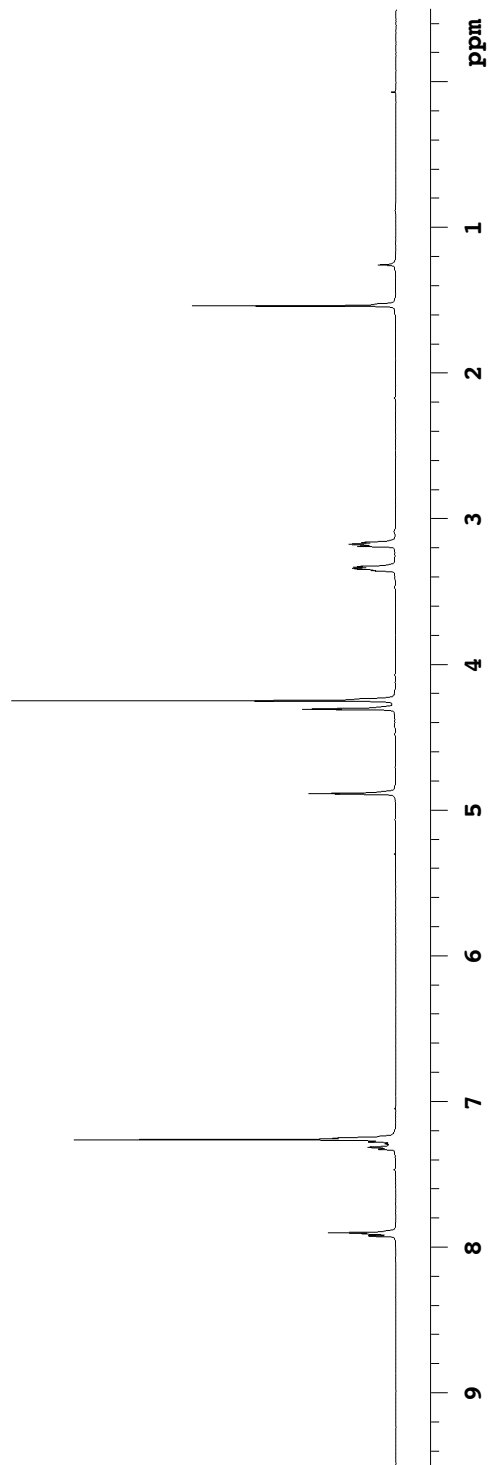
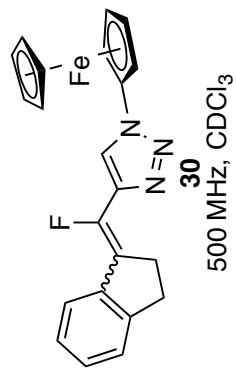
OBSERVE H1, 499.7707217 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 3 min, 10 sec



GS-1231-03-209-pure-cl3-cdcl3

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: Barbara

File: GS-1231-03-209-pure-cl3-cdcl3

INNOVA-500 "riga"

Relax. delay 2.500 sec

Pulse 52.1 degrees

Acq. time 1.300 sec

Width 29996.3 Hz

15188 repetitions

OBSERVE C13, 125.6674223 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 17 hr, 59 min, 35 sec

