Supporting Information

A Mild and One-pot Transformation of Nitroalkanes to Ketones or Aldehydes via a Visible-Light Photocatalysis–Hydrolysis Sequence

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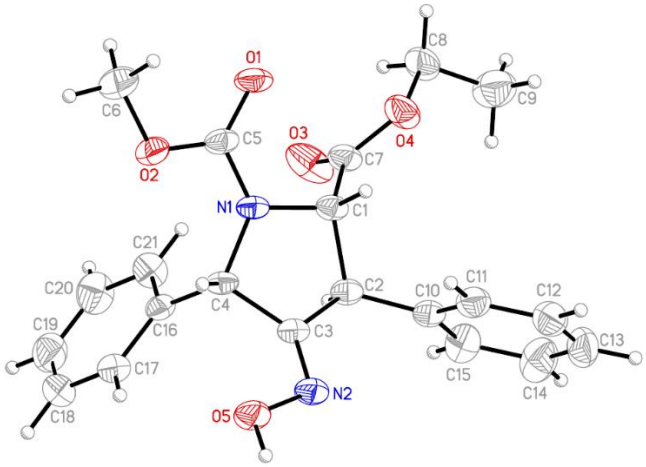
SUPPORTING INFORMATION:

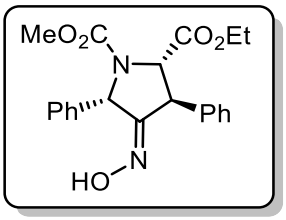
Contents:

Procedure for recrystallization of 2j

Compound **2j** (~5 mg) in a screw-capped vial (4 mL vial) was dissolved in EtOAc (0.5 mL). The vial was placed in another vial (20 mL vial) filled with n-hexane (10 mL). The 20 mL vial was closed gently with a screw cap and stands it for a few days until the formation of the crystals. The crystals formed were subjected to single-crystal X-ray analysis.



Thermal ellipsoids draw at the 50% probability level



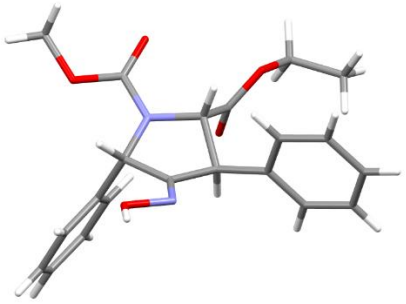


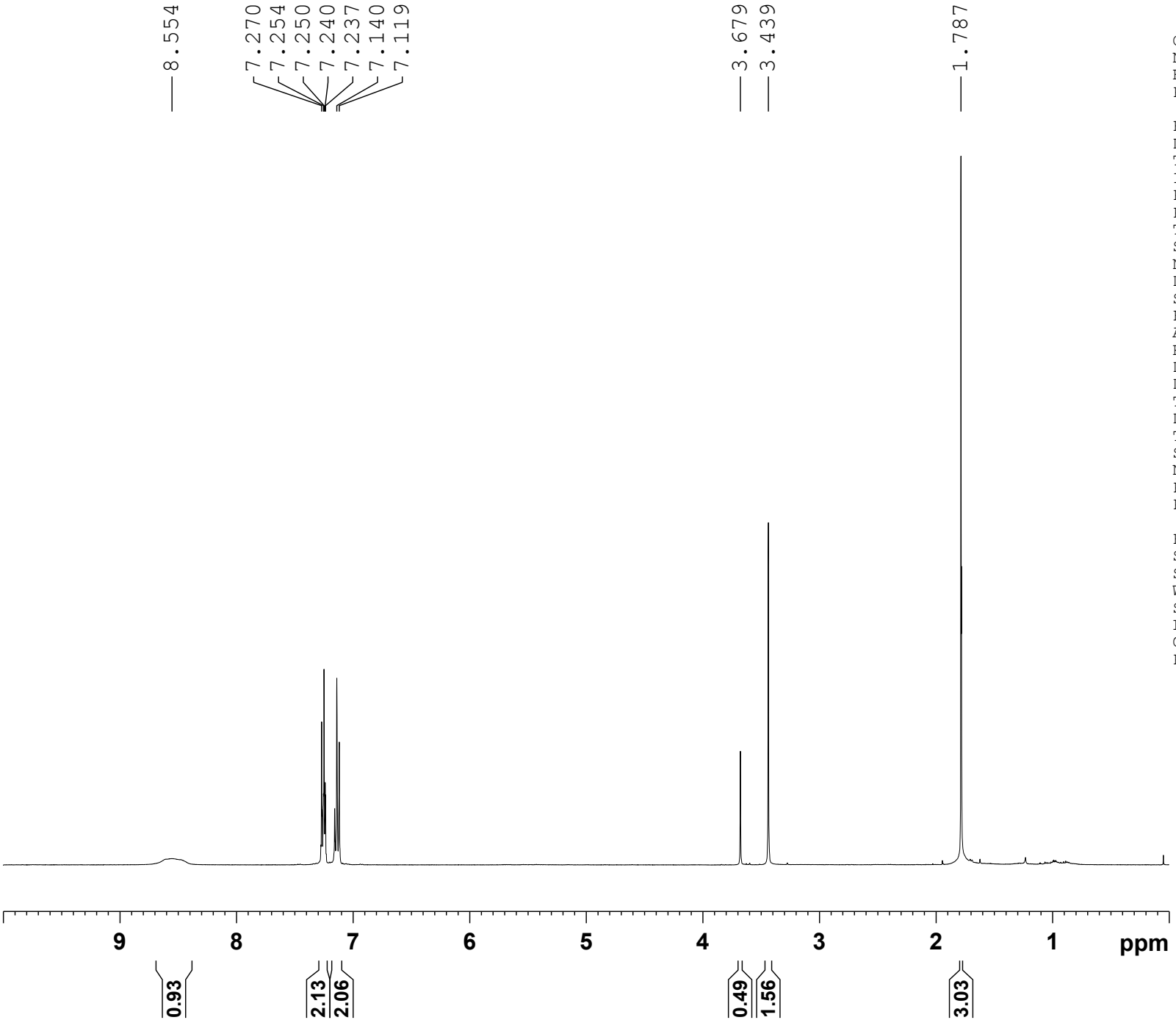
Figure S1. ORTEP and Stereo plots for X-ray crystal structures of **2j** (**ic21150**).

CCDC 2125600 contains the supplementary crystallographic data for **2j** (**ic21150**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S1. Crystal data and structure refinement for **2j** (**ic21150**).

Identification code	ic21150	
Empirical formula	C21 H22 N2 O5	
Formula weight	382.40	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 5.73510(10) Å	α= 90°.
	b = 41.9722(12) Å	β= 107.6440(10)°.
	c = 8.3858(2) Å	γ = 90°.
Volume	1923.63(8) Å^3	
Z	4	
Density (calculated)	1.320 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	808	
Crystal size	0.461 x 0.190 x 0.093 mm^3	
Theta range for data collection	2.595 to 27.498°.	
Index ranges	-6<=h<=7, -54<=k<=54, -10<=l<=10	
Reflections collected	22898	
Independent reflections	4406 [R(int) = 0.0358]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9595 and 0.8936	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4406 / 0 / 256	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.1197	
R indices (all data)	R1 = 0.0602, wR2 = 0.1250	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.313 and -0.209 e.Å^{-3}	

1H NMR (CDCl3, 400 MHz) of compound **2a** (E/Z isomers)

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PROCNO                      1

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TD                     32768
SOLVENT                CDCl3
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DS                         0
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FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                    177.78
DW                    62.400 usec
DE                    16.43 usec
TE                    295.0 K
D1                2.00000000 sec
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NUC1                       1H
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PLW1            12.69999981 W

F2 - Processing parameters
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WDW                        EM
SSB       0
LB        0 Hz
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PC                      1.00
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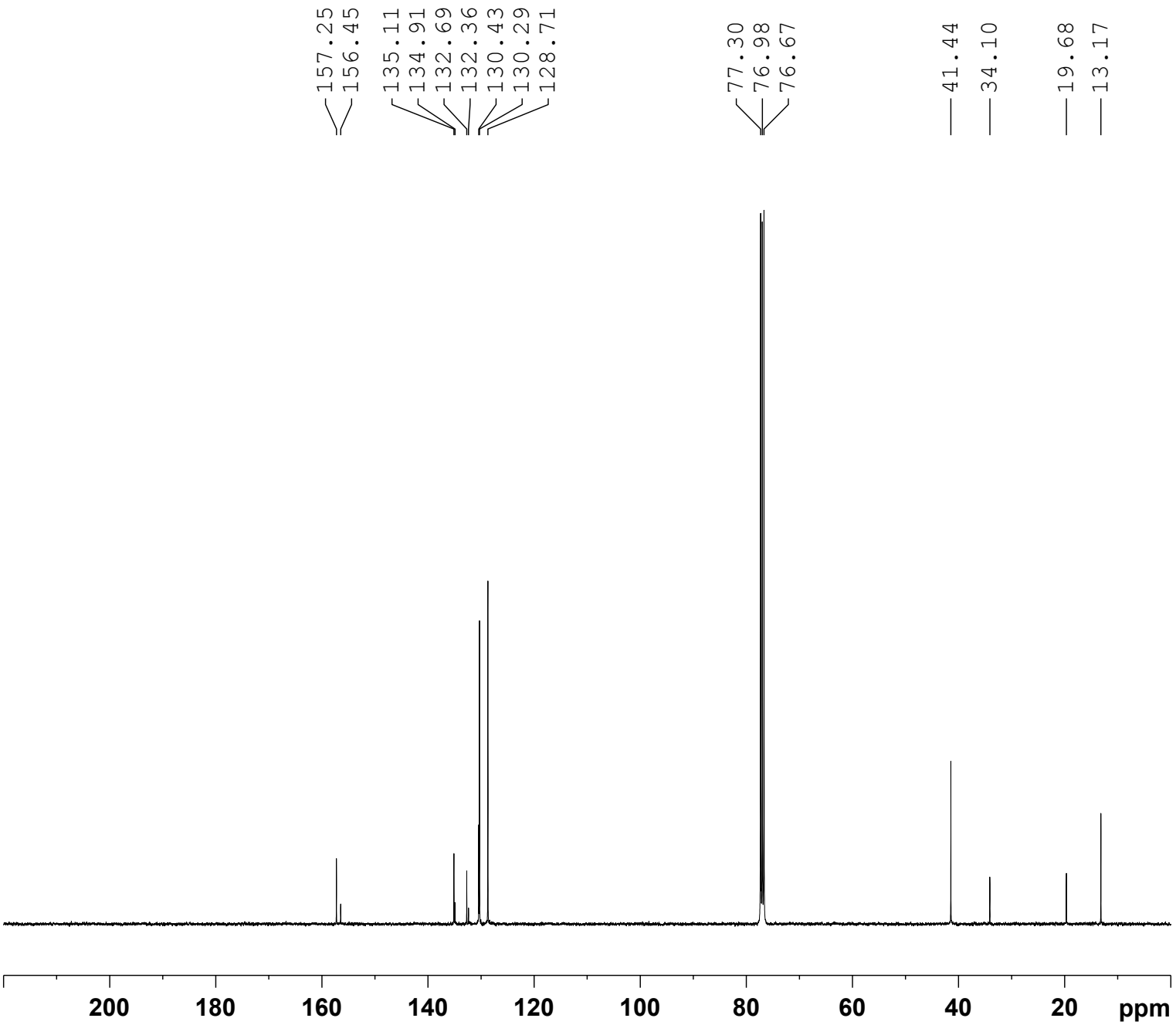
13C NMR (CDCl3, 100 MHz) of compound **2a** (E/Z isomers)

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PROCNO                     1

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TD                    32768
SOLVENT               CDCl3
NS                     4096
DS                        0
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                 0.6815744 sec
RG                    210.28
DW                    20.800 usec
DE                     6.50 usec
TE                    296.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1
SFO1           100.6233329 MHz
NUC1                    13C
P1                    10.50 usec
PLW1           44.09999847 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2                 90.00 usec
PLW2           14.30000019 W
PLW12           0.37118000 W
PLW13           0.18640999 W

F2 - Processing parameters
SI                    32768
SF             100.6127732 MHz
WDW                      EM
SSB       0
LB                     2.00 Hz
GB        0
PC                     1.00
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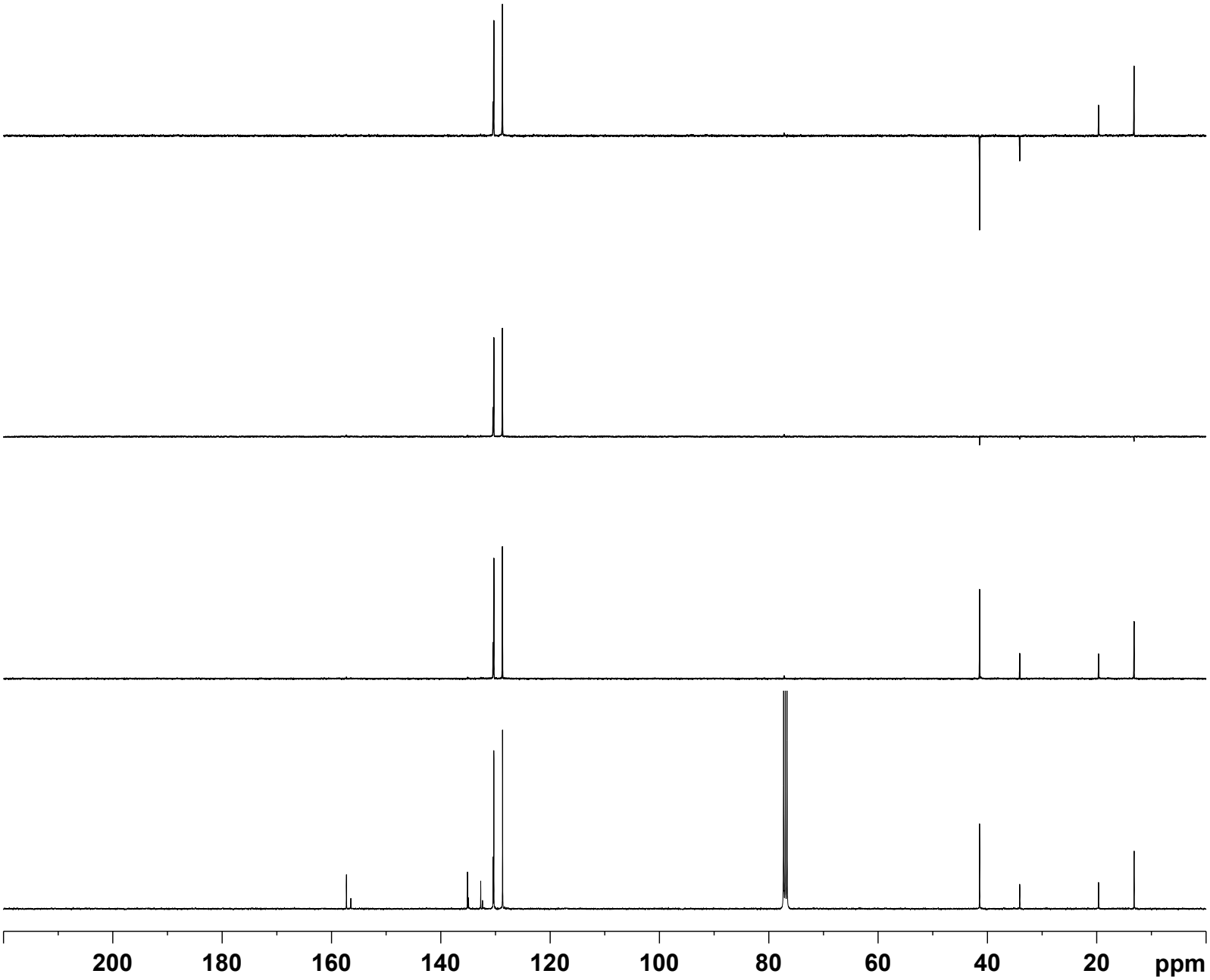
DEPT of compound **2a** (E/Z isomers)

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Current Data Parameters
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EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210129
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INSTRUM           spect
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PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4096
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1                10.50 usec
PLW1         44.09999847 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2         14.30000019 W
PLW12         0.37118000 W
PLW13         0.18640999 W

F2 - Processing parameters
SI                32768
SF          100.6127732 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
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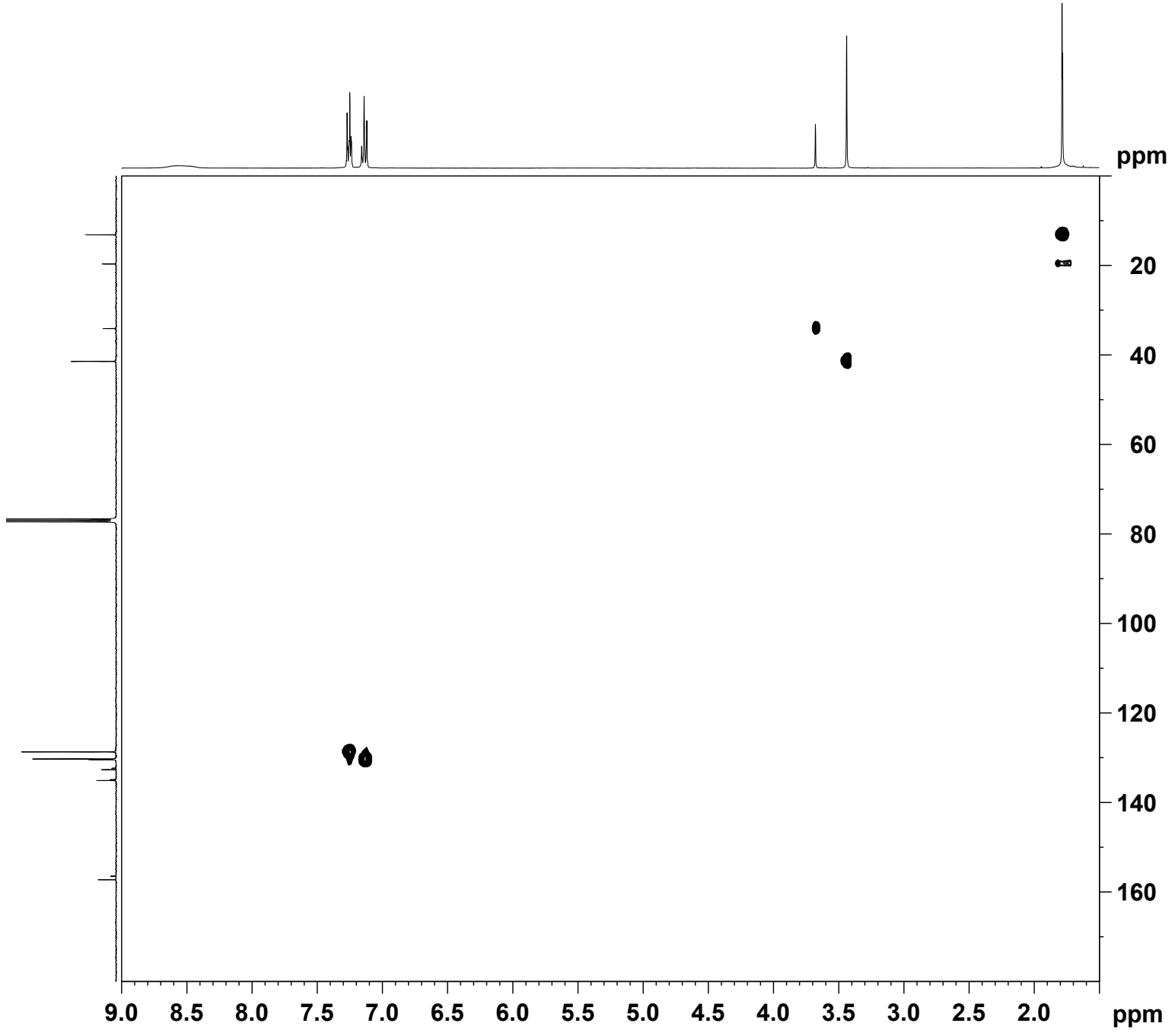
HSQC of compound **2a** (E/Z isomers)

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EXPNO                      6
PROCNO                     1

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PULPROG  hsqcetgpsisp2.2
TD                      2048
SOLVENT                CDCl3
NS                         4
DS                        16
SWH                 8012.820 Hz
FIDRES              7.825020 Hz
AQ                  0.1277952 sec
RG                    210.28
DW                    62.400 usec
DE                     6.50 usec
TE                    294.7 K
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CNST17              -0.5000000
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D1                  1.50000000 sec
D4                  0.00172414 sec
D11                 0.03000000 sec
D16                 0.00020000 sec
D24                 0.00086207 sec
IN0                 0.00002080 sec
TDav                       1
SFO1               400.1324008 MHz
NUC1                      1H
P1                     14.50 usec
P2                     29.00 usec
P28                  1000.00 usec
PLW1               12.69999981 W
SFO2               100.6233329 MHz
NUC2                      13C
CPDPRG[2                garp
P3                     10.50 usec
P14                   500.00 usec
P24                  2000.00 usec
PCPD2                  80.00 usec
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PLW2              44.00000000 W
PLW12              0.75796998 W
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SPOFFS7  0 Hz
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GPNAM[2]      SMSQ10.100
GPZ2                  20.10 %
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GPZ3                  11.00 %
GPNAM[4]      SMSQ10.100
GPZ4                  -5.00 %
P16                 1000.00 usec
P19                  600.00 usec

F1 - Acquisition parameters
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SFO1              100.6233 MHz
FIDRES         187.800476 Hz
SW                238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
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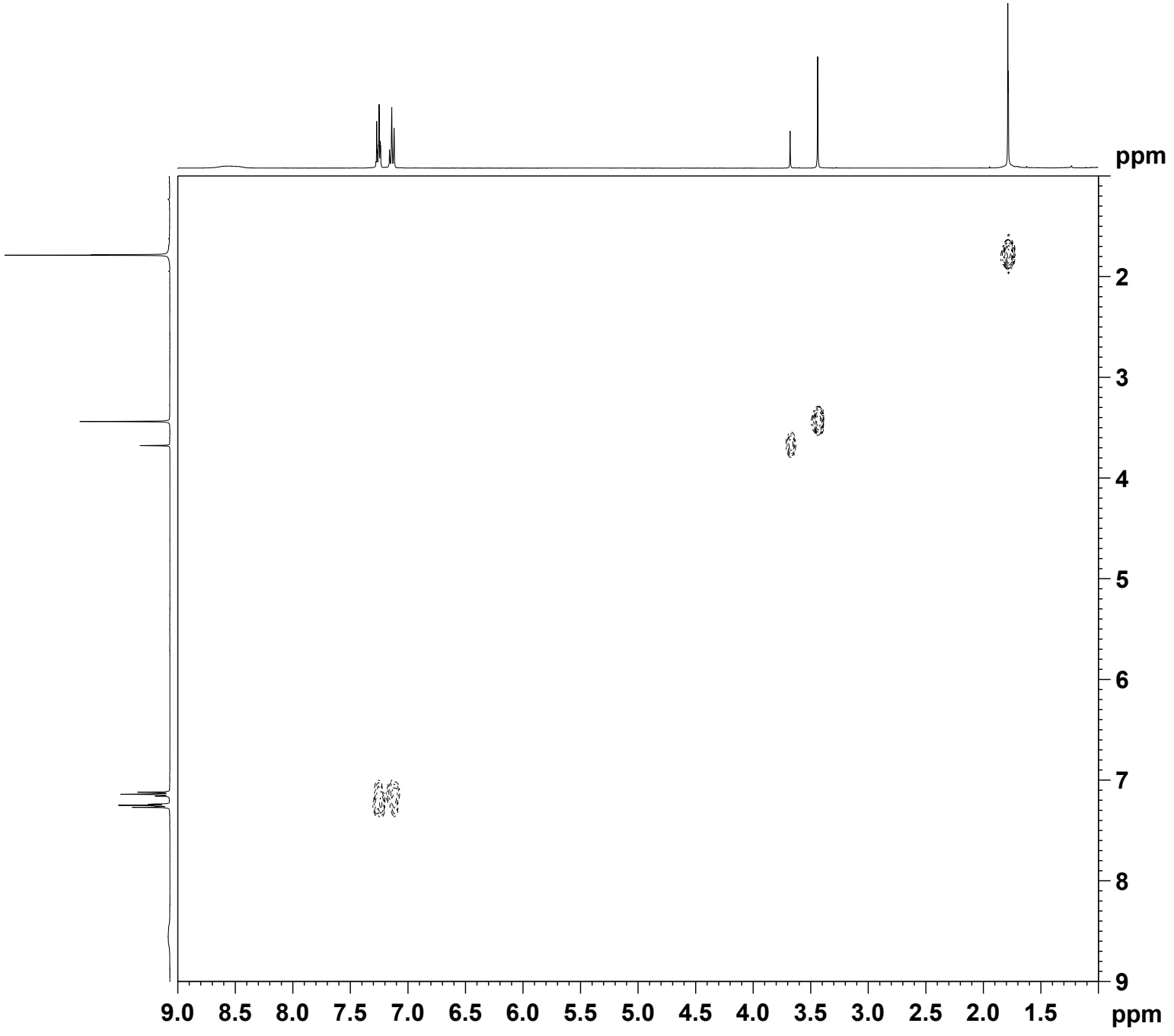
SF             400.1300176 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2         echo-antiecho
SF               100.6127732 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
```

COSY of compound **2a** (E/Z isomers)

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PROCNO                 1

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PULPROG       cosygpppqf
TD                  2048
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                294.6 K
D0             0.00000300 sec
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE               QF

F2 - Processing parameters
SI                  1024
SF           400.1300176 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300176 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
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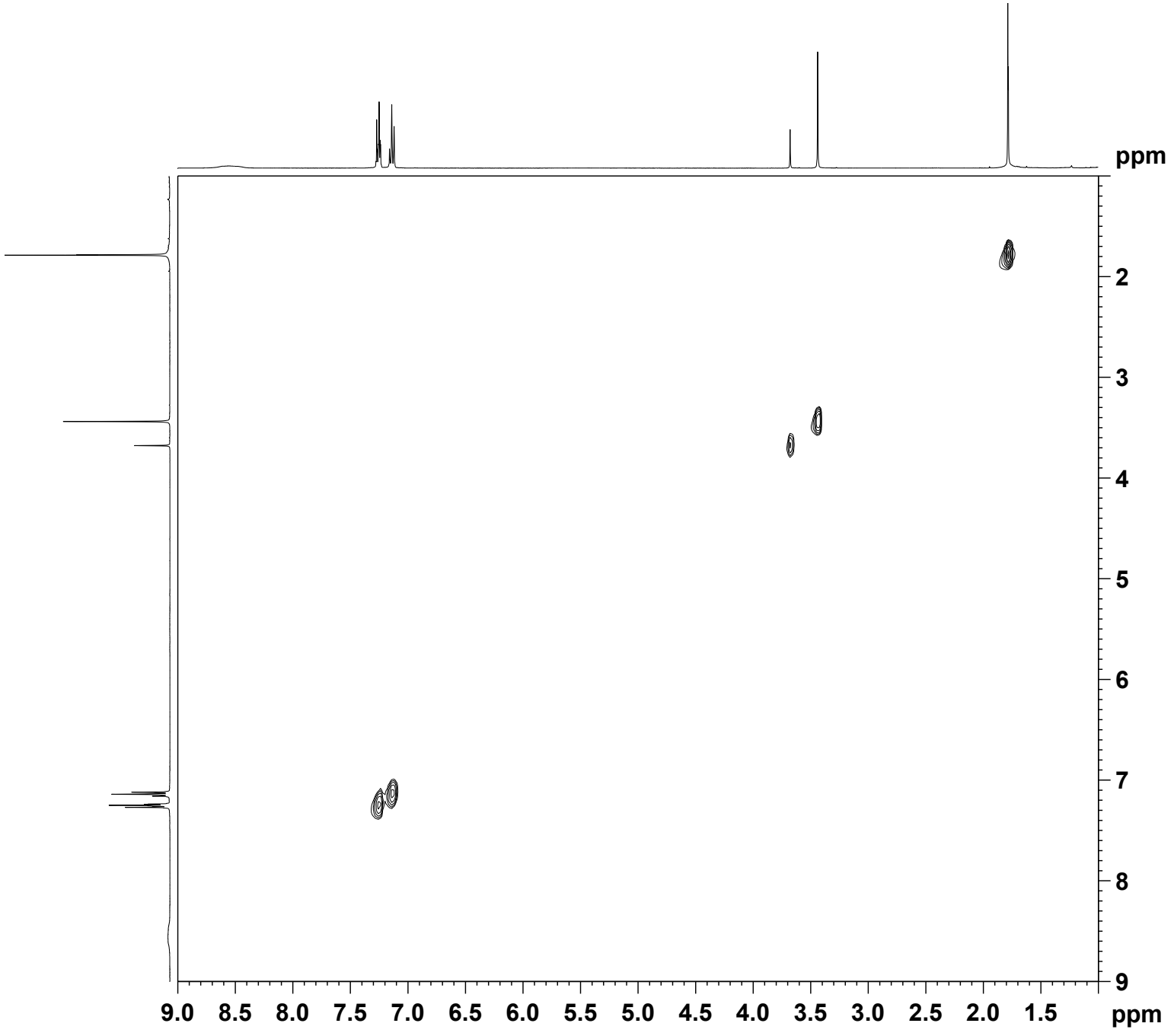
NOESY of compound **2a** (E/Z isomers)

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PROCNO                      1

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Time                     8.01 h
INSTRUM                  spect
PROBHD   Z108618_0922 (
PULPROG          noesygpphpp
TD                       2048
SOLVENT                  CDCl3
NS                          4
DS                         16
SWH                  8012.820 Hz
FIDRES               7.825020 Hz
AQ                   0.1277952 sec
RG                      112.98
DW                      62.400 usec
DE                       6.50 usec
TE                      294.0 K
D0                   0.00004394 sec
D1                   2.00000000 sec
D8                   0.40000001 sec
D11                  0.03000000 sec
D12                  0.00002000 sec
D16                  0.00020000 sec
IN0                  0.00012480 sec
TDav                        1
SFO1               400.1324008 MHz
NUC1                       1H
P1                      14.50 usec
P2                      29.00 usec
P17                   2500.00 usec
PLW1               12.69999981 W
PLW10               2.96690011 W
GPNAM[1]           SMSQ10.100
GPZ1                    40.00 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                        256
SFO1                 400.1324 MHz
FIDRES                62.600159 Hz
SW                    20.025 ppm
FnMODE            States-TPPI

F2 - Processing parameters
SI                       1024
SF                 400.1300176 MHz
WDW                      QSINE
SSB                         2
LB              0 Hz
GB              0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                States-TPPI
SF                 400.1300176 MHz
WDW                      QSINE
SSB                         2
LB              0 Hz
GB              0
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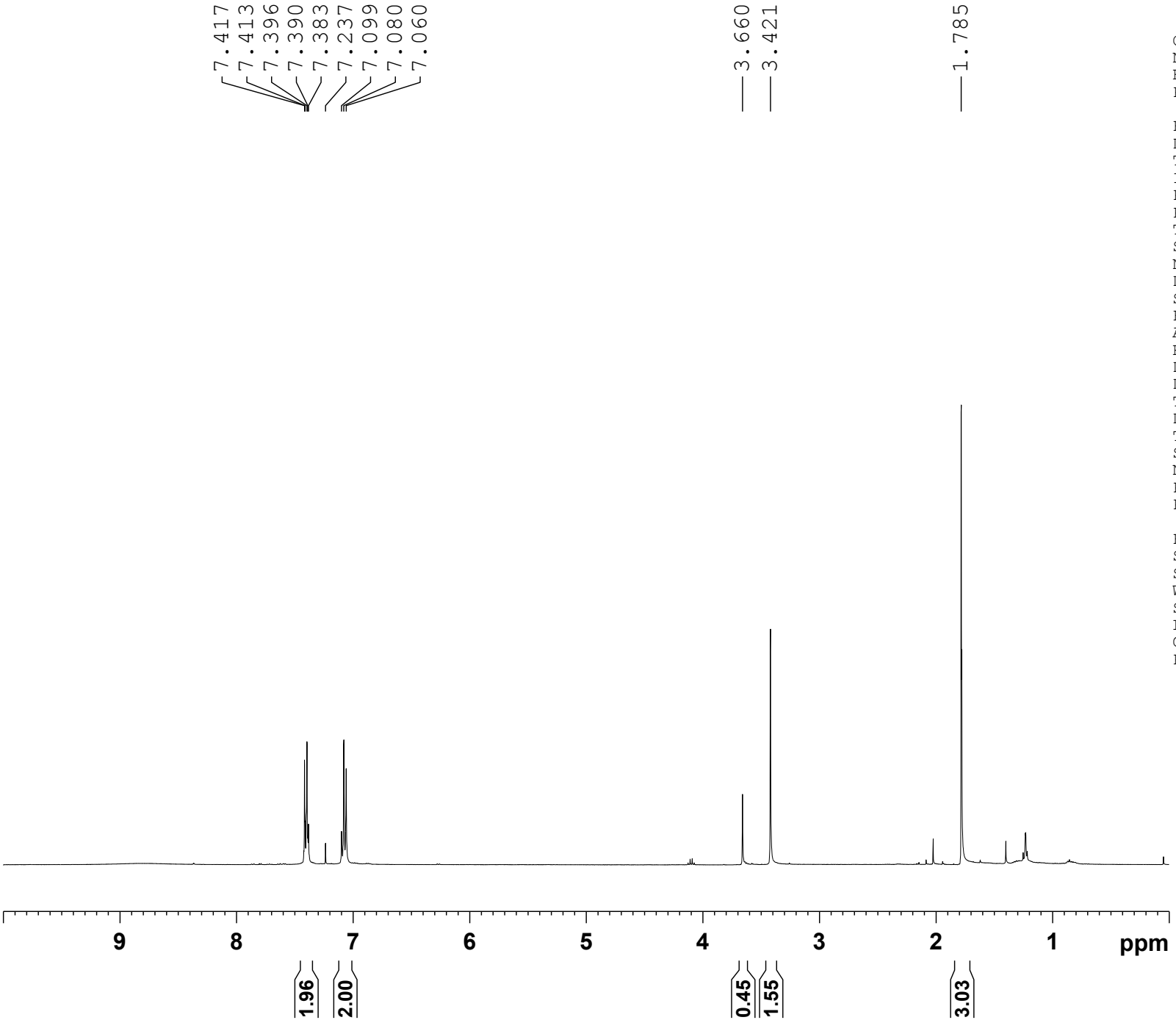
1H NMR (CDCl3, 400 MHz) of compound **2b** (E/Z isomers)

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PROCNO                      1

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PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        15
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                     128.5
DW                    62.400 usec
DE                    16.43 usec
TE                    295.7 K
D1                2.00000000 sec
TD0                        1
SFO1            400.1324008 MHz
NUC1                      1H
P1                    14.50 usec
PLW1            12.69999981 W

F2 - Processing parameters
SI                     16384
SF              400.1300190 MHz
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LB           0 Hz
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PC                      1.00
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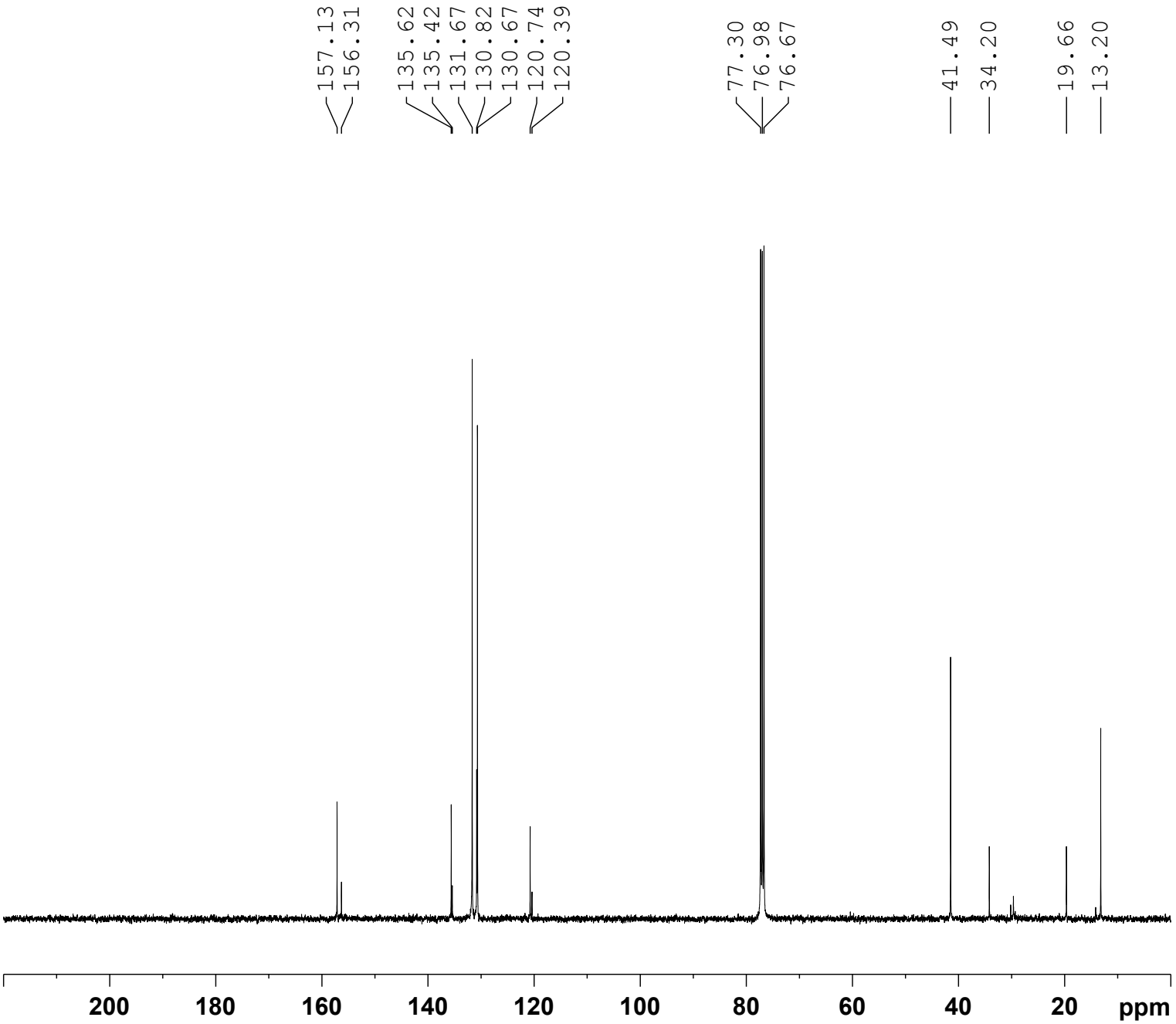
13C NMR (CDCl3, 100 MHz) of compound **2b** (E/Z isomers)

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Current Data Parameters
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EXPNO                      2
PROCNO                     1

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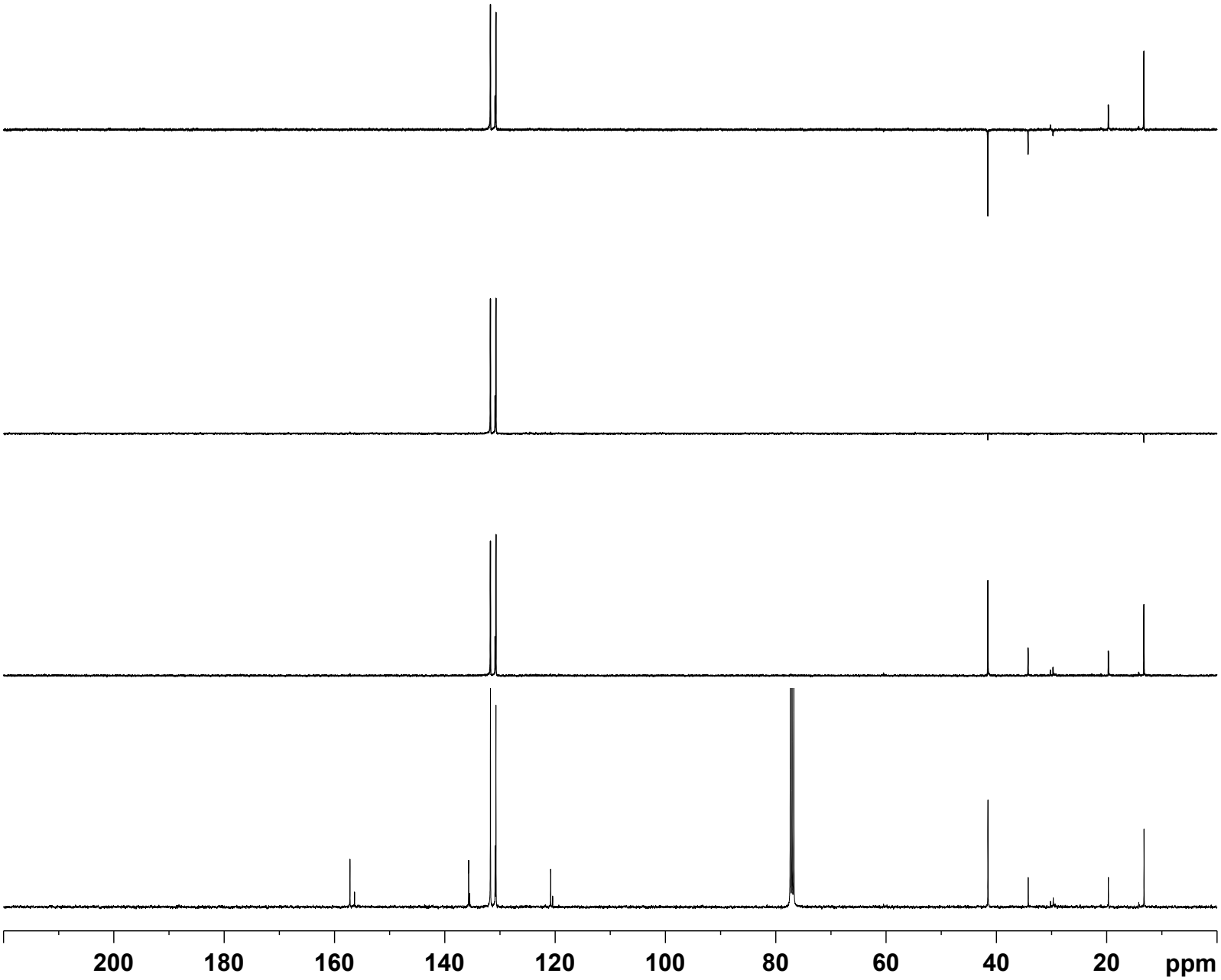
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     1500
DS                        0
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                0.6815744 sec
RG                   210.28
DW                   20.800 usec
DE                    6.50 usec
TE                   296.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1
SFO1           100.6233329 MHz
NUC1                  13C
P1                   10.50 usec
PLW1           44.09999847 W
SFO2           400.1316005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2           14.30000019 W
PLW12           0.37118000 W
PLW13           0.18640999 W

F2 - Processing parameters
SI                    32768
SF             100.6127739 MHz
WDW                     EM
SSB       0
LB                    2.00 Hz
GB        0
PC                    1.00
```

DEPT of compound **2b** (E/Z isomers)

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PROCNO                1

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TD                32768
SOLVENT           CDCl3
NS                 1500
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               296.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1               10.50 usec
PLW1         44.09999847 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
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PLW12         0.37118000 W
PLW13         0.18640999 W

F2 - Processing parameters
SI                32768
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GB        0
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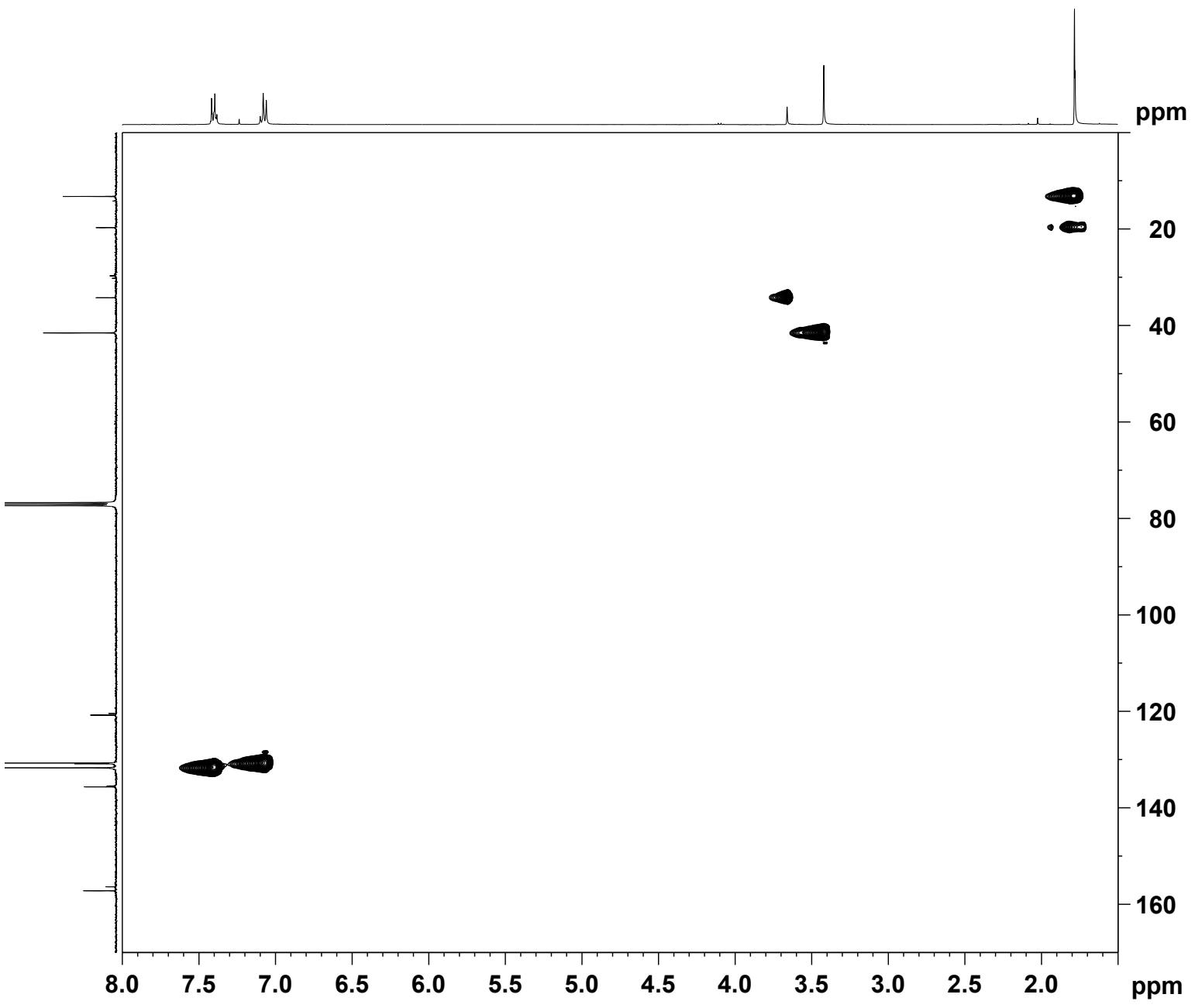
HSQC of compound **2b** (E/Z isomers)

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PROCNO                 1

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PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT             CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                295.9 K
CNST2        145.0000000
CNST17        -0.5000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002080 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         12.69999981 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2            garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0     0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
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SPOFFS3  0 Hz
SPW3          7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7             0.500
SPOFFS7  0 Hz
SPW7          7.41179991 W
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GPZ1               80.00 %
GPNAM[2]      SMSQ10.100
GPZ2               20.10 %
GPNAM[3]      SMSQ10.100
GPZ3               11.00 %
GPNAM[4]      SMSQ10.100
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300190 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127685 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
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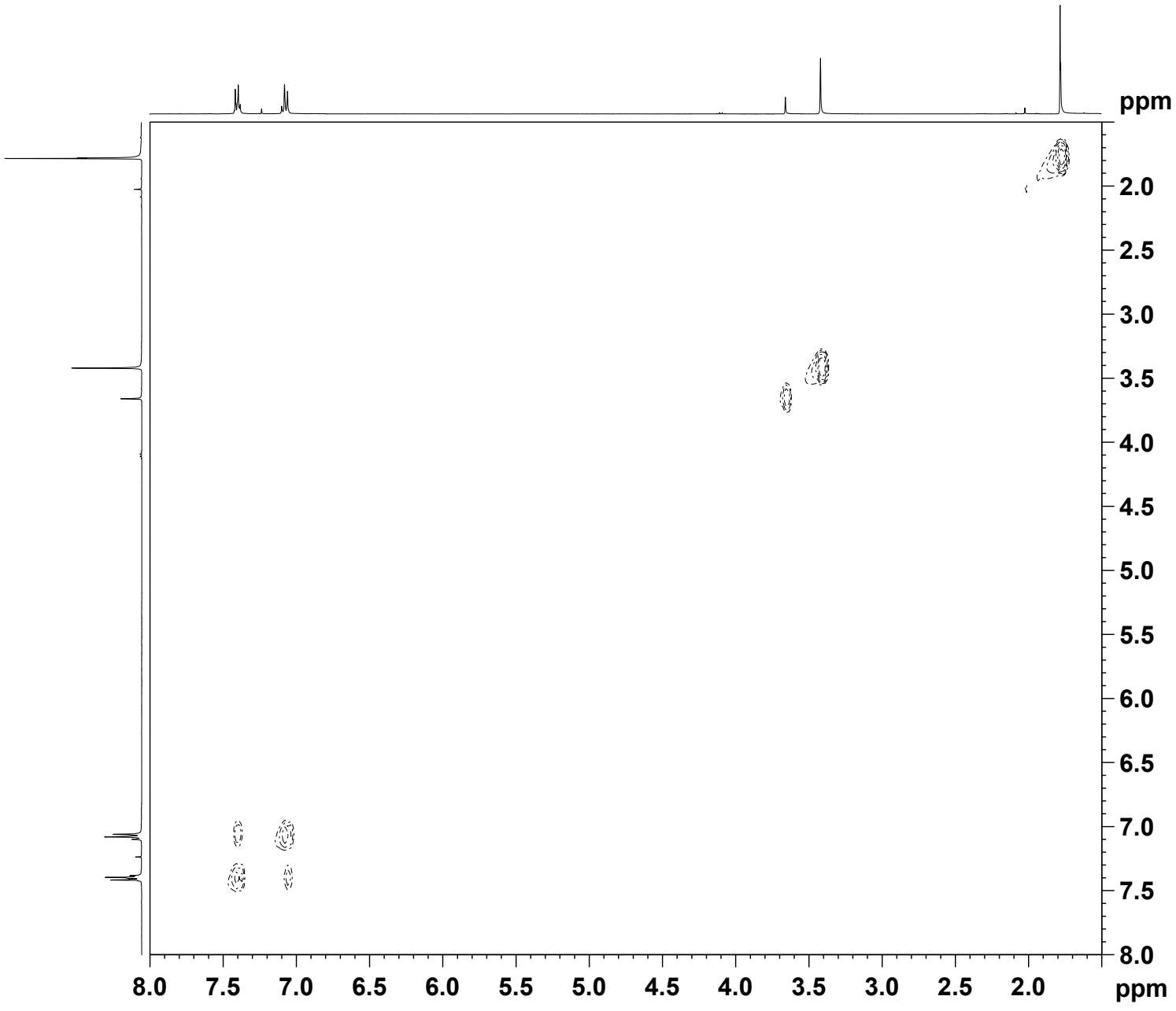
COSY of compound **2b** (E/Z isomers)

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PROCNO                 1

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Time              20.08 h
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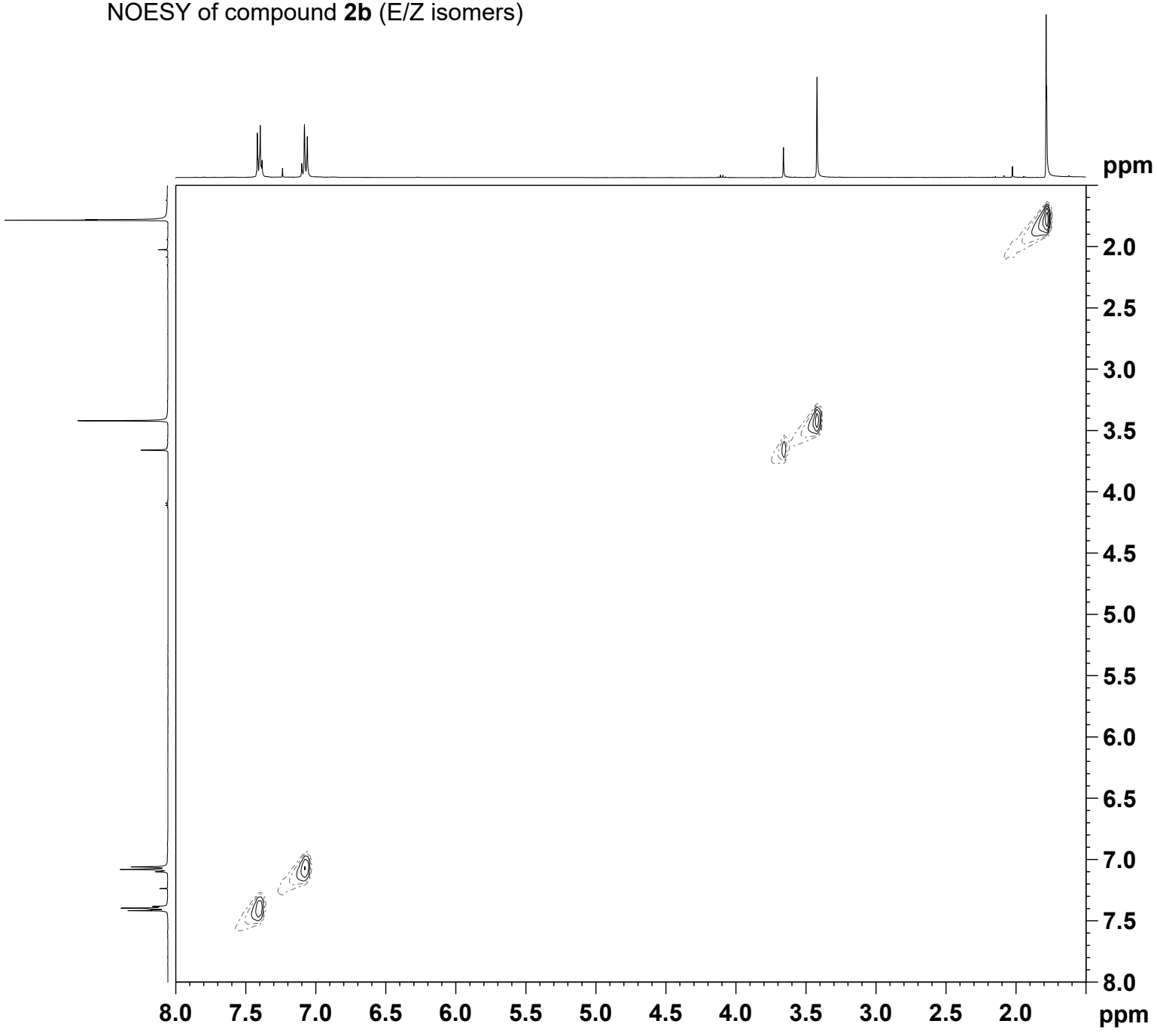
TD                  2048
SOLVENT            CDCl3
NS                     3
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.3 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF           400.1300190 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF           400.1300190 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **2b** (E/Z isomers)




```
Current Data Parameters
NAME                 YYH-066
EXPNO                      8
PROCNO                     1

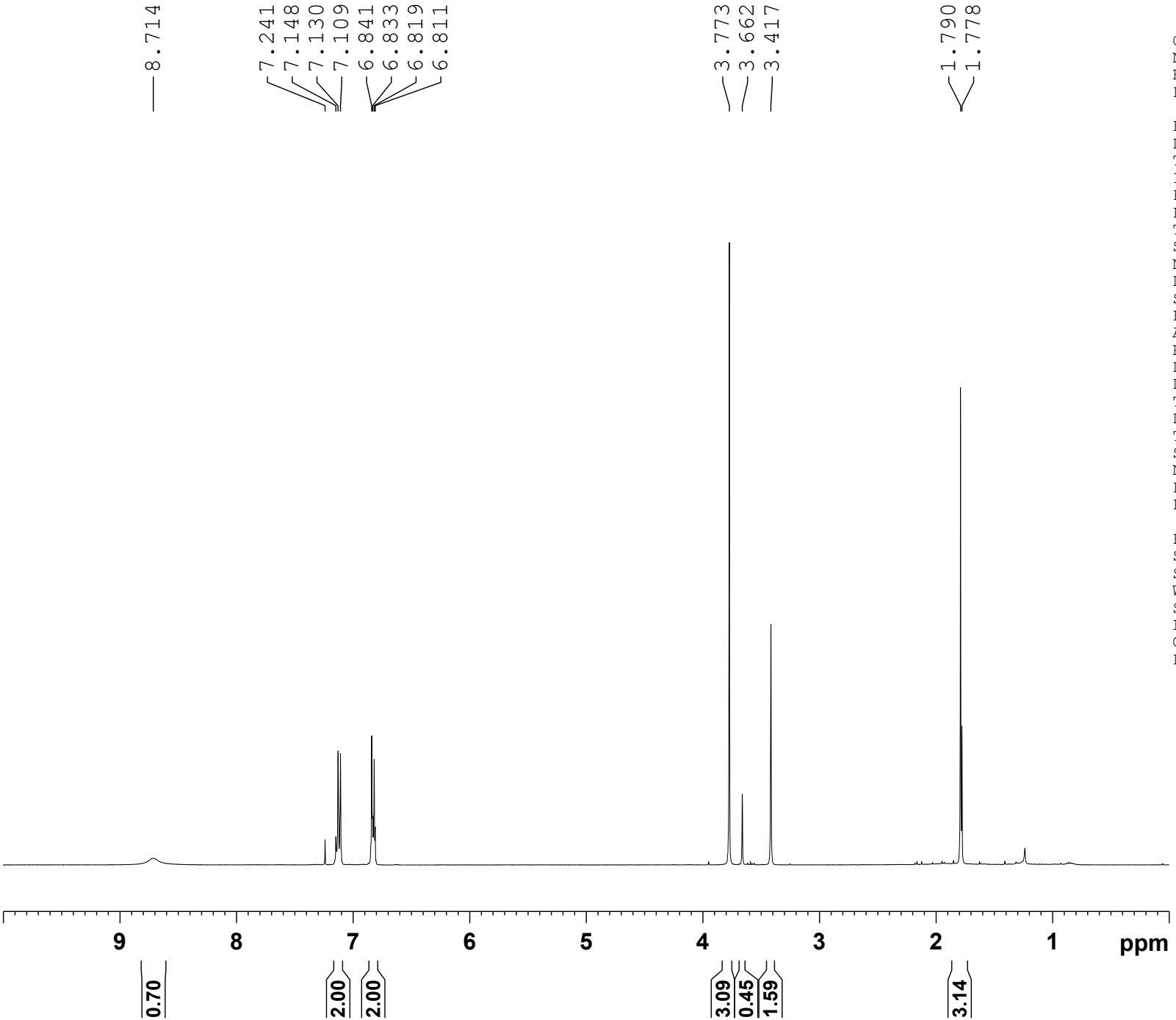
F2 - Acquisition Parameters
Date_               20210422
Time                  20.37 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG       noesygpphpp
TD                      2048
SOLVENT              CDCl3
NS                         3
DS                        16
SWH                8012.820 Hz
FIDRES             7.825020 Hz
AQ                 0.1277952 sec
RG                    112.98
DW                    62.400 usec
DE                     6.50 usec
TE                    295.8 K
D0                 0.00004394 sec
D1                 2.00000000 sec
D8                 0.40000001 sec
D11                0.03000000 sec
D12                0.00002000 sec
D16                0.00020000 sec
IN0                0.00012480 sec
TDav                       1
SFO1            400.1324008 MHz
NUC1                      1H
P1                    14.50 usec
P2                    29.00 usec
P17                 2500.00 usec
PLW1            12.69999981 W
PLW10            2.96690011 W
GPNAM[1]         SMSQ10.100
GPZ1                  40.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                       256
SFO1              400.1324 MHz
FIDRES           62.600159 Hz
SW                  20.025 ppm
FnMODE         States-TPPI

F2 - Processing parameters
SI                      1024
SF              400.1300190 MHz
WDW                    QSINE
SSB                        2
LB         0 Hz
GB         0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2            States-TPPI
SF              400.1300190 MHz
WDW                    QSINE
SSB                        2
LB         0 Hz
GB         0
```

1H NMR (CDCl3, 400 MHz) of compound **2c**

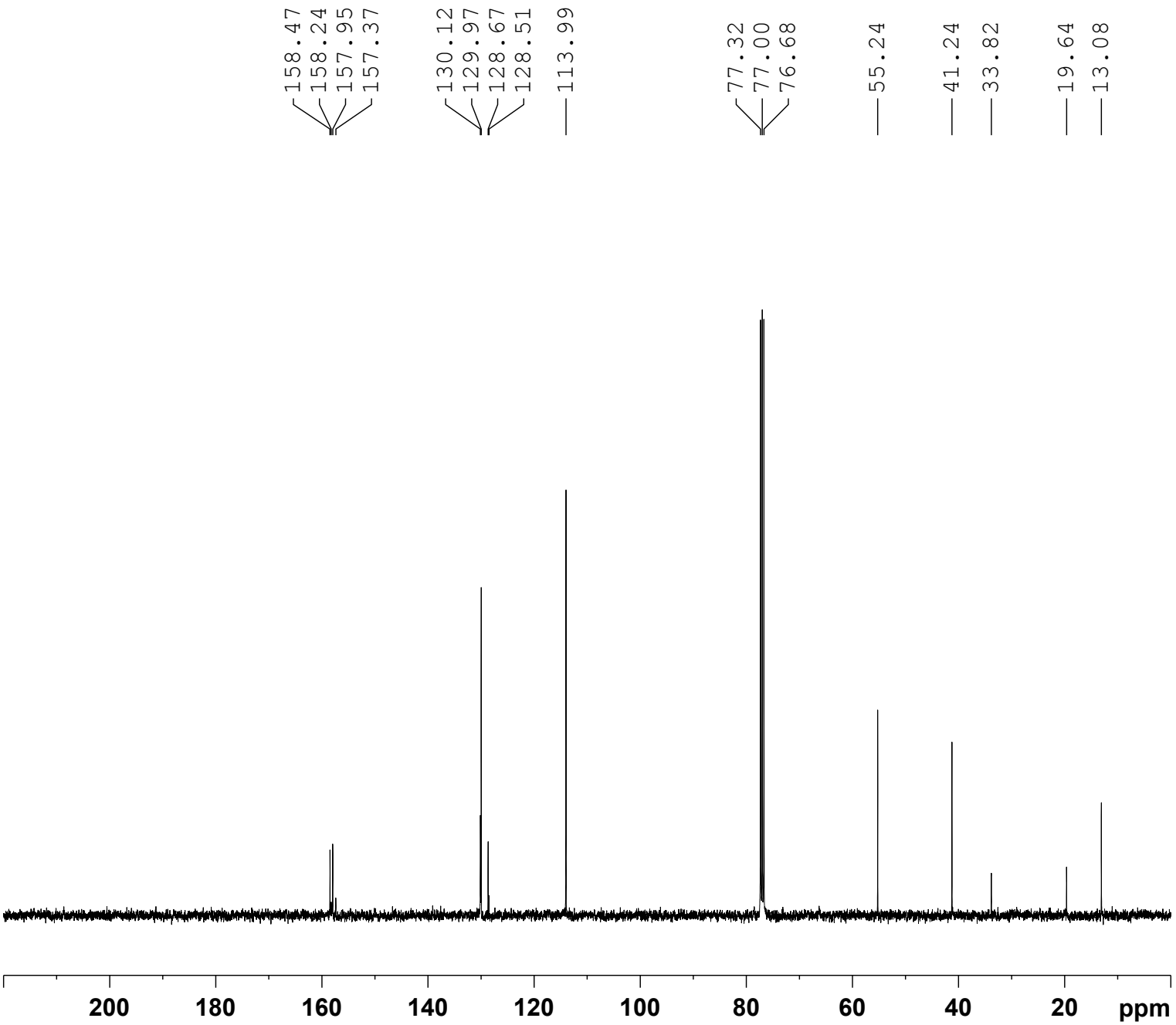



```
Current Data Parameters
NAME                  YYH-067
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210418
Time                   19.02 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                     128.5
DW                    62.400 usec
DE                    16.43 usec
TE                    296.0 K
D1                2.00000000 sec
TD0                         1
SFO1            400.1324008 MHz
NUC1                       1H
P1                    14.50 usec
PLW1            12.69999981 W

F2 - Processing parameters
SI                      16384
SF              400.1300168 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

13C NMR (CDCl3, 100 MHz) of compound **2c**

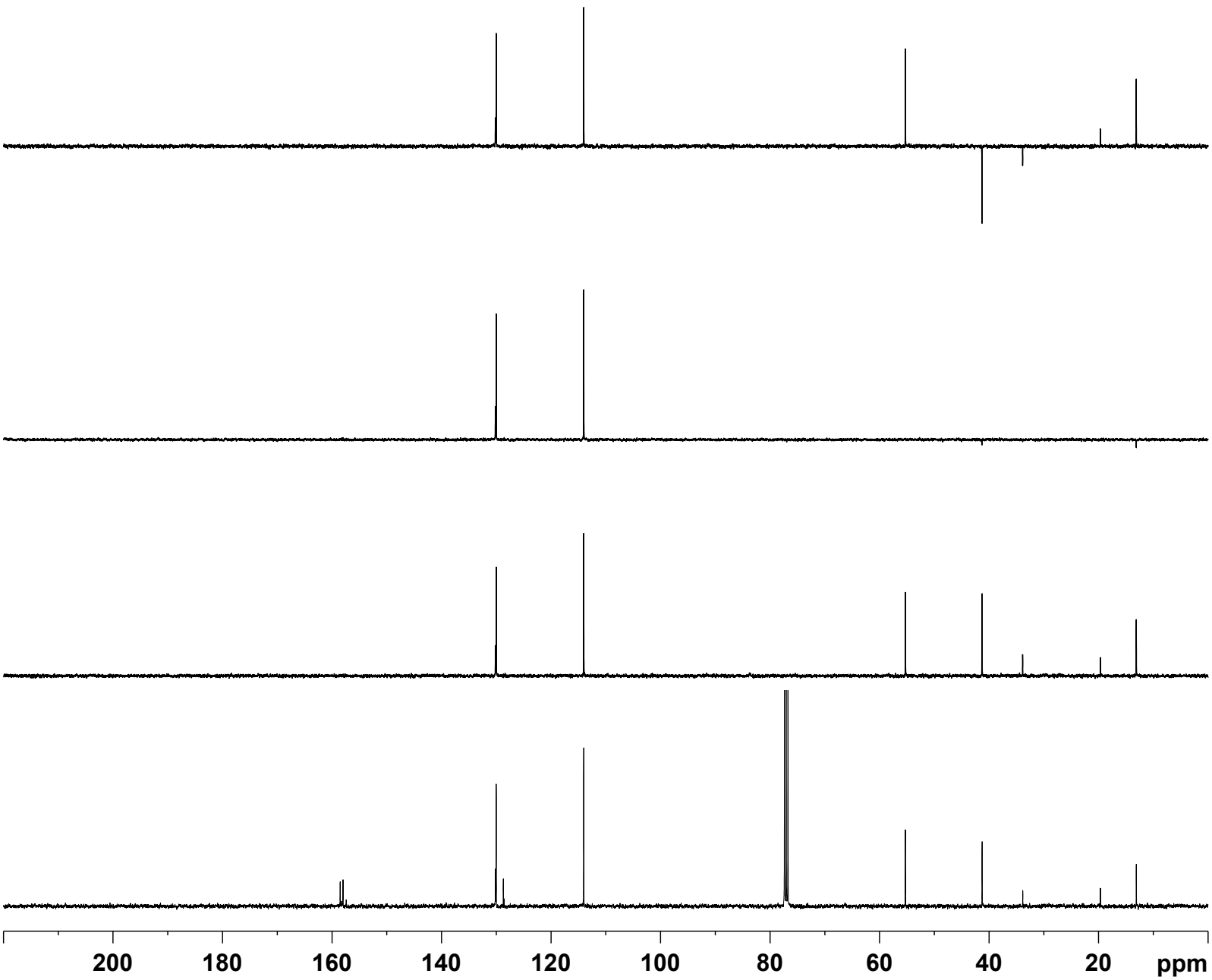



```
Current Data Parameters
NAME                  YYH-067
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210418
Time                   19.11 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      200
DS                        0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     296.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1             100.6233329 MHz
NUC1                     13C
P1                     10.50 usec
PLW1              44.09999847 W
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2              14.30000019 W
PLW12              0.37118000 W
PLW13              0.18640999 W

F2 - Processing parameters
SI                    32768
SF               100.6127723 MHz
WDW                      EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

DEPT of compound **2c**

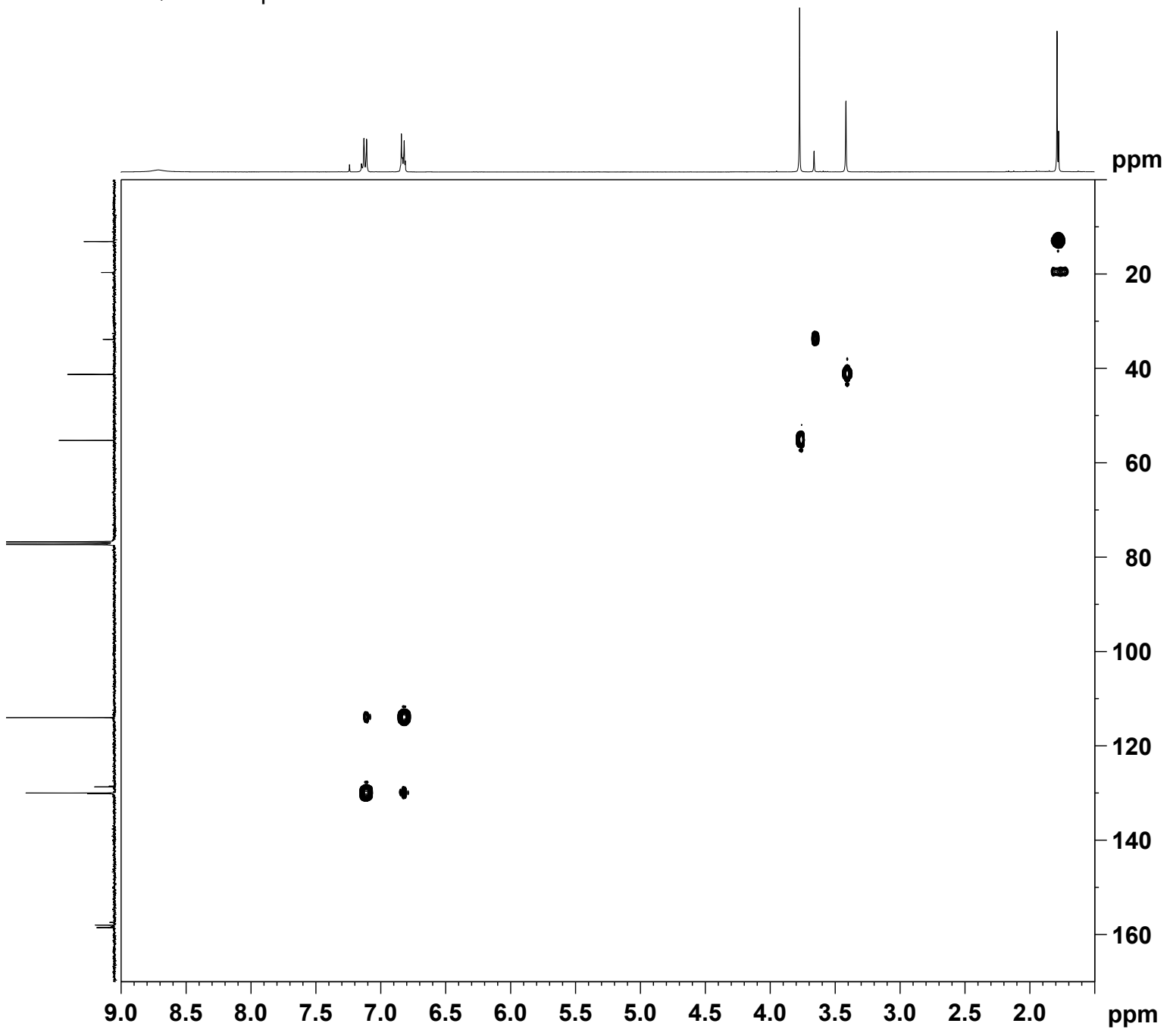



```
Current Data Parameters
NAME            YYH-067
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210418
Time              19.11 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                  200
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               296.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1                10.50 usec
PLW1         44.09999847 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2         14.30000019 W
PLW12         0.37118000 W
PLW13         0.18640999 W

F2 - Processing parameters
SI                32768
SF          100.6127685 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

HSQC of compound **2c**




```
Current Data Parameters
NAME                  YYH-067
EXPNO                       6
PROCNO                      1

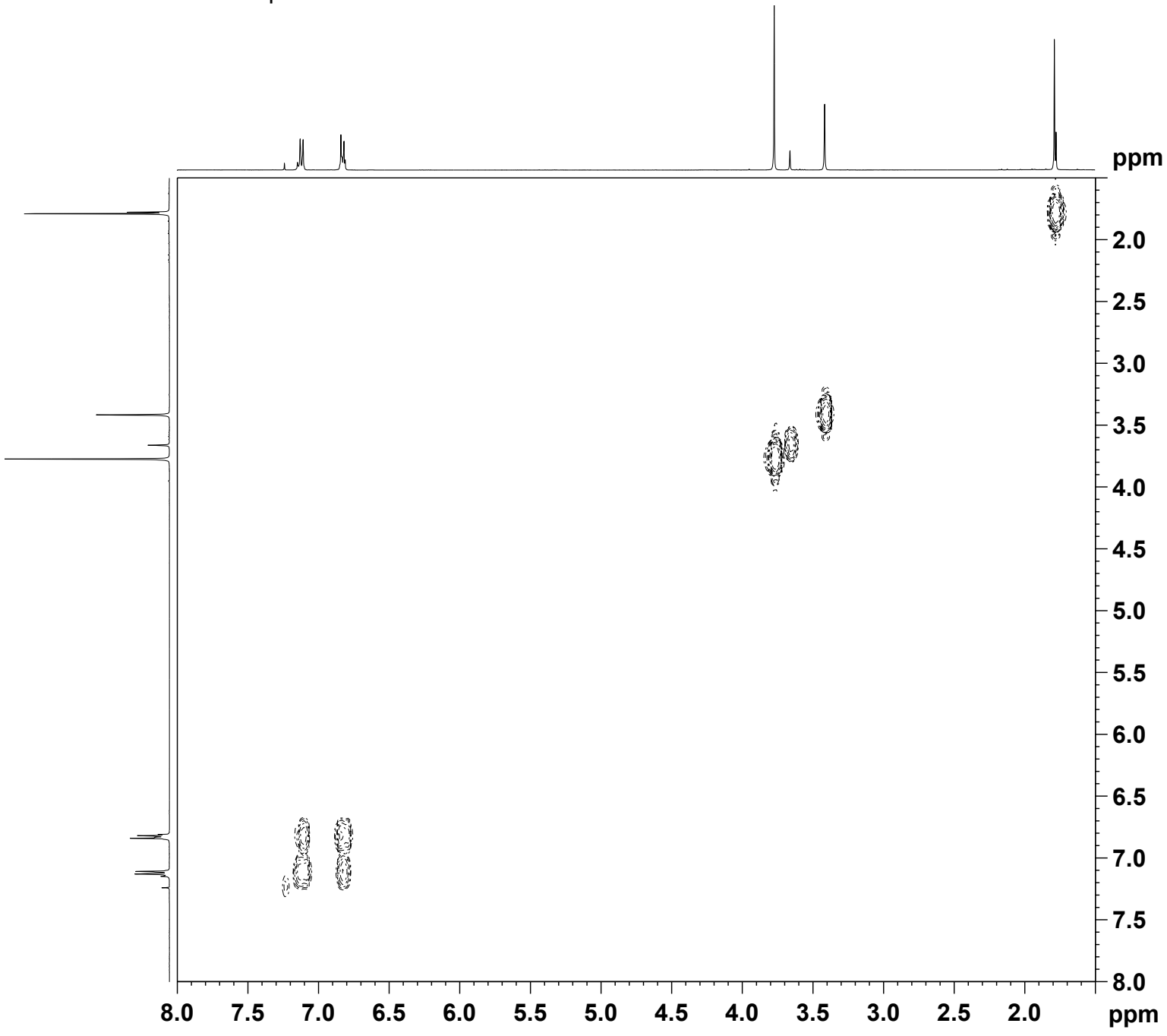
F2 - Acquisition Parameters
Date_               20210418
Time                   19.27 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                       2048
SOLVENT                 CDCl3
NS                          4
DS                         16
SWH                  8012.820 Hz
FIDRES               7.825020 Hz
AQ                   0.1277952 sec
RG                     210.28
DW                      62.400 usec
DE                       6.50 usec
TE                      296.4 K
CNST2              145.0000000
CNST17              -0.5000000
D0                   0.00000300 sec
D1                   1.50000000 sec
D4                   0.00172414 sec
D11                  0.03000000 sec
D16                  0.00020000 sec
D24                  0.00086207 sec
IN0                  0.00002080 sec
TDav                        1
SFO1               400.1324008 MHz
NUC1                       1H
P1                       14.50 usec
P2                       29.00 usec
P28                    1000.00 usec
PLW1               12.69999981 W
SFO2               100.6233329 MHz
NUC2                       13C
CPDPRG[2                 garp
P3                       10.50 usec
P14                     500.00 usec
P24                    2000.00 usec
PCPD2                    80.00 usec
PLW0      0 W
PLW2               44.00000000 W
PLW12               0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                   0.500
SPOFFS3   0 Hz
SPW3                7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7                   0.500
SPOFFS7   0 Hz
SPW7                7.41179991 W
GPNAM[1]      SMSQ10.100
GPZ1                    80.00 %
GPNAM[2]      SMSQ10.100
GPZ2                    20.10 %
GPNAM[3]      SMSQ10.100
GPZ3                    11.00 %
GPNAM[4]      SMSQ10.100
GPZ4                    -5.00 %
P16                   1000.00 usec
P19                    600.00 usec

F1 - Acquisition parameters
TD                          256
SFO1                100.6233 MHz
FIDRES              187.800476 Hz
SW                     238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                         1024
SF                 400.1300168 MHz
WDW                      QSINE
SSB                         2
LB        0 Hz
GB        0
PC                       1.40

F1 - Processing parameters
SI                         1024
MC2              echo-antiecho
SF                 100.6127685 MHz
WDW                      QSINE
SSB                         2
LB        0 Hz
GB        0
```

COSY of compound **2c**




```
Current Data Parameters
NAME             YYH-067
EXPNO                   7
PROCNO                  1

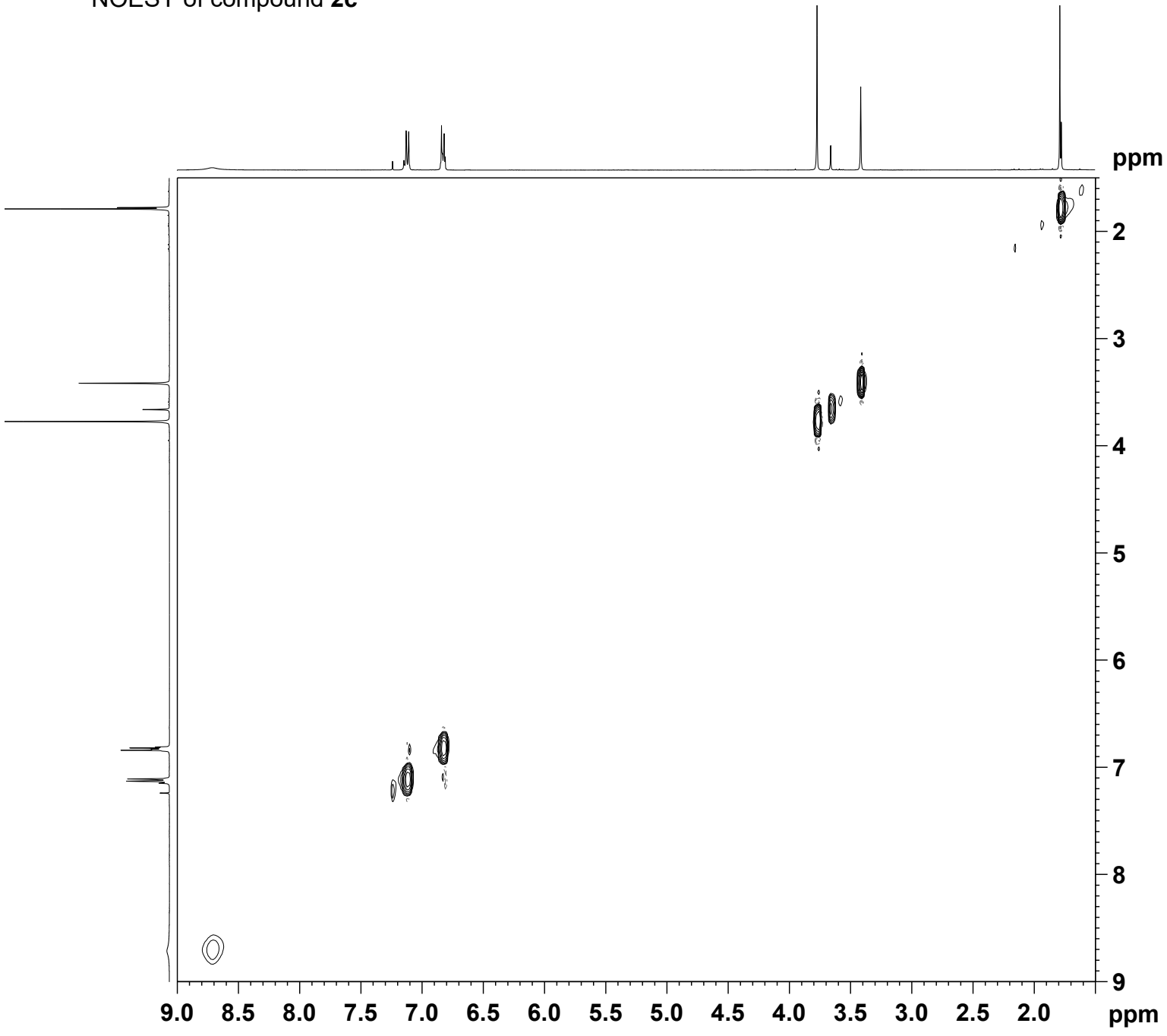
F2 - Acquisition Parameters
Date_            20210418
Time                19.56 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      4
DS                     16
SWH              8012.820 Hz
FIDRES           7.825020 Hz
AQ               0.1277952 sec
RG                 210.28
DW                 62.400 usec
DE                  6.50 usec
TE                 296.4 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                    1
SFO1         400.1324008 MHz
NUC1                   1H
P0                 14.50 usec
P1                 14.50 usec
P17              2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                    256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                 QF

F2 - Processing parameters
SI                   1024
SF           400.1300168 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF           400.1300168 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **2c**




```
Current Data Parameters
NAME                  YYH-067
EXPNO                       8
PROCNO                      1

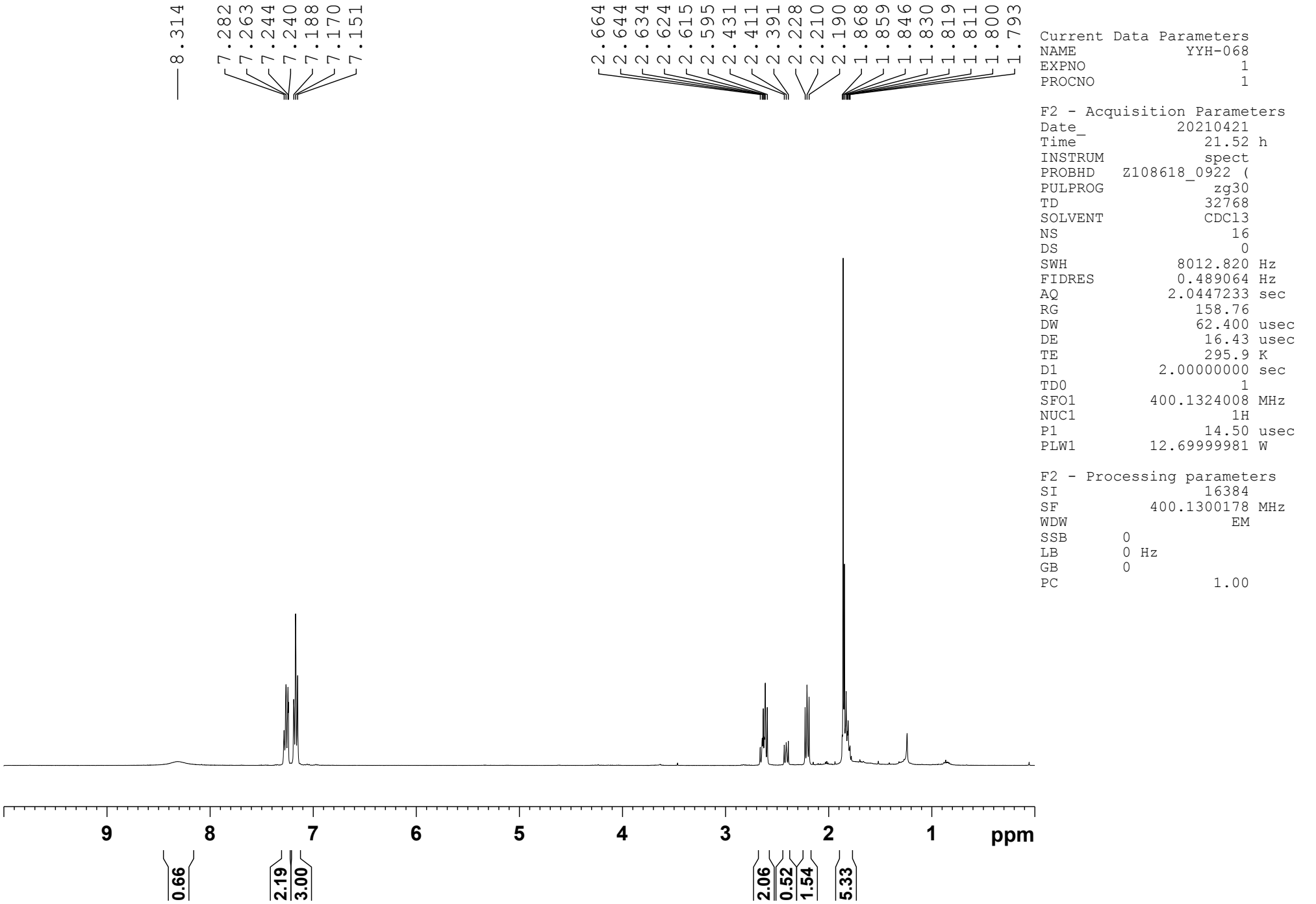
F2 - Acquisition Parameters
Date_              20210418
Time                  20.35 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG       noesygpphpp
TD                       2048
SOLVENT                CDCl3
NS                          5
DS                         16
SWH                 8012.820 Hz
FIDRES              7.825020 Hz
AQ                  0.1277952 sec
RG                     112.98
DW                     62.400 usec
DE                      6.50 usec
TE                     295.8 K
D0                  0.00004394 sec
D1                  2.00000000 sec
D8                  0.40000001 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D16                 0.00020000 sec
IN0                 0.00012480 sec
TDav                        1
SFO1              400.1324008 MHz
NUC1                       1H
P1                     14.50 usec
P2                     29.00 usec
P17                  2500.00 usec
PLW1              12.69999981 W
PLW10              2.96690011 W
GPNAM[1]          SMSQ10.100
GPZ1                  40.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                          256
SFO1                400.1324 MHz
FIDRES              62.600159 Hz
SW                     20.025 ppm
FnMODE           States-TPPI

F2 - Processing parameters
SI                         1024
SF                400.1300168 MHz
WDW                      QSINE
SSB                         2
LB             0 Hz
GB             0
PC                        1.40

F1 - Processing parameters
SI                         1024
MC2              States-TPPI
SF                400.1300168 MHz
WDW                      QSINE
SSB                         2
LB             0 Hz
GB             0
```

1H NMR (CDCl3, 400 MHz) of compound **2d**

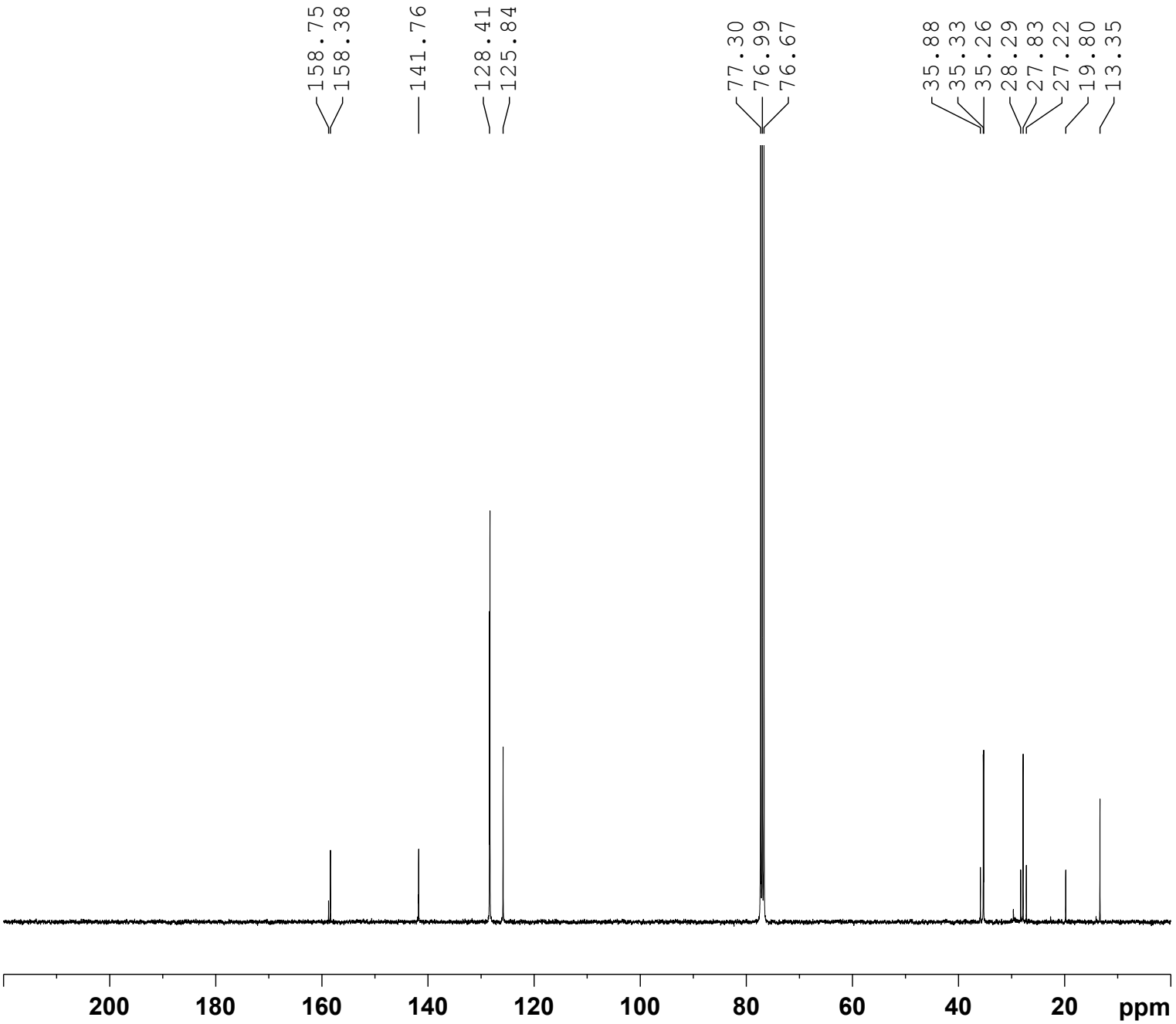



```
Current Data Parameters
NAME                  YYH-068
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210421
Time                   21.52 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                   158.76
DW                   62.400 usec
DE                   16.43 usec
TE                   295.9 K
D1                2.00000000 sec
TD0                         1
SFO1            400.1324008 MHz
NUC1                       1H
P1                   14.50 usec
PLW1            12.69999981 W

F2 - Processing parameters
SI                      16384
SF              400.1300178 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

13C NMR (CDCl3, 100 MHz) of compound **2d**

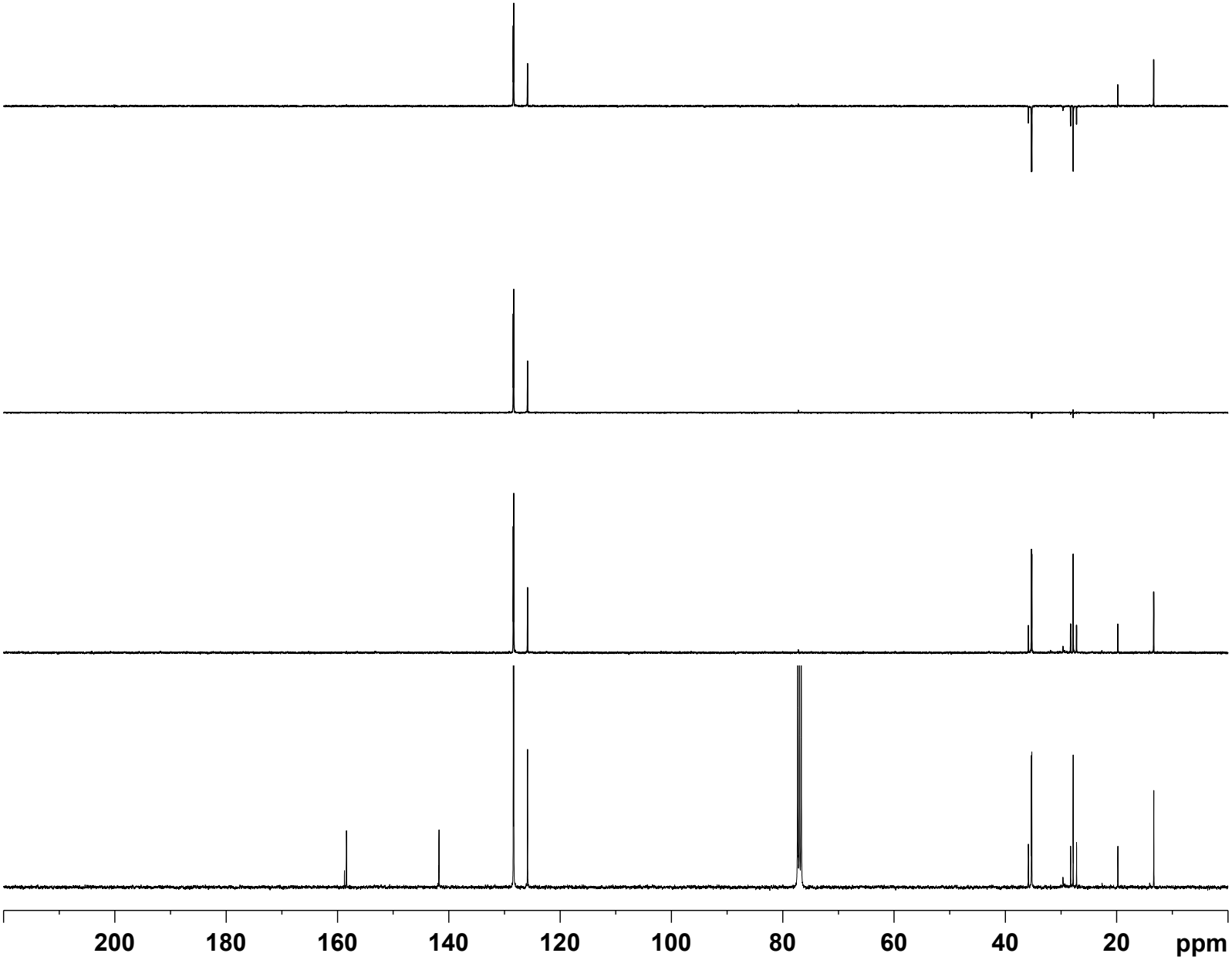



```
Current Data Parameters
NAME                  YYH-068
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210422
Time                    0.13 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       3000
DS                          0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     297.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1             100.6233329 MHz
NUC1                     13C
P1                     10.50 usec
PLW1              44.09999847 W
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2              14.30000019 W
PLW12              0.37118000 W
PLW13              0.18640999 W

F2 - Processing parameters
SI                      32768
SF               100.6127730 MHz
WDW                        EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

DEPT of compound **2d**

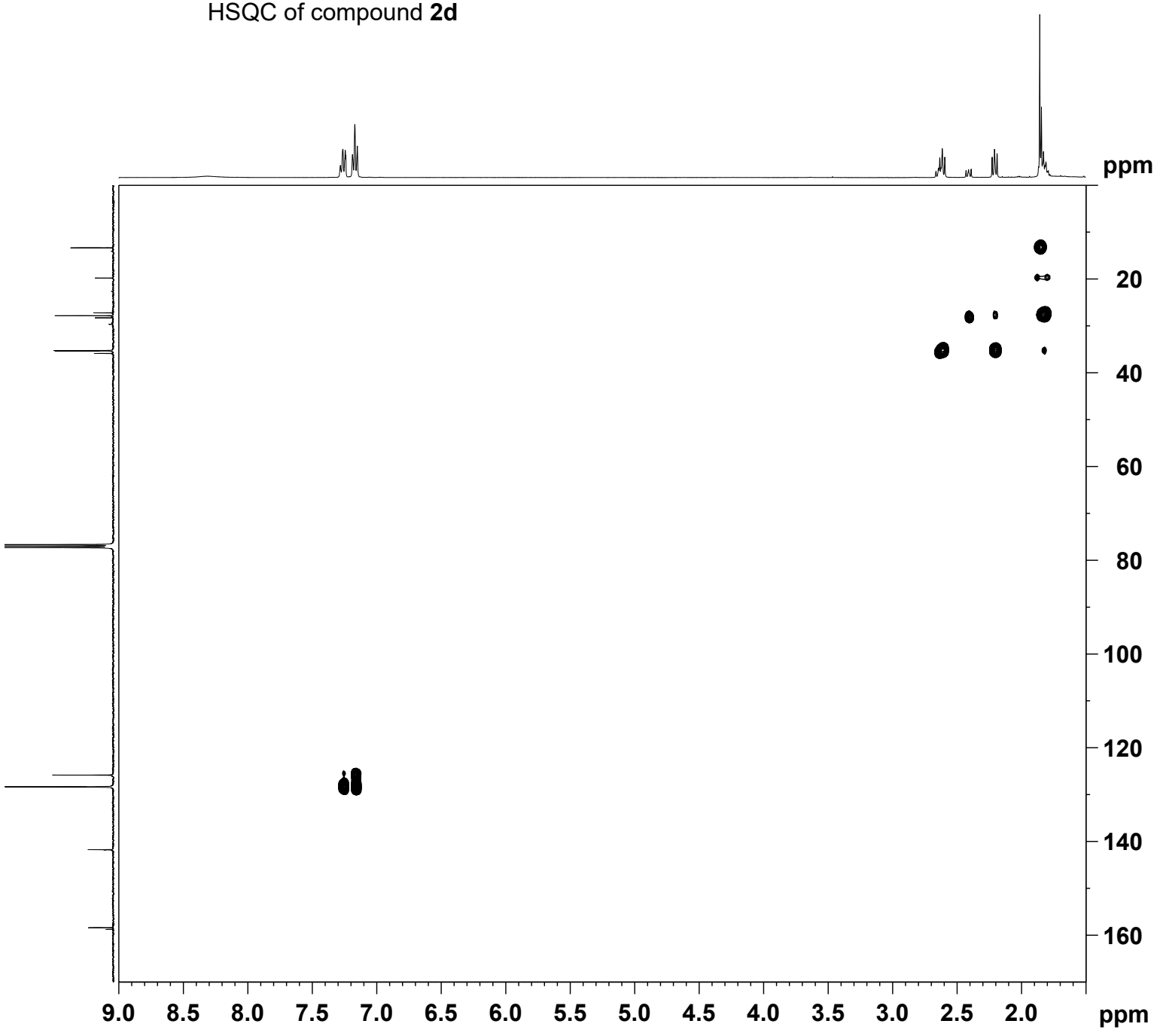



```
Current Data Parameters
NAME                 YYH-068
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20210422
Time                    0.13 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG              zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      3000
DS                         0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     297.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             100.6233329 MHz
NUC1                     13C
P1                     10.50 usec
PLW1              44.09999847 W
SFO2              400.1316005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2              14.30000019 W
PLW12              0.37118000 W
PLW13              0.18640999 W

F2 - Processing parameters
SI                     32768
SF               100.6127730 MHz
WDW                       EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

HSQC of compound **2d**




```
Current Data Parameters
NAME             YYH-068
EXPNO                  6
PROCNO                 1

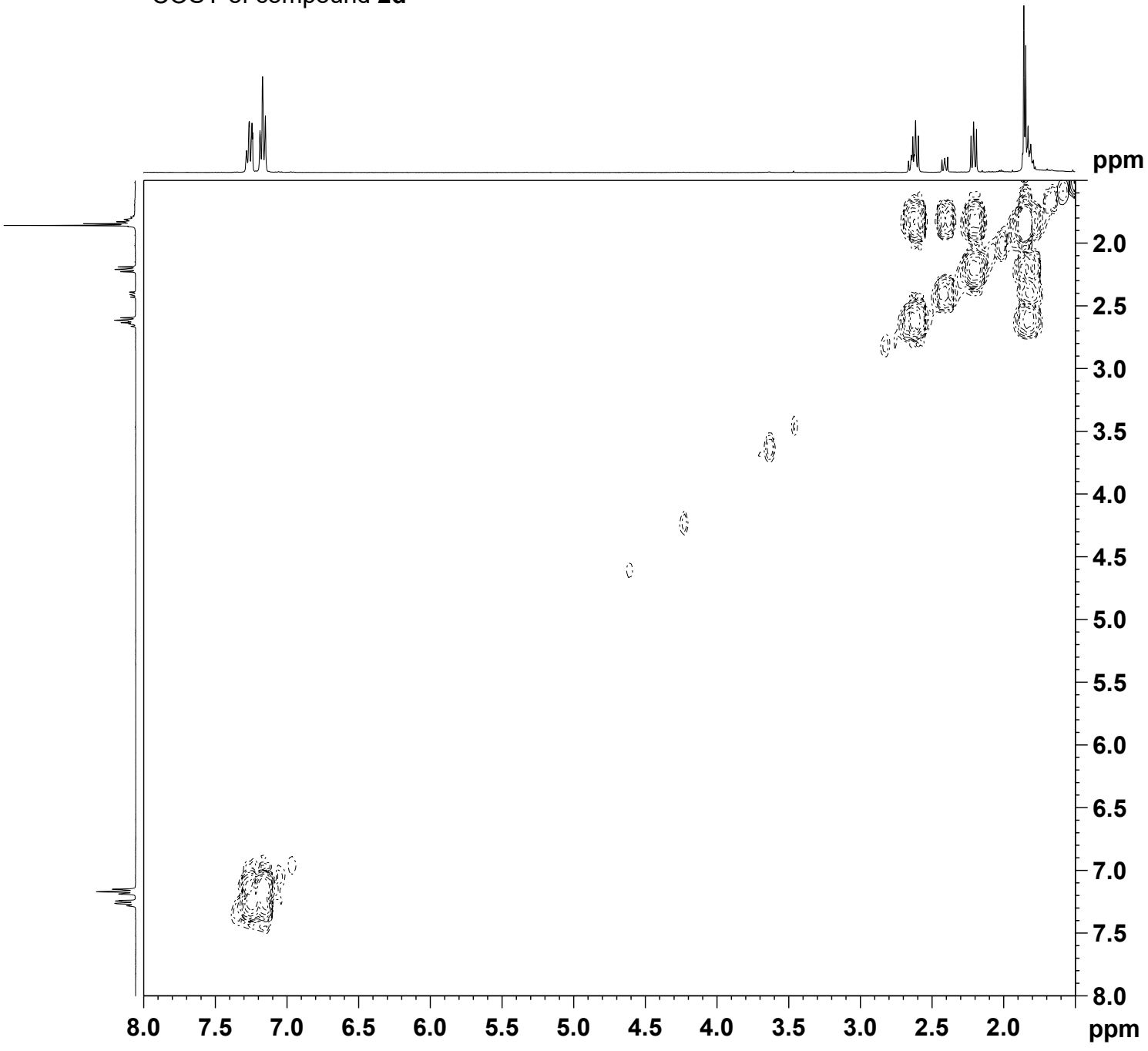
F2 - Acquisition Parameters
Date_           20210422
Time                3.40 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT             CDCl3
NS                     6
DS                    16
SWH              8012.820 Hz
FIDRES           7.825020 Hz
AQ               0.1277952 sec
RG                 210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
CNST2        145.0000000
CNST17        -0.5000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002080 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         12.69999981 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2             garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0     0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3             0.500
SPOFFS3  0 Hz
SPW3          7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7             0.500
SPOFFS7  0 Hz
SPW7          7.41179991 W
GPNAM[1]      SMSQ10.100
GPZ1               80.00 %
GPNAM[2]      SMSQ10.100
GPZ2               20.10 %
GPNAM[3]      SMSQ10.100
GPZ3               11.00 %
GPNAM[4]      SMSQ10.100
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300179 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127730 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

COSY of compound **2d**




```
Current Data Parameters
NAME             YYH-068
EXPNO                  7
PROCNO                 1

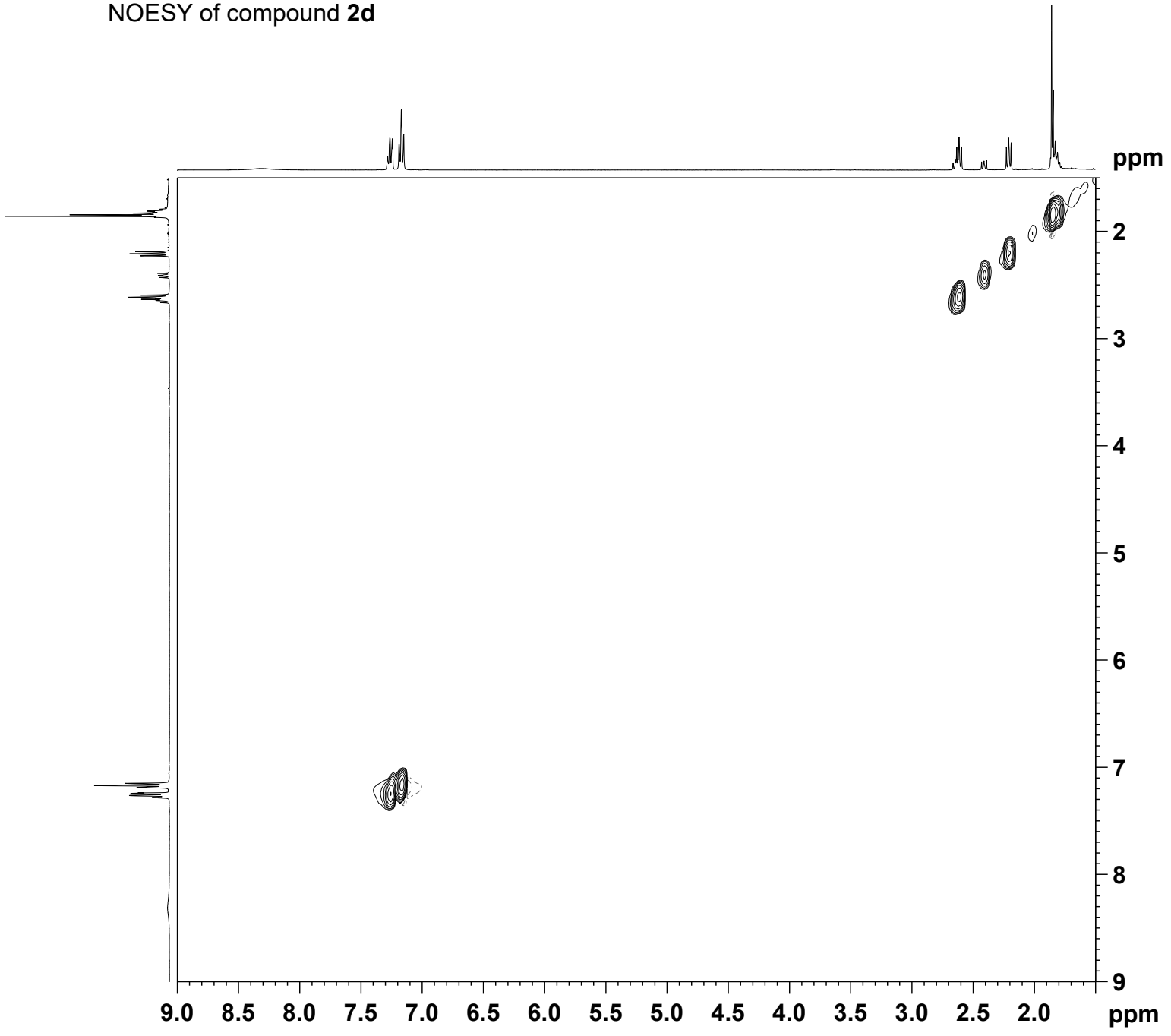
F2 - Acquisition Parameters
Date_           20210422
Time               4.23 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           400.1300179 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300179 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **2d**




```
Current Data Parameters
NAME                 YYH-068
EXPNO                      8
PROCNO                     1

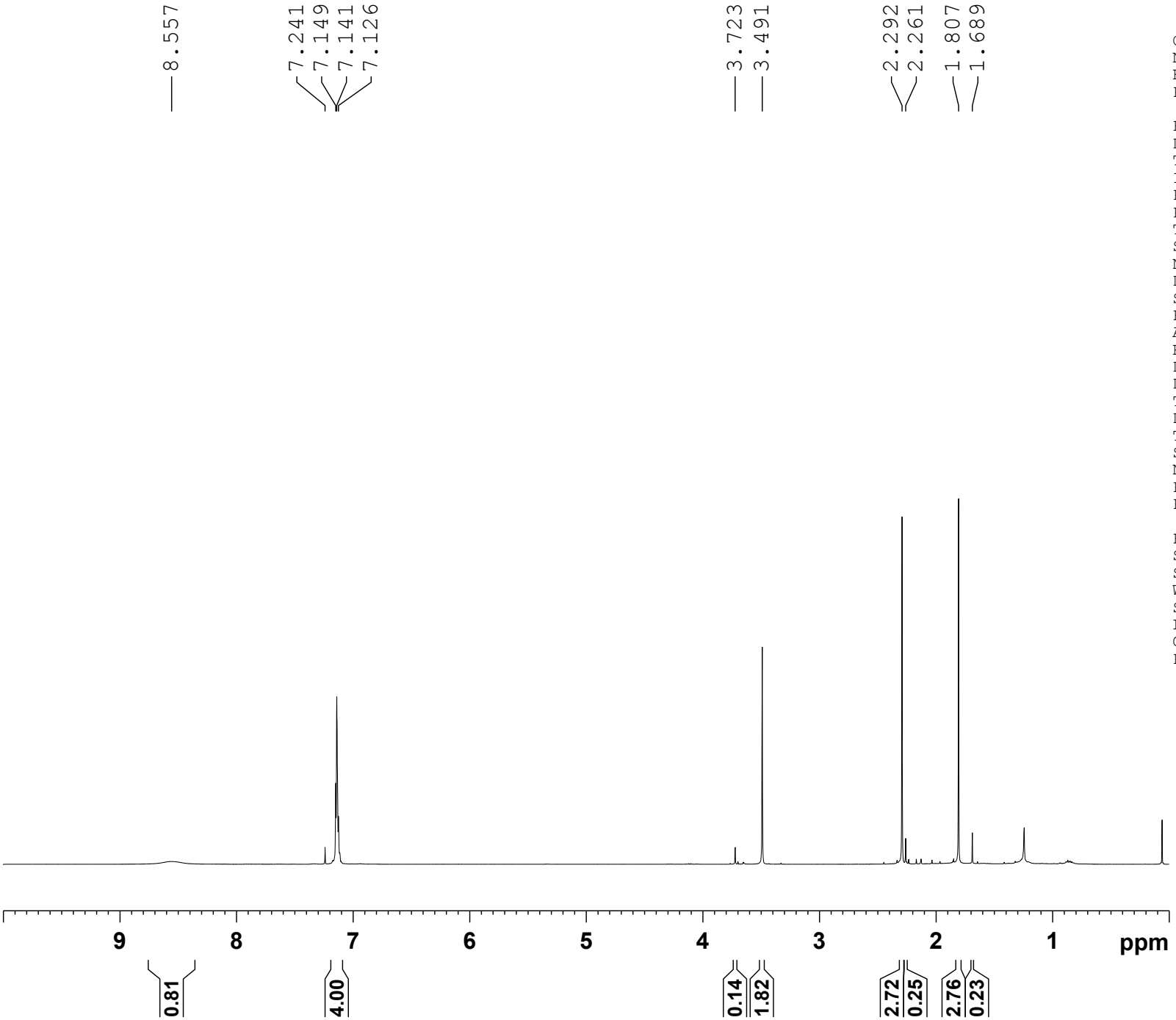
F2 - Acquisition Parameters
Date_               20210422
Time                    5.20 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG       noesygpphpp
TD                      2048
SOLVENT                CDCl3
NS                         6
DS                        16
SWH                 8012.820 Hz
FIDRES              7.825020 Hz
AQ                  0.1277952 sec
RG                     112.98
DW                     62.400 usec
DE                      6.50 usec
TE                     295.8 K
D0                  0.00004394 sec
D1                  2.00000000 sec
D8                  0.40000001 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D16                 0.00020000 sec
IN0                 0.00012480 sec
TDav                       1
SFO1              400.1324008 MHz
NUC1                      1H
P1                     14.50 usec
P2                     29.00 usec
P17                  2500.00 usec
PLW1              12.69999981 W
PLW10              2.96690011 W
GPNAM[1]          SMSQ10.100
GPZ1                  40.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                       256
SFO1               400.1324 MHz
FIDRES            62.600159 Hz
SW                   20.025 ppm
FnMODE          States-TPPI

F2 - Processing parameters
SI                      1024
SF                400.1300179 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
PC                     1.40

F1 - Processing parameters
SI                      1024
MC2             States-TPPI
SF                400.1300179 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
```

1H NMR (CDCl3, 400 MHz) of compound **2e**

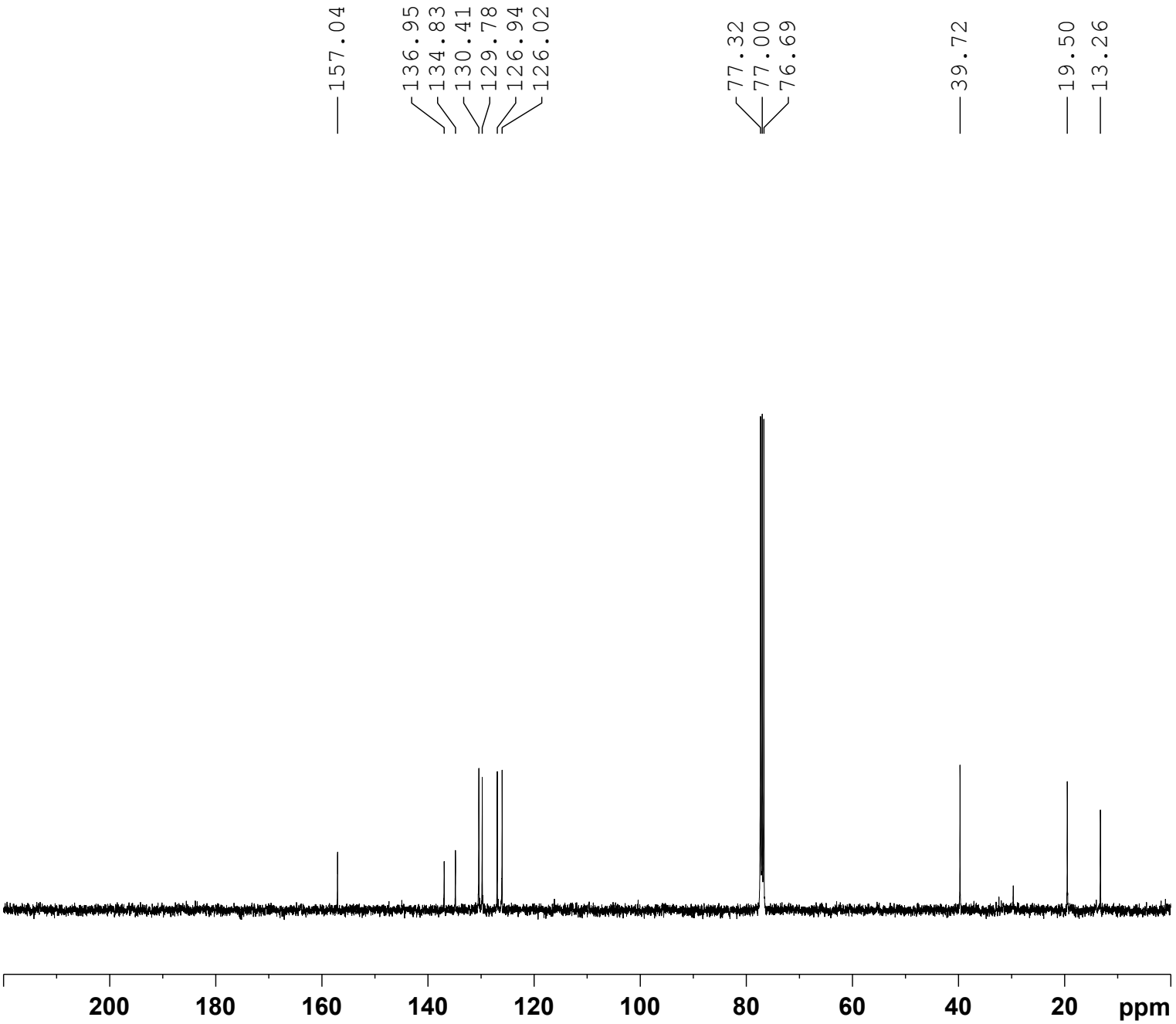



```
Current Data Parameters
NAME                  YYH-074
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20210420
Time                   12.06 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                     128.5
DW                    62.400 usec
DE                    16.43 usec
TE                    296.0 K
D1                2.00000000 sec
TD0                         1
SFO1            400.1324008 MHz
NUC1                       1H
P1                    14.50 usec
PLW1            12.69999981 W

F2 - Processing parameters
SI                      16384
SF              400.1300173 MHz
WDW                        EM
SSB       0
LB        0 Hz
GB        0
PC                      1.00
```

13C NMR (CDCl3, 100 MHz) of compound **2e**

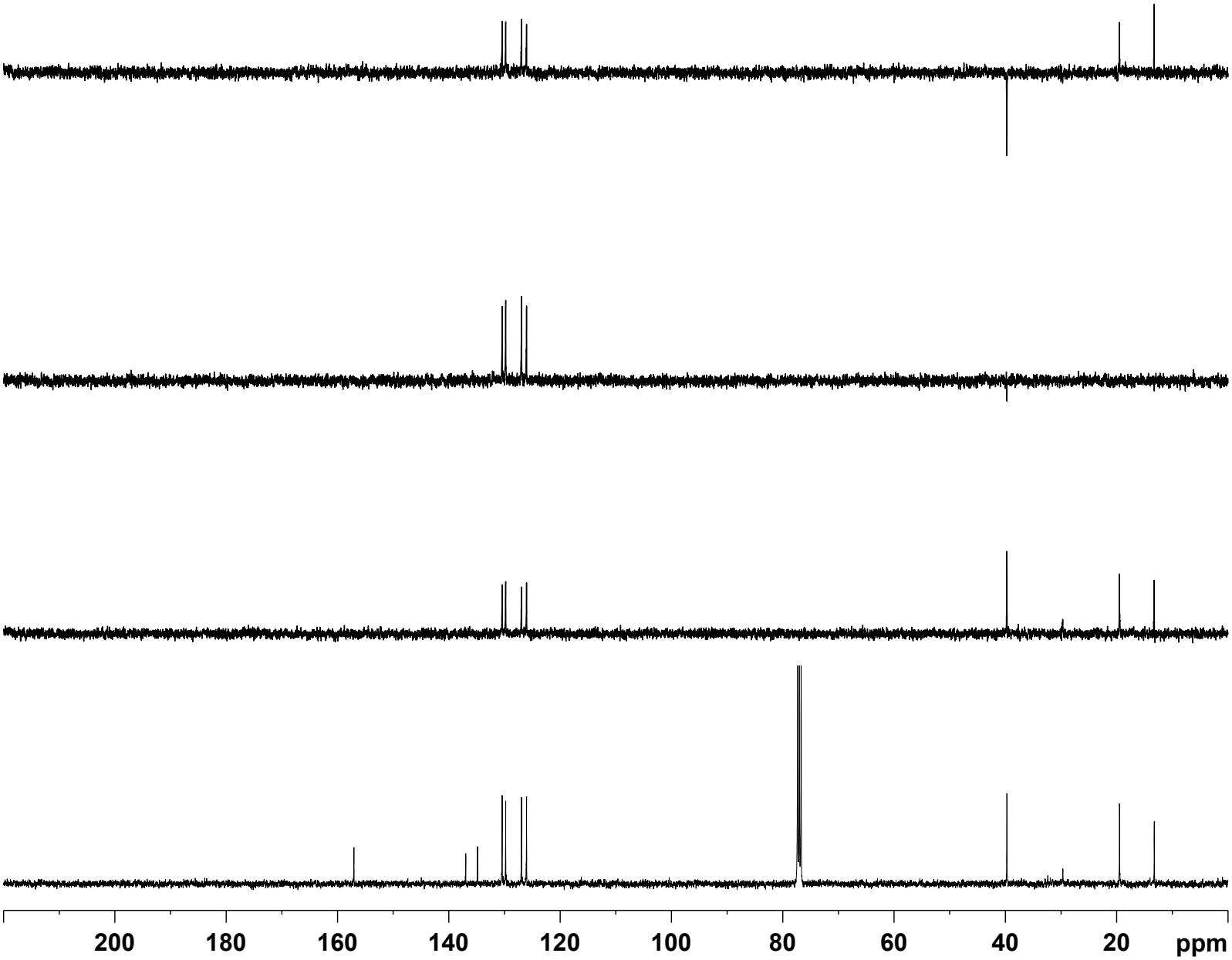



```
Current Data Parameters
NAME                 YYH-074
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20210420
Time                   21.52 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG              zgpg30
TD                     32768
SOLVENT                CDCl3
NS                       200
DS                         0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     296.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1            100.6233329 MHz
NUC1                     13C
P1                     10.50 usec
PLW1              44.09999847 W
SFO2              400.1316005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2              14.30000019 W
PLW12              0.37118000 W
PLW13              0.18640999 W

F2 - Processing parameters
SI                     32768
SF                100.6127729 MHz
WDW                       EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

DEPT of compound **2e**

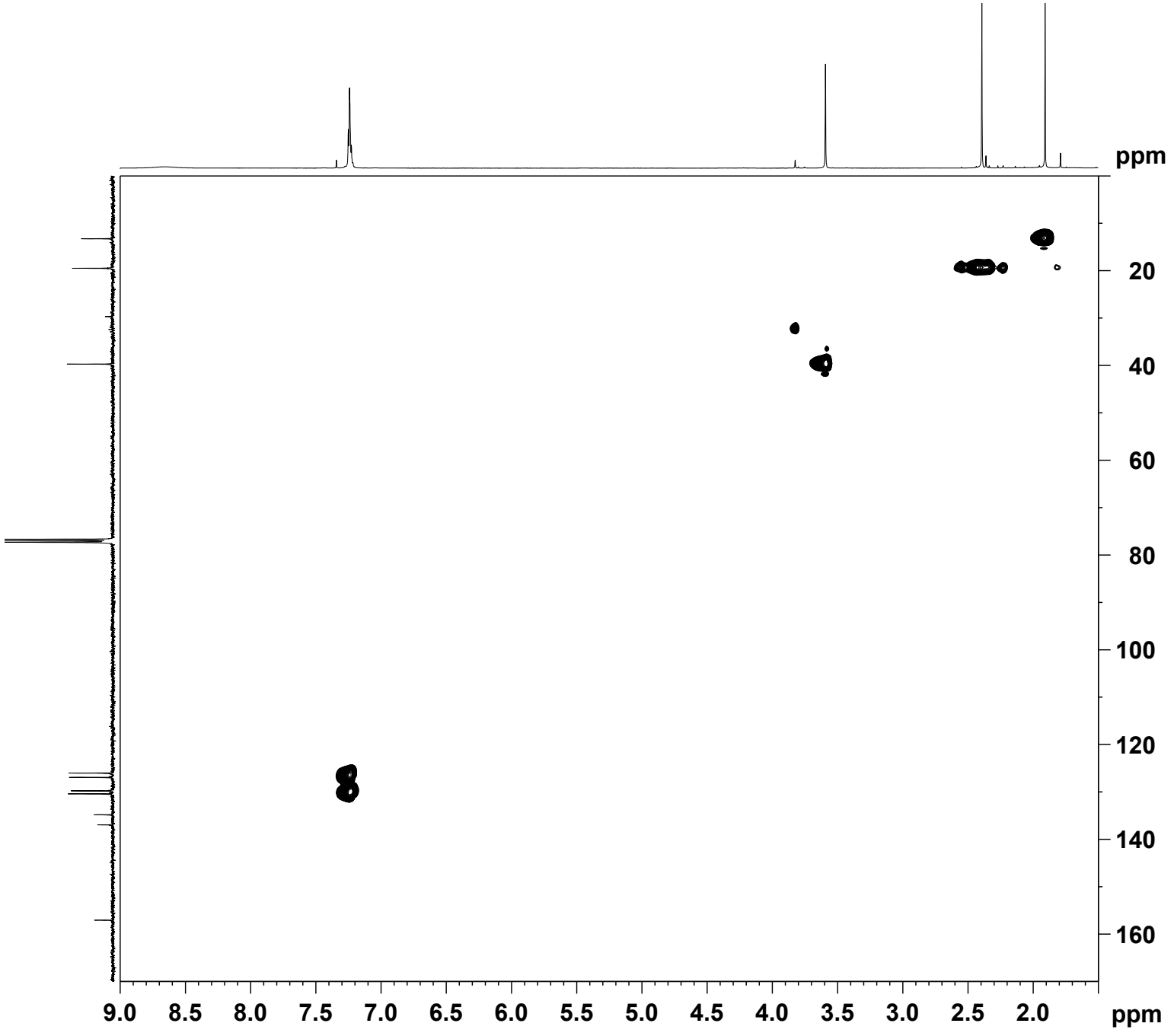



```
Current Data Parameters
NAME                  YYH-074
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210420
Time                   21.52 h
INSTRUM                 spect
PROBHD   Z108618_0922 (
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                        200
DS                          0
SWH                 24038.461 Hz
FIDRES               1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     296.7 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1
SFO1             100.6233329 MHz
NUC1                      13C
P1                     10.50 usec
PLW1               44.09999847 W
SFO2               400.1316005 MHz
NUC2                      1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2               14.30000019 W
PLW12               0.37118000 W
PLW13               0.18640999 W

F2 - Processing parameters
SI                      32768
SF                 100.6127729 MHz
WDW                        EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

HSQC of compound **2e**




```
Current Data Parameters
NAME             YYH-074
EXPNO                  6
PROCNO                 1

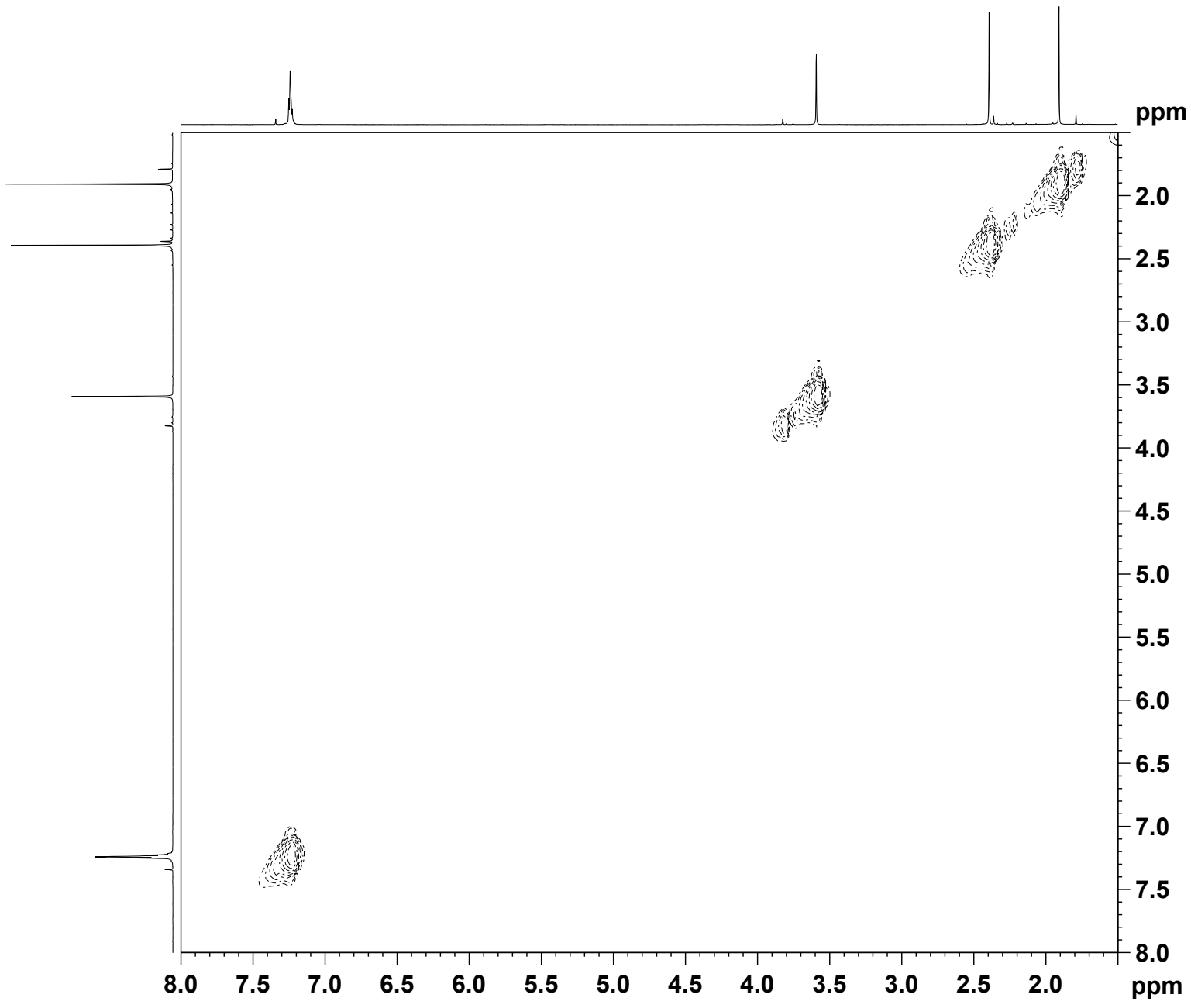
F2 - Acquisition Parameters
Date_           20210420
Time              19.55 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT             CDCl3
NS                     4
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
CNST2        145.0000000
CNST17        -0.5000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00002080 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         12.69999981 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2             garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0      0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3             0.500
SPOFFS3   0 Hz
SPW3          7.41179991 W
SPNAM[7]     Crp60comp.4
SPOAL7             0.500
SPOFFS7   0 Hz
SPW7          7.41179991 W
GPNAM[1]       SMSQ10.100
GPZ1                80.00 %
GPNAM[2]       SMSQ10.100
GPZ2                20.10 %
GPNAM[3]       SMSQ10.100
GPZ3                11.00 %
GPNAM[4]       SMSQ10.100
GPZ4                -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1299767 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127729 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

COSY of compound **2e**




```
Current Data Parameters
NAME             YYH-074
EXPNO                  7
PROCNO                 1

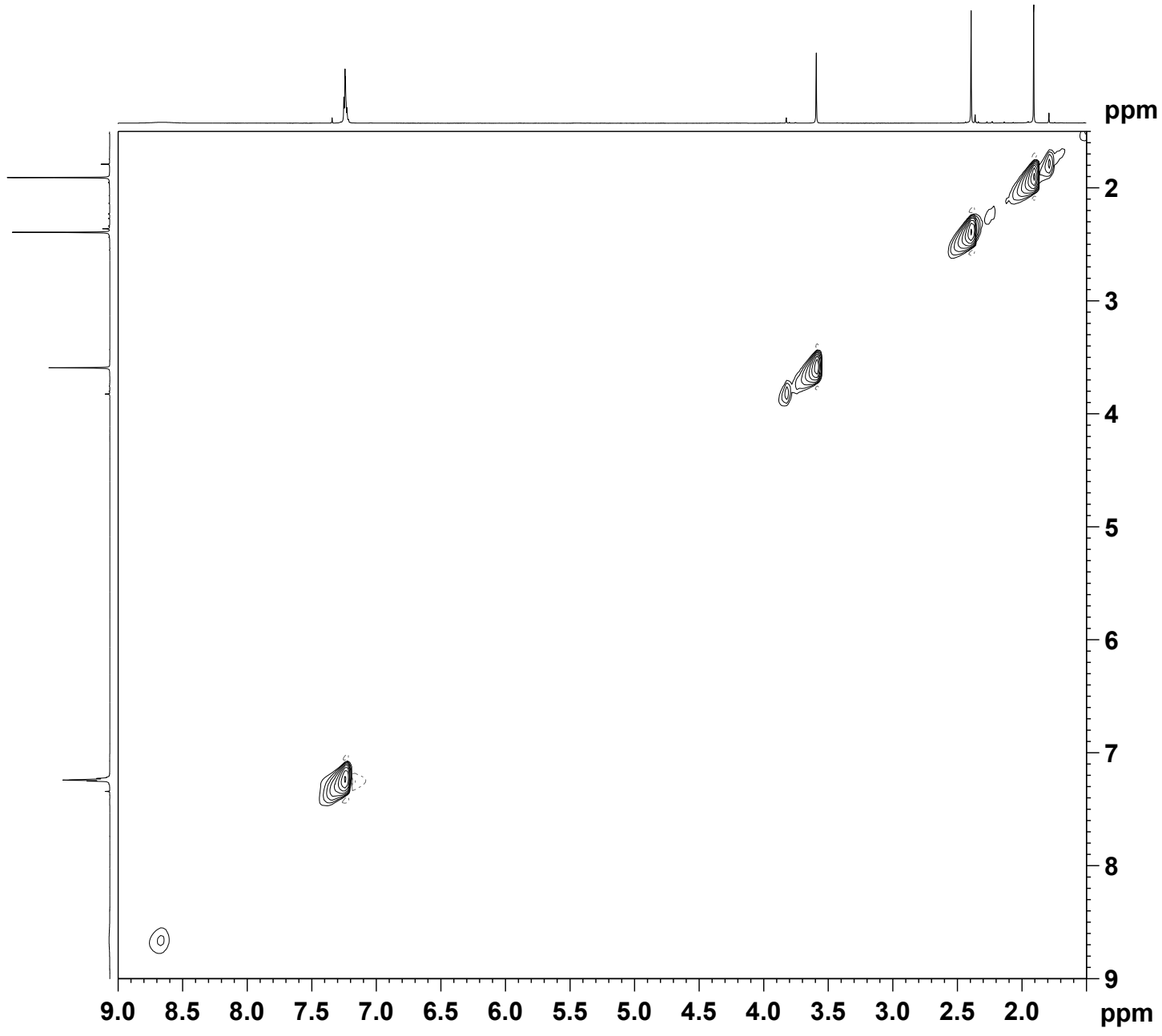
F2 - Acquisition Parameters
Date_           20210420
Time              20.24 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     4
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.3 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF           400.1299767 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF           400.1299767 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **2e**




```
Current Data Parameters
NAME             YYH-074
EXPNO                  8
PROCNO                 1

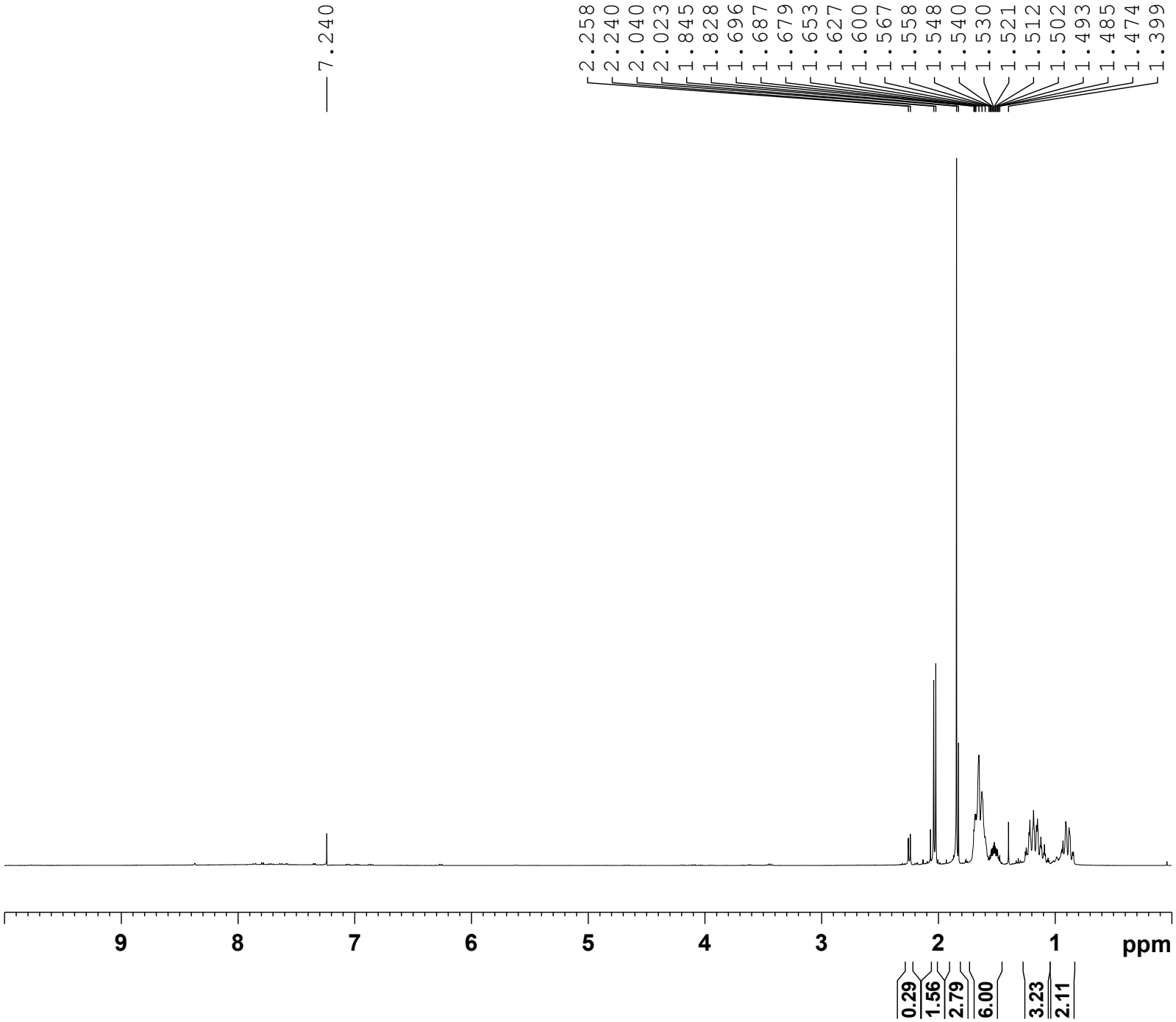
F2 - Acquisition Parameters
Date_           20210420
Time              21.02 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG     noesygpphpp
TD                  2048
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                112.98
DW                62.400 usec
DE                 6.50 usec
TE                295.8 K
D0             0.00004394 sec
D1             2.00000000 sec
D8             0.40000001 sec
D11            0.03000000 sec
D12            0.00002000 sec
D16            0.00020000 sec
IN0            0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                14.50 usec
P2                29.00 usec
P17             2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1              40.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1           400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                  1024
SF           400.1299767 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2          States-TPPI
SF           400.1299767 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

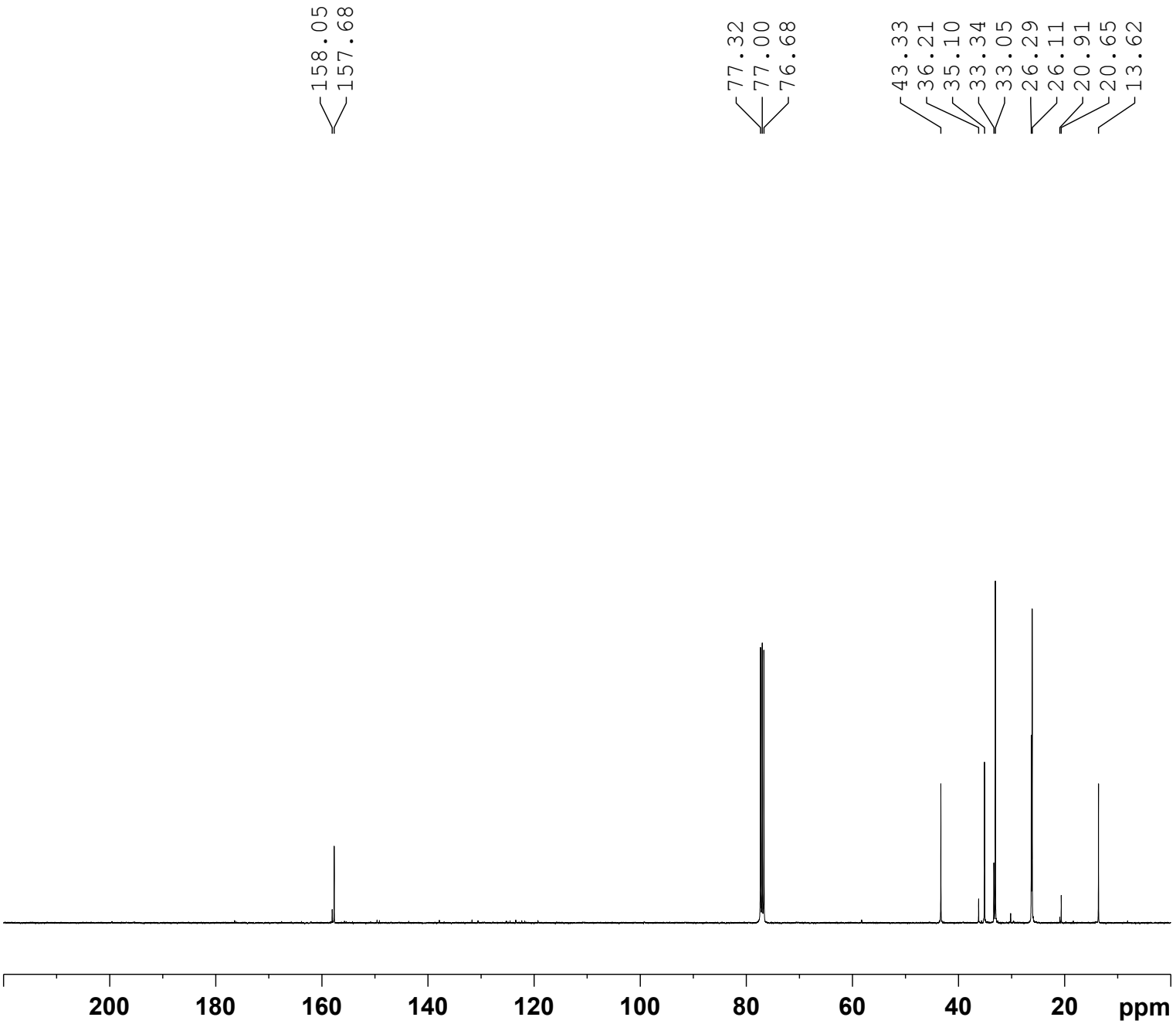
1H NMR (CDCl3, 400 MHz) of compound **2f**




```
Current Data Parameters
NAME                  YYH-069
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210522
Time                   22.07 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                    63.35
DW                   62.400 usec
DE                   16.43 usec
TE                   296.3 K
D1                2.00000000 sec
TD0                         1
SFO1            400.1324008 MHz
NUC1                       1H
P1                    14.50 usec
PLW1            13.10000038 W

F2 - Processing parameters
SI                      16384
SF              400.1300173 MHz
WDW                        EM
SSB       0
LB        0 Hz
GB        0
PC                      1.00
```

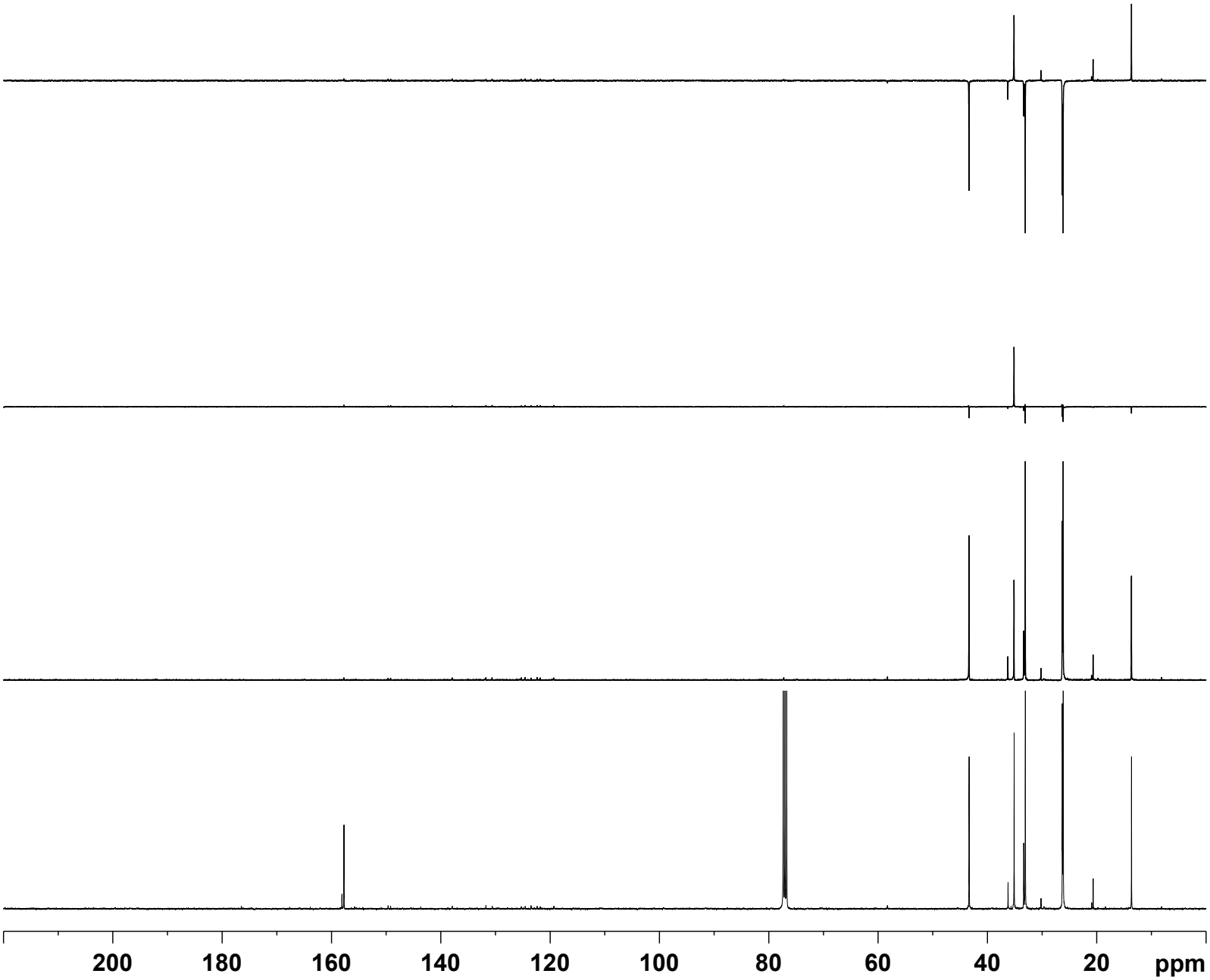



```
Current Data Parameters
NAME                  YYH-069
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210523
Time                     0.48 h
INSTRUM                  spect
PROBHD   Z108618_0922 (
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                        3500
DS                           0
SWH                  24038.461 Hz
FIDRES                1.467191 Hz
AQ                    0.6815744 sec
RG                       210.28
DW                       20.800 usec
DE                        6.50 usec
TE                       297.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1
SFO1               100.6233329 MHz
NUC1                        13C
P1                       10.50 usec
PLW1               44.29999924 W
SFO2               400.1316005 MHz
NUC2                        1H
CPDPRG[2 bi_waltz65_256
PCPD2                    90.00 usec
PLW2               14.60000038 W
PLW12               0.37897000 W
PLW13               0.19032000 W

F2 - Processing parameters
SI                       32768
SF                 100.6127715 MHz
WDW                         EM
SSB          0
LB                        2.00 Hz
GB           0
PC                        1.00
```

13C NMR (CDCl3, 100 MHz) of compound **2f**



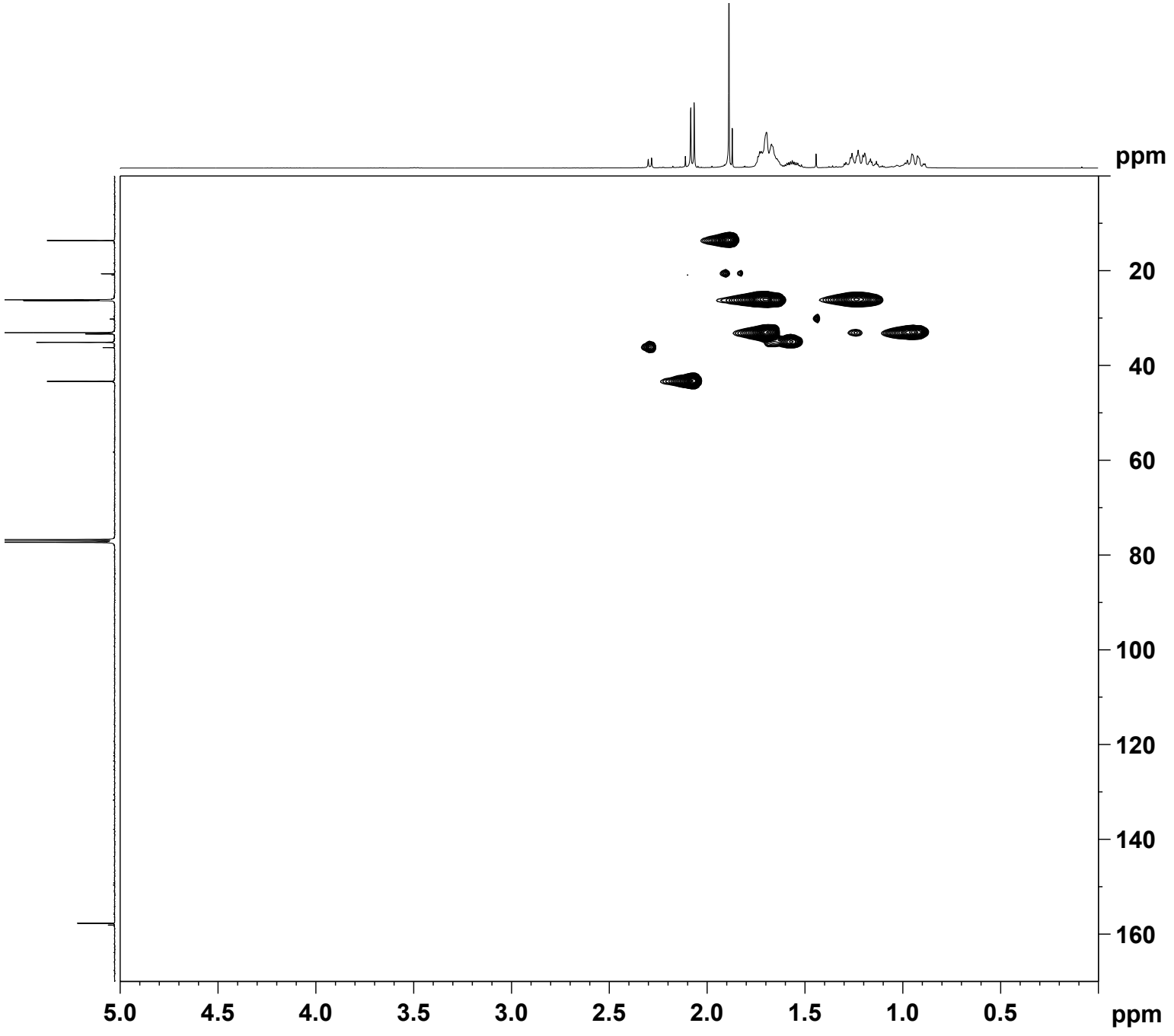

```
Current Data Parameters
NAME                  YYH-069
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210523
Time                     0.48 h
INSTRUM                 spect
PROBHD   Z108618_0922 (
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                        3500
DS                           0
SWH                  24038.461 Hz
FIDRES                1.467191 Hz
AQ                   0.6815744 sec
RG                       210.28
DW                       20.800 usec
DE                        6.50 usec
TE                       297.4 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1
SFO1               100.6233329 MHz
NUC1                        13C
P1                       10.50 usec
PLW1                44.29999924 W
SFO2               400.1316005 MHz
NUC2                        1H
CPDPRG[2 bi_waltz65_256
PCPD2                    90.00 usec
PLW2                14.60000038 W
PLW12                0.37897000 W
PLW13                0.19032000 W

F2 - Processing parameters
SI                       32768
SF                 100.6127685 MHz
WDW                         EM
SSB       0
LB                        2.00 Hz
GB        0
PC                        1.00
```

DEPT of compound **2f**

HSQC of compound **2f**




```
Current Data Parameters
NAME            YYH-069
EXPNO                 6
PROCNO                1

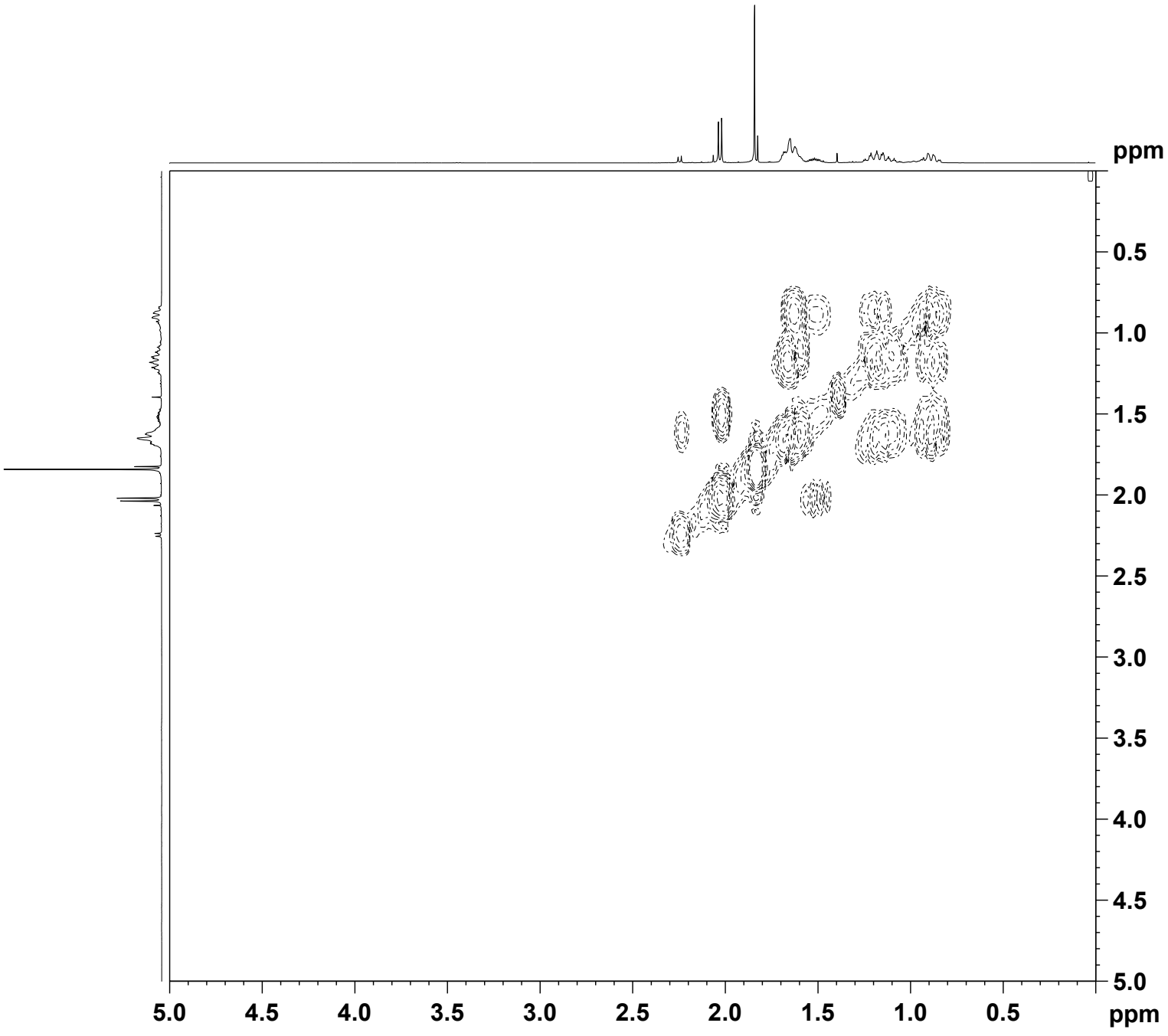
F2 - Acquisition Parameters
Date_          20210612
Time              15.34 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                 2048
SOLVENT            CDCl3
NS                    6
DS                   16
SWH            8012.820 Hz
FIDRES         7.825020 Hz
AQ             0.1277952 sec
RG               210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.9 K
CNST2       145.0000000
CNST17       -0.5000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002080 sec
TDav                  1
SFO1        400.1324008 MHz
NUC1                 1H
P1                14.50 usec
P2                29.00 usec
P28             1000.00 usec
PLW1        13.10000038 W
SFO2        100.6233329 MHz
NUC2                13C
CPDPRG[2           garp
P3                10.50 usec
P14              500.00 usec
P24             2000.00 usec
PCPD2             80.00 usec
PLW0     0 W
PLW2        44.00000000 W
PLW12        0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3              0.500
SPOFFS3  0 Hz
SPW3         7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7              0.500
SPOFFS7  0 Hz
SPW7         7.41179991 W
GPNAM[1]      SMSQ10.100
GPZ1               80.00 %
GPNAM[2]      SMSQ10.100
GPZ2               20.10 %
GPNAM[3]      SMSQ10.100
GPZ3               11.00 %
GPNAM[4]      SMSQ10.100
GPZ4               -5.00 %
P16             1000.00 usec
P19              600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1           100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300000 MHz
WDW                 QSINE
SSB                     2
LB       0 Hz
GB       0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2       echo-antiecho
SF           100.6127685 MHz
WDW                 QSINE
SSB                     2
LB       0 Hz
GB       0
```

COSY of compound **2f**




```
Current Data Parameters
NAME             YYH-069
EXPNO                  7
PROCNO                 1

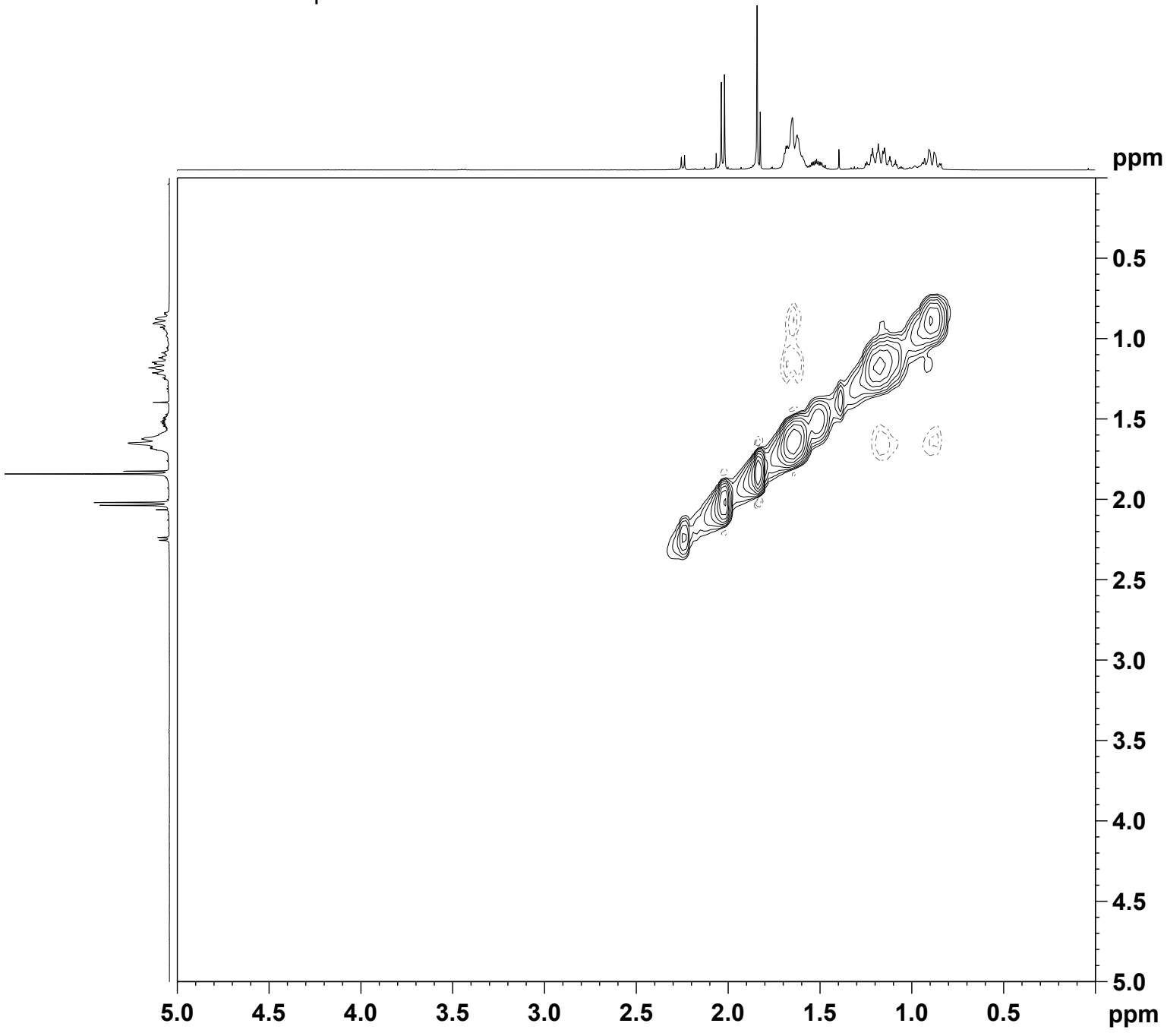
F2 - Acquisition Parameters
Date_           20210523
Time               7.15 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                103.85
DW                62.400 usec
DE                 6.50 usec
TE                296.6 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         13.10000038 W
PLW10         3.06030011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF          400.1300185 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF          400.1300185 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **2f**




```
Current Data Parameters
NAME                  YYH-069
EXPNO                       8
PROCNO                      1

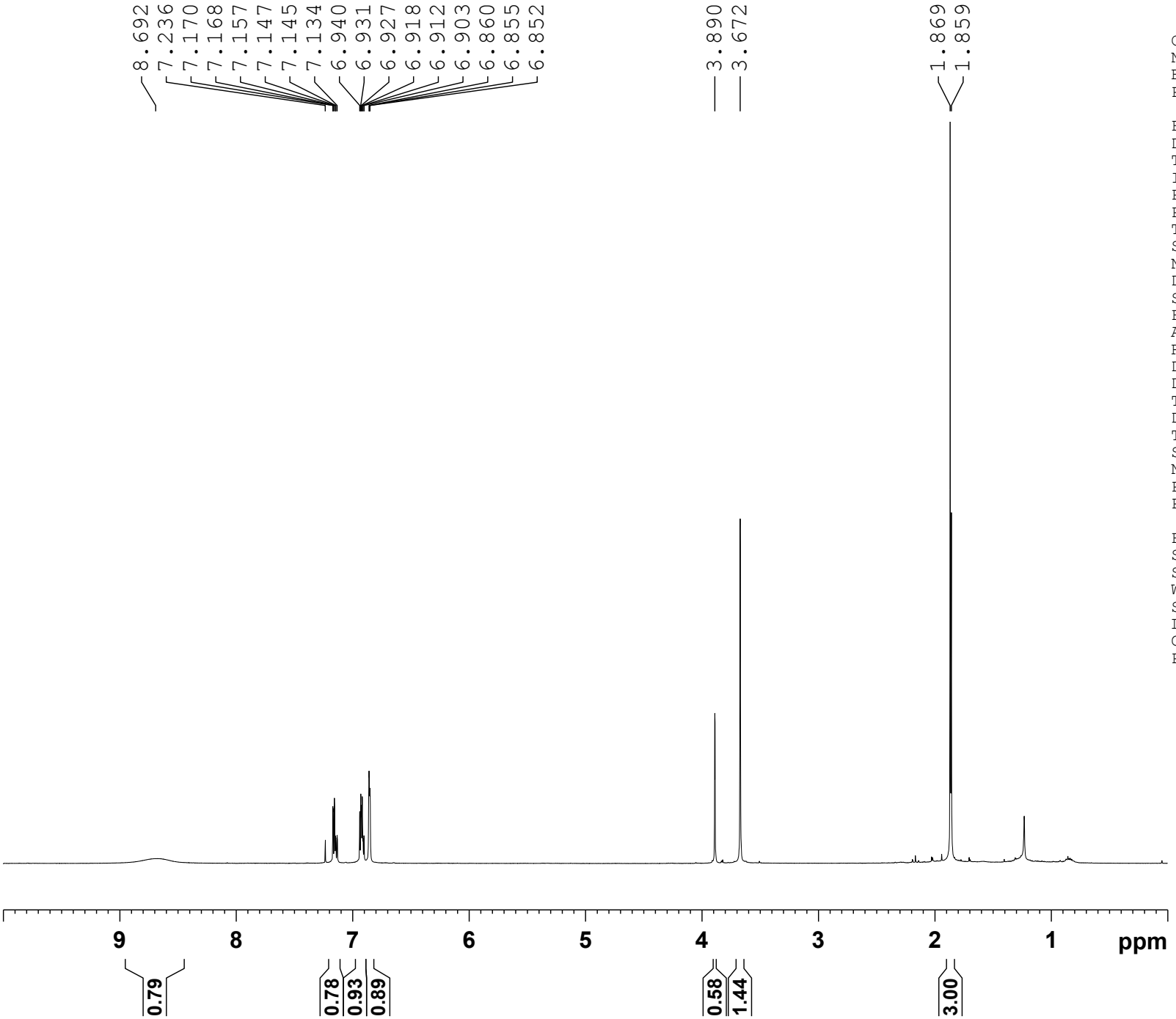
F2 - Acquisition Parameters
Date_               20210523
Time                    8.12 h
INSTRUM                 spect
PROBHD    Z108618_0922 (
PULPROG       noesygpphpp
TD                       2048
SOLVENT                 CDCl3
NS                          6
DS                         16
SWH                 8012.820 Hz
FIDRES              7.825020 Hz
AQ                  0.1277952 sec
RG                      63.35
DW                     62.400 usec
DE                      6.50 usec
TE                     296.0 K
D0                  0.00004394 sec
D1                  2.00000000 sec
D8                  0.40000001 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D16                 0.00020000 sec
IN0                 0.00012480 sec
TDav                        1
SFO1              400.1324008 MHz
NUC1                       1H
P1                      14.50 usec
P2                      29.00 usec
P17                   2500.00 usec
PLW1              13.10000038 W
PLW10              3.06030011 W
GPNAM[1]          SMSQ10.100
GPZ1                    40.00 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                          256
SFO1                400.1324 MHz
FIDRES             62.600159 Hz
SW                    20.025 ppm
FnMODE           States-TPPI

F2 - Processing parameters
SI                         1024
SF                400.1300185 MHz
WDW                       QSINE
SSB                          2
LB             0 Hz
GB             0
PC                        1.40

F1 - Processing parameters
SI                         1024
MC2              States-TPPI
SF                400.1300185 MHz
WDW                       QSINE
SSB                          2
LB             0 Hz
GB             0
```

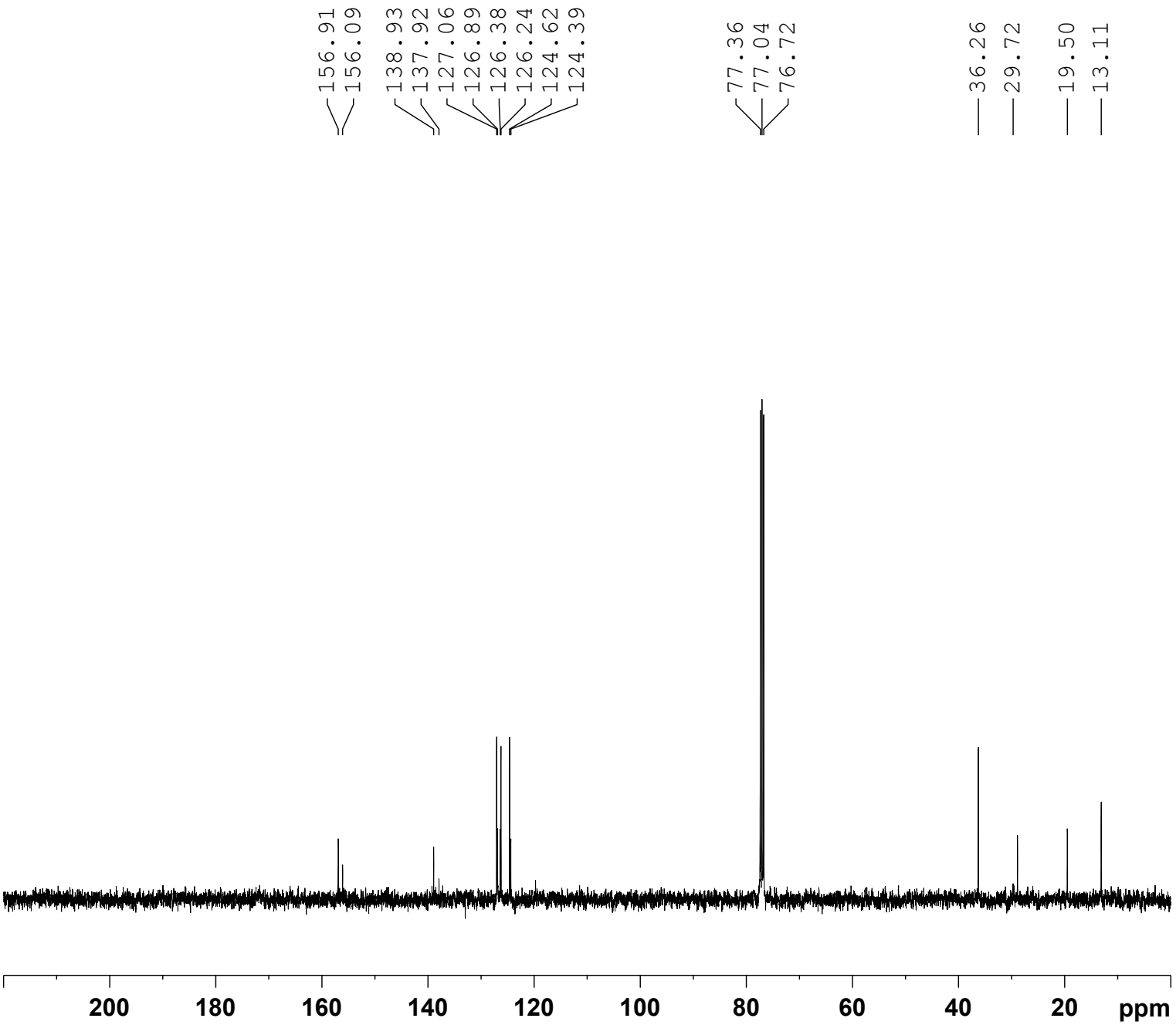
1H NMR (CDCl3, 400 MHz) of compound **2g**




```
Current Data Parameters
NAME                  YYH-070
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210419
Time                   16.54 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                     128.5
DW                    62.400 usec
DE                    16.43 usec
TE                    295.8 K
D1                2.00000000 sec
TD0                         1
SFO1            400.1324008 MHz
NUC1                       1H
P1                    14.50 usec
PLW1            12.69999981 W

F2 - Processing parameters
SI                      16384
SF              400.1300195 MHz
WDW                        EM
SSB       0
LB        0 Hz
GB        0
PC                      1.00
```

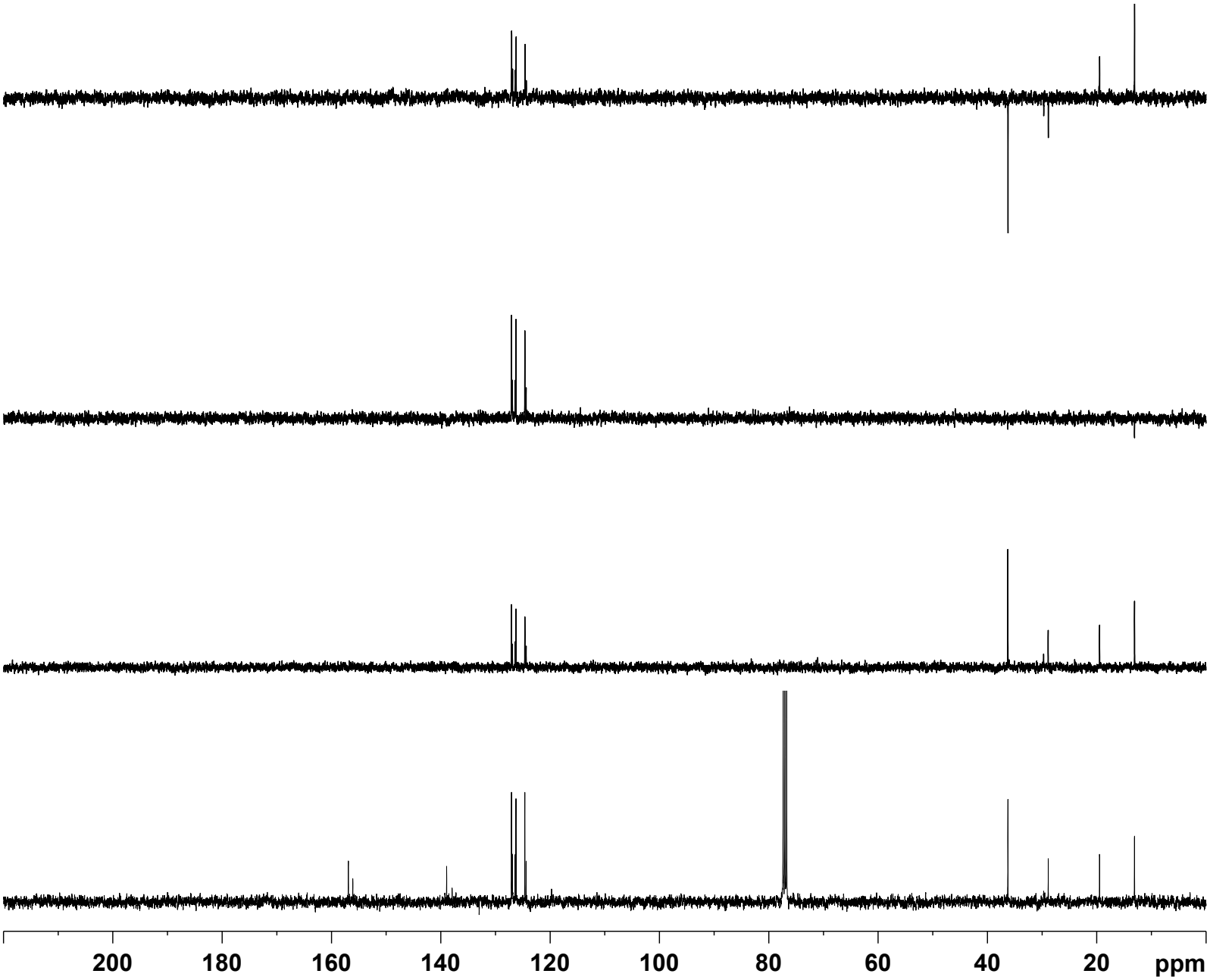



```
Current Data Parameters
NAME                 YYH-070
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210419
Time                  16.57 h
INSTRUM               spect
PROBHD   Z108618_0922 (
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                       64
DS                        0
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                 0.6815744 sec
RG                    210.28
DW                    20.800 usec
DE                     6.50 usec
TE                    296.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1
SFO1           100.6233329 MHz
NUC1                   13C
P1                    10.50 usec
PLW1           44.09999847 W
SFO2           400.1316005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2                 90.00 usec
PLW2           14.30000019 W
PLW12           0.37118000 W
PLW13           0.18640999 W

F2 - Processing parameters
SI                    32768
SF             100.6127685 MHz
WDW                     EM
SSB       0
LB                     2.00 Hz
GB        0
PC                     1.00
```

13C NMR (CDCl3, 100 MHz) of compound **2g**



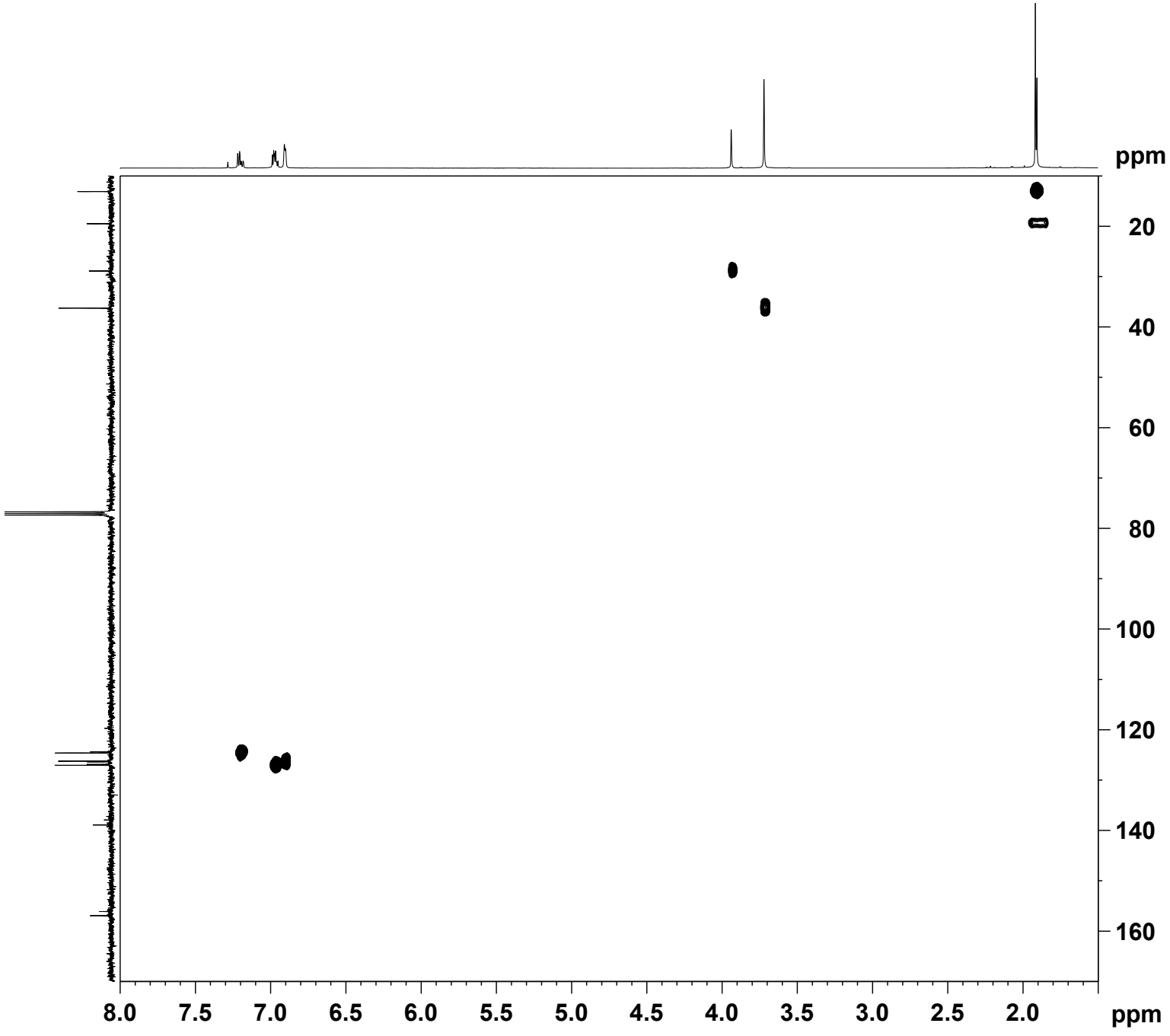

```
Current Data Parameters
NAME                  YYH-070
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210419
Time                   16.57 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG                zgpg30
TD                     32768
SOLVENT                CDCl3
NS                        64
DS                         0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     296.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             100.6233329 MHz
NUC1                     13C
P1                     10.50 usec
PLW1              44.09999847 W
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2              14.30000019 W
PLW12              0.37118000 W
PLW13              0.18640999 W

F2 - Processing parameters
SI                     32768
SF               100.6127685 MHz
WDW                       EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

DEPT of compound **2g**

HSQC of compound **2g**




```
Current Data Parameters
NAME             YYH-070
EXPNO                  6
PROCNO                 1

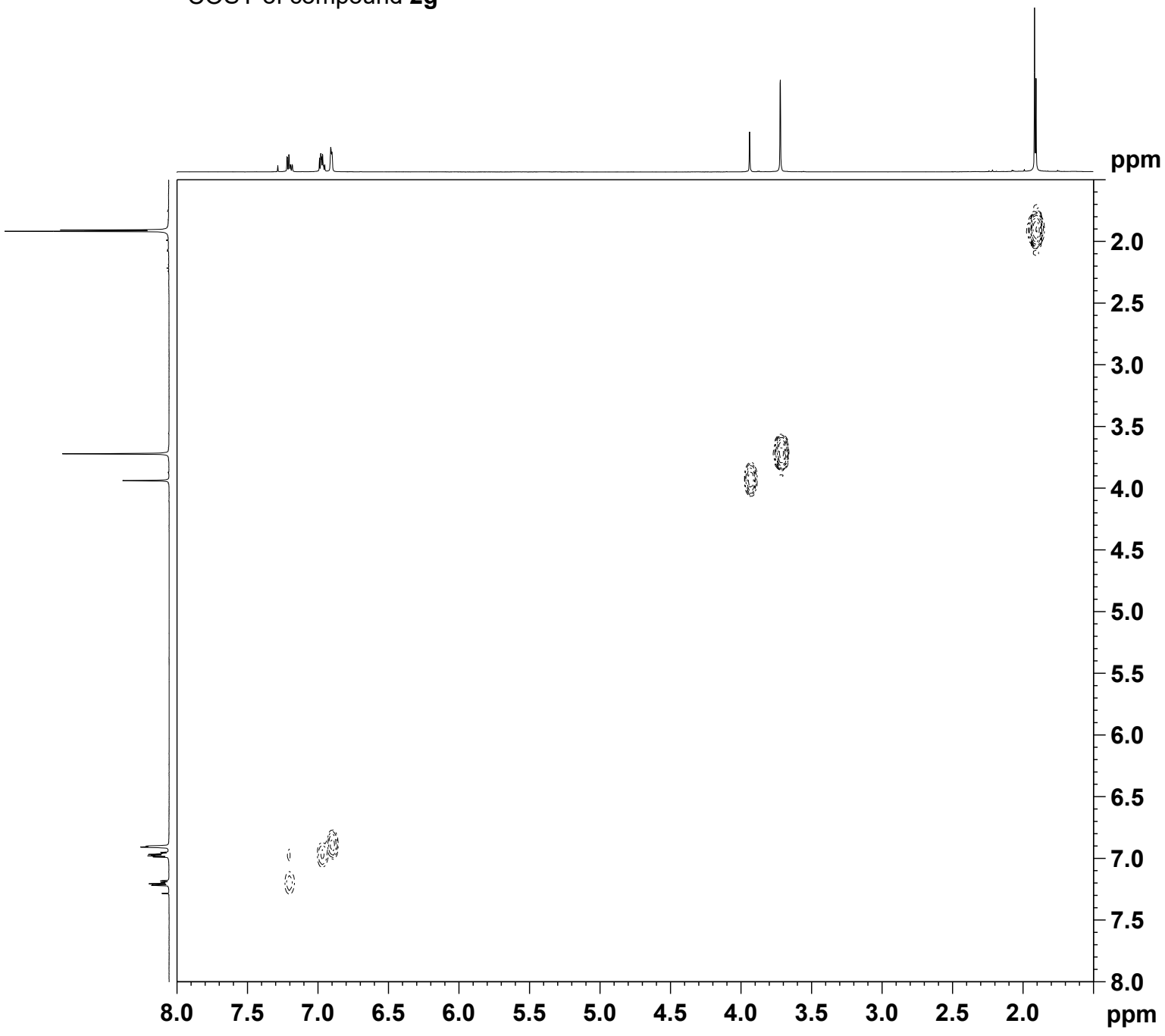
F2 - Acquisition Parameters
Date_           20210419
Time              18.38 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                295.8 K
CNST2        145.0000000
CNST17        -0.5000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00002080 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         12.69999981 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2            garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0      0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3             0.500
SPOFFS3   0 Hz
SPW3          7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7             0.500
SPOFFS7   0 Hz
SPW7          7.41179991 W
GPNAM[1]      SMSQ10.100
GPZ1               80.00 %
GPNAM[2]      SMSQ10.100
GPZ2               20.10 %
GPNAM[3]      SMSQ10.100
GPZ3               11.00 %
GPNAM[4]      SMSQ10.100
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300000 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127685 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

COSY of compound **2g**




```
Current Data Parameters
NAME             YYH-070
EXPNO                  7
PROCNO                 1

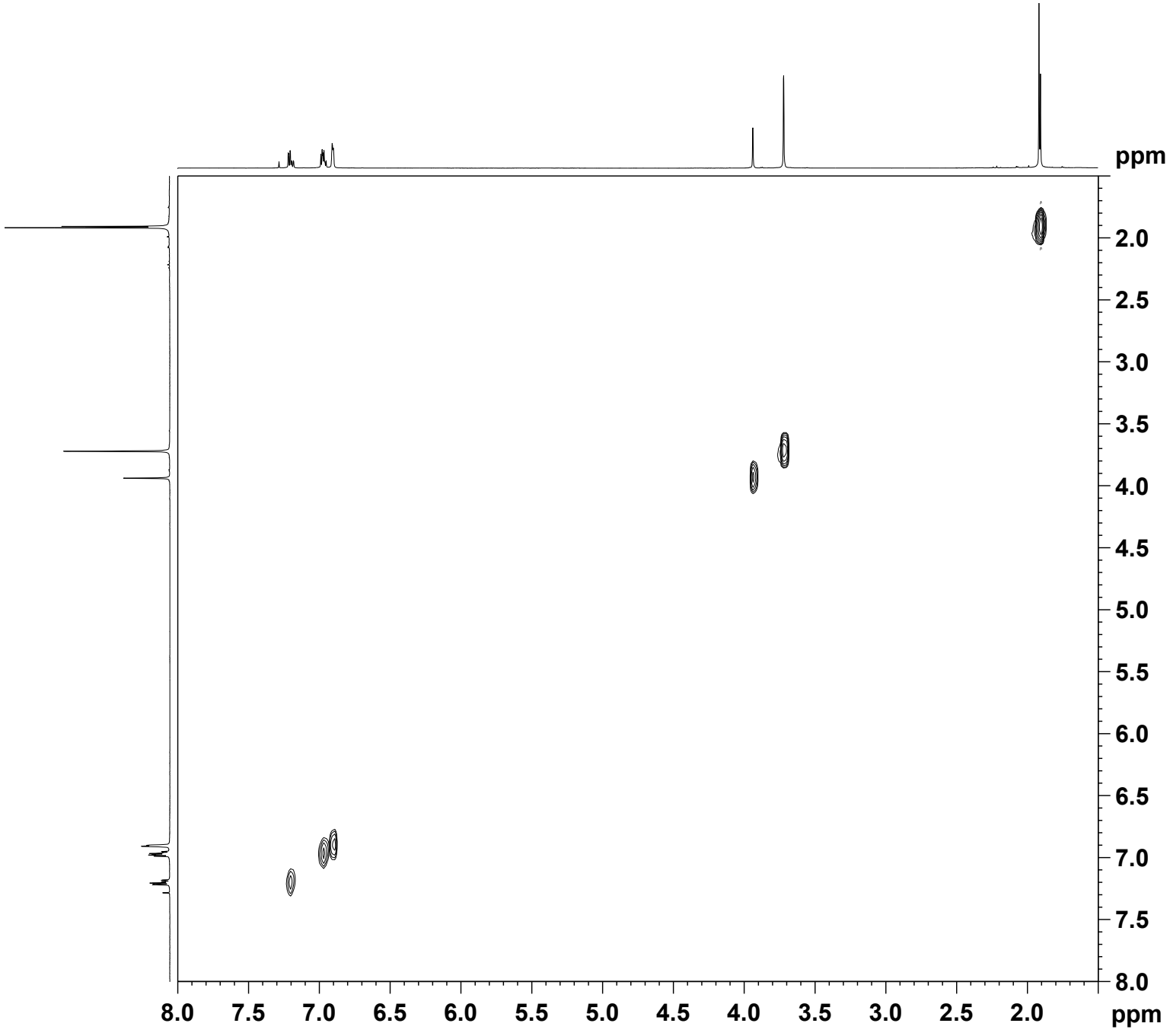
F2 - Acquisition Parameters
Date_           20210419
Time              17.04 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     4
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.2 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **2g**




```
Current Data Parameters
NAME             YYH-070
EXPNO                  8
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210419
Time              17.42 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG     noesygpphpp
TD                  2048
SOLVENT            CDCl3
NS                     5
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                 112.98
DW                 62.400 usec
DE                   6.50 usec
TE                  295.7 K
D0              0.00004394 sec
D1              2.00000000 sec
D8              0.40000001 sec
D11             0.03000000 sec
D12             0.00002000 sec
D16             0.00020000 sec
IN0             0.00012480 sec
TDav                   1
SFO1          400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P17              2500.00 usec
PLW1          12.69999981 W
PLW10          2.96690011 W
GPNAM[1]       SMSQ10.100
GPZ1                40.00 %
P16               1000.00 usec

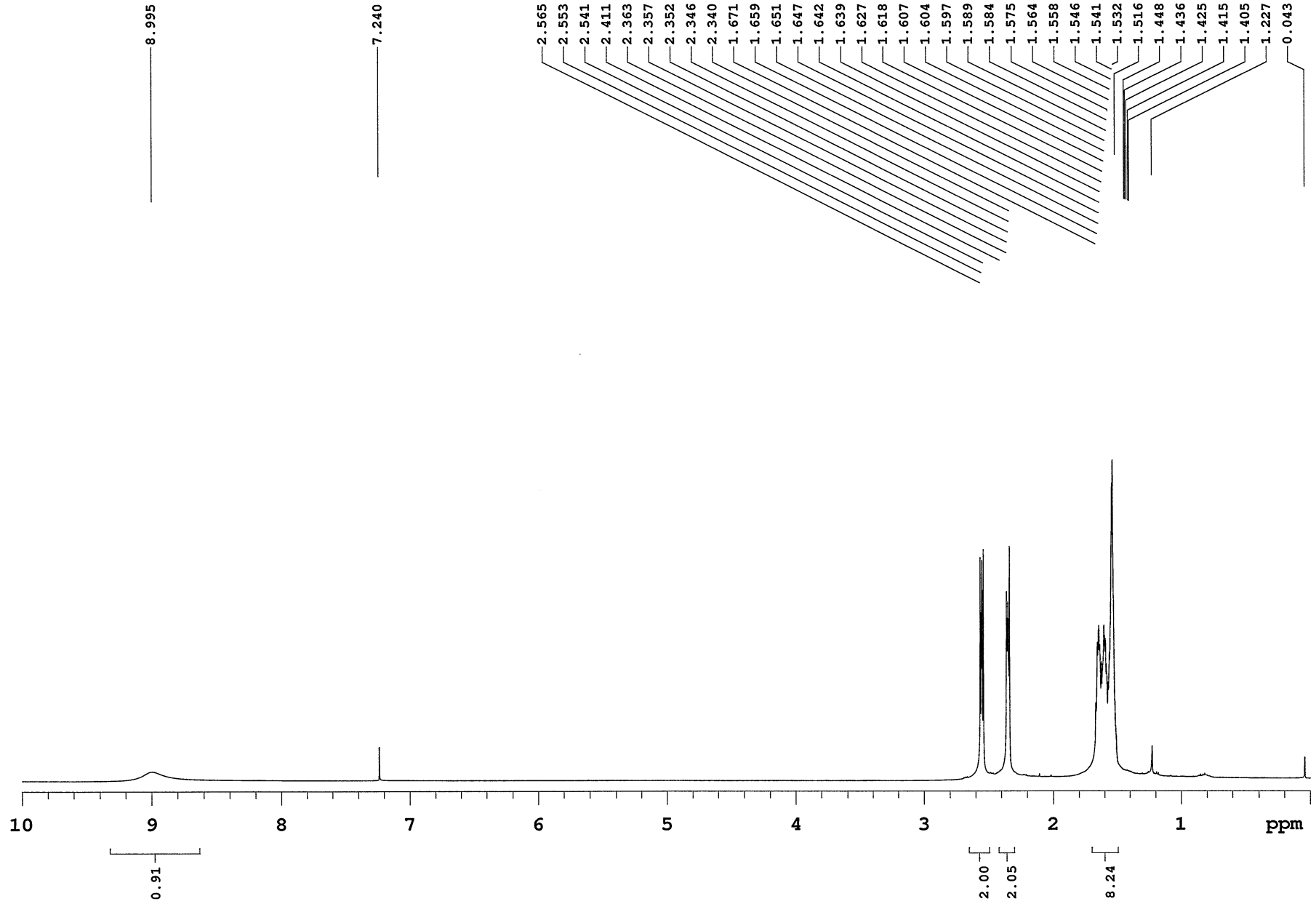
F1 - Acquisition parameters
TD                     256
SFO1            400.1324 MHz
FIDRES          62.600159 Hz
SW                20.025 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                    1024
SF            400.1300000 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2           States-TPPI
SF            400.1300000 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
```

YYH-071

Sample Name **YYH-071**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-05-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



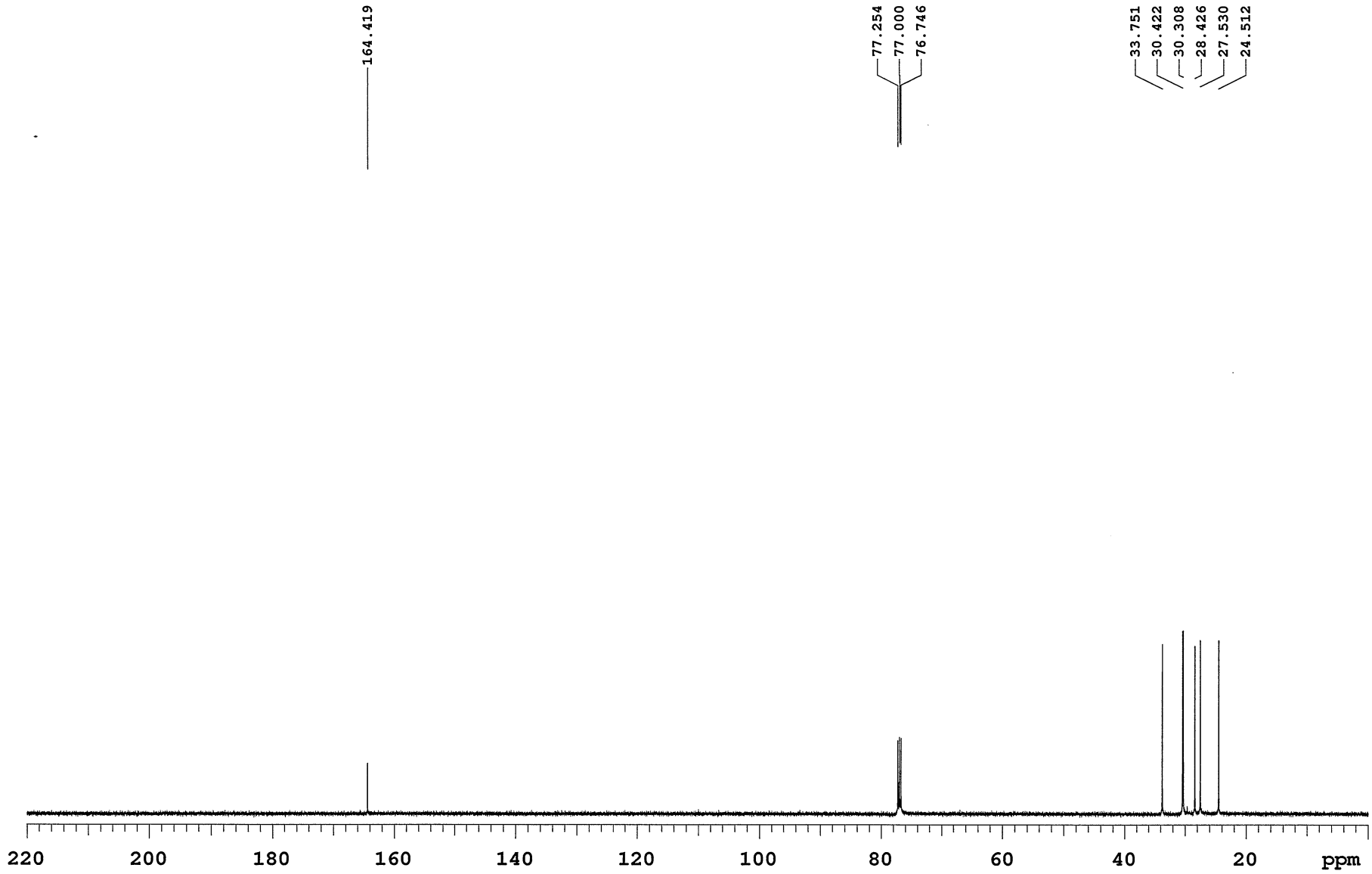
1H NMR (CDCl3, 500 MHz) of compound **2h**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-071/PROTON_03

Plot date 2021-05-28

YYH-071

Sample Name **YYH-071**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-05-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



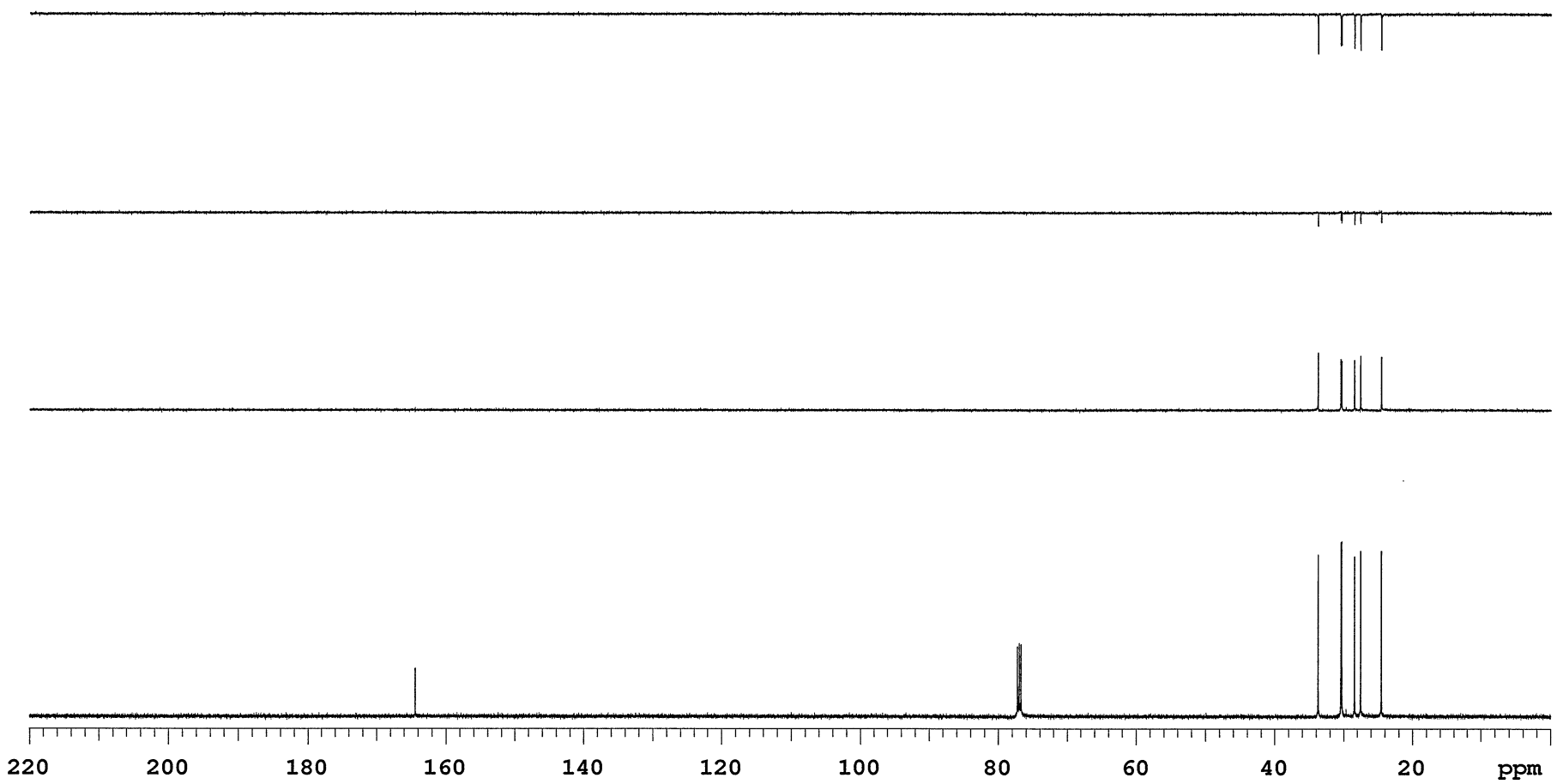
13C NMR (CDCl3, 125 MHz) of compound **2h**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-071/CARBON_02

Plot date 2021-05-27

YYH-071

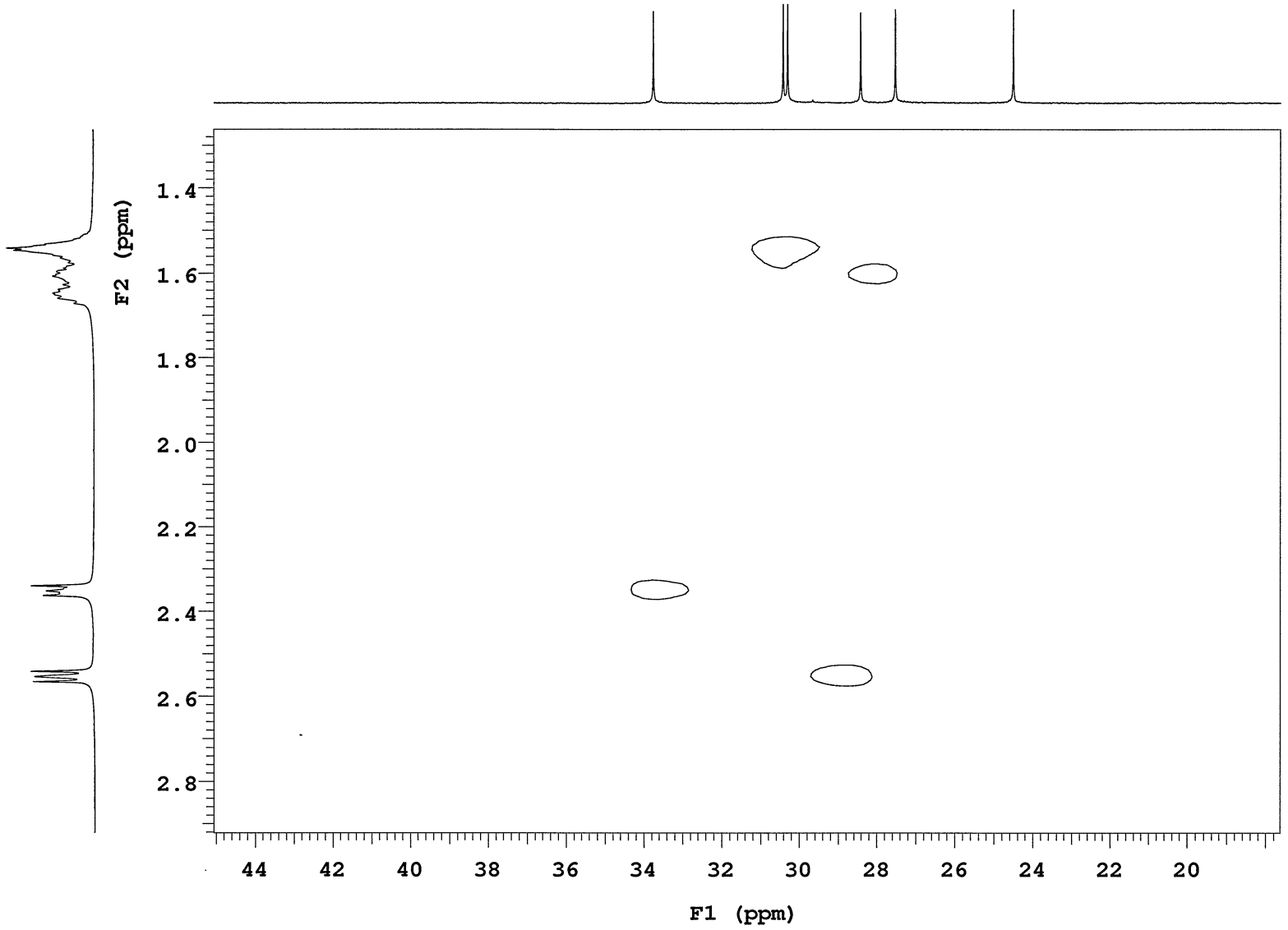
Sample Name **YYH-071**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-05-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **2h**

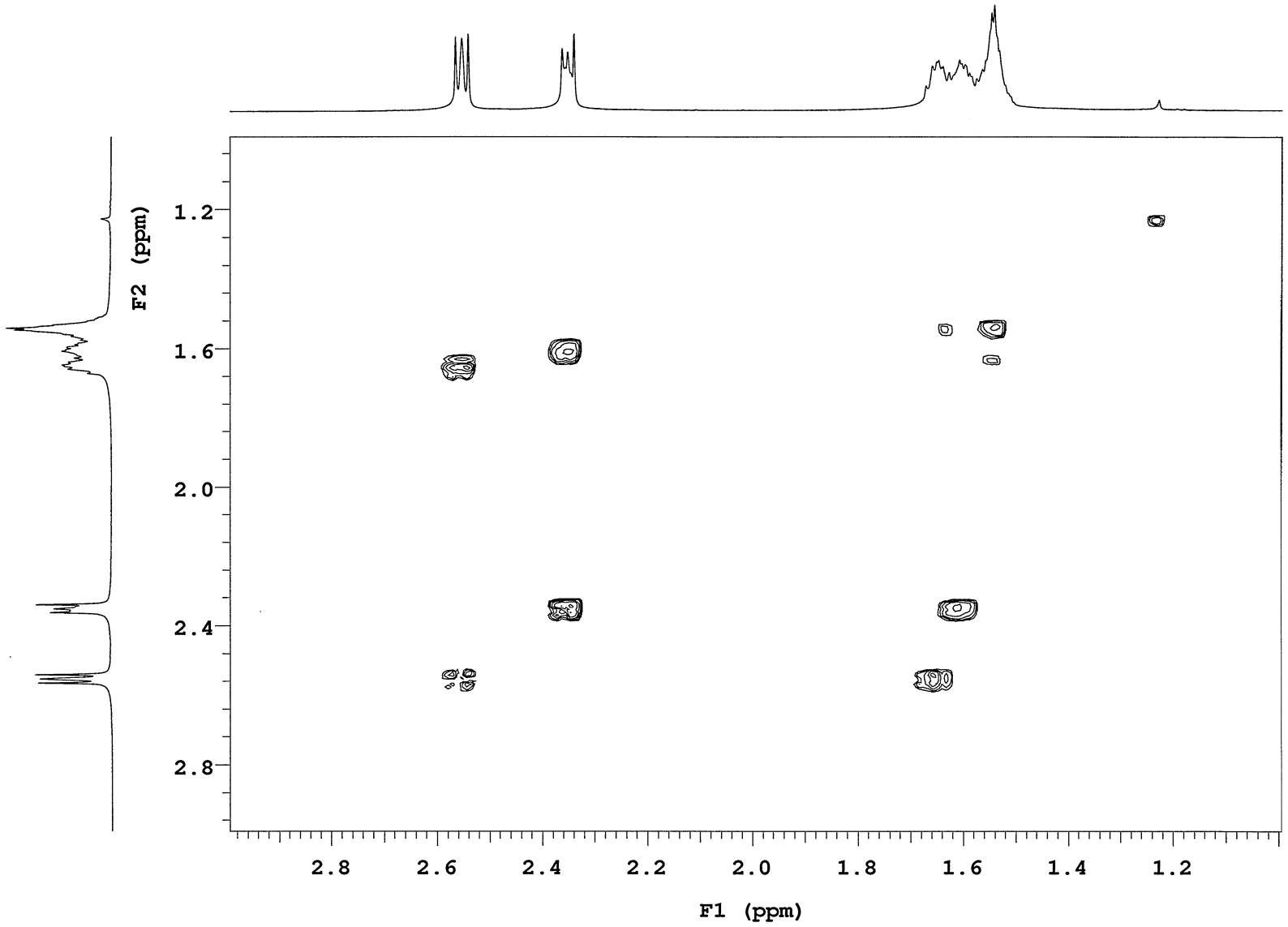
YYH-071

Sample Name **YYH-071**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-05-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



HSQC of compound **2h**

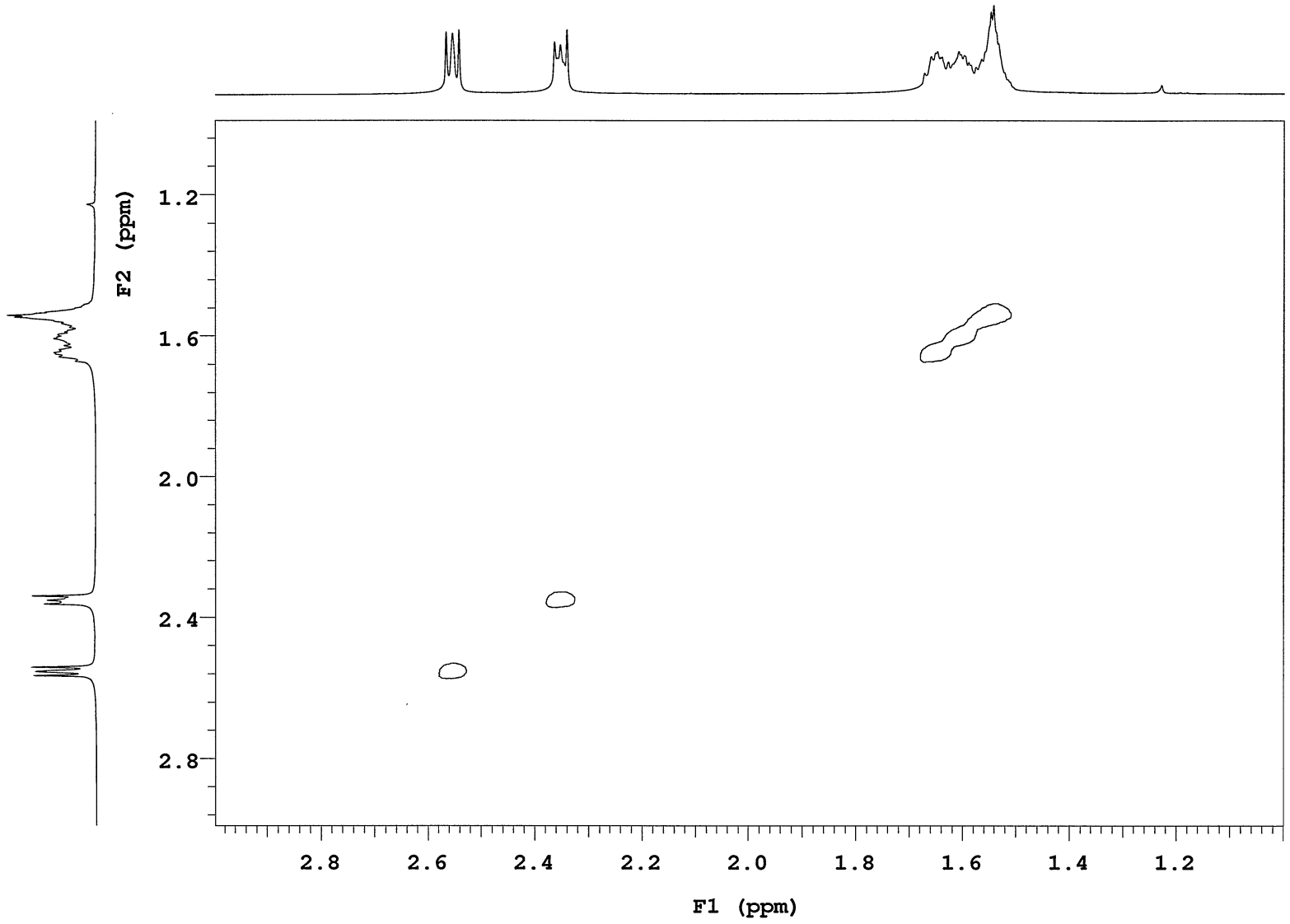
Sample Name **YYH-071**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-05-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



COSY of compound **2h**

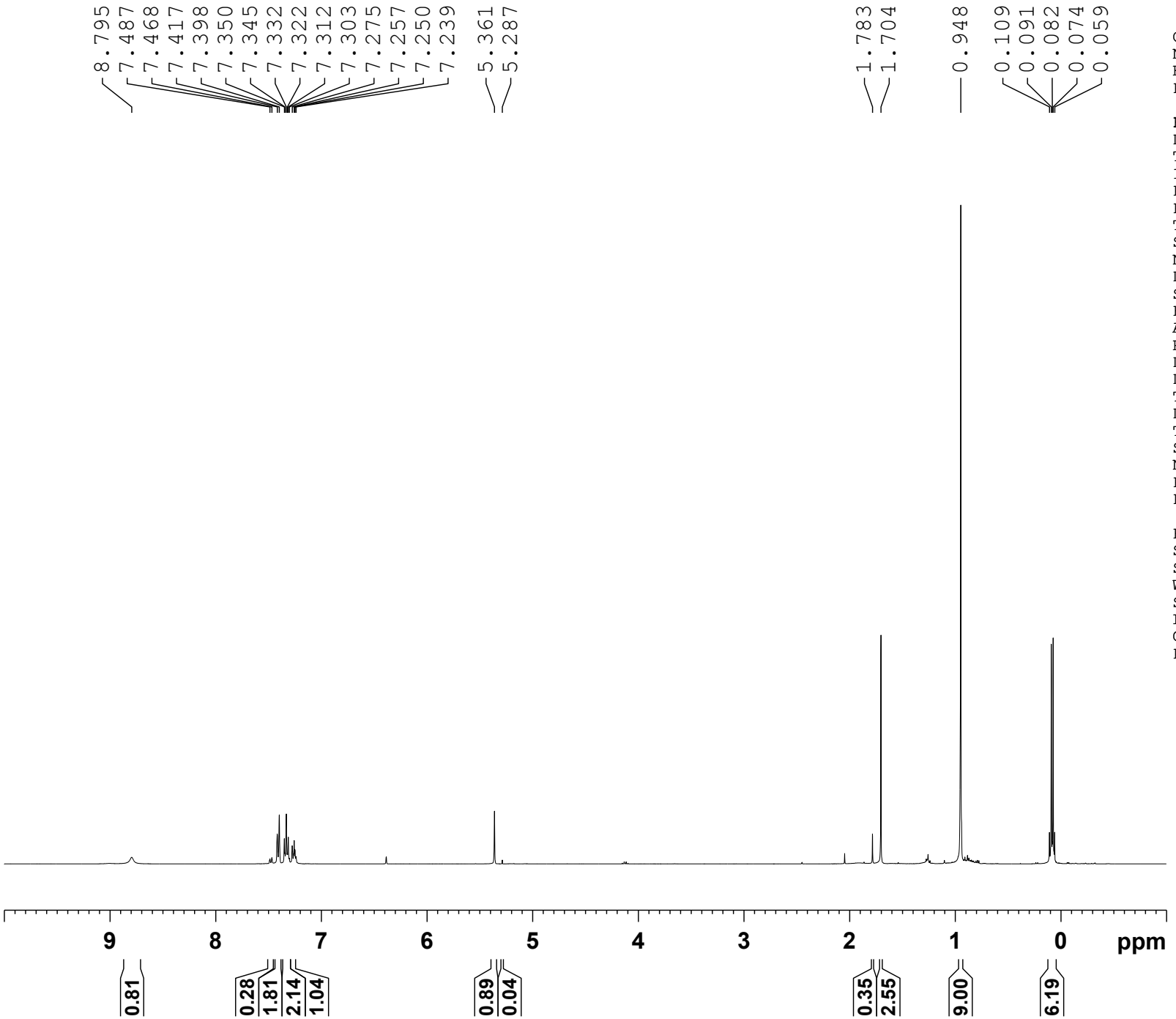
YYH-071

Sample Name **YYH-071**	Pulse sequence **NOESY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-05-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



NOESY of compound **2h**

1H NMR (CDCl3, 400 MHz) of compound **2i**

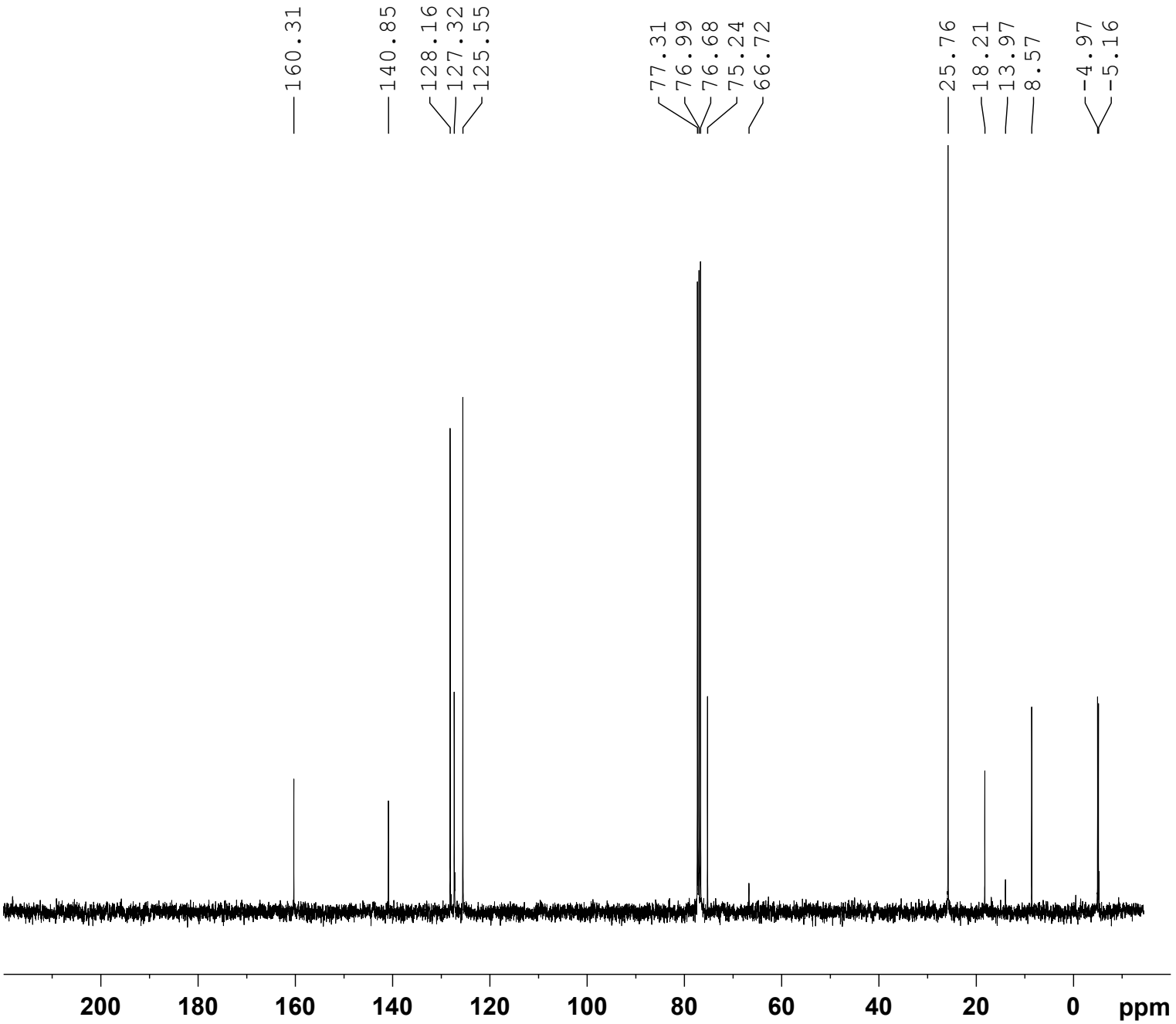



```
Current Data Parameters
NAME                  YYH-075
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20210427
Time                   9.51 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                     63.35
DW                    62.400 usec
DE                    16.43 usec
TE                    295.9 K
D1                2.00000000 sec
TD0                        1
SFO1            400.1324008 MHz
NUC1                      1H
P1                    14.50 usec
PLW1            12.69999981 W

F2 - Processing parameters
SI                     16384
SF              400.1300137 MHz
WDW                       EM
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```

13C NMR (CDCl3, 100 MHz) of compound **2i**

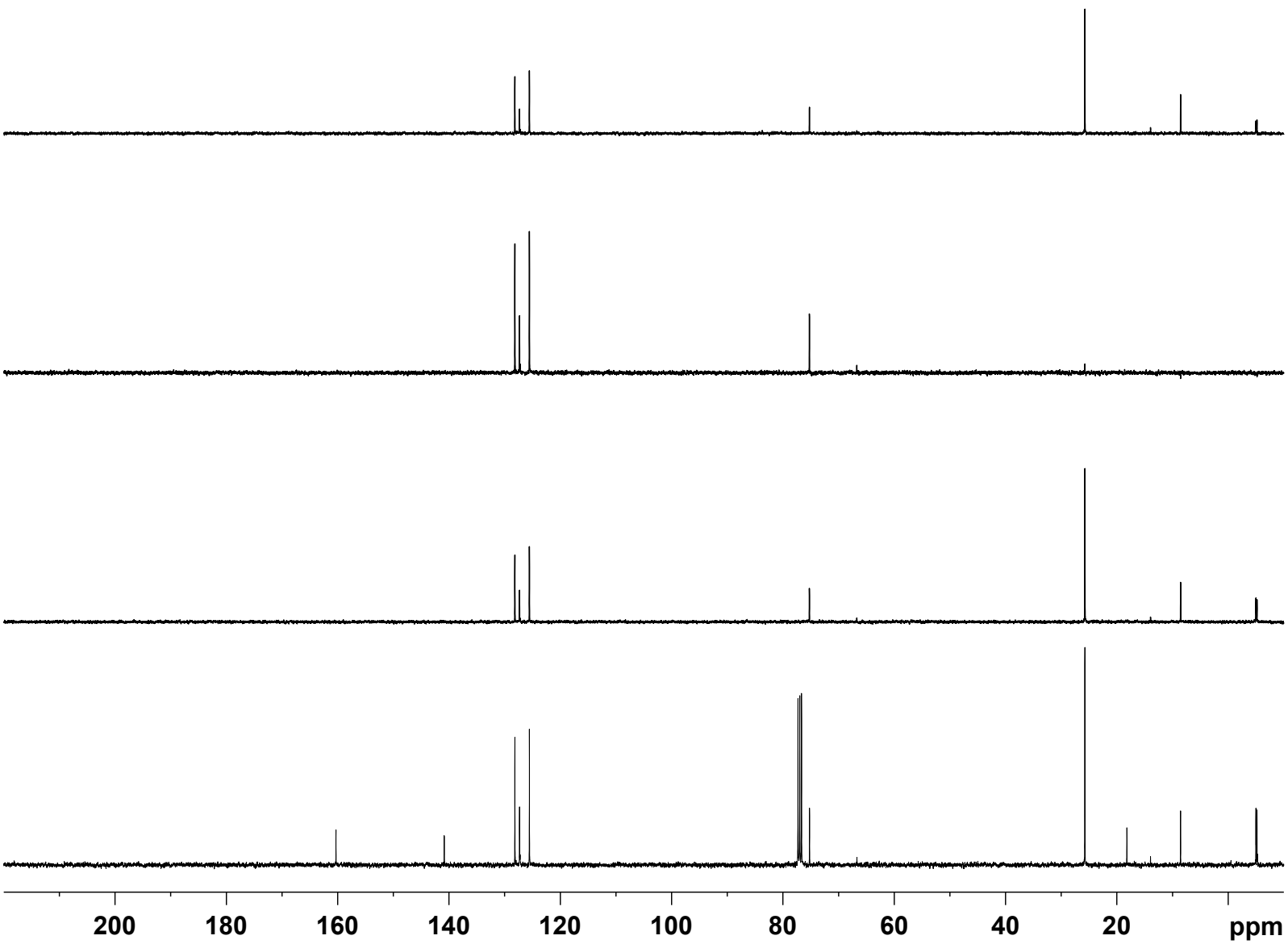



```
Current Data Parameters
NAME                 YYH-075
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210427
Time                  10.04 h
INSTRUM               spect
PROBHD   Z108618_0922 (
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                       64
DS                        0
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                0.6815744 sec
RG                   210.28
DW                   20.800 usec
DE                    6.50 usec
TE                   296.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1
SFO1           100.6233329 MHz
NUC1                   13C
P1                   10.50 usec
PLW1           44.09999847 W
SFO2           400.1316005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2           14.30000019 W
PLW12           0.37118000 W
PLW13           0.18640999 W

F2 - Processing parameters
SI                    32768
SF             100.6127731 MHz
WDW                     EM
SSB       0
LB                    2.00 Hz
GB        0
PC                    1.00
```

DEPT of compound **2i**

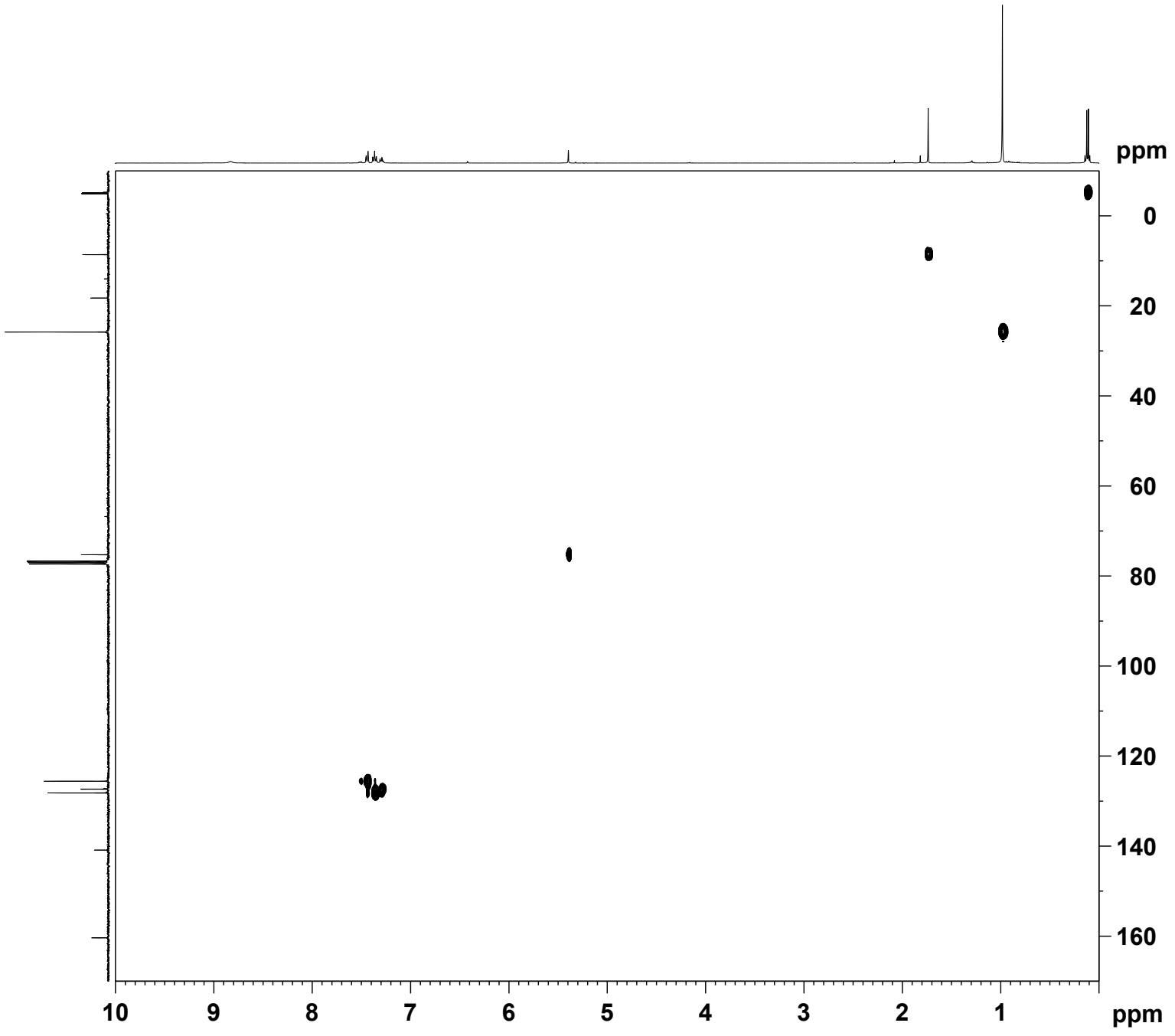



```
Current Data Parameters
NAME            YYH-075
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210427
Time              10.04 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1                10.50 usec
PLW1         44.09999847 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2         14.30000019 W
PLW12         0.37118000 W
PLW13         0.18640999 W

F2 - Processing parameters
SI                32768
SF          100.6127736 MHz
WDW                 EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

HSQC of compound **2i**




```
Current Data Parameters
NAME              YYH-075
EXPNO                   6
PROCNO                  1

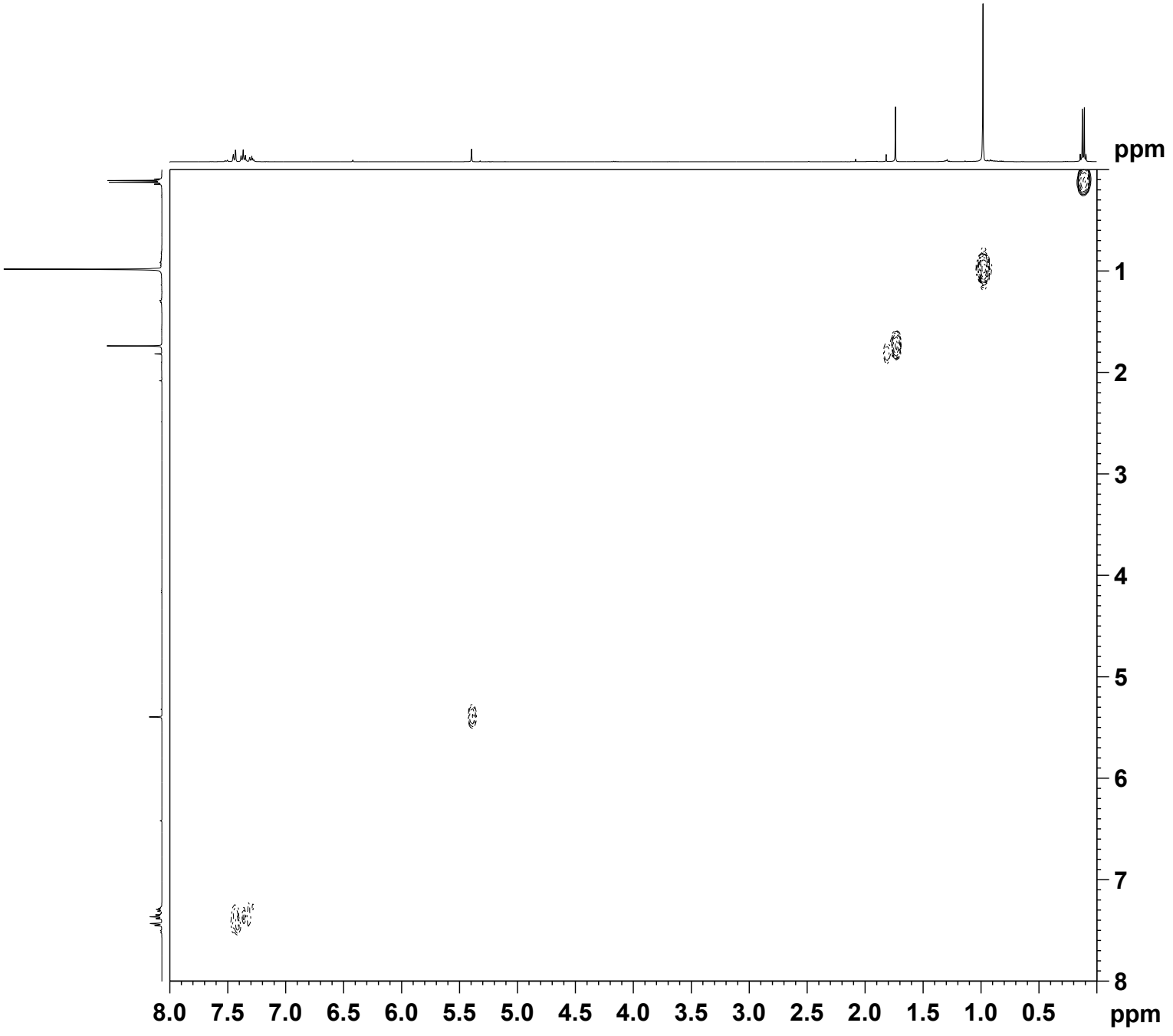
F2 - Acquisition Parameters
Date_           20210427
Time               18.42 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                   2048
SOLVENT             CDCl3
NS                      6
DS                     16
SWH              8012.820 Hz
FIDRES           7.825020 Hz
AQ               0.1277952 sec
RG                 210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.0 K
CNST2        145.0000000
CNST17        -0.5000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002080 sec
TDav                    1
SFO1         400.1324008 MHz
NUC1                 1H
P1                14.50 usec
P2                29.00 usec
P28             1000.00 usec
PLW1         12.69999981 W
SFO2         100.6233329 MHz
NUC2                13C
CPDPRG[2            garp
P3                10.50 usec
P14              500.00 usec
P24             2000.00 usec
PCPD2             80.00 usec
PLW0     0 W
PLW2        44.00000000 W
PLW12        0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3              0.500
SPOFFS3  0 Hz
SPW3         7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7              0.500
SPOFFS7  0 Hz
SPW7         7.41179991 W
GPNAM[1]      SMSQ10.100
GPZ1               80.00 %
GPNAM[2]      SMSQ10.100
GPZ2               20.10 %
GPNAM[3]      SMSQ10.100
GPZ3               11.00 %
GPNAM[4]      SMSQ10.100
GPZ4               -5.00 %
P16             1000.00 usec
P19              600.00 usec

F1 - Acquisition parameters
TD                    256
SFO1           100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF           400.1300000 MHz
WDW                 QSINE
SSB                     2
LB       0 Hz
GB       0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2       echo-antiecho
SF           100.6127685 MHz
WDW                 QSINE
SSB                     2
LB       0 Hz
GB       0
```

COSY of compound **2i**




```
Current Data Parameters
NAME             YYH-075
EXPNO                  7
PROCNO                 1

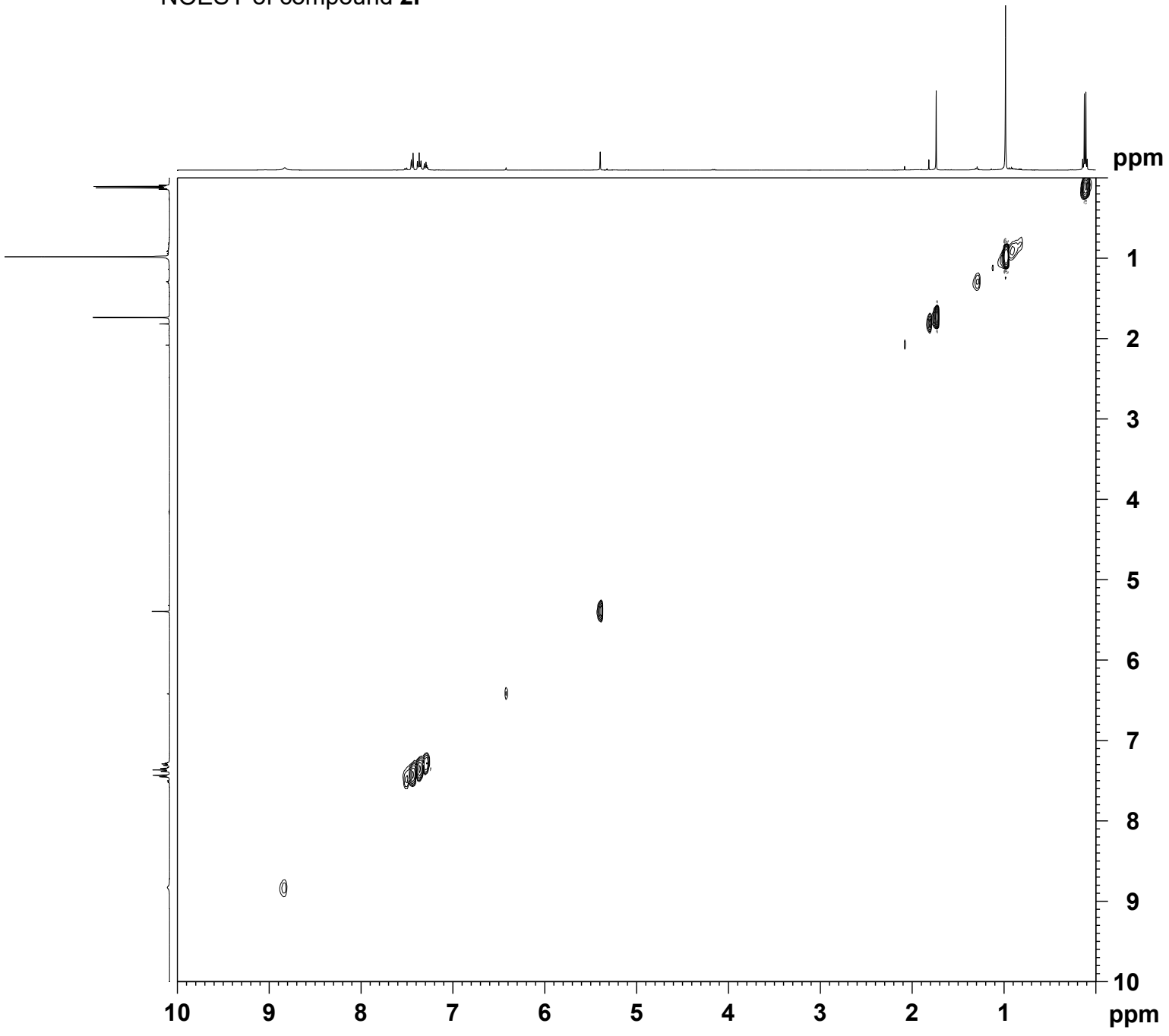
F2 - Acquisition Parameters
Date_           20210503
Time              20.02 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                 63.35
DW                62.400 usec
DE                 6.50 usec
TE                295.9 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF          400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF          400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **2i**




```
Current Data Parameters
NAME                 YYH-075
EXPNO                      8
PROCNO                     1

F2 - Acquisition Parameters
Date_               20210427
Time                  17.35 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG       noesygpphpp
TD                      2048
SOLVENT              CDCl3
NS                         6
DS                        16
SWH                8012.820 Hz
FIDRES             7.825020 Hz
AQ                 0.1277952 sec
RG                     63.35
DW                    62.400 usec
DE                     6.50 usec
TE                    295.9 K
D0                 0.00004394 sec
D1                 2.00000000 sec
D8                 0.40000001 sec
D11                0.03000000 sec
D12                0.00002000 sec
D16                0.00020000 sec
IN0                0.00012480 sec
TDav                       1
SFO1            400.1324008 MHz
NUC1                      1H
P1                     14.50 usec
P2                     29.00 usec
P17                  2500.00 usec
PLW1            12.69999981 W
PLW10            2.96690011 W
GPNAM[1]         SMSQ10.100
GPZ1                  40.00 %
P16                 1000.00 usec

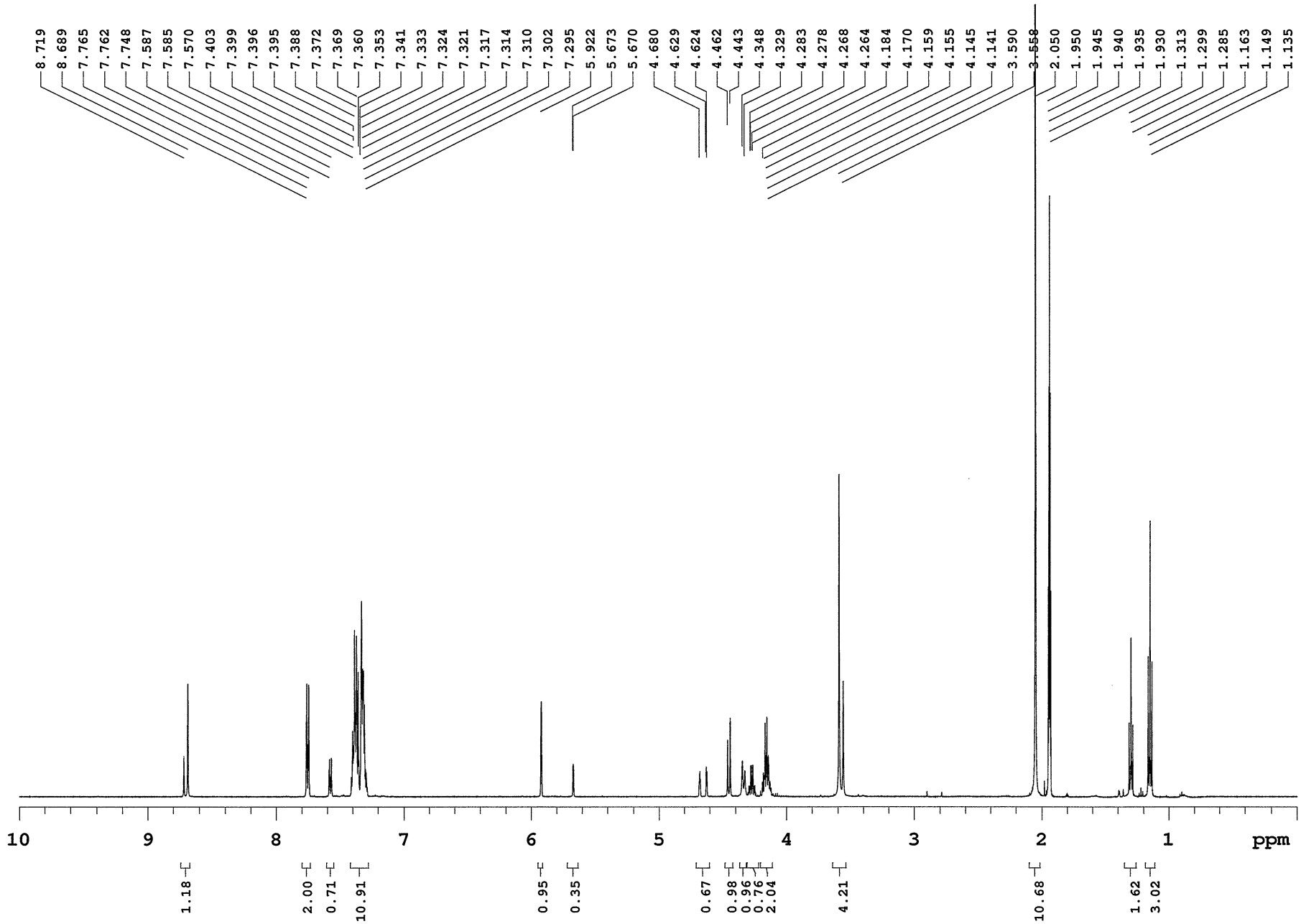
F1 - Acquisition parameters
TD                       256
SFO1              400.1324 MHz
FIDRES           62.600159 Hz
SW                20.025 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                      1024
SF              400.1300000 MHz
WDW                    QSINE
SSB                        2
LB         0 Hz
GB         0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2             States-TPPI
SF              400.1300000 MHz
WDW                    QSINE
SSB                        2
LB         0 Hz
GB         0
```

YYH-120-CD3CN-3

Sample Name	YYH-120-CD3CN-3	Pulse sequence	PROTON	Temperature	50	Study owner	vnmr2
Date collected	2022-01-05	Solvent	cd3cn	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



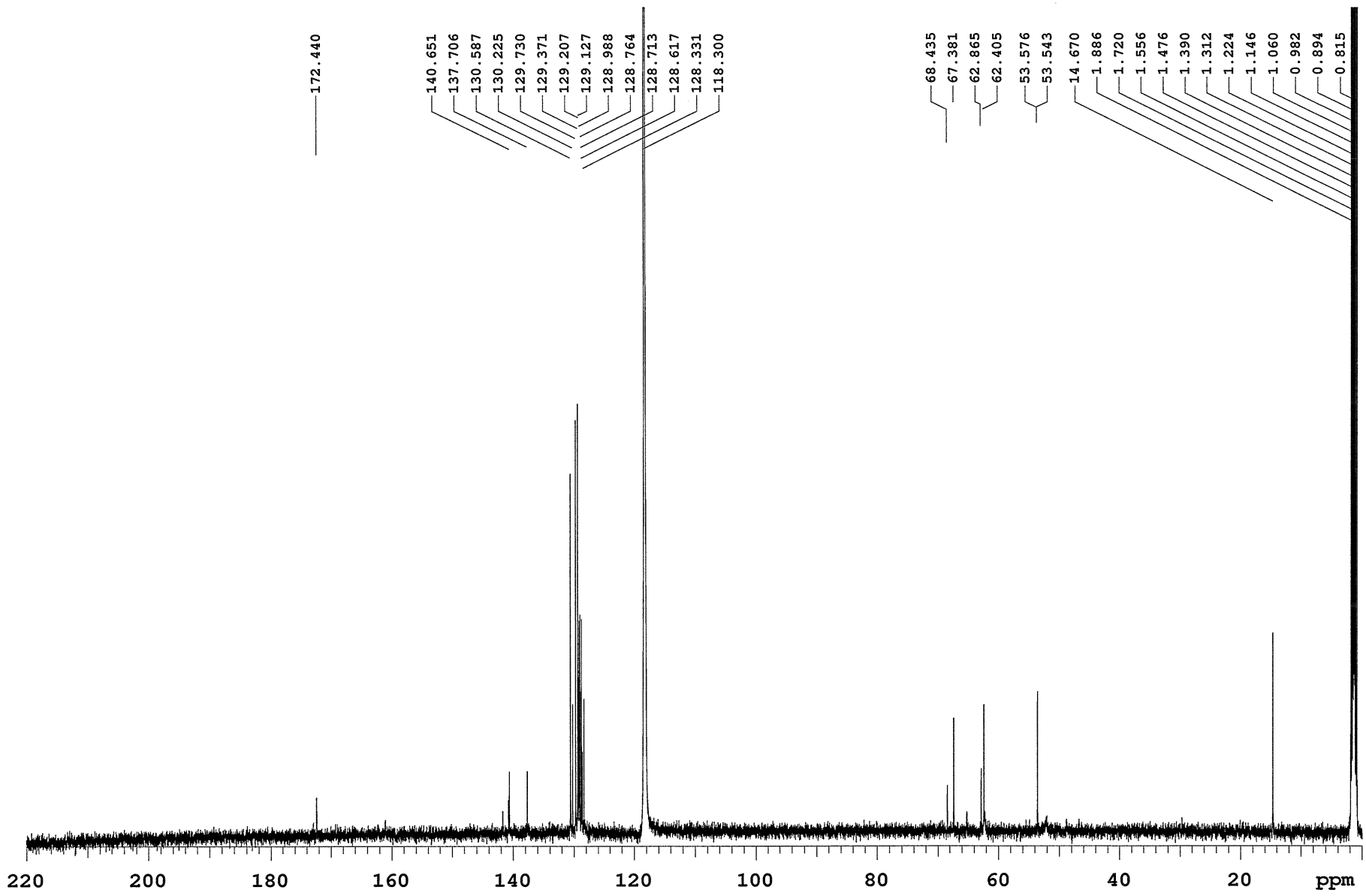
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-120-CD3CN-3/PROTON_03

Plot date 2022-01-06

1H NMR (CD3CN, 500 MHz, 50 centi degrees) of compound **2j**

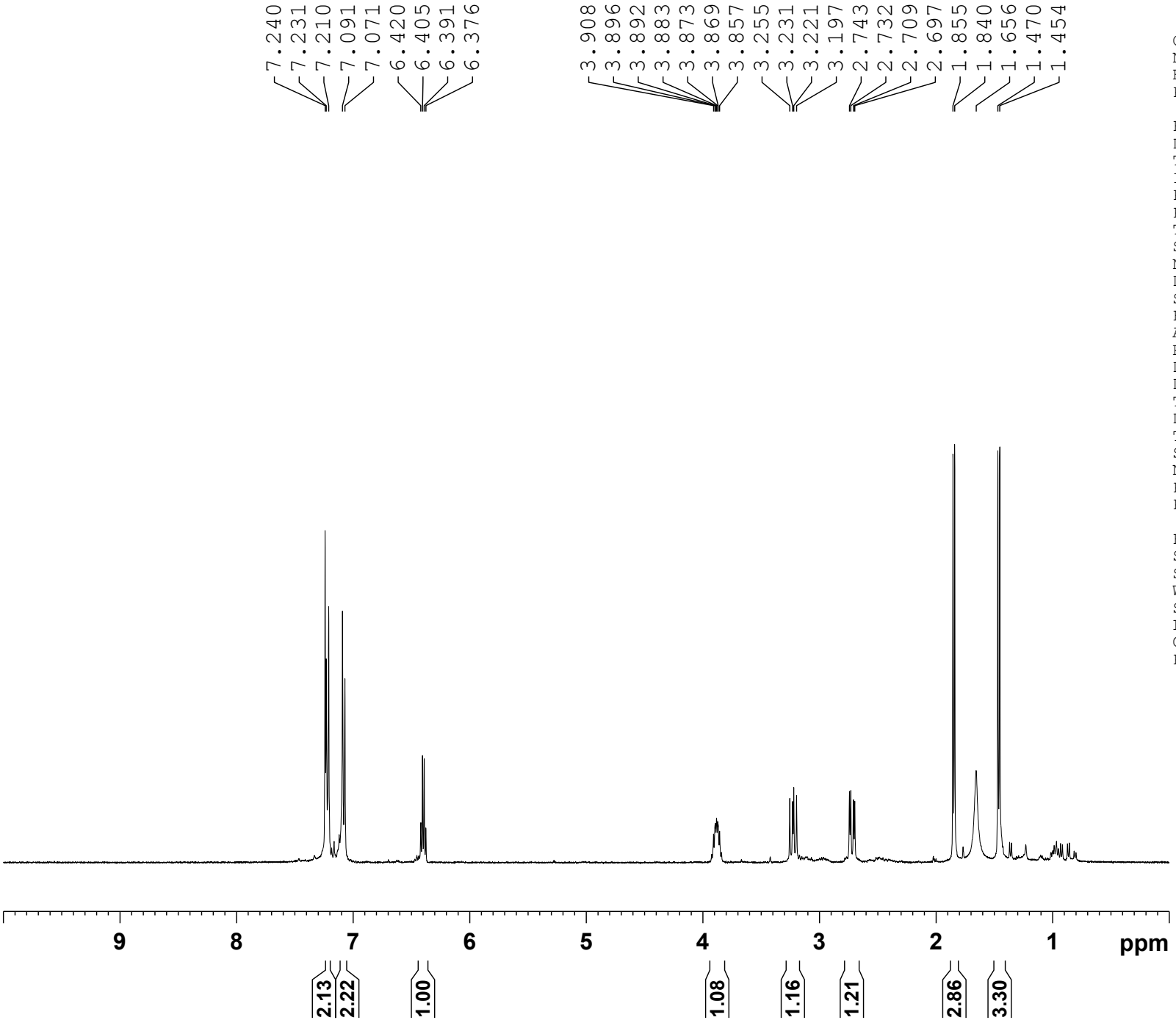
YYH-120-CD3CN-3

Sample Name	YYH-120-CD3CN-3	Pulse sequence	CARBON	Temperature	50	Study owner	vnmr2
Date collected	2022-01-05	Solvent	cd3cn	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



13C NMR (CD3CN, 125 MHz, 50 centi degrees) of compound **2j**

1H NMR (CDCl3, 400 MHz) of compound **3a**

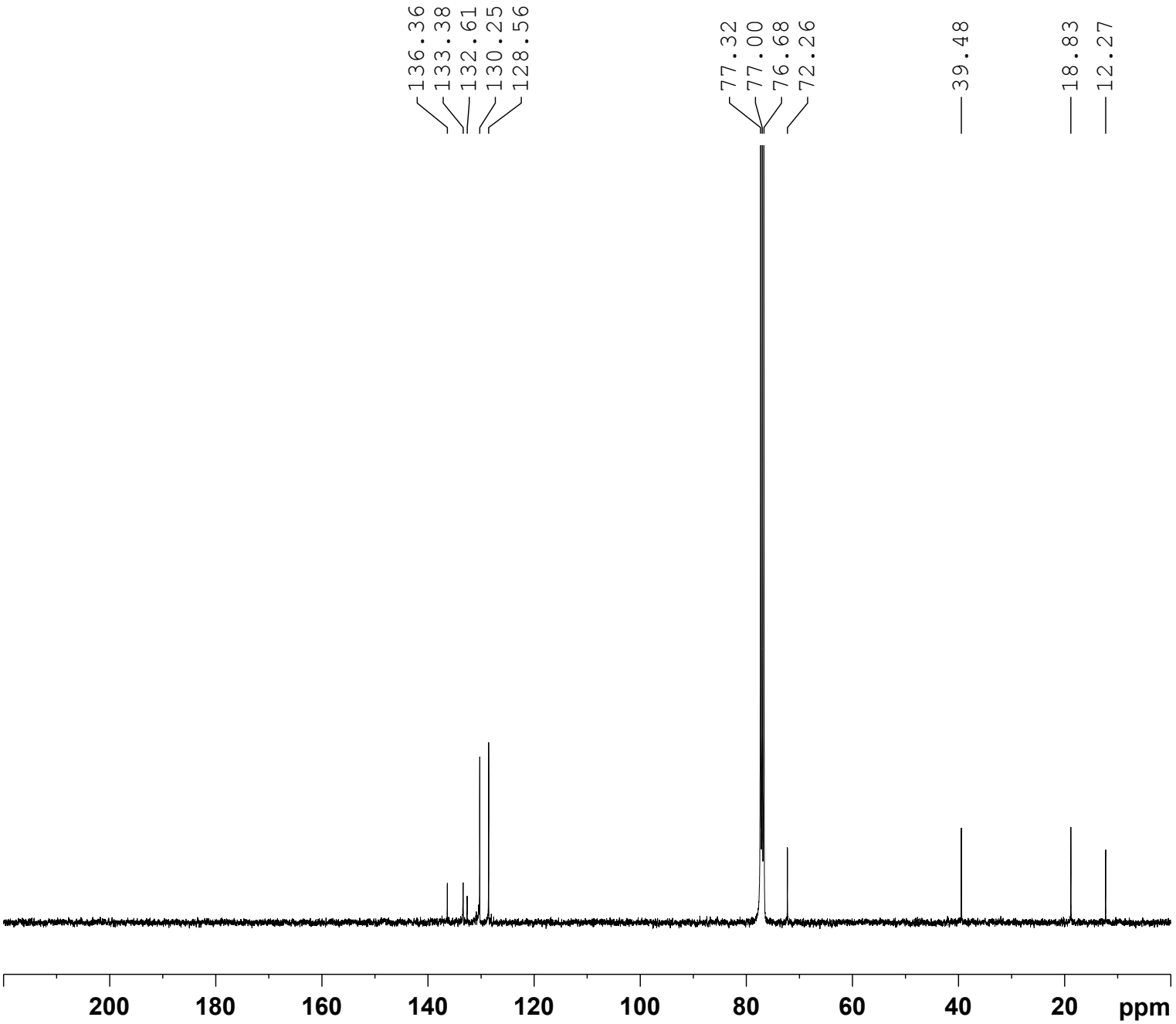



```
Current Data Parameters
NAME          nitrone-3
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20211122
Time              21.56 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ            2.0447233 sec
RG               210.28
DW               62.400 usec
DE               16.43 usec
TE               296.4 K
D1           2.00000000 sec
TD0                   1
SFO1        400.1324008 MHz
NUC1                 1H
P1                14.50 usec
PLW1        12.80000019 W

F2 - Processing parameters
SI                16384
SF          400.1300193 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                1.00
```

13C NMR (CDCl3, 100 MHz) of compound **3a**

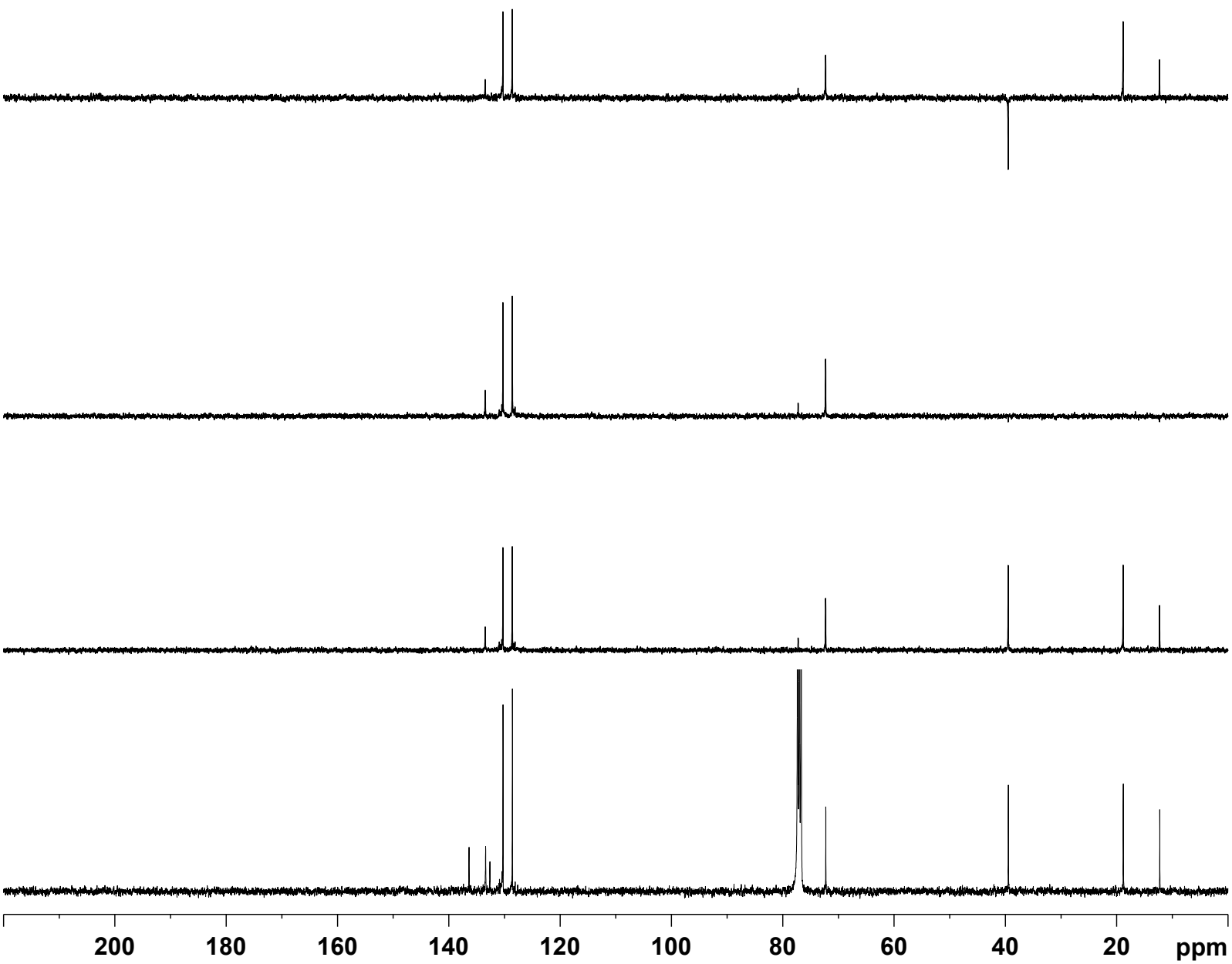



```
Current Data Parameters
NAME          nitrone-3
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20211123
Time               1.45 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                 5000
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               298.5 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1               10.50 usec
PLW1        44.50000000 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.36340001 W
PLW13        0.18250000 W

F2 - Processing parameters
SI                32768
SF          100.6127707 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

DEPT of compound **3a**

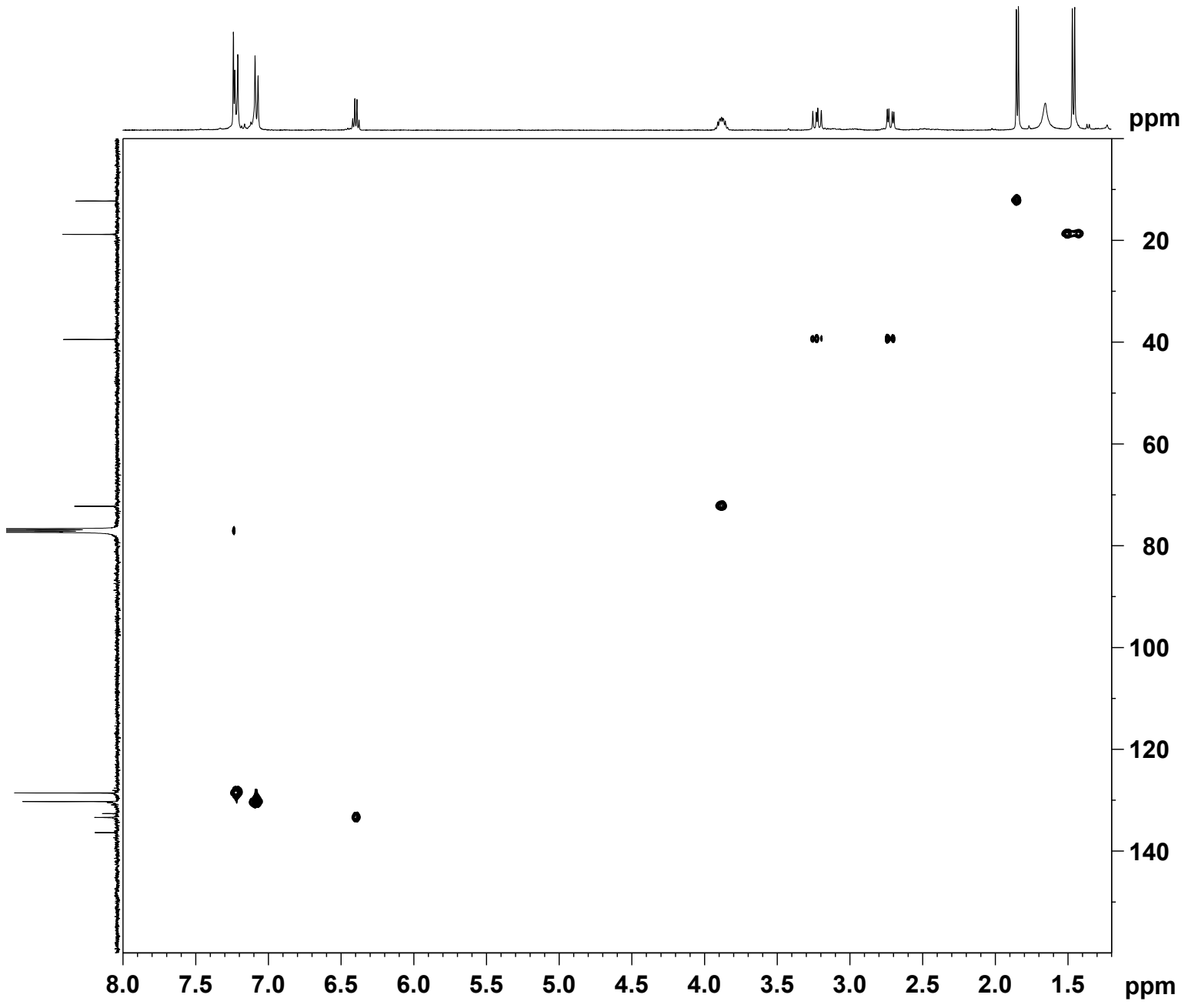



```
Current Data Parameters
NAME          nitrone-3
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20211123
Time               1.45 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 5000
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW                20.800 usec
DE                 6.50 usec
TE                298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1                10.50 usec
PLW1         44.50000000 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.36340001 W
PLW13         0.18250000 W

F2 - Processing parameters
SI                32768
SF          100.6127707 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

HSQC of compound **3a**




```
Current Data Parameters
NAME           nitrone-3
EXPNO                  6
PROCNO                 1

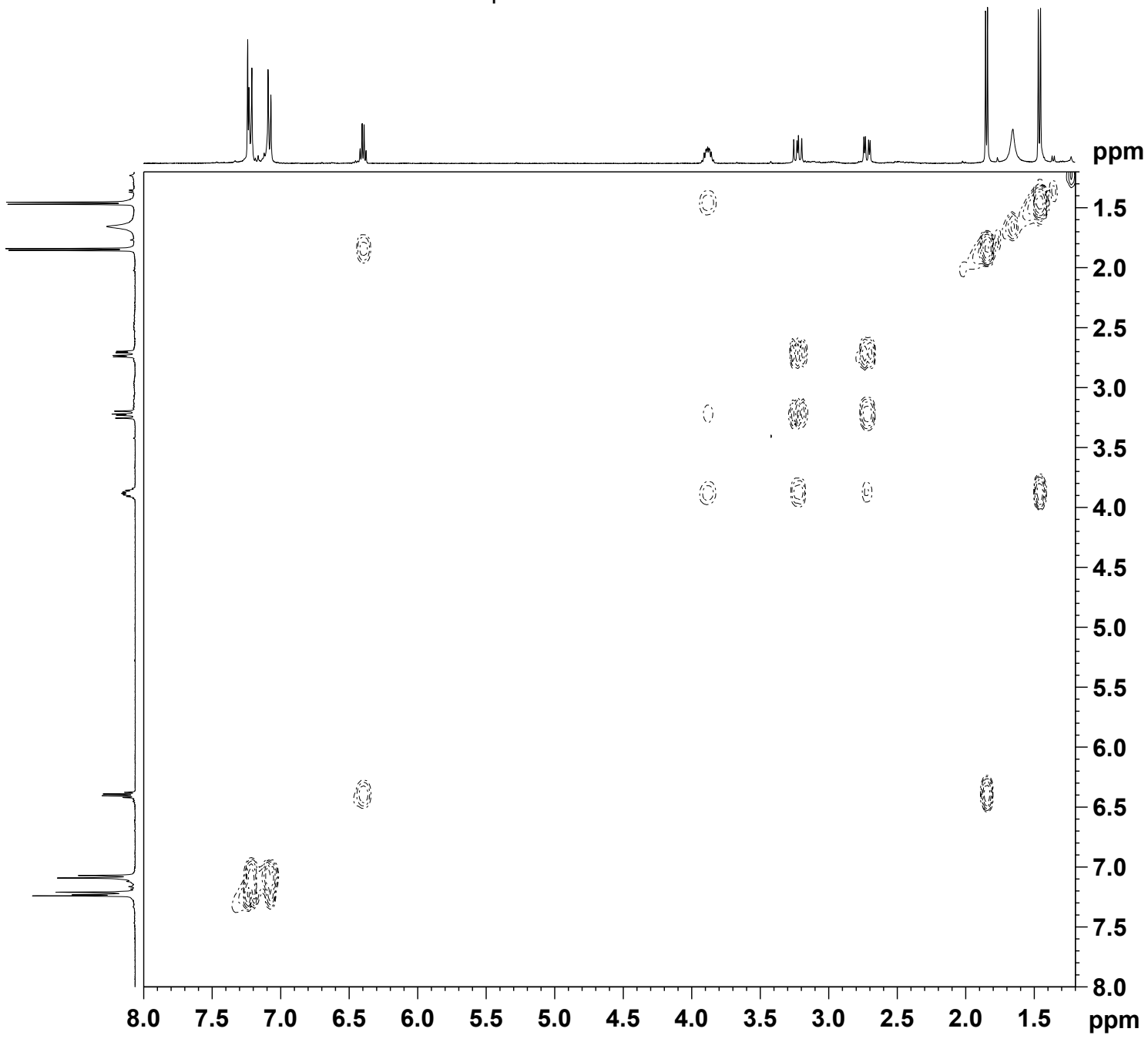
F2 - Acquisition Parameters
Date_           20211123
Time               6.43 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             4000.000 Hz
FIDRES          3.906250 Hz
AQ              0.2560000 sec
RG                 210.28
DW                 125.000 usec
DE                   6.50 usec
TE                  297.6 K
CNST2        145.0000000
CNST17        -0.5000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00002480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         12.80000019 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2             garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0     0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3             0.500
SPOFFS3  0 Hz
SPW3          7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7             0.500
SPOFFS7  0 Hz
SPW7          7.41179991 W
GPNAM[1]      SMSQ10.100
GPZ1               80.00 %
GPNAM[2]      SMSQ10.100
GPZ2               20.10 %
GPNAM[3]      SMSQ10.100
GPZ3               11.00 %
GPNAM[4]      SMSQ10.100
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1           100.6233 MHz
FIDRES       157.510086 Hz
SW              200.364 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300193 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
GB         0
PC                   1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127685 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
GB         0
```

COSY of compound **3a**




```
Current Data Parameters
NAME           nitrone-3
EXPNO                  7
PROCNO                 1

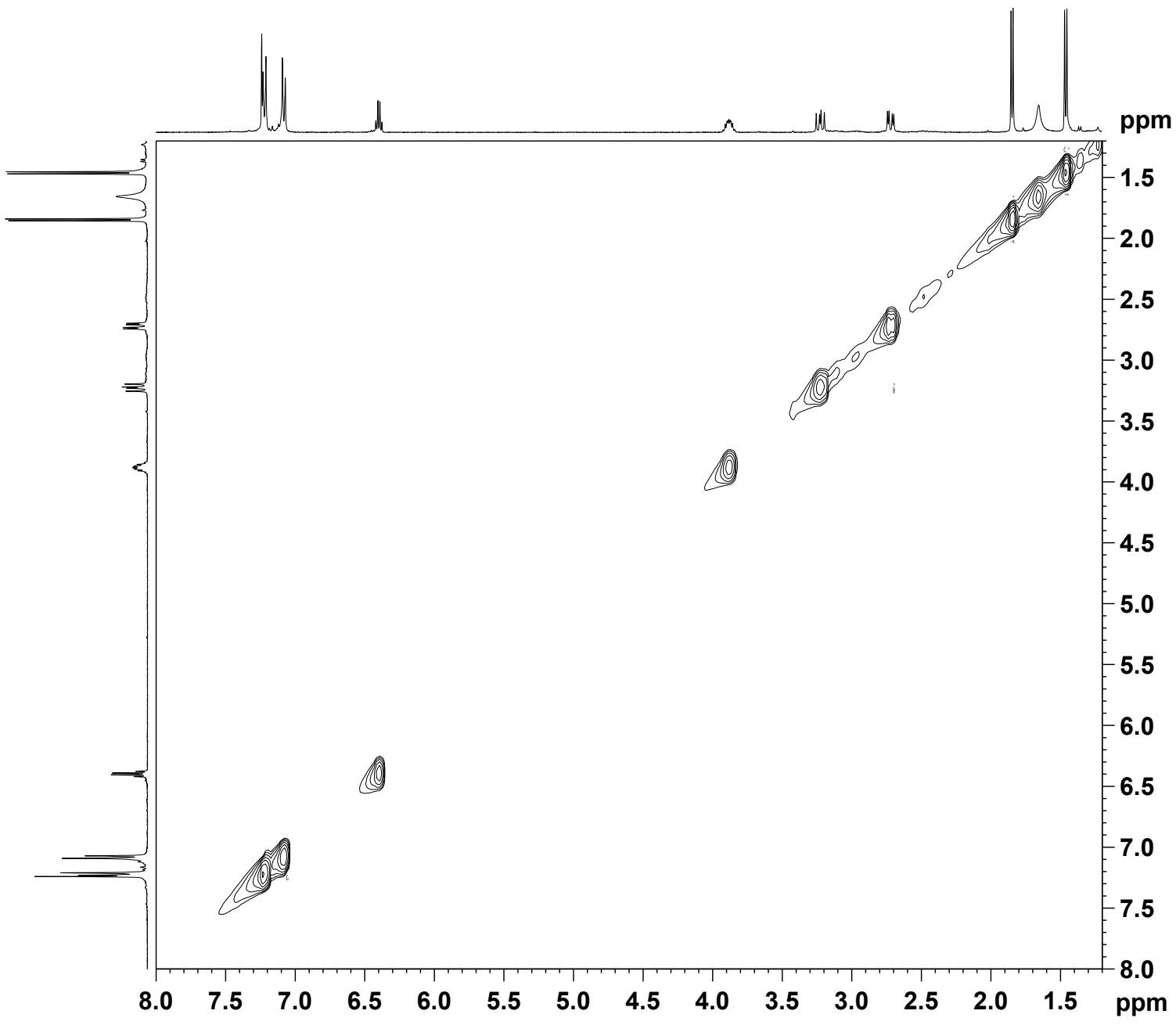
F2 - Acquisition Parameters
Date_           20211123
Time               7.29 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                 210.28
DW                 62.400 usec
DE                  6.50 usec
TE                 297.8 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                 14.50 usec
P1                 14.50 usec
P17              2500.00 usec
PLW1         12.80000019 W
PLW10         2.99020004 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                 20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           400.1300193 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300193 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **3a**




```
Current Data Parameters
NAME           nitrone-3
EXPNO                  8
PROCNO                 1

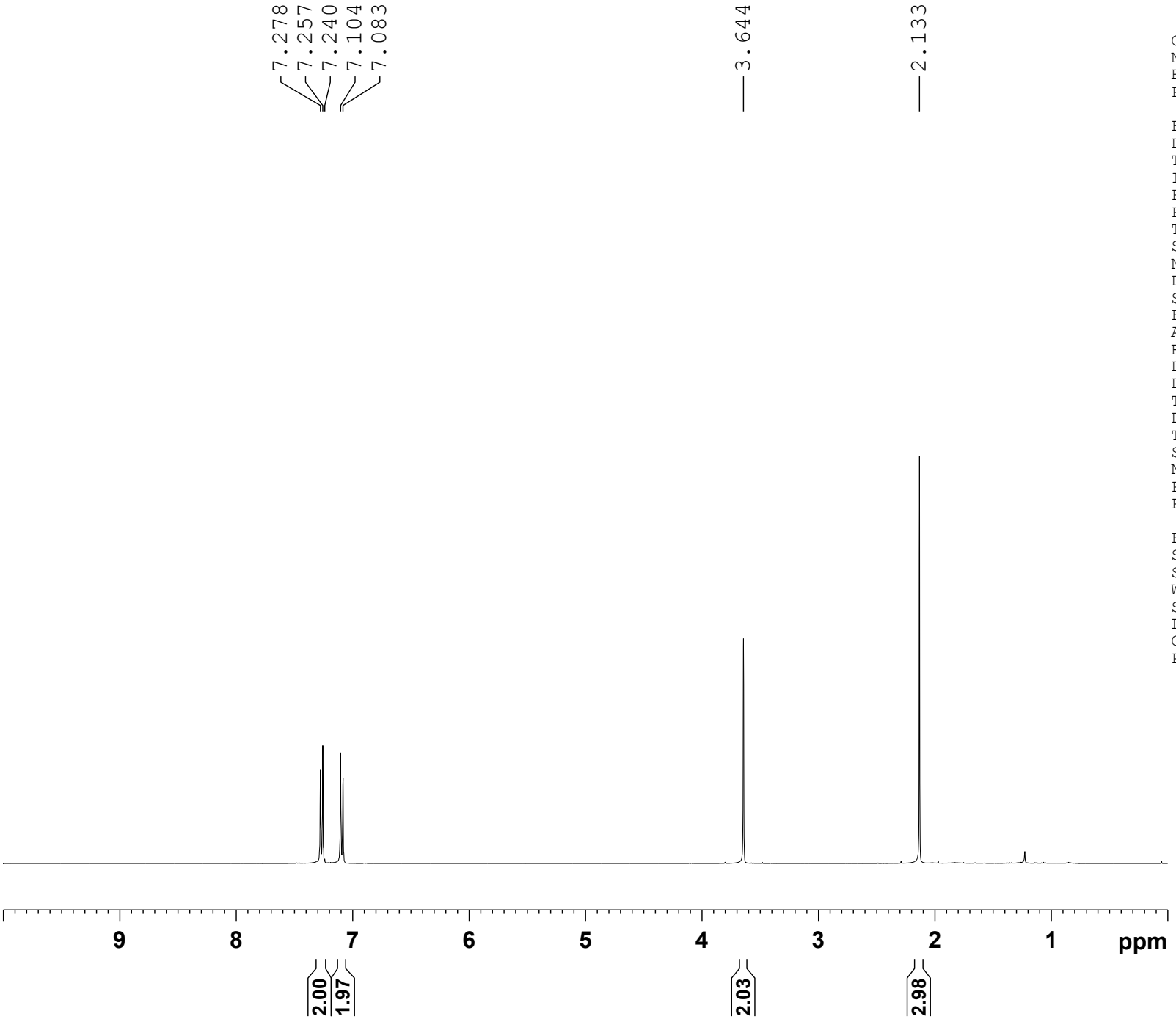
F2 - Acquisition Parameters
Date_           20211123
Time               8.26 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG     noesygpphpp
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                 210.28
DW                 62.400 usec
DE                  6.50 usec
TE                 297.0 K
D0              0.00004394 sec
D1              2.00000000 sec
D8              0.40000001 sec
D11             0.03000000 sec
D12             0.00002000 sec
D16             0.00020000 sec
IN0             0.00012480 sec
TDav                   1
SFO1          400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P17              2500.00 usec
PLW1          12.80000019 W
PLW10          2.99020004 W
GPNAM[1]       SMSQ10.100
GPZ1               40.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1           400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                  1024
SF            400.1300193 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2           States-TPPI
SF            400.1300193 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

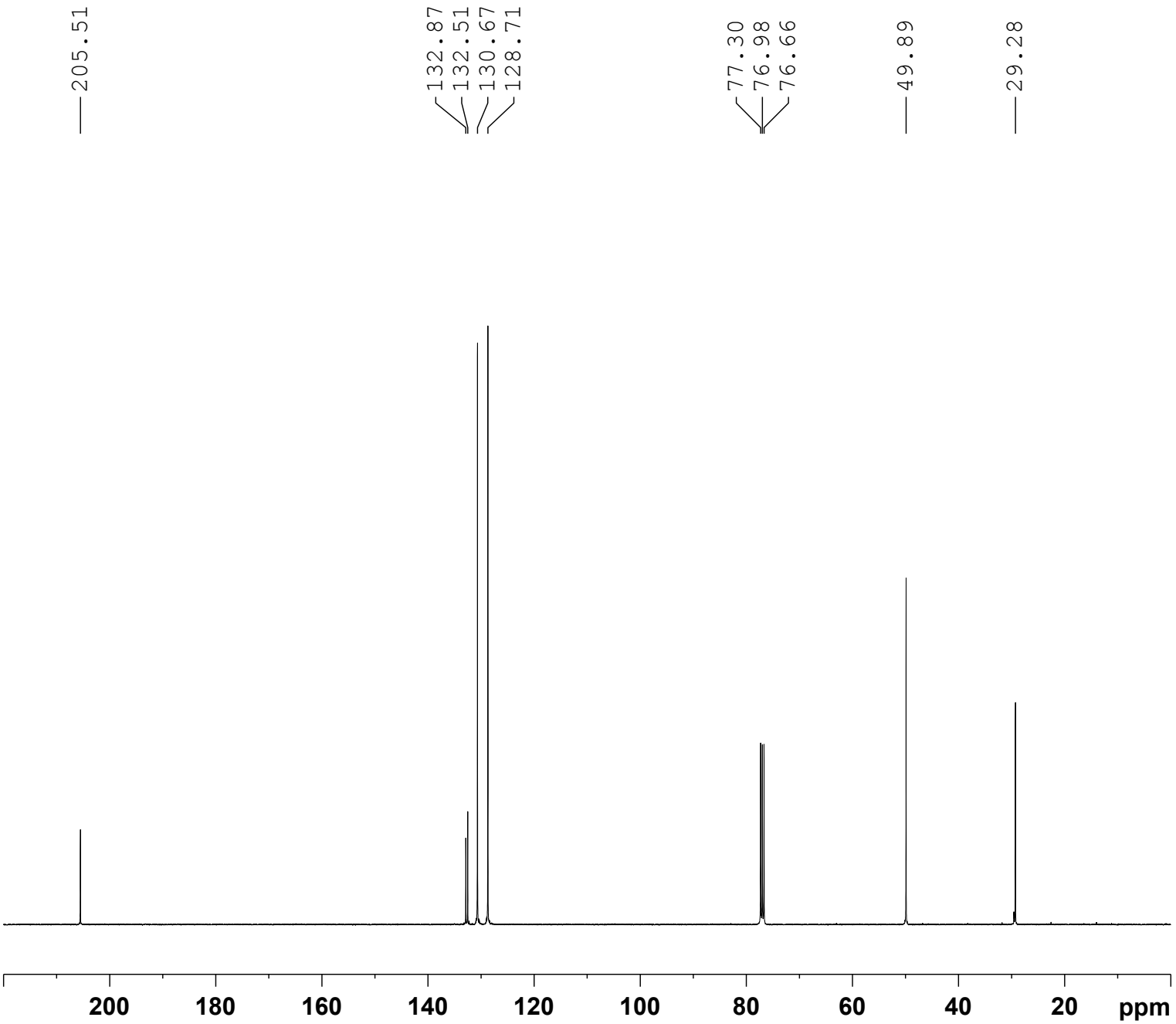
1H NMR (CDCl3, 400 MHz) of compound **4a**




```
Current Data Parameters
NAME             YYH-042
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210218
Time              21.55 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                 63.35
DW                62.400 usec
DE                16.43 usec
TE                294.9 K
D1            2.00000000 sec
TD0                    1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
PLW1         12.69999981 W

F2 - Processing parameters
SI                 16384
SF          400.1300178 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

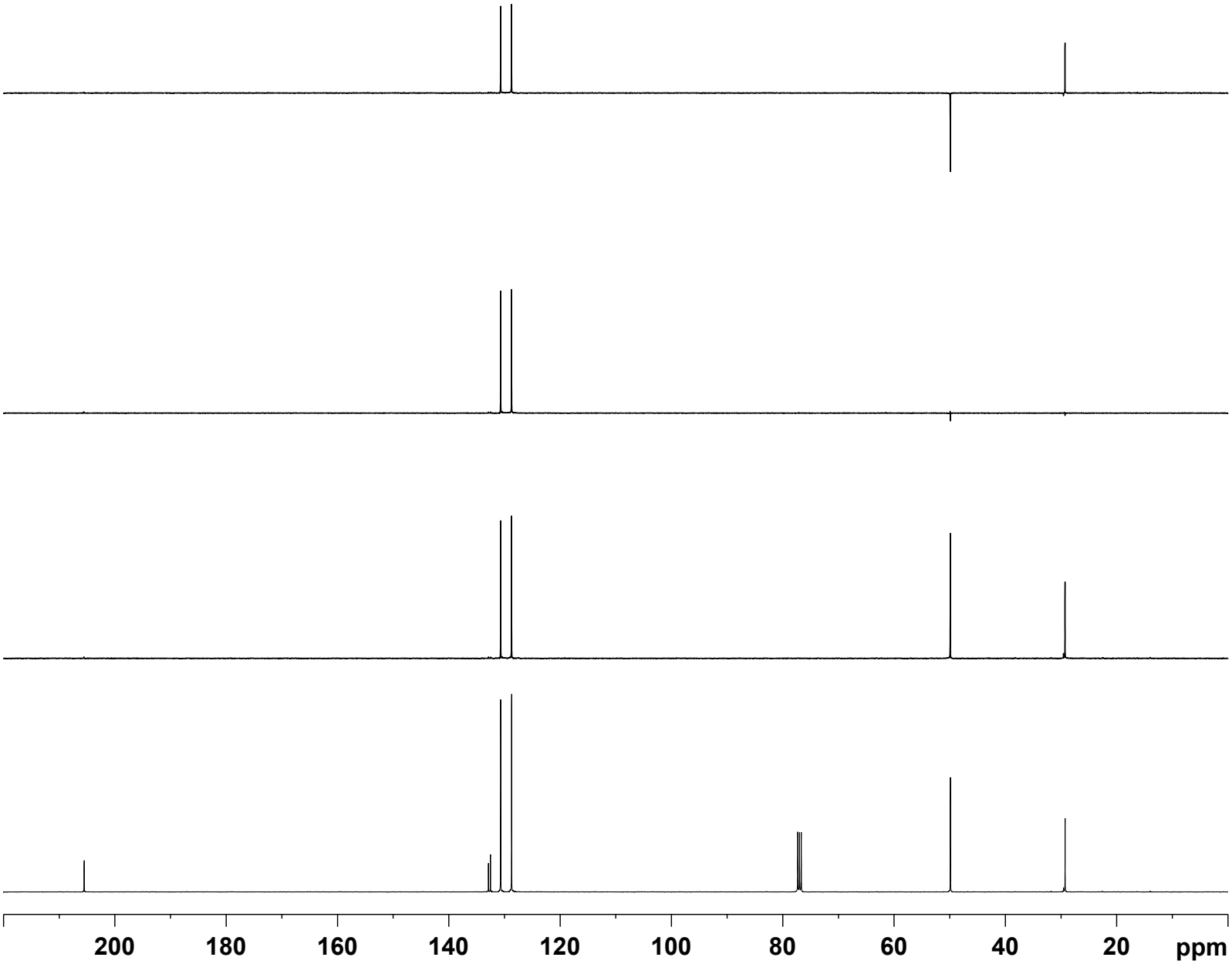



```
Current Data Parameters
NAME                  YYH-042
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210219
Time                     0.14 h
INSTRUM                  spect
PROBHD   Z108618_0922 (
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                        3000
DS                           0
SWH                 24038.461 Hz
FIDRES               1.467191 Hz
AQ                   0.6815744 sec
RG                      210.28
DW                      20.800 usec
DE                       6.50 usec
TE                      295.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1
SFO1               100.6233329 MHz
NUC1                        13C
P1                      10.50 usec
PLW1                44.09999847 W
SFO2               400.1316005 MHz
NUC2                        1H
CPDPRG[2 bi_waltz65_256
PCPD2                   90.00 usec
PLW2                14.30000019 W
PLW12                0.37118000 W
PLW13                0.18640999 W

F2 - Processing parameters
SI                       32768
SF                 100.6127825 MHz
WDW                         EM
SSB       0
LB                       2.00 Hz
GB        0
PC                       1.00
```

13C NMR (CDCl3, 100 MHz) of compound **4a**

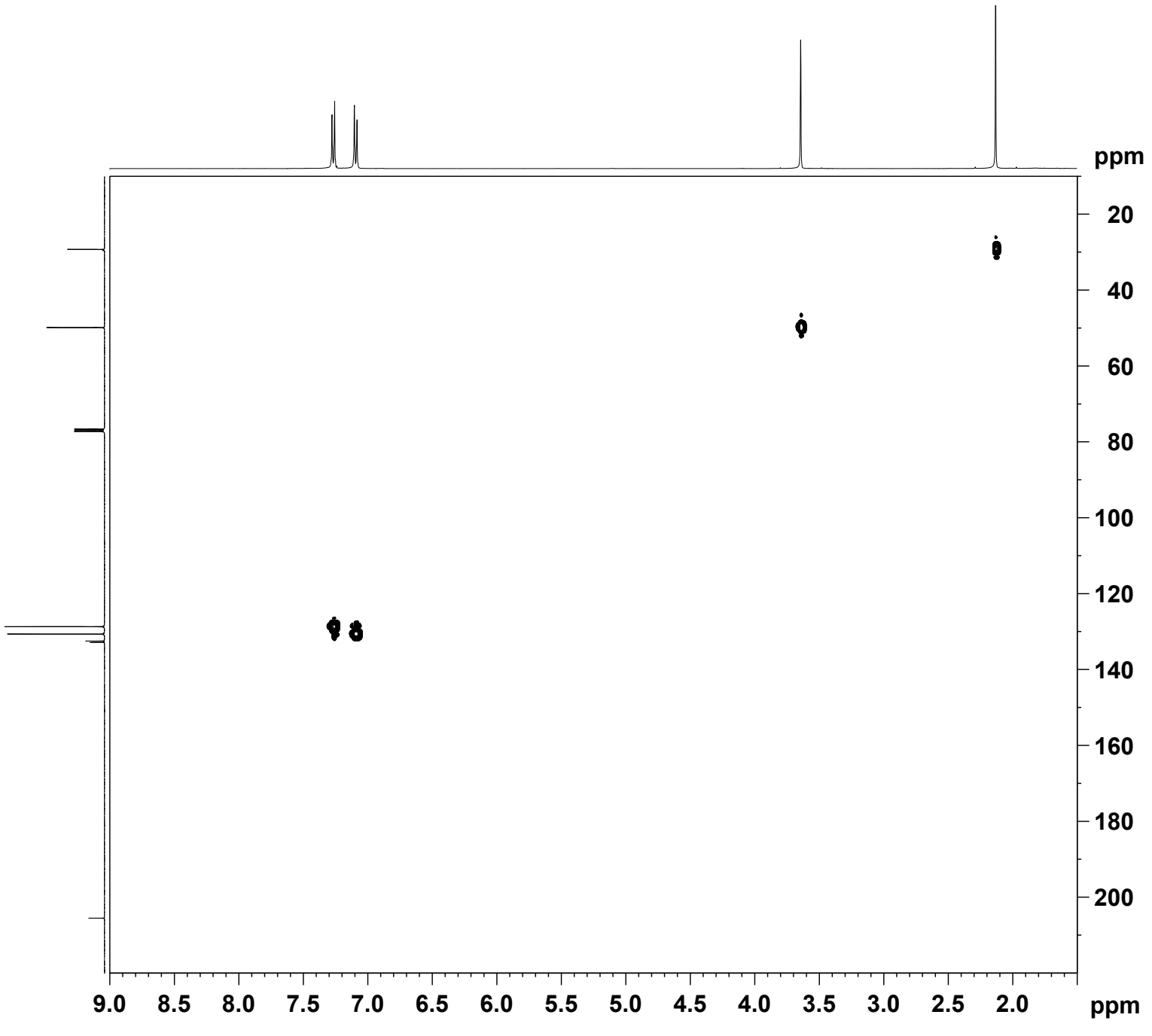



```
Current Data Parameters
NAME            YYH-042
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210219
Time               0.14 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                 3000
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW                20.800 usec
DE                 6.50 usec
TE                295.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1                10.50 usec
PLW1         44.09999847 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2         14.30000019 W
PLW12         0.37118000 W
PLW13         0.18640999 W

F2 - Processing parameters
SI                32768
SF          100.6127825 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

DEPT of compound **4a**



HSQC of compound **4a**

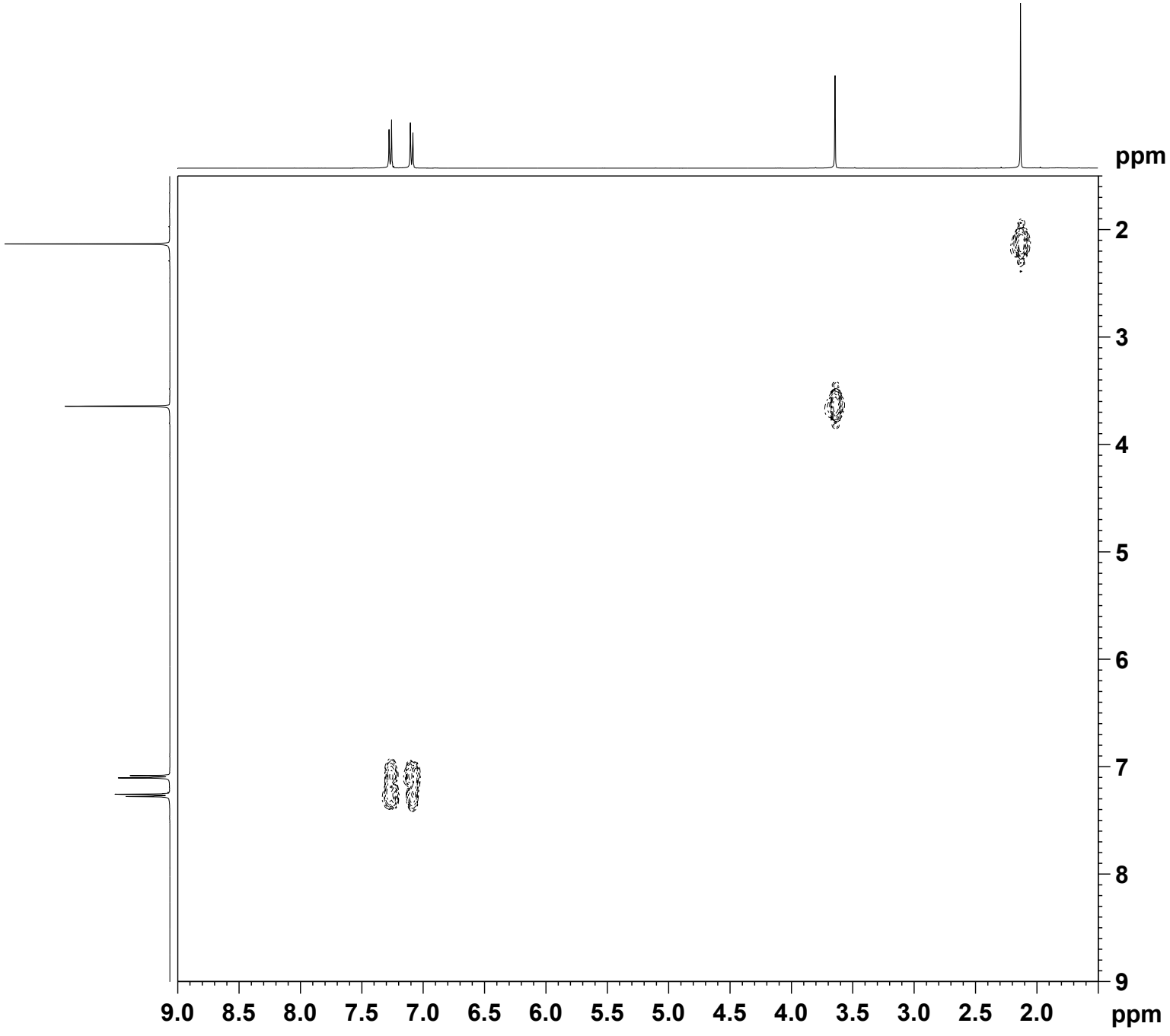
```
Current Data Parameters
NAME             YYH-042
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210219
Time                2.33 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH              8012.820 Hz
FIDRES           7.825020 Hz
AQ               0.1277952 sec
RG                 210.28
DW                  62.400 usec
DE                   6.50 usec
TE                  295.0 K
CNST2        145.0000000
CNST17        -0.5000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00002080 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         12.69999981 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2             garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0      0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3             0.500
SPOFFS3   0 Hz
SPW3          7.41179991 W
SPNAM[7]     Crp60comp.4
SPOAL7             0.500
SPOFFS7   0 Hz
SPW7          7.41179991 W
GPNAM[1]       SMSQ10.100
GPZ1                80.00 %
GPNAM[2]       SMSQ10.100
GPZ2                20.10 %
GPNAM[3]       SMSQ10.100
GPZ3                11.00 %
GPNAM[4]       SMSQ10.100
GPZ4                -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300178 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127825 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```



COSY of compound **4a**

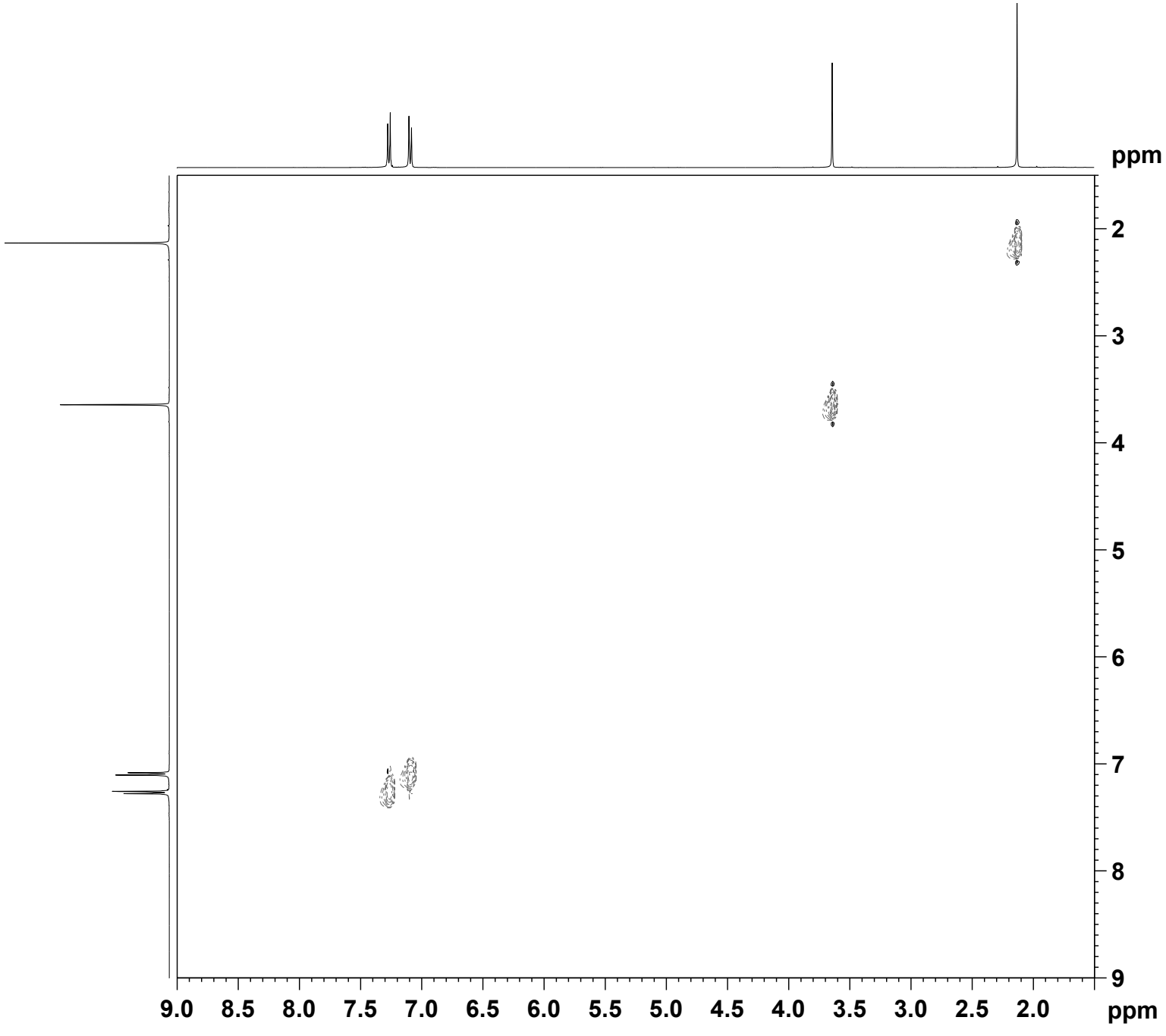
```
Current Data Parameters
NAME             YYH-042
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210219
Time               3.16 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                144.47
DW                62.400 usec
DE                 6.50 usec
TE                295.0 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         12.69999981 W
PLW10         2.96690011 W
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           400.1300178 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300178 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```



NOESY of compound **4a**

```
Current Data Parameters
NAME                  YYH-042
EXPNO                       8
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210219
Time                     4.13 h
INSTRUM                 spect
PROBHD   Z108618_0922 (
PULPROG          noesygpphpp
TD                       2048
SOLVENT                 CDCl3
NS                          6
DS                         16
SWH                  8012.820 Hz
FIDRES               7.825020 Hz
AQ                   0.1277952 sec
RG                       63.35
DW                     62.400 usec
DE                      6.50 usec
TE                      294.3 K
D0                   0.00004394 sec
D1                   2.00000000 sec
D8                   0.40000001 sec
D11                  0.03000000 sec
D12                  0.00002000 sec
D16                  0.00020000 sec
IN0                  0.00012480 sec
TDav                        1
SFO1               400.1324008 MHz
NUC1                       1H
P1                       14.50 usec
P2                       29.00 usec
P17                    2500.00 usec
PLW1               12.69999981 W
PLW10               2.96690011 W
GPNAM[1]           SMSQ10.100
GPZ1                    40.00 %
P16                   1000.00 usec

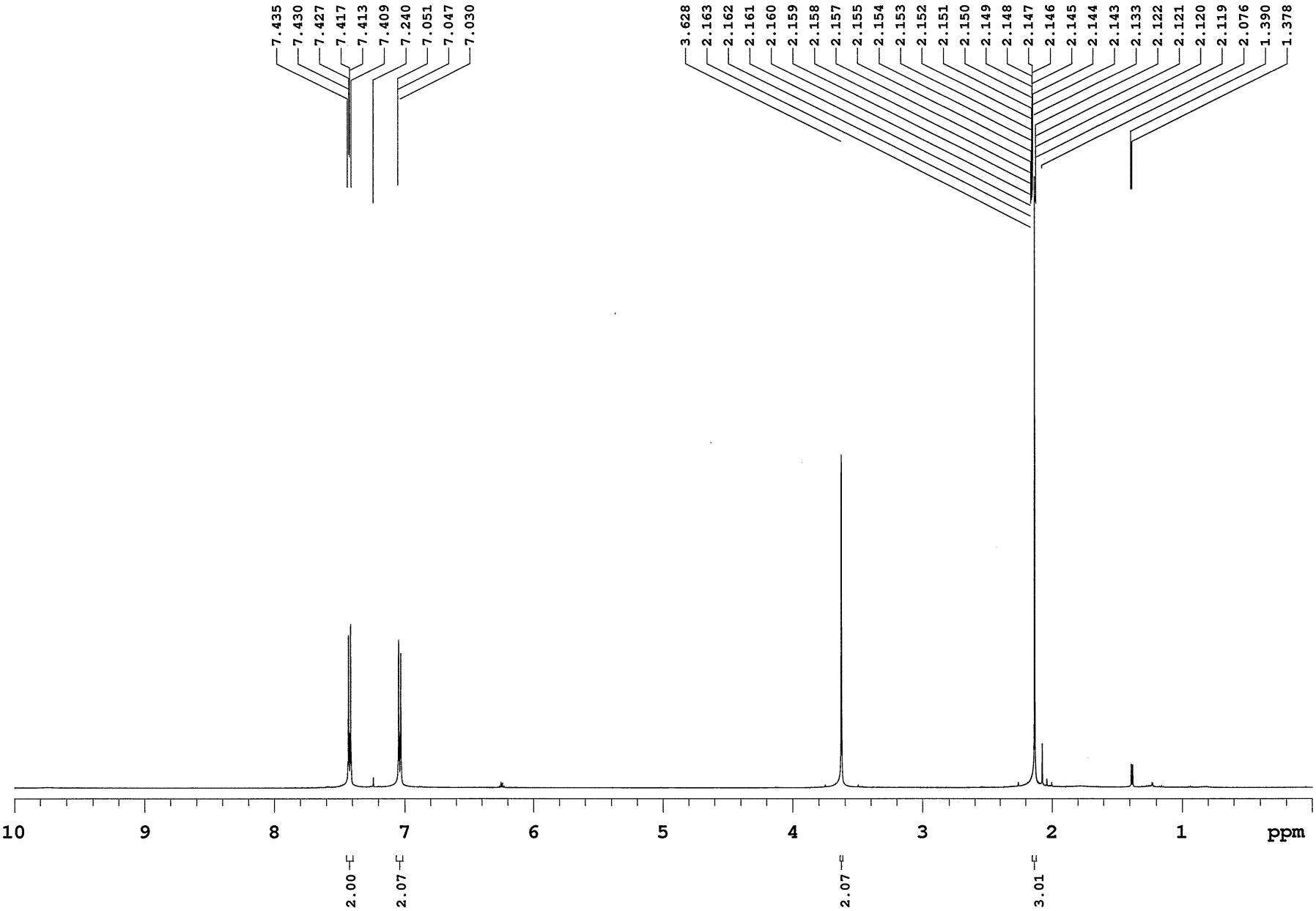
F1 - Acquisition parameters
TD                          256
SFO1                 400.1324 MHz
FIDRES              62.600159 Hz
SW                     20.025 ppm
FnMODE            States-TPPI

F2 - Processing parameters
SI                         1024
SF                 400.1300178 MHz
WDW                       QSINE
SSB                          2
LB              0 Hz
GB              0
PC                        1.40

F1 - Processing parameters
SI                         1024
MC2               States-TPPI
SF                 400.1300178 MHz
WDW                       QSINE
SSB                          2
LB              0 Hz
GB              0
```

YYH-063

Sample Name **YYH-063**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-02**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



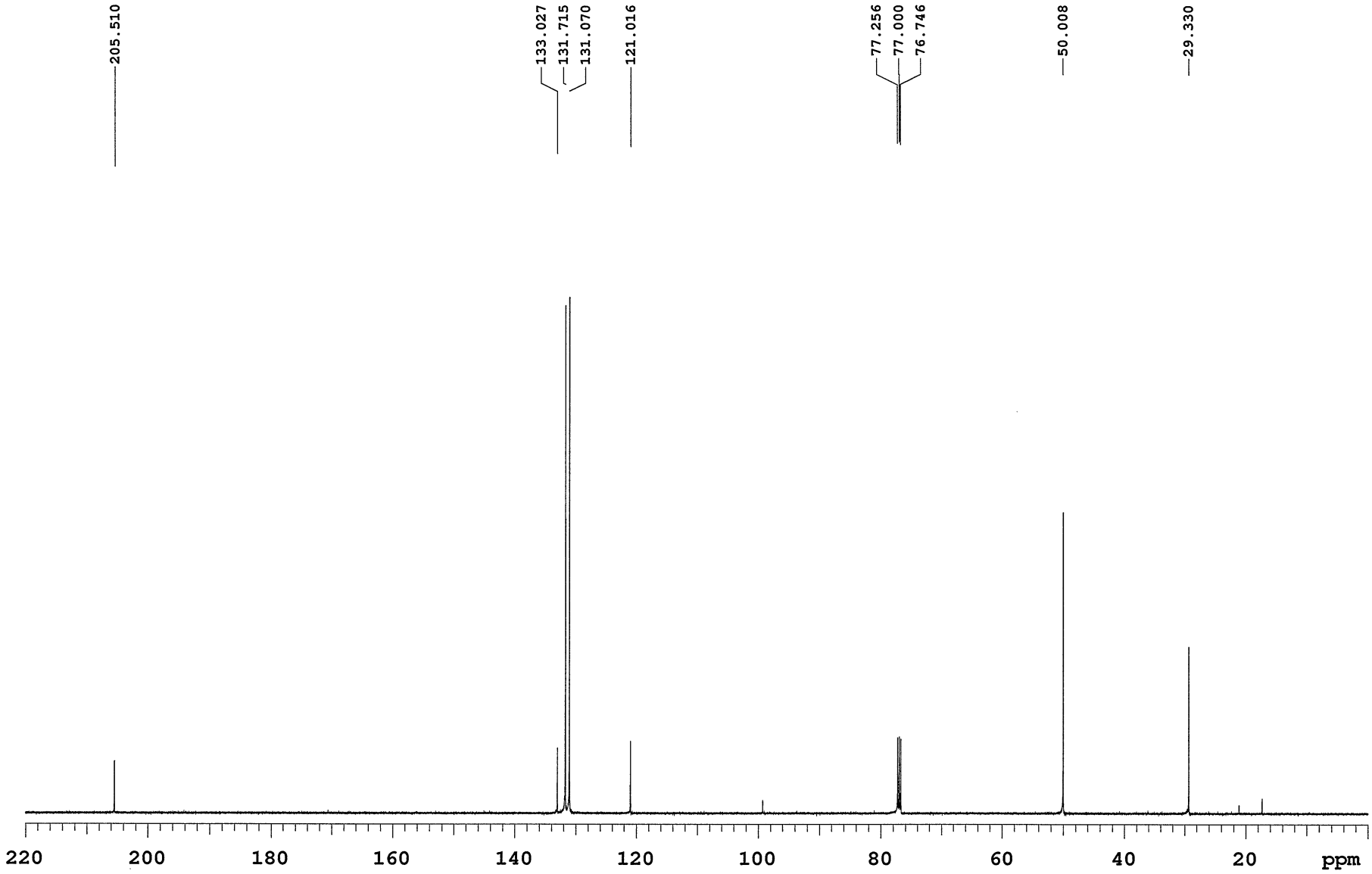
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-063/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4b**

Plot date 2021-08-04

YYH-063

Sample Name **YYH-063**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-02**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



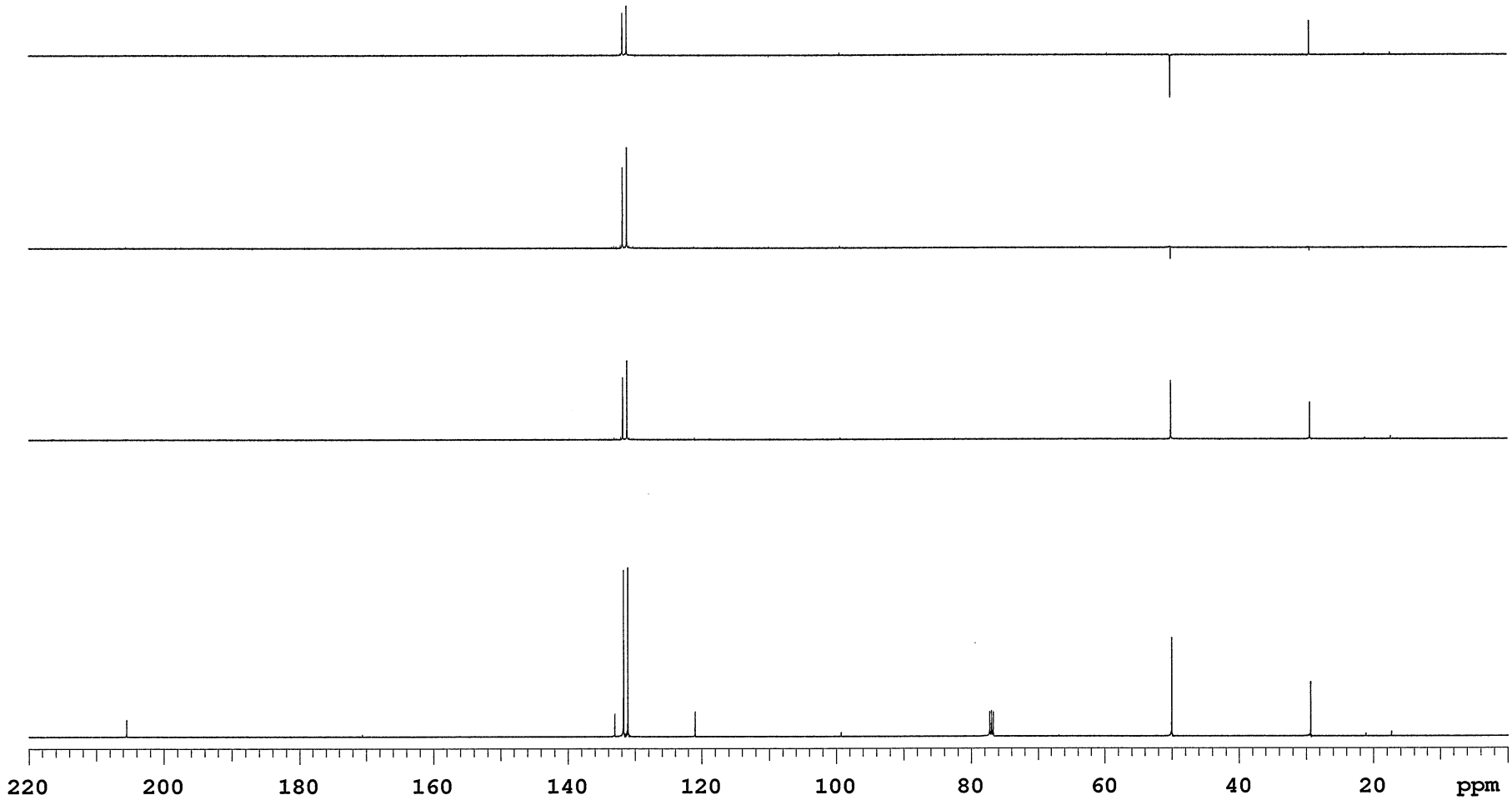
1H NMR (CDCl3, 125 MHz) of compound **4b**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-063/CARBON_02

Plot date 2021-06-03

YYH-063

Sample Name **YYH-063**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-02**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



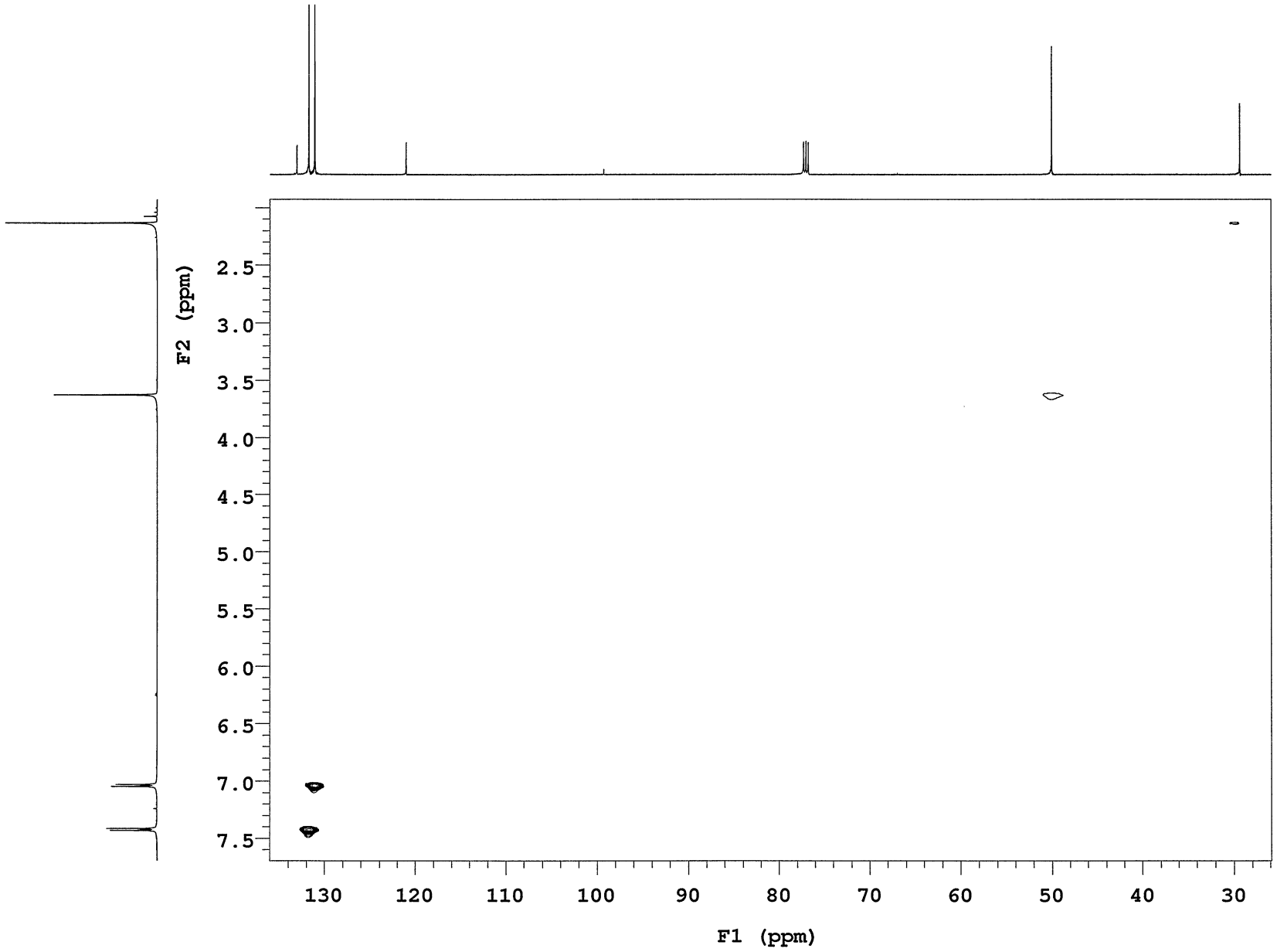
DEPT of compound **4b**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-063/DEPT_01

Plot date 2021-06-03

YYH-063

Sample Name **YYH-063**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-03**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



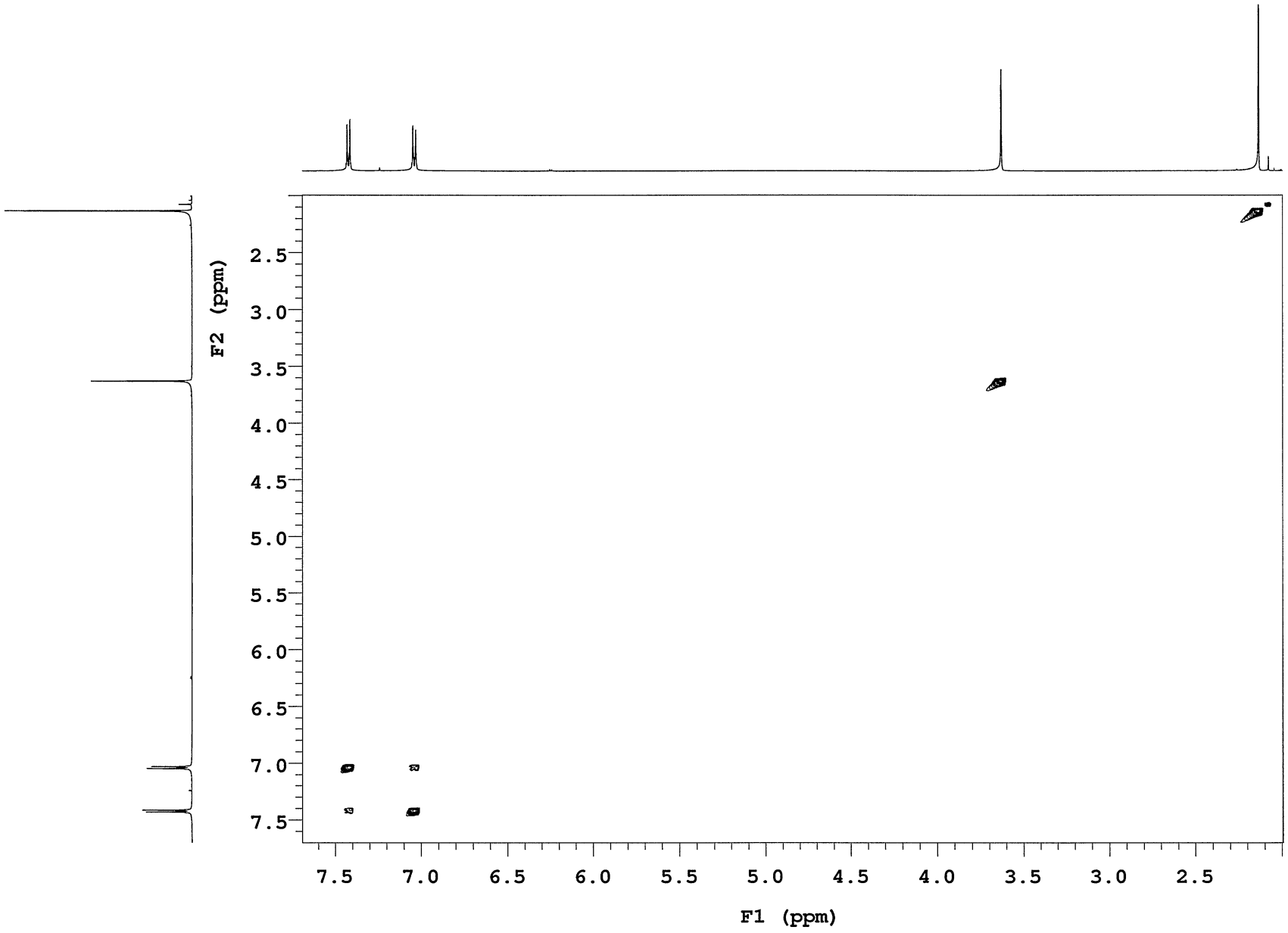
HSQC of compound **4b**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-063/gHSQC_01

Plot date 2021-06-03

YYH-063

Sample Name **YYH-063**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-03**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



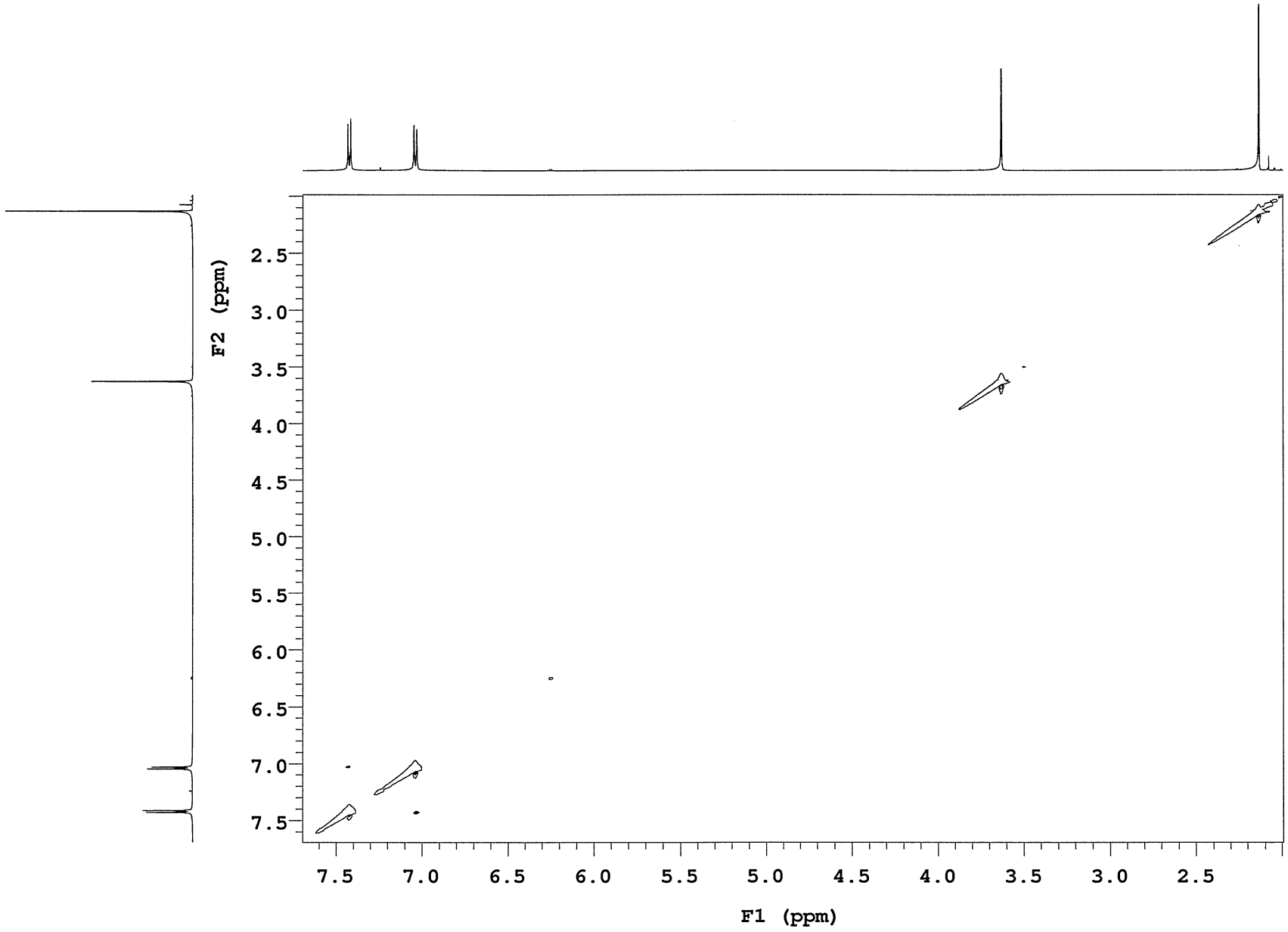
COSY of compound **4b**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-063/gCOSY_01

Plot date 2021-06-03

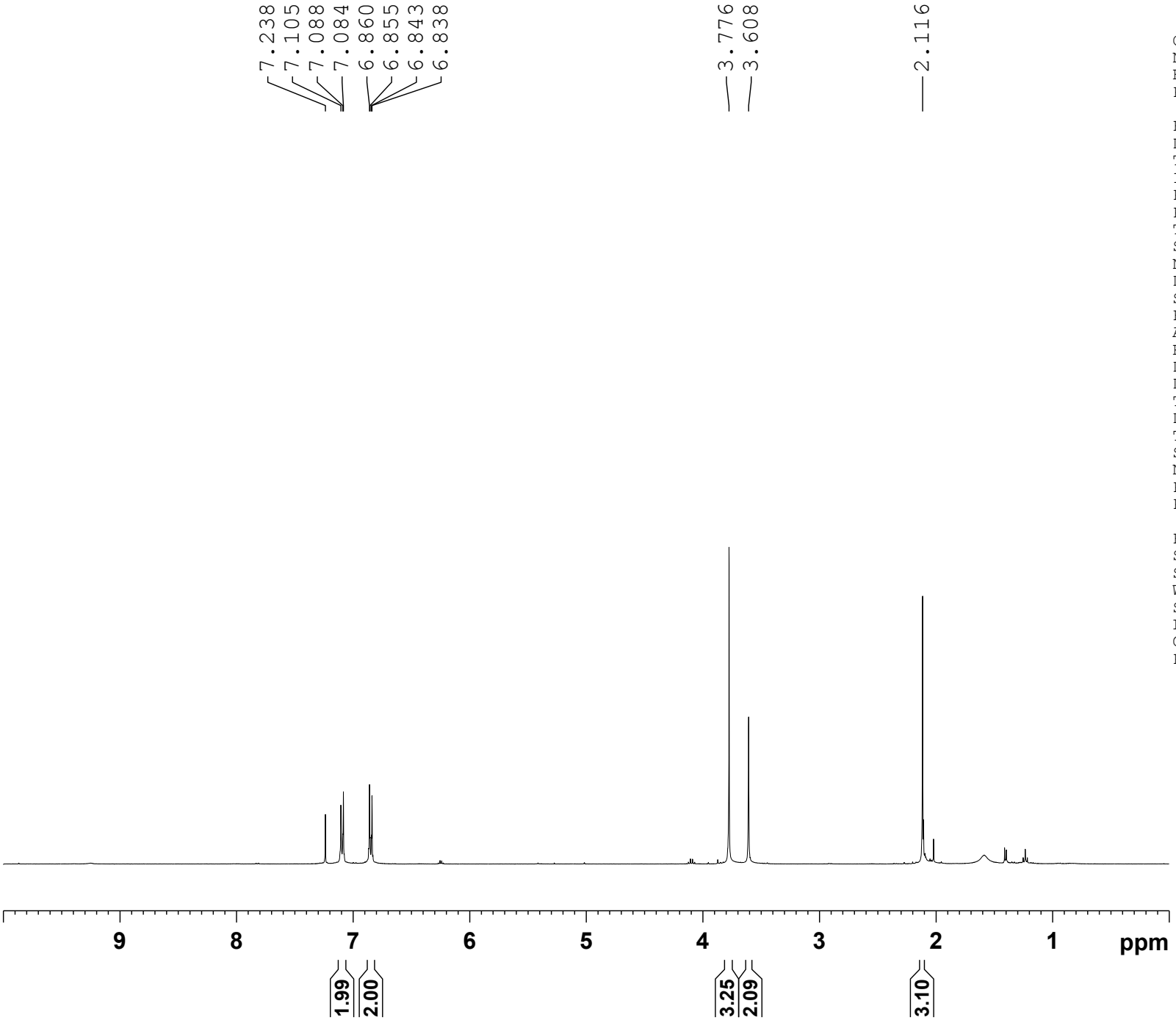
YYH-063

Sample Name **YYH-063**	Pulse sequence **NOESY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-03**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



NOESY of compound **4b**

1H NMR (CDCl3, 400 MHz) of compound **4c**

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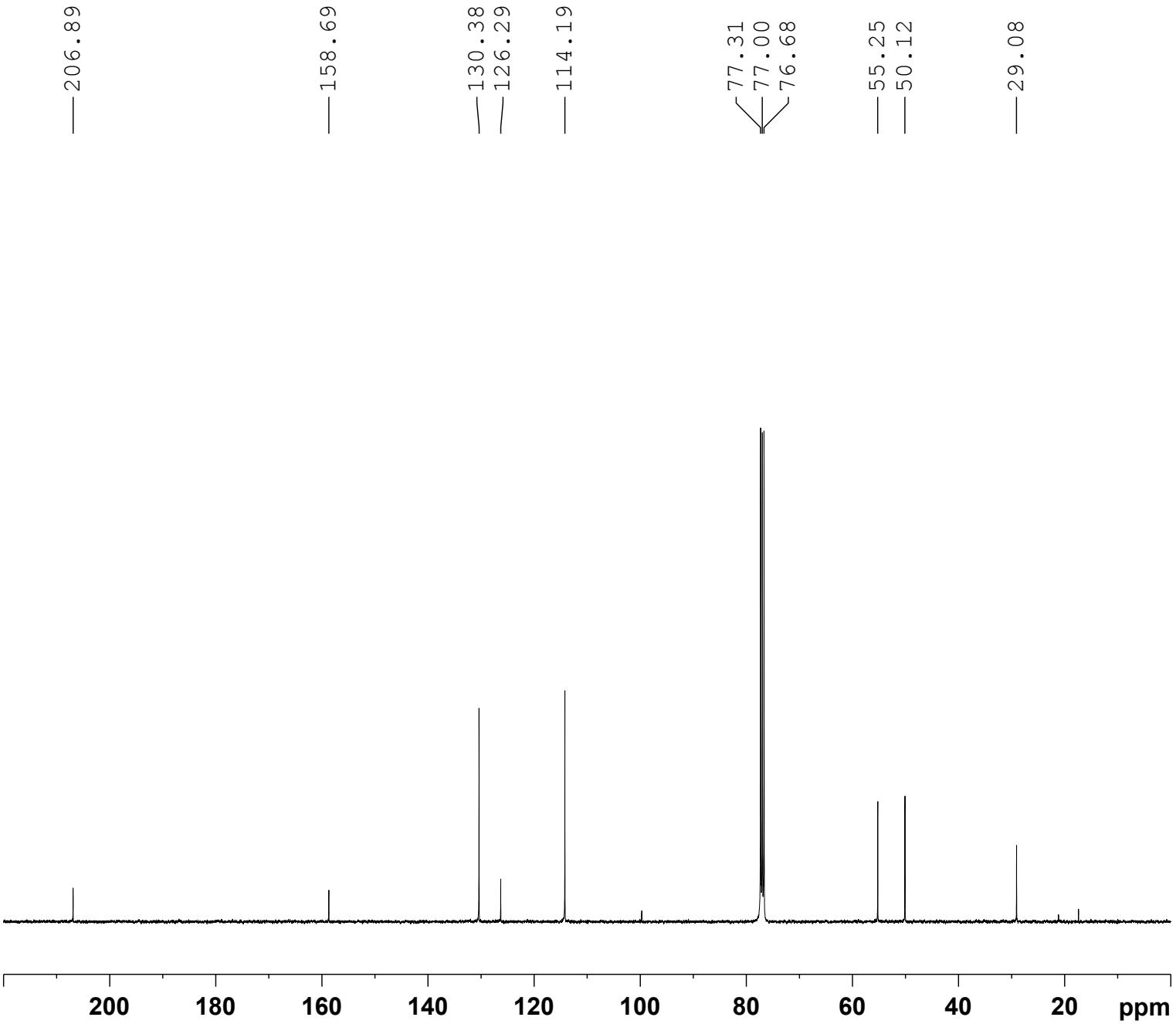
Current Data Parameters
NAME                  YYH-077
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20210819
Time                  22.56 h
INSTRUM               spect
PROBHD   Z108618_0922 (
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                2.0447233 sec
RG                   210.28
DW                   62.400 usec
DE                   16.43 usec
TE                   297.5 K
D1              2.00000000 sec
TD0                       1
SFO1           400.1324008 MHz
NUC1                    1H
P1                   14.50 usec
PLW1           13.10000038 W

F2 - Processing parameters
SI                    16384
SF             400.1300189 MHz
WDW                     EM
SSB       0
LB        0 Hz
GB        0
PC                    1.00
```

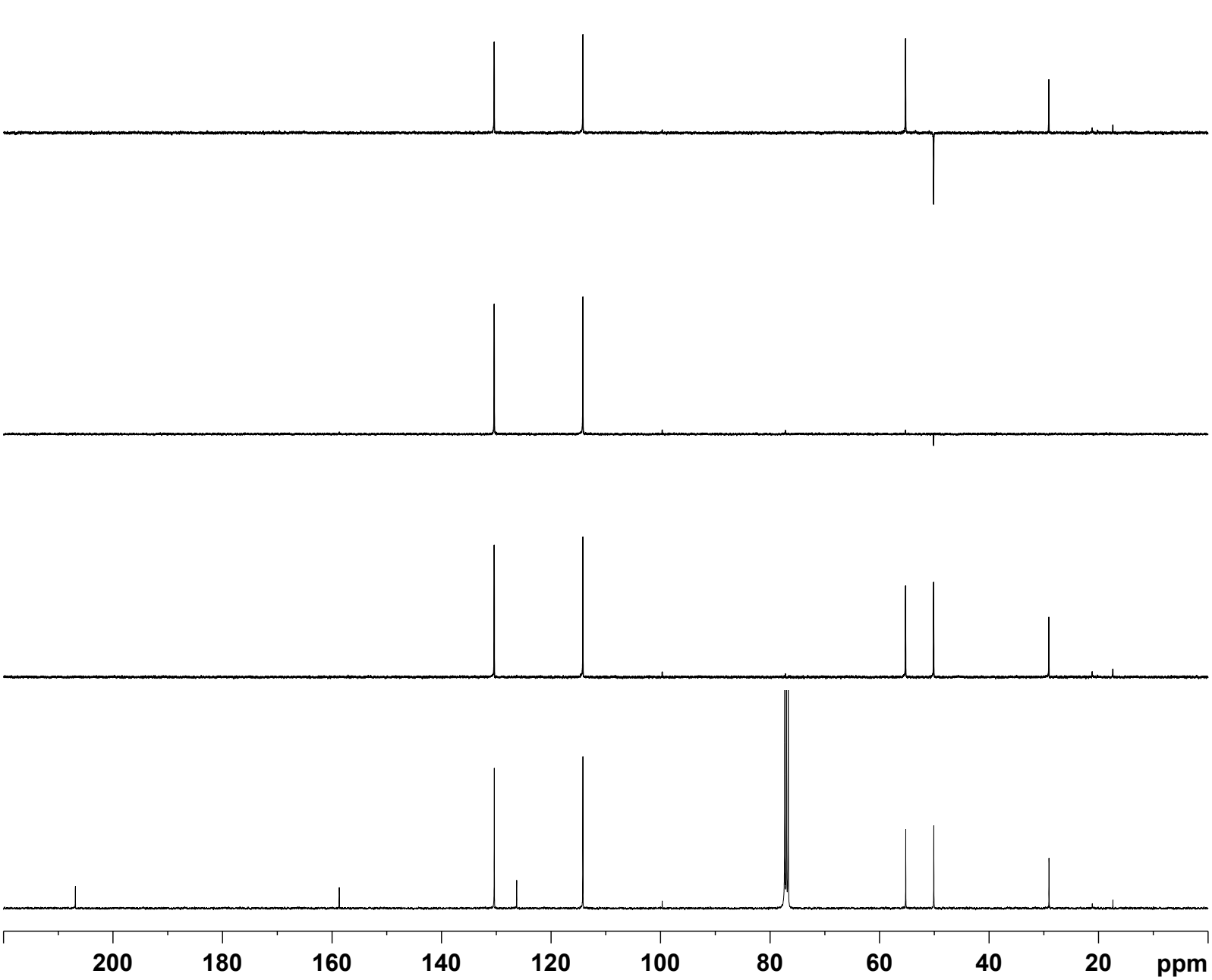



```
Current Data Parameters
NAME                  YYH-077
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210604
Time                    1.03 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       4000
DS                          0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     296.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1             100.6233329 MHz
NUC1                     13C
P1                     10.50 usec
PLW1              44.29999924 W
SFO2              400.1316005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2              14.60000038 W
PLW12              0.37897000 W
PLW13              0.19032000 W

F2 - Processing parameters
SI                      32768
SF               100.6127712 MHz
WDW                       EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

13C NMR (CDCl3, 100 MHz) of compound **4c**



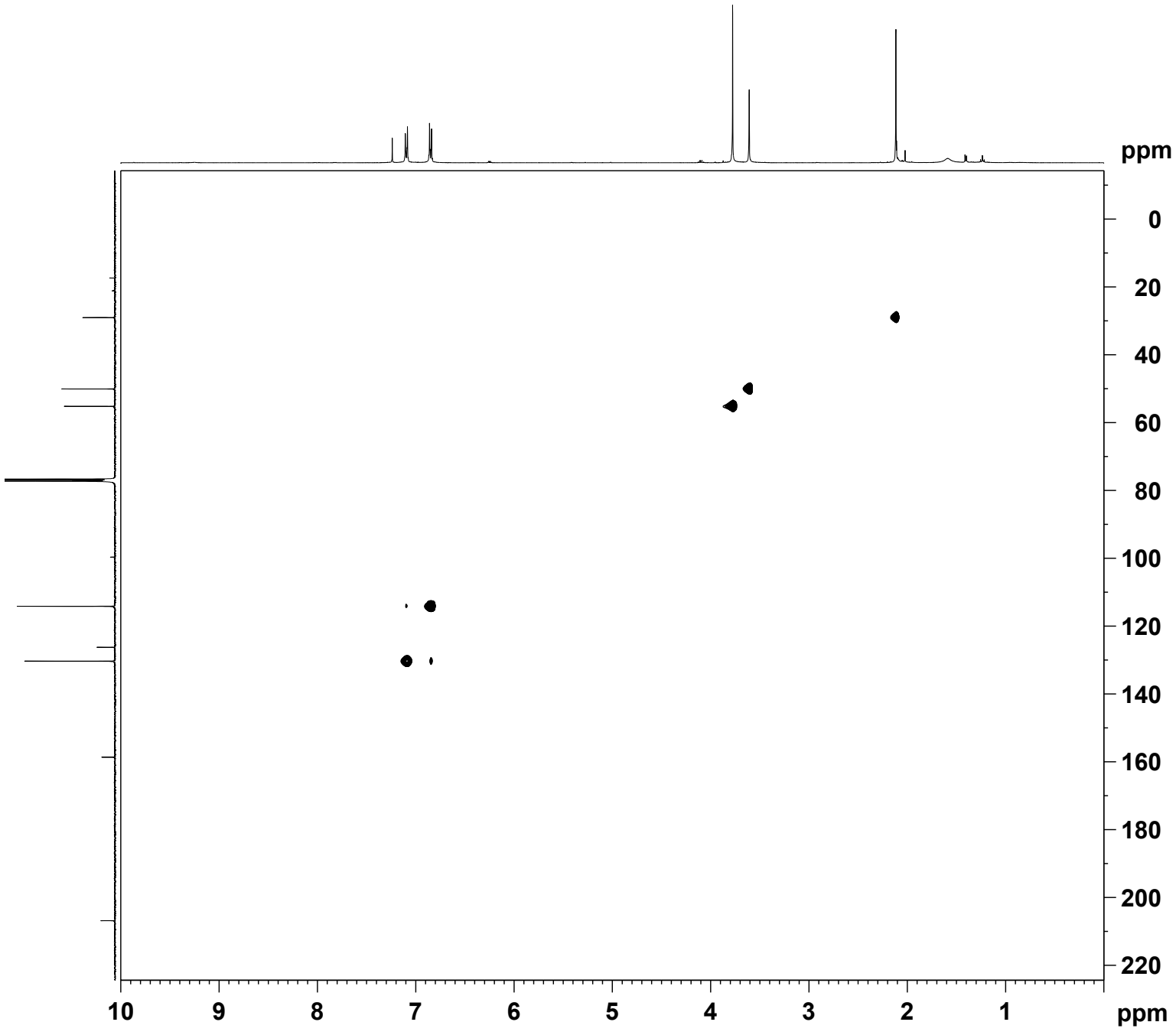

```
Current Data Parameters
NAME            YYH-077
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210604
Time               1.03 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4000
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               296.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1               10.50 usec
PLW1         44.29999924 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2         14.60000038 W
PLW12         0.37897000 W
PLW13         0.19032000 W

F2 - Processing parameters
SI                32768
SF          100.6127730 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

DEPT of compound **4c**

HSQC of compound **4c**




```
Current Data Parameters
NAME            YYH-077
EXPNO                 6
PROCNO                1

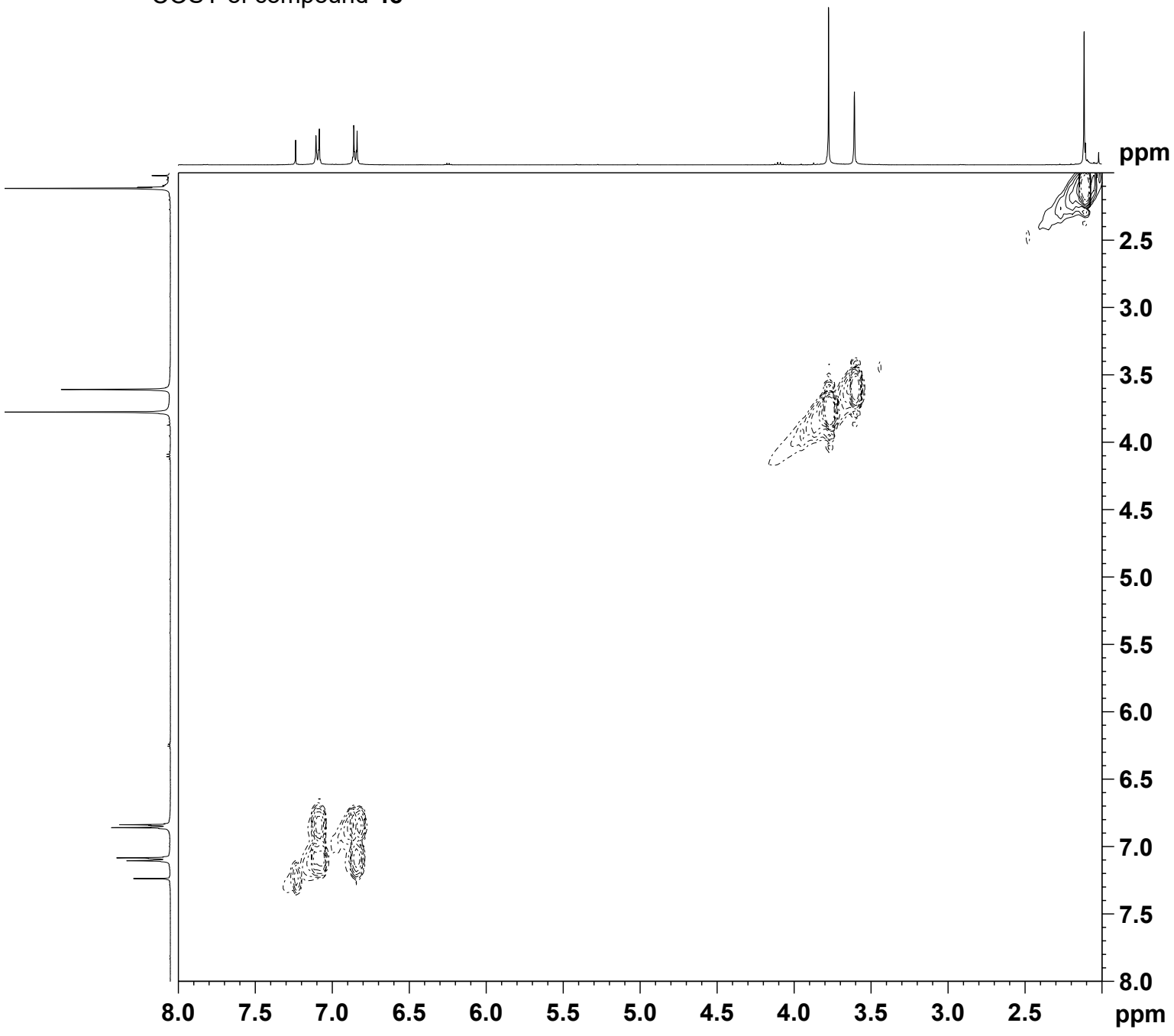
F2 - Acquisition Parameters
Date_          20210604
Time               5.38 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                 2048
SOLVENT           CDCl3
NS                    6
DS                   16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                297.3 K
CNST2       145.0000000
CNST17       -0.5000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002080 sec
TDav                  1
SFO1        400.1324008 MHz
NUC1                 1H
P1                14.50 usec
P2                29.00 usec
P28             1000.00 usec
PLW1        13.10000038 W
SFO2        100.6233329 MHz
NUC2                13C
CPDPRG[2           garp
P3                10.50 usec
P14              500.00 usec
P24             2000.00 usec
PCPD2             80.00 usec
PLW0     0 W
PLW2        44.00000000 W
PLW12        0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3            0.500
SPOFFS3  0 Hz
SPW3          7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7            0.500
SPOFFS7  0 Hz
SPW7          7.41179991 W
GPNAM[1]      SMSQ10.100
GPZ1              80.00 %
GPNAM[2]      SMSQ10.100
GPZ2              20.10 %
GPNAM[3]      SMSQ10.100
GPZ3              11.00 %
GPNAM[4]      SMSQ10.100
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

F1 - Acquisition parameters
TD                  256
SFO1           100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300188 MHz
WDW                QSINE
SSB                    2
LB       0 Hz
GB       0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2       echo-antiecho
SF          100.6127730 MHz
WDW                QSINE
SSB                    2
LB       0 Hz
GB       0
```

COSY of compound **4c**




```
Current Data Parameters
NAME             YYH-077
EXPNO                  7
PROCNO                 1

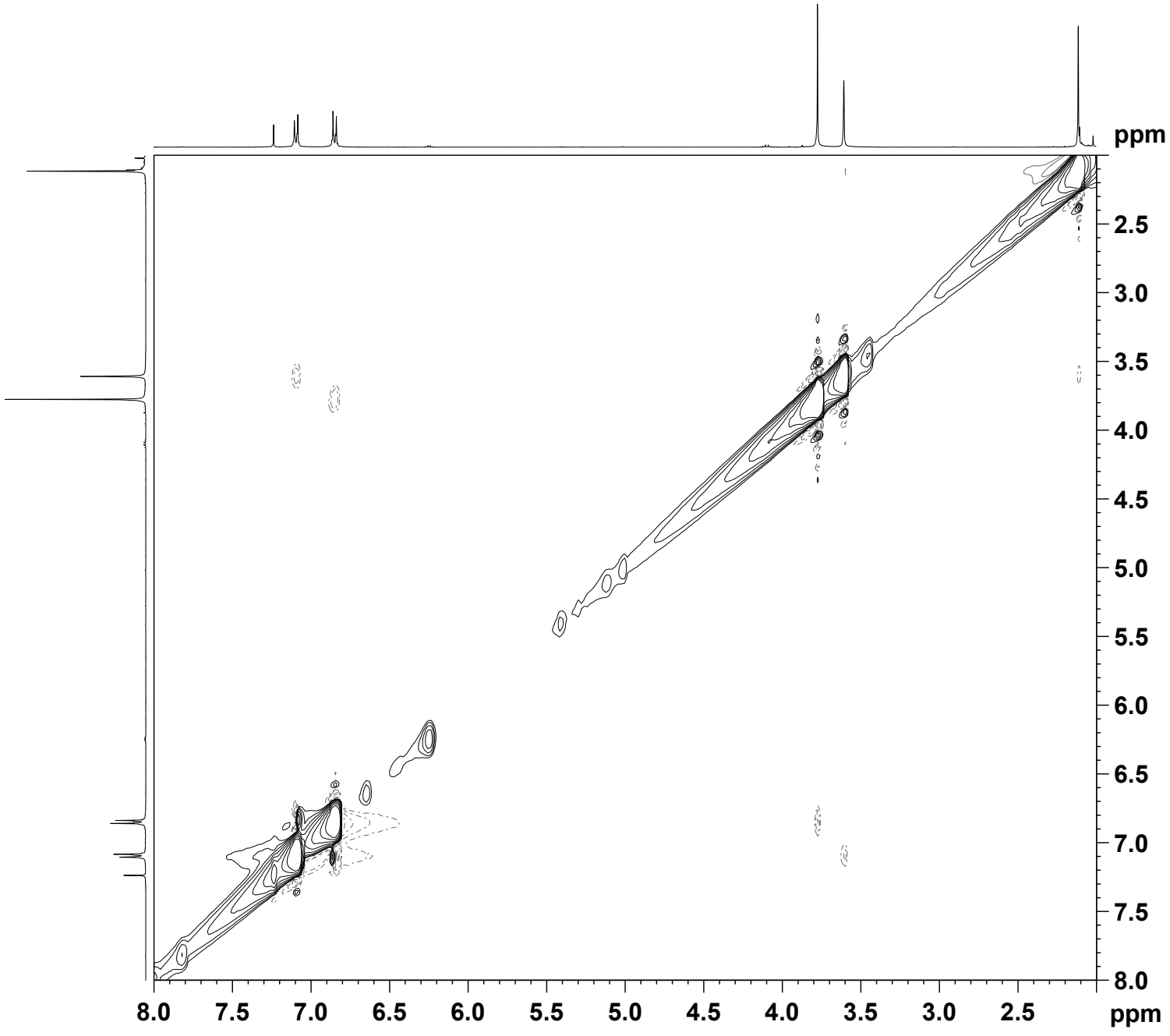
F2 - Acquisition Parameters
Date_           20210604
Time               6.22 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG      cosygpppqf
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                297.3 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         13.10000038 W
PLW10         3.06030011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE              QF

F2 - Processing parameters
SI                  1024
SF           400.1300188 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300188 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **4c**




```
Current Data Parameters
NAME                  YYH-077
EXPNO                       8
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210604
Time                    7.18 h
INSTRUM                 spect
PROBHD    Z108618_0922 (
PULPROG       noesygpphpp
TD                       2048
SOLVENT                 CDCl3
NS                          6
DS                         16
SWH                  8012.820 Hz
FIDRES               7.825020 Hz
AQ                   0.1277952 sec
RG                      210.28
DW                      62.400 usec
DE                       6.50 usec
TE                      296.7 K
D0                   0.00004394 sec
D1                   2.00000000 sec
D8                   0.40000001 sec
D11                  0.03000000 sec
D12                  0.00002000 sec
D16                  0.00020000 sec
IN0                  0.00012480 sec
TDav                        1
SFO1               400.1324008 MHz
NUC1                       1H
P1                      14.50 usec
P2                      29.00 usec
P17                   2500.00 usec
PLW1                13.10000038 W
PLW10                3.06030011 W
GPNAM[1]             SMSQ10.100
GPZ1                    40.00 %
P16                   1000.00 usec

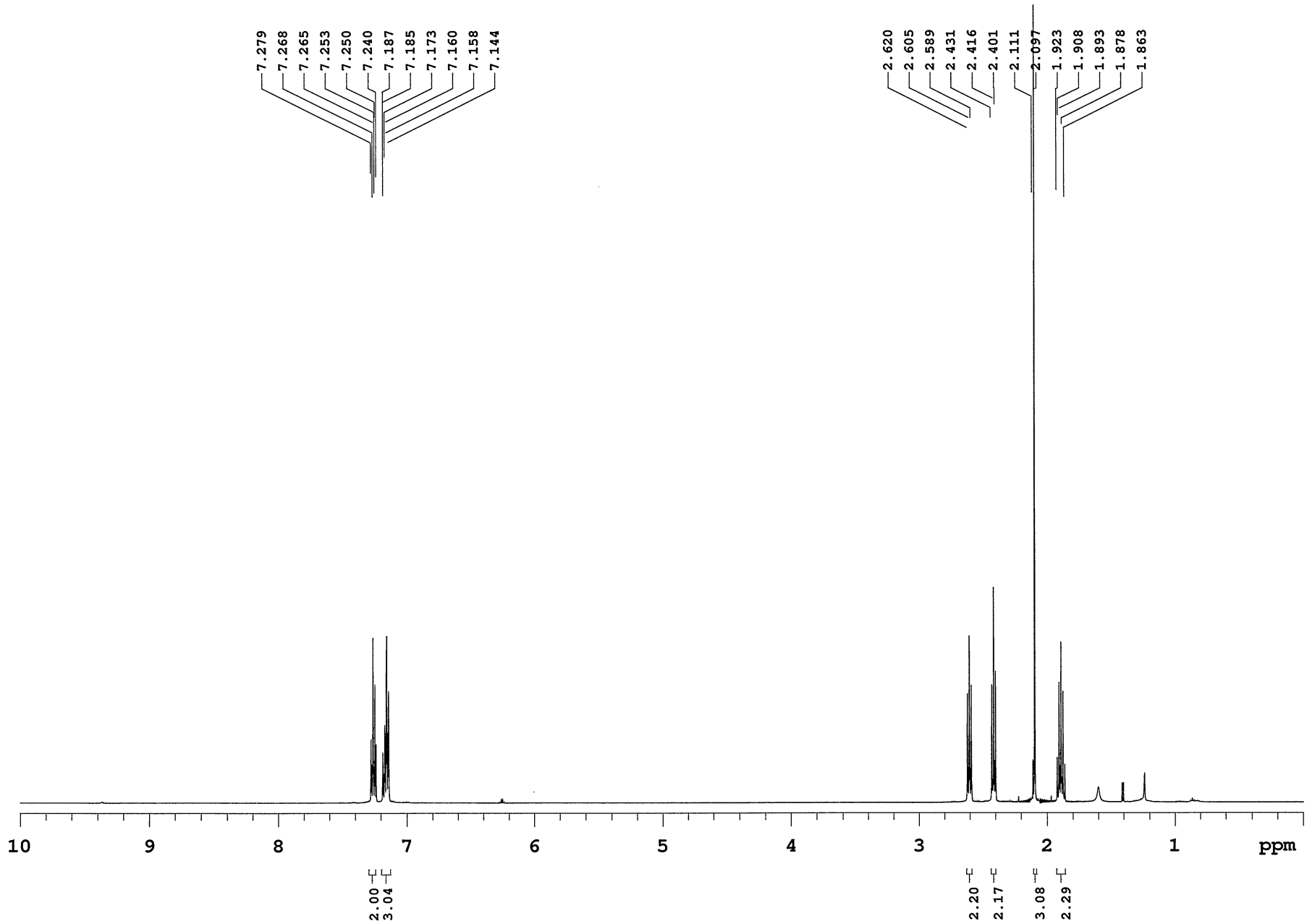
F1 - Acquisition parameters
TD                        256
SFO1                 400.1324 MHz
FIDRES                62.600159 Hz
SW                       20.025 ppm
FnMODE             States-TPPI

F2 - Processing parameters
SI                       1024
SF                 400.1300188 MHz
WDW                      QSINE
SSB                         2
LB              0 Hz
GB              0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                States-TPPI
SF                 400.1300188 MHz
WDW                      QSINE
SSB                         2
LB              0 Hz
GB              0
```

YYH-076

Sample Name **YYH-076**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



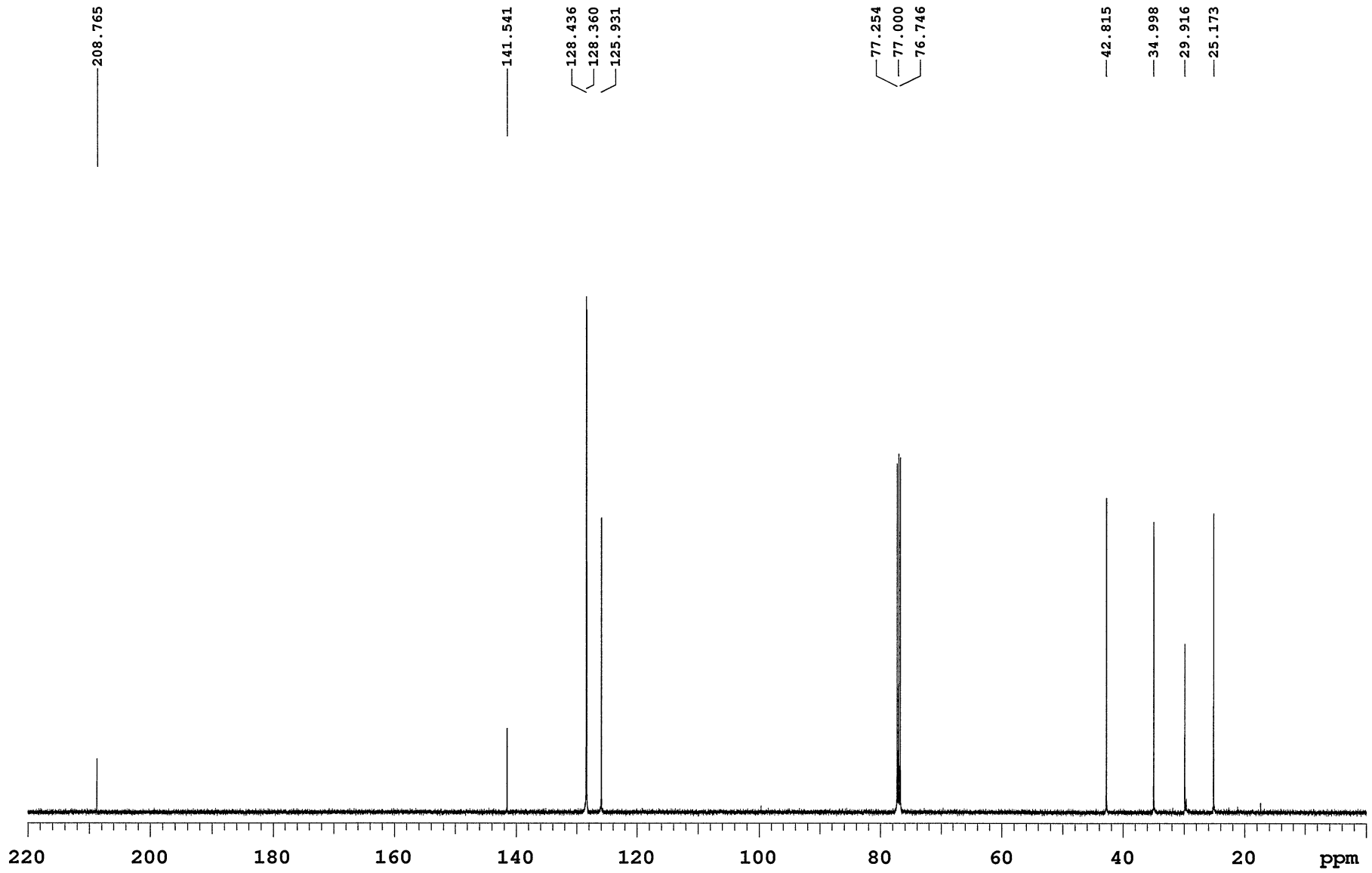
1H NMR (CDCl3, 500 MHz) of compound **4d**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-076/PROTON_03

Plot date 2021-06-10

YYH-076

Sample Name **YYH-076**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



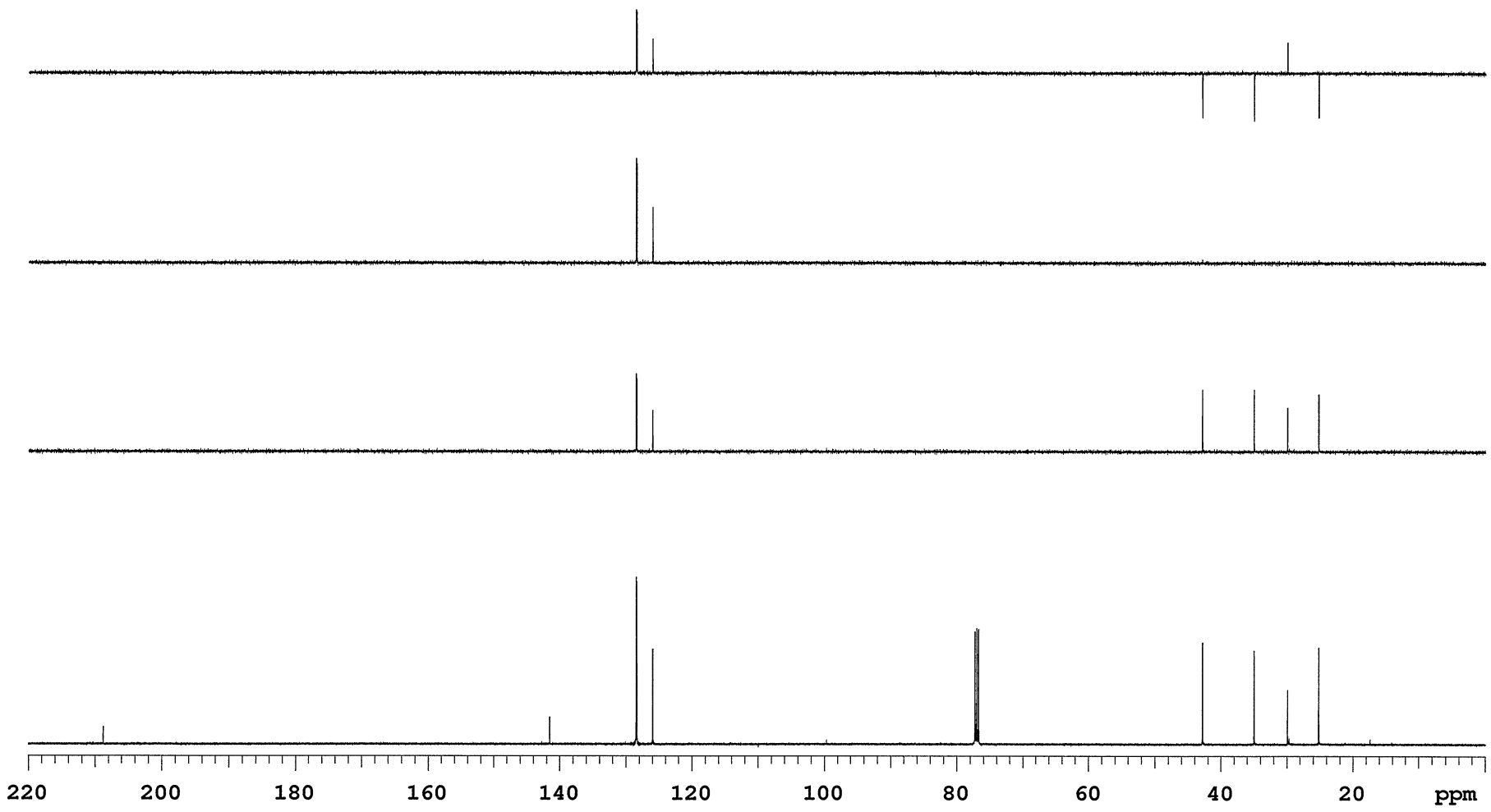
13C NMR (CDCl3, 125 MHz) of compound **4d**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-076/CARBON_02

Plot date 2021-06-10

YYH-076

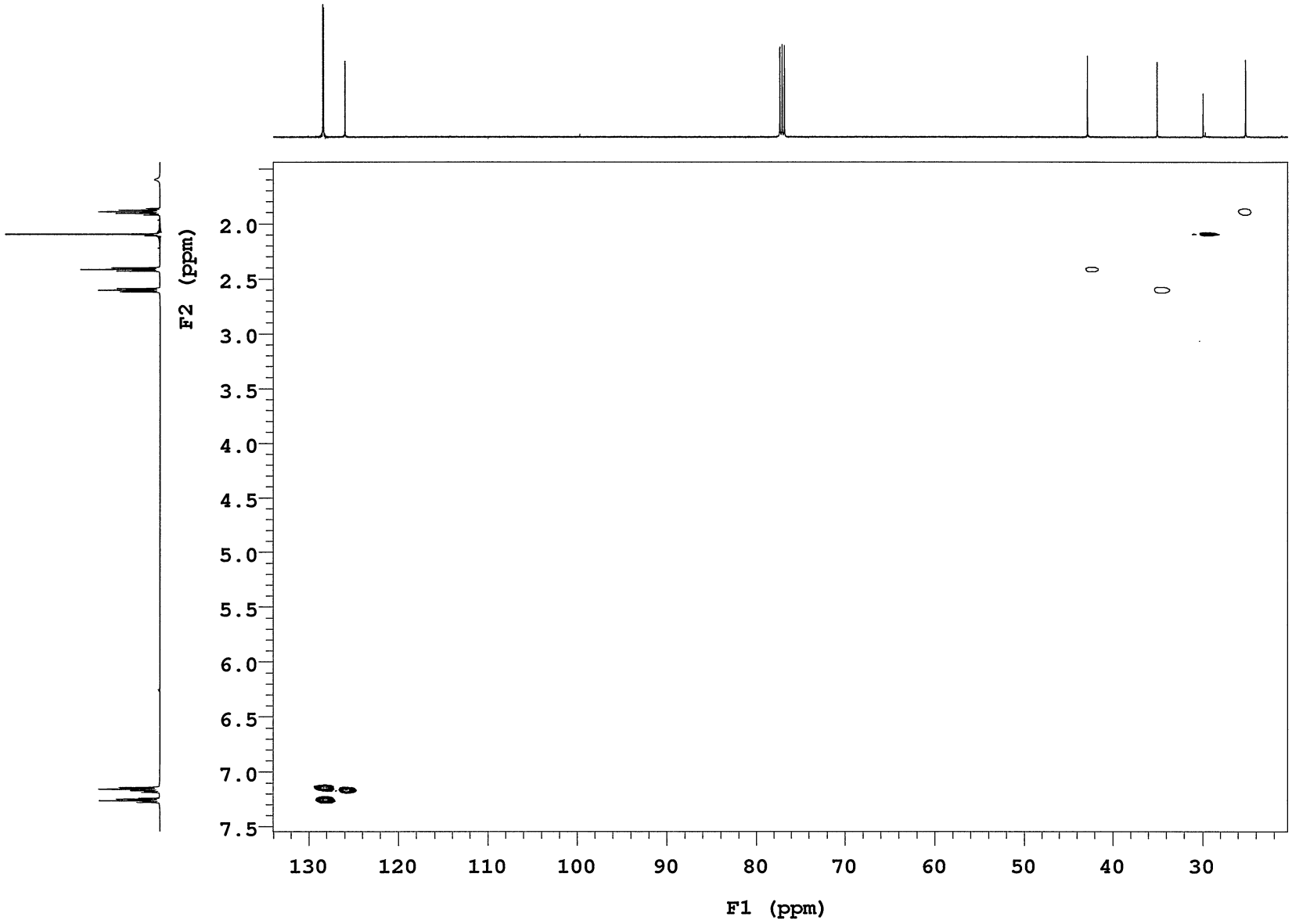
Sample Name **YYH-076**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **4d**

YYH-076

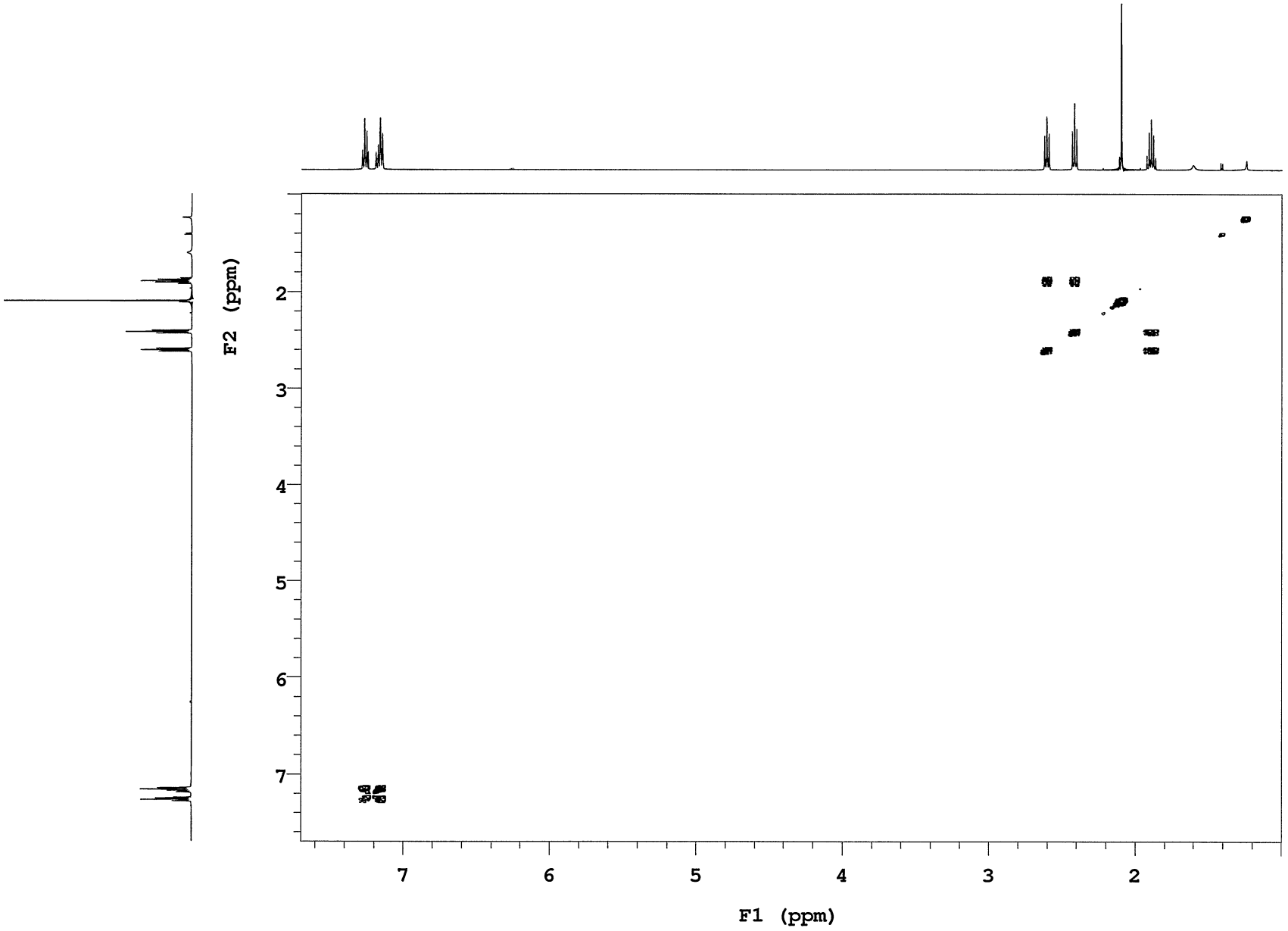
Sample Name	**YYH-076**	Pulse sequence	**gHSQC**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2021-06-10**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



HSQC of compound **4d**

YYH-076

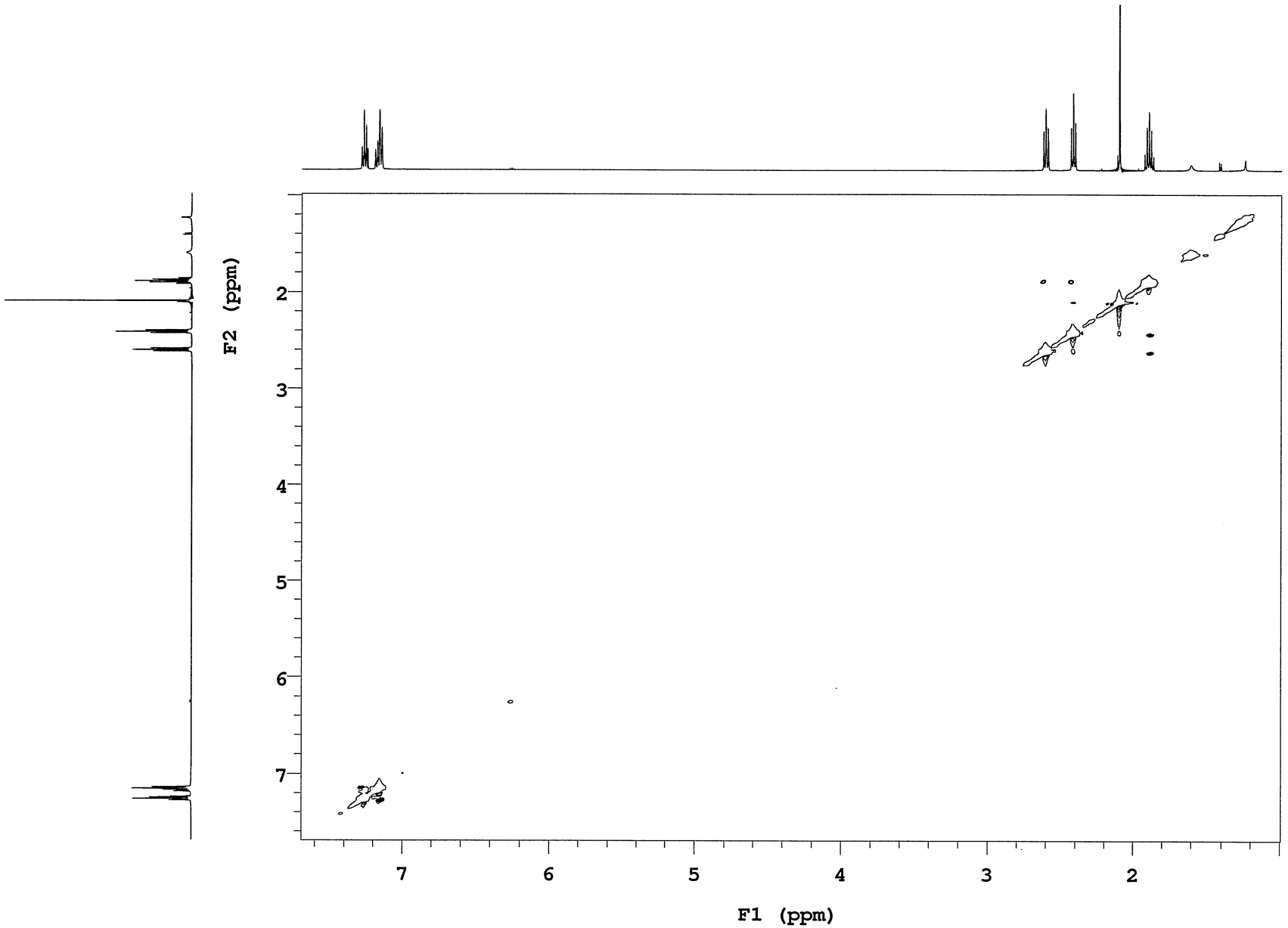
Sample Name **YYH-076**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-10**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



COSY of compound **4d**

YYH-076

Sample Name	**YYH-076**	Pulse sequence	**NOESY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2021-06-10**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

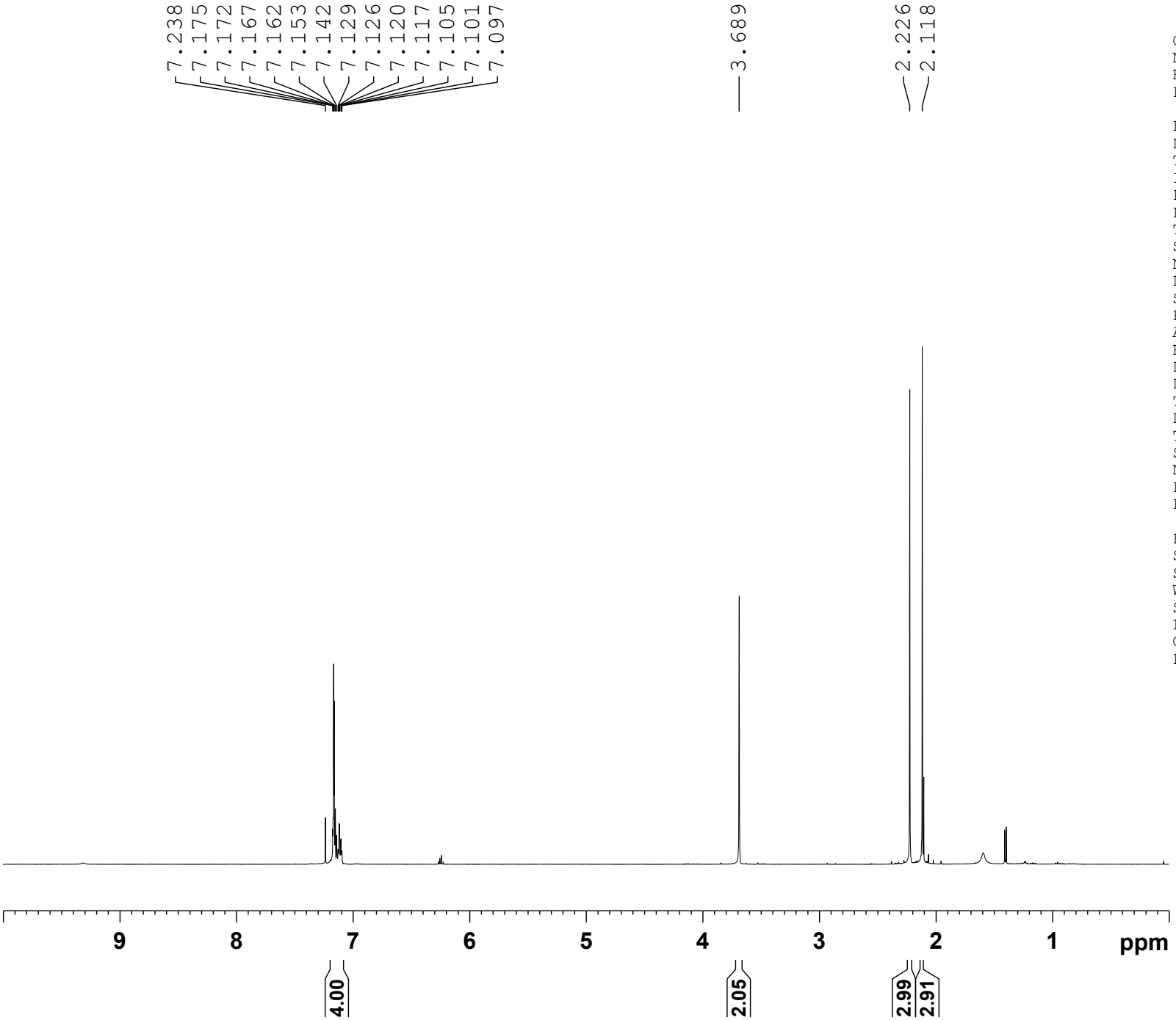


NOESY of compound **4d**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-076/NOESY_01

Plot date 2021-06-10

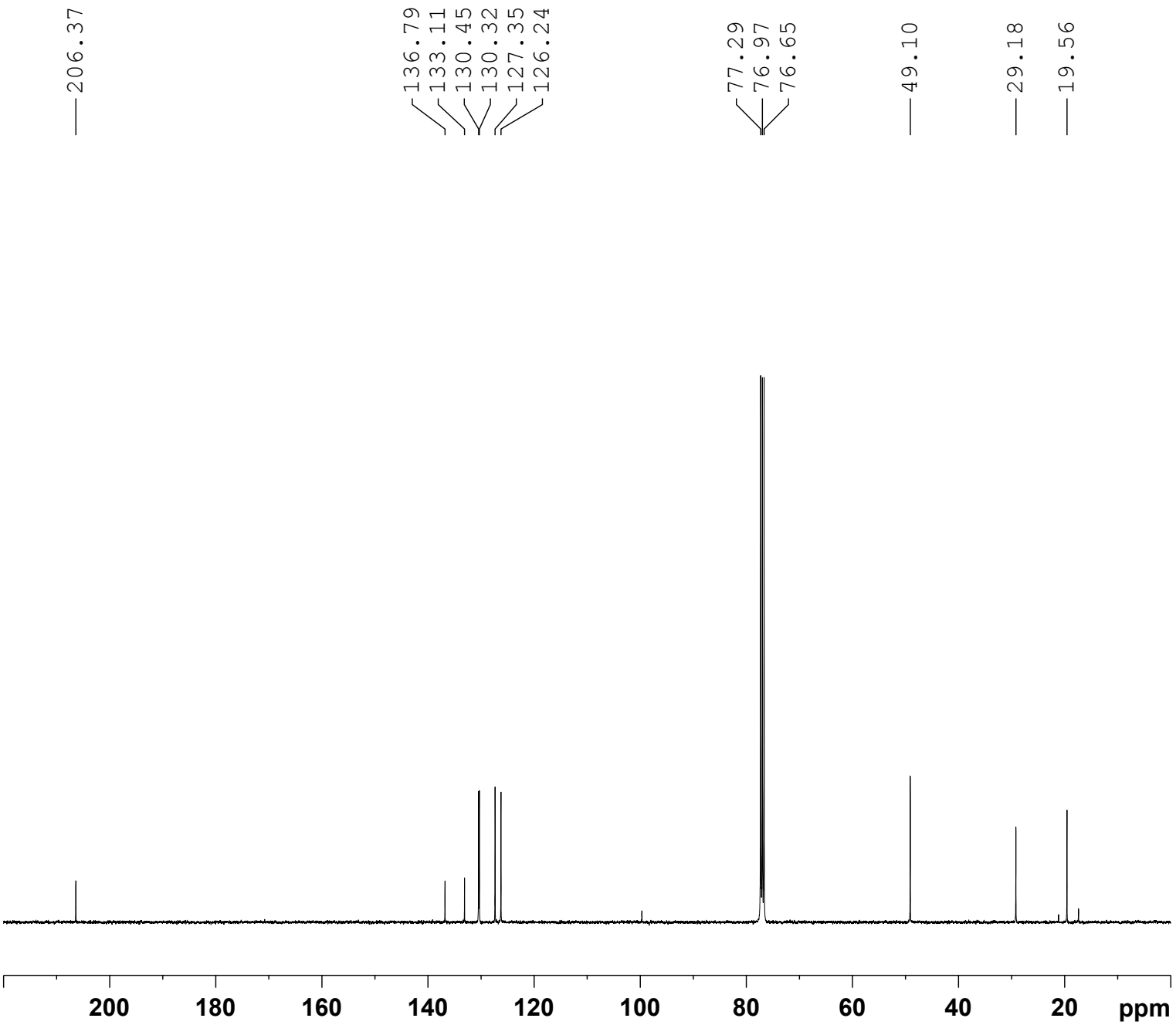
1H NMR (CDCl3, 400 MHz) of compound **4e**




```
Current Data Parameters
NAME                 YYH-084
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210607
Time                  23.08 h
INSTRUM               spect
PROBHD    Z108618_0922 (
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                2.0447233 sec
RG                   177.78
DW                   62.400 usec
DE                   16.43 usec
TE                   297.7 K
D1               2.00000000 sec
TD0                        1
SFO1           400.1324008 MHz
NUC1                      1H
P1                   14.50 usec
PLW1           13.10000038 W

F2 - Processing parameters
SI                    16384
SF             400.1300189 MHz
WDW                      EM
SSB       0
LB        0 Hz
GB        0
PC                    1.00
```



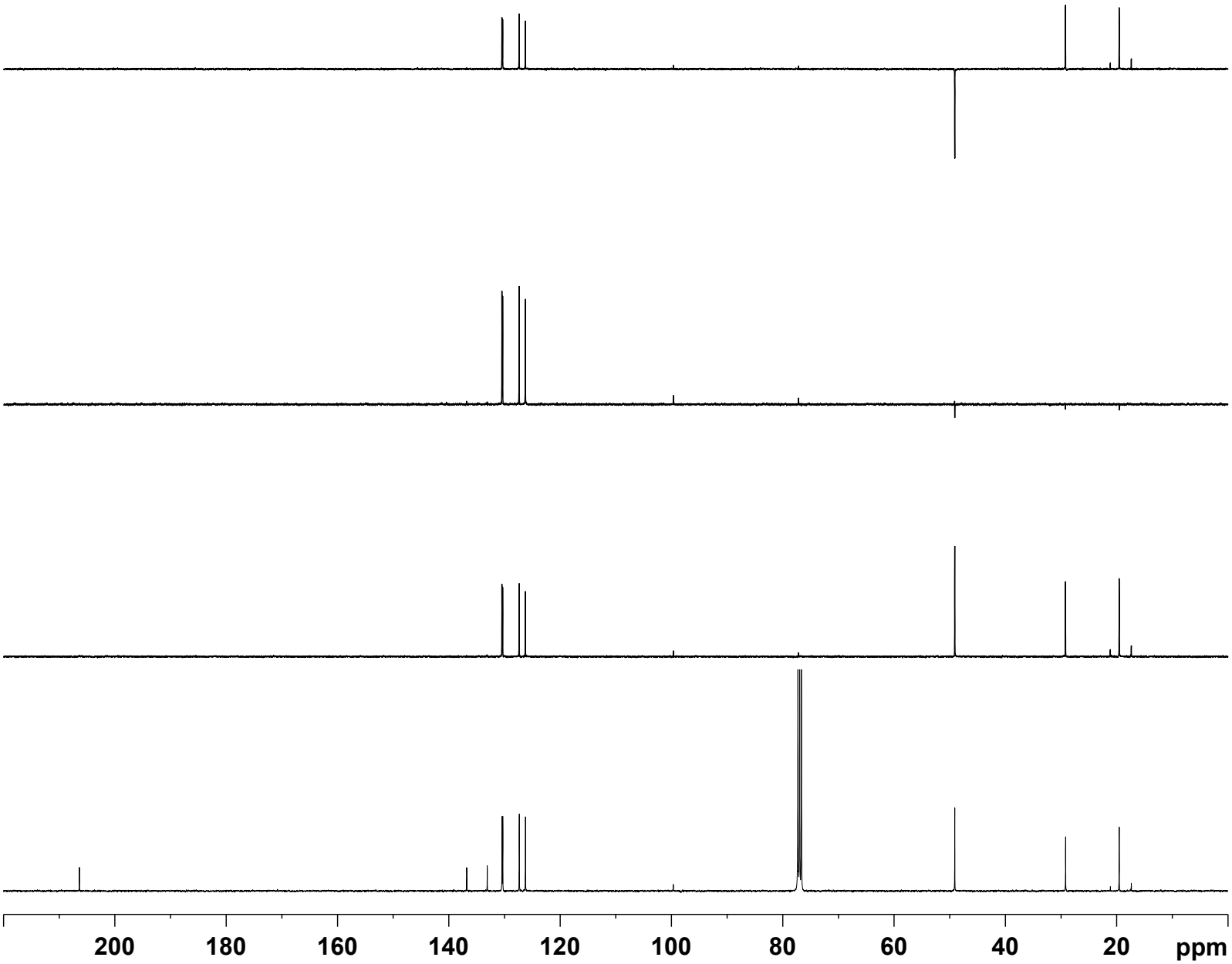

```
Current Data Parameters
NAME                  YYH-084
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210608
Time                    9.34 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG               zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      4000
DS                         0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     299.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             100.6233329 MHz
NUC1                     13C
P1                     10.50 usec
PLW1              44.29999924 W
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2              14.60000038 W
PLW12              0.37897000 W
PLW13              0.19032000 W

F2 - Processing parameters
SI                     32768
SF               100.6127747 MHz
WDW                       EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

13C NMR (CDCl3, 100 MHz) of compound **4e**

DEPT of compound **4e**




```
Current Data Parameters
NAME            YYH-084
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210608
Time               9.34 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4000
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW                20.800 usec
DE                 6.50 usec
TE                299.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1                10.50 usec
PLW1         44.29999924 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2         14.60000038 W
PLW12         0.37897000 W
PLW13         0.19032000 W

F2 - Processing parameters
SI                32768
SF          100.6127747 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
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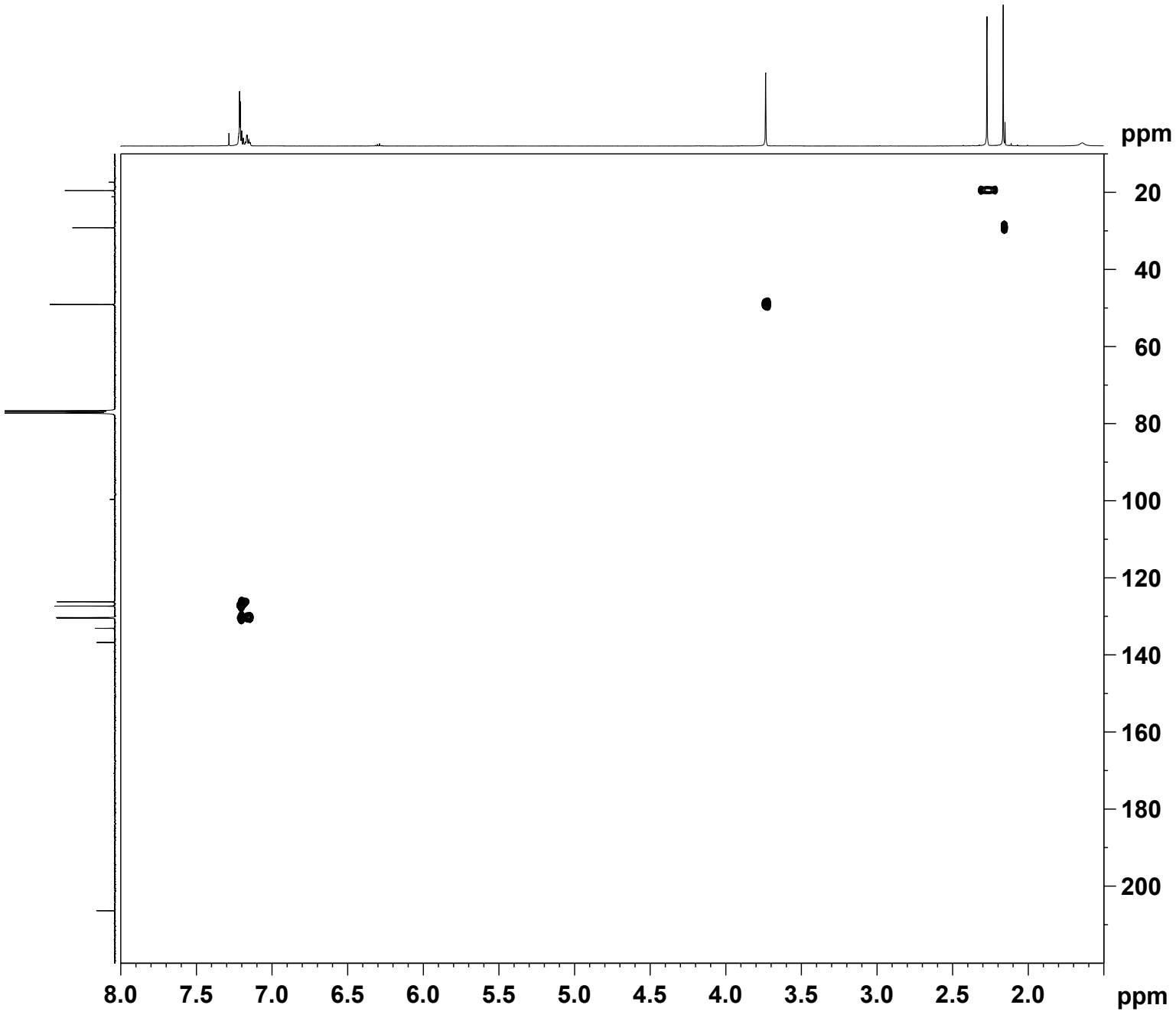
HSQC of compound **4e**

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Current Data Parameters
NAME             YYH-084
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
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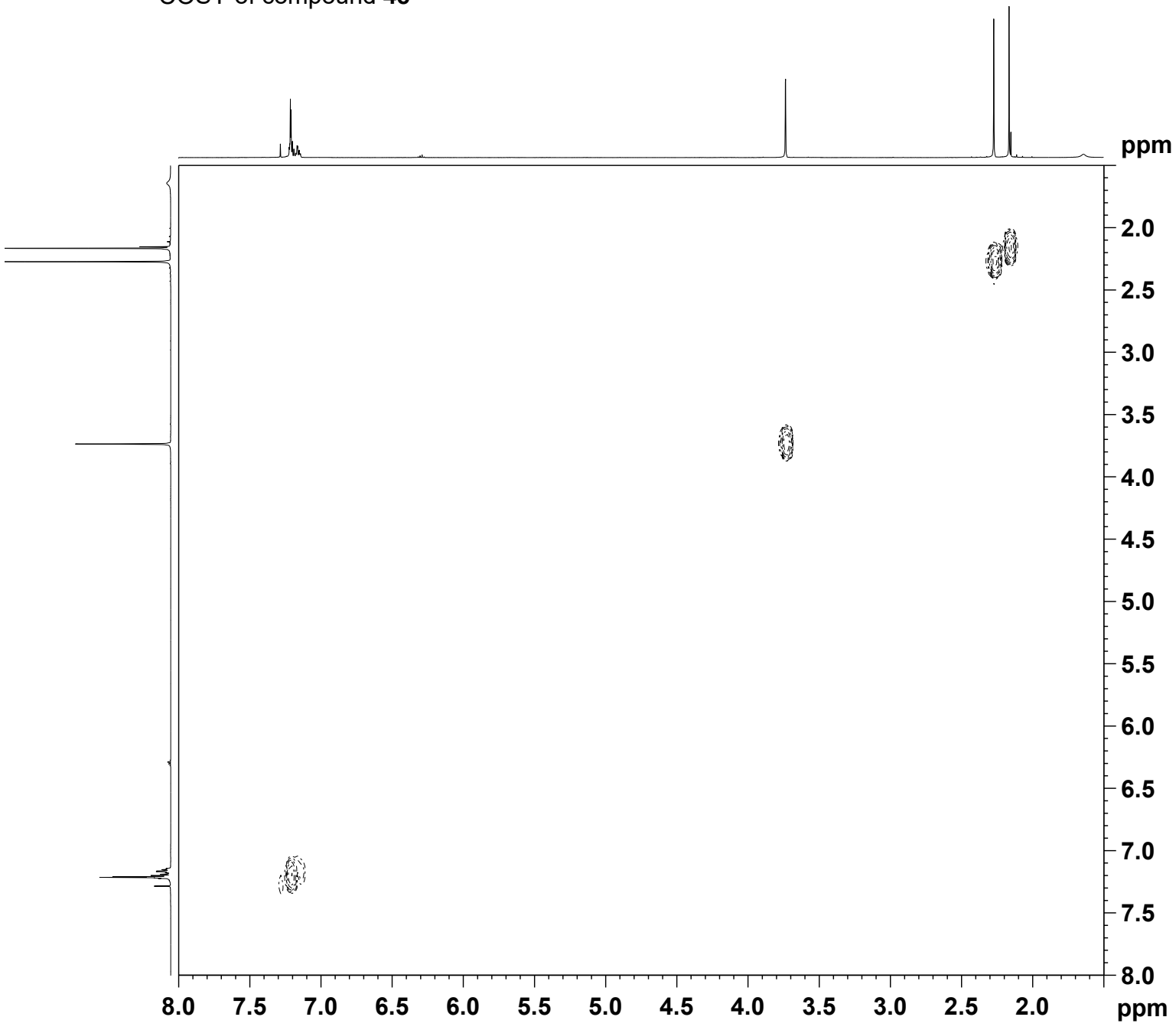
Time                3.45 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH              8012.820 Hz
FIDRES           7.825020 Hz
AQ               0.1277952 sec
RG                 210.28
DW                62.400 usec
DE                 6.50 usec
TE                298.1 K
CNST2        145.0000000
CNST17        -0.5000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002080 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         13.10000038 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2             garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0      0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3              0.500
SPOFFS3   0 Hz
SPW3          7.41179991 W
SPNAM[7]     Crp60comp.4
SPOAL7              0.500
SPOFFS7   0 Hz
SPW7          7.41179991 W
GPNAM[1]       SMSQ10.100
GPZ1                80.00 %
GPNAM[2]       SMSQ10.100
GPZ2                20.10 %
GPNAM[3]       SMSQ10.100
GPZ3                11.00 %
GPNAM[4]       SMSQ10.100
GPZ4                -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                    256
SFO1            100.6233 MHz
FIDRES        187.800476 Hz
SW               238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF            400.1300000 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF            100.6127747 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

COSY of compound **4e**

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Current Data Parameters
NAME             YYH-084
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210608
Time               4.28 h
INSTRUM            spect
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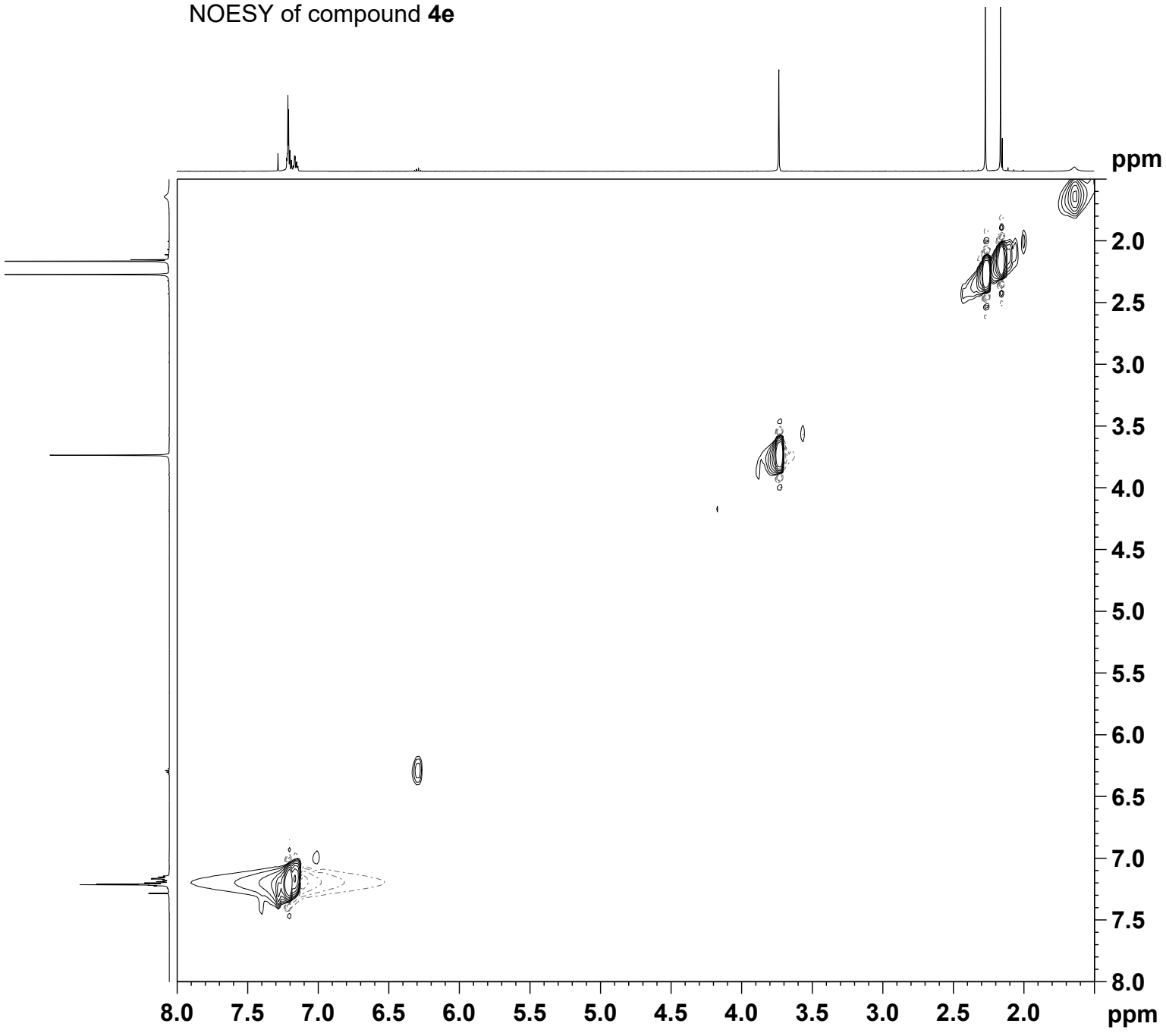
PULPROG       cosygpppqf
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                298.1 K
D0             0.00000300 sec
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         13.10000038 W
PLW10         3.06030011 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF           400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF           400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **4e**

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Current Data Parameters
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EXPNO                  8
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210608
Time               5.25 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG     noesygpphpp
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                 210.28
DW                 62.400 usec
DE                  6.50 usec
TE                 297.5 K
D0              0.00004394 sec
D1              2.00000000 sec
D8              0.40000001 sec
D11             0.03000000 sec
D12             0.00002000 sec
D16             0.00020000 sec
IN0             0.00012480 sec
TDav                   1
SFO1          400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P17              2500.00 usec
PLW1          13.10000038 W
PLW10          3.06030011 W
GPNAM[1]      SMSQ10.100
GPZ1              40.00 %
P16             1000.00 usec

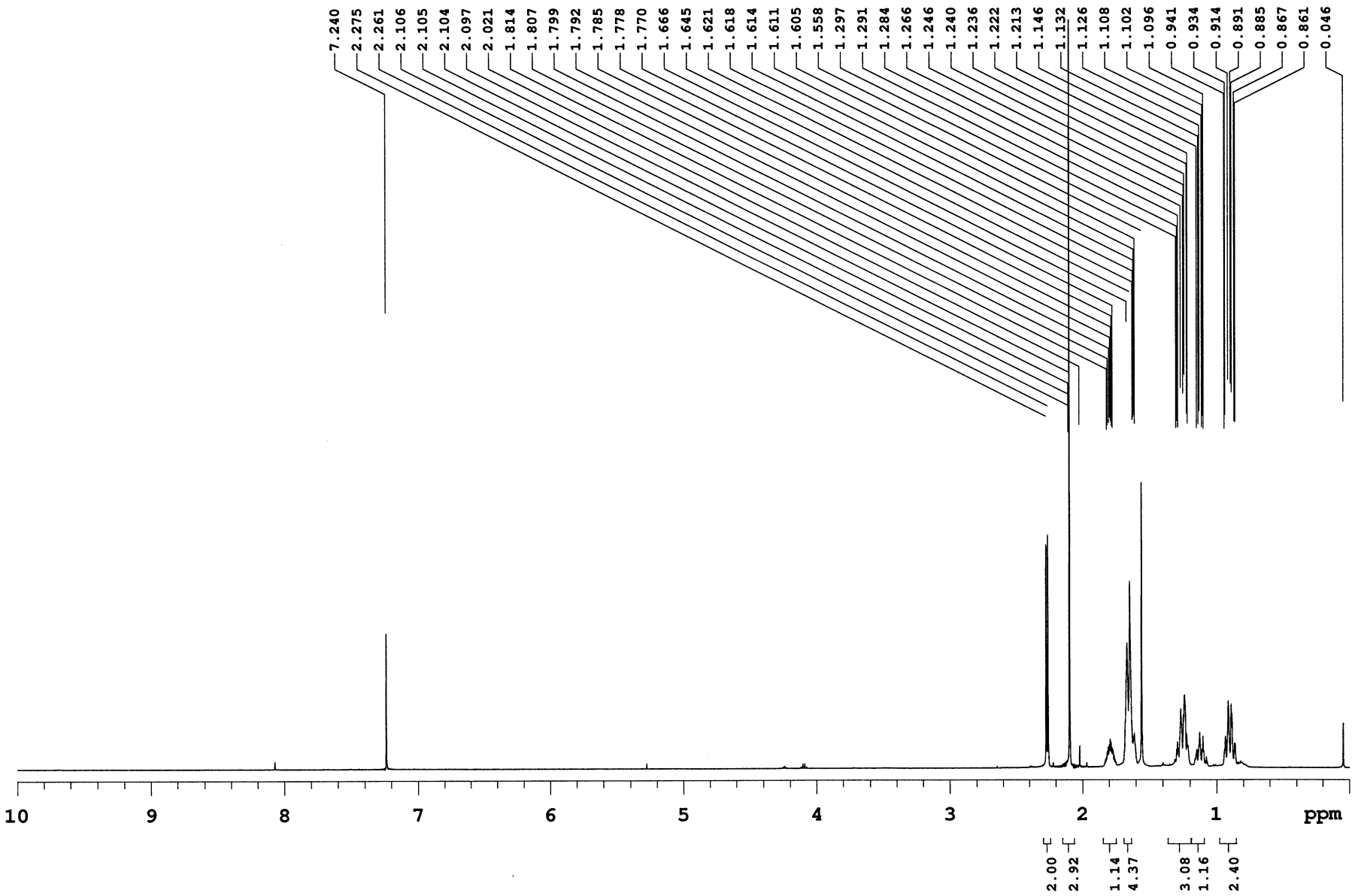
F1 - Acquisition parameters
TD                   256
SFO1           400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                  1024
SF           400.1300000 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2          States-TPPI
SF           400.1300000 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

YYH-079

Sample Name **YYH-079**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-26**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



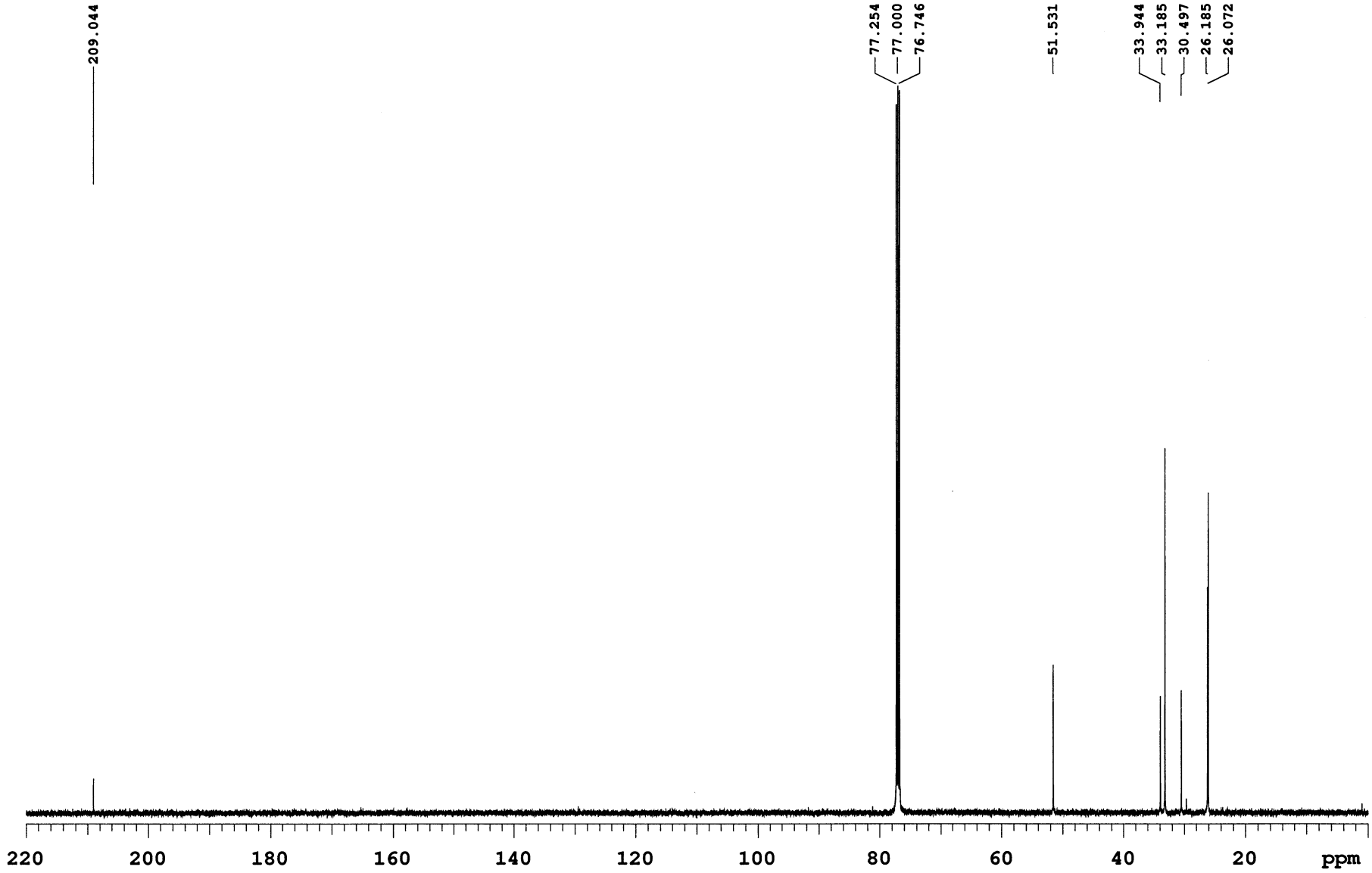
1H NMR (CDCl3, 500 MHz) of compound **4f**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-079/PROTON_03

Plot date 2021-07-28

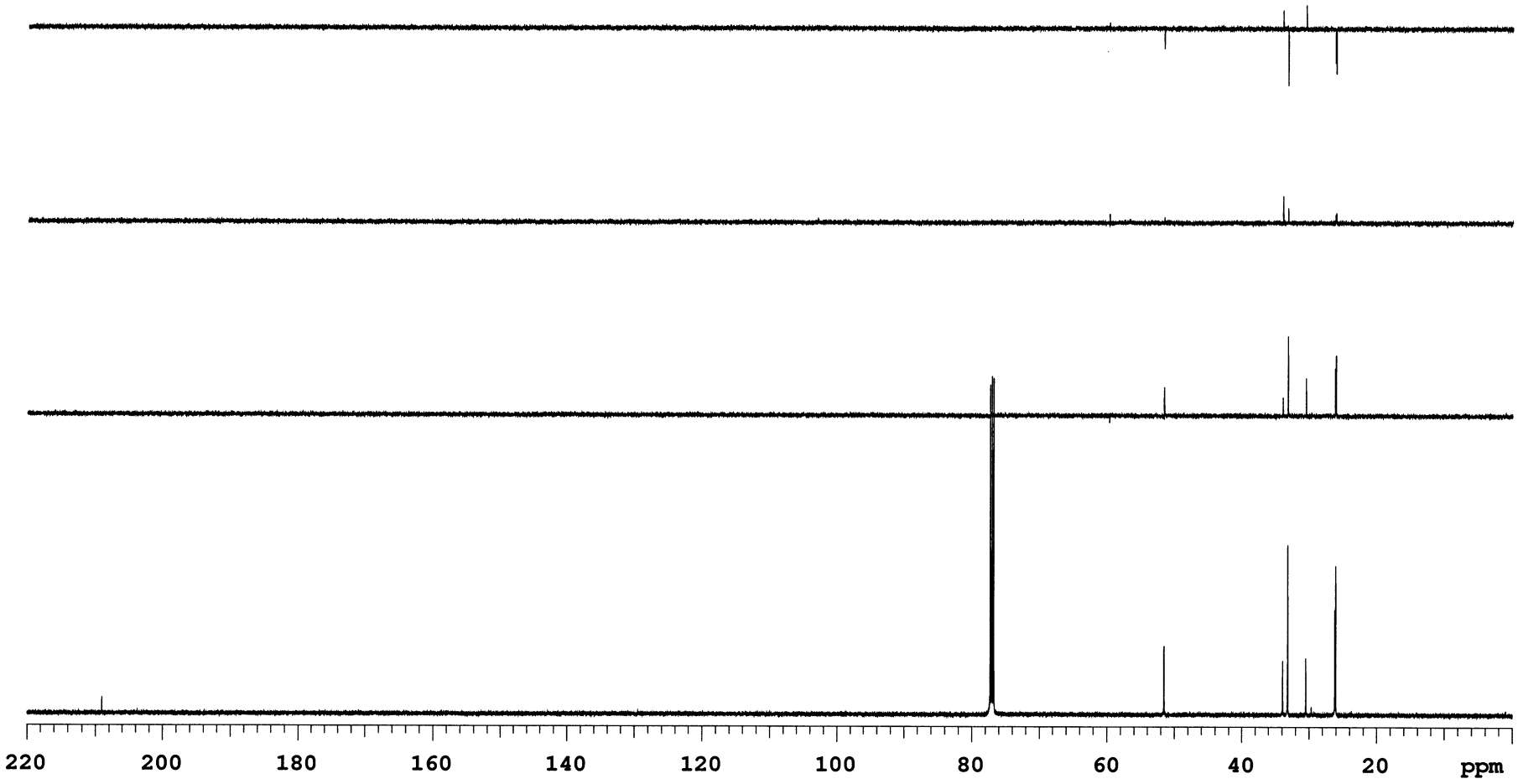
YYH-079

Sample Name **YYH-079**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-26**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



13C NMR (CDCl3, 125 MHz) of compound **4f**

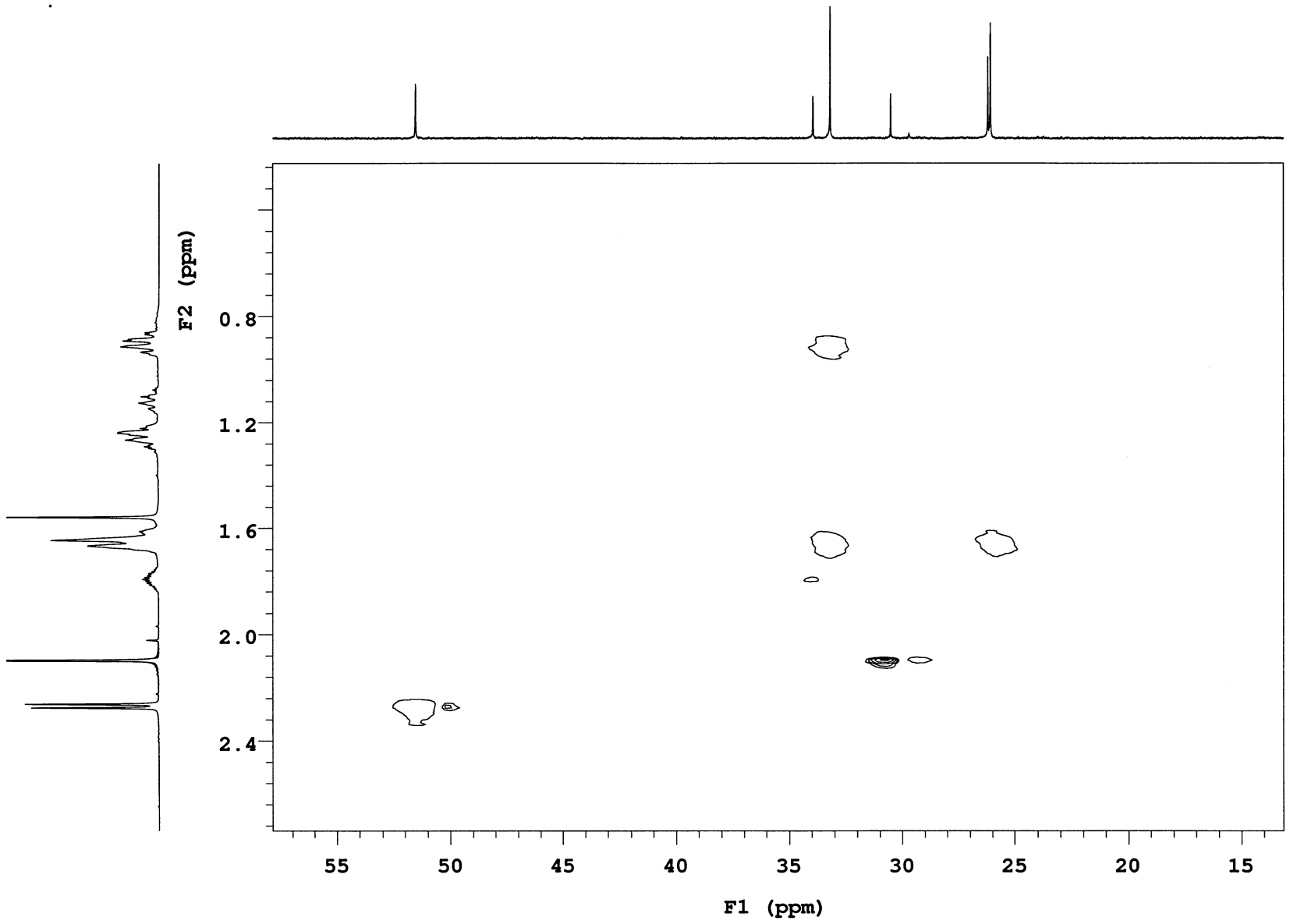
Sample Name **YYH-079** | Pulse sequence **DEPT** | Temperature **25** | Study owner **vnmr2**
Date collected **2021-08-06** | Solvent **cdcl3** | Spectrometer **Agilent-NMR-inova500** | Operator **vnmr2**



DEPT of compound **4f**

YYH-079

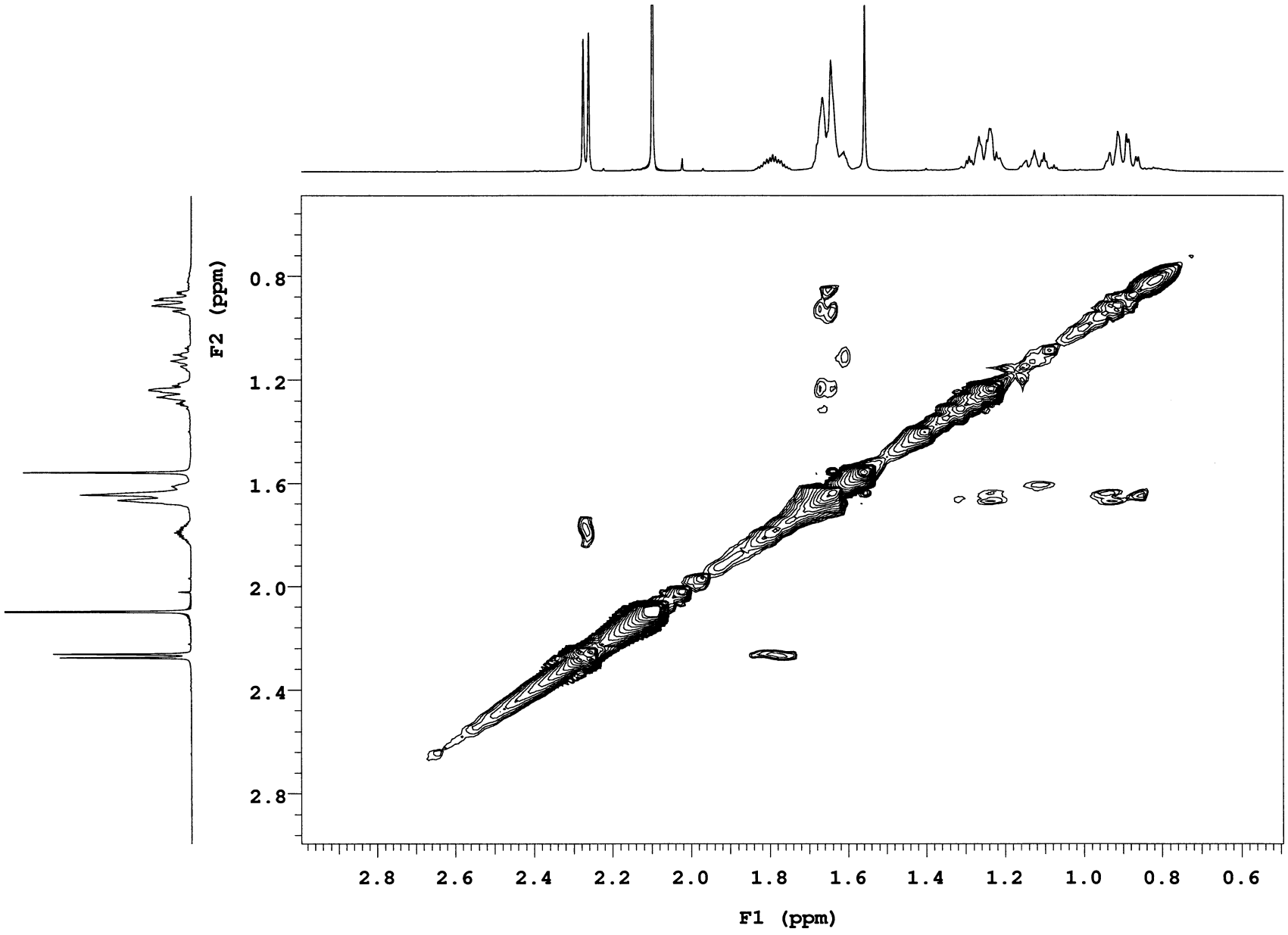
Sample Name **YYH-079**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



HSQC of compound **4f**

YYH-079

Sample Name **YYH-079**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



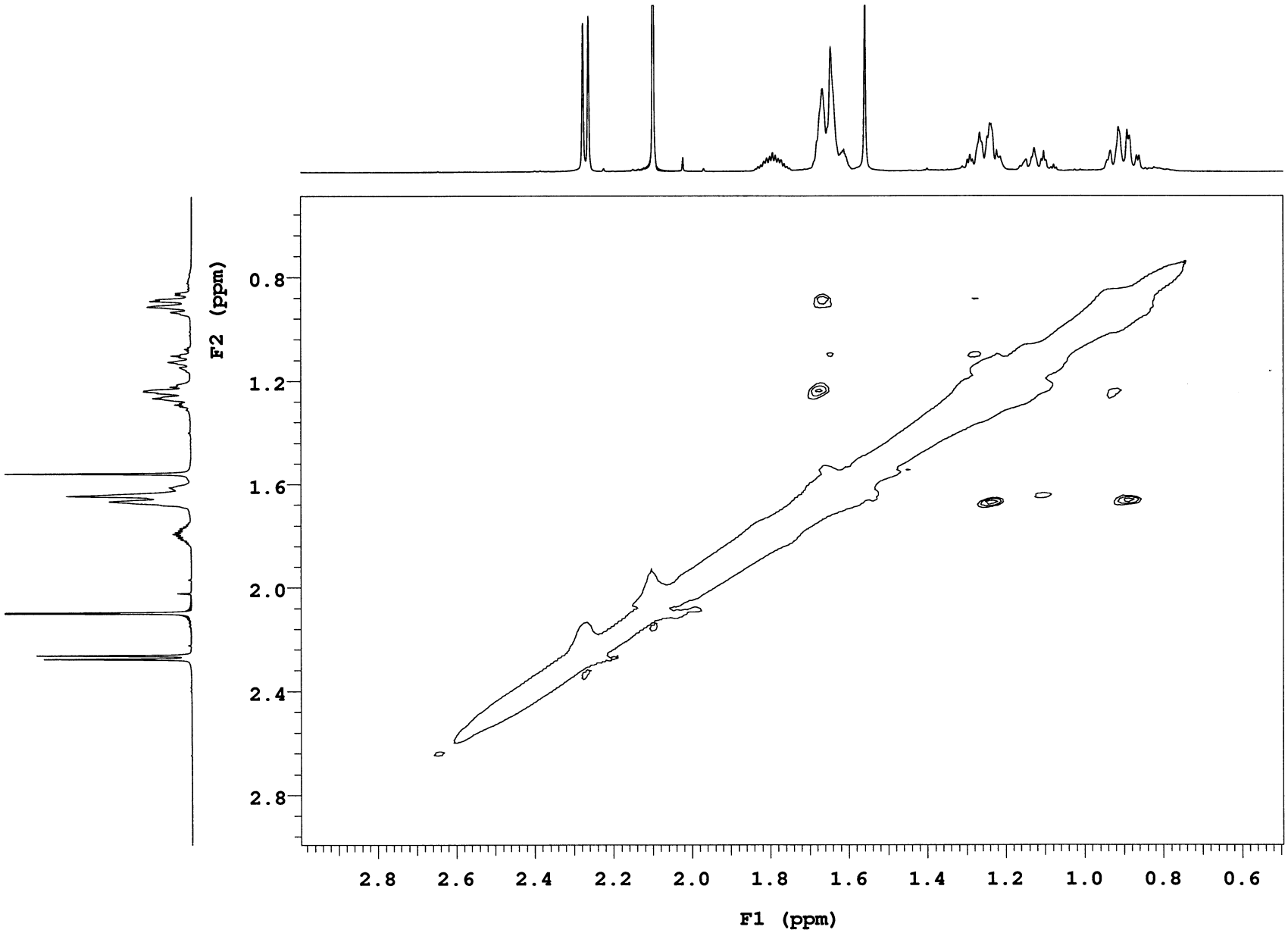
COSY of compound **4f**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-079/gCOSY_01

Plot date 2021-07-28

YYH-079

Sample Name **YYH-079**	Pulse sequence **NOESY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



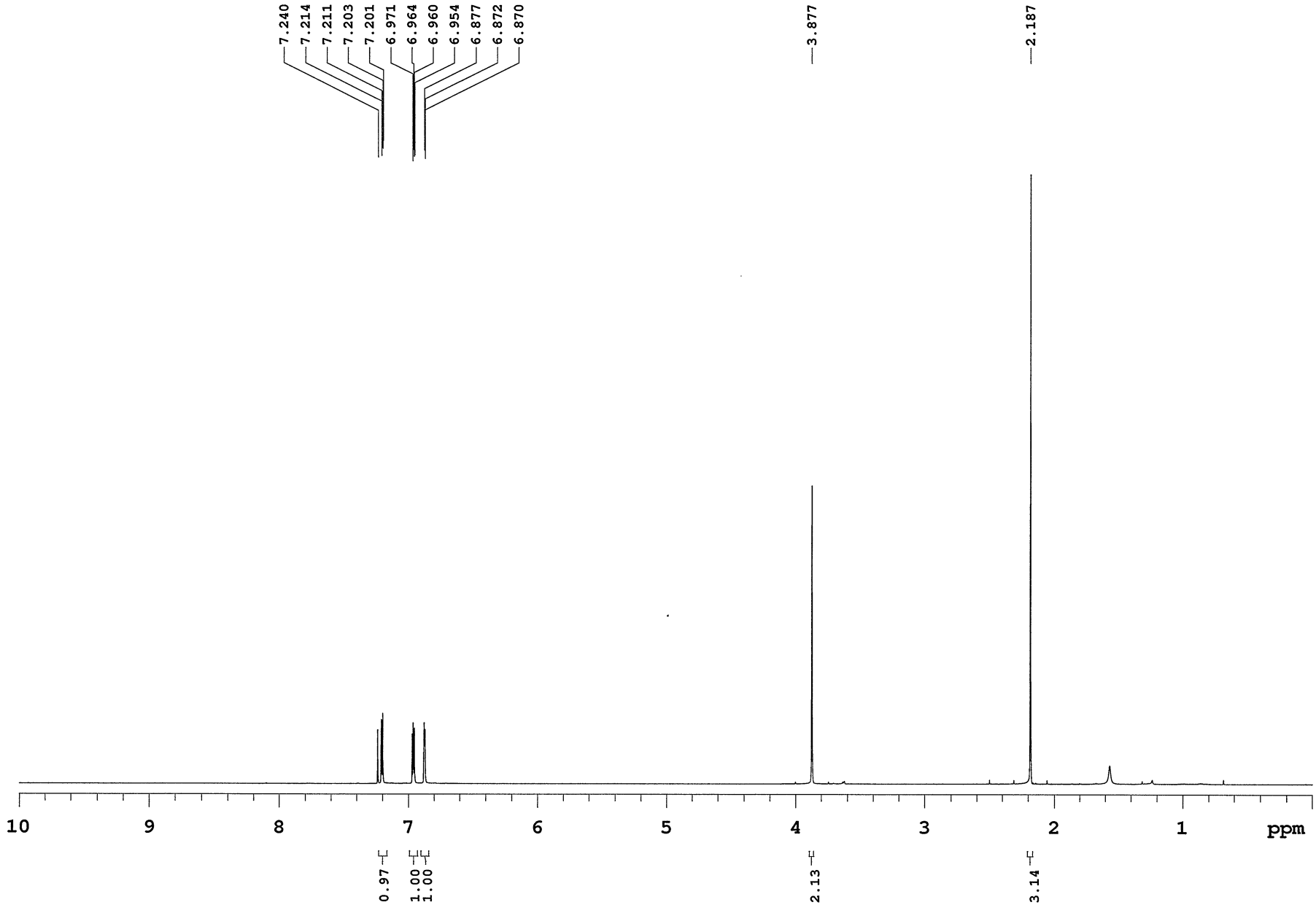
NOESY of compound **4f**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-079/NOESY_01

Plot date 2021-07-28

YYH-080

Sample Name **YYH-080**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-23**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



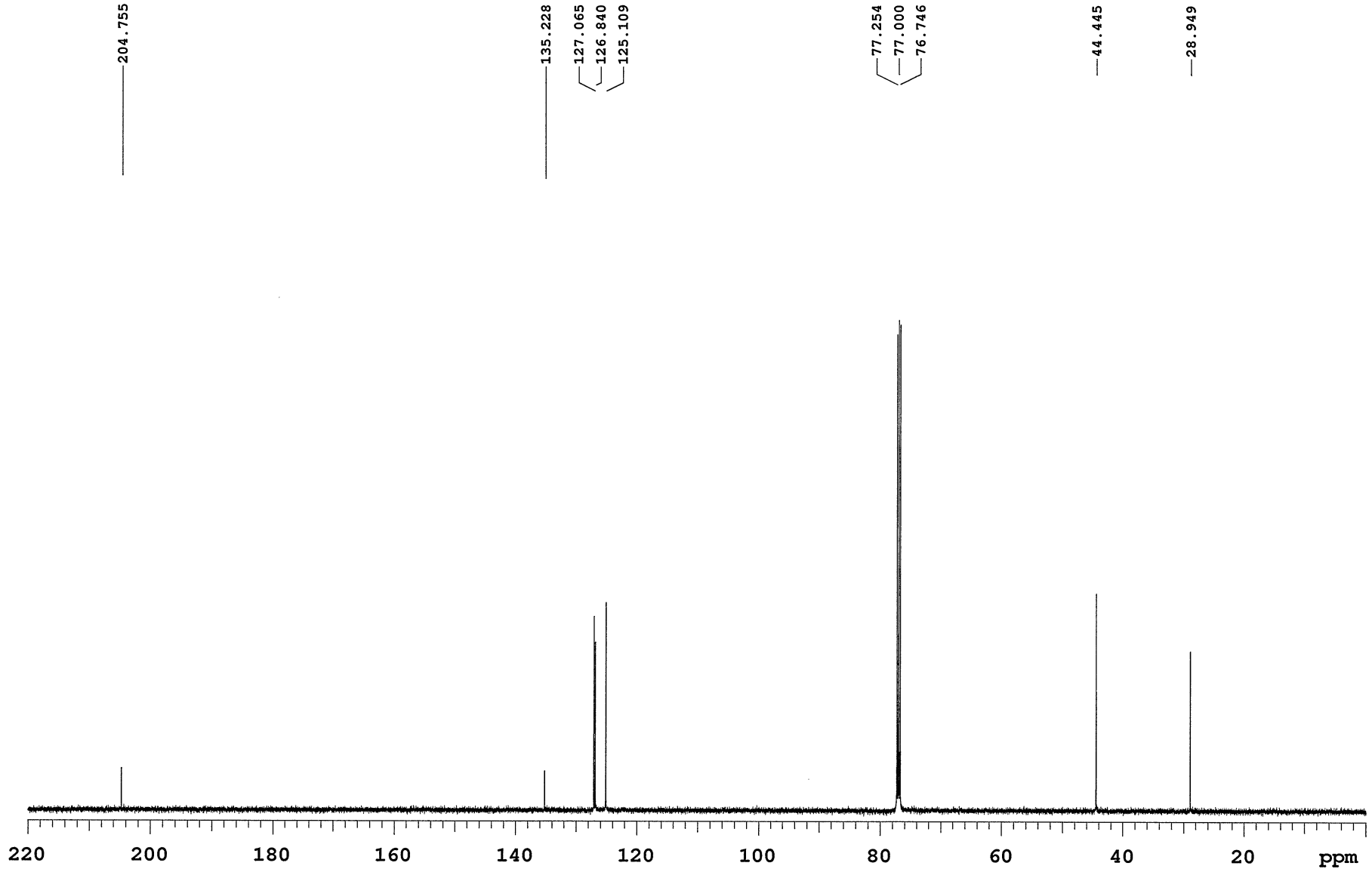
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-080/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4g**

Plot date 2021-06-28

YYH-080

Sample Name **YYH-080**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-23**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



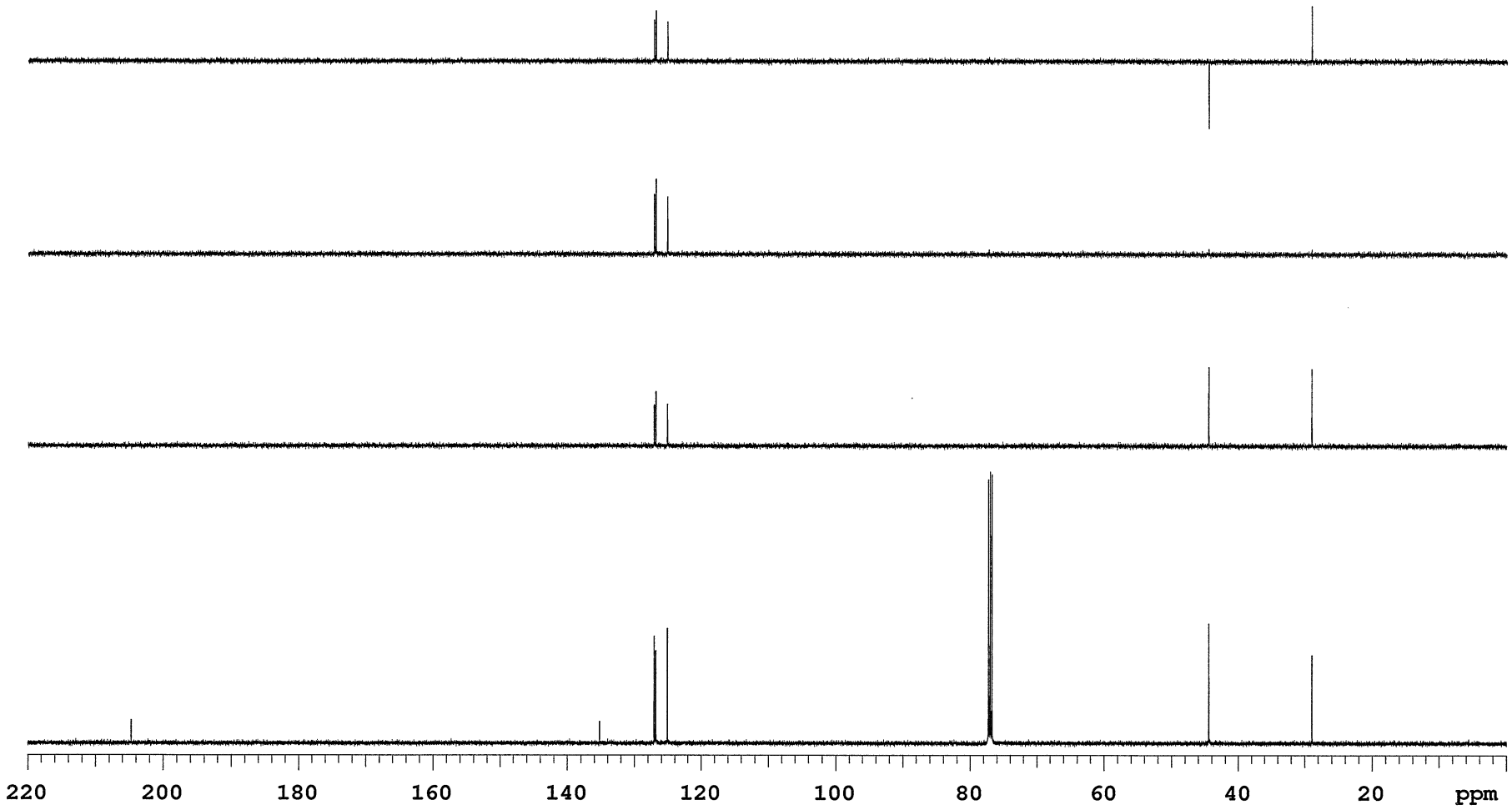
13C NMR (CDCl3, 125 MHz) of compound **4g**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-080/CARBON_02

Plot date 2021-06-28

YYH-080

Sample Name **YYH-080**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-24**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



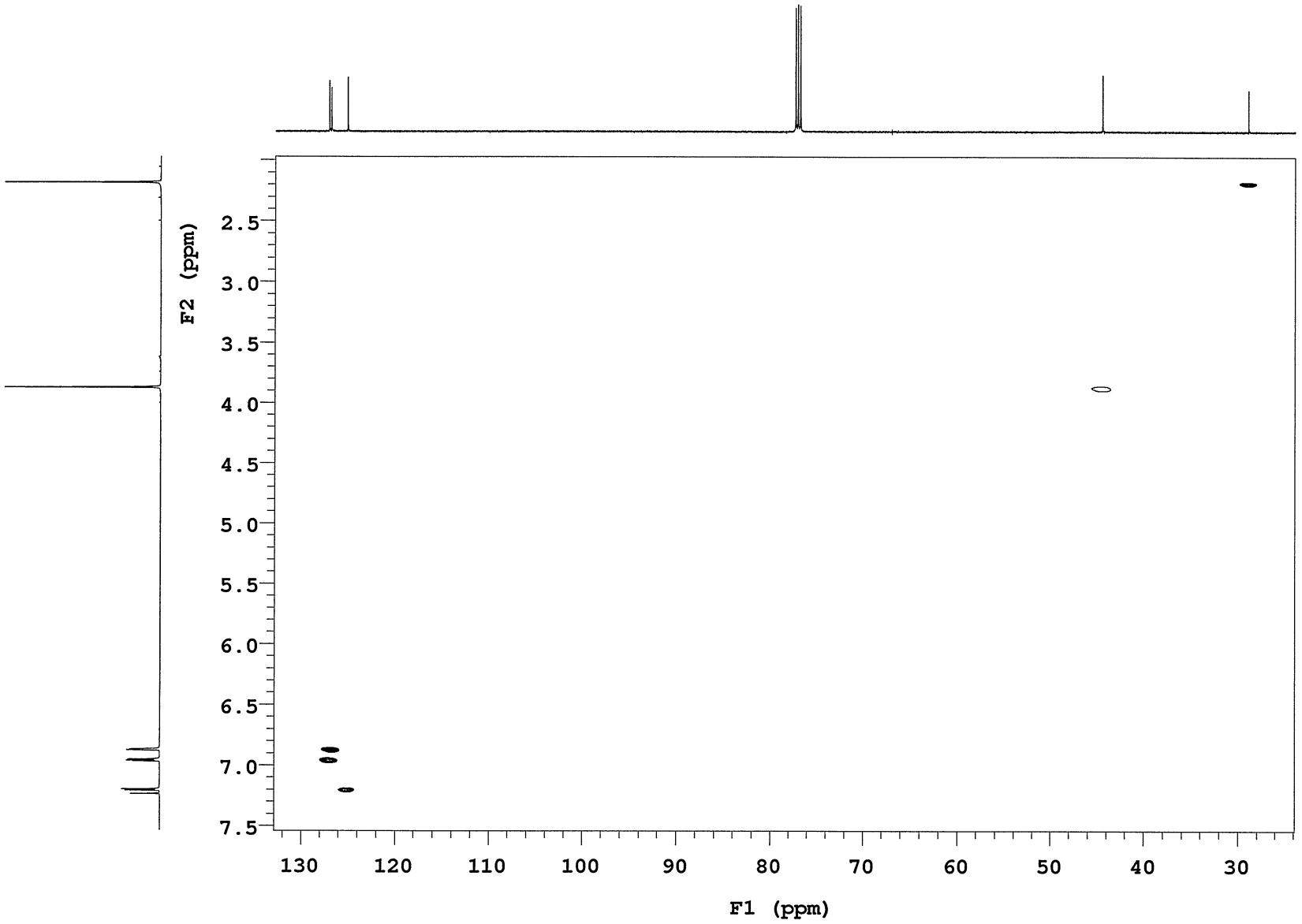
DEPT of compound **4g**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-080/DEPT_01

Plot date 2021-06-28

YYH-080

Sample Name	**YYH-080**	Pulse sequence	**gHSQC**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2021-06-24**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



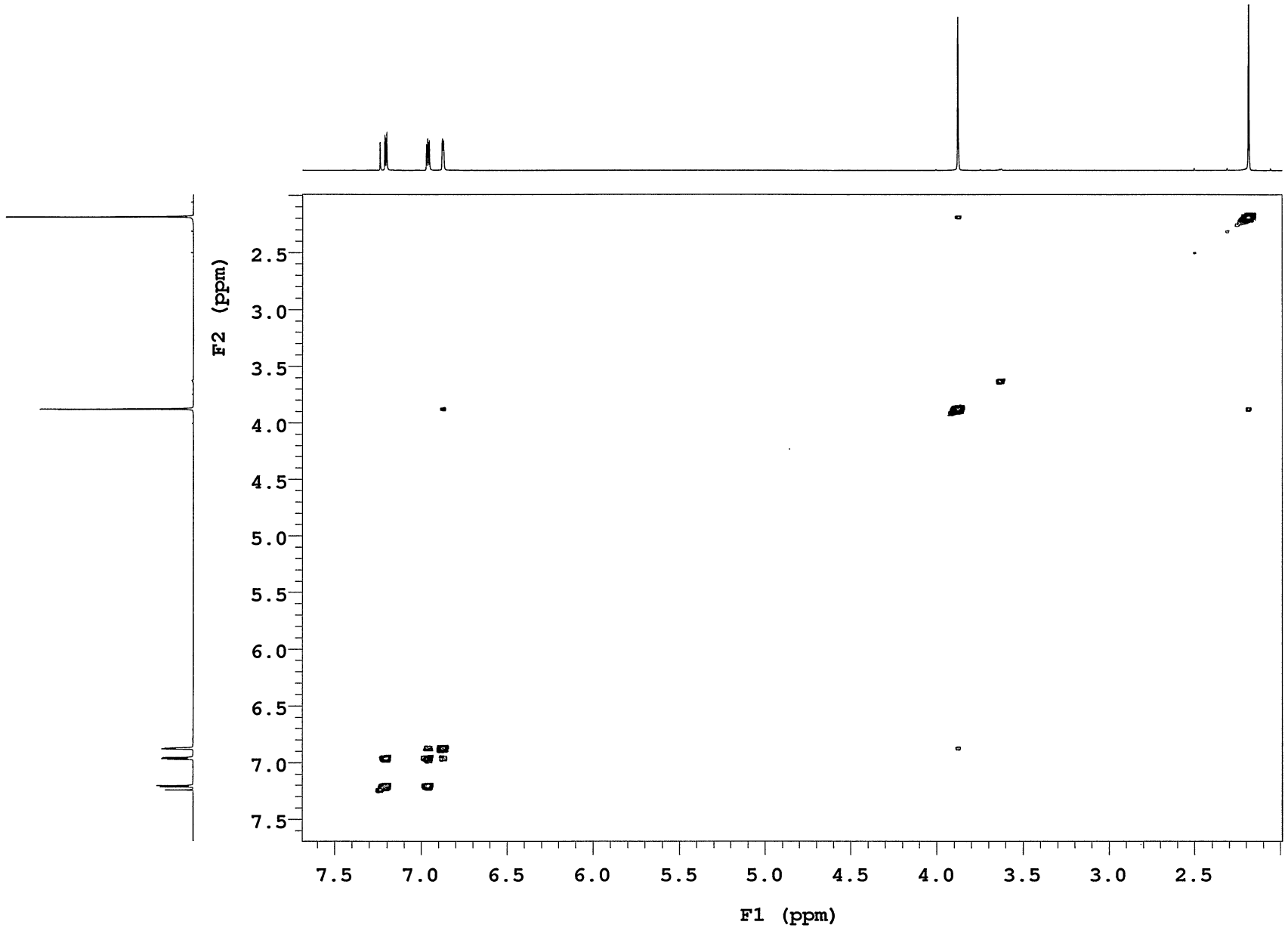
HSQC of compound **4g**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-080/gHSQC_01

Plot date 2021-06-28

YYH-080

Sample Name	YYH-080	Pulse sequence	gCOSY	Temperature	25	Study owner	vnmr2
Date collected	2021-06-24	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



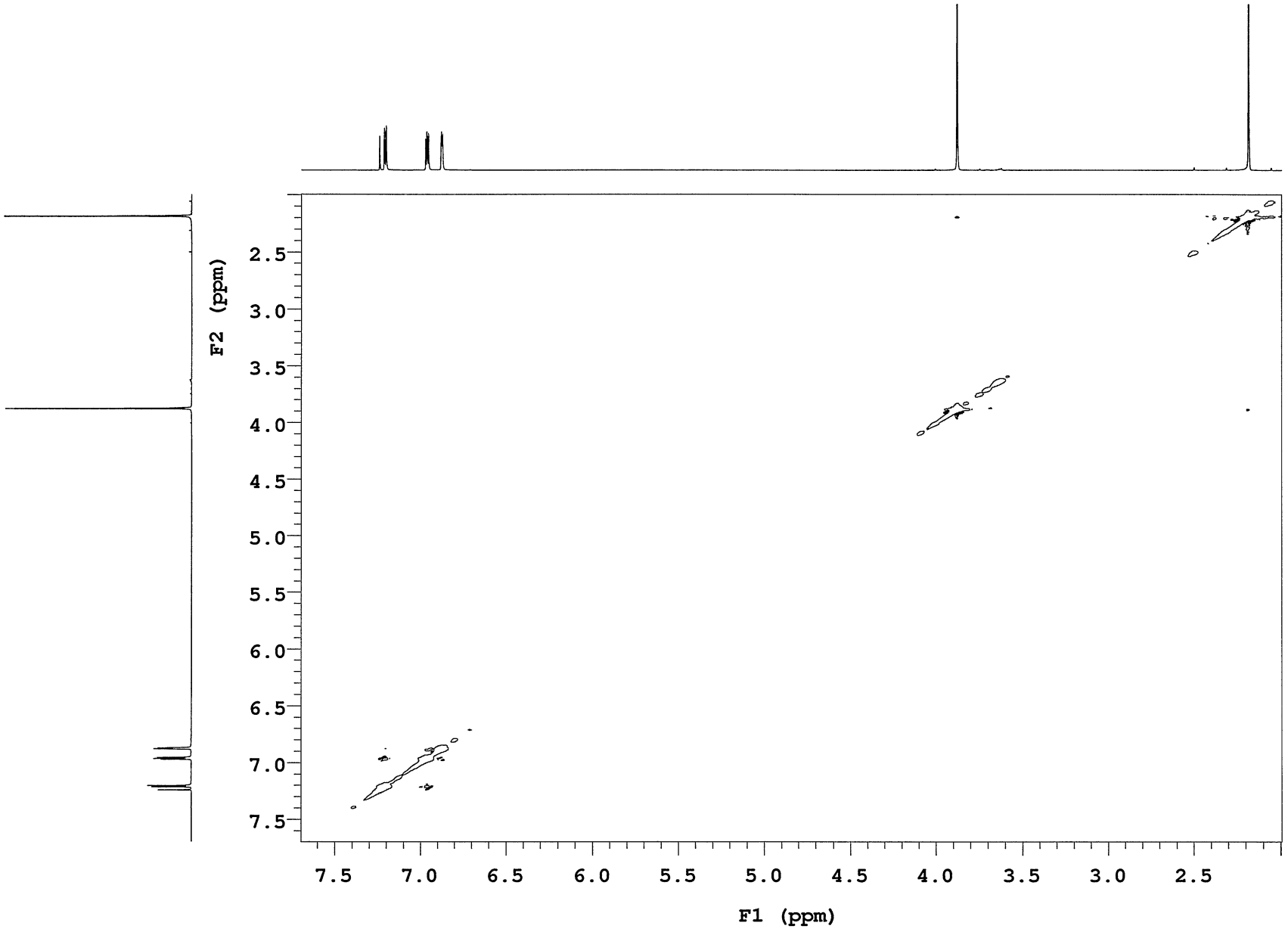
COSY of compound **4g**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-080/gCOSY_01

Plot date 2021-06-28

YYH-080

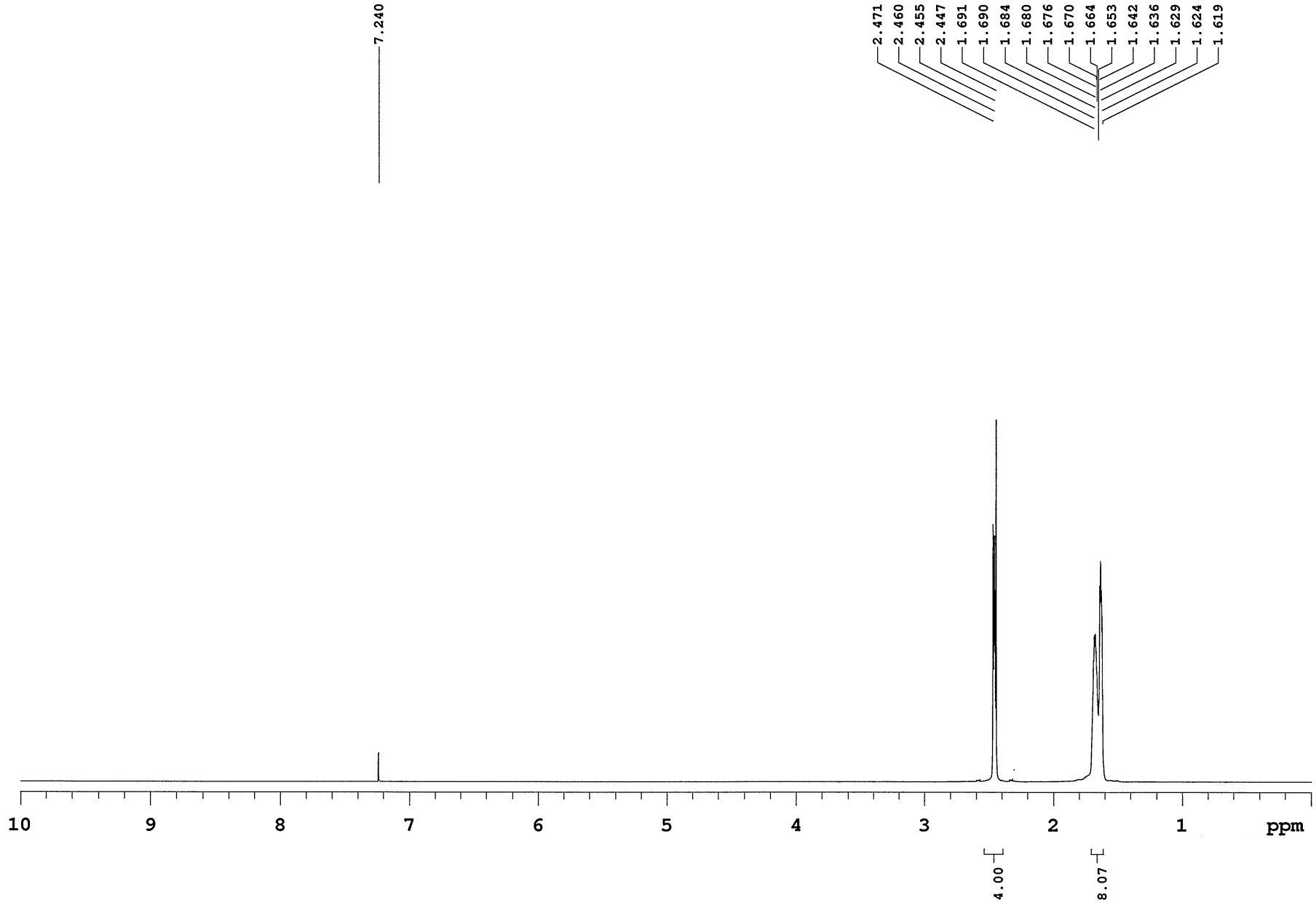
Sample Name	YYH-080	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr2
Date collected	2021-06-24	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



NOESY of compound **4g**

YYH-081

Sample Name	YYH-081	Pulse sequence	PROTON	Temperature	25	Study owner	vnmr2
Date collected	2021-06-16	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



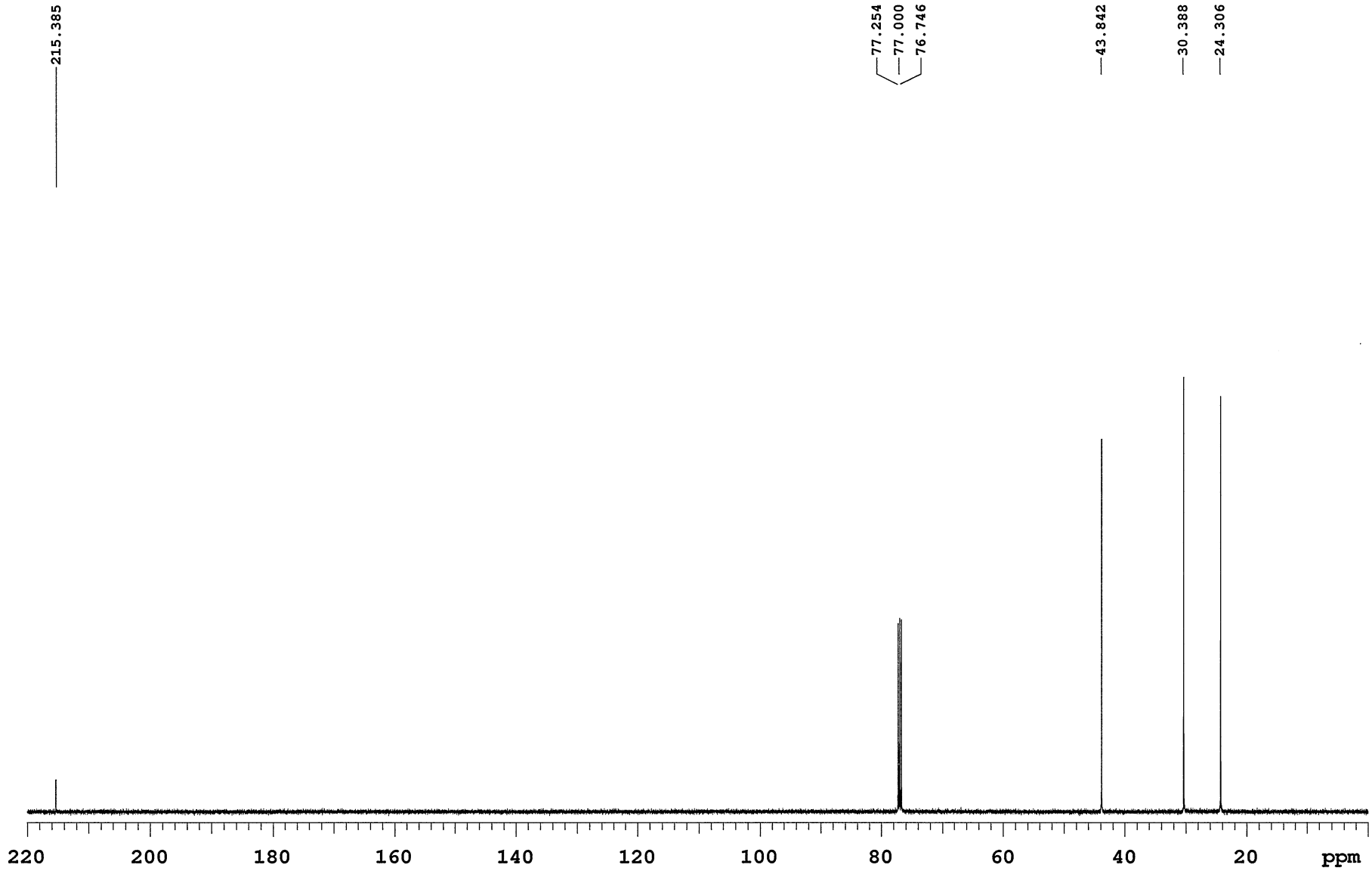
1H NMR (CDCl3, 500 MHz) of compound **4h**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-081/PROTON_04

Plot date 2021-06-17

YYH-081

Sample Name **YYH-081**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-16**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



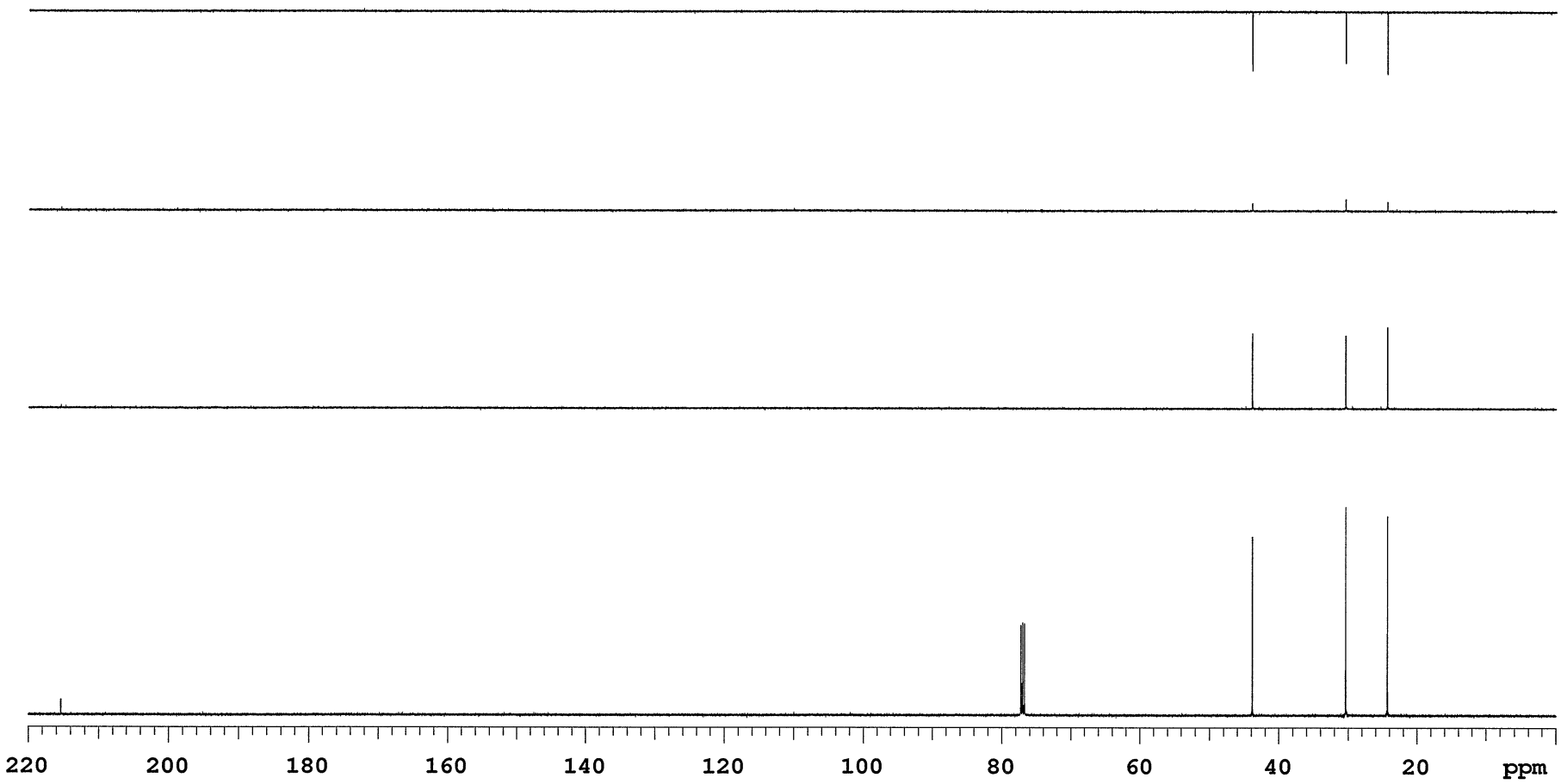
13C NMR (CDCl3, 125 MHz) of compound **4h**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-081/CARBON_02

Plot date 2021-06-17

YYH-081

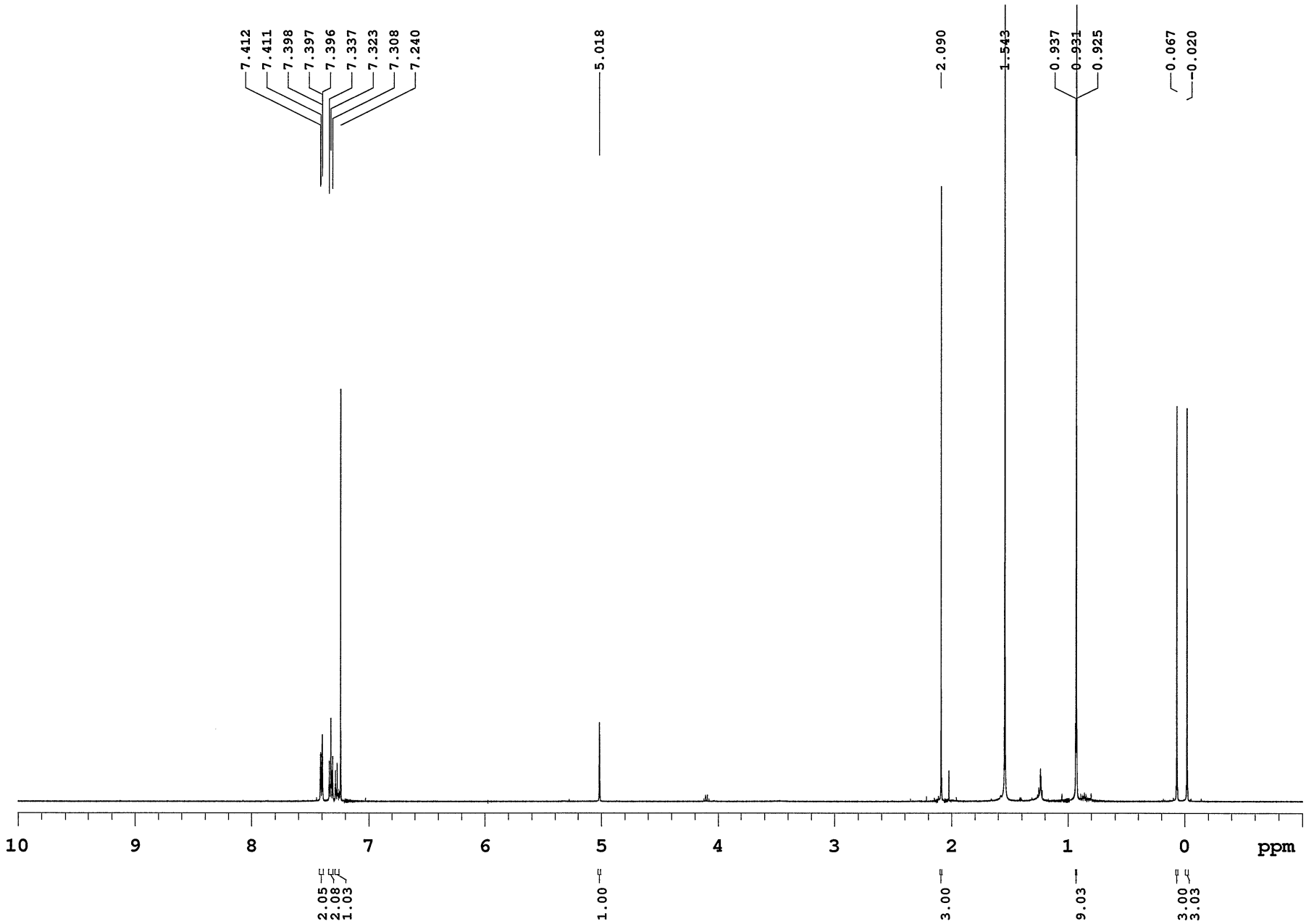
Sample Name **YYH-081**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-16**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **4h**

YYH-085

Sample Name **YYH-085**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



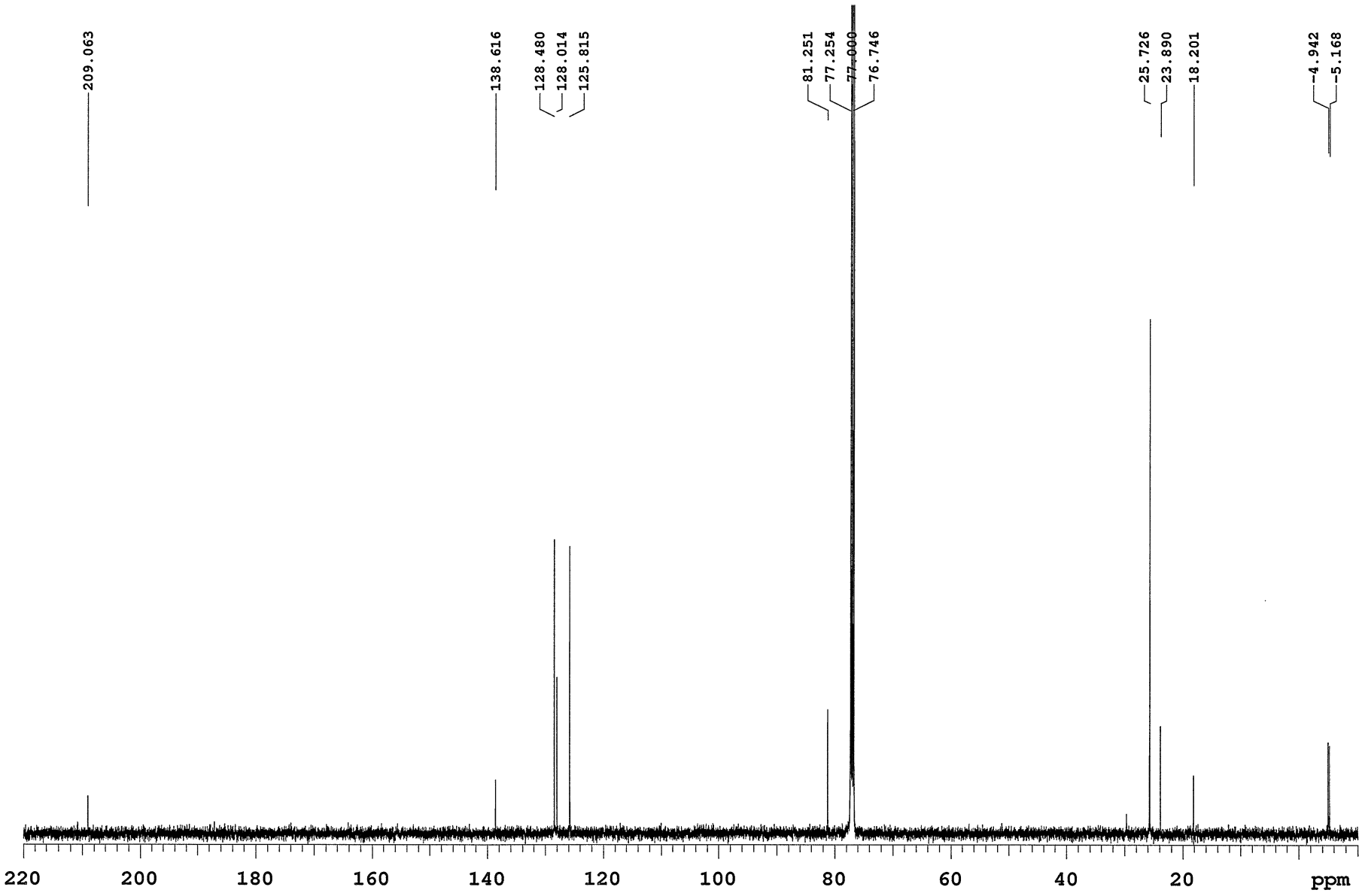
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-085/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4i**

Plot date 2021-06-09

YYH-085

Sample Name **YYH-085**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



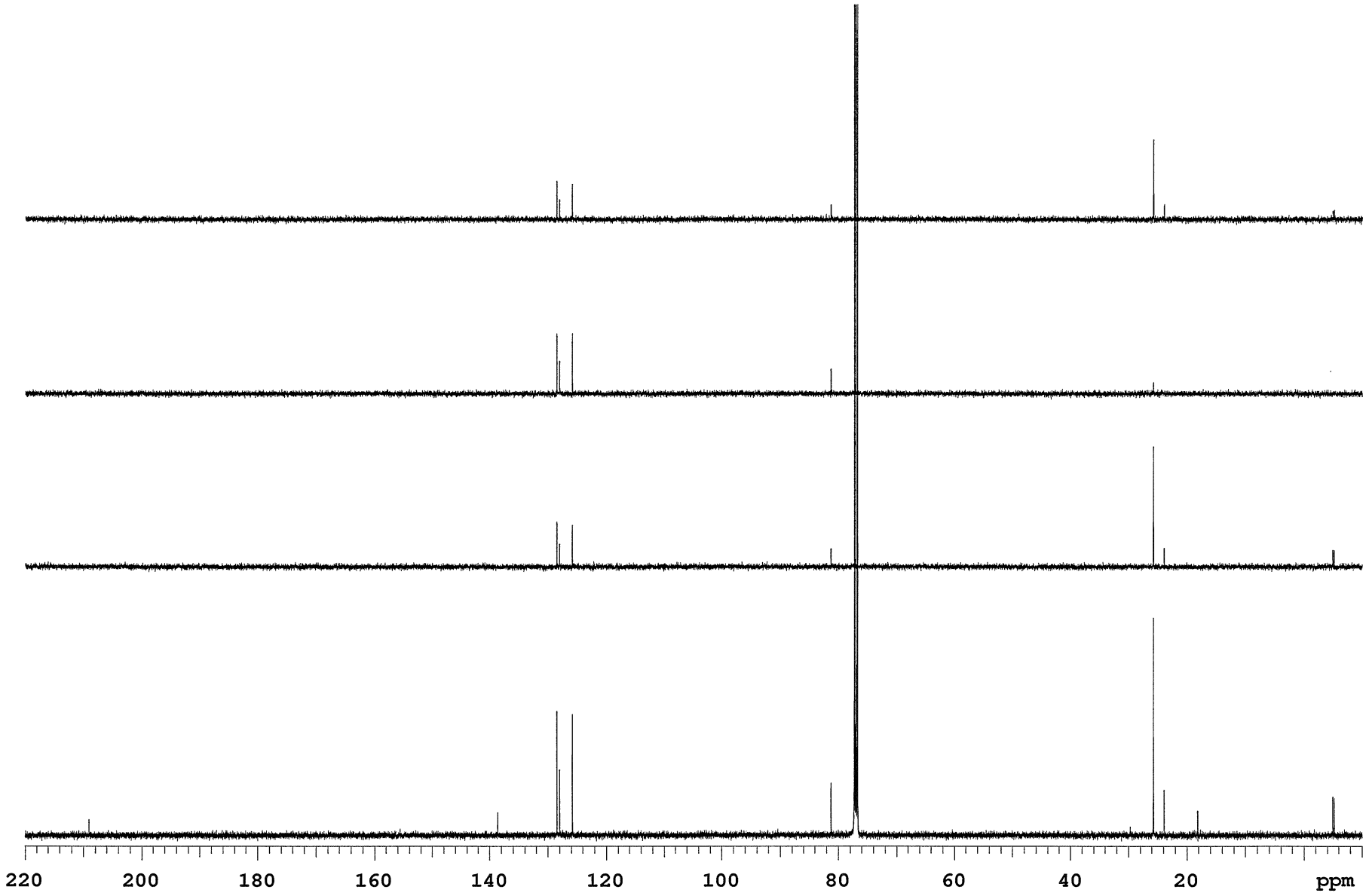
13C NMR (CDCl3, 125 MHz) of compound **4i**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-085/CARBON_02

Plot date 2021-06-09

YYH-085

Sample Name **YYH-085**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



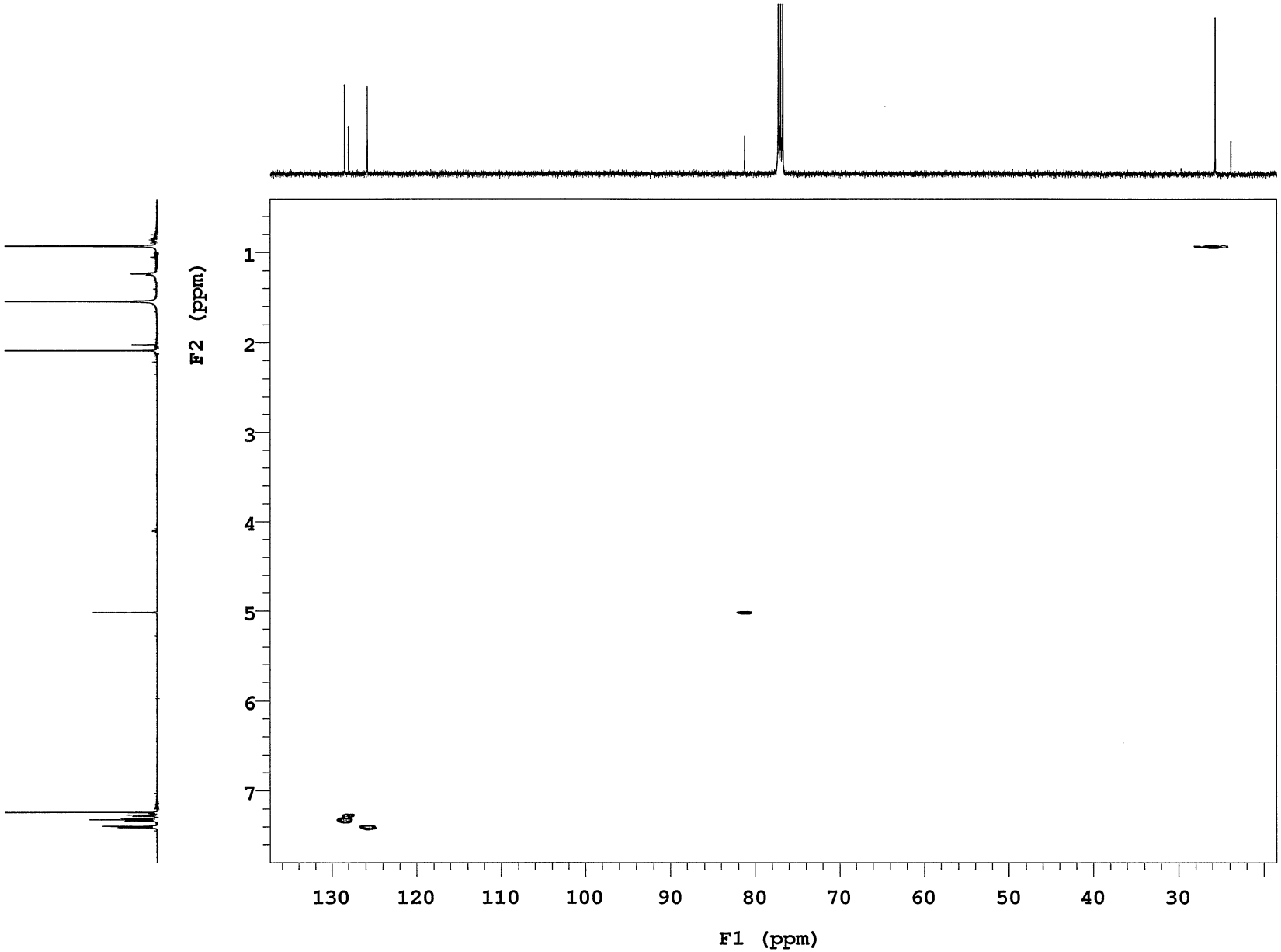
DEPT of compound **4i**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-085/DEPT_01

Plot date 2021-07-14

YYH-085

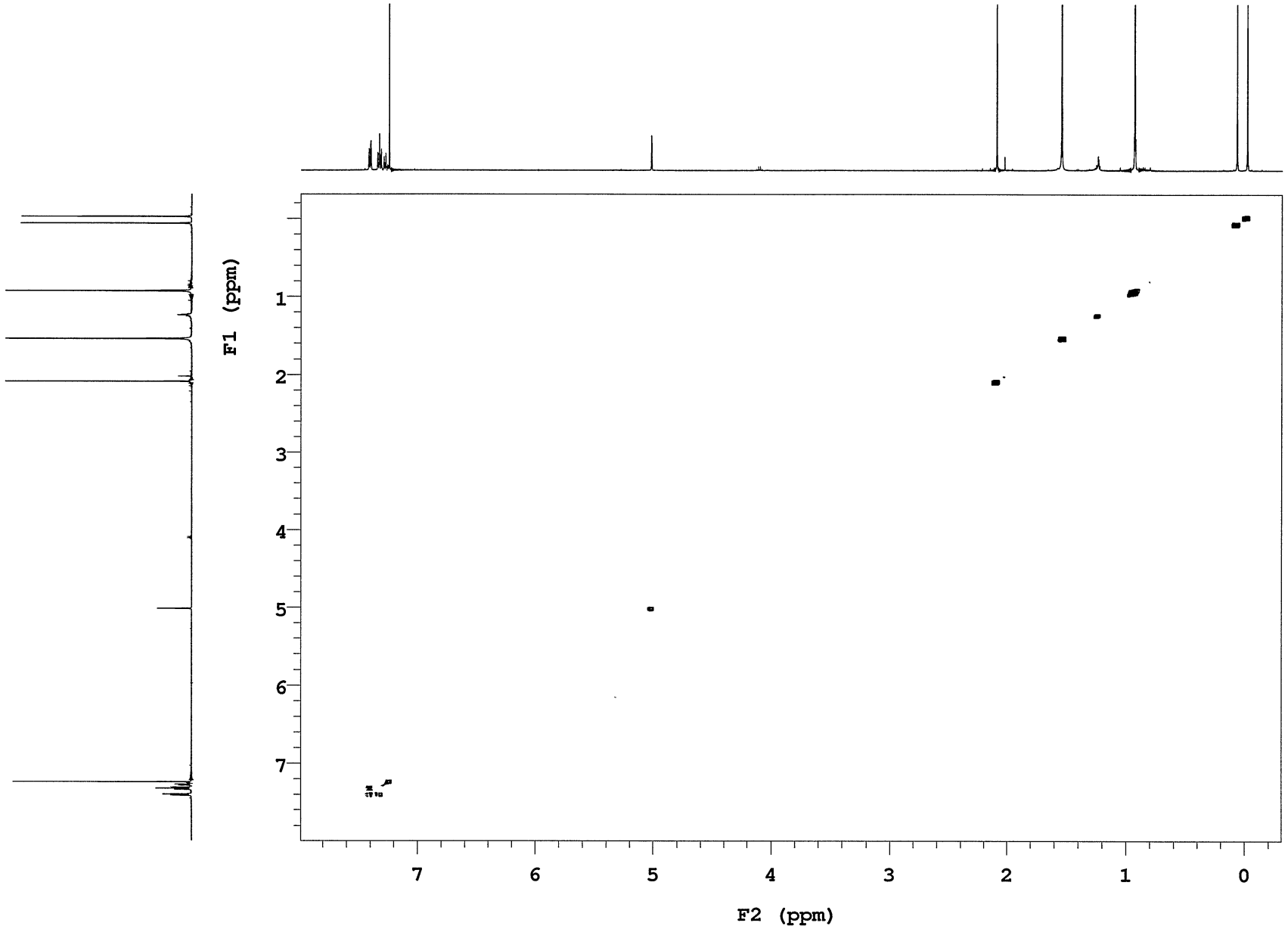
Sample Name **YYH-085**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



HSQC of compound **4i**

YYH-085

Sample Name **YYH-085** | Pulse sequence **gCOSY** | Temperature **25** | Study owner **vnmr2**
Date collected **2021-06-09** | Solvent **cdcl3** | Spectrometer **Agilent-NMR-inova500** | Operator **vnmr2**



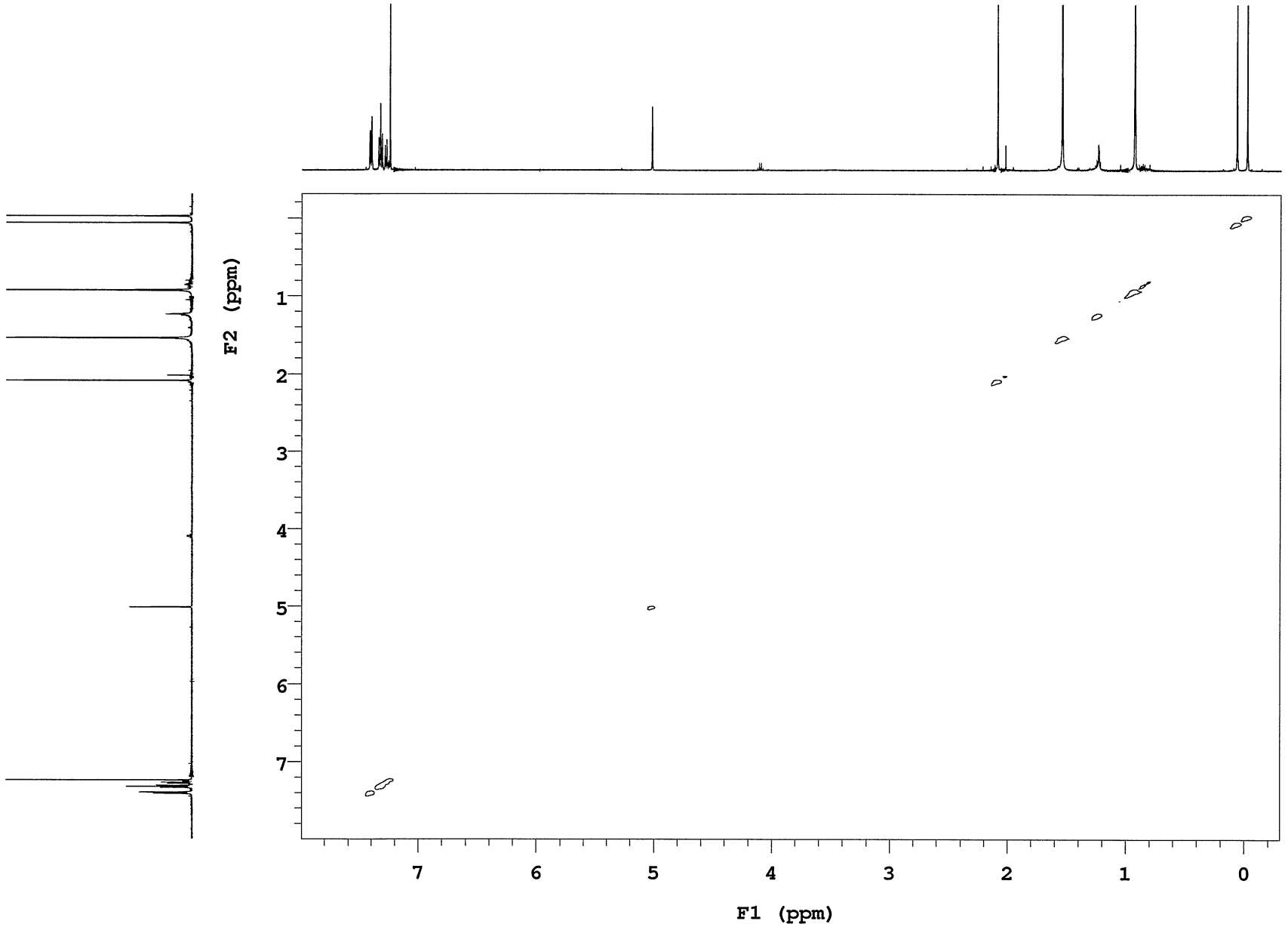
COSY of compound **4i**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-085/gCOSY_01

Plot date 2021-06-09

YYH-085

Sample Name **YYH-085**	Pulse sequence **NOESY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

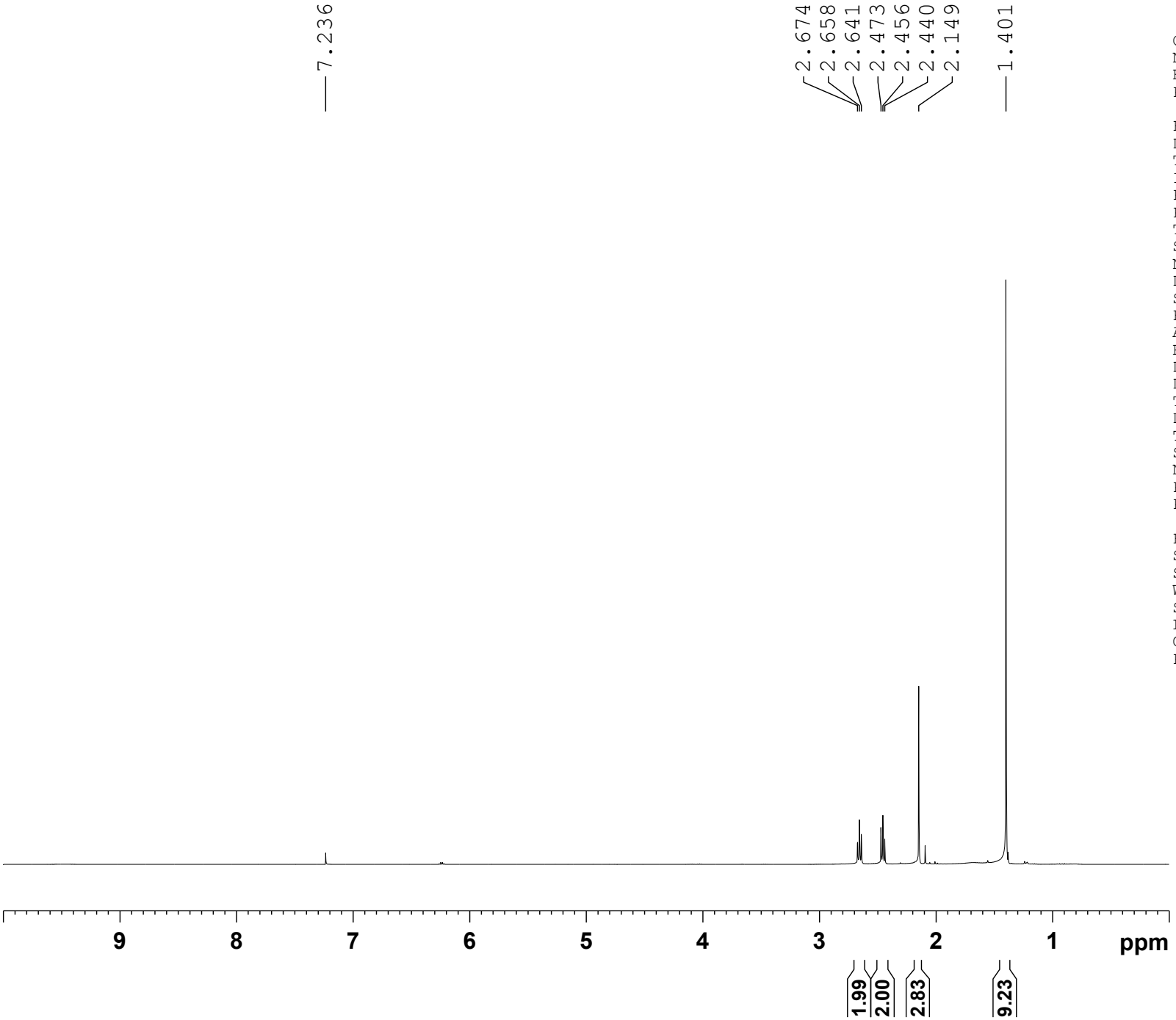


NOESY of compound **4i**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-085/NOESY_01

Plot date 2021-06-09

1H NMR (CDCl3, 400 MHz) of compound **4k**

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Current Data Parameters
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EXPNO                       1
PROCNO                      1

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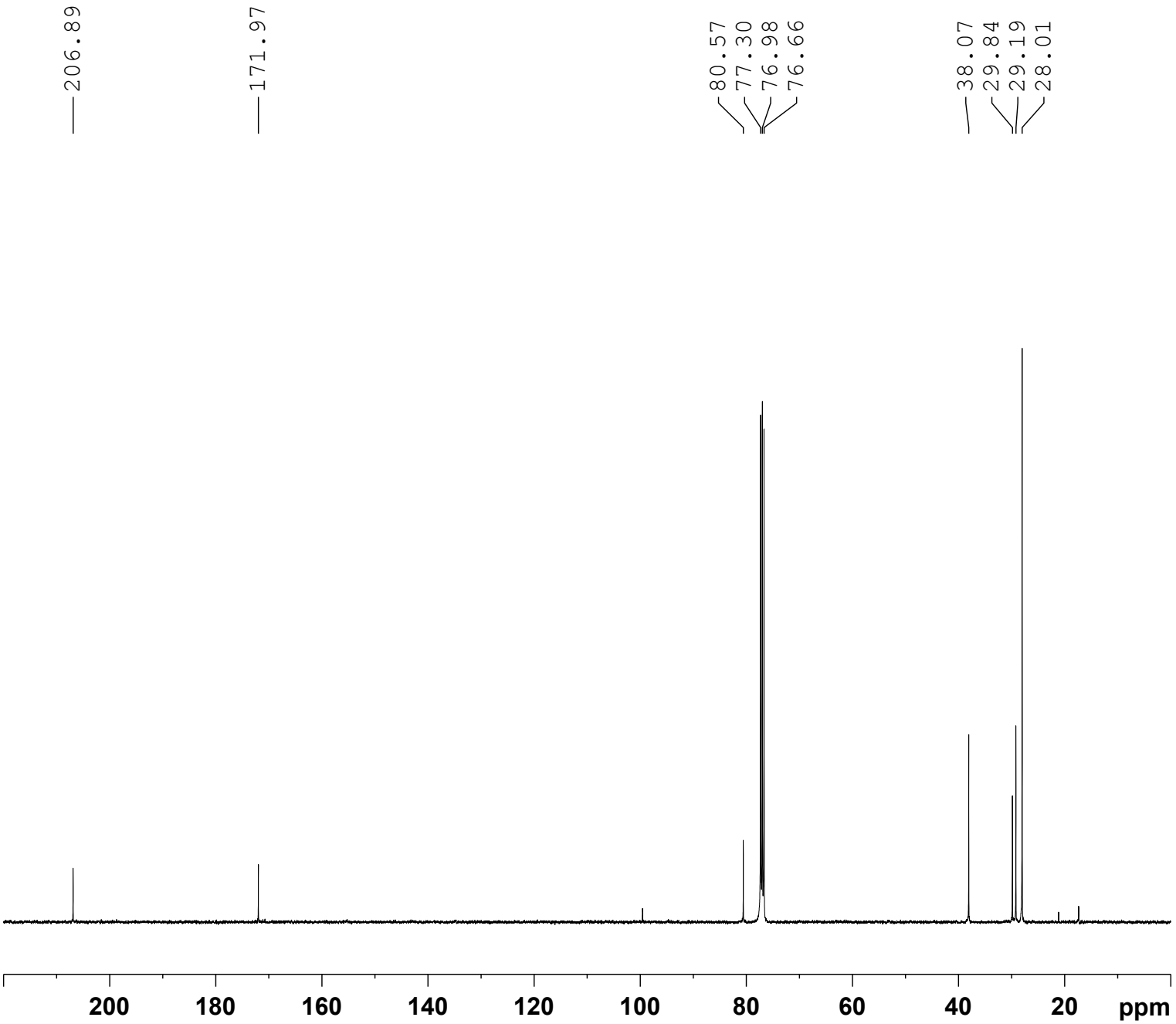
Time                   22.22 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                     128.5
DW                    62.400 usec
DE                    16.43 usec
TE                    297.6 K
D1                2.00000000 sec
TD0                         1
SFO1            400.1324008 MHz
NUC1                       1H
P1                    14.50 usec
PLW1            13.10000038 W

F2 - Processing parameters
SI                      16384
SF              400.1300197 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

13C NMR (CDCl3, 100 MHz) of compound **4k**

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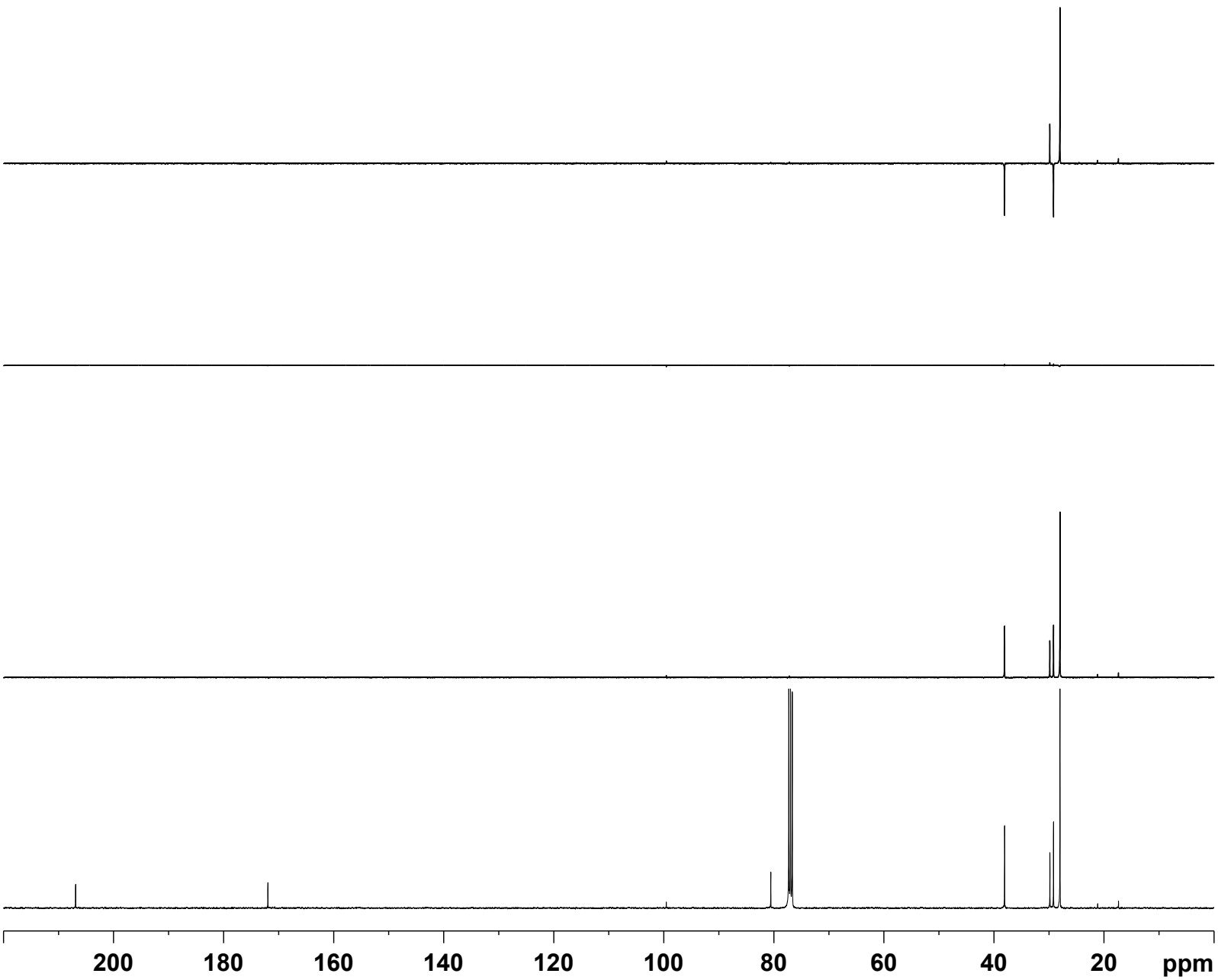
Current Data Parameters
NAME                 YYH-083
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20210609
Time                    1.26 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG               zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      4000
DS                         0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     298.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1            100.6233329 MHz
NUC1                    13C
P1                     10.50 usec
PLW1               44.29999924 W
SFO2               400.1316005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2               14.60000038 W
PLW12               0.37897000 W
PLW13               0.19032000 W

F2 - Processing parameters
SI                     32768
SF                100.6127726 MHz
WDW                       EM
SSB          0
LB                      2.00 Hz
GB           0
PC                      1.00
```

DEPT of compound **4k**

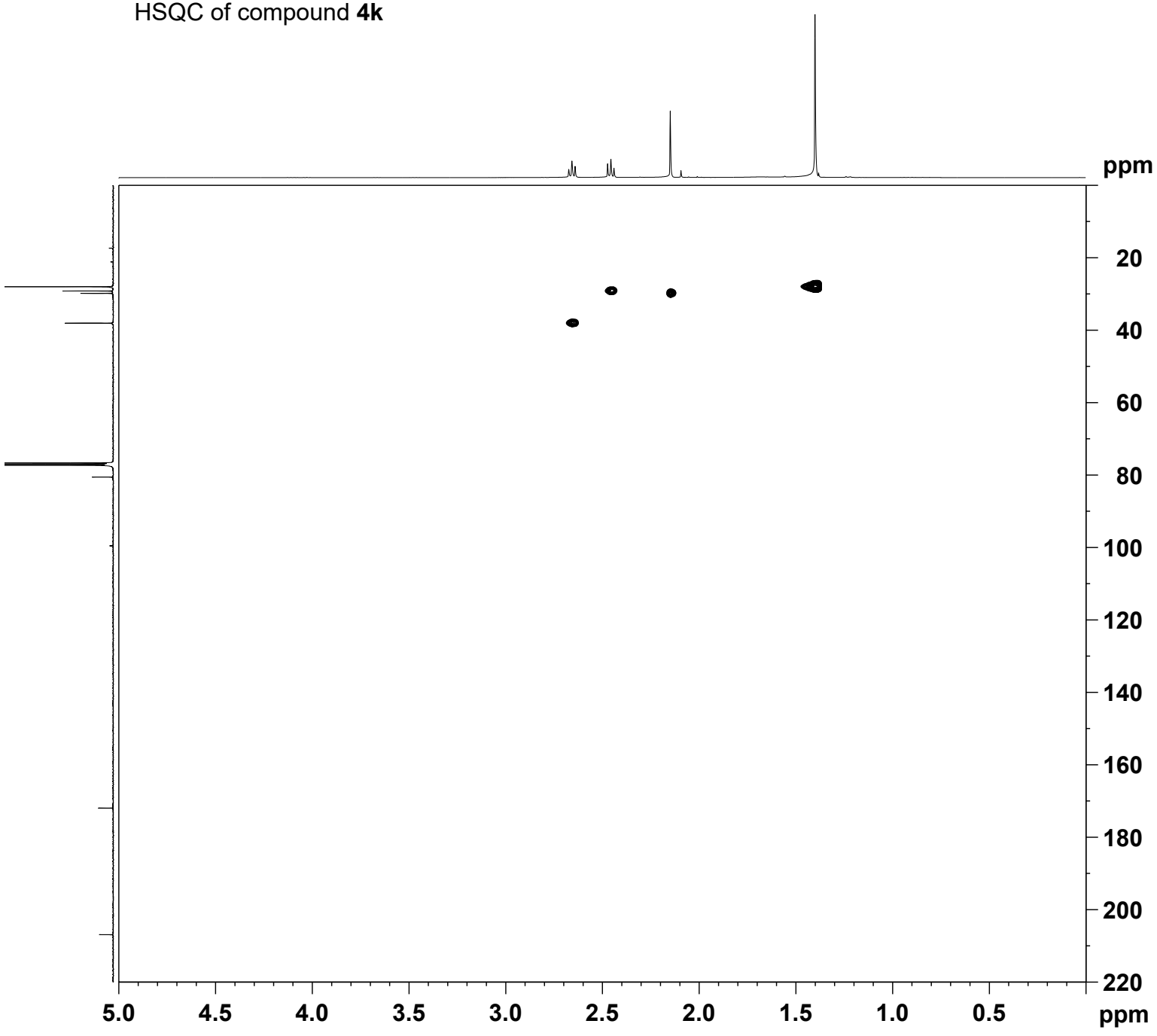



```
Current Data Parameters
NAME            YYH-083
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210609
Time               1.26 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4000
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1               10.50 usec
PLW1        44.29999924 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2            90.00 usec
PLW2        14.60000038 W
PLW12        0.37897000 W
PLW13        0.19032000 W

F2 - Processing parameters
SI                32768
SF          100.6127726 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

HSQC of compound **4k**

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Current Data Parameters
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EXPNO                  6
PROCNO                 1

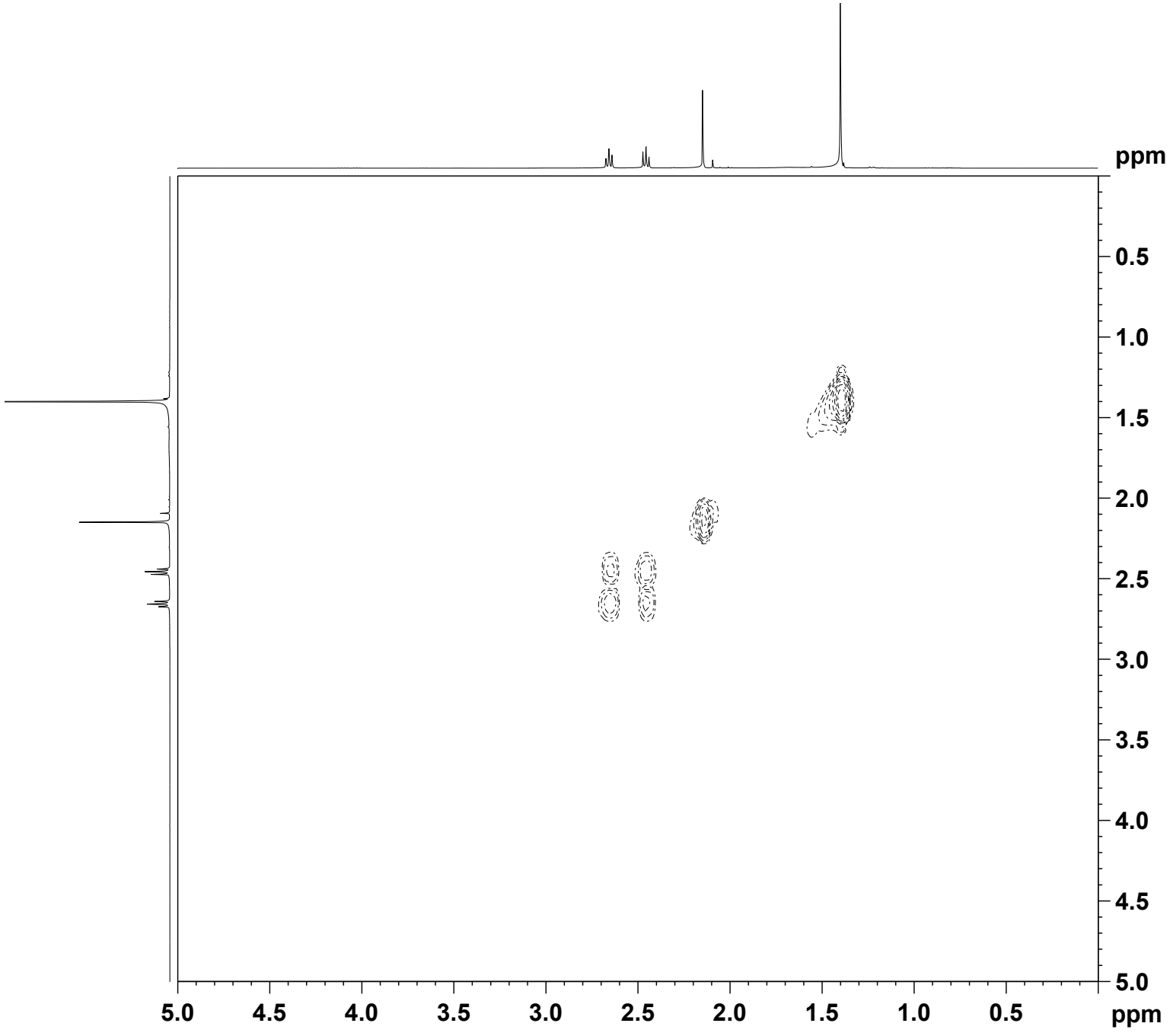
F2 - Acquisition Parameters
Date_           20210609
Time               6.01 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                298.3 K
CNST2        145.0000000
CNST17        -0.5000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00002080 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         13.10000038 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2            garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0     0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3             0.500
SPOFFS3  0 Hz
SPW3          7.41179991 W
SPNAM[7]    Crp60comp.4
SPOAL7             0.500
SPOFFS7  0 Hz
SPW7          7.41179991 W
GPNAM[1]      SMSQ10.100
GPZ1               80.00 %
GPNAM[2]      SMSQ10.100
GPZ2               20.10 %
GPNAM[3]      SMSQ10.100
GPZ3               11.00 %
GPNAM[4]      SMSQ10.100
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1           100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300197 MHz
WDW                 QSINE
SSB                     2
LB       0 Hz
GB       0
PC                   1.40

F1 - Processing parameters
SI                  1024
MC2       echo-antiecho
SF           100.6127726 MHz
WDW                 QSINE
SSB                     2
LB       0 Hz
GB       0
```

COSY of compound **4k**

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Current Data Parameters
NAME             YYH-083
EXPNO                  7
PROCNO                 1

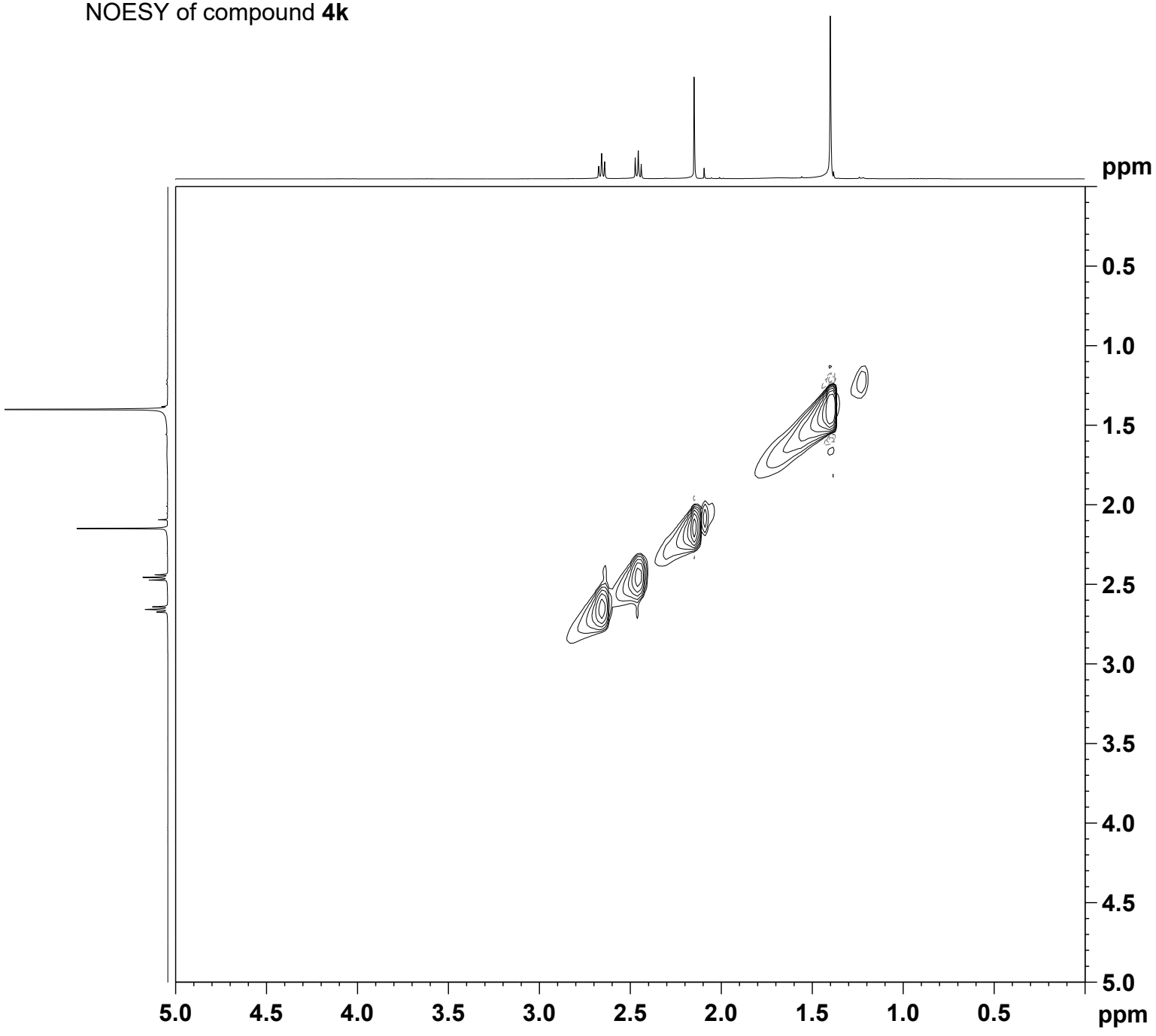
F2 - Acquisition Parameters
Date_           20210609
Time               6.44 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     6
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                 63.35
DW                62.400 usec
DE                 6.50 usec
TE                298.3 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         13.10000038 W
PLW10         3.06030011 W
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF          400.1300197 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF          400.1300197 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **4k**




```
Current Data Parameters
NAME                 YYH-083
EXPNO                      8
PROCNO                     1

F2 - Acquisition Parameters
Date_               20210609
Time                   7.41 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG         noesygpphpp
TD                      2048
SOLVENT                CDCl3
NS                         6
DS                        16
SWH                 8012.820 Hz
FIDRES              7.825020 Hz
AQ                  0.1277952 sec
RG                     112.98
DW                     62.400 usec
DE                      6.50 usec
TE                     297.7 K
D0                  0.00004394 sec
D1                  2.00000000 sec
D8                  0.40000001 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D16                 0.00020000 sec
IN0                 0.00012480 sec
TDav                       1
SFO1              400.1324008 MHz
NUC1                       1H
P1                     14.50 usec
P2                     29.00 usec
P17                  2500.00 usec
PLW1              13.10000038 W
PLW10              3.06030011 W
GPNAM[1]           SMSQ10.100
GPZ1                  40.00 %
P16                 1000.00 usec

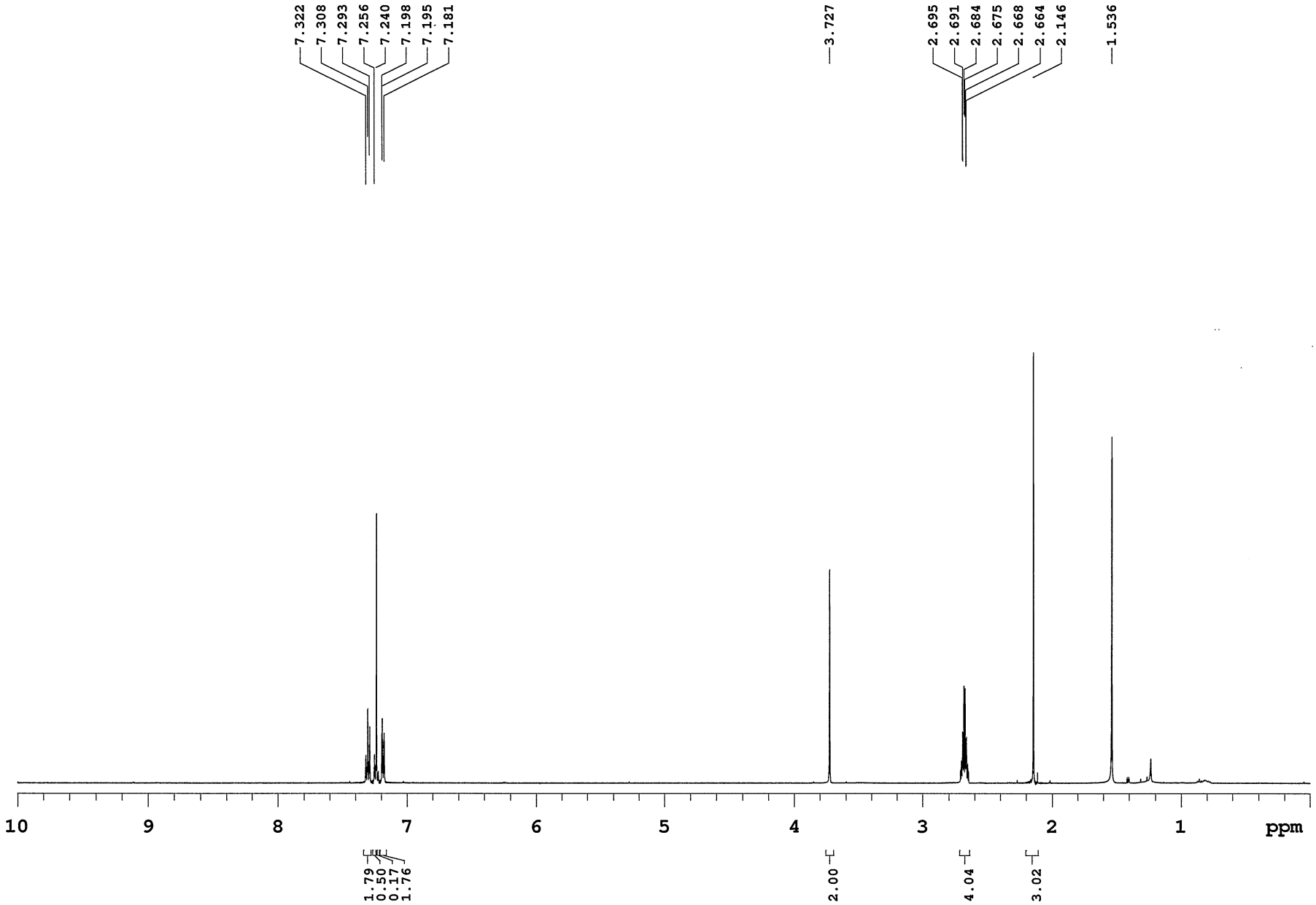
F1 - Acquisition parameters
TD                       256
SFO1                400.1324 MHz
FIDRES              62.600159 Hz
SW                     20.025 ppm
FnMODE           States-TPPI

F2 - Processing parameters
SI                      1024
SF                400.1300197 MHz
WDW                     QSINE
SSB                        2
LB             0 Hz
GB             0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2               States-TPPI
SF                400.1300197 MHz
WDW                     QSINE
SSB                        2
LB             0 Hz
GB             0
```

YYH-082

Sample Name **YYH-082**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-10**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



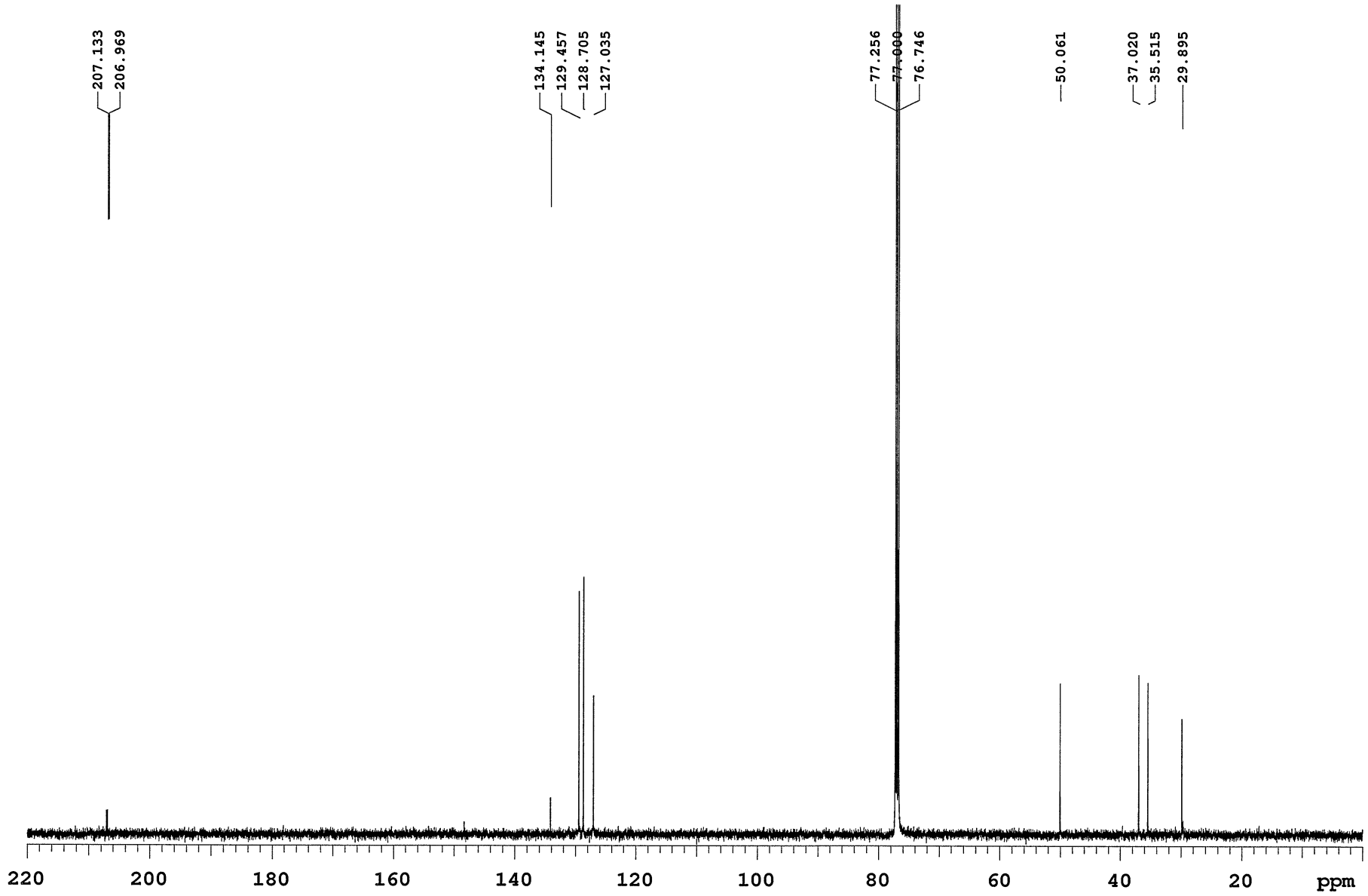
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-082/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4l**

Plot date 2021-06-11

YYH-082

Sample Name	YYH-082	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2021-06-10	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



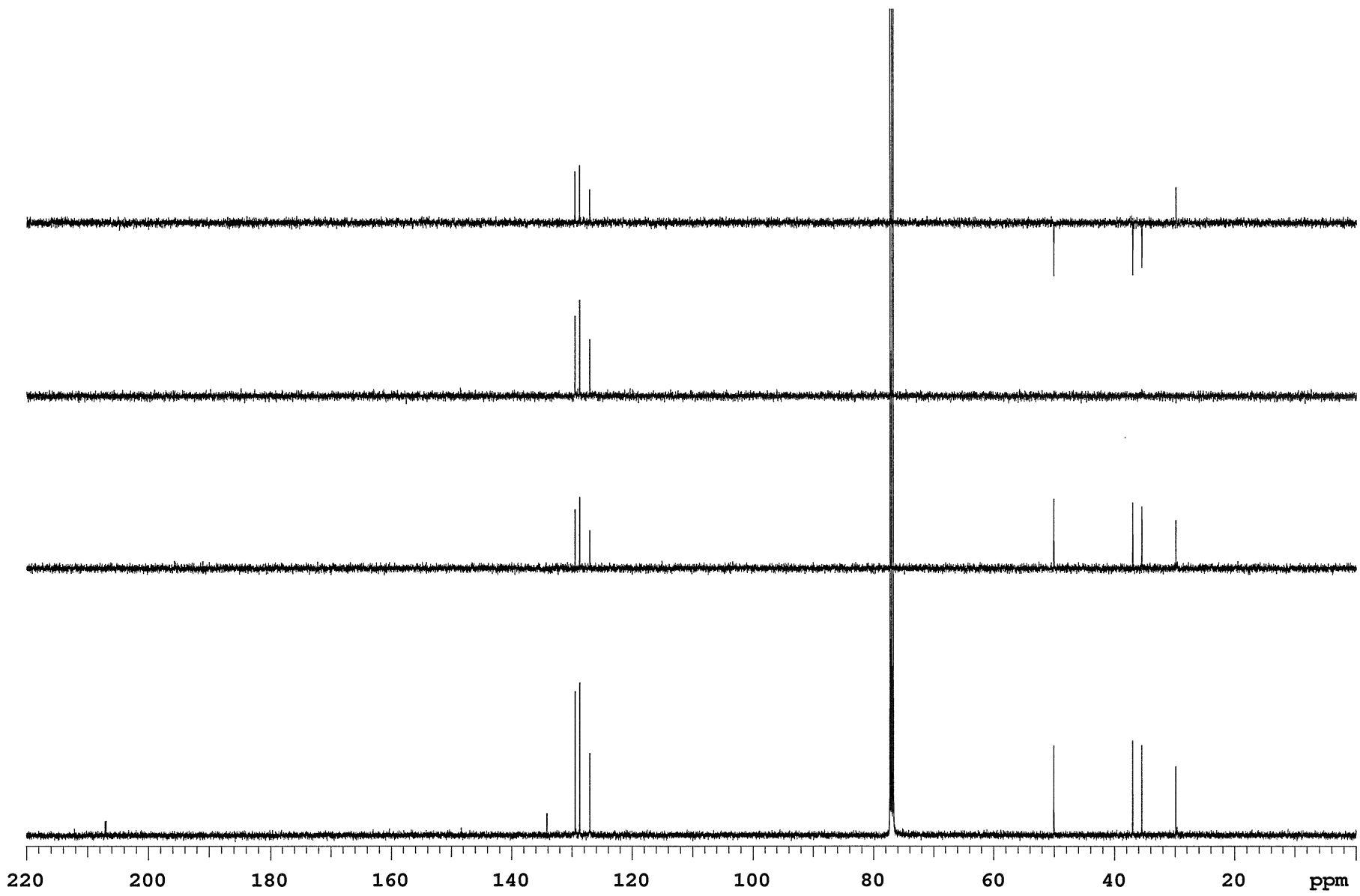
13C NMR (CDCl3, 125 MHz) of compound **4l**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-082/CARBON_02

Plot date 2021-06-11

YYH-082

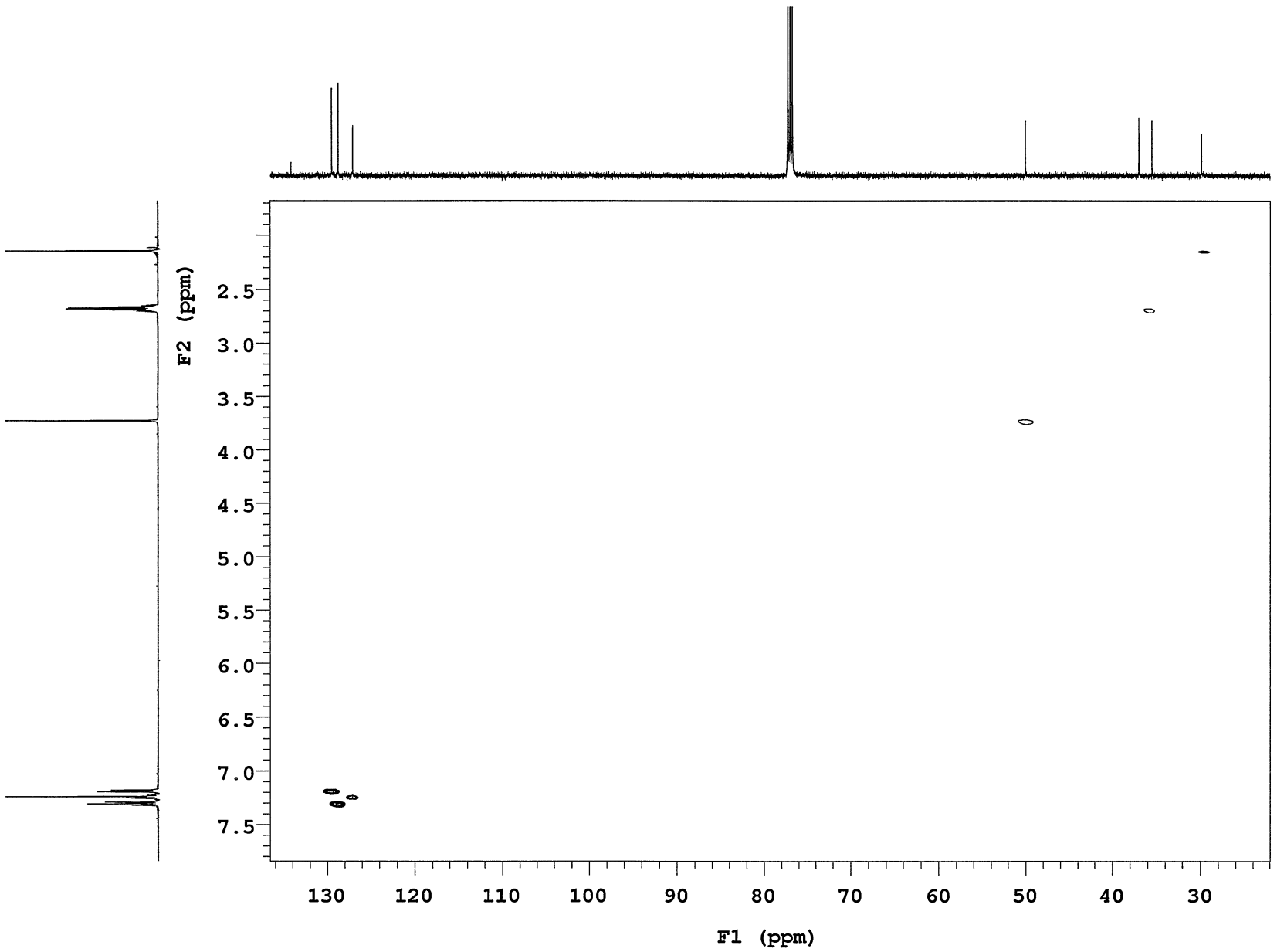
Sample Name **YYH-082**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-11**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **4l**

YYH-082

Sample Name **YYH-082**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-11**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



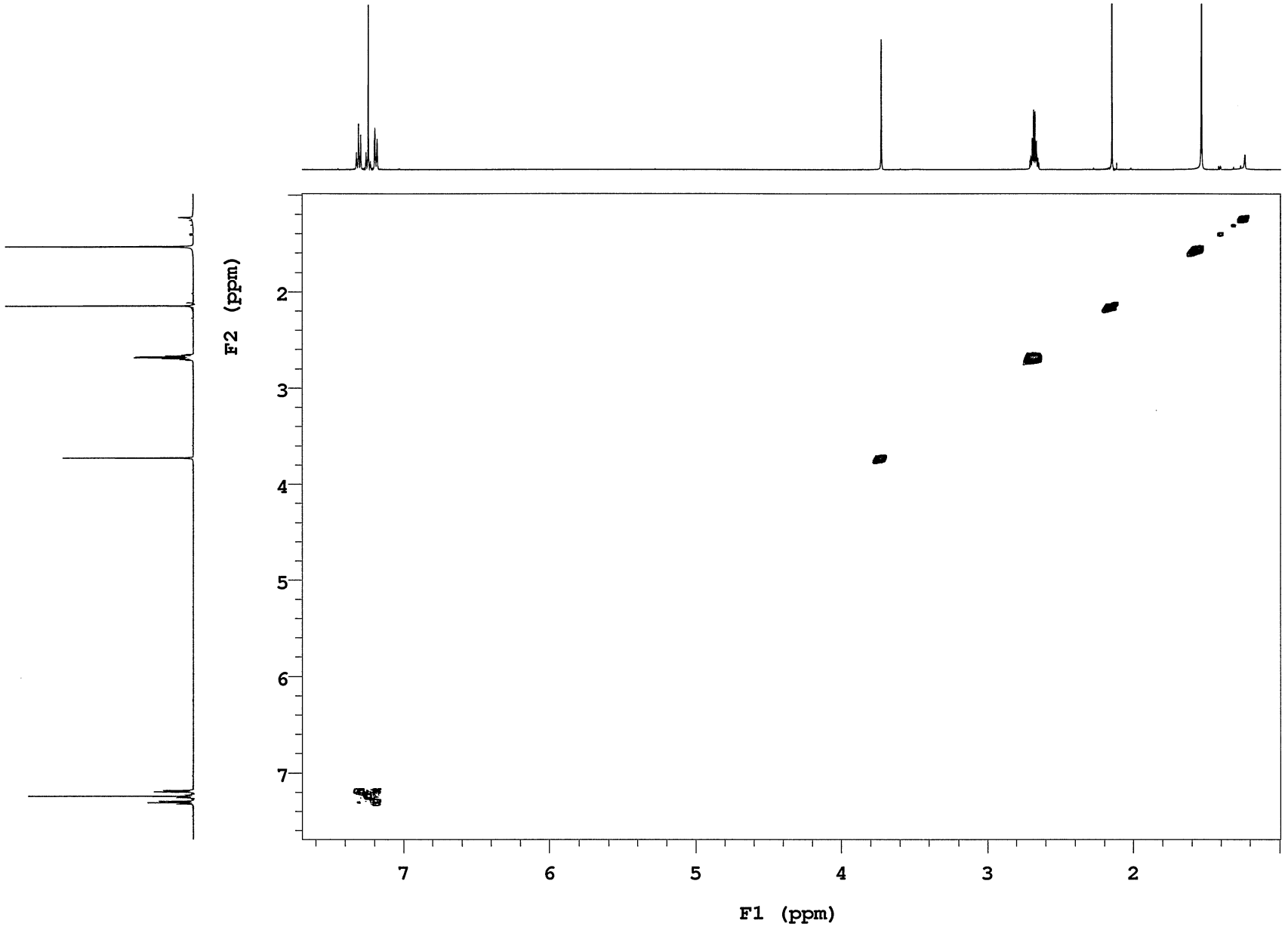
HSQC of compound **4l**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-082/gHSQC_01

Plot date 2021-06-11

YYH-082

Sample Name **YYH-082**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-06-11**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



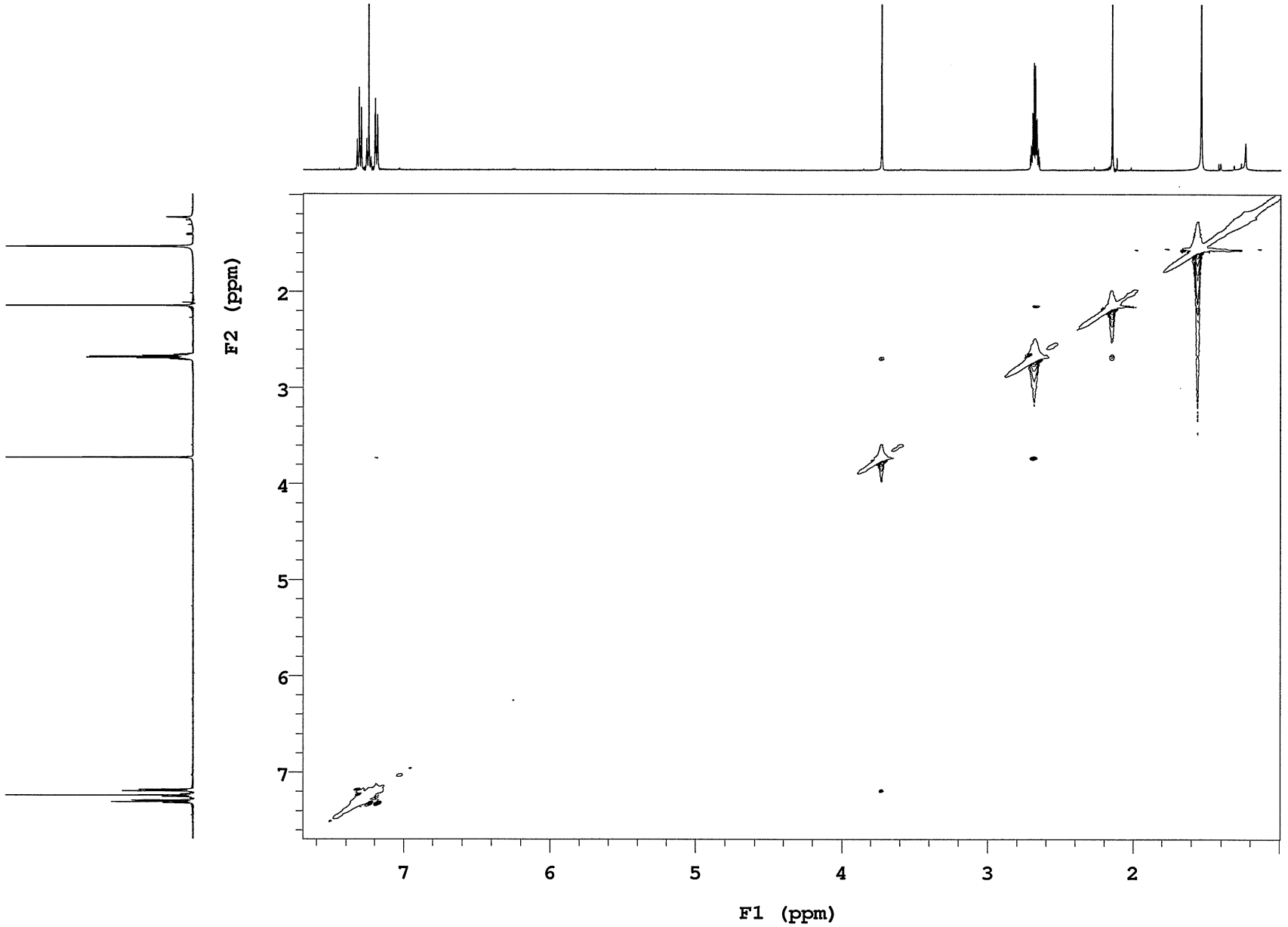
COSY of compound **4l**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-082/gCOSY_01

Plot date 2021-06-11

YYH-082

Sample Name	YYH-082	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr2
Date collected	2021-06-11	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



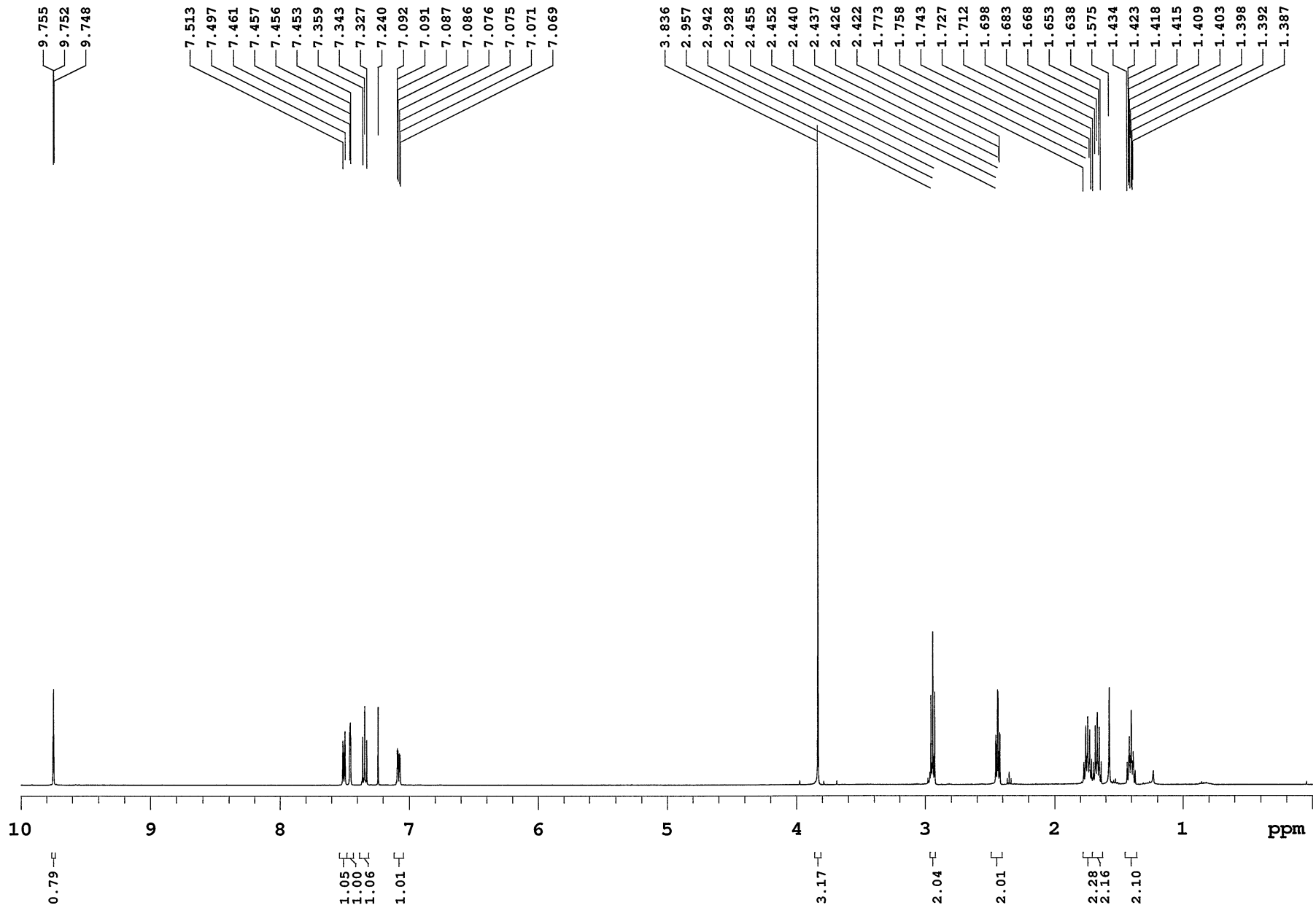
NOESY of compound **4l**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-082/NOESY_01

Plot date 2021-06-11

YYH-088-2

Sample Name **YYH-088-2**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-16**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



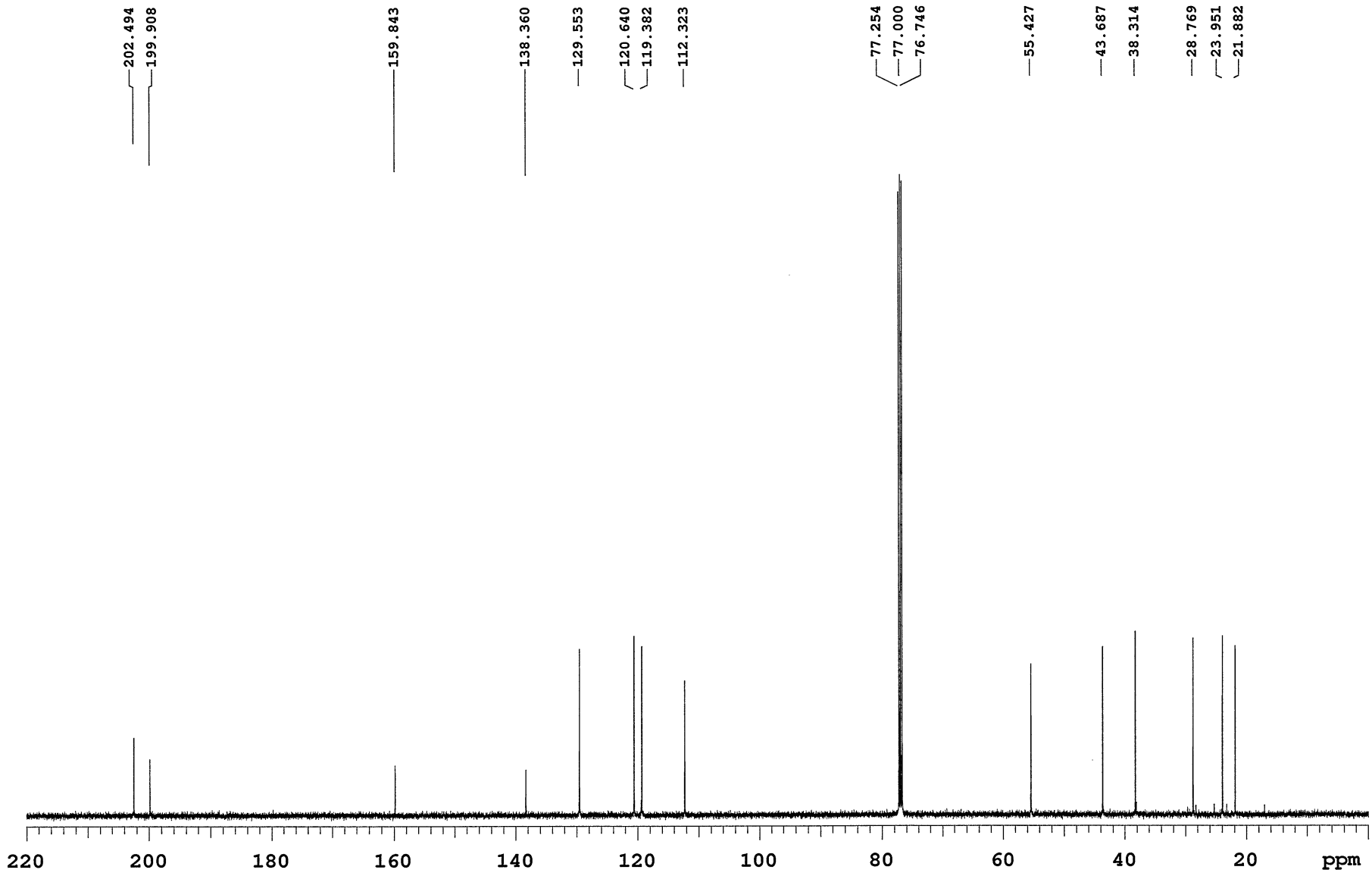
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-088-2/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4m**

Plot date 2021-07-16

YYH-088-2

Sample Name	YYH-088-2	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2021-07-16	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



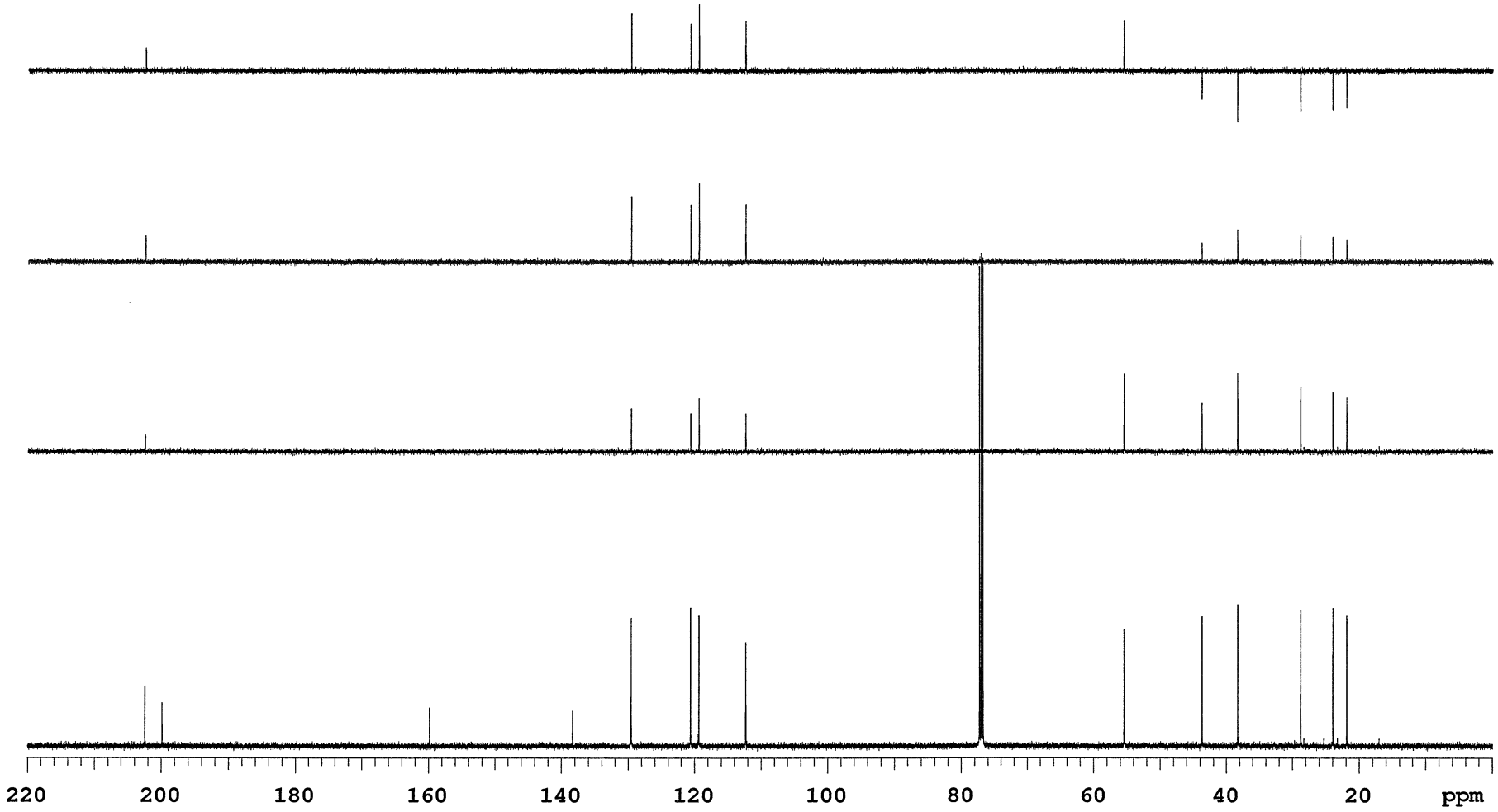
13C NMR (CDCl3, 125 MHz) of compound **4m**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-088-2/CARBON_02

Plot date 2021-07-16

YYH-088-2

Sample Name **YYH-088-2**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-16**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



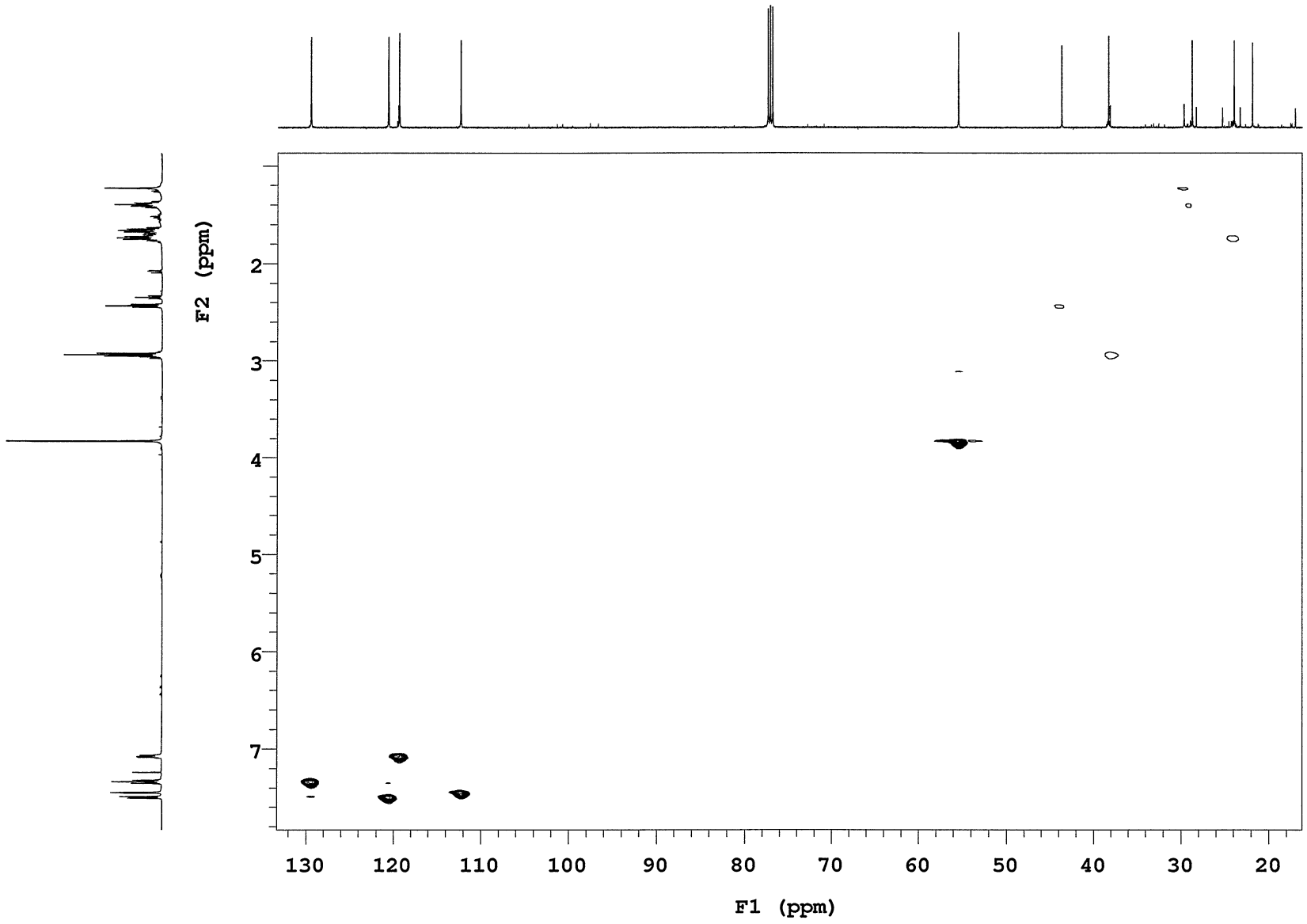
DEPT of compound **4m**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-088-2/DEPT_01

Plot date 2021-07-16

YYH-088

Sample Name **YYH-088**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-02**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



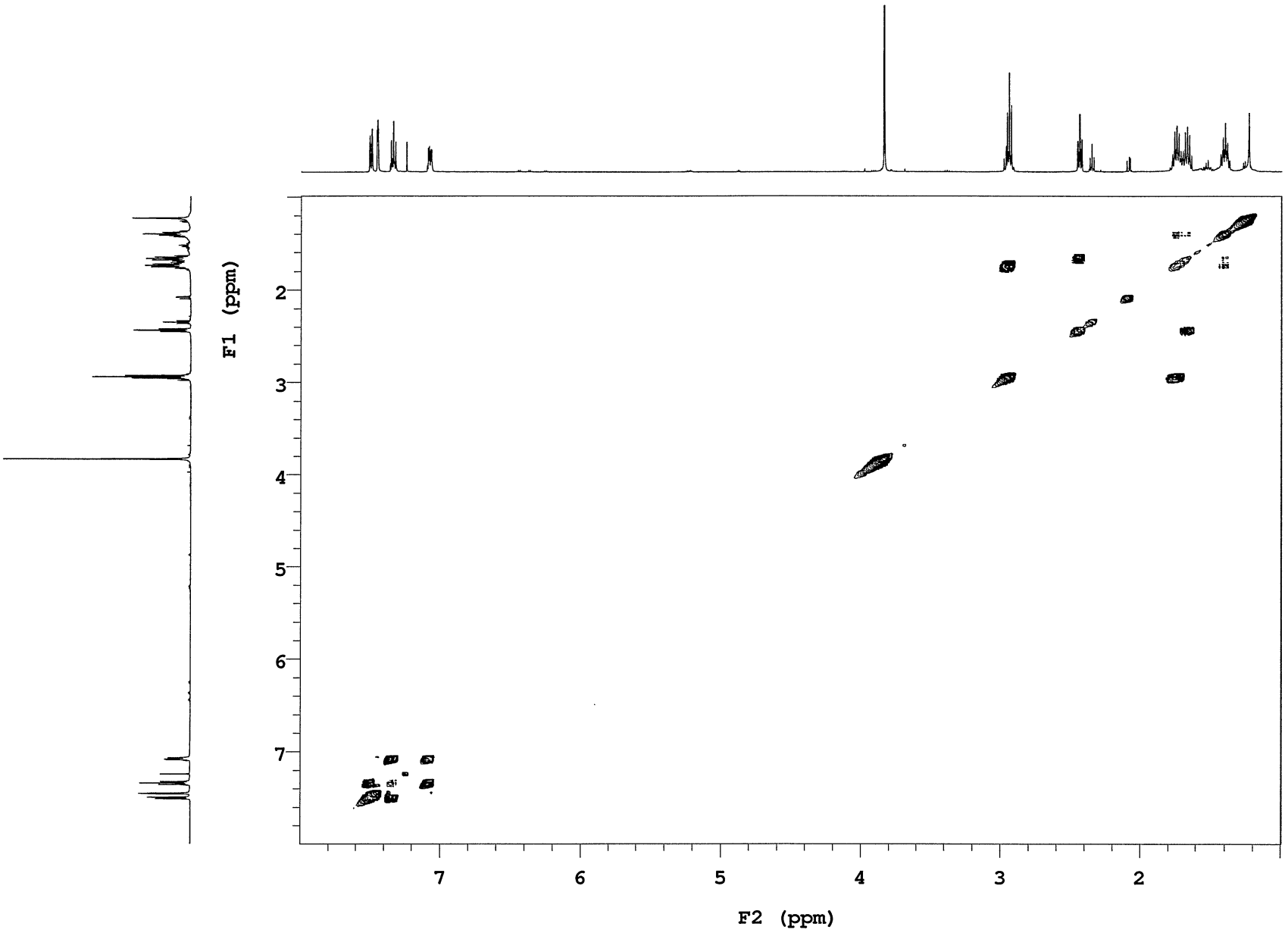
HSQC of compound **4m**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-088/gHSQC_01

Plot date 2021-07-02

YYH-088

Sample Name	**YYH-088**	Pulse sequence	**gCOSY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2021-07-02**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



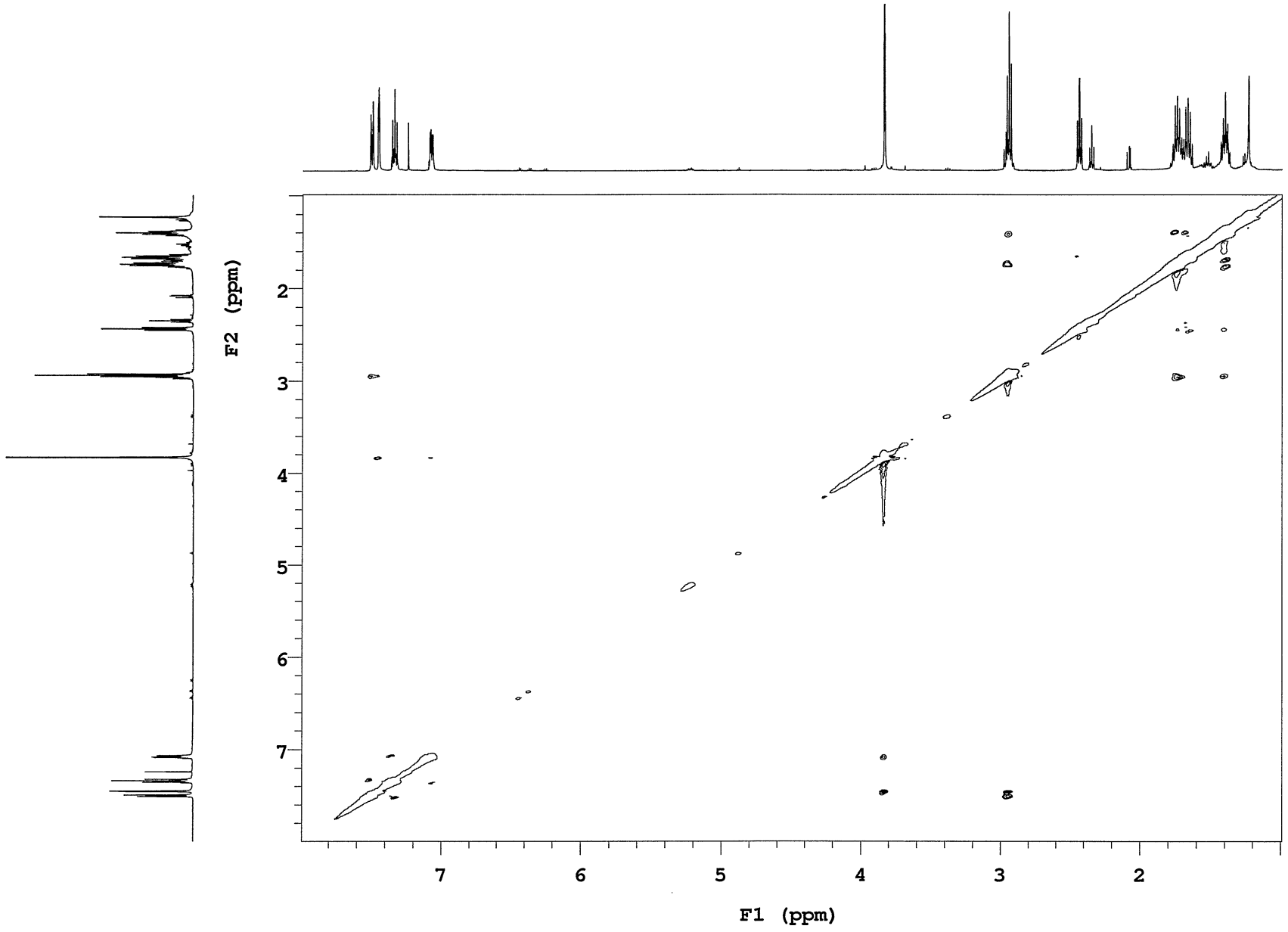
COSY of compound **4m**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-088/gCOSY_01

Plot date 2021-07-02

YYH-088

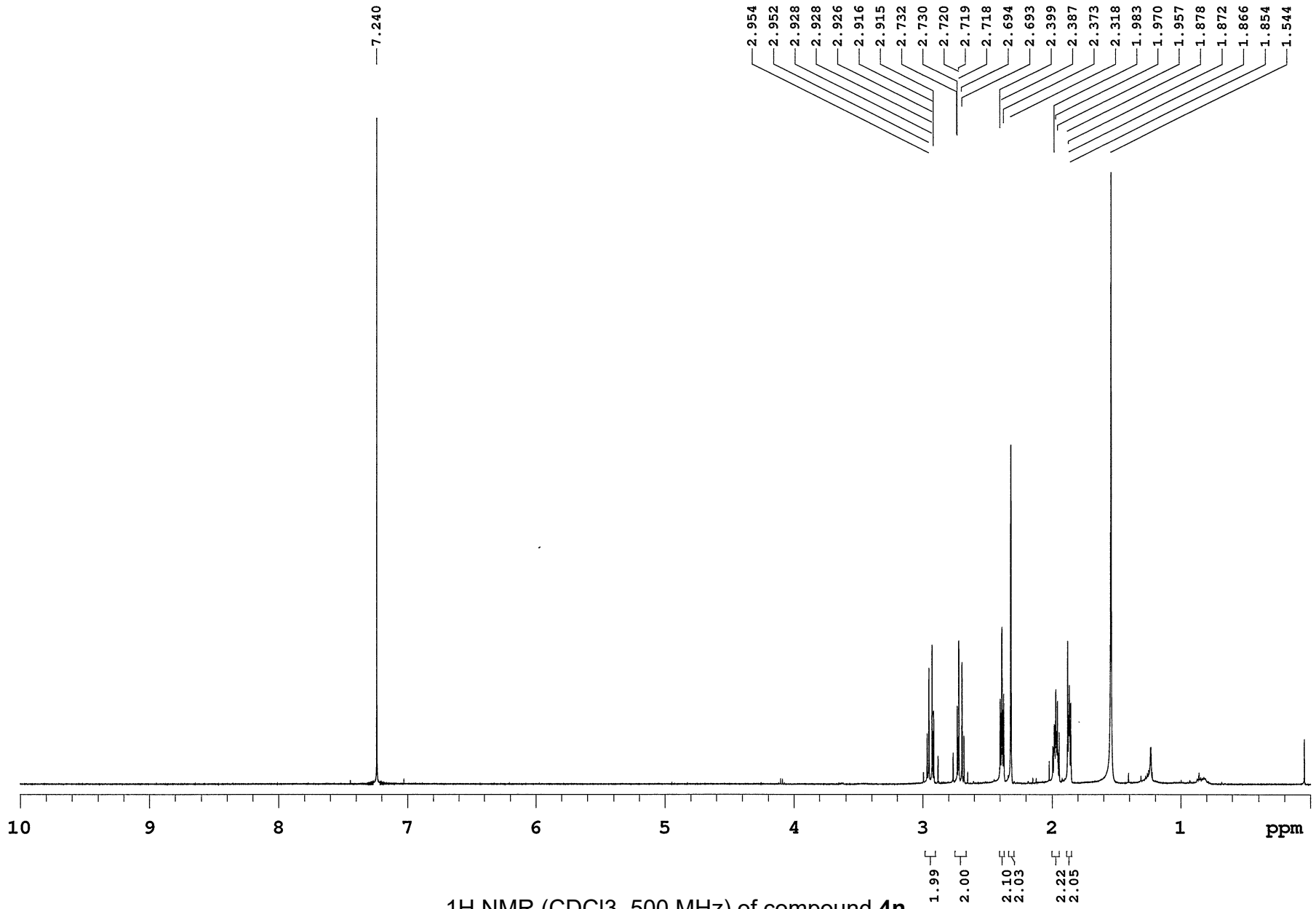
Sample Name	YYH-088	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr2
Date collected	2021-07-02	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



NOESY of compound **4m**

YYH-090

Sample Name	YYH-090	Pulse sequence	PROTON	Temperature	25	Study owner	vnmr2
Date collected	2021-08-27	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



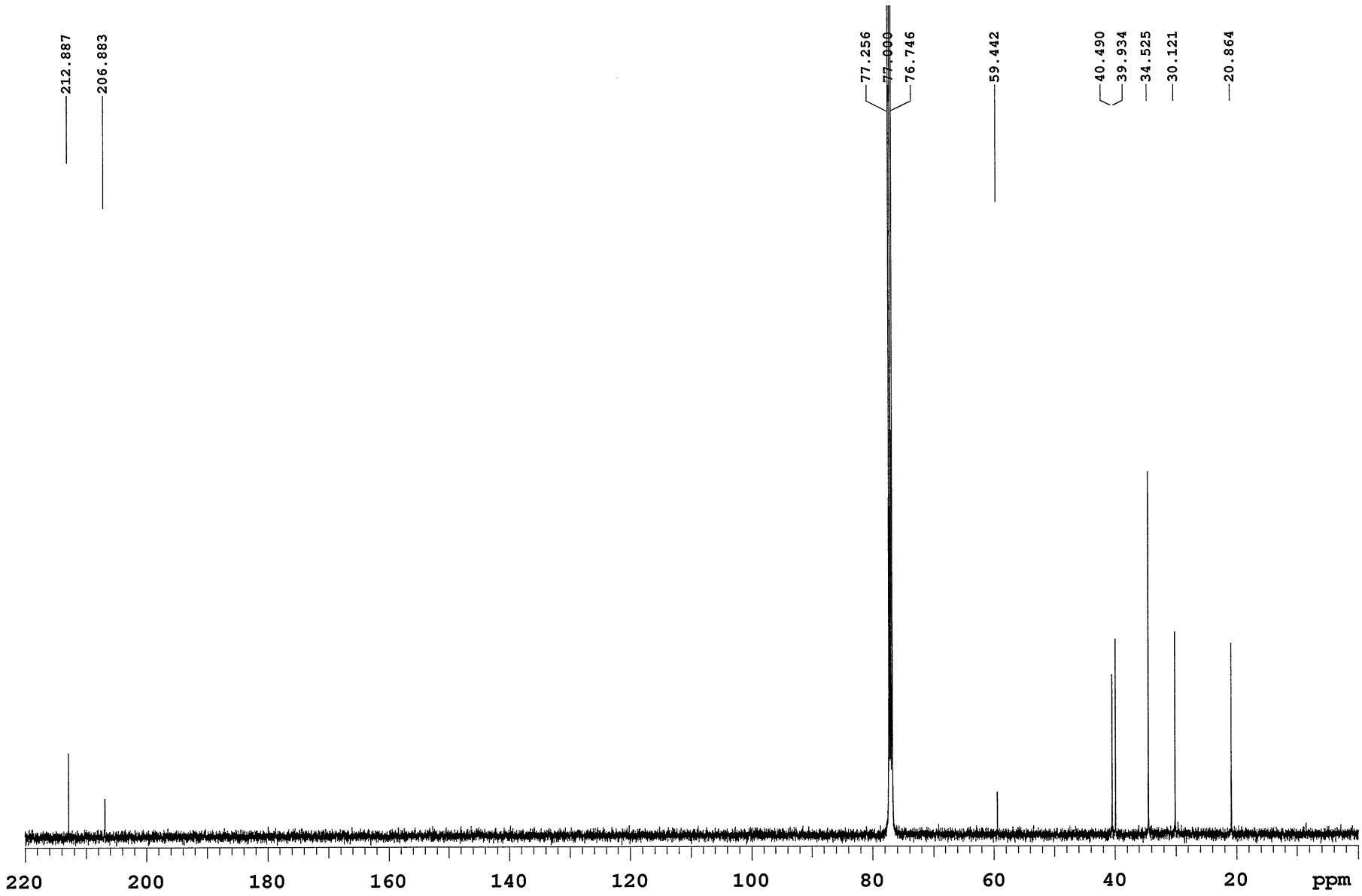
1H NMR (CDCl3, 500 MHz) of compound **4n**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-090/PROTON_03

Plot date 2021-08-30

YYH-090

Sample Name **YYH-090**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



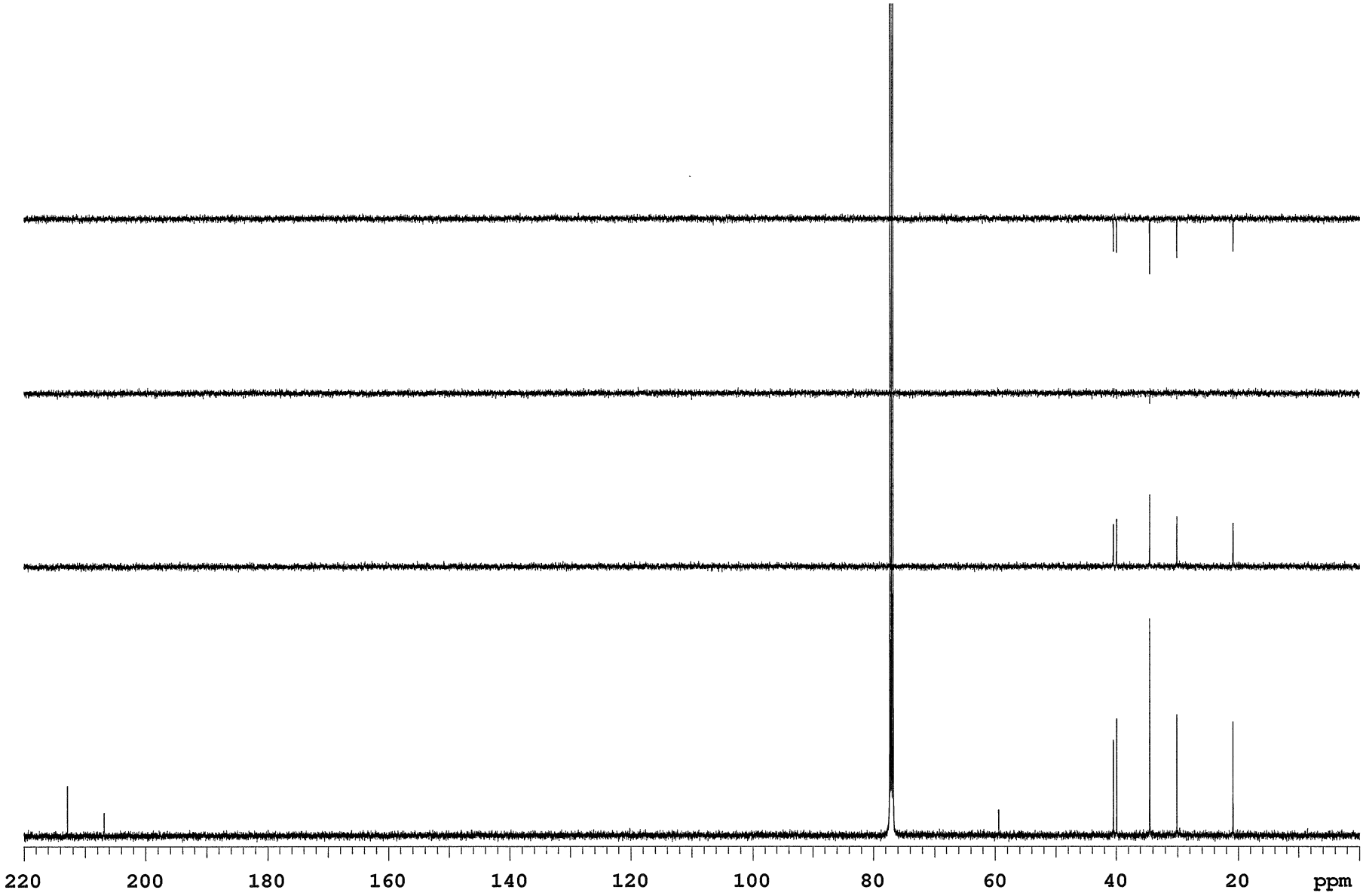
13C NMR (CDCl3, 125 MHz) of compound **4n**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-090/CARBON_02

Plot date 2021-08-30

YYH-090

Sample Name **YYH-090**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



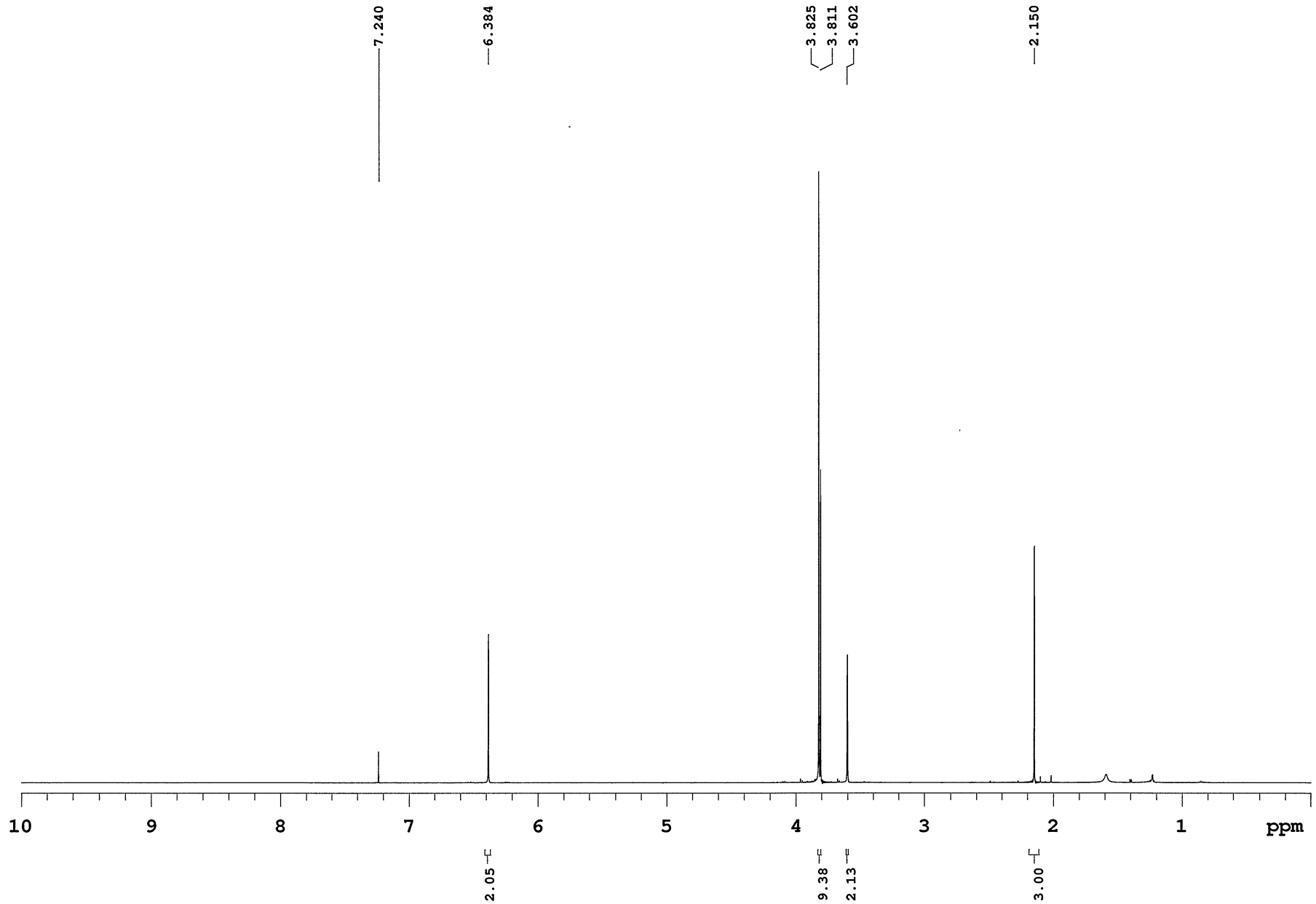
DEPT of compound **4n**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-090/DEPT_01

Plot date 2021-08-30

YYH-102

Sample Name **YYH-102**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-01**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



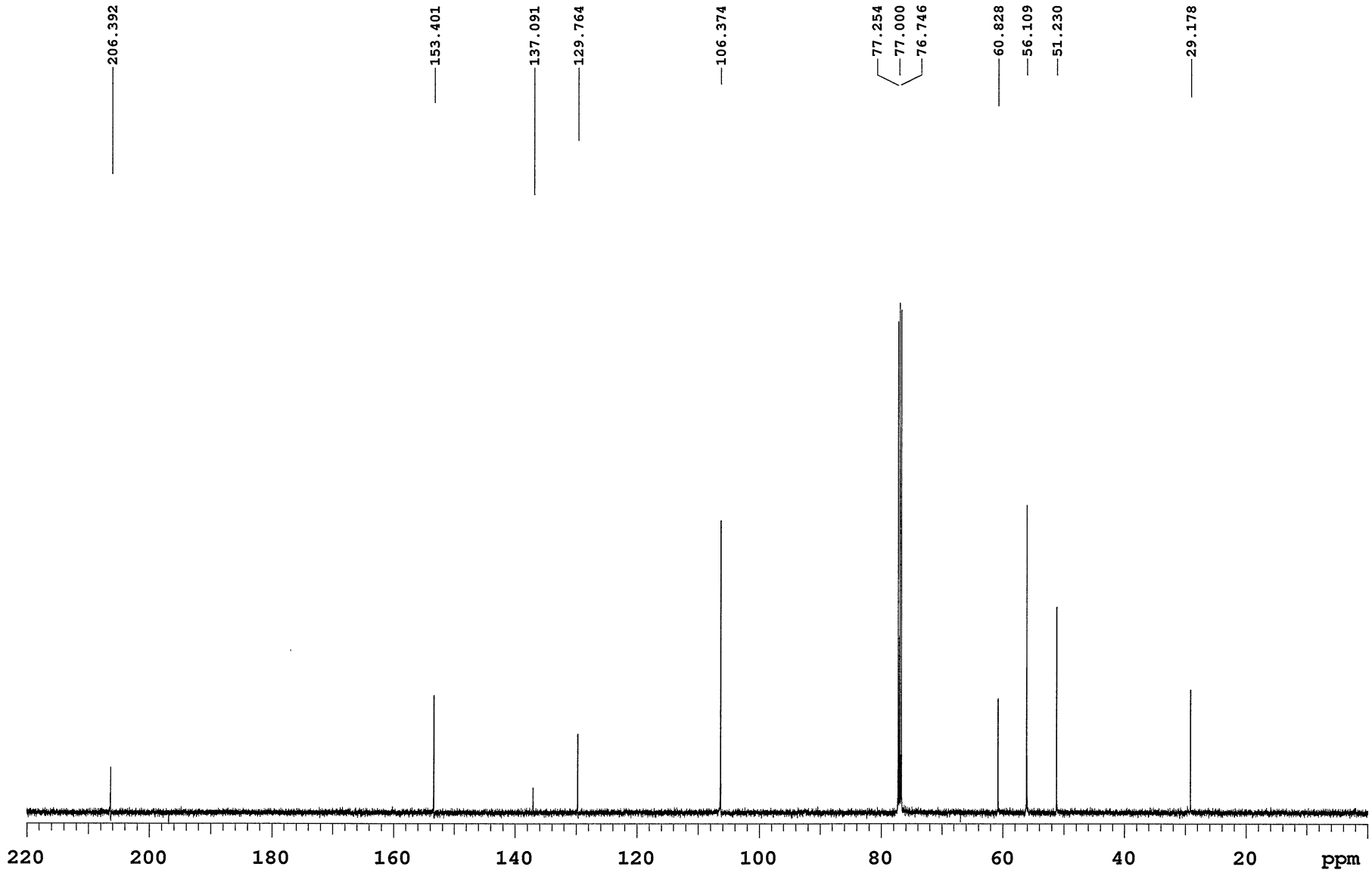
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-102/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4o**

Plot date 2021-07-01

YYH-102

Sample Name	YYH-102	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2021-07-01	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



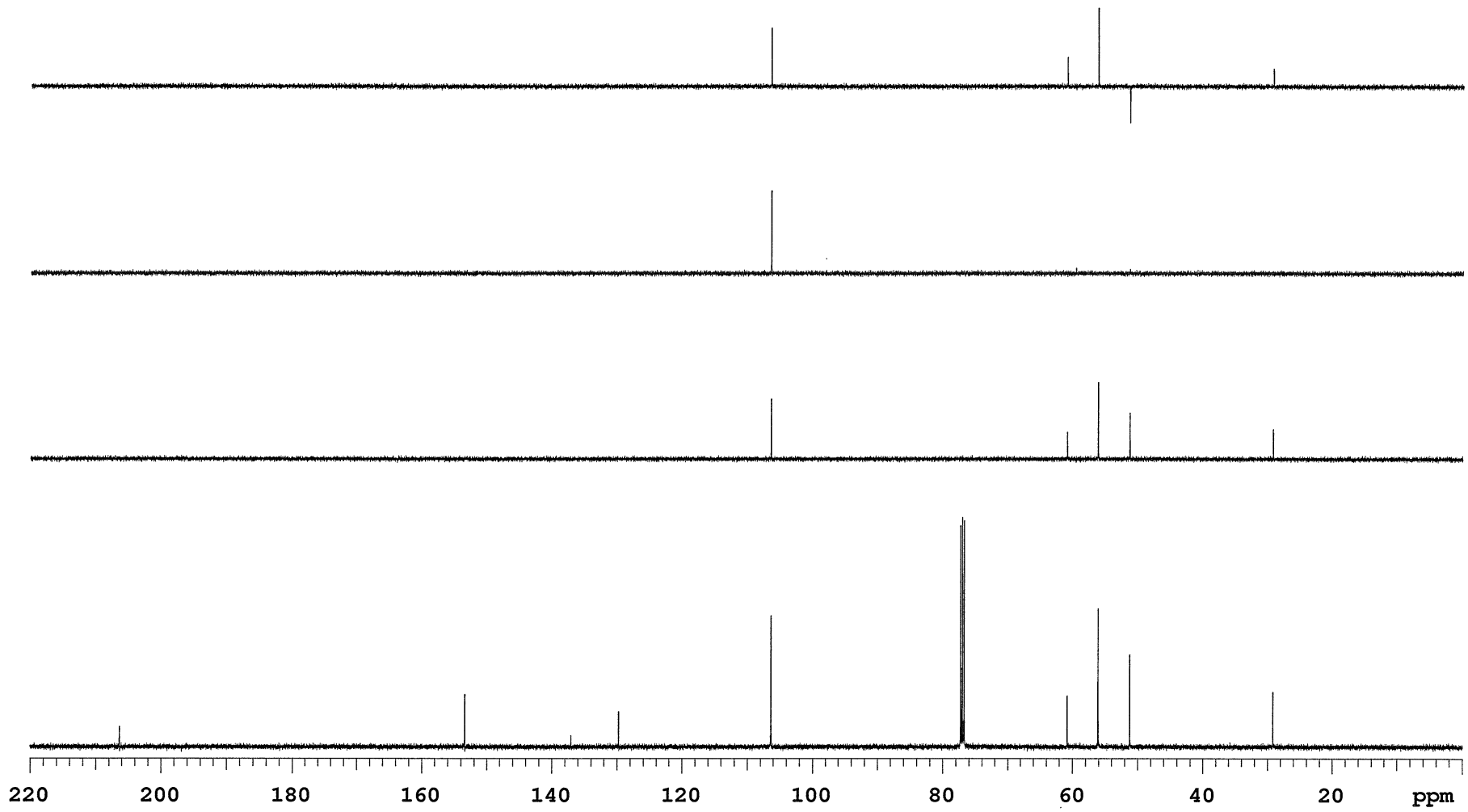
13C NMR (CDCl3, 125 MHz) of compound **4o**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-102/CARBON_02

Plot date 2021-07-01

YYH-102

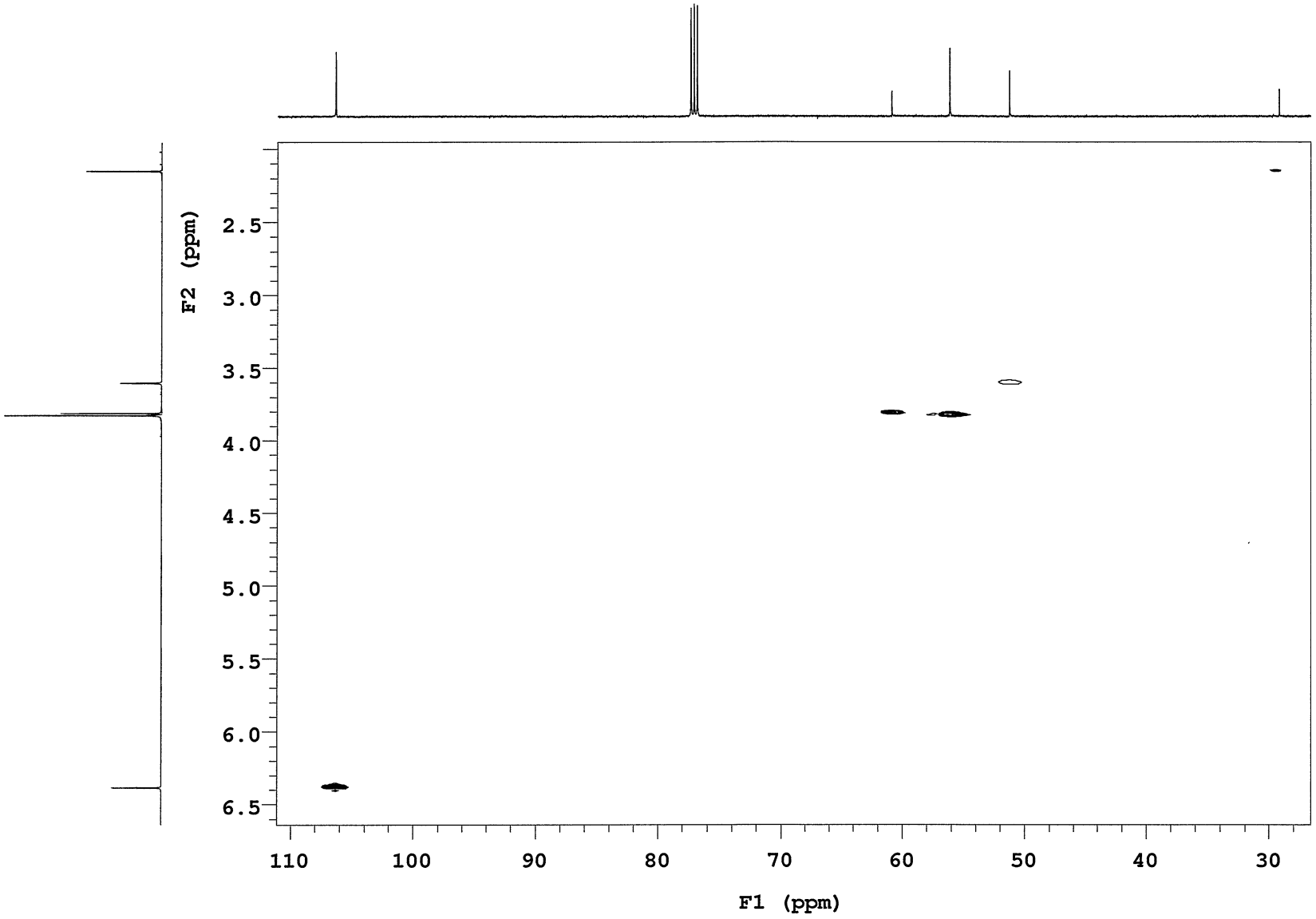
Sample Name **YYH-102**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-01**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **4o**

YYH-102

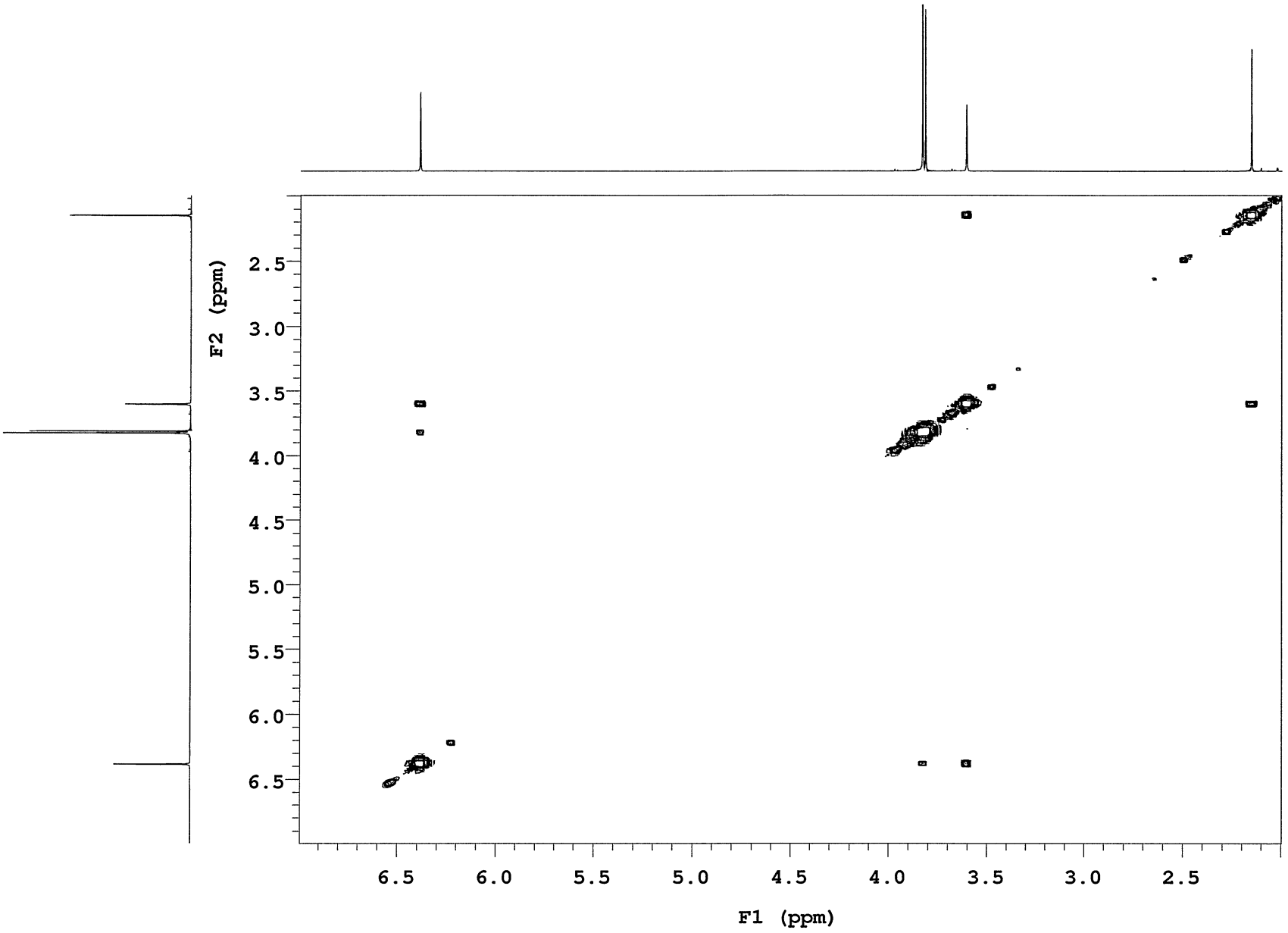
Sample Name **YYH-102**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-01**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



HSQC of compound **4o**

YYH-102

Sample Name	**YYH-102**	Pulse sequence	**gCOSY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2021-07-01**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



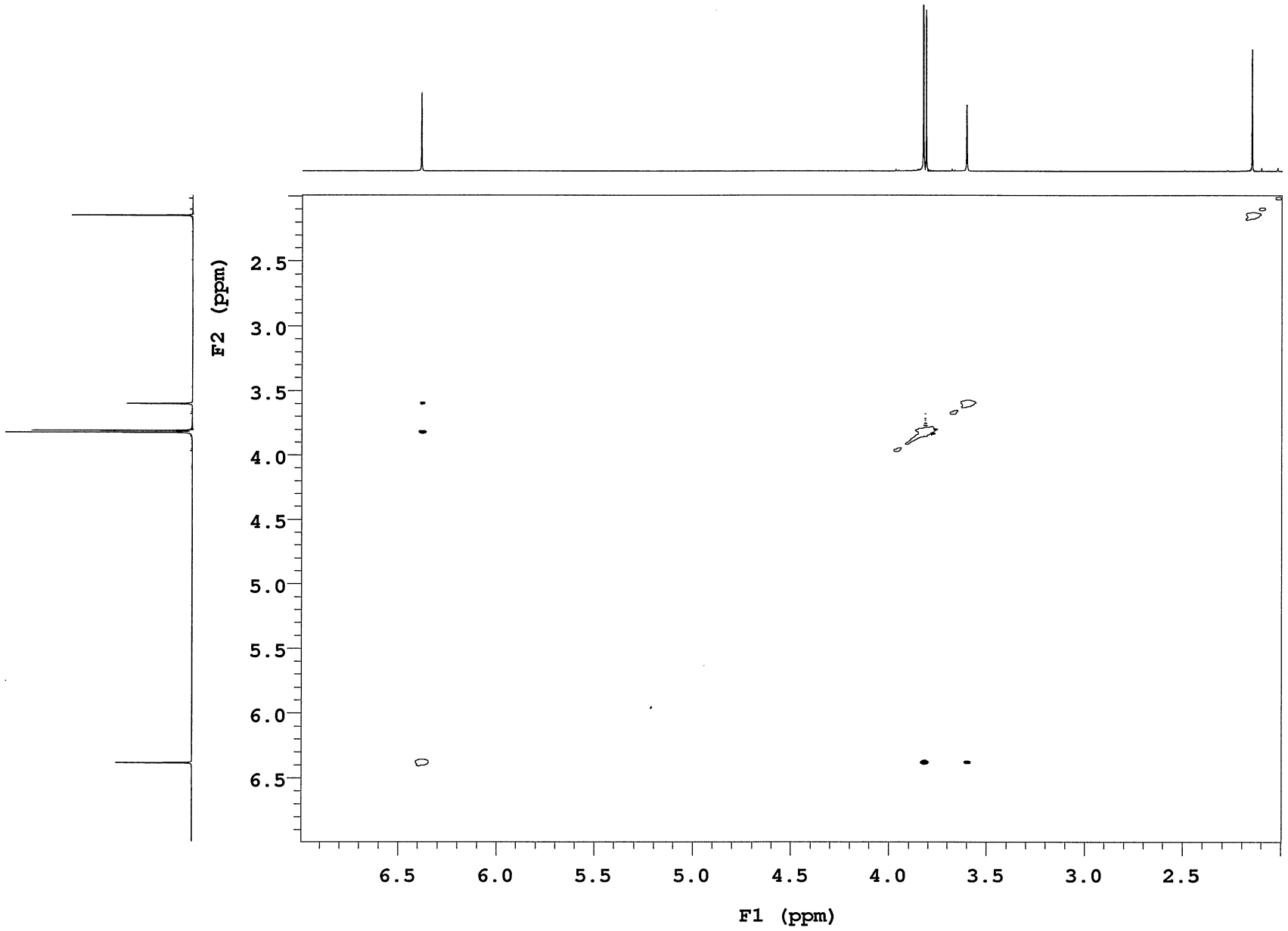
COSY of compound **4o**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-102/gCOSY_01

Plot date 2021-07-01

YYH-102

Sample Name	**YYH-102**	Pulse sequence	**NOESY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2021-07-01**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



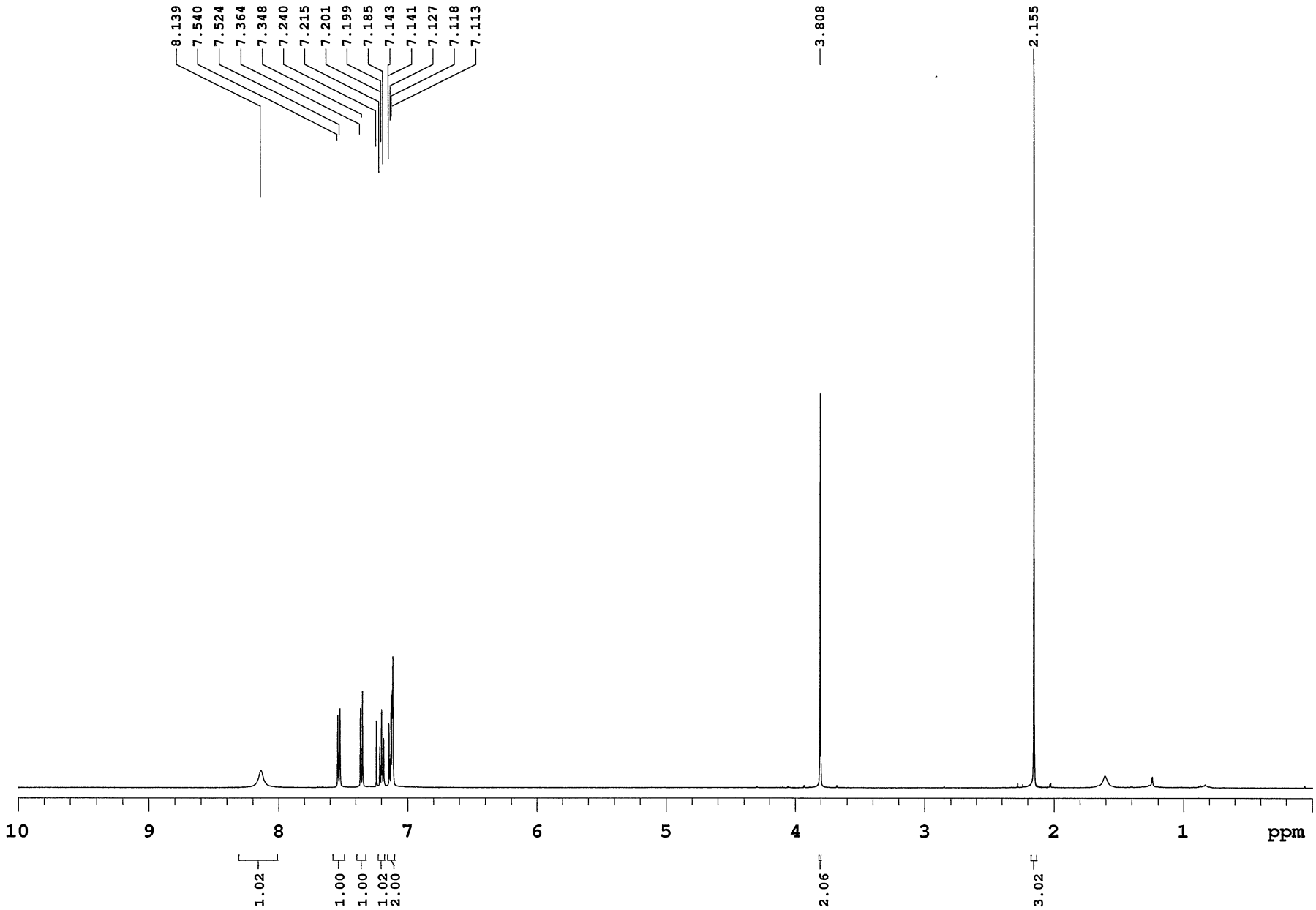
NOESY of compound **4o**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-102/NOESY_01

Plot date 2021-07-01

YYH-104

Sample Name **YYH-104**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-07**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



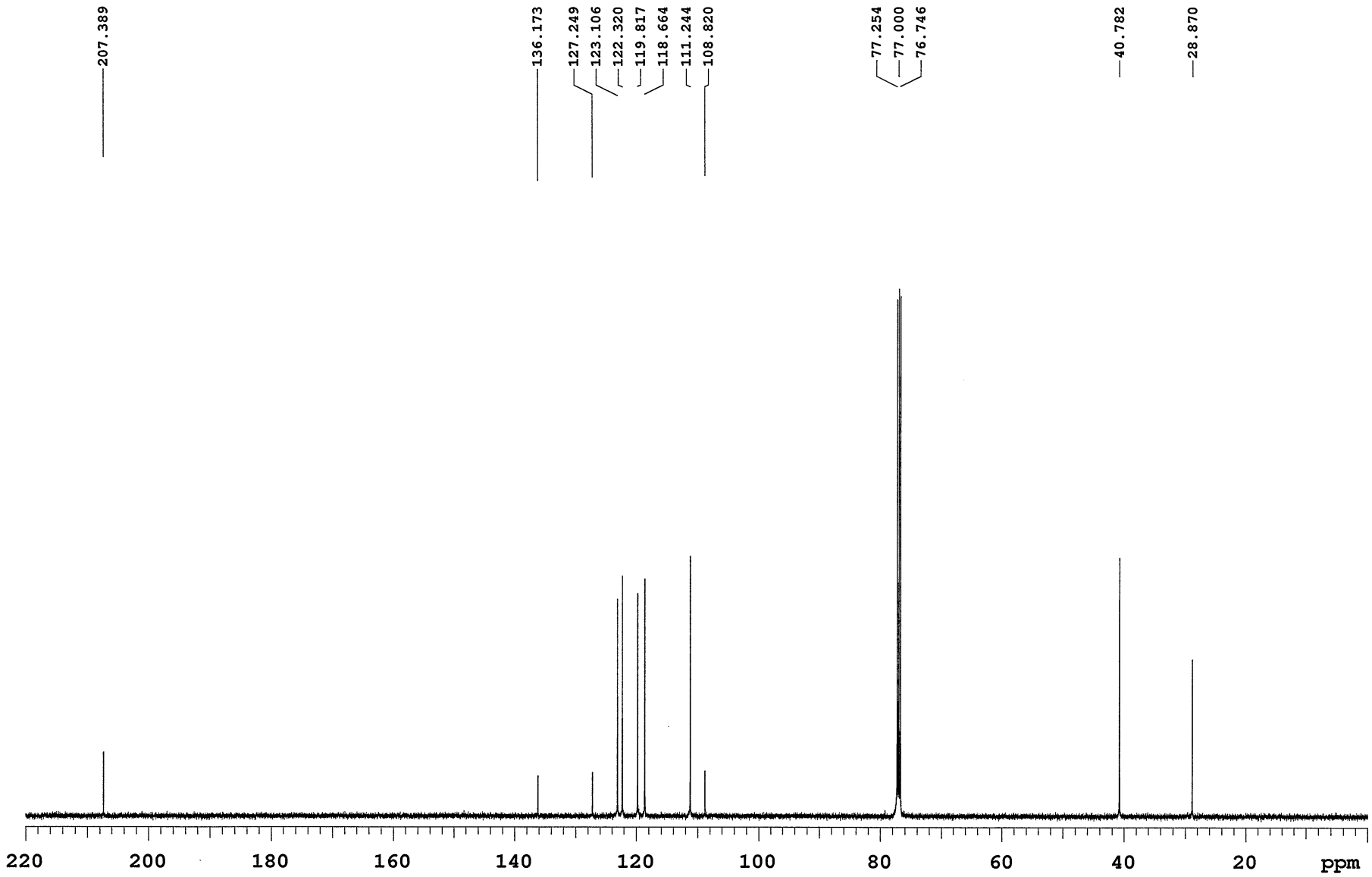
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-104/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4p**

Plot date 2021-07-08

YYH-104

Sample Name **YYH-104**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-07**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



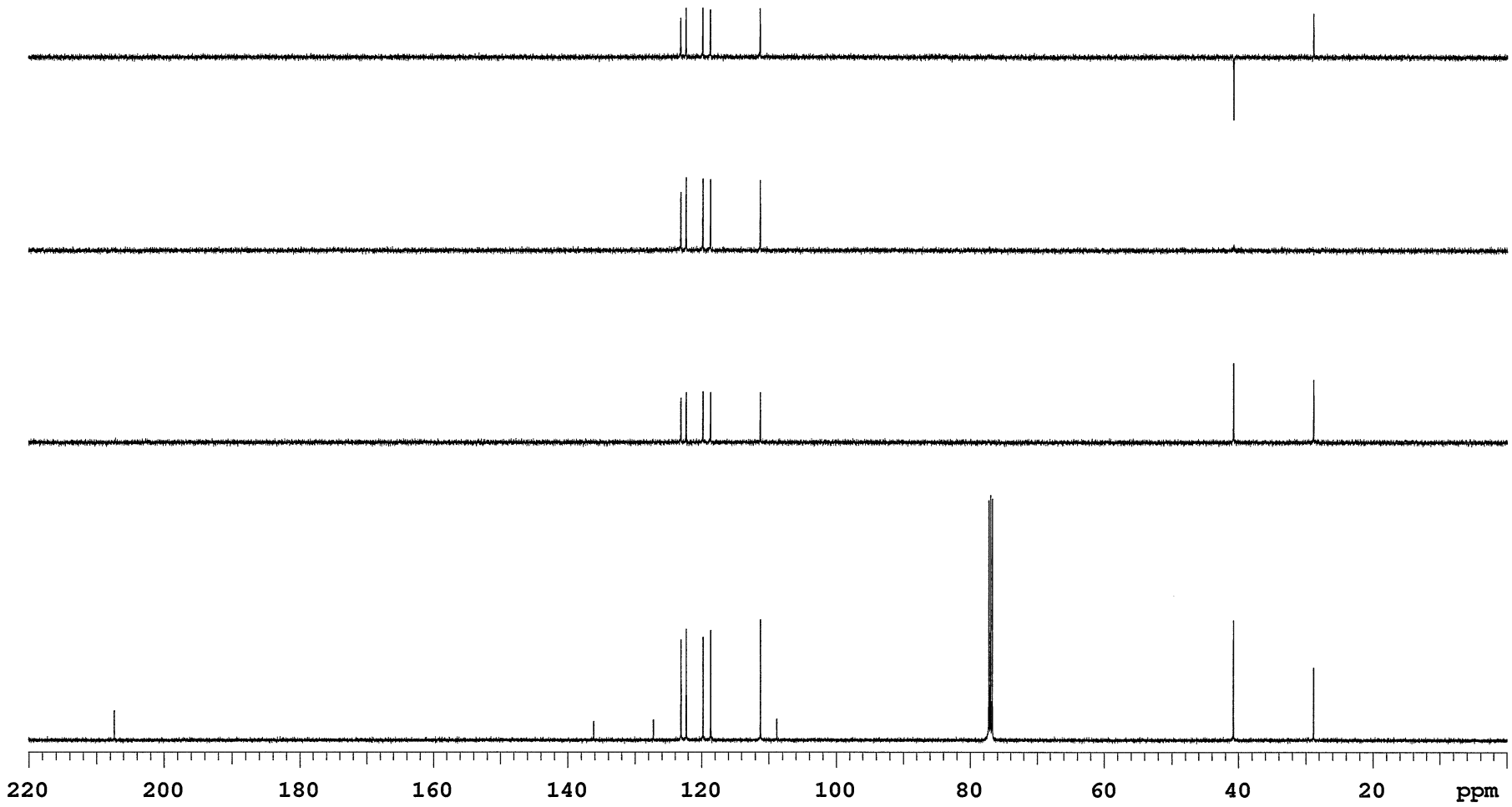
13C NMR (CDCl3, 125 MHz) of compound **4p**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-104/CARBON_02

Plot date 2021-07-08

YYH-104

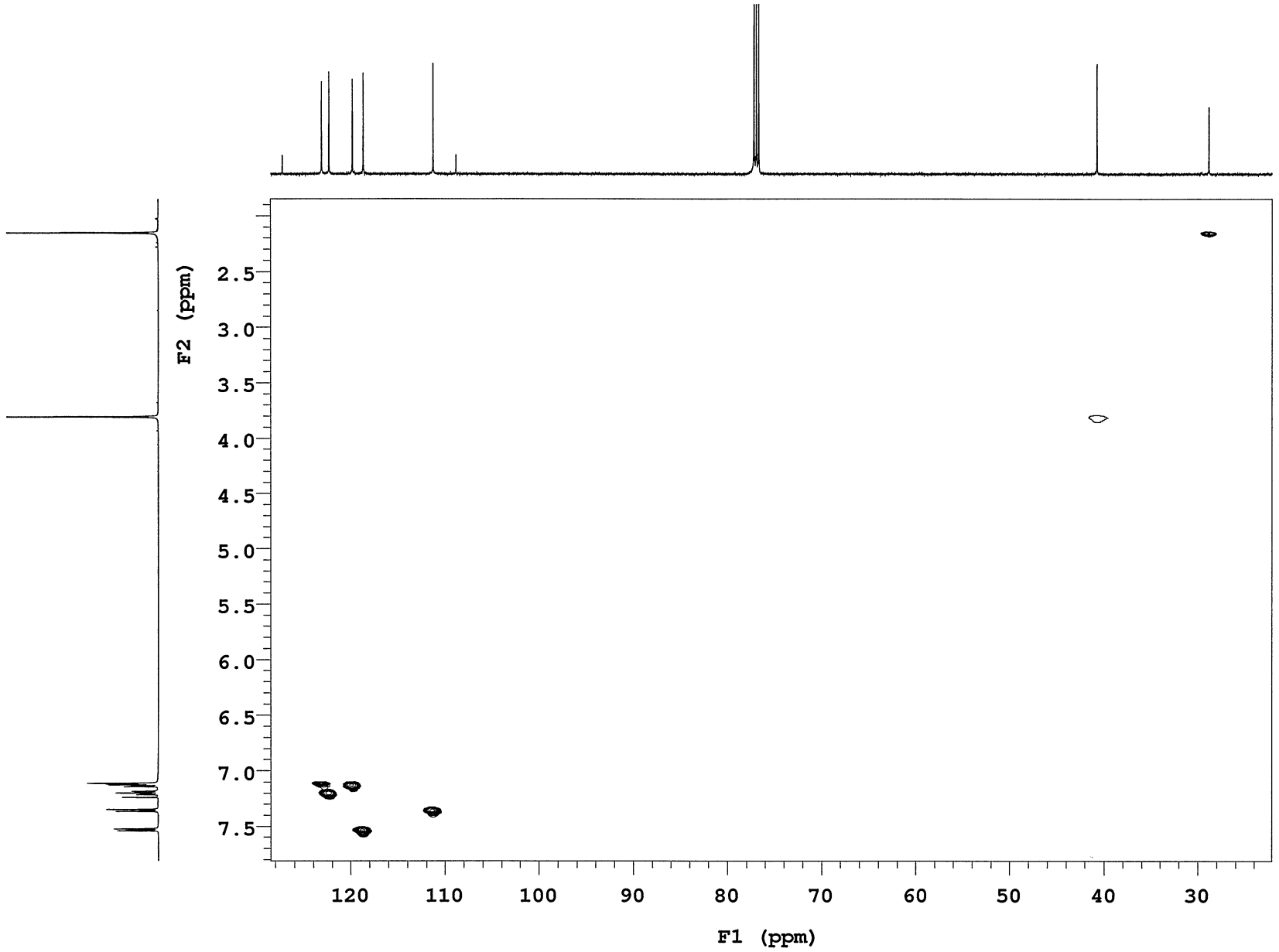
Sample Name **YYH-104**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-07-07**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **4p**

YYH-104

Sample Name	YYH-104	Pulse sequence	gHSQC	Temperature	25	Study owner	vnmr2
Date collected	2021-07-08	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



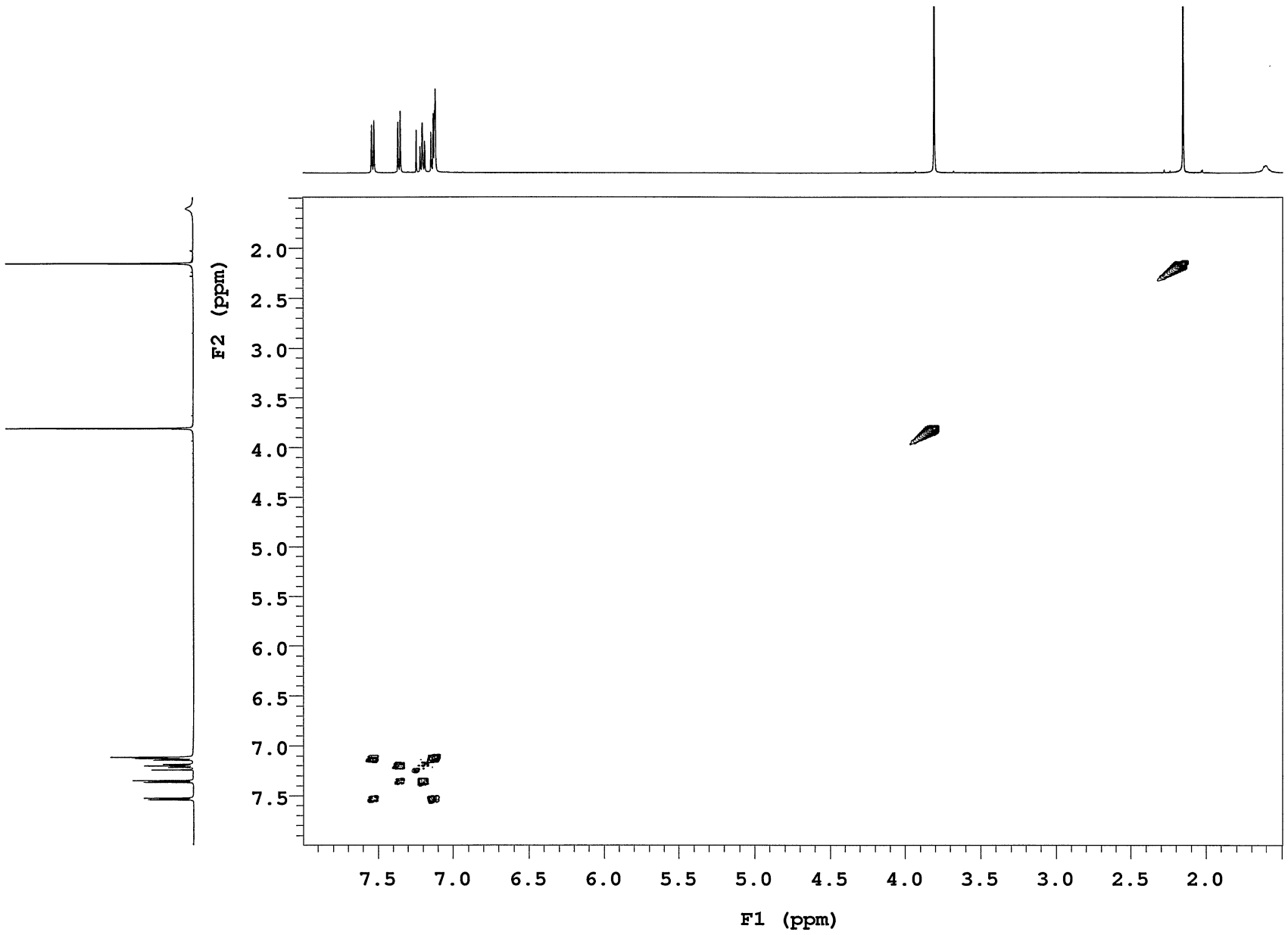
HSQC of compound **4p**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-104/gHSQC_01

Plot date 2021-07-08

YYH-104

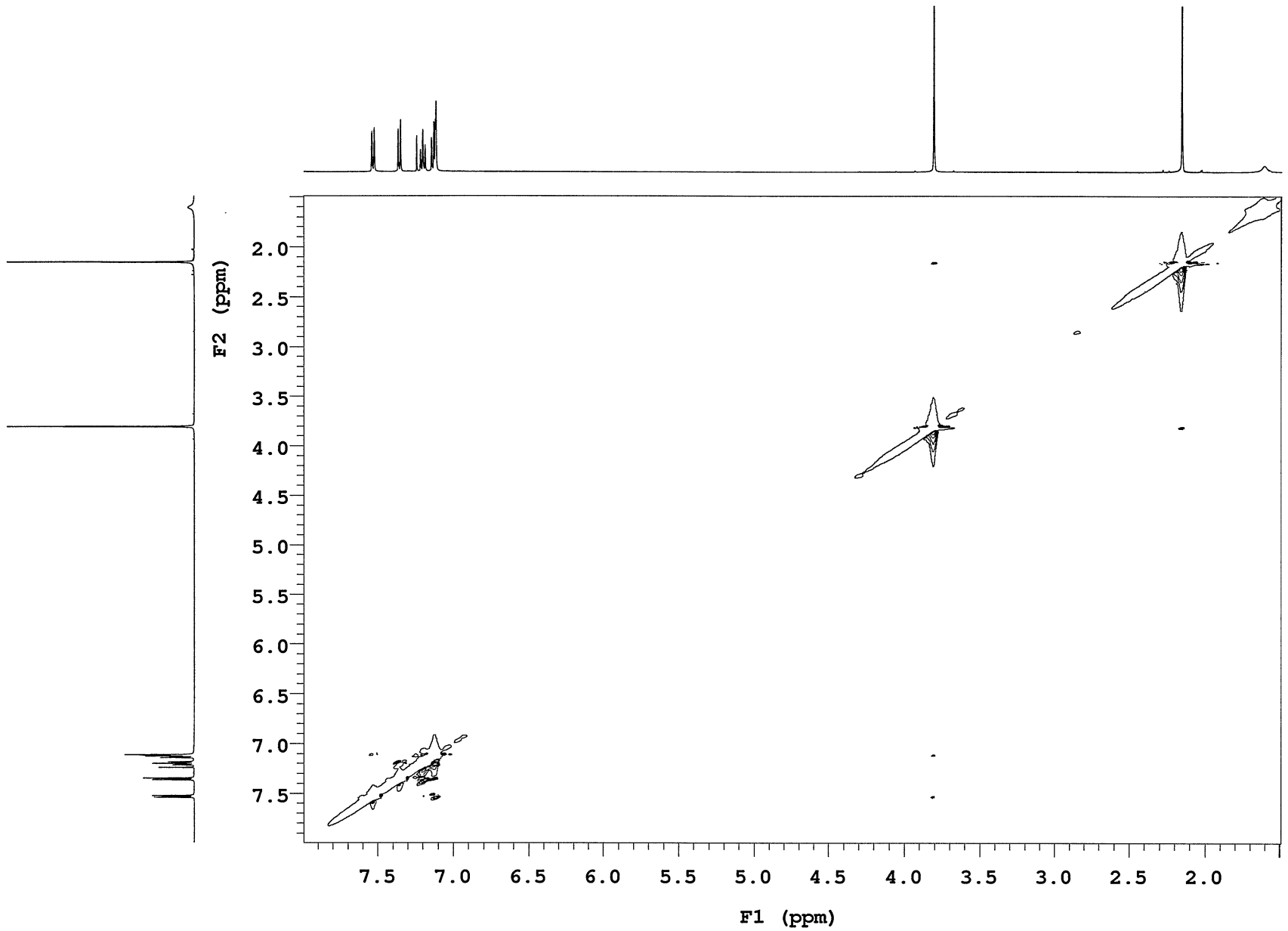
Sample Name	YYH-104	Pulse sequence	gCOSY	Temperature	25	Study owner	vnmr2
Date collected	2021-07-08	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



COSY of compound **4p**

YYH-104

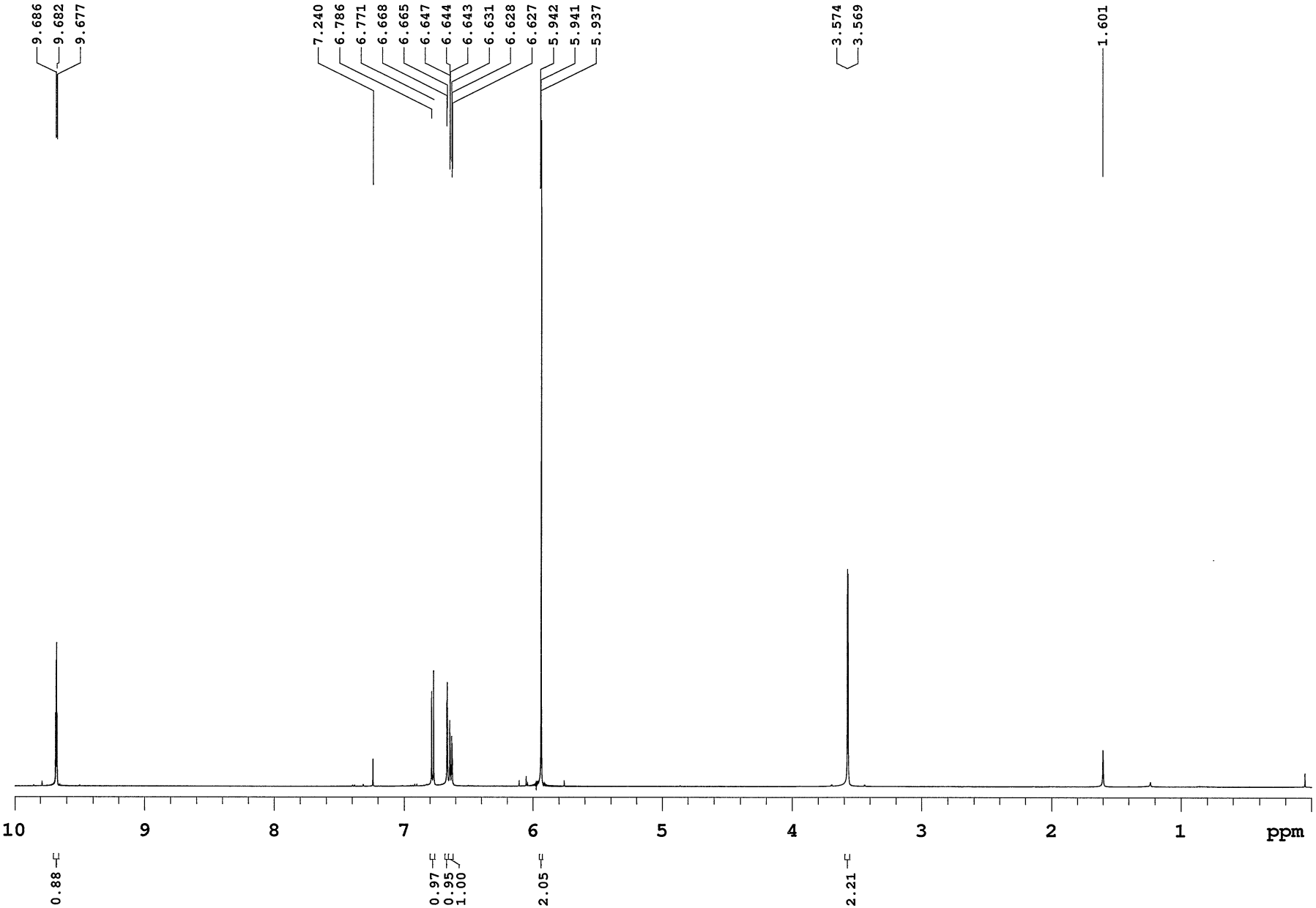
Sample Name	YYH-104	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr2
Date collected	2021-07-08	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



NOESY of compound **4p**

YYH-105

Sample Name **YYH-105**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-26**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



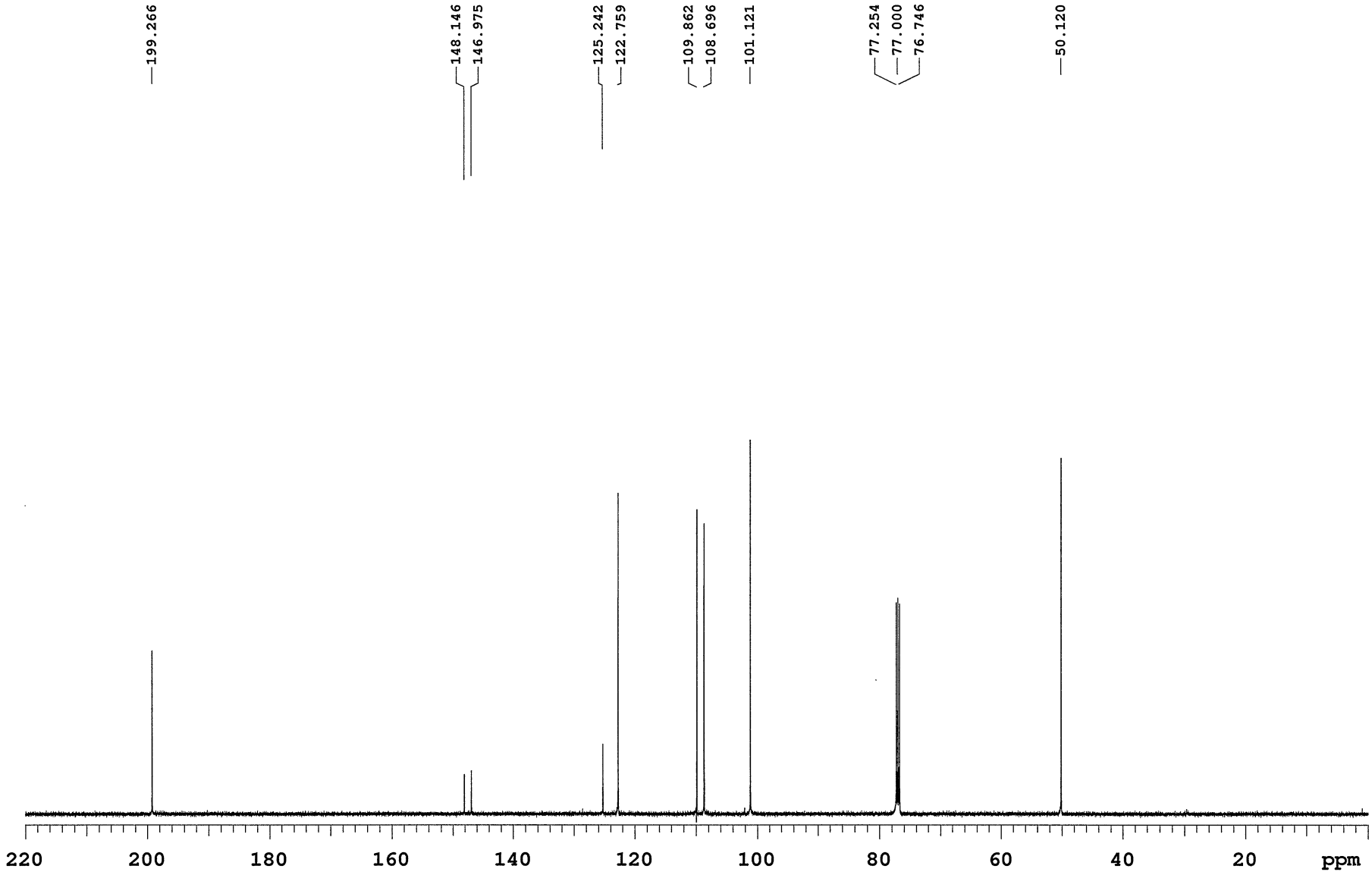
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-105/PROTON_07

1H NMR (CDCl3, 500 MHz) of compound **4q**

Plot date 2021-08-27

YYH-105

Sample Name **YYH-105**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-26**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

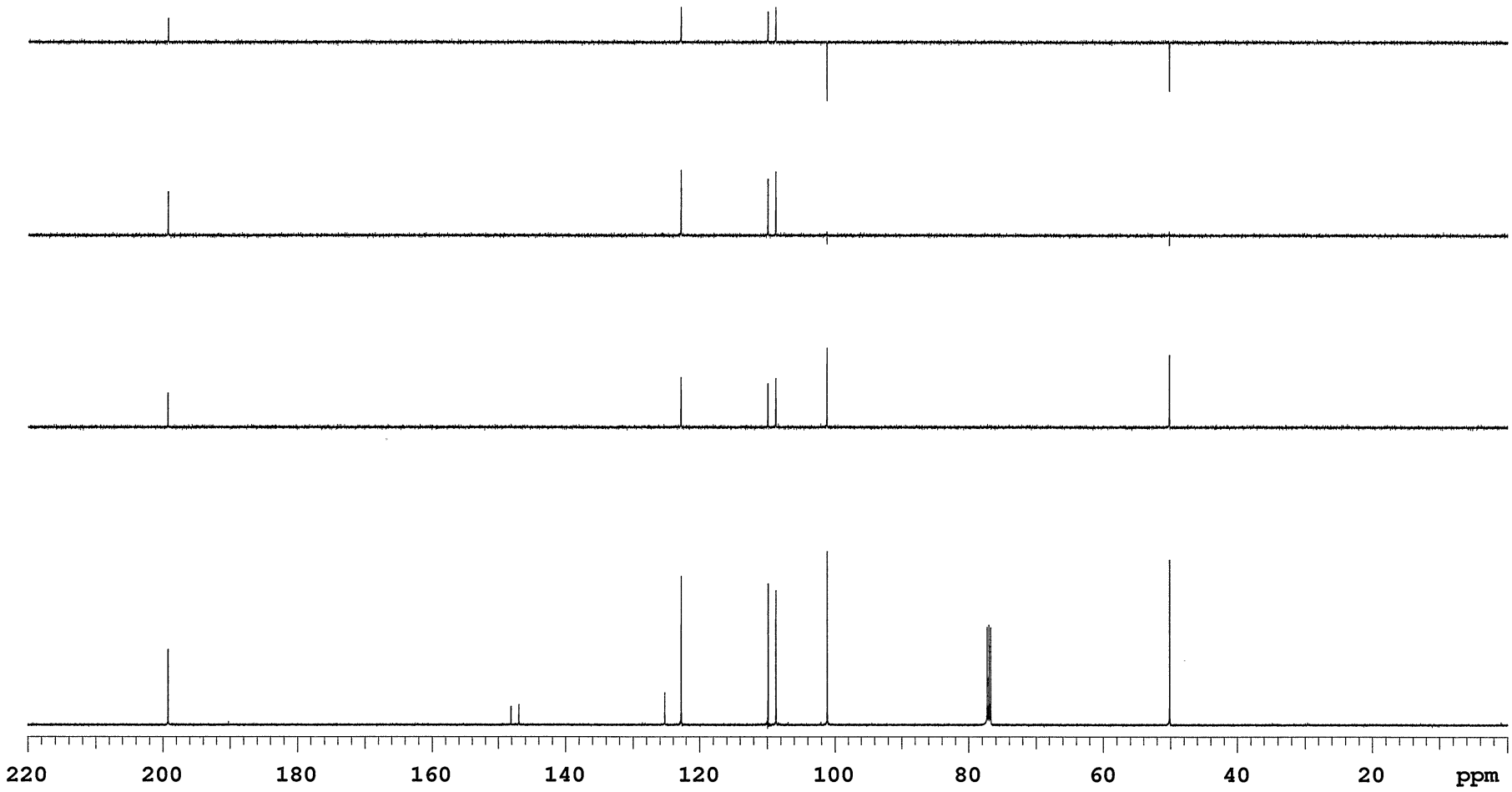


13C NMR (CDCl3, 125 MHz) of compound **4q**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-105/CARBON_04

Plot date 2021-08-27

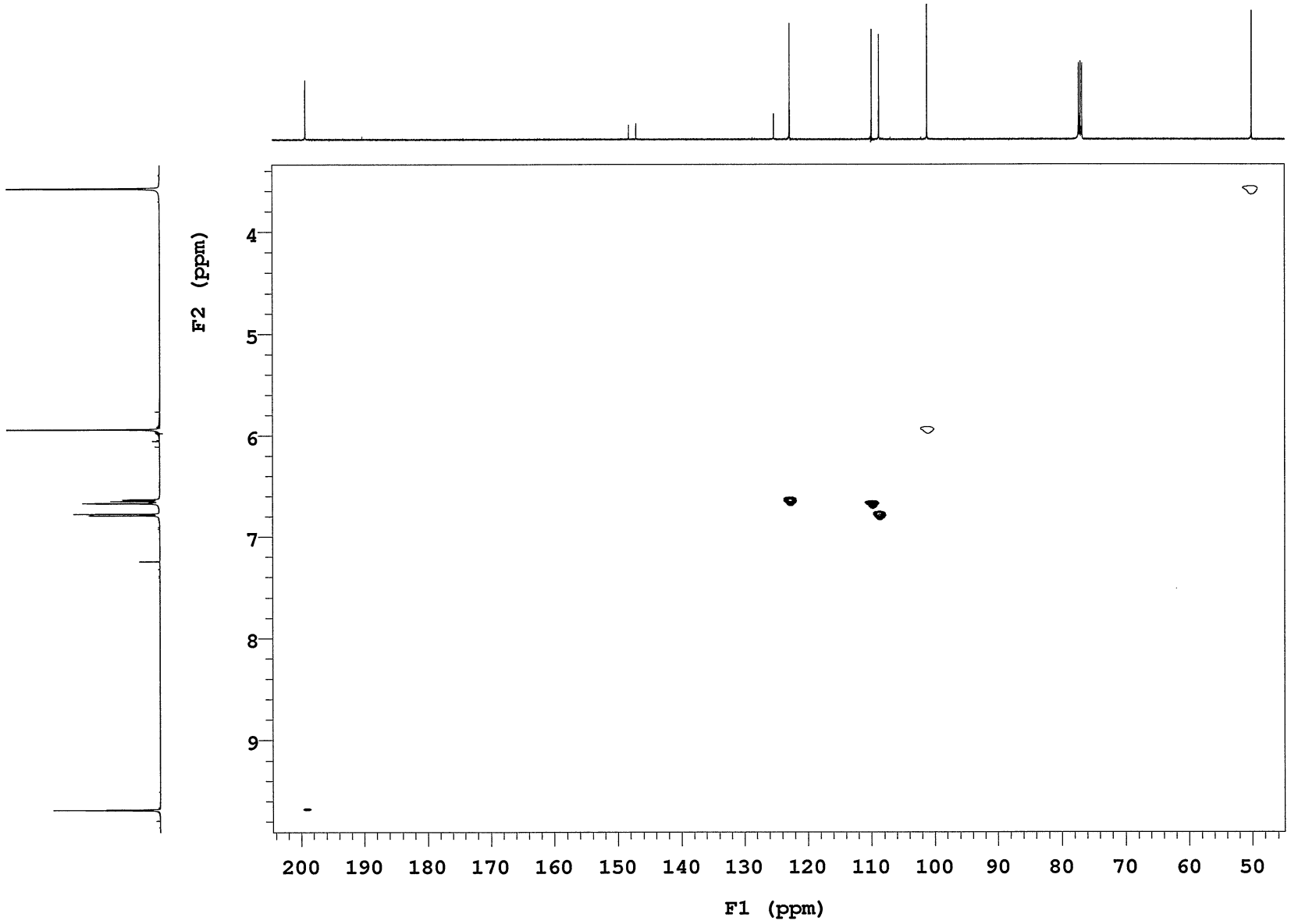
Sample Name **YYH-105**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-26**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **4q**

YYH-105

Sample Name **YYH-105**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



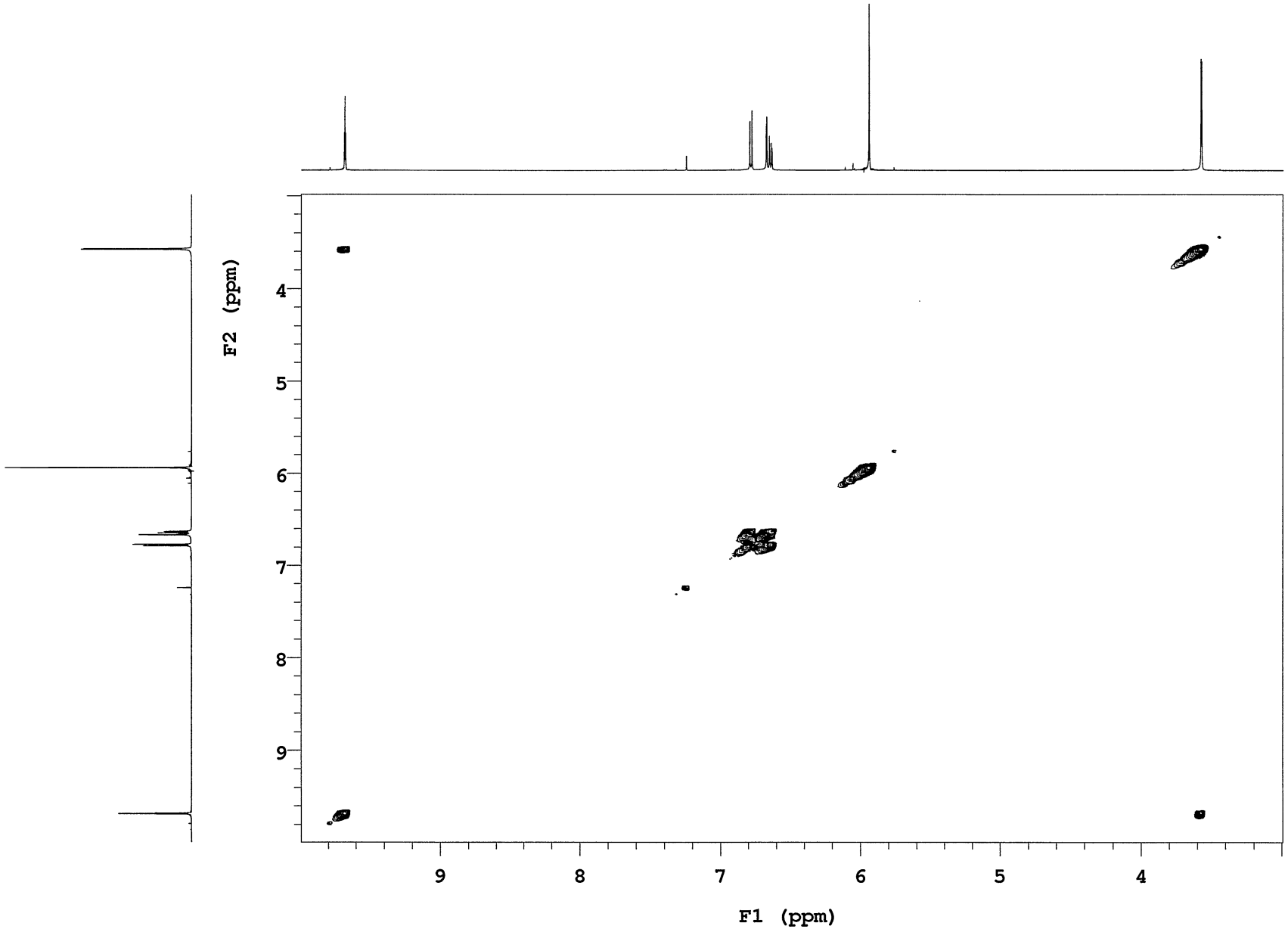
HSQC of compound **4q**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-105/gHSQC_02

Plot date 2021-08-27

YYH-105

Sample Name **YYH-105**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



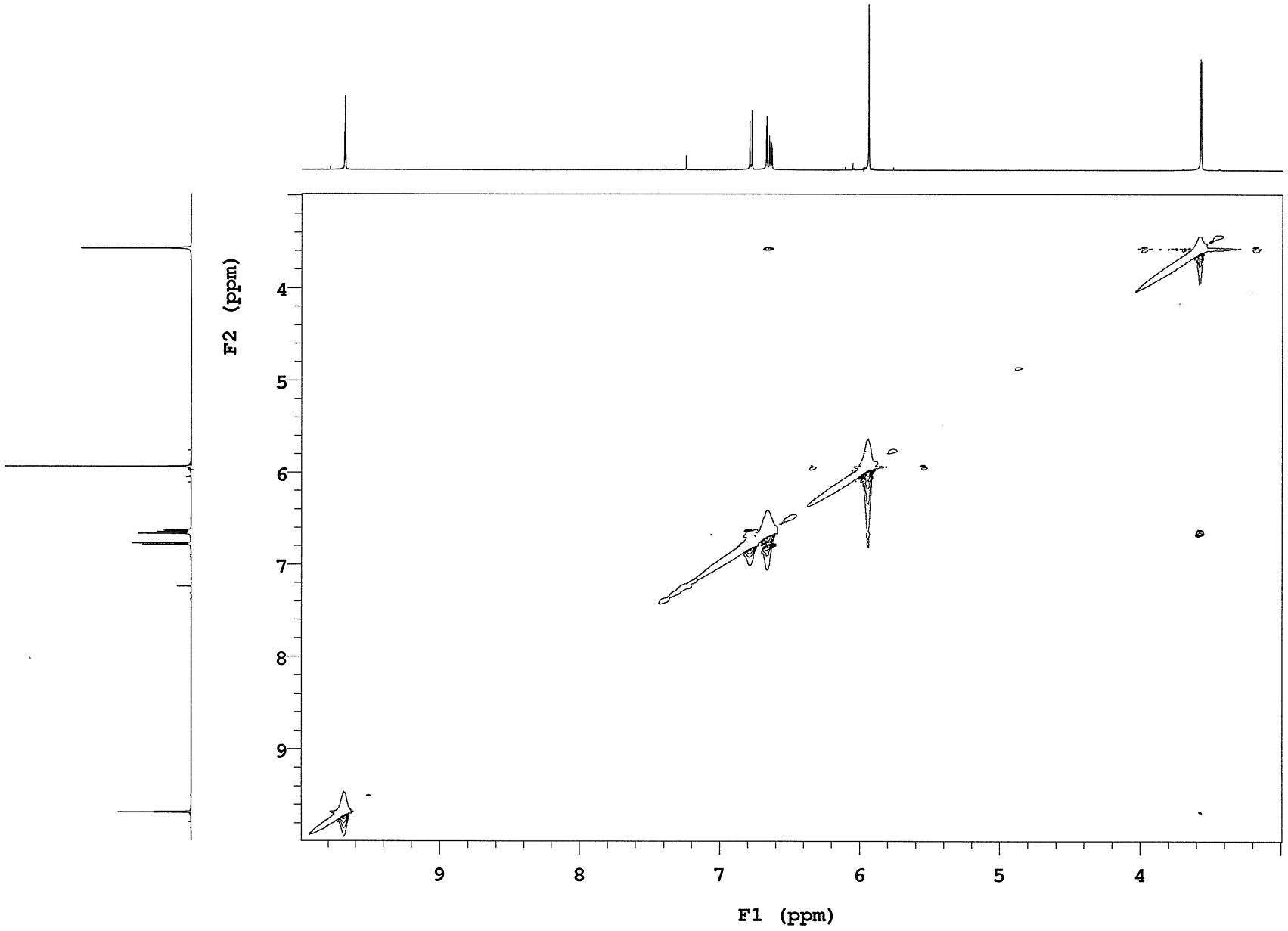
COSY of compound **4q**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-105/gCOSY_02

Plot date 2021-08-27

YYH-105

Sample Name	YYH-105	Pulse sequence	NOESY	Temperature	25	Study owner	vnmr2
Date collected	2021-08-27	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



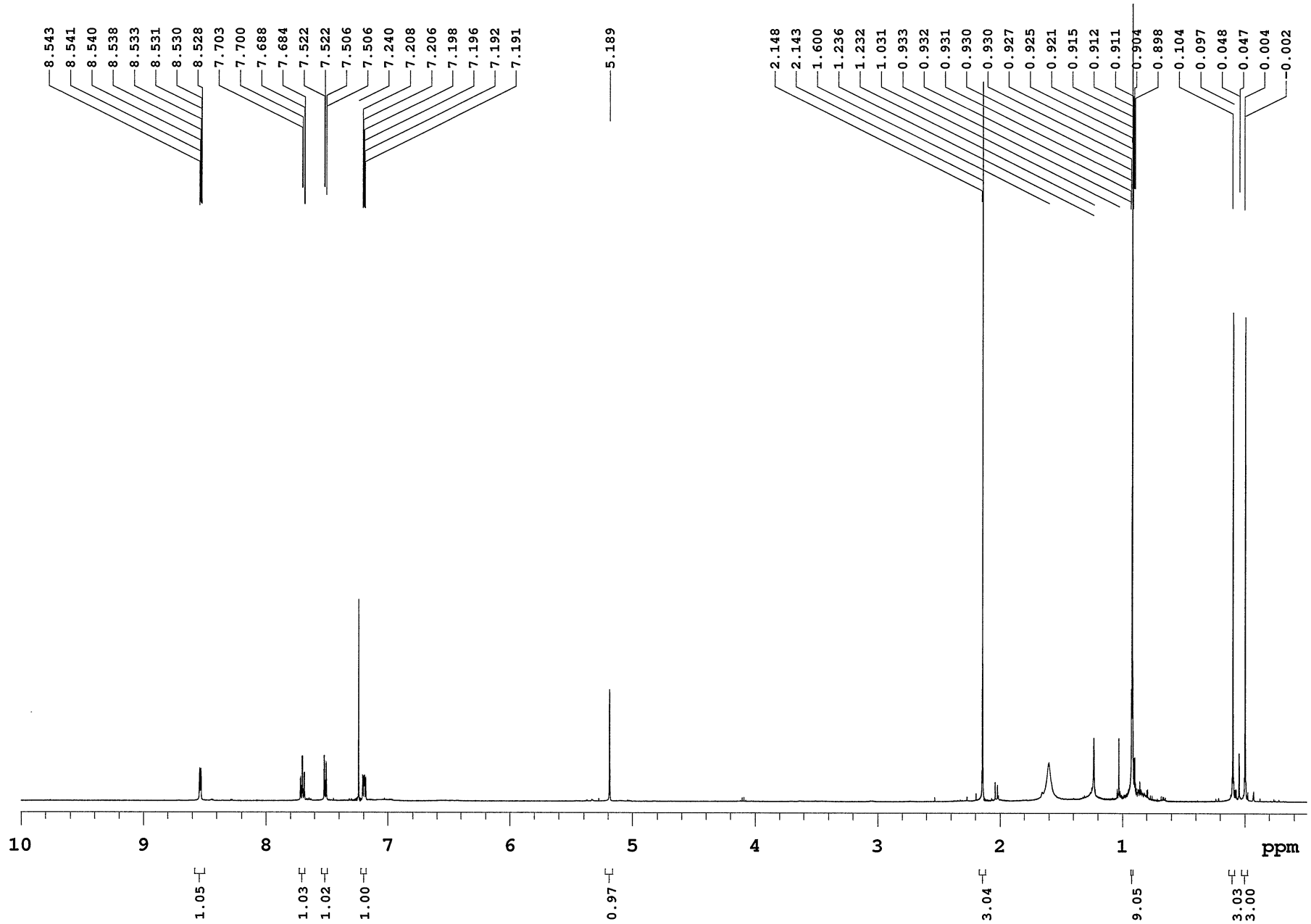
NOESY of compound **4q**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-105/NOESY_02

Plot date 2021-08-27

YYH-116

Sample Name **YYH-116** | Pulse sequence **PROTON** | Temperature **25** | Study owner **vnmr2**
Date collected **2021-09-09** | Solvent **cdcl3** | Spectrometer **Agilent-NMR-inova500** | Operator **vnmr2**



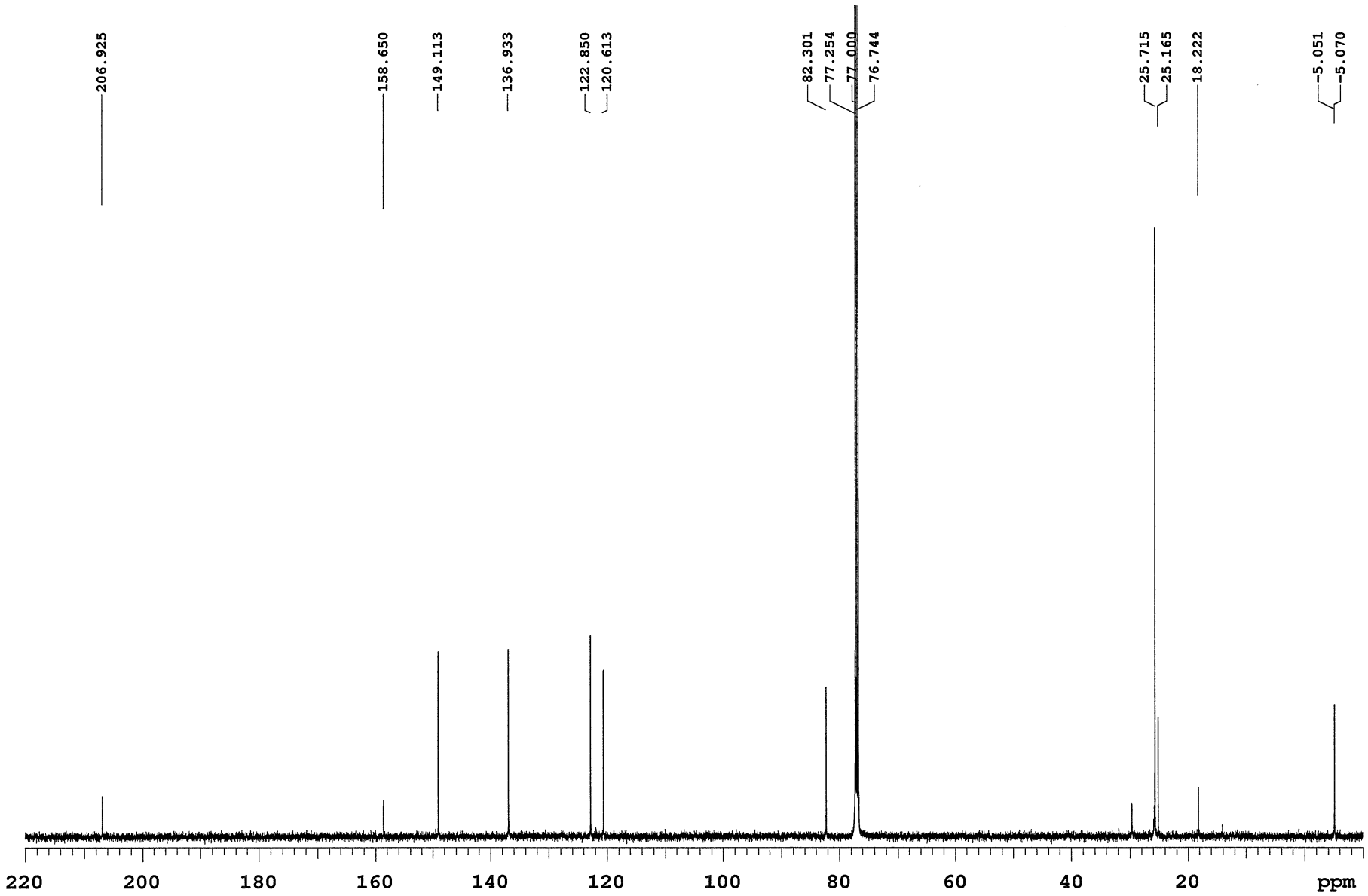
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-116/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4r**

Plot date 2021-09-14

YYH-116

Sample Name **YYH-116** | Pulse sequence **CARBON** | Temperature **25** | Study owner **vnmr2**
Date collected **2021-09-09** | Solvent **cdcl3** | Spectrometer **Agilent-NMR-inova500** | Operator **vnmr2**



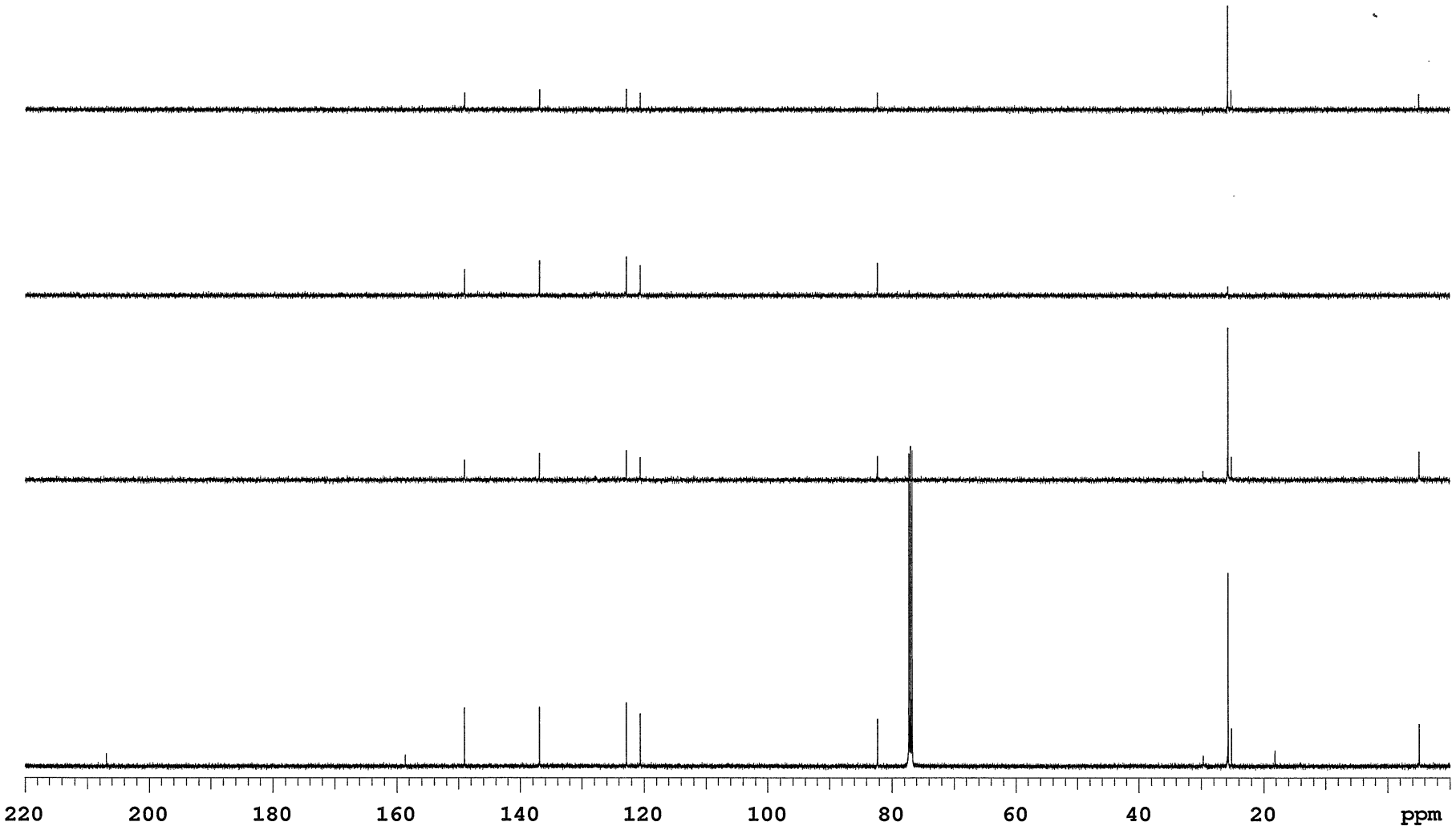
13C NMR (CDCl3, 125 MHz) of compound **4r**

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-116/CARBON_02

Plot date 2021-09-28

YYH-116

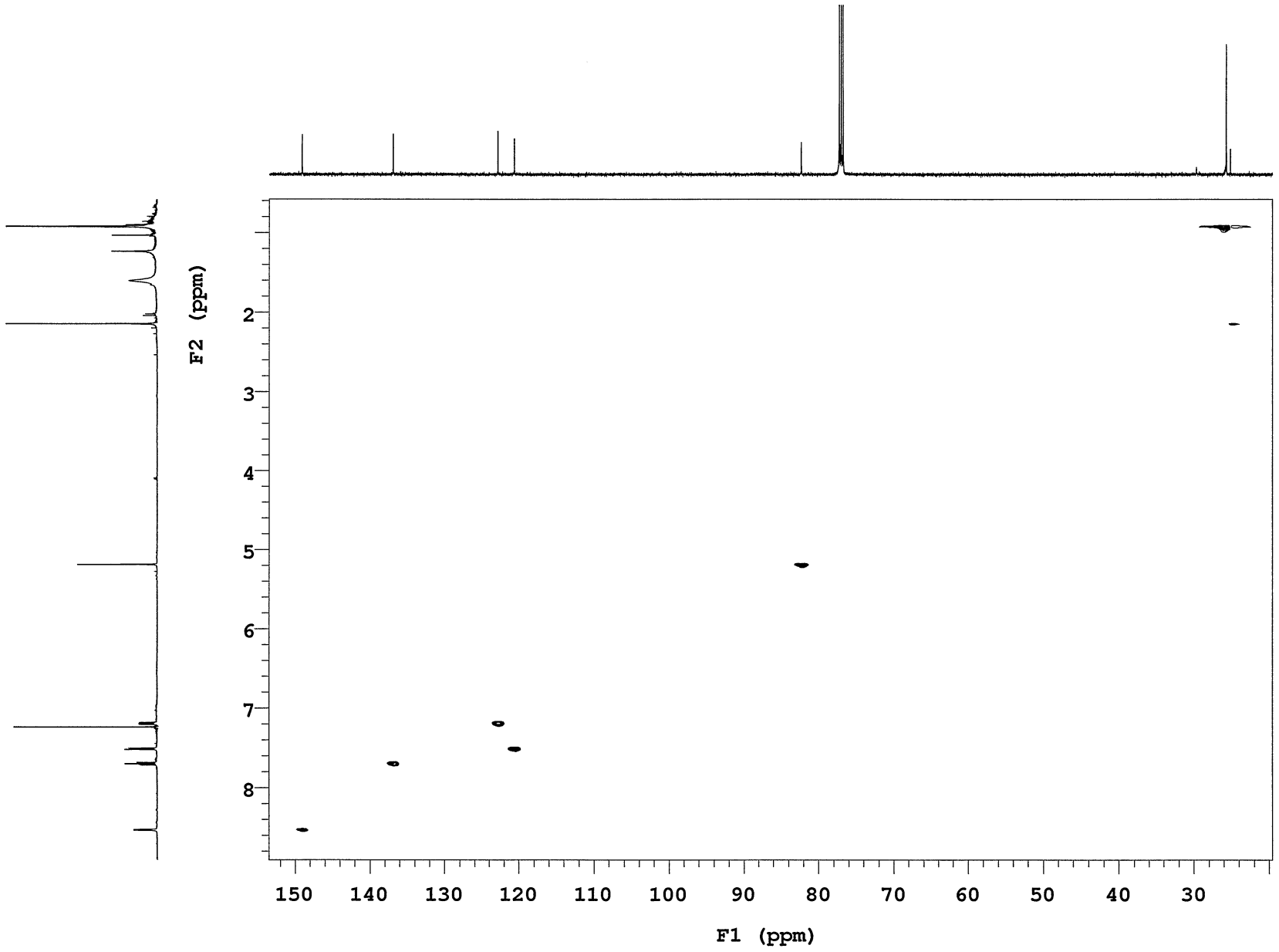
Sample Name **YYH-116**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-09-09**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **4r**

YYH-116

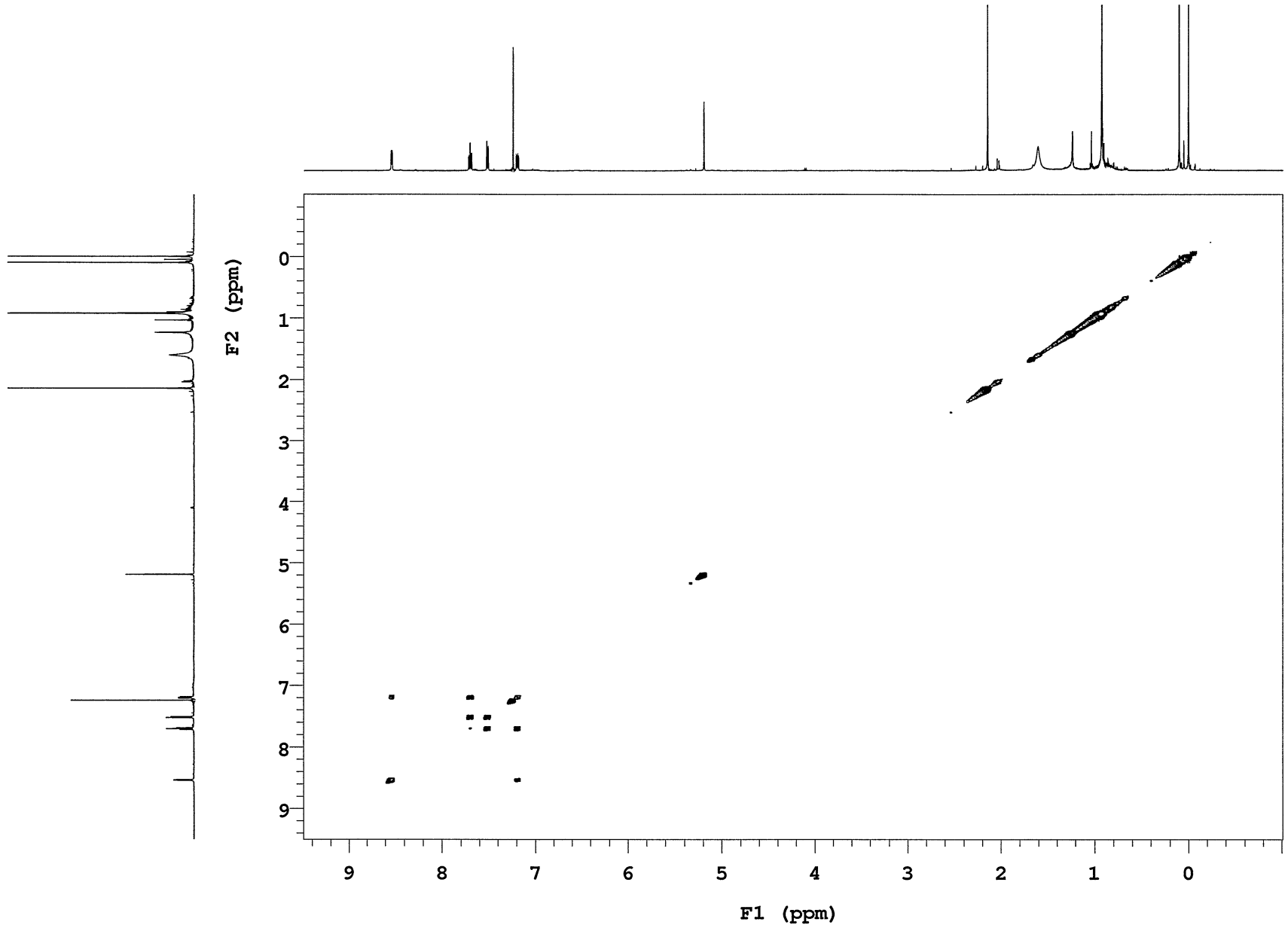
Sample Name	**YYH-116**	Pulse sequence	**gHSQC**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2021-09-10**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



HSQC of compound **4r**

YYH-116

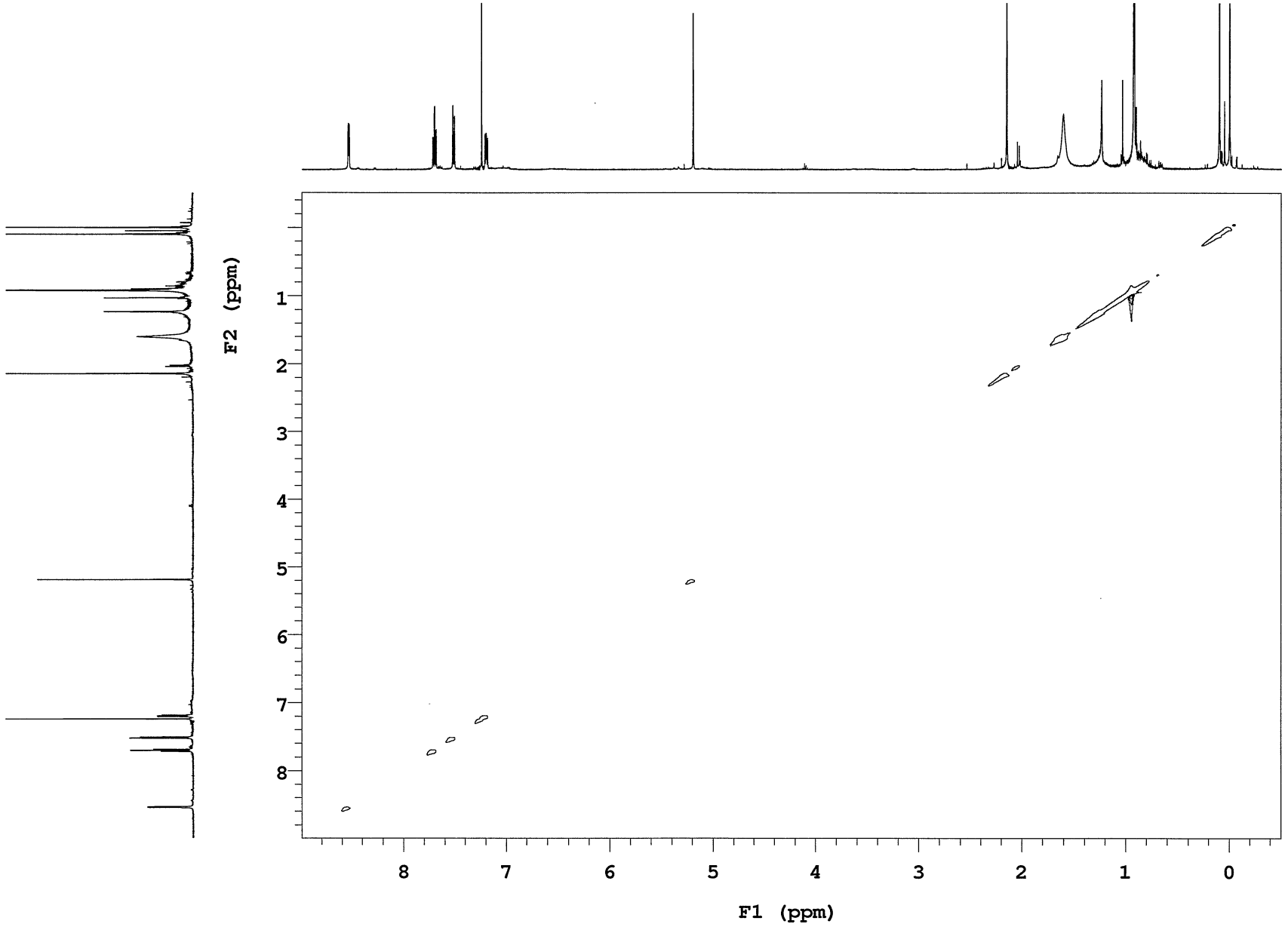
Sample Name **YYH-116**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-09-10**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



COSY of compound **4r**

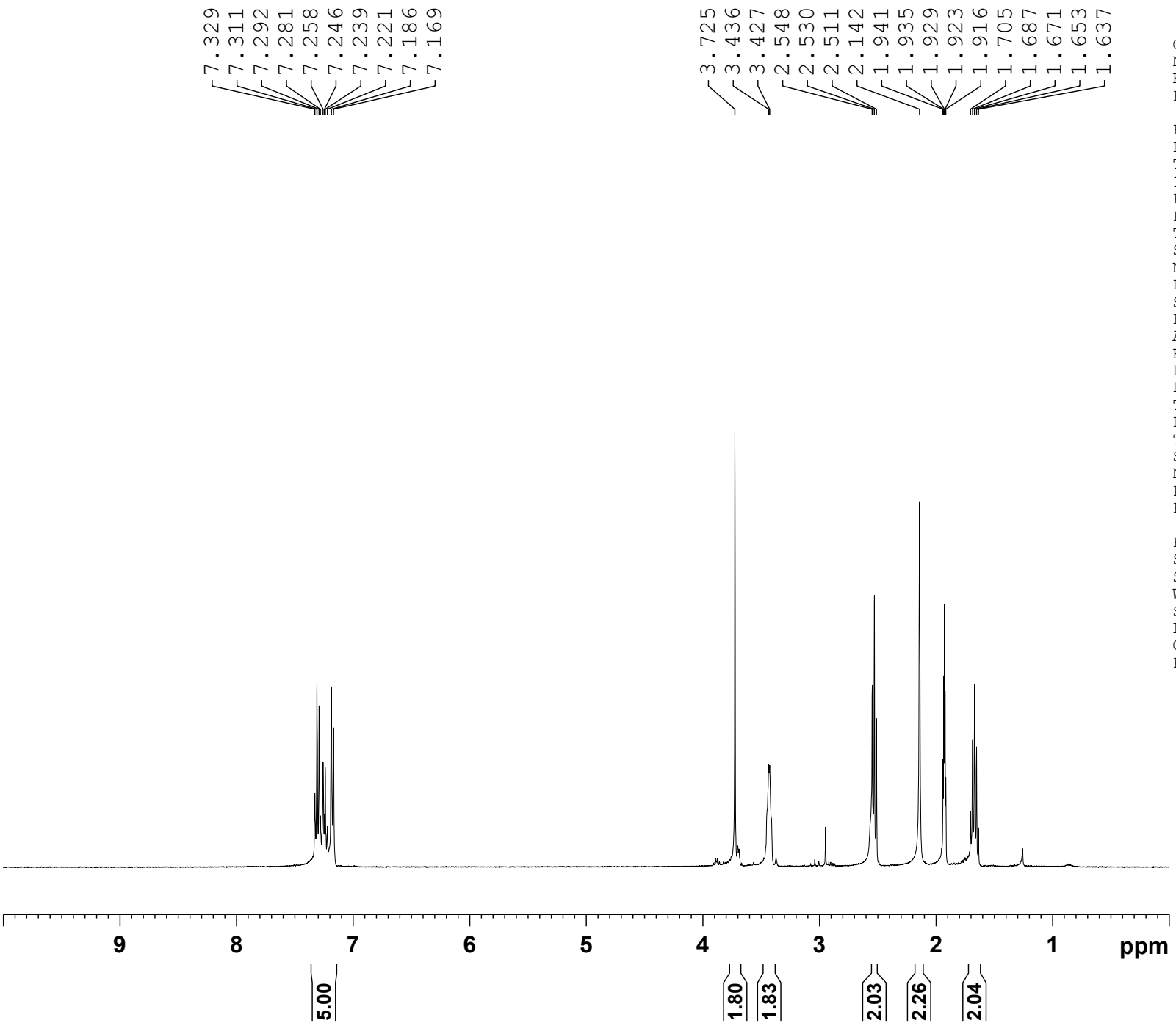
YYH-116

Sample Name **YYH-116**	Pulse sequence **NOESY**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-09-10**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



NOESY of compound **4r**

1H NMR (CD3CN, 400 MHz) of compound **4s**

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Current Data Parameters
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EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
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Time                   13.51 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CD3CN
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                   210.28
DW                    62.400 usec
DE                    16.43 usec
TE                    296.2 K
D1                2.00000000 sec
TD0                        1
SFO1            400.1324008 MHz
NUC1                      1H
P1                    14.50 usec
PLW1            12.80000019 W

F2 - Processing parameters
SI                     16384
SF              400.1300158 MHz
WDW                       EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
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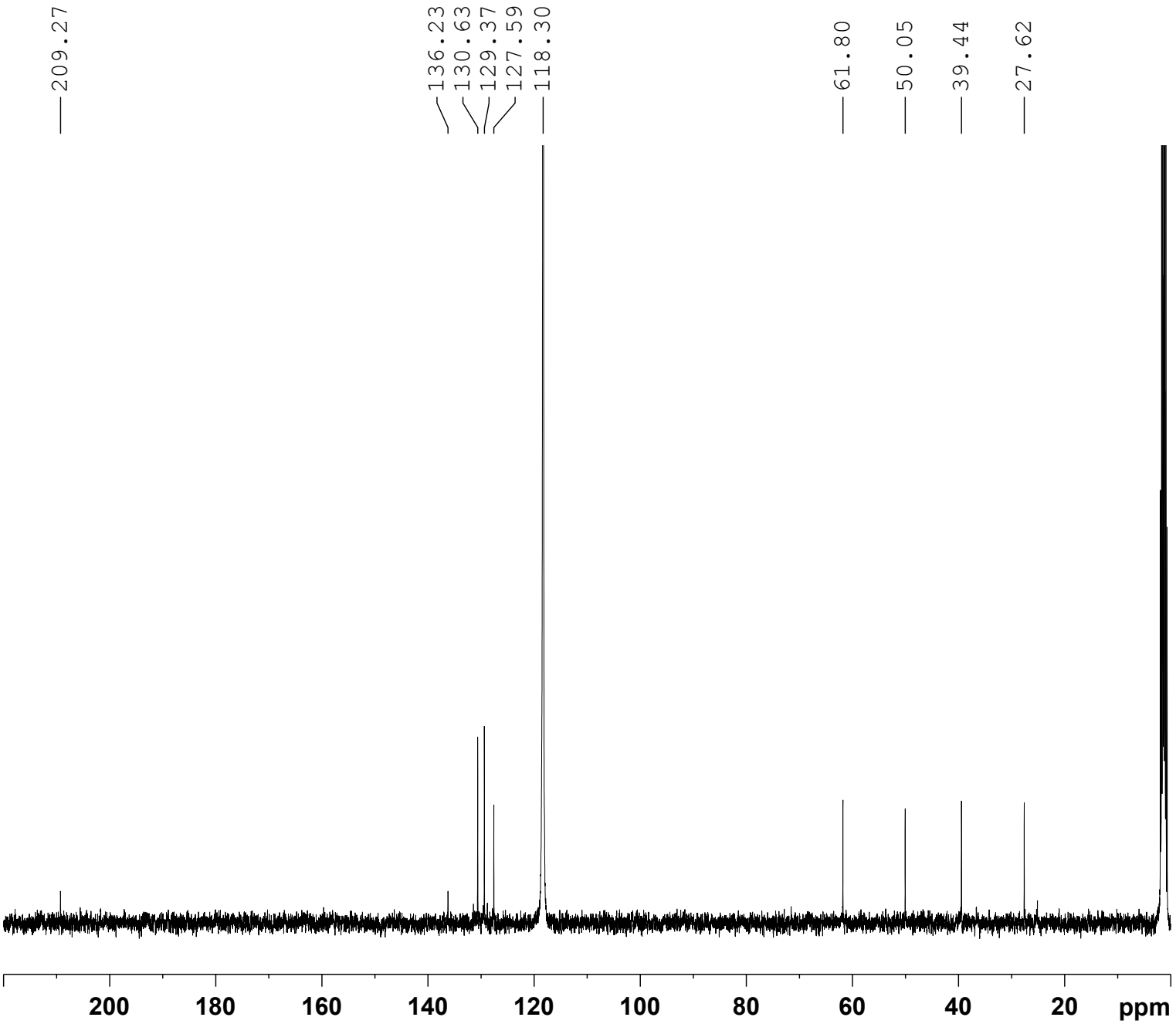


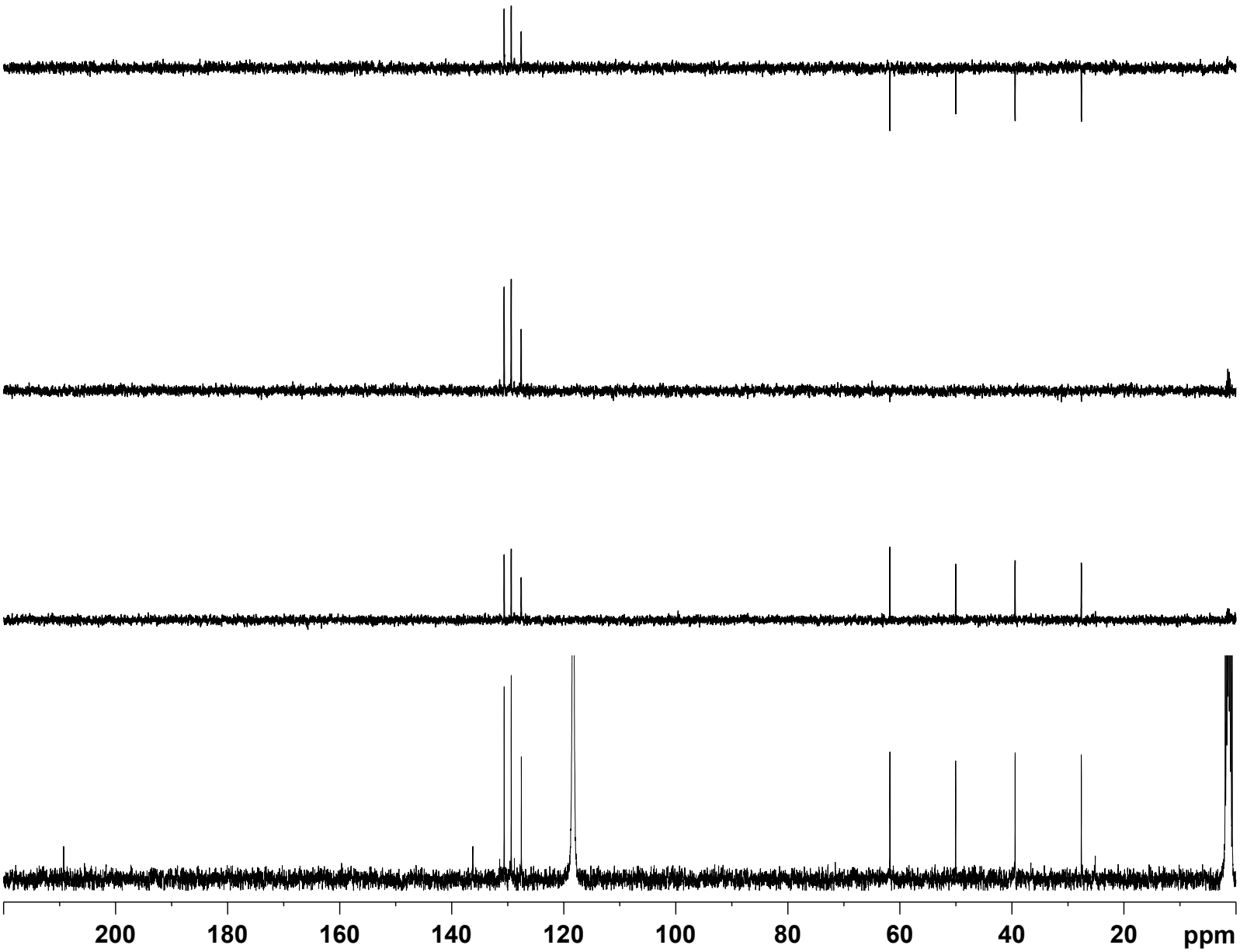
13C NMR (CD3CN, 100 MHz) of compound **4s**

```
Current Data Parameters
NAME                  YYH-122
EXPNO                       5
PROCNO                      1

F2 - Acquisition Parameters
Date_                20211117
Time                    14.11 h
INSTRUM                  spect
PROBHD   Z108618_0922 (
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CD3CN
NS                         400
DS                           0
SWH                  24038.461 Hz
FIDRES                1.467191 Hz
AQ                    0.6815744 sec
RG                       210.28
DW                       20.800 usec
DE                        6.50 usec
TE                       296.8 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1
SFO1               100.6233329 MHz
NUC1                        13C
P1                       10.50 usec
PLW1                44.50000000 W
SFO2               400.1316005 MHz
NUC2                        1H
CPDPRG[2 bi_waltz65_256
PCPD2                    90.00 usec
PLW2                14.00000000 W
PLW12                0.36340001 W
PLW13                0.18250000 W

F2 - Processing parameters
SI                       32768
SF                 100.6126697 MHz
WDW                         EM
SSB       0
LB                        2.00 Hz
GB        0
PC                        1.00
```

DEPT of compound **4s**

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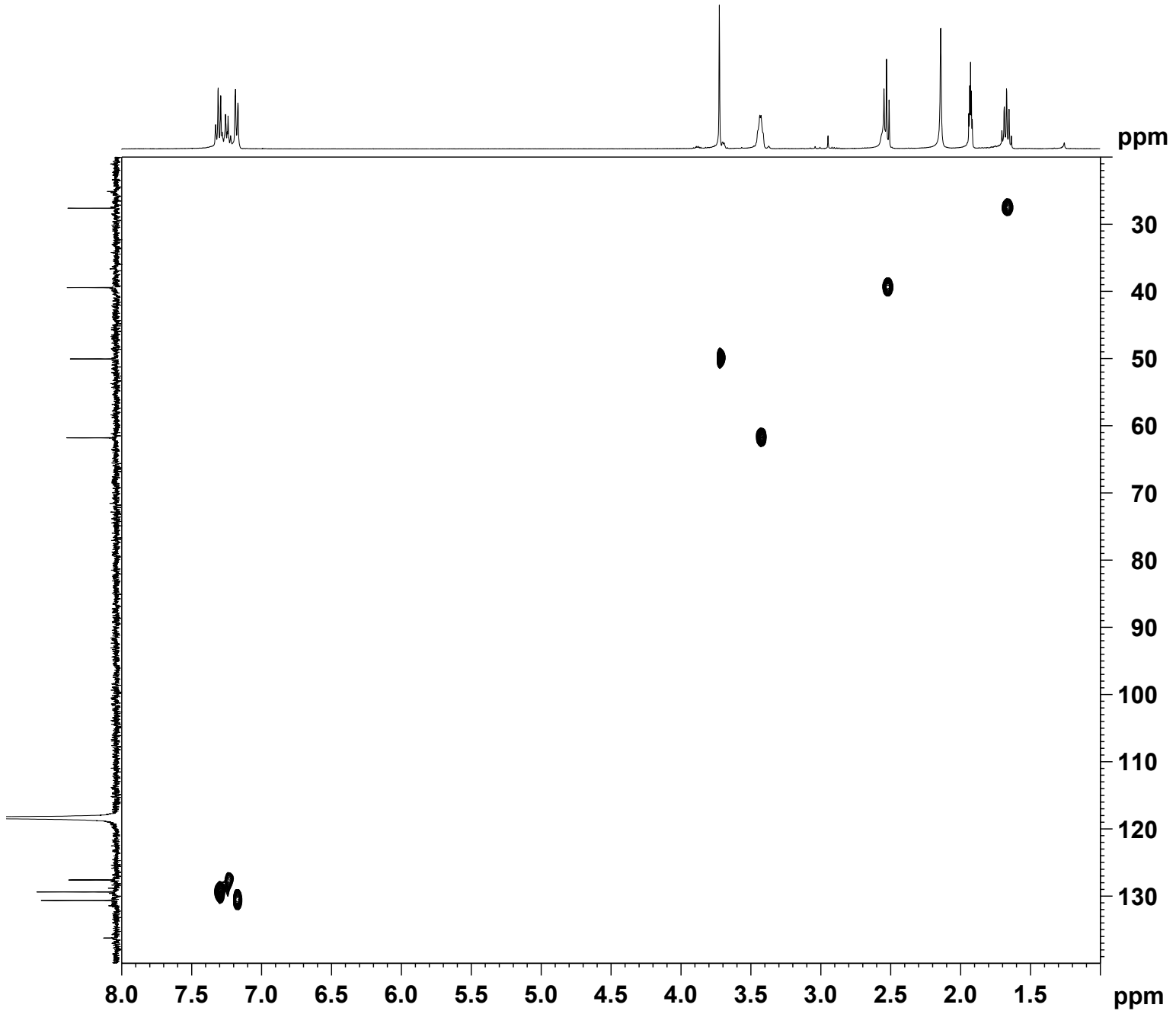
Current Data Parameters
NAME                 YYH-122
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_               20211117
Time                  14.11 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG              zgpg30
TD                    32768
SOLVENT               CD3CN
NS                      400
DS                        0
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                0.6815744 sec
RG                   210.28
DW                   20.800 usec
DE                    6.50 usec
TE                   296.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1
SFO1           100.6233329 MHz
NUC1                    13C
P1                   10.50 usec
PLW1           44.50000000 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2           14.00000000 W
PLW12           0.36340001 W
PLW13           0.18250000 W

F2 - Processing parameters
SI                    32768
SF             100.6126697 MHz
WDW                      EM
SSB       0
LB                    2.00 Hz
GB        0
PC                    1.00
```

HSQC of compound **4s**

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Current Data Parameters
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EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
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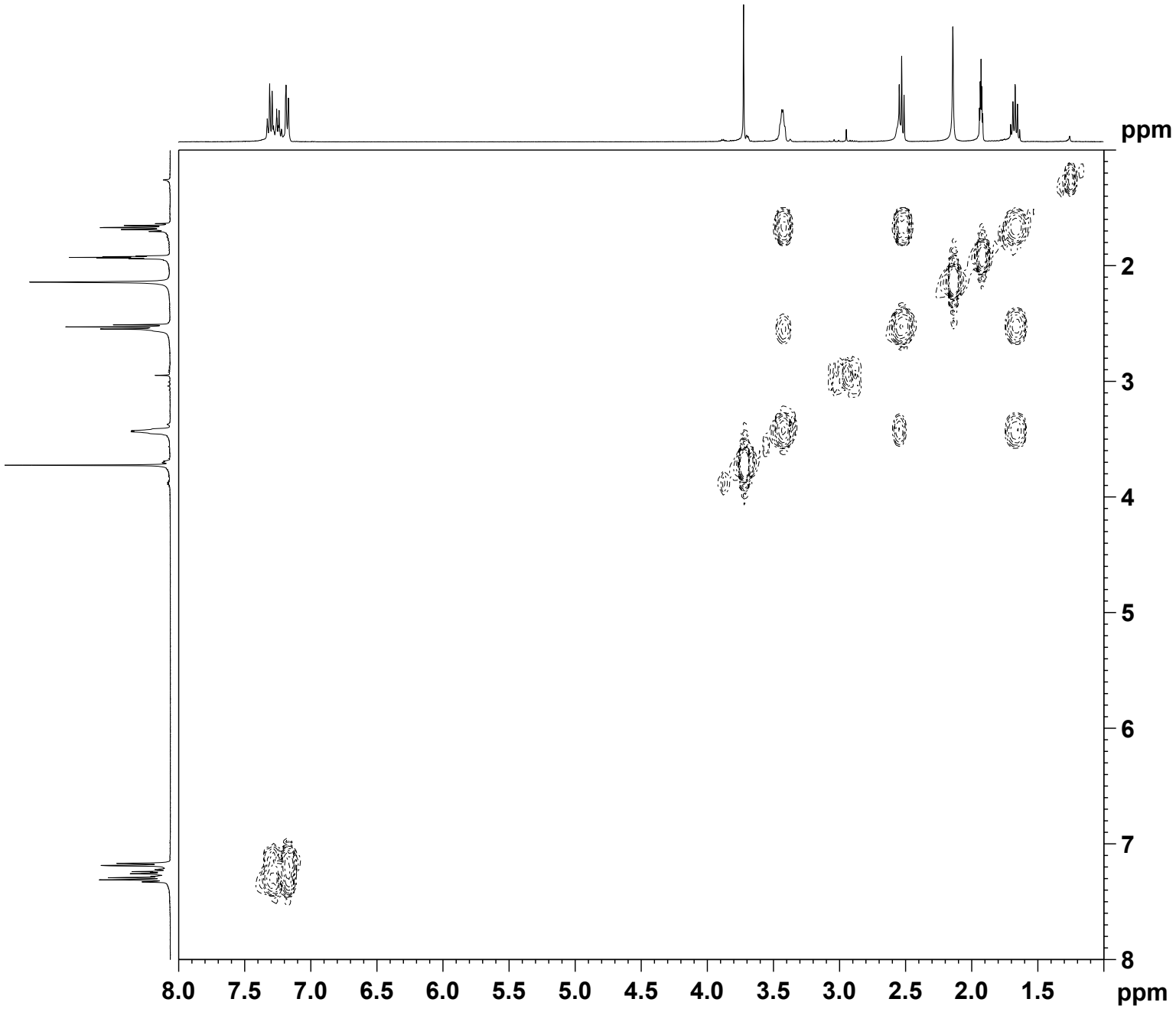
Time               22.58 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG  hsqcetgpsisp2.2
TD                  2048
SOLVENT            CD3CN
NS                     8
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ              0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                296.5 K
CNST2        145.0000000
CNST17        -0.5000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00002080 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
P2                 29.00 usec
P28              1000.00 usec
PLW1         12.80000019 W
SFO2         100.6233329 MHz
NUC2                 13C
CPDPRG[2             garp
P3                 10.50 usec
P14               500.00 usec
P24              2000.00 usec
PCPD2              80.00 usec
PLW0      0 W
PLW2         44.00000000 W
PLW12         0.75796998 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3             0.500
SPOFFS3   0 Hz
SPW3           7.41179991 W
SPNAM[7]     Crp60comp.4
SPOAL7             0.500
SPOFFS7   0 Hz
SPW7           7.41179991 W
GPNAM[1]       SMSQ10.100
GPZ1                80.00 %
GPNAM[2]       SMSQ10.100
GPZ2                20.10 %
GPNAM[3]       SMSQ10.100
GPZ3                11.00 %
GPNAM[4]       SMSQ10.100
GPZ4                -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6233 MHz
FIDRES       187.800476 Hz
SW              238.896 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300158 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6126697 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

COSY of compound **4s**

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EXPNO                 10
PROCNO                 1

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INSTRUM             spect
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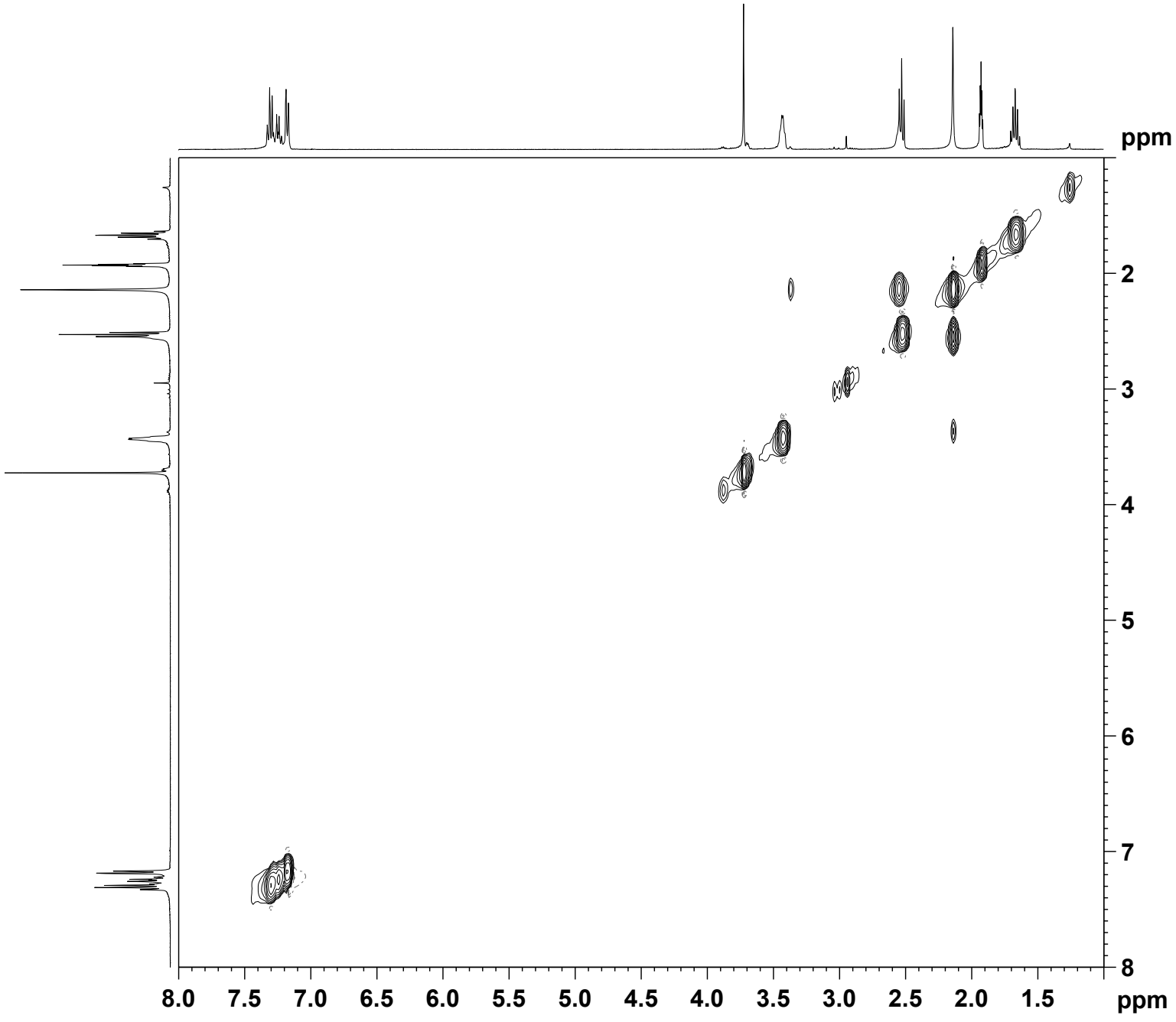
PULPROG       cosygpppqf
TD                  2048
SOLVENT            CD3CN
NS                     8
DS                    16
SWH             8012.820 Hz
FIDRES          7.825020 Hz
AQ             0.1277952 sec
RG                210.28
DW                62.400 usec
DE                 6.50 usec
TE                297.0 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012480 sec
TDav                   1
SFO1         400.1324008 MHz
NUC1                  1H
P0                14.50 usec
P1                14.50 usec
P17             2500.00 usec
PLW1         12.80000019 W
PLW10         2.99020004 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1324 MHz
FIDRES         62.600159 Hz
SW                20.025 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF           400.1300158 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF           400.1300158 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

NOESY of compound **4s**




```
Current Data Parameters
NAME                  YYH-122
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_               20211119
Time                    1.11 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG       noesygpphpp
TD                       2048
SOLVENT                CD3CN
NS                          8
DS                         16
SWH                 8012.820 Hz
FIDRES              7.825020 Hz
AQ                  0.1277952 sec
RG                     210.28
DW                     62.400 usec
DE                      6.50 usec
TE                     296.5 K
D0                  0.00004394 sec
D1                  2.00000000 sec
D8                  0.40000001 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D16                 0.00020000 sec
IN0                 0.00012480 sec
TDav                        1
SFO1              400.1324008 MHz
NUC1                       1H
P1                     14.50 usec
P2                     29.00 usec
P17                  2500.00 usec
PLW1              12.80000019 W
PLW10              2.99020004 W
GPNAM[1]          SMSQ10.100
GPZ1                   40.00 %
P16                  1000.00 usec

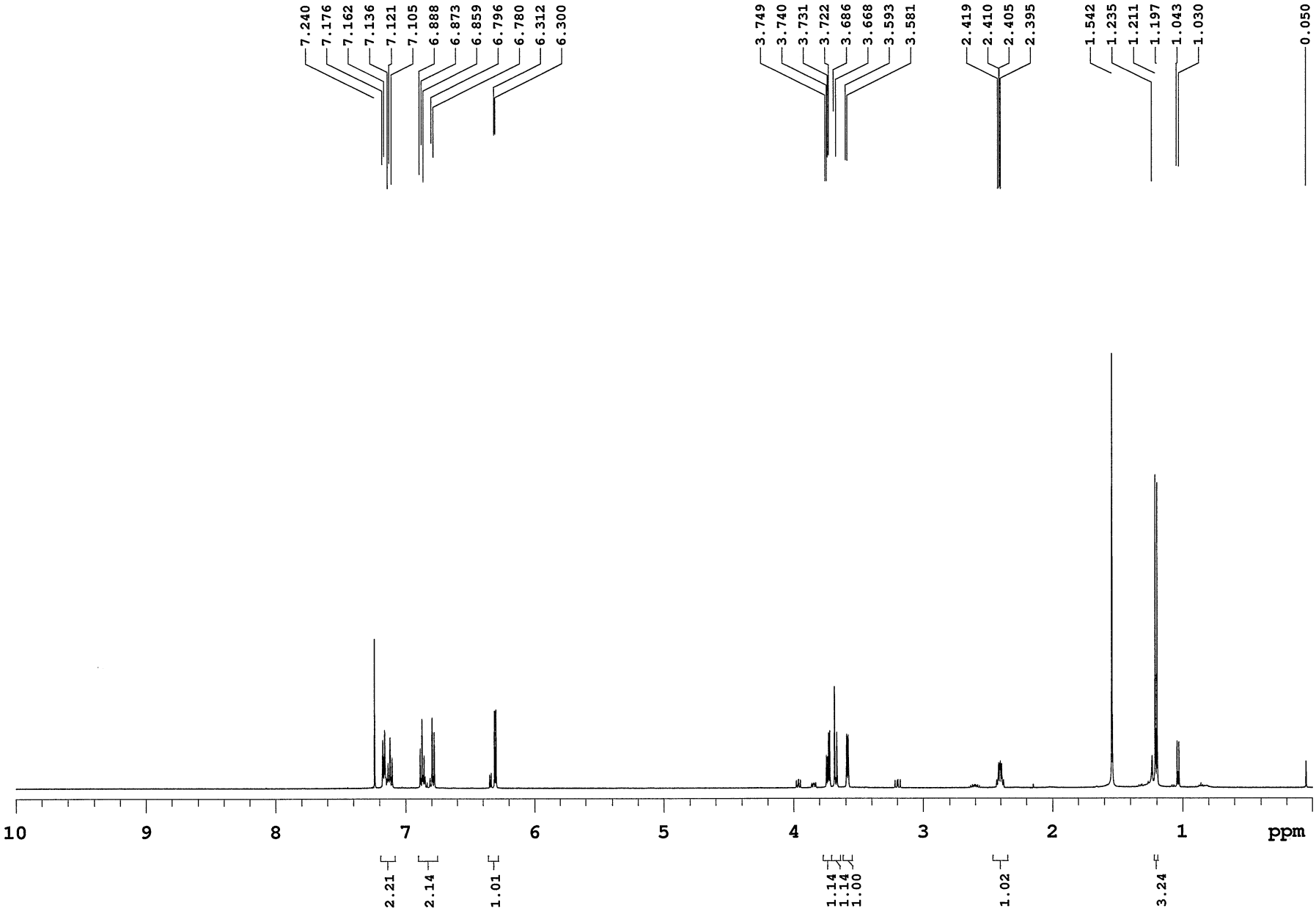
F1 - Acquisition parameters
TD                          256
SFO1                400.1324 MHz
FIDRES              62.600159 Hz
SW                     20.025 ppm
FnMODE           States-TPPI

F2 - Processing parameters
SI                         1024
SF                400.1300158 MHz
WDW                      QSINE
SSB                         2
LB             0 Hz
GB             0
PC                        1.40

F1 - Processing parameters
SI                         1024
MC2              States-TPPI
SF                400.1300158 MHz
WDW                      QSINE
SSB                         2
LB             0 Hz
GB             0
```

YYH-106

Sample Name **YYH-106**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-03**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



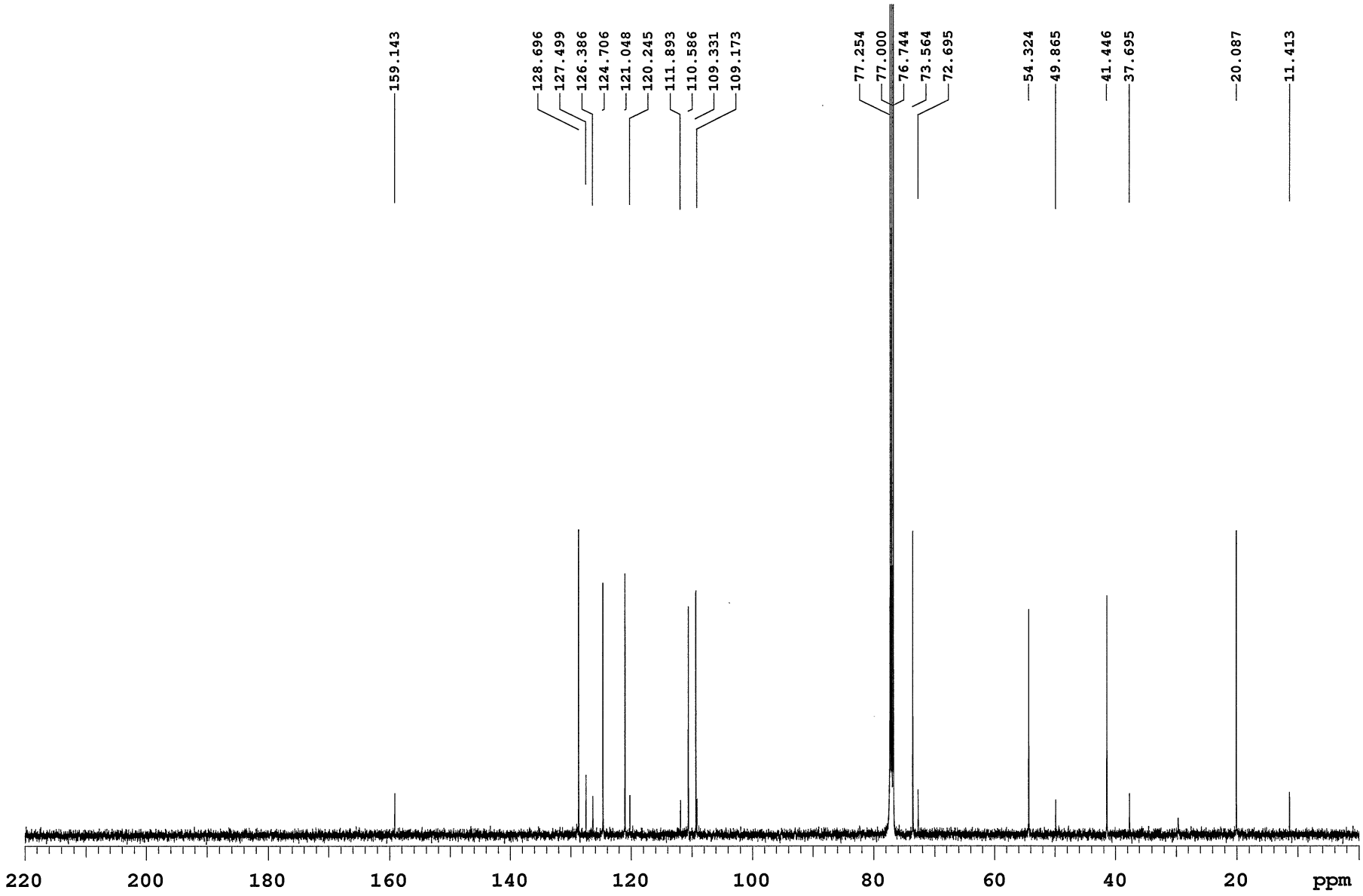
Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-106/PROTON_03

1H NMR (CDCl3, 500 MHz) of compound **4t,** with dr

Plot date 2021-08-04

YYH-106

Sample Name **YYH-106** | Pulse sequence **CARBON** | Temperature **25** | Study owner **vnmr2**
Date collected **2021-08-03** | Solvent **cdcl3** | Spectrometer **Agilent-NMR-inova500** | Operator **vnmr2**



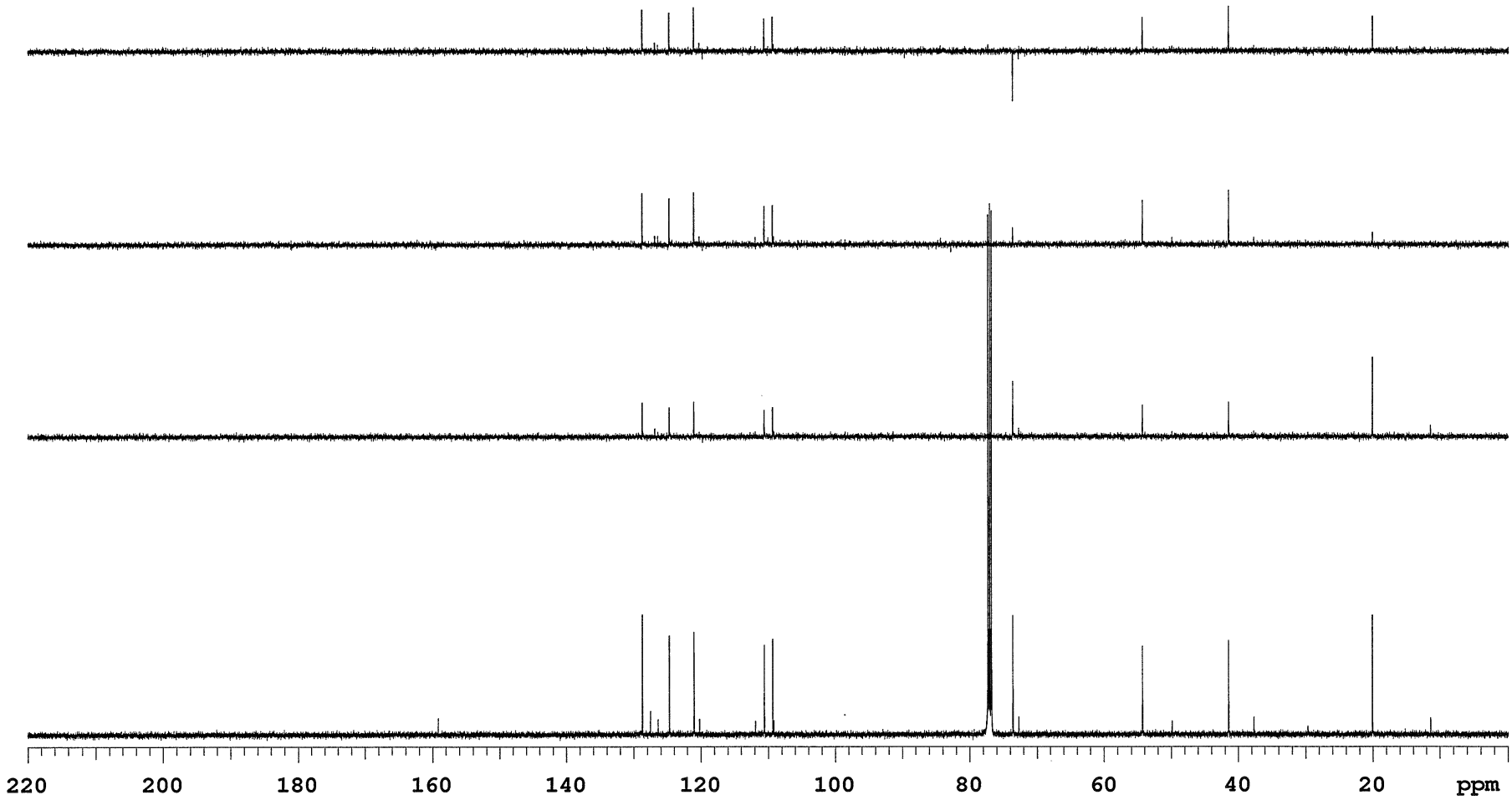
13C NMR (CDCl3, 125 MHz) of compound **4t**, with dr

Data file /home/vnmr2/vnmrsys/data/511/YYH/YYH-106/CARBON_02

Plot date 2021-08-17

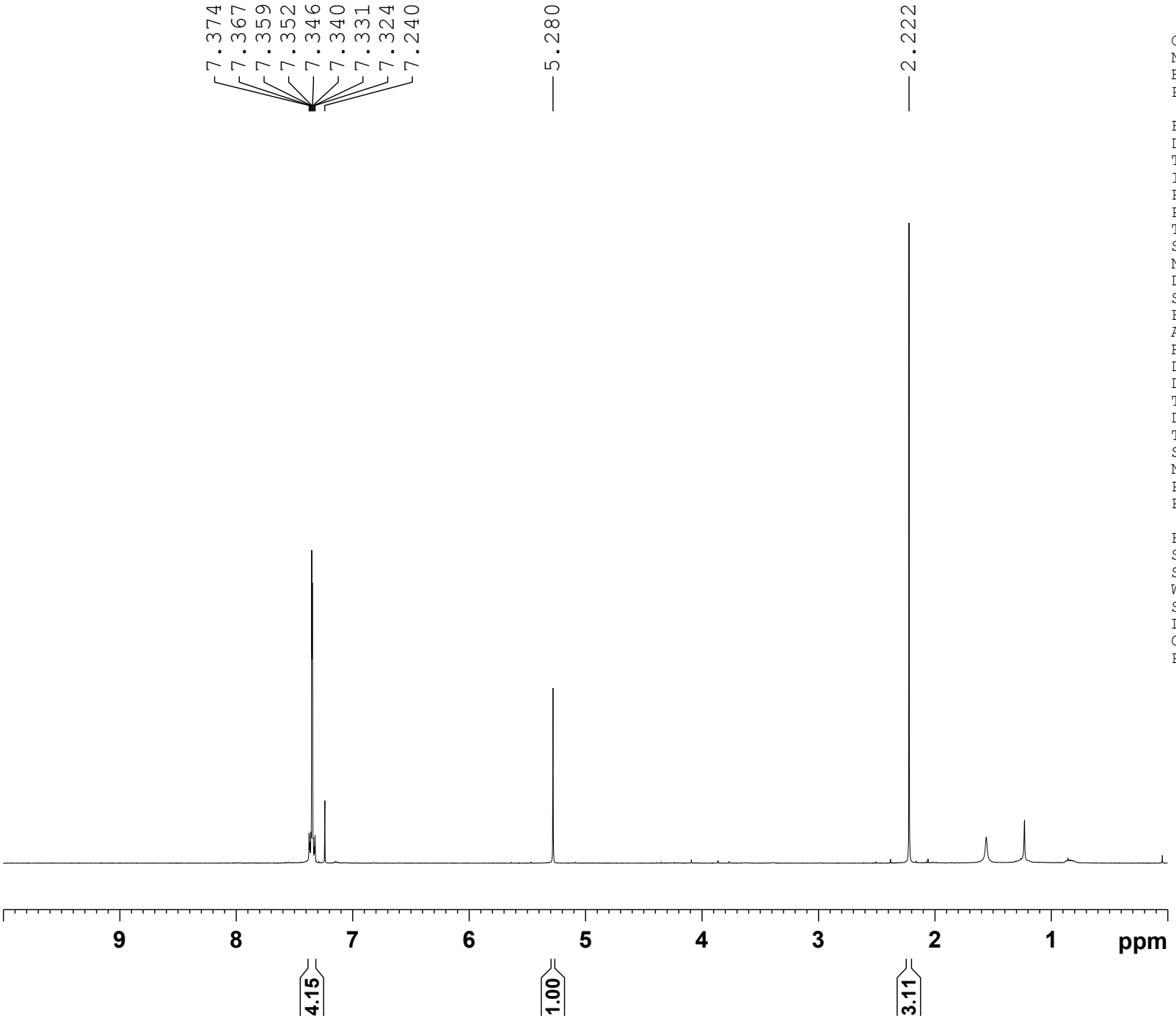
YYH-106

Sample Name **YYH-106**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2021-08-03**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



DEPT of compound **4t,** with dr

1H NMR (CDCl3, 400 MHz) of compound **5a**

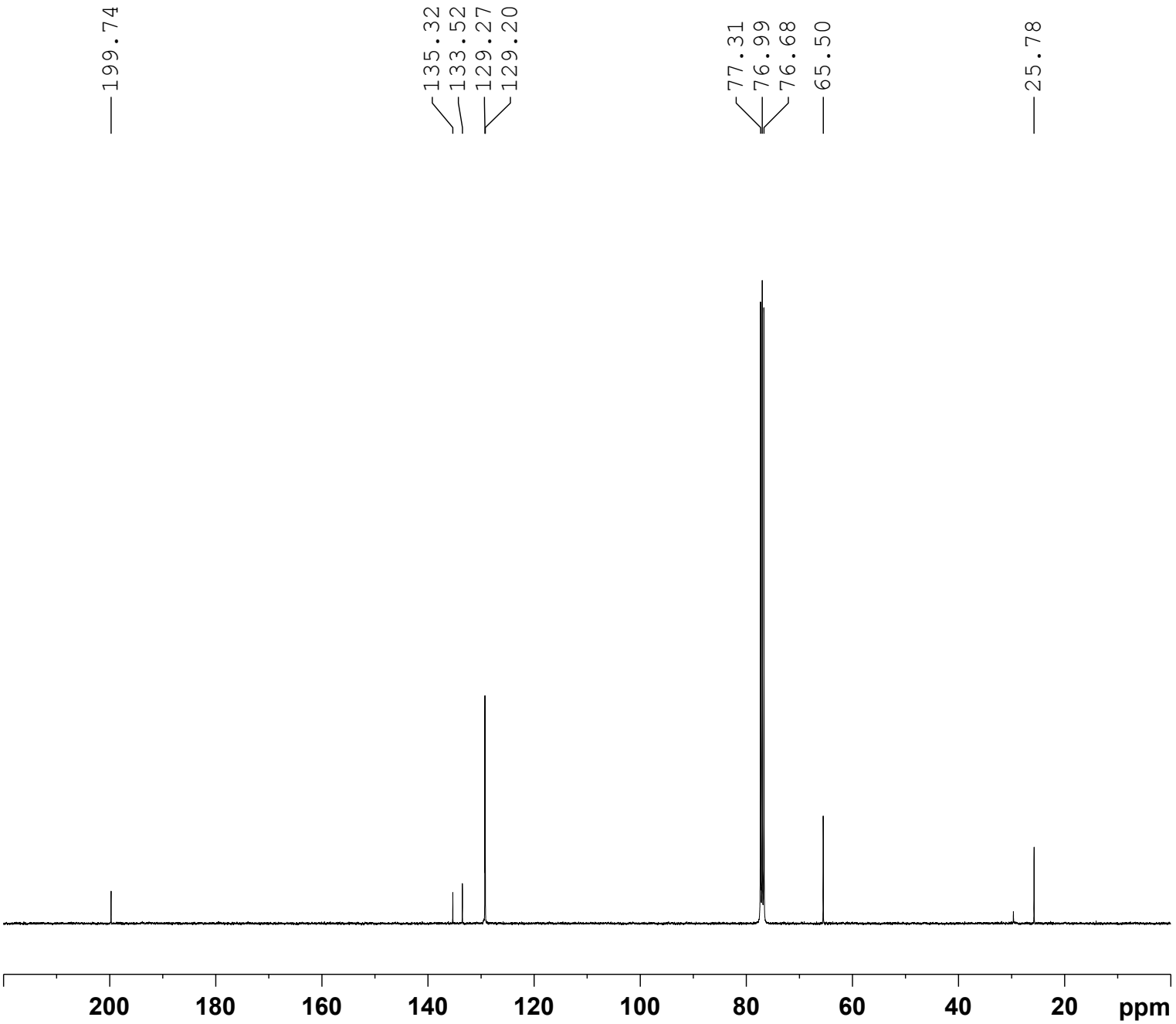



```
Current Data Parameters
NAME        YYH-3-464-f1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211028
Time              21.58 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                210.28
DW                62.400 usec
DE                16.43 usec
TE                296.2 K
D1           2.00000000 sec
TD0                    1
SFO1         400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
PLW1         13.10000038 W

F2 - Processing parameters
SI                 16384
SF          400.1300174 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

13C NMR (CDCl3, 100 MHz) of compound **5a**

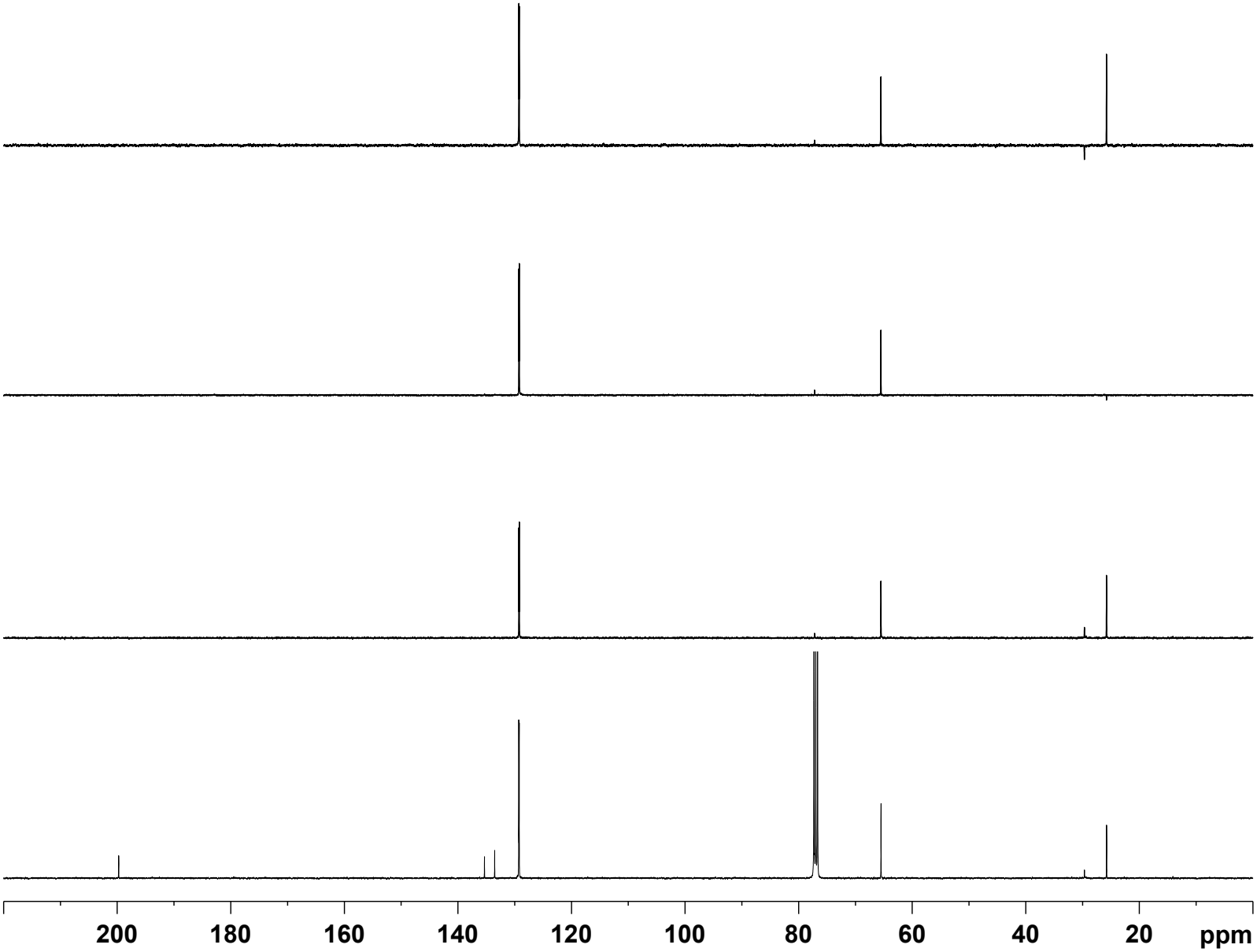



```
Current Data Parameters
NAME       YYH-3-464-f1
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20211029
Time               2.34 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                 6000
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               297.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1               10.50 usec
PLW1        44.29999924 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2        14.60000038 W
PLW12        0.37897000 W
PLW13        0.19032000 W

F2 - Processing parameters
SI                32768
SF          100.6127713 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

DEPT of compound **5a**

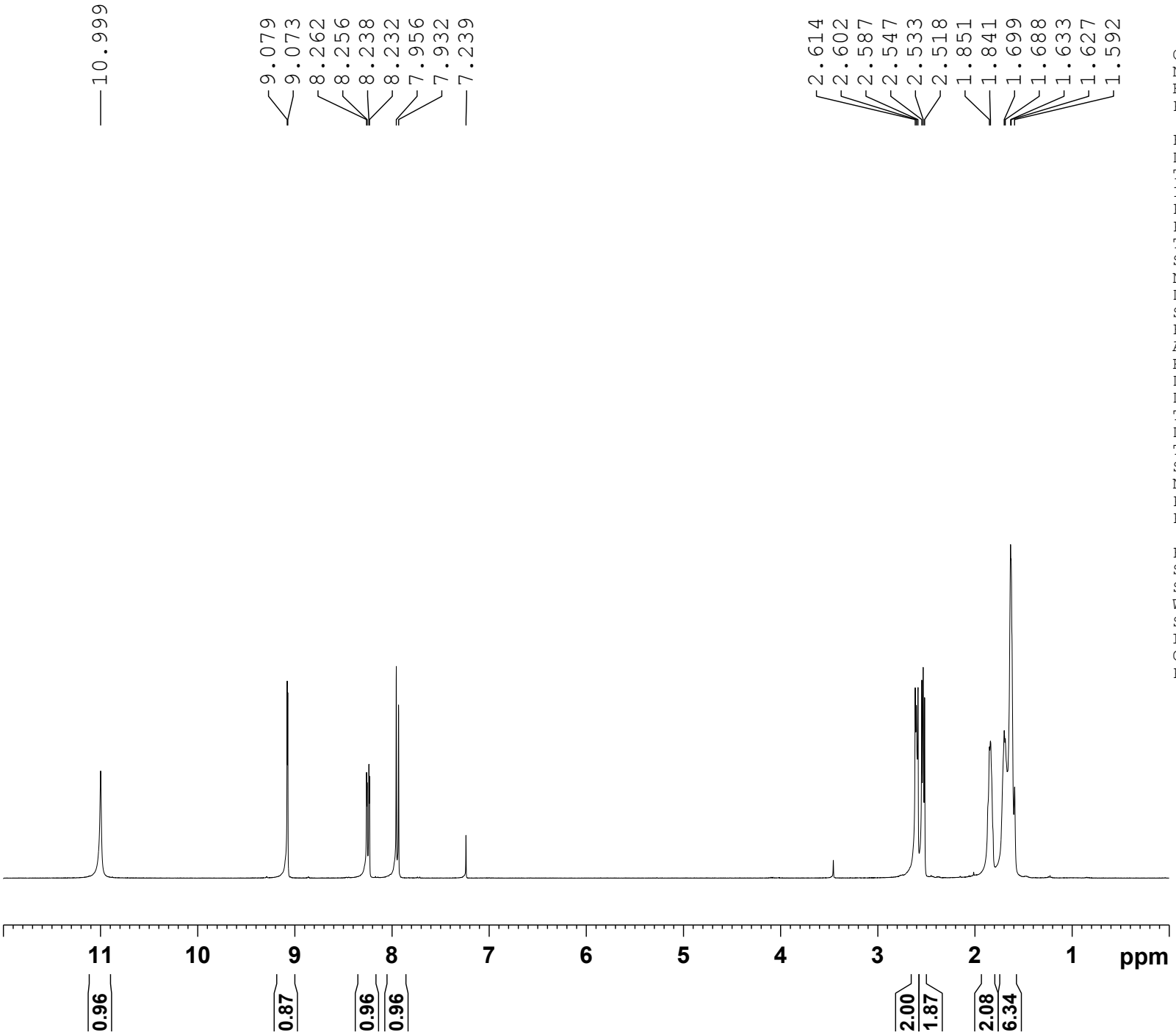



```
Current Data Parameters
NAME       YYH-3-464-f1
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20211029
Time              2.34 h
INSTRUM           spect
PROBHD   Z108618_0922 (
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 6000
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               297.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1               10.50 usec
PLW1         44.29999924 W
SFO2         400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2            90.00 usec
PLW2         14.60000038 W
PLW12         0.37897000 W
PLW13         0.19032000 W

F2 - Processing parameters
SI                32768
SF          100.6127713 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

1H NMR (CDCl3, 400 MHz) of compound **6h**

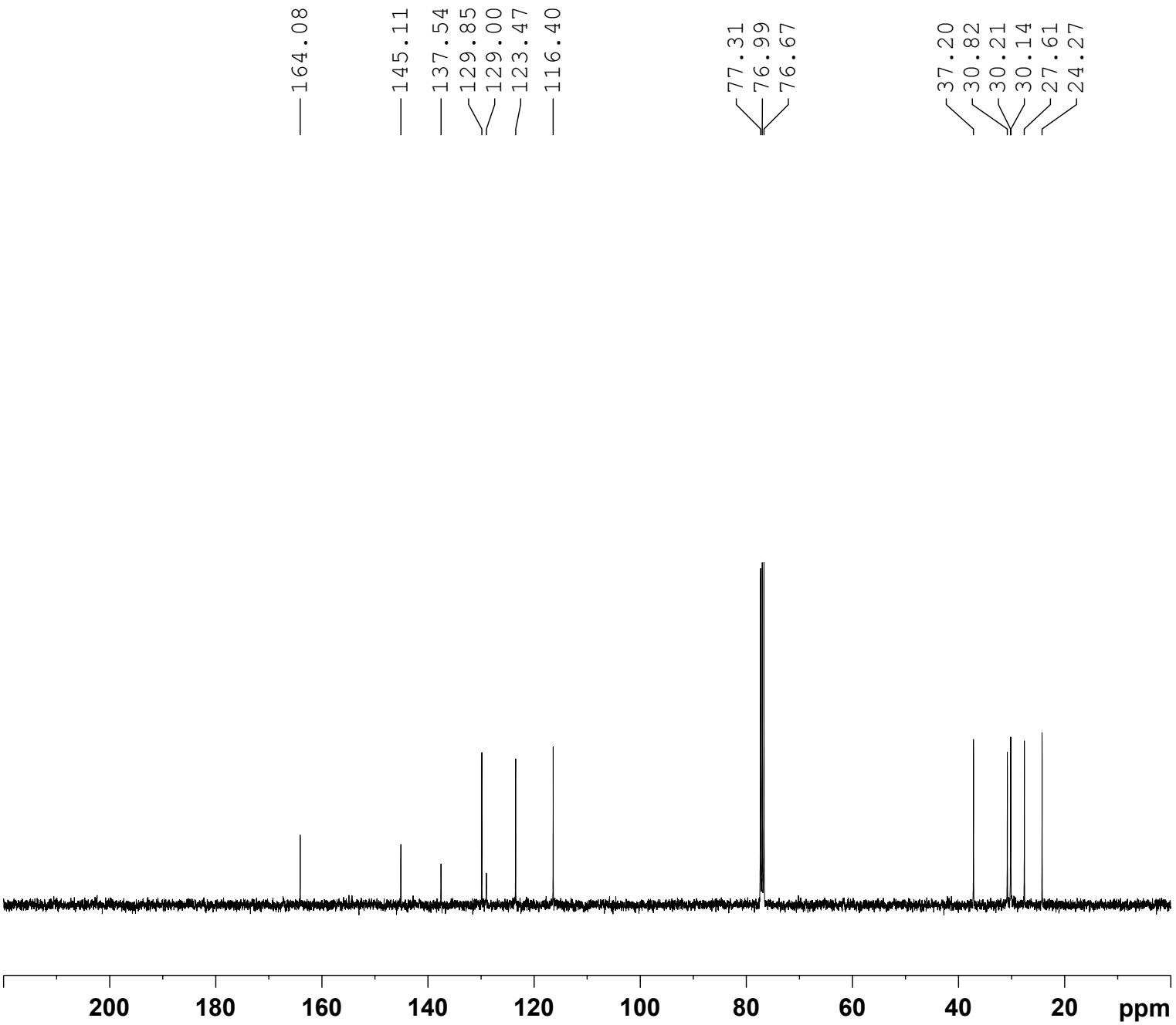



```
Current Data Parameters
NAME                  YYH-114
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210910
Time                   13.32 h
INSTRUM                spect
PROBHD    Z108618_0922 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                2.0447233 sec
RG                    103.85
DW                    62.400 usec
DE                    16.43 usec
TE                    298.5 K
D1                2.00000000 sec
TD0                         1
SFO1            400.1324008 MHz
NUC1                       1H
P1                    14.50 usec
PLW1            13.10000038 W

F2 - Processing parameters
SI                      16384
SF              400.1300174 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

13C NMR (CDCl3, 100 MHz) of compound **6h**

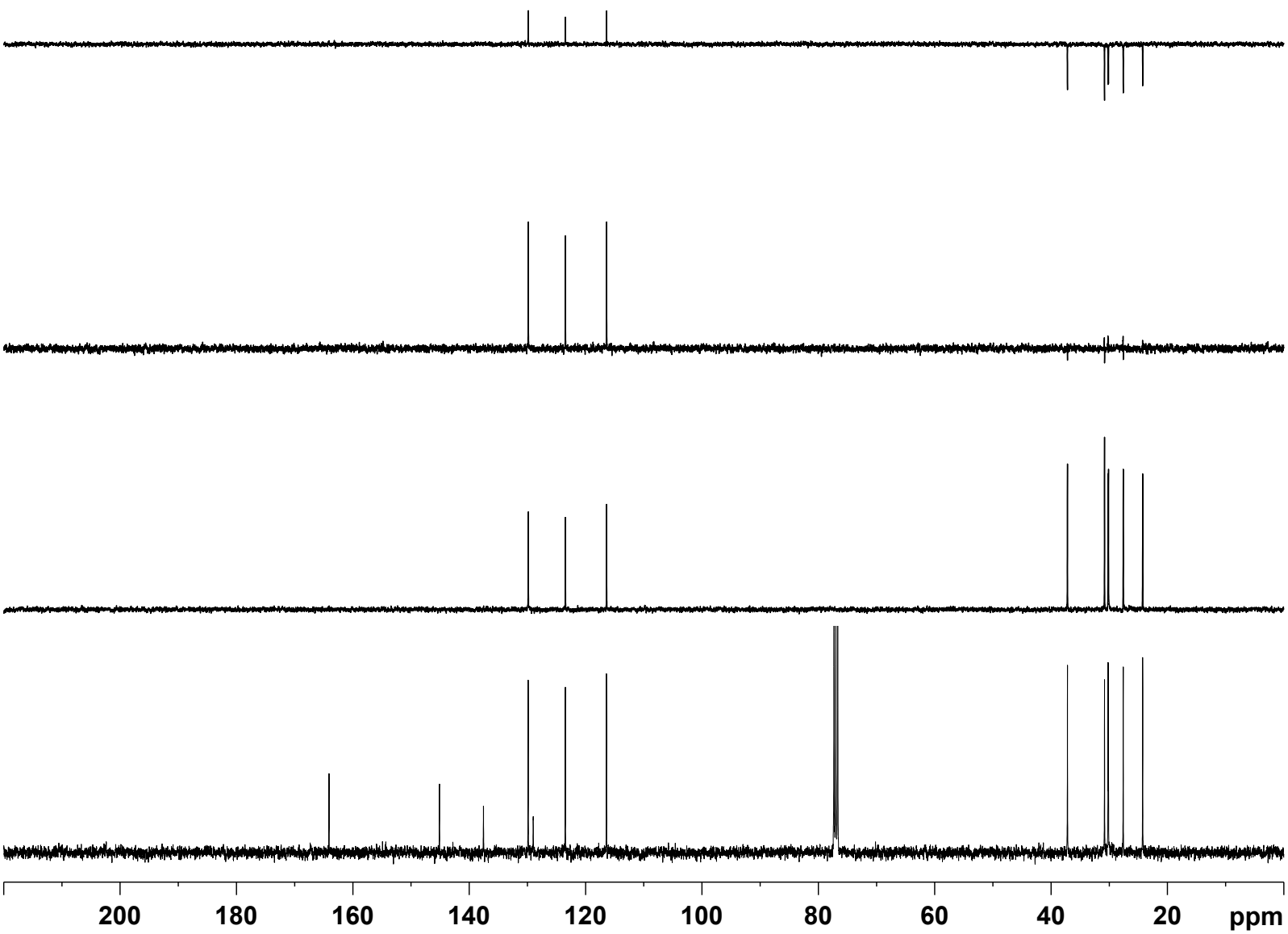



```
Current Data Parameters
NAME                  YYH-114
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210910
Time                   13.39 h
INSTRUM                spect
PROBHD   Z108618_0922 (
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      135
DS                        0
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                  0.6815744 sec
RG                     210.28
DW                     20.800 usec
DE                      6.50 usec
TE                     299.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1             100.6233329 MHz
NUC1                     13C
P1                     10.50 usec
PLW1              44.29999924 W
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2              14.60000038 W
PLW12              0.37897000 W
PLW13              0.19032000 W

F2 - Processing parameters
SI                    32768
SF               100.6127742 MHz
WDW                      EM
SSB       0
LB                      2.00 Hz
GB        0
PC                      1.00
```

DEPT of compound **6h**




```
Current Data Parameters
NAME             YYH-114
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210910
Time              13.39 h
INSTRUM            spect
PROBHD   Z108618_0922 (
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  135
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               299.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1               10.50 usec
PLW1         44.29999924 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2            90.00 usec
PLW2         14.60000038 W
PLW12         0.37897000 W
PLW13         0.19032000 W

F2 - Processing parameters
SI                32768
SF           100.6127742 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```