

Supporting Information

Mechanistic Studies on the *Cis* to *Trans* Epimerization of Trisubstituted-1,2,3,4-Tetrahydro- β -Carbolines

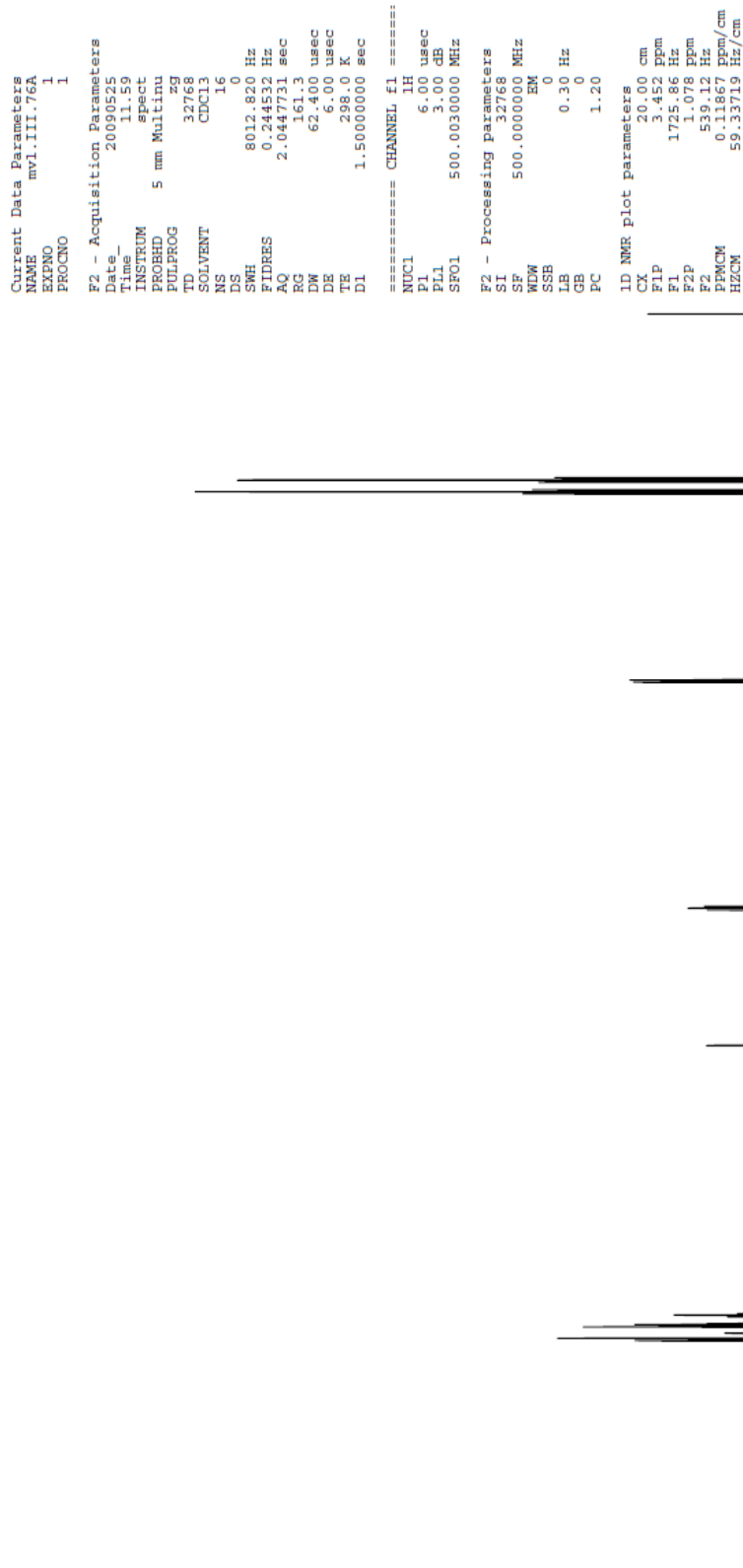
*Michael L. Van Linn and James M. Cook**

Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee, 3210 N.
Cramer Street, Milwaukee, WI, 53211

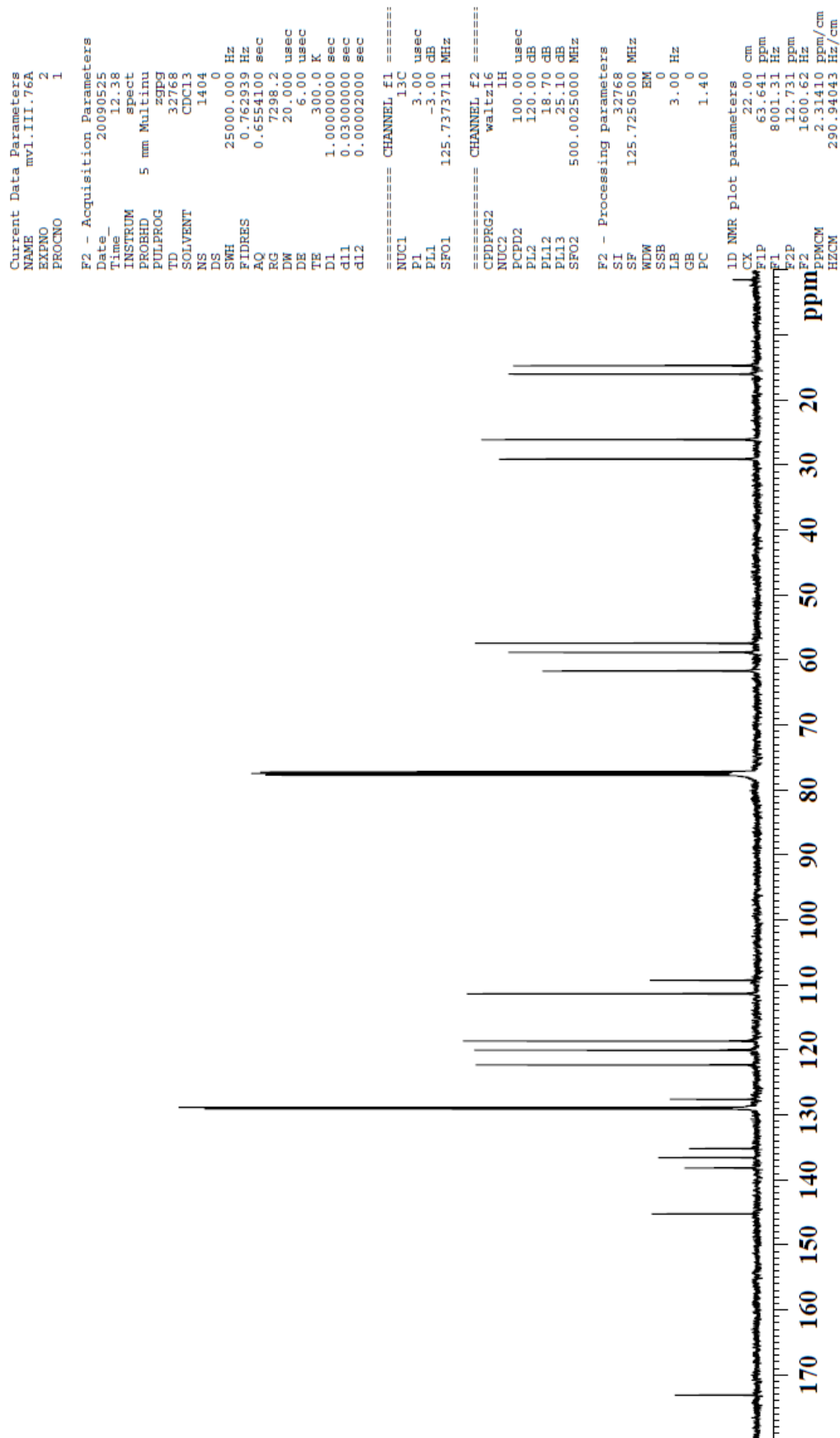
^1H and ^{13}C NMR spectra for all compounds

NMR spectra for Compound 5a

proton spectrum



carbon spectrum



NMR spectra for Compound **5b**

proton spectrum

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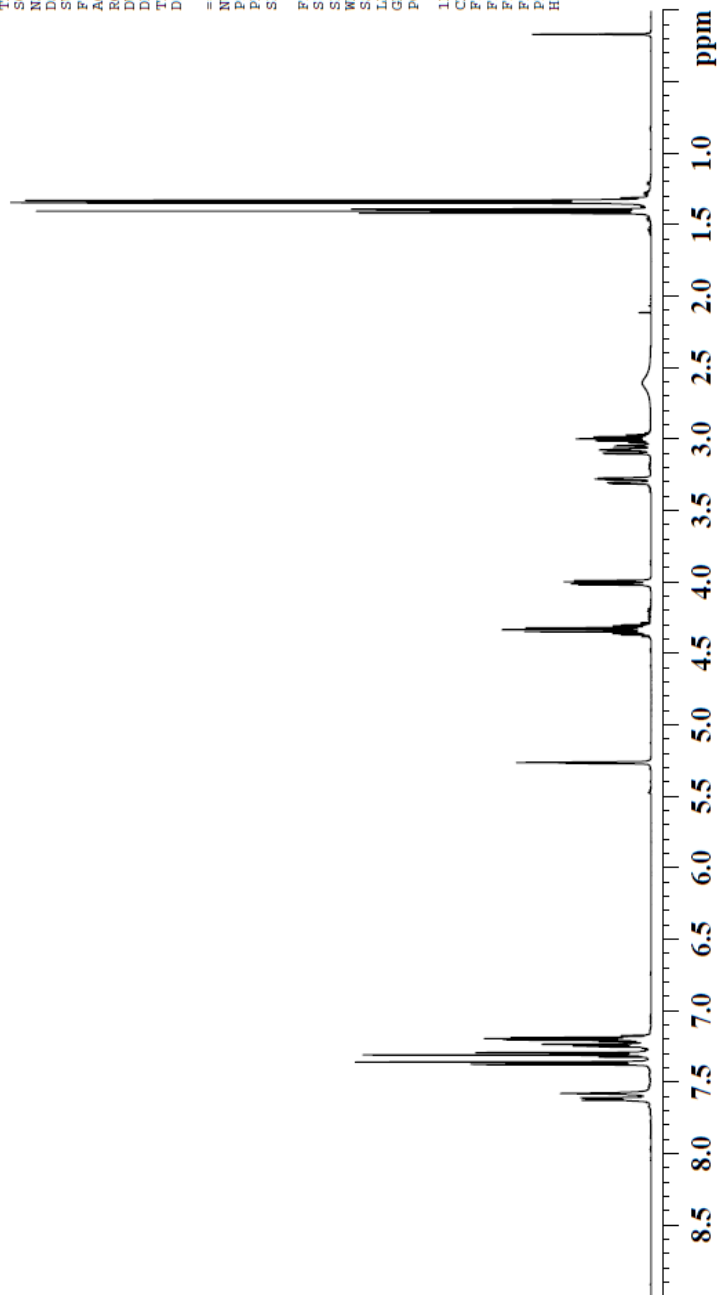
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EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20090525
Time      9.07
INSTRUM   spect
PROBHD    5 mm Multinu
PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         16
DS         0
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.044731 sec
RG         50.8
DW         62.400 usec
DE         6.00 usec
TE         298.0 K
D1         1.50000000 sec

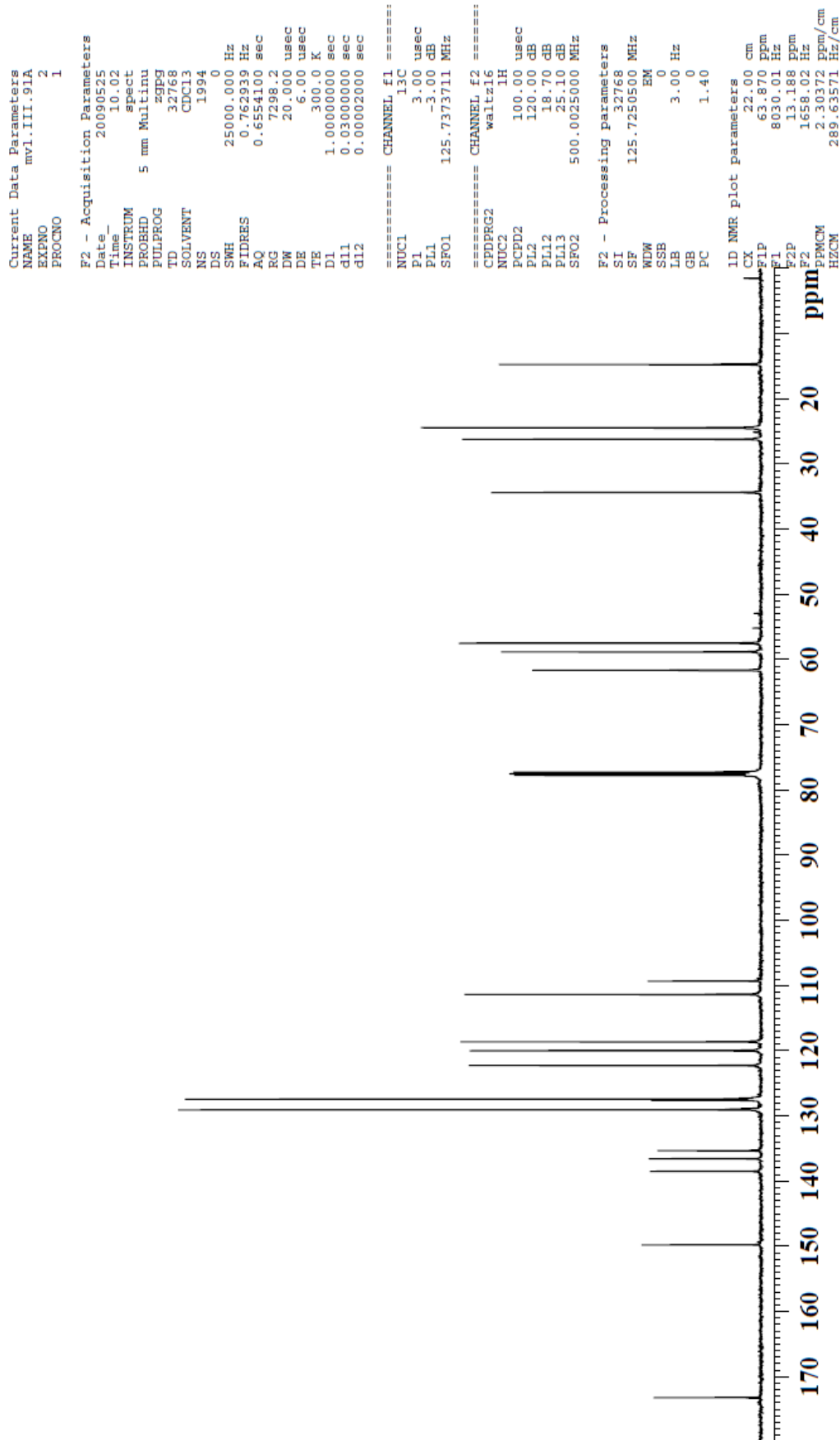
===== CHANNEL f1 =====
NUC1       1H
P1         5.00 usec
PL1        3.00 dB
SFO1       500.0030000 MHz

F2 - Processing parameters
SI         32768
SF         500.0000000 MHz
WDW         EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.20

1D NMR plot parameters
CX         20.00 cm
F1P        3.415 ppm
F1         1707.46 Hz
F2P        1.152 ppm
F2         575.91 Hz
PQCM       0.11315 ppm/cm
HZCM       56.57732 Hz/cm
  
```



carbon spectrum



NMR spectra for Compound **5c**

proton spectrum

```

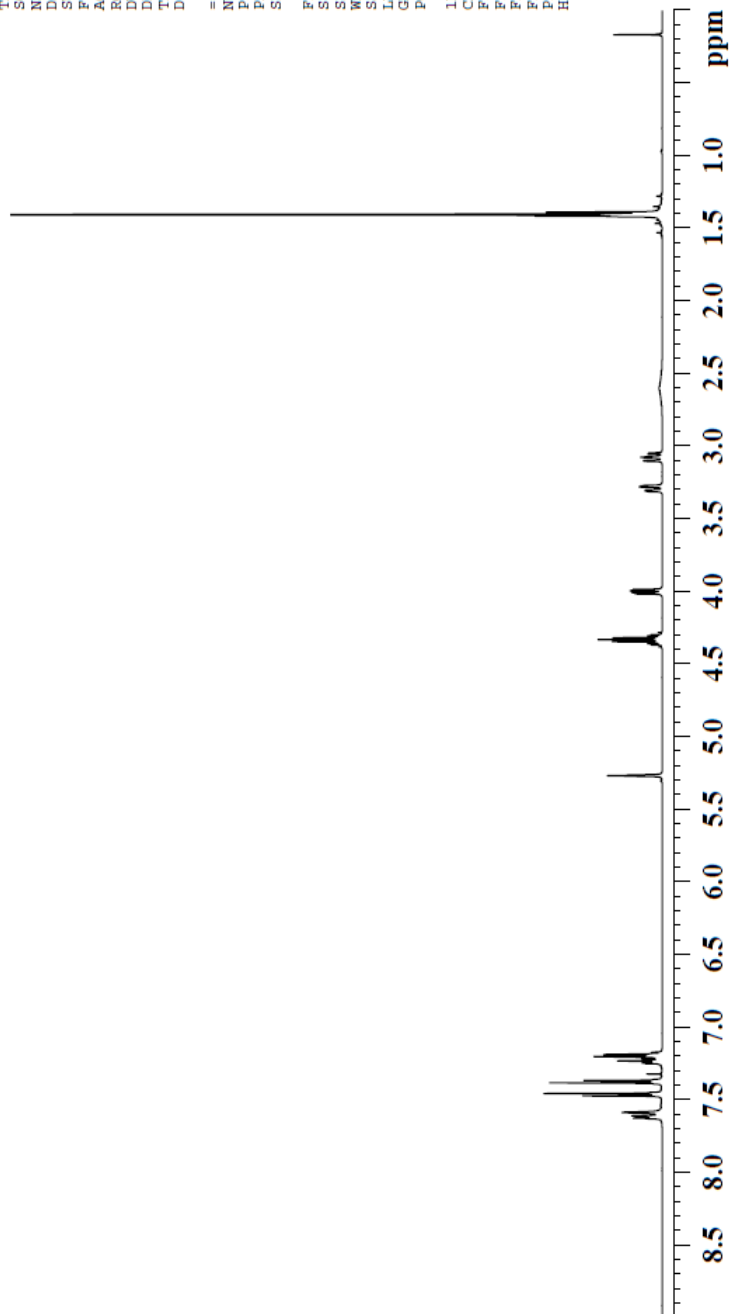
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NAME      mv1.1v.22A
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20090525
Time      11.04
INSTRUM   spect
PROBHD    5 mm Multinu
PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         16
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SWH        8012.820 Hz
FIDRES     0.244532 Hz
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DW         62.400 usec
DE         6.00 usec
TE         298.0 K
D1         1.5000000 sec

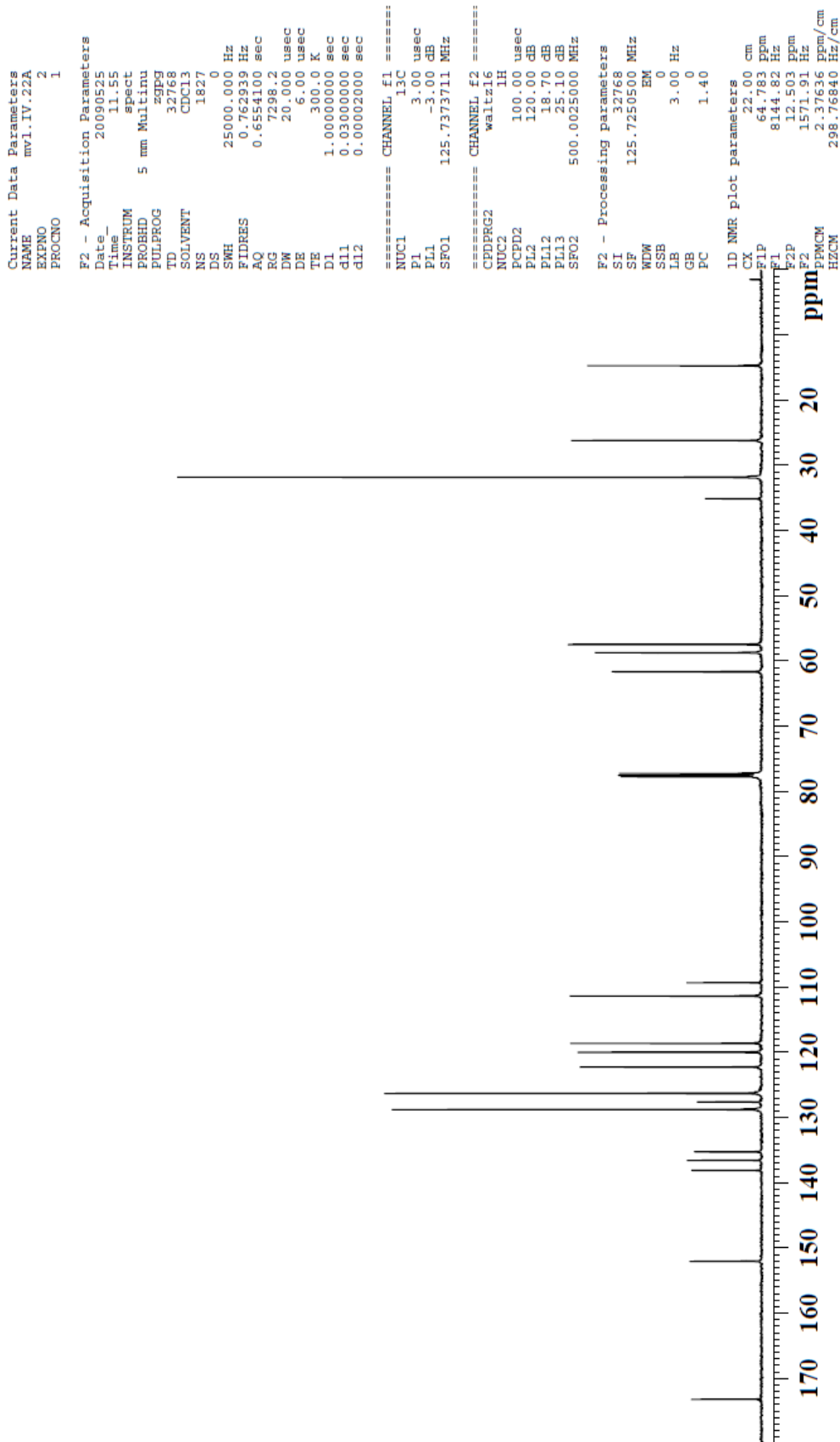
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P1         6.00 usec
PL         3.00 dB
SFO1       500.0030000 MHz

F2 - Processing parameters
SI         32768
SF         500.0000000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.20

1D NMR plot parameters
CX         20.00 cm
FLP        3.370 ppm
F1         1685.24 Hz
F2P        3.006 ppm
F2         1502.81 Hz
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```



carbon spectrum



NMR spectra for Compound **5d**

proton spectrum

```

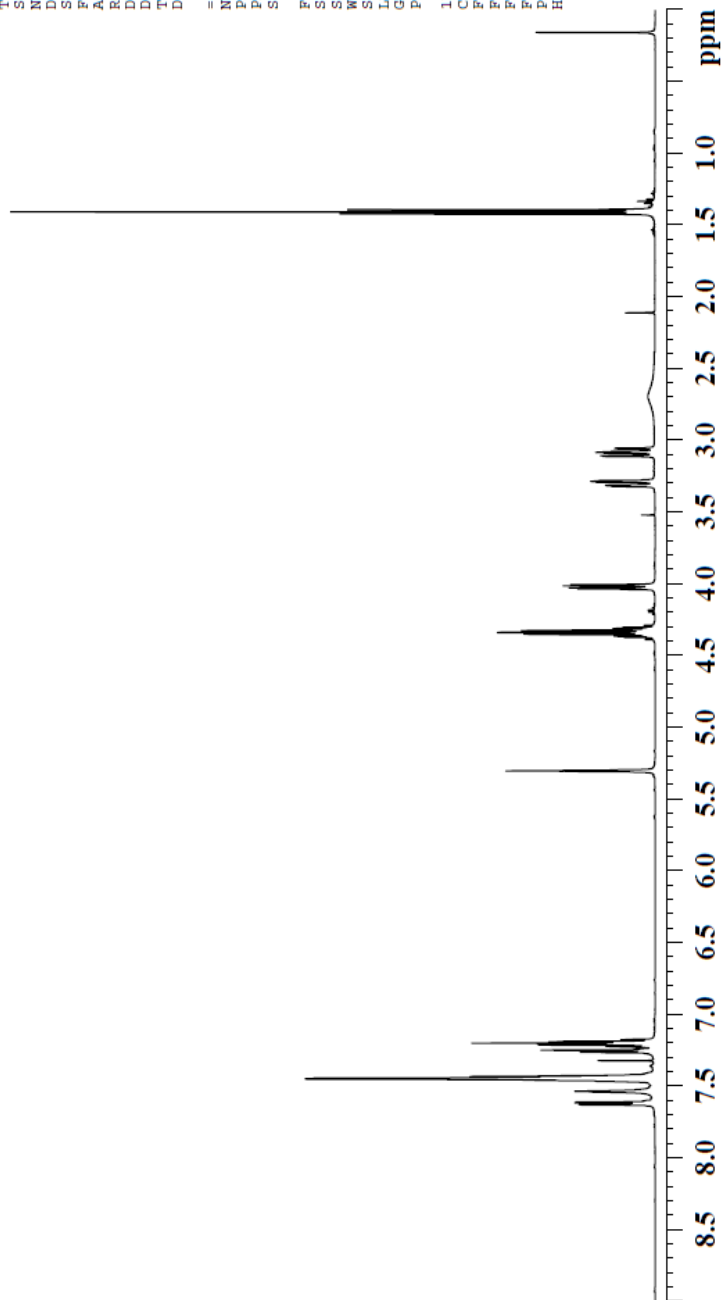
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EXPNO     1
PROCNO    1

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INSTRUM   spect
PROBHD    5 mm Multinu
PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         16
DS         0
SMH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG         80.6
DW         62.400 usec
DE         6.00 usec
TE         298.0 K
D1         1.5000000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         6.00 usec
PL1        3.00 dB
SFO1       500.0030000 MHz

F2 - Processing parameters
SI         32768
SF         500.0000000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.20

ID NMR plot parameters
CX         20.00 cm
FLP        3.452 ppm
F1         1725.86 Hz
F2P        1.207 ppm
F2         603.51 Hz
PPMCM      0.11223 ppm/cm
HZCM       56.11734 Hz/cm
  
```



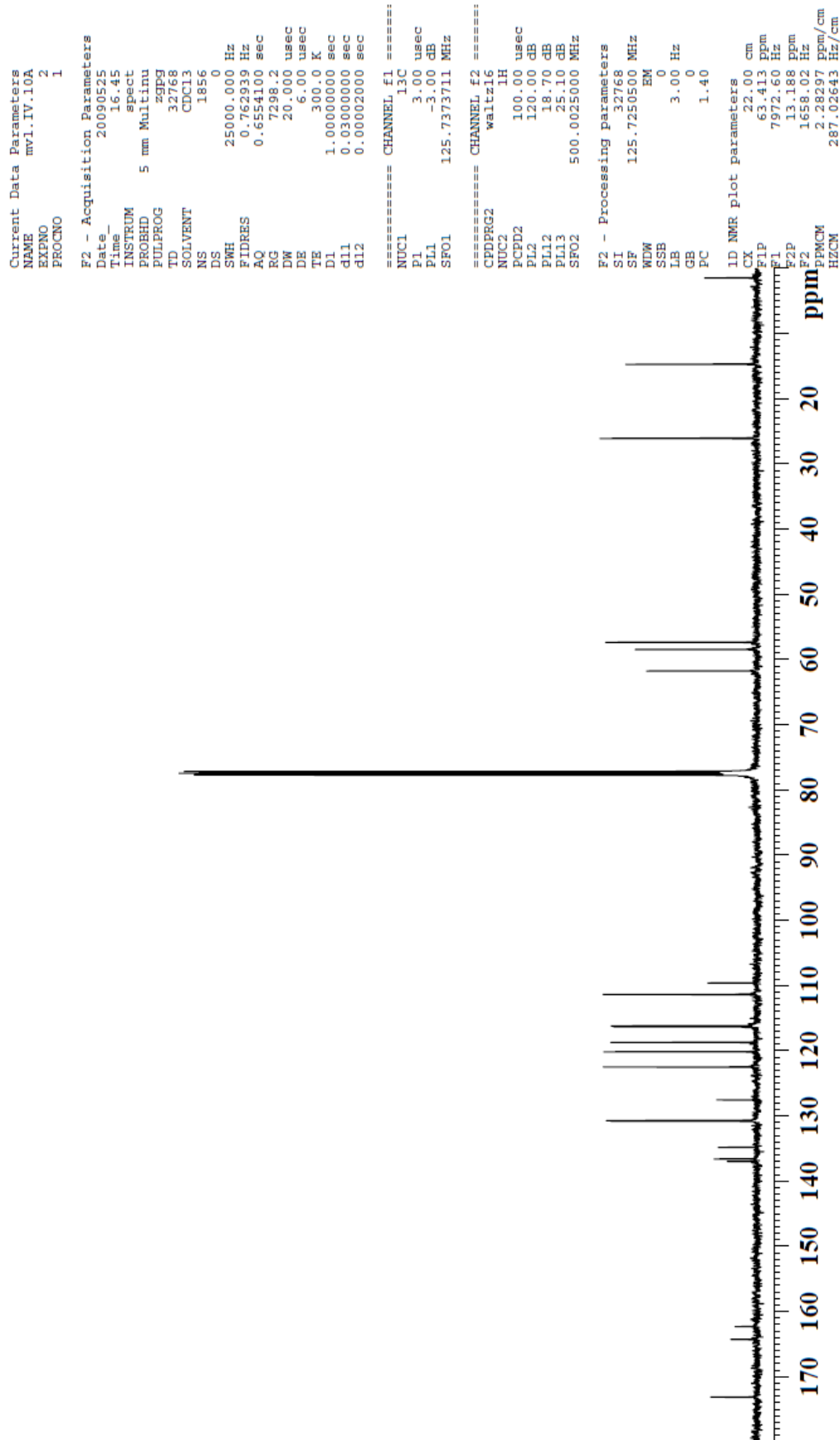
S76

NMR spectra for Compound 5e

proton spectrum



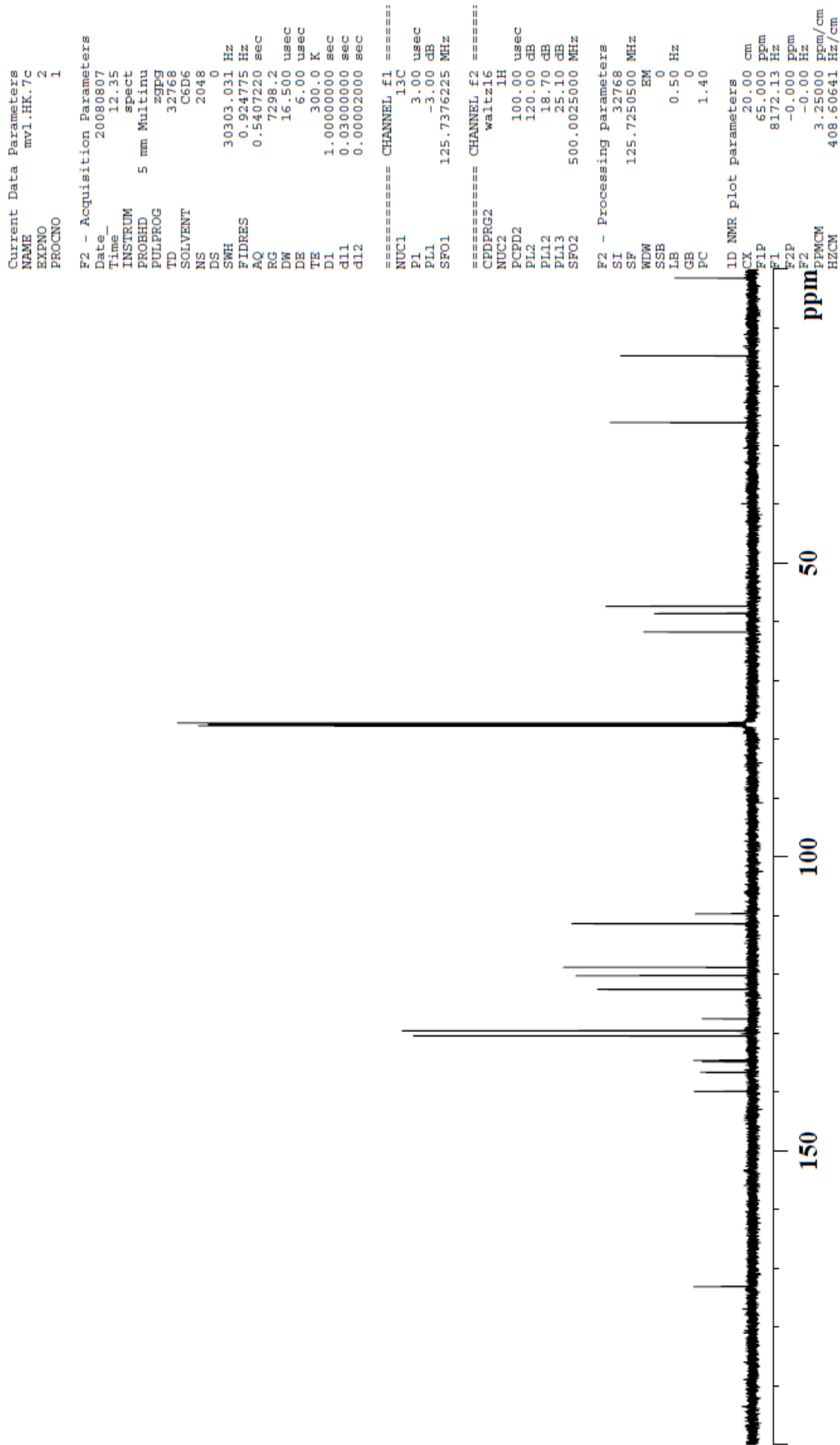
carbon spectrum



proton spectrum



carbon spectrum



NMR spectra for Compound **5g**

proton spectrum

```

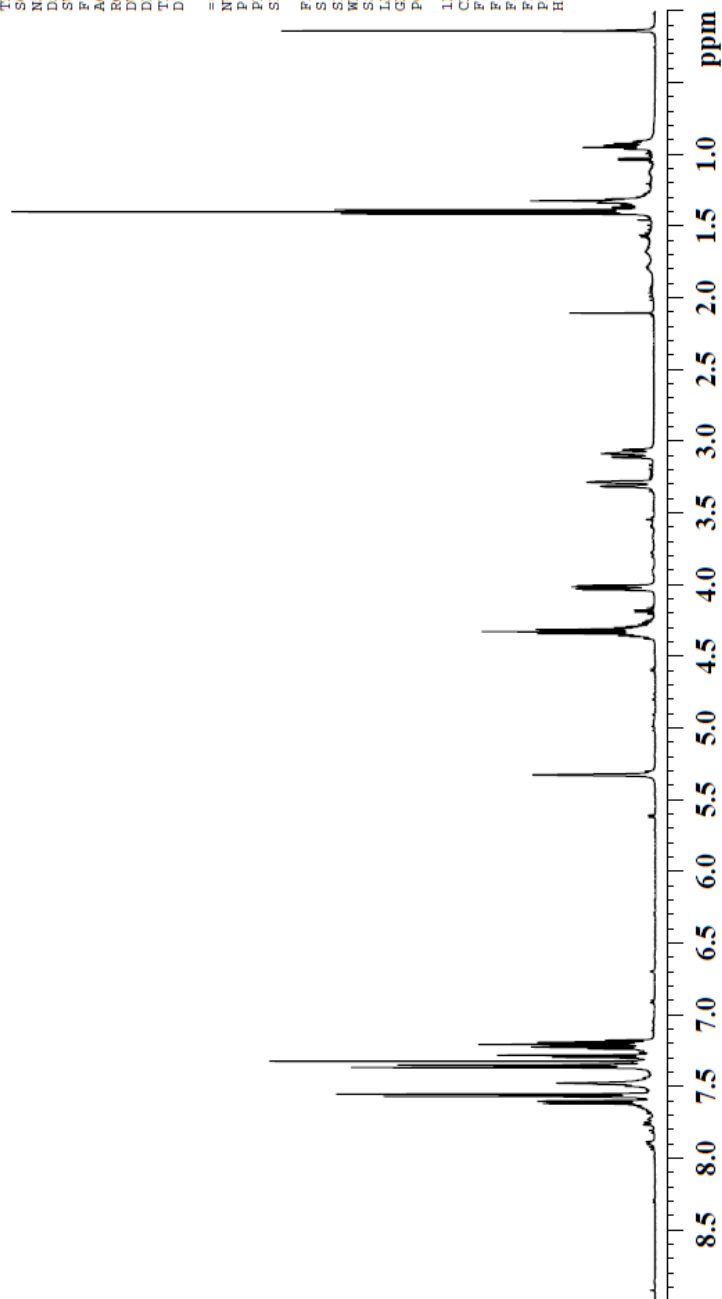
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EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
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Time      18.01
INSTRUM   spect
PROBHD    5 mm Multinu
PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         16
DS         0
SWH        8012.820 Hz
FIDRES     0.244532 Hz
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RG         324.5
DW         62.400 usec
DE         6.00 usec
TE         298.0 K
D1         1.50000000 sec

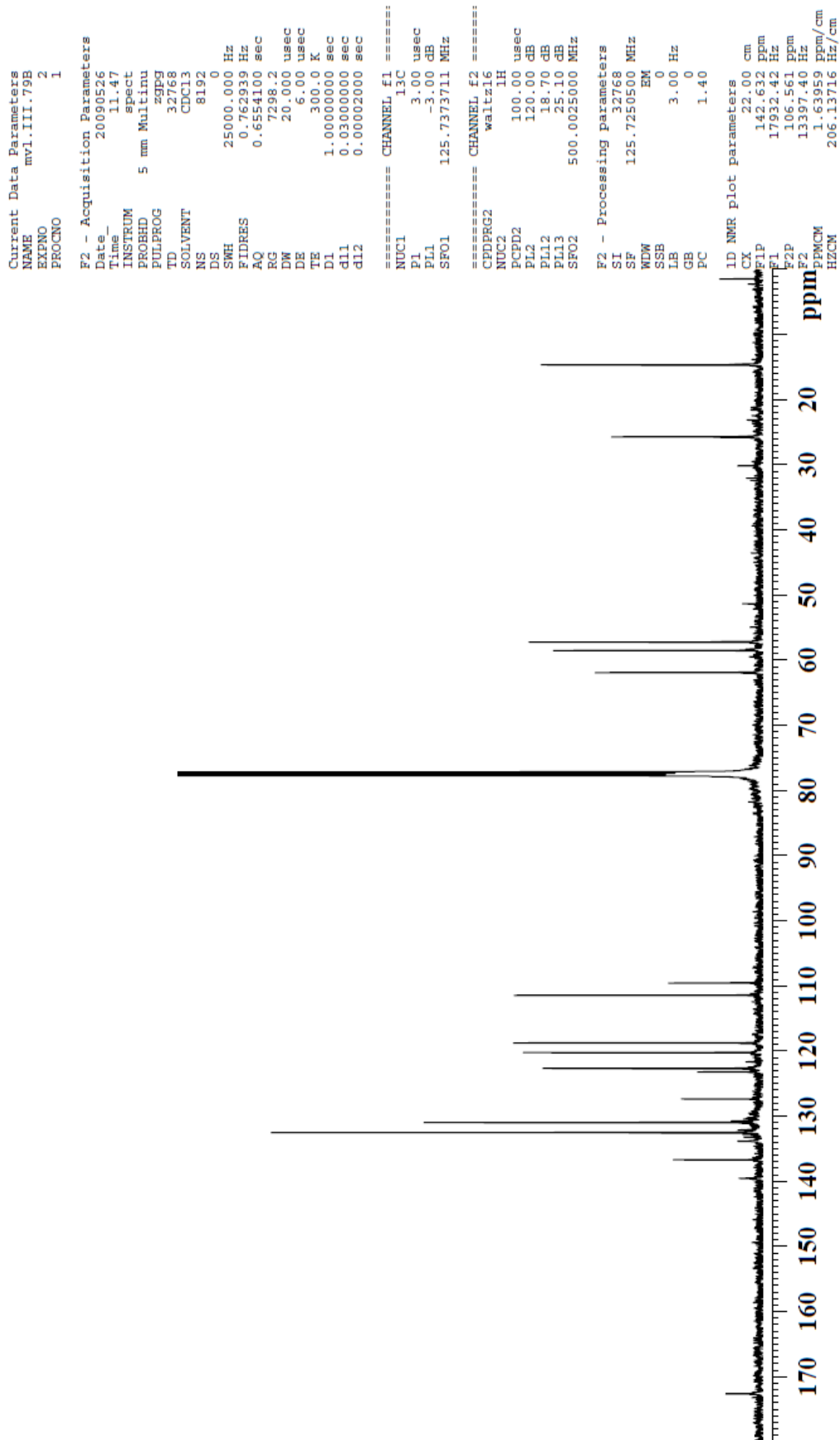
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NUC1       1H
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PL1        3.00 dB
SFO1       500.0030000 MHz

F2 - Processing parameters
SI         32768
SF         500.0000000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.20

ID NMR plot parameters
CX         20.00 cm
FLP        3.470 ppm
F1         1735.06 Hz
F2P        1.133 ppm
F2         566.72 Hz
PDMCM      0.11683 ppm/cm
HZCM       58.41723 Hz/cm
    
```



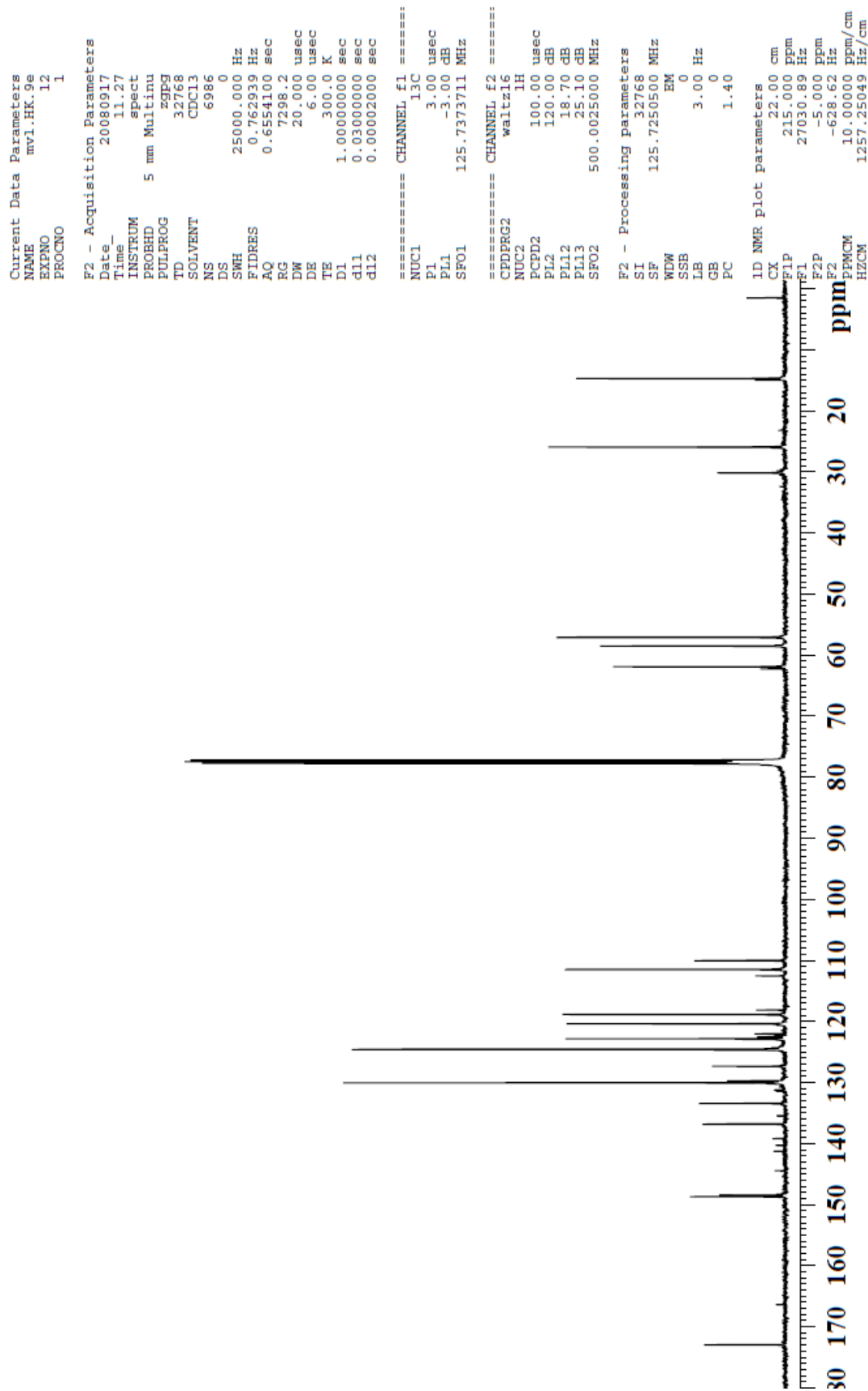
carbon spectrum



proton spectrum

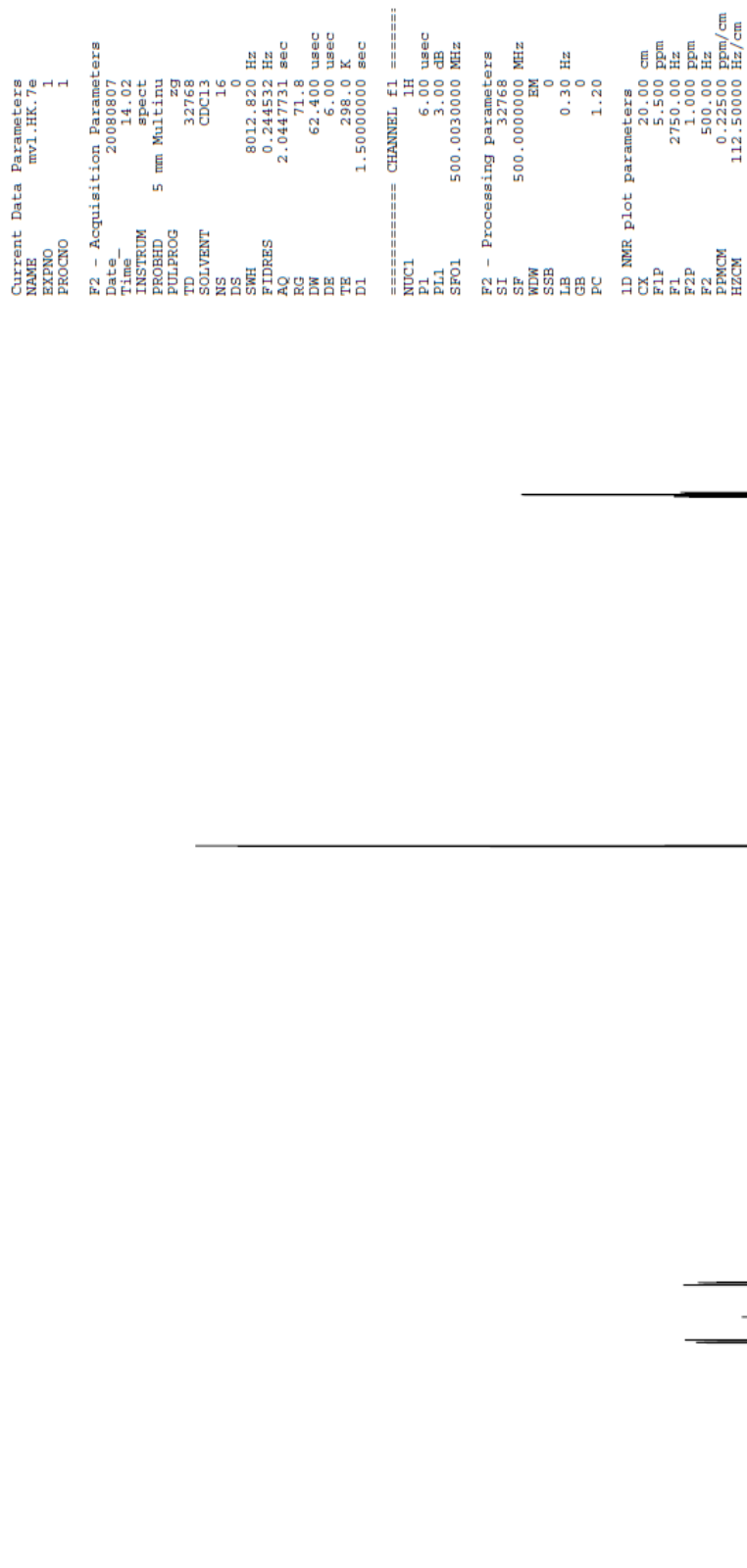


carbon spectrum

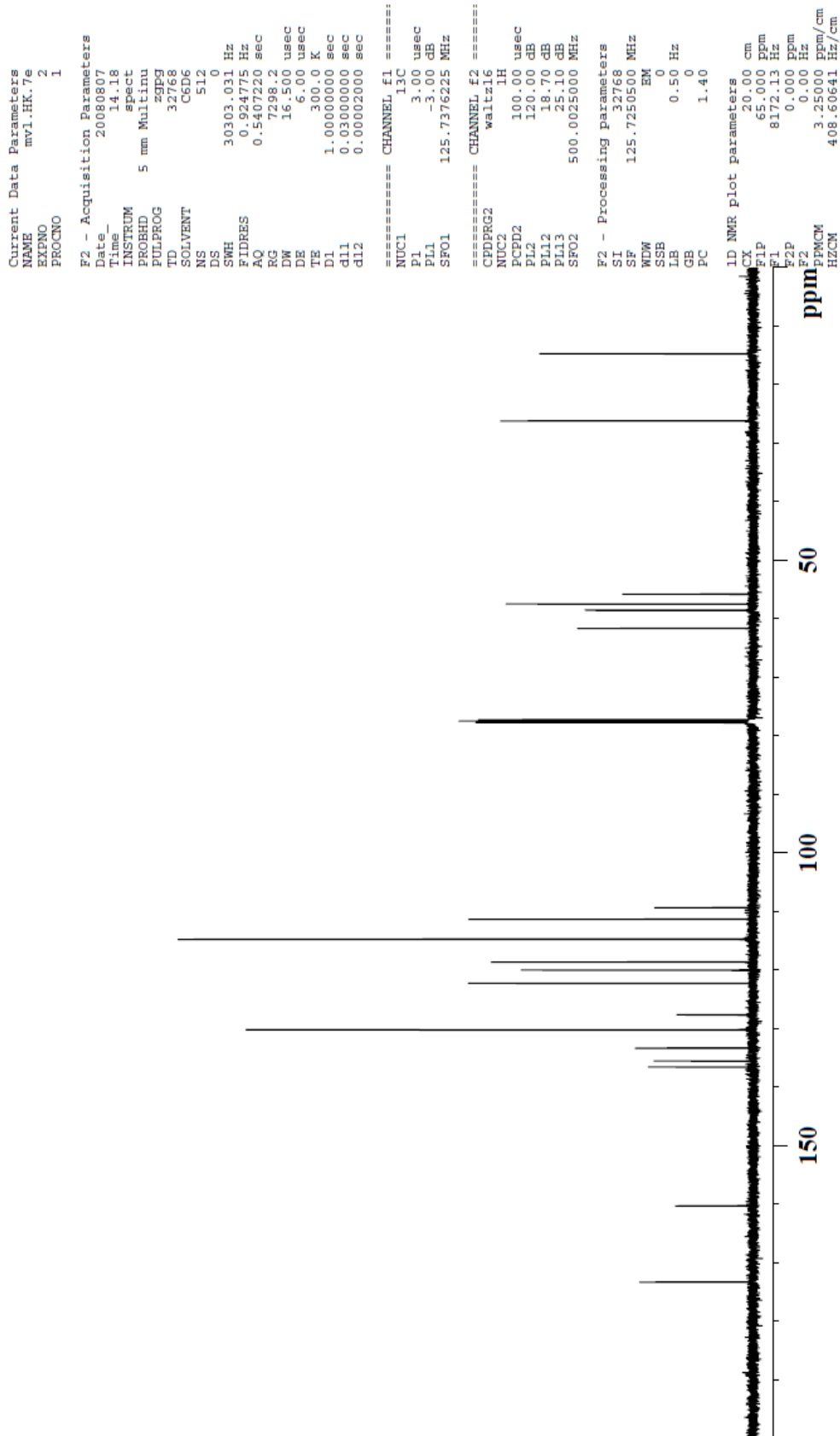


NMR spectra for Compound **5i**

proton spectrum



carbon spectrum



NMR spectra for Compound **6a**

proton spectrum

```

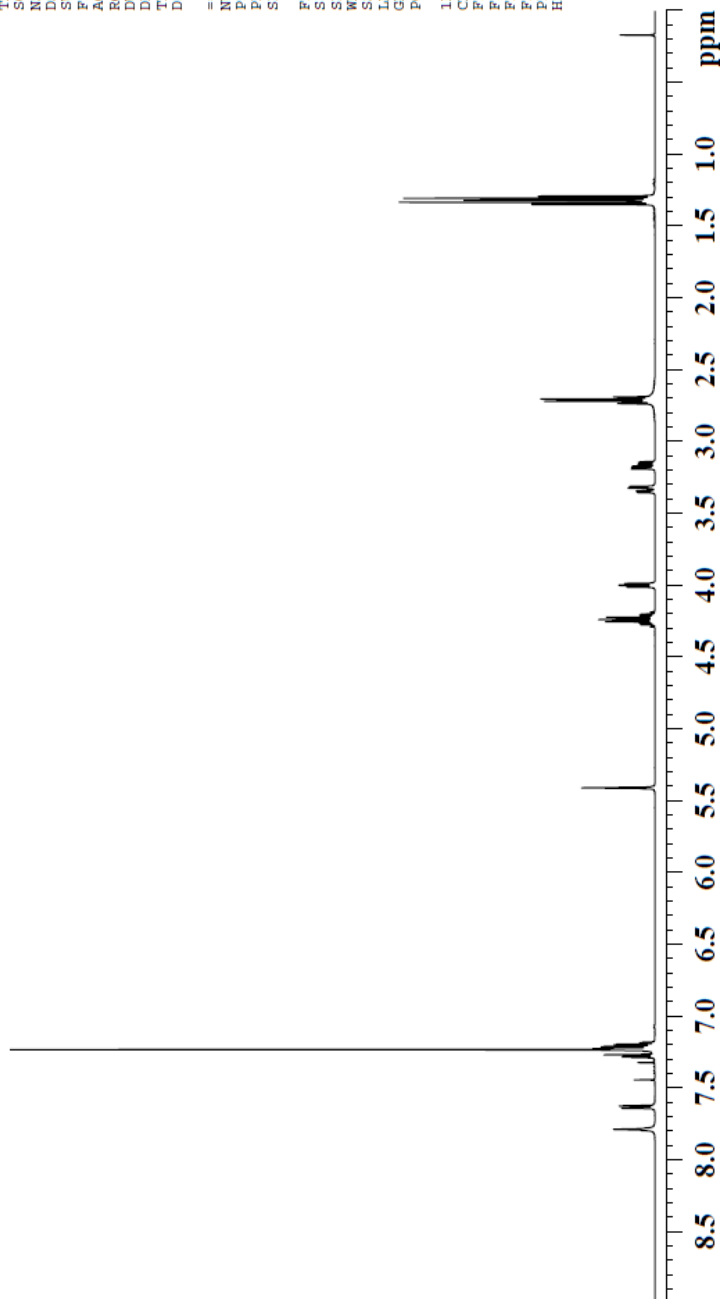
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EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20090525
Time      10.06
INSTRUM   spect
PROBHD    5 mm Multinu
PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         16
DS         0
SWH        8012.820 Hz
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AQ         2.0447731 sec
RG         57
DE         62.400 usec
TE         298.0 K
D1         1.50000000 sec

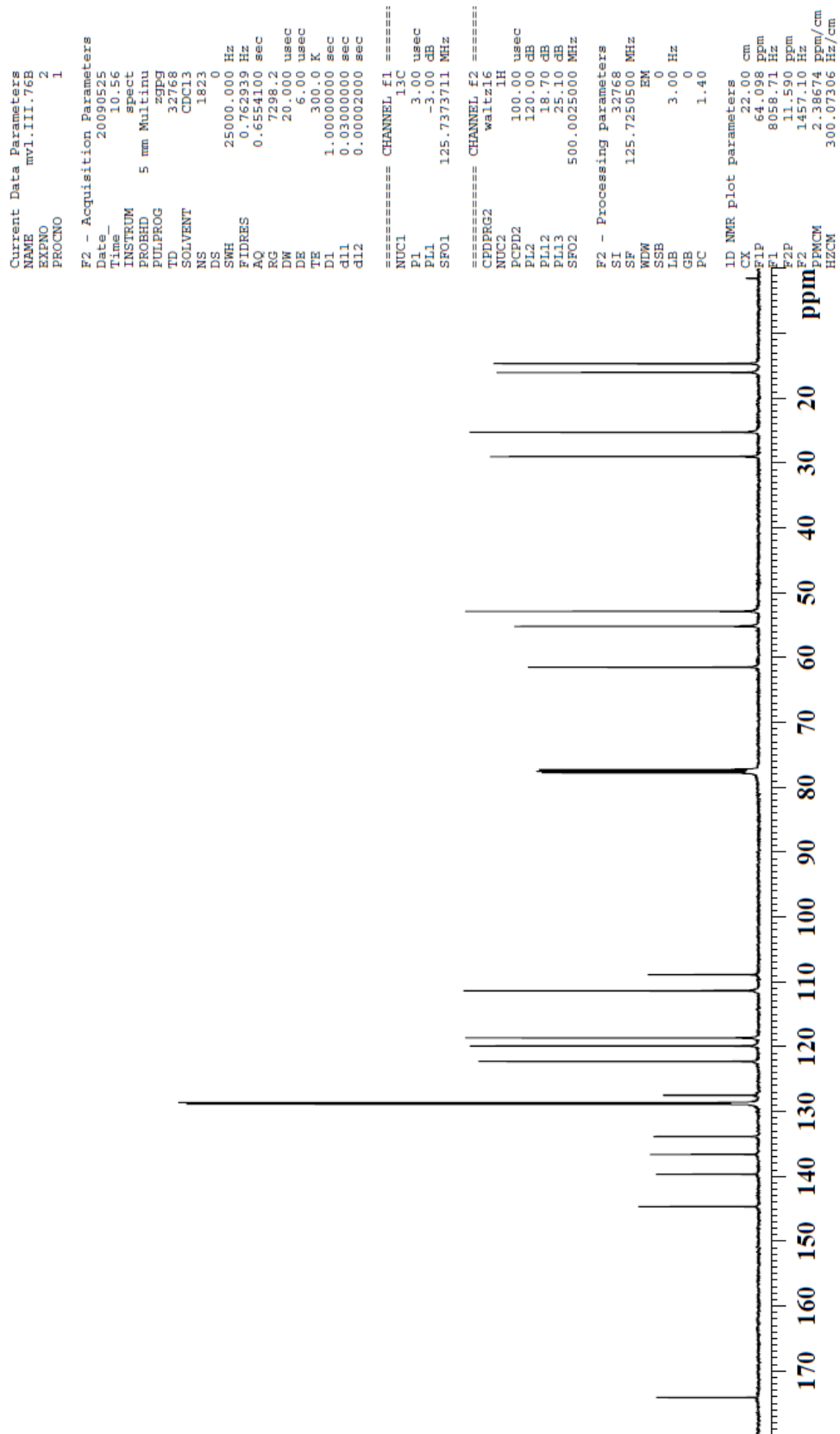
===== CHANNEL f1 =====
NUC1       1H
P1         6.00 usec
PL1        3.00 dB
SFO1       500.0030000 MHz

F2 - Processing parameters
SI         32768
SF         500.0000000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.20

1D NMR plot parameters
CX         20.00 cm
F1P        3.470 ppm
F1         1735.06 Hz
F2P        1.152 ppm
F2         575.91 Hz
PPMCM      0.11591 ppm/cm
HZCM       57.95726 Hz/cm
  
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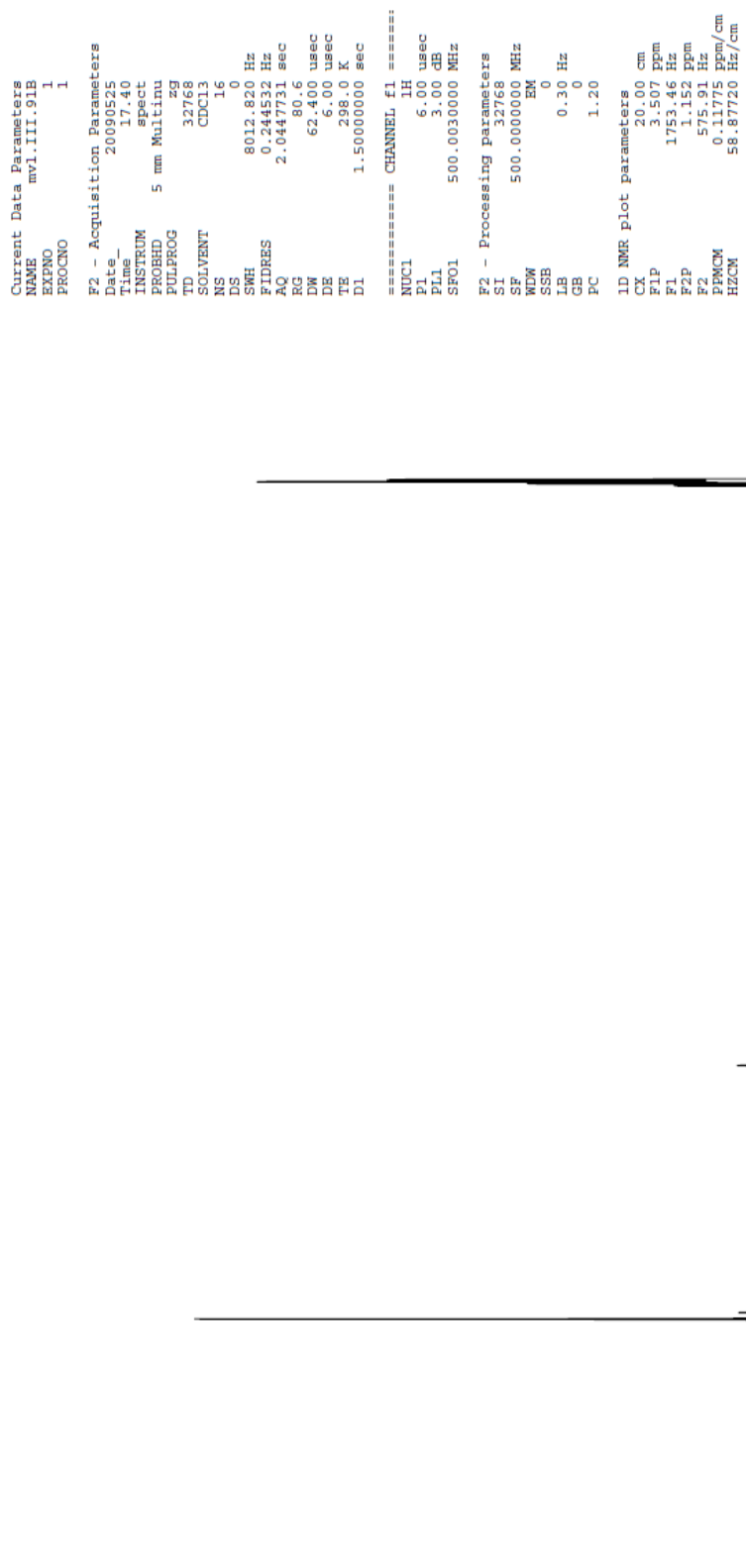


carbon spectrum

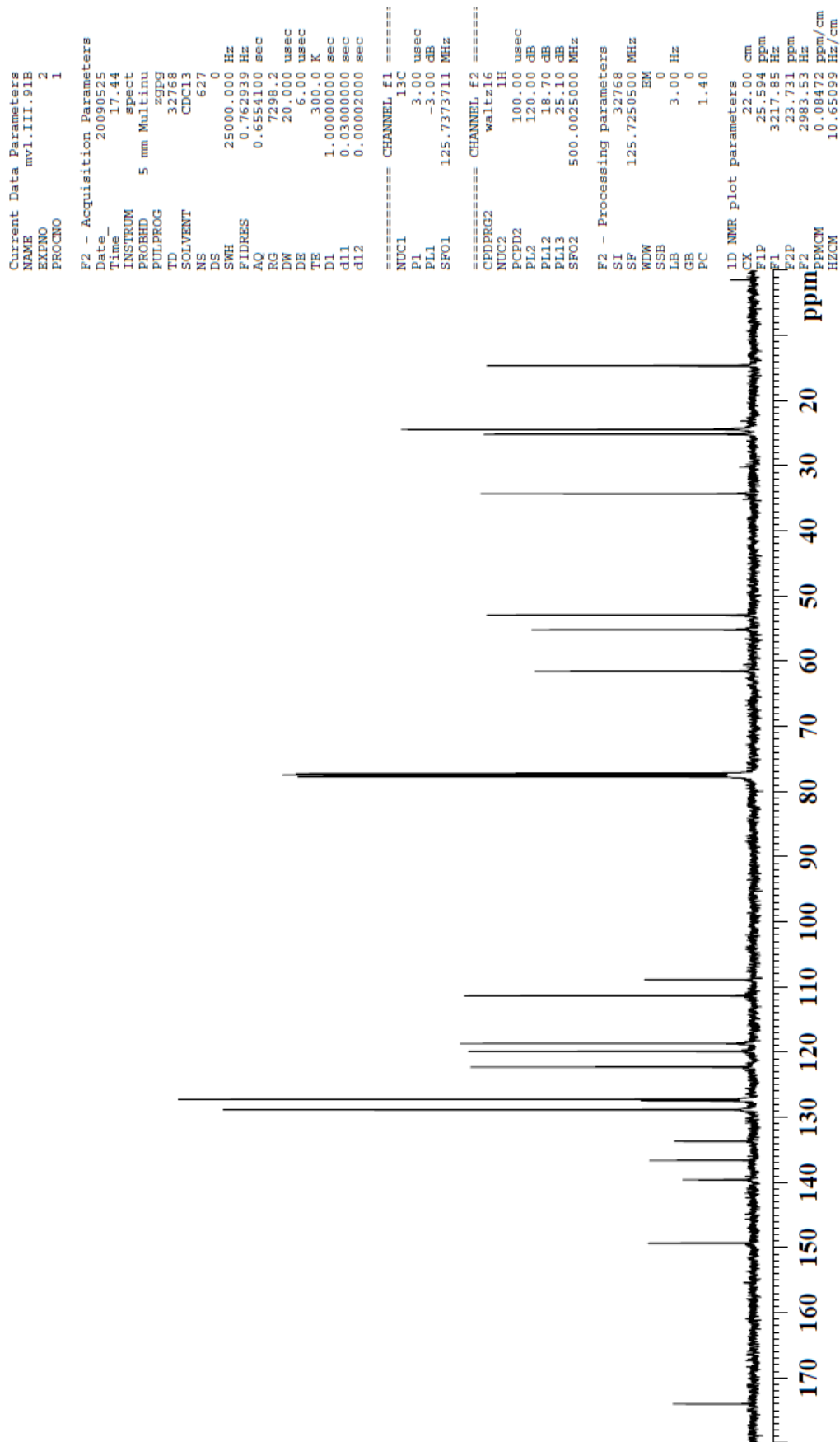


NMR spectra for Compound **6b**

proton spectrum



carbon spectrum

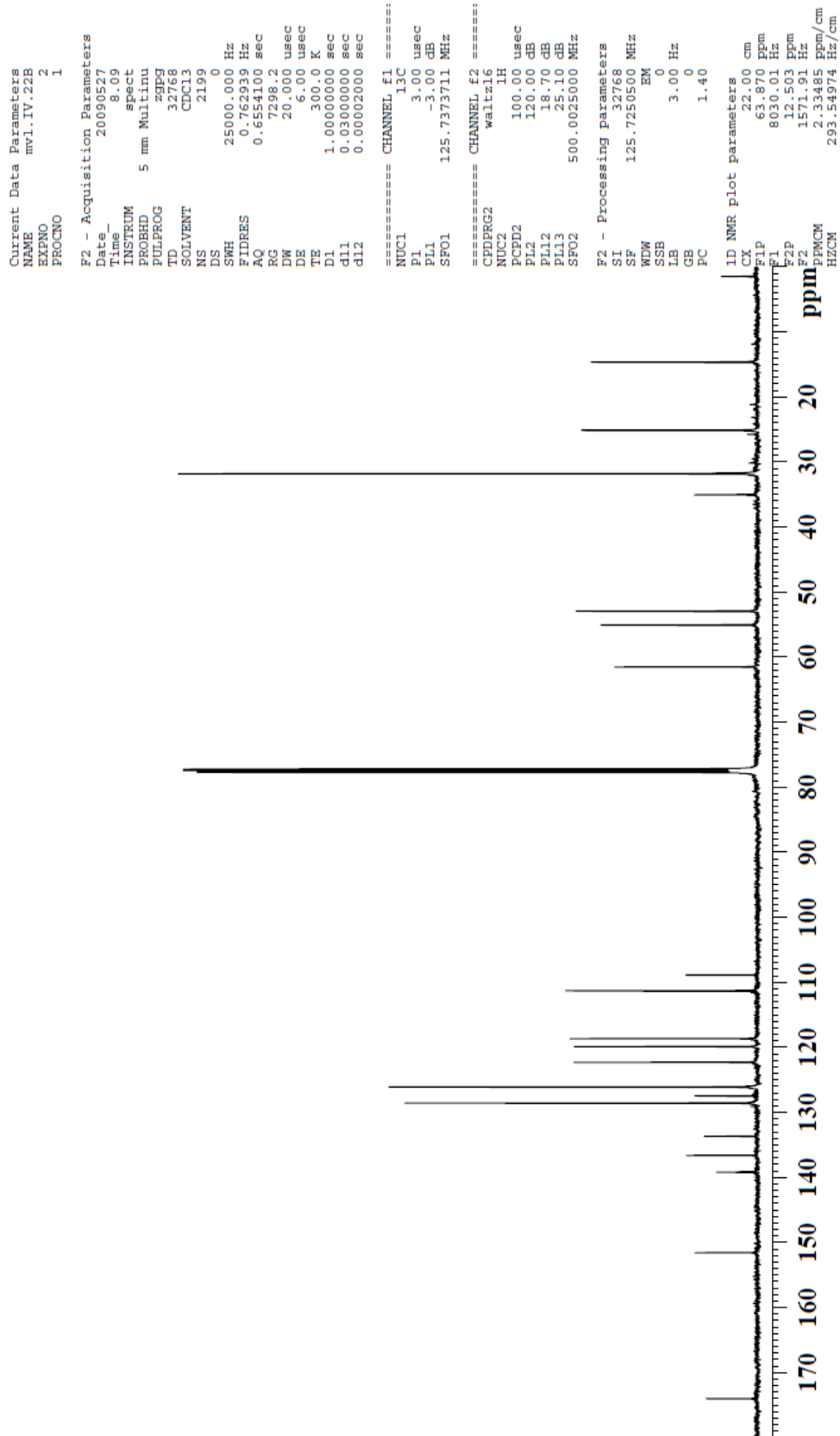


NMR spectra for Compound **6c**

proton spectrum

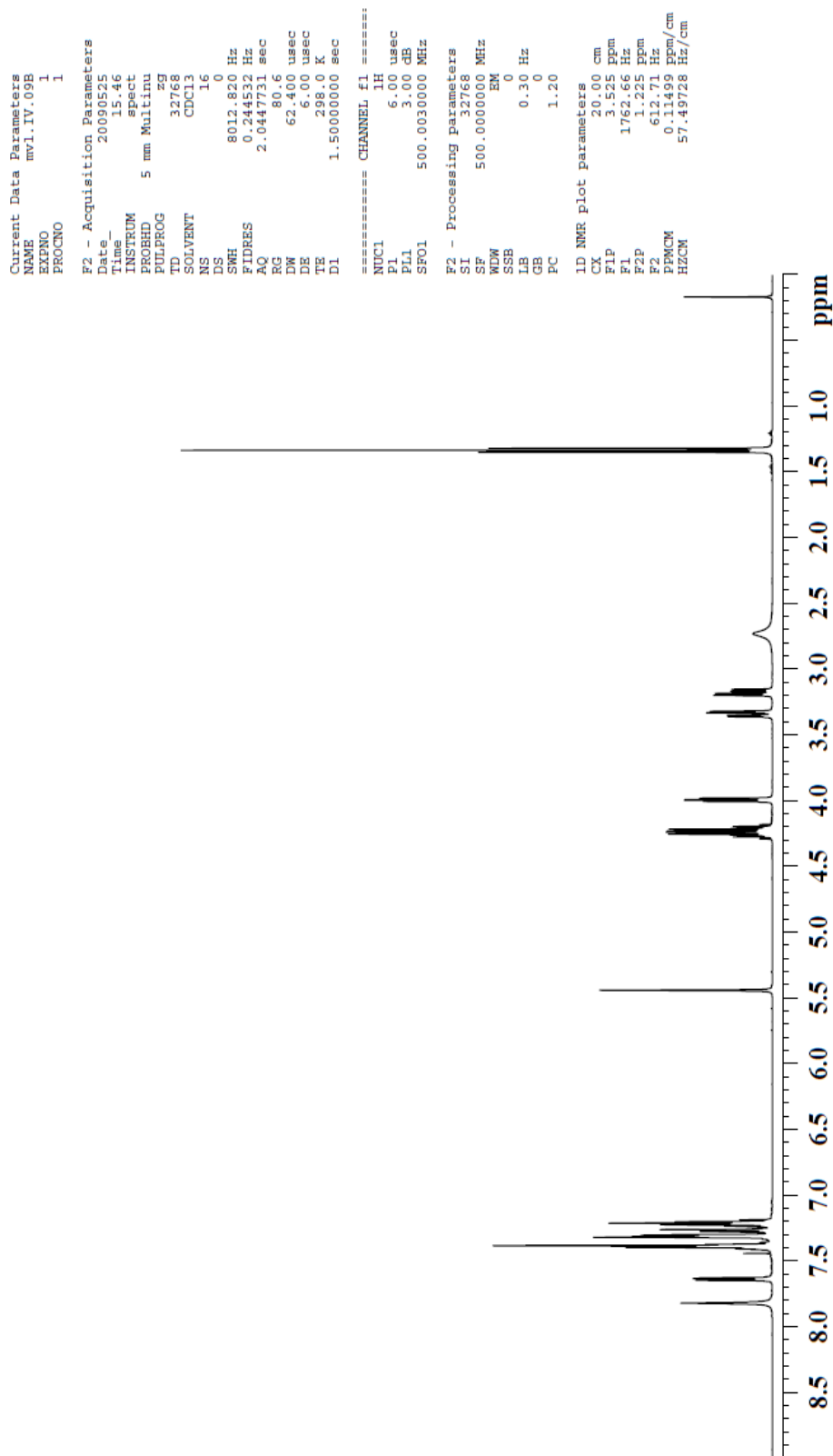


carbon spectrum

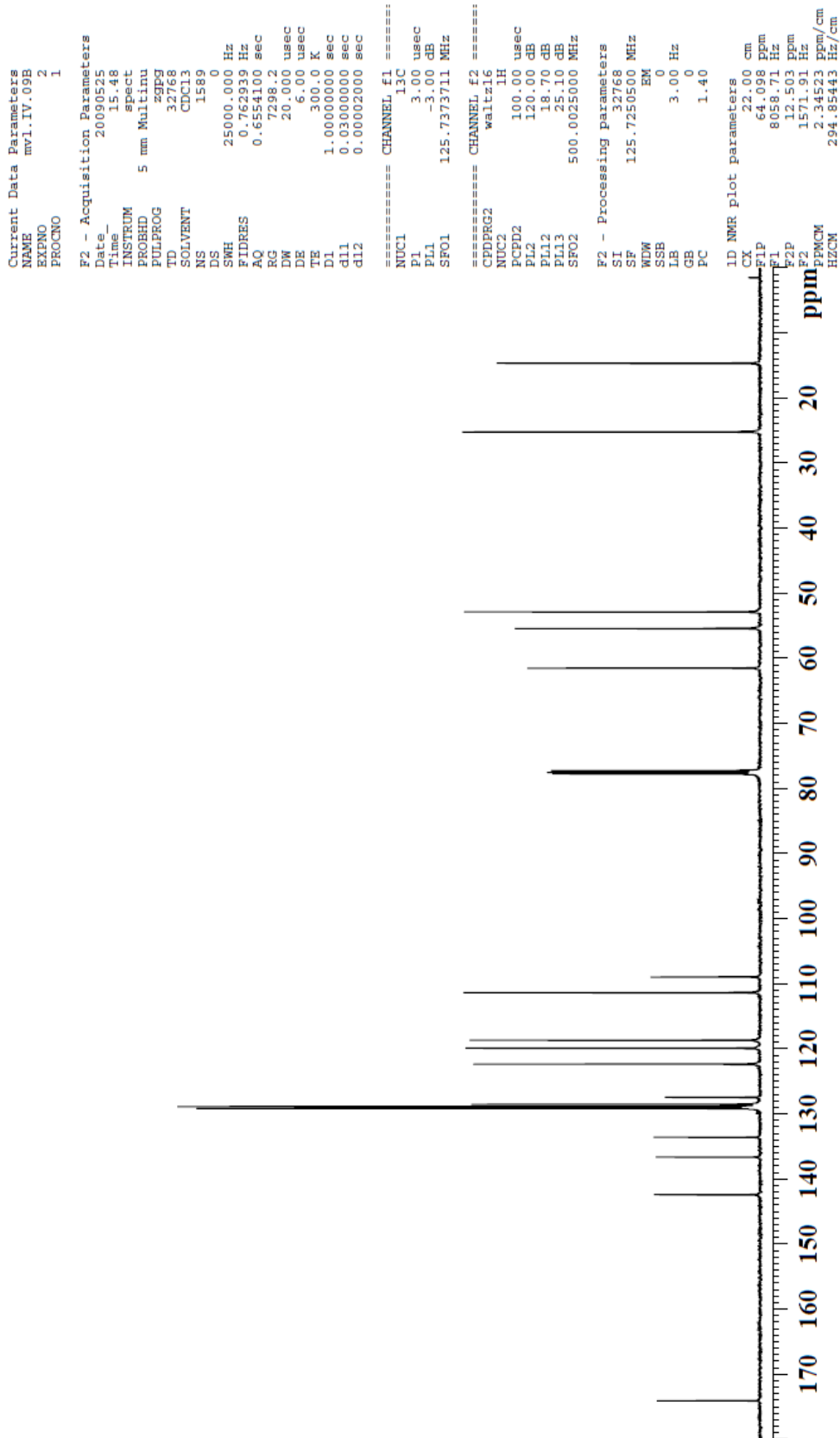


NMR spectra for Compound **6d**

proton spectrum

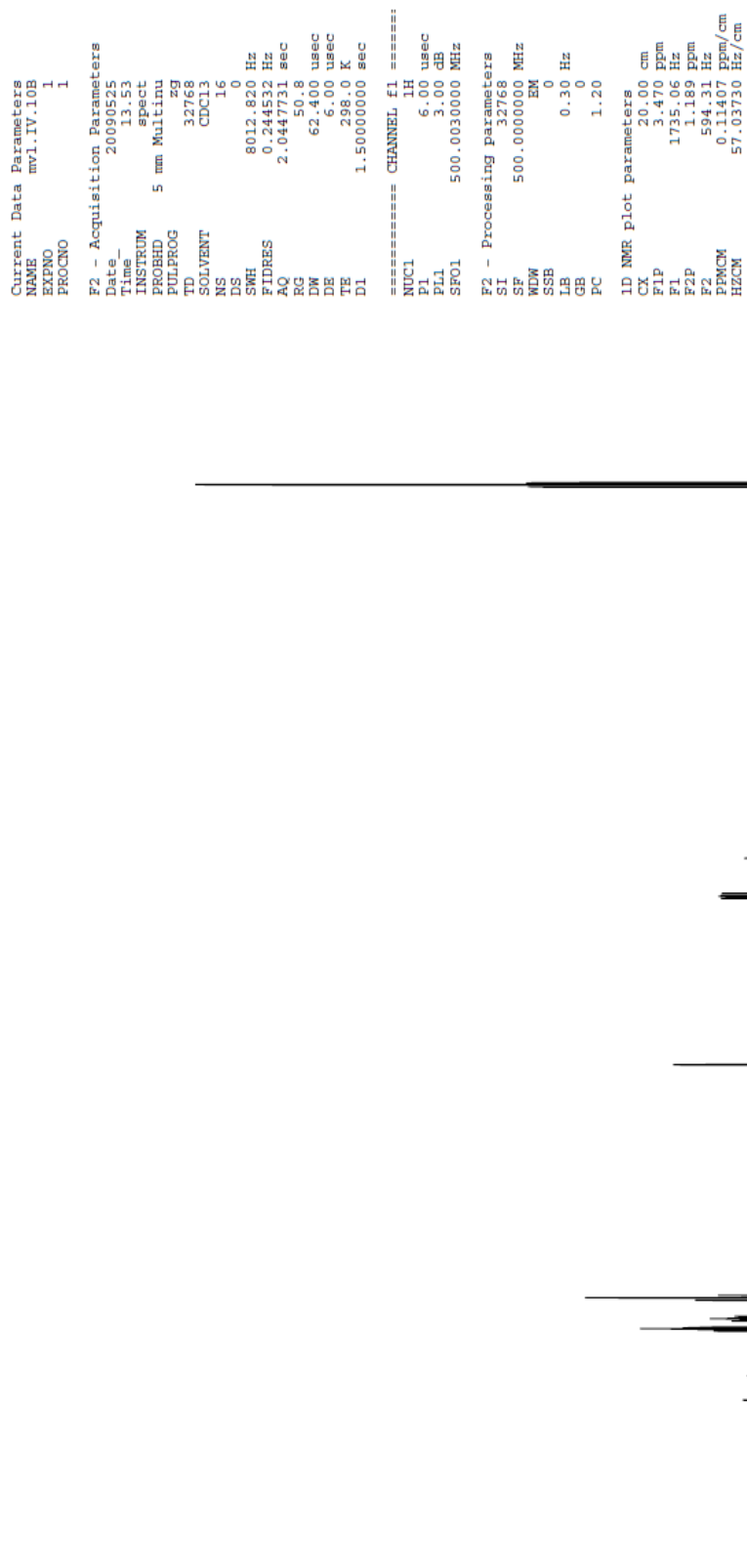


carbon spectrum

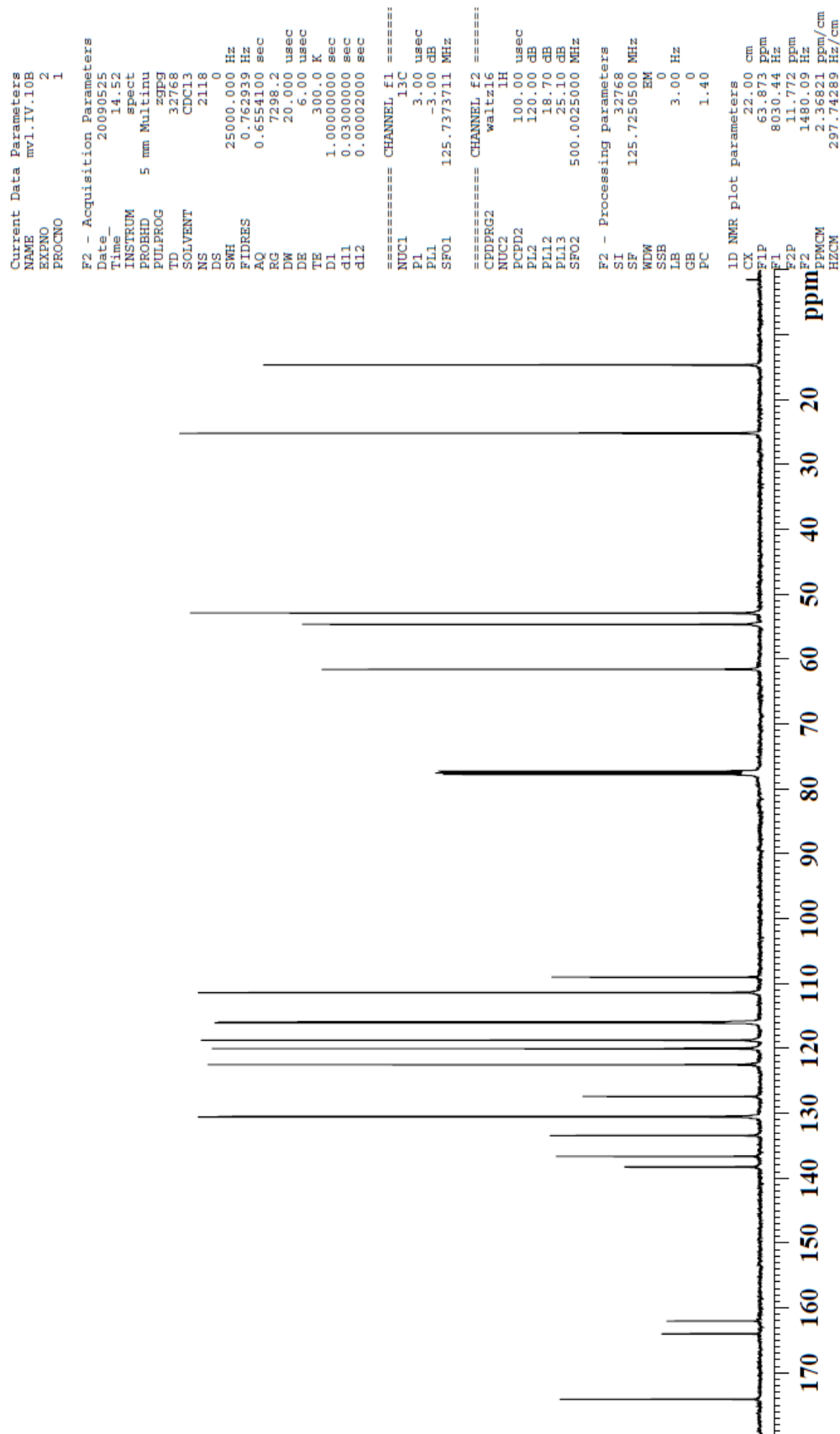


NMR spectra for Compound **6e**

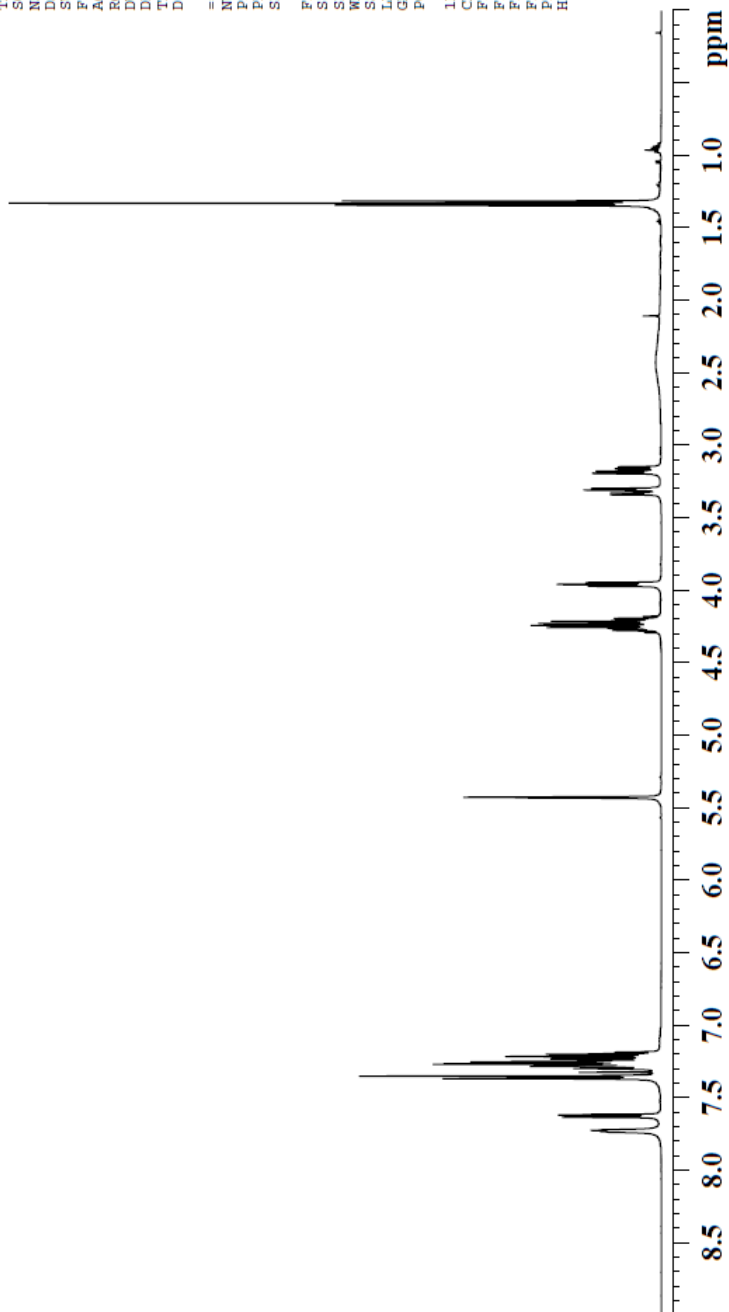
proton spectrum



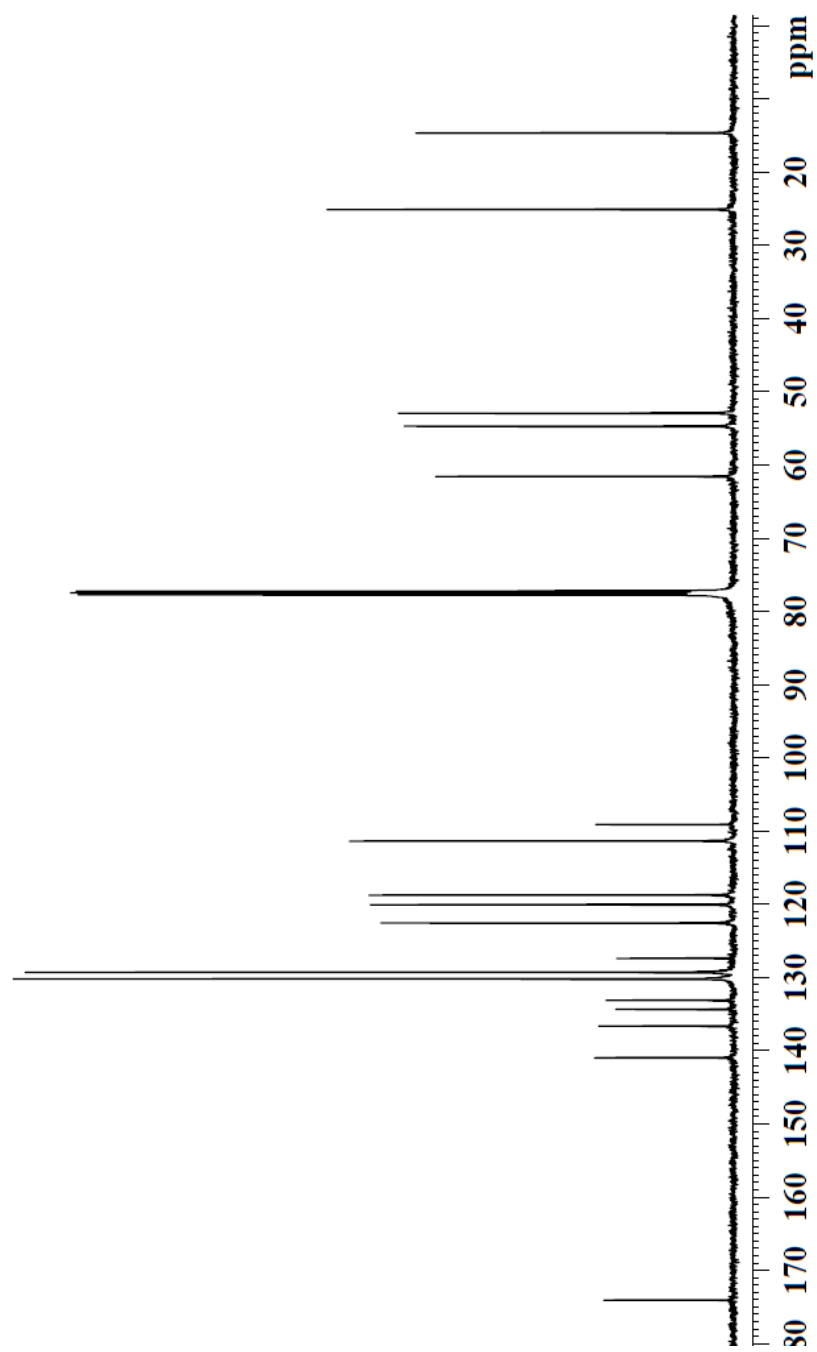
carbon spectrum



NMR spectra for Compound **6f**

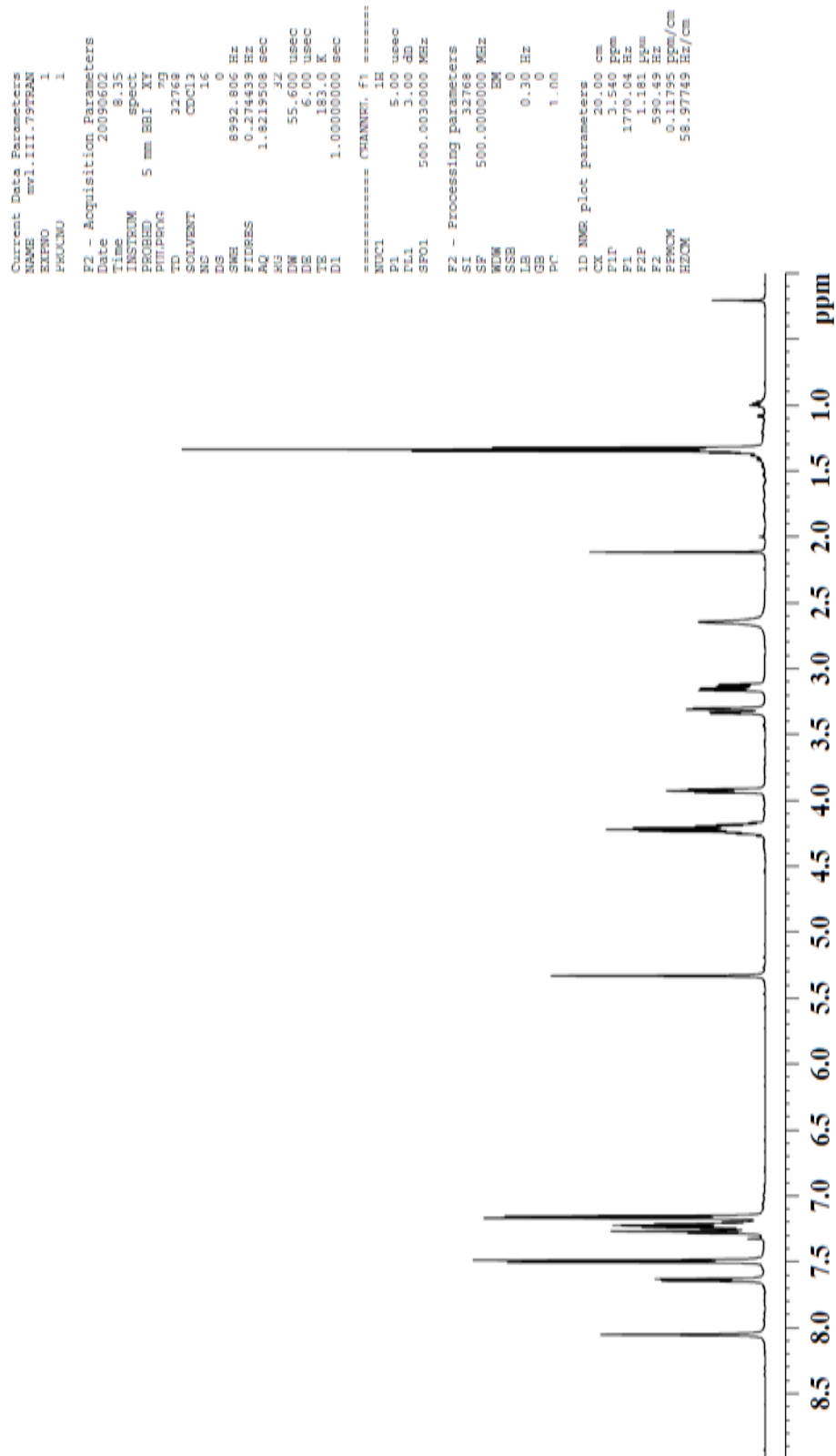


carbon spectrum

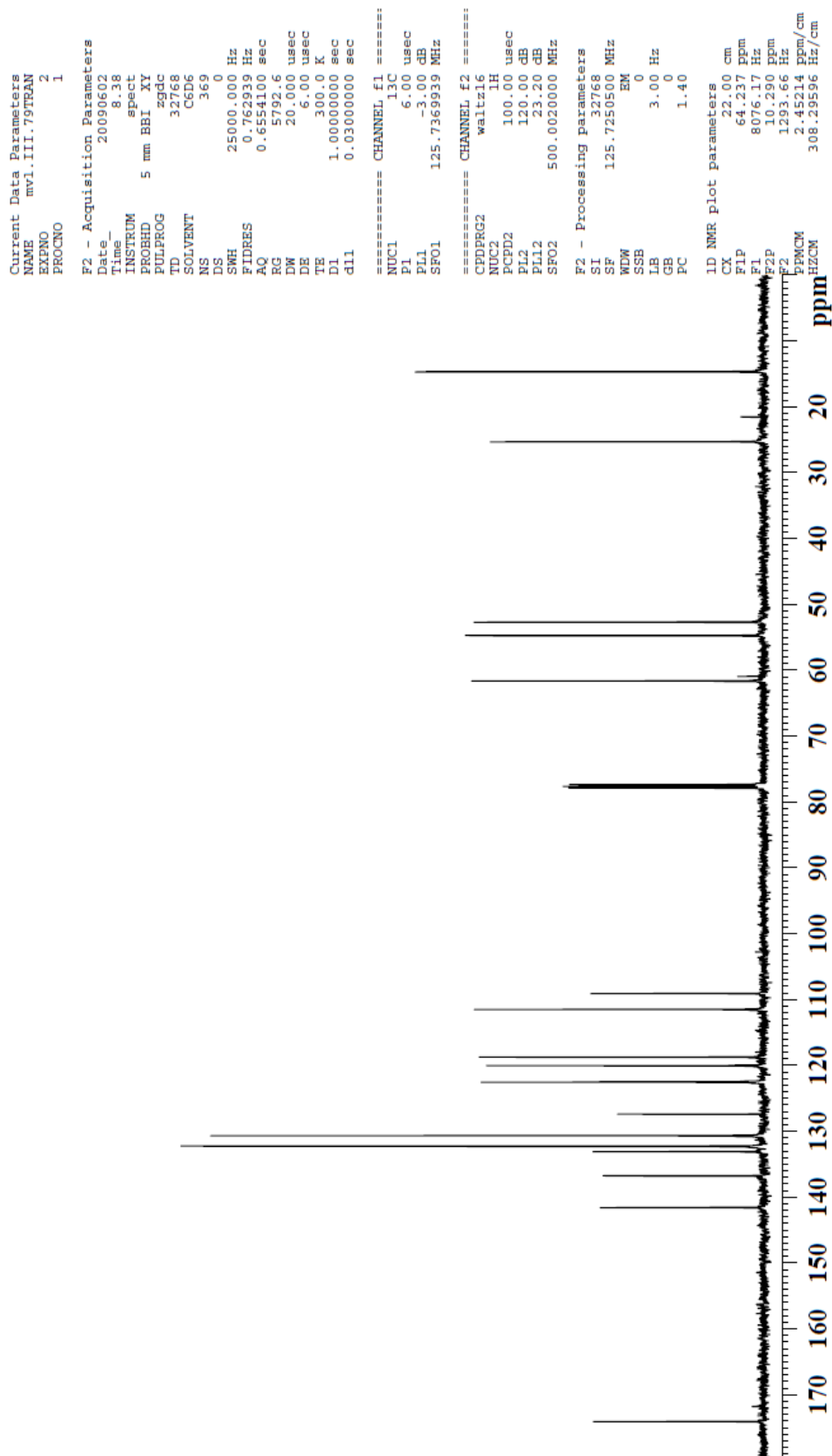


NMR spectra for Compound **6g**

proton spectrum



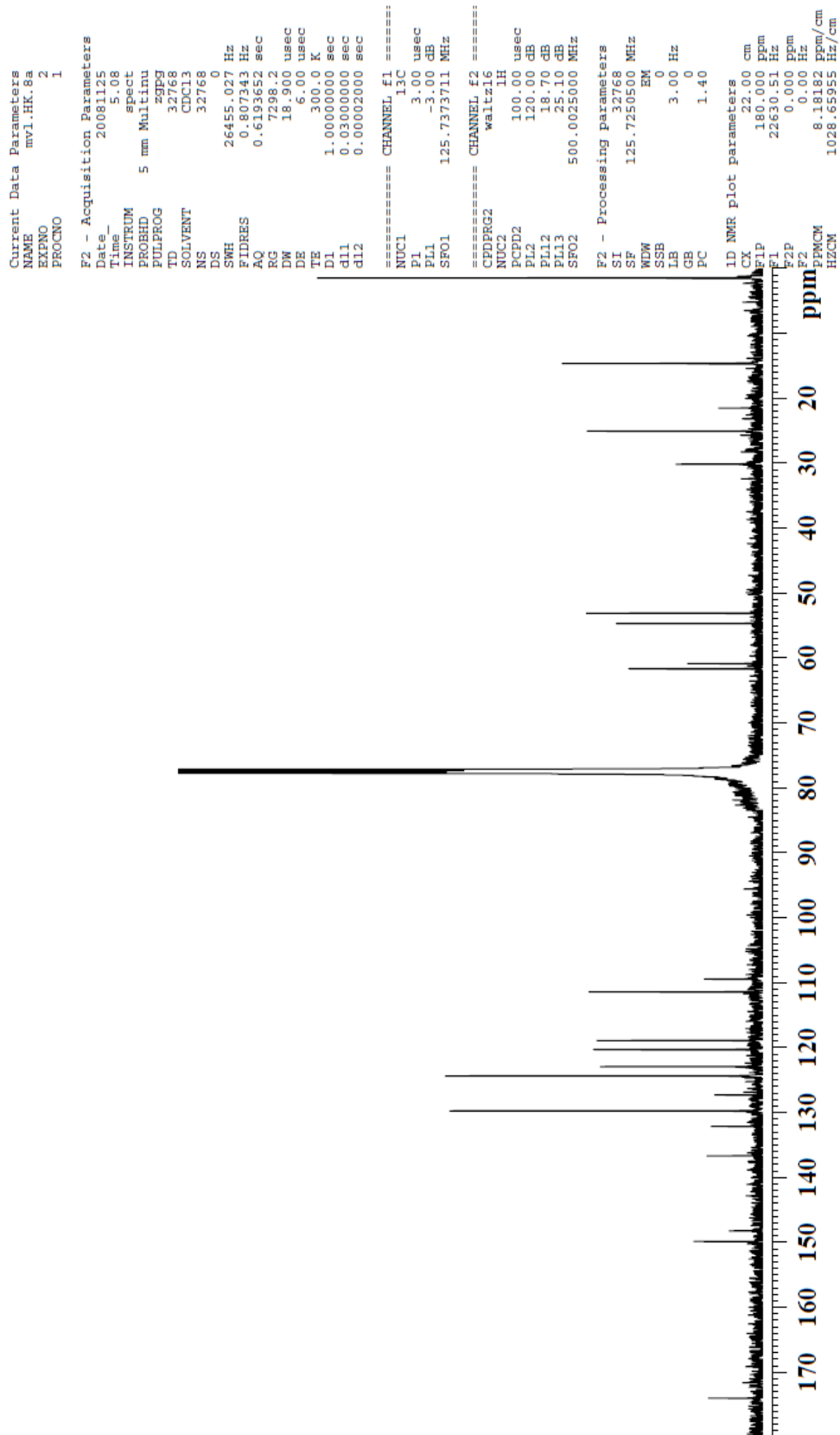
carbon spectrum



proton spectrum

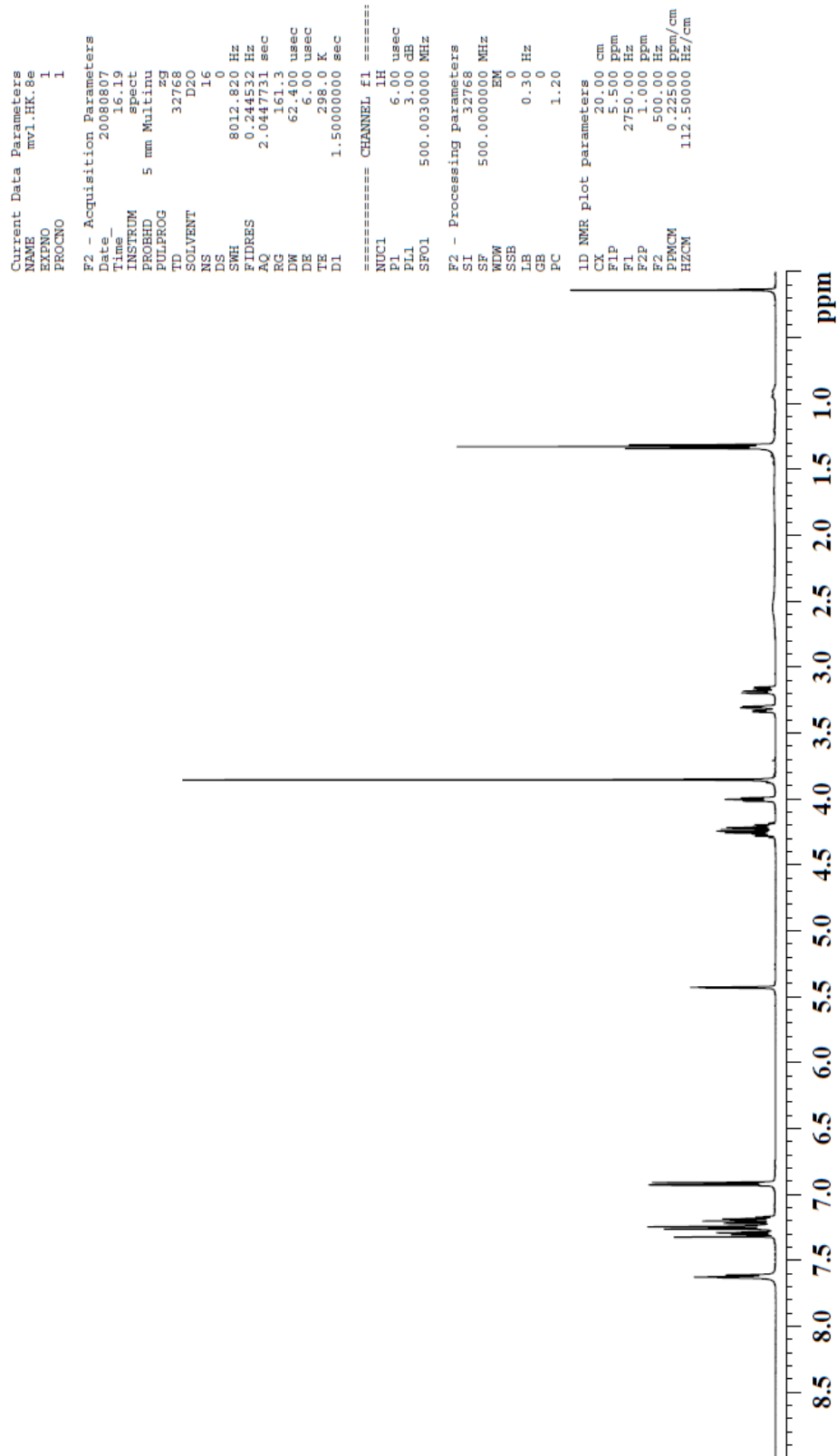


carbon spectrum

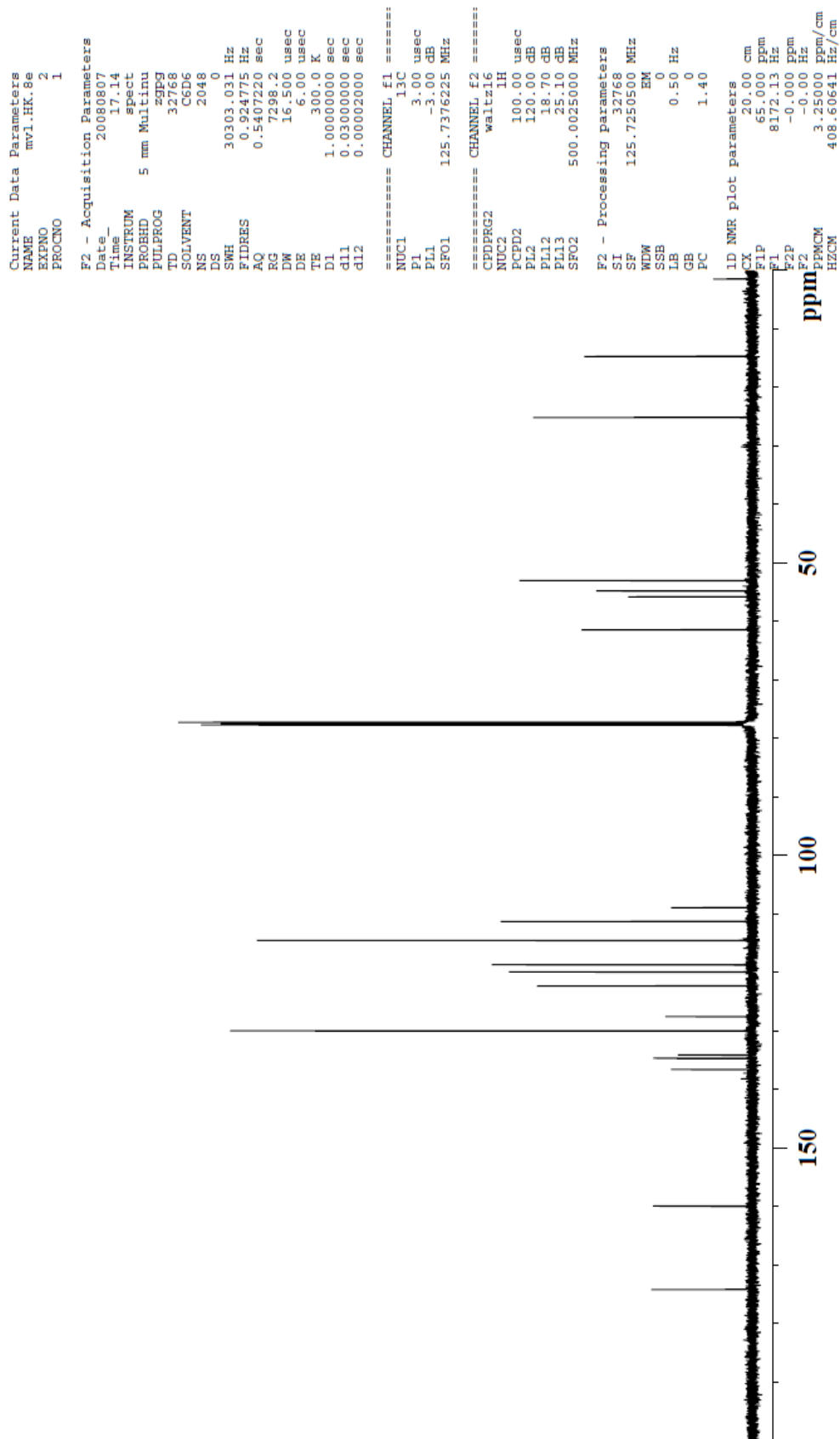


NMR spectra for Compound **6i**

proton spectrum



carbon spectrum



NMR spectra for Compound 7a

proton spectrum

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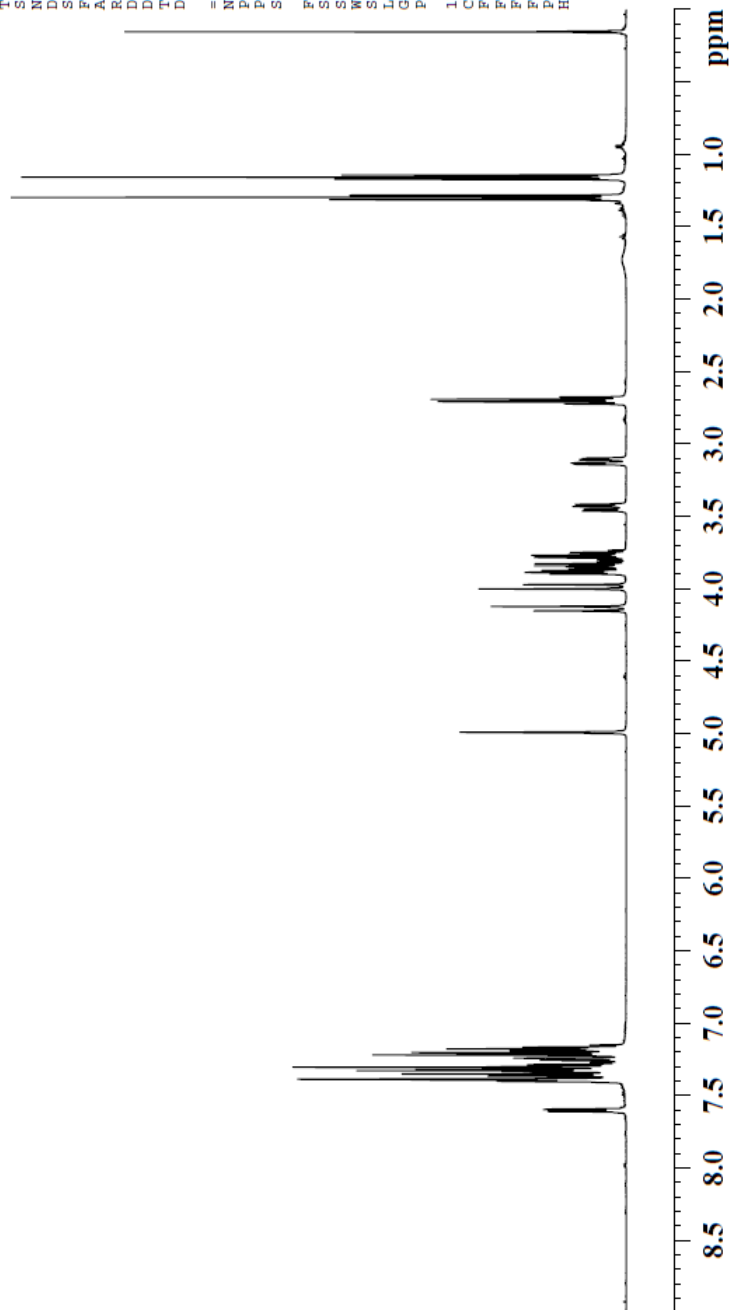
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EXPNO     10
PROCNO    1

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PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         16
DS         0
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FIDRES     0.274439 Hz
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DE         55.600 usec
TE         183.0 K
D1         1.00000000 sec

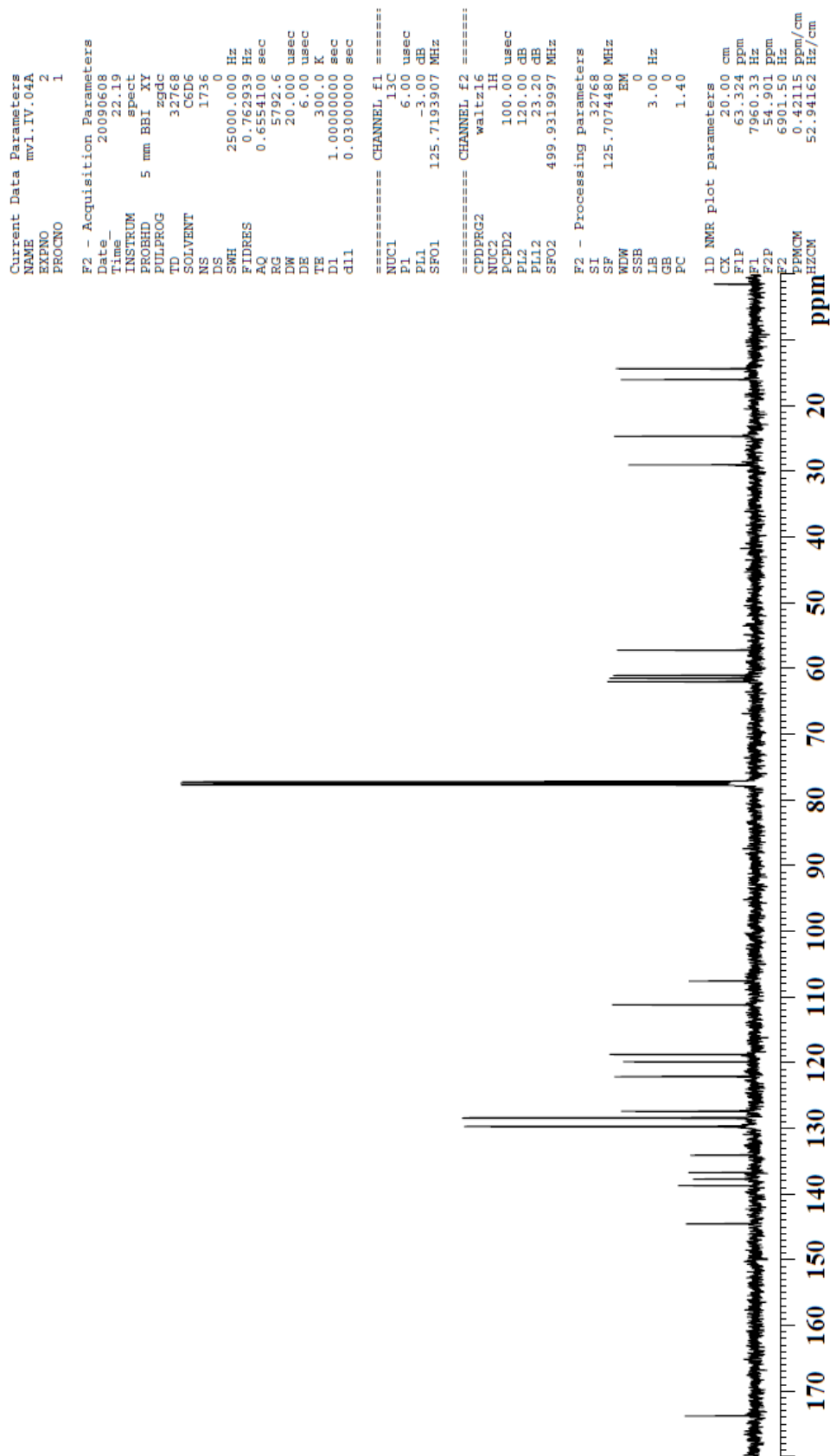
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P1         5.00 usec
PL1        3.00 dB
SFO1       499.9329996 MHz

F2 - Processing parameters
SI         32768
SF         499.9300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         20.00 cm
FLP        3.493 ppm
F1         1746.14 Hz
F2P        1.091 ppm
F2         545.33 Hz
PQCM       0.12010 ppm/cm
HZCM       60.04047 Hz/cm
  
```

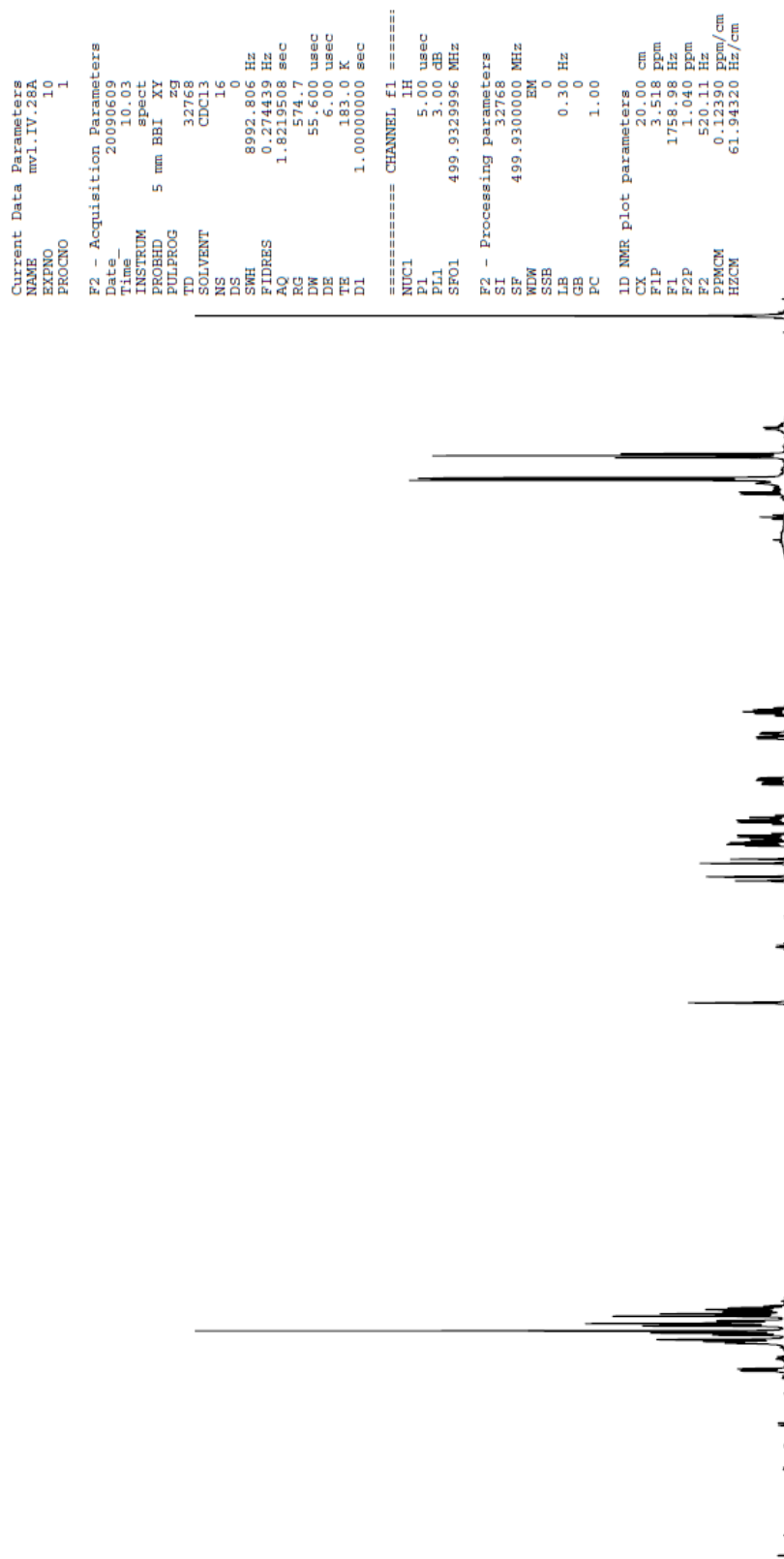


carbon spectrum



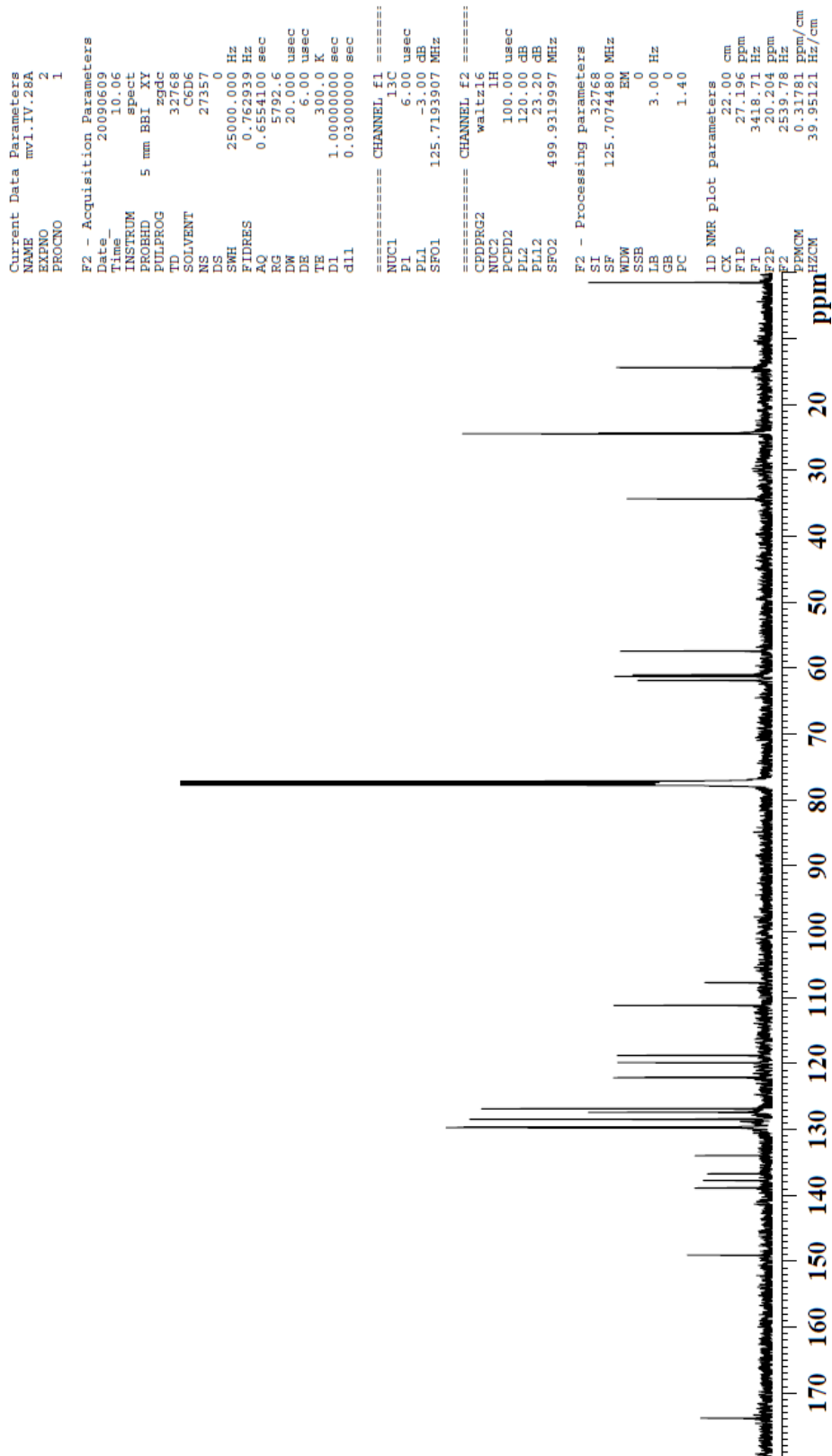
NMR spectra for Compound **7b**

proton spectrum



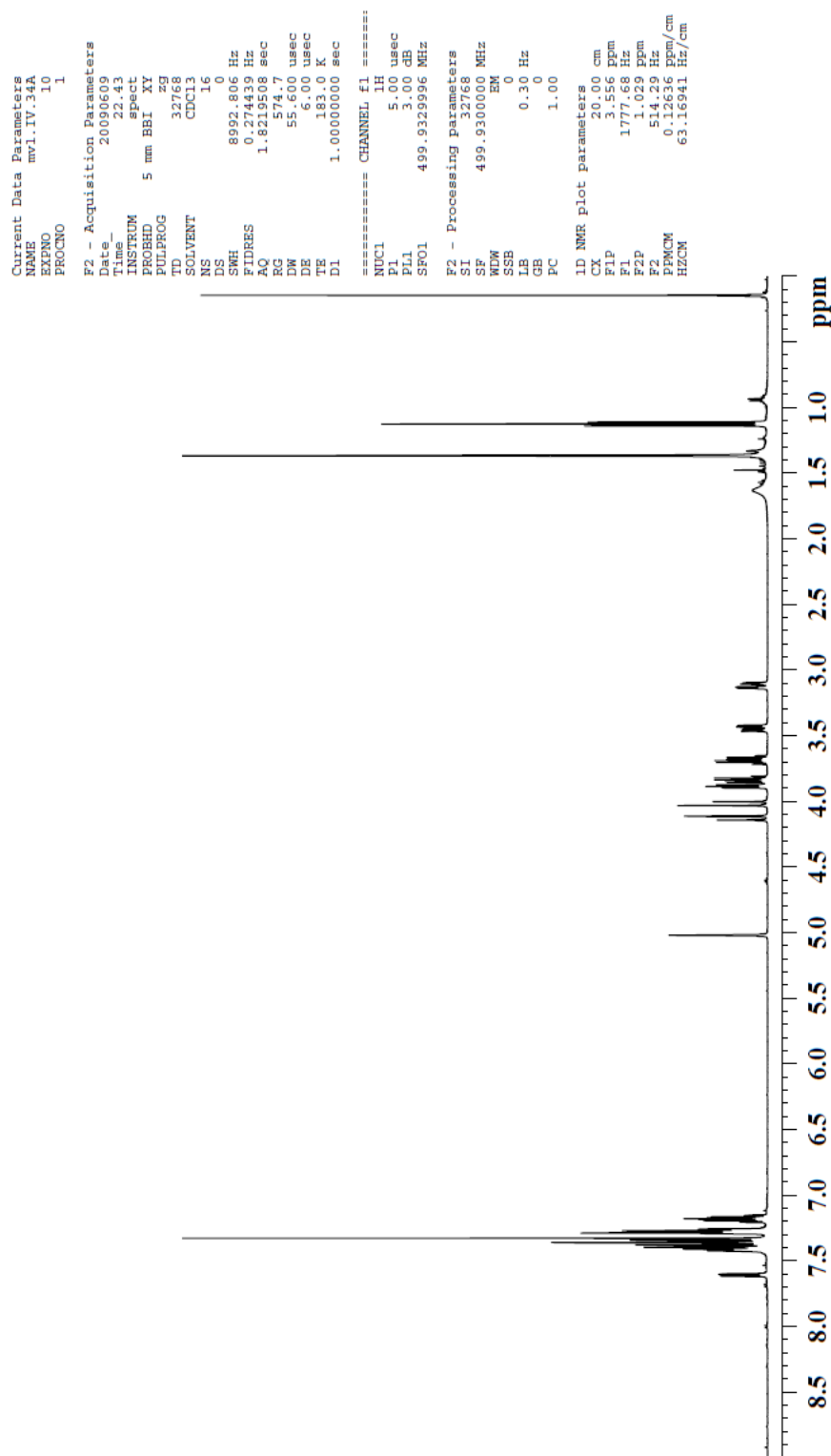
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

carbon spectrum

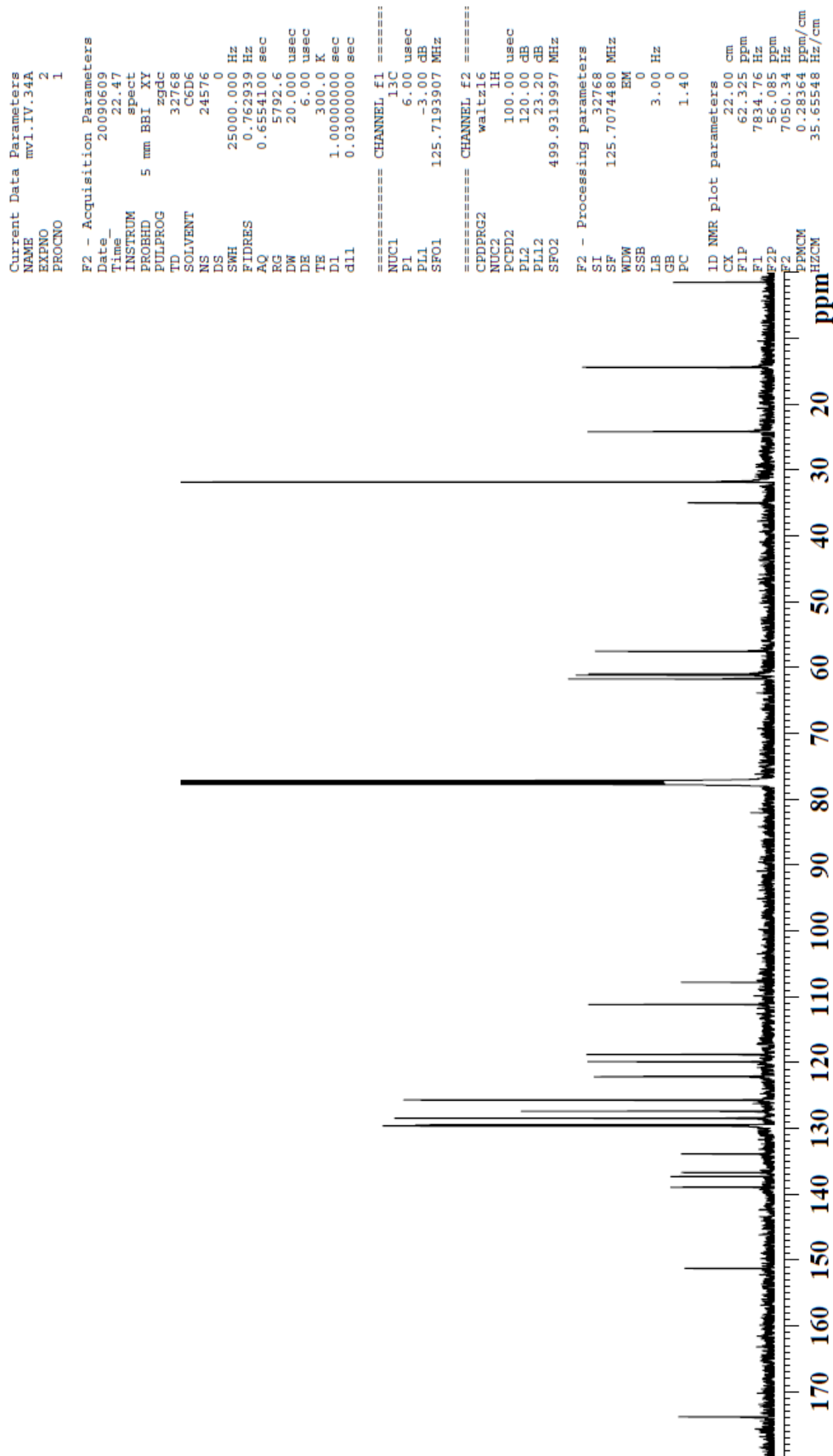


NMR spectra for Compound **7c**

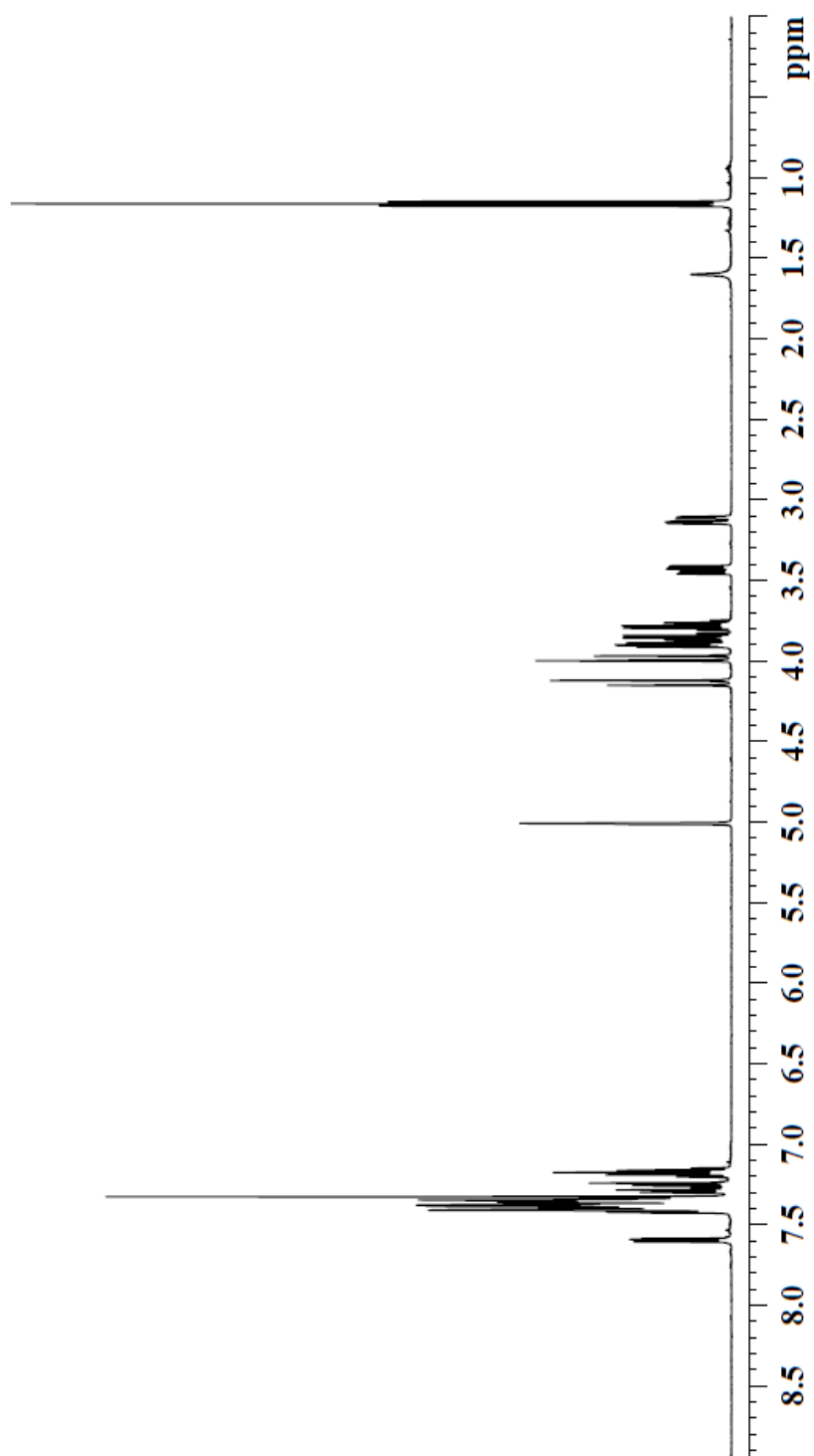
proton spectrum



carbon spectrum



proton spectrum



NMR spectra for Compound **7e**

proton spectrum

```

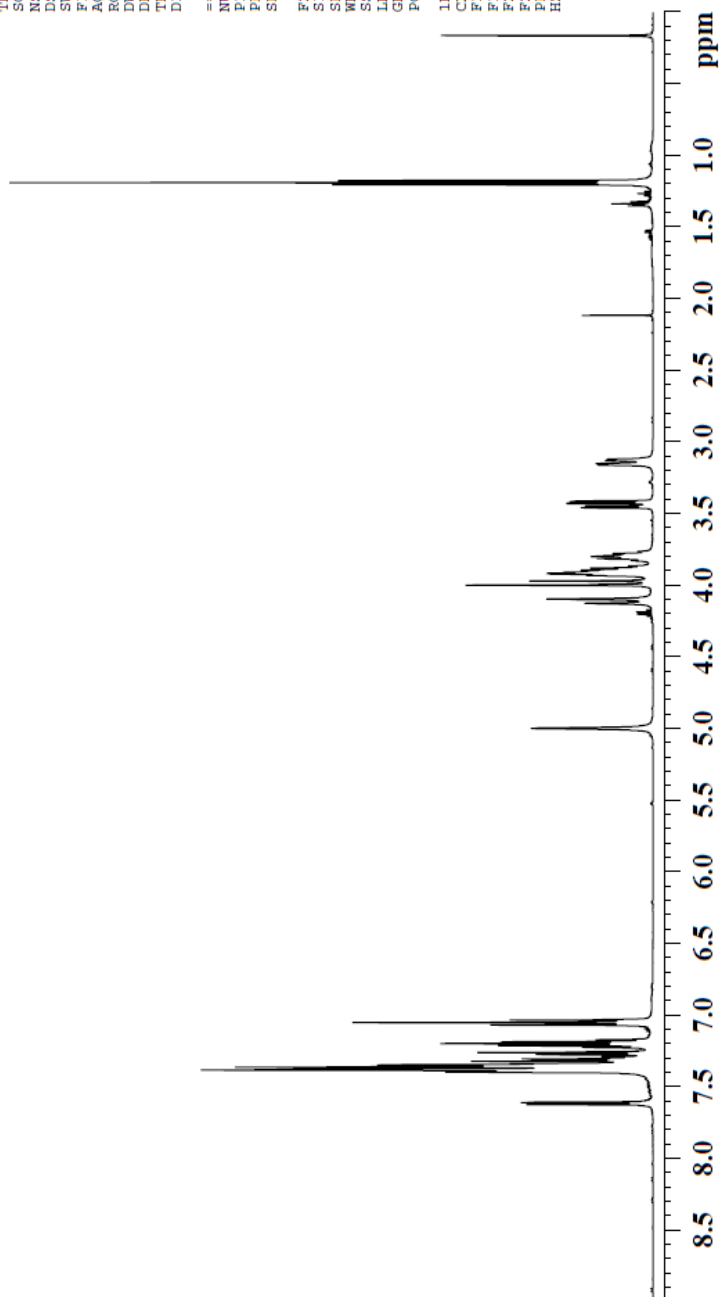
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EXPNO     1
PROCNO    1

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PULPROG   zg
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SOLVENT   CDCl3
NS         16
DS         0
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG         80.6
DE         62.400 usec
TE         298.0 K
D1         1.50000000 sec

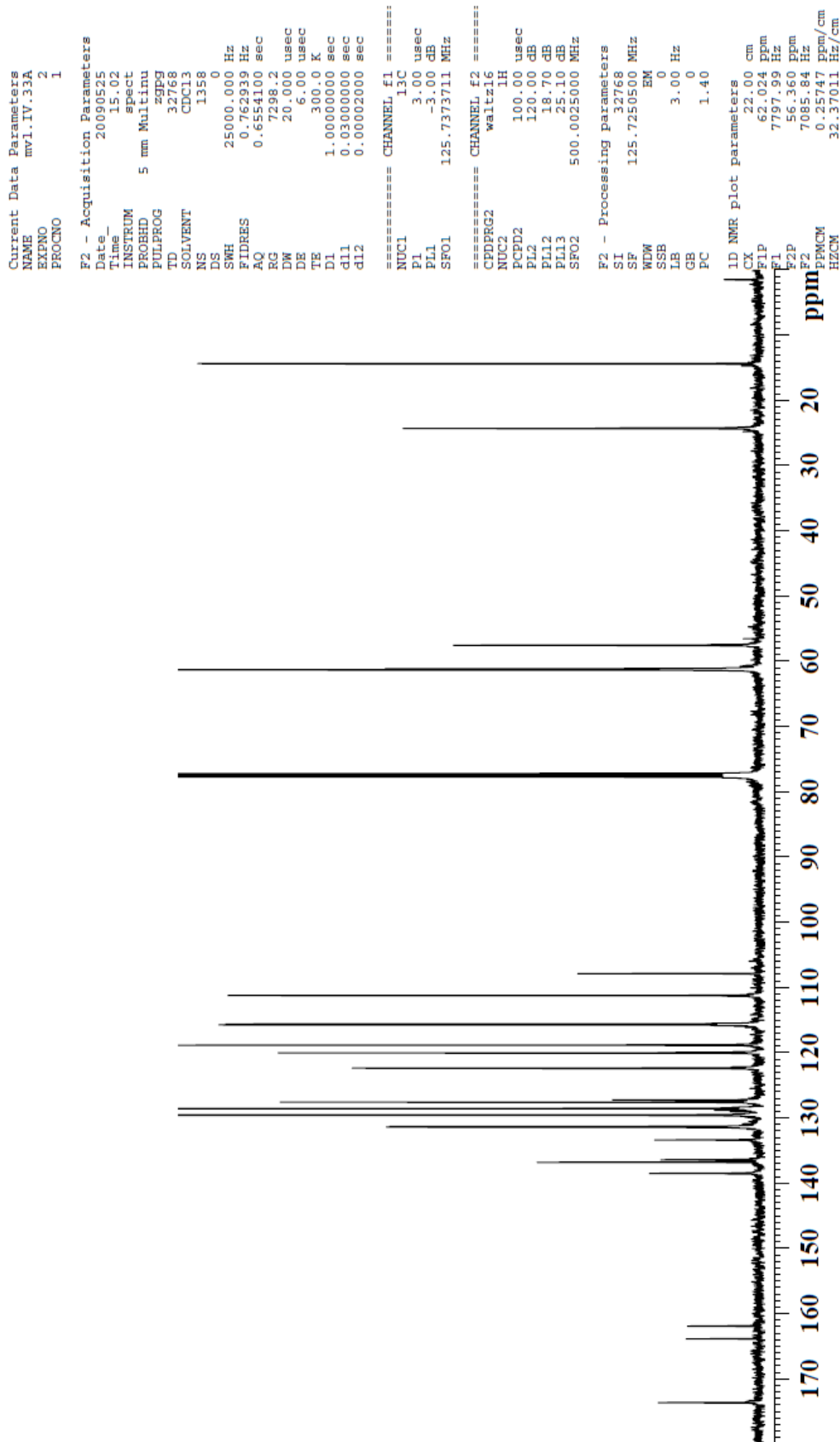
===== CHANNEL f1 =====
NUC1       1H
P1         6.00 usec
PL1        3.00 dB
SFO1       500.0030000 MHz

F2 - Processing parameters
SI         32768
SF         500.0000000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.20

1D NMR plot parameters
CX         20.00 cm
FIP        3.599 ppm
F1         1799.46 Hz
F2P        1.005 ppm
F2         502.32 Hz
PPMCM      0.12971 ppm/cm
HZCM       64.85693 Hz/cm
  
```



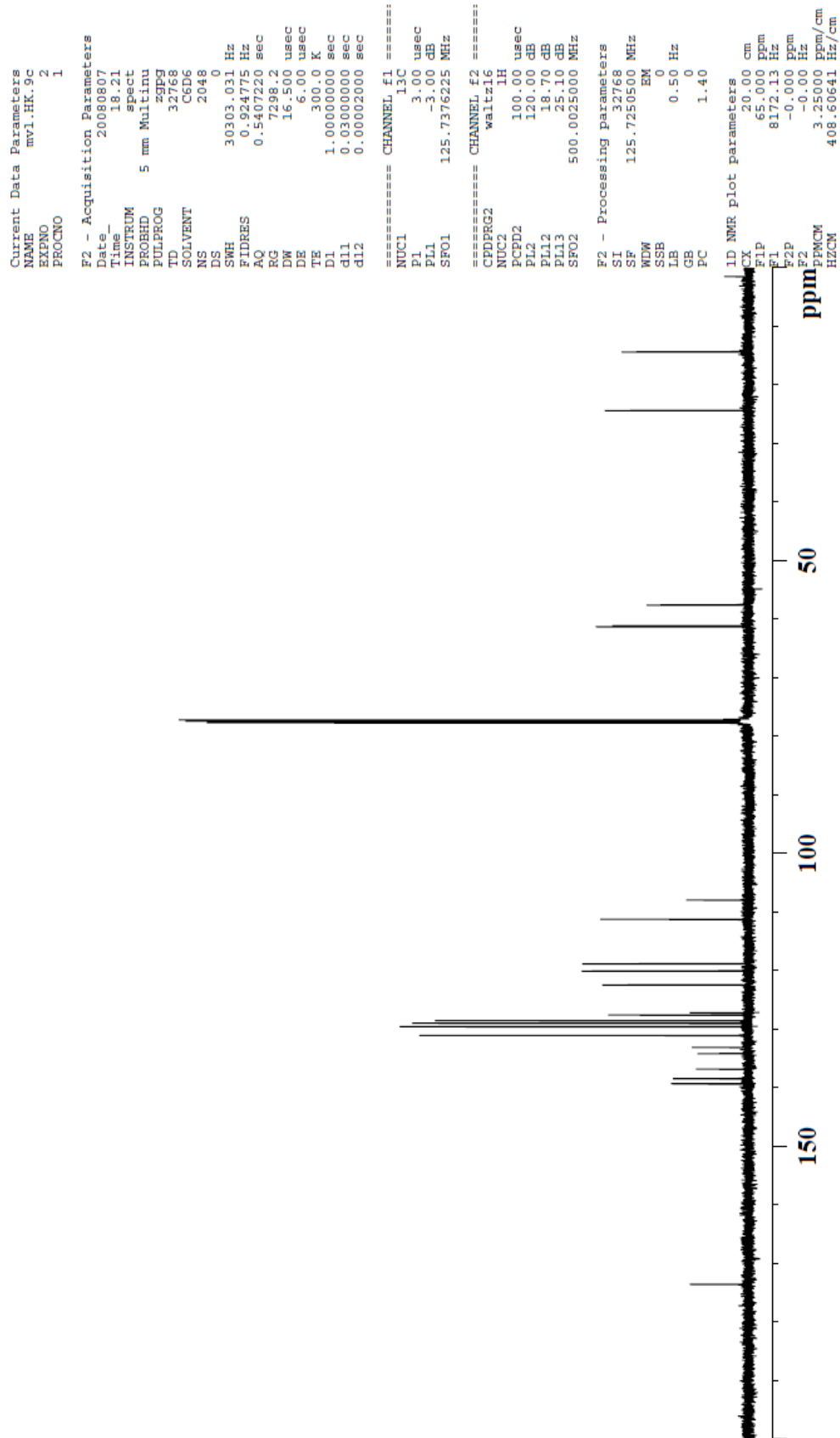
carbon spectrum



proton spectrum



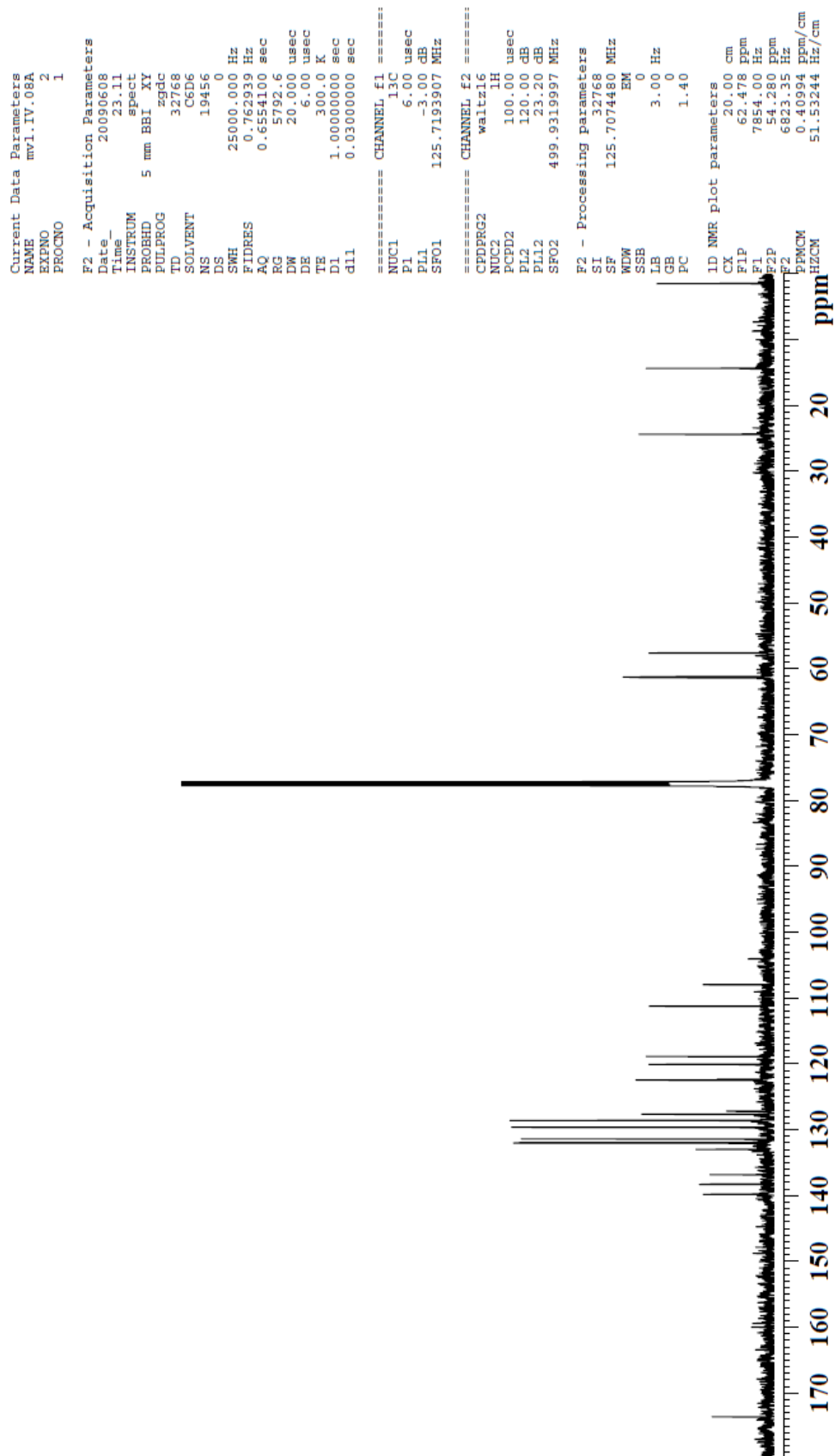
carbon spectrum



proton spectrum

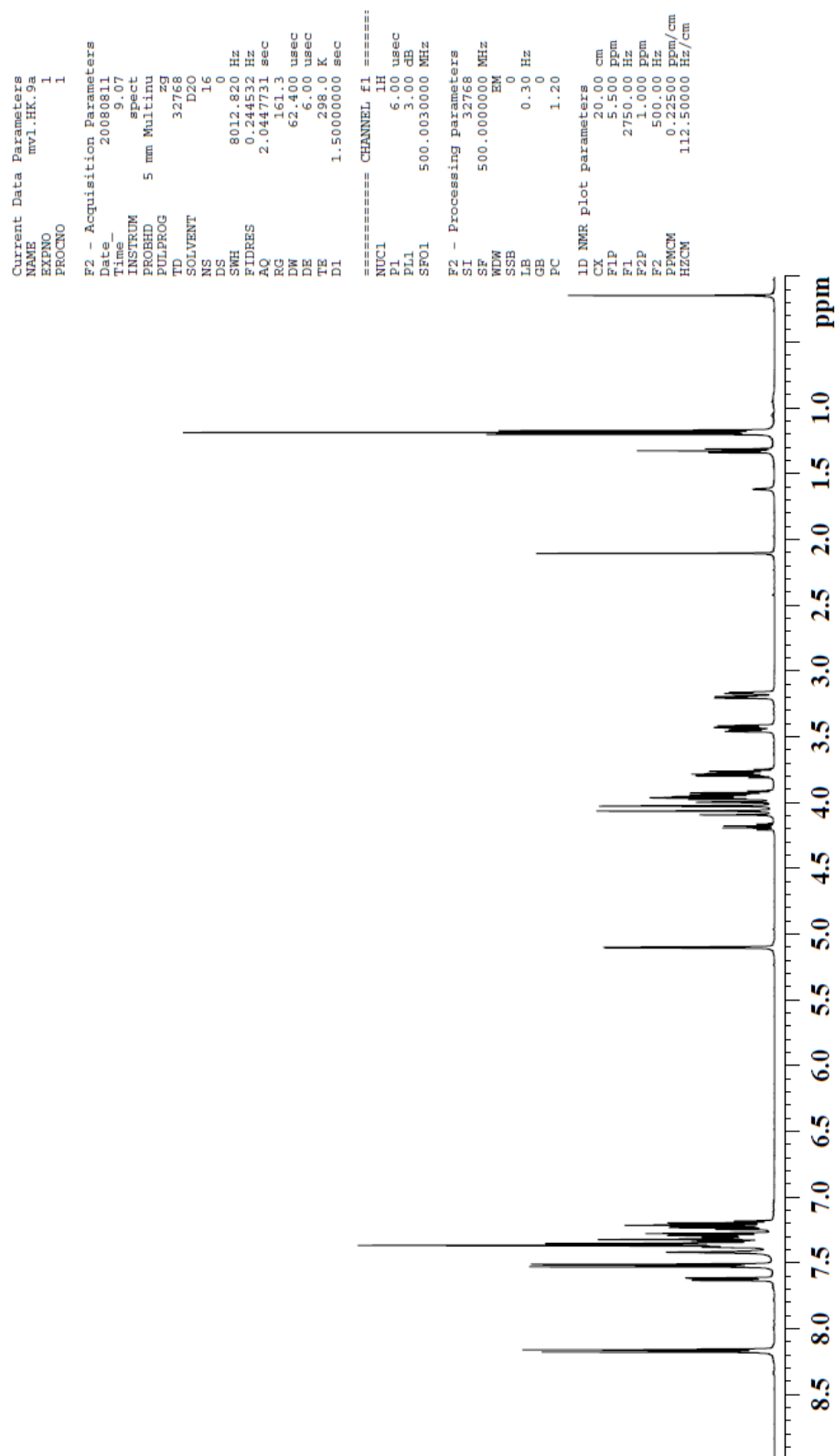


carbon spectrum

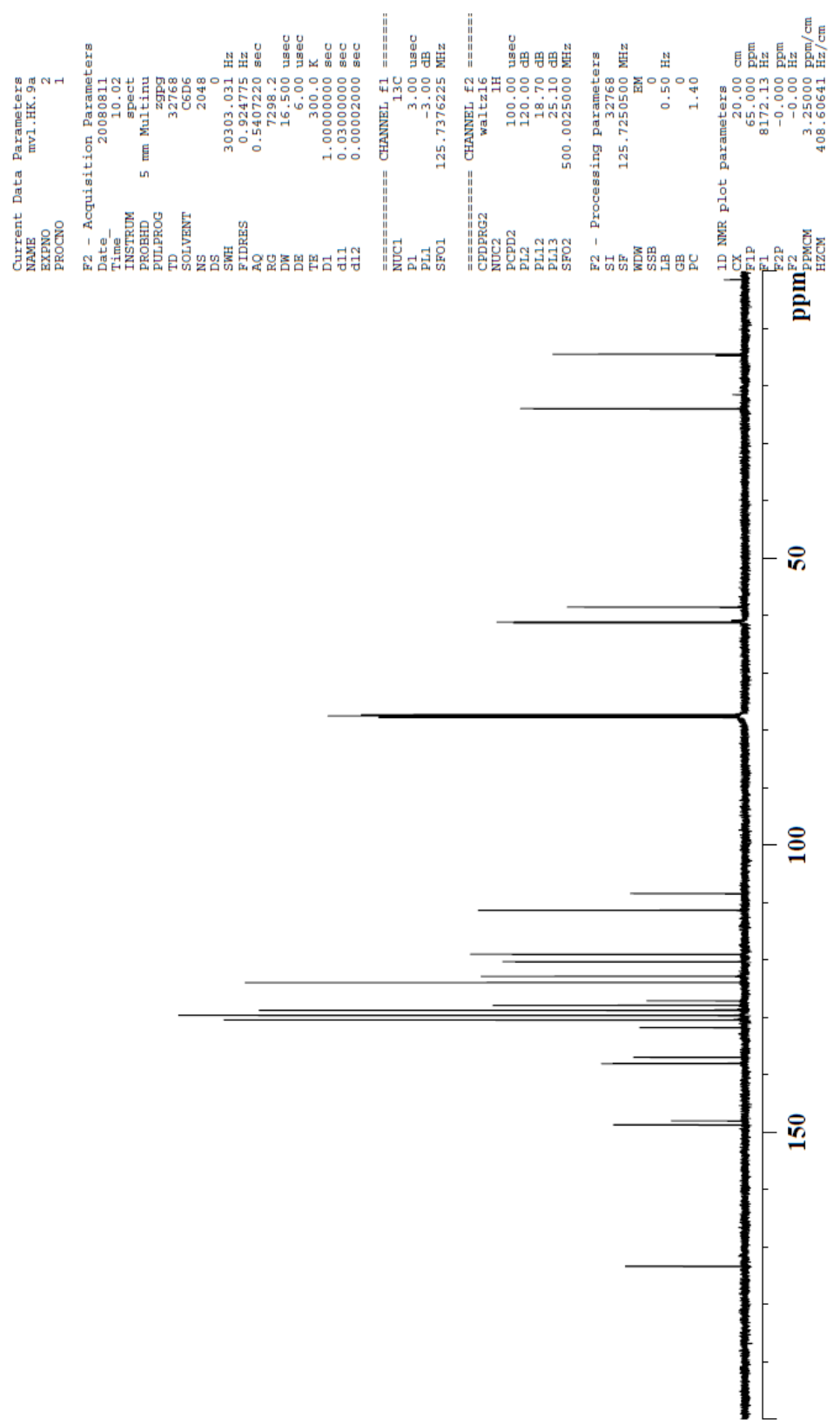


NMR spectra for Compound **7h**

proton spectrum

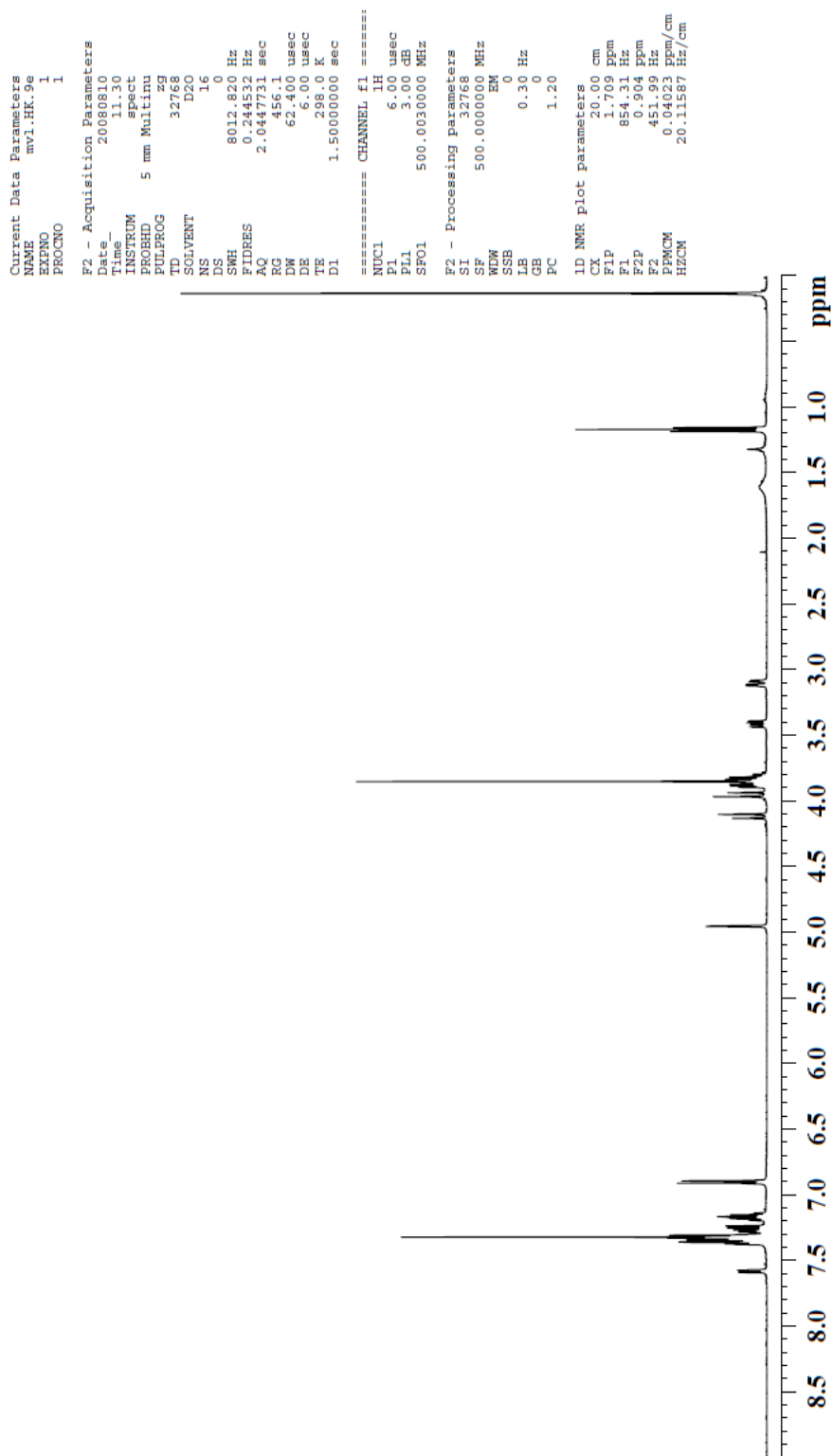


carbon spectrum

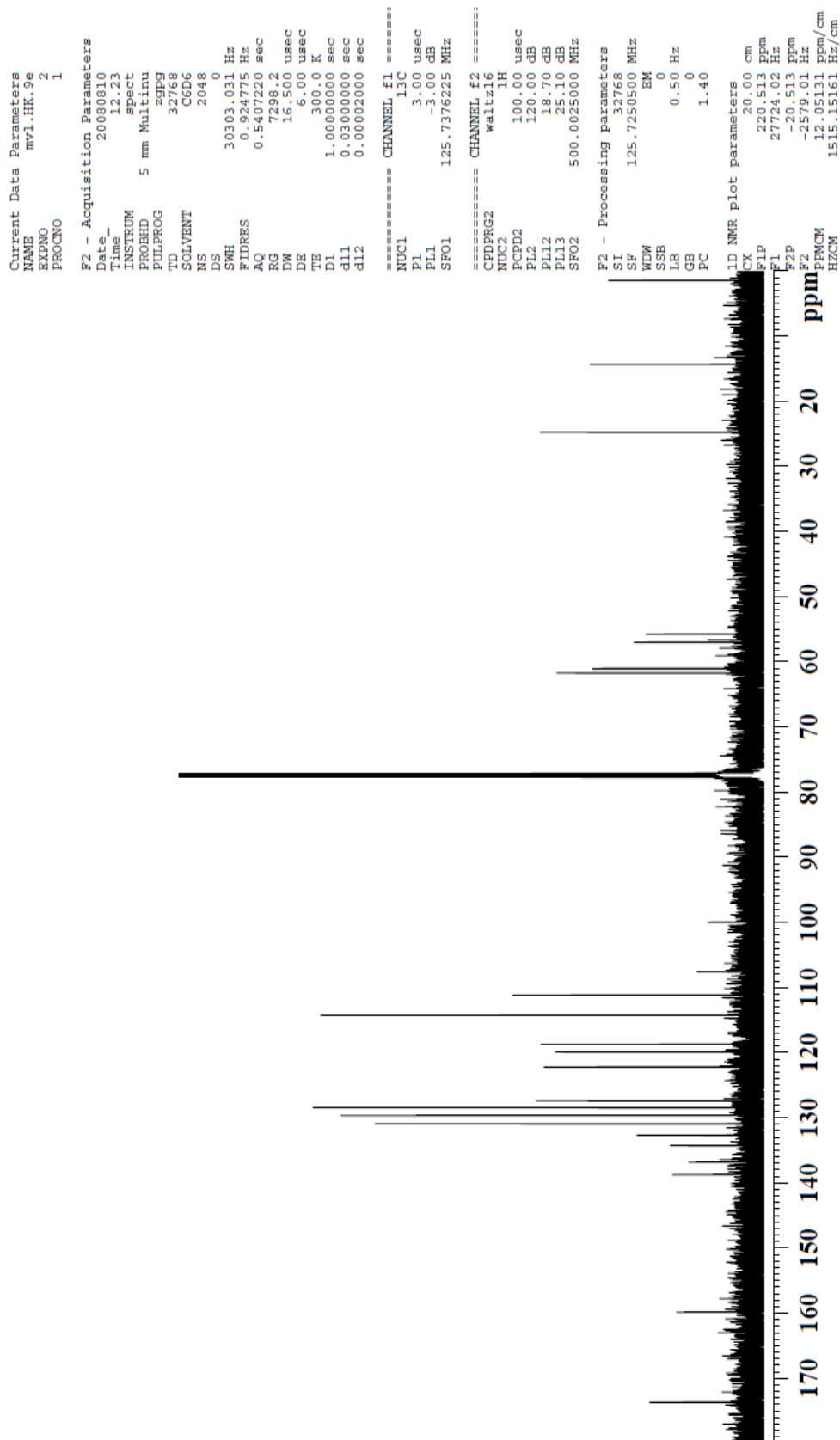


NMR spectra for Compound **7i**

proton spectrum



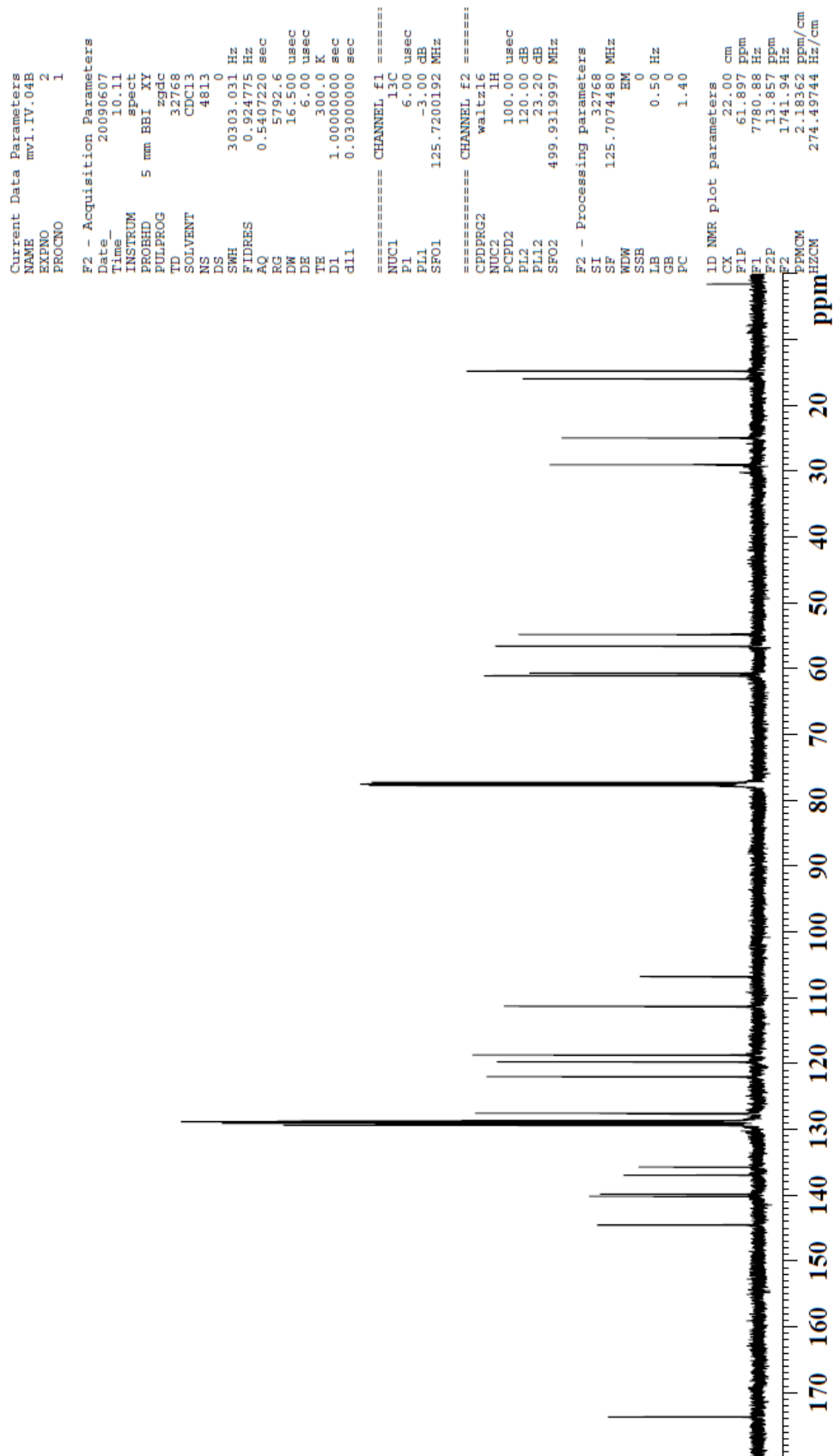
carbon spectrum



proton spectrum

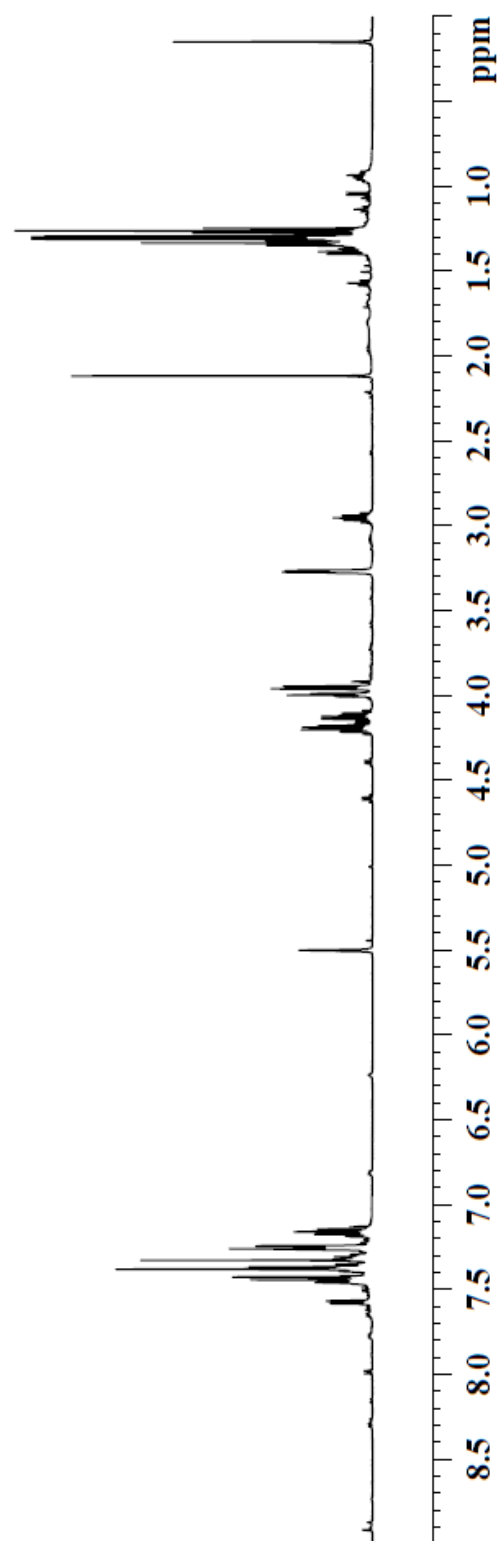


carbon spectrum

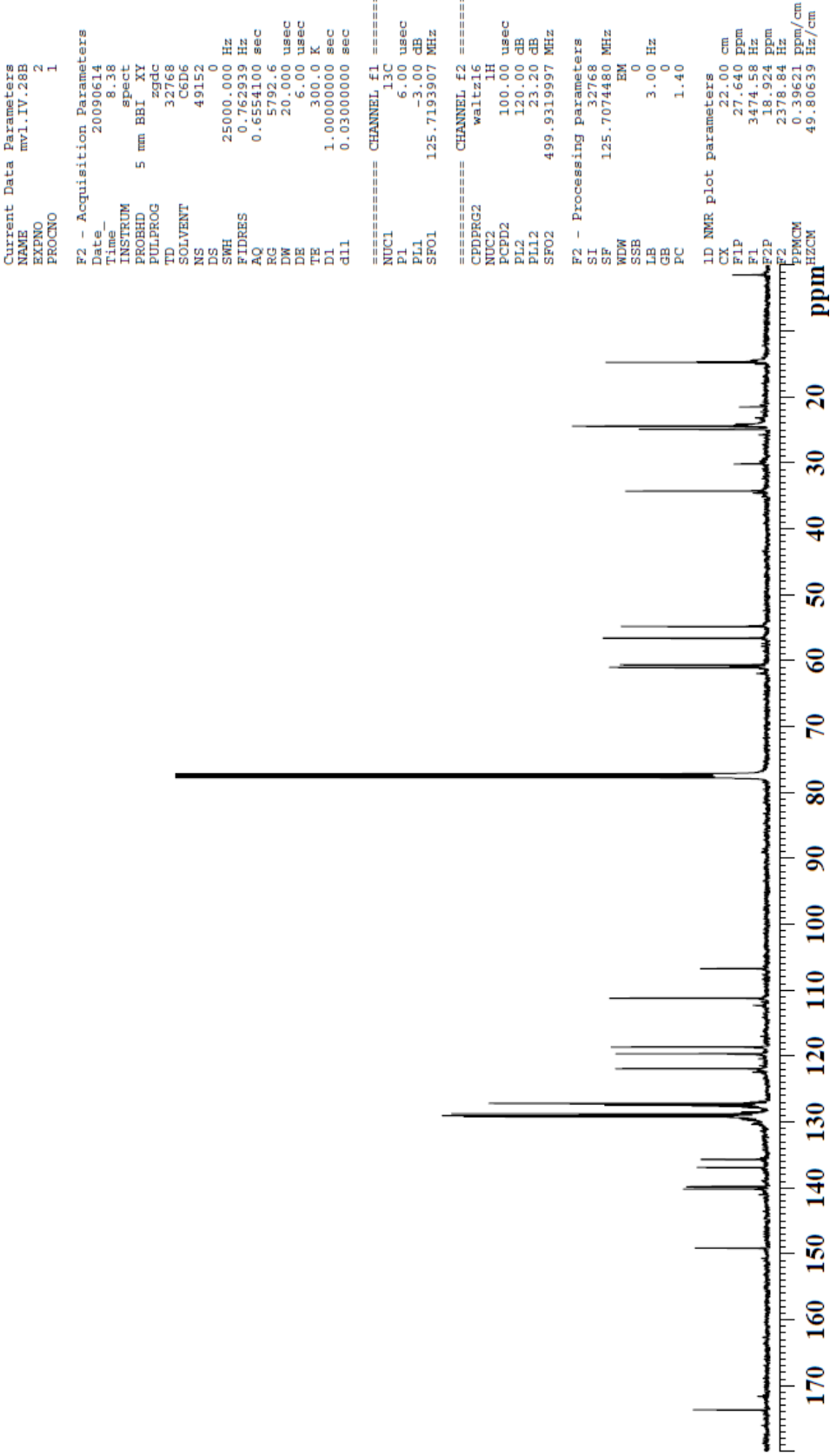


NMR spectra for Compound **8b**

proton spectrum

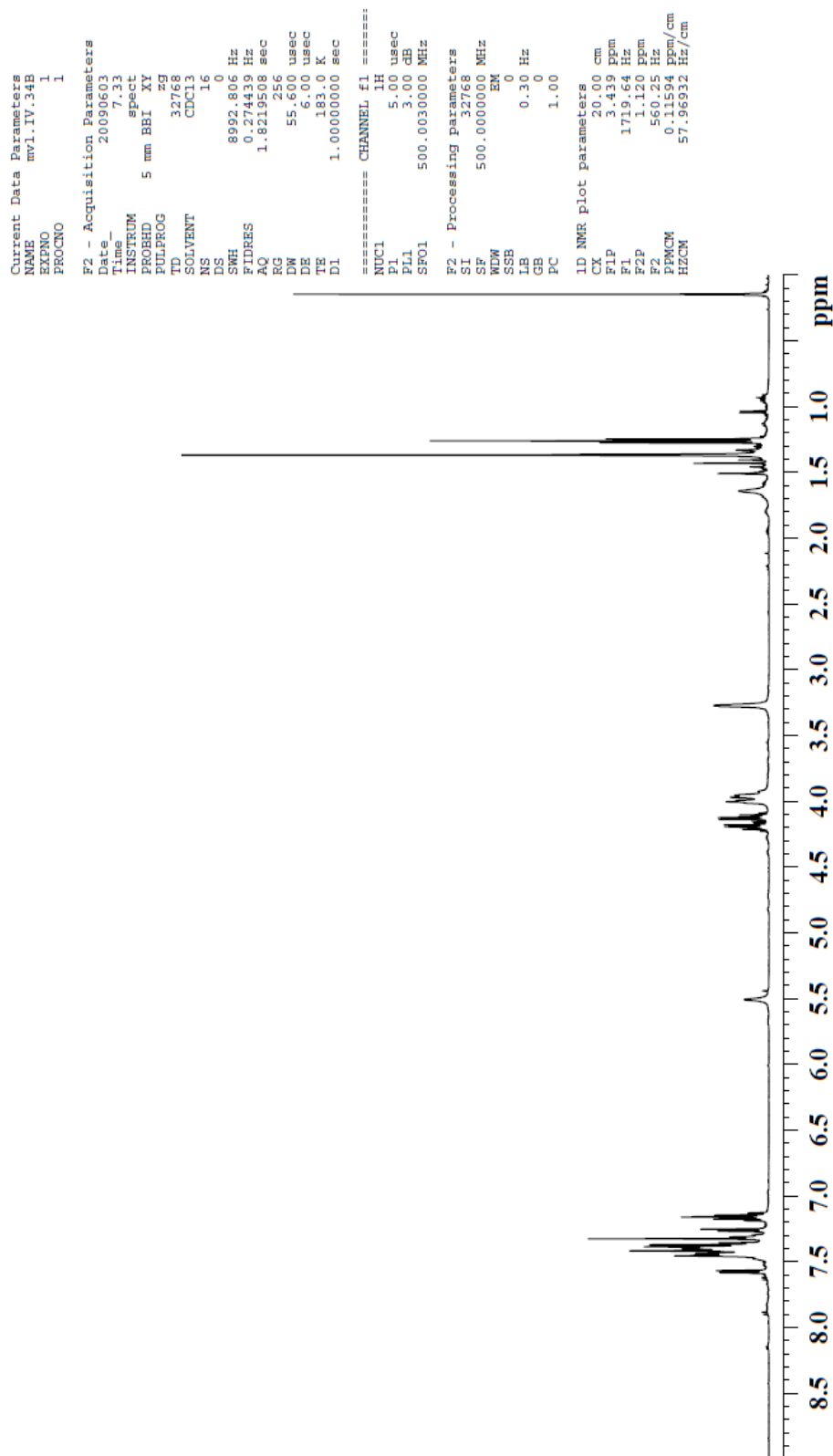


carbon spectrum

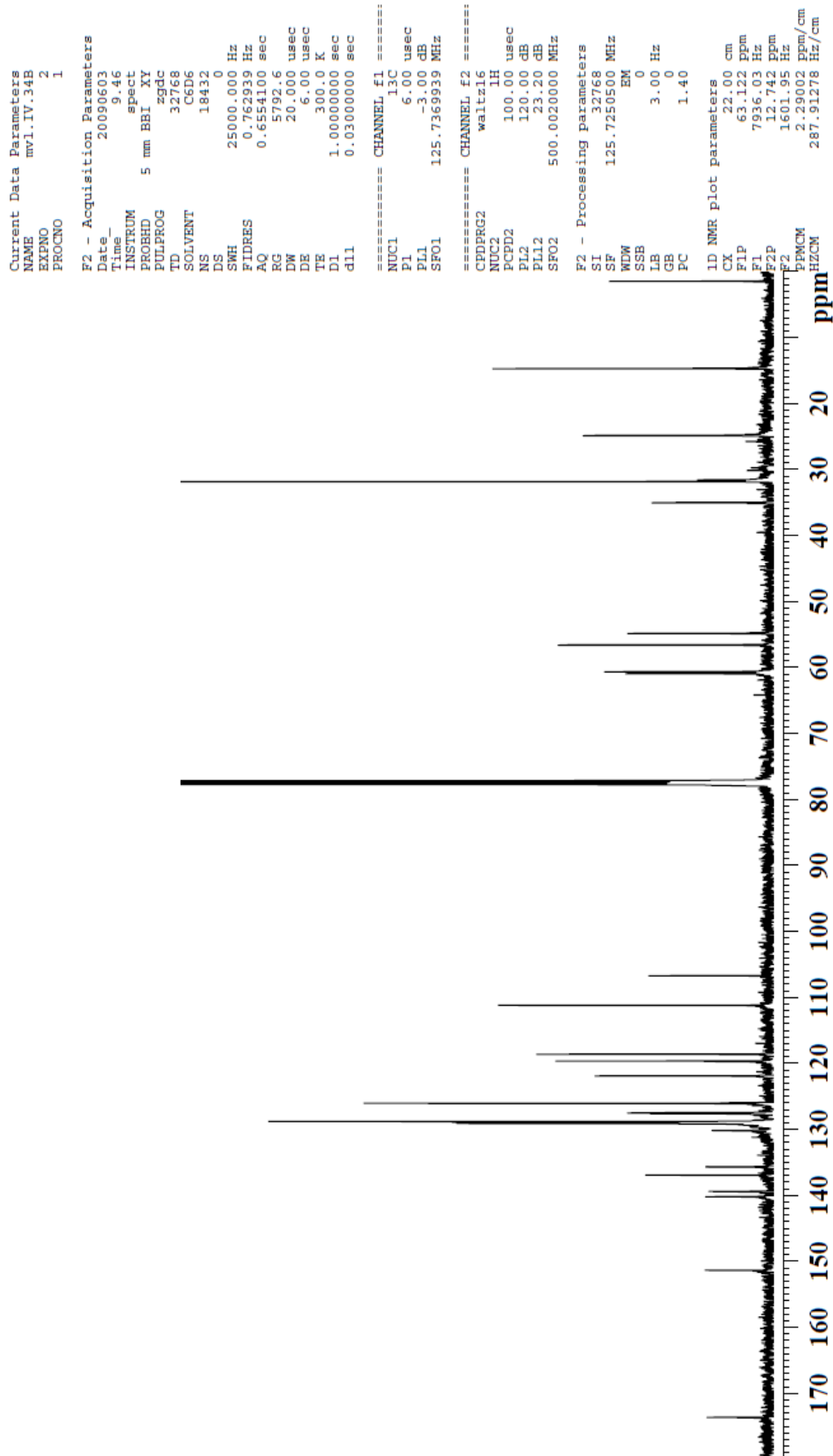


NMR spectra for Compound **8c**

proton spectrum



carbon spectrum



NMR spectra for Compound **8d**

proton spectrum

```

Current Data Parameters
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PROCNO    1

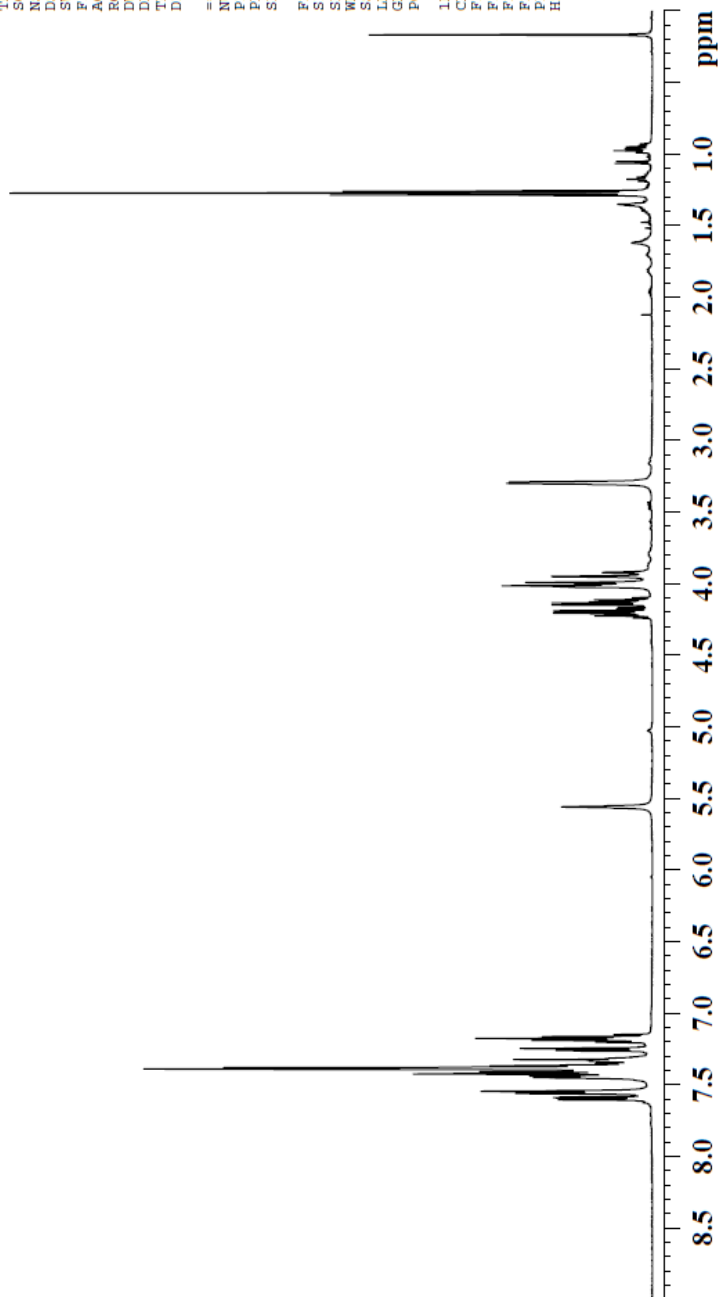
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PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         16
DS         0
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG          80.6
DM         62.400 usec
DE         6.00 usec
TE         298.0 K
D1         1.5000000 sec

===== CHANNEL f1 =====
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P1         6.00 usec
PL1        3.00 dB
SFO1       500.0030000 MHz

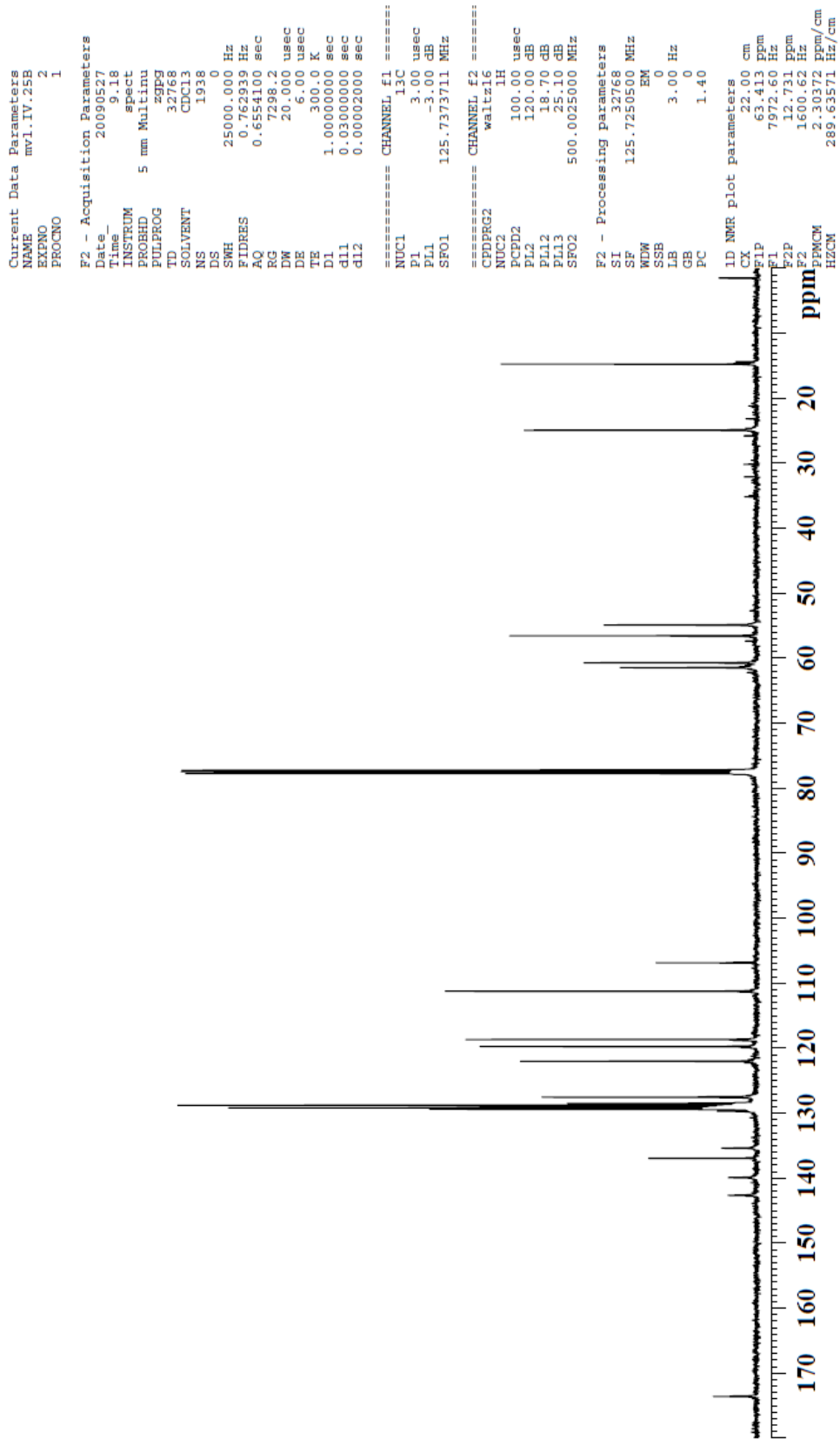
F2 - Processing parameters
SI         32768
SF         500.0000000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.20

1D NMR plot parameters
CX         20.00 cm
FLP        3.470 Ppm
F1         1735.06 Hz
F2P        1.115 Ppm
F2         557.52 Hz
FREQM      0.11175 Ppm/cm
HZCN       58.87720 Hz/cm

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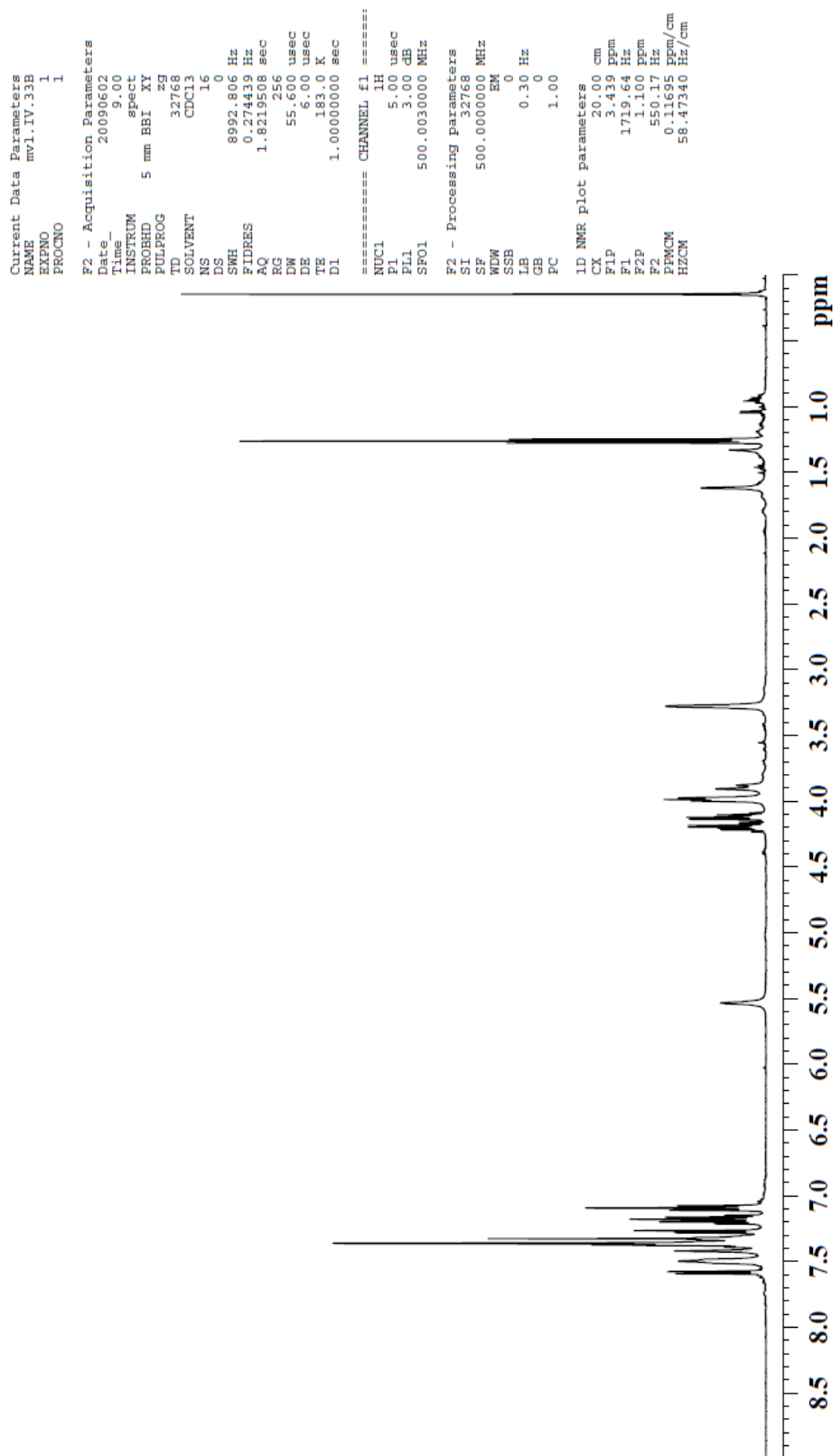


carbon spectrum

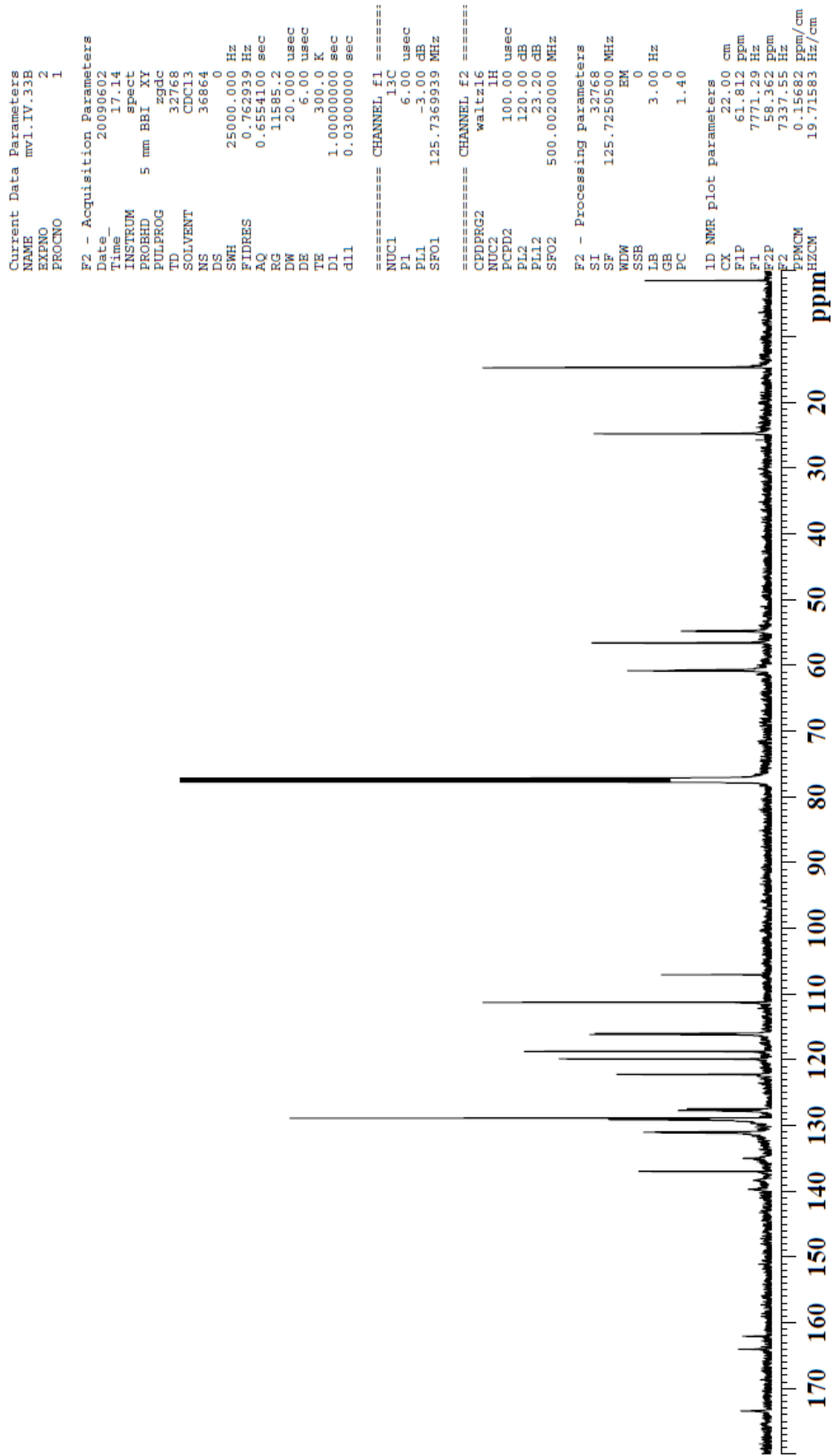


NMR spectra for Compound **8e**

proton spectrum

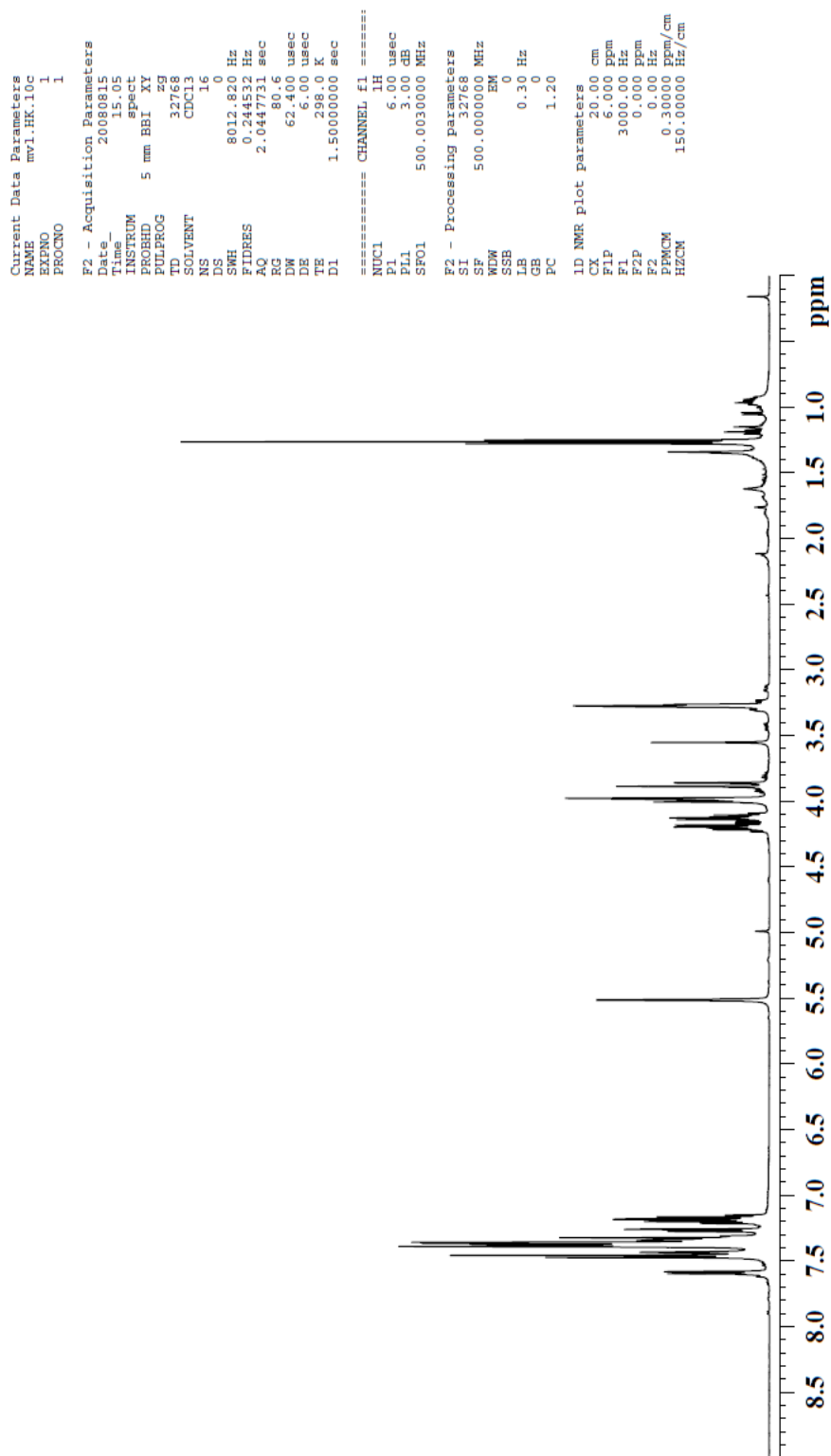


carbon spectrum

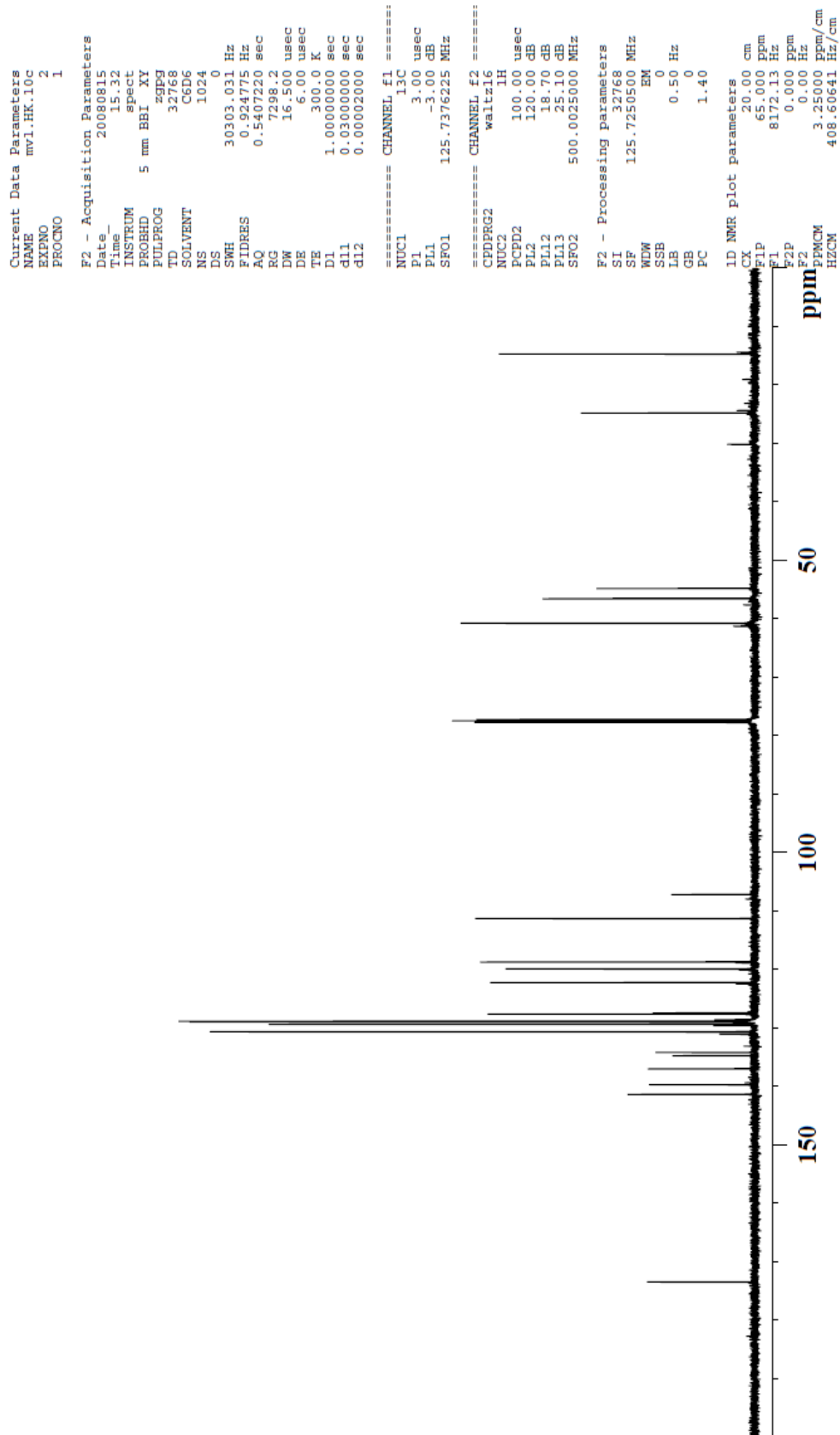


NMR spectra for Compound **8f**

proton spectrum



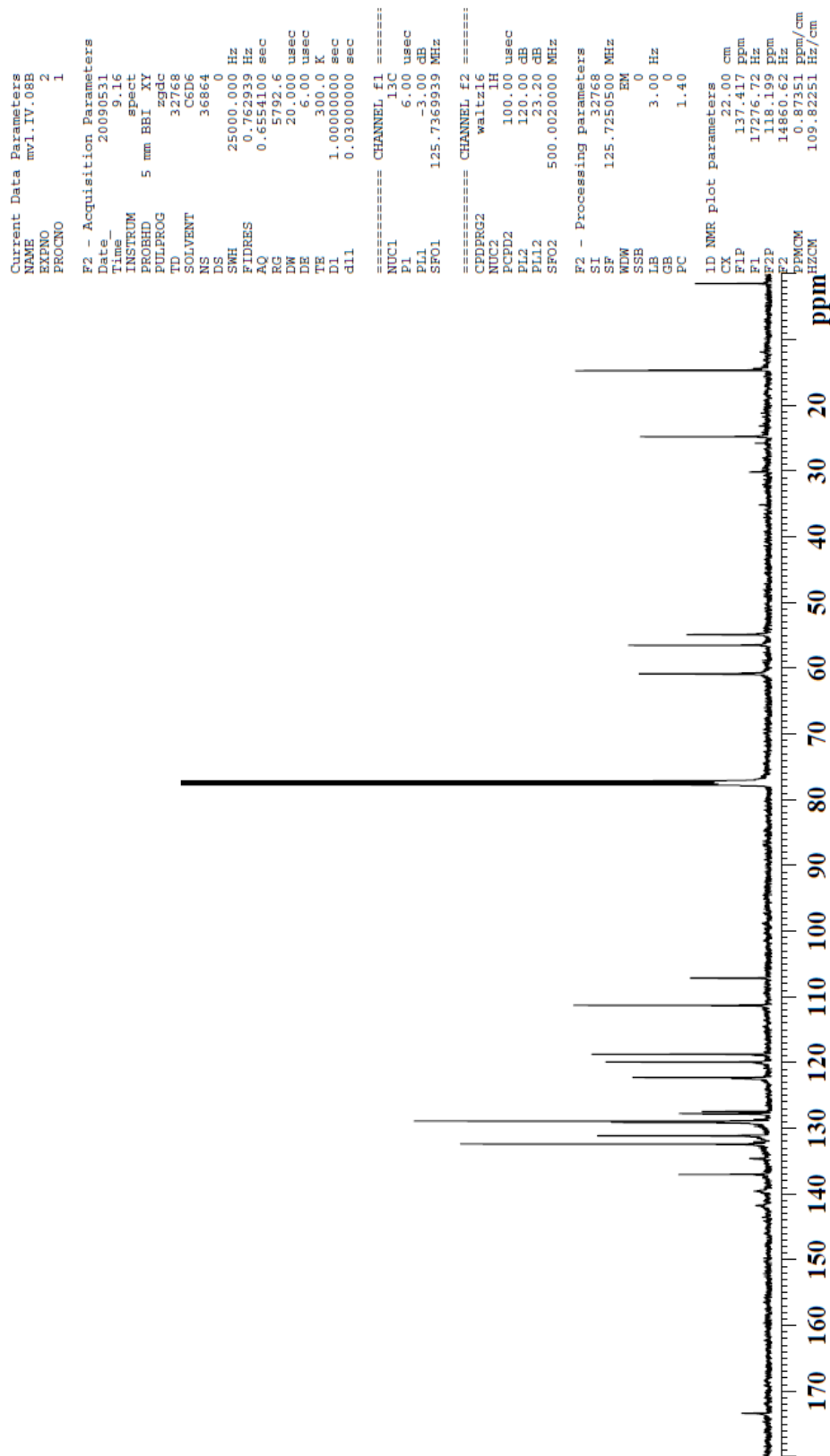
carbon spectrum



proton spectrum



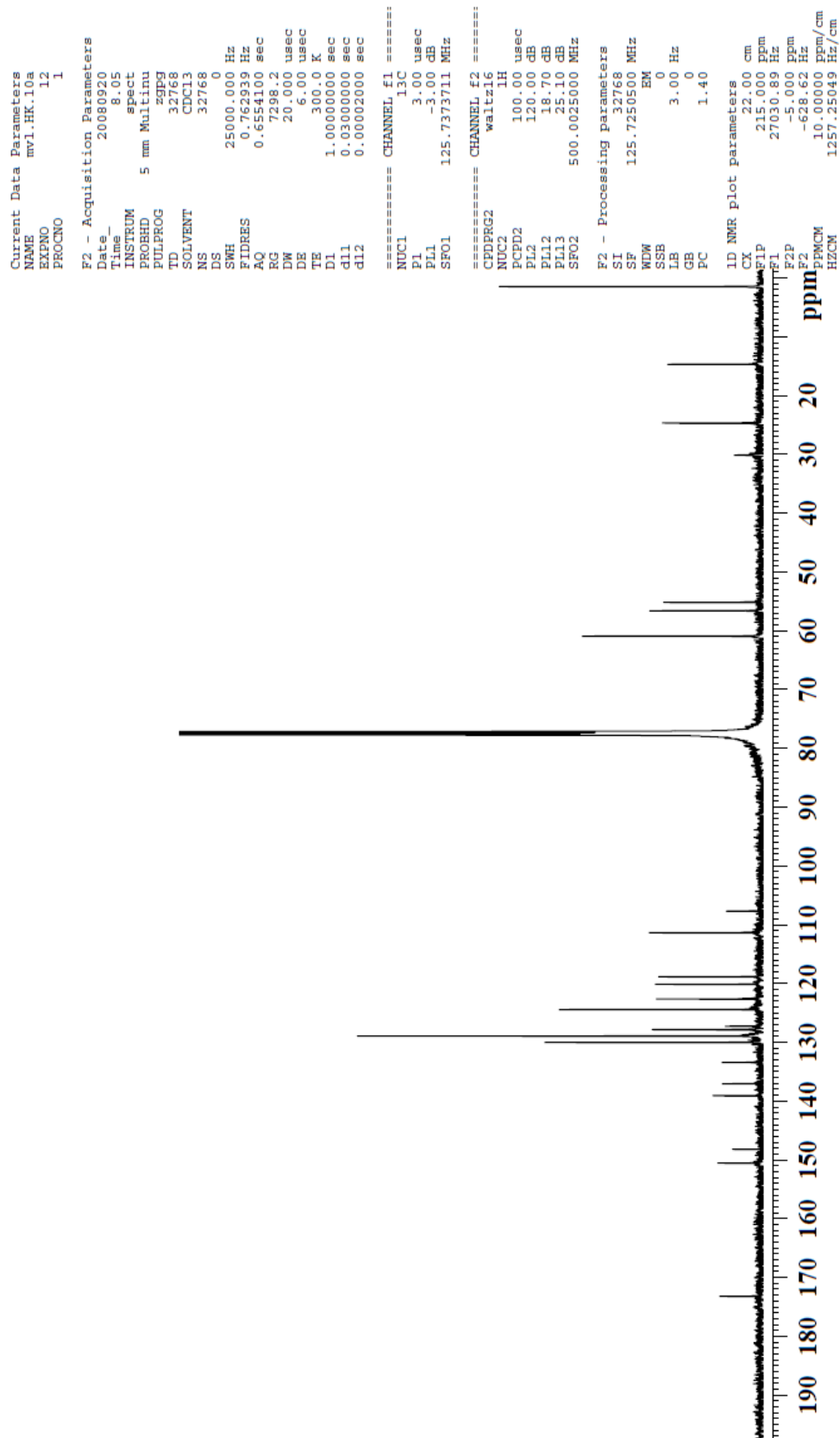
carbon spectrum



proton spectrum

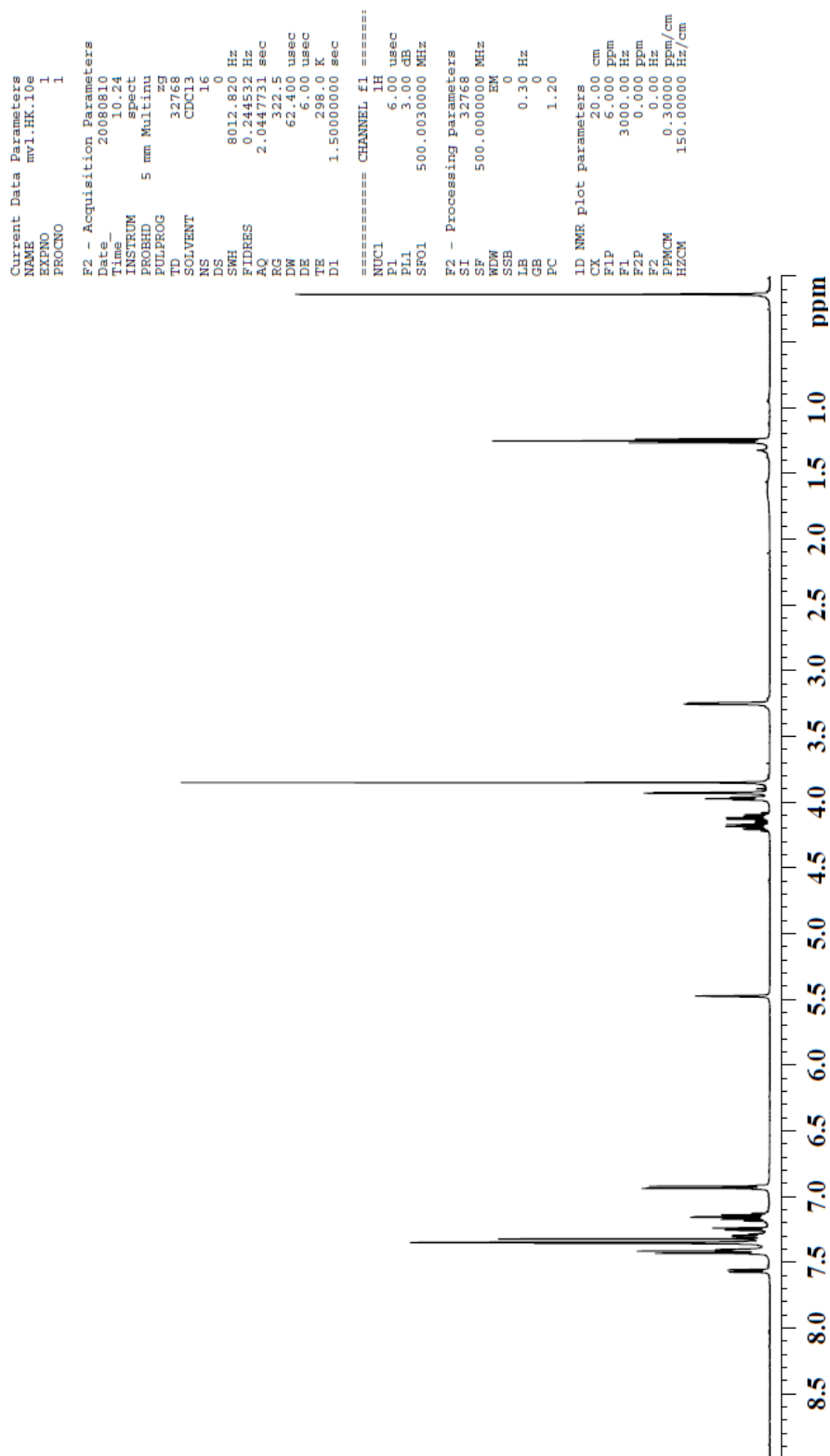


carbon spectrum



NMR spectra for Compound **8i**

proton spectrum



carbon spectrum

