NAME_____

Chem 203

Organic Spectroscopy

Midterm Examination, Part II (60 points total)

Problem 4 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.

4. Analyze the spectra and solve the structure of the molecule for which data are provided. The following data are provided: EI-MS; IR (KBr pellet); 500 MHz ^{1}H NMR in CD_3SOCD_3; 125.8 MHz ^{13}C NMR, DEPT 90, and DEPT 135 in CD_3SOCD_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):

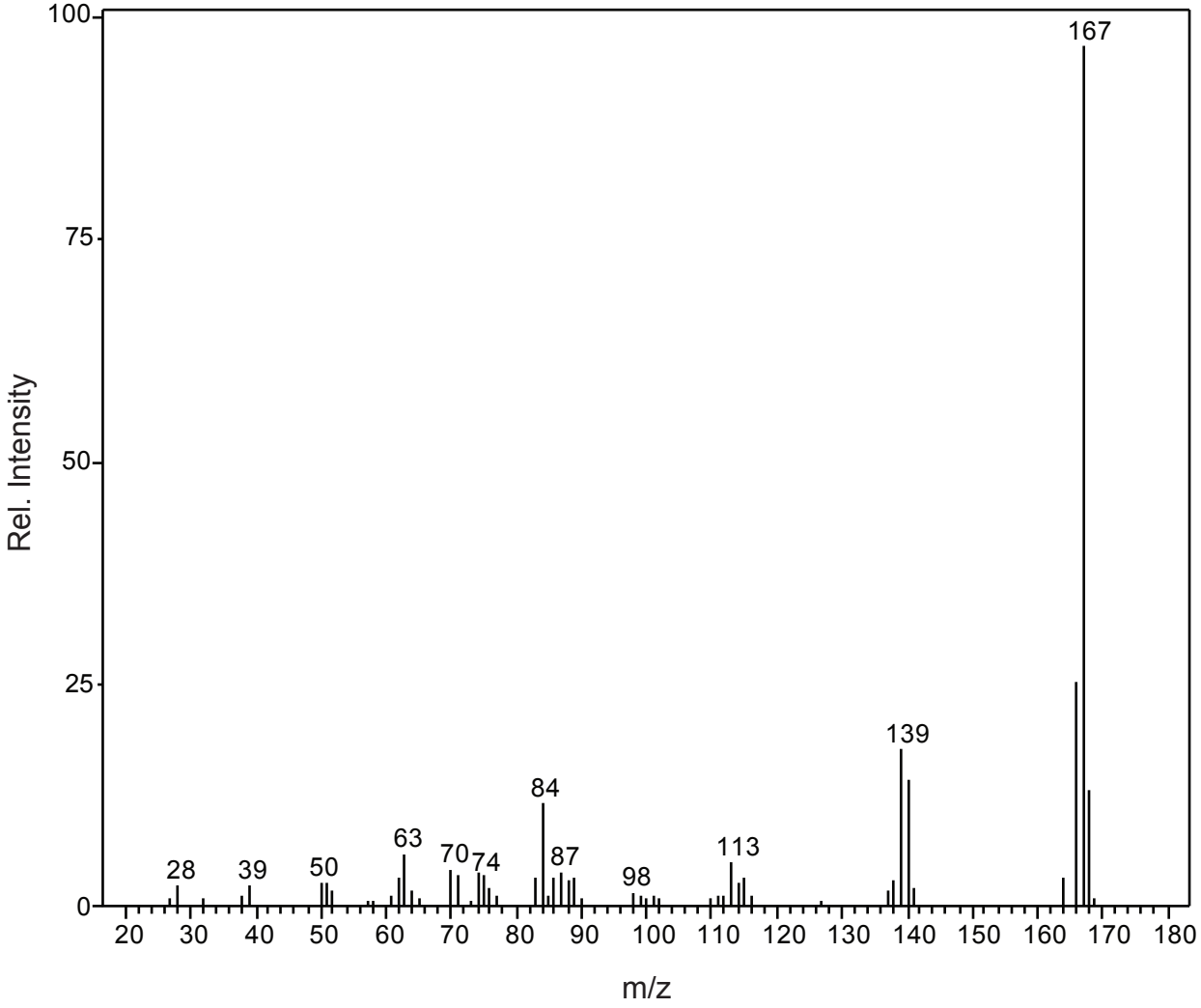
Fragments (from NMR):

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

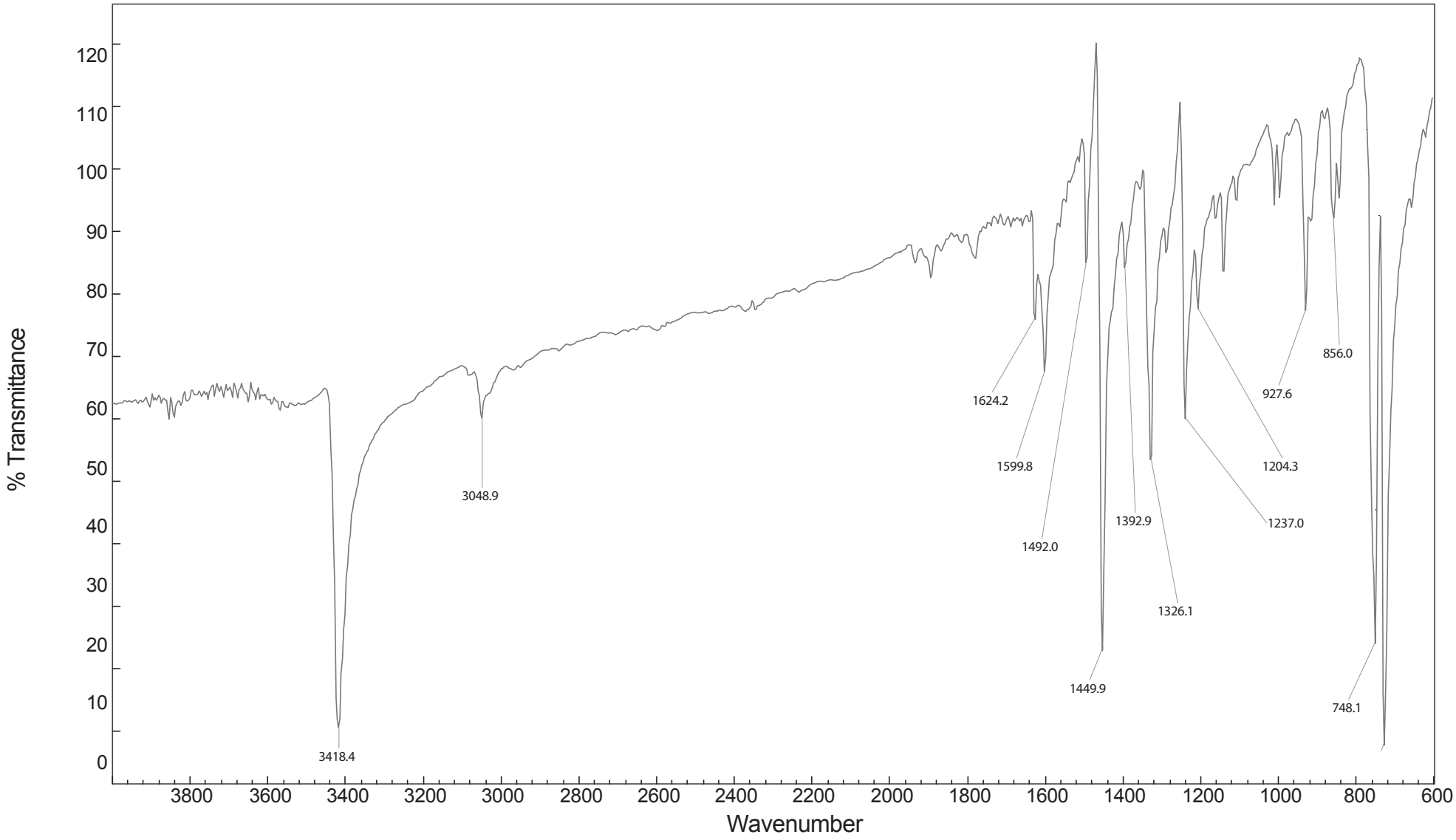
Structure with ^{1}H NMR resonances lettered from the most downfield to the most upfield (a, b, c, d, etc.): (Note: Not all resonances can be assigned with certainty. If assignments are uncertain, indicate so by showing possible letters.)

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.)

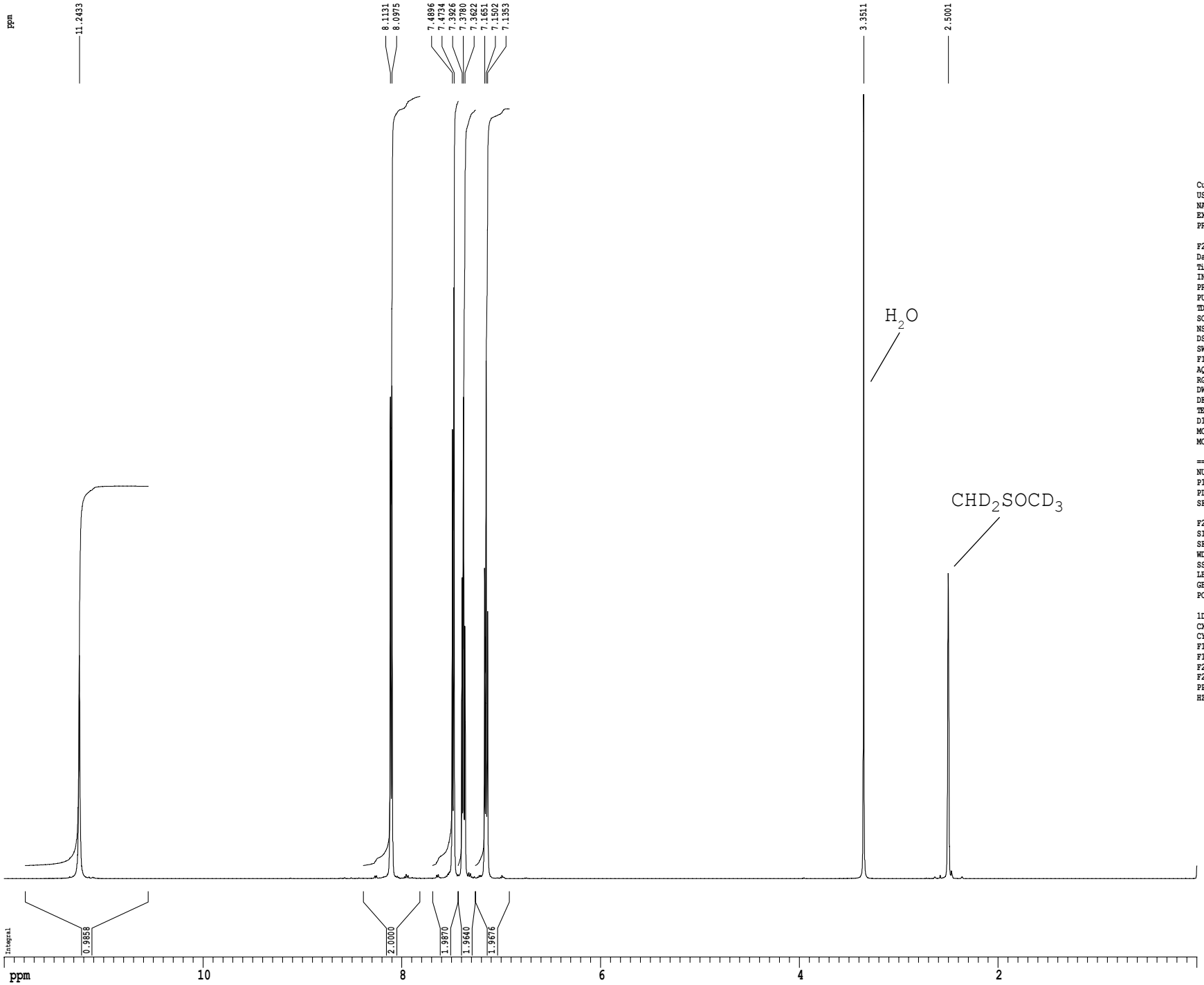
Electron ionization (EI-MS)



Varian Resolutions Pro



1H spectrum

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PROCNO                  1

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PULPROG              zg30
TD                  81728
SOLVENT              DMSO
NS                     32
DS                      2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                      5
DW                 62.400 usec
DE                  6.00 usec
TE                 298.0 K
D1              0.10000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

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NUC1                   1H
P1                  7.50 usec
PL1                 1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameter
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SF            500.2200130 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                12.000 ppm
F1                6002.64 Hz
F2P                -0.000 ppm
F2                  -0.00 Hz
PPMCM            0.52632 ppm/cm
HZCM           263.27368 Hz/cm
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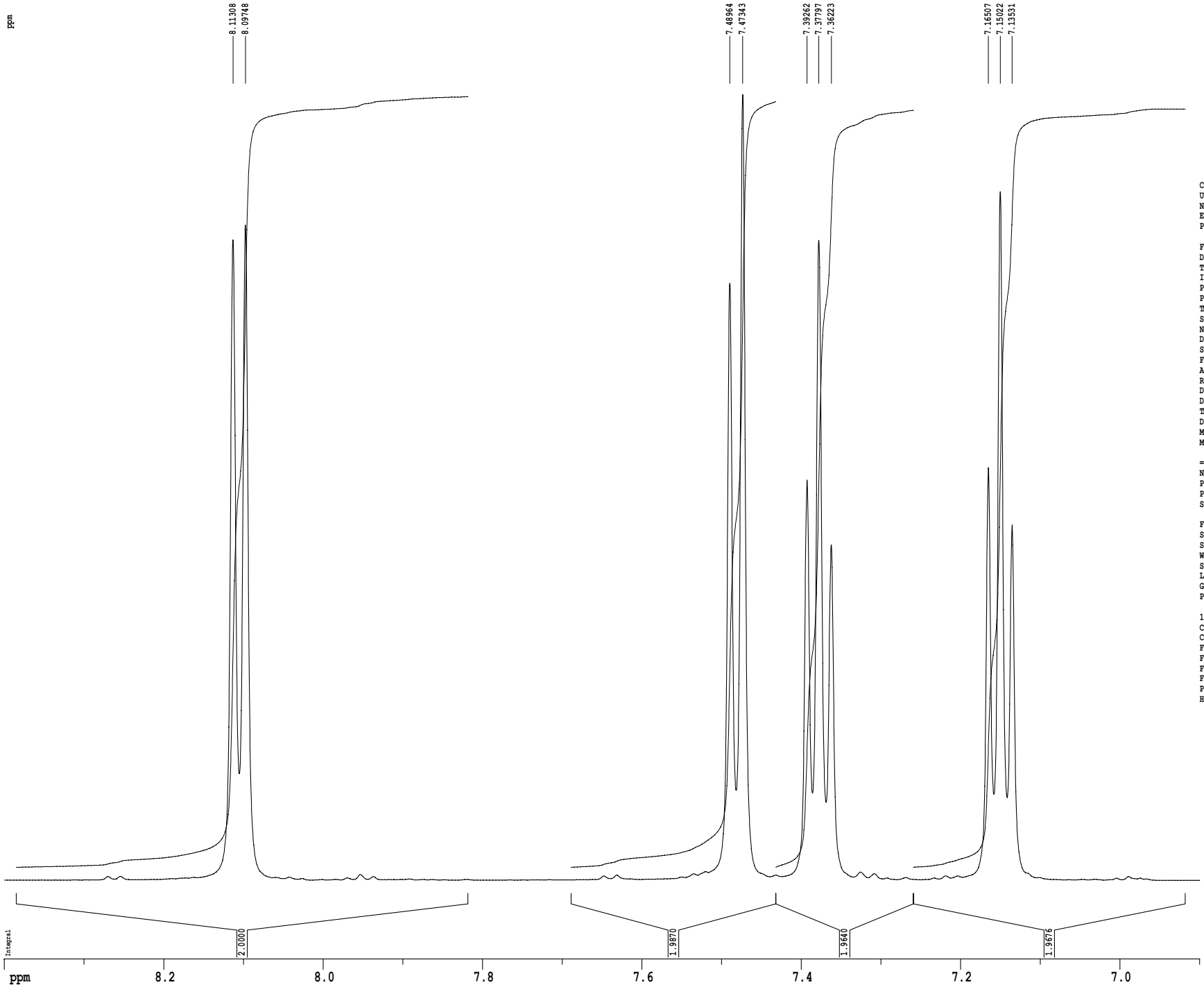
#	ADDRESS	FREQUENCY [Hz]	[PPM]	INTENSITY
1	15301.2	5624.100	11.2433	4.27
2	28107.5	4058.324	8.1131	9.22
3	28171.3	4050.520	8.0975	9.42
4	30658.1	3746.467	7.4896	8.59
5	30724.4	3738.359	7.4734	11.31
6	31055.0	3697.938	7.3926	5.75
7	31115.0	3690.608	7.3780	9.20
8	31179.4	3682.737	7.3622	4.83
9	31986.0	3584.111	7.1651	5.93
10	32046.8	3576.682	7.1502	9.90
11	32107.8	3569.224	7.1353	5.11
12	47589.7	1676.307	3.3511	15.00
13	51071.5	1250.609	2.5001	5.84

1H spectrum

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Current Data Parameters
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NAME          midterm I d
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141030
Time                21.09
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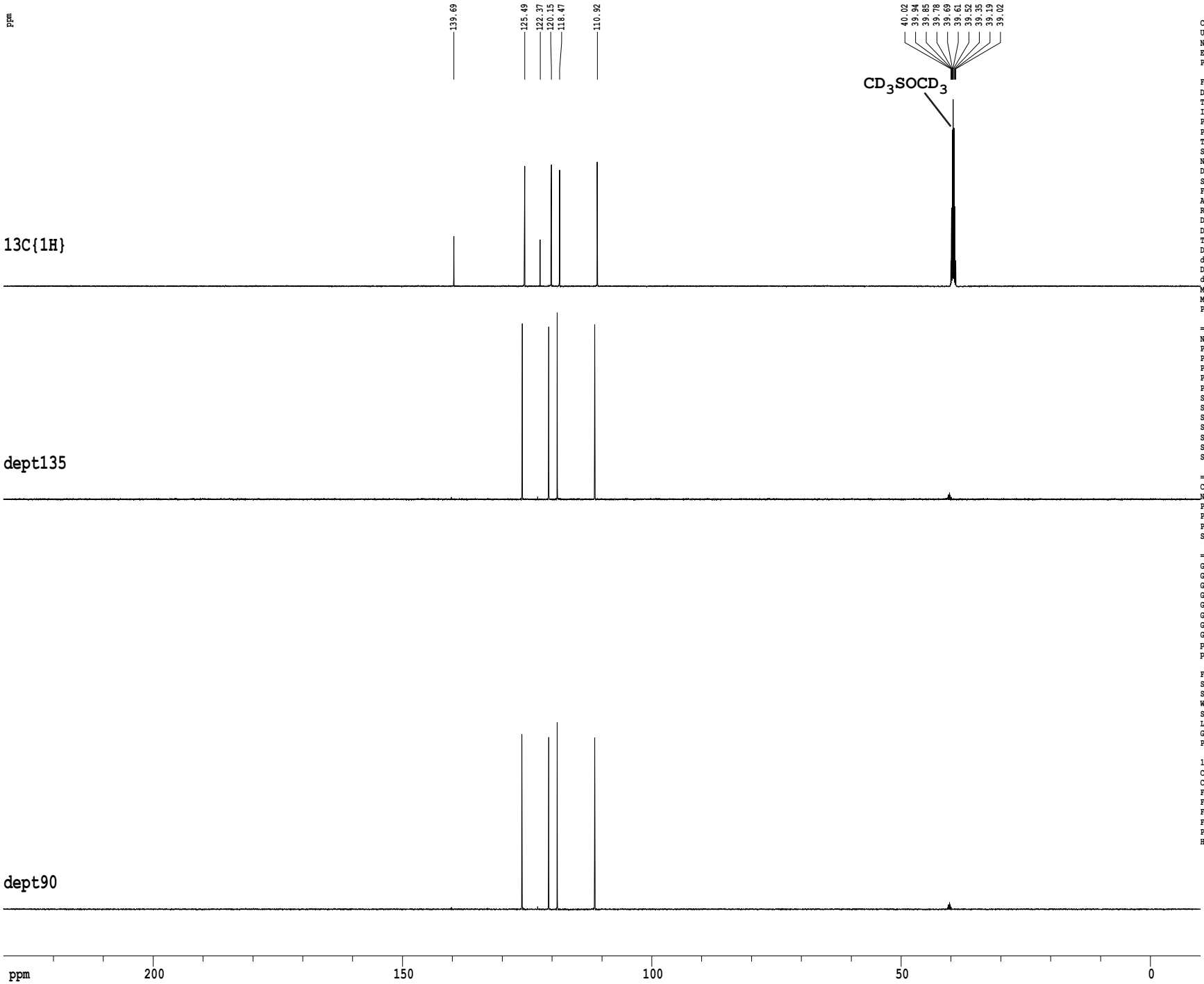
PULPROG              zg30
TD                  81728
SOLVENT              DMSO
NS                     32
DS                      2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                      5
DW                 62.400 usec
DE                  6.00 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            500.2200130 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                  8.400 ppm
F1                 4201.85 Hz
F2P                  6.900 ppm
F2                 3451.52 Hz
PPMCM             0.06579 ppm/cm
HZCM             32.90920 Hz/cm
```

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

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PROCNO                1

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Time              21.13
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PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                65536
SOLVENT            CDCl3
NS                  608
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           125.7804792 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             28929.51 Hz
F2P              -10.000 ppm
F2             -1257.80 Hz
PPMCM           10.52632 ppm/cm
HZCM          1324.00513 Hz/cm
```