Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

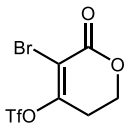
General Information

All reactions were carried out under an argon atmosphere using dry solvents under anhydrous conditions, unless otherwise stated. All chemicals were purchased commercially, and used without further purification. Anhydrous toluene, dichloromethane, tetrahydrofuran, *N*,*N*-dimethylformamide were purchased from Sigma-Aldrich Corporation and used without further purification. Flash chromatography was performed using 230-400 mesh Silica Flash 60® silica gel (Silicycle Inc.). Reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm plates (60F-254) coated with silica gel, using UV light and an aqueous solution of potassium permanganate and sodium carbonate as well as heat as visualizing agents. Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator. Yields refer to chromatographically purified compounds, unless otherwise stated.

NMR spectra were recorded on either a Bruker Avance 400 (^{1}H: 400 MHz, ^{13}C: 100 MHz), or a Bruker Avance III HD 600 (^{13}C:150 MHz), and were internally referenced based on solvent peaks (for $CDCl_3$, referenced as 7.26 (^{1}H) and 77.0 ppm (^{13}C)). High-resolution mass spectrometric data were obtained using Agilent Technologies 6530 Accurate-Mass Q-TOF LC/MS. Infrared spectra were recorded using a Perkin-Elmer Spectrum Two IR spectrometer.

The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad.

5-bromo-6-oxo-3,6-dihydro-2H-pyran-4-yl trifluoromethanesulfonate (5)

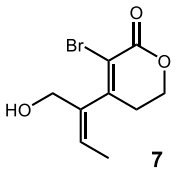


5

N-bromosuccinimide (1.2 g, 6.4 mmol) was added to a solution of dihydro-2H-pyran-2,4(3H)-dione (**4**) (730 mg, 6.40 mmol) in *t*-BuOH (10 mL) under argon. The reaction mixture was concentrated after stirring at room temperature for 2 h. The residue was dissolved in dry DCM (30 mL). Triethylamine (1.3 g, 13 mmol) was added to the mixture under argon. Then trifluoromethanesulfonic anhydride (2.17 g, 7.68 mmol) was added to the mixture dropwise at 0 ^{o}C. The mixture was stirred at 0 ^{o}C for 20 min. After being concentrated *in vacuo*, the residue

was purified by column chromatography (hexanes: ethyl acetate = 5:1) to give compound **5** (1.3 g, 62%) as a light yellow oil, R_f = 0.4 (hexanes/ethyl acetate = 2:1); **IR** ν_{max} (film)/cm^{-1} 1744, 1643, 1432, 1222, 1134, 1089; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.51 (t, J = 6.4 Hz, 2H), 2.99 (t, J = 6.4 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.1, 158.2, 119.7 (q, J = 319 Hz), 107.1, 64.2, 29.1; **HR-MS** *m/z* calcd for $C_6H_5BrF_3O_5S$ $[M + H]^+$ 324.8988 and 326.8967, found 324.8975 and 326.8964.

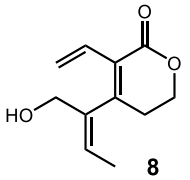
(*E*)-3-bromo-4-(1-hydroxybut-2-en-2-yl)-5,6-dihydro-2H-pyran-2-one (7)



7

A Schlenk tube (250 mL) was charged with lithium chloride (712 mg; 16.9 mmol) and flame-dried under high vacuum. Upon cooling, CuCl (2.5 g; 25 mmol) was added and then degassed with Argon (four times). A solution of compound **5** (914 mg, 2.81 mmol) and (*Z*)-2-(tributylstannyl)but-2-en-1-ol (**6**) (1.53 g, 4.22 mmol) in THF/toluene (1:1, 50 mL) was added to the Schlenk tube under argon, followed by tetrakis(triphenylphosphine)palladium(0) (162 mg, 0.14 mmol). After the reaction mixture was heated at 60 ^{o}C for 30 min, the mixture was poured into water, and extracted with ethyl acetate (three times). The combined organic layer was dried and evaporated *in vacuo*, and the residue was purified by column chromatography (hexanes: ethyl acetate = 5:1 to dichloromethane: ethyl acetate = 7:1) to give (*E*)-3-bromo-4-(1-hydroxybut-2-en-2-yl)-5,6-dihydro-2H-pyran-2-one (**7**) (558 mg, 80%) as a light yellow oil; R_f = 0.5 (dichloromethane/ethyl acetate = 2:1); **IR** ν_{max} (film)/cm^{-1} 3442, 2954, 2923, 2852, 1725, 1397, 1276, 1112, 1073; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.71 (q, J = 6.8 Hz, 1H), 4.47 (t, J = 6.0 Hz, 2H), 4.24 (s, 2H), 2.67 (br.s, 2H), 2,18 (br.s, 1H), 1.62 (d, J = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.2, 155.9, 138.6, 125.3, 112.3, 66.0, 65.0, 31.2, 14.6; **HRMS** *m/z* calcd for $C_9H_{12}BrO_3$ $[M+H]^+$ 246.9964 and 248.9944, found 246.9964 and 248.9943.

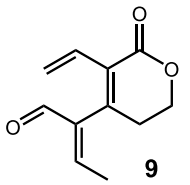
(*E*)-4-(1-hydroxybut-2-en-2-yl)-3-vinyl-5,6-dihydro-2H-pyran-2-one (8)



8

A Schlenk tube (25 mL) was charged with LiCl (172 mg, 4.05 mmol) and flame-dried under high vacuum. Upon cooling, (*t*-$Bu_3P)_2Pd$ (21 mg, 0.04 mmol) was added, and the mixture was degassed four times under high vacuum with an argon purge. DMF (3 mL) was introduced while stirring, followed by tributylvinylstannane (257 mg, 0.81 mmol) and a solution of **5** (100 mg, 0.41 mmol) in DMF (2 mL). The resulting mixture was rigorously degassed four times by the freeze-pump-thaw process (–78 °C to 25 °C, Ar). The reaction mixture was then stirred at 60 °C for 3 h. After completion of the reaction, as indicated by MS, the reaction mixture was cooled, diluted with EtOAc (20 mL), and washed with water (20 mL). The aqueous layer was extracted with EtOAc (3 × 10 mL), and the combined organic layer was washed with brine (2 × 10 mL) and dried over Na_2SO_4. The solvent was removed *in vacuo*, and the residue was purified by flash column chromatography on silica gel (hexanes: ethyl acetate = 3:1, then dichloromethane: ethyl acetate = 7:1) to give the desired product **8** (63 mg, 80%) as a light yellow oil, R_f = 0.5 (dichloromethane/ethyl acetate = 2:1); **IR** ν_{max}(film)/cm^{-1} 3418, 3020, 2981, 2938, 2856, 1700, 1396, 1301, 1143, 1052; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.31 (dd, *J* = 17.6, 11.6 Hz, 1H), 6.07 (d, *J* = 17.6 Hz, 1H), 5.75 (q, *J* = 6.8 Hz, 1H), 5.34 (d, *J* = 11.6 Hz, 1H), 4.36 (t, *J* = 6.0 Hz, 2H), 4.20 (s, 1H), 2.56 (t, *J* = 6.0 Hz, 2H), 1.73 (br.s, 1H), 1.58 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.5, 151.5, 138.1, 128.9, 125.5, 124.9, 120.0, 65.4, 65.1, 29.3, 14.5; HRMS *m/z* calcd for $C_{11}H_{15}O_3$ $[M + H]^+$ 195.1016, found 195.1011.

(*E*)-2-(6-oxo-5-vinyl-3,6-dihydro-2H-pyran-4-yl)but-2-enal (9)

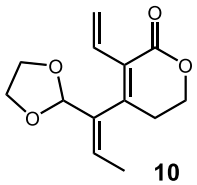


9

To a solution of compound **8** (63 mg, 0.21 mmol) in DCM (5 mL) was added Dess-Martin periodinane (182 mg, 0.43 mmol) at room temperature. The reaction mixture was stirred for 30 min under argon atmosphere. The reaction was quenched with saturated $Na_2S_2O_3$ and stirred for 20 min. The organic layer was washed by brine, dried with Na_2SO_4 and concentrated. The

residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 3/1) to give **7** (60 mg) in 95% yield as a colorless oil, R_f = 0.5 (hexane/ethyl acetate = 1:1); **IR** ν_{max} (film)/cm^{-1} 2833, 2712, 1717, 1682, 1627, 1299, 1143; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.47 (s, 1H), 6.83 (q, *J* = 7.2 Hz, 1H), 6.11 (dd, *J* = 17.6, 11.2 Hz, 1H), 6.01 (d, *J* = 17.6 Hz, 1H), 5.34 (d, *J* = 11.2 Hz, 1H), 4.41-4.03 (m, 2H), 2.49 (br.s, 2H), 1.92 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.8, 162.8, 151.5, 145.6, 142.4, 128.2, 127.4, 121.0, 65.3, 28.9, 16.1; HRMS m/z calcd for $C_{11}H_{13}O_3$ $[M + H]^+$ 193.0859, found 193.0854.

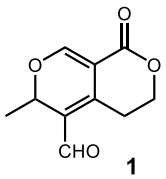
(*E*)-4-(1-(1,3-dioxolan-2-yl)prop-1-en-1-yl)-3-vinyl-5,6-dihydro-2H-pyran-2-one (10)



10

To a solution of compound **9** (138 mg, 0.72 mmol), ethylene glycol (444 mg, 7.2 mmol) and trimethyl orthoformate (381 mg, 3.6 mmol) in DCM (10 mL) was added *p*-toluenesulfonic acid monohydrate (12 mg, 0.07 mmol). The reaction mixture was stirred at room temperature for 2 h under argon atmosphere. The reaction mixture was quenched by triethylamine (0.2 mL), and washed with brine and dried over Na_2SO_4. The solvent was removed *in vacuo*, and the residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 7:1) to give the desired product **10** (146 mg, 84%) as a colorless oil. R_f = 0.6 (hexane/ethyl acetate = 1:1); **IR** ν_{max} (film)/cm^{-1} 3024, 2981, 2950, 2891, 1717, 1299, 1143, 1124, 1077, 1038, 940; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.36 (dd, *J* = 17.6, 12.0 Hz, 1H), 6.10 (dd, *J* = 17.6, 2.0 Hz, 1H), 5.95 (q, *J* = 6.8 Hz, 1H), 5.33-5.30 (m, 2H), 4.32 (t, *J* = 6.0 Hz, 2H), 3.93-3.87 (m, 4H), 2.59-2.56 (m, 2H), 1.60 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.0,149.4, 135.4, 129.3, 128.9, 126.6, 119.7, 105.6, 65.1, 64.9 (2C), 30.1, 14.2; HRMS m/z calcd for $C_{13}H_{17}O_4$ $[M + H]^+$ 237.1121, found 237.1118.

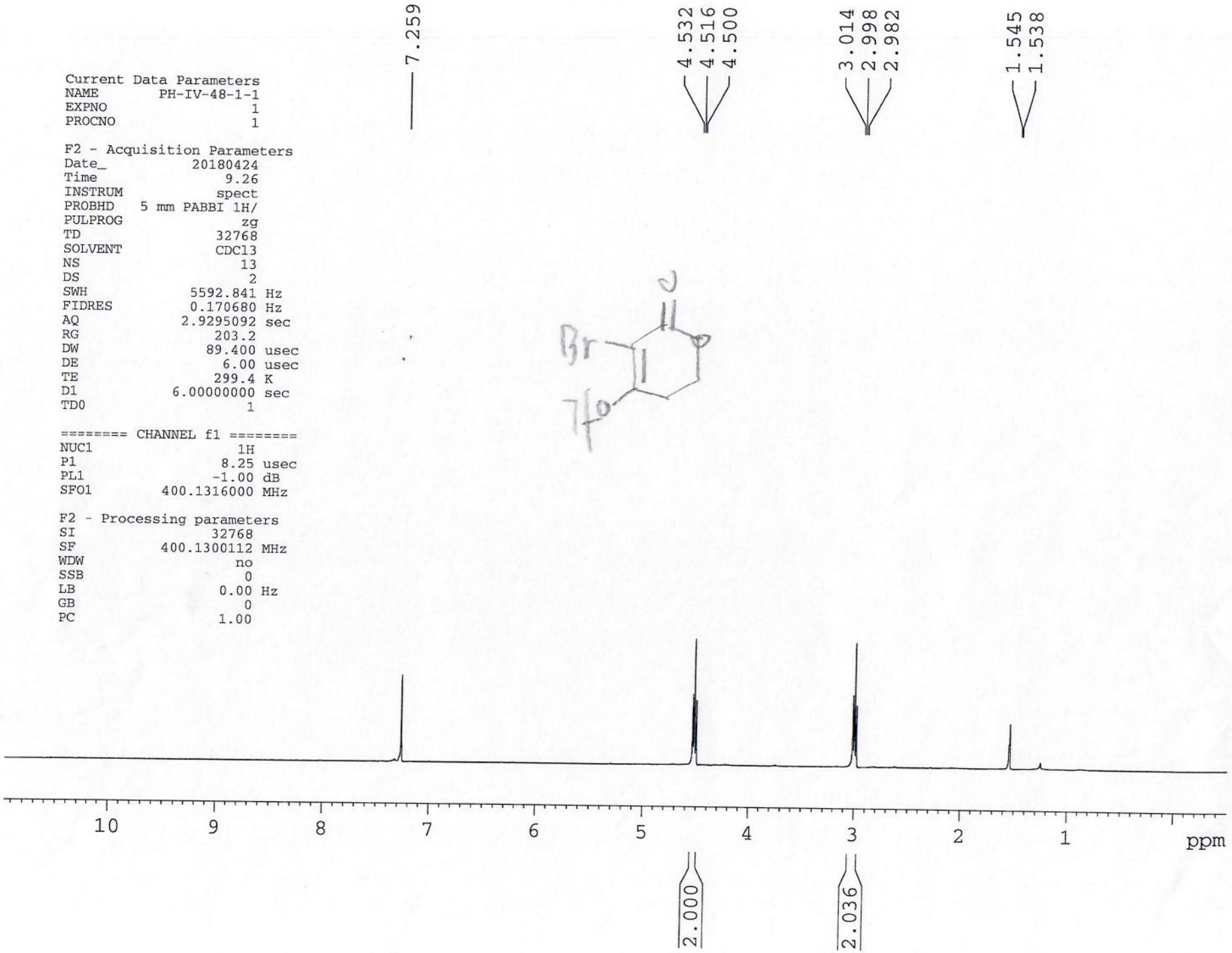
Swermirin (1)



1

To a stirred solution of compound **10** (16 mg, 0.068 mmol) in acetone/water (1:1, 5 mL) was

added osmium tetroxide as a 2.5% weight solution in *t*-BuOH (50 μL, 0.004 mmol) and 4-methylmorpholine *N*-oxide (16 mg, 0.136 mmol) at 0 °C. The mixture was stirred at room temperature for 2 h. After completion of the reaction, as indicated by TLC, sodium periodate (44 mg, 0.204 mmol) was added and the reaction mixture was stirred for another 20 min. The reaction mixture was diluted with water (10 mL), and extracted with EtOAc (3×10 mL), and the combined organic layer was washed with brine (2 × 10 mL) and dried over Na_2SO_4. After the drying agent was filtered off, *p*-toluenesulfonic acid monohydrate (1.3 mg, 0.007 mmol) was added to the organic solution. The mixture was stirred at room temperature for 10 min, quenched by triethylamine (0.1 mL), and concentrated. The residue was purified by flash column chromatography on silica gel (dichloromethane/ethyl acetate = 9:1) to give the desired product **1** (7 mg, 54%) as a light yellow solid. R_f = 0.6 (DCM/ethyl acetate = 2:1); **IR** ν_{max} (film)/cm^{-1} 1721, 1651, 1636, 1557, 1472, 1448, 1399, 1370, 1360, 1336, 1301, 1279, 1166, 1109, 1033, 976, 949; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 7.93 (s, 1H), 5.64 (q, J = 6.4 Hz, 1H), 4.46-4.34 (m, 2H), 3.14-3.03 (m, 2H), 1.40 (d, 6.4 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 185.4, 163.6, 163.1, 142.4, 120.4, 104.0, 73.2, 65.0, 22.8, 19.8; HRMS m/z calcd for $C_{10}H_{11}O_4$ $[M + H]^+$ 195.0652, found 195.0668.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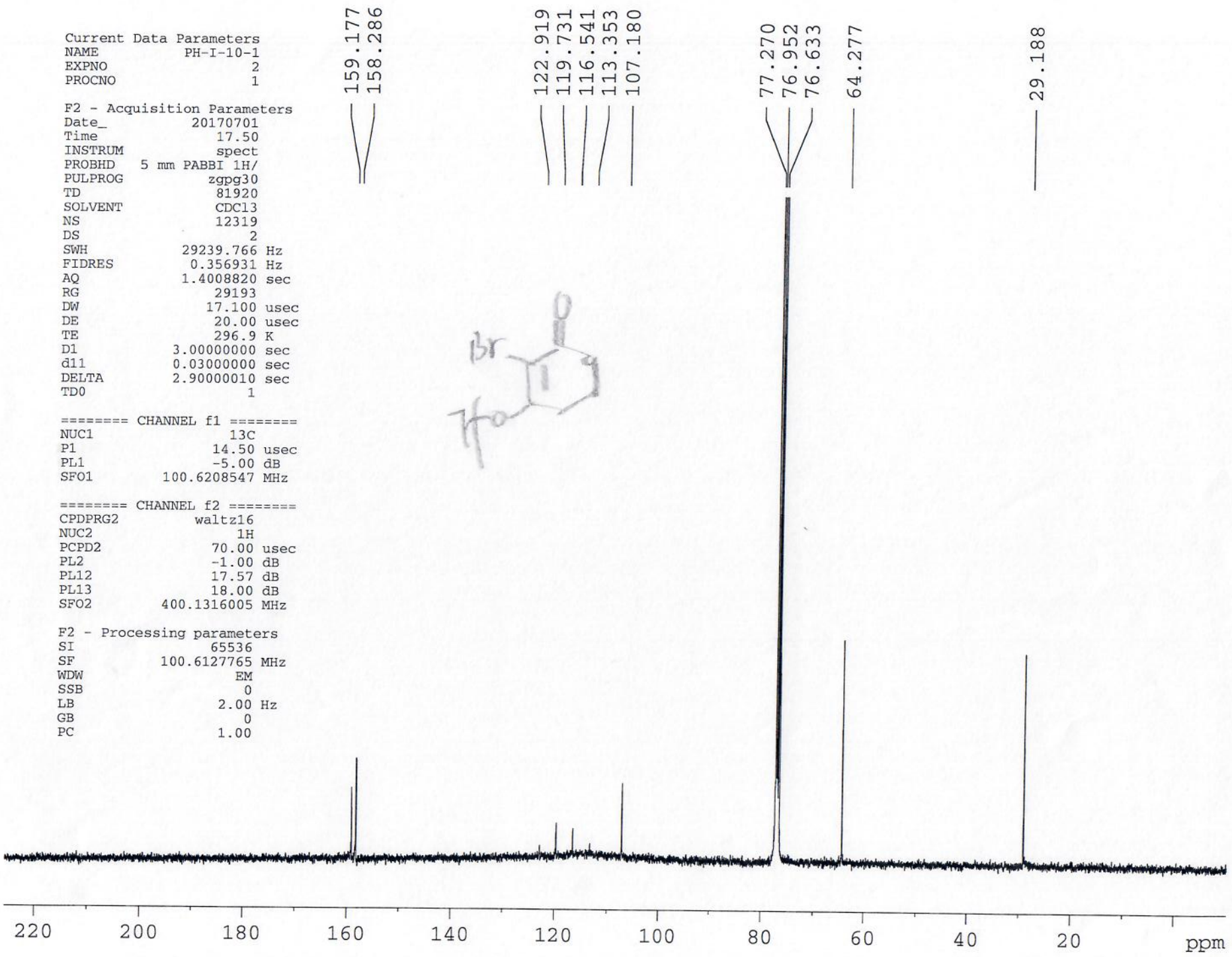

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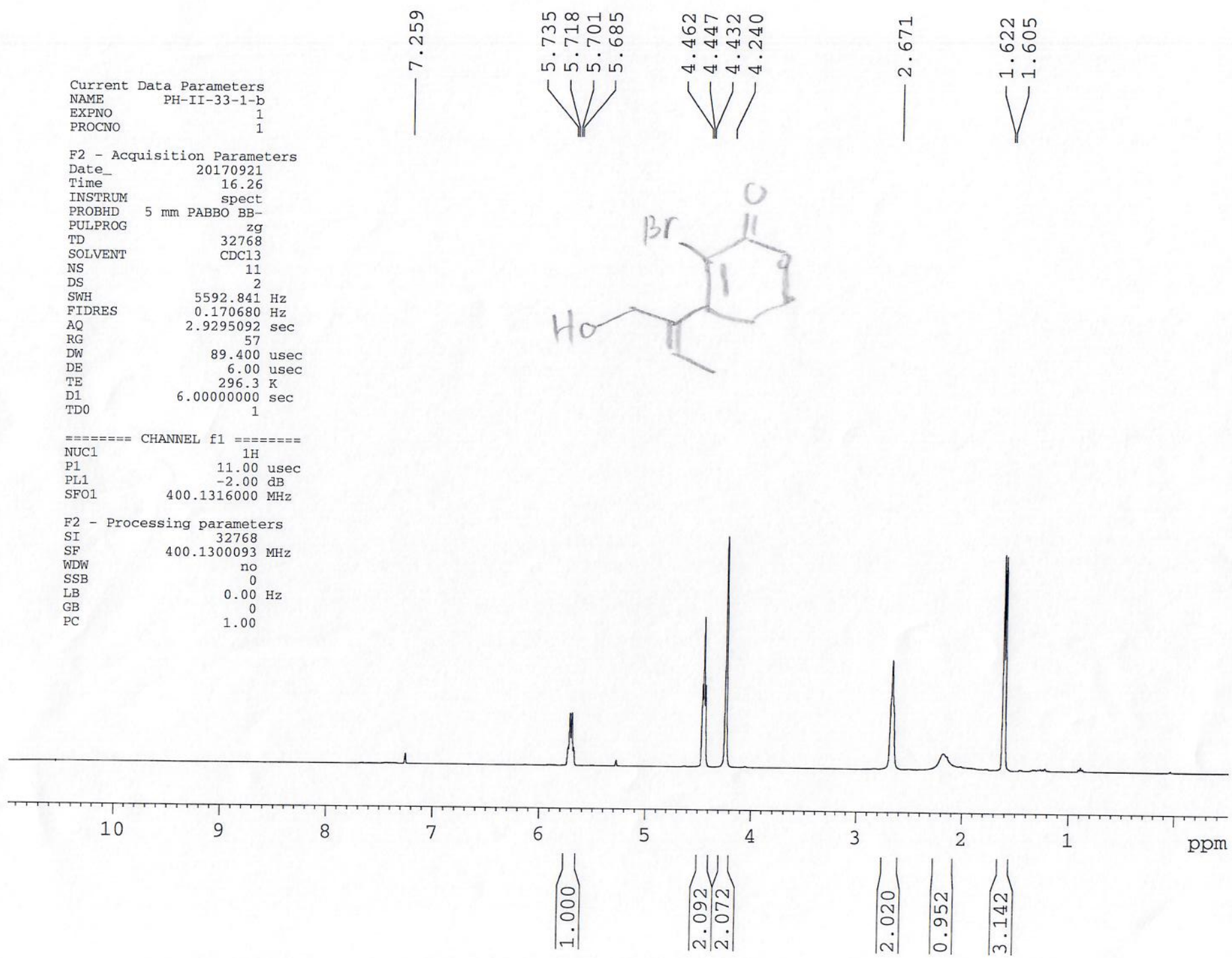

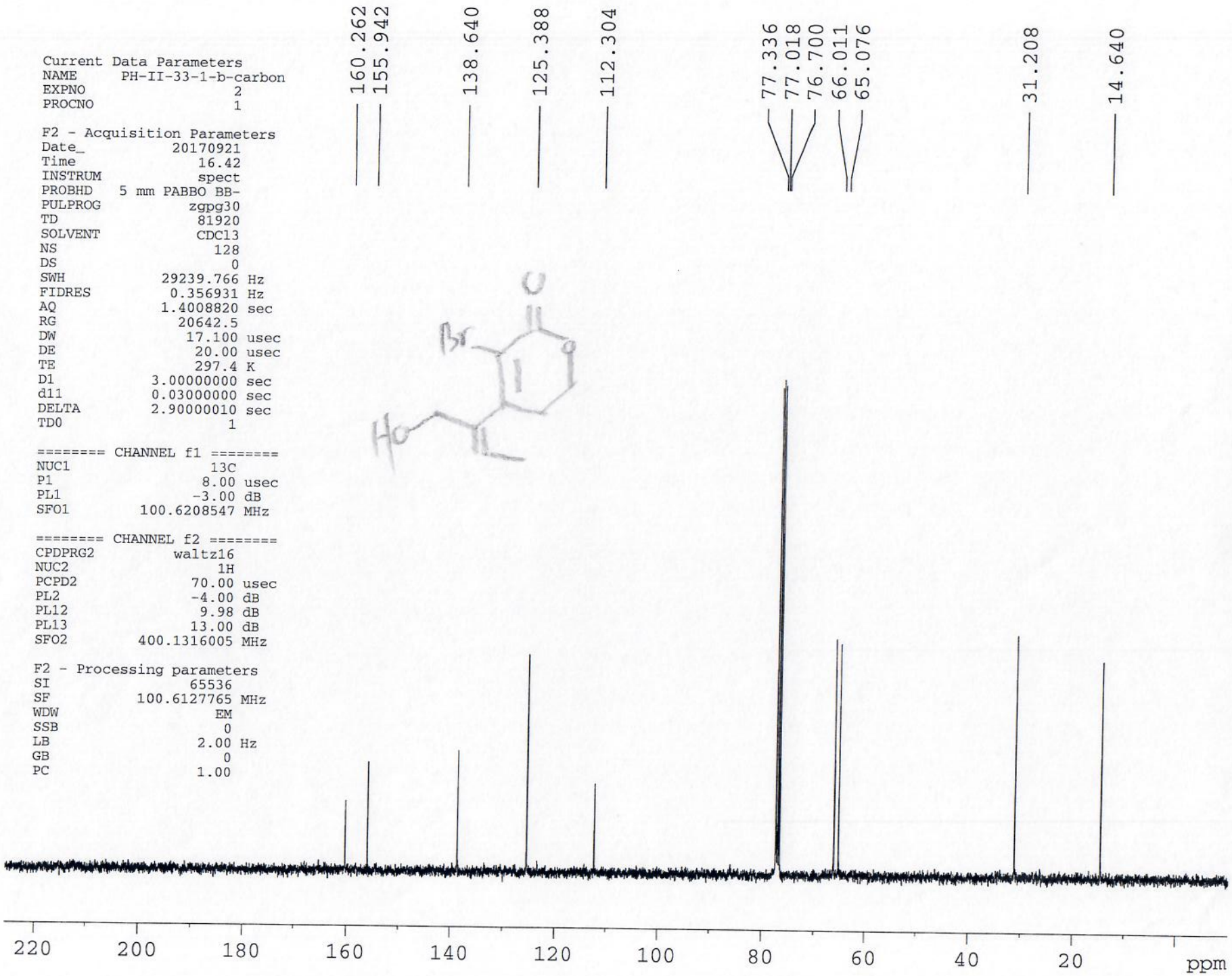
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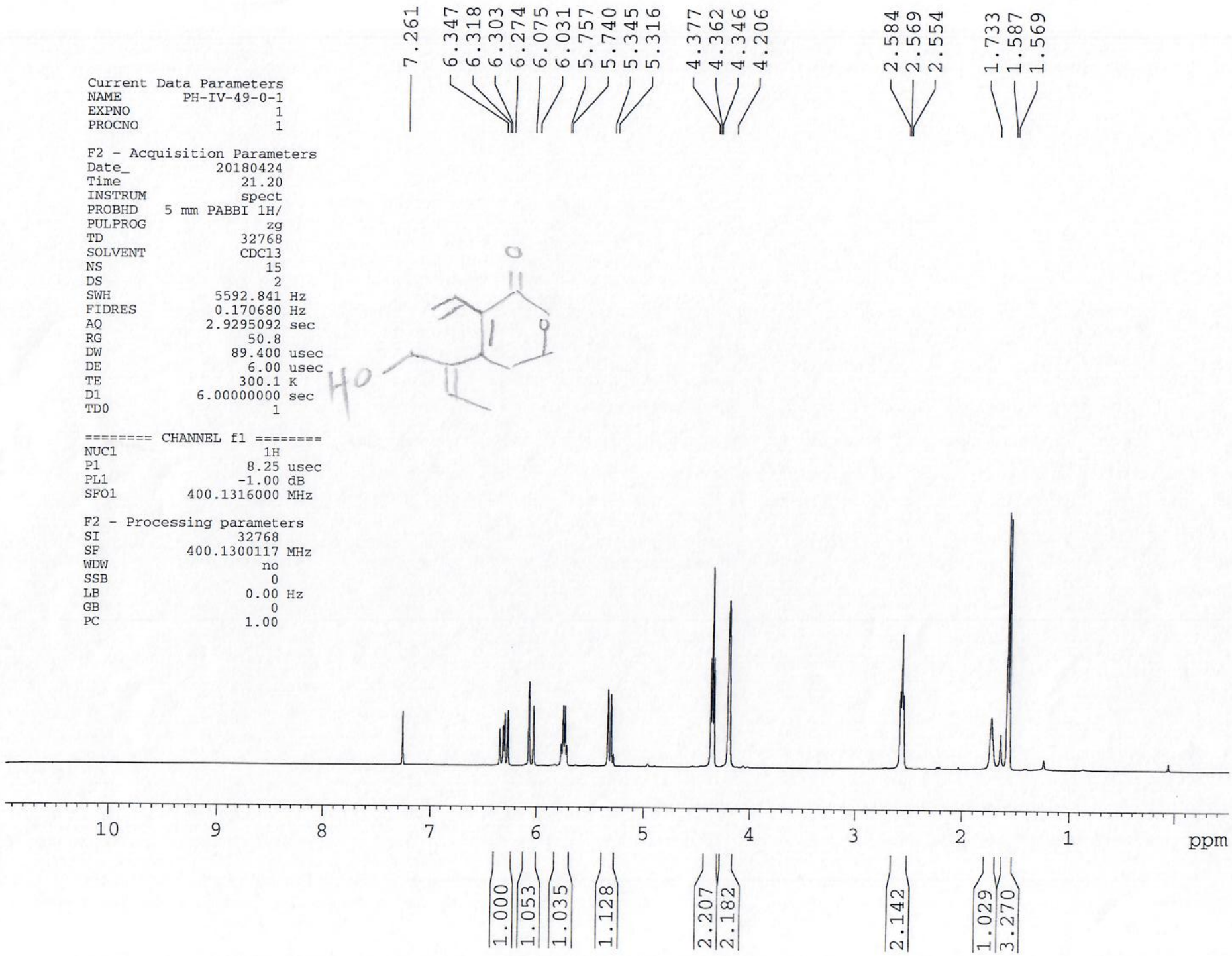
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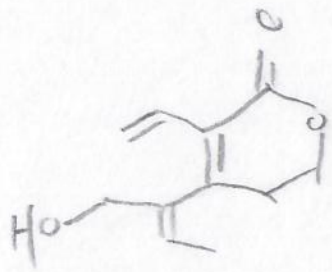

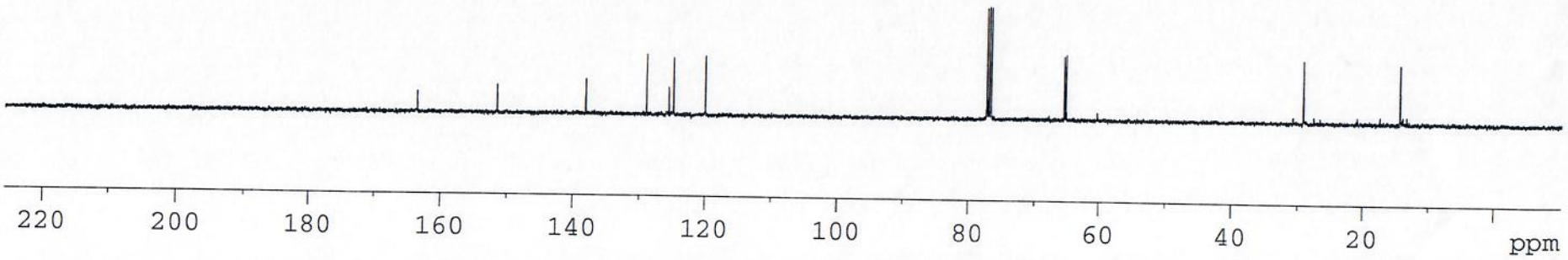

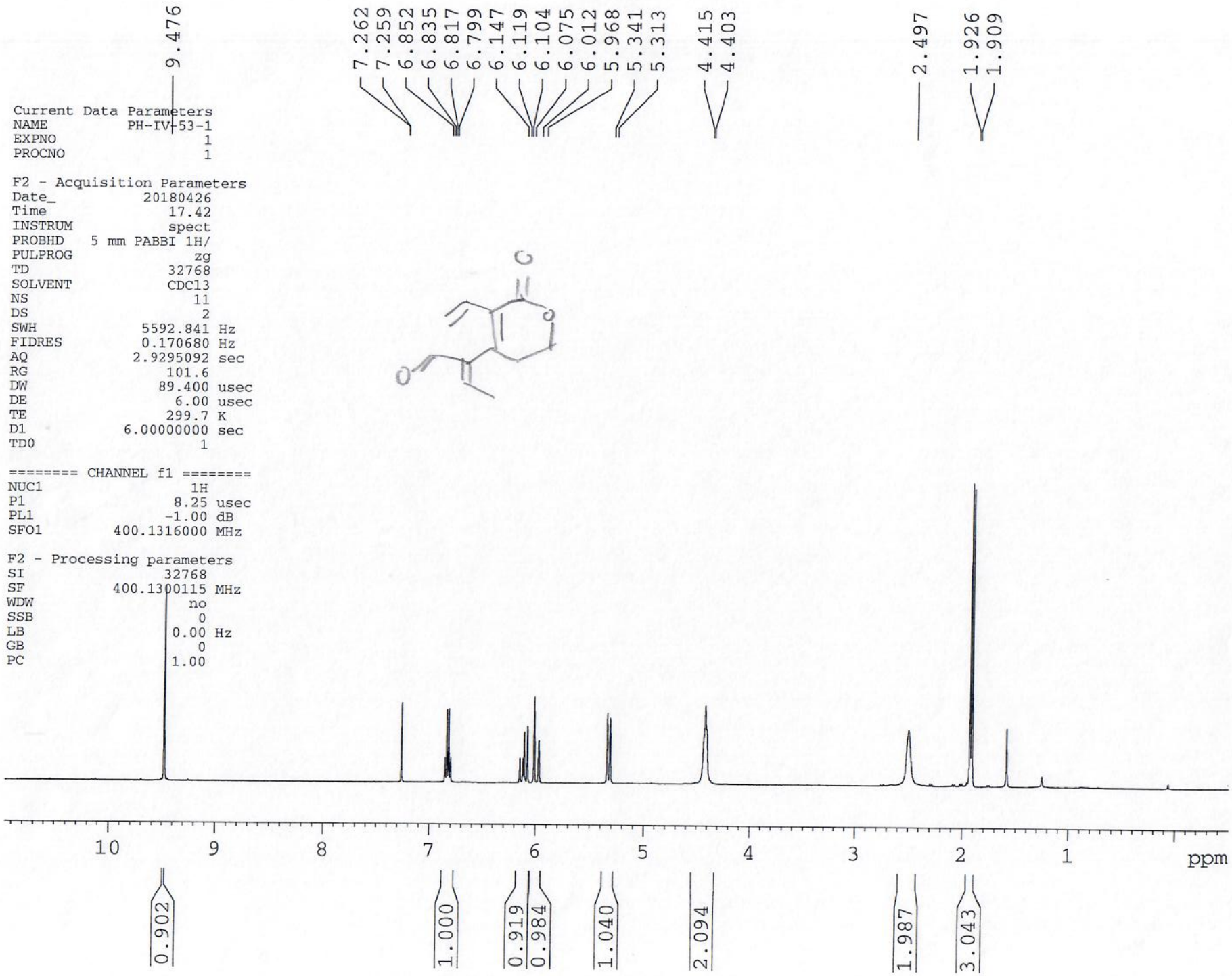
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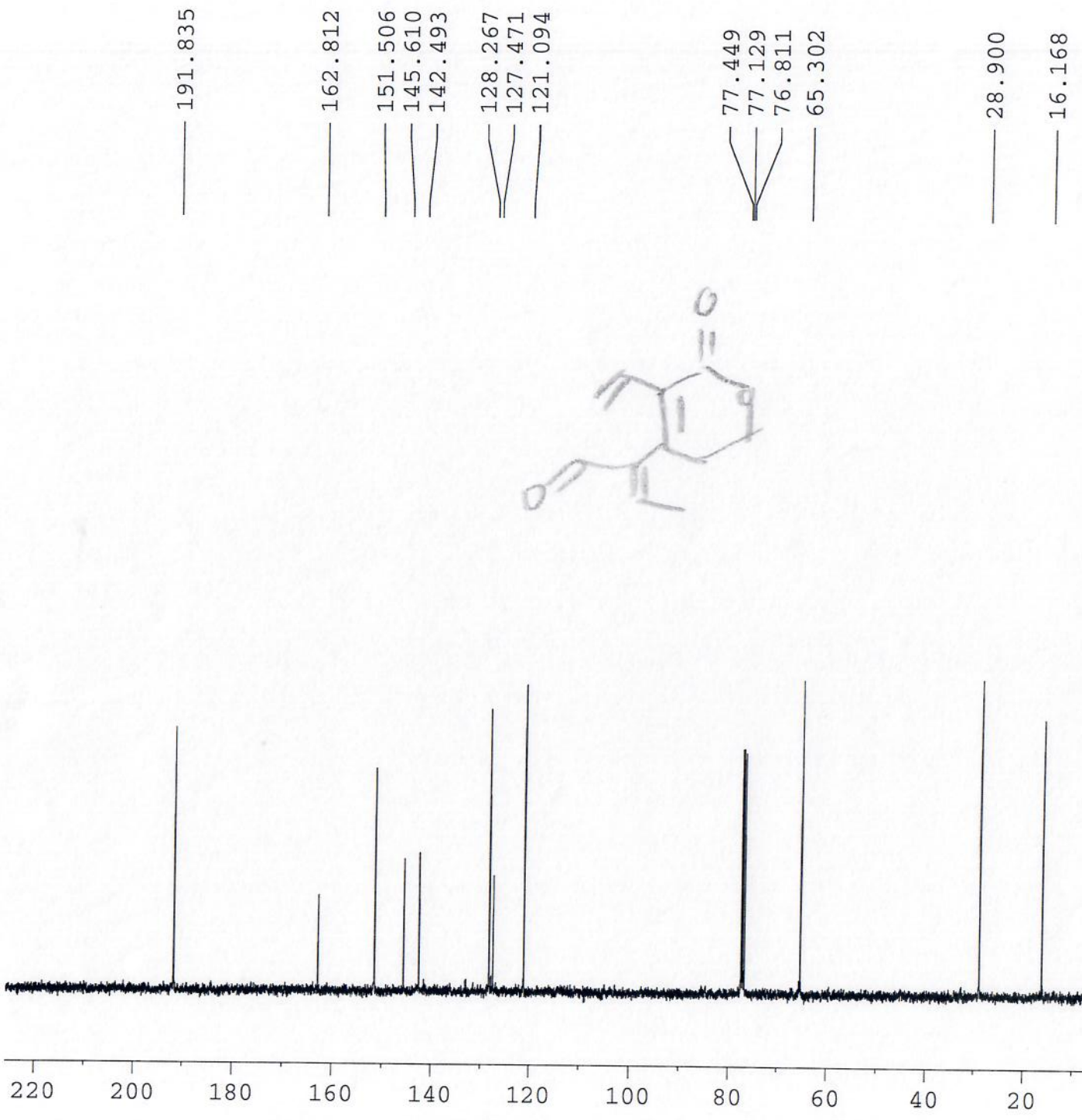
RG 101.6
DW 89.400 usec
DE 6.00 usec
TE 299.7 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.25 usec
PL1 -1.00 dB
SFO1 400.1316000 MHz
F2 - Processing parameters
SI 32768
SF 400.1300115 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
0.902
1.000
0.919
0.984
1.040
2.094
1.987
3.043



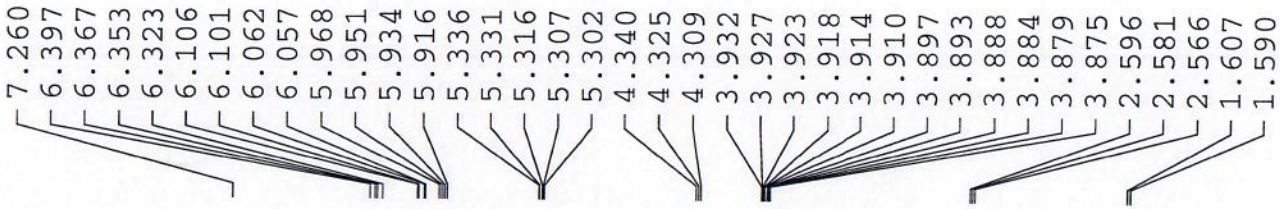
Current Data Parameters
NAME PH-II-60-1-Carbon
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171012
Time 17.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 81920
SOLVENT CDCl3
NS 46
DS 0
SWH 29239.766 Hz
FIDRES 0.356931 Hz
AQ 1.4008820 sec
RG 20642.5
DW 17.100 usec
DE 20.00 usec
TE 296.7 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
TD0 1

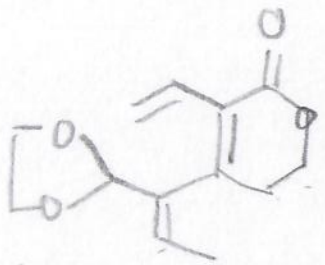
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 -3.00 dB
SFO1 100.6208547 MHz

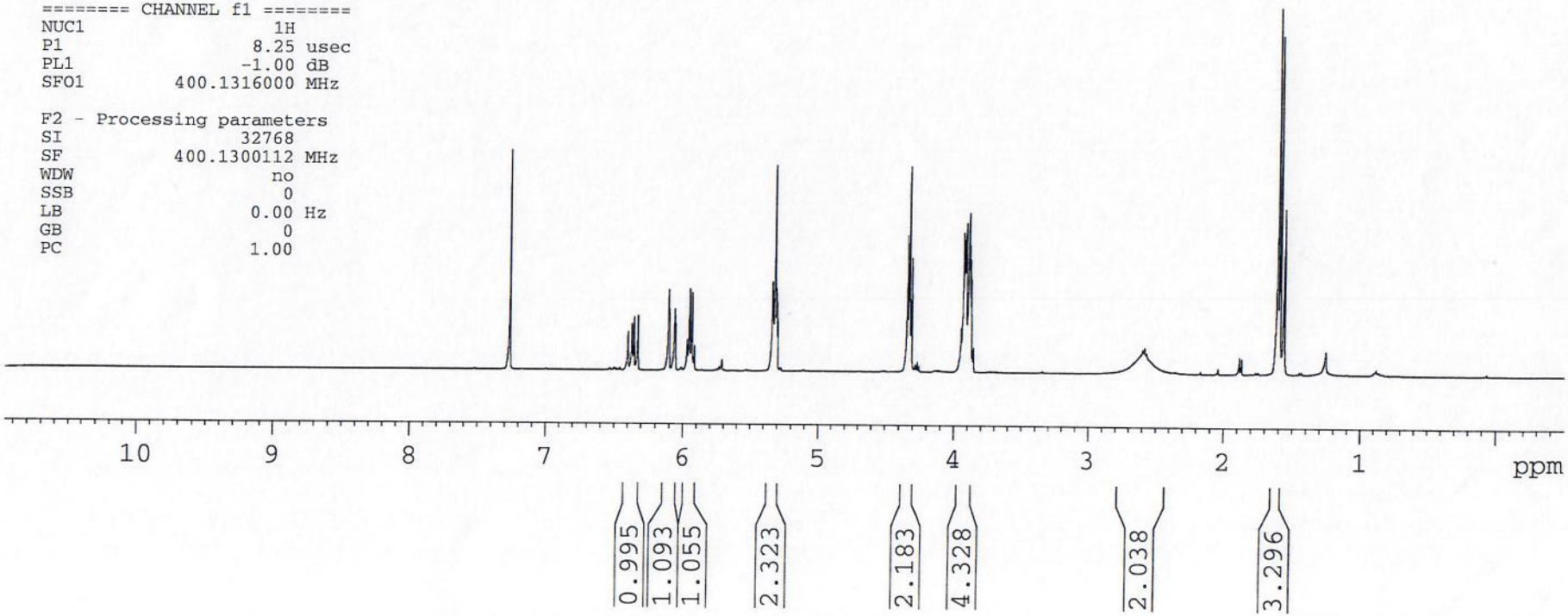
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -4.00 dB
PL12 9.98 dB
PL13 13.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127765 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



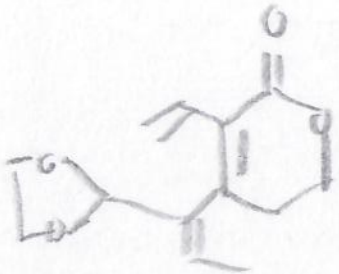

```
Current Data Parameters
NAME        PH-IV-50-1-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180425
Time               21.05
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    12
DS                     2
SWH             5592.841 Hz
FIDRES          0.170680 Hz
AQ              2.9295092 sec
RG                   128
DW                89.400 usec
DE                 6.00 usec
TE                301.1 K
D1           6.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  8.25 usec
PL1                -1.00 dB
SFO1         400.1316000 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300112 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

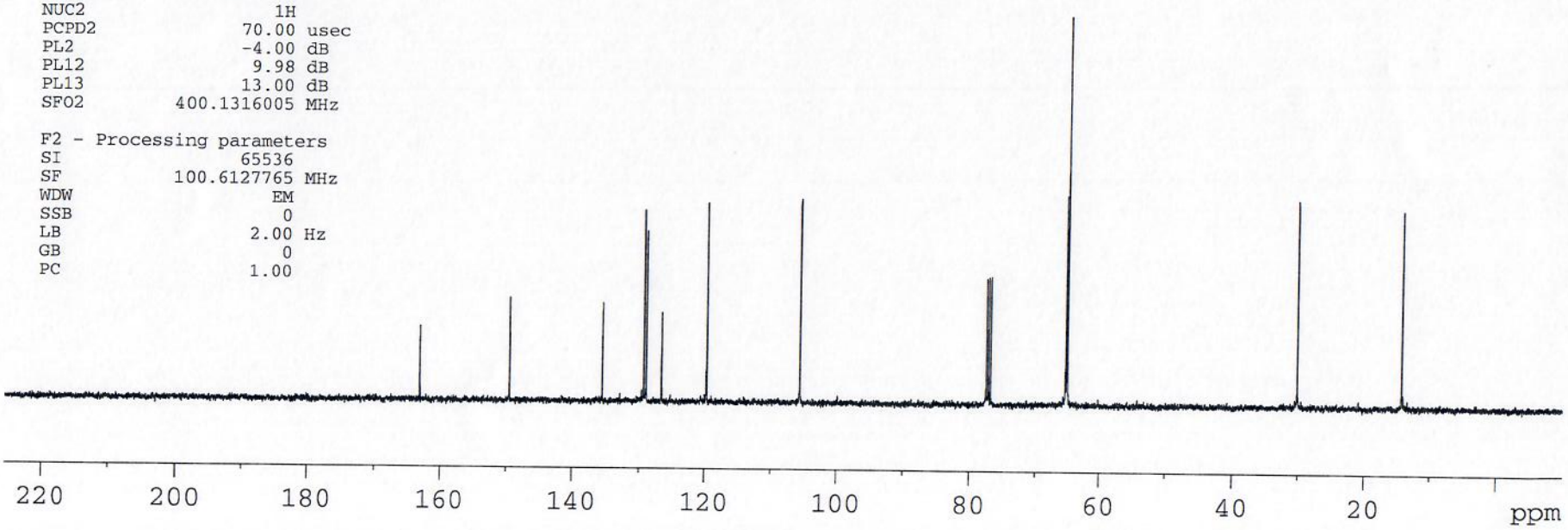




```
Current Data Parameters
NAME      PH-II-61-1-Carbon
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171013
Time              13.18
INSTRUM           spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                81920
SOLVENT           CDCl3
NS                   49
DS                    0
SWH           29239.766 Hz
FIDRES         0.356931 Hz
AQ             1.4008820 sec
RG               20642.5
DW                17.100 usec
DE                20.00 usec
TE                297.0 K
D1            3.00000000 sec
d11           0.03000000 sec
DELTA         2.90000010 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  8.00 usec
PL1                -3.00 dB
SFO1         100.6208547 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL2               -4.00 dB
PL12               9.98 dB
PL13              13.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                65536
SF         100.6127765 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

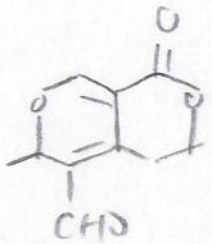
163.073
149.491
135.459
129.308
128.949
126.637
119.701
105.614
77.500
77.181
76.861
65.186
64.928
30.110
14.232

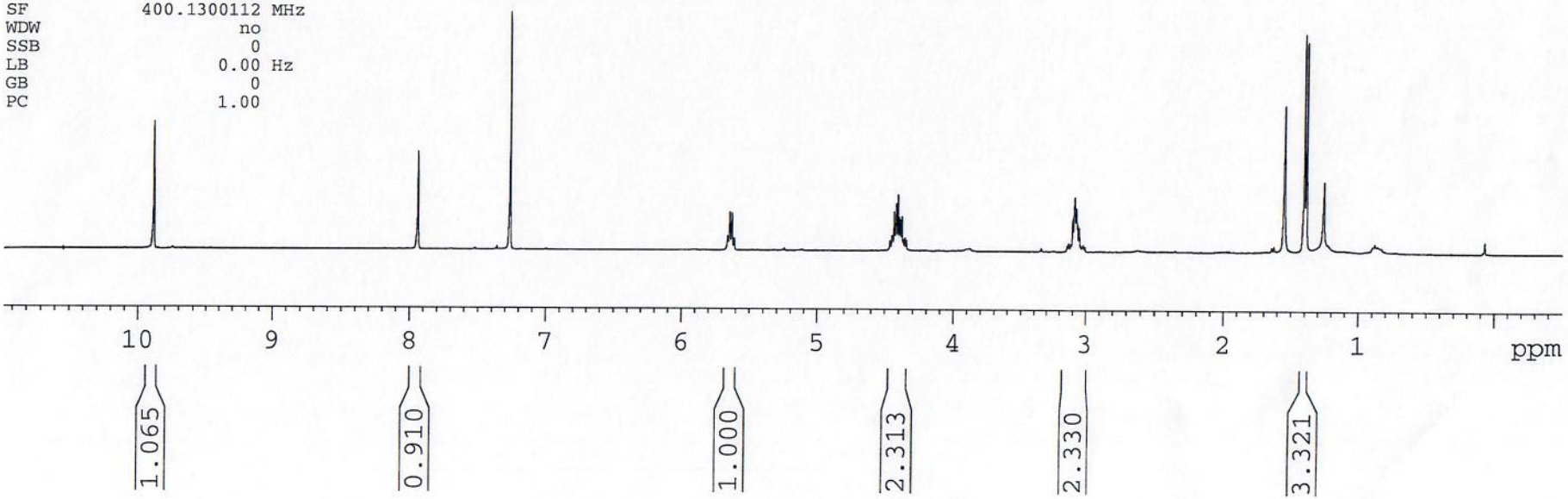




9.880
7.939
7.261
5.659
5.643
5.627
5.611
4.462
4.450
4.434
4.419
4.407
4.396
4.388
4.377
4.368
4.359
4.348
3.142
3.131
3.116
3.100
3.085
3.074
3.063
3.051
3.041
3.021
3.010
1.403
1.387

```
Current Data Parameters
NAME       PH-IV-52-NP-3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180426
Time               10.58
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   15
DS                    2
SWH            5592.841 Hz
FIDRES        0.170680 Hz
AQ            2.9295092 sec
RG                  256
DW               89.400 usec
DE                6.00 usec
TE               300.5 K
D1           6.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.25 usec
PL1               -1.00 dB
SFO1        400.1316000 MHz

F2 - Processing parameters
SI                32768
SF        400.1300112 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```





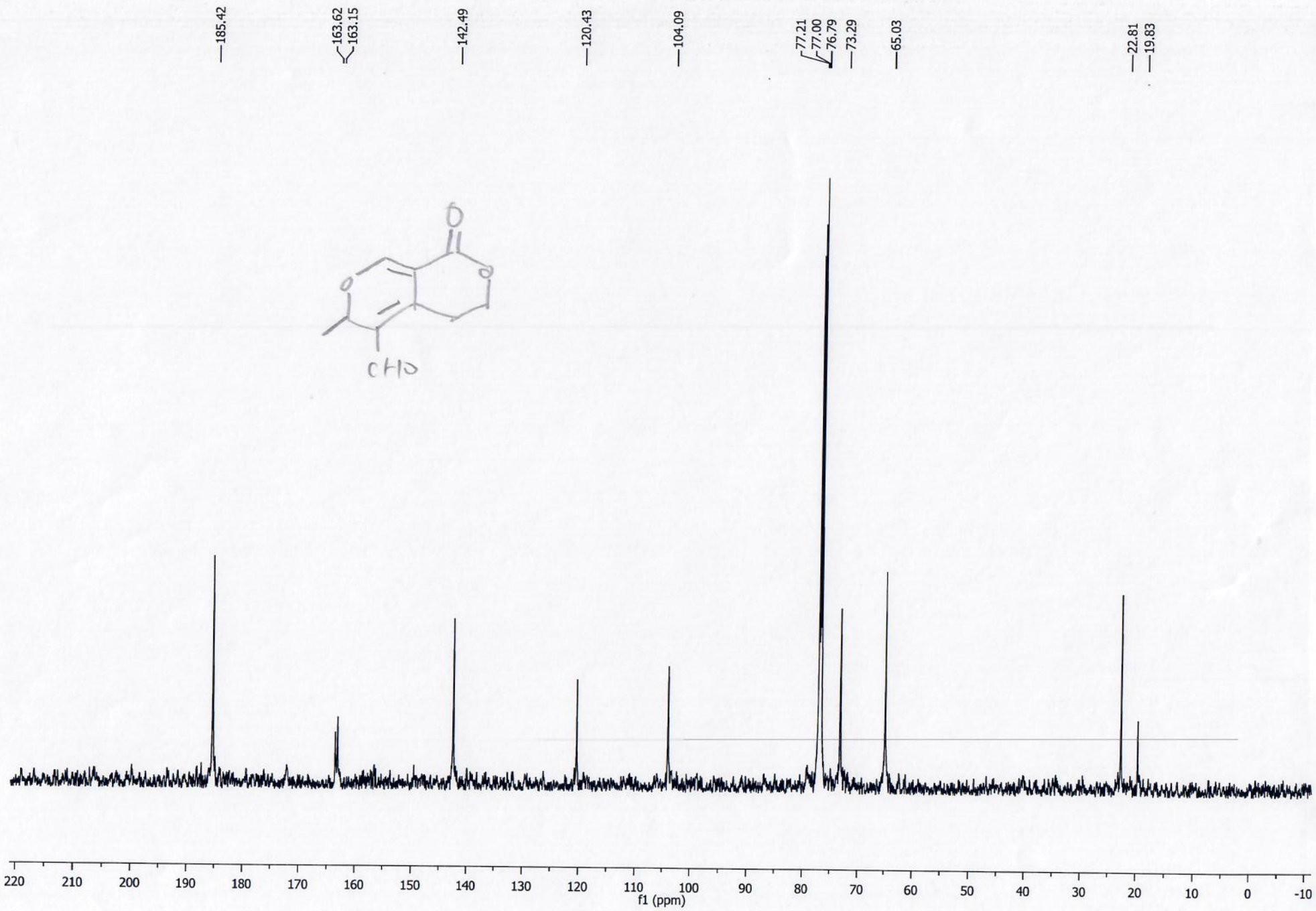

185.42
163.62
163.15
142.49
120.43
104.09
77.21
77.00
76.79
73.29
65.03
22.81
19.83
CHO
f1 (ppm)

Table 1. The comparison of ^{1}H NMR data of natural swermirin, gentiogenal and synthetic swermirin

Natural swermirin ($CDCl_3$)*	Gentiogenal (90 MHz, $CDCl_3$) *	Synthetic swerimirin (400 MHz, $CDCl_3$)
9.88 (s, 1H)	9.88 (s, 1H)	9.88 (s, 1H)
7.93 (s, 1H)	7.95 (s, 1H)	7.93 (s, 1H)
5.63 (q, *J* = 7.0, 1H)	5.64 (q, *J* = 6.5, 1H)	5.64 (q, *J* = 6.4 Hz, 1H)
4.41 (t, *J* = 5.9 Hz, 2 H)	4.43-4.44 (t, *J* = 4.9 Hz, 2 H)	4.46-4.34 (m, 2H)
3.08 (t, *J* = 5.9 Hz, 2H)	3.09-3.11 (t, *J* = 4.9 Hz, 2H)	3.14-3.03 (m, 2H)
1.4 (d, *J* = 7.0 Hz, 3H)	1.39 (d, *J* = 6.5 Hz, 3H)	1.40 (d, *J* = 6.4 Hz, 3H)

*TMS as internal standard;

Table 2. The comparison of ^{13}C NMR data of natural swerimirin, gentiogenal and synthetic swerimirin.

Natural swerimirin ($CDCl_3$)*	Gentiogenal (75.5 MHz, $CDCl_3$) *	Synthetic swerimirin (150 MHz, $CDCl_3$)
19.81	19.8	19.8
22.82	22.6	22.8
65.15	65.1	65.0
73.29	73.1	73.2
104.2	103.9	104.0
120.44	120.2	120.4
142.63	142.7	142.4
163.02	163.3	163.1
163.64	163.9	163.6
185.63	185.7	185.4

*TMS as internal standard;