

NAME _____

Chem 203

Organic Spectroscopy

Midterm Examination, Part II (50 points total)

Problem 1 of 3 (two out of three required, 25 points)

Saturday, November 5, 2011, 9 am - ???

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

1. 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: 151.0633

Noteworthy Heteroatoms:

Molecular Formula:

Unsaturation Number:

Functional Groups (be as specific as possible):

Fragments (from NMR):

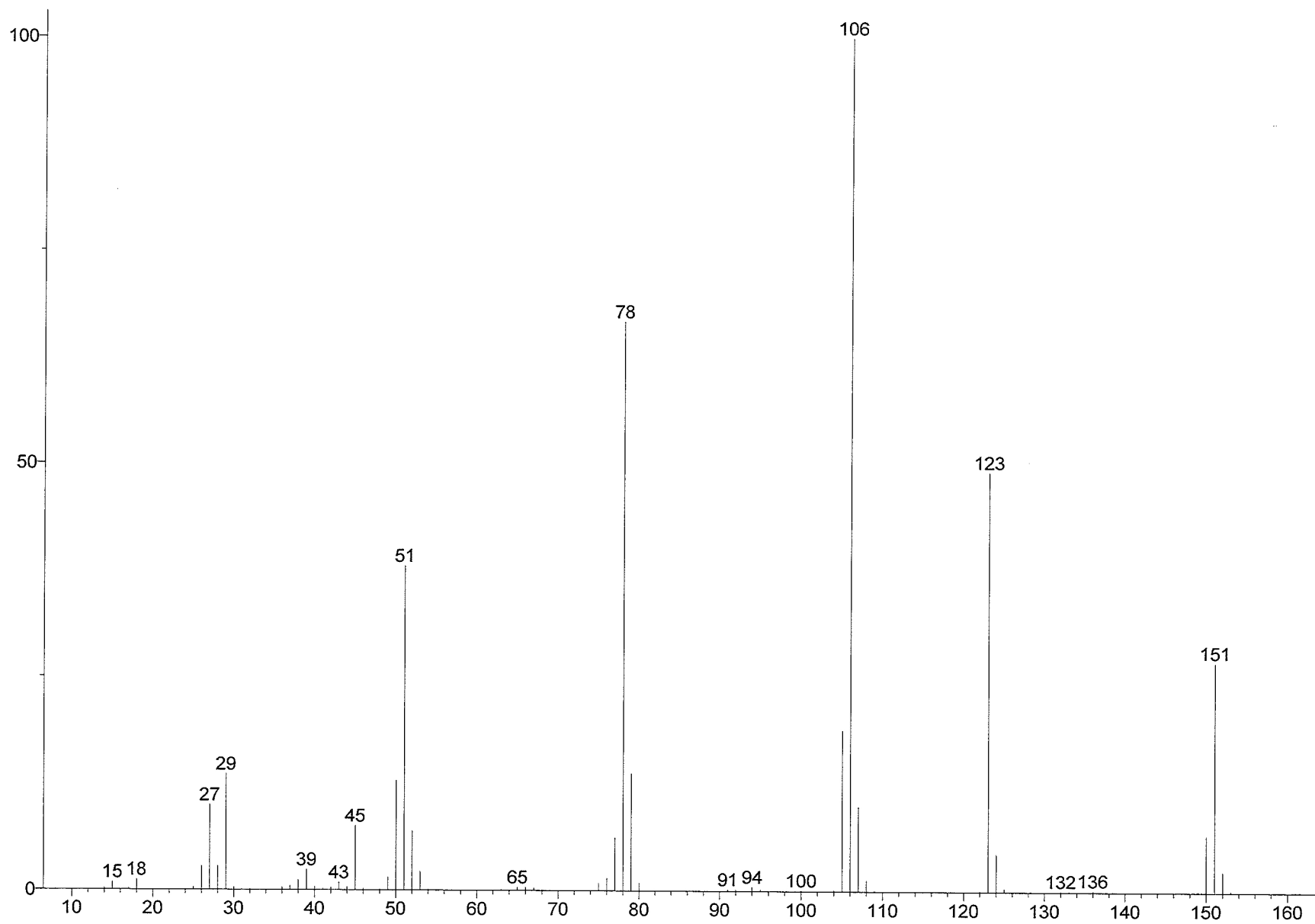
Structure (Make sure to properly indicate stereochemistry, if applicable):

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.)

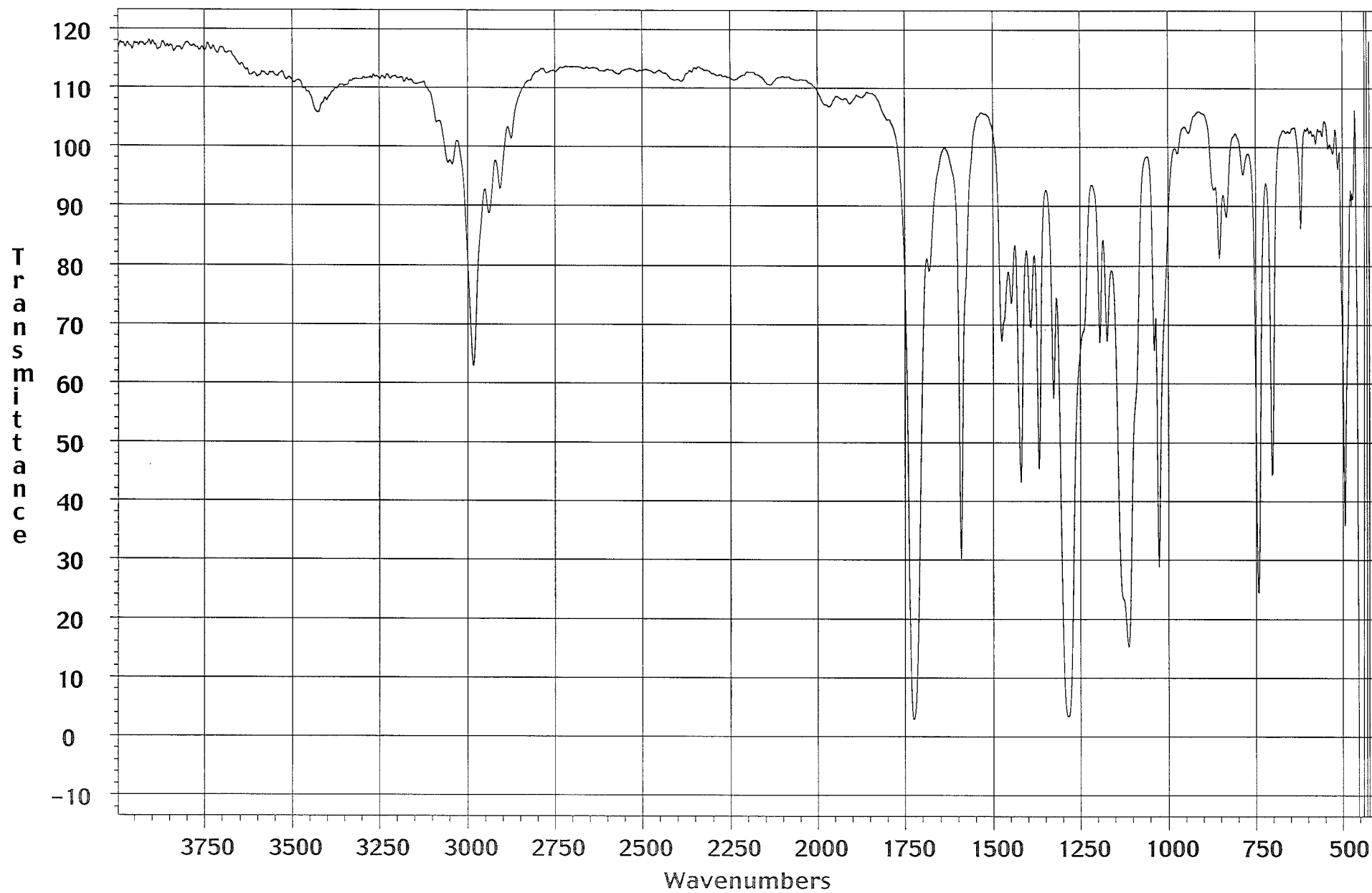
Structure with ^{13}C NMR resonances numbered from the most downfield to the most upfield (1, 2, 3, 4, etc.): (Note: Not all resonances can be assigned with certainty. If assignments are uncertain, indicate so by showing possible numbers.)

Molecular Model: Build an energy-minimized molecular model of the structure using PyMOL and the "clean" function. Save the .pse files as structure1.pse. E-mail the .pse file to me (jsnowick@uci.edu).

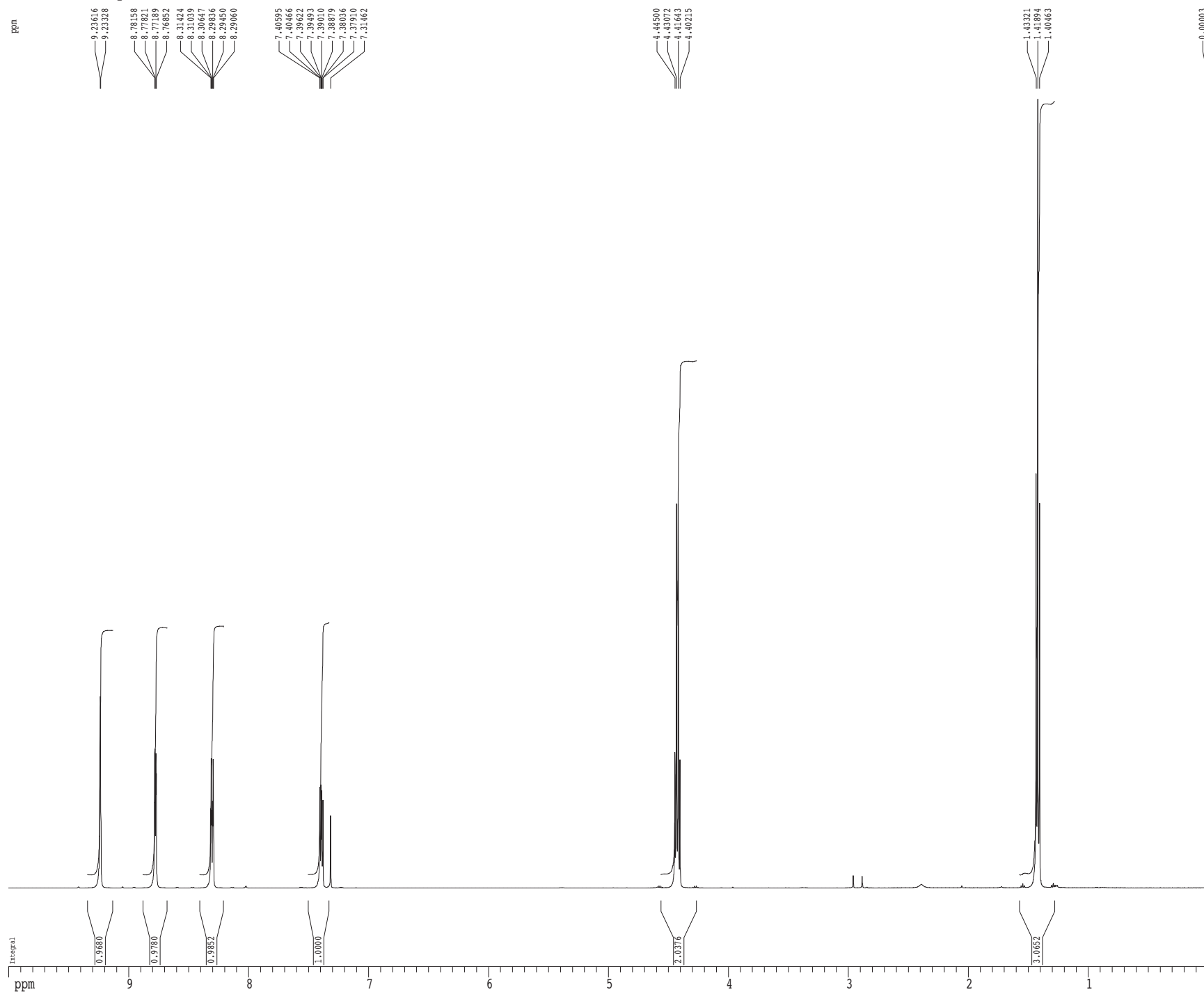
EIMS



Thin Film NaCl plates



500 MHz ¹H spectrum in CDCl₃



Current Data Parameters

USER	nmrlit
NAME	nmrlit-X-sample2
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	2011012
Time	19.12
INSTRUM	gn500
PROBHD	5 mm broadband
PULPROG	zg30
TD	81728
SOLVENT	CDCl3
NS	8
DS	2
SWH	8012.820 Hz
FIDRES	0.098043 Hz
AQ	5.0998774 sec
RG	71.8
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	¹ H
P1	12.20 usec
PL1	-5.00 dB
SFO1	499.5134966 MHz

F2 - Processing parameters

SI	65536
SF	499.5100003 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

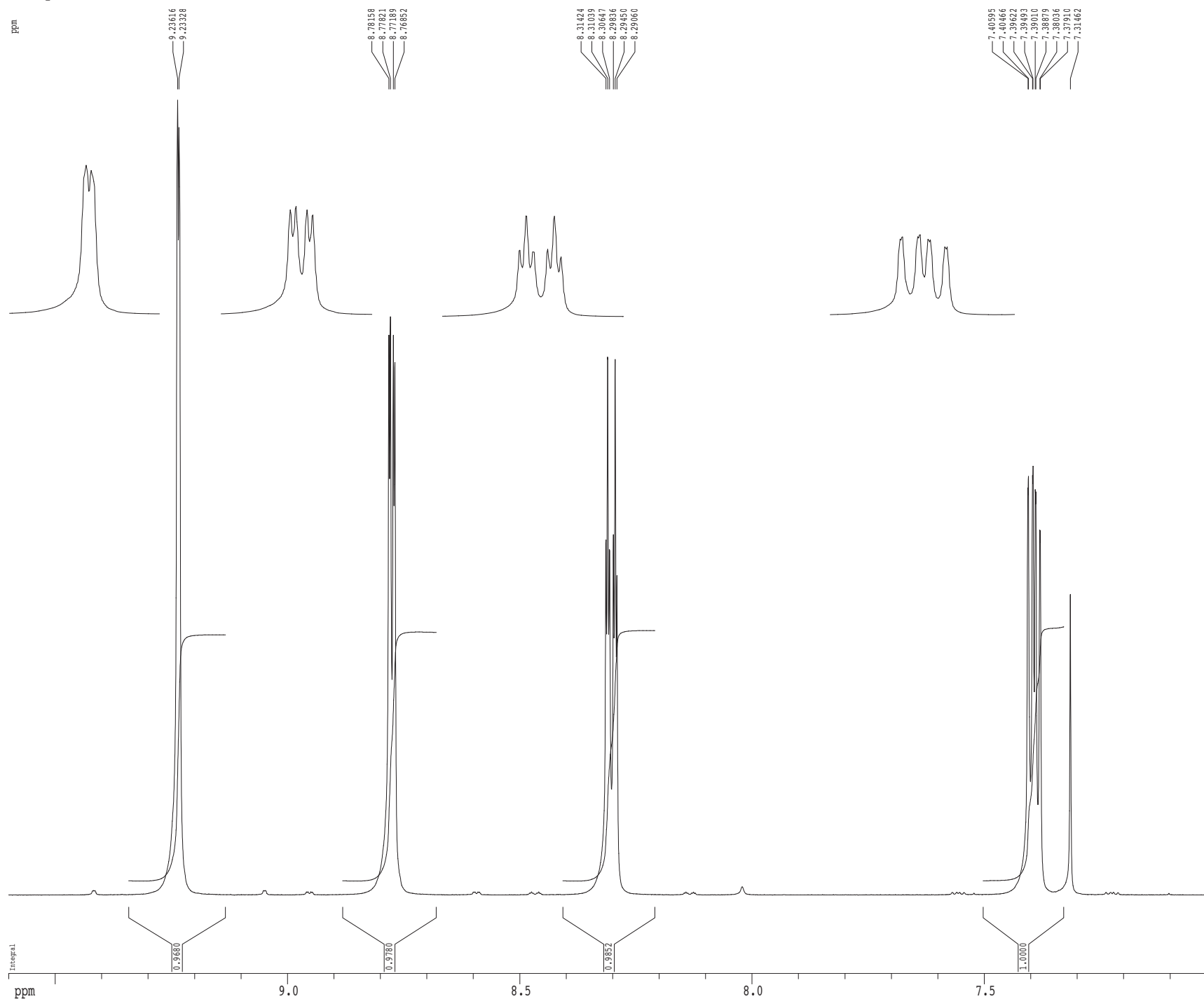
1D NMR plot parameters

CX	22.80 cm
CY	15.00 cm
F1P	10.000 ppm
F1	4995.10 Hz
F2P	0.000 ppm
F2	0.00 Hz
PPMCM	0.43860 ppm/cm
HZCM	219.08334 Hz/cm

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 F1=15.020ppm, F2=-1.021ppm, MI=0.40cm, MAXI=10000.00cm, PC=1.000

#	ADDRESS	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	23630.2	4613.554	9.2362	3.64
2	23642.0	4612.116	9.2333	3.51
3	25487.4	4386.486	8.7816	2.57
4	25501.2	4384.801	8.7782	2.64
5	25526.9	4381.649	8.7719	2.56
6	25540.8	4379.962	8.7685	2.44
7	27396.7	4153.044	8.3142	1.63
8	27412.4	4151.125	8.3104	2.46
9	27428.4	4149.166	8.3065	1.58
10	27461.6	4145.112	8.2984	1.65
11	27477.3	4143.184	8.2945	2.45
12	27493.3	4141.236	8.2906	1.46
13	31107.4	3699.345	7.4059	1.87
14	31112.7	3698.701	7.4047	1.92
15	31147.2	3694.485	7.3962	1.92
16	31152.5	3693.841	7.3949	1.96
17	31172.2	3691.427	7.3901	1.85
18	31177.5	3690.774	7.3888	1.85
19	31212.0	3686.565	7.3804	1.67
20	31217.1	3685.932	7.3791	1.66
21	31480.6	3653.725	7.3146	1.38
22	43204.2	2220.323	4.4450	2.58
23	43262.6	2213.188	4.4307	7.36
24	43320.9	2206.053	4.4164	7.30
25	43379.3	2198.916	4.4021	2.45
26	55508.7	715.902	1.4332	7.90
27	55567.0	708.773	1.4189	15.00
28	55625.5	701.626	1.4046	7.37
29	61363.9	0.013	0.0000	0.87

¹H spectrum



Current Data Parameters

USER	nmrlit
NAME	nmrlit-X-sample2
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20111012
Time	19.12
INSTRUM	gn500
PROBHD	5 mm broadband
PULPROG	zg30
TD	81728
SOLVENT	CDCl3
NS	8
DS	2
SWH	8012.820 Hz
FIDRES	0.098043 Hz
AQ	5.0998774 sec
RG	71.8
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	12.20 usec
PL1	-5.00 dB
SFO1	499.5134966 MHz

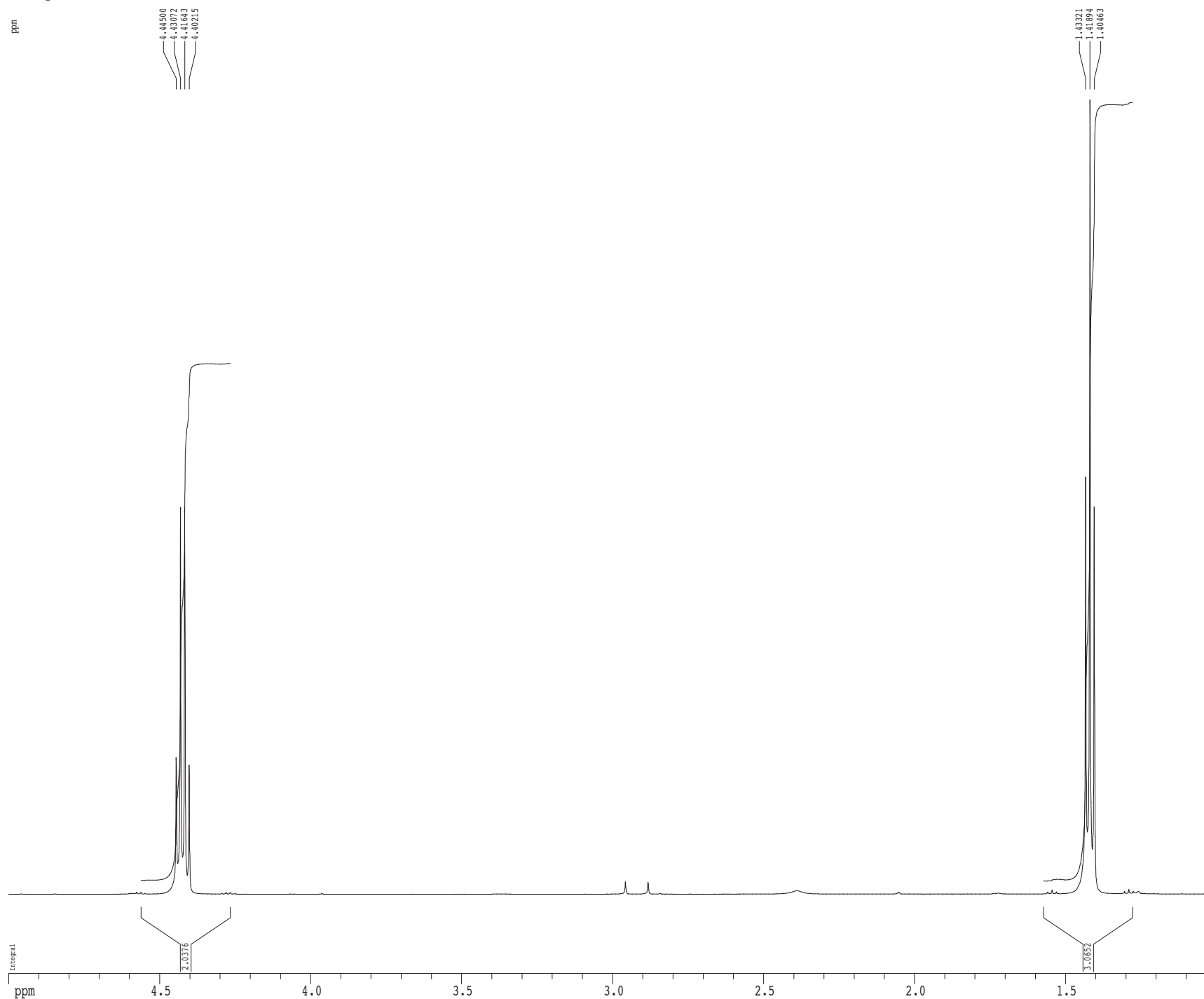
F2 - Processing parameters

SI	65536
SF	499.5100003 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.80 cm
CY	15.00 cm
F1P	9.600 ppm
F1	4795.30 Hz
F2P	7.000 ppm
F2	3496.57 Hz
PPMCM	0.11404 ppm/cm
HZCM	56.96168 Hz/cm

¹H spectrum



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Current Data Parameters
USER          nmrl1t
NAME          nmrl1t-X-sample2
EXPNO         1
PROCNO        1

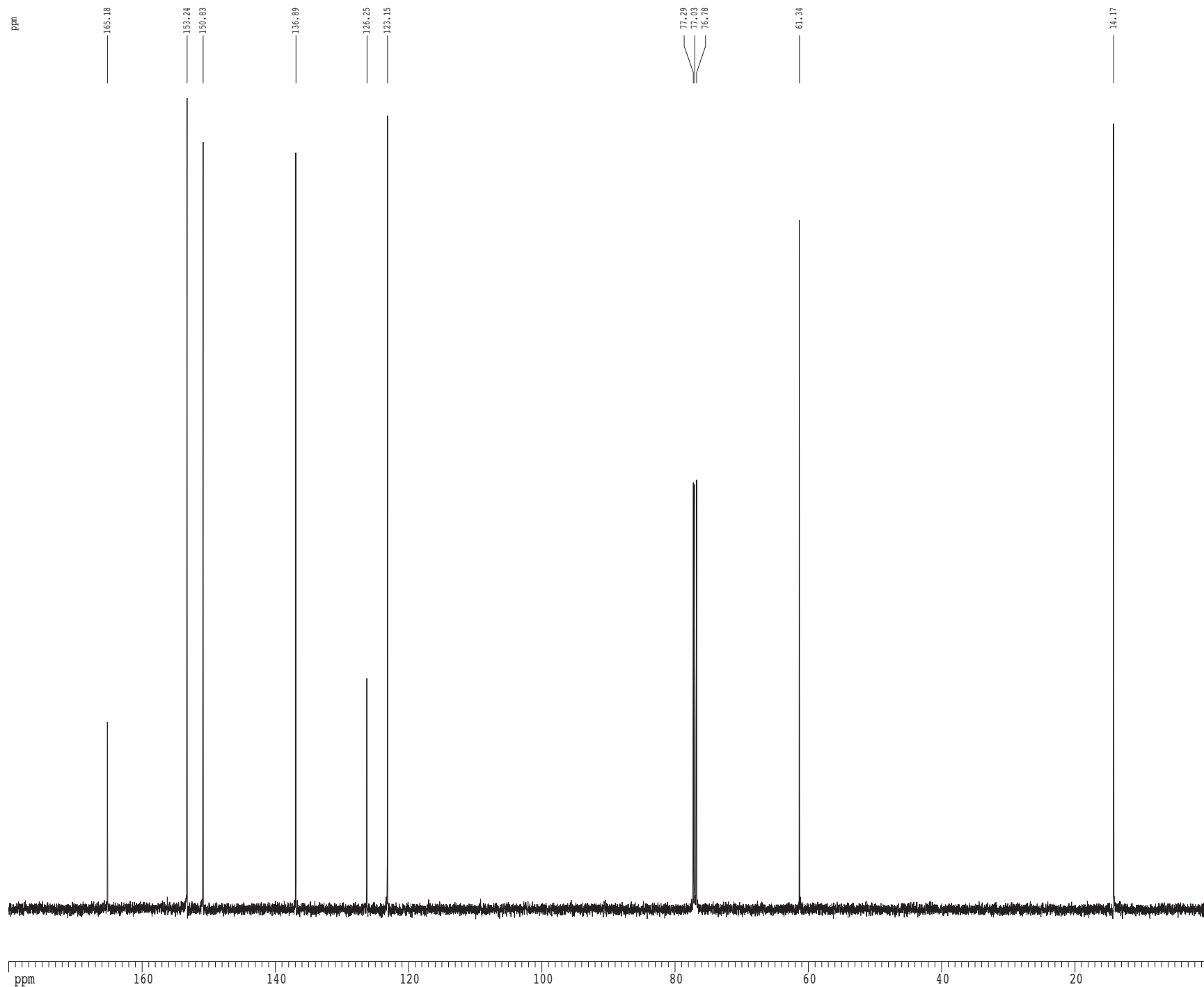
F2 - Acquisition Parameters
Date_         20111012
Time          19.12
INSTRUM       gn500
PROBHD        5 mm broadband
PULPROG       zg30
TD            81728
SOLVENT       CDCl3
NS            8
DS            2
SWH           8012.820 Hz
FIDRES        0.098043 Hz
AQ            5.0998774 sec
RG            71.8
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            12.20 usec
PL1           -5.00 dB
SFO1          499.5134966 MHz

F2 - Processing parameters
SI            65536
SF            499.5100003 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

ID NMR plot parameters
CX            22.80 cm
CY            15.00 cm
FIP           5.000 ppm
F1            2497.55 Hz
F2P           1.000 ppm
F2            499.51 Hz
PPMCM         0.17544 ppm/cm
HZCM          87.63334 Hz/cm
    
```

125.6 MHz ¹³C spectrum with ¹H decoupling in CDCl₃



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Current Data Parameters
USER          nmrl1t
NAME          nmrl1t-X-sample2
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20111012
Time          19.17
INSTRUM       gn500
PROBHD        5 mm broadband
PULPROG       zgdc30
TD            65536
SOLVENT       CDCl3
NS            184
DS            4
SWH           30303.031 Hz
FIDRES        0.462388 Hz
AQ            1.0813940 sec
RG            4597.6
DW            16.500 usec
DE            4.50 usec
TE            298.0 K
D1            0.25000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

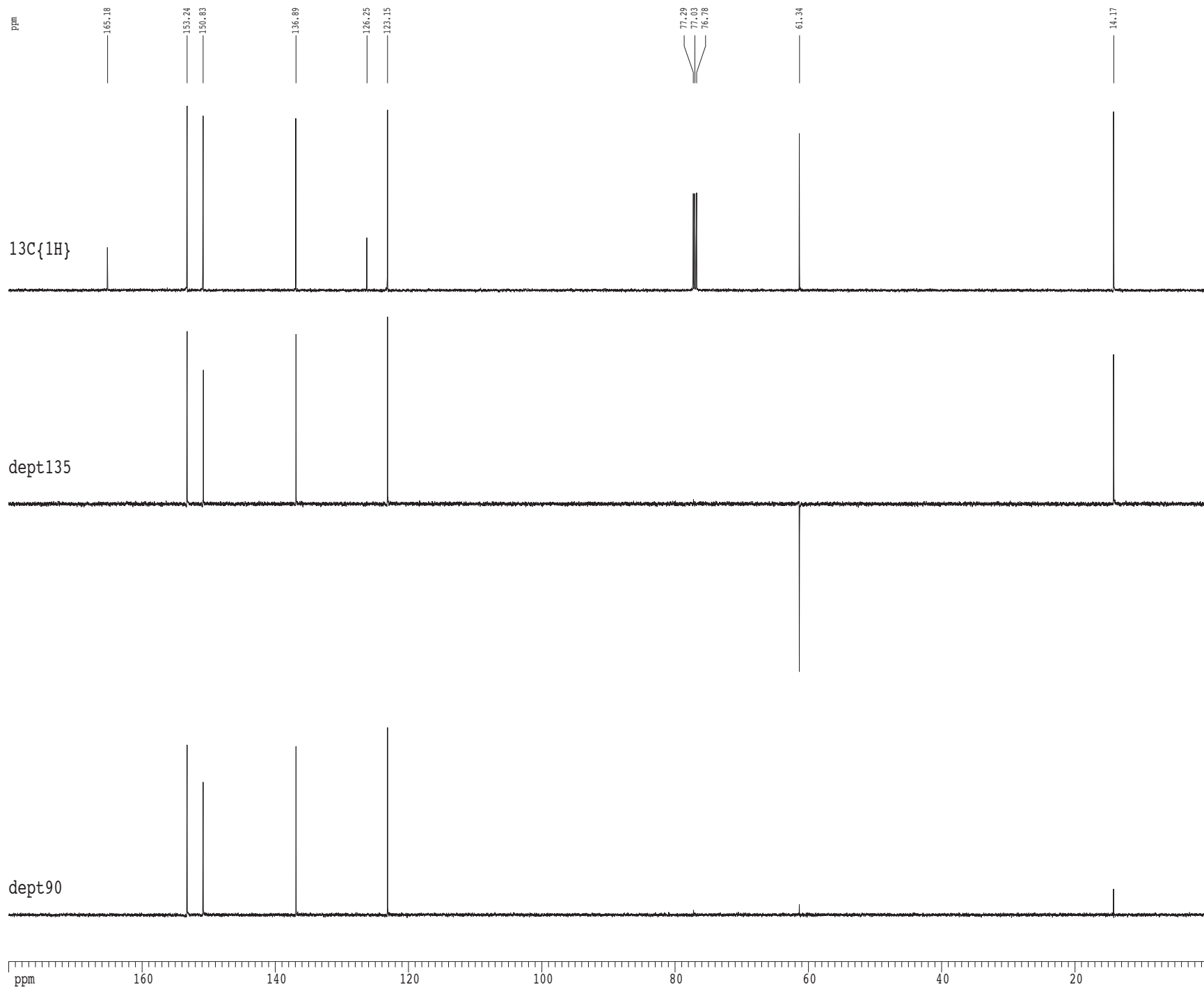
===== CHANNEL f1 =====
NUC1           13C
P1             7.70 usec
PL1            0.00 dB
SF01          125.6157052 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2          80.00 usec
PL2            -3.00 dB
PL12           13.20 dB
SF02          499.5124975 MHz

F2 - Processing parameters
SI            65536
SF            125.6019001 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            2.00

1D NMR plot parameters
CX            22.80 cm
CY            15.65 cm
F1P           180.000 ppm
F1            22608.34 Hz
F2P           0.000 ppm
F2            0.00 Hz
PPMCM         7.89474 ppm/cm
HZCM          991.59399 Hz/cm
    
```

¹³C spectrum with ¹H decoupling



Current Data Parameters

USER	nmr11t
NAME	nmr11t-X-sample2
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20111012
Time	19.17
INSTRUM	gn500
PROBHD	5 mm broadband
PULPROG	zgdc30
TD	65536
SOLVENT	CDCl3
NS	184
DS	4
SWH	30303.031 Hz
FIDRES	0.462388 Hz
AQ	1.0813940 sec
RG	4597.6
DW	16.500 usec
DE	4.50 usec
TE	298.0 K
D1	0.25000000 sec
d11	0.03000000 sec
MCREST	0.00000000 sec
MCNRK	0.01500000 sec

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

NUC1	¹³ C
P1	7.70 usec
PL1	0.00 dB
SFO1	125.6157052 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	¹ H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	13.20 dB
SFO2	499.5124975 MHz

F2 - Processing parameters

SI	65536
SF	125.6019001 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	180.000 ppm
F1	22608.34 Hz
F2P	0.000 ppm
F2	0.00 Hz
PPMCM	7.89474 ppm/cm
HZCM	991.59399 Hz/cm