

Supporting information

Acetylcholinesterase Inhibitory Meroterpenoids from a Mangrove Endophytic Fungus *Aspergillus* sp. 16-5c

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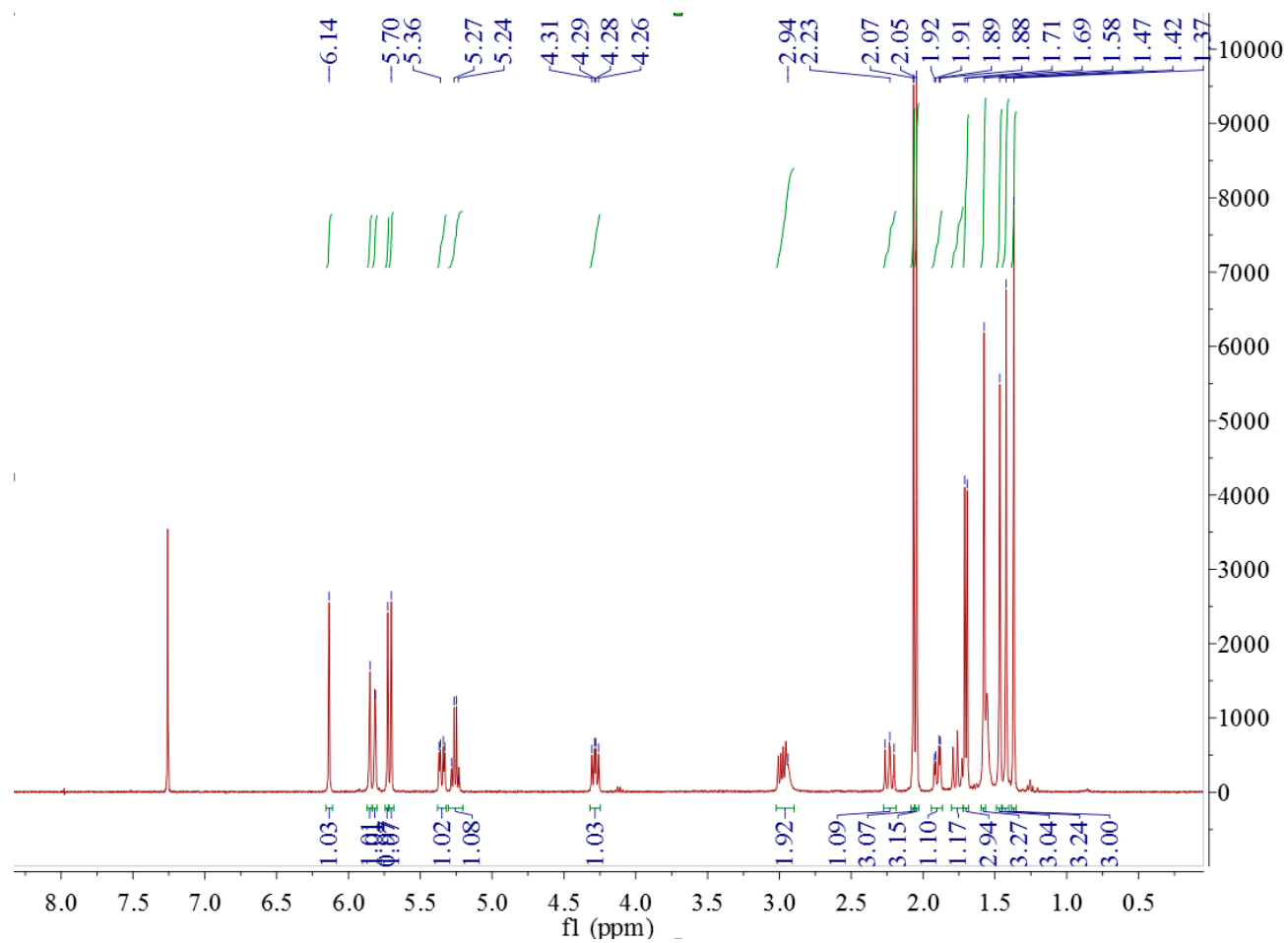
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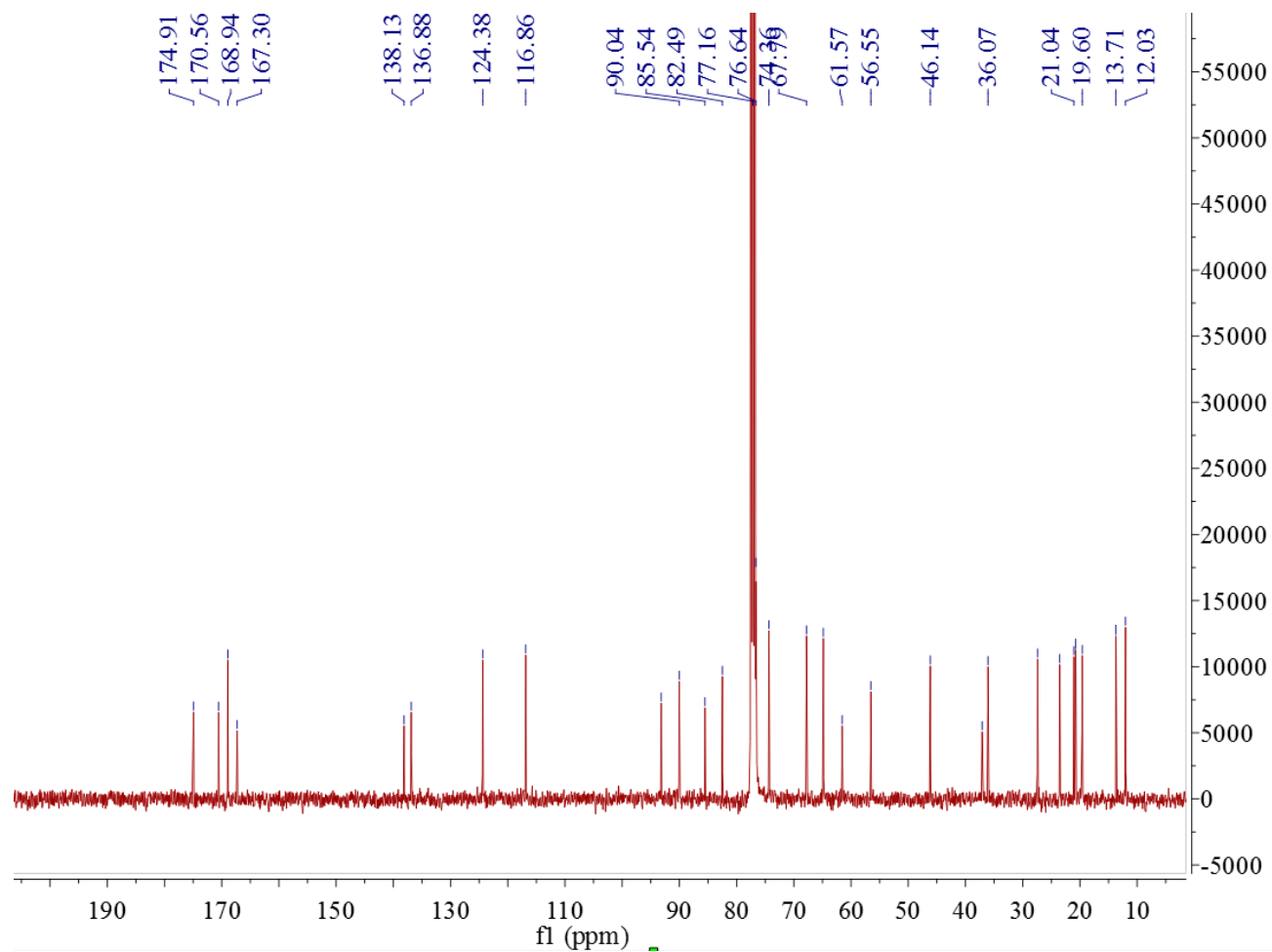
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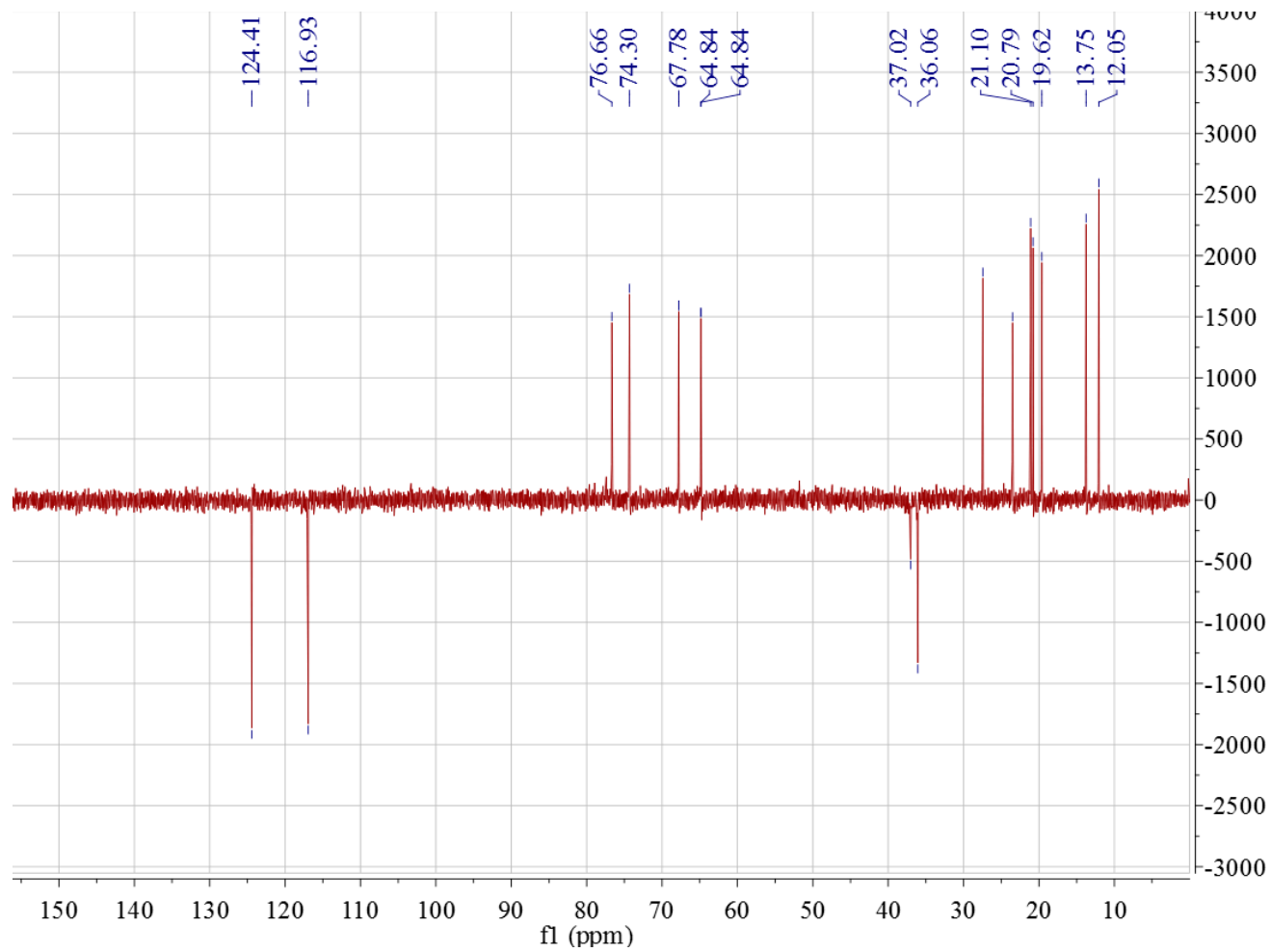
The $^1\text{H-NMR}$ (400 MHz) spectrum of Compound 1 in CDCl_3



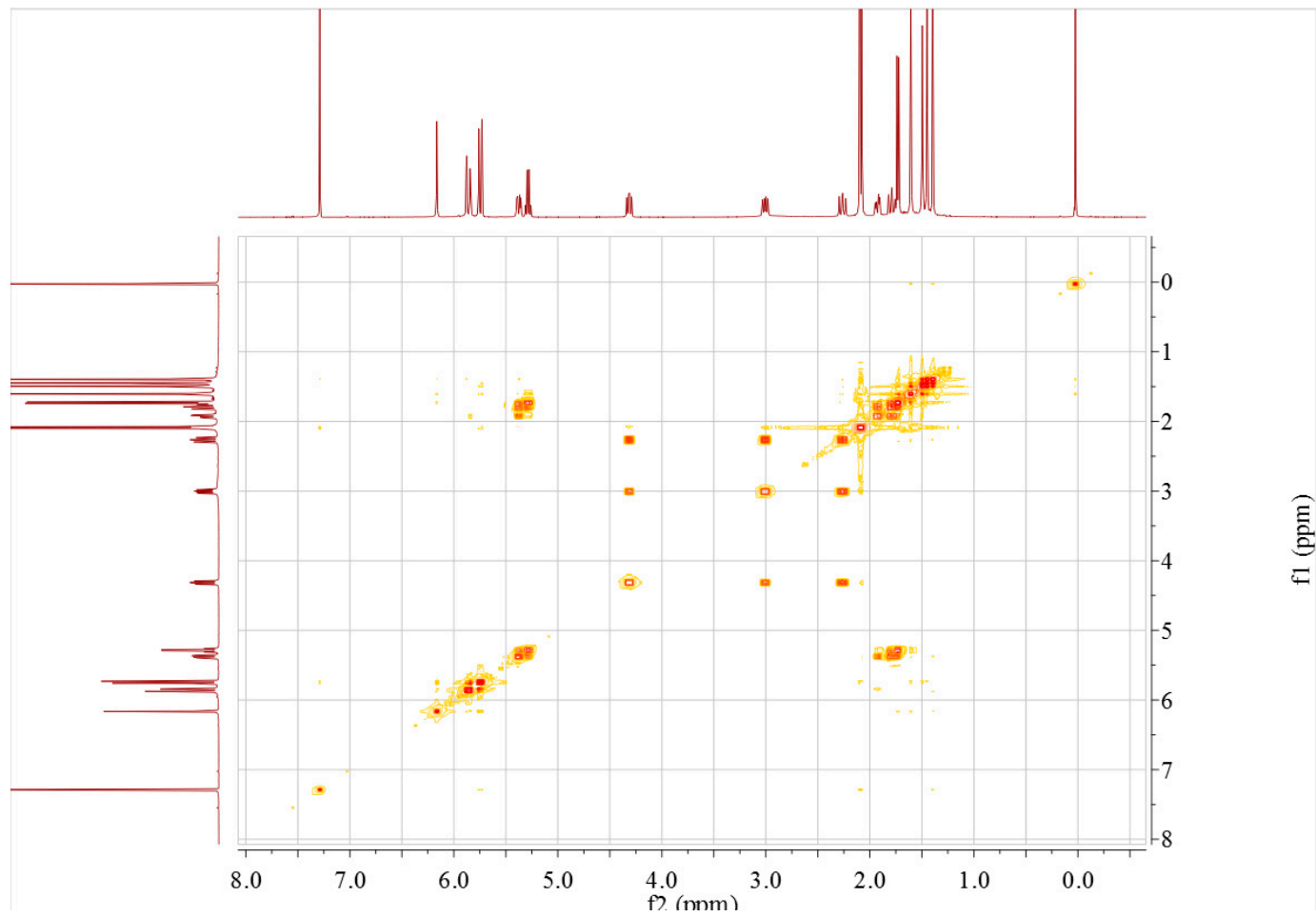
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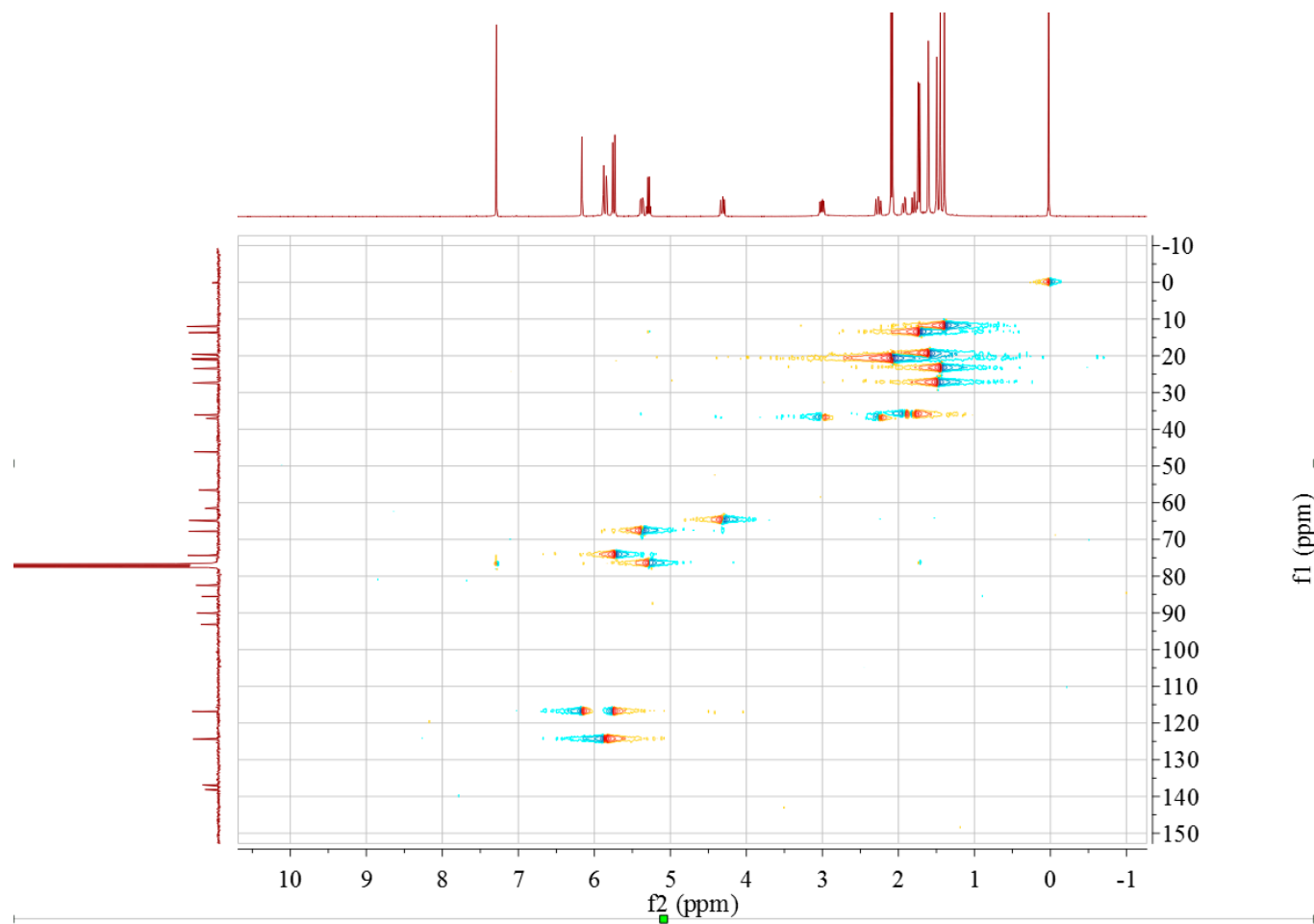
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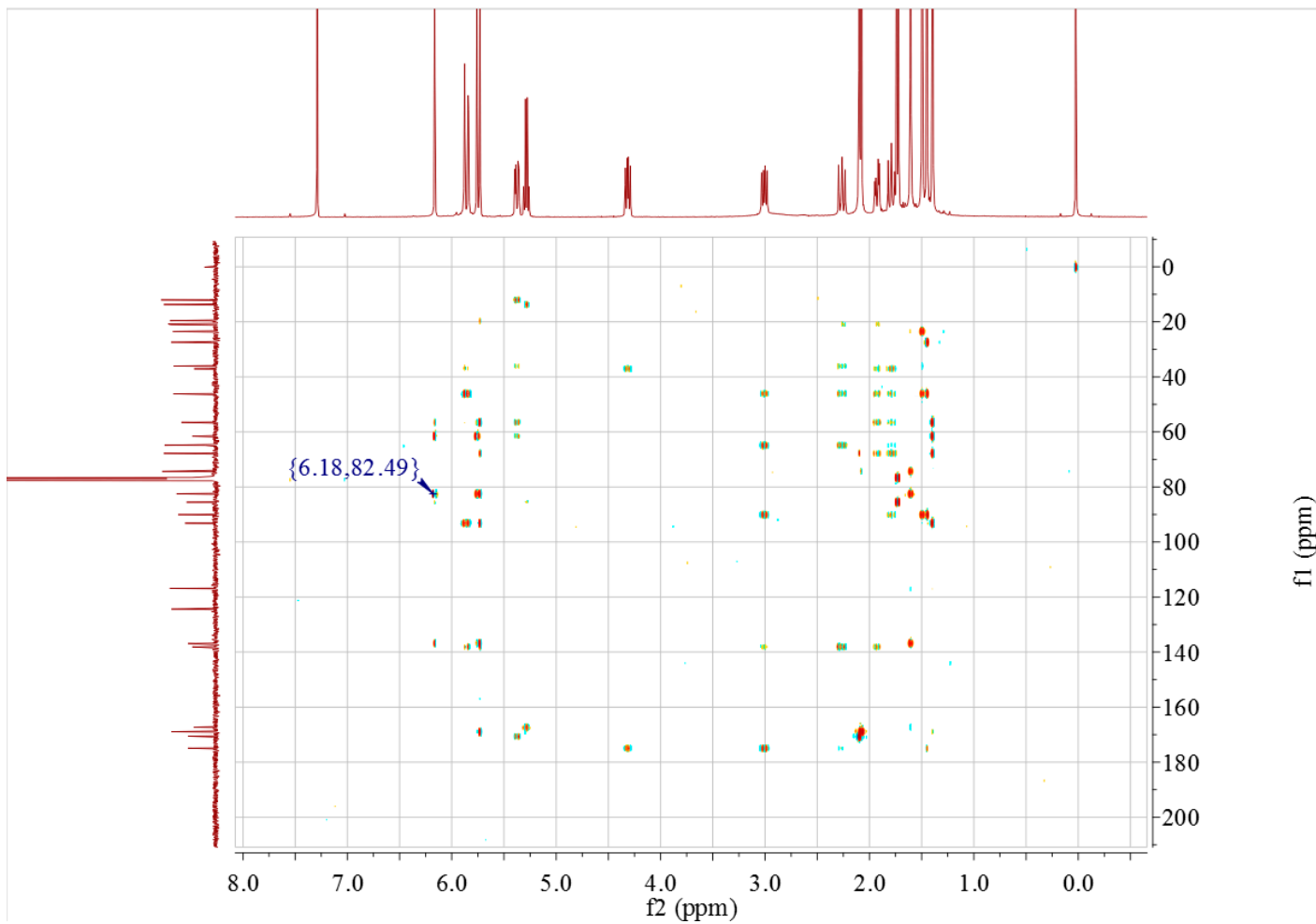
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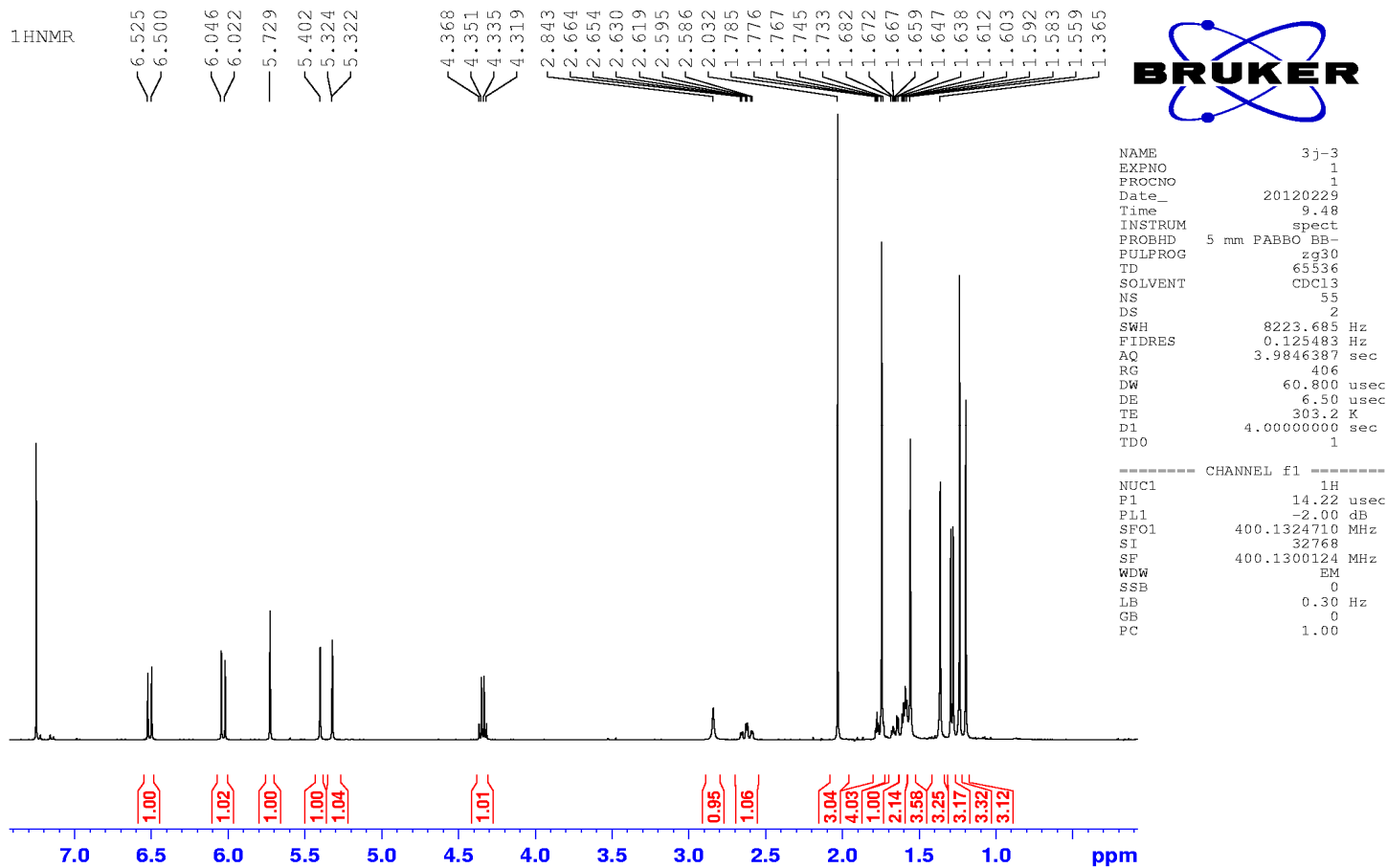
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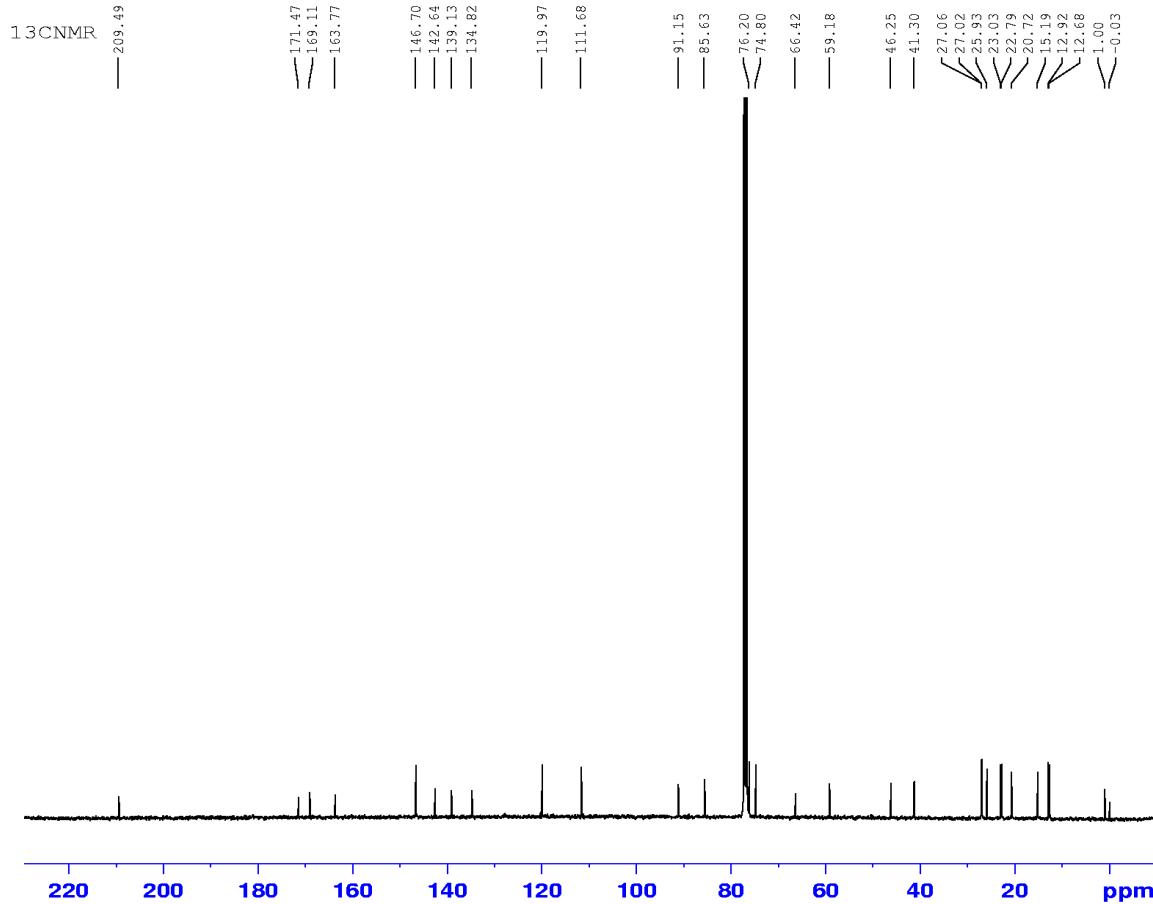
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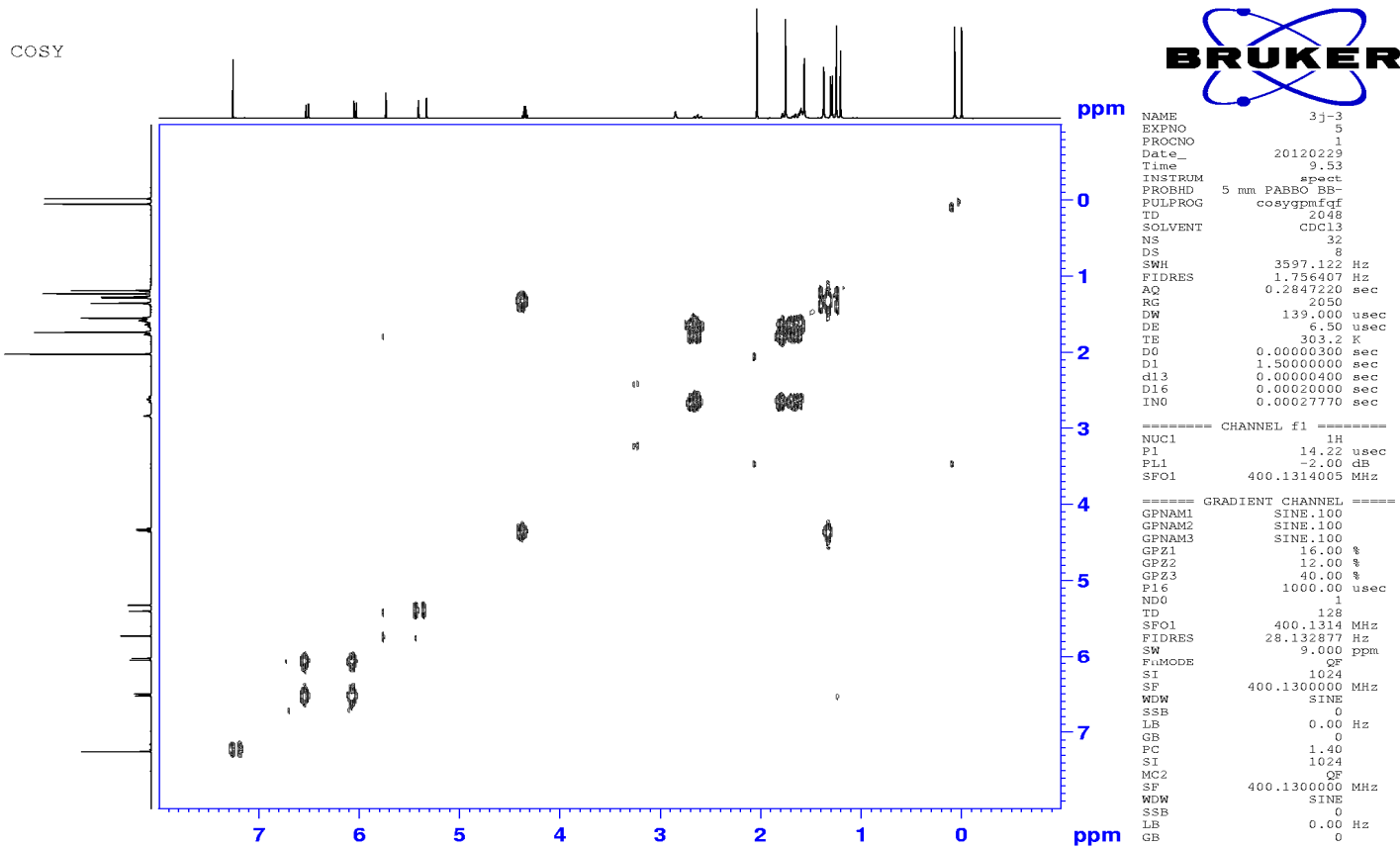
The $^1\text{H-NMR}$ (400 MHz) spectrum of Compound 2 in CDCl_3



The ^{13}C -NMR (400 MHz) spectrum of Compound 2 in CDCl_3

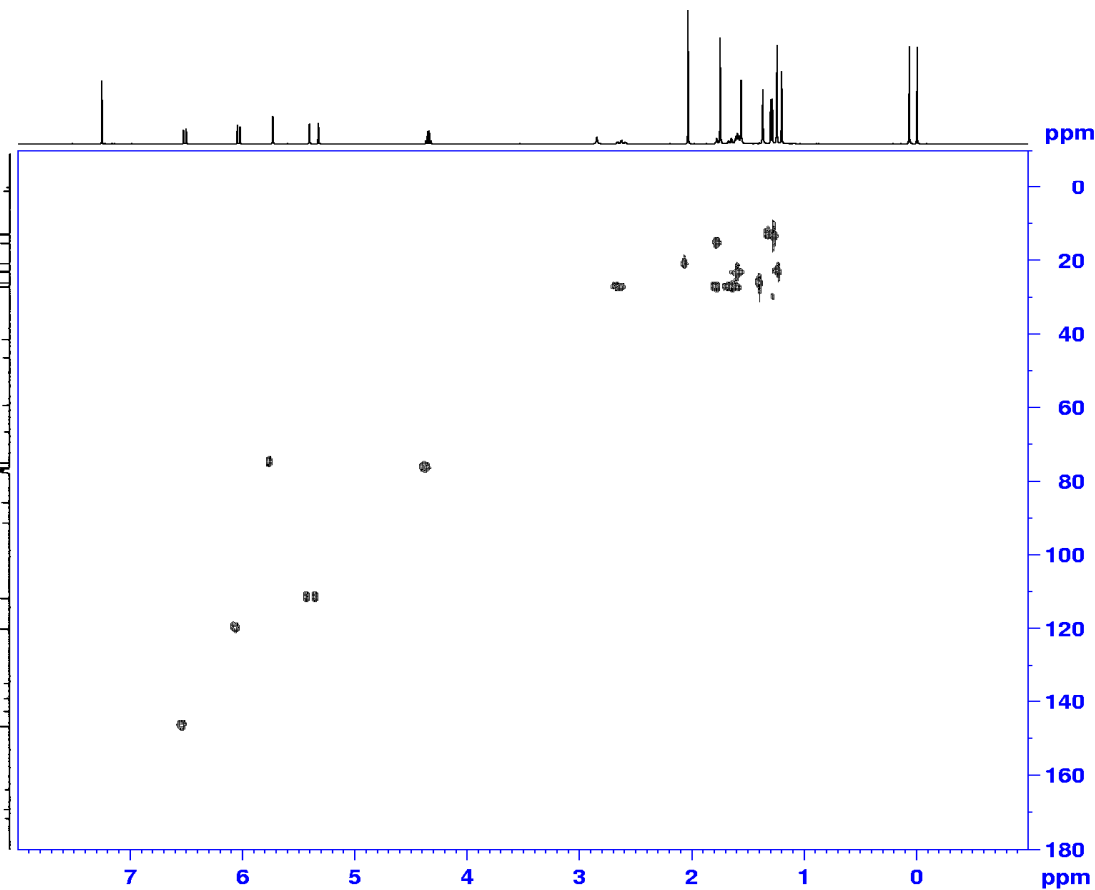


The ^1H - ^1H COSY (400 MHz) spectrum of Compound 2 in CDCl_3



The HSQC (400 MHz) spectrum of Compound 2 in CDCl₃

HSQC



```

NAME          3j-3
EXPNO         6
PROCNO       1
Date_        20120229
Time         17.10
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      hsqcetgp
TD           1024
SOLVENT      CDCl3
NS           32
DS           16
SWH          3597.122 Hz
FIDRES       3.512815 Hz
AQ           0.1423860 sec
RG           2050
DW           139.000 usec
DE           6.40 usec
TE           303.3 K
CHST2        145.0000000
d0           0.0000000 sec
d1           1.0000000 sec
d11          0.1300000 sec
d13          0.00000400 sec
d16          0.00020000 sec
d21          0.00349000 sec
d4           0.00172414 sec
DELTA        0.00221556 sec
DELTA1       0.00071614 sec
THO          0.00002615 sec
STICUP       0
ZGORTHS

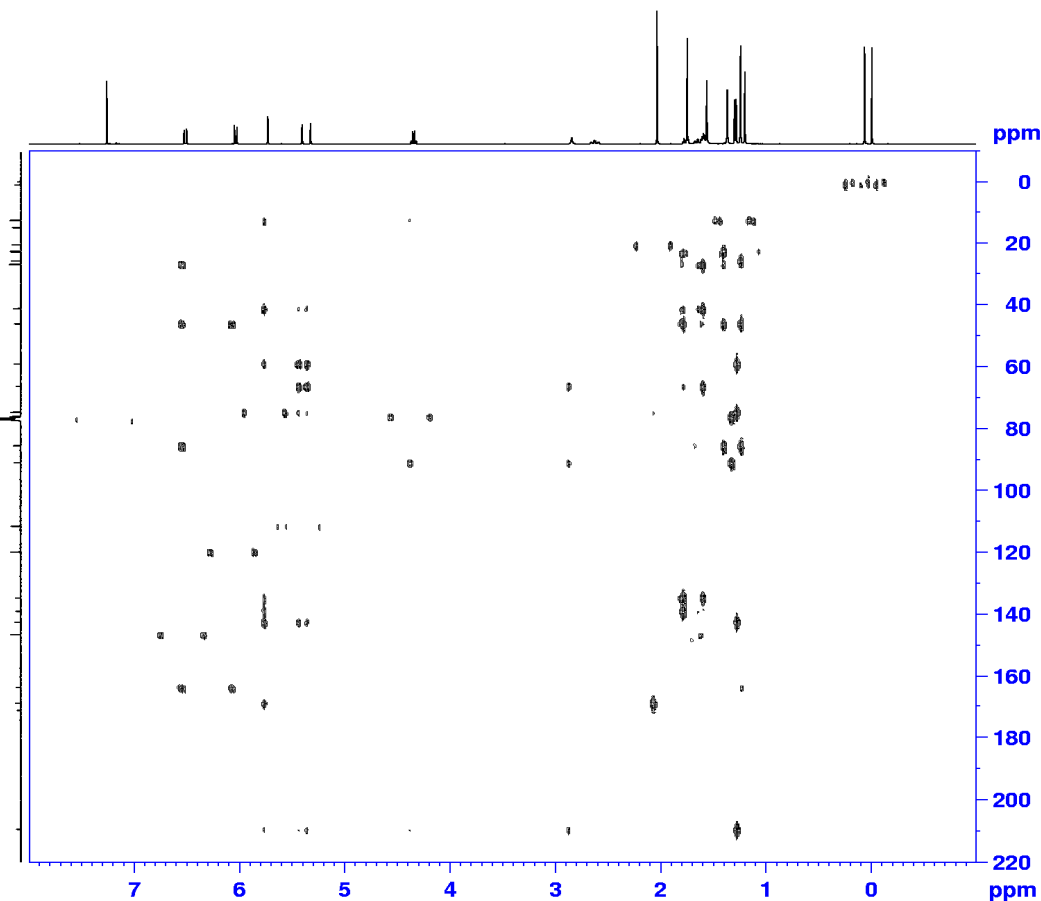
----- CHANNEL f1 -----
NUC1          1H
P1           14.22 usec
P2           28.44 usec
P28          1000.00 usec
PL1          -2.00 dB
SFO1         400.1314005 MHz

----- CHANNEL f2 -----
CPDPRG2      gpcp
NUC2          13C
P3           9.57 usec
P4           19.14 usec
PCPD2        80.00 usec
PL12         21.44 dB
PL2          3.00 dB
SFO2         100.6213211 MHz

----- GRADIENT CHANNEL -----
GPI1AM1      SINE.100
GPI1AM2      SINE.100
GPZ1         80.00 %
GPZ2         20.10 %
PL6          1000.00 usec
H2O          2
TD           128
SFO1         100.6213 MHz
FIDRES       149.378586 Hz
SW           190.024 ppm
FMODE        Echo-Antiecho
SI           1024
SF           400.1300000 MHz
WDW          QSHINE
SSB          2
LB           0.00 Hz
GB           0
PC           1.40
SI           1024
MC2          echo-antiecho
SF           100.6127690 MHz
WDW          QSHINE
SSB          2
LB           0.00 Hz
GB           0
    
```

The HMBC (400 MHz) spectrum of Compound 2 in CDCl₃

HMBC



```

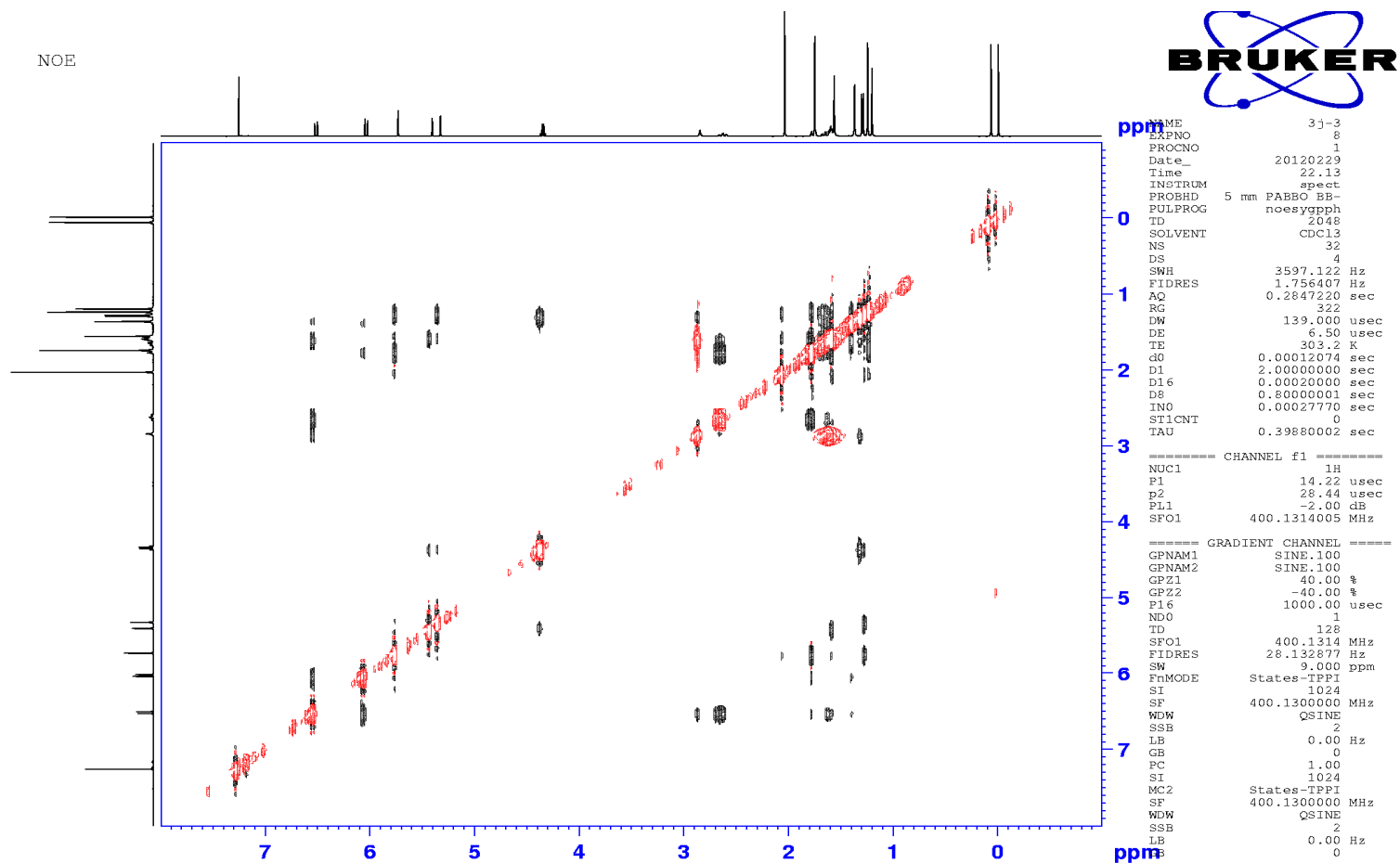
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EXPNO         7
PROCNO        1
Date_         20120229
Time          18.33
INSTRUM       spect
PROBHD        5 mm PAHRO BH-
PULPROG       hmbcpgndgf
TD            4096
SOLVENT       CDCl3
NS            48
DS            16
SWH           3597.122 Hz
FIDRES        0.878204 Hz
AQ            0.5693940 sec
RG            2050
DW            139.000 usec
DE            6.50 usec
TE            303.2 K
CNST13        8.0000000
d0            0.0000300 sec
D1            1.5000000 sec
D16           0.0002000 sec
d6            0.0625000 sec
IN0           0.00002160 sec

===== CHANNEL f1 =====
NUC1          1H
P1            14.22 usec
P2            28.44 usec
PL1           -2.00 dB
SFO1          400.1314005 MHz

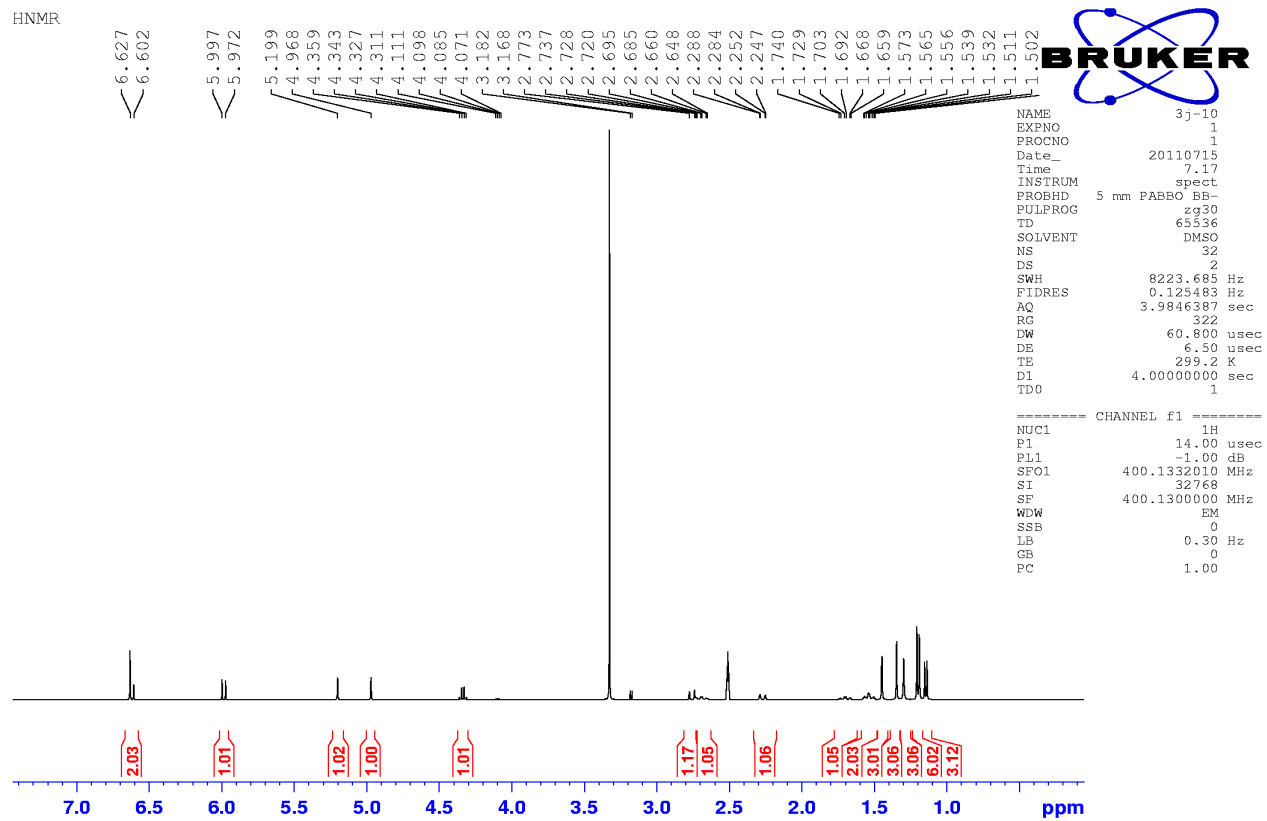
===== CHANNEL f2 =====
NUC2          13C
P3            9.57 usec
PL2           3.00 dB
SFO2          100.6233333 MHz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GPZ1          50.00 %
GPZ2          30.00 %
GPZ3          40.10 %
P16           1000.00 usec
ND0           2
TD            128
SFO1          100.6233 MHz
FIDRES        180.844910 Hz
SW            230.048 ppm
EnMODE        QP
SI            1024
SF            400.1300000 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QP
SF            100.6127690 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
    
```

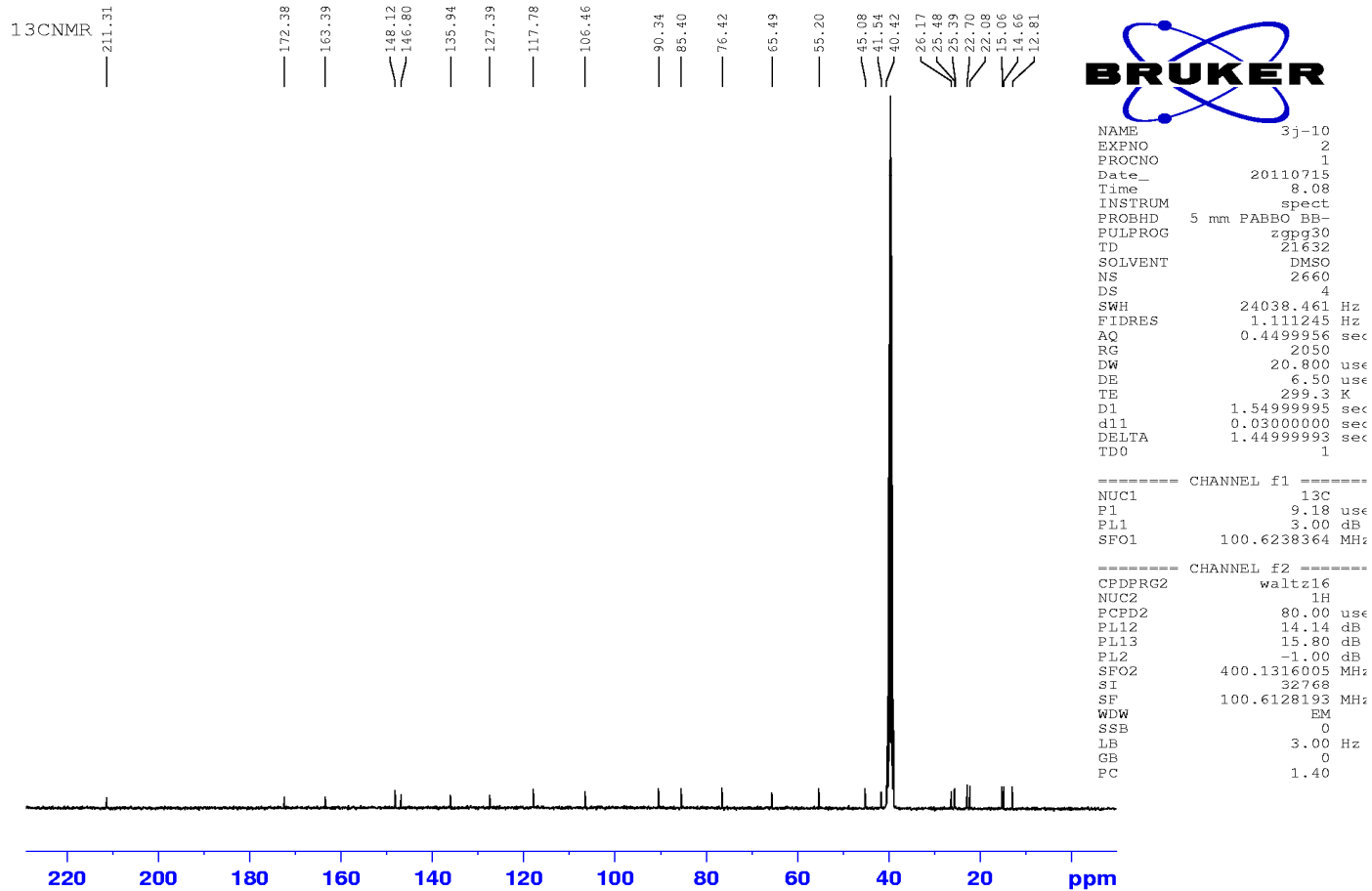
The NOE (400 MHz) spectrum of Compound 2 in CDCl₃



The ¹H-NMR (400 MHz) spectrum of Compound 3 in CDCl₃

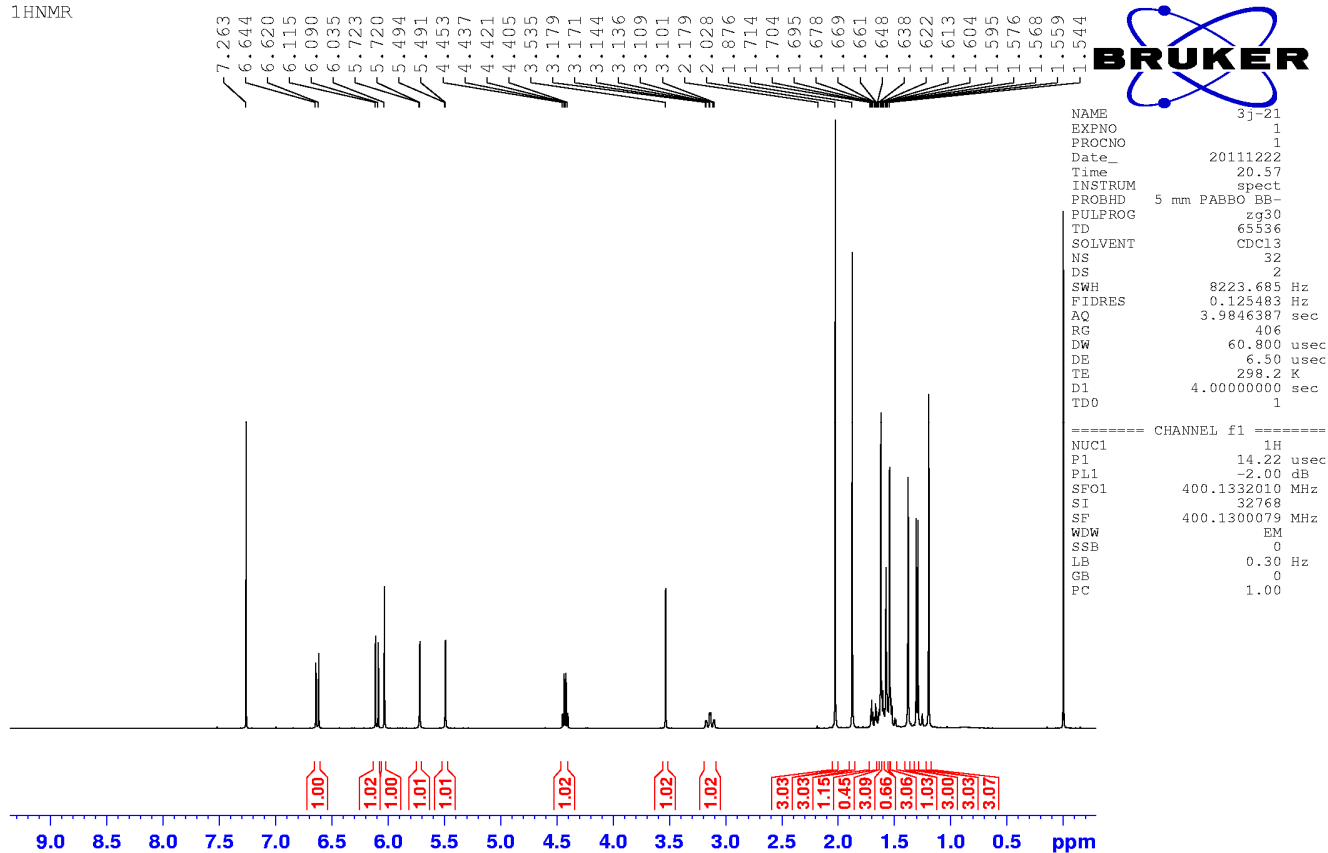


The ^{13}C -NMR (400 MHz) spectrum of Compound 3 in CDCl_3

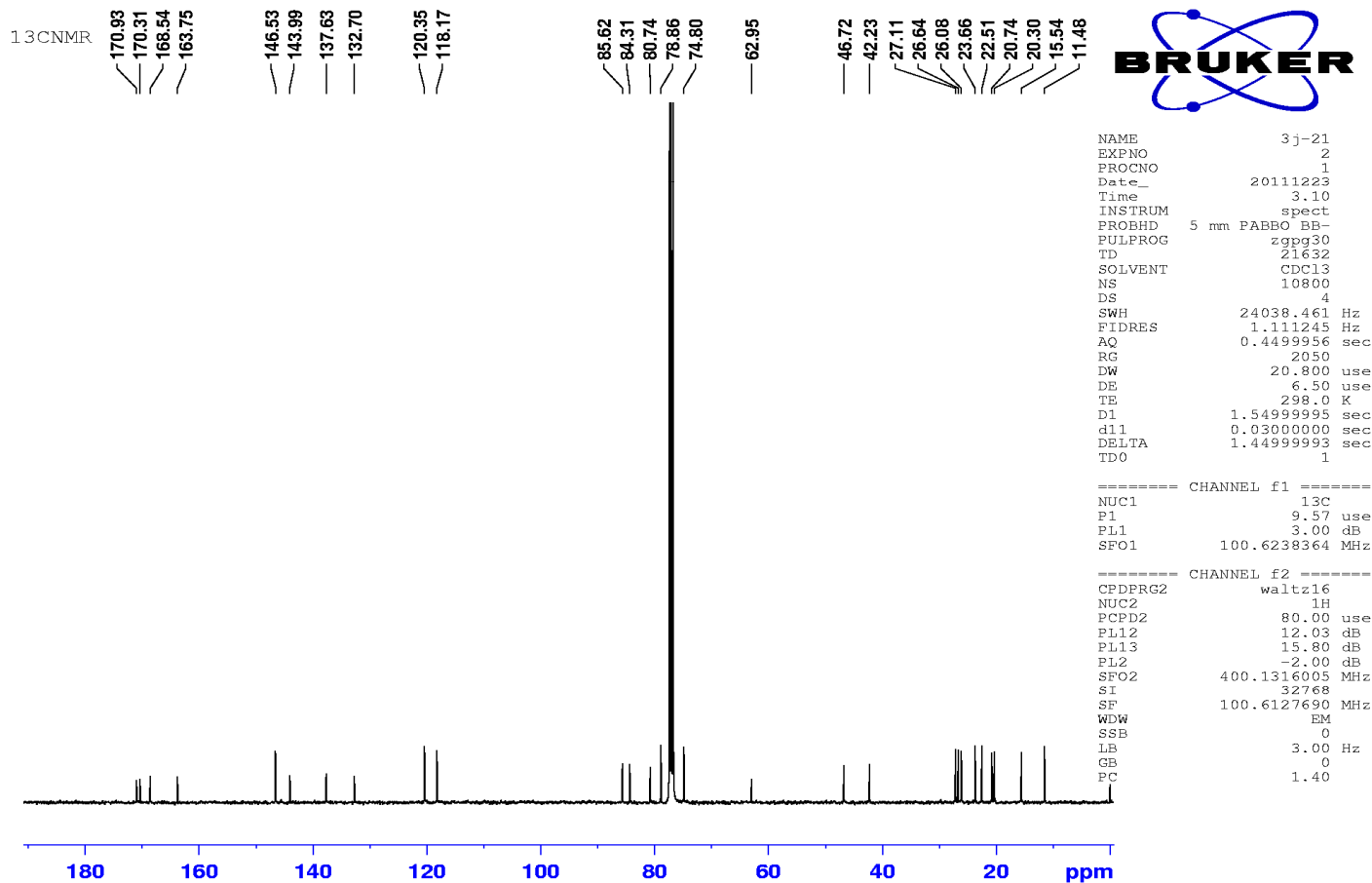


The ¹H-NMR (400 MHz) spectrum of Compound 4 in CDCl₃

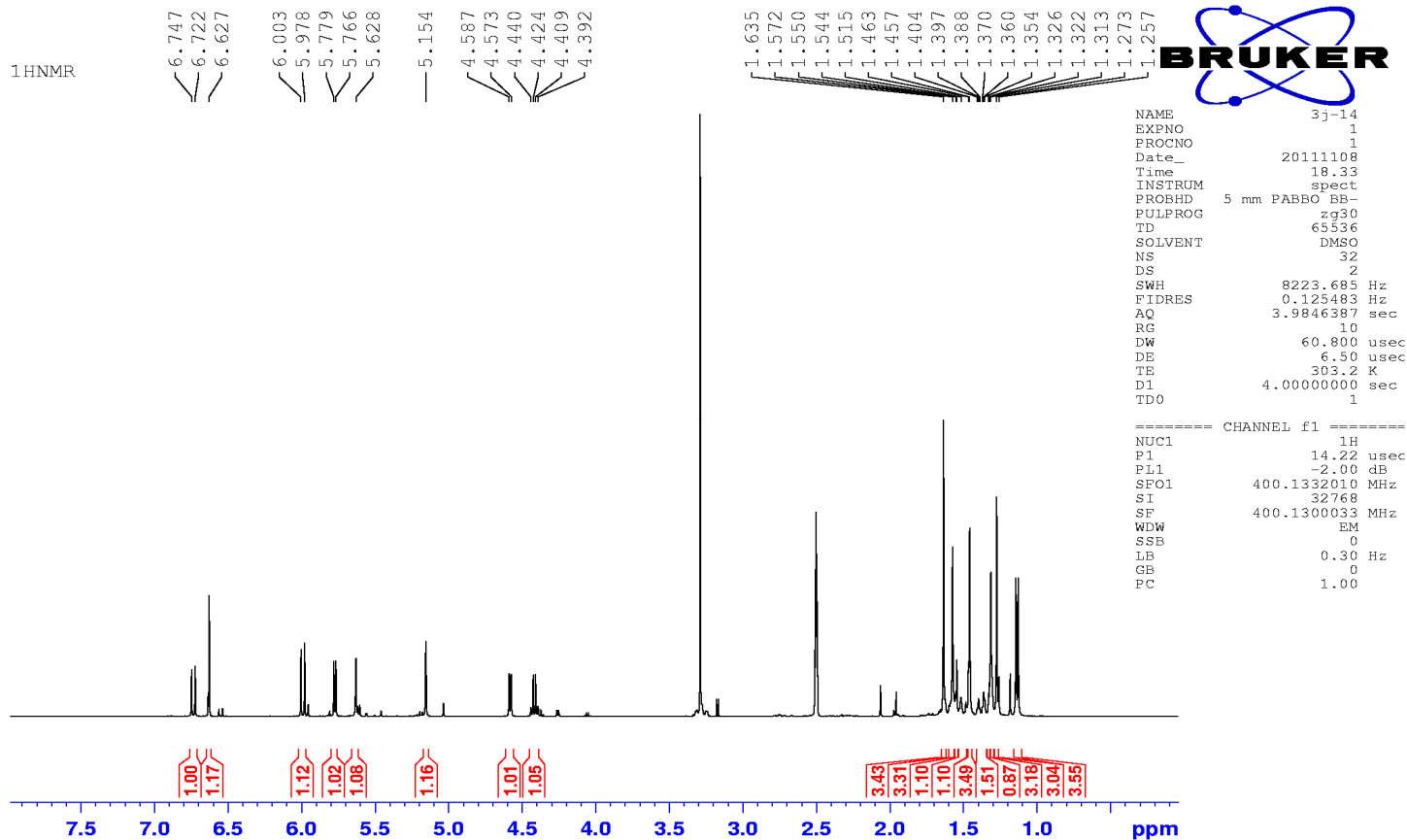
¹HNMR



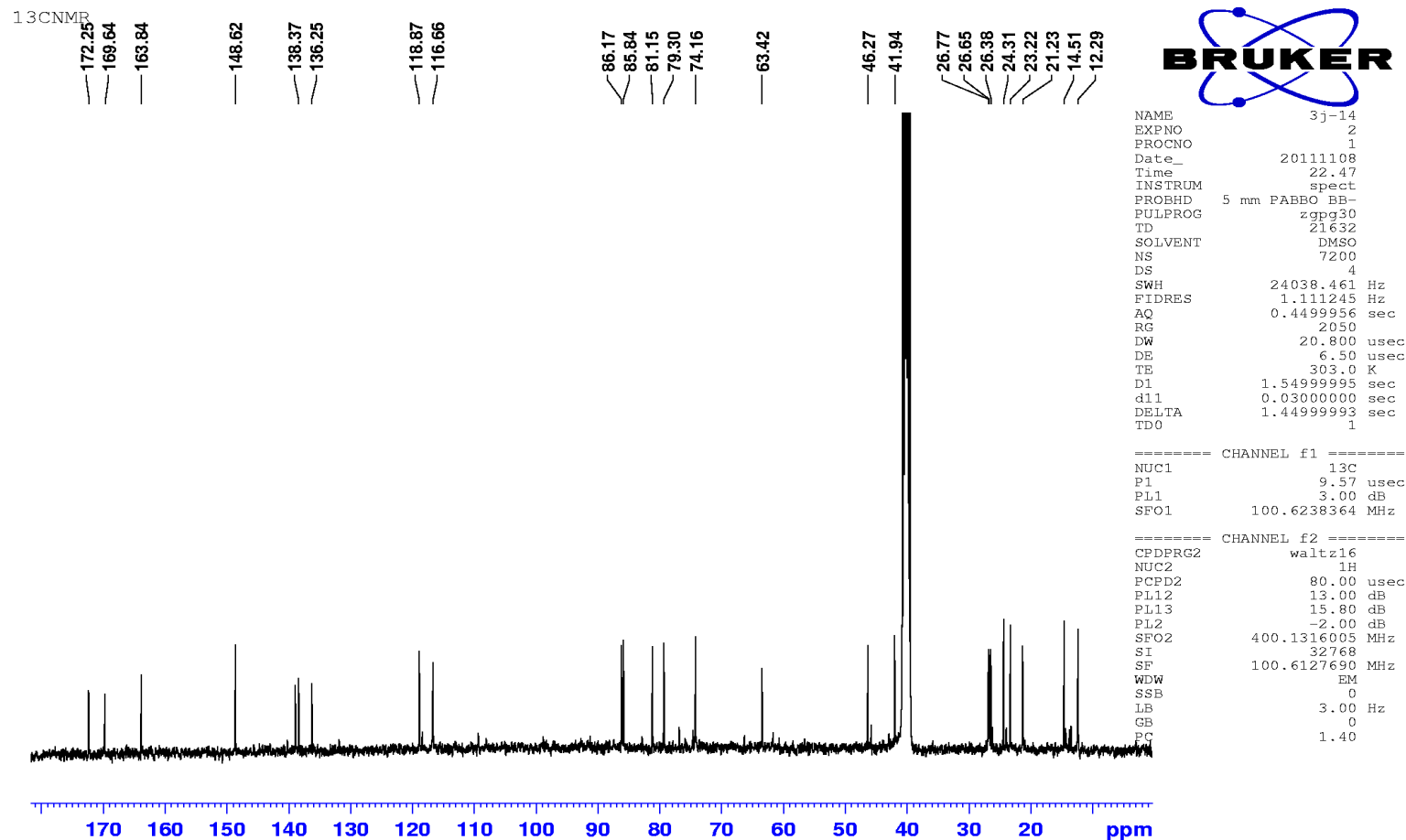
The ¹³C-NMR (400 MHz) spectrum of Compound 4 in CDCl₃



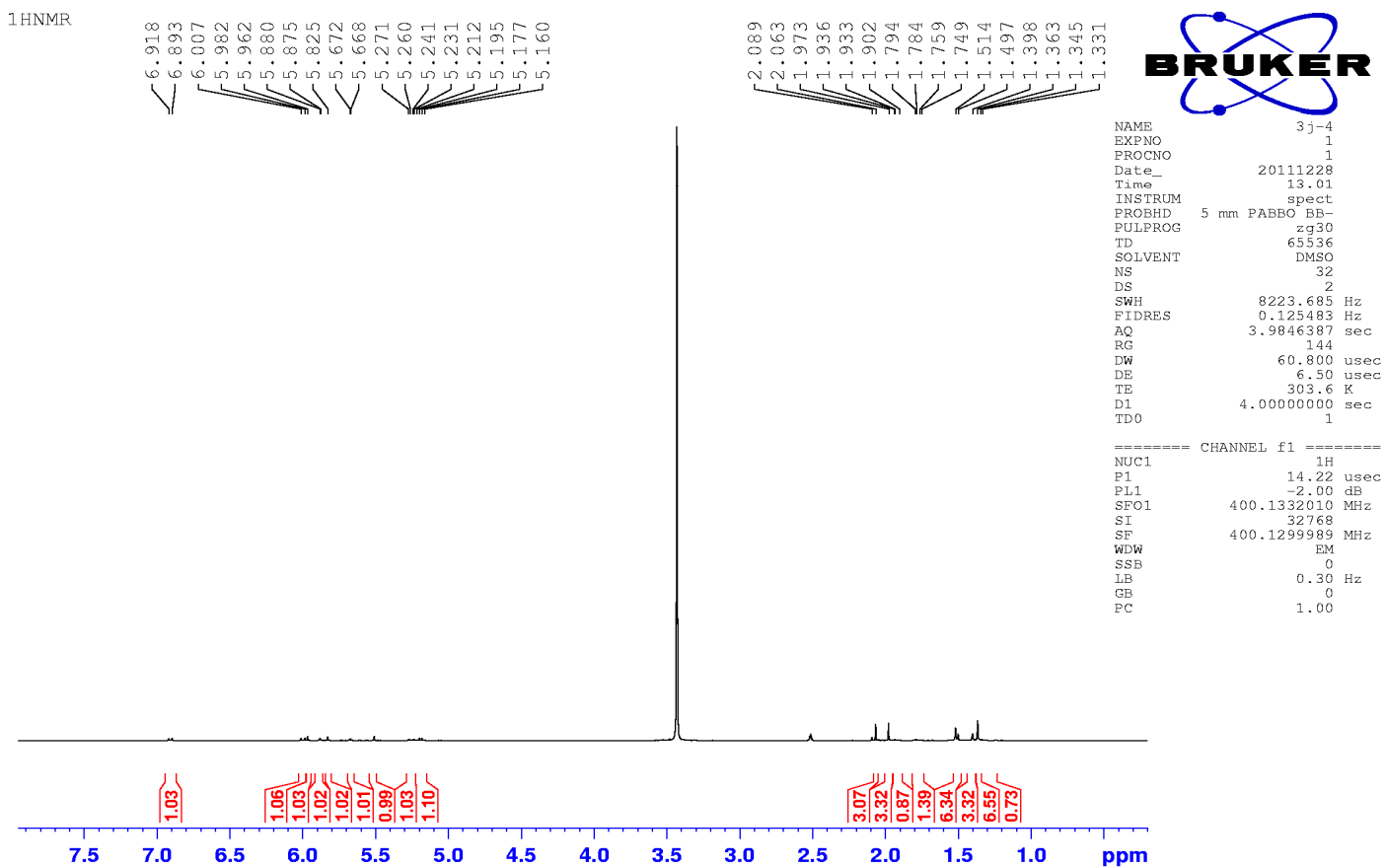
The ¹H-NMR (400 MHz) spectrum of Compound 5 in DMSO



The ^{13}C -NMR (400 MHz) spectrum of Compound 5 in DMSO



The ¹H NMR (400 MHz) spectrum of Compound 6 in DMSO



The ^{13}C NMR (400 MHz) spectrum of Compound 6 in DMSO

^{13}C NMR



```

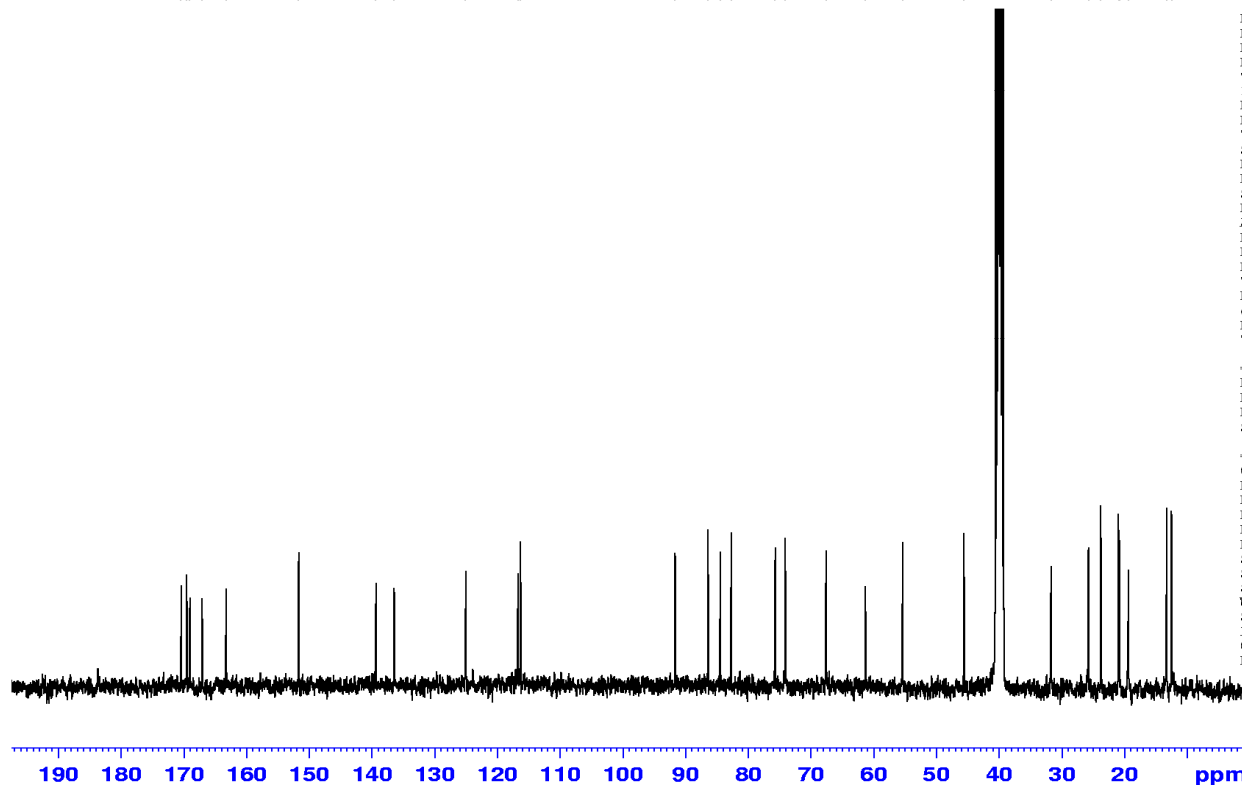
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EXPNO                2
PROCNO              1
Date_               20111228
Time_               14.45
INSTRUM             spect
PROBHD              5 mm PABBO BB-
PULPROG             zgpg30
TD                  21632
SOLVENT             DMSO
NS                   3612
DS                   4
SWH                 24038.461 Hz
FIDRES              1.111245 Hz
AQ                  0.4499956 sec
RG                   2050
DW                  20.800 usec
DE                   6.50 usec
TE                   303.2 K
D1                  1.54999995 sec
d11                  0.03000000 sec
DELTA               1.44999993 sec
TD0                  1
    
```

```

----- CHANNEL f1 -----
NUC1                 13C
P1                    9.57 usec
PL1                    3.00 dB
SFO1                 100.6238364 MHz
    
```

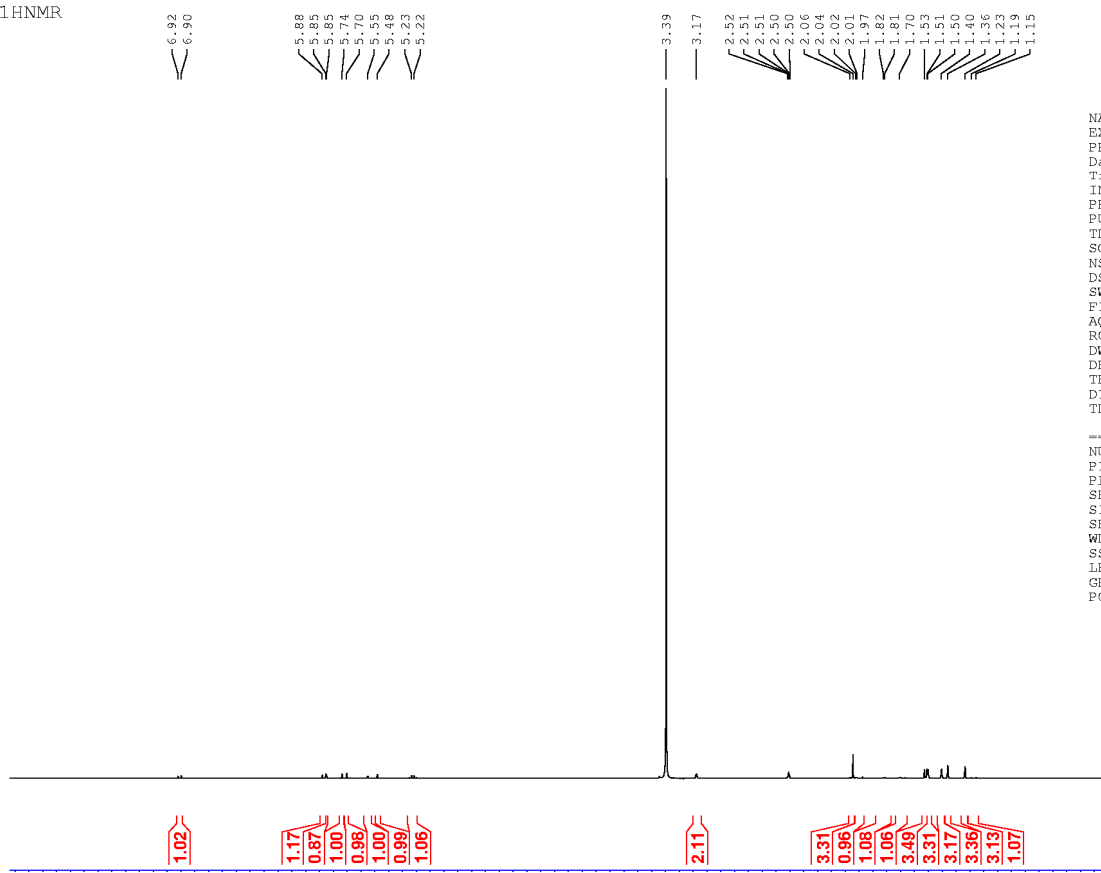
```

----- CHANNEL f2 -----
CPDPRG2              waltz16
NUC2                  1H
PCPD2                 80.00 usec
PL12                  12.03 dB
PL13                  15.80 dB
PL2                   -2.00 dB
SFO2                  400.1316005 MHz
SI                    32768
SF                    100.6127690 MHz
WDW                    EM
SSB                     0
LB                      3.00 Hz
GB                       0
PC                      1.40
    
```



The ¹H-NMR (400 MHz) spectrum of Compound 7 in DMSO

¹H NMR



```

NAME          3j-5
EXPNO         1
PROCNO        1
Date_         20120223
Time          17.02
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            32
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            128
DW            60.800 usec
DE            6.50 usec
TE            303.0 K
D1            4.0000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          1H
P1            14.22 usec
PL1           -2.00 dB
SF01         400.1332010 MHz
SI            32768
SF            400.1300002 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

The ¹³C-NMR (400 MHz) spectrum of Compound 7 in DMSO

¹³CNMR

169.62
169.56
167.57
163.61
152.94
140.77
137.14
123.92
115.30
114.98
89.94
86.69
84.87
83.00
76.16
74.28
64.18
50.74
49.06
44.18
26.76
26.50
26.50
25.80
23.78
20.92
19.22
17.36
13.43



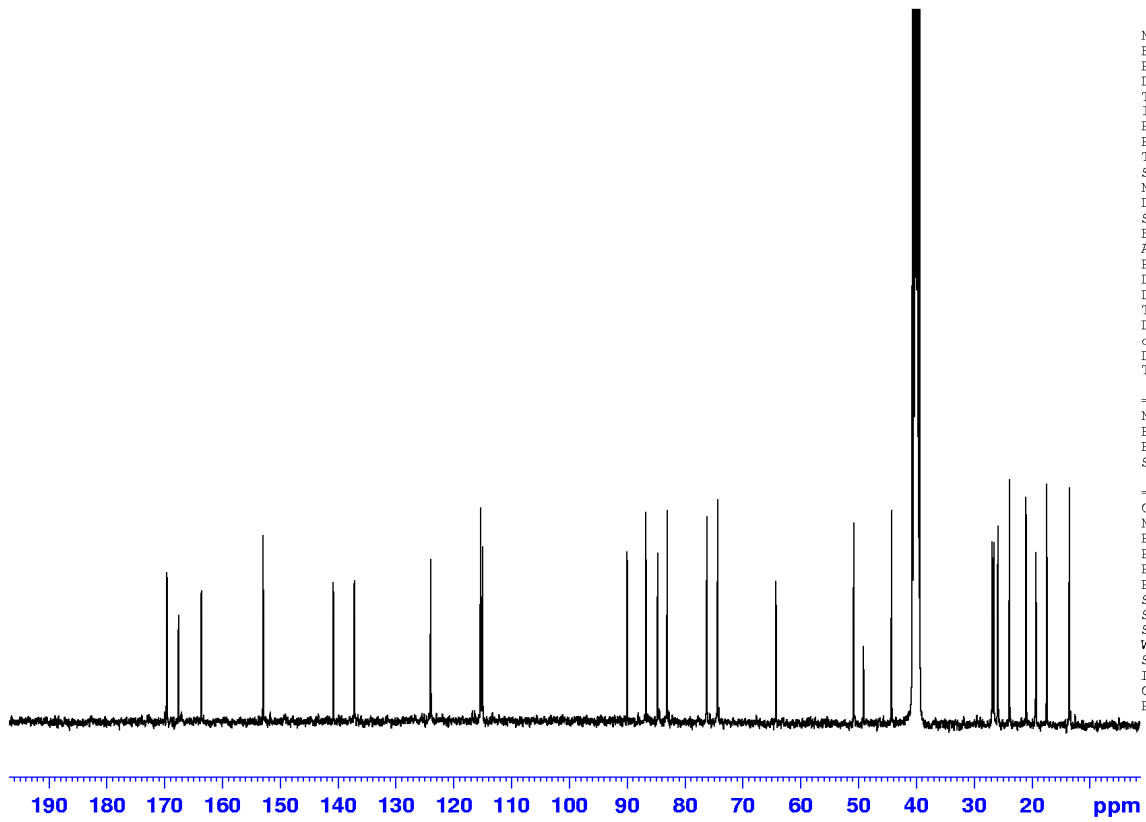
```

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EXPNO         2
PROCNO        1
Date_         20120224
Time          2.35
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            21632
SOLVENT       DMSO
NS            10800
DS            4
SWH           24038.461 Hz
FIDRES        1.111245 Hz
AQ            0.4499956 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            302.9 K
D1            1.54999995 sec
d11           0.03000000 sec
DELTA         1.44999993 sec
TDO          1
    
```

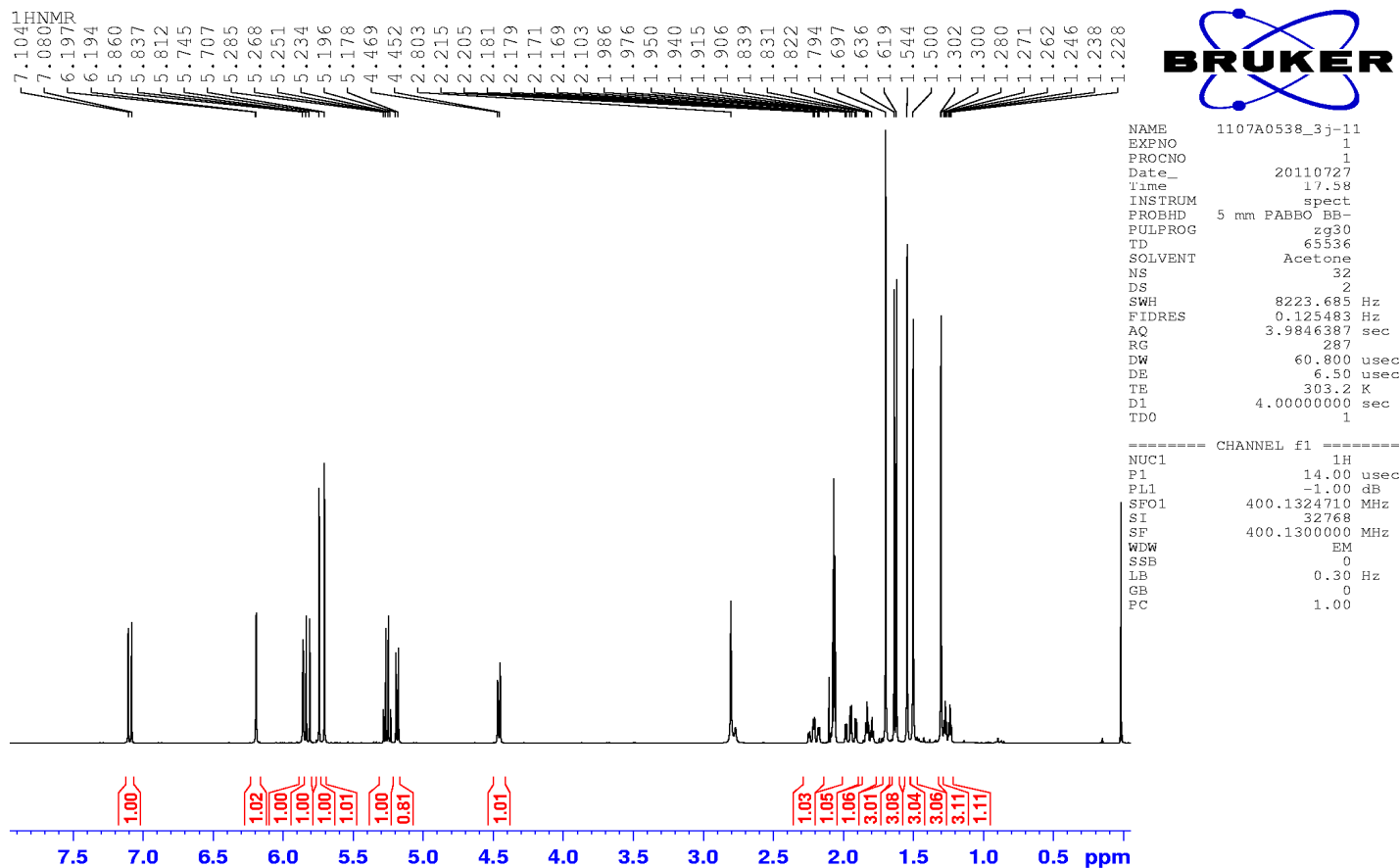
```

===== CHANNEL f1 =====
NUC1           13C
P1             9.57 usec
PL1            3.00 dB
SFO1           100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2            1H
PCPD2          80.00 usec
PL12           12.03 dB
PL13           15.80 dB
PL2            -2.00 dB
SFO2           400.1316005 MHz
SI             32768
SF             100.6127690 MHz
WDW            EM
SSB            0
LB             3.00 Hz
GB             0
PC             1.40
    
```

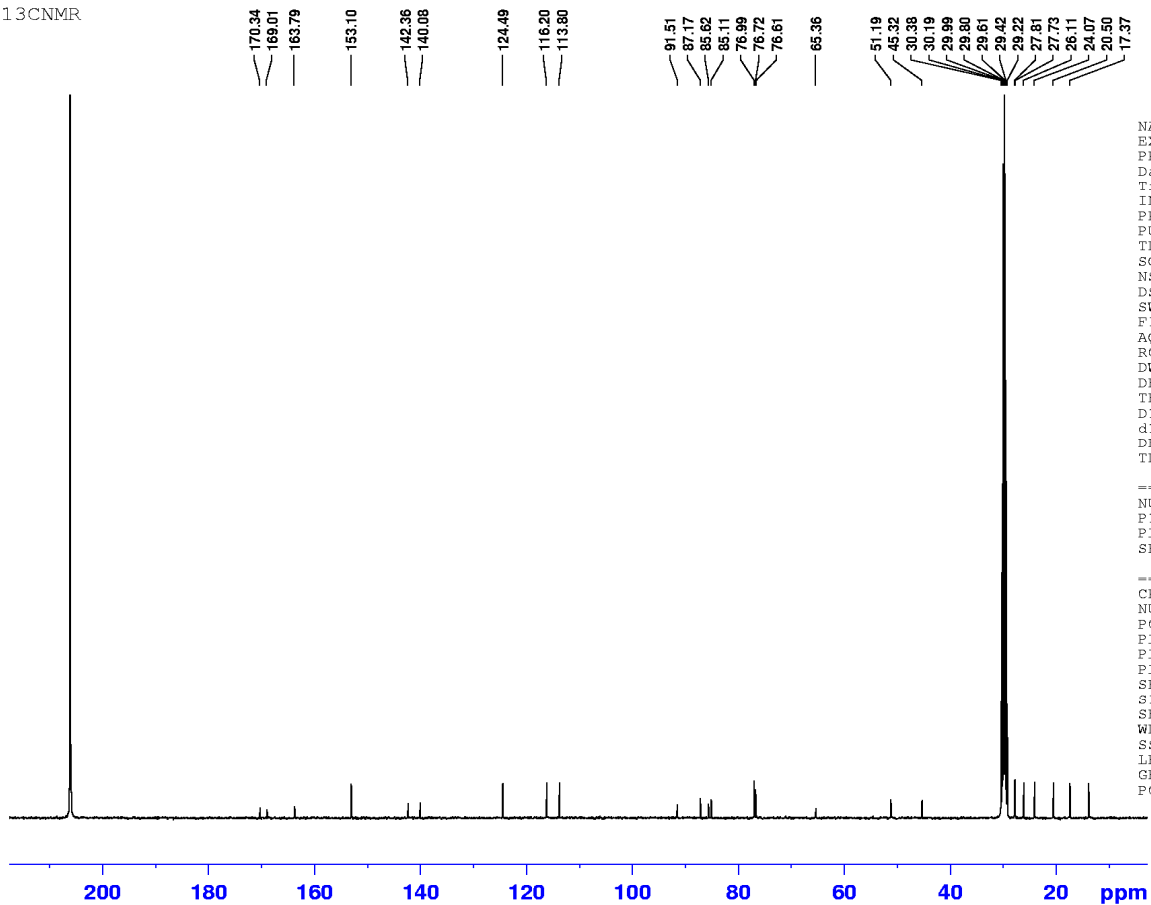


The ¹H-NMR (400 MHz) spectrum of Compound 8 in Acetone-d₆



The ^{13}C -NMR (400 MHz) spectrum of Compound 8 in Acetone- d_6

^{13}C NMR



```

NAME      1107A0538_3j-11
EXPNO     2
PROCNO    1
Date_     20110727
Time      20.15
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         21632
SOLVENT   Acetone
NS         4004
DS         4
SWH        24038.461 Hz
FIDRES     1.111245 Hz
AQ         0.4499956 sec
RG         2050
DW         20.800 usec
DE         6.50 usec
TE         303.2 K
D1         1.54999995 sec
d11        0.03000000 sec
DELTA     1.44999993 sec
TD0        1
    
```

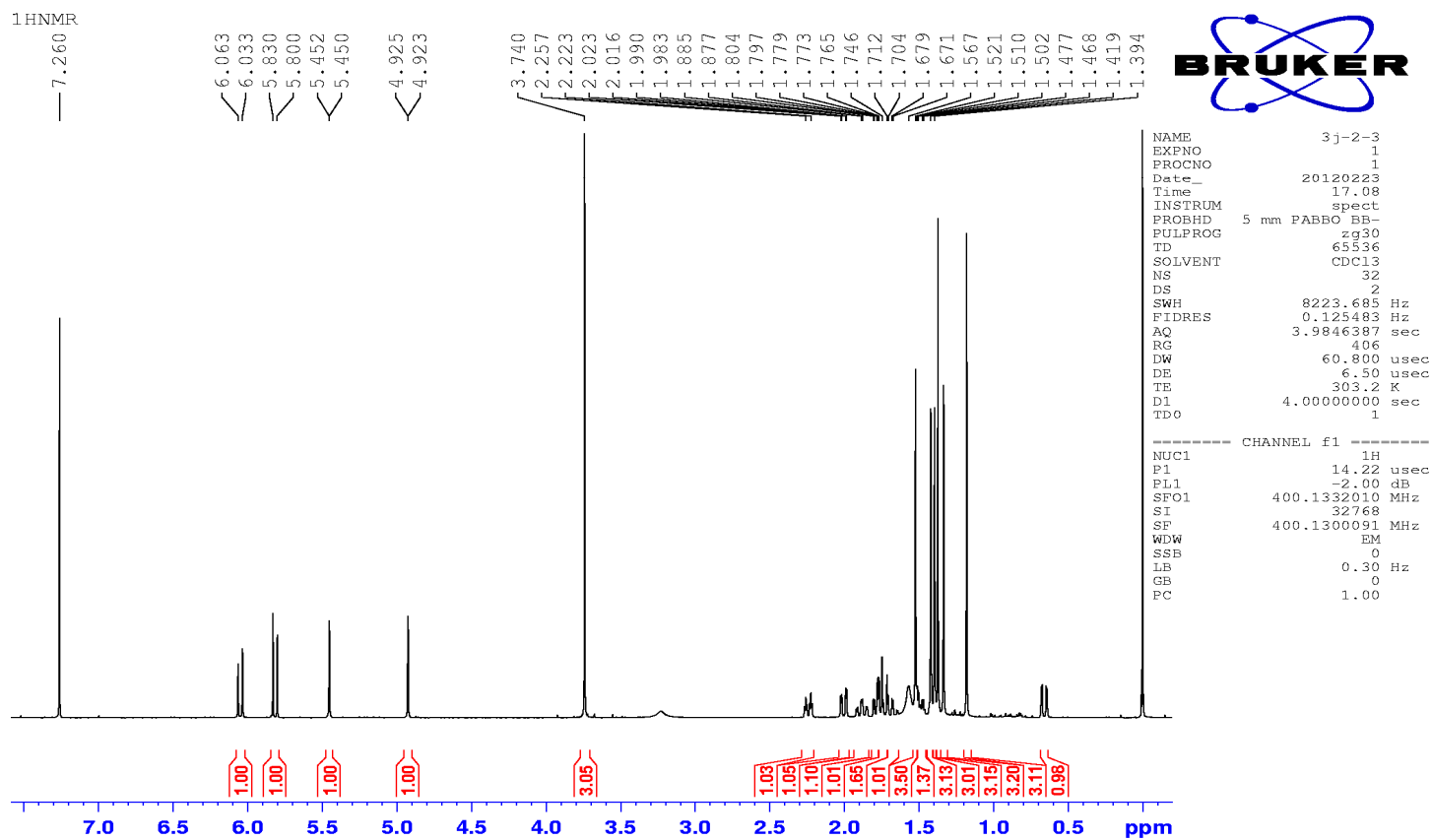
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===== CHANNEL f1 =====
NUC1      13C
P1        9.18 usec
PL1       3.00 dB
SFO1     100.6238364 MHz
    
```

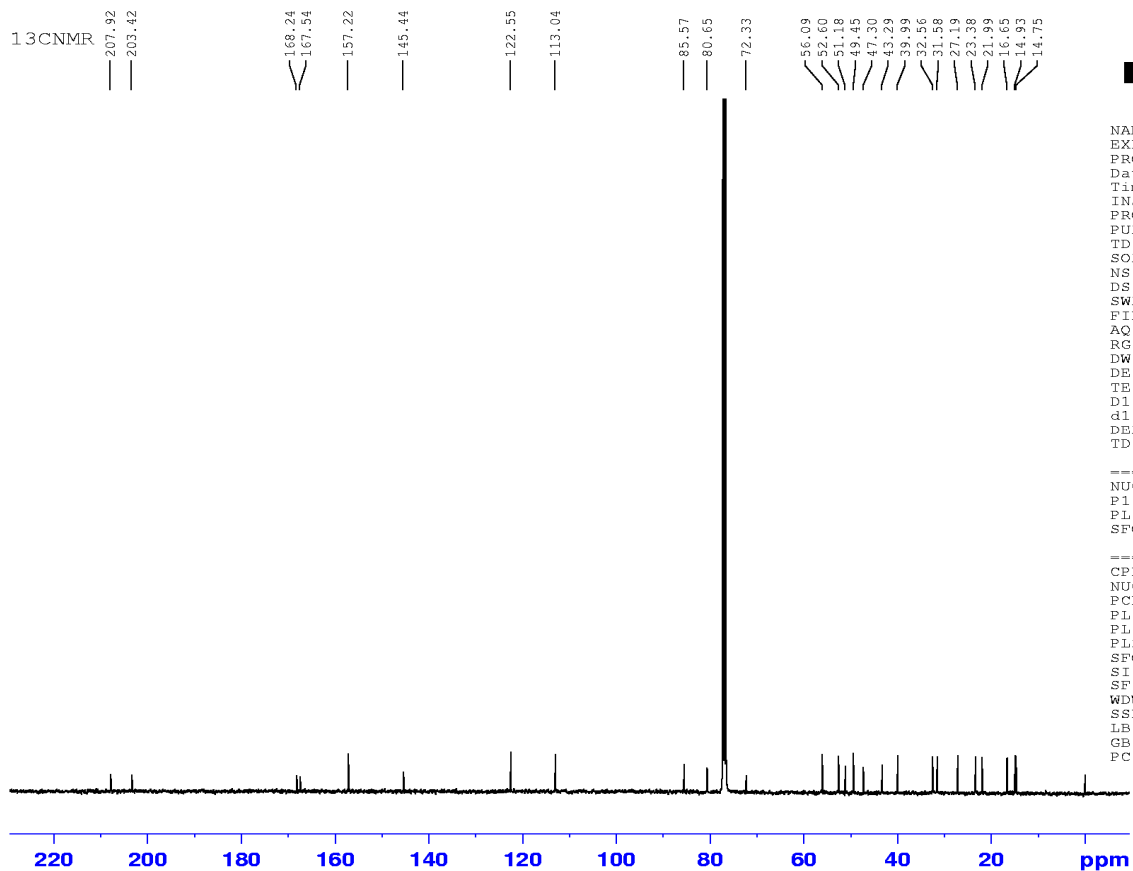
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===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL12      14.14 dB
PL13      15.80 dB
PL2        -1.00 dB
SFO2     400.1316005 MHz
SI        32768
SF        100.6126794 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
    
```

The ¹H-NMR (400 MHz) spectrum of Compound 9 in CDCl₃



The ^{13}C -NMR (400 MHz) spectrum of Compound 9 in CDCl_3



```

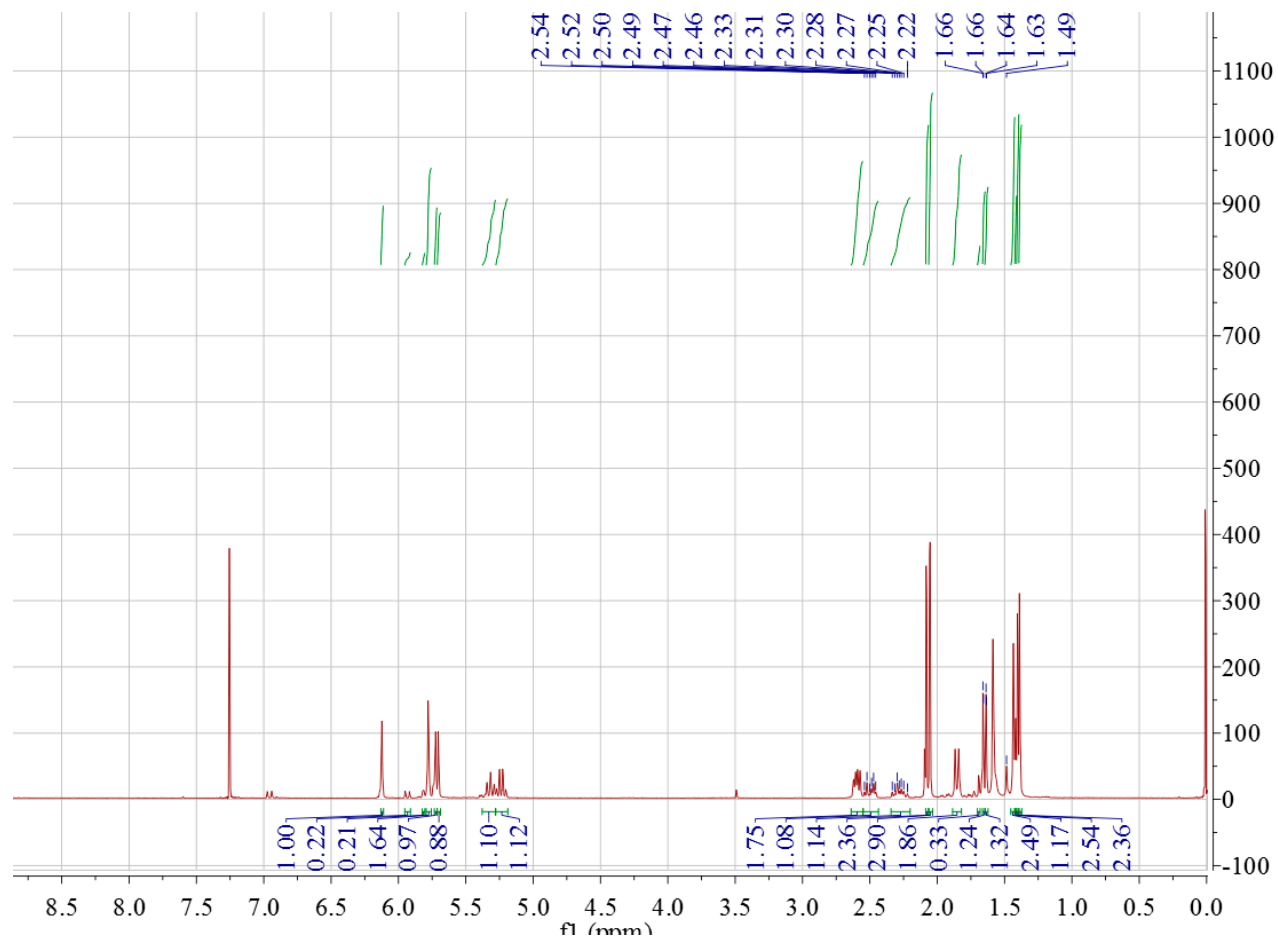
NAME          3j-2-3
EXPNO         2
PROCNO        1
Date_         20120224
Time_         8.03
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            21632
SOLVENT       CDCl3
NS            7218
DS            4
SWH           24038.461 Hz
FIDRES        1.111245 Hz
AQ            0.4499956 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            303.2 K
D1            1.54999995 sec
d11           0.03000000 sec
DELTA         1.44999993 sec
TDO           1
    
```

```

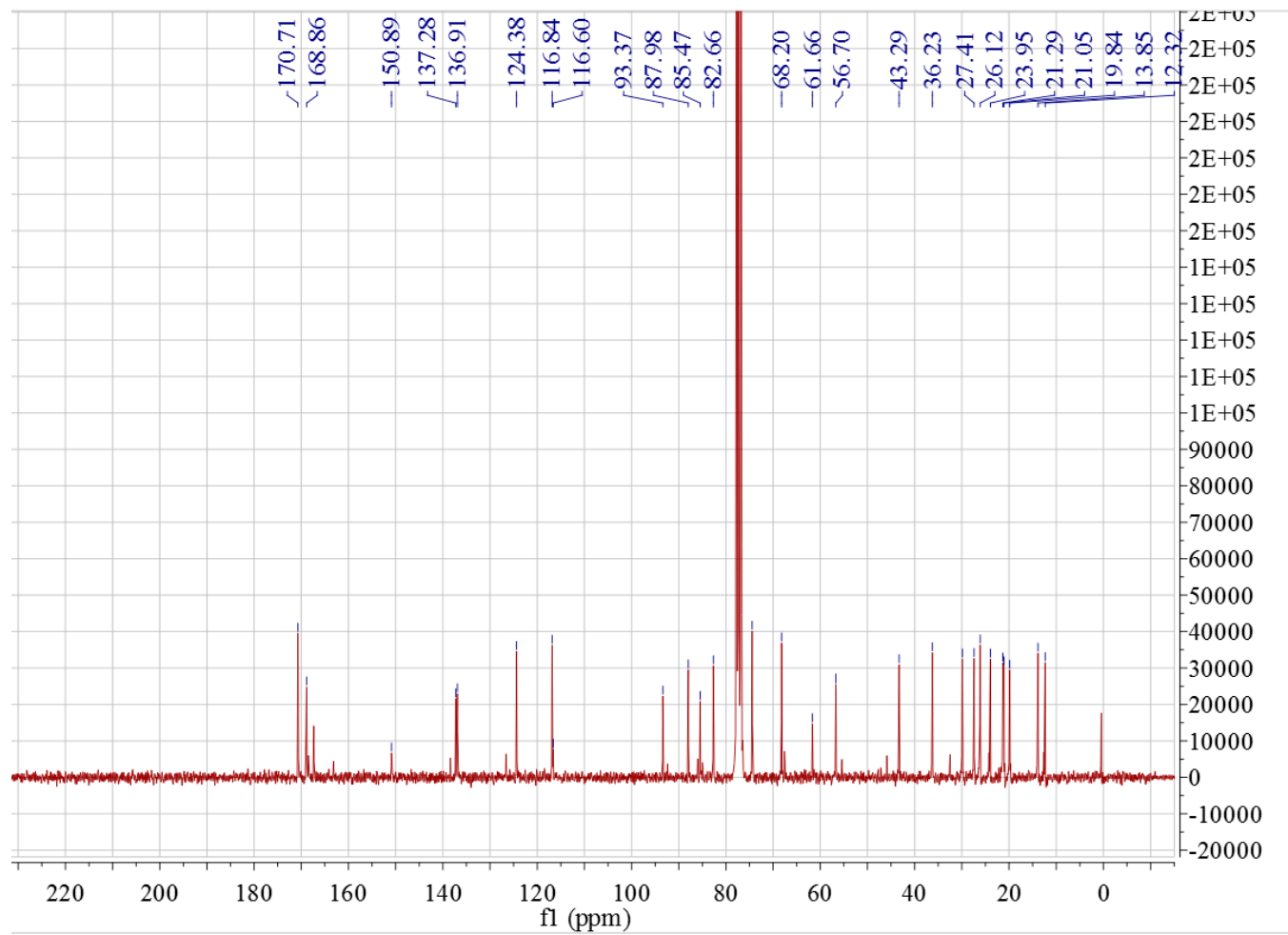
----- CHANNEL f1 -----
NUC1          13C
P1            9.57 usec
PL1           3.00 dB
SF01         100.6238364 MHz

----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          12.03 dB
PL13          15.80 dB
PL2           -2.00 dB
SF02         400.1316005 MHz
SI            32768
SF            100.6127682 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40
    
```

The ^1H -NMR (400 MHz) spectrum of Compound 10 in CDCl_3

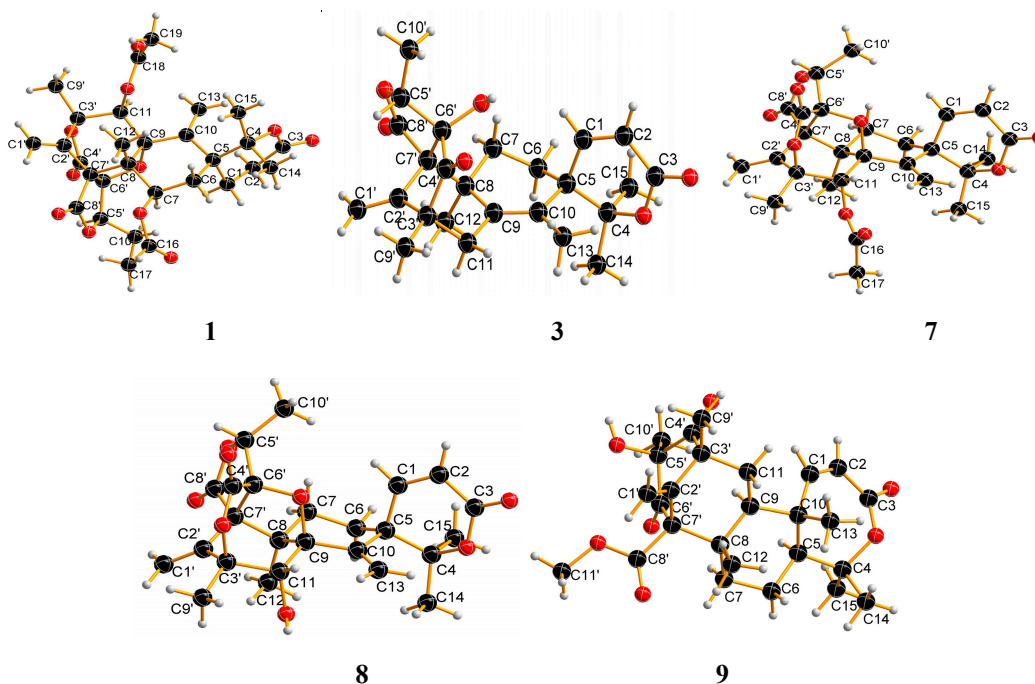


The ^{13}C -NMR (400 MHz) spectrum of Compound 10 in CDCl_3

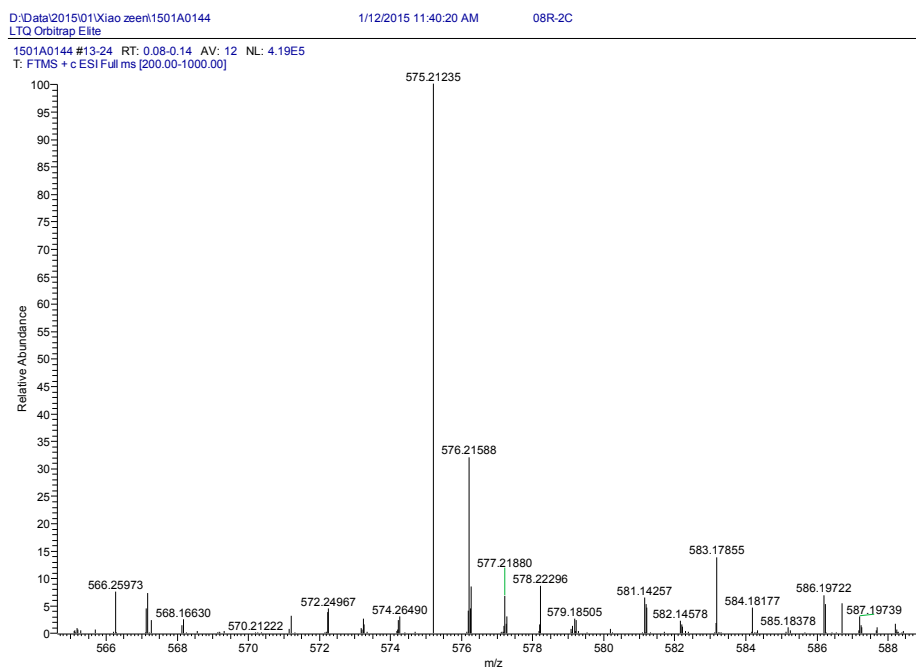


X-ray Crystallographic

Perspective ORTEP drawings for Compounds 1,3,7,8, 9

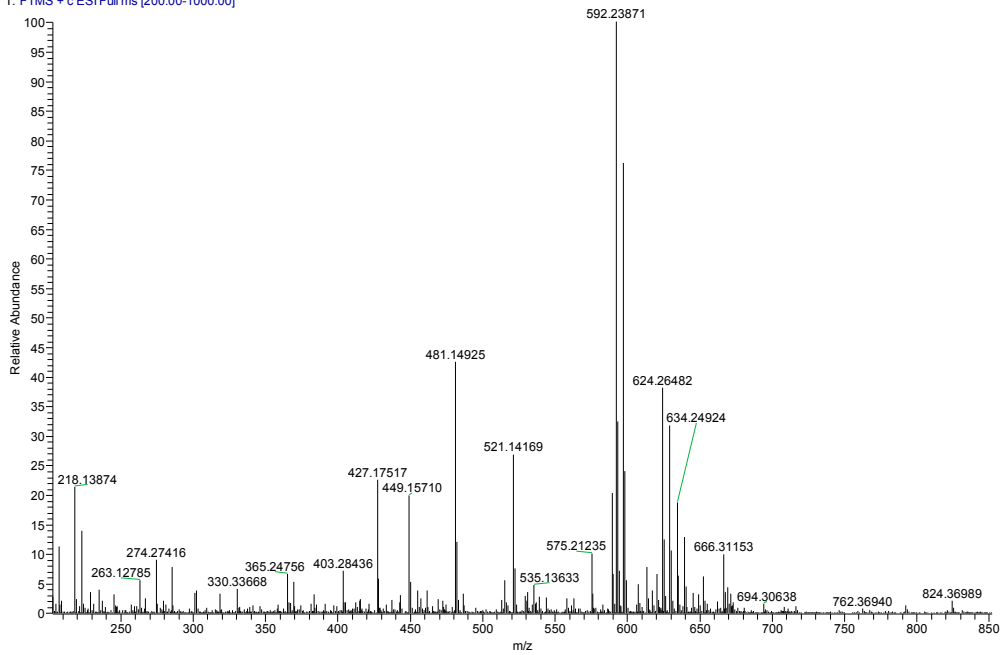


The ESIMS of Compound 1



The HRESIMS of Compound 1

1501A0144 #13-24 RT: 0.08-0.14 AV: 12 NL: 4.20E6
T: FTMS + c ESI Full ms [200.00-1000.00]



The ESIMS of Compound 2

Formula Predictor Report - 3j-3.lcd

Page 1 of 1

Data File: F:\data\wangjun\ly ul\20120621\3j-3.lcd

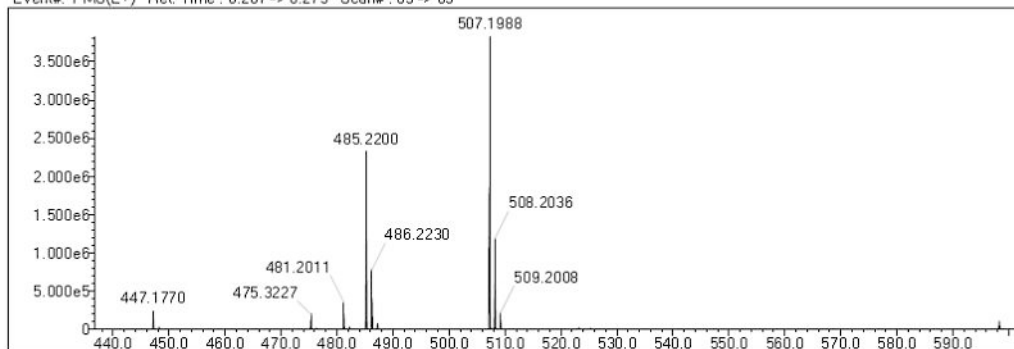
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	35	O	2	0	11	S	2	0	0	Pt	2	0	0	H
B	3	0	0	18O	2	0	0	Cl	1	0	5					Na
C	4	0	30	F	1	0	0	Br	1	0	5					
N	3	0	0	P	3	0	0	I	3	0	0					

Error Margin (ppm): 500
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

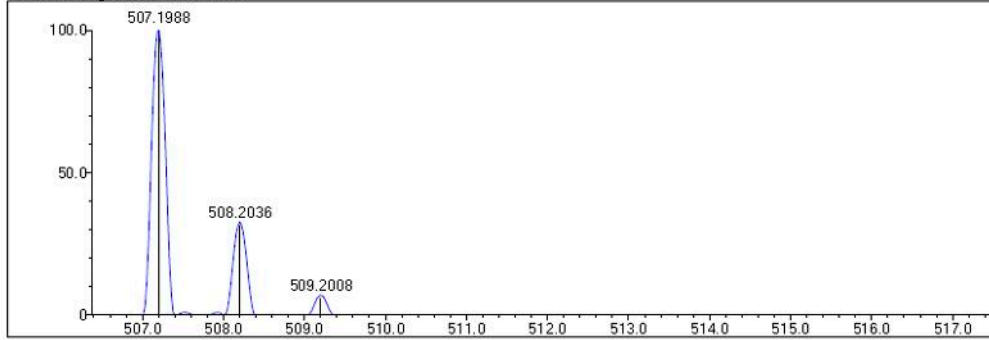
Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 500

Event#: 1 MS(E+) Ret. Time : 0.207-> 0.273 Scan#: 63-> 83

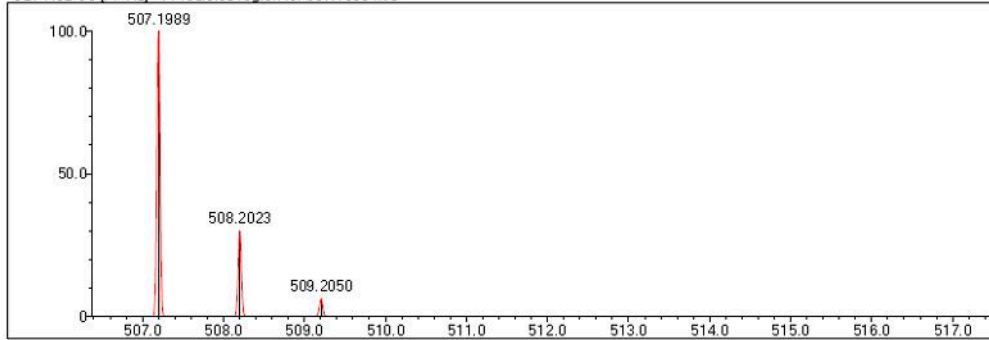


The HRESIMS of Compound 2

Measured region for 507.1988 m/z



C27 H32 O8 [M+Na]⁺: Predicted region for 507.1989 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	71.25	C27 H32 O8	[M+Na] ⁺	507.1988	507.1989	-0.1	-0.20	71.25	12.0