ELECTRONIC SUPPORTING INFORMATION (ESI)

Design and synthesis of sugar-triazole based uracil appended sugar-imine derivatives – An application in DNA binding studies

Arasappan Hemamalini[a], Ettayapuram Ramaprasad Azhagiya Singham[b], Sathish kumar Mudedla[b], Venkatesan Subramanian[b], Thangamuthu Mohan Das[a,c]*

[a]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai – 600 025, INDIA.
[b]Chemical Laboratory, Central Leather Research Institute (CSIR) Adyar, Chennai- 600 020, INDIA
[b]Department of Chemistry, School of Basic and Applied Sciences, Central University of Tamil Nadu, Thiruvarur -610 004; Ph. No. +919489054278; Fax 04366 – 225312; E-mail: tmohandas@cutn.ac.in

Table 1 Spectral data and optimization of reaction condition of sugar-triazole derivatives, **6-9**

Compound No.	R	Time (h)	Yield (%)	NMR data				
				δ Ano-H /ppm	δ Ald-H /ppm	δ Trz-H /ppm	δ Trz-C /ppm	Δ (δ_{C4}-δ_{C5})
6	-H	24	85	5.91-5.88	10.48	7.92	121.5, 144.1	23
7	-OCH_3	26	79	5.89-5.86	9.86	7.91	144.0, 121.7	22
8	-Cl	20	74	5.90-5.87	10.39	7.91	143.6, 121.6	22
9	-OH	24	83	5.91-5.88	9.98	7.88	144.4, 121.2	23

Table 2 Spectroscopic data and optimization of reaction condition of sugar-imine derivatives, **11-14**

Entry	R	Time (h)	Yield (%)	NMR data			
				δ Ano-H/ppm, J_{H1H2} Hz	δ Trz-H /ppm	δ Imin-H /ppm	δ Imin-C /ppm
11	-H	1	56	5.79, 9.0	7.27	7.61	165
12	-OCH_3	3	58	5.58, 9.3	7.69	8.01	168
13	-Cl	3	35	5.60,_[a]	7.67	7.93	167
14	-H	4	52	5.60-5.53,_*	7.50	8.01	167

*Peaks merged with saccharide proton, [a]merged with alkene proton

General procedure for the synthesis of *O*-propargylated derivative, 2-5

To the corresponding hydroxy benzaldehydes (1 mmol) in dry DMF, (5 mmol) anhydrous K_2CO_3 was added and stirred for 10 minutes. To the reaction mixture was added propargyl bromide (1.2 mmol) and stirred for 24 hours. After the completion of the reaction, work up was done using chloroform. The organic layer was evaporated and the product was purified using silica gel column chromatography.

Spectral data of 2-(prop-2-ynyloxy)-1-benzaldehyde (2):

Pale yellow solid; Mp: 64-66 ^oC; Yield: 0.12 g (75%); ^1H NMR (300 MHz, $CDCl_3$): δ 10.49 (s, 1H, -CHO), 7.87 (d, J = 7.8 Hz, 1H, Ar-H), 7.61-7.55 (m, 1H, Ar-H), 7.14-7.07 (m, 2H, Ar-H), 4.9 (s, 2H, $-OCH_2$), 2.57 (t, J = 2.4 Hz, 1H, -C≡CH); ^{13}C NMR (75 MHz, $CDCl_3$): δ 189.5, 159.8, 135.7, 128.6, 125.5, 121.7, 113.2, 77.7, 76.5, 56.4.

Spectral data of 2-methoxy-4-(prop-2-ynyloxy)-1-benzaldehyde (3):

Pale yellow solid; Mp: 86-88 ^oC; Yield: 0.16 g (84%); ^1H NMR (300 MHz, $CDCl_3$): δ 9.88 (s, 1H, -CHO), 7.49-7.45 (m, 2H, Ar-H), 7.15 (d, J = 8.1 Hz, 1H, Ar-H), 4.87 (d, J = 2.4 Hz, 2H, $-OCH_2$), 3.95 (s, 3H, $-OCH_3$), 2.57 (t, J = 2.3 Hz, 1H, -C≡CH); ^{13}C NMR (75 MHz, $CDCl_3$): δ 190.8, 152.2, 150.1, 131.0, 126.2, 112.7, 109.6, 77.0, 76.6, 56.6, 56.0.

Spectral data of 5-chloro-2-(prop-2-ynyloxy)-1-benzaldehyde (4):

Yellow solid; Mp: 60-62 ^oC; Yield: 0.14 g (74%); ^1H NMR (300 MHz, $CDCl_3$): δ 10.41 (s, 1H, -CHO), 7.81 (s, 1H, Ar-H), 7.51 (d, J = 9.0 Hz, 1H, Ar-H), 7.09 (d, J = 9.0 Hz, 1H, Ar-H), 4.83 (d, J = 2.4 Hz, 2H, $-OCH_2$), 2.59 (t, J = 2.4 Hz, 1H, -C≡CH); ^{13}C NMR (75 MHz, $CDCl_3$): δ 188.2, 158.1, 135.2, 128.1, 127.5, 126.5, 115.0, 77.2, 76.9, 56.8.

Spectral data of 3-(prop-2-ynyloxy)-1-benzaldehyde (5):

Yield 0.13 g, (81%); ^1H NMR (300 MHz, $CDCl_3$): δ 9.97 (s, 1H, -CHO), 7.52-7.44 (m, 3H, Ar-H), 7.28-7.23 (m, 1H, Ar-H), 4.76 (d, J = 2.4 Hz, 2H, $-OCH_2$), 2.57 (t, J = 2.4 Hz, 1H, -C≡CH); ^{13}C NMR (75 MHz, $CDCl_3$): δ 192.0, 158.1, 137.8, 130.2, 124.1, 122.1, 113.6, 77.9, 76.2, 56.0.

^1H NMR, ^{13} C NMR, DEPT-135, Mass spectrum are available in the ESI

Contents

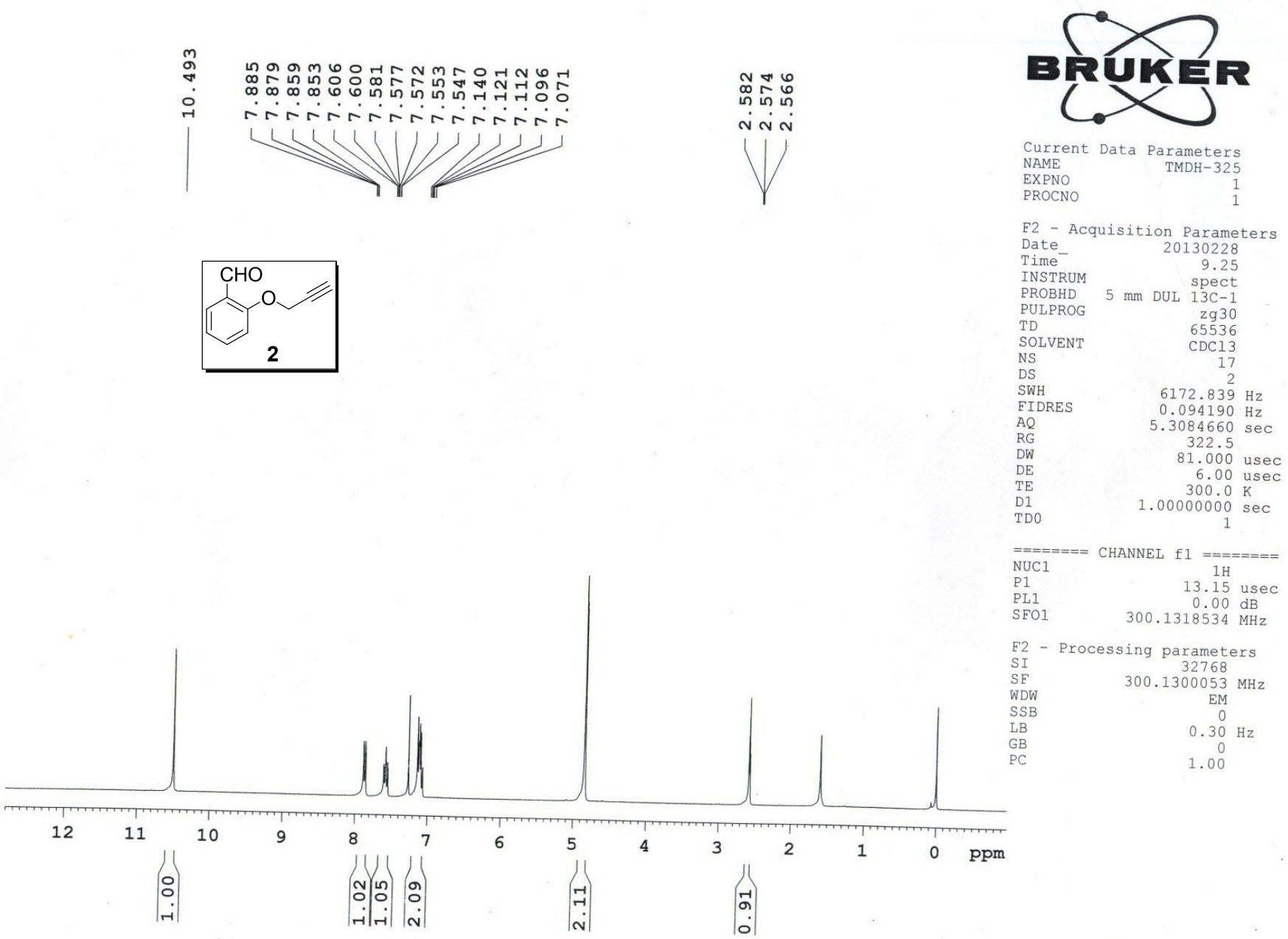

Figure 1 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 2.

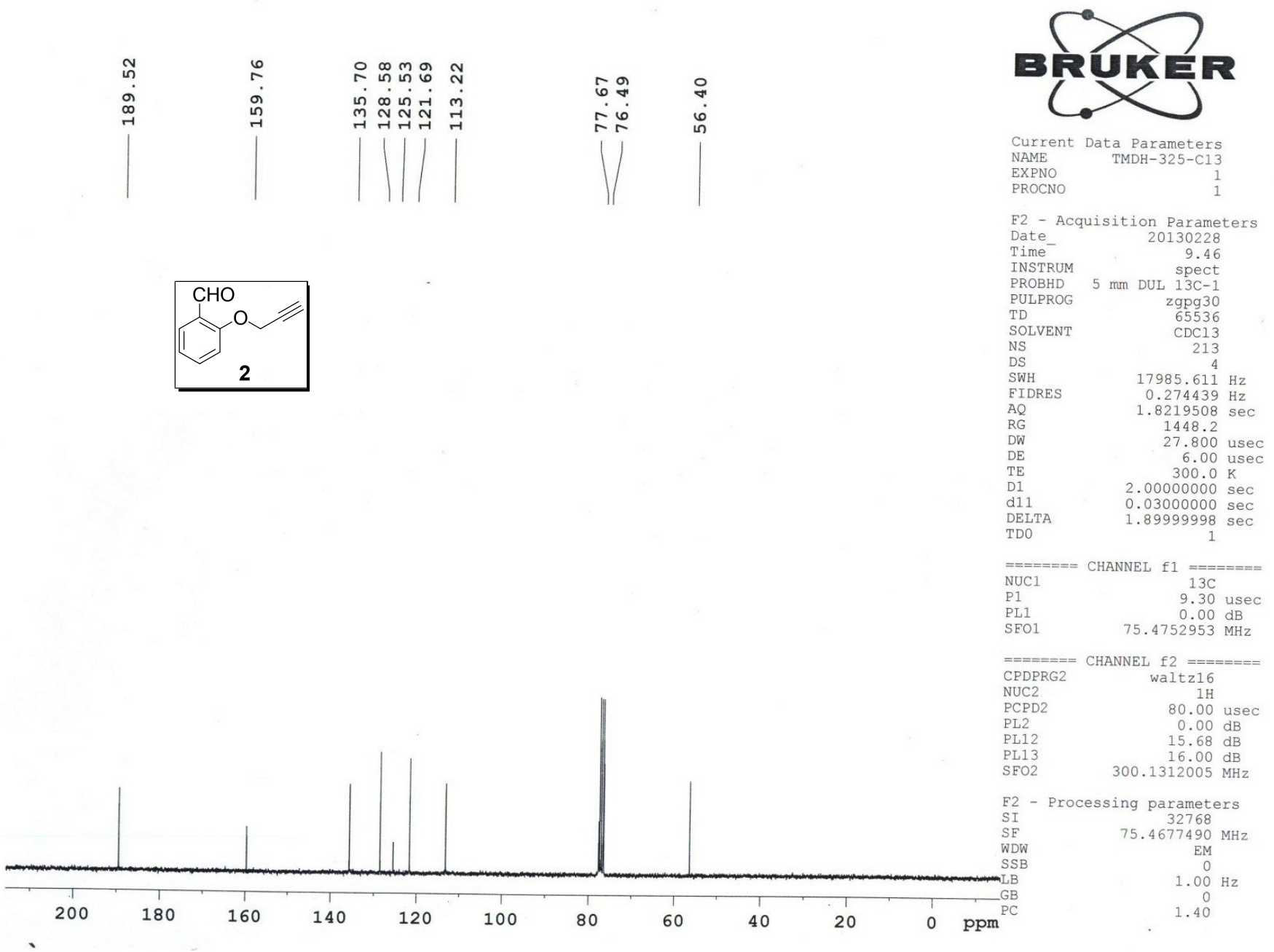

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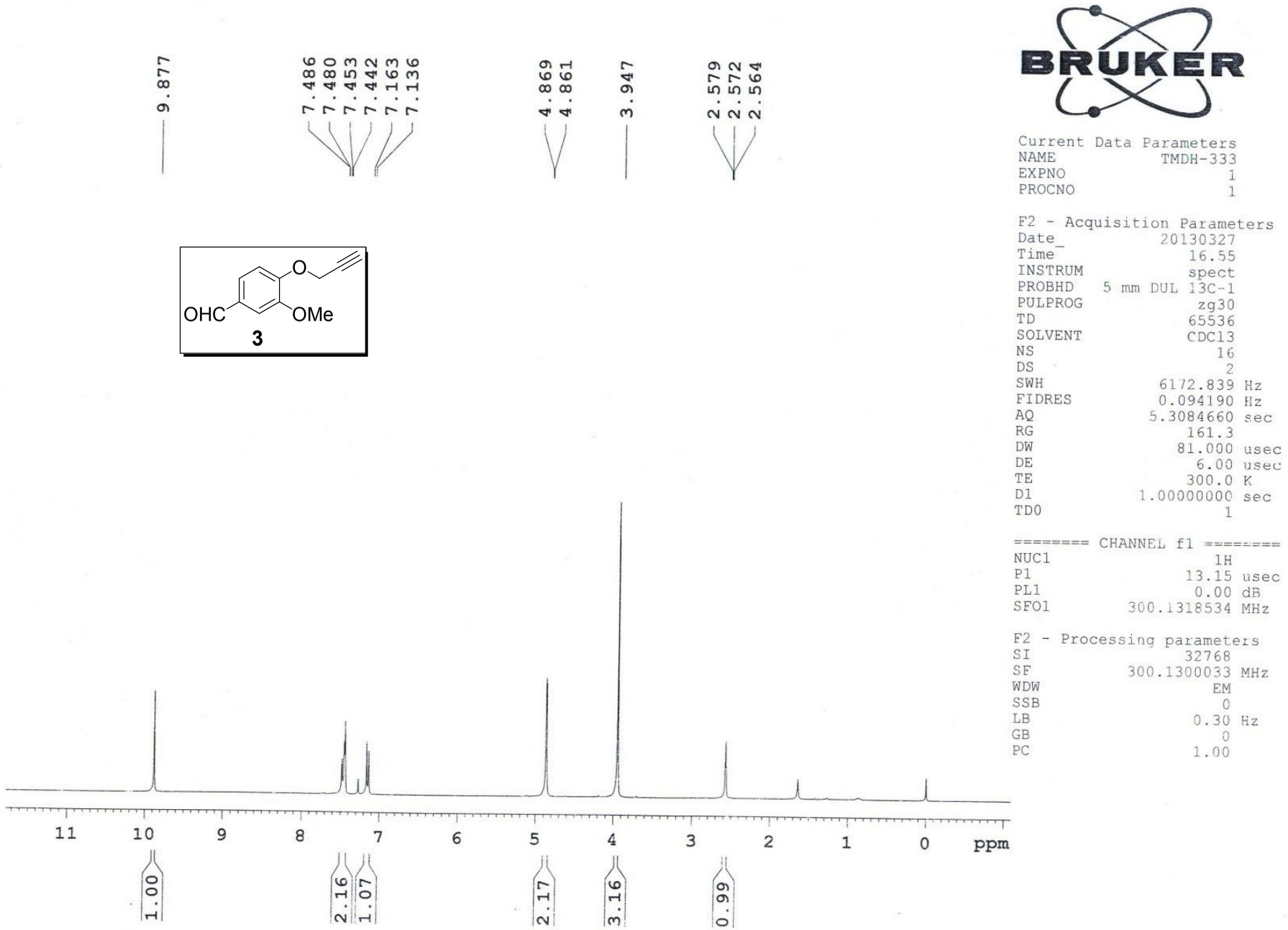
Figure 2 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 2



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DS 2
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FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 161.3
DW 81.000 usec
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TE 300.0 K
D1 1.00000000 sec
TD0 1

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F2 - Processing parameters
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Figure 3 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 3.

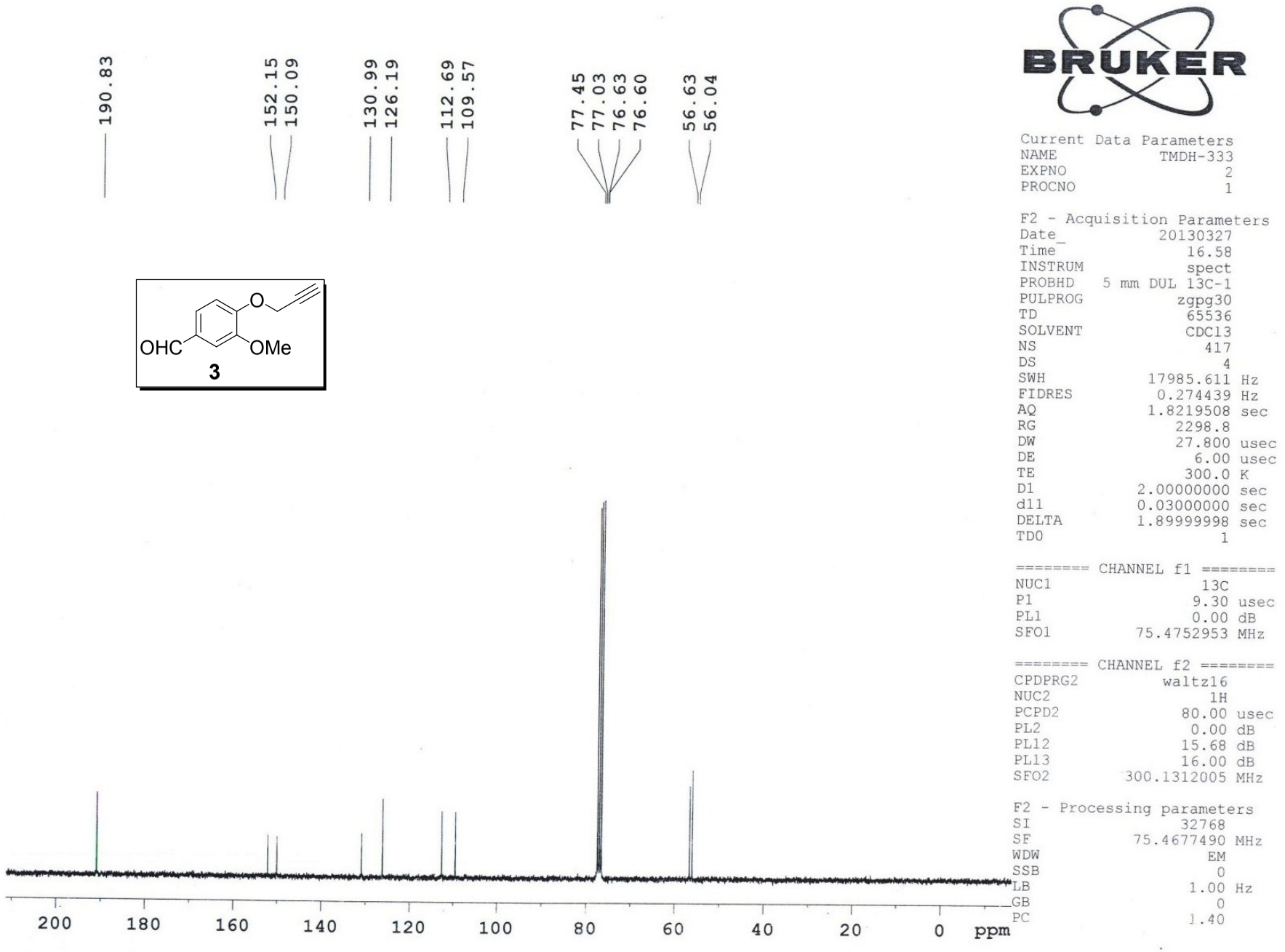


Figure 4 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 3

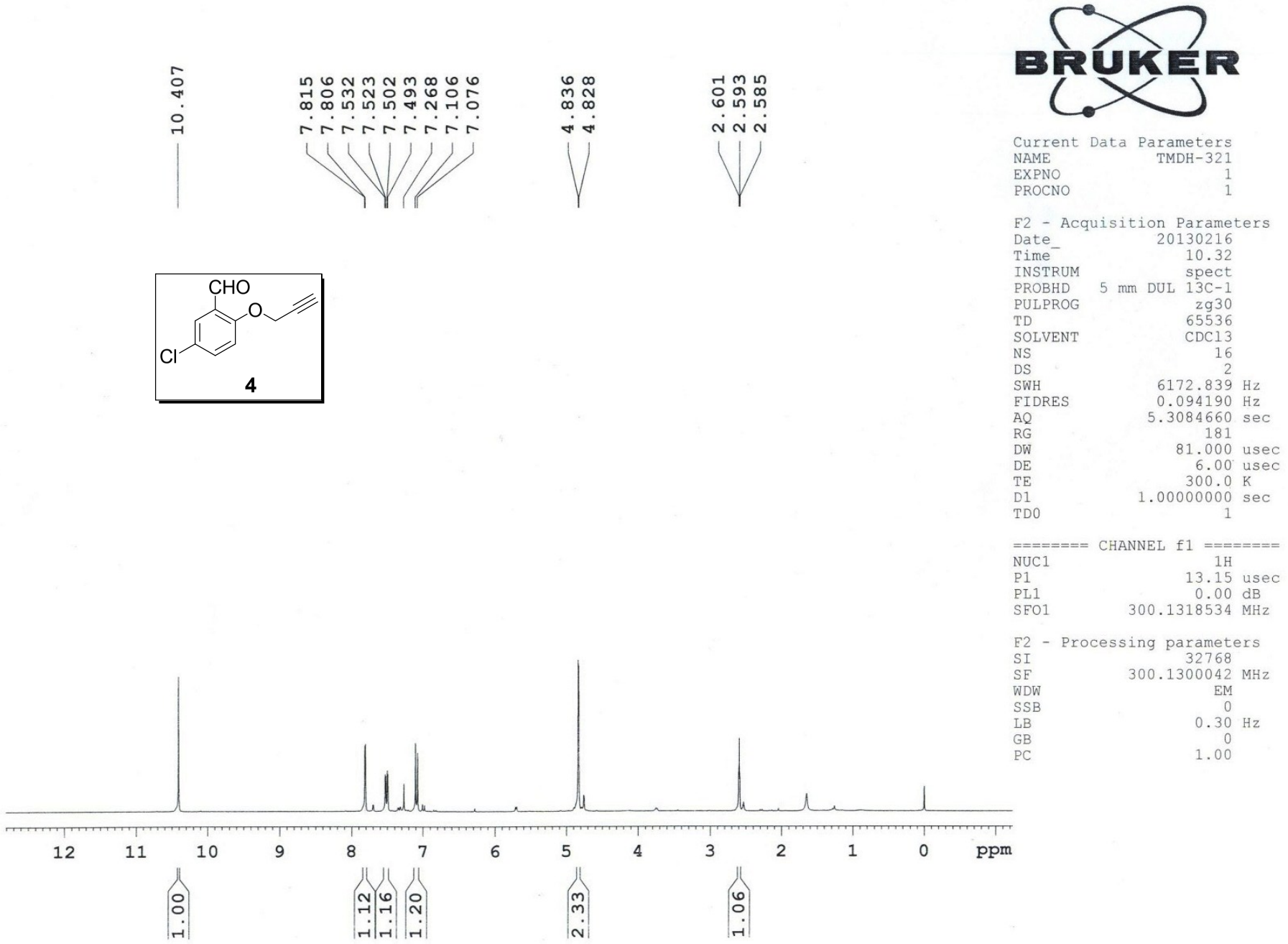


Figure 5 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 4.

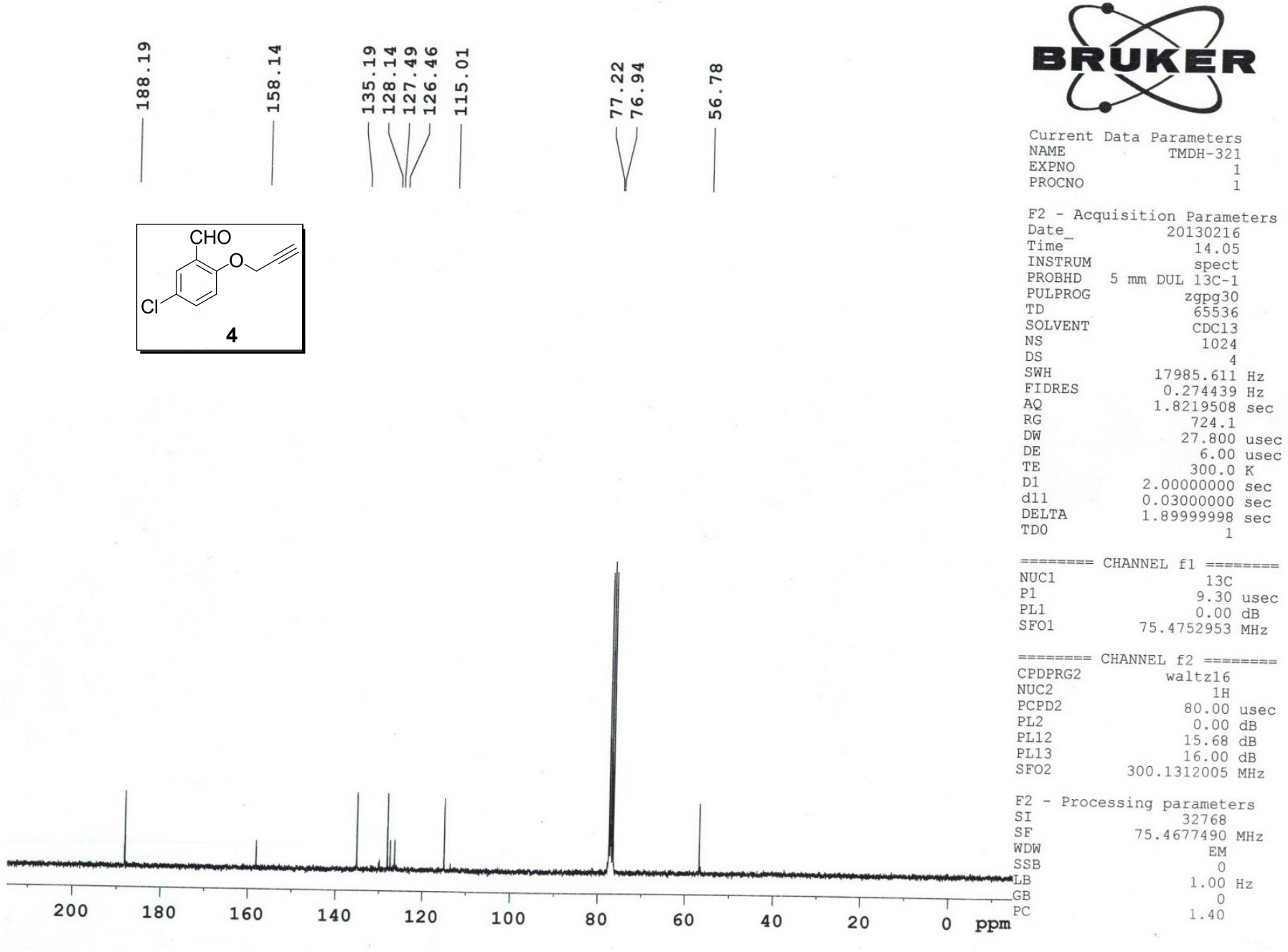
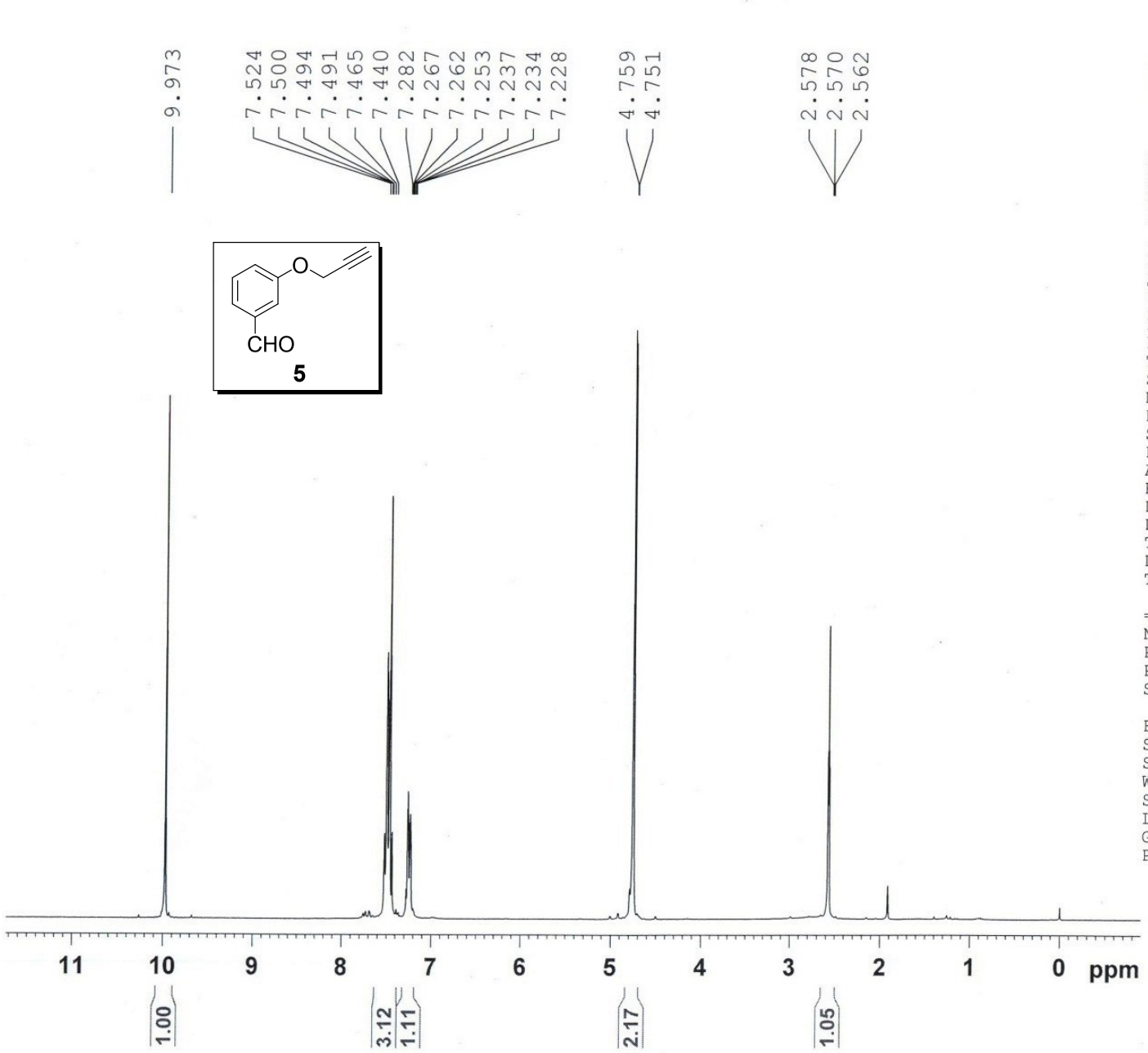


Figure 6 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 4.



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SOLVENT	CDCl3
NS	16
DS	2
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FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	57
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TD0	1

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PL1	0.00 dB
SFO1	300.1318534 MHz

F2 - Processing parameters

SI	32768
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Figure 7 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 5.

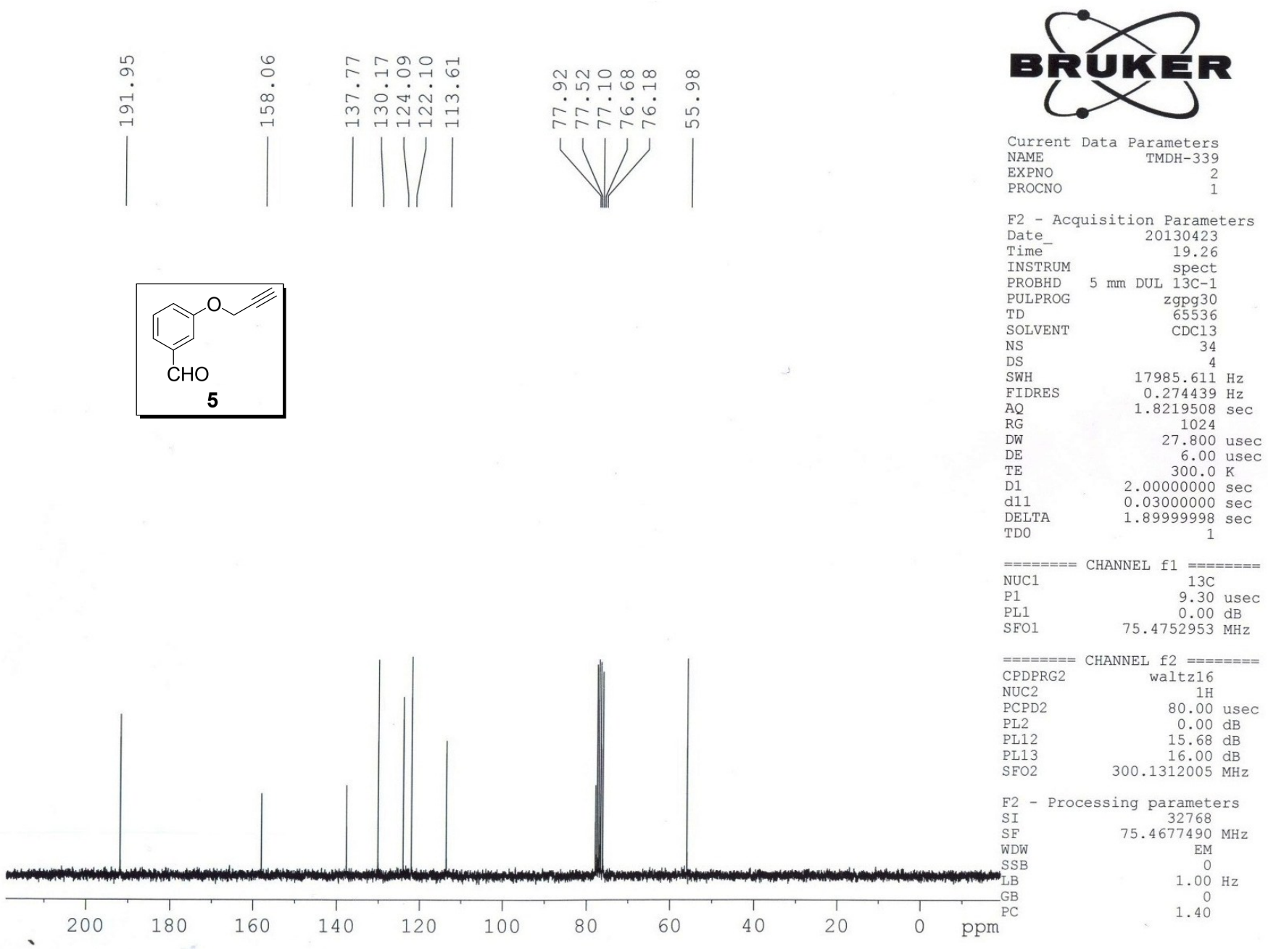


Figure 8 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 5.

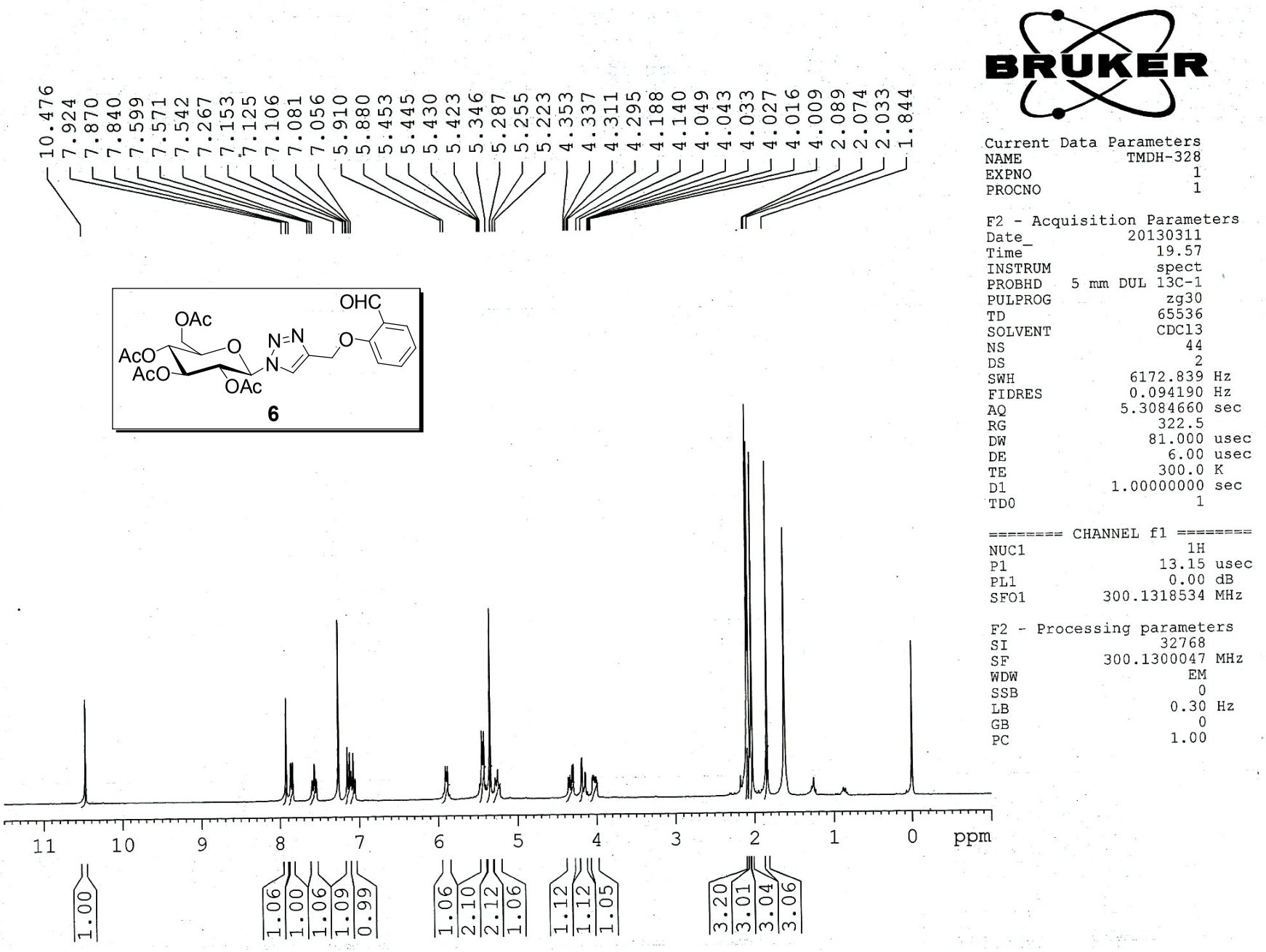


Figure 9 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 6.

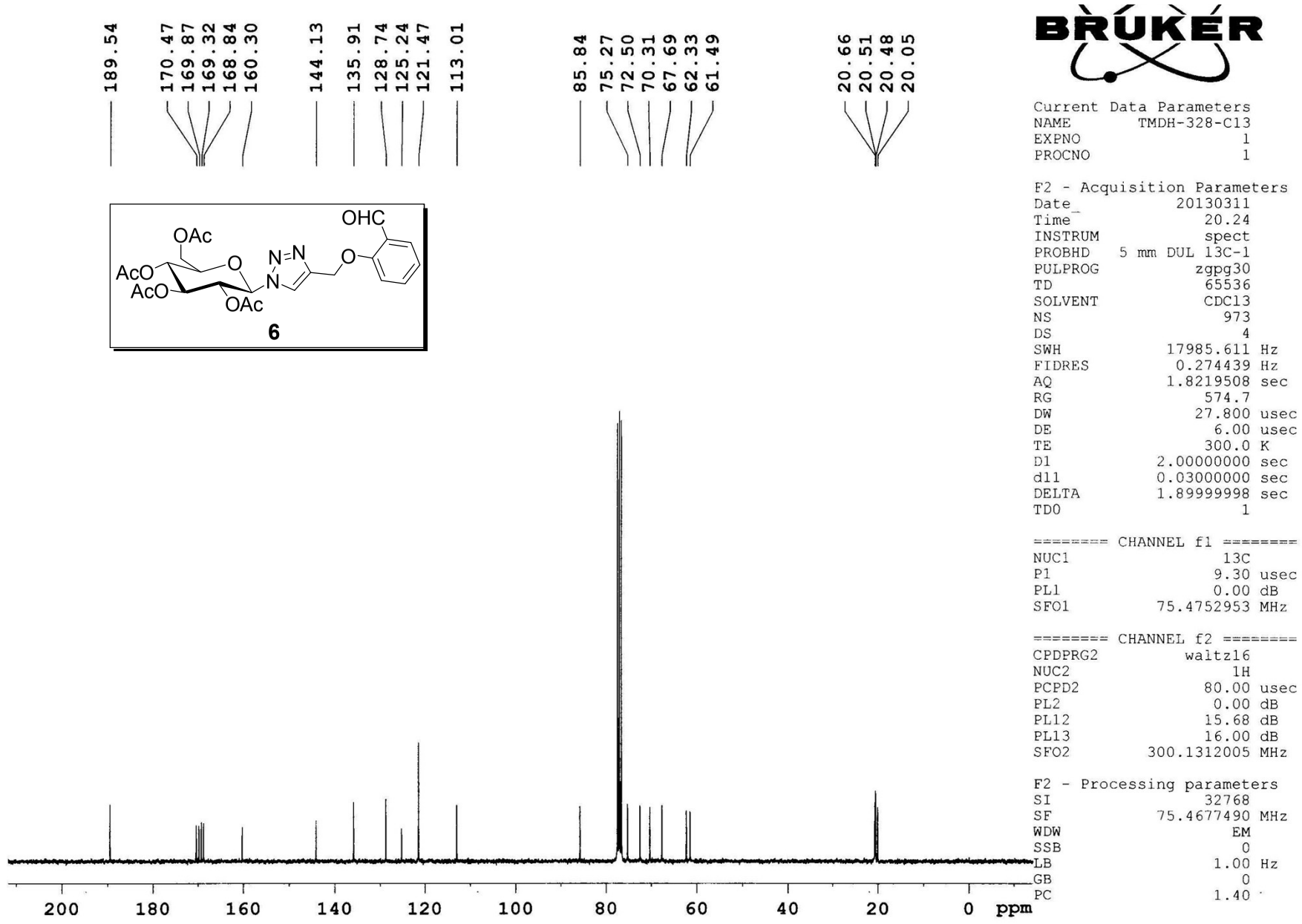
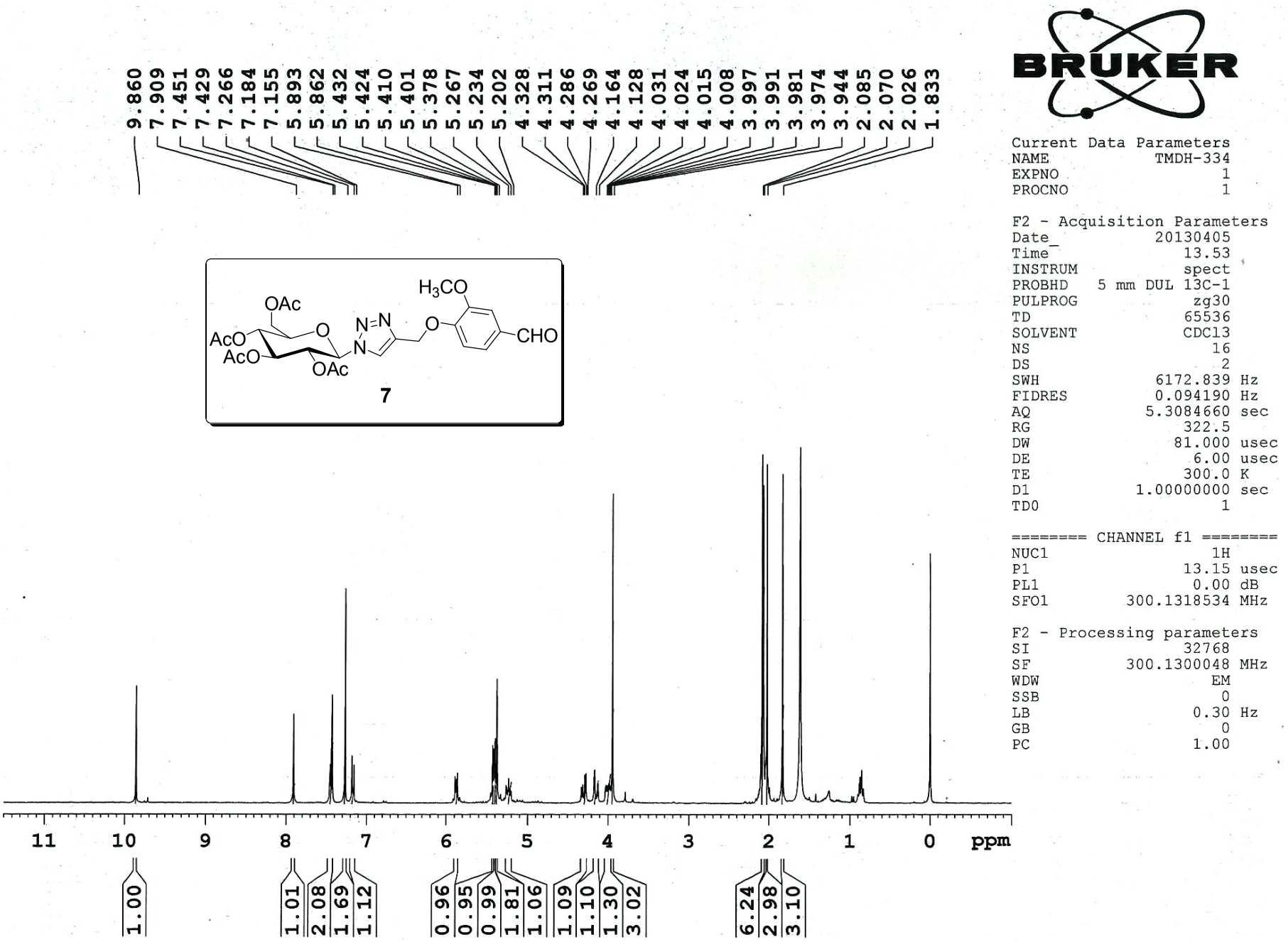


Figure 10 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 6

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SOLVENT                 CDCl3
NS                         16
DS                          2
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FIDRES               0.094190 Hz
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RG                       322.5
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P1                       13.15 usec
PL1                       0.00 dB
SFO1              300.1318534 MHz

F2 - Processing parameters
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Figure 11 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 7.

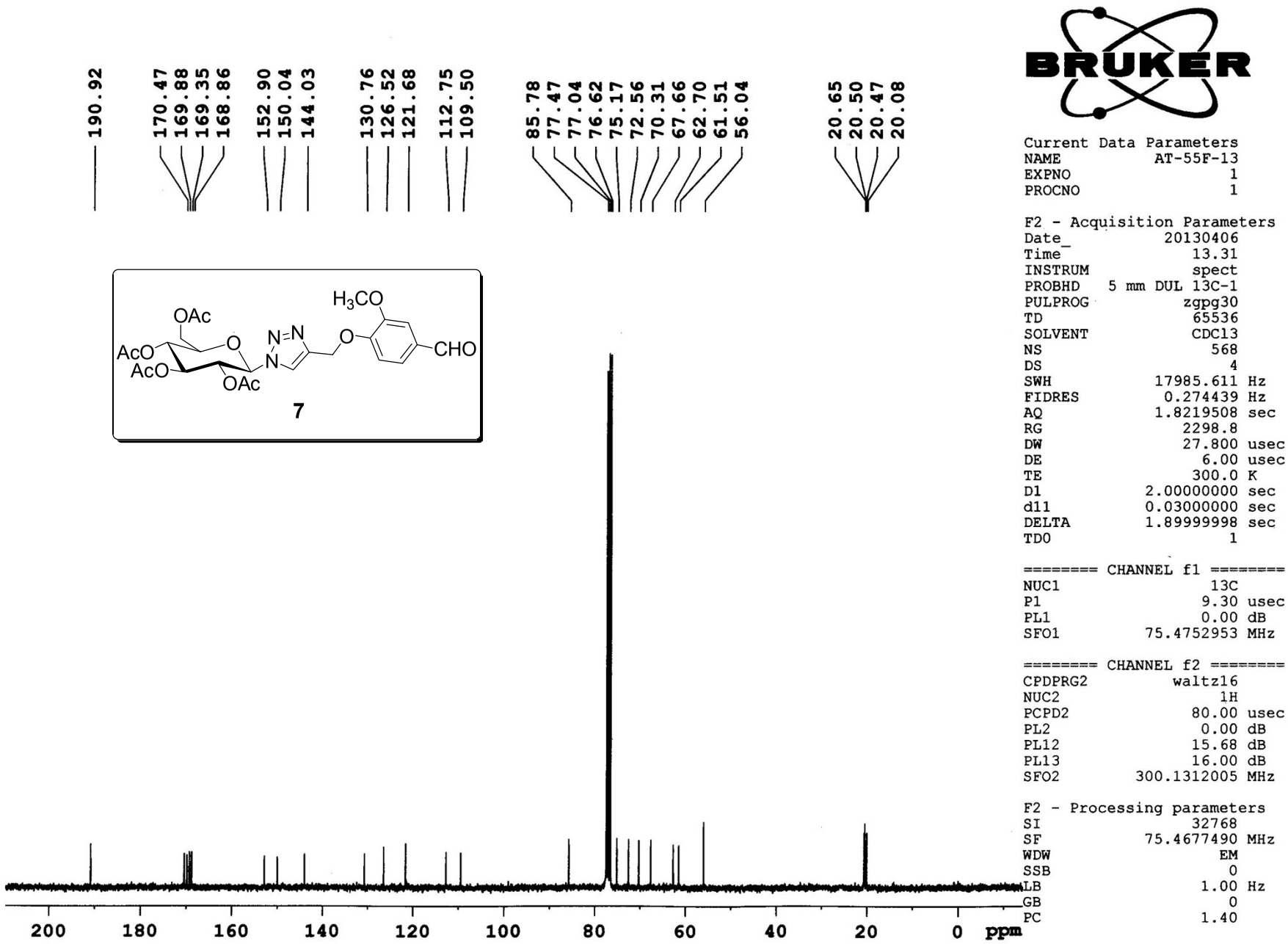

Figure 12 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 7.

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CNO                     1

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                  27.800 usec
                   6.00 usec
                  300.0 K
2           145.0000000
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                0.00344828 sec
                0.00002000 sec
A               0.00001184 sec
                        1

===== CHANNEL f1 ========
                      13C
                    9.30 usec
                   18.60 usec
                    0.00 dB
             75.4752953 MHz

===== CHANNEL f2 ========
PRG2              waltz16
                      1H
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                   26.30 usec
2                  80.00 usec
                    0.00 dB
                   15.68 dB
            300.1312005 MHz

- Processing parameters
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             75.4677490 MHz
                      EM
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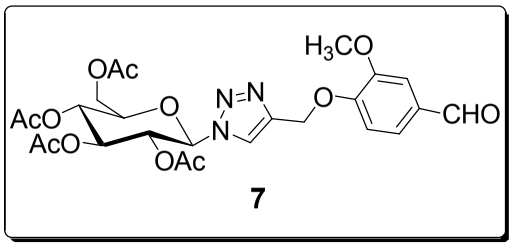

7

Figure 13 DEPT-135 spectrum (75 MHz, $CDCl_3$) of compound, 7.

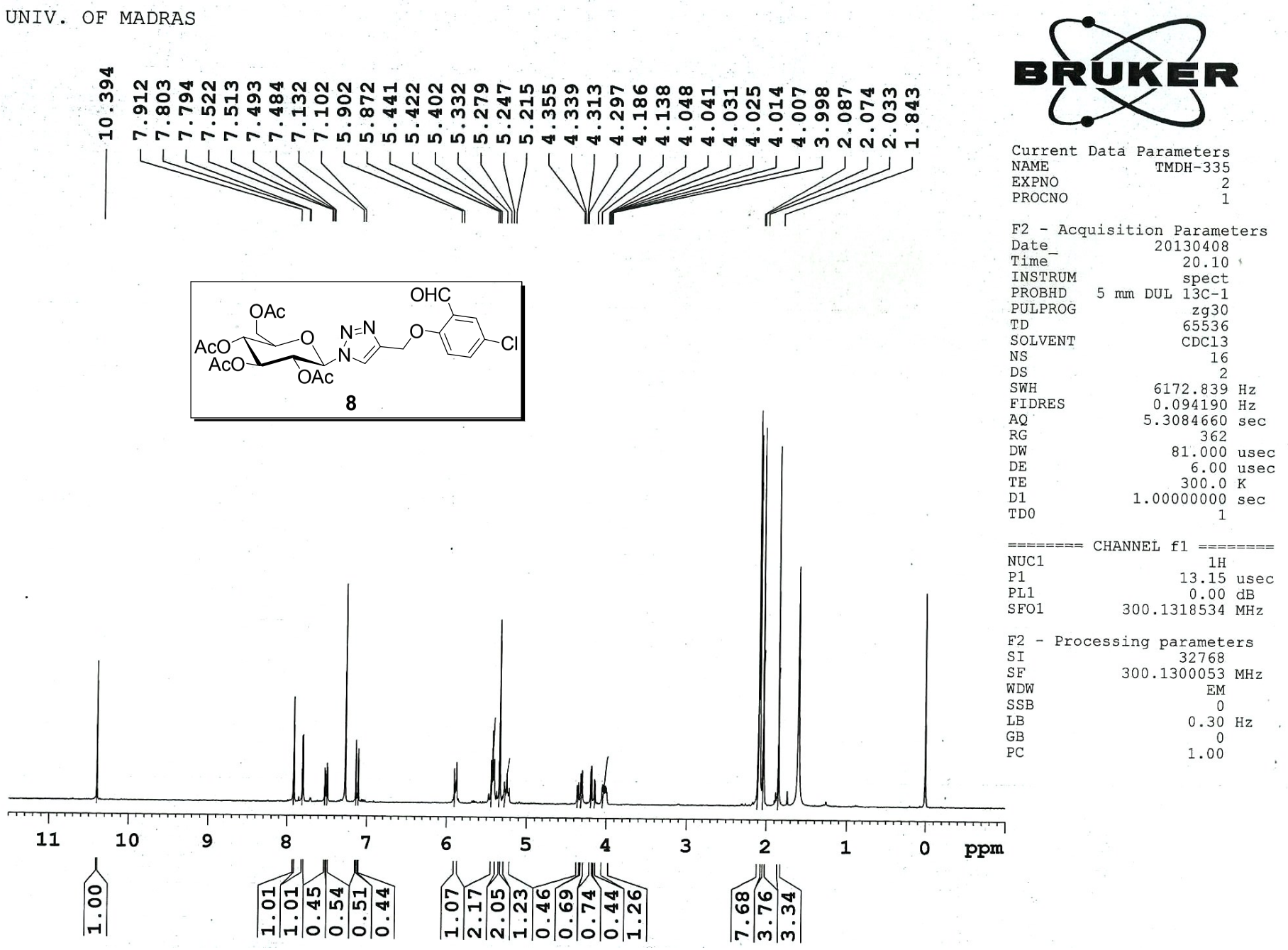

Figure 14 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 8.

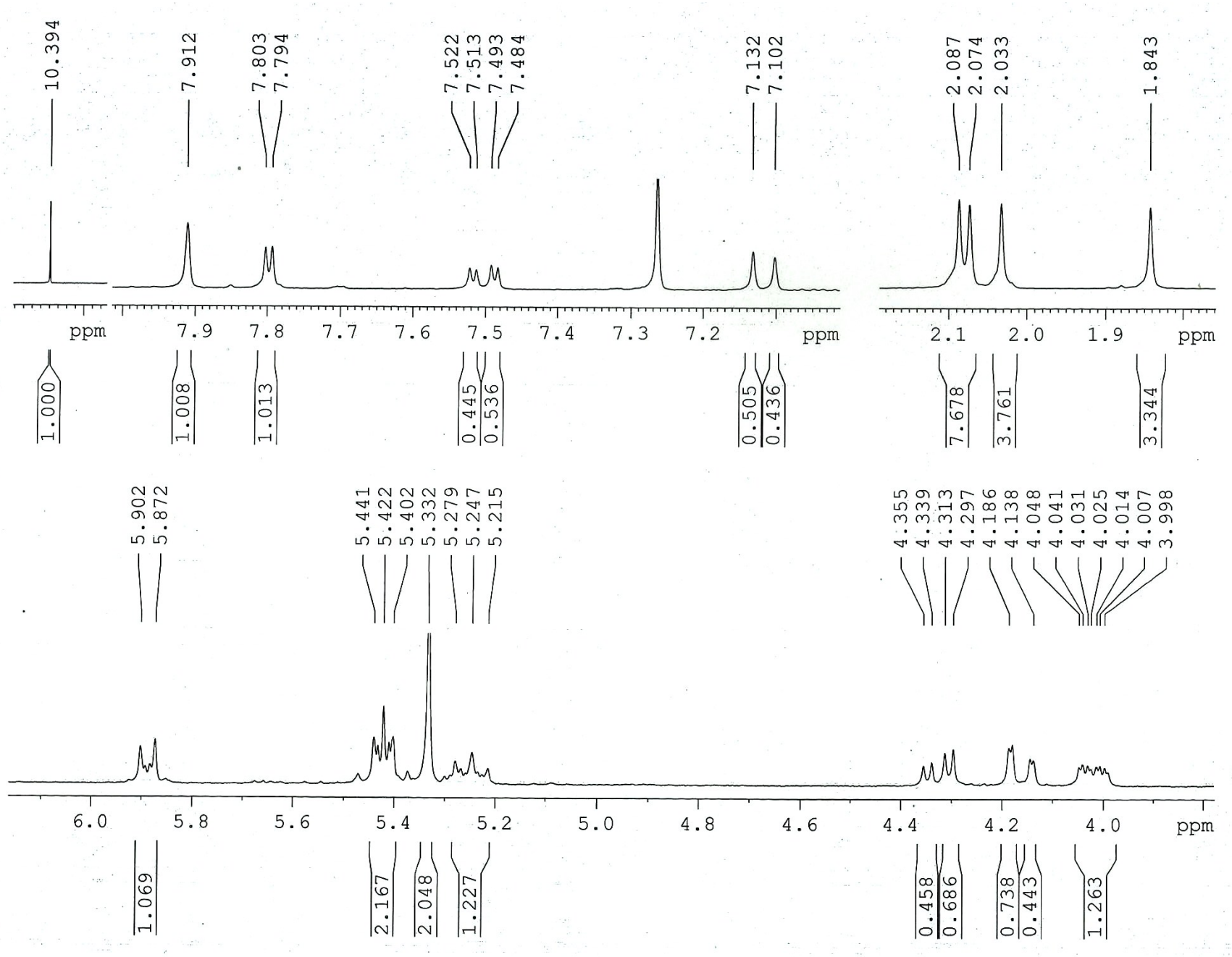

Figure 15 ^{1}H NMR expansion spectrum (300 MHz, $CDCl_3$) of compound, 8.

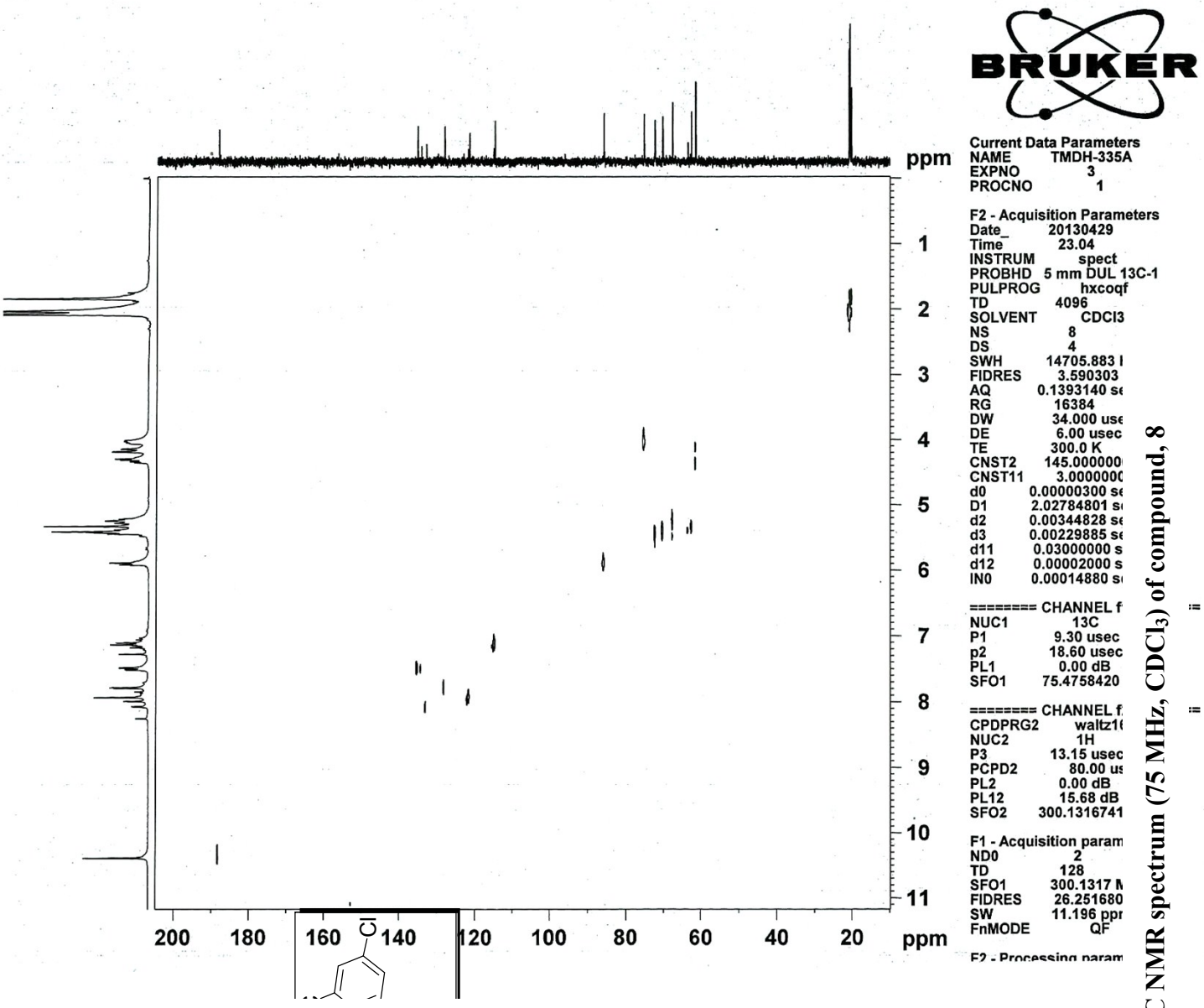

Figure 17 ^{1}H - ^{13}C COSY spectrum ($CDCl_3$) of compound, 8


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SFO1       75.4758420

======== CHANNEL f
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NUC2              1H
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PCPD2          80.00 us
PL2            0.00 dB
PL12           15.68 dB
SFO2       300.1316741

F1 - Acquisition param
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F2 - Processing param
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Figure 16 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 8

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FIDRES        0.274439 Hz
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RG                1625.5
DW            27.800 usec
DE             6.00 usec
TE             300.0 K
CNST2          2.000000000 sec
CNST11         0.030000000 sec
d0             1.89999998 sec
D1                   1

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PL1            0.00 dB
SFO1       75.4752953 MHz

======== CHANNEL f2 ========
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PL12           15.68 dB
PL13           16.00 dB
SFO2       300.1312005 MHz

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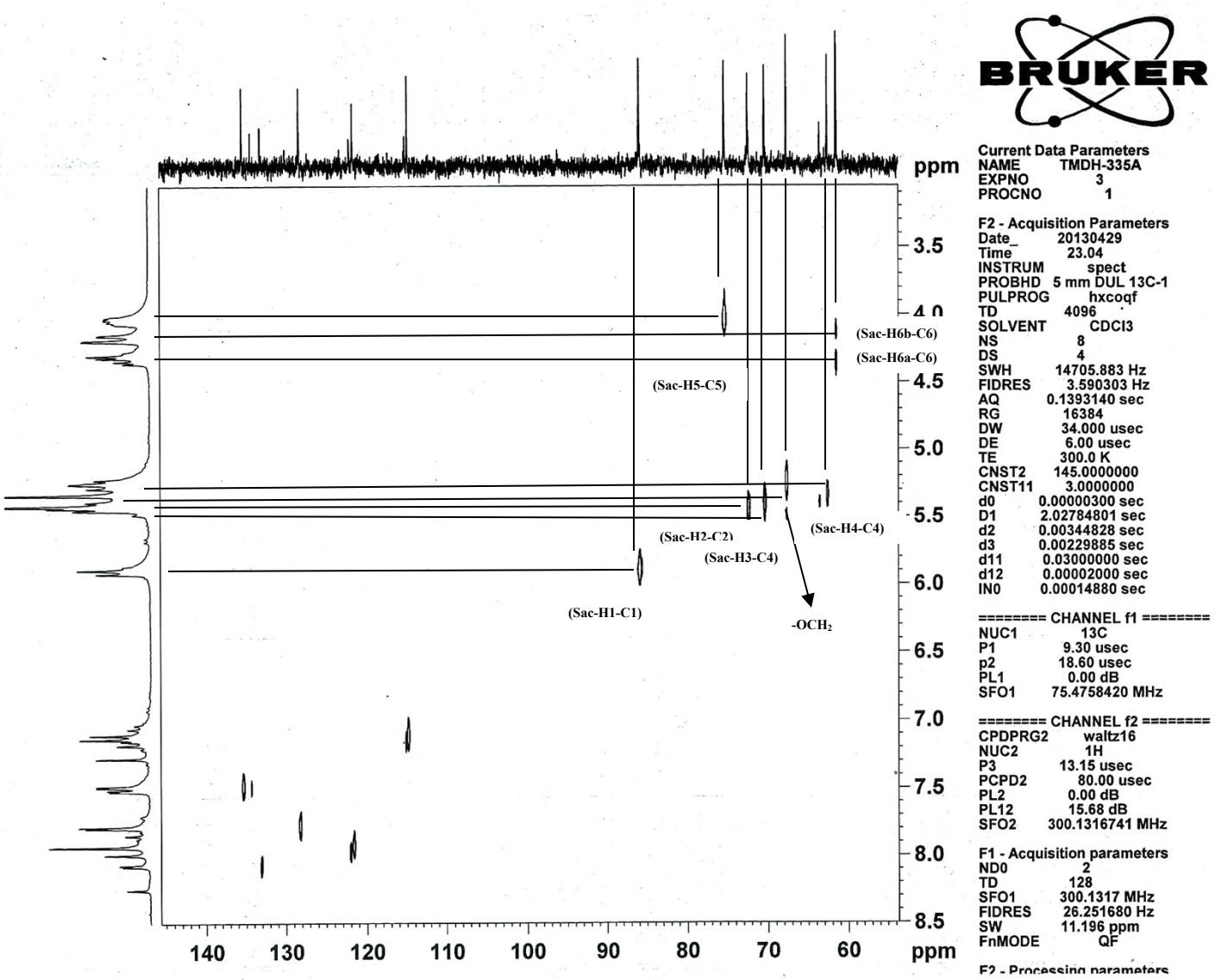
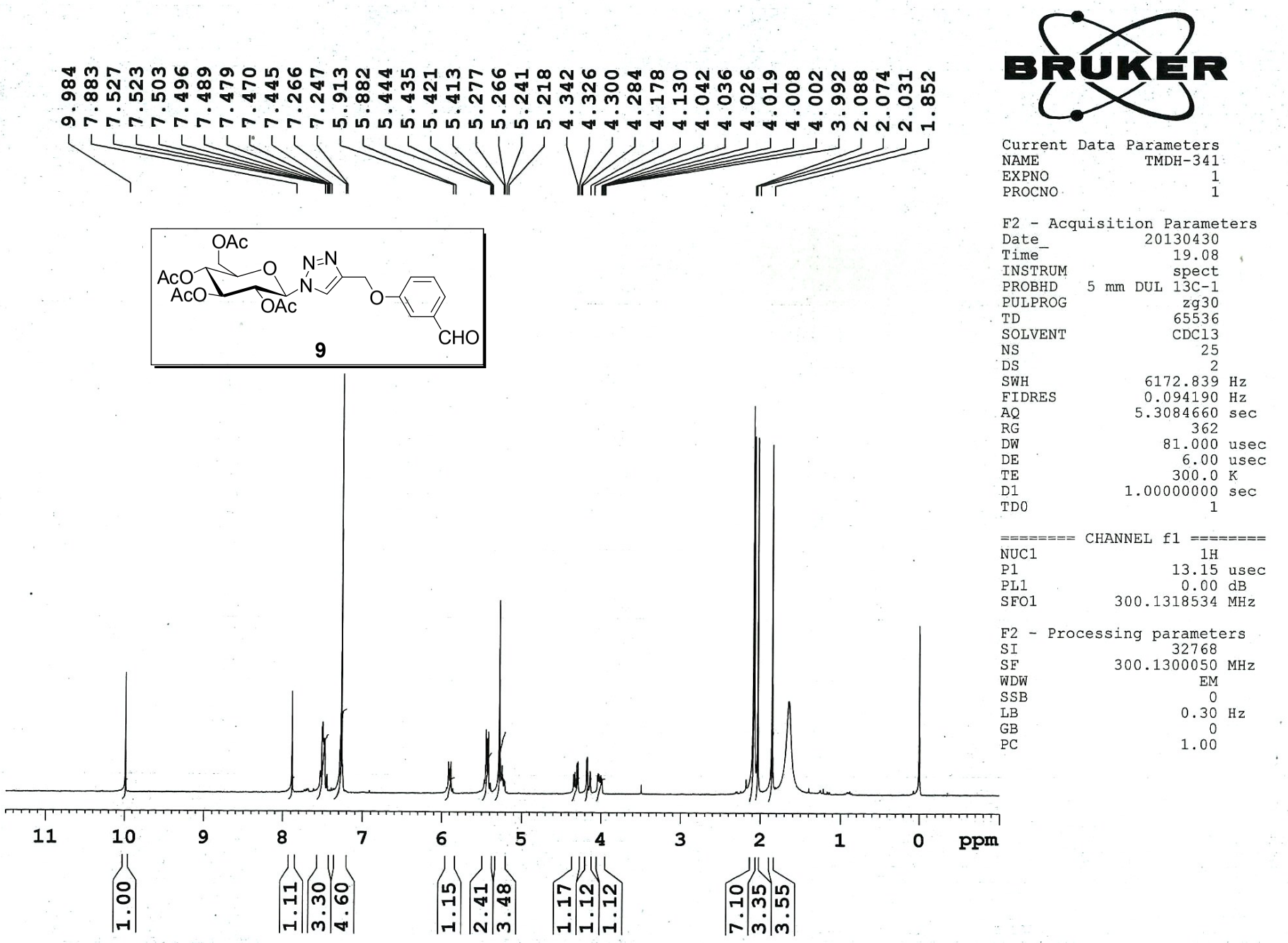


Figure 18 ^{1}H - ^{13}C COSY expansion spectrum ($CDCl_3$) of compound, 8



BRUKER

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SOLVENT                CDCl3
NS                        25
DS                         2
SWH                 6172.839 Hz
FIDRES              0.094190 Hz
AQ                  5.3084660 sec
RG                       362
DW                    81.000 usec
DE                     6.00 usec
TE                     300.0 K
D1                1.00000000 sec
TD0                        1

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PL1                     0.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
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Figure 19 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 9.

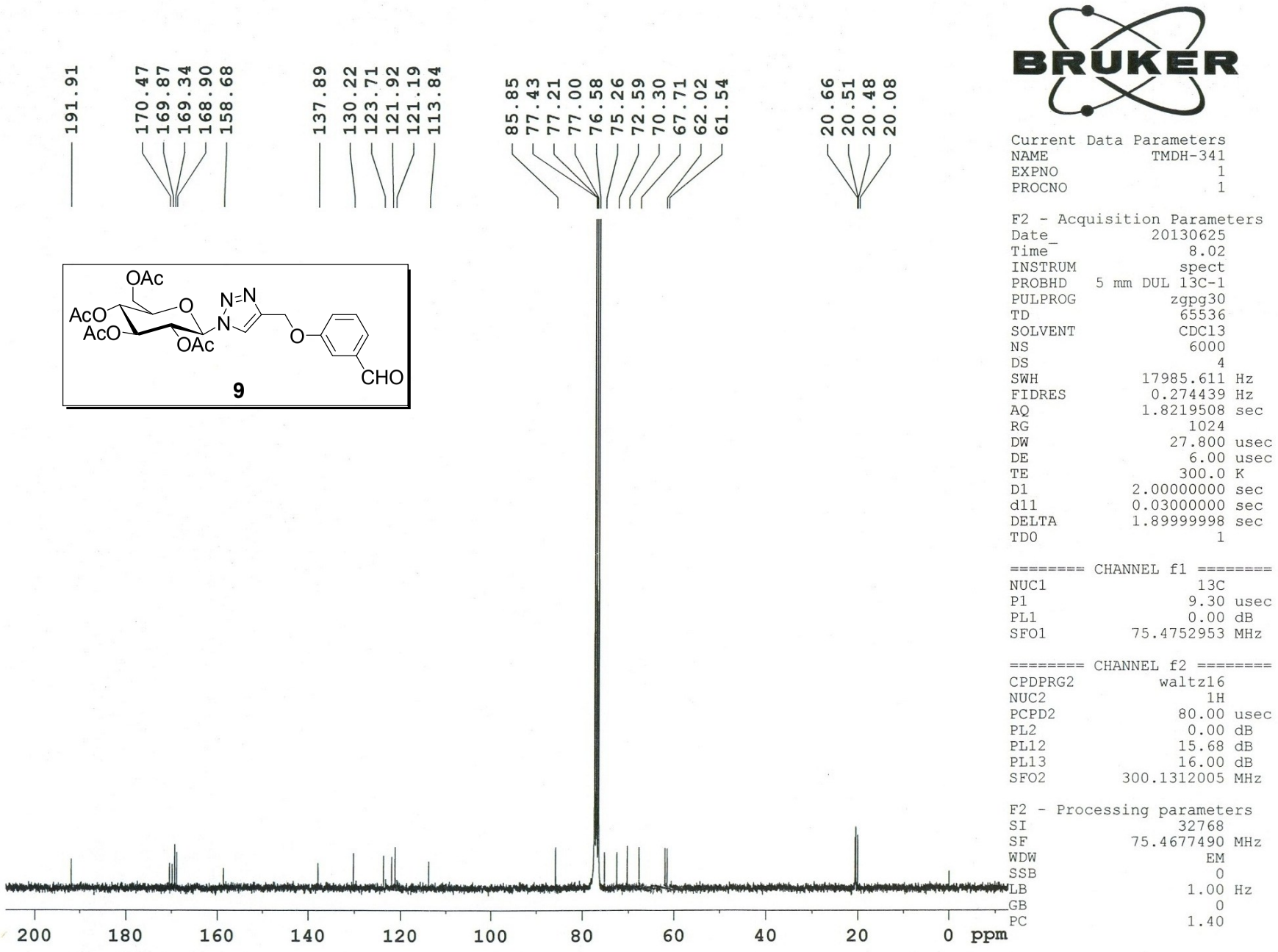


Figure 20 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 9.

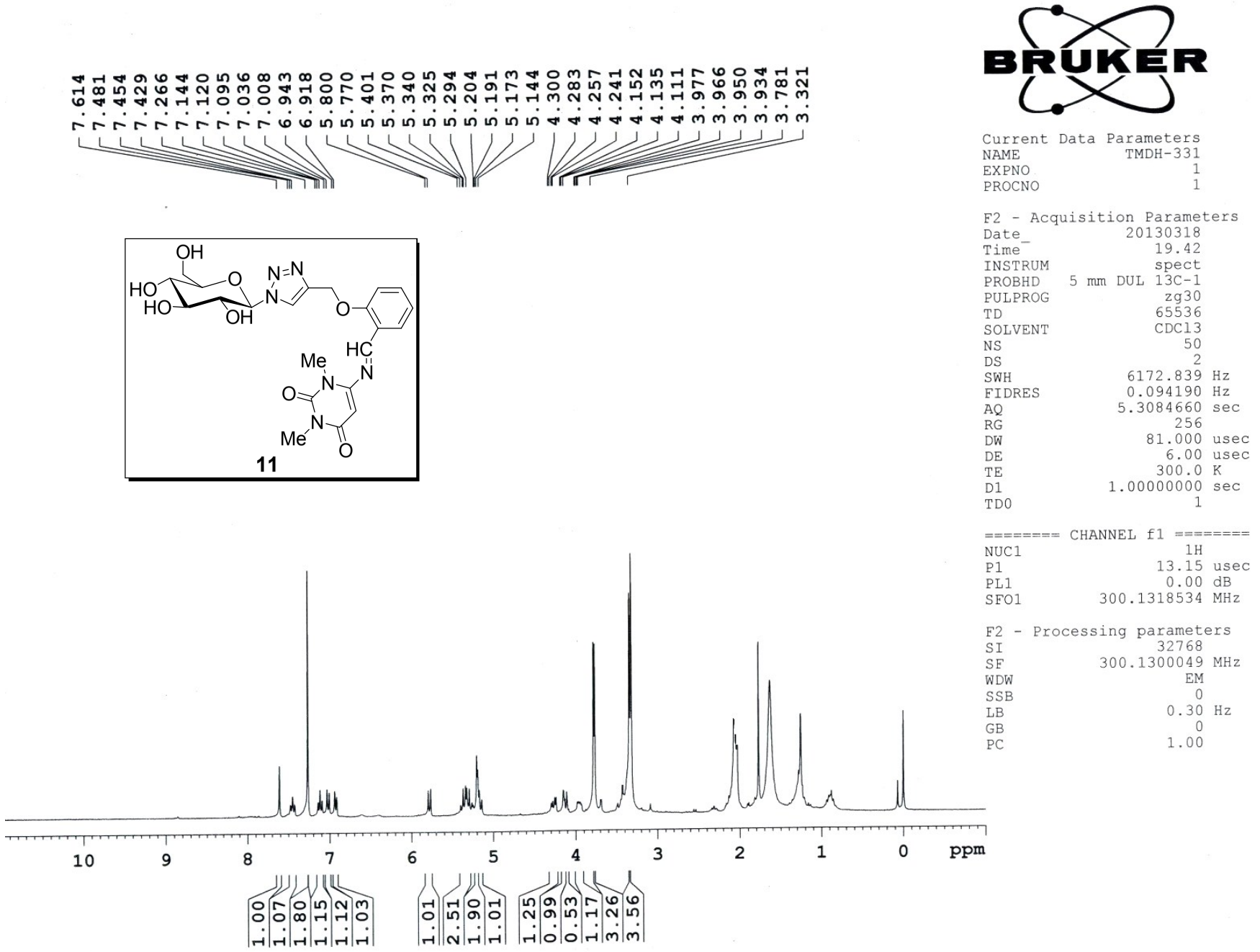


Figure 21 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 11.

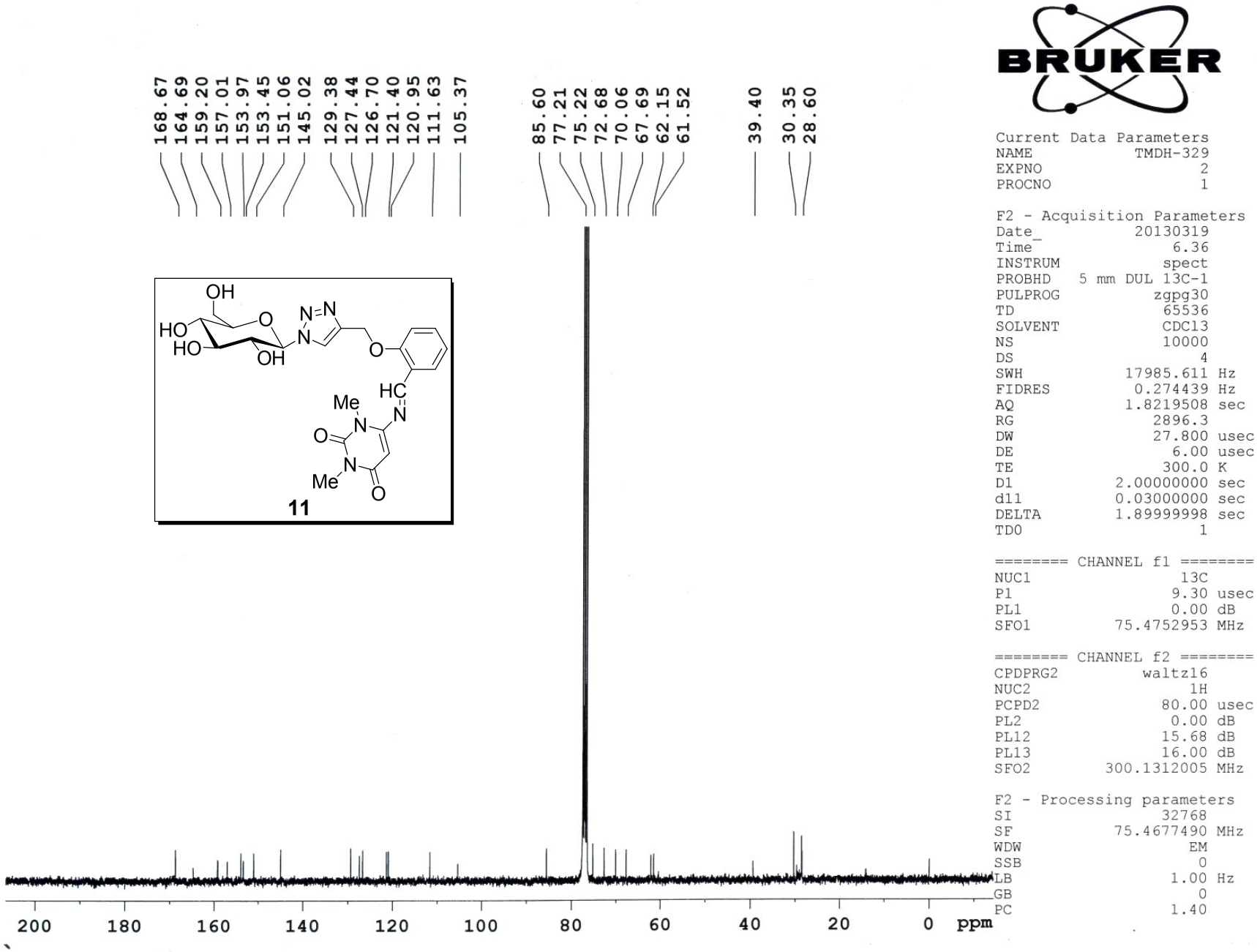


Figure 22 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 11.

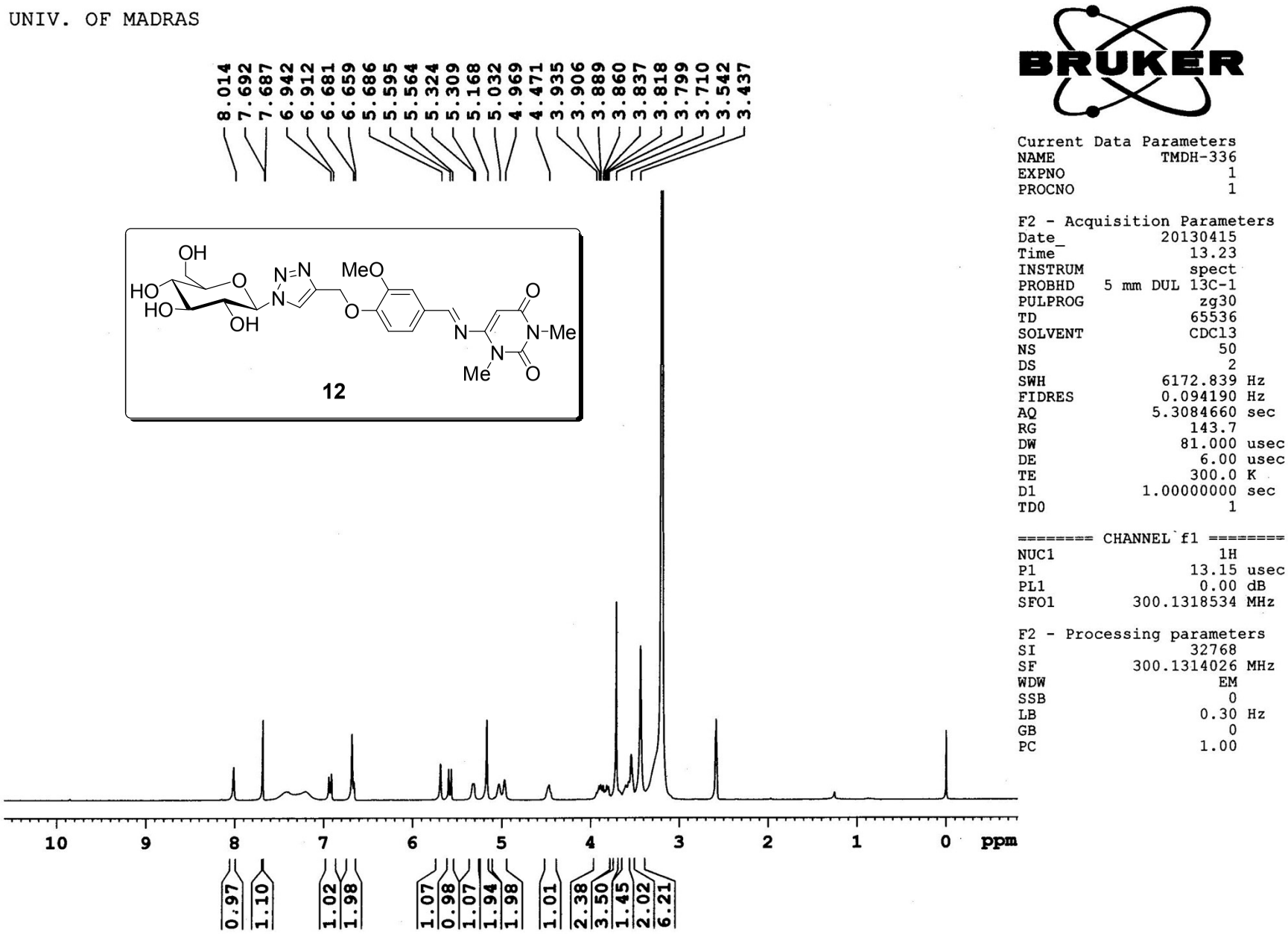


Figure 23 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 12.

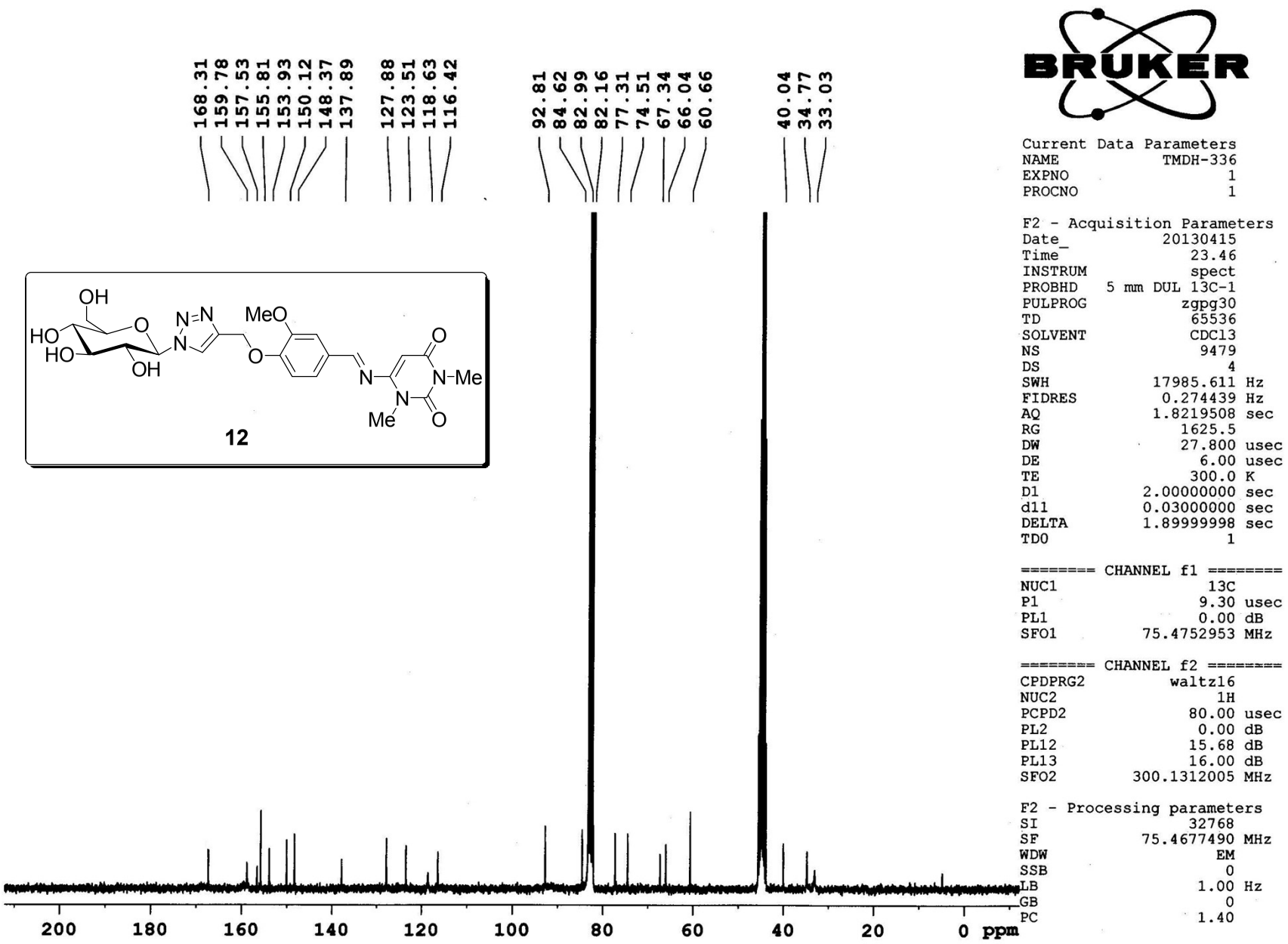


Figure 24 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 12.

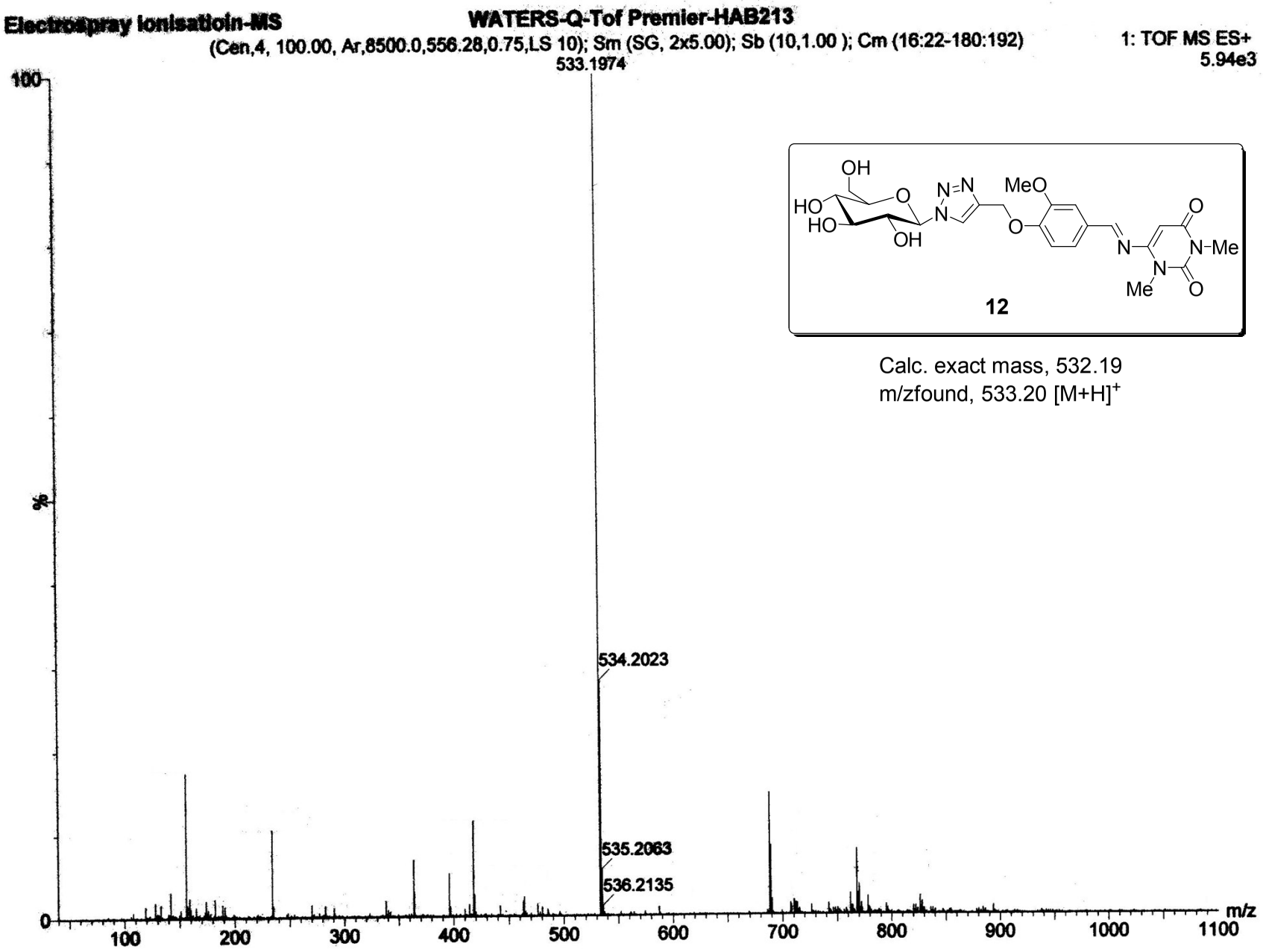


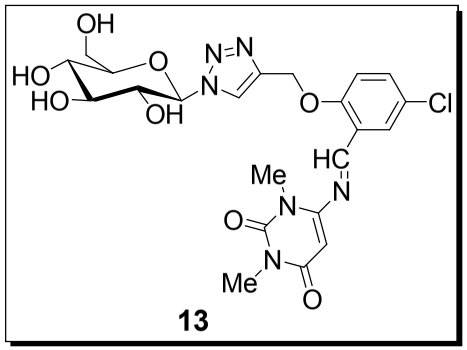
Figure 25 Mass spectrum of compound, 12.

```
Current Data Parameters
NAME            TMDH-338
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130422
Time               19.55
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    50
DS                     2
SWH              6172.839 Hz
FIDRES           0.094190 Hz
AQ               5.3084660 sec
RG                 203.2
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.15 usec
PL1                 0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1314005 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



ppm

Figure 26 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 13.

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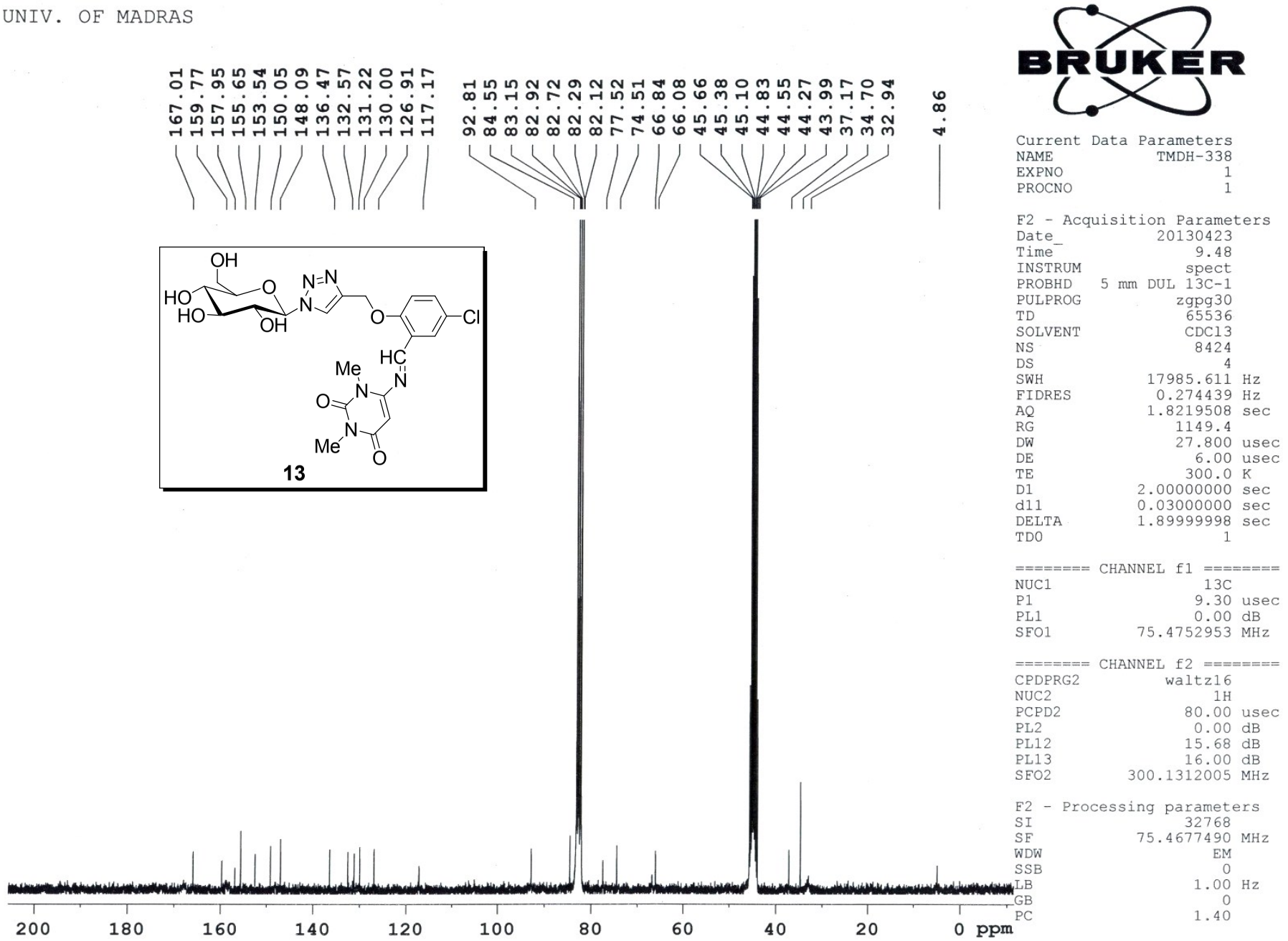


BRUKER

Current Data Parameters
NAME TMDH-338
EXPNO 1
PROCNO 1

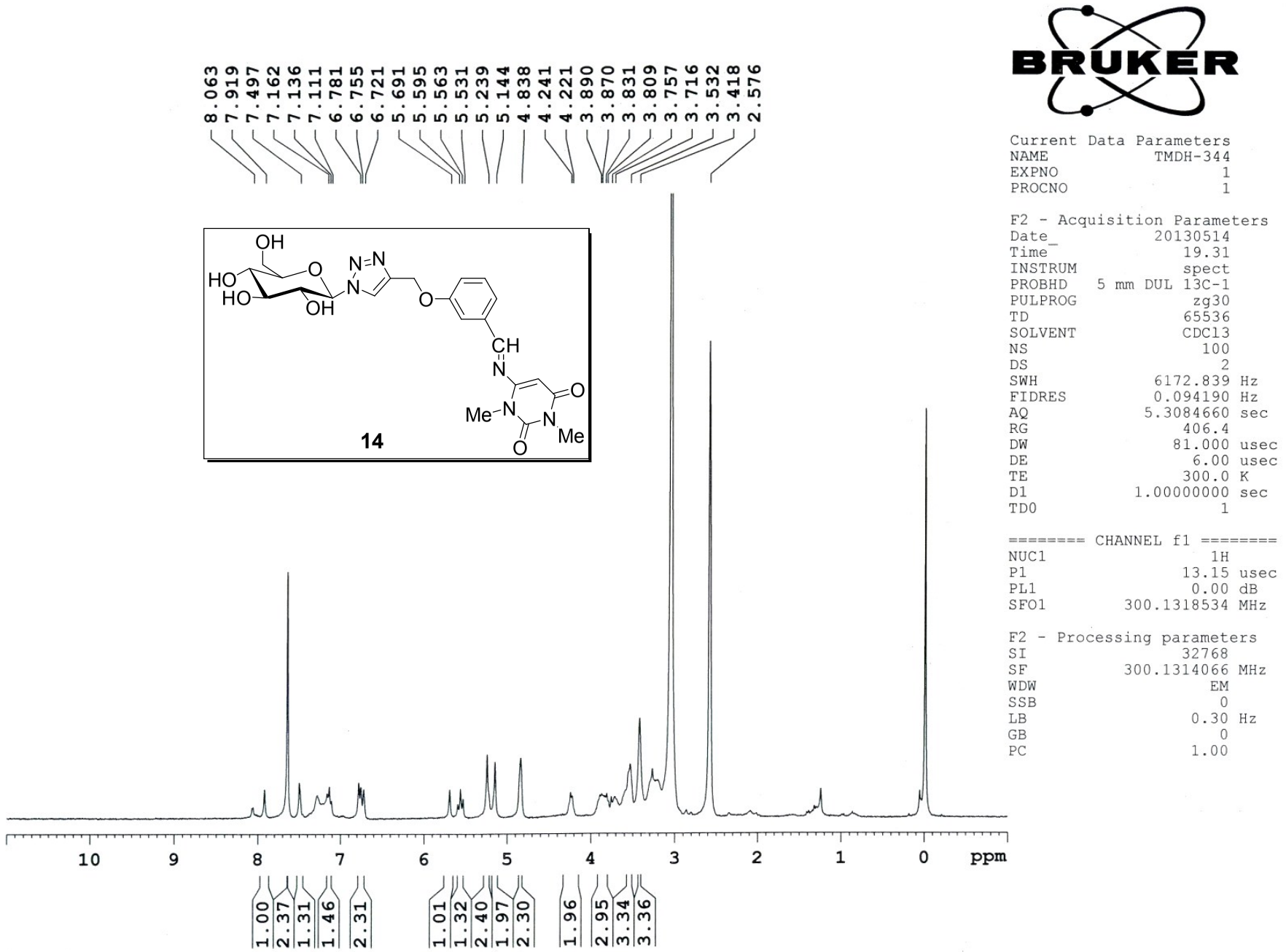
F2 - Acquisition Parameters
Date_ 20130423
Time 9.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8424
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1149.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 27 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 13.



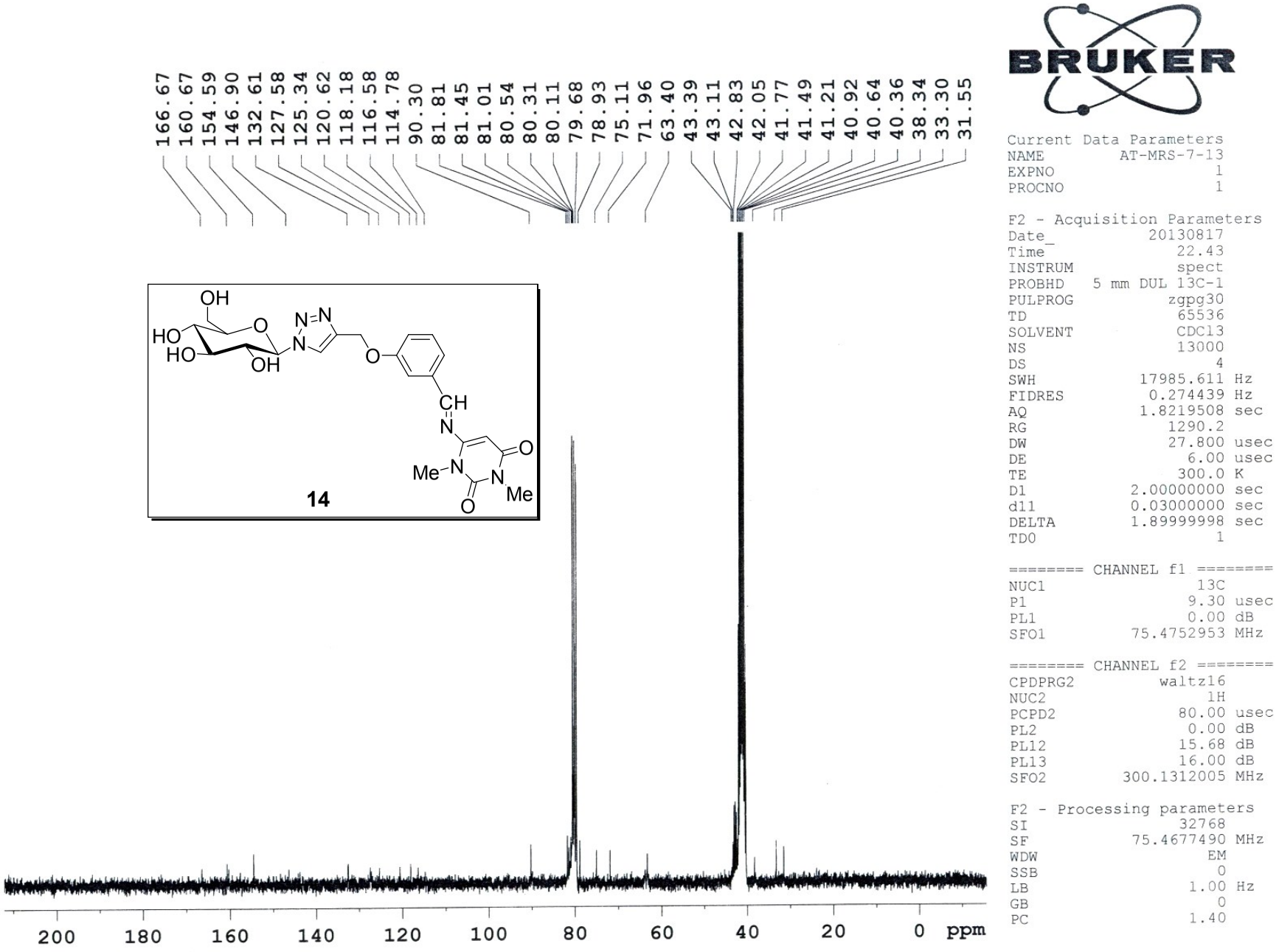

```
Current Data Parameters
NAME            TMDH-344
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130514
Time               19.31
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                   100
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                 406.4
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.15 usec
PL1                0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1314066 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00
```

Figure 28 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 14.



BRUKER

```
Current Data Parameters
NAME          AT-MRS-7-13
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130817
Time                22.43
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                 13000
DS                     4
SWH           17985.611 Hz
FIDRES         0.274439 Hz
AQ            1.8219508 sec
RG               1290.2
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.30 usec
PL1                  0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.68 dB
PL13               16.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Figure 29 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 14.

Docking Studies:

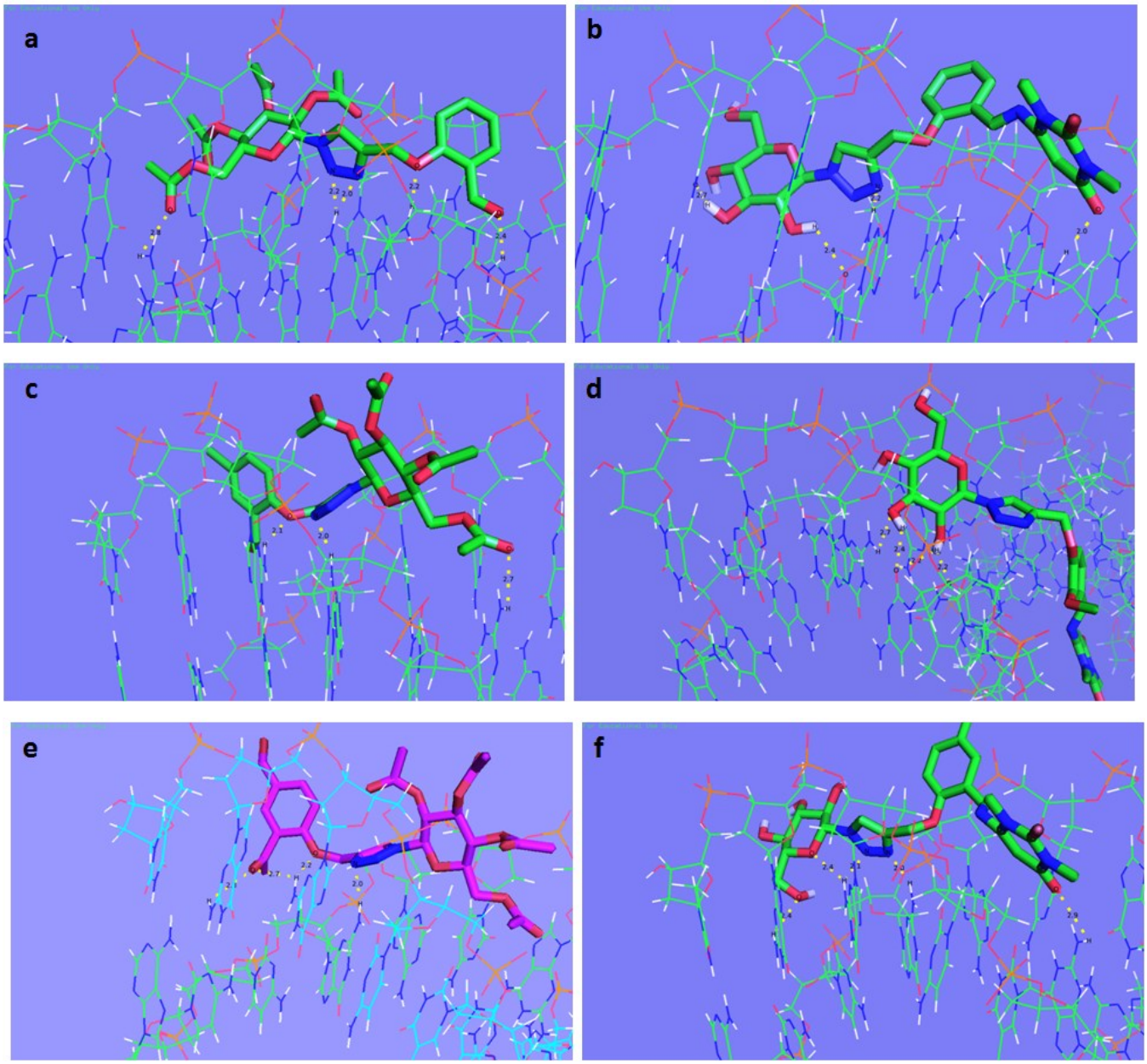


Figure 30 Hydrogen bonding interaction of compounds (a) **6**, (b) **11**,(c) ,**7** (d) **12**, (e) ,**8** (f) **13**.