NAME_____

Chem 203

Organic Spectroscopy

Midterm Examination, Part II (60 points total)

Problem 1 of 4 (three out of four required, 20 points)

Saturday, November 15, 2014, 9 am - ???

SUBMIT THREE OF THE FOUR PROBLEMS FOR GRADING AND DO NOT SUBMIT THE PROBLEM THAT YOU DO NOT WANT GRADED. IF FOUR PROBLEMS ARE SUBMITTED, ONLY THE FIRST THREE (PROBLEMS 1, 2, AND 3) 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 DISHNONESTY, 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.

1. Analyze the spectra and solve the structure of the molecule for which data are provided. The following data are provided: EI-MS; IR (thin film on NaCl plates); 500 MHz ^{1}H NMR in $CDCl_3$; 125.8 MHz ^{13}C NMR, DEPT 90, and DEPT 135 in $CDCl_3$.

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}H NMR and ^{13}C NMR resonances to the respective atoms in the molecules. Mass spectra are EI-MS, 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):

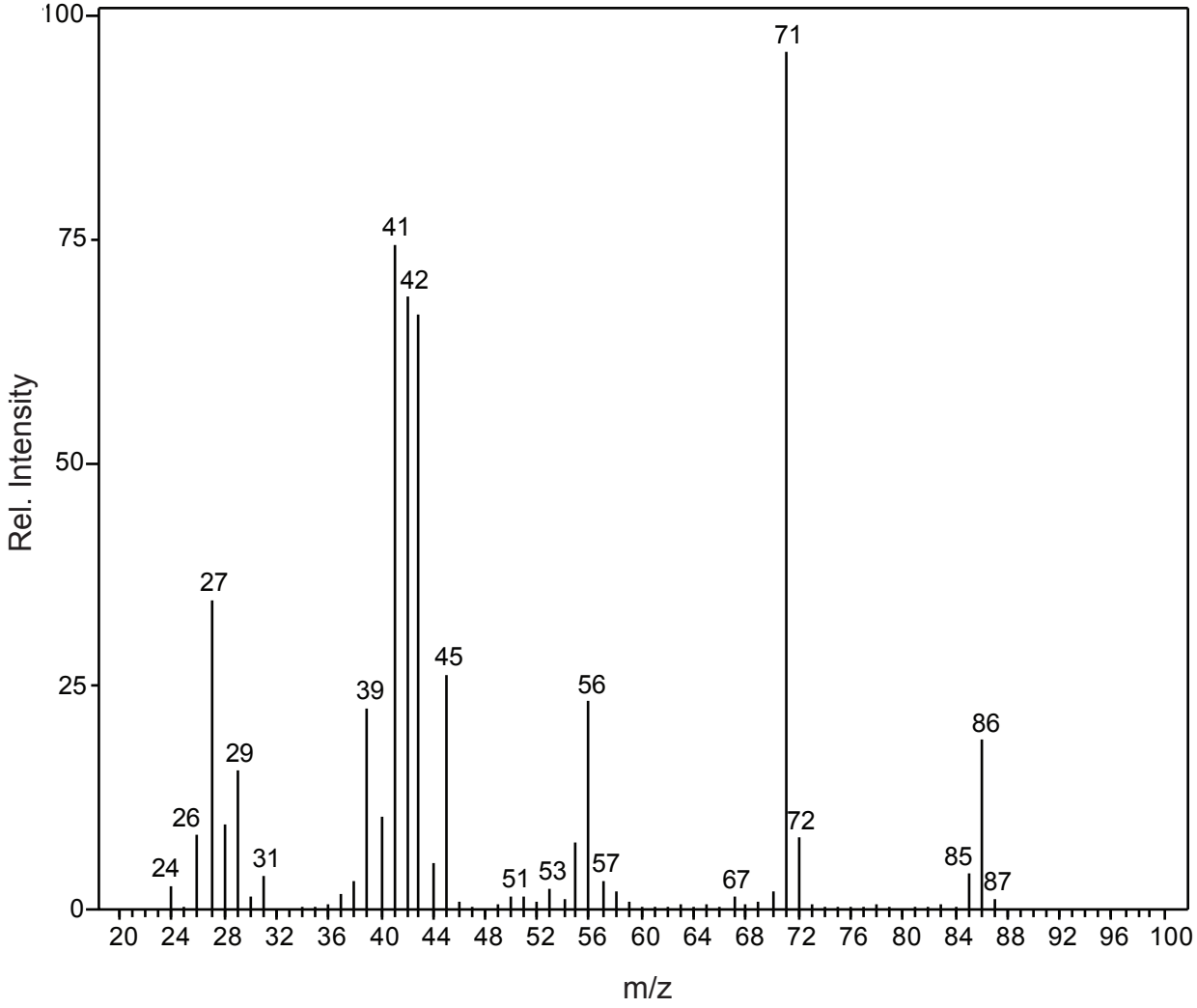
Fragments (from NMR):

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

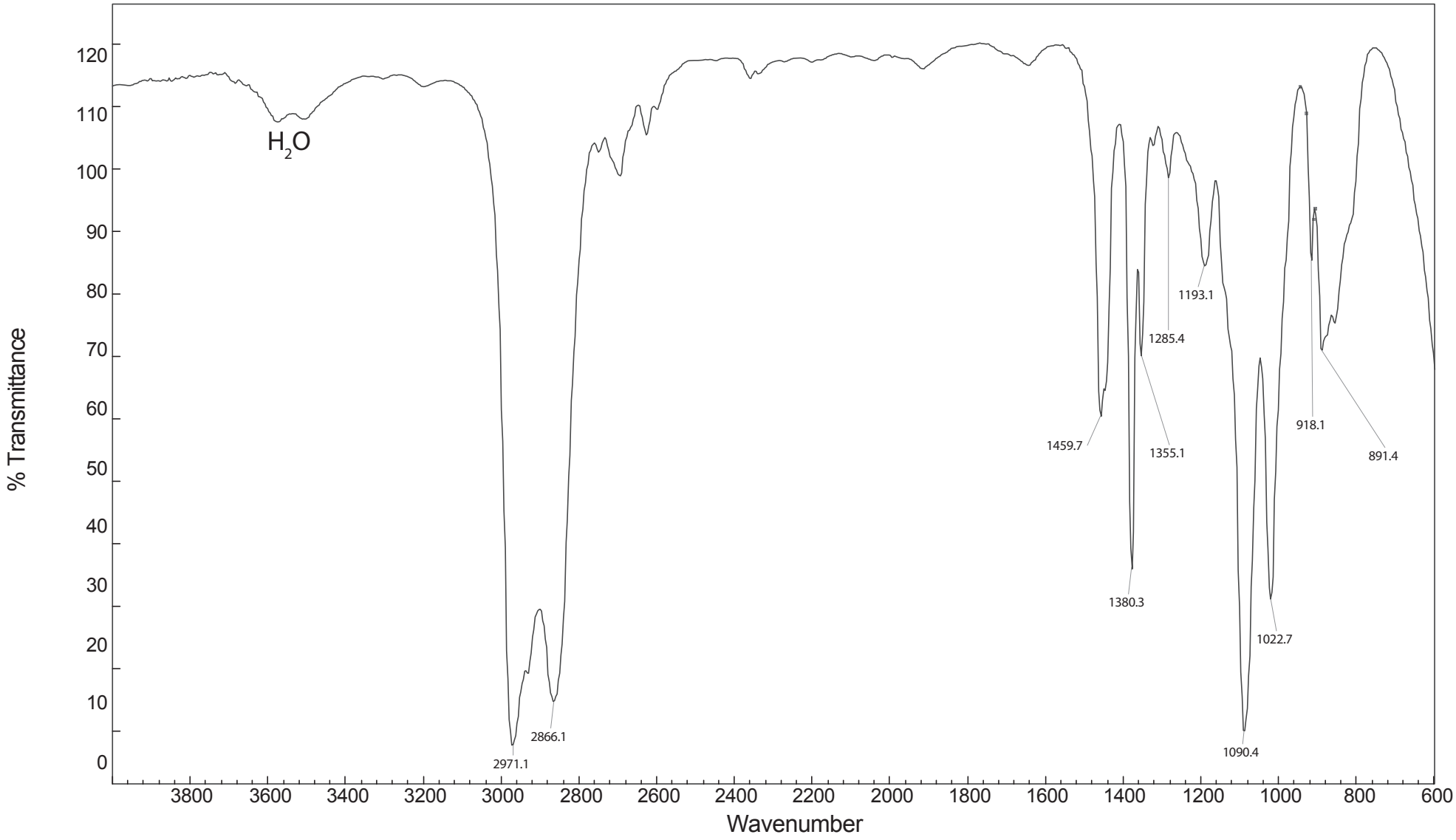
Structure with ^{1}H NMR resonances lettered from the most downfield to the most upfield (a, b, c, d, etc.): (Note: Not all resonances can be assigned with certainty. If assignments are uncertain, indicate so by showing possible letters.)

Structure with ^{13}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.)

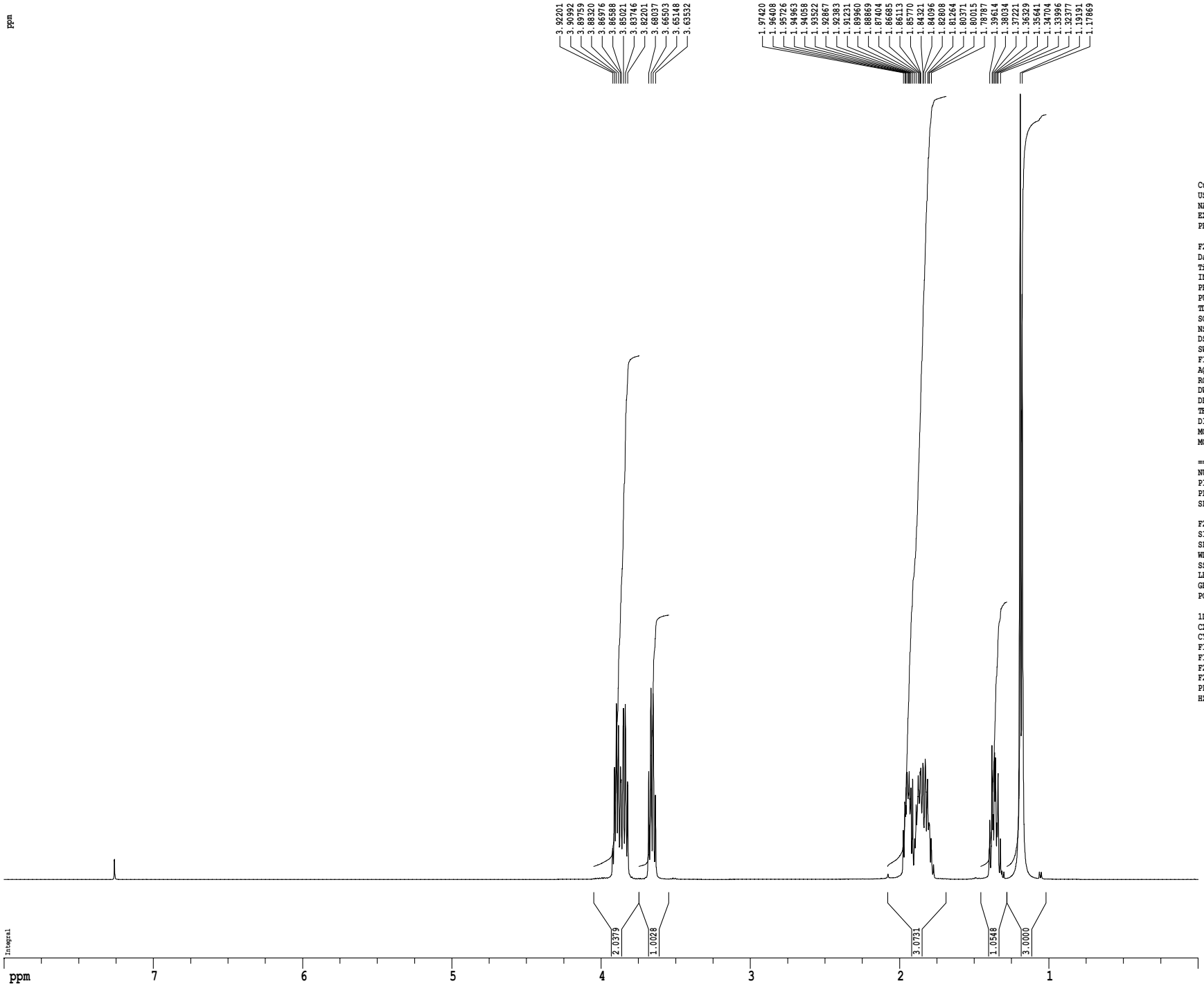
Electron ionization (EI-MS)



Varian Resolutions Pro



1H spectrum

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EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
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PROBHD   5 mm CPTCI 1H-
PULPROG               zg30
TD                   81728
SOLVENT              CDCl3
NS                       8
DS                       2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                     3.2
DW                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                  7.50 usec
PL1                 1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameter
SI                   65536
SF            500.2200308 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                 8.000 ppm
F1                4001.76 Hz
F2P                 0.000 ppm
F2                   0.00 Hz
PPMCM            0.35088 ppm/cm
HZCM           175.51581 Hz/cm
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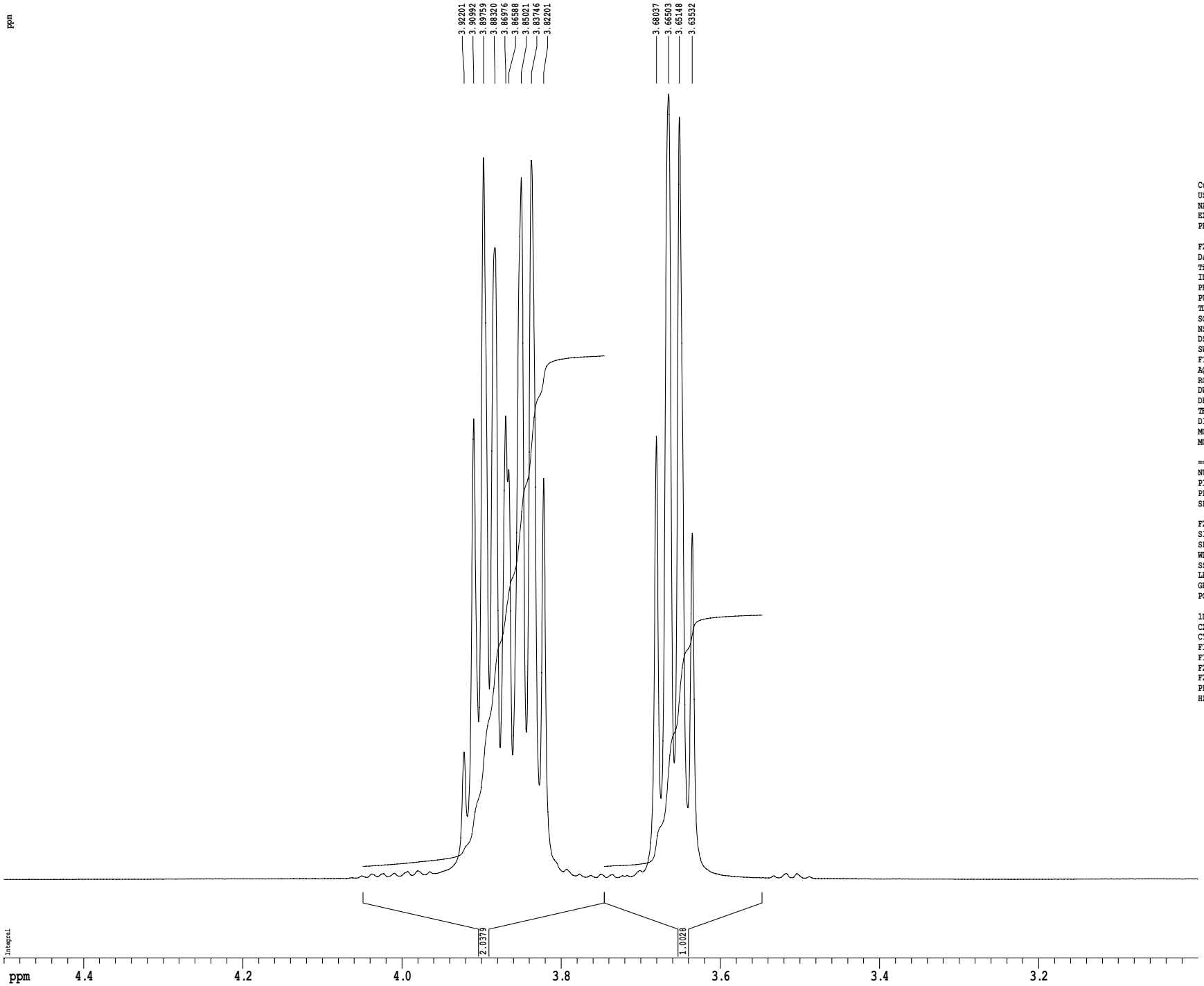
1	45108.5	1961.867	3.9220	0.60
2	45158.0	1955.822	3.9099	2.15
3	45208.4	1949.651	3.8976	3.37
4	45267.3	1942.454	3.8832	2.94
5	45322.3	1935.730	3.8698	2.16
6	45338.2	1933.788	3.8659	1.91
7	45402.3	1925.952	3.8502	3.27
8	45454.4	1919.576	3.8375	3.35
9	45517.7	1911.845	3.8220	1.87
10	46097.1	1840.994	3.6804	2.07
11	46159.9	1833.323	3.6650	3.66
12	46215.3	1826.542	3.6515	3.55
13	46281.4	1818.461	3.6353	1.62
14	53077.5	987.534	1.9742	0.94
15	53118.9	982.470	1.9641	1.48
16	53146.8	979.059	1.9573	1.42
17	53178.0	975.241	1.9496	2.05
18	53215.0	970.719	1.9406	1.65
19	53237.0	968.036	1.9352	2.07
20	53263.8	964.759	1.9287	1.37
21	53283.6	962.335	1.9238	1.75
22	53330.7	956.576	1.9123	1.92
23	53382.7	950.217	1.8996	0.78
24	53427.4	944.758	1.8887	1.43
25	53487.3	937.432	1.8740	1.99
26	53516.7	933.835	1.8668	1.54
27	53540.1	930.976	1.8611	2.06
28	53554.1	929.260	1.8577	2.13
29	53613.4	922.012	1.8432	2.23
30	53622.6	920.887	1.8410	2.19
31	53675.3	914.443	1.8281	2.30
32	53738.5	906.718	1.8126	1.92
33	53775.0	902.249	1.8037	1.09
34	53789.6	900.472	1.8002	1.06
35	53839.8	894.329	1.7879	0.79
36	55442.5	698.375	1.3961	1.14
37	55507.1	690.471	1.3803	2.56
38	55540.4	686.406	1.3722	1.24
39	55576.9	681.947	1.3633	2.43
40	55605.0	678.501	1.3564	2.32
41	55643.4	673.816	1.3470	1.08
42	55672.3	670.275	1.3400	2.03
43	55738.6	662.175	1.3238	0.78
44	56278.0	596.216	1.1919	15.00
45	56332.1	589.604	1.1787	11.18

1H spectrum

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Current Data Parameter
USER                nmr14t
NAME          midterm I a
EXPNO                   1
PROCNO                  1

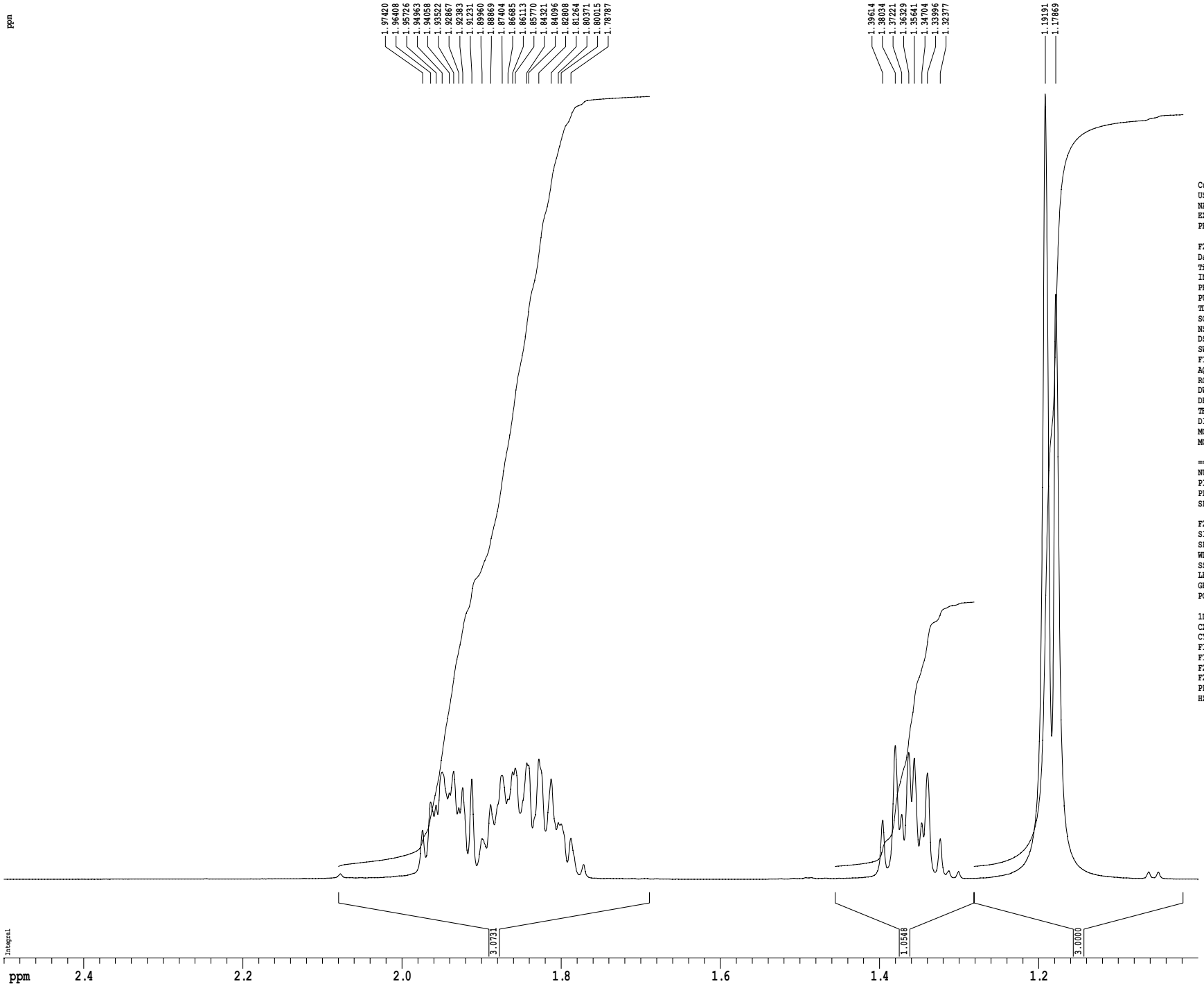
F2 - Acquisition Parameters
Date_            20141106
Time                18.59
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG               zg30
TD                   81728
SOLVENT              CDCl3
NS                       8
DS                       2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                     3.2
DW                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                  7.50 usec
PL1                 1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameter
SI                   65536
SF            500.2200308 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                 4.500 ppm
F1                2250.99 Hz
F2P                 3.000 ppm
F2                1500.66 Hz
PPMCM             0.06579 ppm/cm
HZCM             32.90921 Hz/cm
```

1H spectrum



Current Data Parameter

USER	nmr14t
NAME	midterm I a
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20141106
Time	18.59
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	zg30
TD	81728
SOLVENT	CDCl3
NS	8
DS	2
SWH	8012.820 Hz
FIDRES	0.098043 Hz
AQ	5.0998774 sec
RG	3.2
DW	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	7.50 usec
PL1	1.60 dB
SFO1	500.2235015 MHz

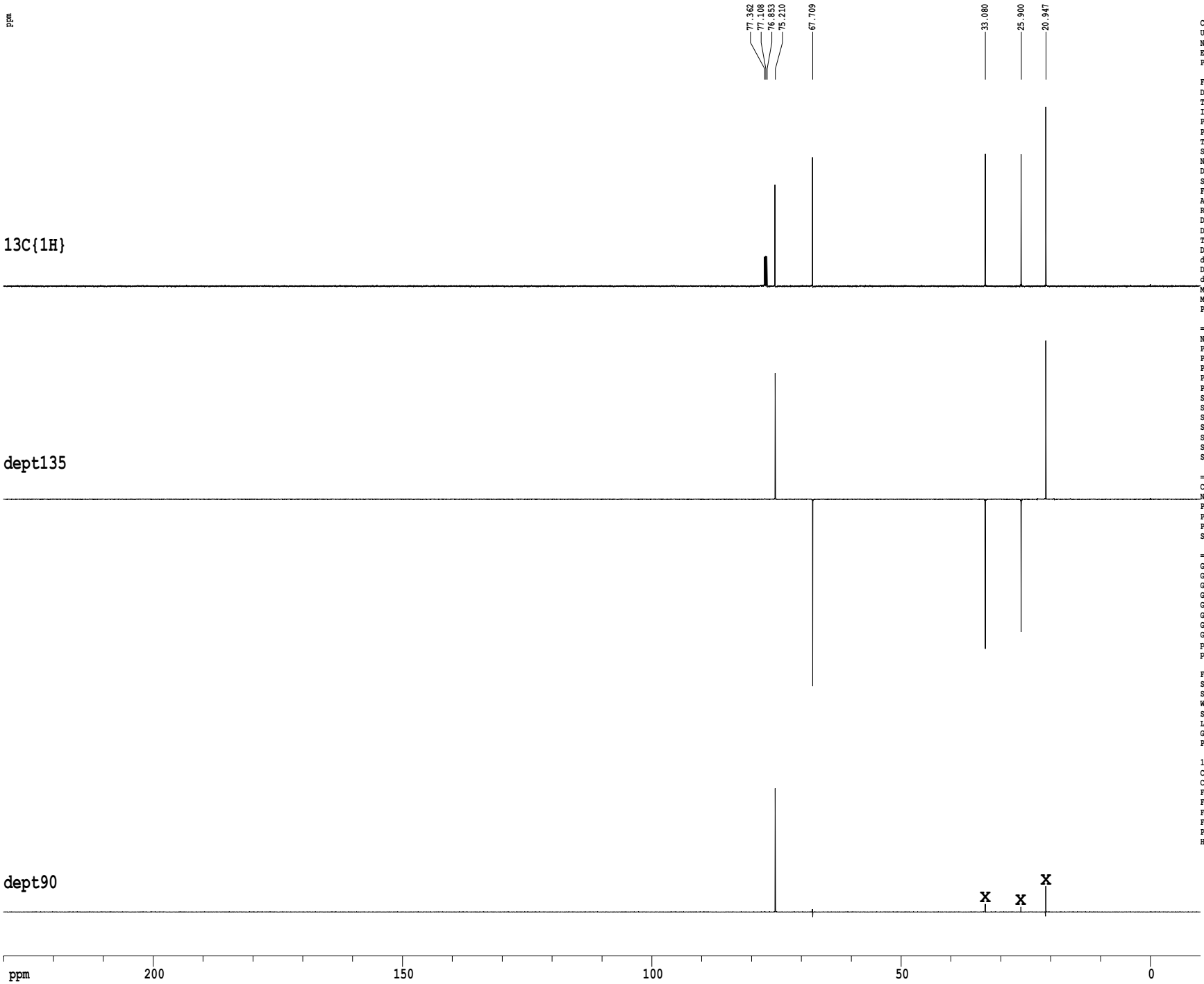
F2 - Processing parameter

SI	65536
SF	500.2200308 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

1D NMR plot parameters

CX	22.80 cm
CY	15.00 cm
F1P	2.500 ppm
F1	1250.55 Hz
F2P	1.000 ppm
F2	500.22 Hz
PPMCM	0.06579 ppm/cm
HZCM	32.90921 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling

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Current Data Parameters
USER                nmr14t
NAME          midterm I a
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20141106
Time                 19.02
INSTRUM            cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     112
DS                      16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                 7298.2
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1            0.25000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2                 31.00 usec

======== CHANNEL f1 =======
NUC1                 13C
P1                 15.50 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1          125.7942548 MHz
SP1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 =======
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12               24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                   65536
SF            125.7804190 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                230.000 ppm
F1                 28929.50 Hz
F2P                -10.000 ppm
F2                -1257.80 Hz
PPMCM             10.52632 ppm/cm
HZCM           1324.00439 Hz/cm
```