

NAME _____

Chem 203

Organic Spectroscopy

Midterm Examination, Part II (60 points total)

Problem 3 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 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 ^1H 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: 112.0160

Noteworthy Heteroatoms:

Molecular Formula:

Unsaturation Number:

Functional Groups (be as specific as possible):

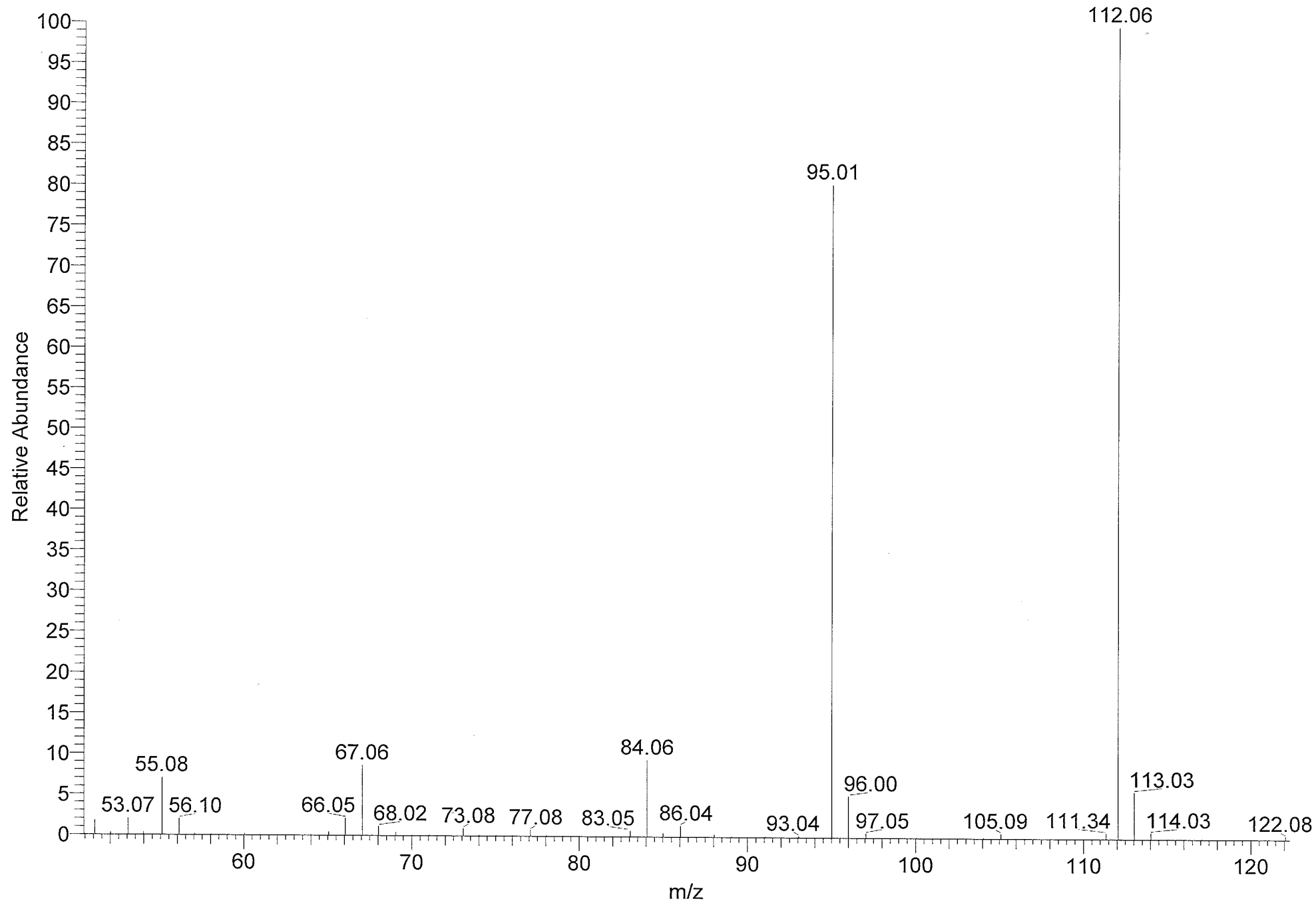
Fragments (from NMR):

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

Structure with ^1H 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.)

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

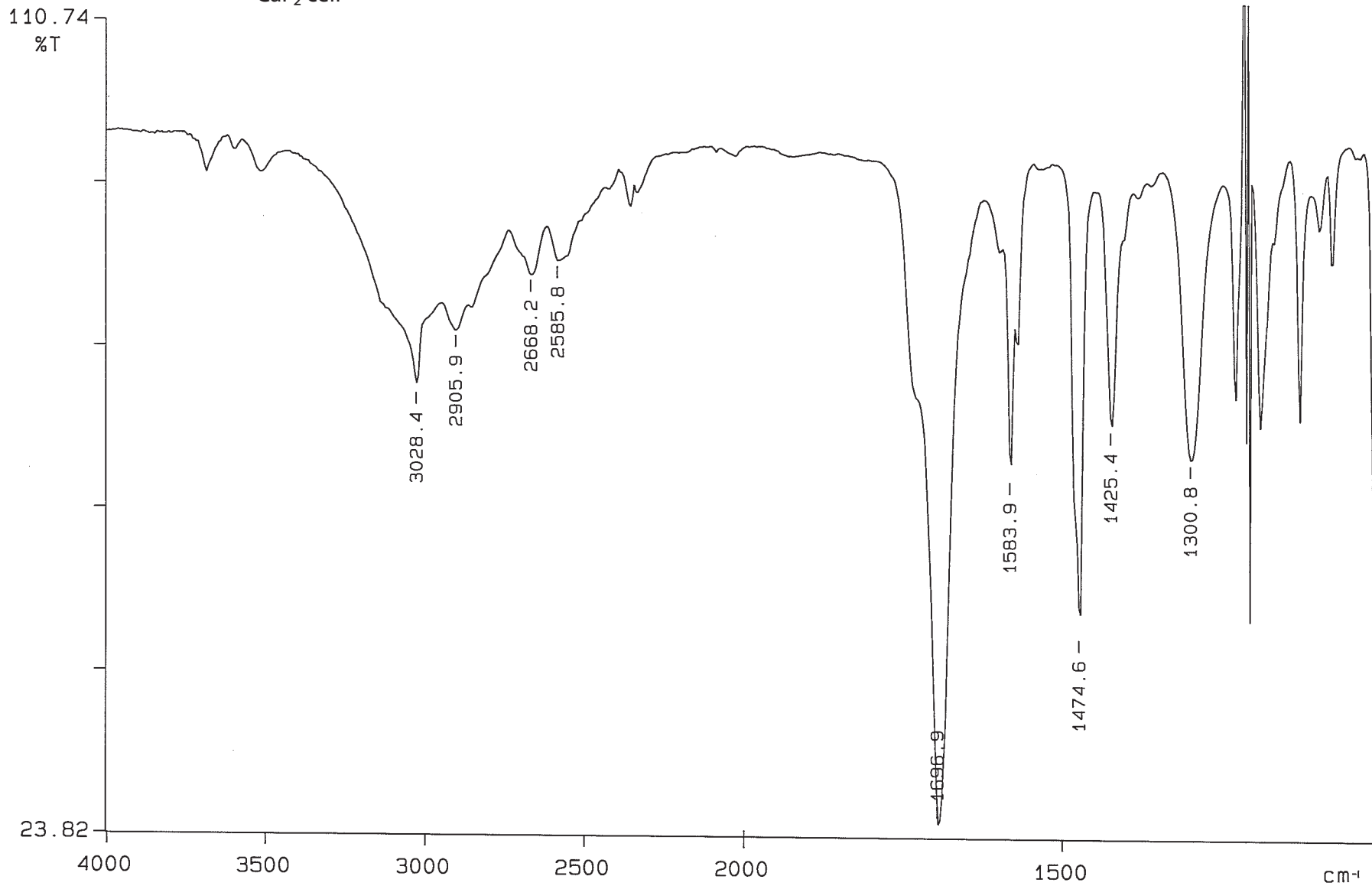


#3

PERKIN ELMER

5% solution in CHCl_3

CaF_2 cell

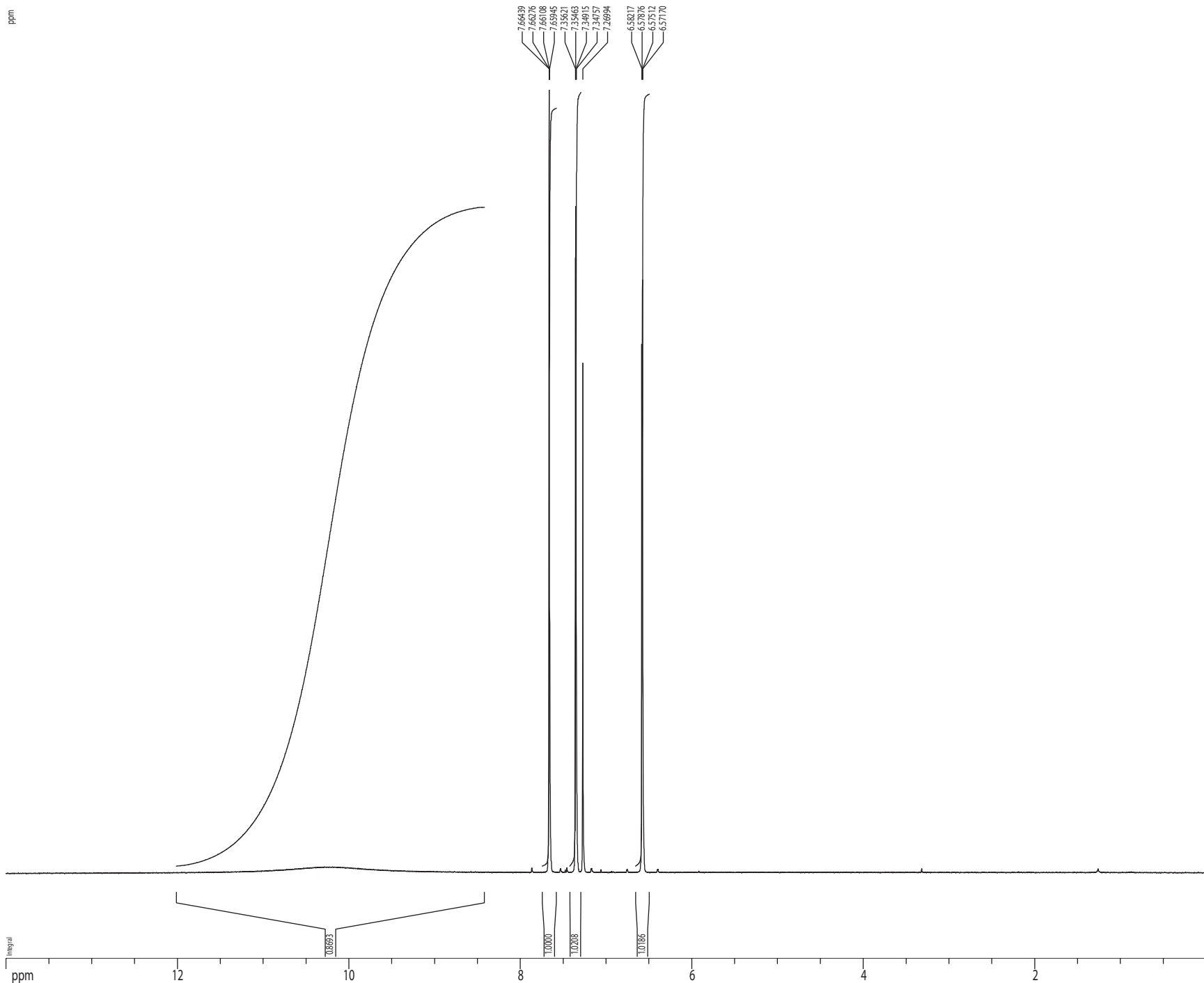


12/10/31 12:58

X: 4 scans, 4.0cm-1

500 MHz ¹H NMR spectrum in CDCl₃

ppm



Current Data Parameters
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 NAME Mid_3_500_CDCL3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121101
 Time 8.52
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG zg30
 TD 81728
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 8
 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 500.2200258 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

Integral

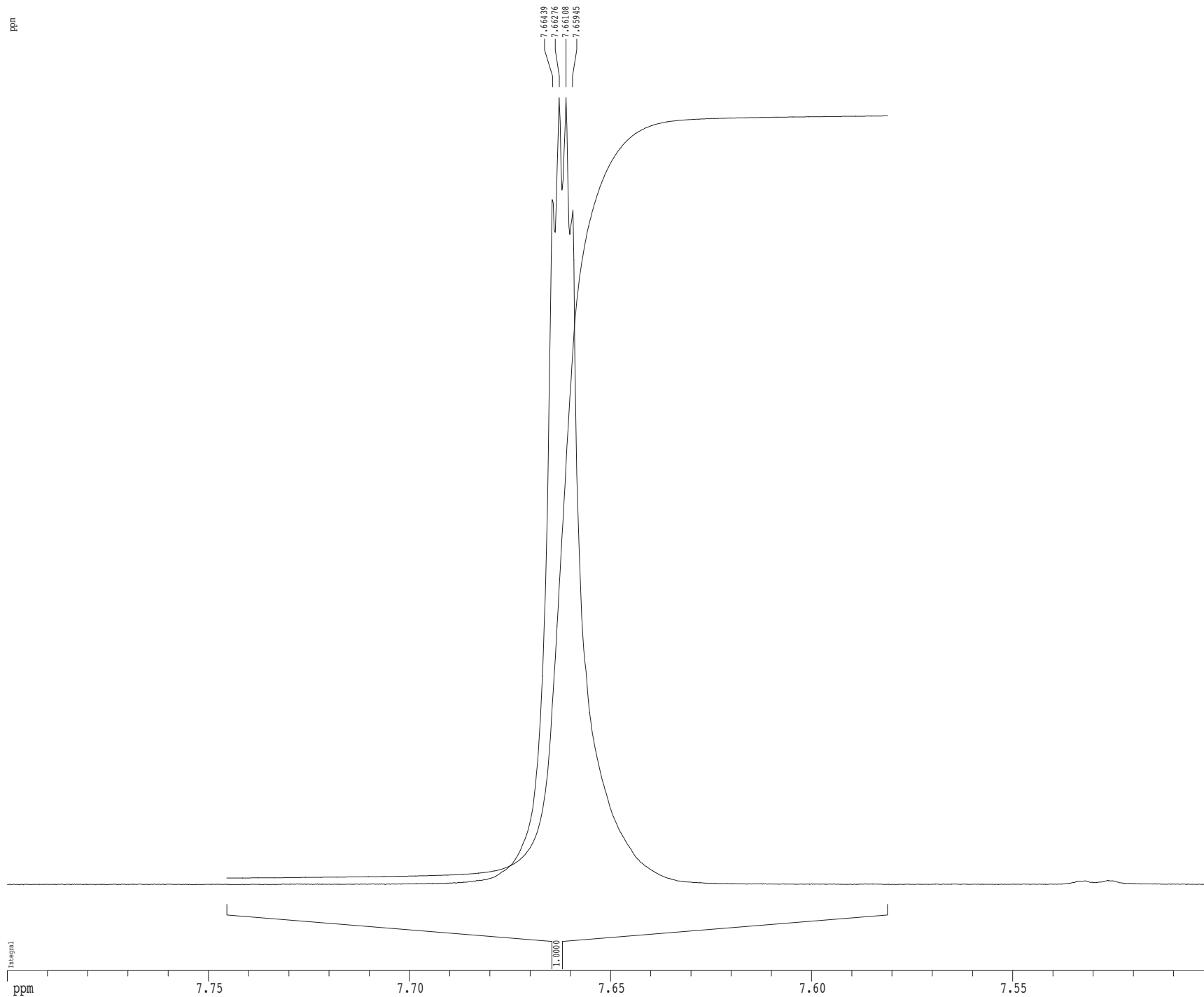
ppm

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	[Hz]	[PPM]	
1	29838.4	3833.881	7.6644 13.19
2	29845.1	3833.066	7.6628 15.00
3	29852.0	3832.224	7.6611 14.99
4	29858.7	3831.409	7.6594 12.94
5	31099.3	3679.724	7.3562 11.86
6	31105.7	3678.934	7.3546 11.50
7	31128.2	3676.189	7.3491 12.81
8	31134.6	3675.401	7.3476 11.91
9	31452.2	3636.571	7.2699 9.84
10	34266.1	3292.533	6.5822 10.17
11	34280.0	3290.825	6.5788 11.19
12	34294.9	3289.008	6.5751 11.40
13	34308.9	3287.296	6.5717 10.51

1H spectrum

ppm



Current Data Parameters
USER nmrl2t
NAME Mid_3_500_CDCL3
EXPNO 1
PROCNO 1

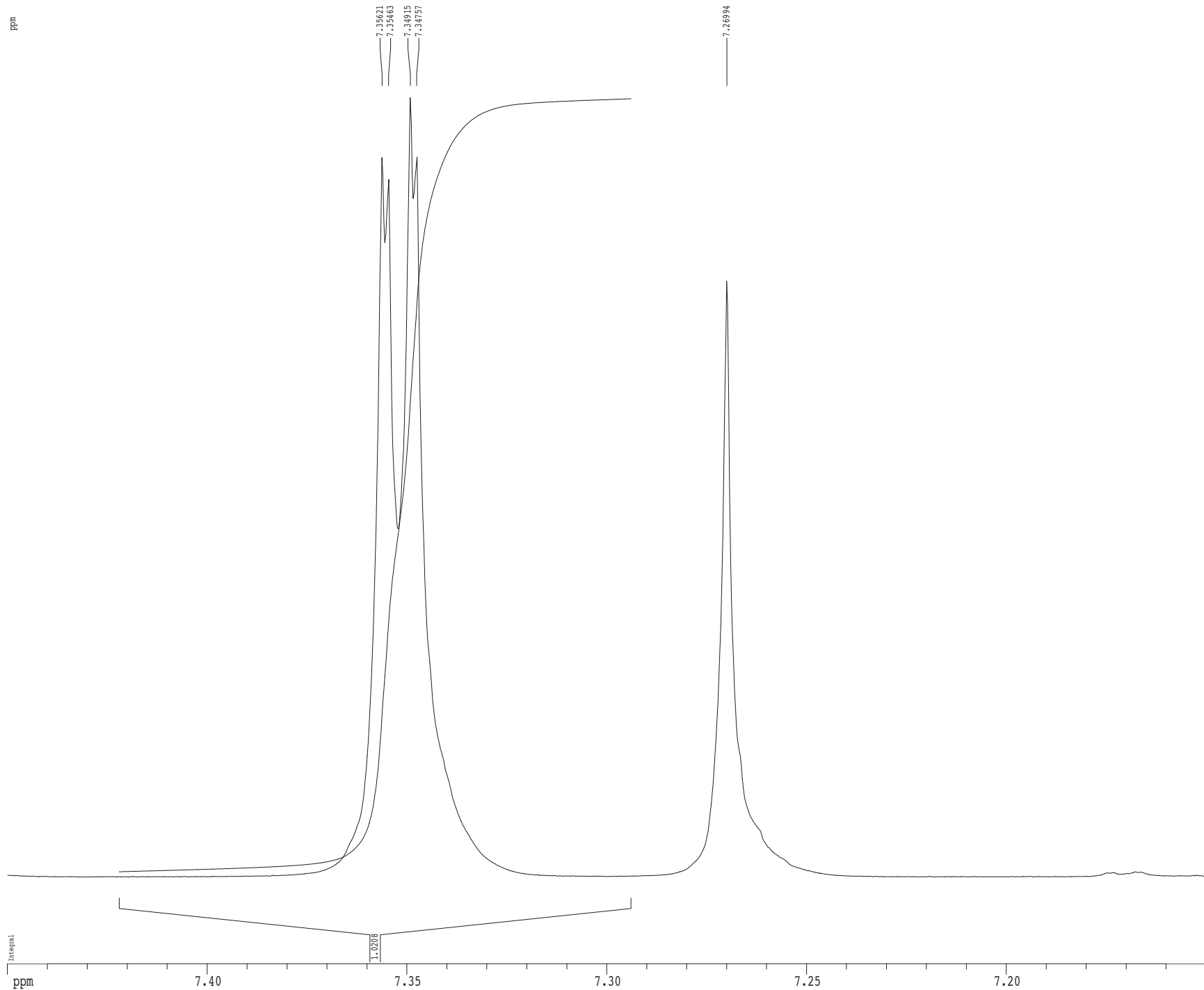
F2 - Acquisition Parameters
Date_ 20121101
Time 8.52
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCL3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 8
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRX 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SF01 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200258 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 7.800 ppm
F1 3901.72 Hz
F2P 7.500 ppm
F2 3751.65 Hz
PPMCM 0.01316 ppm/cm
HZCM 6.58185 Hz/cm

1H spectrum



Current Data Parameters
USER nmrl2t
NAME Mid_3_500_CDCL3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121101
Time 8.52
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCL3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 8
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRX 0.01500000 sec

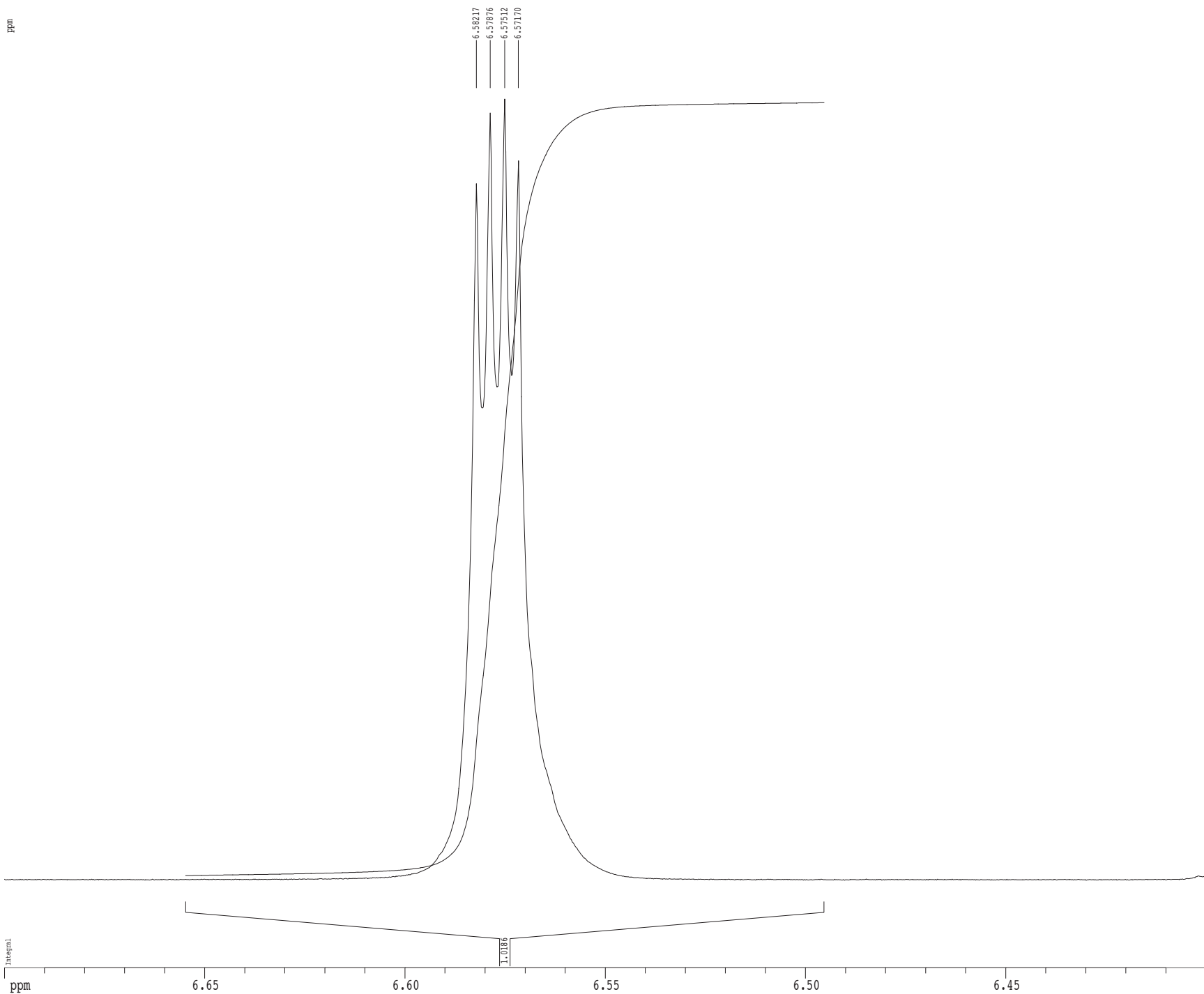
===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SF01 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200258 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 7.450 ppm
F1 3726.64 Hz
F2P 7.150 ppm
F2 3576.57 Hz
PPMCM 0.01316 ppm/cm
HZCM 6.58184 Hz/cm

1H spectrum

ppm



Current Data Parameters
USER nmrl2t
NAME Mid_3_500_CDCL3
EXPNO 1
PROCNO 1

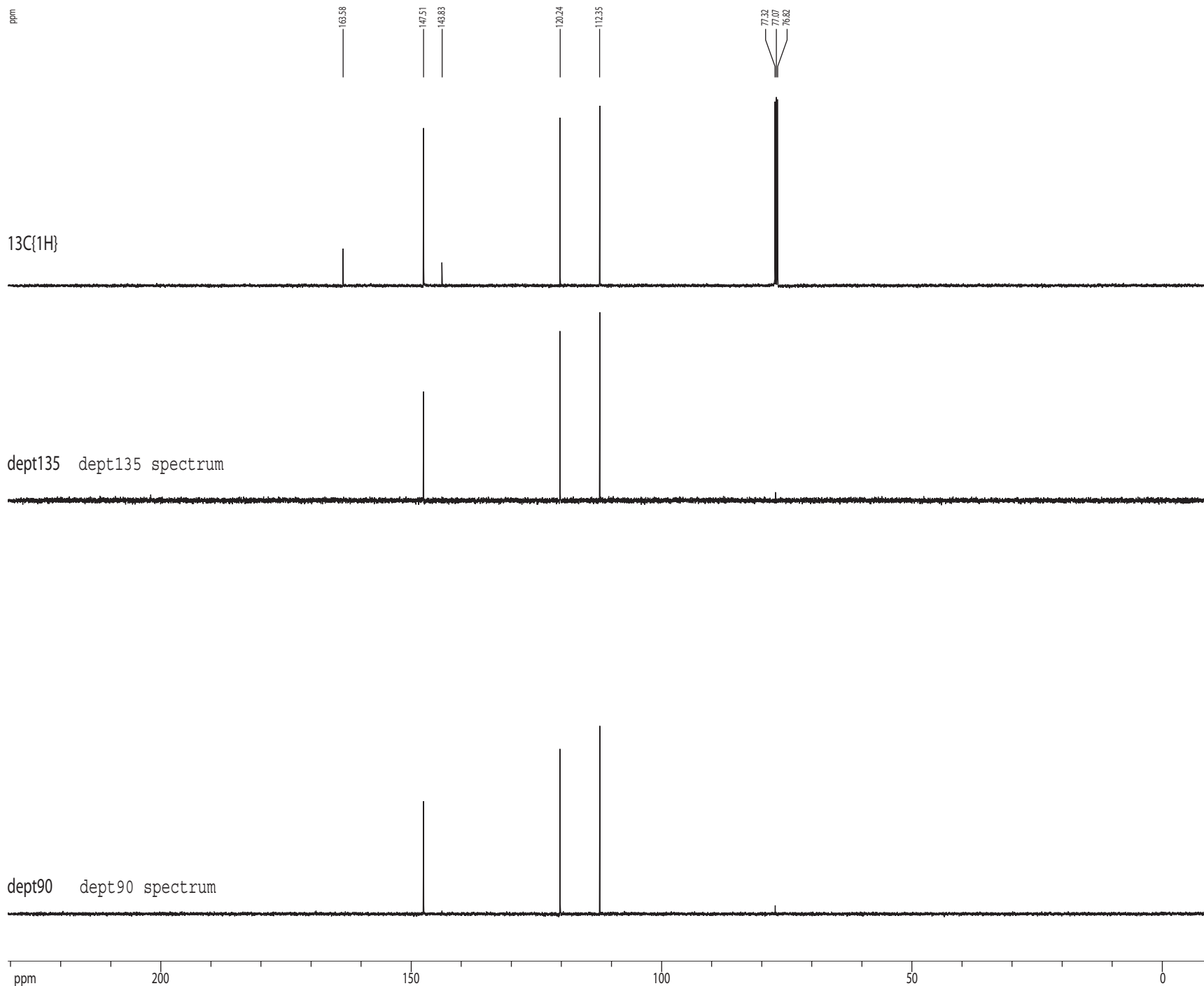
F2 - Acquisition Parameters
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Time 8.52
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PULPROG zg30
TD 81728
SOLVENT CDCL3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 8
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRX 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SF01 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200258 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 6.700 ppm
F1 3351.47 Hz
F2P 6.400 ppm
F2 3201.41 Hz
PPMCM 0.01316 ppm/cm
HZCM 6.58184 Hz/cm

125.8 MHz ¹³C NMR spectrum with ¹H decoupling in CDCl₃



Current Data Parameters
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 NAME Mid_3_500_CDCl3
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
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 Time 9:01
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG SpinEchogg30gp.prd
 TD 65536
 SOLVENT CDCl3
 NS 500
 DS 16
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0814105 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
 MCWRR 0.00000000 sec
 MCWRR 0.01500000 sec
 P2 31.00 usec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 15.50 usec
 P11 500.00 usec
 P12 2000.00 usec
 PLO 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 3.58 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