NAME_____

Chem 203

Organic Spectroscopy

Midterm Examination, Part II (60 points total)

Problem 2 of 4 (three out of four required, 20 points)

Saturday, November 10, 2012, 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.

2. 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}H NMR and ^{13}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: 169.0294

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.)

C:\Xcalibur\Data\RKS_2 10/31/2012 12:54:10 PM

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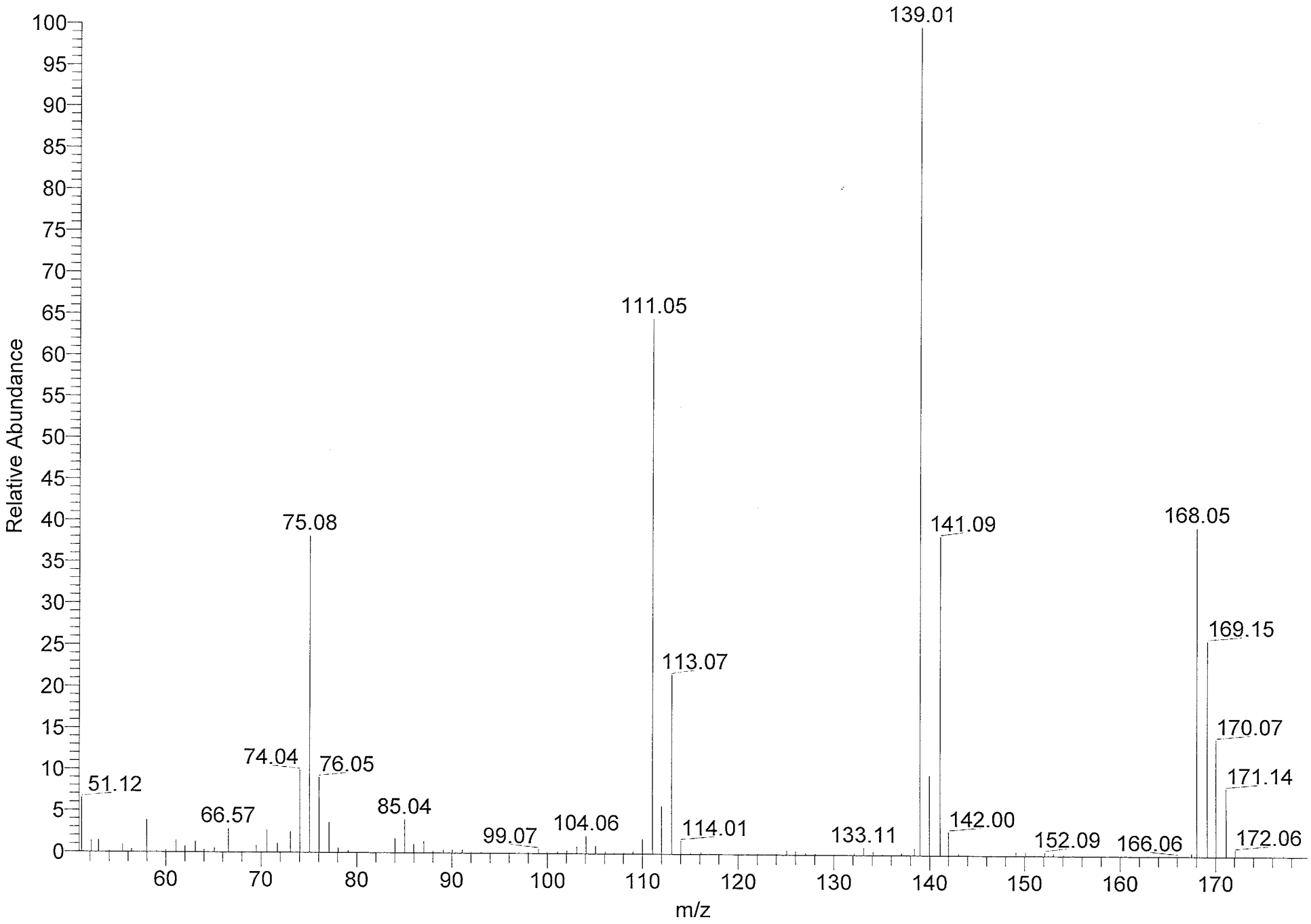
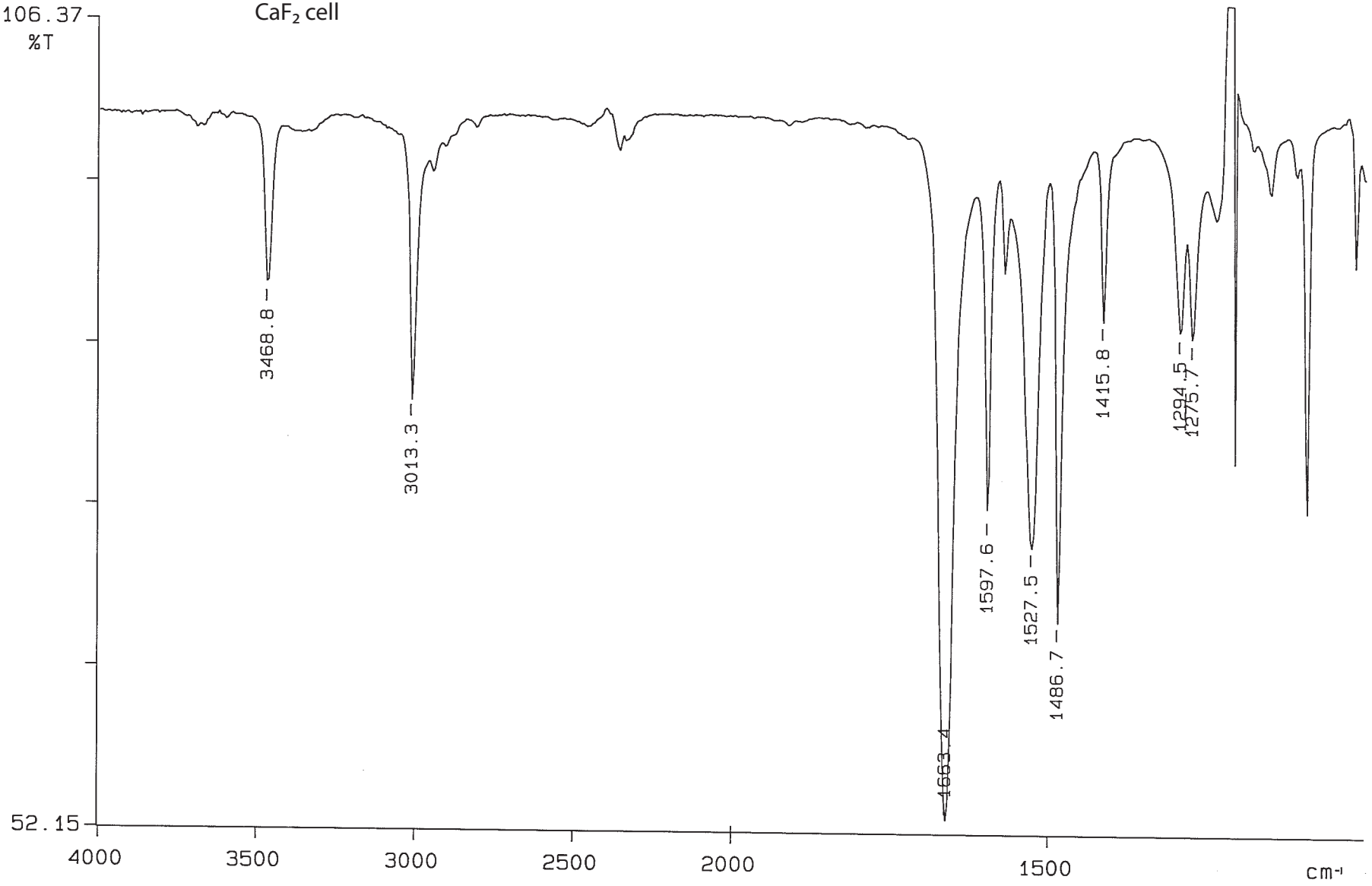
T: {0,0} + c EI Full ms [50.00-600.00]



PERKIN ELMER #2

5% solution in $CHCl_3$
CaF_2 cell



12/10/31 13:03
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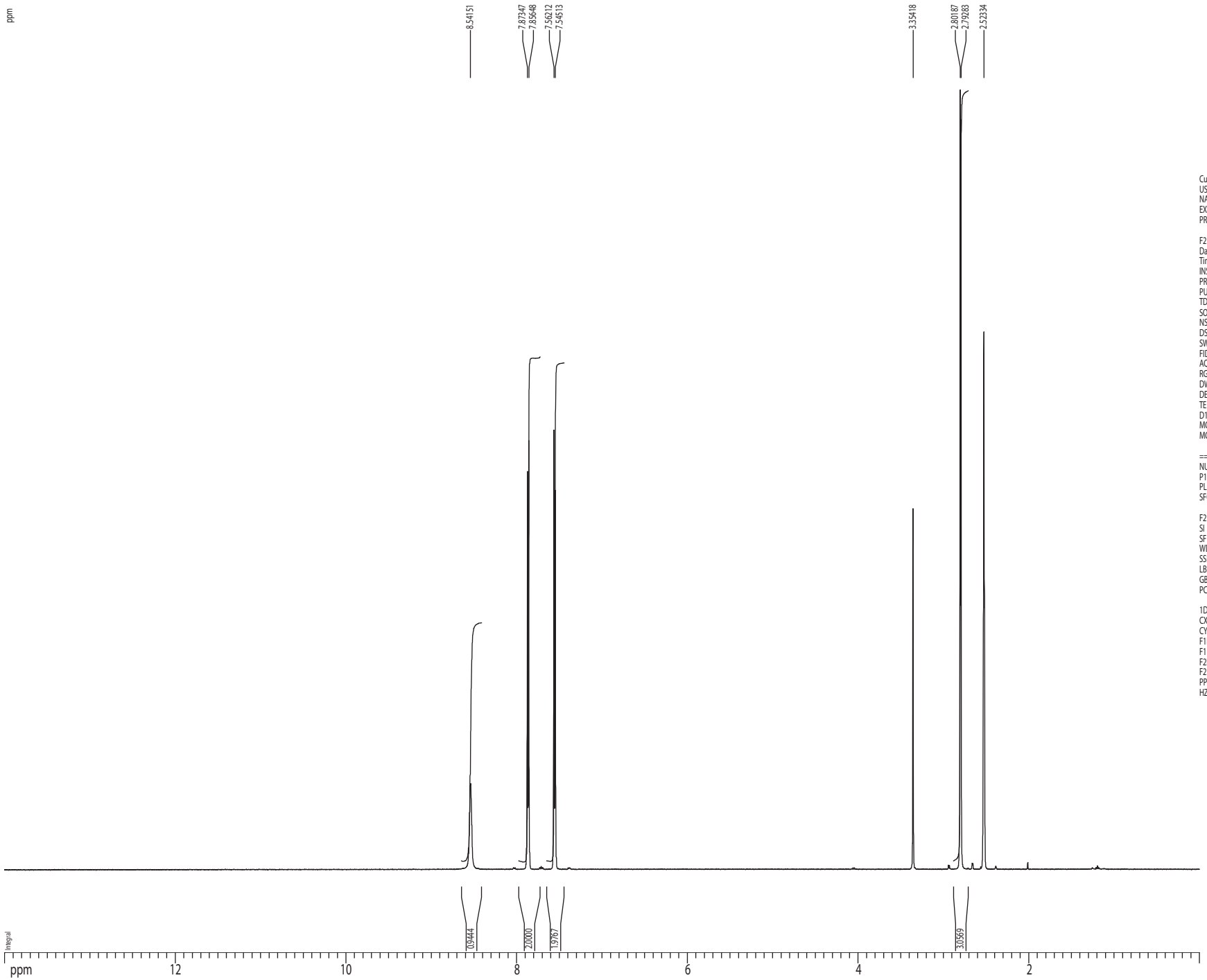
500 MHZ 1H NMR Spectrum in CD3SOCD3



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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 DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 12.7
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 parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 14.000 ppm
F1 7003.08 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.61404 ppm/cm
HZCM 307.15265 Hz/cm

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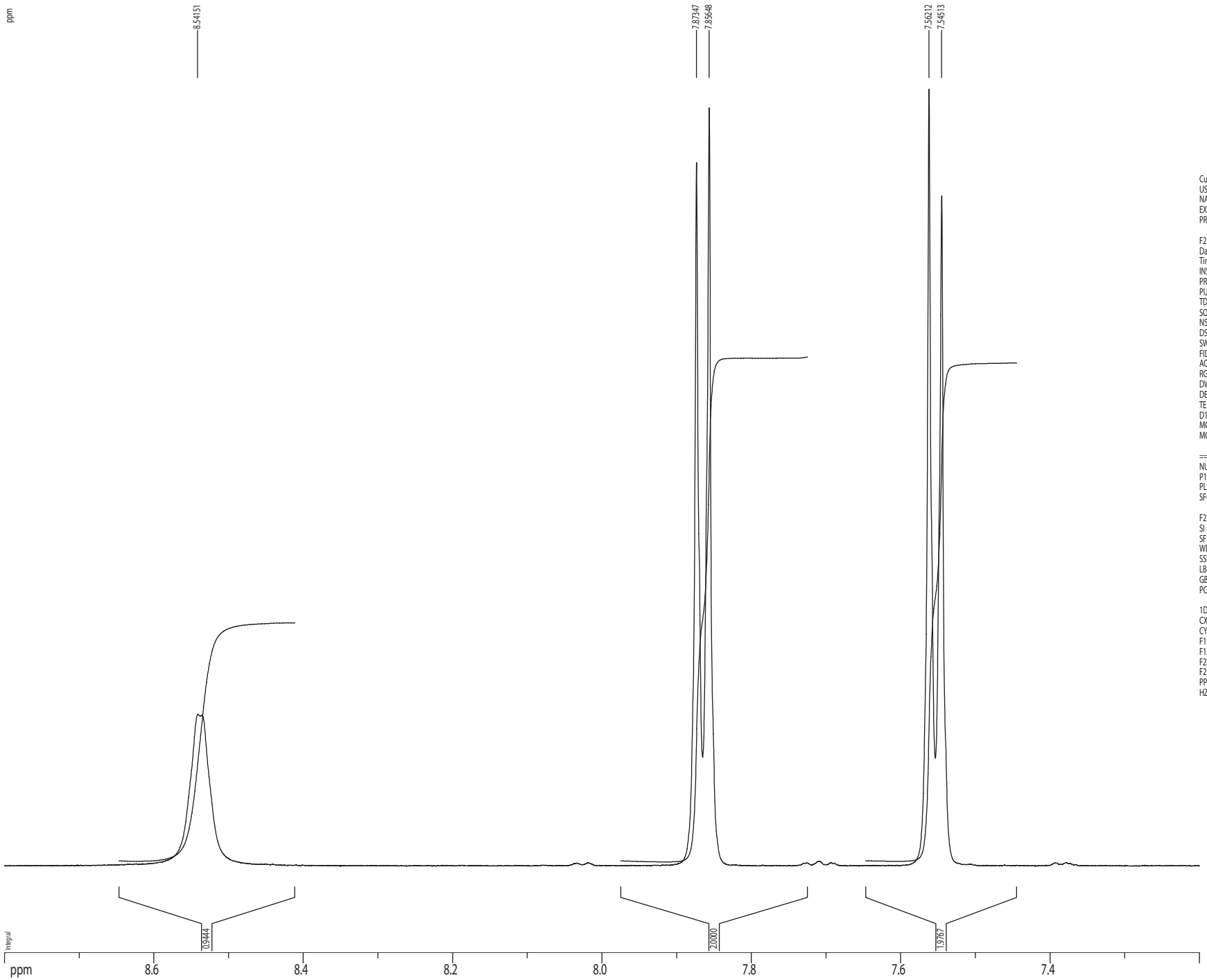
1	26461.3	4272.634	8.5415	1.73
2	29194.4	3938.467	7.8735	7.71
3	29263.9	3929.970	7.8565	8.28
4	30468.3	3782.722	7.5621	8.49
5	30537.8	3774.225	7.5451	7.33
6	47684.0	1677.828	3.3542	6.97
7	49943.6	1401.553	2.8019	15.00
8	49980.6	1397.028	2.7928	14.43
9	51083.1	1262.223	2.5233	10.35

1H spectrum



Current Data Parameters
USER nmr12t
NAME Mid_2_500_DMSO
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121101
Time 10.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 12.7
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 parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 8.800 ppm
F1 4401.94 Hz
F2P 7.200 ppm
F2 3601.58 Hz
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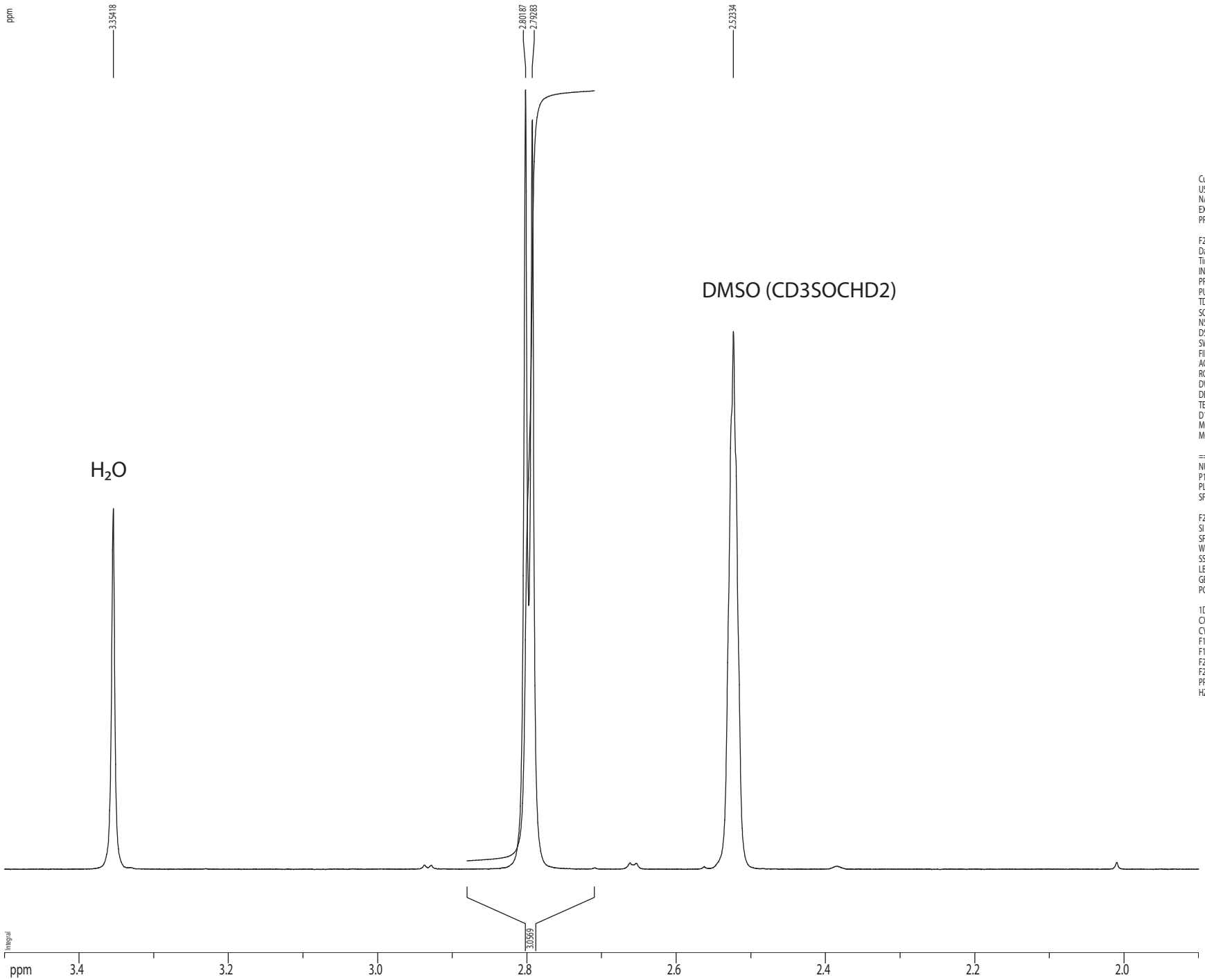
HZCM 35.10317 Hz/cm

1H spectrum



Current Data Parameters
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NAME Mid_2_500_DMSO
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 10.27
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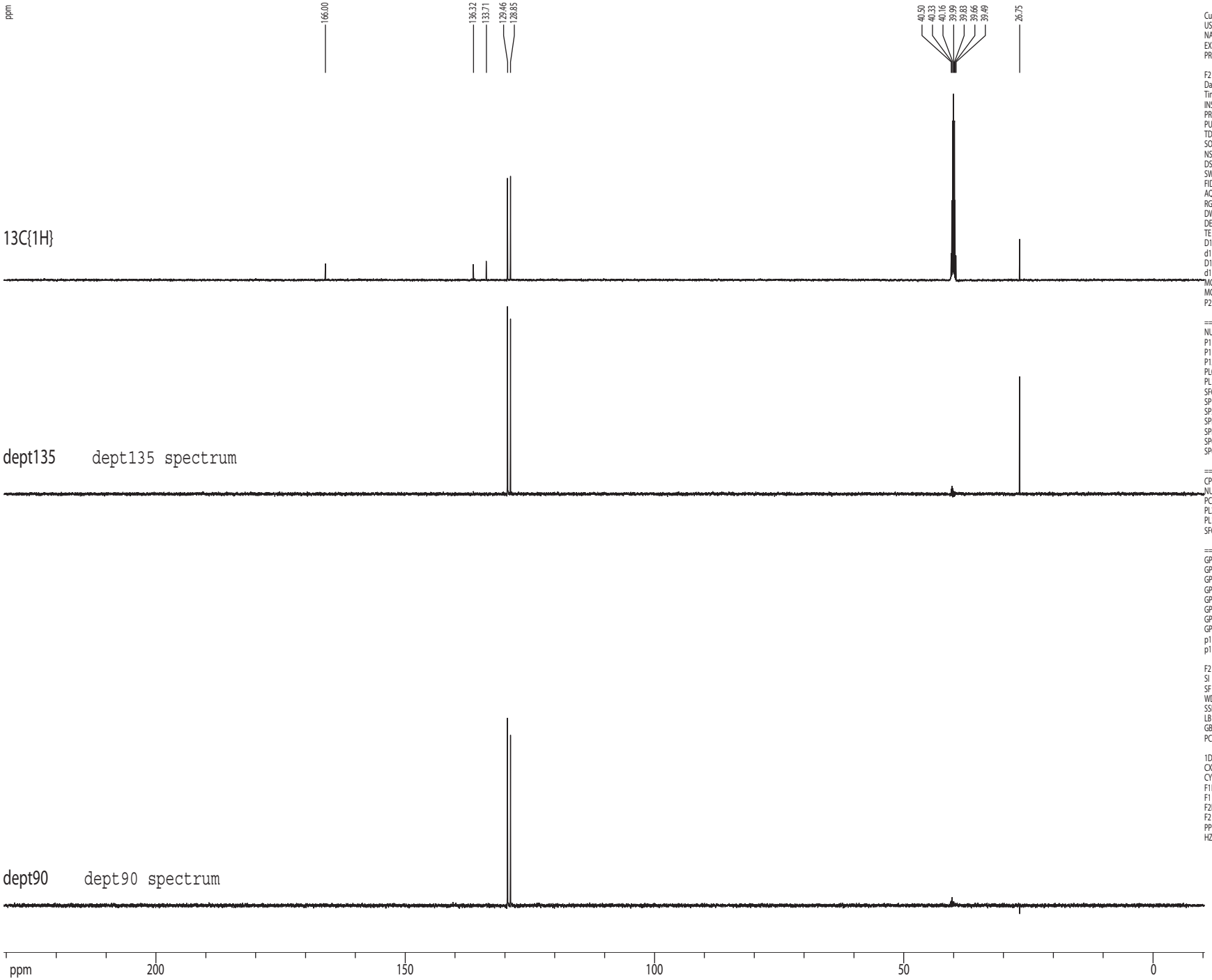
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 12.7
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 3.500 ppm
F1 1750.77 Hz
F2P 1.900 ppm
F2 950.42 Hz
PPMCM 0.07018 ppm/cm
HZCM 35.10316 Hz/cm

125.8 MHz 13C NMR spectrum with 1H decoupling in CD3SOCD3



Current Data Parameters
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PROCNO 1

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PULPROG SpinEchopg30gp.prd
TD 65536
SOLVENT CDCl3
NS 137
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 =====
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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 230.637 ppm
F1 29009.68 Hz
F2P -10.287 ppm
F2 -1293.96 Hz
PPMCM 10.56688 ppm/cm
HZCM 1329.10706 Hz/cm