

**CHE 344L   Spectroscopic Analysis of an Unknown   Spring 2014**

<b>Section L1—Dr. Fisher   9 students</b>
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- 1**   Benzaldehyde
- 2**   2-Propanol
- 3**   Methyl ethyl ketone (2-butanone)
- 4**   1-Hexene
- 5**   1-Propanol
- 6**   Methylbenzylamine
- 7**   Ethyl acetate
- 8**   Propanoic acid
- 9**   tert-Butanol

<b>Section L2—Dr. Fisher   10 students</b>
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- 10**   Propanoic acid
- 11**   tert-Butanol
- 12**   Benzaldehyde
- 13**   1-Hexene
- 14**   1-Propanol
- 15**   Ethyl acetate
- 16**   2-Propanol
- 17**   Methylbenzylamine
- 18**   Benzoic acid
- 19**   Methyl ethyl ketone

<b>Section L3—Dr. Fisher    10 students</b>
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- 20    Propanoic acid
- 21    2-Propanol
- 22    Benzaldehyde
- 23    1-Propanol
- 24    Methylbenzylamine
- 25    1-Hexene
- 26    Ethyl acetate
- 27    Benzoic acid
- 28    tert-Butanol
- 29    Methylbenzylamine

<b>Section L4—Ms Tsesarskaia    13 students</b>
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- 30    Benzoic acid
- 31    Benzaldehyde
- 32    Methylbenzylamine
- 33    1-Propanol
- 34    Methyl ethyl ketone (2-butanone)
- 35    1-Hexene
- 36    Ethyl acetate
- 37    Propanoic acid
- 38    Methyl ethyl ketone

- 39 2-Propanol
- 40 Methylbenzylamine
- 41 tert-Butanol
- 42 1-Hexene



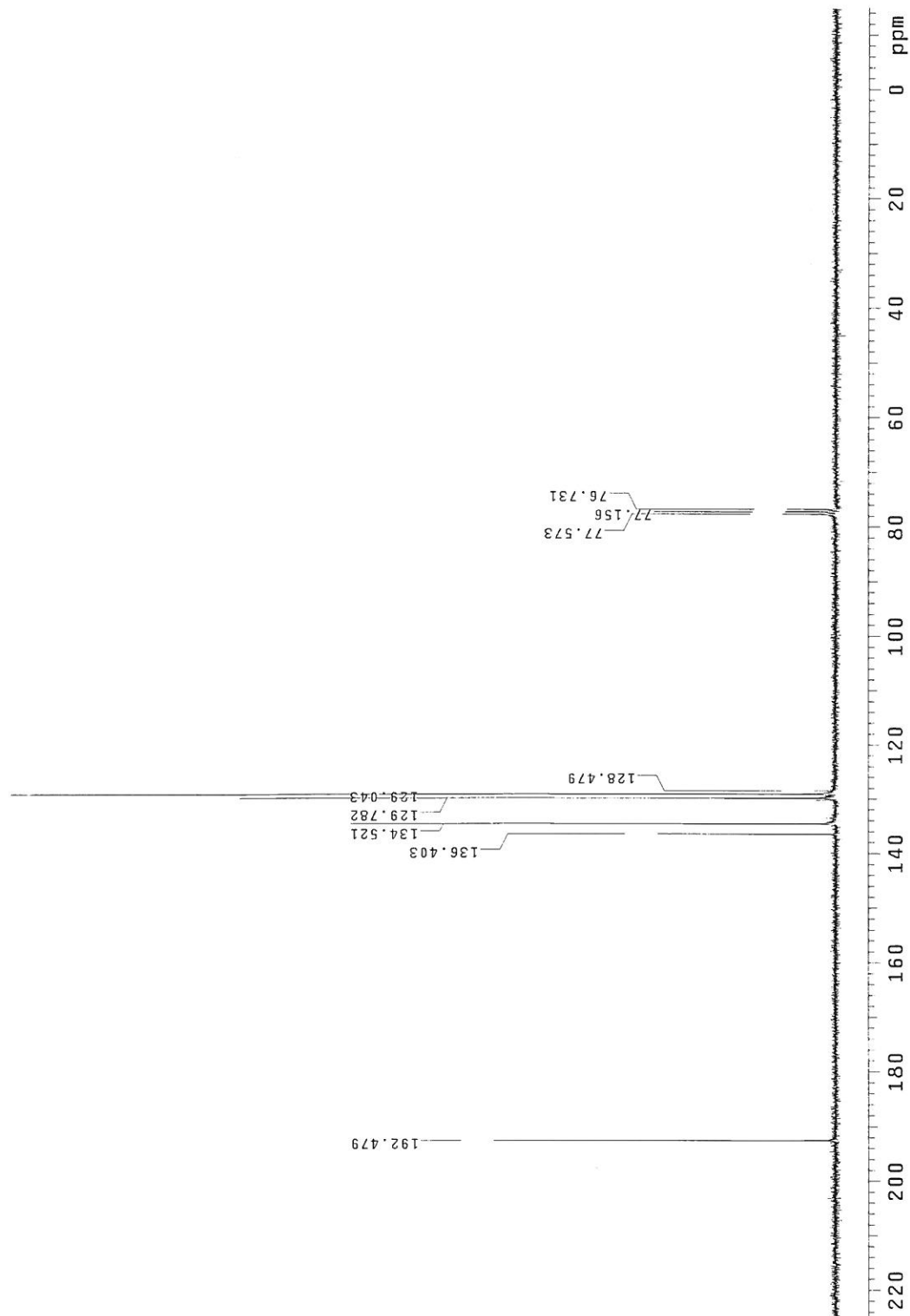
unk 1 spring 2014

Sample: unk 1 spring 2014  
Sample ID: s20140404\_05  
File: 0049.fid

Pulse Sequence: s2pul

Solvent: cdc13  
Temp: 20.0 C / 293.1 K  
Operator: che344  
File: 0049 "nmr300"  
INOVA-300

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
512 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 19 min, 42 sec





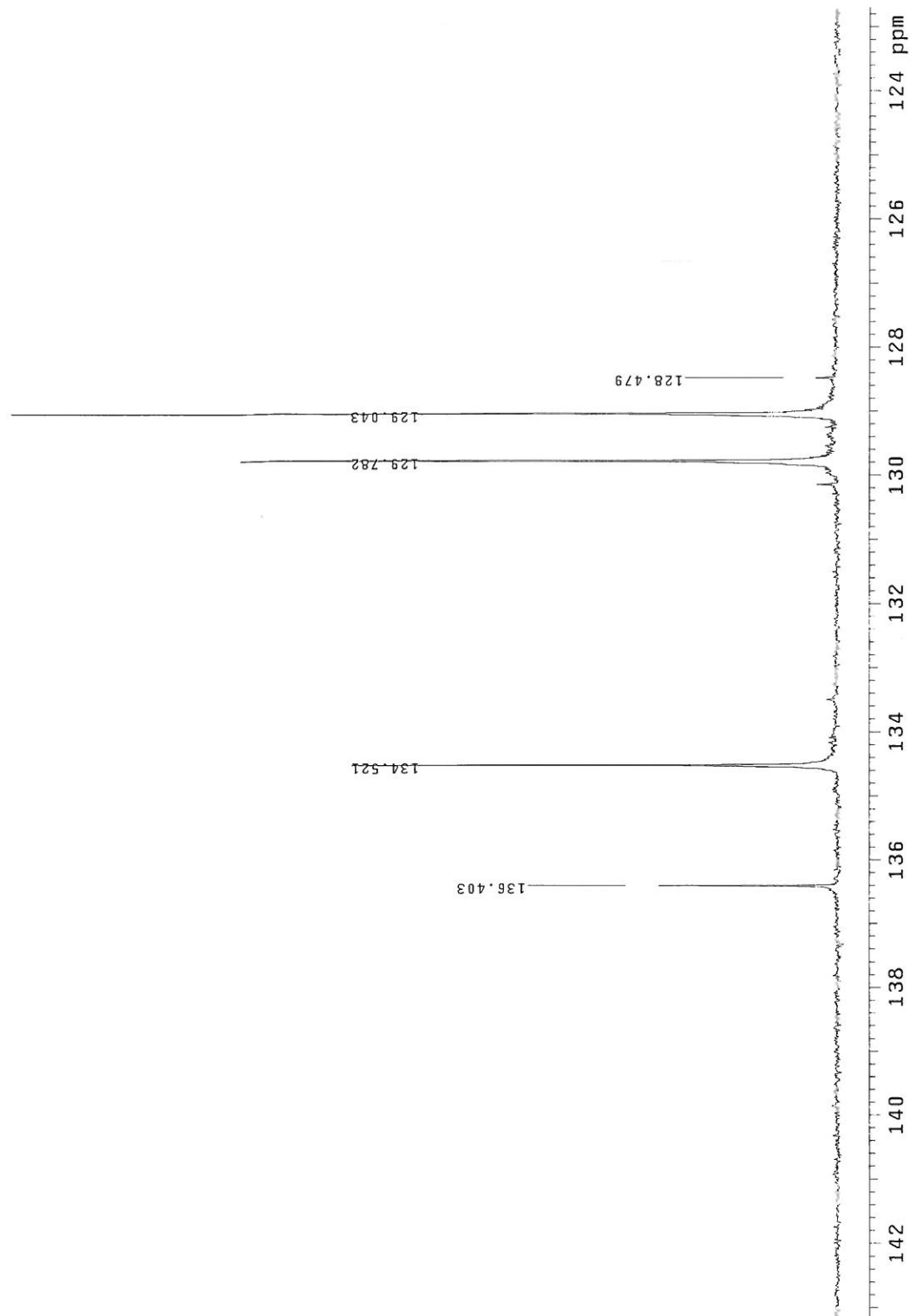
unk 1 spring 2014

Sample: unk 1 spring 2014  
Sample ID: s\_20140404\_05  
File: 0049.fid

Pulse Sequence: s2pul

Solvent: cdc13  
Temp: 20.0 C / 293.1 K  
Operator: che344  
File: 0049  
INNOVA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
512 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 19 min, 42 sec







unk 2 spring 2014

Sample: unk 2 spring 2014

Sample ID: s\_20140404\_07

File: /home/che344/vnmrSYS/data/che344spring2014/unk2c13-256scans.fid

Pulse Sequence: s2pu1

Solvent: cdCl3

Temp: 20.0 C / 293.1 K

Operator: che344

File: unk2c13-256scans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

256 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

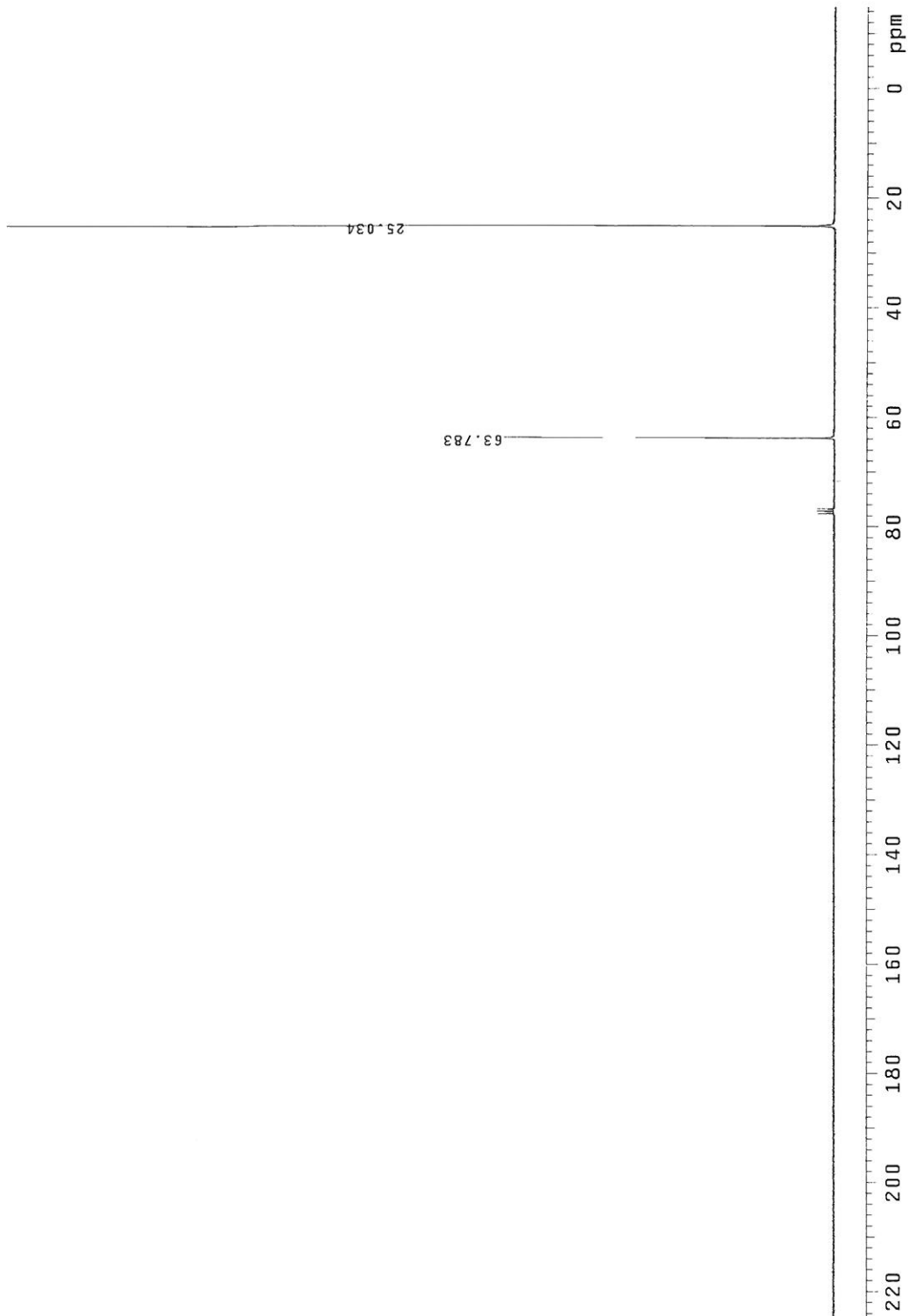
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 51 sec





unk 2 spring 2014

Sample: unk 2 spring 2014

Sample ID: s\_20140404\_07

File: /home/che344/vnmrSYS/data/che344spring2014/unk2c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 20.0 C / 293.1 K

Operator: che344

File: unk2c13-256scans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

256 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

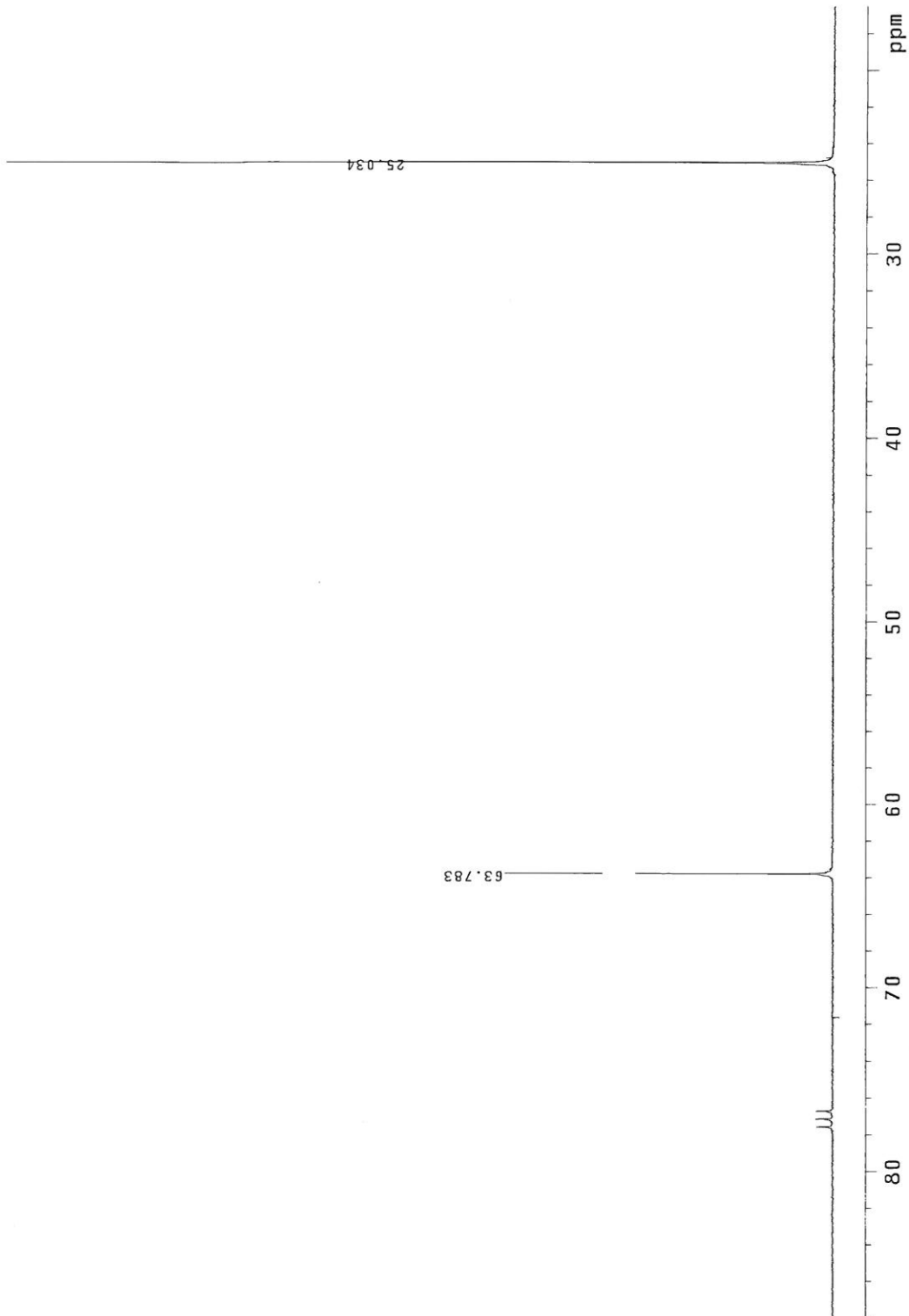
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 51 sec





unk 3 spring 2014

Sample: unk 3 spring 2014

Sample ID: s\_20140404\_08

File: /home/che344/vnmrsys/data/che344spring2014/unk3c13-5kscans.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp: 20.0 C / 293.1 K

Operator: che344

File: unk3c13-5kscans

INNOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

5000 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

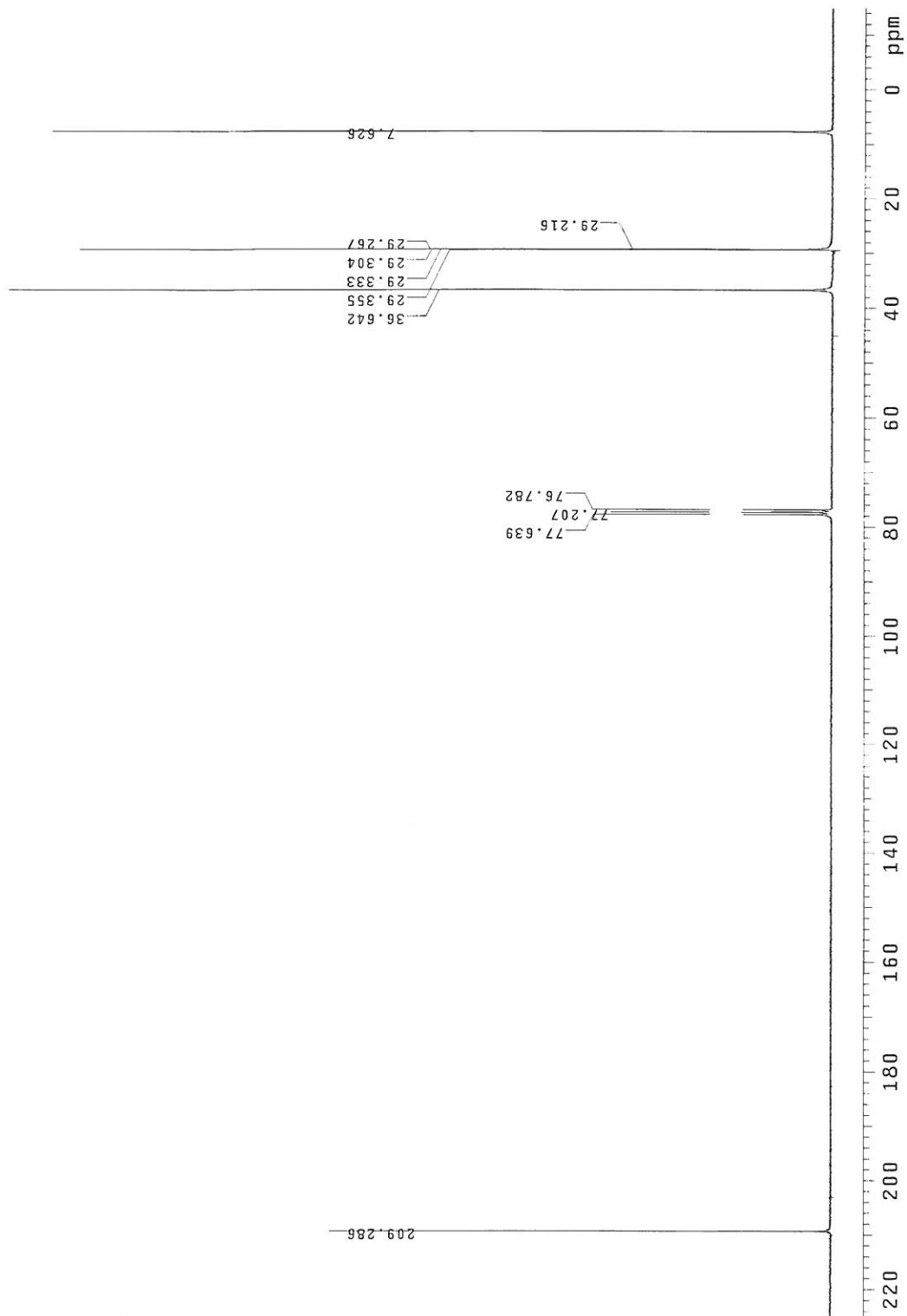
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 3 hr, 12 min, 27 sec





unk 3 spring 2014

Sample: unk 3 spring 2014

Sample ID: S\_20140404\_08

File: /home/che344/vnmrSYS/data/che344spring2014/unk3c13-5kscans.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 20.0 C / 293.1 K

Operator: che344

File: unk3c13-5kscans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

5000 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

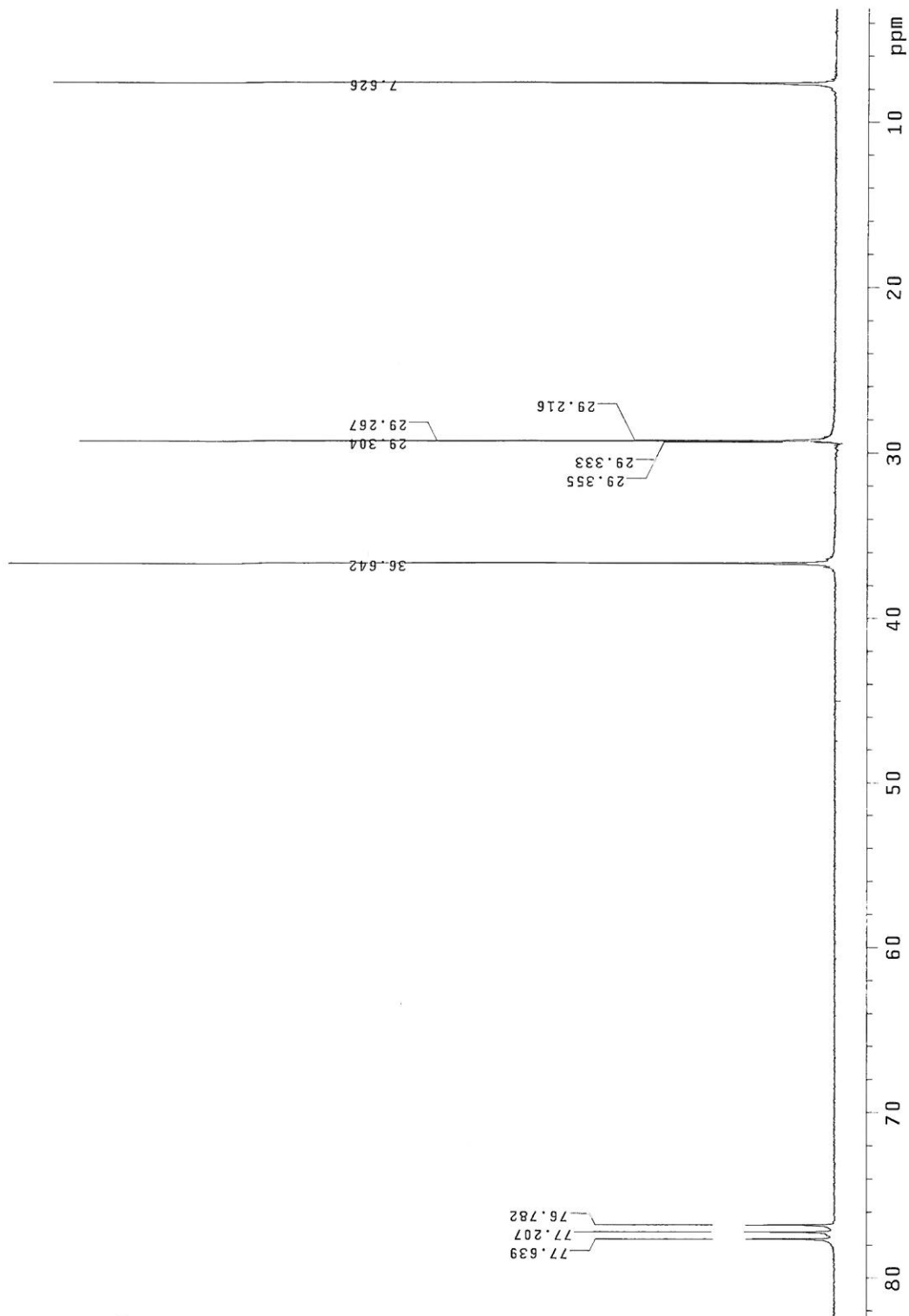
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 3 hr, 12 min, 27 sec







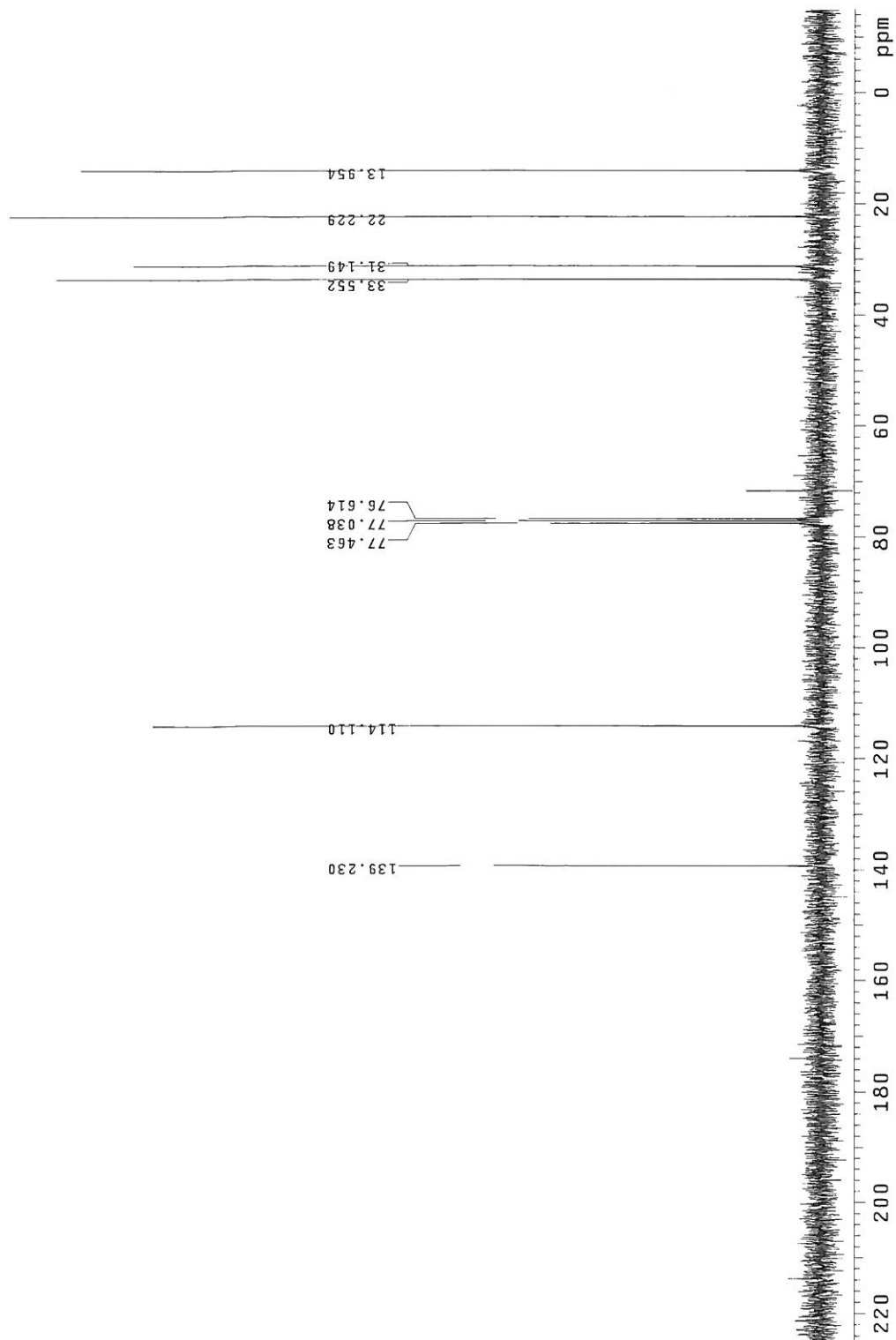
unk 4spring 2014

Sample: unk 4 spring 2014  
Sample ID: s.20140406.01  
File: /home/che344/vnmrSYS/data/che344spring2014/unk4c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdcl3  
Temp: 20.0 C / 293.1 K  
Operator: che344  
File: unk4c13-256scans  
INOVA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
256 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec





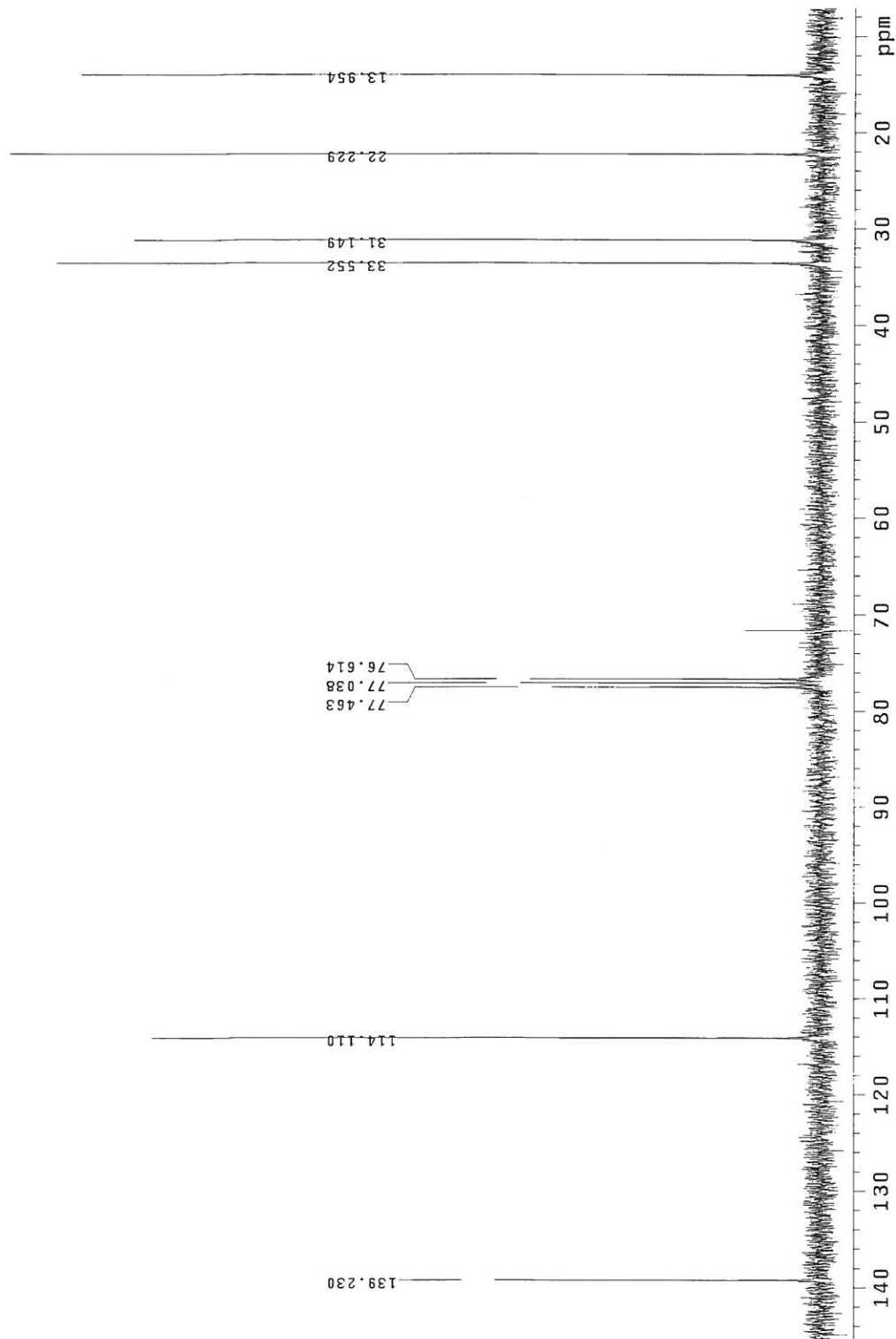
unk 4spring 2014

Sample: unk 4 spring 2014  
Sample ID: s\_20140406\_01  
File: /home/che344/vnmrSYS/data/che344spring2014/unk4c13-256scans.fid

Pulse Sequence: s2pu1

Solvent: cdcl3  
Temp: 20.0 C / 293.1 K  
Operator: che344  
File: unk4c13-256scans  
INOVA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
256 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec





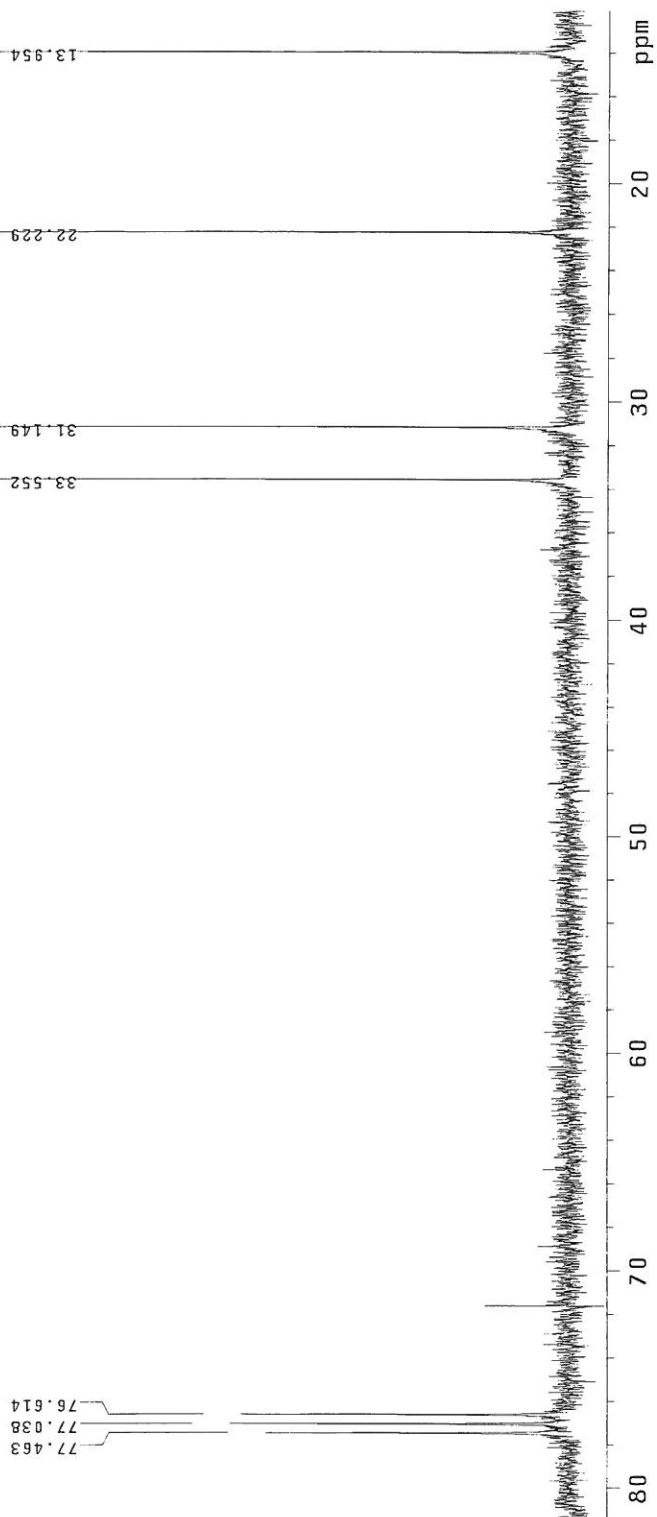
unk 4spring 2014

Sample: unk 4 spring 2014  
Sample ID: s\_20140406\_01  
File: /home/che344/vnmrsys/data/che344spring2014/unk4c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdcl3  
Temp. 20.0 C / 293.1 K  
Operator: che344  
File: unk4c13-256scans  
INOVA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
256 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec





unk 5spring 2014

Sample: unk 5 spring 2014

Sample ID: s\_20140406\_02

File: /home/che344/vnmrsys/data/che344spring2014/unk5c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp: 20.0 C / 293.1 K

Operator: che344

File: unk5c13-256scans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

256 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

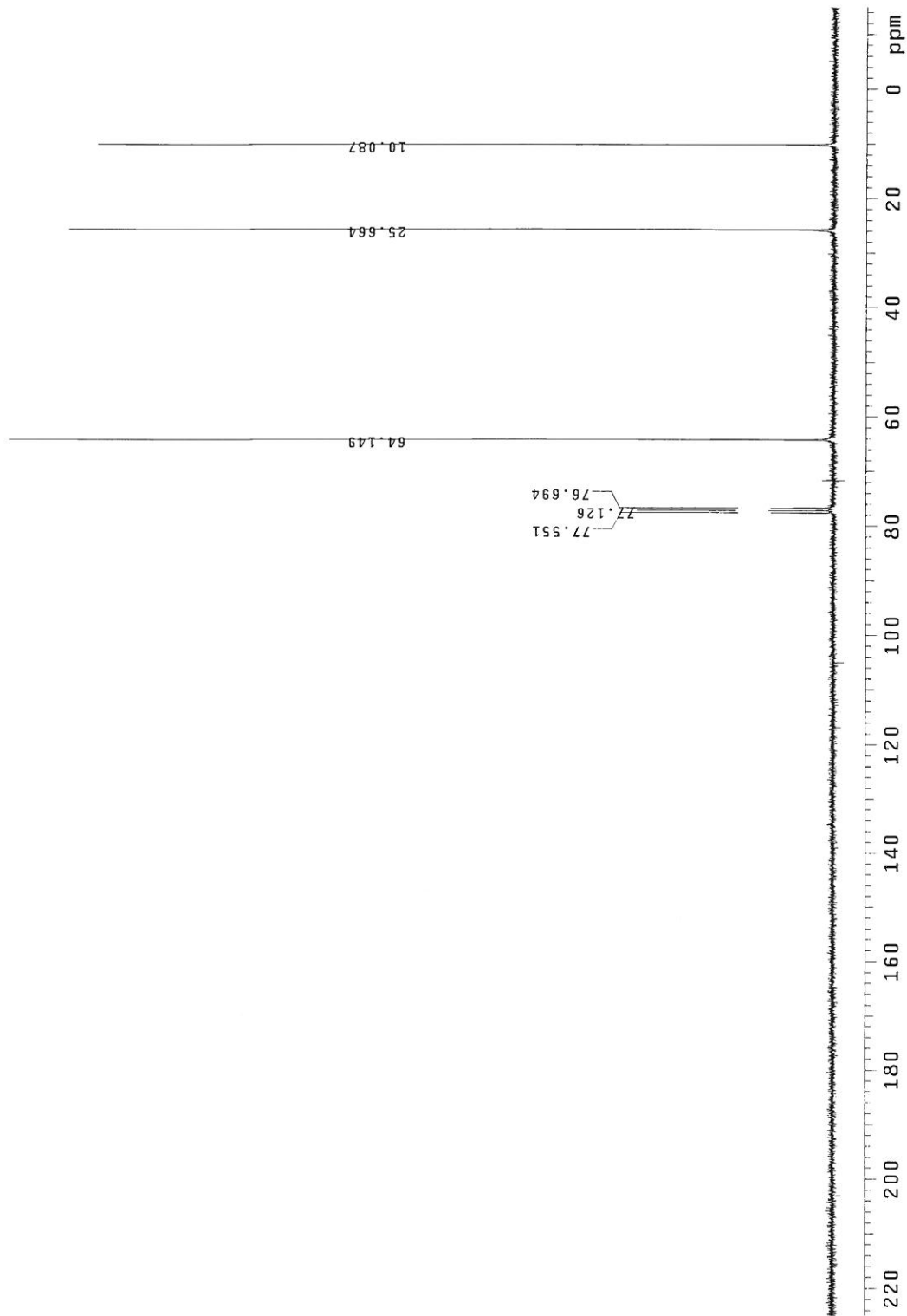
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 51 sec



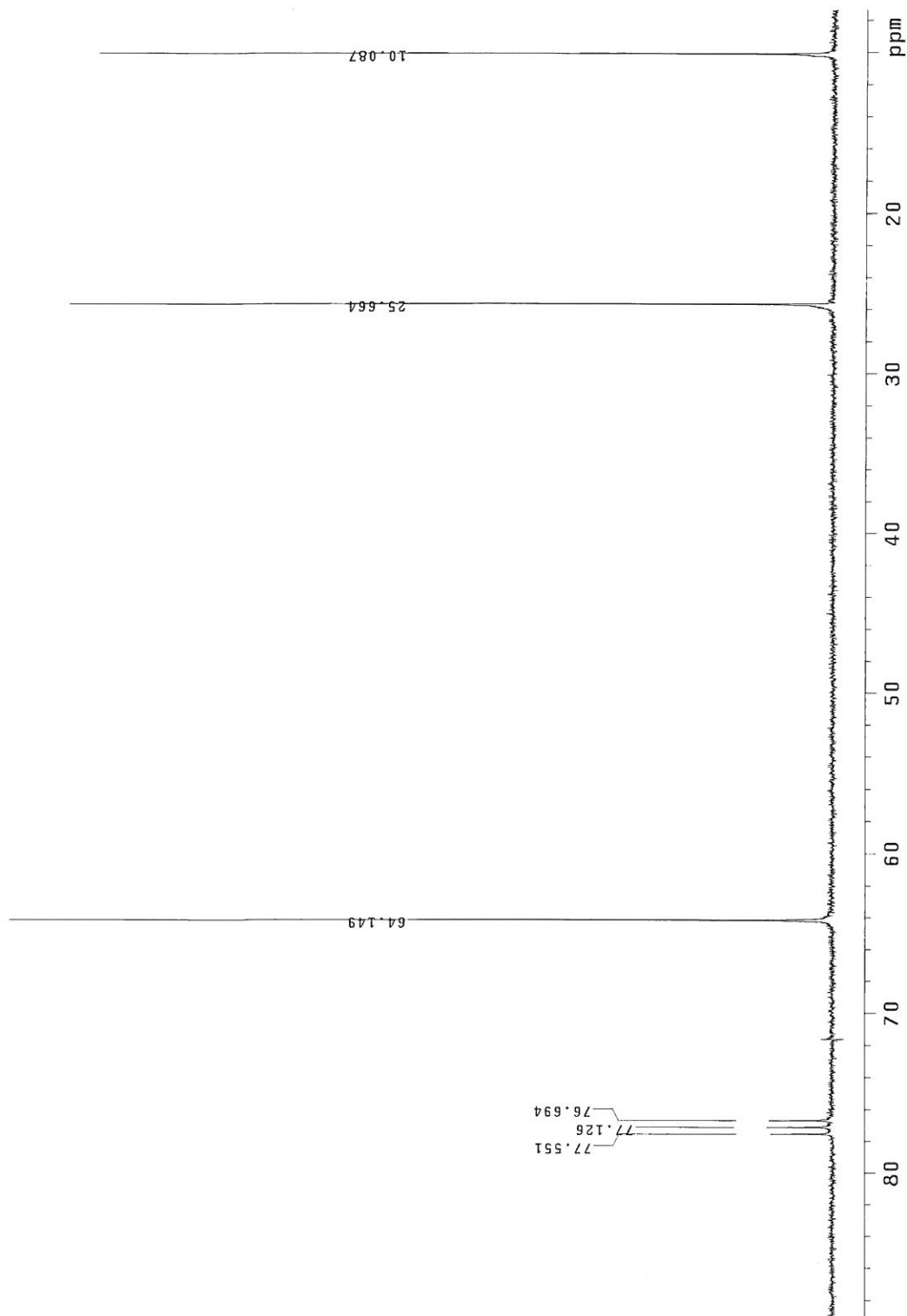




unk 5spring 2014

Sample: unk 5 spring 2014  
Sample ID: s.20140406.02  
File: /home/che344/vnmrSYS/data/che344spring2014/unk5c13-256scans.fid  
Pulse Sequence: s2pu1  
Solvent: cdc13  
Temp: 20.0 C / 293.1 K  
Operator: che344  
File: unk5c13-256scans  
INOVA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
256 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec





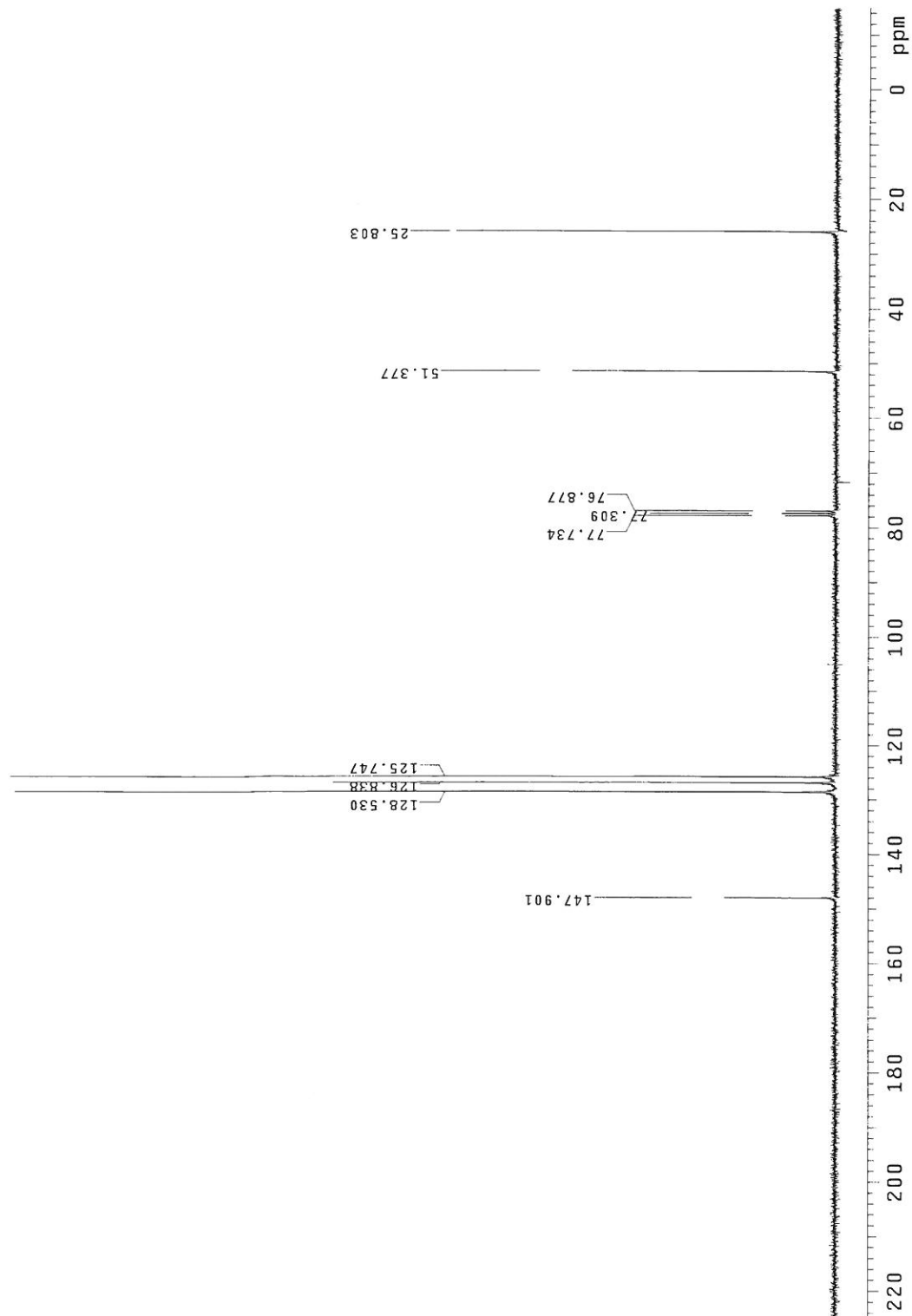
unk 6spring 2014

Sample: unk 6 spring 2014  
Sample ID: s\_20140406\_03  
File: /home/che344/vnmrsys/data/che344spring2014/unk6c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdc13  
Temp. 20.0 C / 293.1 K  
Operator: che344  
File: unk6c13-256scans  
INNOVA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
256 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec

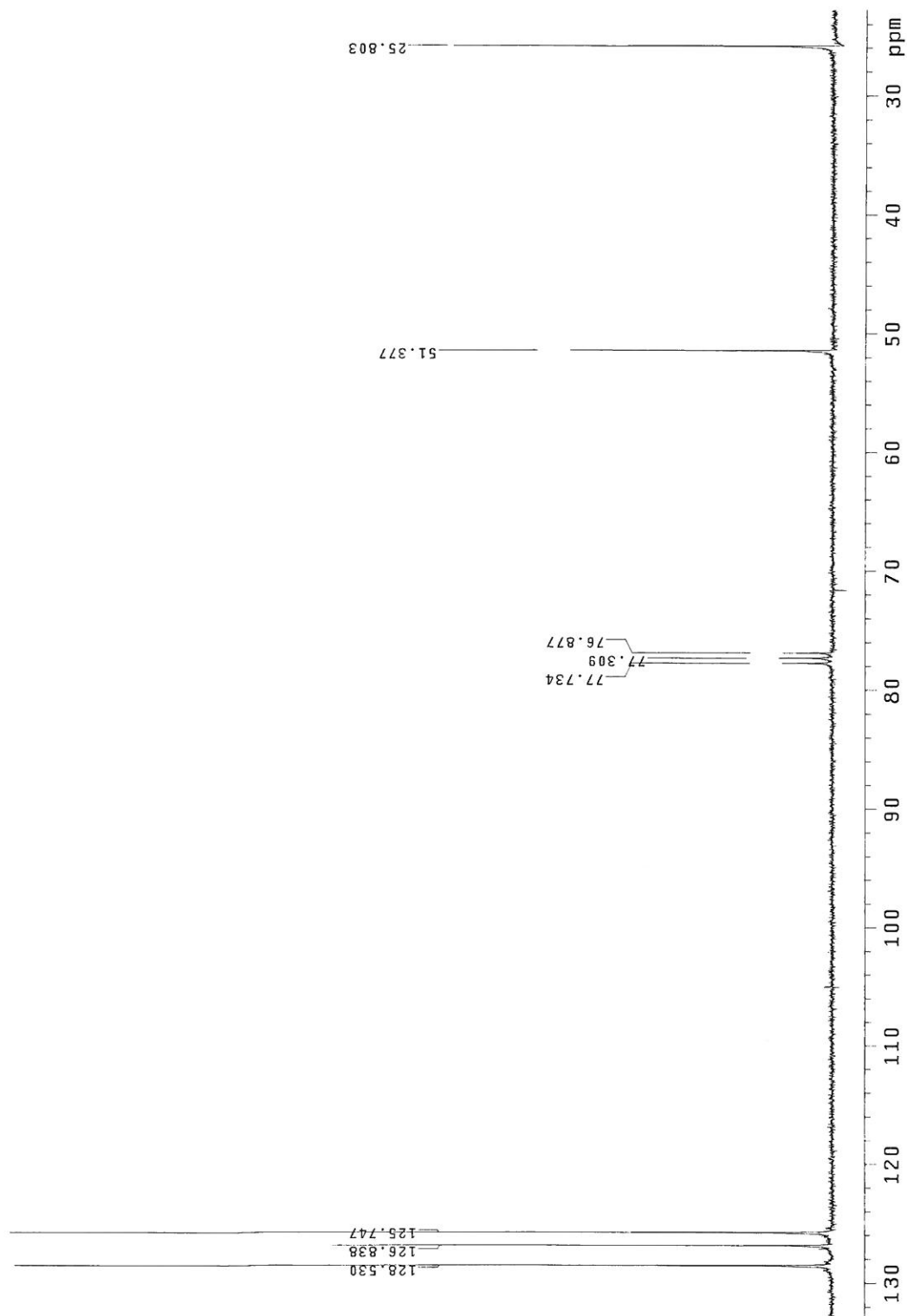




unk 6spring 2014

Sample: unk 6 spring 2014  
Sample ID: s\_20140406\_03  
File: /home/che344/vnmrSYS/data/che344spring2014/unk6c13-256scans.fid  
Pulse Sequence: s2pul  
Solvent: cdc13  
Temp. 20.0 C / 293.1 K  
Operator: che344  
File: unk6c13-256scans  
INQVA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
256 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec





unk 7spring 2014

Sample: unk 7 spring 2014

Sample ID: s\_20140406\_04

File: /home/che344/vnmrSYS/data/che344spring2014/unk7c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 20.0 C / 293.1 K

Operator: che344

File: unk7c13-256scans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

256 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

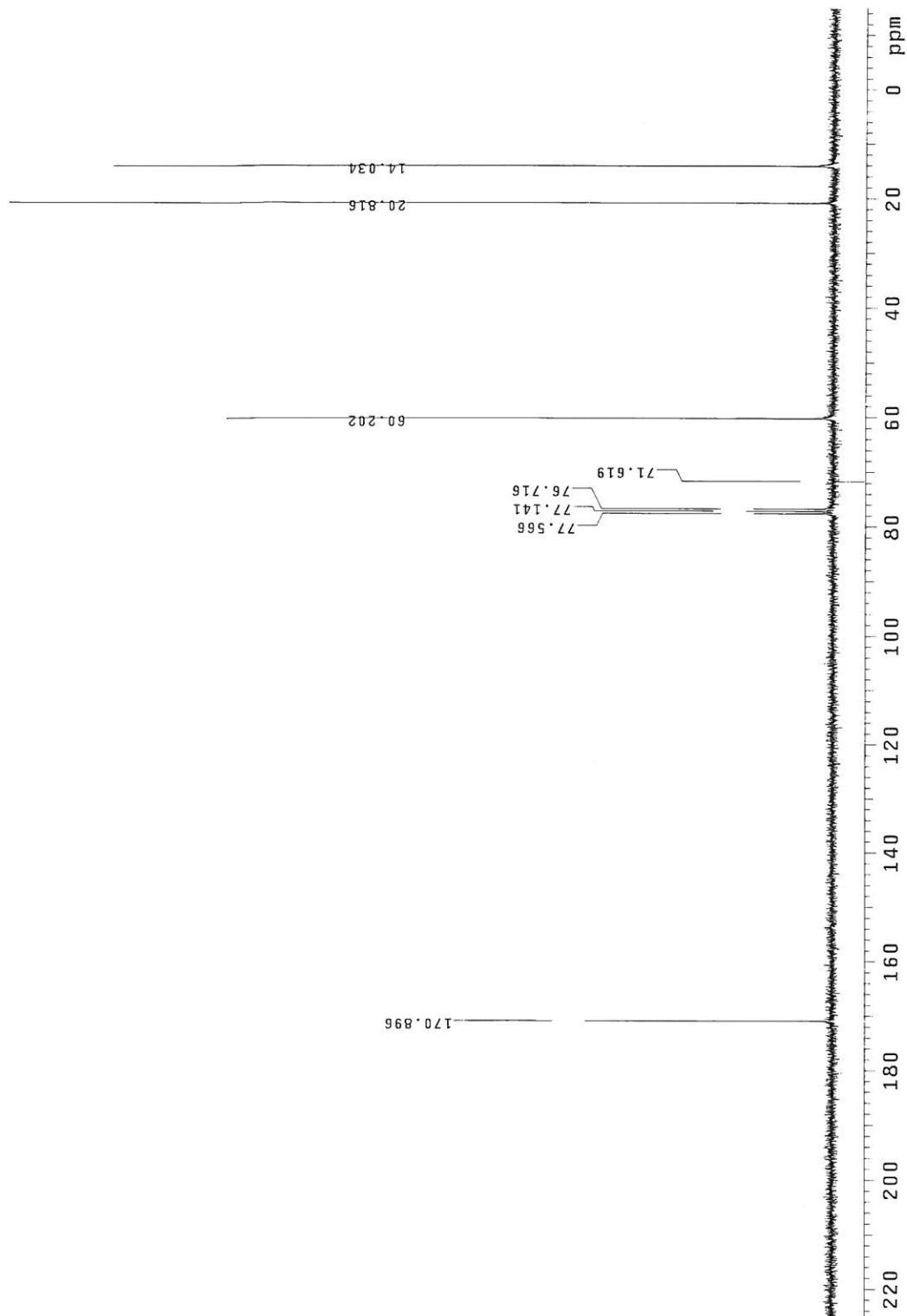
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 51 sec







unk 7spring 2014

Sample: unk 7 spring 2014

Sample ID: s\_20140406\_04

File: /home/che344/vnmrSYS/data/che344spring2014/unk7c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp: 20.0 C / 293.1 K

Operator: che344

File: unk7c13-256scans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

256 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB,

continuously on

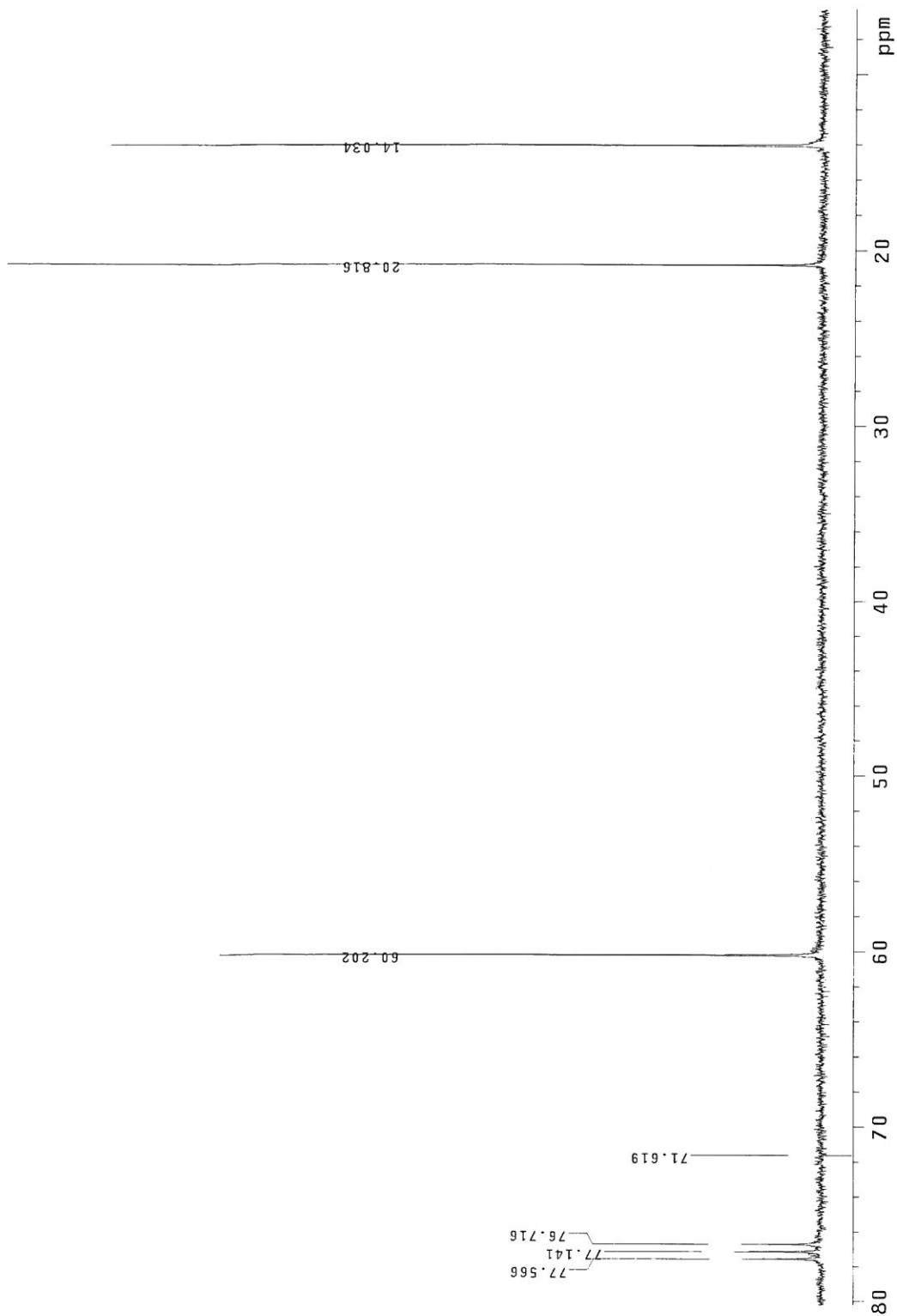
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 51 sec





unk 8spring 2014

Sample: unk 8 spring 2014

Sample ID: s\_20140406\_05

File: /home/che344/vnmrSYS/data/che344spring2014/unk8c13-5kscans.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 20.0 C / 293.1 K

Operator: che344

File: unk8c13-5kscans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

5000 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

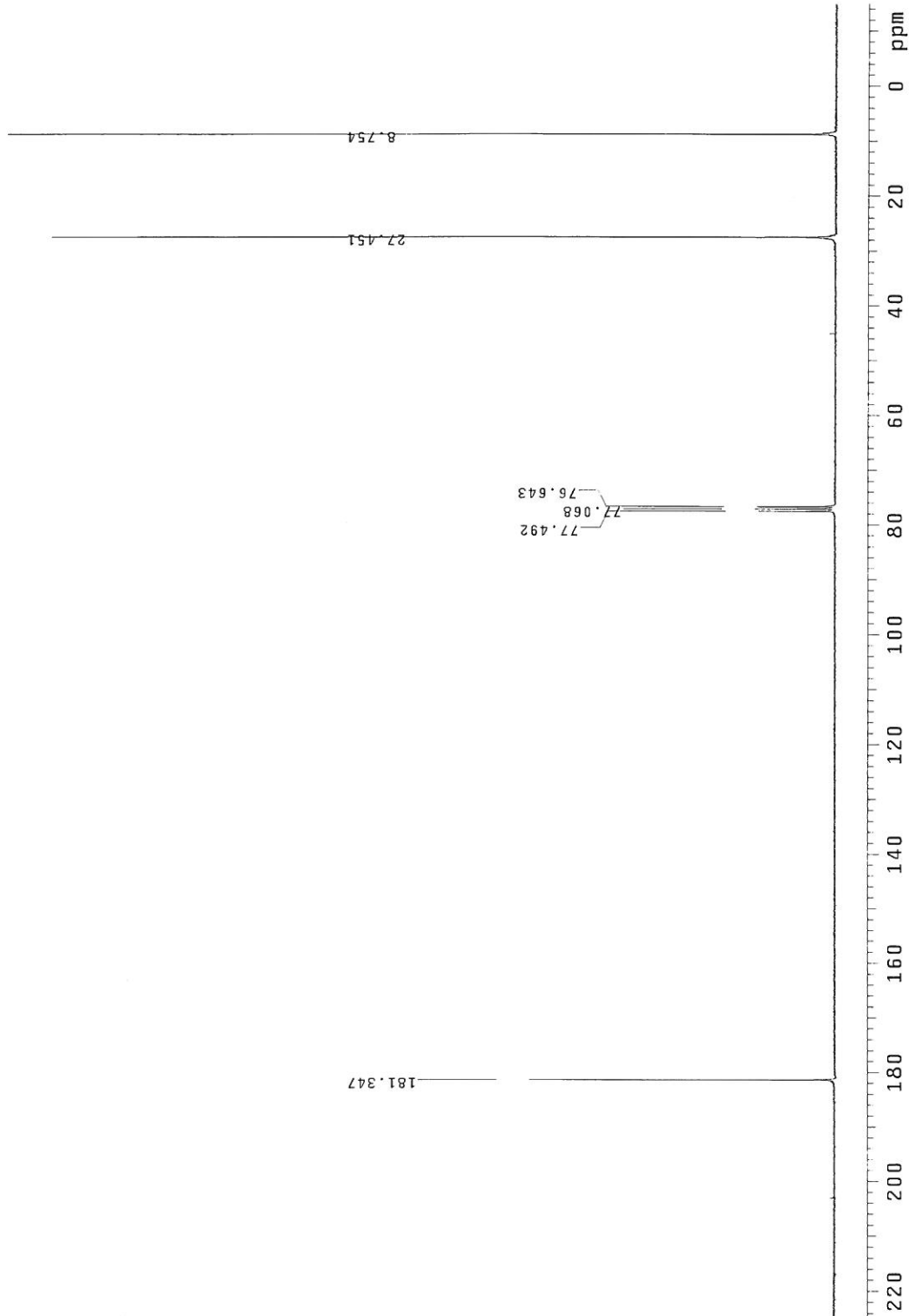
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 3 hr, 12 min, 27 sec





unk 8spring 2014

Sample: unk 8 spring 2014

Sample ID: s\_20140406\_05

File: /home/che344/vnmrsys/data/che344spring2014/unk8c13-5kscans.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 20.0 C / 293.1 K

Operator: che344

File: unk8c13-5kscans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

5000 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

WALTZ-16 modulated

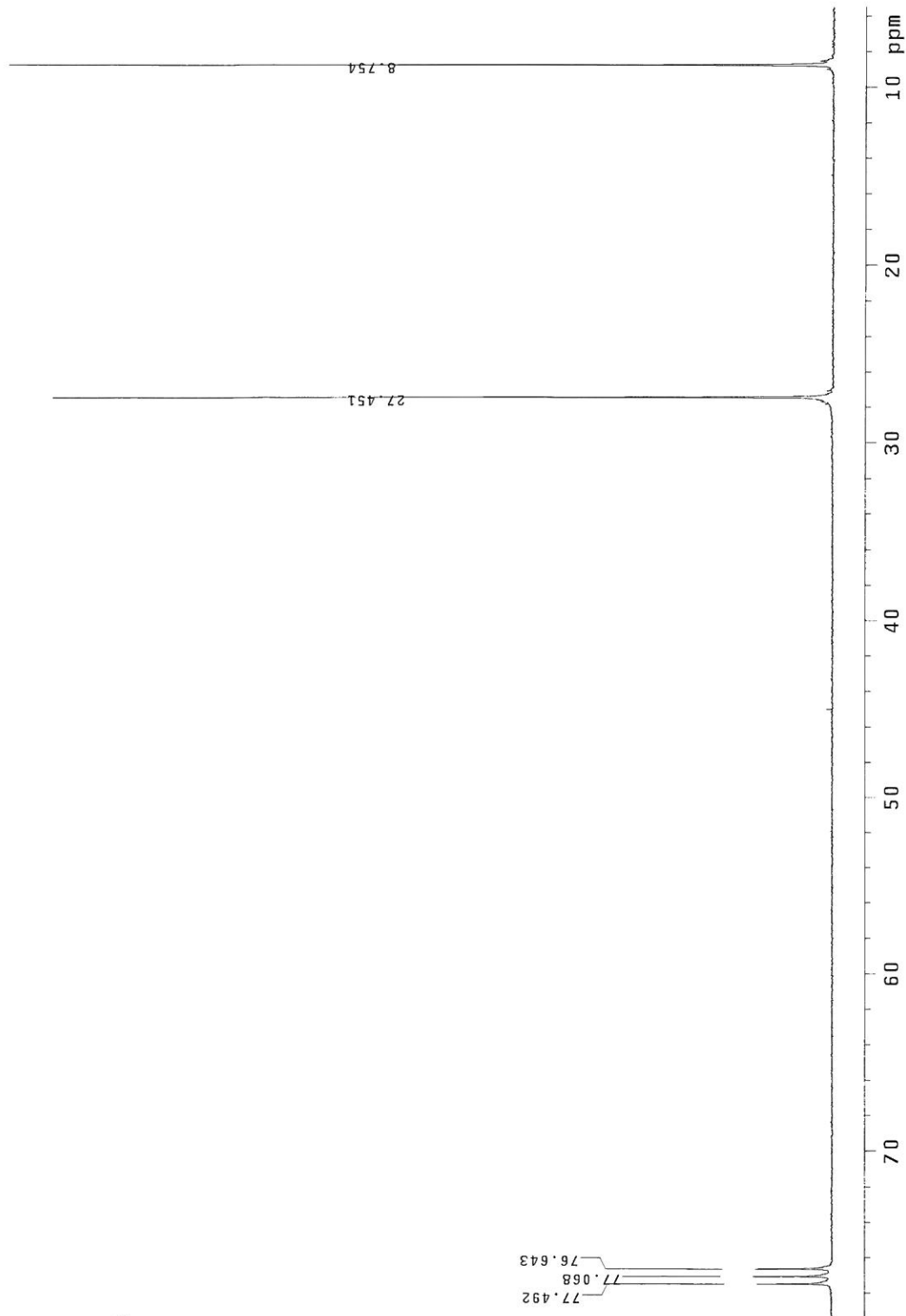
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 3 hr, 12 min, 27 sec

77.492  
77.068  
76.643





unk 9spring 2014

Sample: unk 9 spring 2014

Sample ID: s\_20140407\_01

File: /home/che344/vnmrSYS/data/che344spring2014/unk9c13-256scans.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp: 20.0 C / 293.1 K

Operator: che344

File: unk9c13-256scans

INOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

256 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

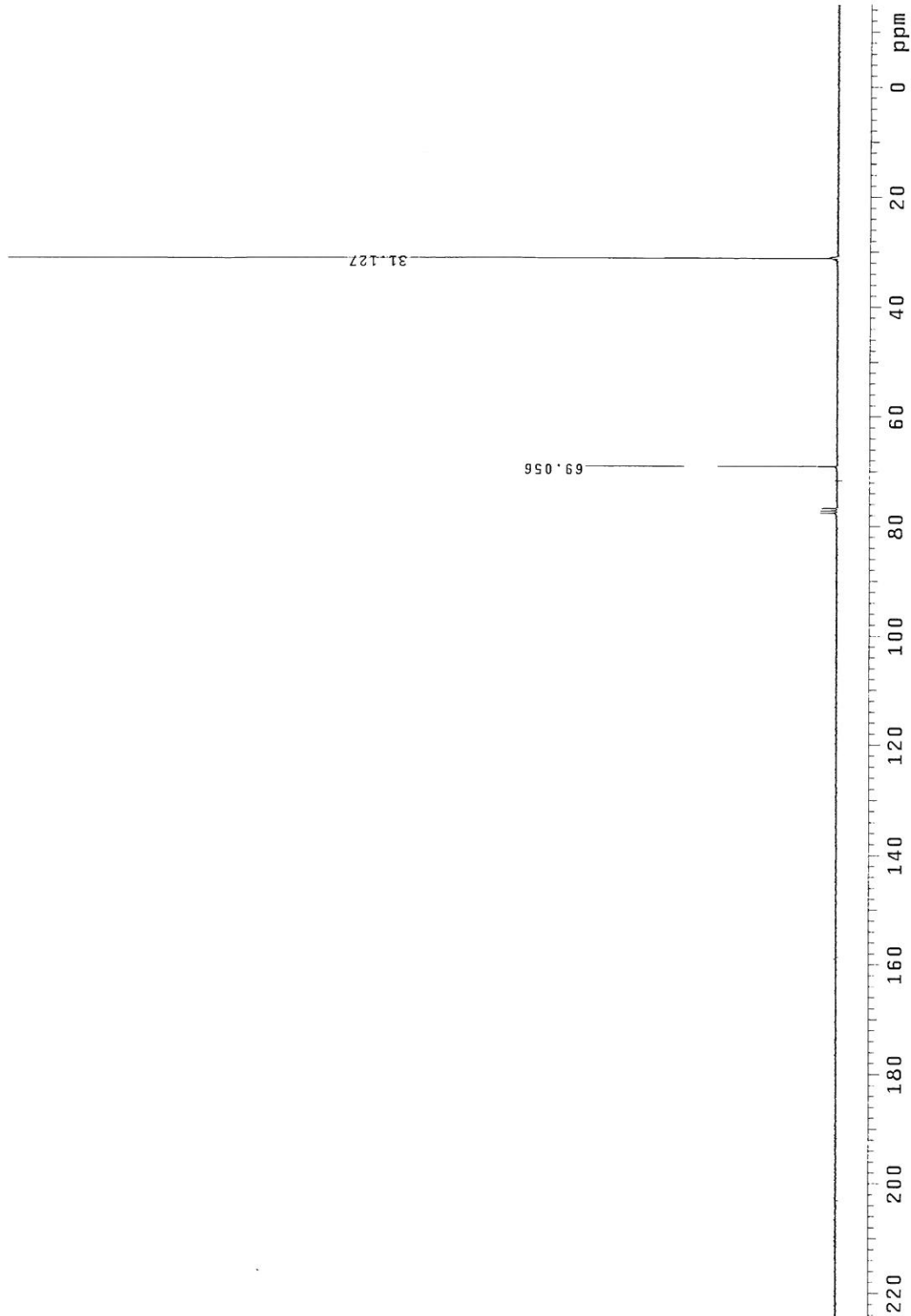
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 51 sec







unk 9spring 2014

Sample: unk 9 spring 2014

Sample ID: s\_20140407\_01

File: /home/che344/vnmrSYS/data/che344spring2014/unk9c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 20.0 C / 293.1 K

Operator: che344

File: unk9c13-256scans

INNOVA-300 "nmr300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 18095.5 Hz

256 repetitions

OBSERVE C13, 75.4051517 MHz

DECOUPLE H1, 299.8825561 MHz

Power 34 dB

continuously on

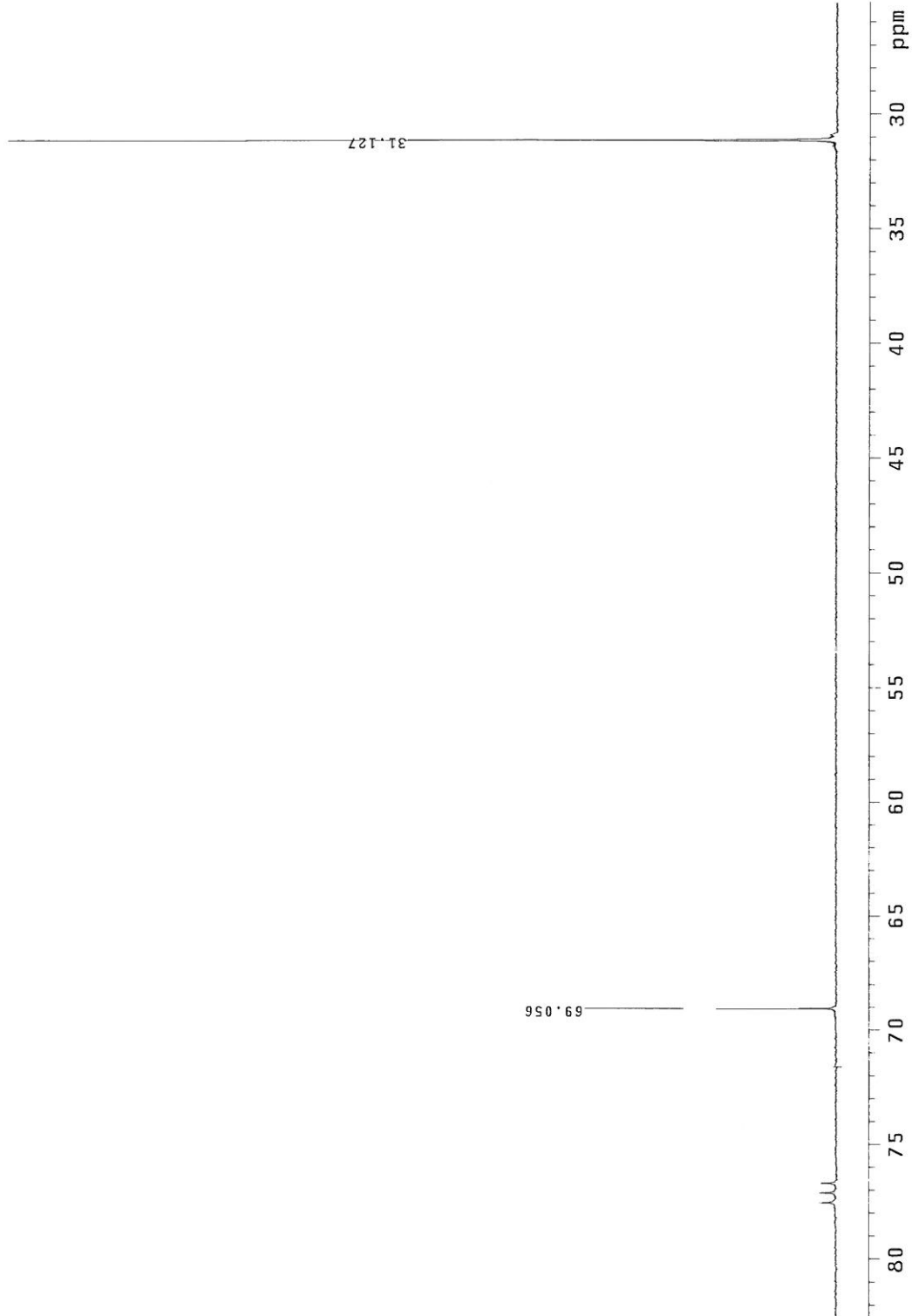
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 51 sec





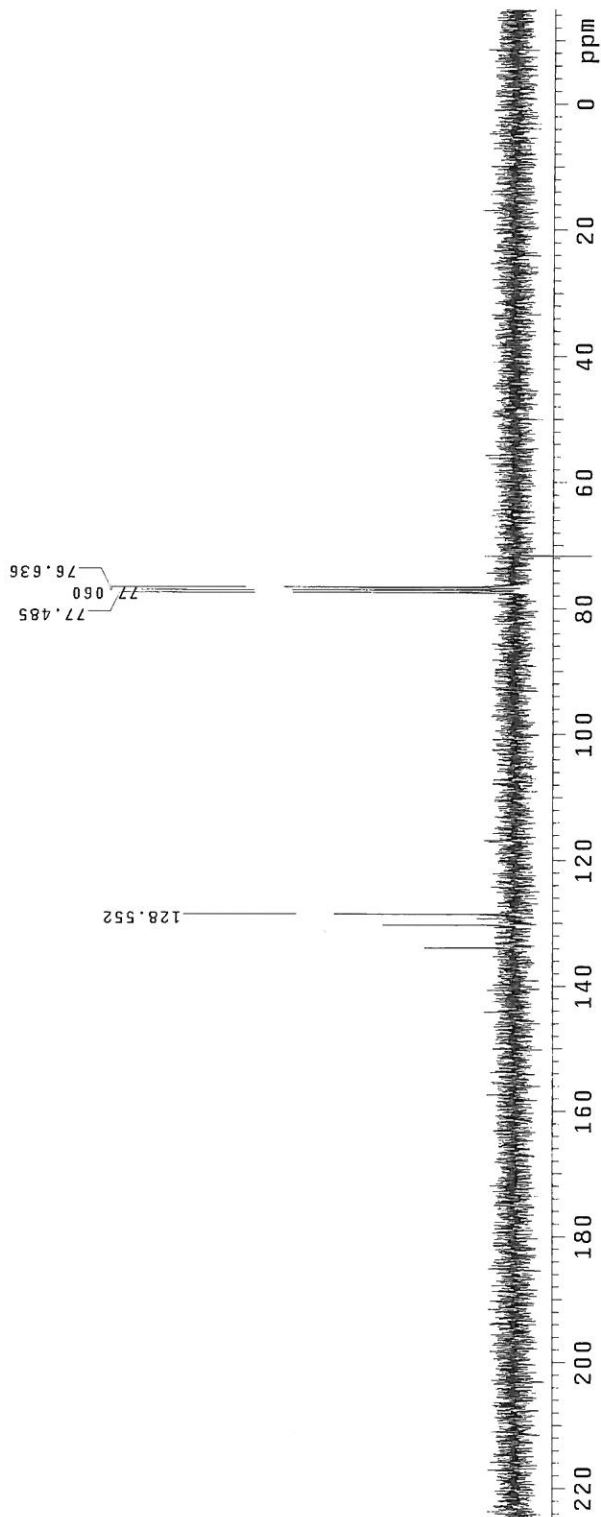
unk 18 spring 2014

Sample: unk 18 spring 2014  
Sample ID: s\_20140407\_02  
File: /home/che344/vnmrsys/data/che344spring2014/unk18c13-256scans.fid

Pulse Sequence: s2pul

Solvent: cdcl3  
Temp: 20.0 C / 293.1 K  
Operator: che344  
File: unk18c13-256scans  
INOVA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
256 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB,  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec





unk 18 spring 2014

Sample: unk 18 spring 2014

Sample ID: s\_20140407\_02

File: /home/che344/vnmrSYS/data/che344spring2014/unk18c13-256scans.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 20.0 C / 293.1 K

Operator: che344

File: unk18c13-256scans

INOVIA-300 "nmr300"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 18095.5 Hz  
256 repetitions  
OBSERVE C13, 75.4051517 MHz  
DECOUPLE H1, 299.8825561 MHz  
Power 34 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec

