

NAME \_\_\_\_\_

**Chem 203**

**Organic Spectroscopy**

Midterm Examination, Part II (50 points total)

Problem 3 of 3 (two out of three required, 25 points)

Saturday, November 5, 2011, 9 am - ???

**SUBMIT TWO OF THE THREE PROBLEMS FOR GRADING AND DO NOT SUBMIT THE PROBLEM THAT YOU DO NOT WANT GRADED. IF THREE PROBLEMS ARE SUBMITTED, ONLY THE FIRST TWO (PROBLEMS 1 AND 2) WILL BE GRADED**

Books, notes, calculators, rulers, and laptop computers are permitted as is wireless (or wired) internet access and appropriate software (e.g., PyMOL, Maestro/MacroModel, Excel, ChemDoodle, Chemdraw, ElComp, MolE, etc.). Communication with other students by e-mail, text, or in person is not permitted. Catalogs of molecular structures (e.g., the Aldrich catalog, the Merck Index, etc.) or databases of molecular structures (such as wireless access to SciFinder Scholar, the Sigma-Aldrich website, etc.) are NOT PERMITTED. INAPPROPRIATE COMMUNICATION OR USE OF SUCH ITEMS CONSTITUTES ACADEMIC DISHONESTY, WILL RESULT IN A FAILING GRADE (F) IN THE CLASS, AND MAY RESULT IN EXPULSION FROM THE Ph.D. PROGRAM.

If you wish to use a laptop computer, please be willing to share briefly with others when needed.

3. Analyze the spectra and solve the structure of the molecule for which data are provided.

Identify any noteworthy heteroatoms present. Determine the molecular formula and unsaturation number. Identify functional groups that are present from the IR and other spectra. Identify key fragments from NMR. Assign the  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR resonances to the respective atoms in the molecules. Mass spectra are EIMS, unless otherwise indicated.

ONLY WORK SHOWN ON THIS PAGE WILL BE GRADED.

Exact Mass: Not available

Noteworthy Heteroatoms:

Molecular Formula:

Unsaturation Number:

Functional Groups (be as specific as possible):

Fragments (from NMR):

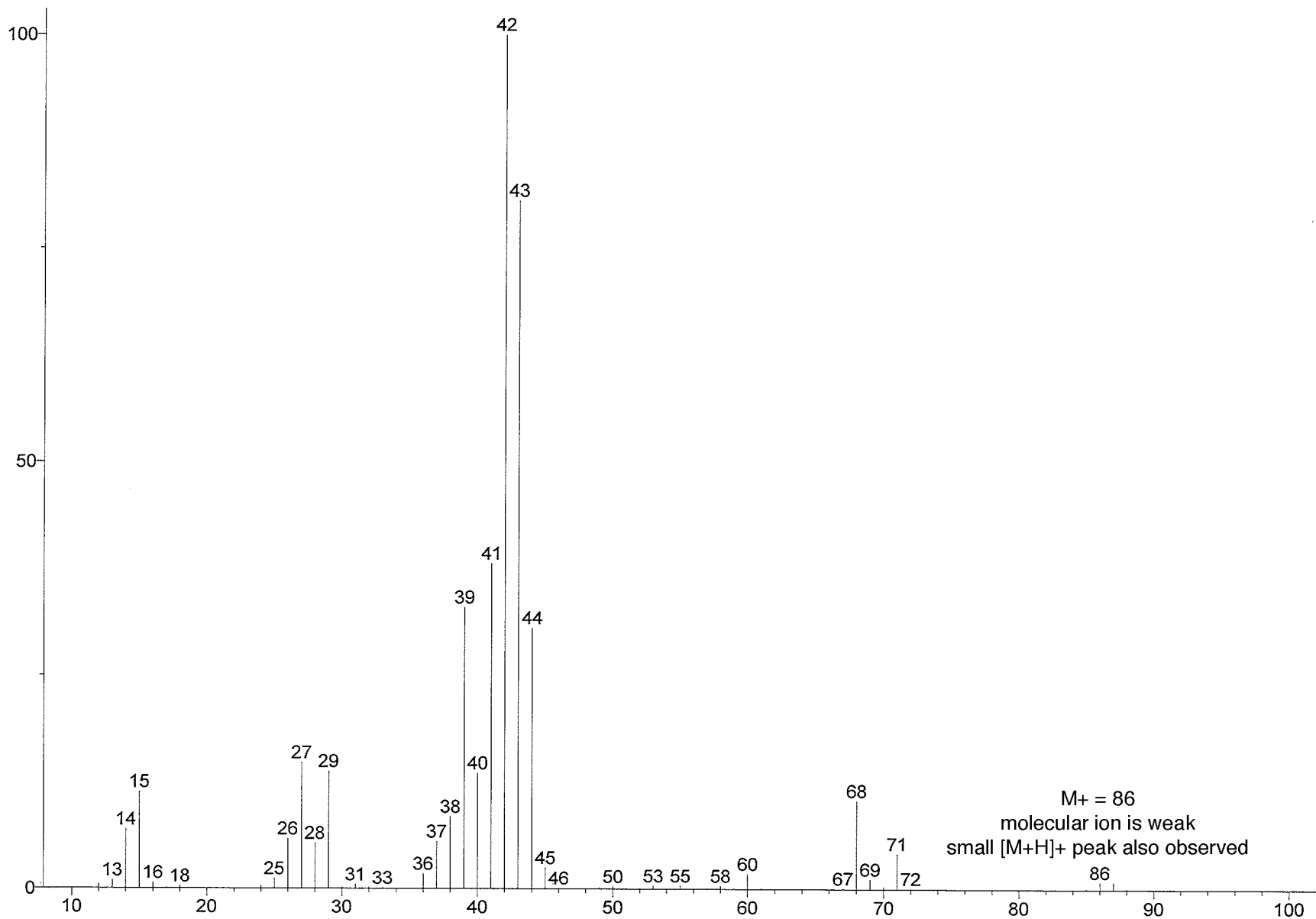
Structure (Make sure to properly indicate stereochemistry, if applicable):

Structure with  $^1\text{H}$  NMR resonances lettered from the most downfield to the most upfield (a, b, c, d, etc.): (Note: Not all resonances can be assigned with certainty. If assignments are uncertain, indicate so by showing possible letters.)

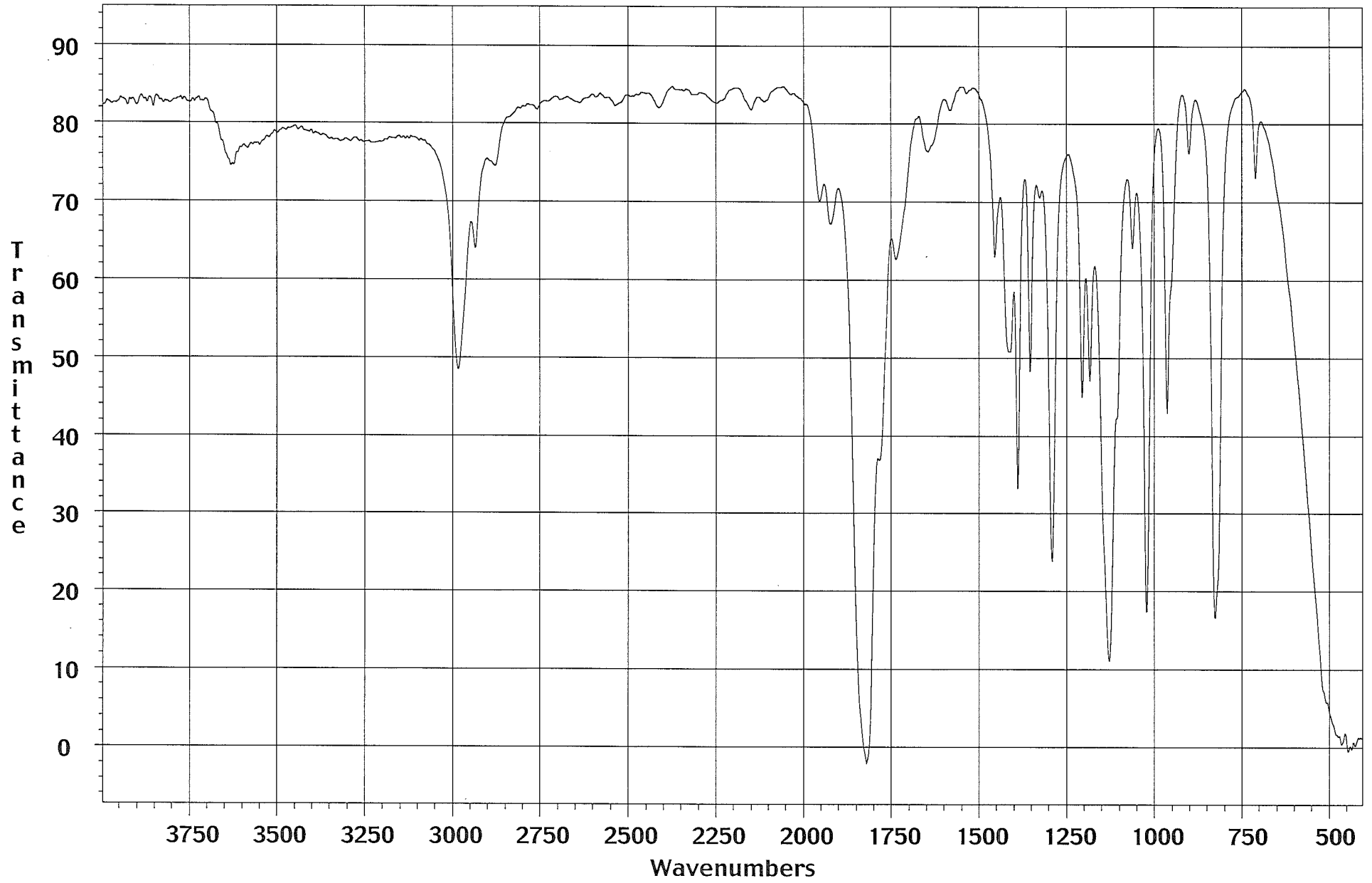
Structure with  $^{13}\text{C}$  NMR resonances numbered from the most downfield to the most upfield (1, 2, 3, 4, etc.): (Note: Not all resonances can be assigned with certainty. If assignments are uncertain, indicate so by showing possible numbers.)

Molecular Model: Build an energy-minimized molecular model of the structure using PyMOL and the "clean" function. Save the .pse files as structure3.pse. E-mail the .pse file to me (jsnowick@uci.edu).

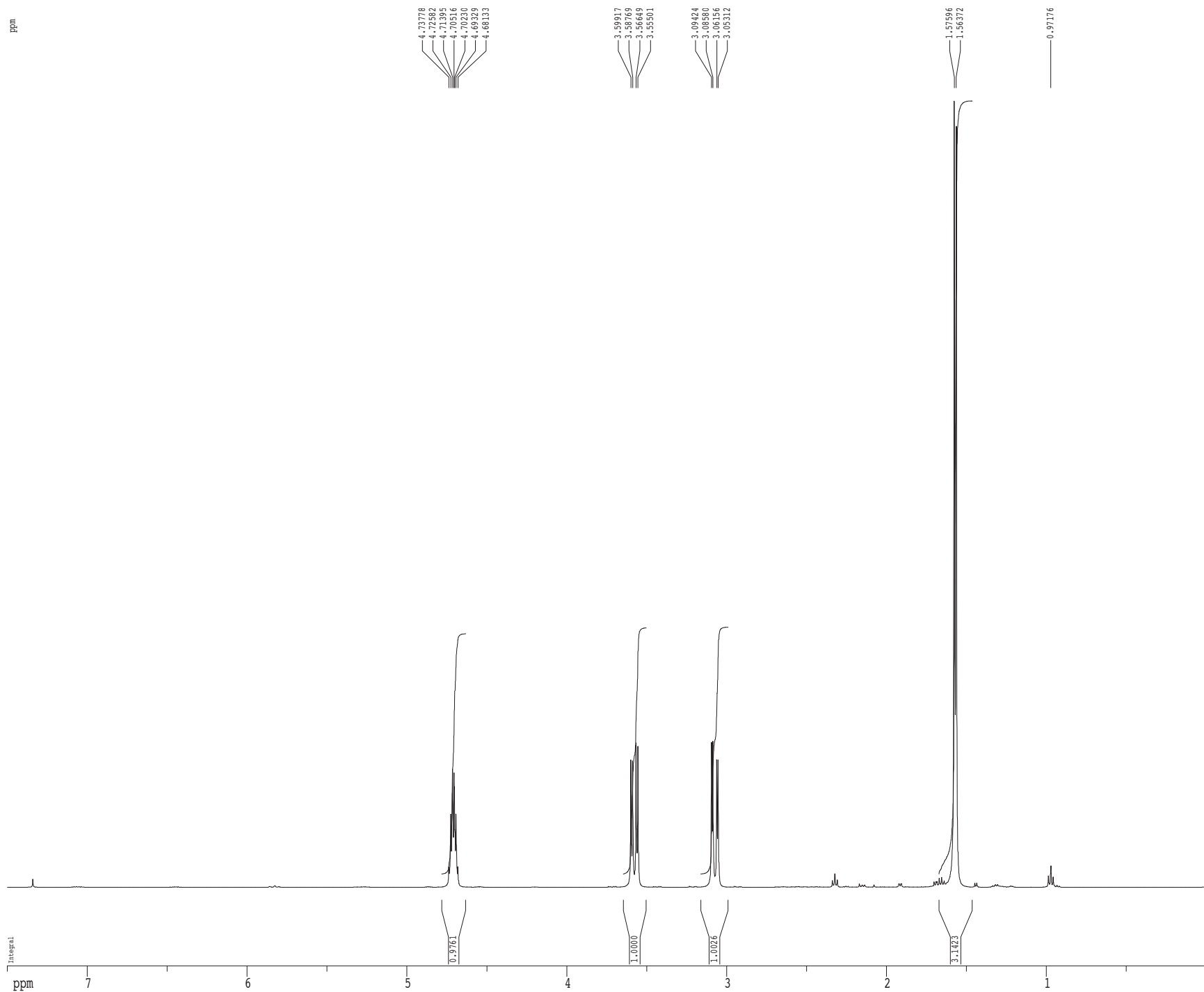
EIMS



# Thin film NaCL plates



1H spectrum



Current Data Parameters  
USER nmrlit  
NAME nmrl1-X-sample5  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111101  
Time 14.37  
INSTRUM gn500  
PROBHD 5 mm broadband  
PULPROG zg30  
TD 81728  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.098043 Hz  
AQ 5.0998774 sec  
RG 40.3  
DN 62.400 usec  
DE 6.00 usec  
TE 298.0 K  
D1 0.10000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 12.20 usec  
PL1 -5.00 dB  
SF01 499.5134966 MHz

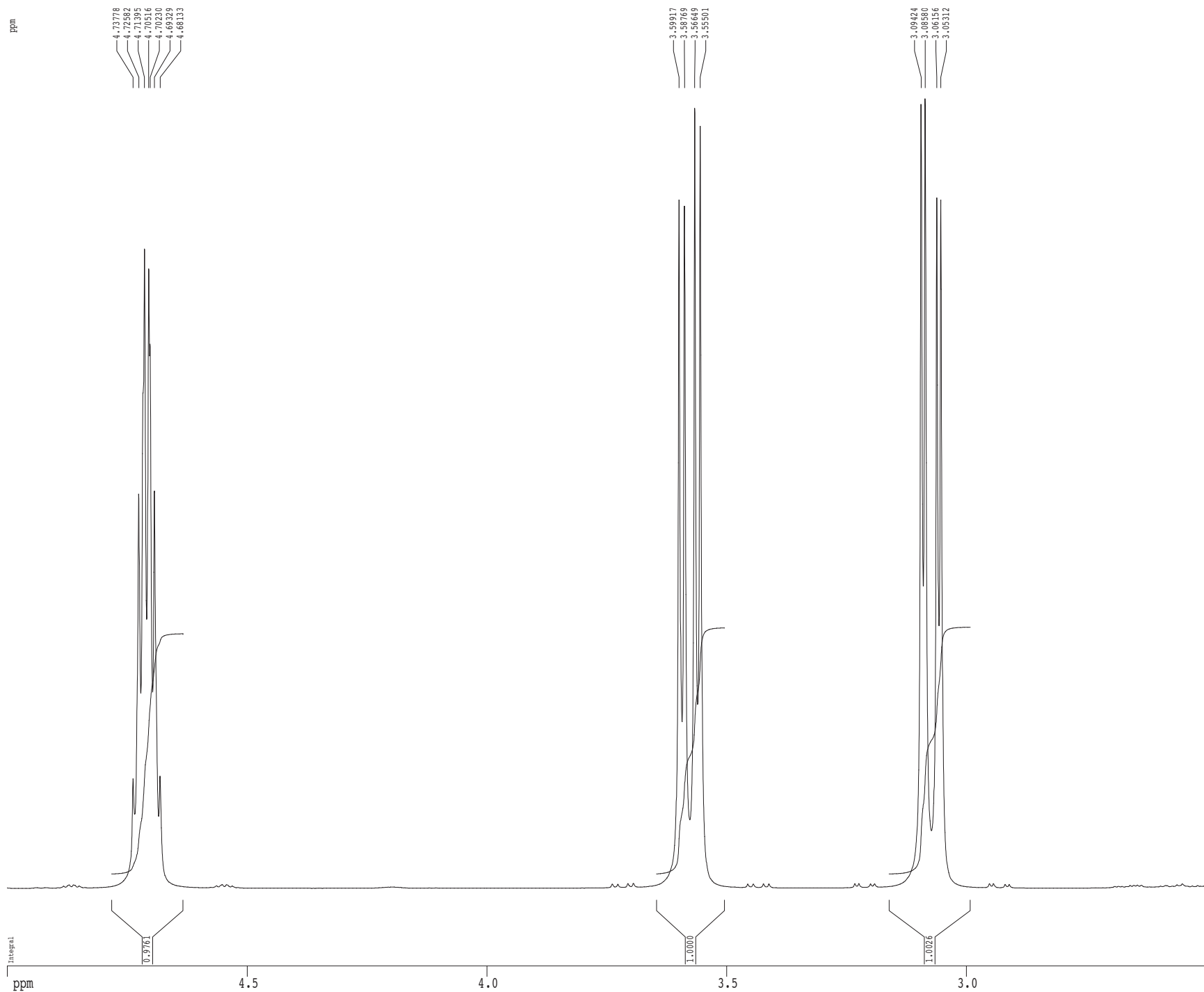
F2 - Processing parameters  
SI 65536  
SF 499.5099869 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 22.80 cm  
CY 15.00 cm  
FIP 7.500 ppm  
F1 3746.32 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PPMCM 0.32895 ppm/cm  
HZCM 164.31250 Hz/cm

DU=/v, USER=nmr11t, NAME=nmr11-X-sample5, EXPNO=1, PROCNO=1  
F1=15.047ppm, F2=-0.995ppm, MI=0.30cm, MAXI=10000.00cm, PC=1.000

#	ADDRESS	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	42117.1	2366.568	4.7378	0.38
2	42166.0	2360.592	4.7258	1.38
3	42214.4	2354.667	4.7140	2.25
4	42250.3	2350.276	4.7052	2.18
5	42262.0	2348.847	4.7023	1.91
6	42298.8	2344.345	4.6933	1.39
7	42347.7	2338.372	4.6813	0.39
8	46768.8	1797.819	3.5992	2.42
9	46815.7	1792.086	3.5877	2.40
10	46902.3	1781.497	3.5665	2.75
11	46949.2	1775.764	3.5550	2.68
12	48831.7	1545.601	3.0942	2.76
13	48866.1	1541.388	3.0858	2.78
14	48965.2	1529.277	3.0616	2.43
15	48999.6	1525.064	3.0531	2.42
16	55034.5	787.210	1.5760	15.00
17	55084.5	781.093	1.5637	14.52
18	57502.9	485.402	0.9718	0.41

1H spectrum



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Current Data Parameters
USER          nmrl1t
NAME          nmrl1-X-sample5
EXPNO         1
PROCNO        1

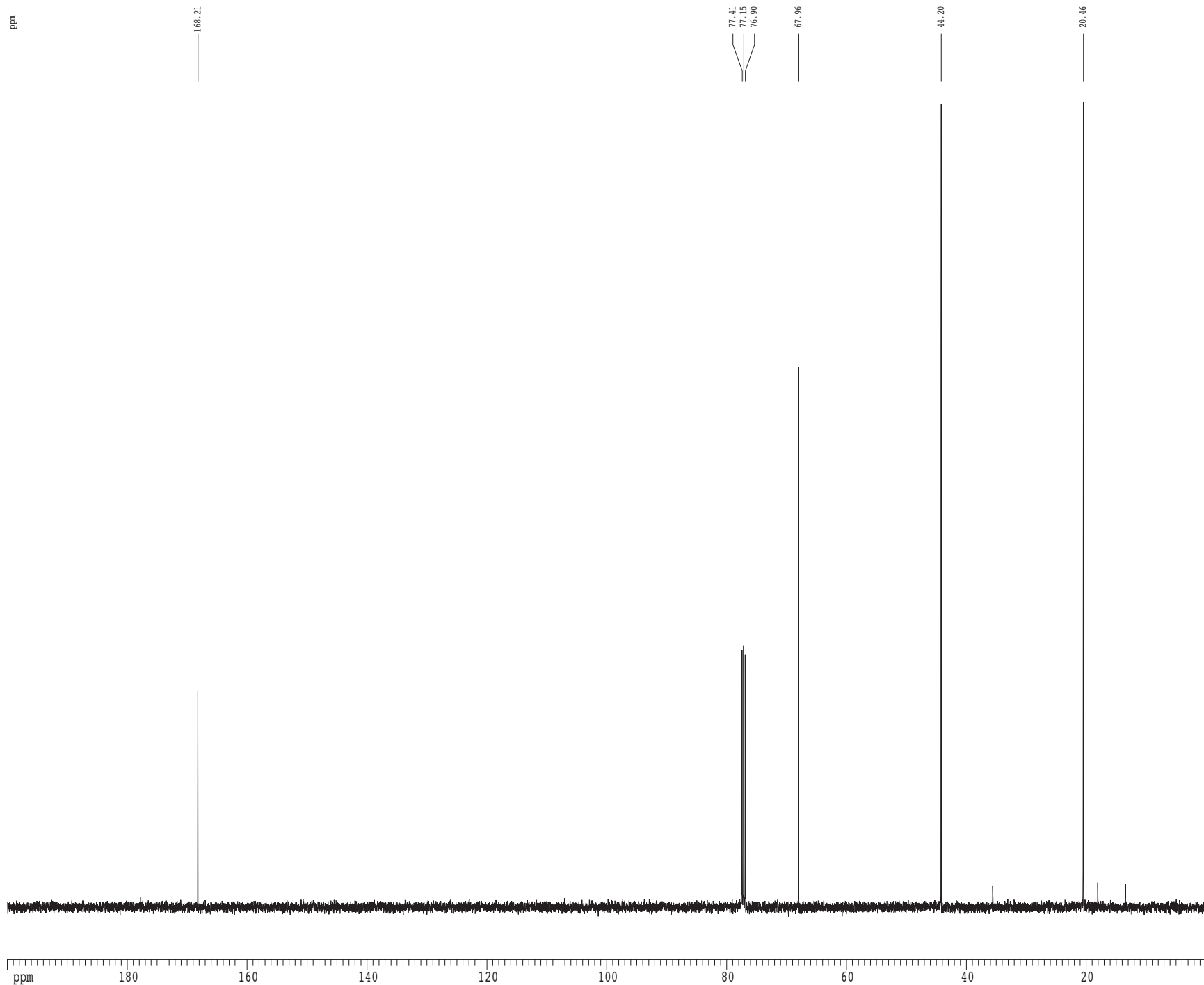
F2 - Acquisition Parameters
Date_         20111101
Time          14.37
INSTRUM       gn500
PROBHD        5 mm broadband
PULPROG       zg30
TD            81728
SOLVENT       CDCl3
NS            32
DS            2
SWH           8012.820 Hz
FIDRES        0.098043 Hz
AQ            5.0998774 sec
RG            40.3
DN            62.400 usec
DE            6.00 usec
TE            298.0 K
D1            0.10000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            12.20 usec
PL1           -5.00 dB
SF01          499.5134966 MHz

F2 - Processing parameters
SI            65536
SF            499.5099869 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00

ID NMR plot parameters
CX            22.80 cm
CY            15.00 cm
FIP           5.000 ppm
F1            2497.55 Hz
F2P           2.500 ppm
F2            1248.77 Hz
PPMCM         0.10965 ppm/cm
HZCM          54.77083 Hz/cm
    
```

125.6 MHz <sup>13</sup>C spectrum with <sup>1</sup>H decoupling in CDCl<sub>3</sub>



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Current Data Parameters
USER          nmr11t
NAME          nmr11-X-sample5
EXPNO        2
PROCNO       1

F2 - Acquisition Parameters
Date_        2011101
Time_        14.39
INSTRUM      qn500
PROBHD       5 mm broadband
PULPROG      zgdc30
TD           65536
SOLVENT      CDCl3
NS           46
DS           4
SWH          30303.031 Hz
FIDRES       0.462388 Hz
AQ           1.0813940 sec
RG           46341
DW           16.500 usec
DE           4.50 usec
TE           298.0 K
D1           0.25000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            7.70 usec
PL1           0.00 dB
SF01         125.6157052 MHz

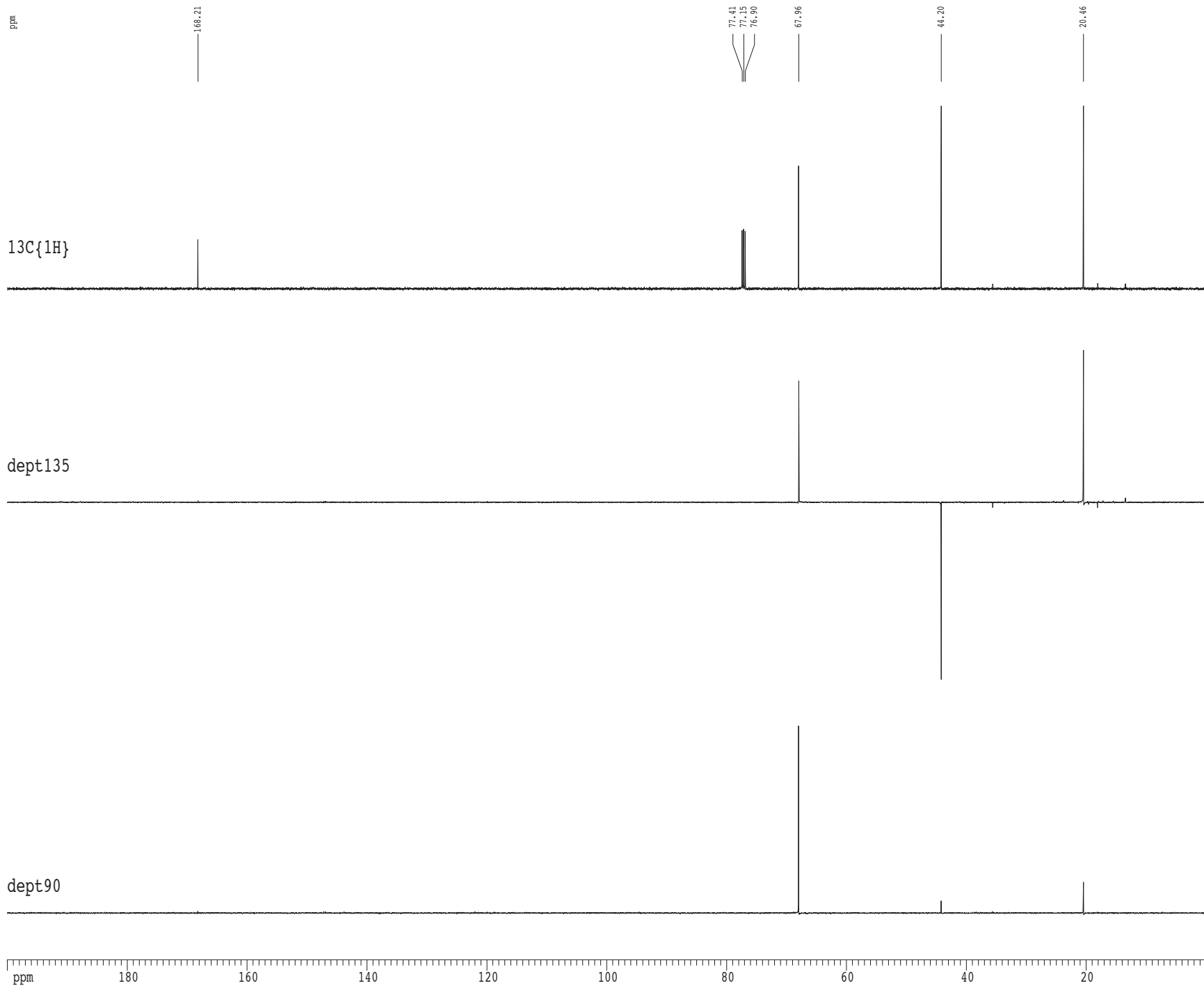
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           -3.00 dB
PL12         13.20 dB
SF02         499.5124975 MHz

F2 - Processing parameters
S1            65536
SF           125.6019001 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            2.00

1D NMR plot parameters
CX            22.80 cm
CY            15.65 cm
F1P          200.000 ppm
F1           25120.38 Hz
F2P           0.000 ppm
F2            0.00 Hz
PPMCM        8.77193 ppm/cm
HZCM         1101.77112 Hz/cm
    
```



13C spectrum with 1H decoupling



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Current Data Parameters
USER      nmr11t
NAME      nmr11-X-sample5
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     2011101
Time      14.39
INSTRUM   gn500
PROBHD    5 mm broadband
PULPROG   zgdc30
TD         65536
SOLVENT   CDCl3
NS         46
DS         4
SWH        30303.031 Hz
FIDRES     0.462388 Hz
AQ         1.0813940 sec
RG         46341
DW         16.500 usec
DE         4.50 usec
TE         298.0 K
D1         0.25000000 sec
d11        0.03000000 sec
MCREST     0.00000000 sec
MCWRK     0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         7.70 usec
PL1        0.00 dB
SF01       125.6157052 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -3.00 dB
PL12       13.20 dB
SF02       499.5124975 MHz

F2 - Processing parameters
S1         65536
SF         125.6019001 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         2.00

1D NMR plot parameters
CX         22.80 cm
CY         3.56 cm
F1P        200.000 ppm
F1         25120.38 Hz
F2P        0.000 ppm
F2         0.00 Hz
PPMCM      8.77193 ppm/cm
HZCM       1101.77112 Hz/cm
    
```