Supporting Information for

Use of the Diels-Alder Adduct of Pyrrole in Organic Synthesis. Formal Synthesis of Tamiflu

Akio Kamimura* and Toshiki Nakano

Department of Applied Molecular Bioscience, Graduate School of Medicine, Yamaguchi University, Ube 755-8611 Japan,

Contents

tn-Diels

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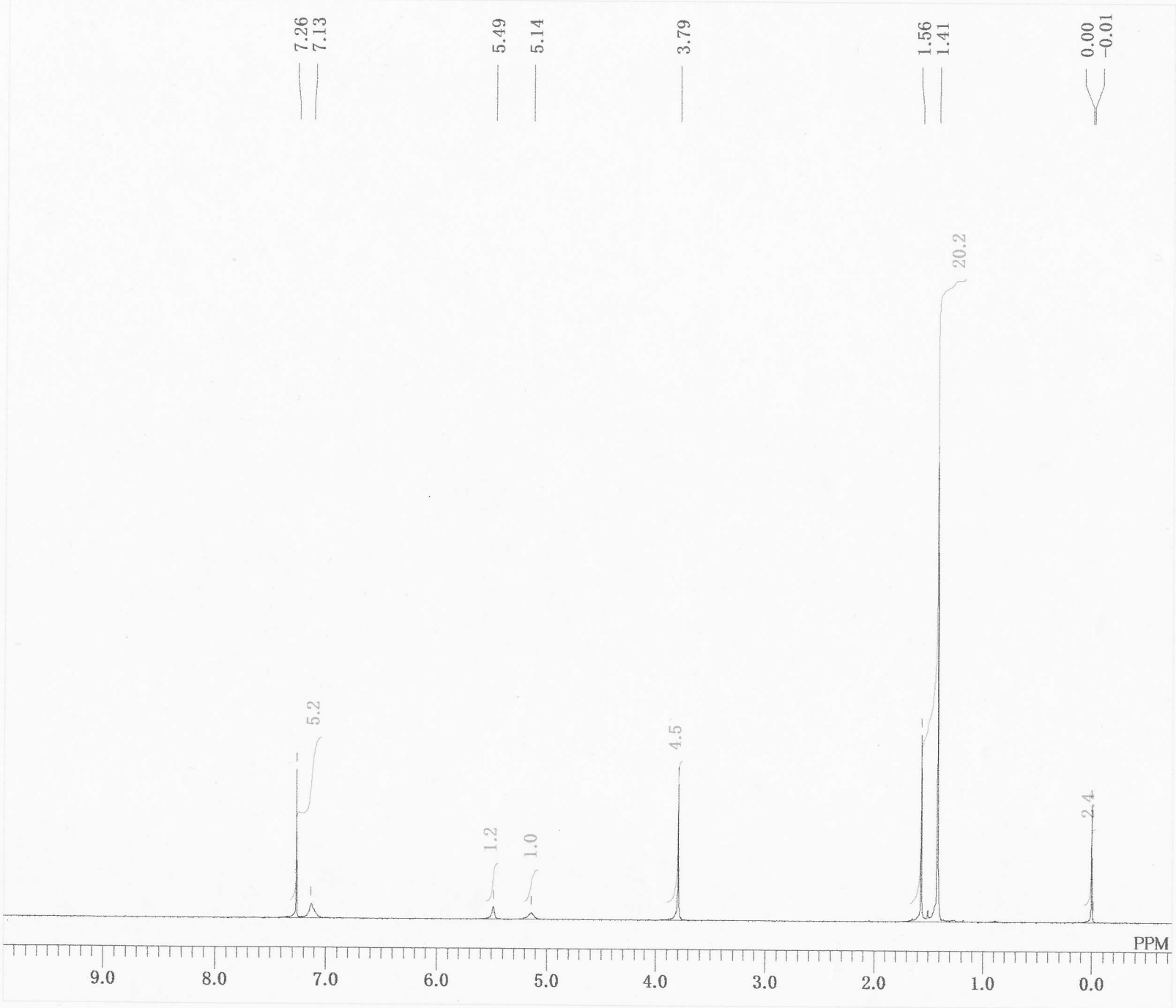

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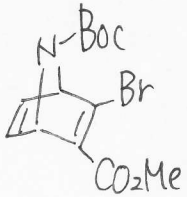

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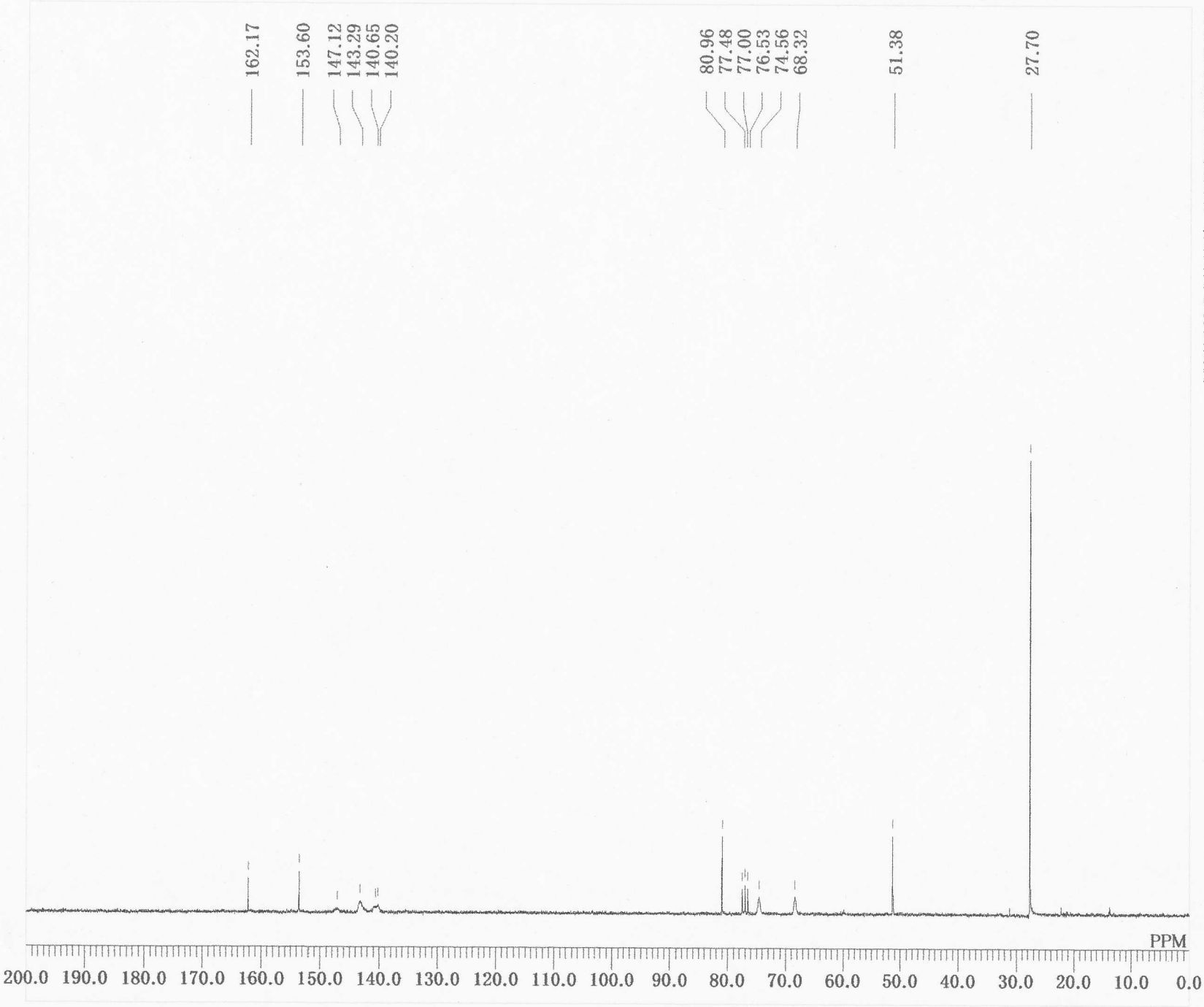
tn03006pr1-13C



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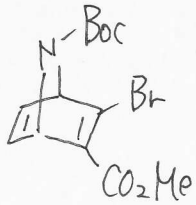

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tn-(epoxy)

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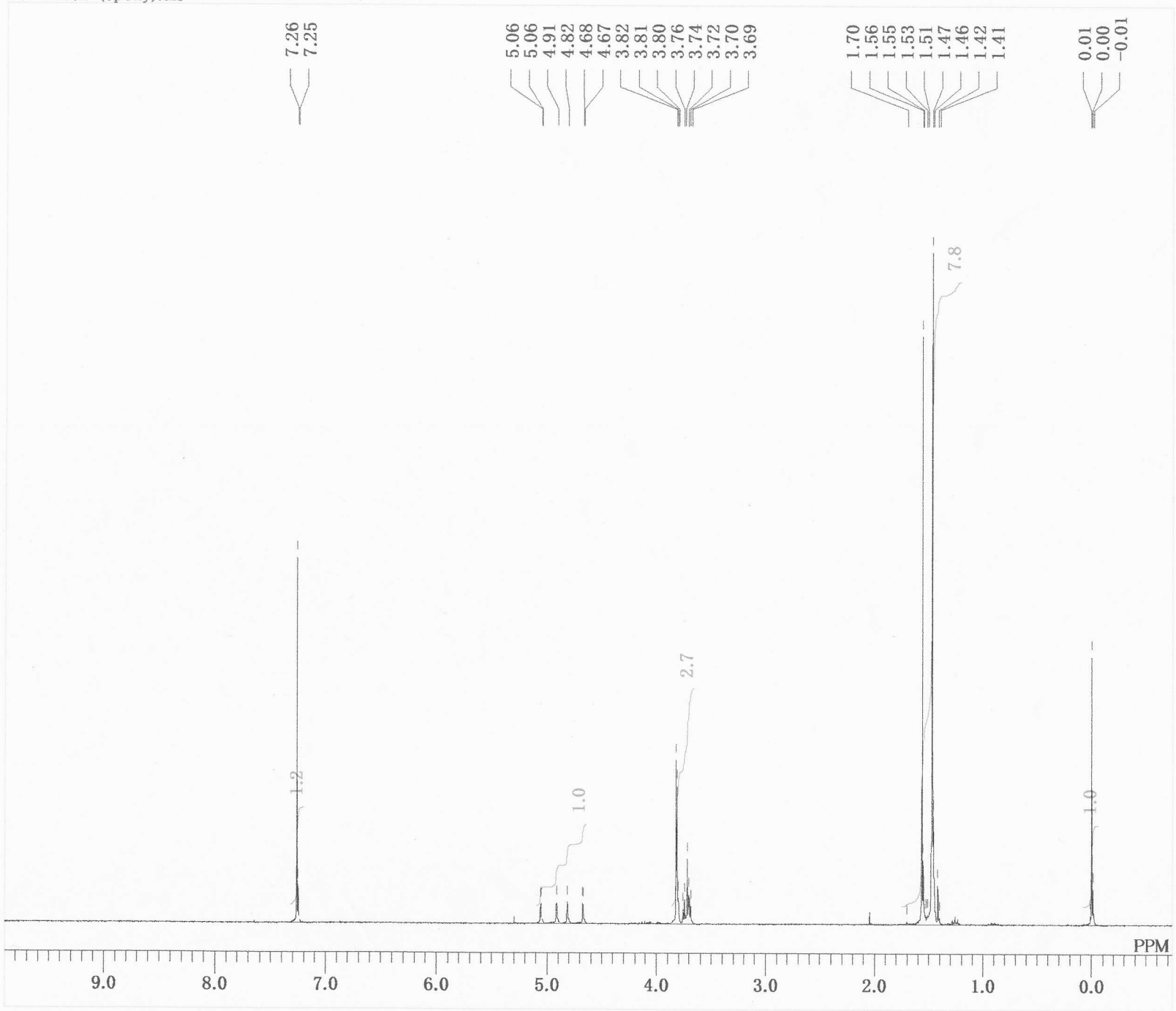

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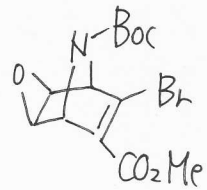

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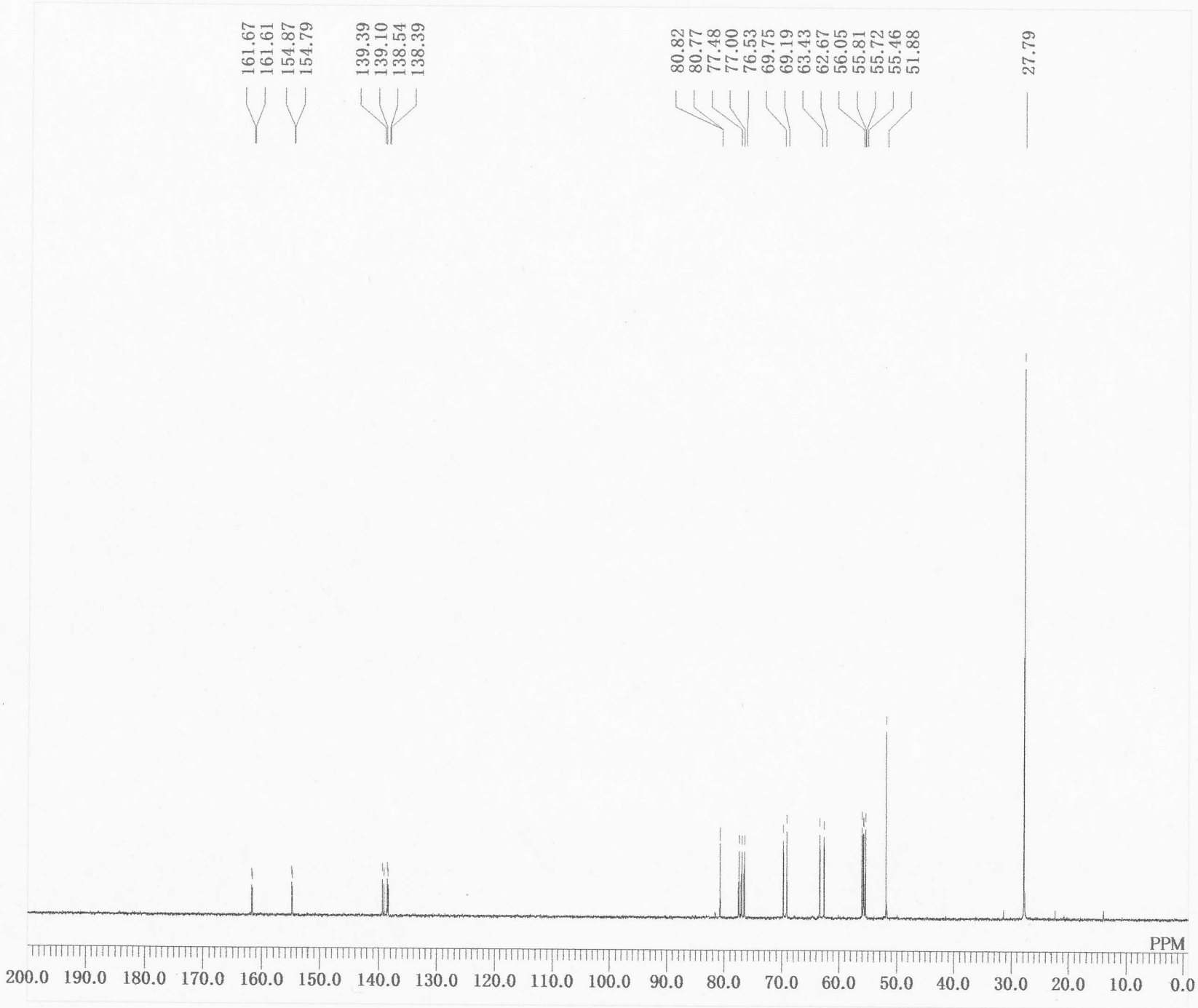

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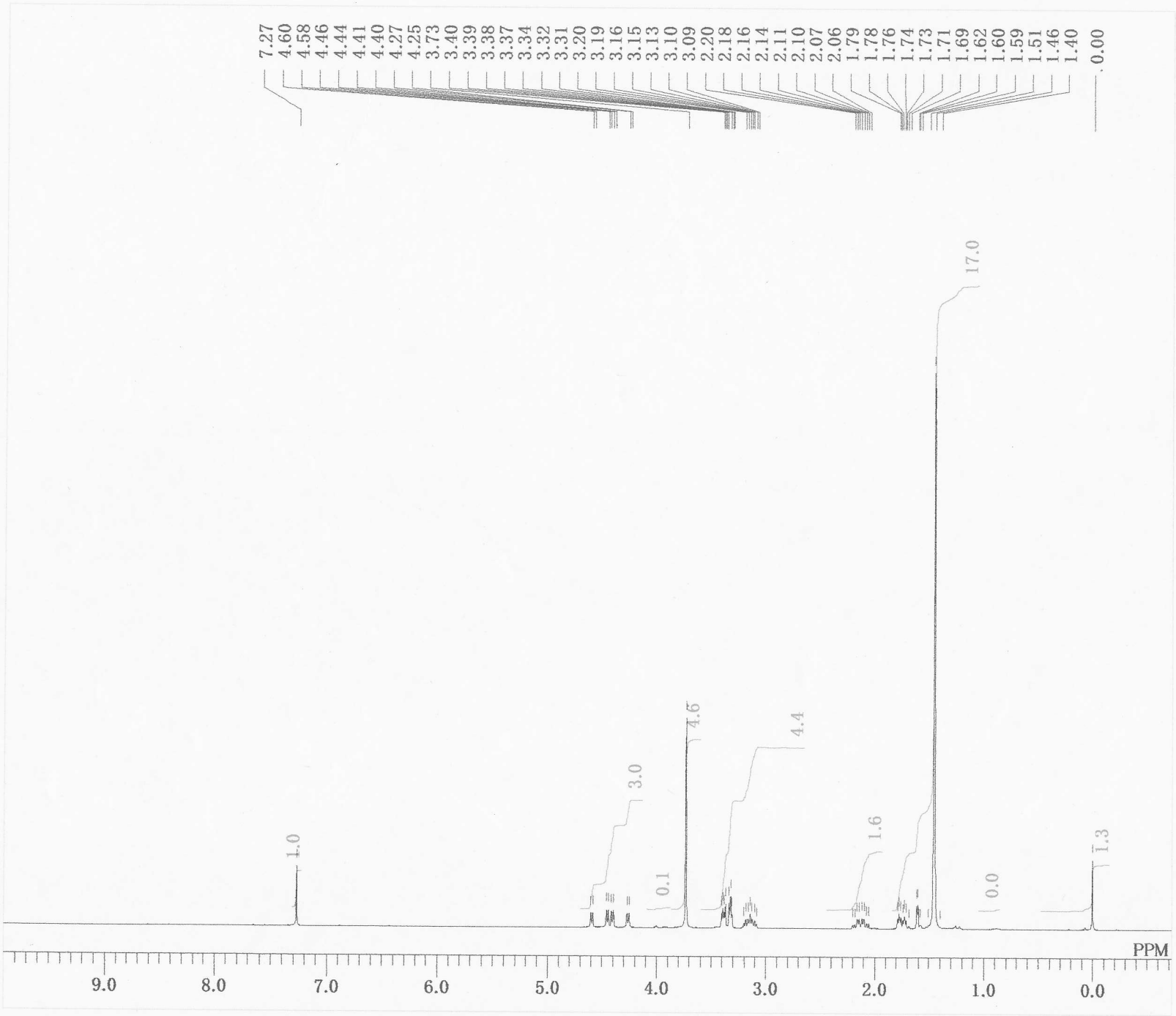
4

tn-(Endo)



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PD	3.9670 sec
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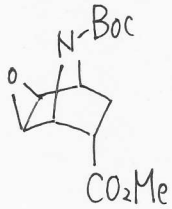

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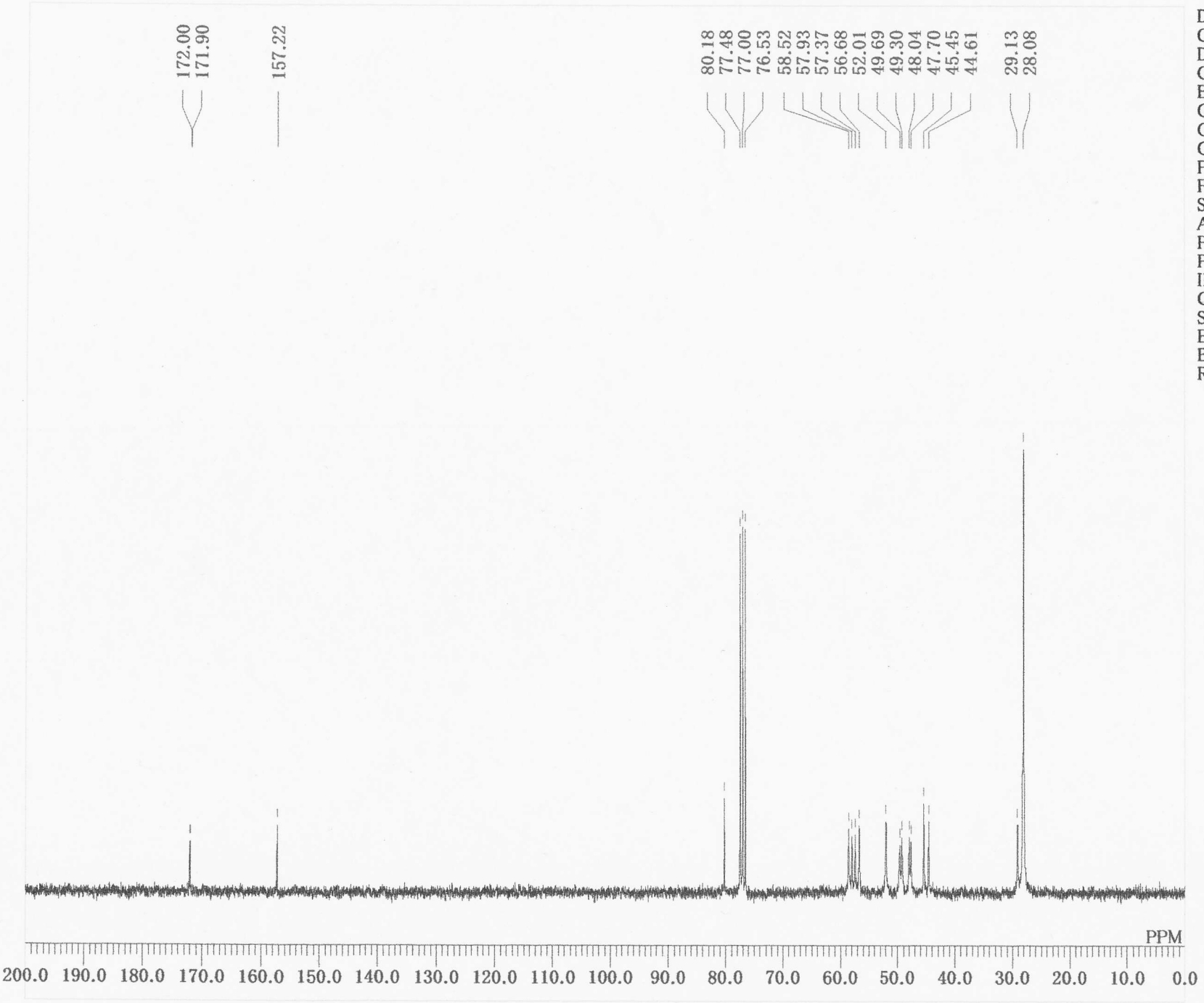

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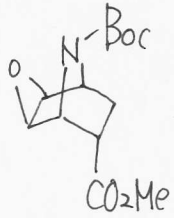

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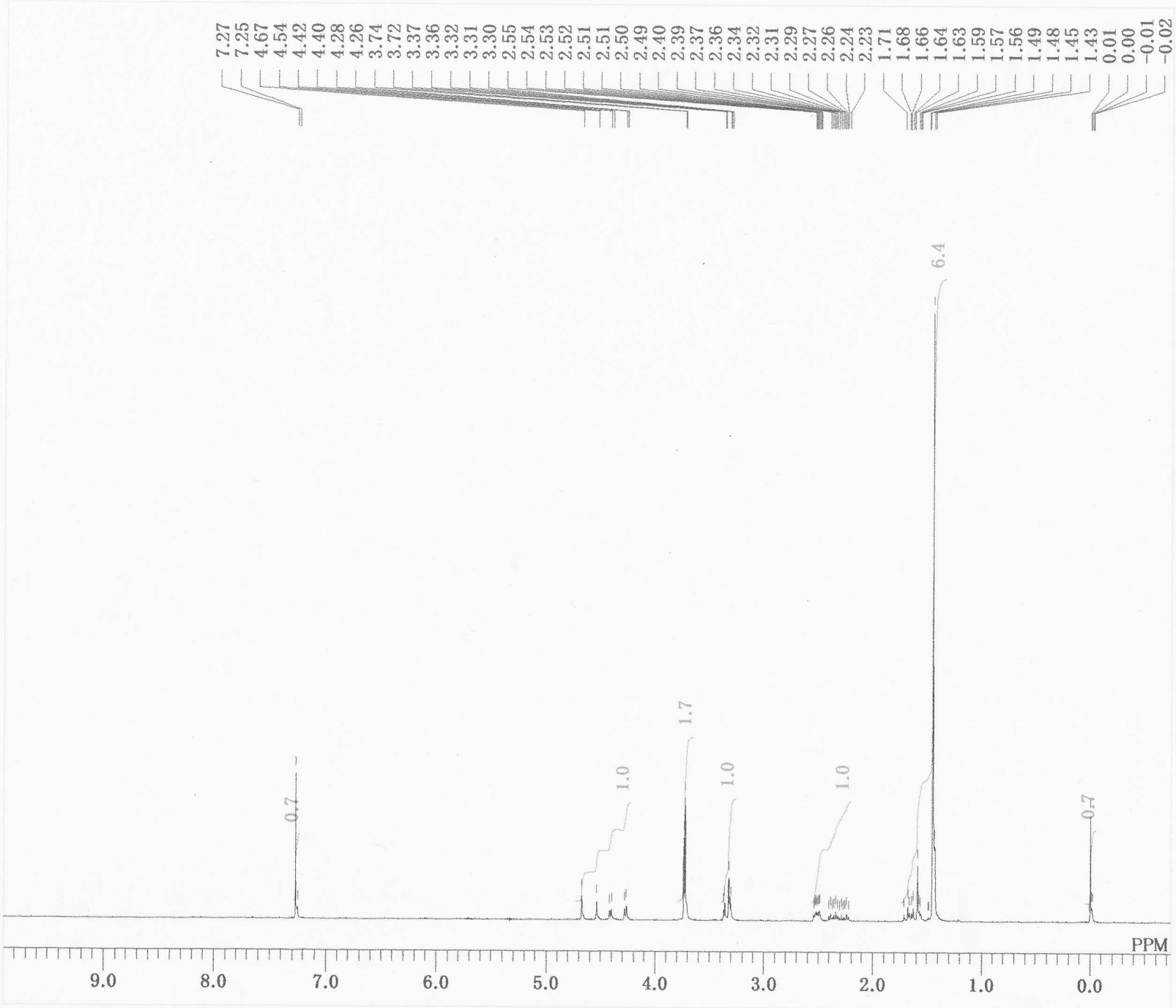
S8



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POINT	16384
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SCANS	16
ACQTM	3.0331 sec
PD	3.9670 sec
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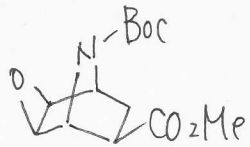

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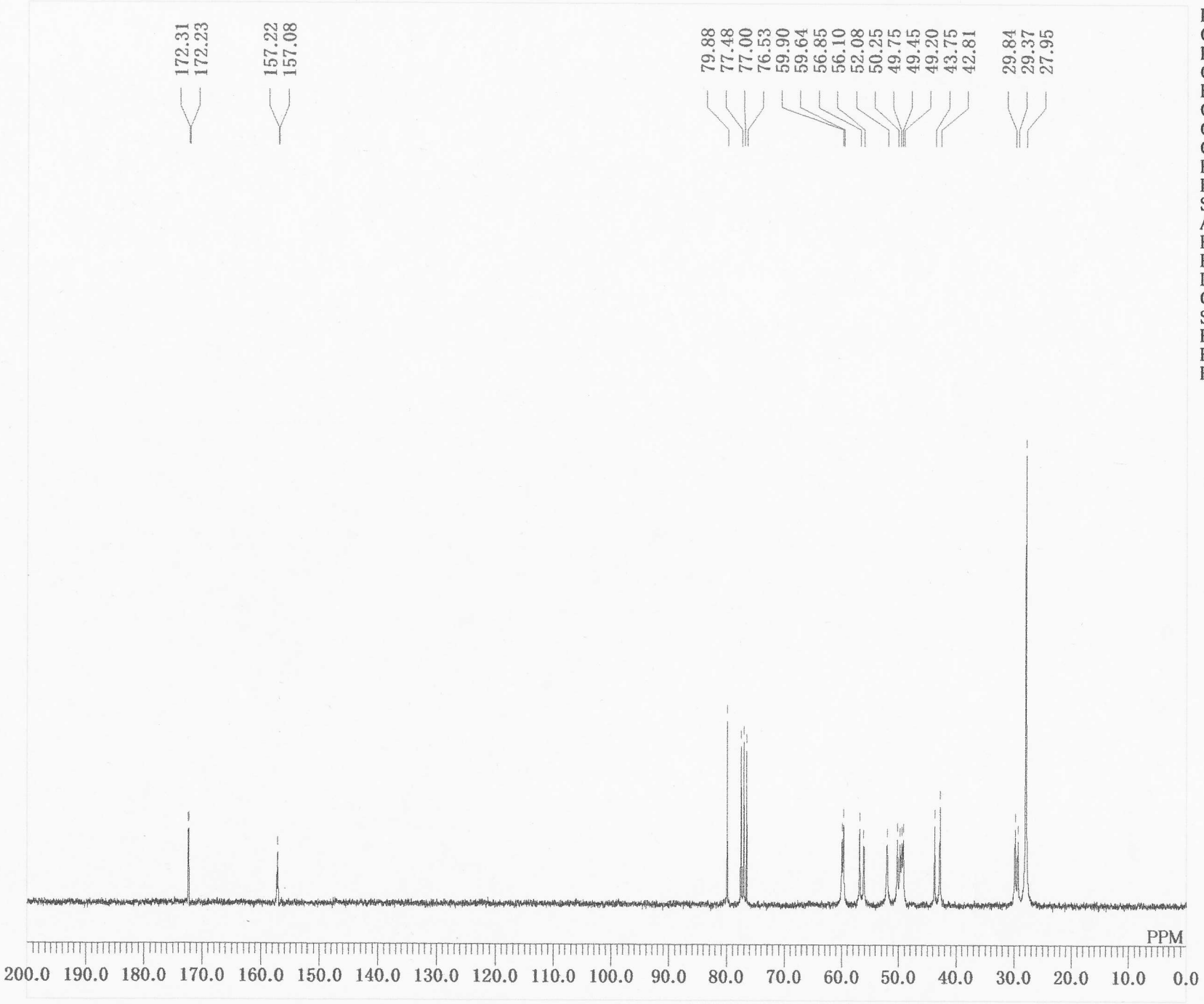

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OBFIN	5200.00 Hz
POINT	32768
FREQU	18306.64 Hz
SCANS	1024
ACQTM	1.7900 sec
PD	1.2100 sec
PW1	4.10 usec
IRNUC	1H
CTEMP	32.1 c
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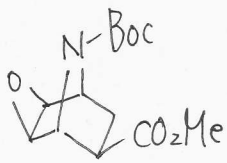
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	26



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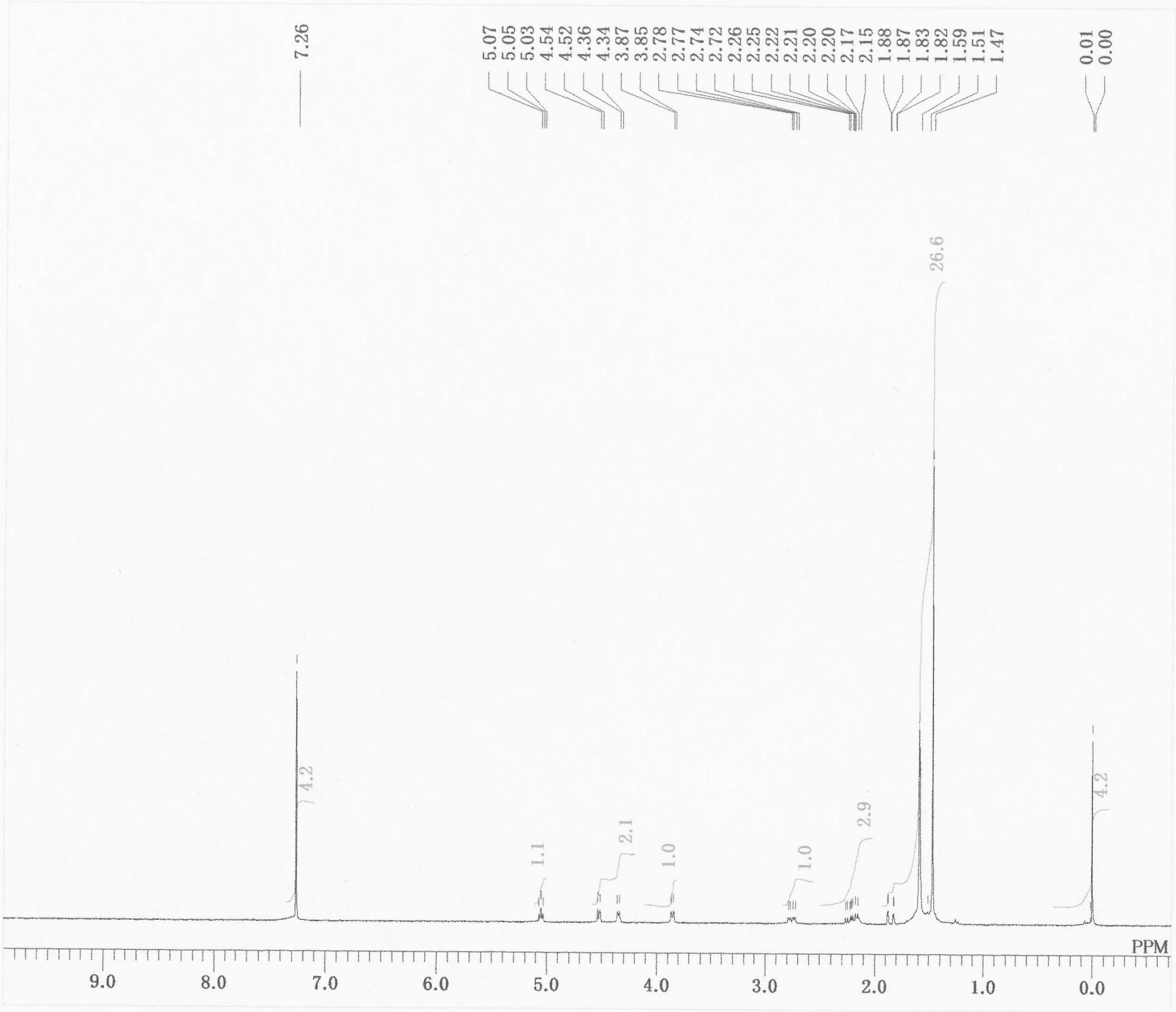

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SCANS	16
ACQTM	3.0331 sec
PD	3.9670 sec
PW1	5.00 usec
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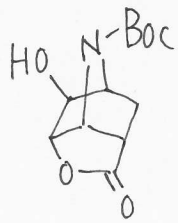
BF	0.12 Hz
RGAIN	23



6

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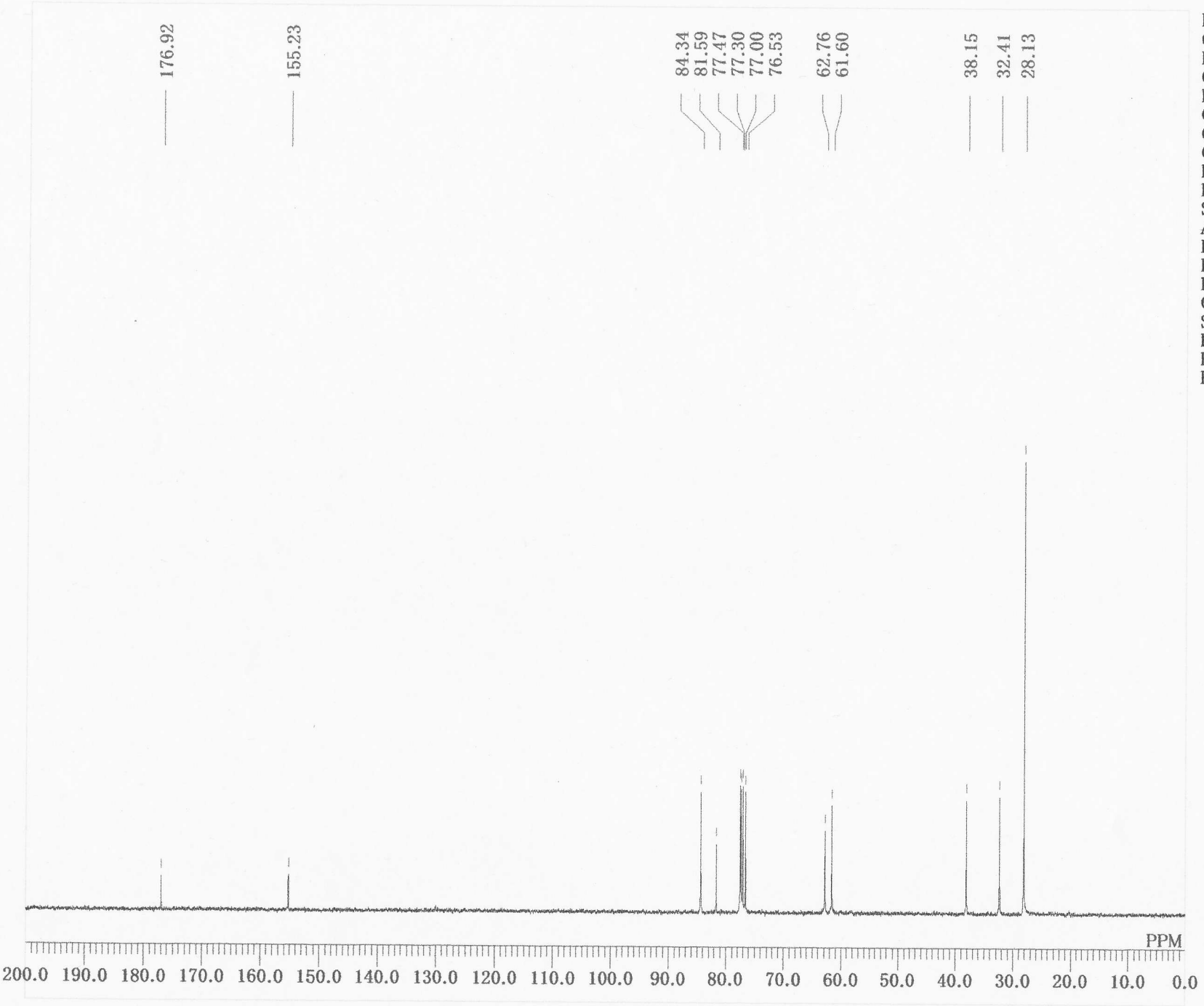

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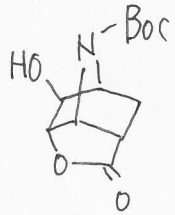
OBFIN	5200.00 Hz
POINT	32768
FREQU	18306.64 Hz
SCANS	2048
ACQTM	1.7900 sec
PD	1.2100 sec
PW1	4.20 usec
IRNUC	1H
CTEMP	29.6 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	26



6

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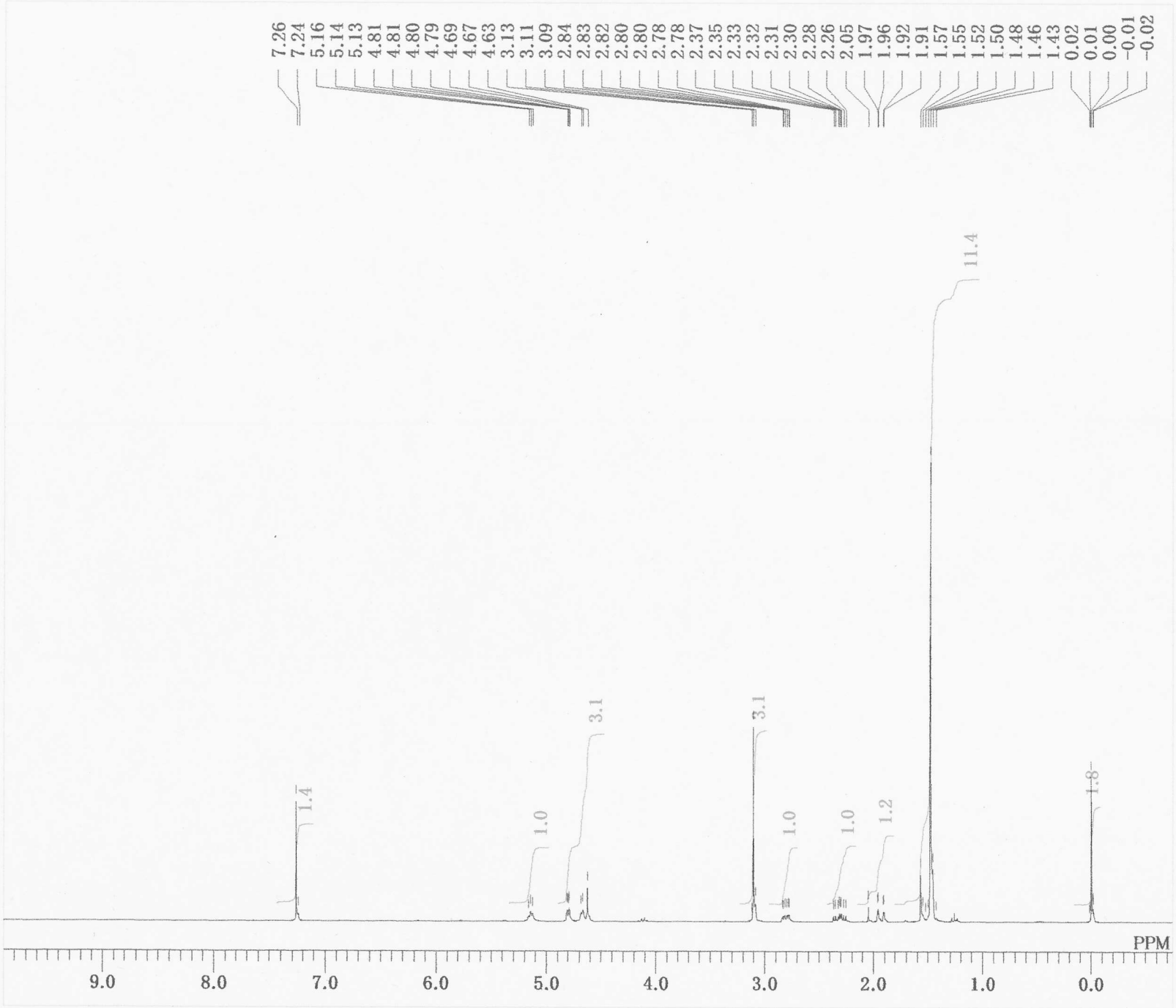

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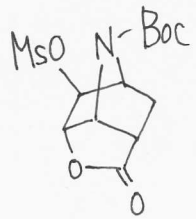
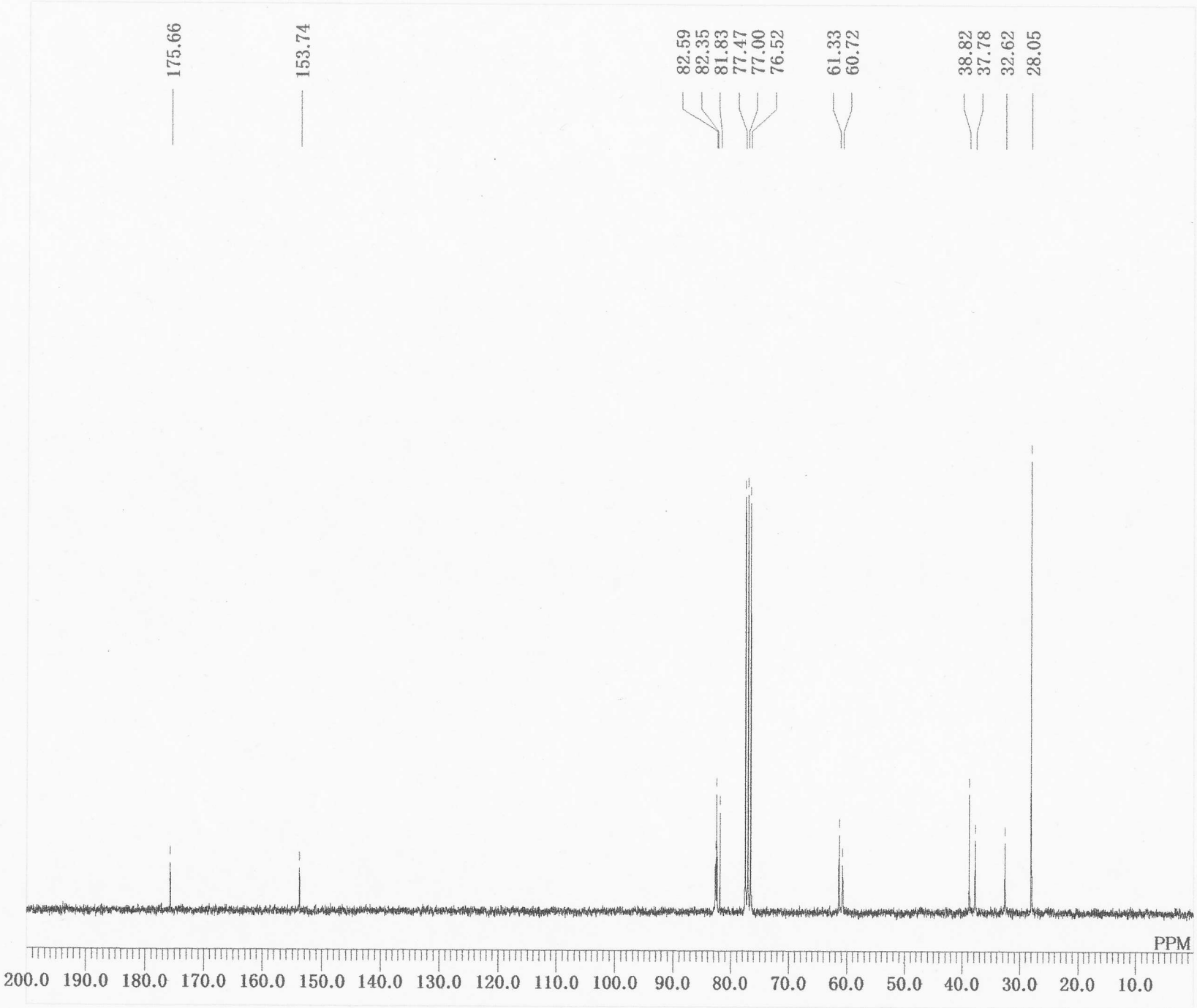
OBFIN	5800.00 Hz
POINT	16384
FREQU	5401.76 Hz
SCANS	16
ACQTM	3.0331 sec
PD	3.9670 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	23.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	21



7

13C

S13



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SCANS	1024
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PD	1.2100 sec
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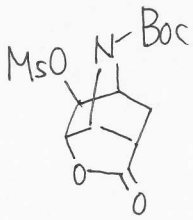
RGAIN	26



7

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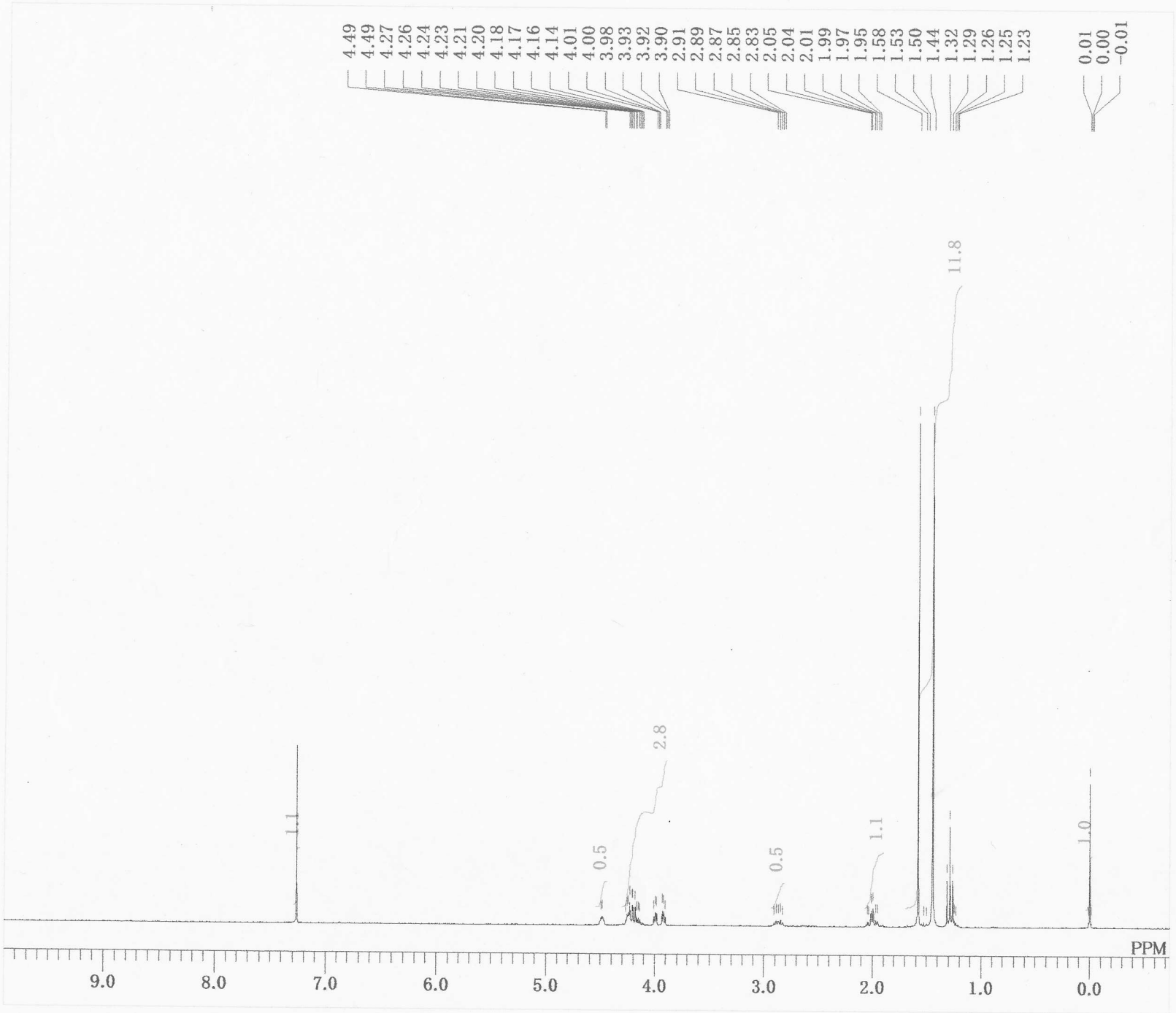

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POINT	16384
FREQU	5401.76 Hz
SCANS	16
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PD	3.9670 sec
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IRNUC	1H
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SLVNT	CDCL3
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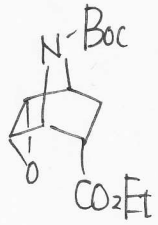

8

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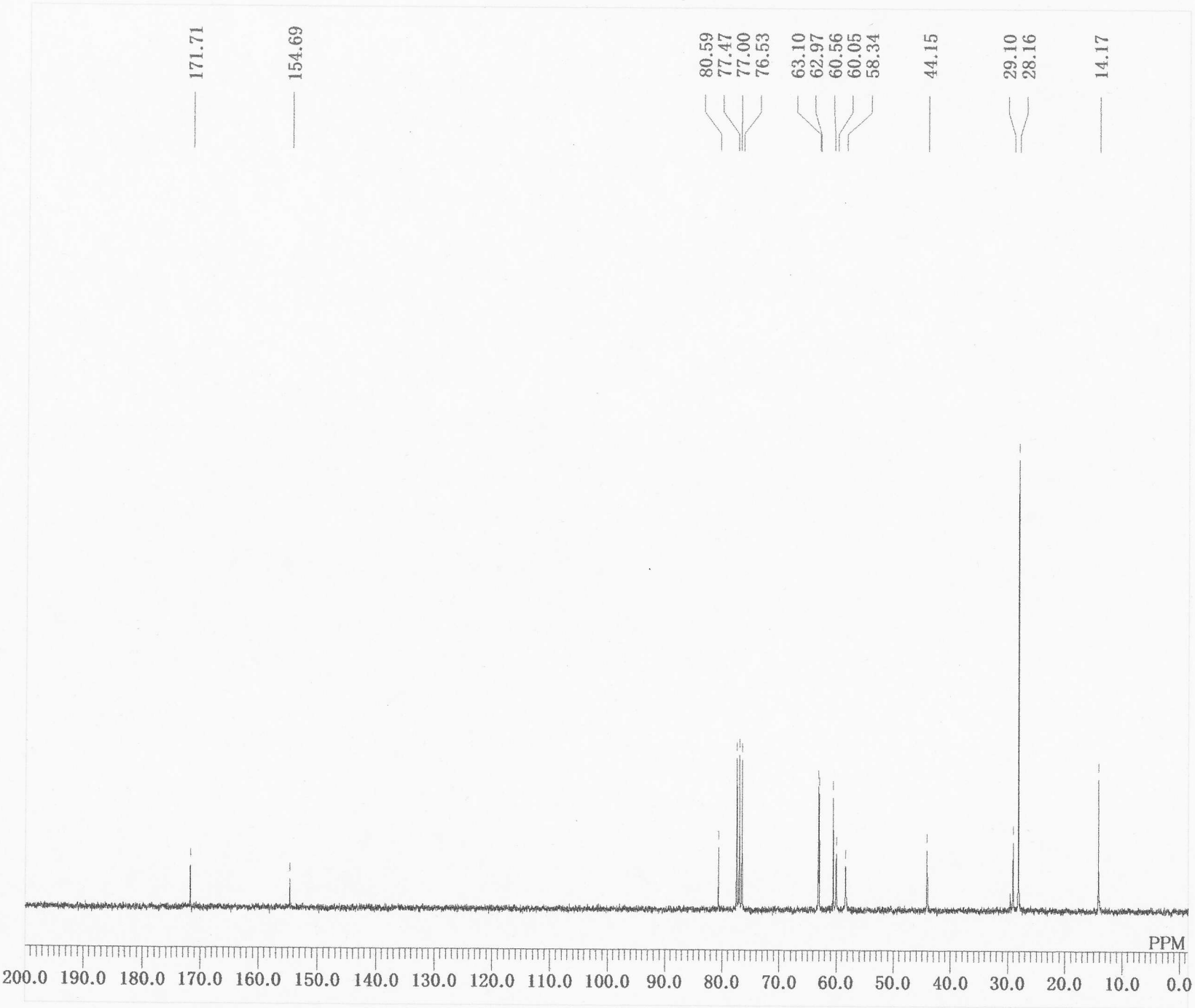

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SCANS	1024
ACQTM	1.7900 sec
PD	1.2100 sec
PW1	4.20 usec
IRNUC	1H
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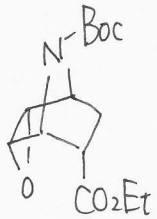
RGAIN	25



8

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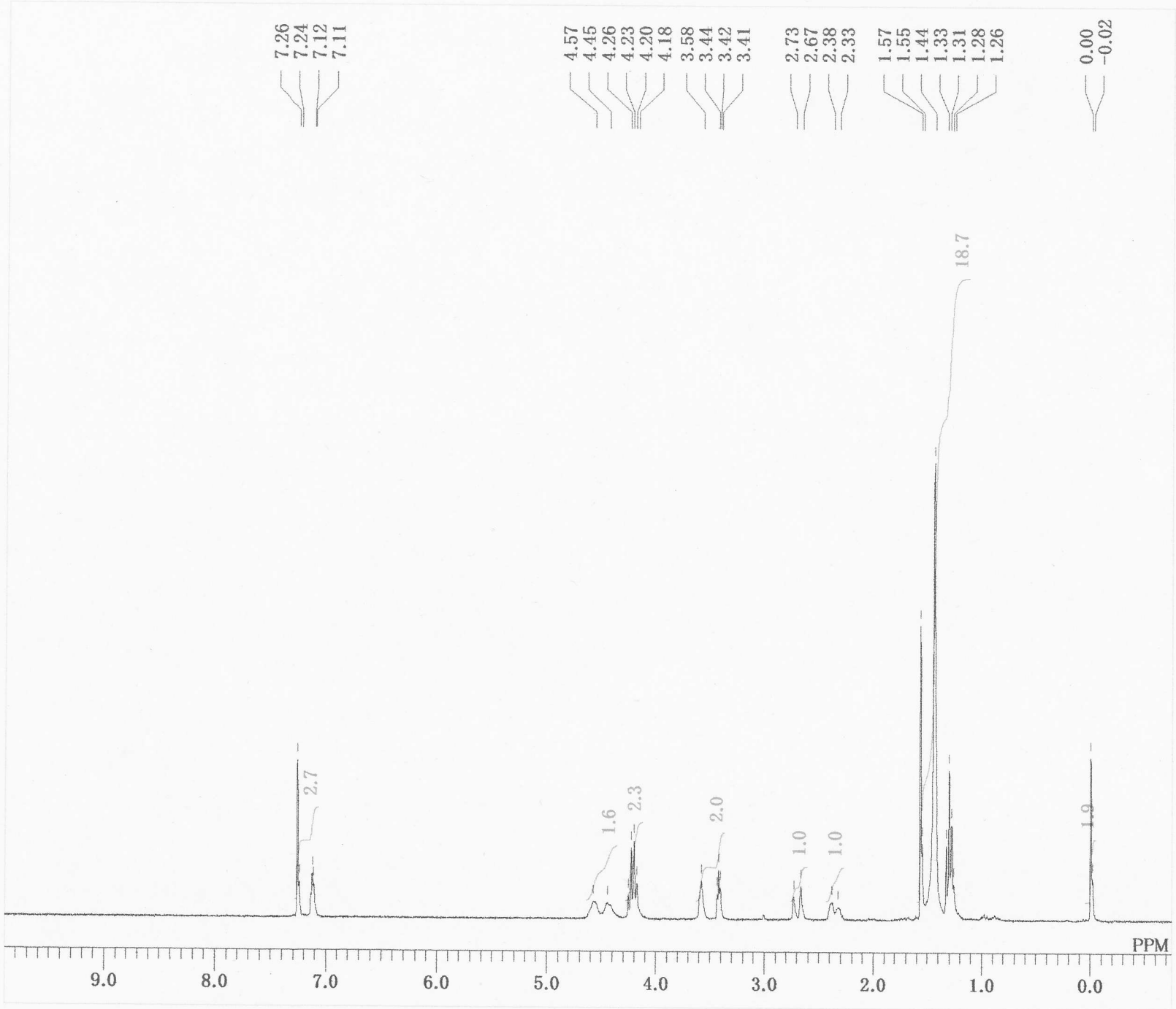

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OBFIN	5800.00 Hz
POINT	16384
FREQU	5401.76 Hz
SCANS	16
ACQTM	3.0331 sec
PD	3.9670 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	25.7 c
SLVNT	CDCL3
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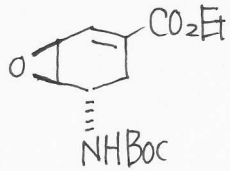
BF	0.12 Hz
RGAIN	21



9

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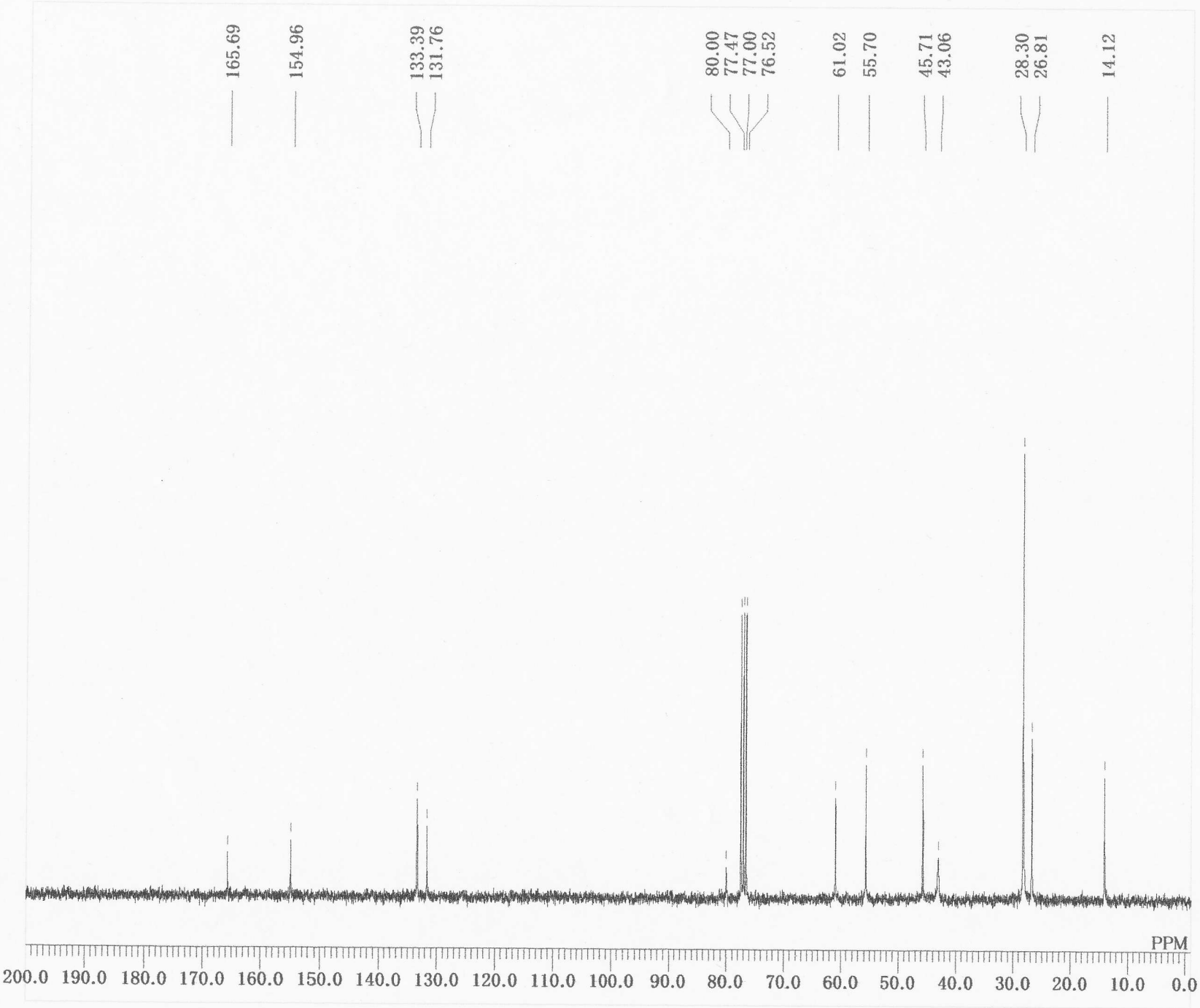

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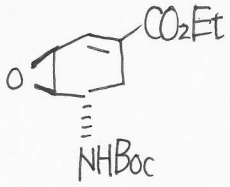
OBSET	135.00 KHz
OBFIN	5200.00 Hz
POINT	32768
FREQU	18306.64 Hz
SCANS	1024
ACQTM	1.7900 sec
PD	1.2100 sec
PW1	4.10 usec
IRNUC	1H
CTEMP	34.8 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	27



9

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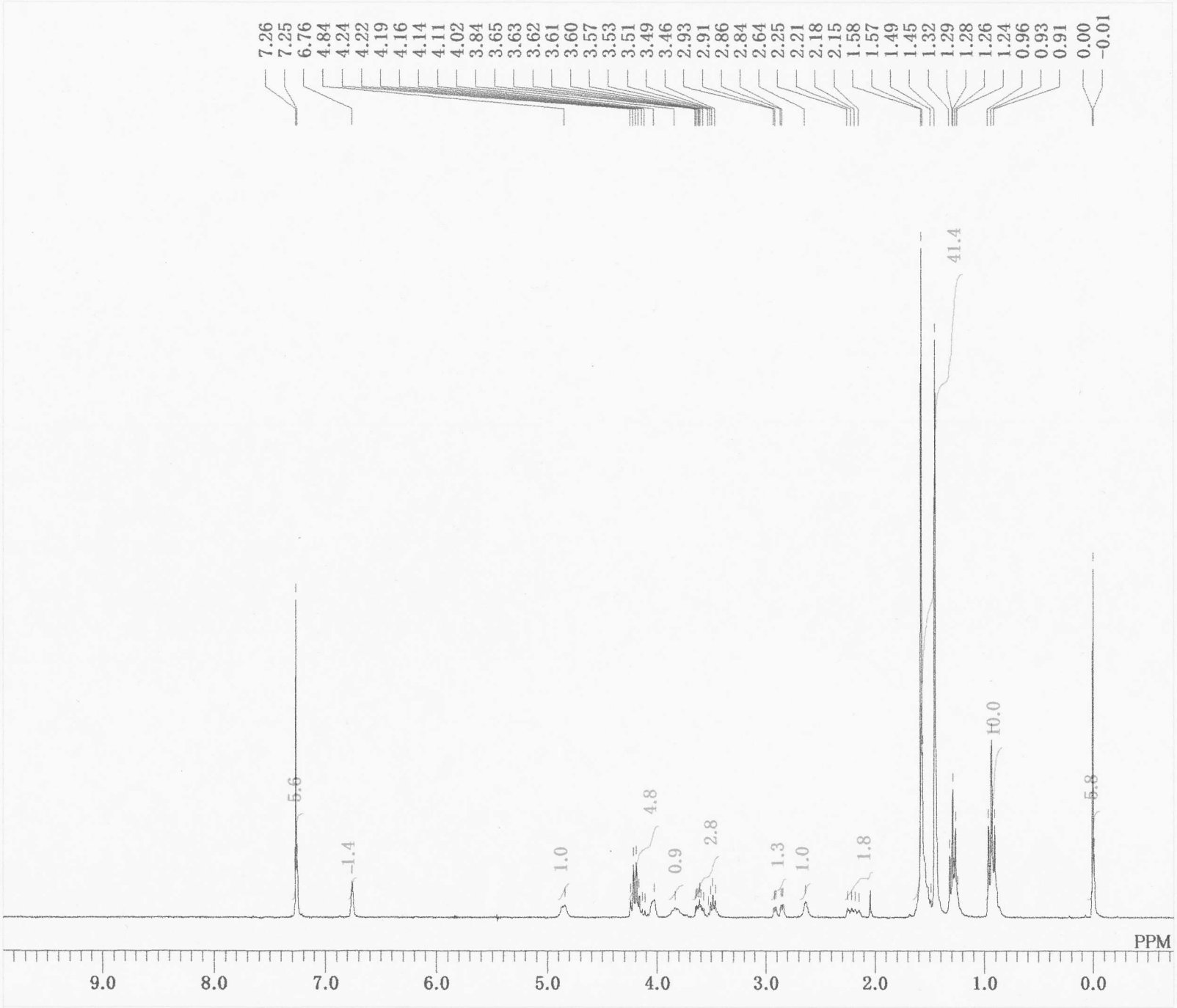

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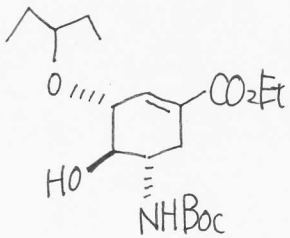
OBFIN	5800.00 Hz
POINT	16384
FREQU	5401.76 Hz
SCANS	64
ACQTM	3.0331 sec
PD	3.9670 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	23.9 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	23



10

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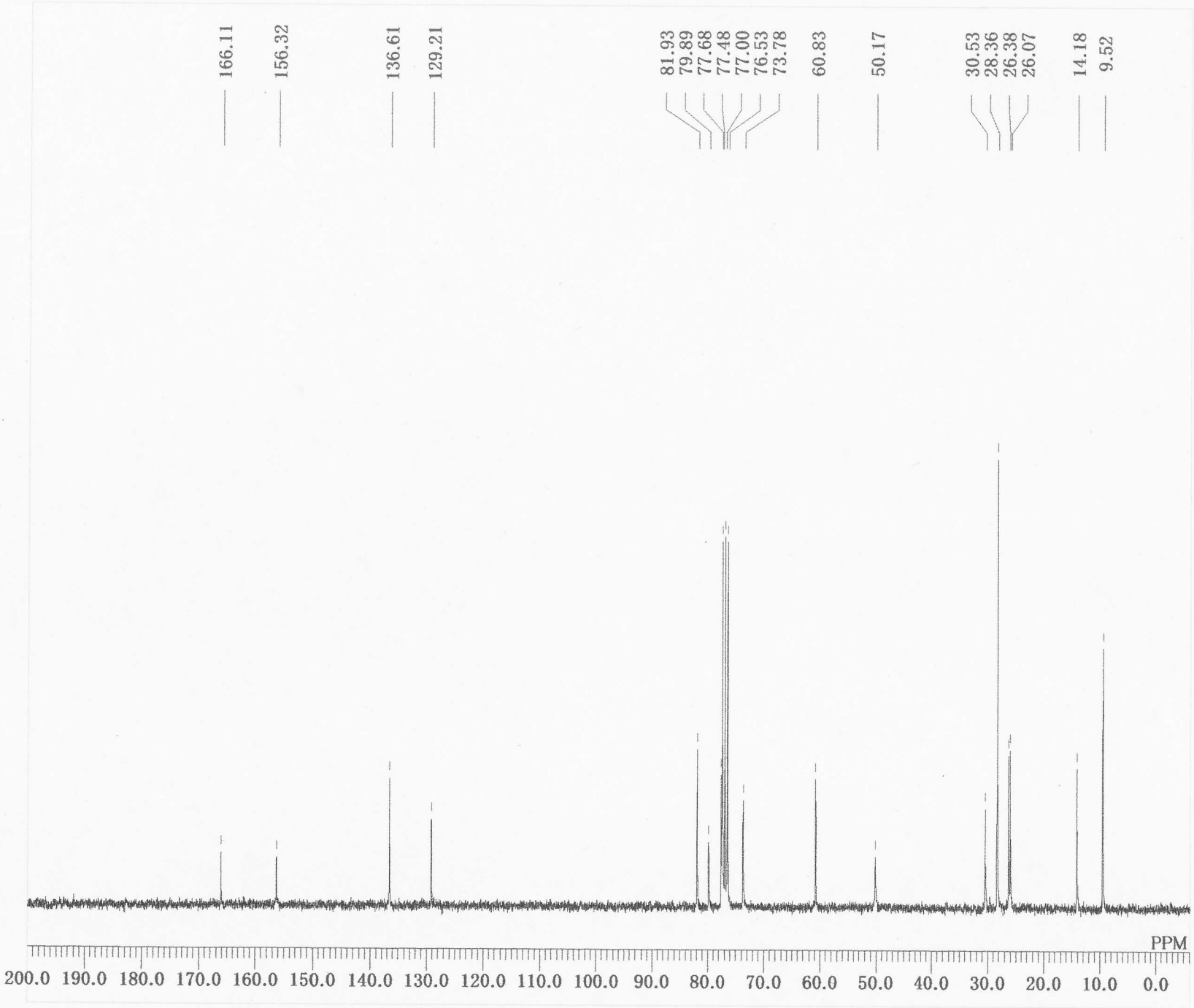

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OBFIN	5200.00 Hz
POINT	32768
FREQU	18306.64 Hz
SCANS	4096
ACQTM	1.7900 sec
PD	1.2100 sec
PW1	4.10 usec
IRNUC	1H
CTEMP	34.3 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
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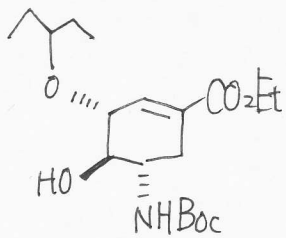
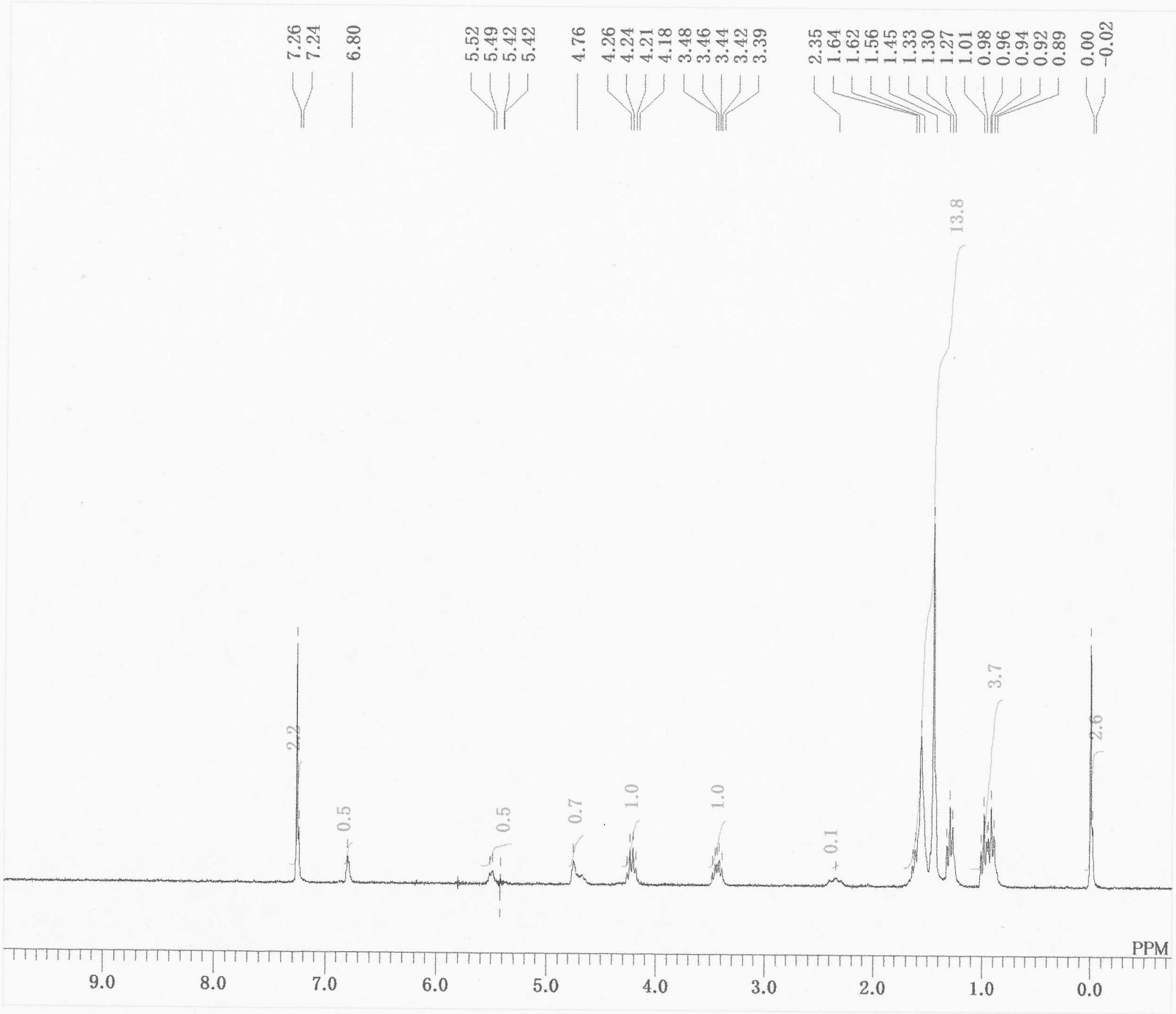
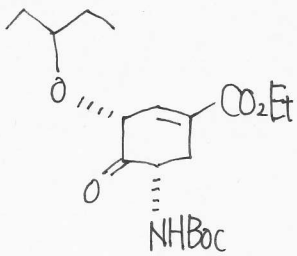


10

tn04078pr1

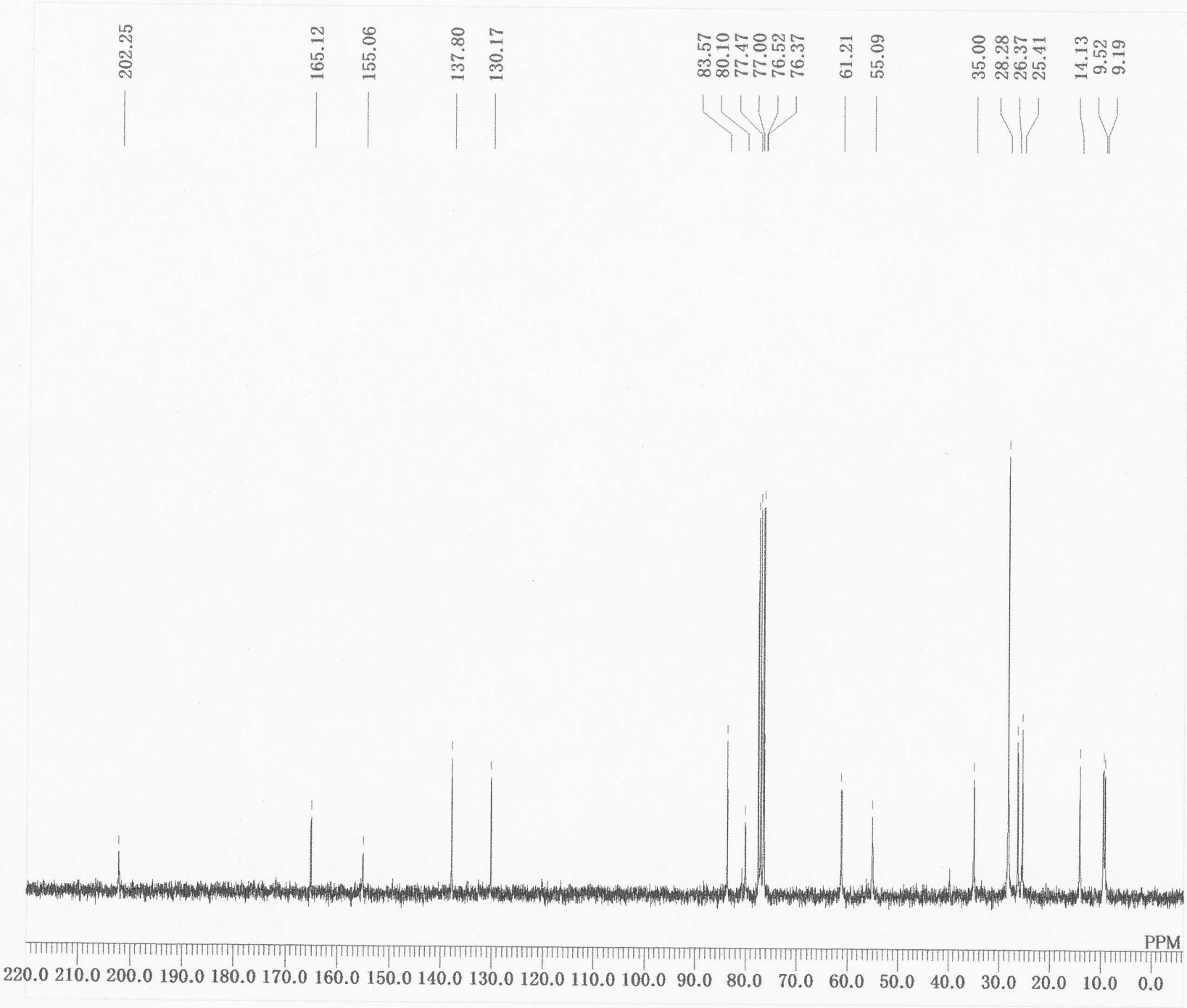


DFILE	tn04078pr1.als
COMNT	tn04078pr1
DATIM	Fri Dec 04 04:13:54 2009
OBNUC	1H
EXMOD	NON
OBFRQ	270.05 MHz
OBSET	112.00 KHz
OBFIN	5800.00 Hz
POINT	16384
FREQU	5401.76 Hz
SCANS	16
ACQTM	3.0331 sec
PD	3.9670 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	24.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	24

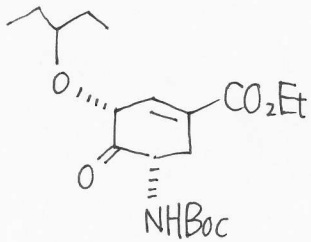


11

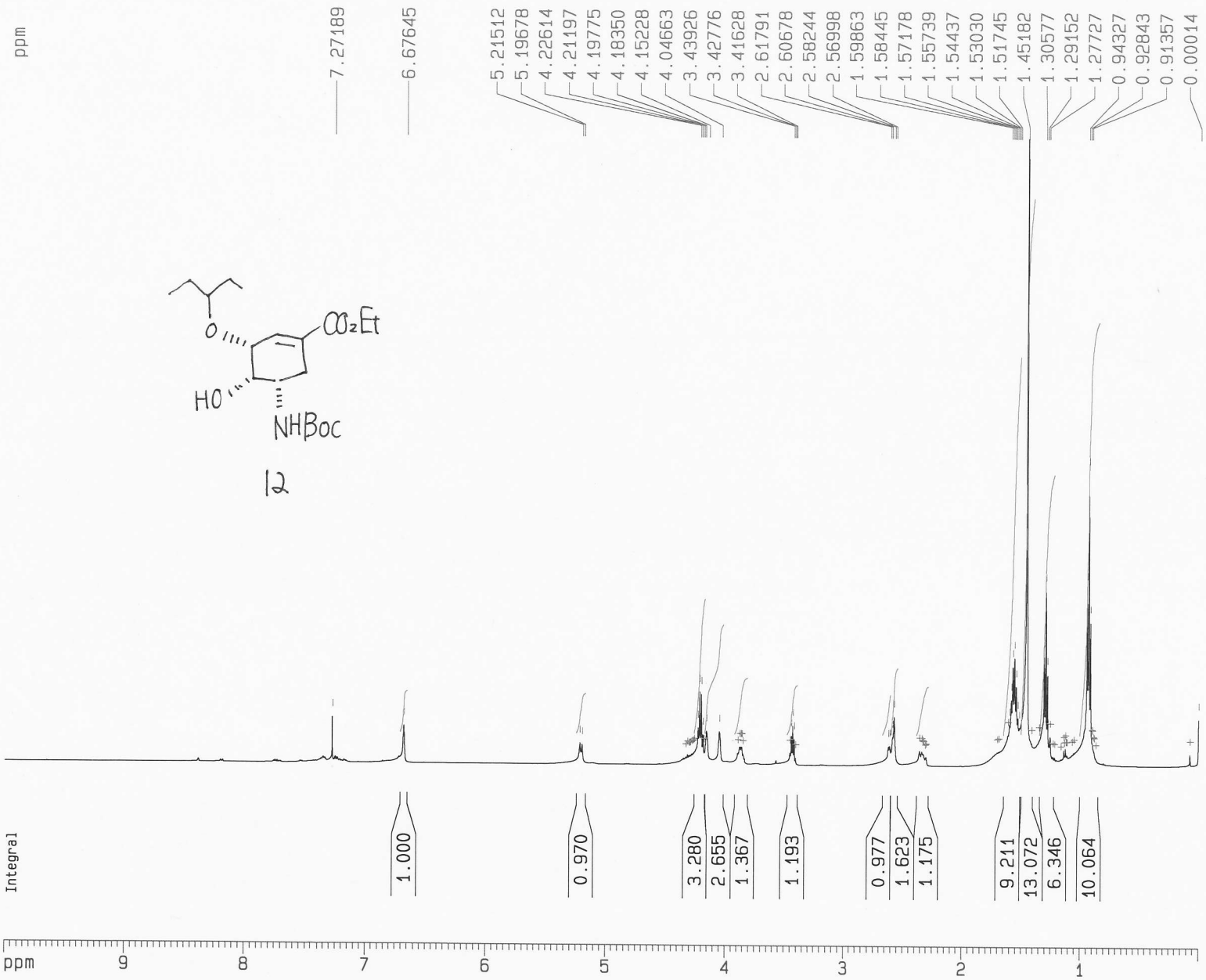
tn04073pr1-13C



DFILE	tn04073pr1-13C.als
COMNT	tn04073pr1-13C
DATIM	Mon Nov 30 17:31:48 2009
OBNUC	13C
EXMOD	BCM
OBFRQ	67.80 MHz
OBSET	135.00 KHz
OBFIN	5200.00 Hz
POINT	32768
FREQU	18306.64 Hz
SCANS	2048
ACQTM	1.7900 sec
PD	1.2100 sec
PW1	4.10 usec
IRNUC	1H
CTEMP	34.7 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	24



11



12

Current Data Parameters
NAME tn04076PR1
EXPNO 13
PROCNO 1

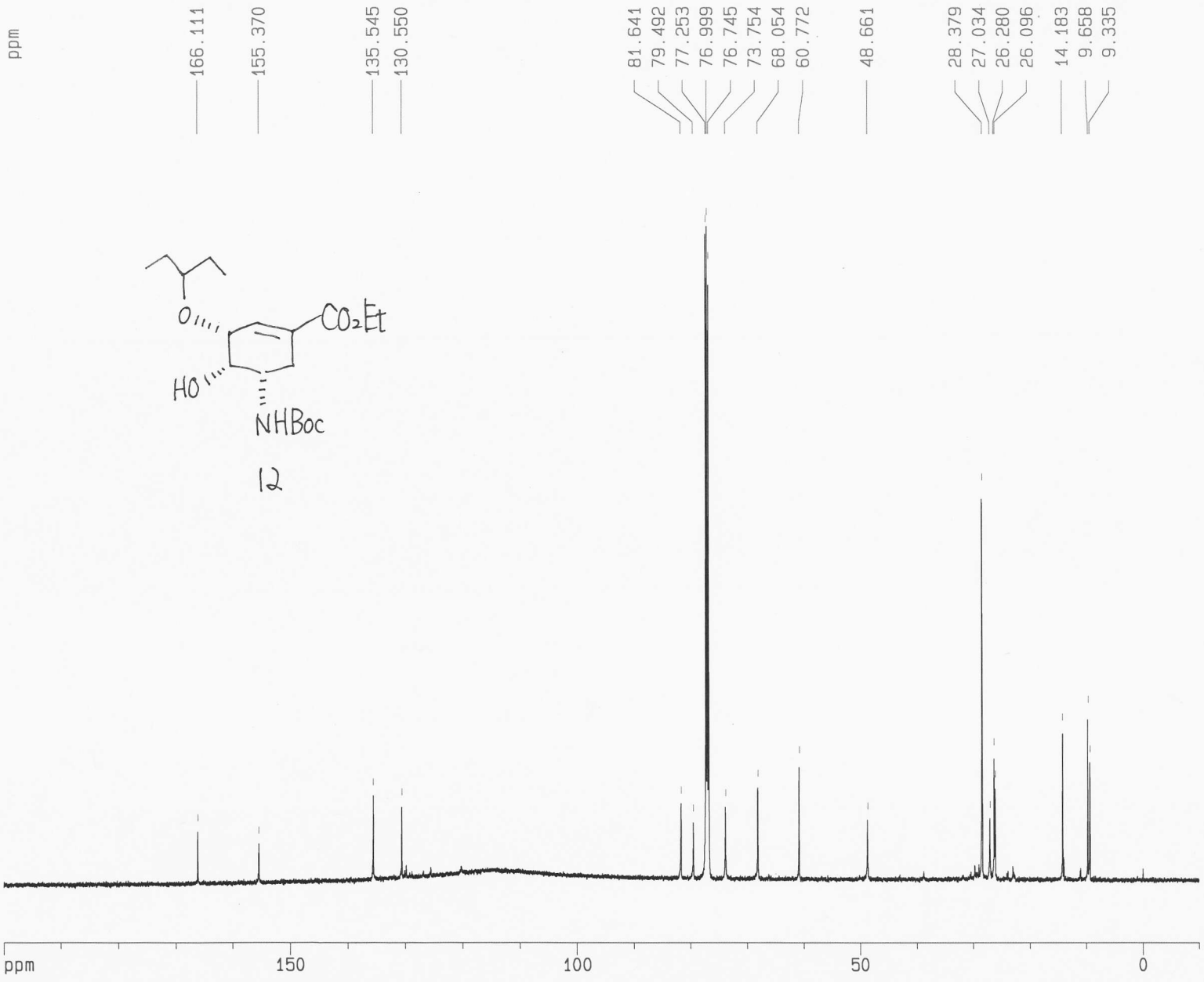
F2 - Acquisition Parameters
Date_ 20091219
Time 17.02
INSTRUM drx500
PROBHD 5 mm TXI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 12531.328 Hz
FIDRES 0.191213 Hz
AQ 2.6149364 sec
RG 64
DW 39.900 usec
DE 7.50 usec
TE 300.0 K
D1 1.00000000 sec

========== CHANNEL f1 ==========
NUC1 1H
P1 8.20 usec
PL1 -2.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.50000 ppm/cm
HZCM 250.06500 Hz/cm

tn04076PR1

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Current Data Parameters
NAME          tn04076PR1
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20091219
Time               13.49
INSTRUM          drx500
PROBHD     5 mm TXI 1H-
PULPROG             zgpg
TD                 65536
SOLVENT            CDCl3
NS                 17408
DS                     4
SWH            31446.541 Hz
FIDRES          0.479836 Hz
AQ             1.0420724 sec
RG               14596.5
DW                15.900 usec
DE                 6.00 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

============ CHANNEL f1 =============
NUC1                 13C
P1                 13.50 usec
PL1                -4.00 dB
SFO1         125.7715719 MHz

============ CHANNEL f2 =============
CPDPRG2          waltz16
NUC2                  1H
PCPD2              75.00 usec
PL2                -2.00 dB
PL12               10.50 dB
PL13               10.50 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577907 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P               200.000 ppm
F1              25151.56 Hz
F2P               -10.000 ppm
F2              -1257.58 Hz
PPMCM           10.50000 ppm/cm
HZCM          1320.45679 Hz/cm
```