JOC The Journal of Organic Chemistry

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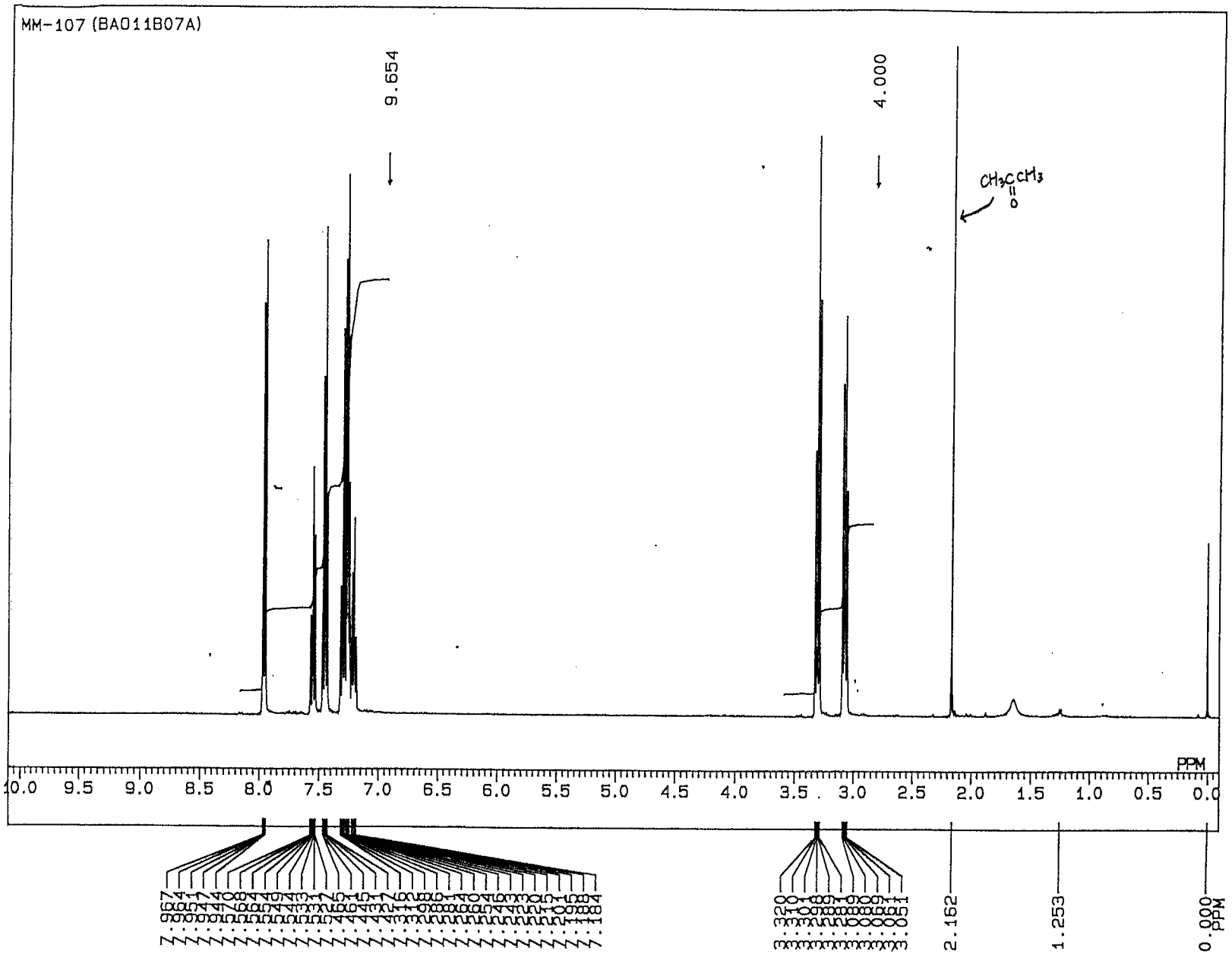
G 379-1



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FREQU 8000.0 Hz
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PD 4.000 sec
PW1 7.7 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 60 us
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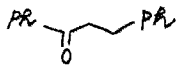
MM-107



2a

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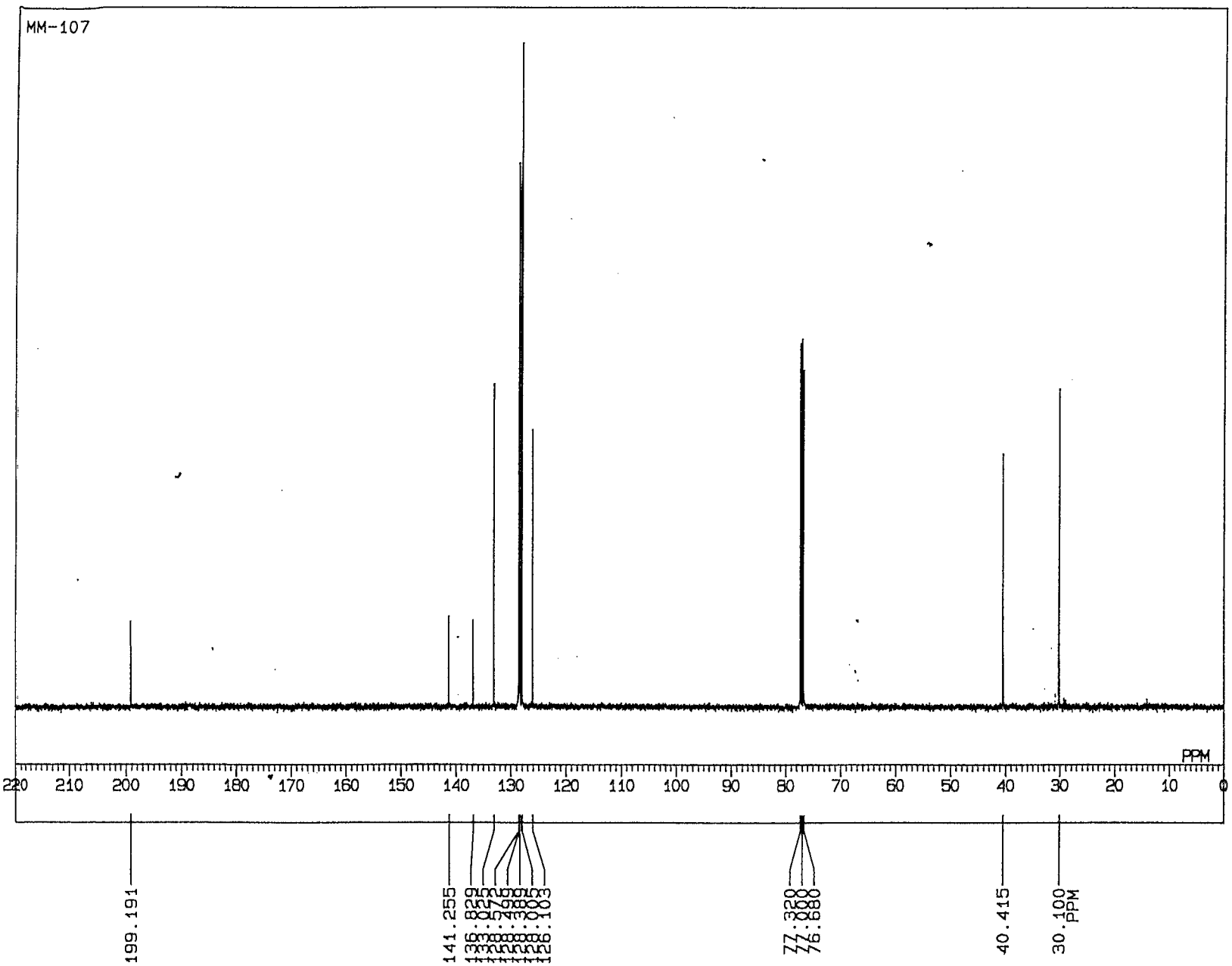

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PD 1.912 sec
PW1 5.2 us
IRFIN 10300.0 Hz
IRATN 20
IRRPW 50 us
TEMP. 27.0 c
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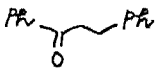
MM-107



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G 379-2

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G379-3

Acquisition Parameters for DAT File: DR0:[100,100]HR.DAT;10

Acquisition Date:	22-JUN-1992 15:00		
Sample :	M2-44		
Scan Range :	110.000-300.000	Data Type :	PS,HE
Scan Slope :	5.0 sec.	Cycle Time :	2.1 sec.
Scan Type :	MF,LI,UP,DA	Accel. Voltage :	3.0 kv/DAC
Maximum Run Time:	20 min.	Run Time :	7'20.9"
Valve open/close:			
Ionization Mode :	EI	Polarity :	POS.
Resolving Power :		Filter setting :	
Inlet Source :	PAC	Magnetic Field :	Auto
Temp. Points :	GC	Pre_amp Control :	HS
Threshold Level :	1000-1000	Valley :	1, Fix
Tic Range :	110.000-300.000		25%
Dynamic Calibration File:			
Static Calibration File :			

CH-TEMP. 250°C

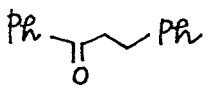
Elemental Composition

Data File: [100,100]HR.DAT;10 Date: 22-JUN-92(Mon) 15:00:29
Sample: M2-44
RT 6'49", EI(+), GC 234.8c, BP: m/z 210.1024, Int. 91.46, Lv 0.00
Scan# 196

----> for sample peak, U.S. 0/15, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/50, H 0/100, O 0/10

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
210.1024	100.00	-2.1	9.0	1:	C15 H14 O



calcd. 210.10452

2a

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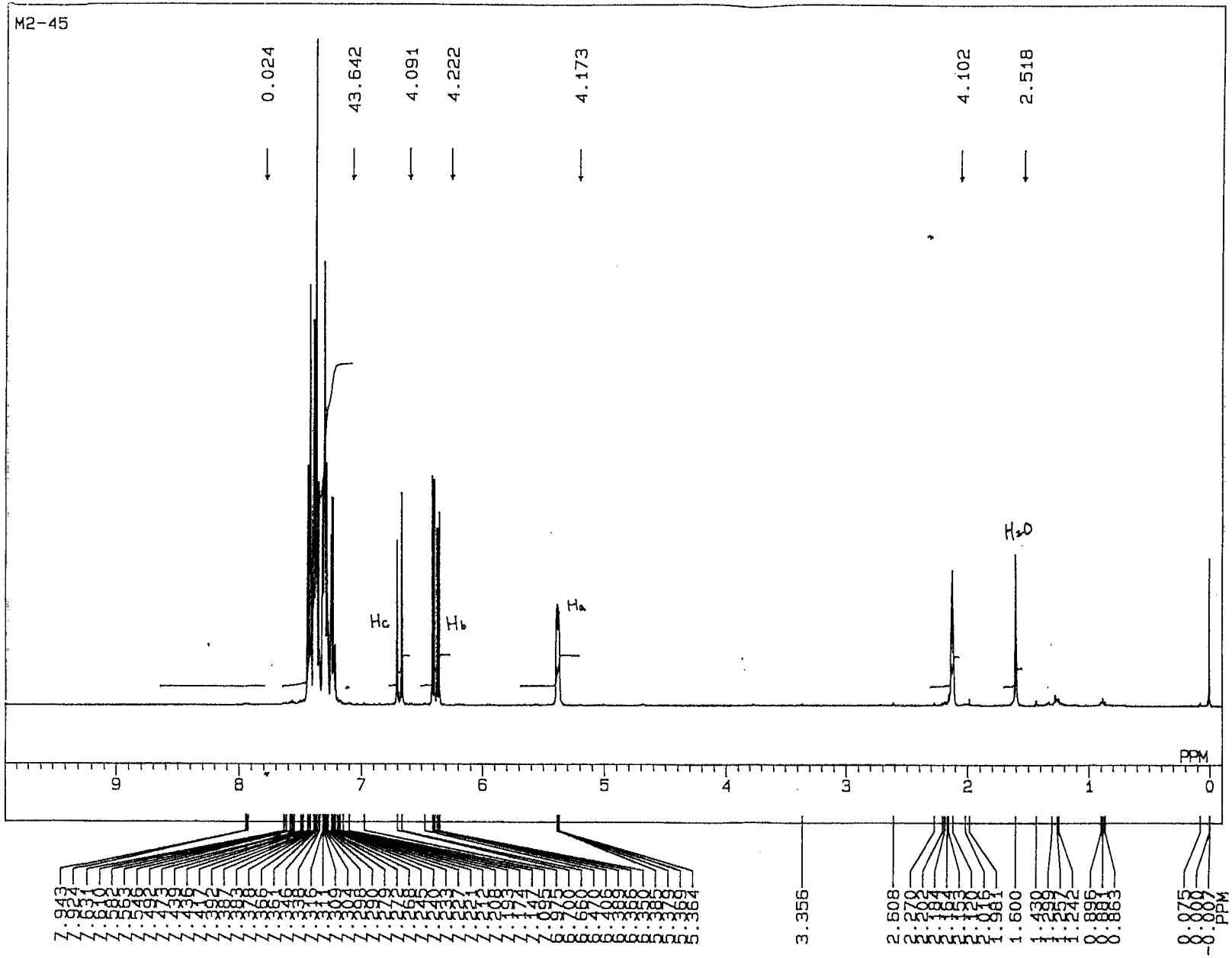
G 379-4



JEOL

11-JUN-92 18: 49: 24
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COMNT M2-45
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OBFIN 10300.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 4.000 sec
PW1 7.3 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 60 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 15
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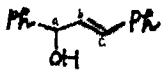
XS -174.2667 Hz

M2-45 PTLC F3



3a

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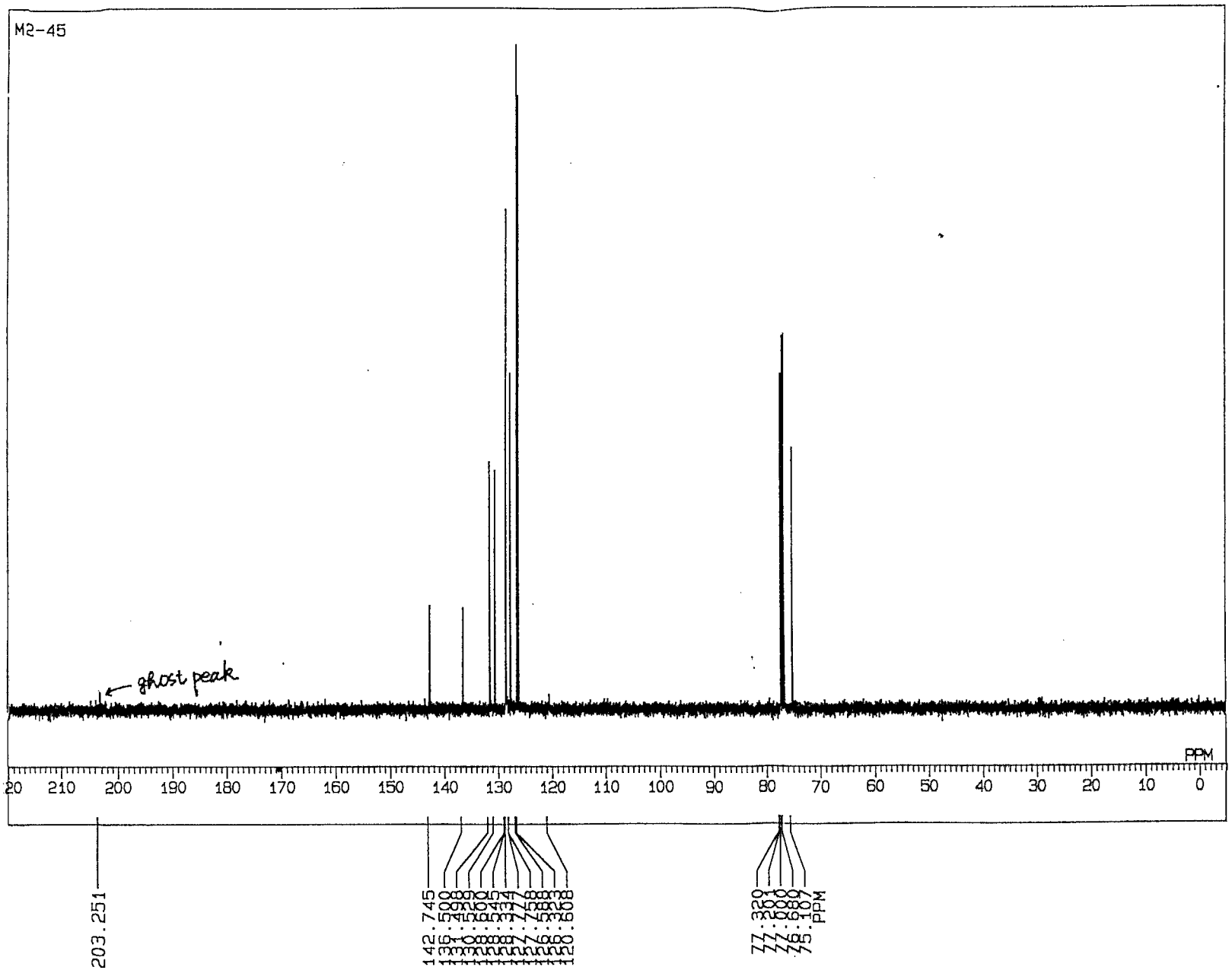

JEOL

11-JUN-92 19:04:00
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COMNT M2-45
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OBFIN 10244.0 Hz
POINT 65536
FREQU 30120.5 Hz
SCANS 168
ACQTM 1.088 sec
PD 1.912 sec
PW1 5.0 us
IRFIN 10300.0 Hz
IRATN 20
IRRPW 60 us
TEMP. 27.0 c
SLVNT CDCL3
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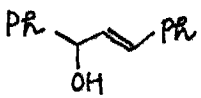
BF 0.92 Hz
RGAIN 28
XE 22618.2200 Hz
XS -957.3691 Hz



3a

G379-5

G379-6

Acquisition Parameters for DAT File: DR0:[100,100]HR.DAT;7

Acquisition Date:	22-JUN-1992 14:45		
Sample :	M2-45		
Scan Range :	110.000-300.000	Data Type :	PS,HE
Scan Slope :	5.0 sec.	Cycle Time :	2.1 sec.
Scan Type :	MF,LI,UP,DA	Accel. Voltage :	3.0 kv/DAC
Maximum Run Time:	20 min.	Run Time :	7'54.5"
Valve open/close:			
Ionization Mode :	EI	Polarity :	POS.
Resolving Power :		Filter setting :	Auto
Inlet Source :	PAC	Magnetic Field :	HS
Temp. Points :	GC	Pre_amp Control :	1. Fine
Threshold Level :	1000-1000	Valley :	25%
Tic Range :	110.000-300.000		
Dynamic Calibration File:			
Static Calibration File :			

CH.TEMP. 250°C

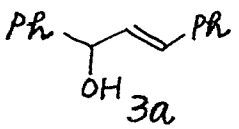
Elemental Composition

Data File: [100,100]HR.DAT;7 Date: 22-JUN-92(Mon) 14:45:43
Sample: M2-45
RT 7'21", EI(+), GC 245.2c, BP: m/z 118.9920, Int. 74.84, Lv 0.00
Scan# 211

----> for sample peak, U.S. 0/15, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/50, H 0/100, O 0/10

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
210.1038	44.74	-0.7	9.0	1:	C15 H14 O



3a

calcd. 210.10452

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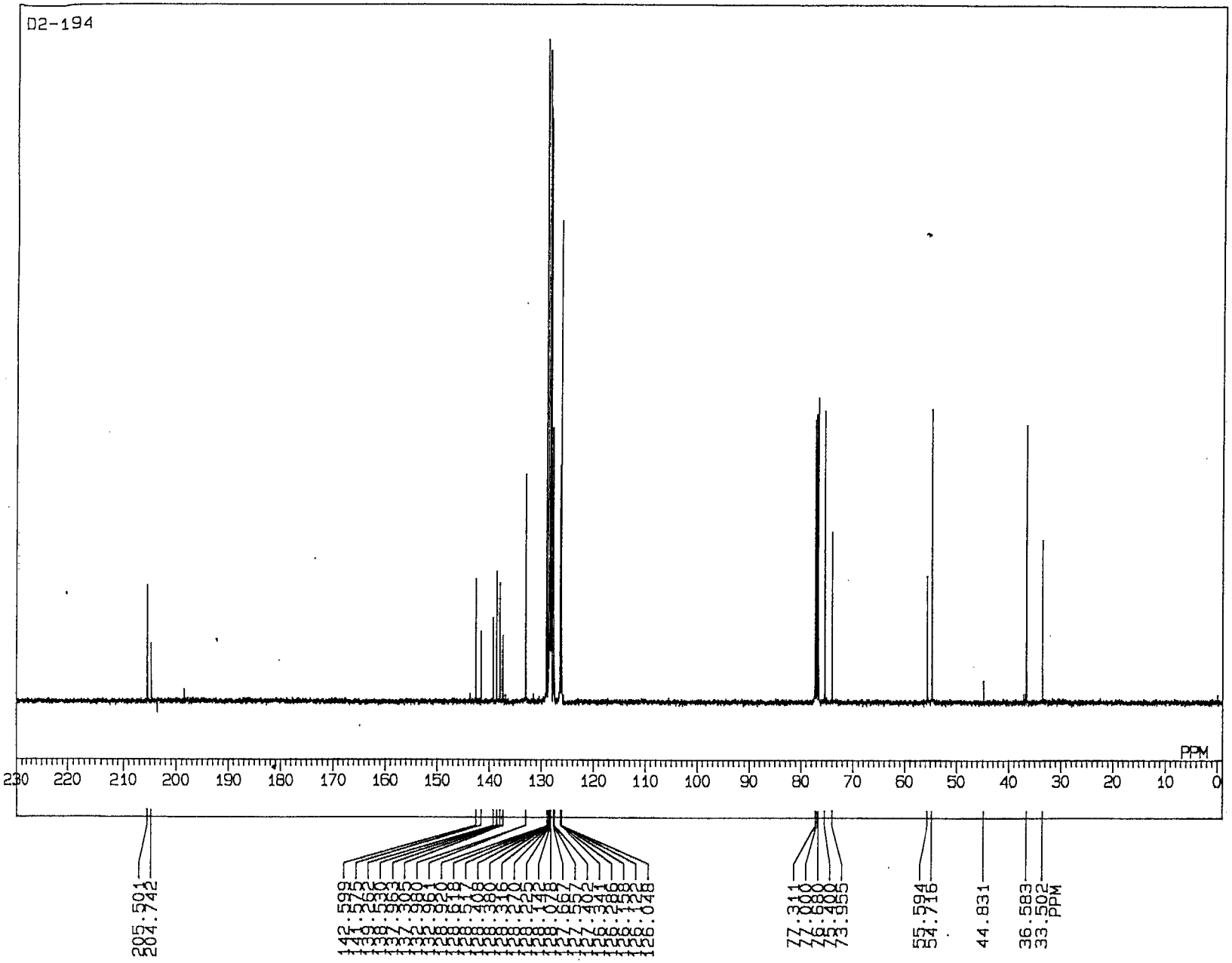
G 379-7



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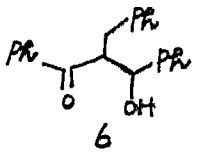
OBFIN 10244.0 Hz
POINT 65536
FREQU 30120.5 Hz
SCANS 600
ACQTM 1.088 sec
PD 1.912 sec
PW1 5.2 us
IRFIN 10300.0 Hz
IRATN 20
IRRPW 50 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 25
XE 23221.3700 Hz
XS -1666.5620 Hz

D2-194



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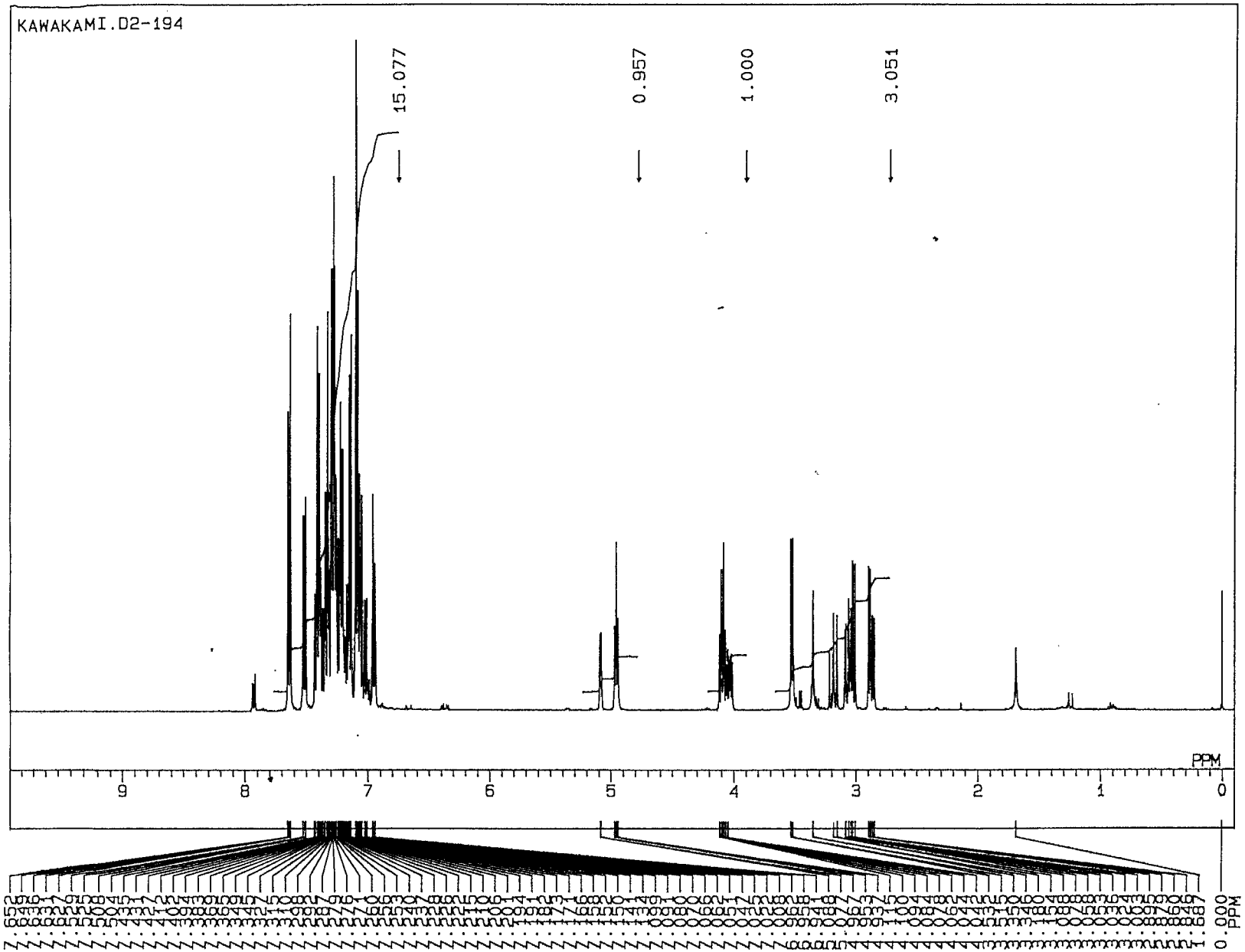

09-JUN-95 12: 48: 54
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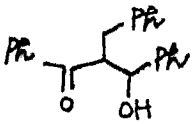
COMNT KAWAKAMI.D2-194
EXMOD SGNON
OBNUC 1H
OBFIN 10300.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 4.000 sec
PW1 7.7 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 60 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 9
XE 3997.8250 Hz
XS -179.6378 Hz

D2-194



6

G 379-B

G 379-9

Acquisition Parameters for DAT File: DR0:[100,100]HR.DAT;2

Acquisition Date:	21-JUN-1995 10:50		
Sample :	D2-194		
Scan Range :	250.000-370.000	Data Type :	PS,HE
Scan Slope :	9.0 sec.	Cycle Time :	2.0 sec.
Scan Type :	MF,LI,UP,DA	Accel. Voltage :	3.0 kv/DAC
Maximum Run Time:	20 min.	Run Time :	2'52.1"
Valve open/close:			
Ionization Mode :	×9× CI	Polarity :	POS.
Resolving Power :	5000	Filter setting :	3000
Inlet Source :	DIR	Magnetic Field :	HS
Temp. Points :	DI	Pre_amp Control :	
Threshold Level :	1000-1000	Valley :	25%
Tic Range :	250.000-370.000		
Dynamic Calibration File:			
Static Calibration File :			

CH. TEMP. 100°C

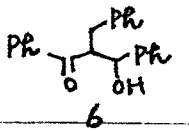
Elemental Composition

Data File: [100,100]HR.DAT;2 Date: 21-JUN-95(Wed) 10:50:53
Sample: D2-194
RT 1'58", CI(+), GC 57.6c, BP: m/z 292.9824, Int. 40.69, Lv 0.00
Scan# 60

----> for sample peak, U.S. 0/15, Def. 5.0 mmu, Formula, up to 1000 mass
C 11/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
317.1537	14.47	-0.5	12.5	1:	C22 H21 O2



calcd. [CI] = 317.1541
$C_{22}H_{21}O_2$

Elemental Composition

Data File: [100,100]HR.DAT;2 Date: 21-JUN-95(Wed) 10:50:53
Sample: D2-194
RT 2'00", CI(+), GC 57.6c, BP: m/z 292.9824, Int. 45.32, Lv 0.00
Scan# 61

----> for sample peak, U.S. 0/15, Def. 5.0 mmu, Formula, up to 1000 mass
C 11/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
317.1526	15.60	-1.5	12.5	1:	C22 H21 O2

Elemental Composition

Data File: [100,100]HR.DAT;2 Date: 21-JUN-95(Wed) 10:50:53
Sample: D2-194
RT 2'02", CI(+), GC 57.7c, BP: m/z 318.9792, Int. 46.22, Lv 0.00
Scan# 62

----> for sample peak, U.S. 0/15, Def. 5.0 mmu, Formula, up to 1000 mass
C 11/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
317.1529	20.16	-1.3	12.5	1:	C22 H21 O2

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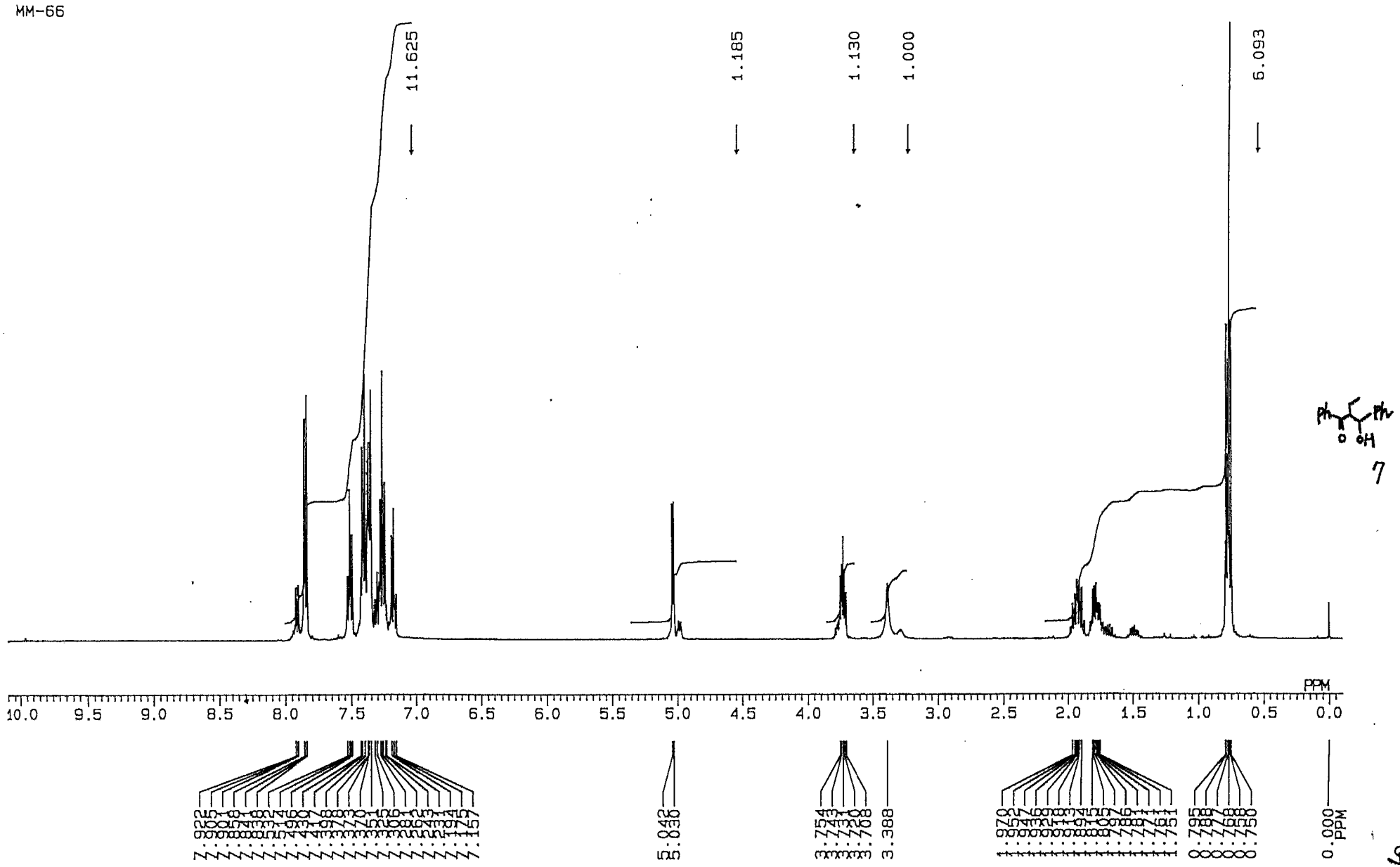

G379-10

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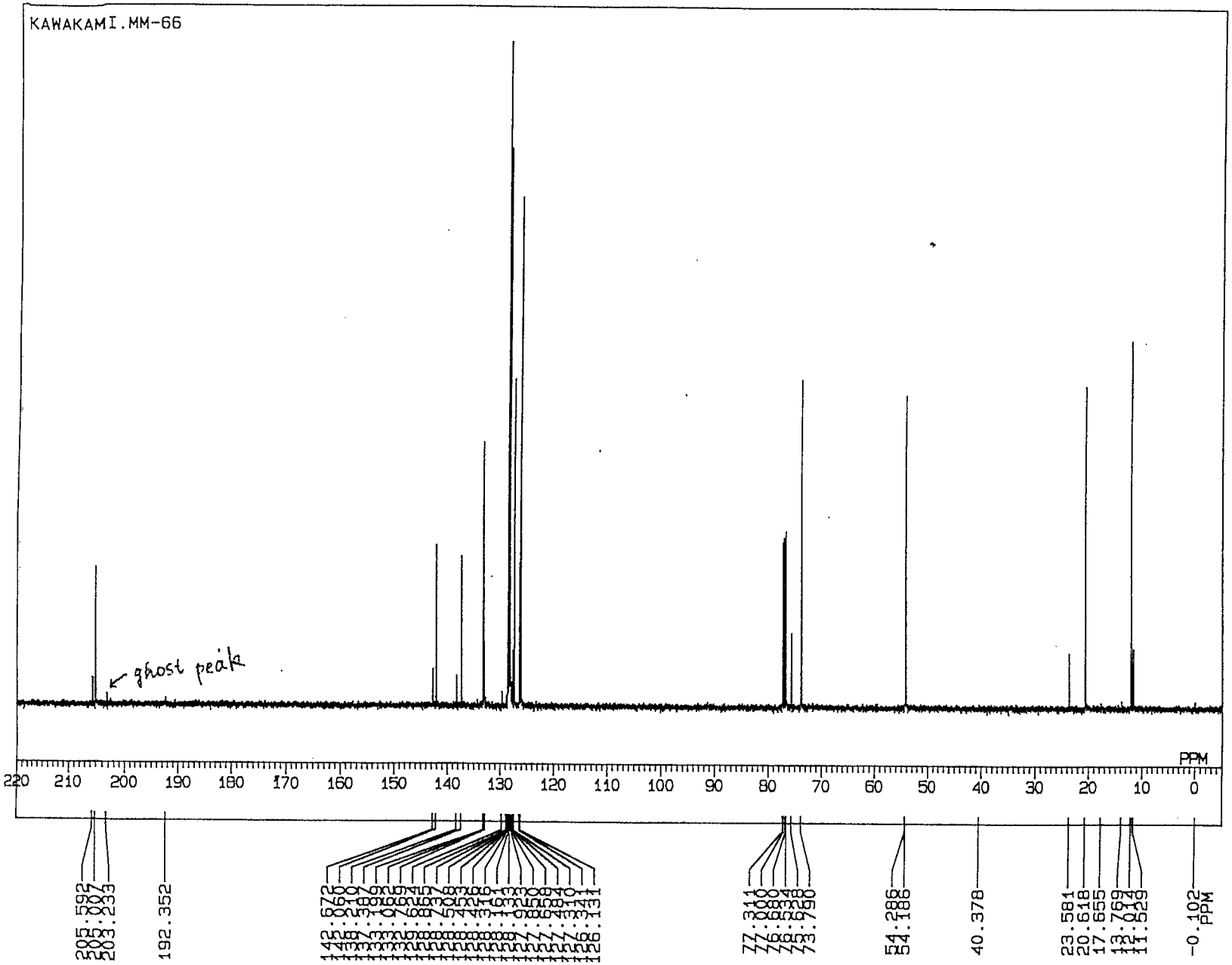
G 379-11



18-AUG-94 14:24:16
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COMNT KAWAKAMI.MM-66
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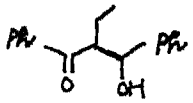
OBNUC 13C
OBFIN 10244.0 Hz
POINT 65536
FREQU 30120.5 Hz
SCANS 169
ACQTM 1.088 sec
PD 1.912 sec
PW1 5.2 us
IRFIN 10300.0 Hz
IRATN 20
IRRPW 50 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.92 Hz
RGAIN 25
XE 22618.2200 Hz
XS -987.4814 Hz

MM - 66



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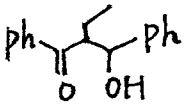
G 379-12



7

Acquisition Parameters for DAT File: DRO:[100,100]HR.DAT;14

Acquisition Date:	21-SEP-1994 10:37		
Sample :	MM-66		
Scan Range :	160.000-340.000	Data Type :	PS,HE
Scan Slope :	5.0 sec.	Cycle Time :	2.0 sec.
Scan Type :	MF,LI,UP,DA	Accel. Voltage :	3.0 kv/DAC
Maximum Run Time:	30 min.	Run Time :	2'42.1"
Valve open/close:			
Ionization Mode :	EI	Polarity :	POS.
Resolving Power :	3000	Filter setting :	3000
Inlet Source :	DIR	Magnetic Field :	HS
Temp. Points :	DI	Pre_amp Control :	
Threshold Level :		Valley :	25%
Tic Range :	160.000-340.000		
Dynamic Calibration File:			
Static Calibration File :			

Elemental Composition

Data File: [100,100]HR.DAT;14 Date: 21-SEP-94(Wed) 10:37:04
Sample: MM-66
RT 1'04", EI(+), GC 41.1c, BP: m/z 168.9888, Int. 75.65, Lv 0.00
Scan# 33

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 6/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
254.1302	10.45	-0.4	9.0	1:	C17 H18 O2

Elemental Composition

Data File: [100,100]HR.DAT;14 Date: 21-SEP-94(Wed) 10:37:04
Sample: MM-66
RT 1'06", EI(+), GC 41.1c, BP: m/z 168.9888, Int. 76.08, Lv 0.00
Scan# 34

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 6/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
254.1310	11.68	0.3	9.0	1:	C17 H18 O2

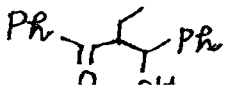
Elemental Composition

Data File: [100,100]HR.DAT;14 Date: 21-SEP-94(Wed) 10:37:04
Sample: MM-66
RT 1'08", EI(+), GC 42.1c, BP: m/z 168.9888, Int. 73.25, Lv 0.00
Scan# 35

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 6/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
254.1304	14.13	-0.2	9.0	1:	C17 H18 O2



calcd. 254.1307

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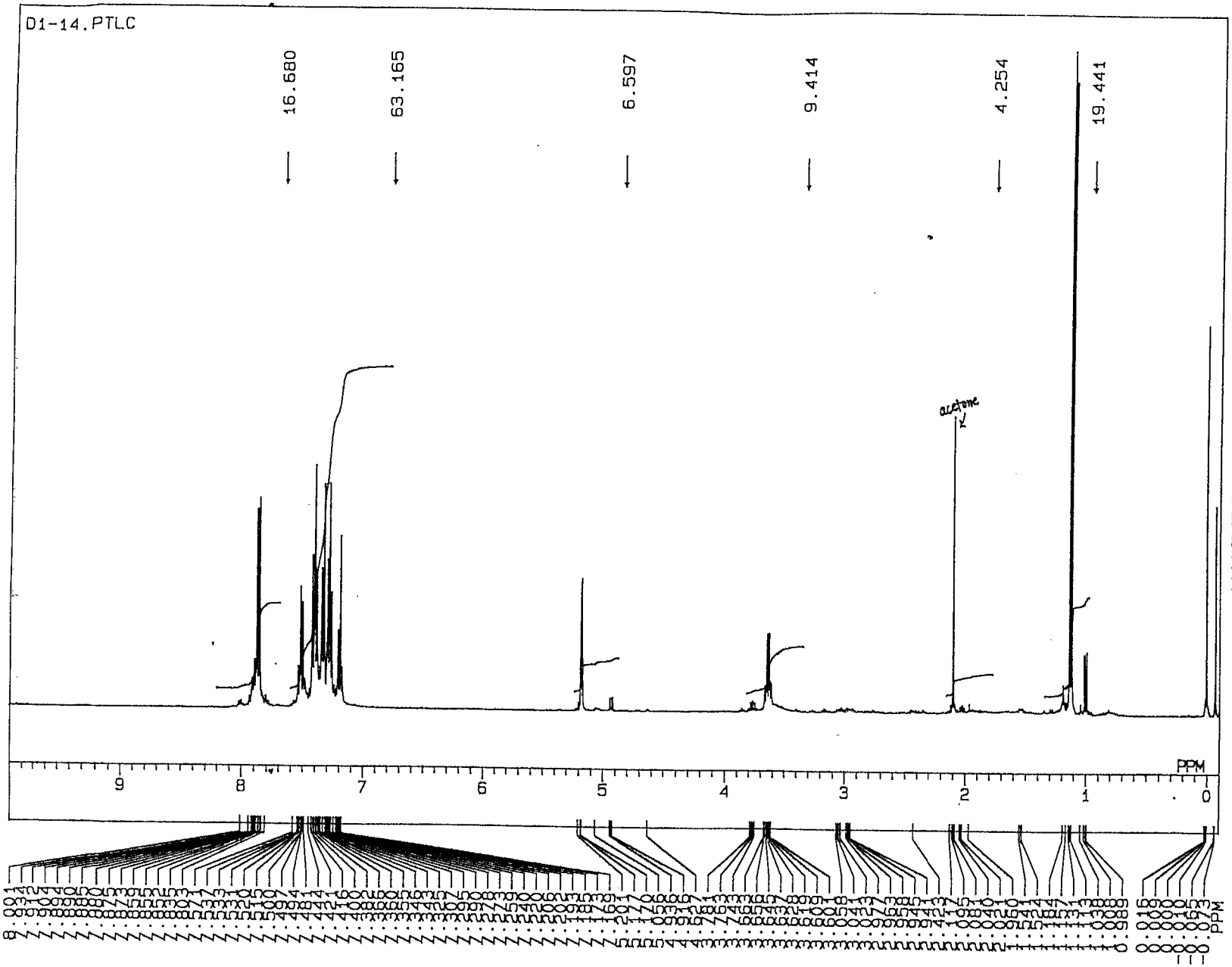
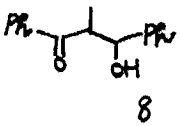
G 379-13



JEOL

08-MAR-93 15:04:28
DFILE 08MAR0801
COMNT D1-14.PTLC
EXMOD SGNON
OBNUC 1H
OBFIN 10300.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 4.000 sec
PW1 7.5 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 60 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 17
XE 3997.8250 Hz
XS -196.2394 Hz



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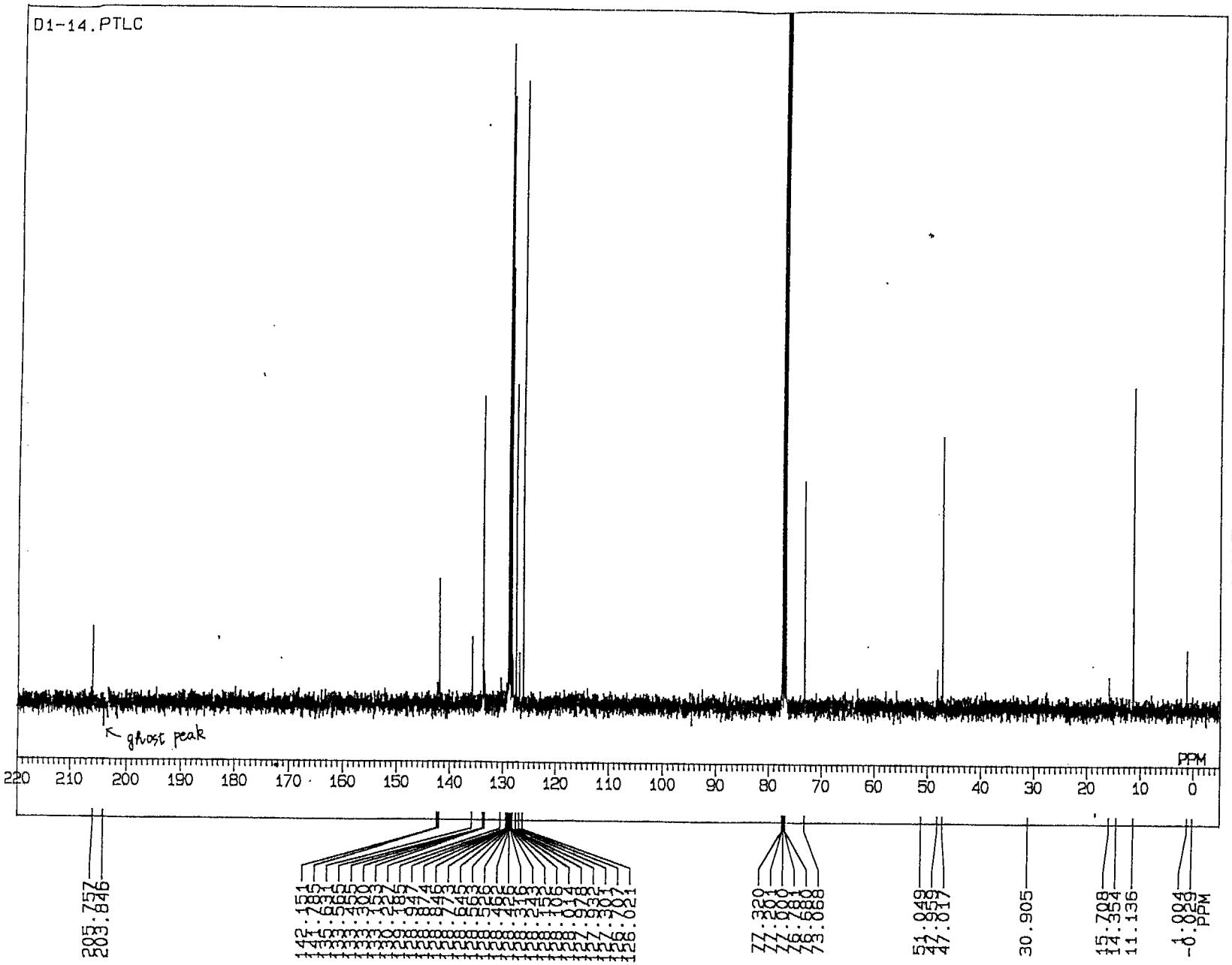
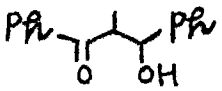


JEOL

08-MAR-93 15:33:38
DFILE 08MAR0803
COMNT D1-14.PTLC
EXMOD SGBCM
OBNUC 13C
OBFIN 10244.0 Hz
POINT 65536
FREQU 30120.5 Hz
SCANS 438
ACQTM 1.088 sec
PD 1.912 sec
PW1 5.2 us
IRFIN 10300.0 Hz
IRATN 25
IRRPW 65 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.92 Hz
RGAIN 28
XE 22618.2100 Hz
XS -955.5313 Hz



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G376-14

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G379-15

Acquisition Parameters for DAT File: DR0:[100,100]HR.DAT;4

Acquisition Date:	10-MAY-1993 16:19		
Sample :	D1-14 PTLC		
Scan Range :	140.000-320.000	Data Type :	PS,HE
Scan Slope :	5.0 sec.	Cycle Time :	2.0 sec.
Scan Type :	MF,LI,UP,DA	Accel. Voltage :	3.0 kv/DAC
Maximum Run Time:	20 min.	Run Time :	1'14.1"
Valve open/close:			
Ionization Mode :	EI	Polarity :	POS.
Resolving Power :	5,000	Filter setting :	
Inlet Source :	DIR	Magnetic Field :	HS
Temp. Points :	DI	Pre_amp Control :	
Threshold Level :	1000-1000	Valley :	25%
Tic Range :	140.000-320.000		
Dynamic Calibration File:			
Static Calibration File :			

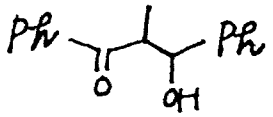
Elemental Composition

Data File: [100,100]HR.DAT;4 Date: 10-MAY-93(Mon) 16:19:51
Sample: D1-14 PTLC
RT 0'54", EI(+), GC 27.0c, BP: m/z 222.1025, Int. 61.27, Lv 0.00
Scan# 28

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/50, H 0/100, O 0/10

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
240.1148	47.22	-0.2	9.0	1:	C16 H16 O2



8

calcd. 240.11508

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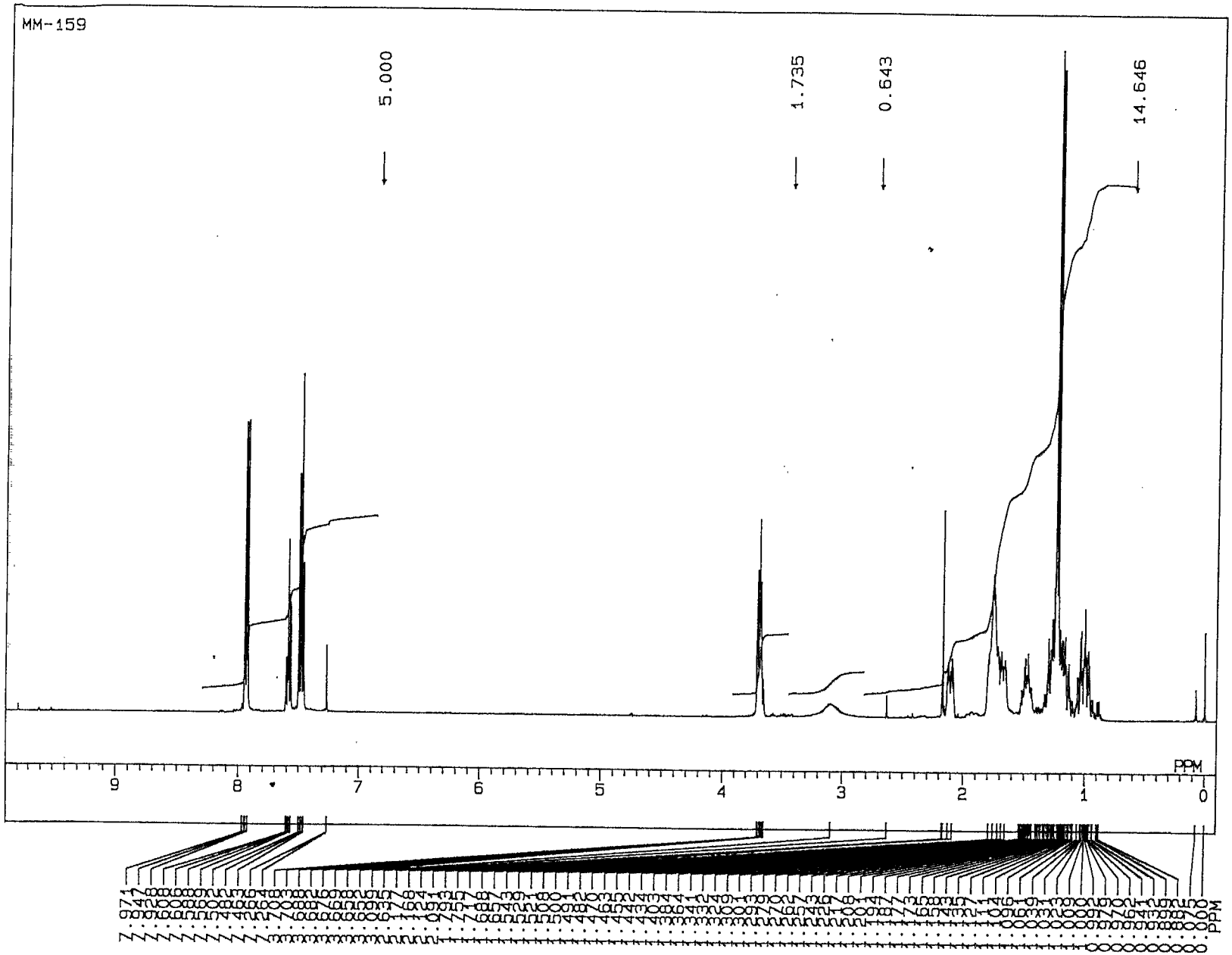
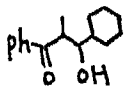


31-JAN-95 19: 05: 37
DFILE DU: 231BAB7
COMNT MM-159
EXMOD SGNON
OBNUC 1H
OBFIN 10300.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 4.000 sec
PW1 7.7 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 60 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 12
XE 3997.8250 Hz
XS -164.0125 Hz



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G379-16

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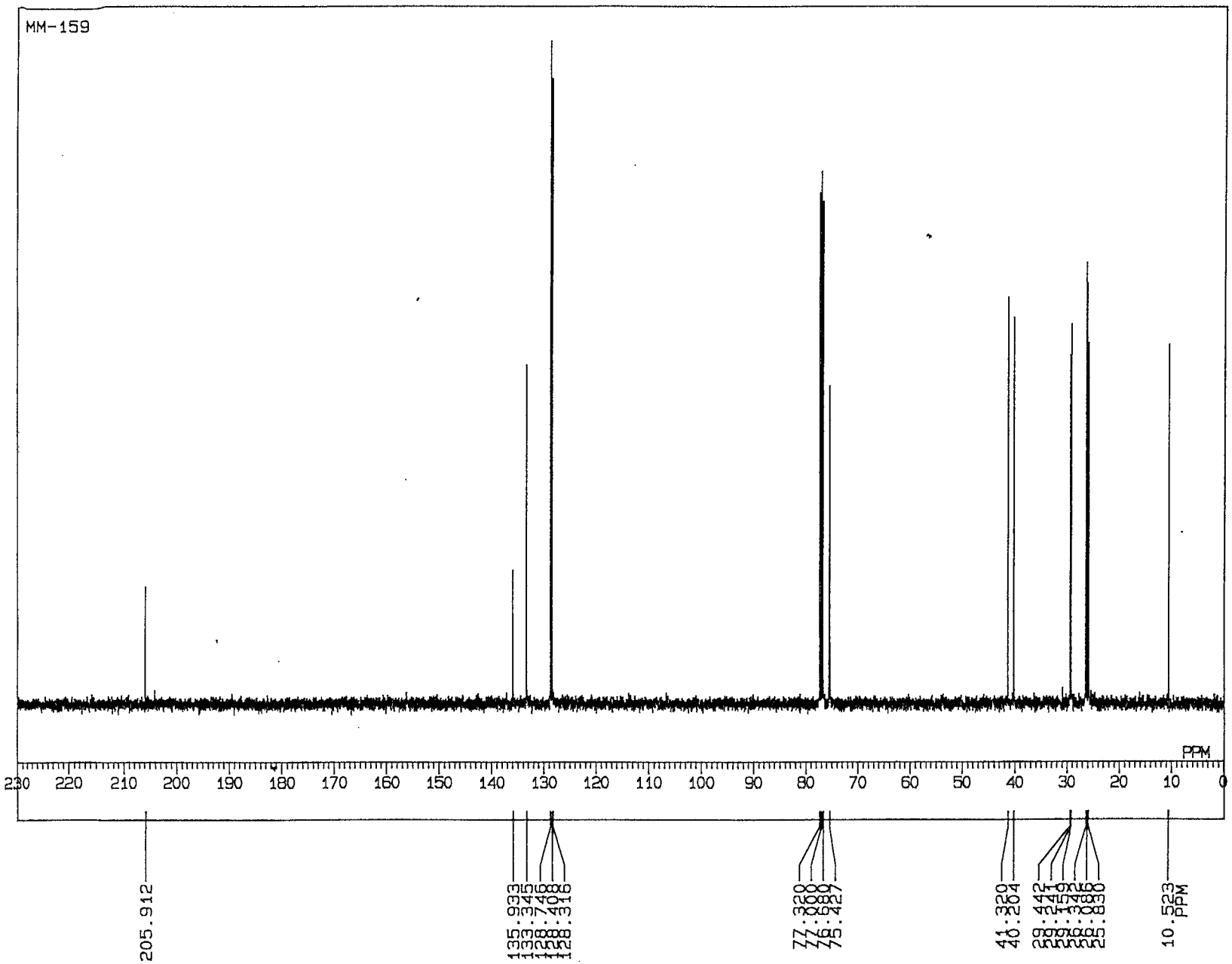
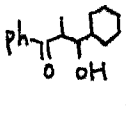


26-JAN-95 20:51:42
DFILE DU:231BAB8
COMNT MM-159
EXMOD SGBCM
OBNUC 13C
OBFIN 10244.0 Hz
POINT 65536
FREQU 30120.5 Hz
SCANS 300
ACQTM 1.088 sec
PD 1.912 sec
PW1 5.2 us
IRFIN 10300.0 Hz
IRATN 20
IRRPW 50 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 25
XE 23130.8800 Hz
XS -1704.4450 Hz

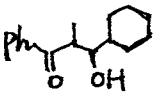


9

G379-17

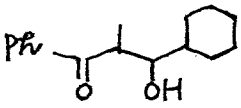
G 379-18

Acquisition Parameters for DAT File: DR0:[100,100]HR.DAT;23



9

Acquisition Date:	26-JAN-1995 11:08		
Sample :	MM-159		
Scan Range :	190.000-300.000	Data Type :	PS,HE
Scan Slope :	8.0 sec.	Cycle Time :	2.0 sec.
Scan Type :	MF,LI,UP,DA	Accel. Voltage :	3.0 kv/DAC
Maximum Run Time:	30 min.	Run Time :	2' 2.1"
Valve open/close:			
Ionization Mode :	EI	Polarity :	POS.
Resolving Power :	5000	Filter setting :	Auto
Inlet Source :	DIR	Magnetic Field :	HS
Temp. Points :	DI	Pre_amp Control :	
Threshold Level :	1500-1500	Valley :	25%
Tic Range :	190.000-300.000		
Dynamic Calibration File:			
Static Calibration File :			



9

$C_{16}H_{22}O_2$

calcd. 246.16206

Elemental Composition

Data File: [100,100]HR.DAT;23 Date: 26-JAN-95(Thu) 11:08:14
Sample: MM-159
RT 1'58", EI(+), GC 44.1c, BP: m/z 218.9856, Int. 42.20, Lv 0.00
Scan# 60

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 5/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
246.1623	43.47	0.3	6.0	1:	C16 H22 O2

Elemental Composition

Data File: [100,100]HR.DAT;23 Date: 26-JAN-95(Thu) 11:08:14
Sample: MM-159
RT 2'00", EI(+), GC 44.3c, BP: m/z 218.9856, Int. 42.75, Lv 0.00
Scan# 61

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 5/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
246.1616	41.06	-0.3	6.0	1:	C16 H22 O2

Elemental Composition

Data File: [100,100]HR.DAT;23 Date: 26-JAN-95(Thu) 11:08:14
Sample: MM-159
RT 2'02", EI(+), GC 44.6c, BP: m/z 228.1525, Int. 42.03, Lv 0.00
Scan# 62

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 5/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
246.1631	50.04	1.2	6.0	1:	C16 H22 O2

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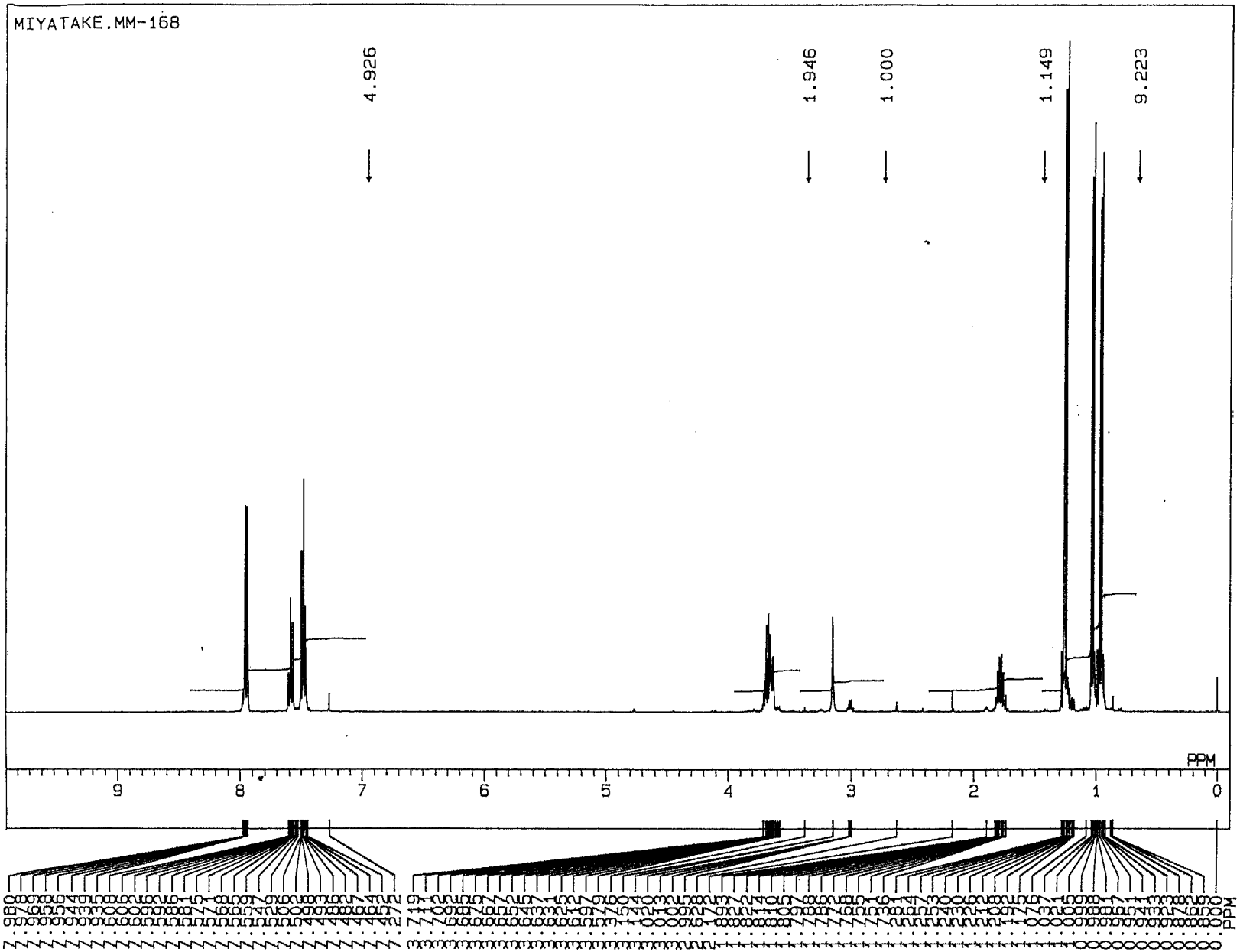
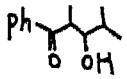


06-FEB-95 21: 10: 29
DFILE DU: 022BAB7
COMNT MIYATAKE.MM-168
EXMOD SGNON
OBNUC 1H
OBFIN 10300.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 4.000 sec
PW1 7.7 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 60 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 9
XE 3997.8250 Hz
XS -160.5945 Hz



10

G 379-1c

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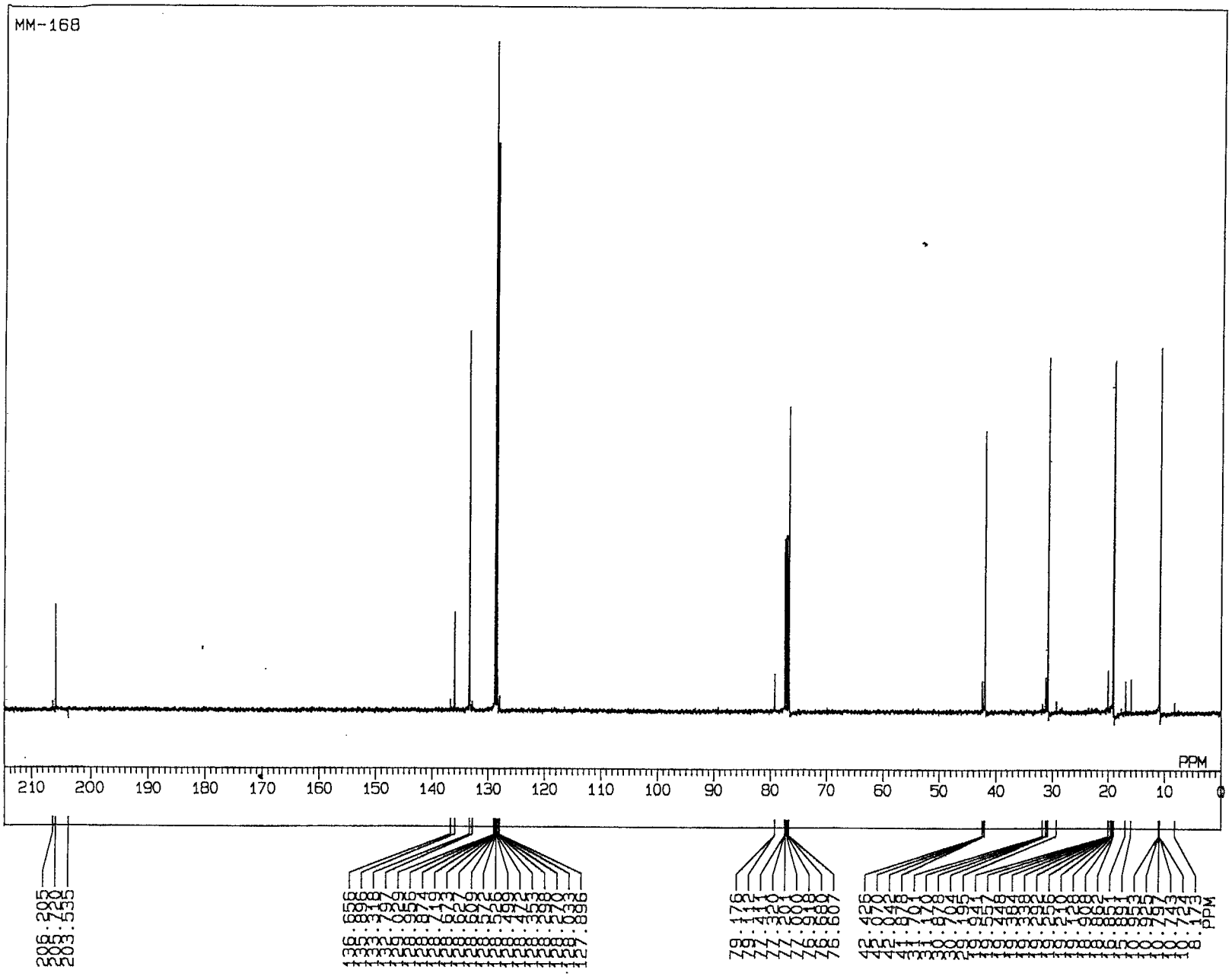
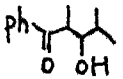


06-FEB-95 21:59:58
DFILE DU:022BAB8
COMNT MM-168
EXMOD SGBCM
OBNUC 13C
OBFIN 10244.0 Hz
POINT 65536
FREQU 30120.5 Hz
SCANS 300
ACQTM 1.088 sec
PD 1.912 sec
PW1 5.2 us
IRFIN 10300.0 Hz
IRATN 20
IRRPW 50 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 25
XE 21612.9600 Hz
XS -959.2090 Hz

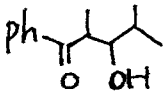


10

G 379-2

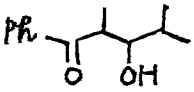
67379-2t

Acquisition Parameters for DAT File: DR0:[100,100]HR.DAT;15



10

Acquisition Date:	20-FEB-1995 10:17		
Sample :	MM-168		
Scan Range :	150.000-260.000	Data Type :	PS,HE
Scan Slope :	7.0 sec.	Cycle Time :	2.0 sec.
Scan Type :	MF,LI,UP,DA	Accel. Voltage :	3.0 kv/DAC
Maximum Run Time:	20 min.	Run Time :	1'26.1"
Valve open/close:			
Ionization Mode :	EI	Polarity :	POS.
Resolving Power :	5000	Filter setting :	3000
Inlet Source :	DIR	Magnetic Field :	HS
Temp. Points :	DI	Pre_amp Control :	
Threshold Level :	1000-1000	Valley :	
Tic Range :	150.000-260.000		
Dynamic Calibration File:			
Static Calibration File :			



10

$C_{13}H_{18}O_2$
calcd. 206.1307

Elemental Composition

Data File: [100,100]HR.DAT;15 Date: 20-FEB-95(Mon) 10:17:12
Sample: MM-168
RT 0'34", EI(+), GC 32.6c, BP: m/z 168.9888, Int. 53.25, Lv 0.00
Scan# 18

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 2/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
205.1300	5.83	-0.7	5.0	1:	C13 H18 O2

Elemental Composition

Data File: [100,100]HR.DAT;15 Date: 20-FEB-95(Mon) 10:17:12
Sample: MM-168
RT 0'36", EI(+), GC 32.9c, BP: m/z 168.9888, Int. 53.29, Lv 0.00
Scan# 19

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 2/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
206.1301	5.71	-0.6	5.0	1:	C13 H18 O2

Elemental Composition

Data File: [100,100]HR.DAT;15 Date: 20-FEB-95(Mon) 10:17:12
Sample: MM-168
RT 0'38", EI(+), GC 32.9c, BP: m/z 168.9888, Int. 53.76, Lv 0.00
Scan# 20

----> for sample peak, U.S. 0/20, Def. 5.0 mmu, Formula, up to 1000 mass
C 2/50, H 0/100, O 0/5

----> for standard peak, U.S. 0/10, Def. 5.0 mmu, Formula, up to 1000 mass
C 0/20, H 0/1, F 0/30

Mass	Int.	mmu	U.S.	No:	Elemental Formula
206.1299	9.10	-0.8	5.0	1:	C13 H18 O2