

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 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 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. The following data are provided: EI-MS; IR (thin film on NaCl plates); 500 MHz ^1H 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 ^1H 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):

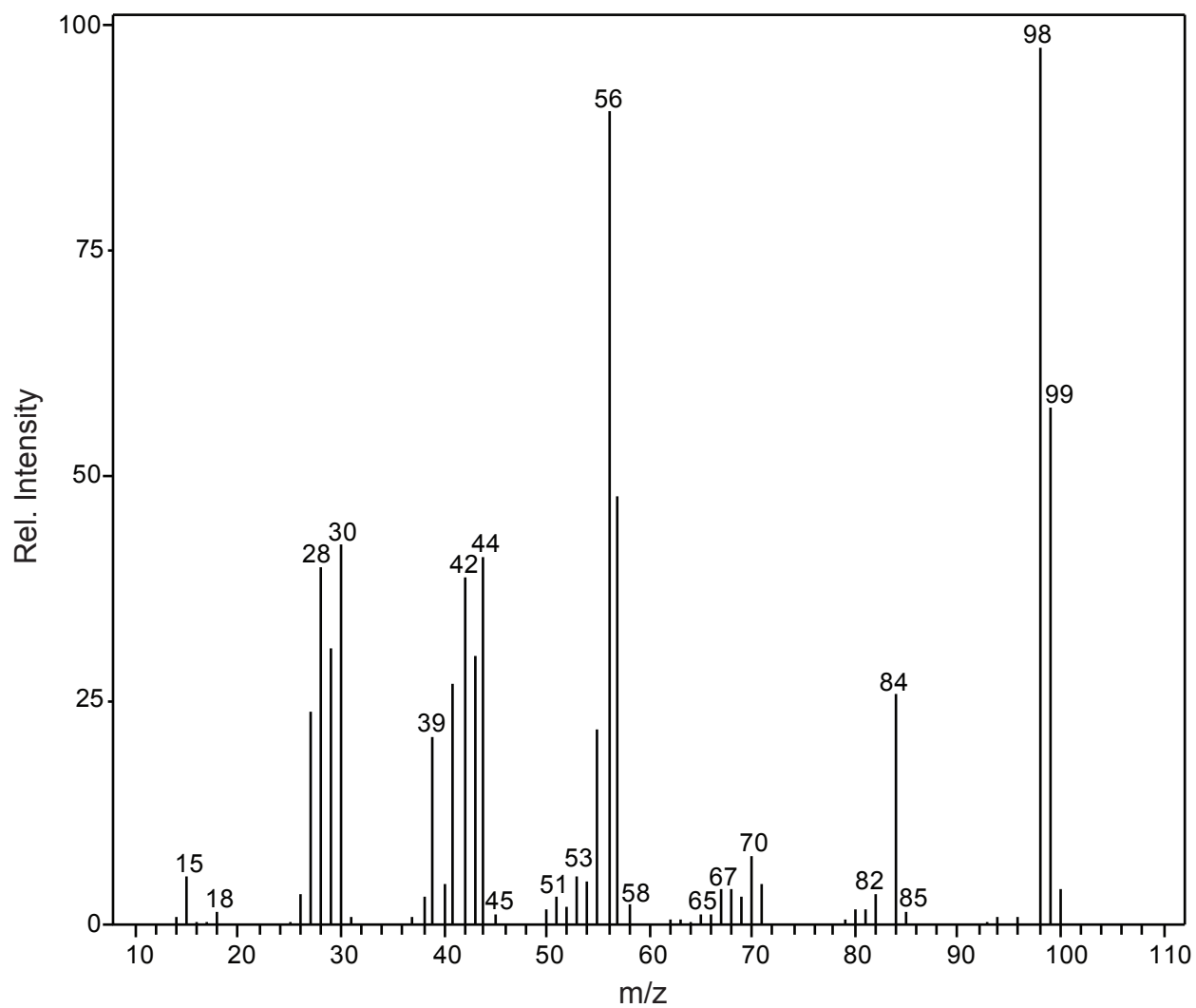
Fragments (from NMR):

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

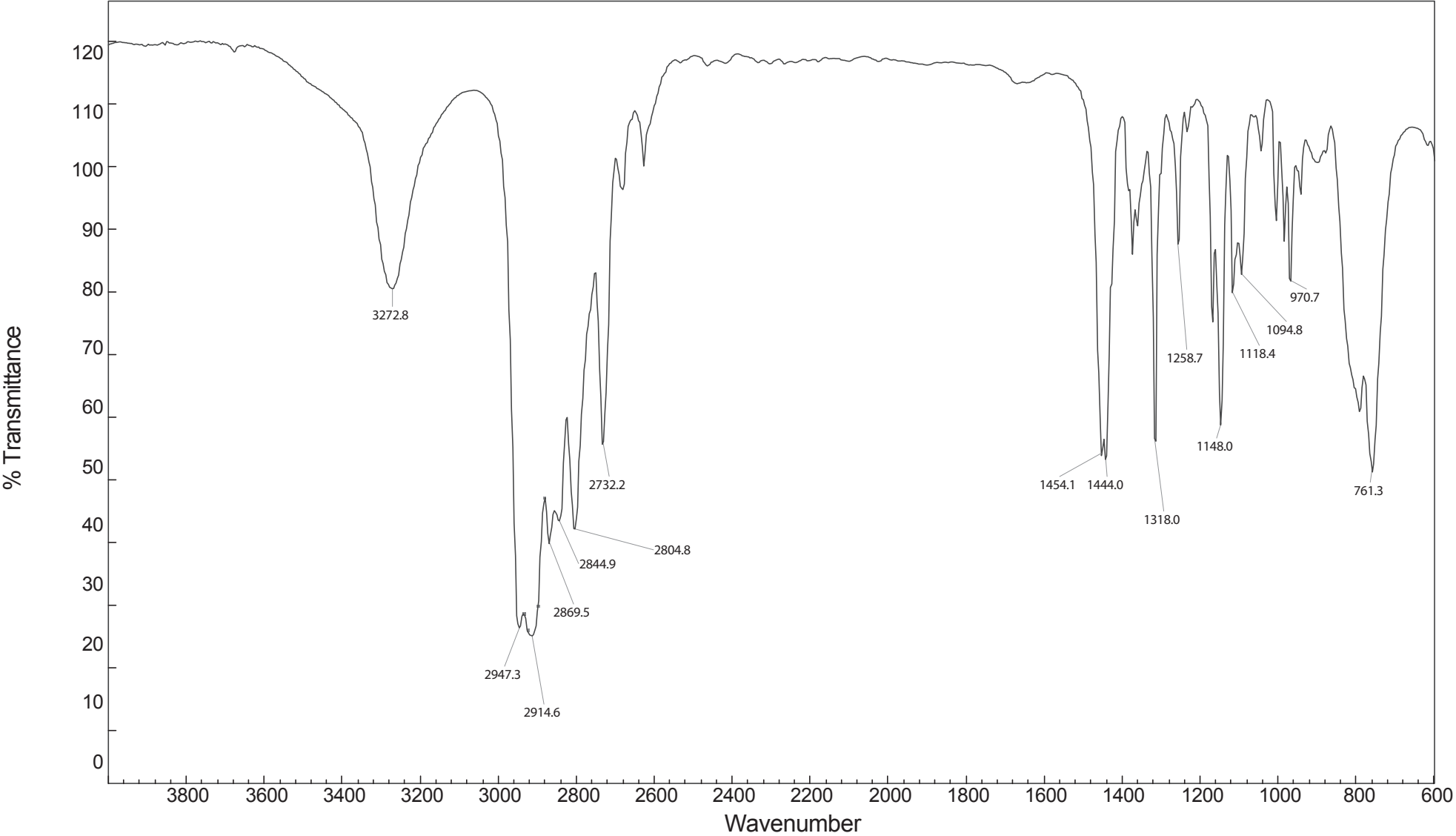
Structure with ^1H NMR resonances lettered from the most downfield to the most upfield (a, b, c, d, etc.): (Note: Not all resonances can be assigned with certainty. If assignments are uncertain, indicate so by showing possible letters.)

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.)

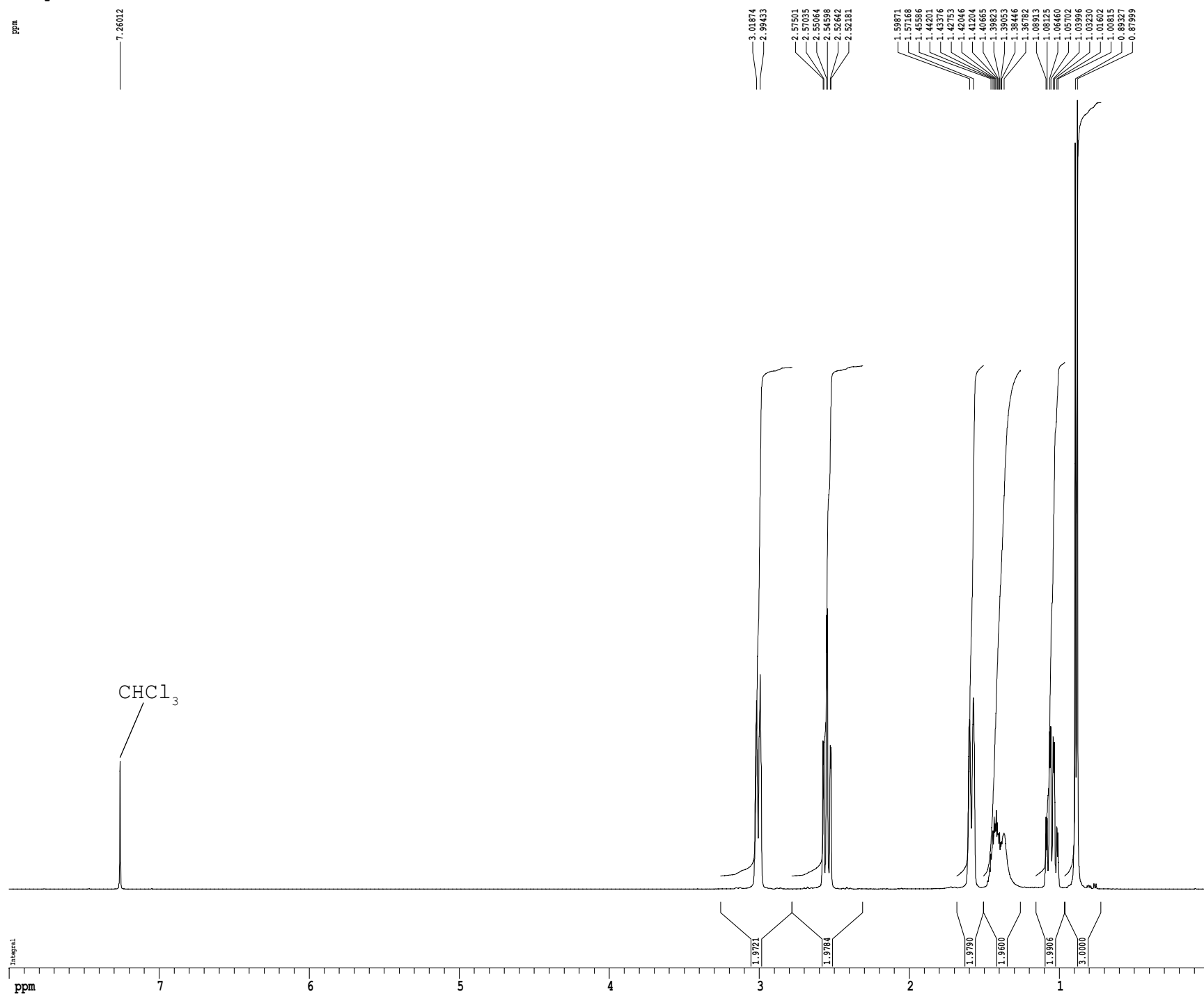
Electron ionization (EI-MS)



Varian Resolutions Pro



¹H spectrum



Current Data Parameters

USER	nmr14t
NAME	midterm 1 c
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20141030
Time	21.27
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	6.3
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	500.2200316 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

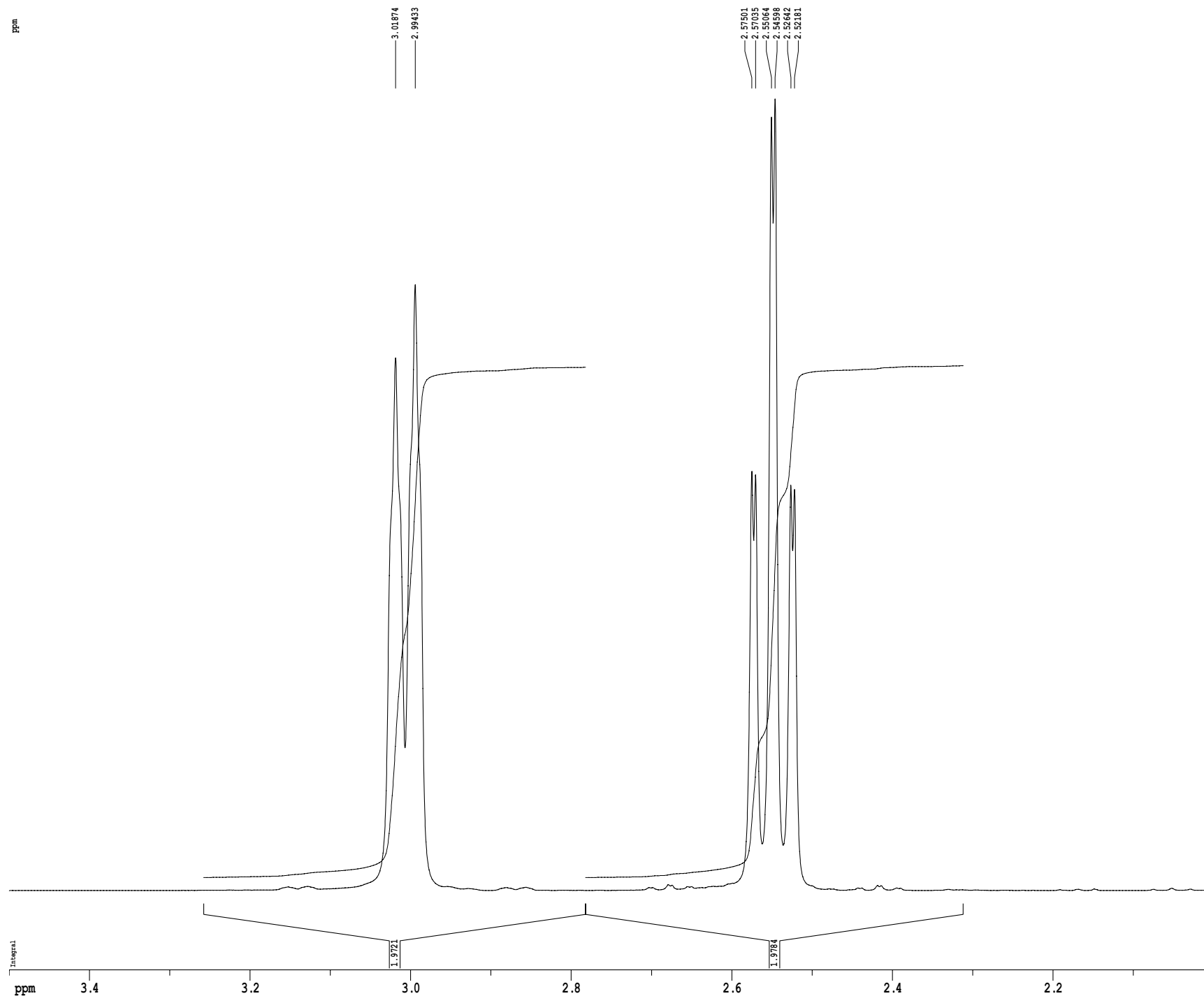
1D NMR plot parameters

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

DU=/v, USER=nmr14t, NAME=midterm I c, EXPNO=1, PROCNO=1
 F1=14.946ppm, F2=-1.072ppm, MI=0.50cm, MAXI=10000.00cm, PC=4.000

#	ADDRESS	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	31445.5	3631.659	7.2601	2.44
2	48798.0	1510.034	3.0187	3.59
3	48897.9	1497.826	2.9943	4.08
4	50613.4	1288.069	2.5750	2.83
5	50632.5	1285.739	2.5703	2.80
6	50713.1	1275.882	2.5506	5.21
7	50732.2	1273.551	2.5460	5.33
8	50812.2	1263.765	2.5264	2.73
9	50831.1	1261.459	2.5218	2.70
10	54607.7	799.705	1.5987	3.23
11	54718.3	786.186	1.5717	3.64
12	55192.2	728.248	1.4559	0.67
13	55248.8	721.321	1.4420	1.11
14	55282.6	717.194	1.4338	1.37
15	55308.1	714.078	1.4275	1.24
16	55337.0	710.543	1.4205	1.50
17	55371.4	706.330	1.4120	1.26
18	55393.5	703.632	1.4066	1.06
19	55427.9	699.421	1.3982	1.08
20	55459.4	695.571	1.3905	0.89
21	55484.3	692.534	1.3845	0.90
22	55552.3	684.210	1.3678	1.06
23	56692.5	544.804	1.0891	1.37
24	56724.7	540.865	1.0813	1.35
25	56792.9	532.535	1.0646	3.00
26	56823.9	528.741	1.0570	3.09
27	56893.7	520.208	1.0400	2.90
28	56925.0	516.379	1.0323	2.79
29	56991.6	508.232	1.0160	1.18
30	57023.8	504.296	1.0081	1.08
31	57493.8	446.830	0.8933	14.19
32	57548.2	440.188	0.8800	15.00

¹H spectrum



Current Data Parameters

USER	nmr14t
NAME	midterm 1 c
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20141030
Time	21.27
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	6.3
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

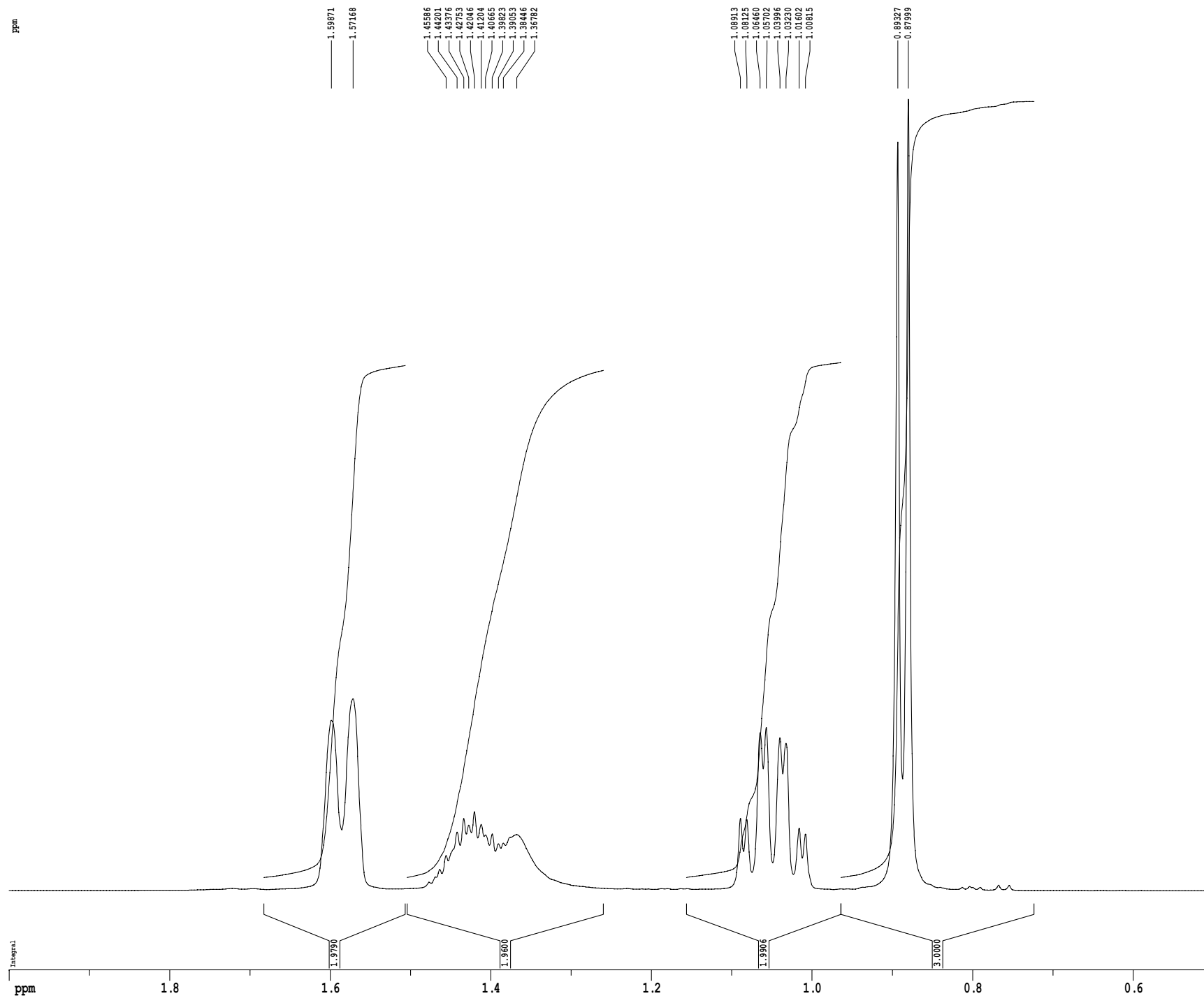
F2 - Processing parameter

SI	65536
SF	500.2200316 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	3.500 ppm
F1	1750.77 Hz
F2P	2.000 ppm
F2	1000.44 Hz
PPMCM	0.06579 ppm/cm
HZCM	32.90921 Hz/cm

¹H spectrum



Current Data Parameters

USER	nmr14t
NAME	midterm 1 c
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20141030
Time	21.27
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	zg30
TD	81728
SOLVENT	CDC13
NS	32
DS	2
SWH	8012.820 Hz
FIDRES	0.098043 Hz
AQ	5.0998774 sec
RG	6.3
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

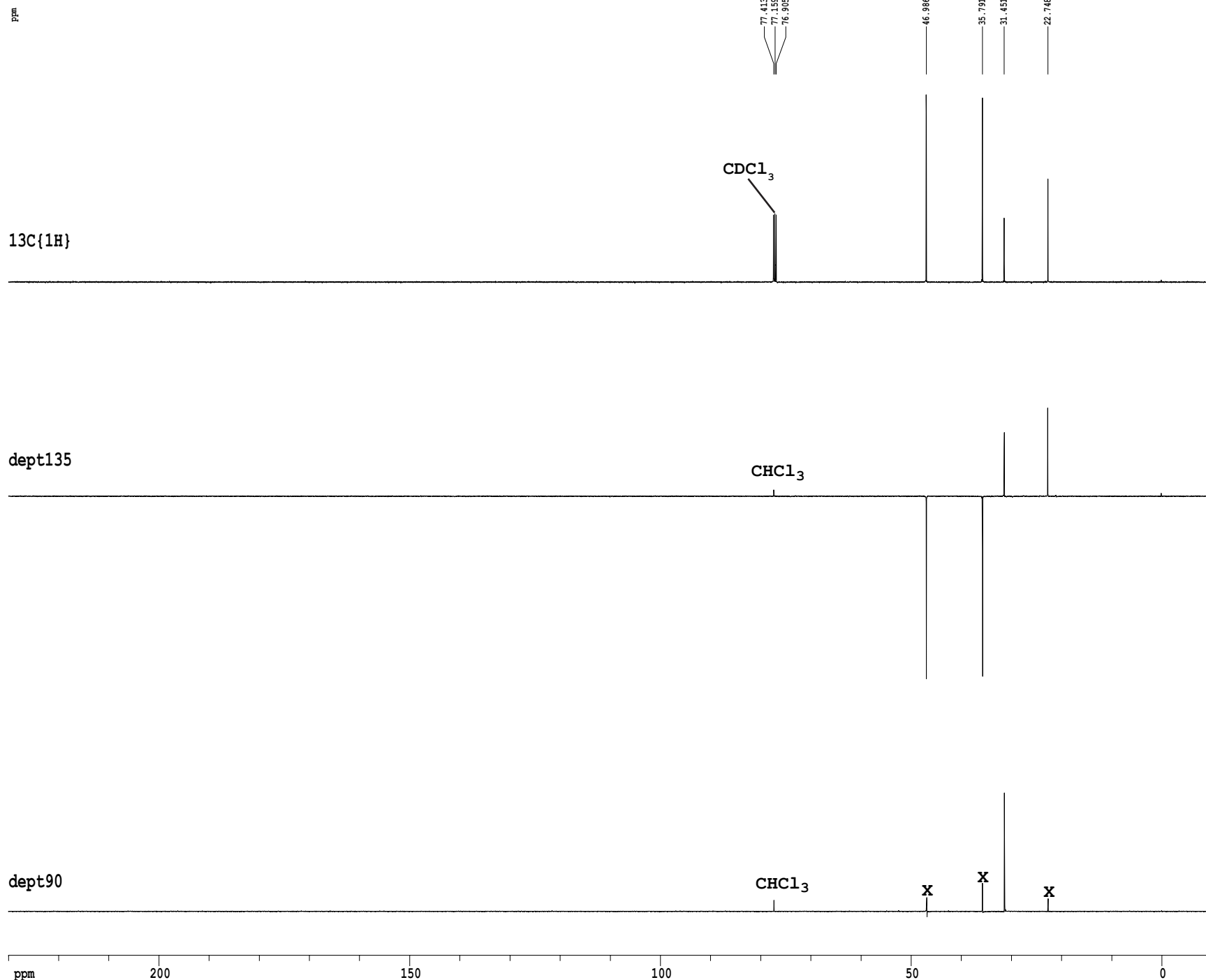
F2 - Processing parameter

SI	65536
SF	500.2200316 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	2.000 ppm
F1	1000.44 Hz
F2P	0.500 ppm
F2	250.11 Hz
PPMCM	0.06579 ppm/cm
HZCM	32.90921 Hz/cm

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



Current Data Parameters

USER	nmrl4t
NAME	midterm 1 c
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20141030
Time	21.44
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	SpinEcho30p-prd
TD	65536
SOLVENT	CDCl3
NS	640
DS	16
SWH	30303.031 Hz
FIDRES	0.462388 Hz
AQ	1.0813940 sec
RG	72.98 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
MCWRR	0.01500000 sec
F2	31.00 usec

===== CHANNEL f1 =====

NUC1	13C
P1	15.50 usec
PL1	500.00 usec
P12	2000.00 usec
PL2	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 =====

CPNAM1	SINE.100
CPNAM2	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	125.7804103 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	28929.49 Hz
F2P	-10.000 ppm
F2	-1257.80 Hz
PPMCM	10.52632 ppm/cm
HZCM	1324.00439 Hz/cm