

Fig. 1. 4-Hydroxy-3-(3-methylbut-2-enyl)benzaldehyde (**6**) 的¹H-NMR圖譜

— 191.284

— 160.198

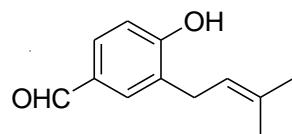
— 135.736
— 131.869
— 130.491
— 129.891
— 127.845

— 120.676
— 116.034

— 77.252
— 77.000
— 76.744

— 29.266
— 25.796

— 17.905



CC

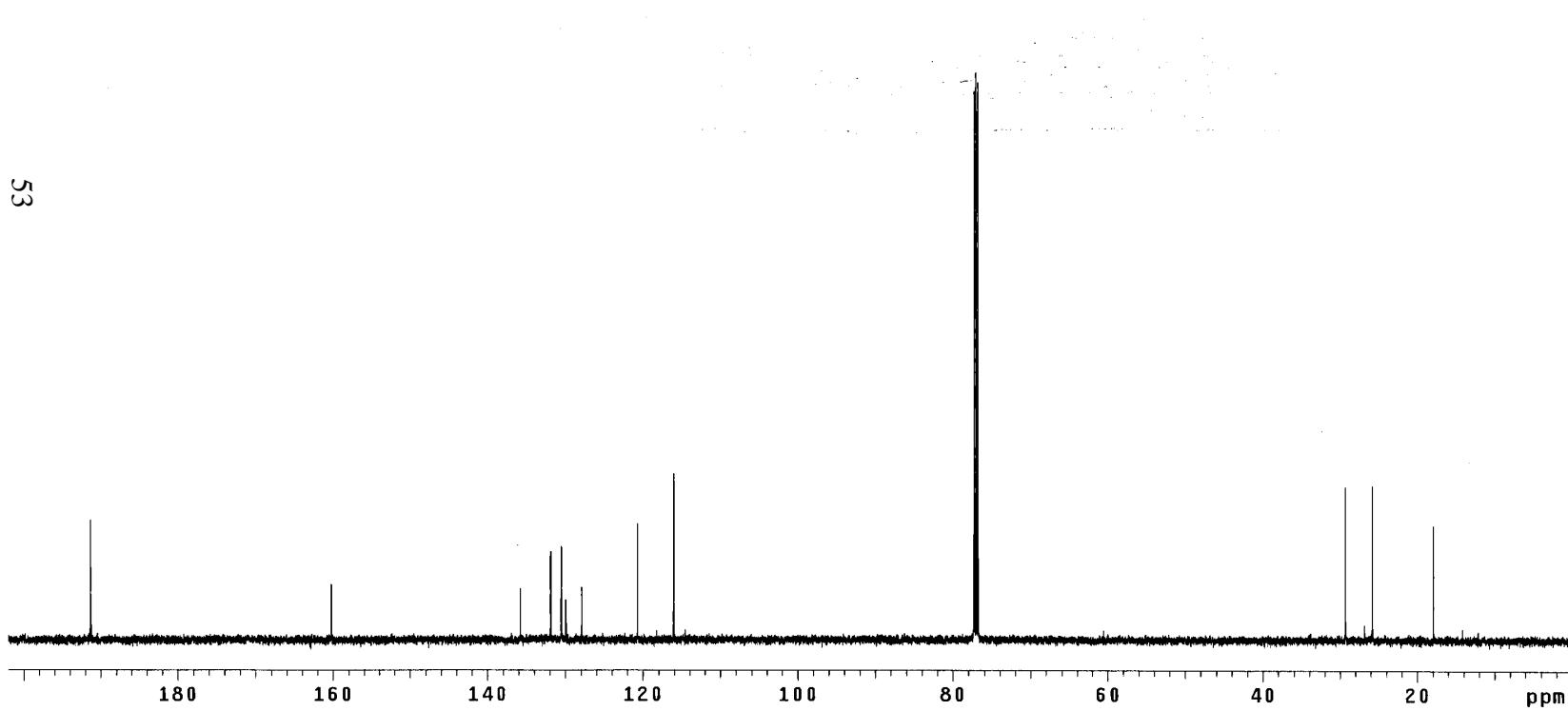


Fig. 2. 4-Hydroxy-3-(3-methylbut-2-enyl)benzaldehyde (**6**) 的¹³C-NMR圖譜

54

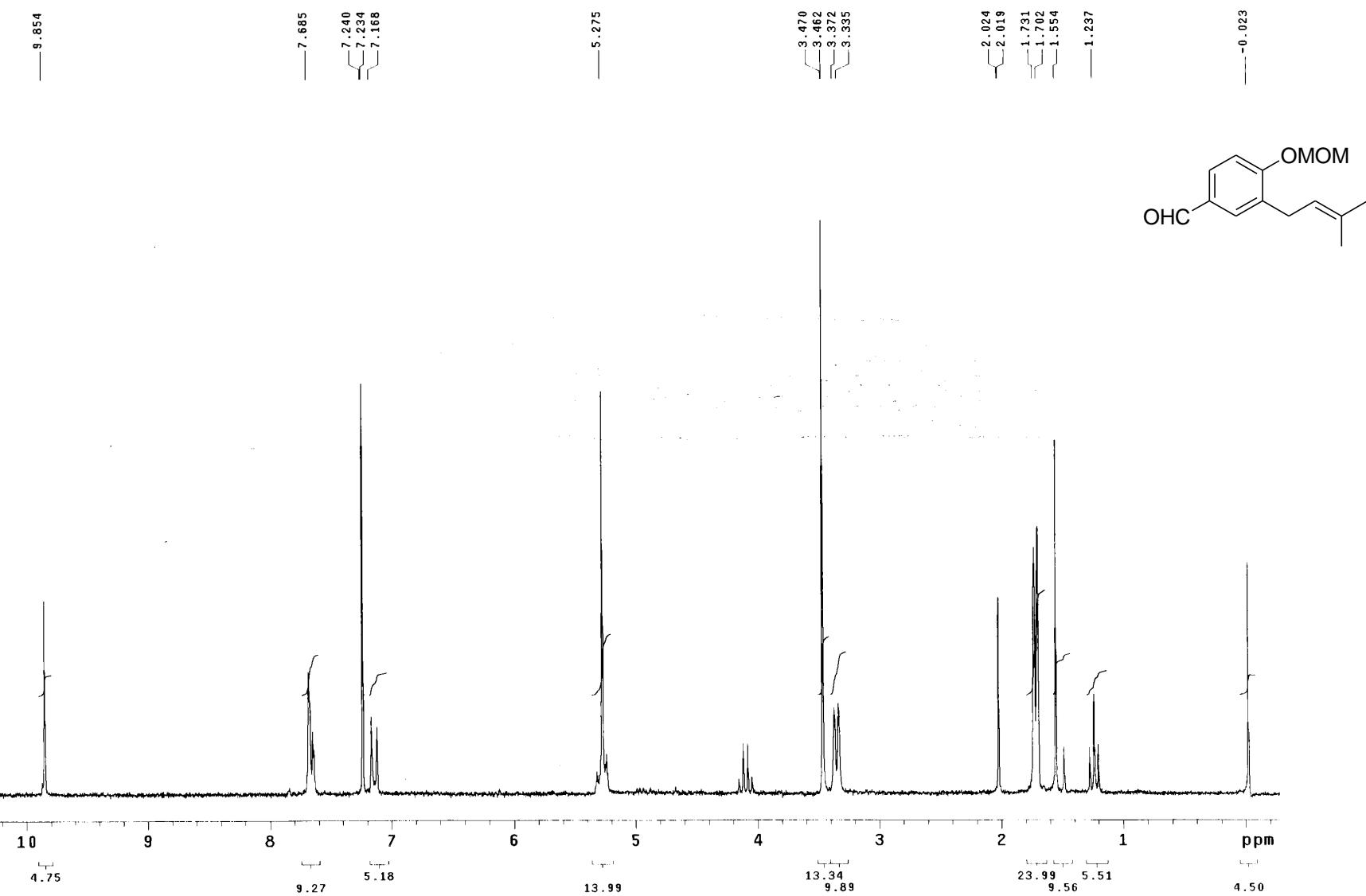


Fig. 3. 4-(Methoxymethoxy)-3-(3-methylbut-2-enyl)benzaldehyde (7) 的¹H-NMR圖譜

C:\Xcalibur\data\MJD\CJY-50

12/23/2011 2:19:08 PM

DIP-EI-70ev

CJY-50 #24 RT: 0.51 AV: 1 NL: 5.30E4

T: + c Full ms [50.00-650.00]

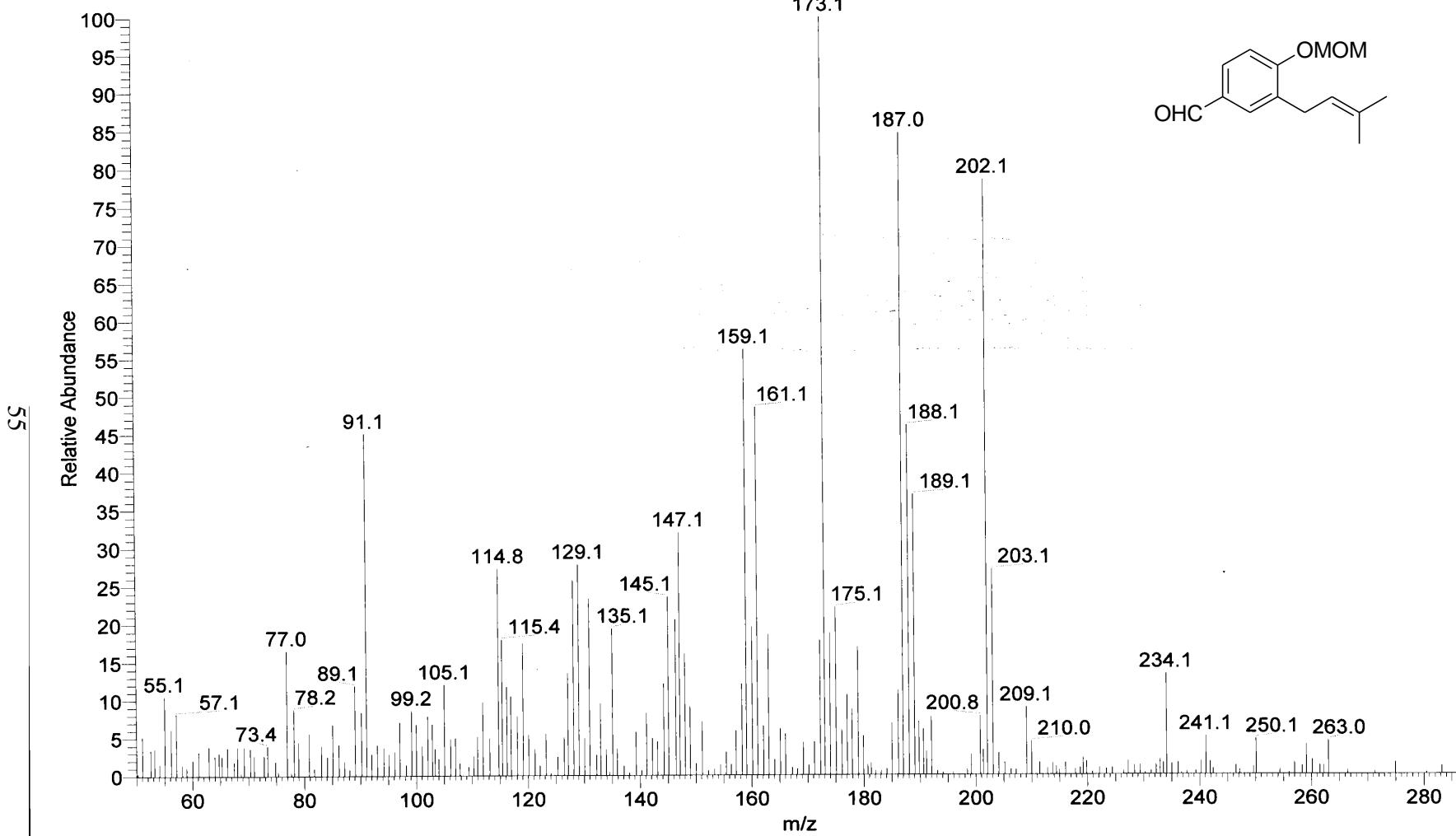


Fig. 4. 4-(Methoxymethoxy)-3-(3-methylbut-2-enyl)benzaldehyde (7) 的 EI-MS 圖譜

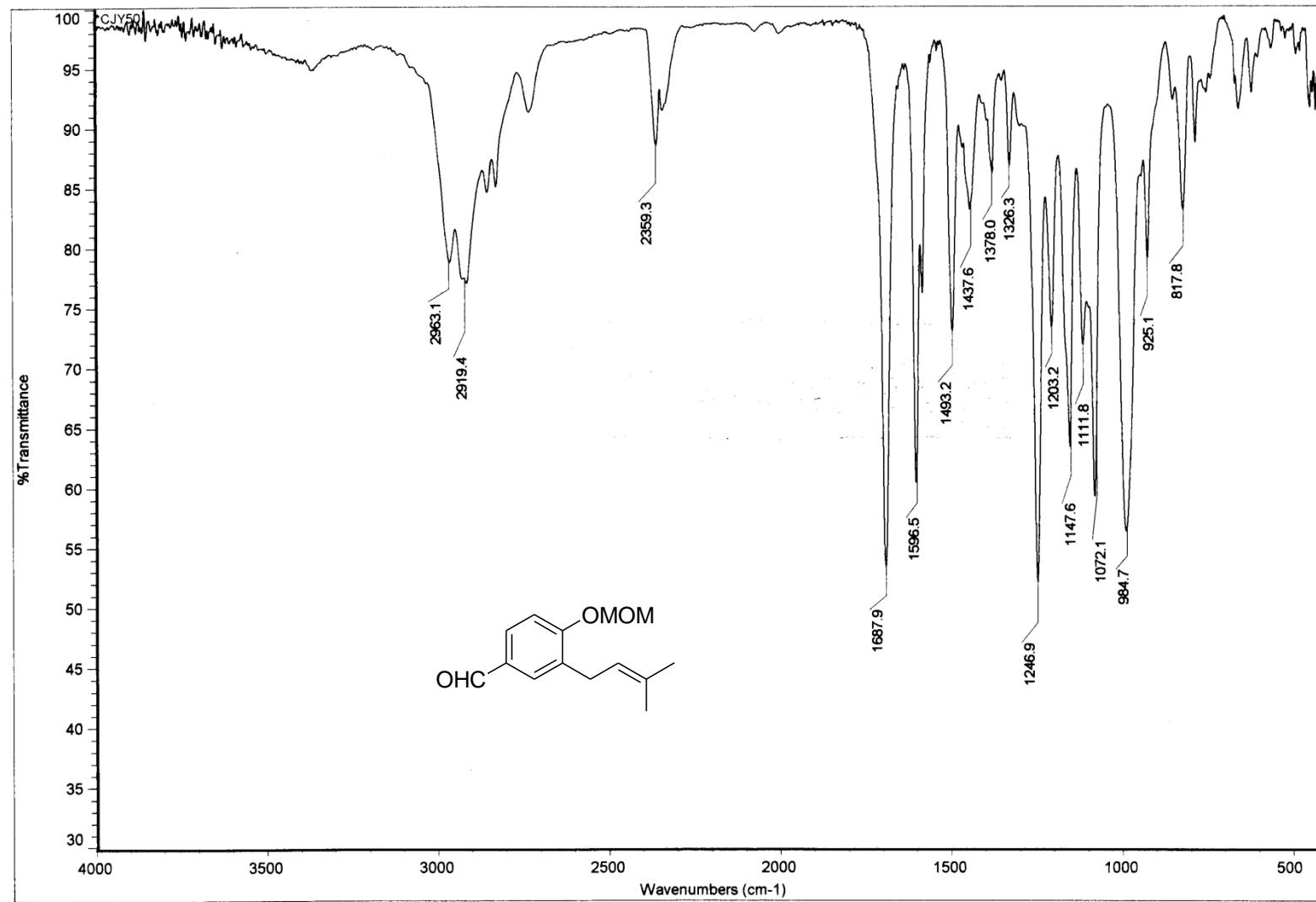


Fig. 5. 4-(Methoxymethoxy)-3-(3-methylbut-2-enyl)benzaldehyde (7) 的FTIR圖譜

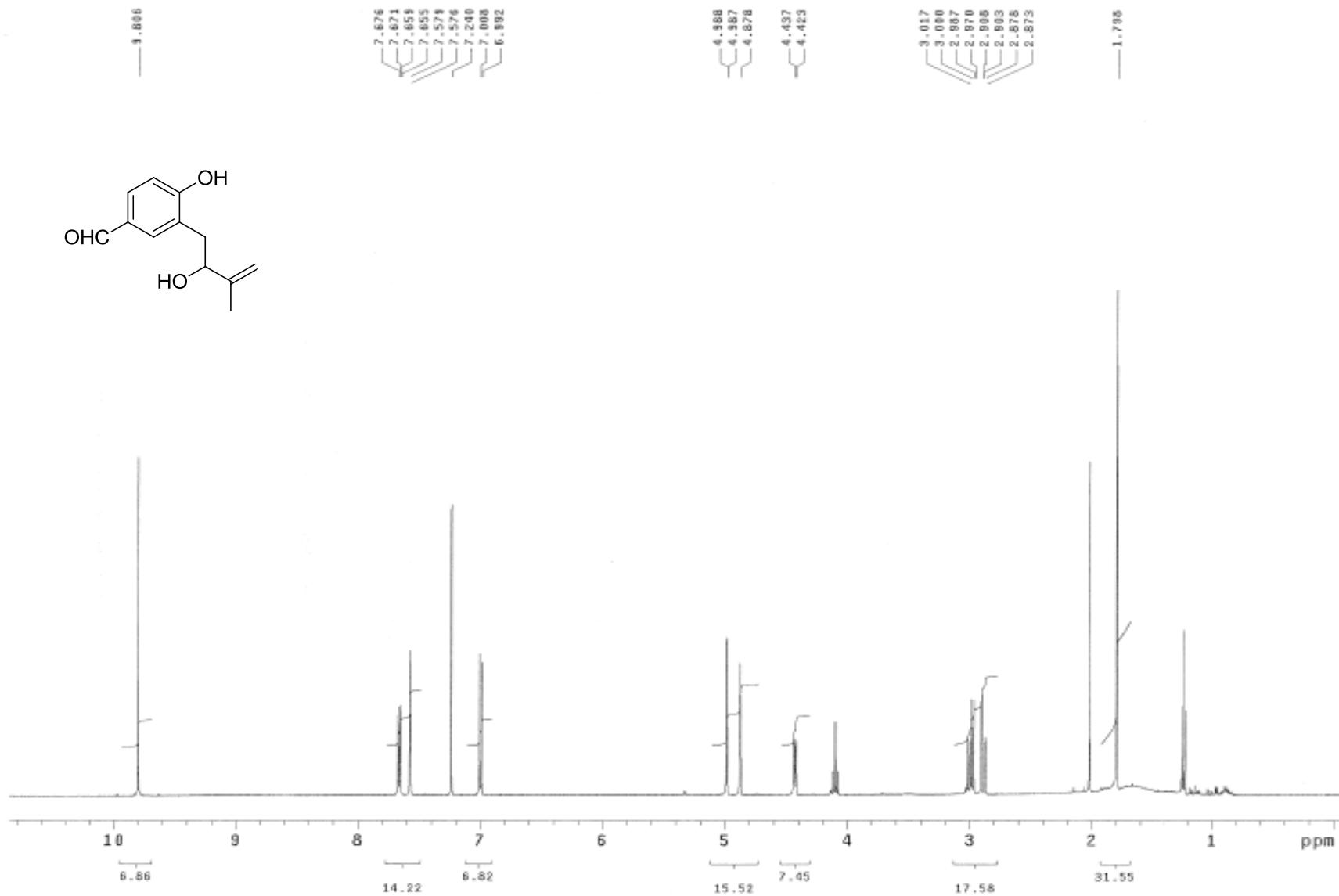
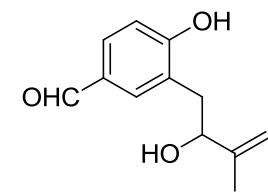


Fig. 6. 4-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)benzaldehyde (**8**) 的¹H-NMR圖譜

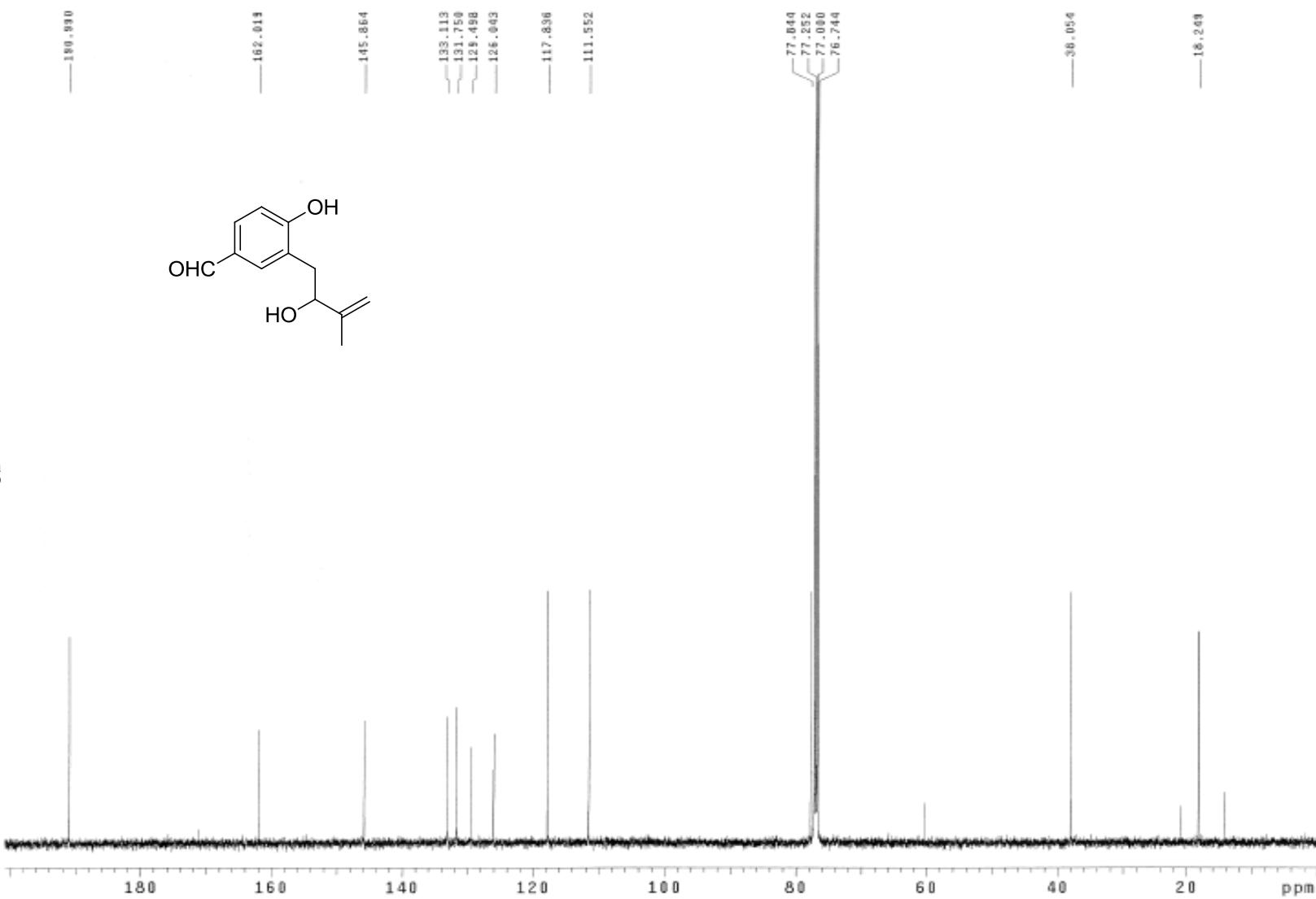


Fig. 7. 4-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)benzaldehyde (8) 的 ^{13}C -NMR 圖譜

C:\Xcalibur\data\MJD\CSH-233

12/23/2011 11:09:23 AM

DIP-EI-70ev

CSH-233 #131 RT: 2.69 AV: 1 NL: 6.88E7

T: + c Full ms [50.00-650.00]

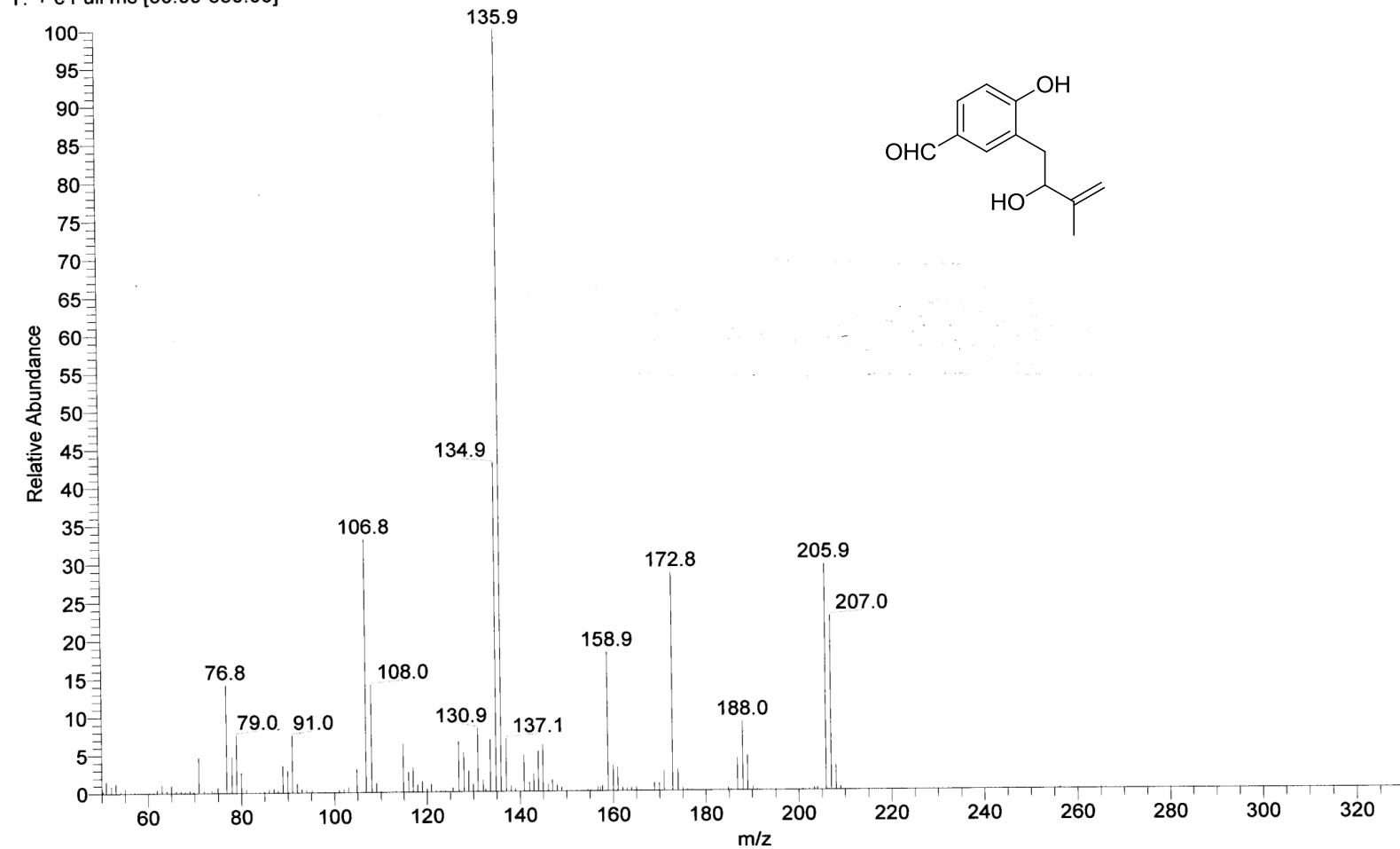


Fig. 8. 4-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)benzaldehyde (8) 的 EI-MS 圖譜

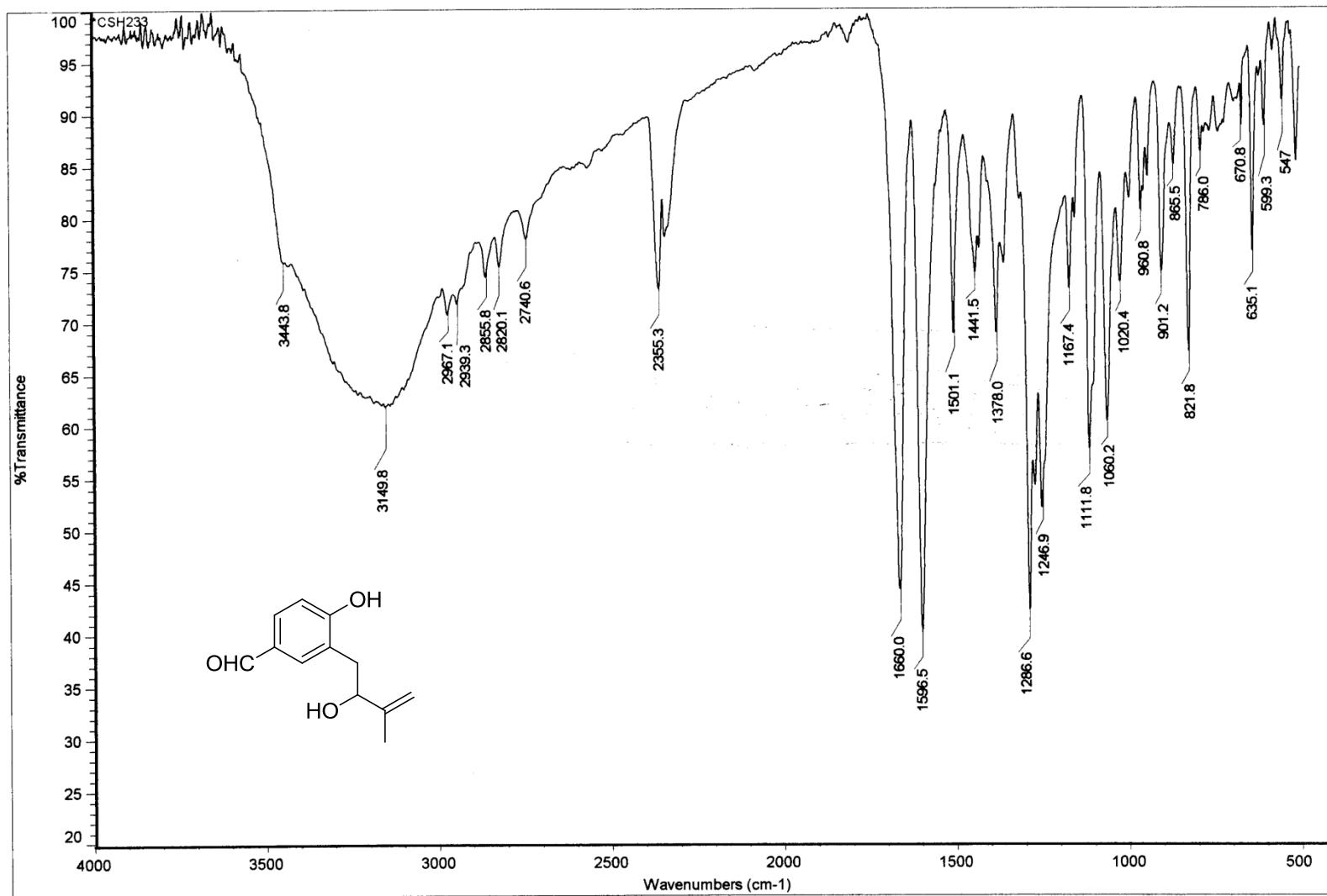
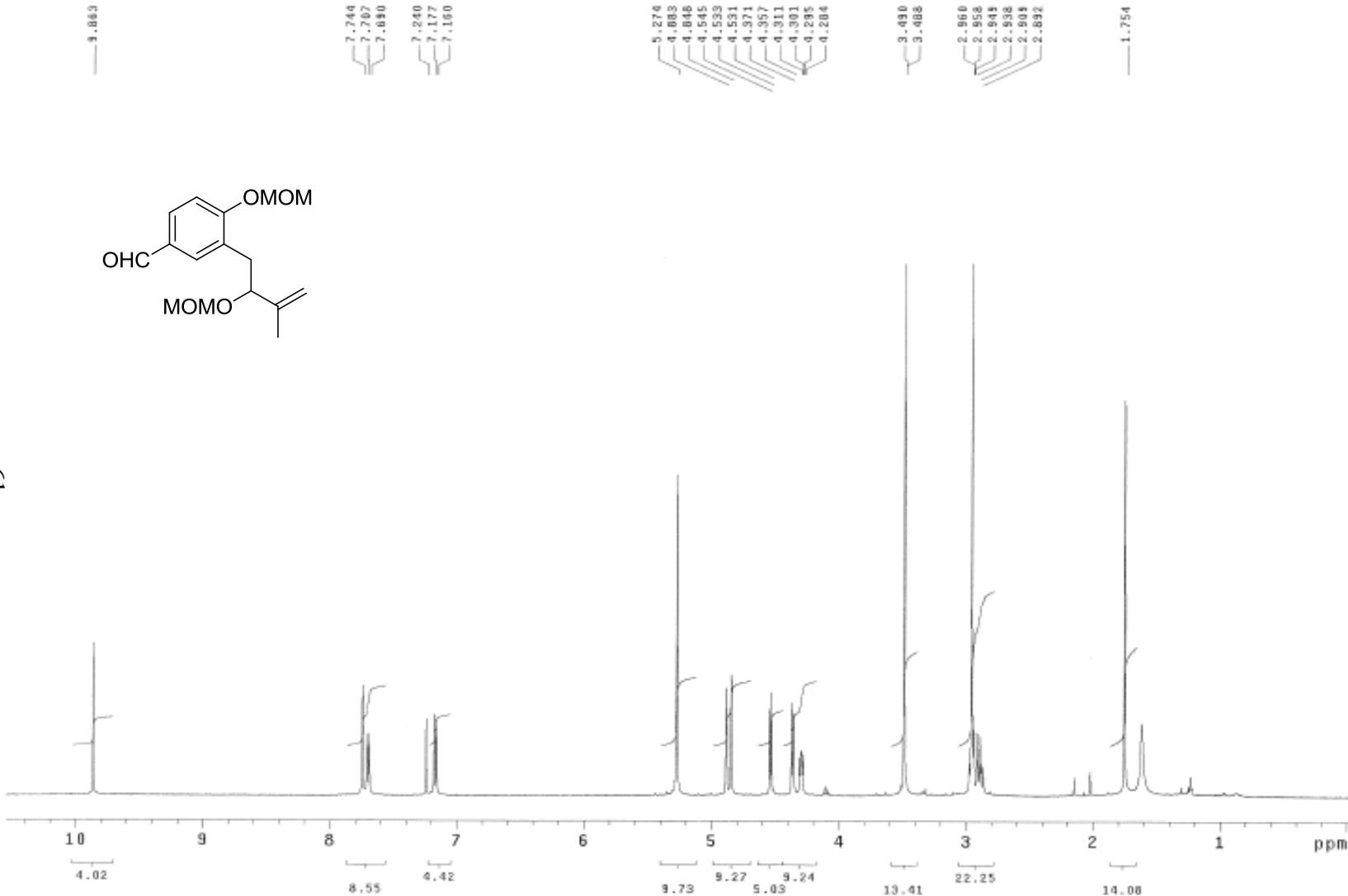
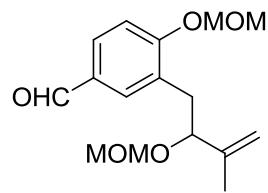


Fig. 9. 4-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)benzaldehyde (8) 的FTIR圖譜



CSH234 125 MHz

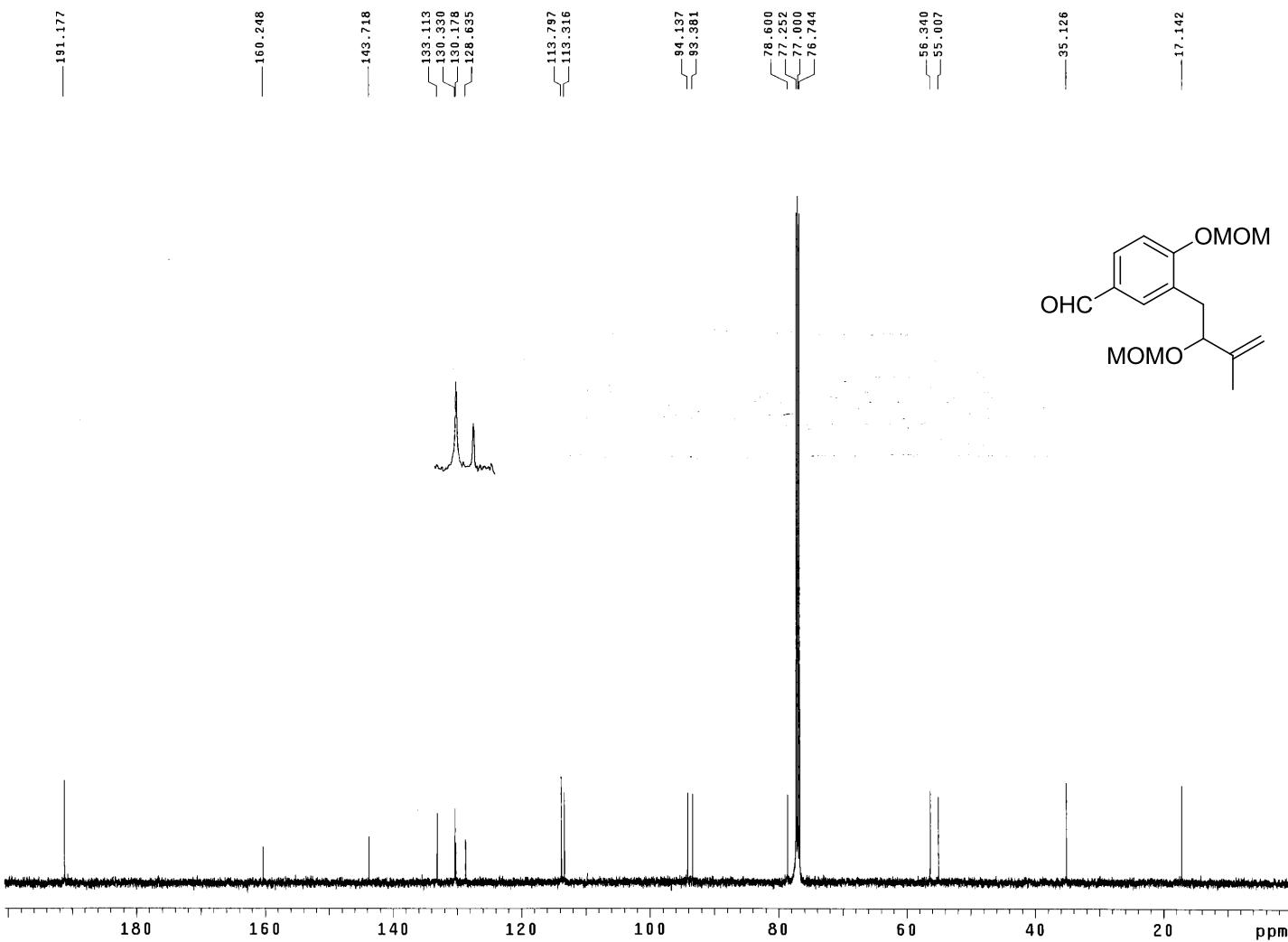


Fig. 11. 4-(Methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)-benzaldehyde (**9**) 的¹³C-NMR 圖譜

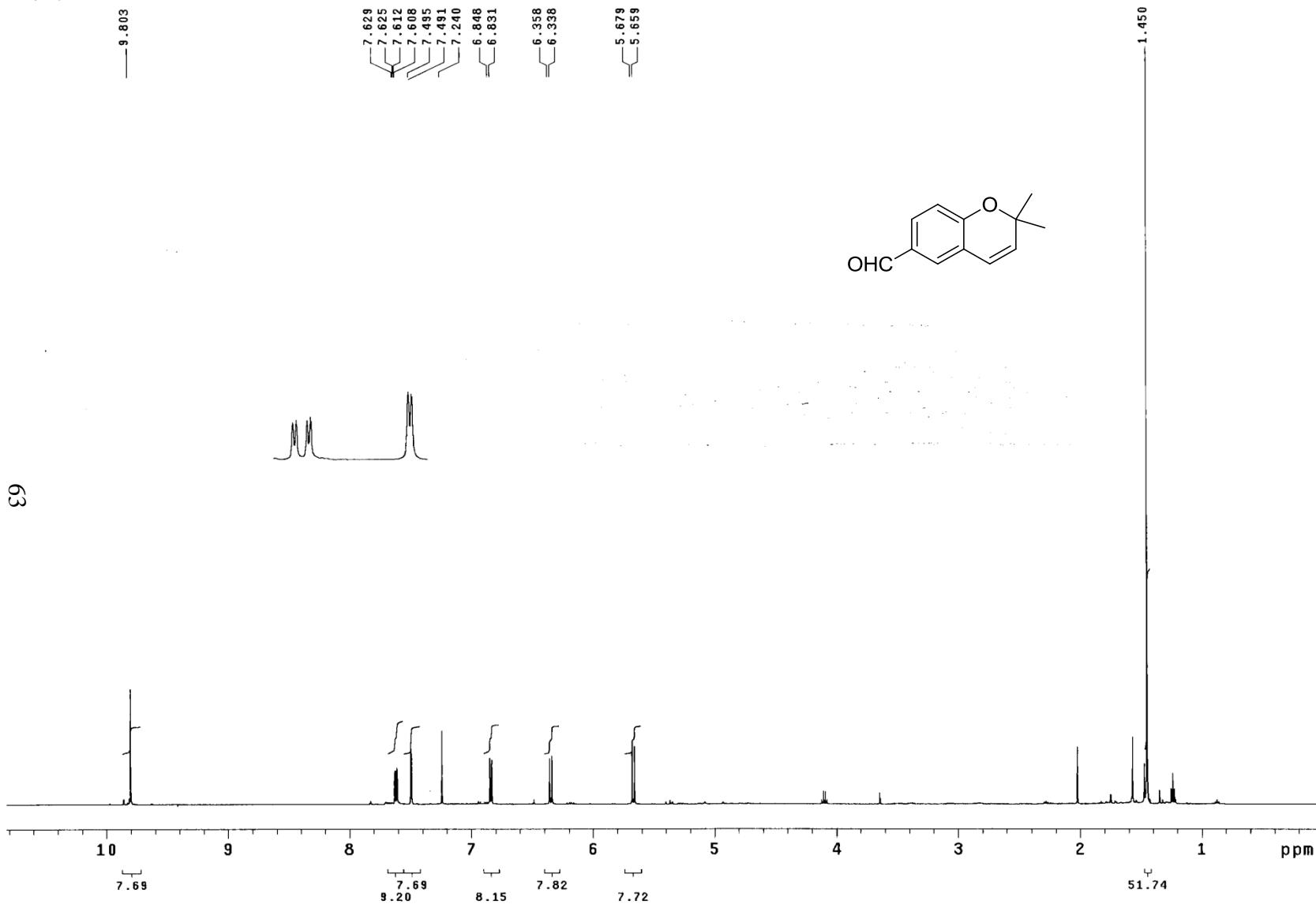


Fig. 12. 2,2-Dimethyl-2H-chromene-6-carbaldehyde (**10**) 的¹H-NMR 圖譜

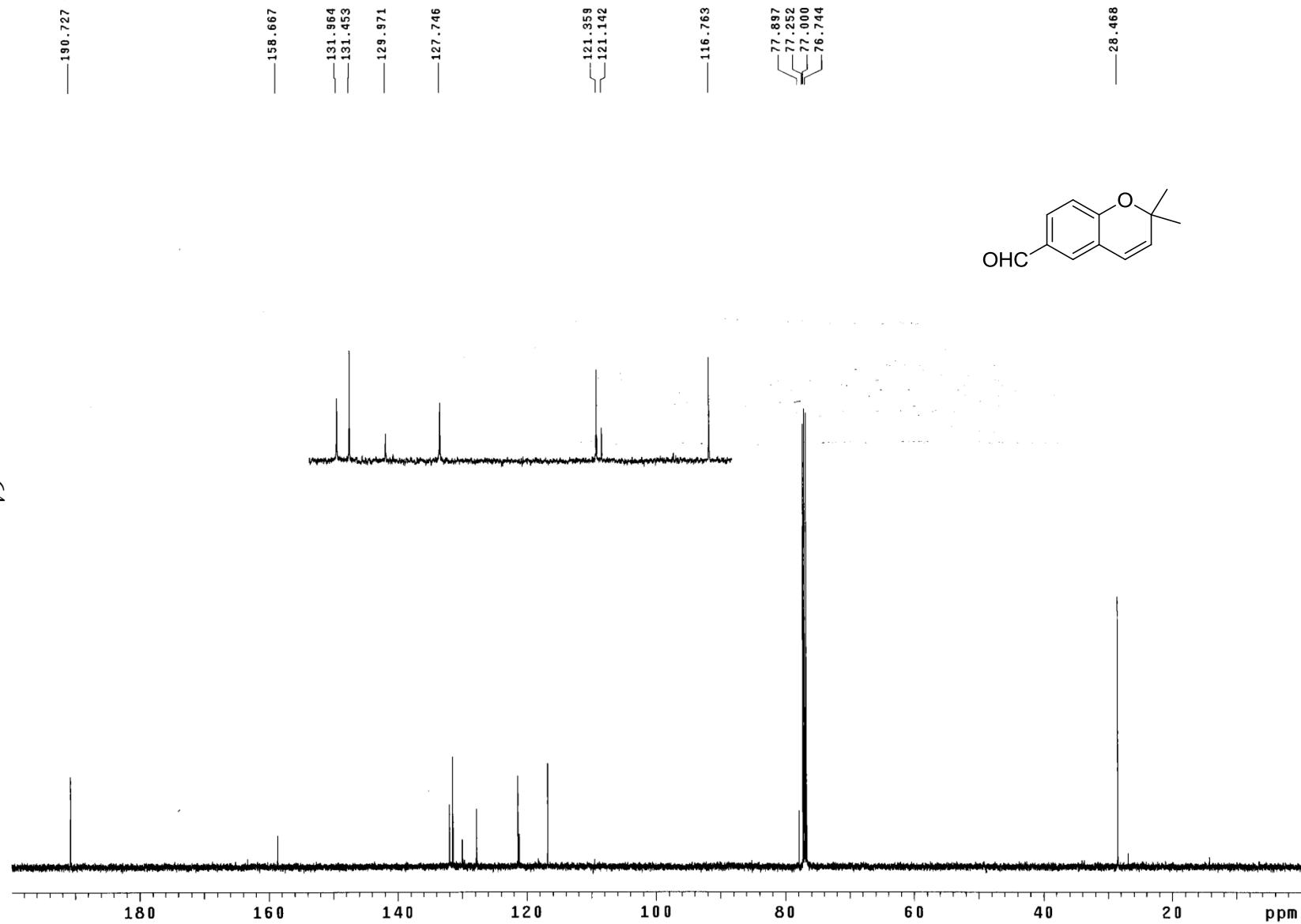


Fig. 13. 2,2-Dimethyl-2H-chromene-6-carbaldehyde (**10**) 的¹³C-NMR 圖譜

C:\Xcalibur\data\MJD\CSH-233c

DIP-EI-70ev

CSH-233c #7 RT: 0.16 AV: 1 NL: 3.06E8

T: + c Full ms [50.00-650.00]

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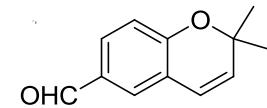
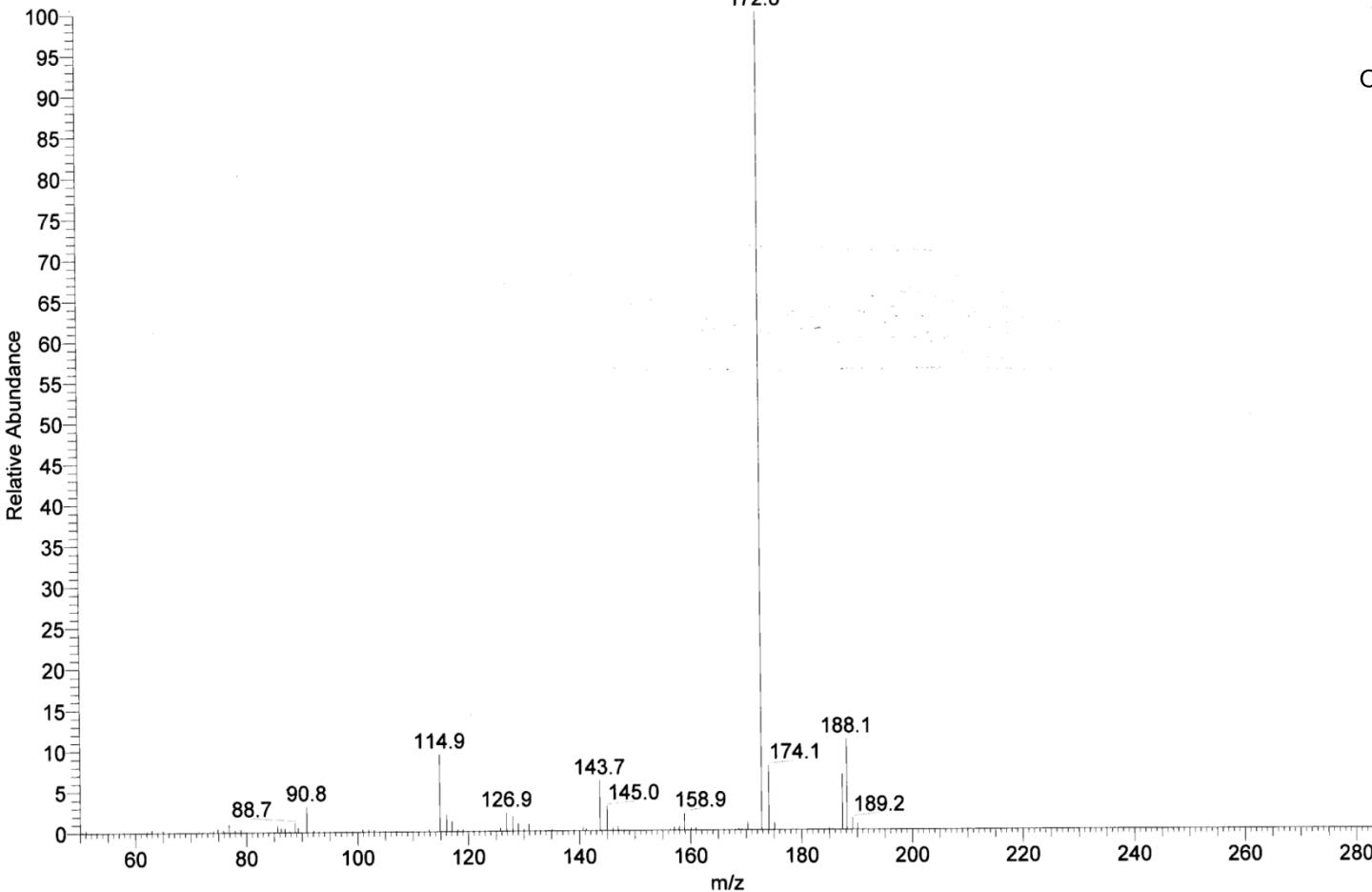


Fig. 14. 2,2-Dimethyl-2H-chromene-6-carbaldehyde (**10**) 的 EI-MS 圖譜

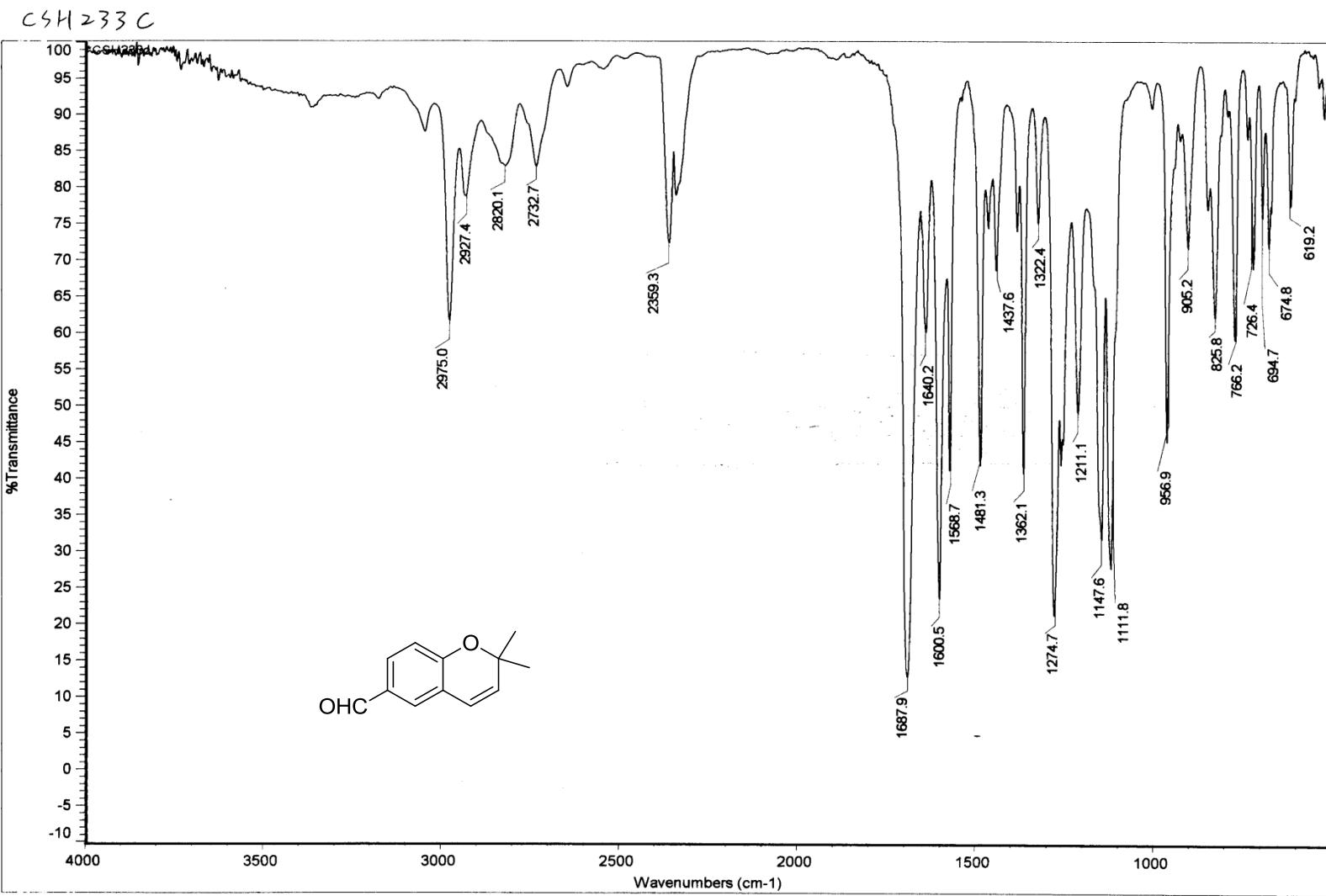


Fig. 15. 2,2-Dimethyl-2H-chromene-6-carbaldehyde (**10**) 的 FTIR 圖譜

CJY6}

— 13.032

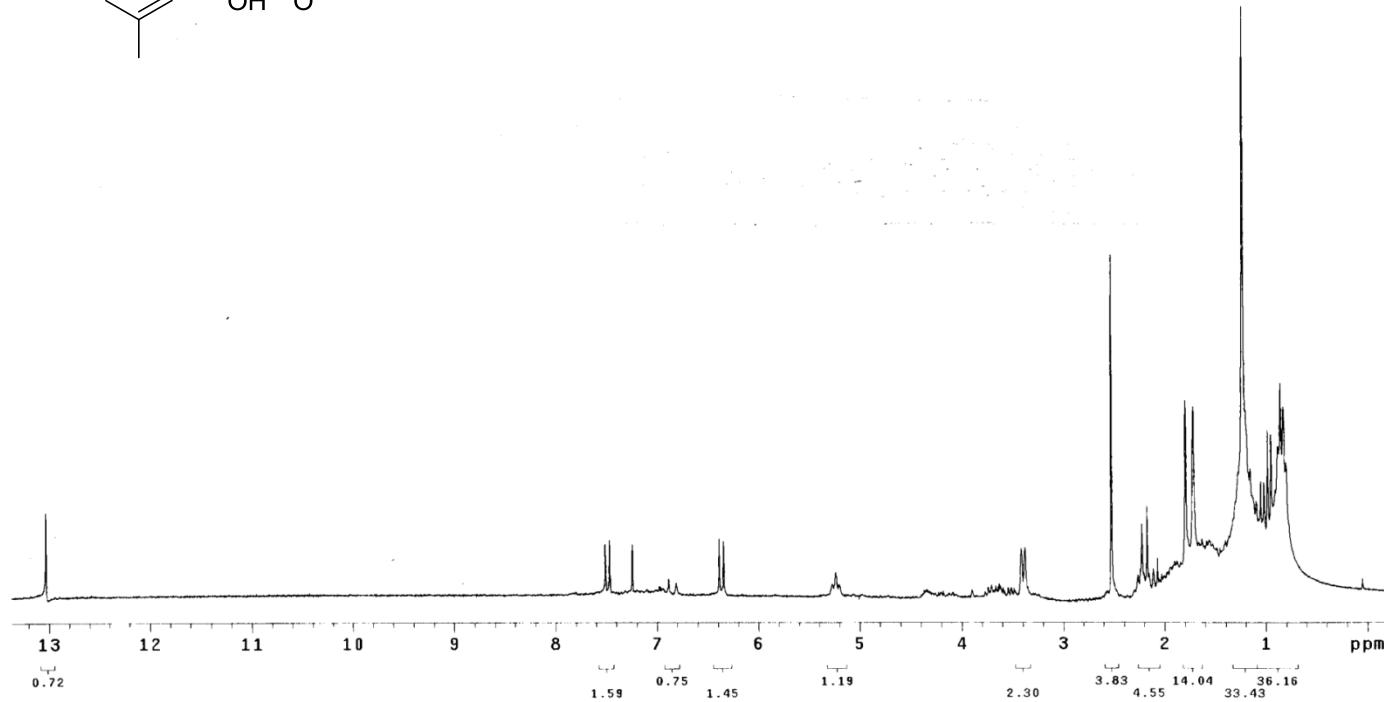
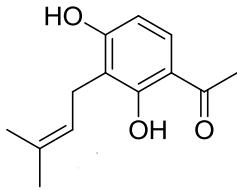


Fig. 16. 1-(2,4-Dihydroxy-3-(3-methylbut-2-enyl)phenyl)ethanone (**11**) 的¹H-NMR圖譜

C:\Xcalibur\data\MJD\CJY-03

DIP-EI-70ev

CJY-03 #43 RT: 0.90 AV: 1 NL: 3.82E5

T: + c Full ms [50.00-650.00]

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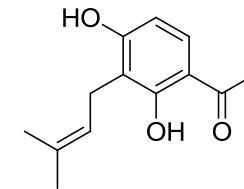
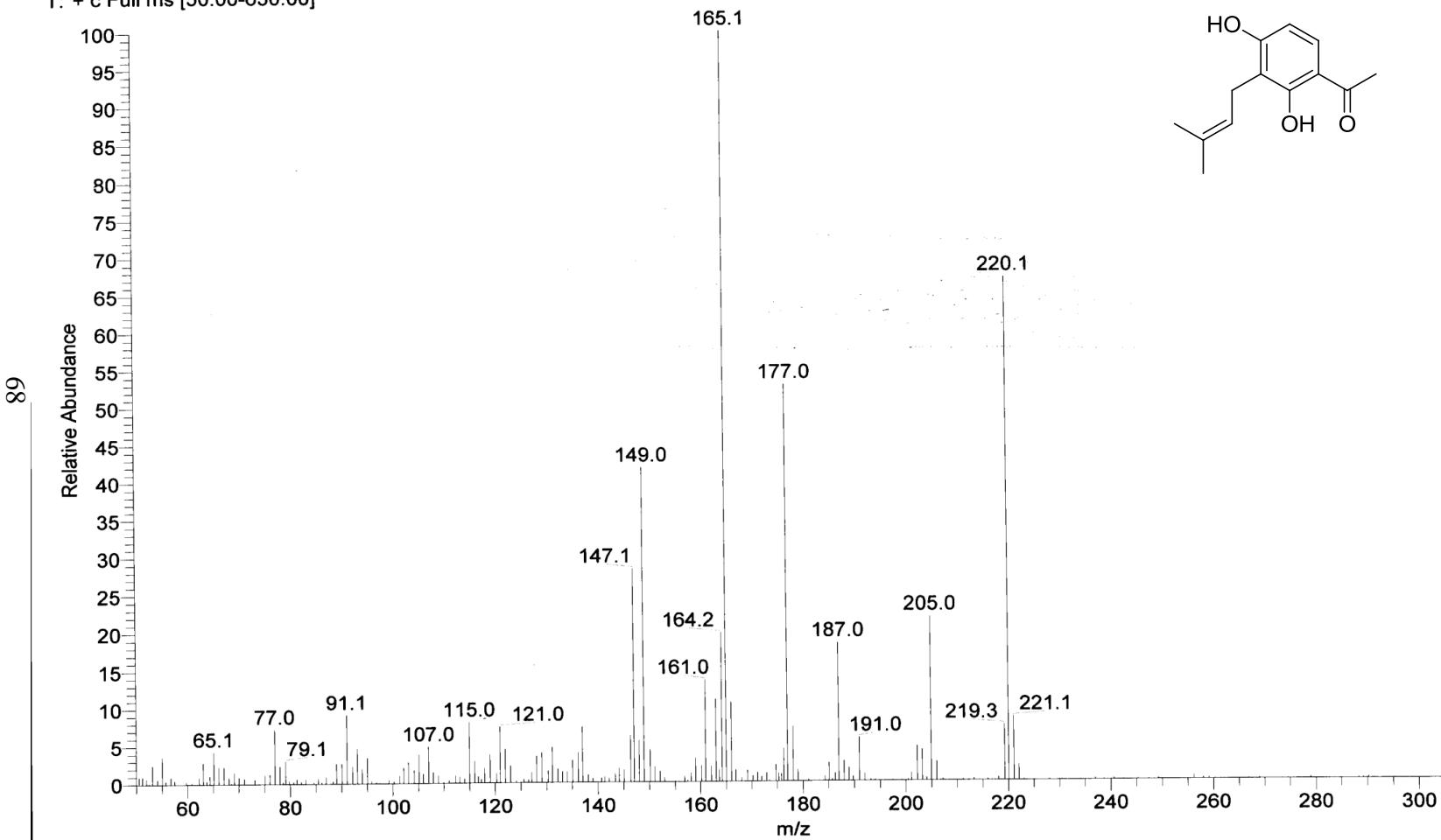


Fig. 17. 1-(2,4-Dihydroxy-3-(3-methylbut-2-enyl)phenyl)ethanone (**11**) 的EI-MS圖譜

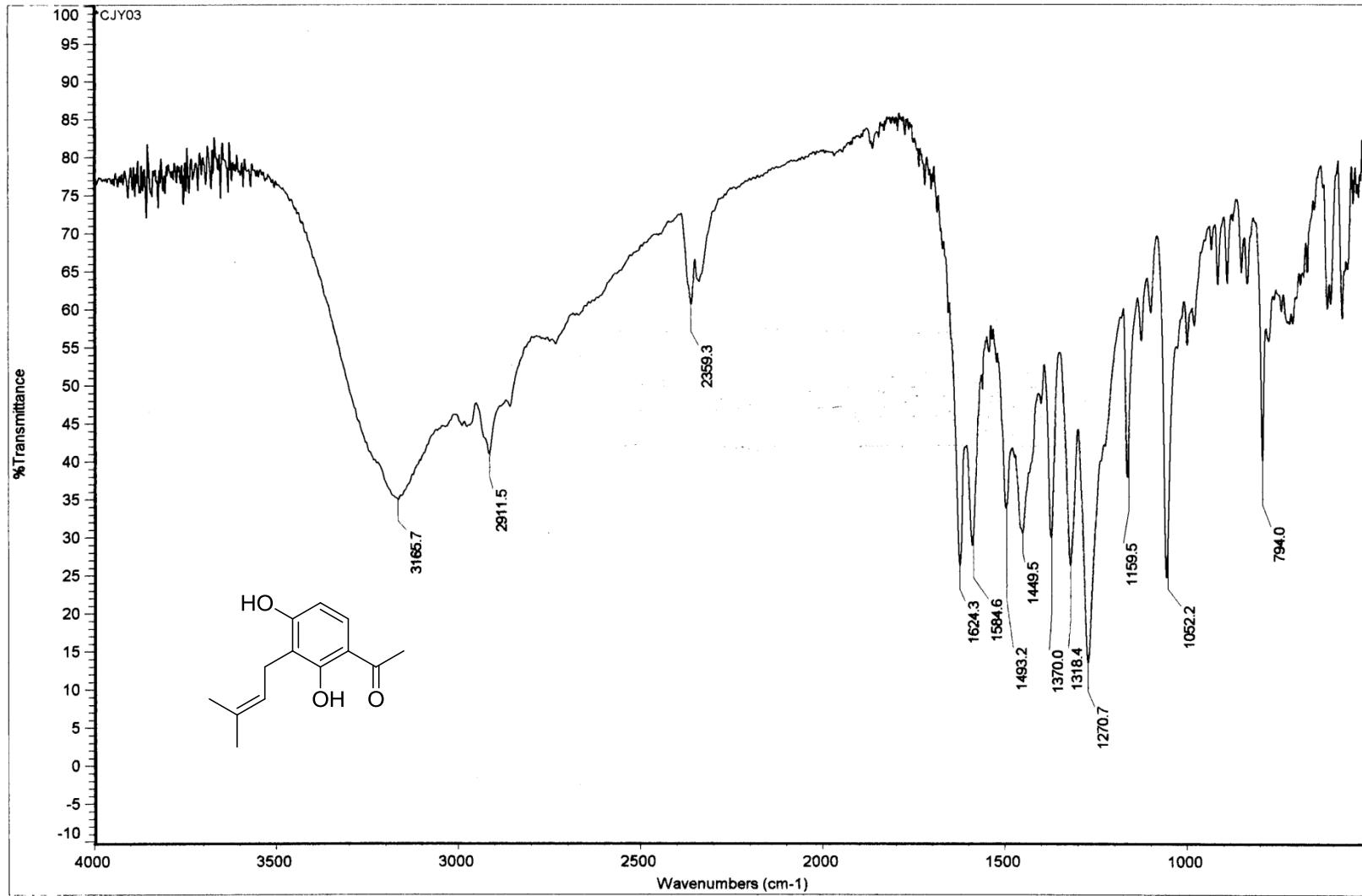


Fig. 18. 1-(2,4-Dihydroxy-3-(3-methylbut-2-enyl)phenyl)ethanone (**11**) 的FTIR圖譜

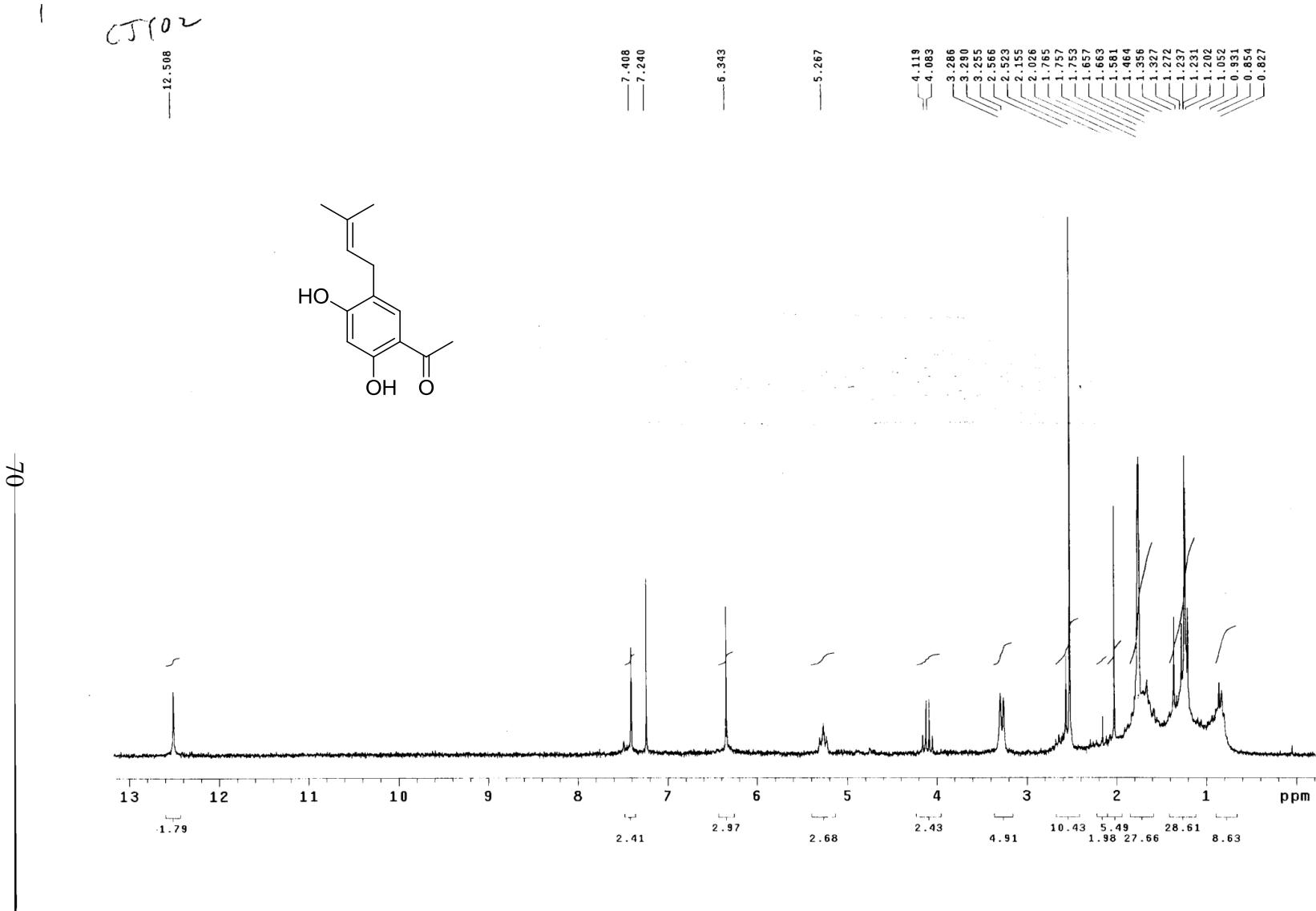


Fig. 19. 1-(2,4-Dihydroxy-5-(3-methylbut-2-enyl)phenyl)ethanone (**12**) 的¹H-NMR圖譜

C:\Xcalibur\data\MJD\CJY-02
DIP-EI-70ev

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CJY-02 #128 RT: 2.63 AV: 1 NL: 4.59E7
T: + c Full ms [50.00-650.00]

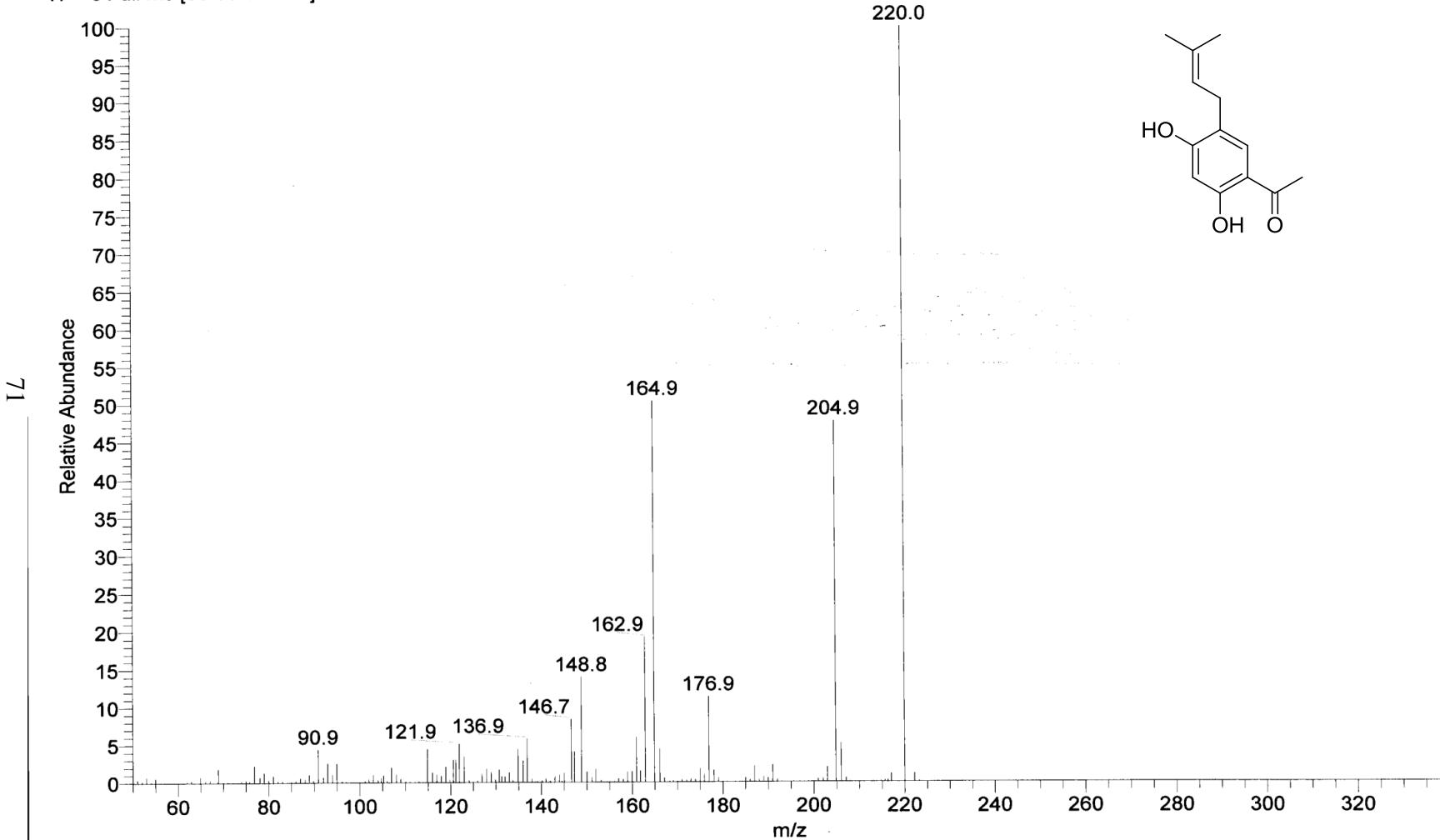


Fig. 20. 1-(2,4-Dihydroxy-5-(3-methylbut-2-enyl)phenyl)ethanone (**12**) 的 EI-MS 圖譜

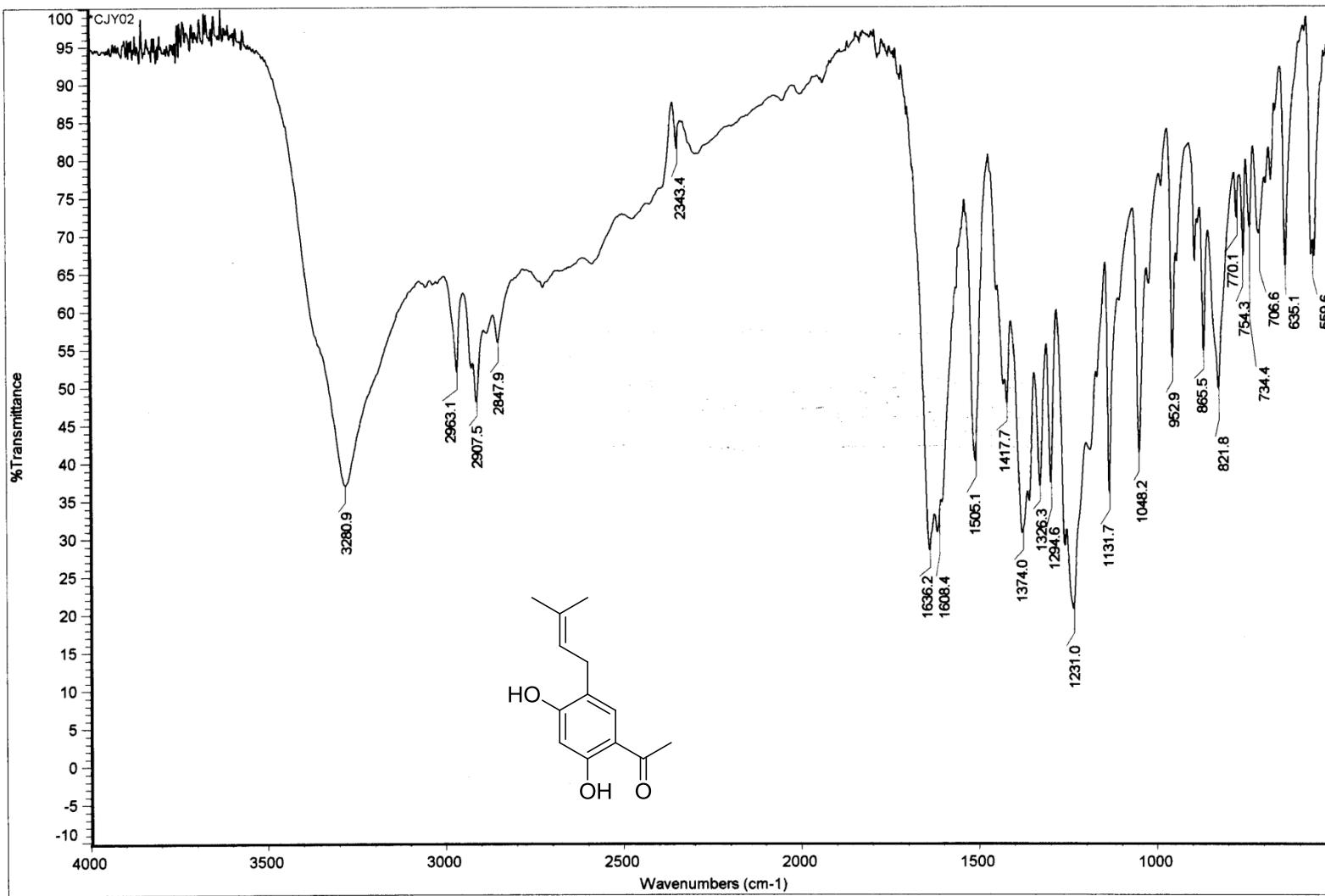
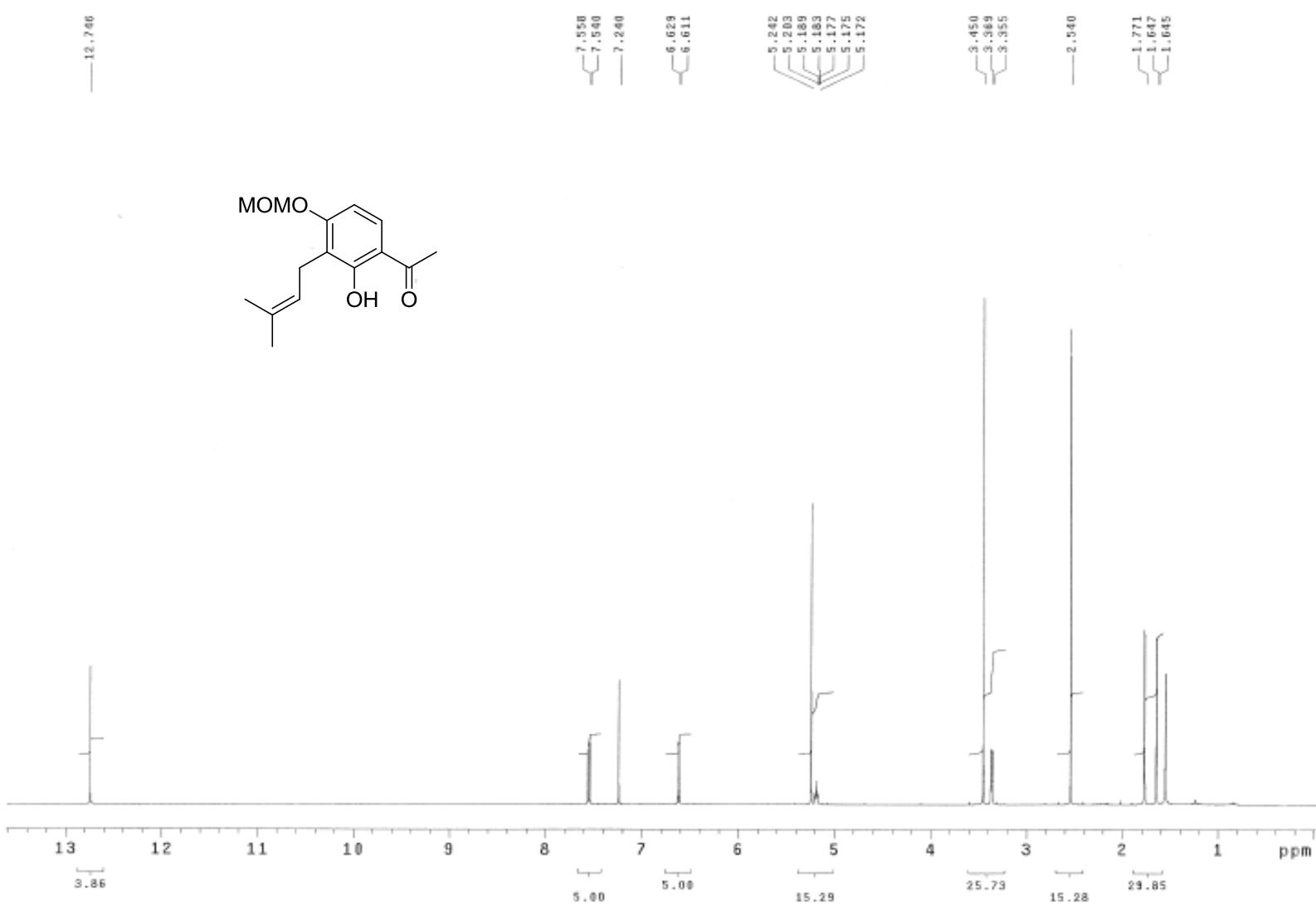


Fig. 21. 1-(2,4-Dihydroxy-5-(3-methylbut-2-enyl)phenyl)ethanone (**12**) 的FTIR圖譜



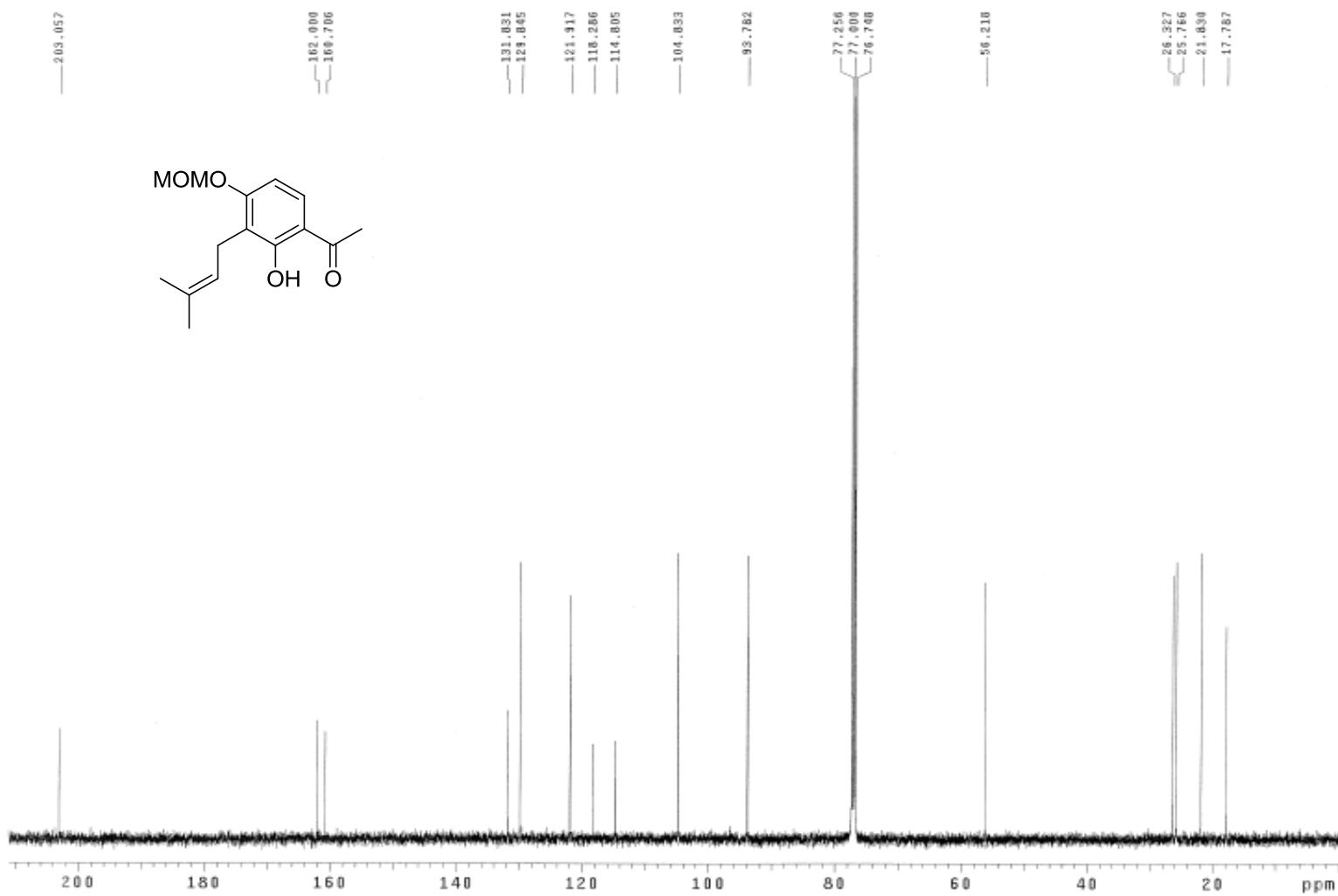


Fig. 23. 1-(2-Hydroxy-4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)ethanone (**13**) 的¹³C-NMR 圖譜

C:\Xcalibur\data\MJD\CJY-31
DIP-EI-70ev
CJY-31 #8 RT: 0.18 AV: 1 NL: 1.63E6
T: + c Full ms [50.00-650.00]

12/23/2011 3:21:52 PM

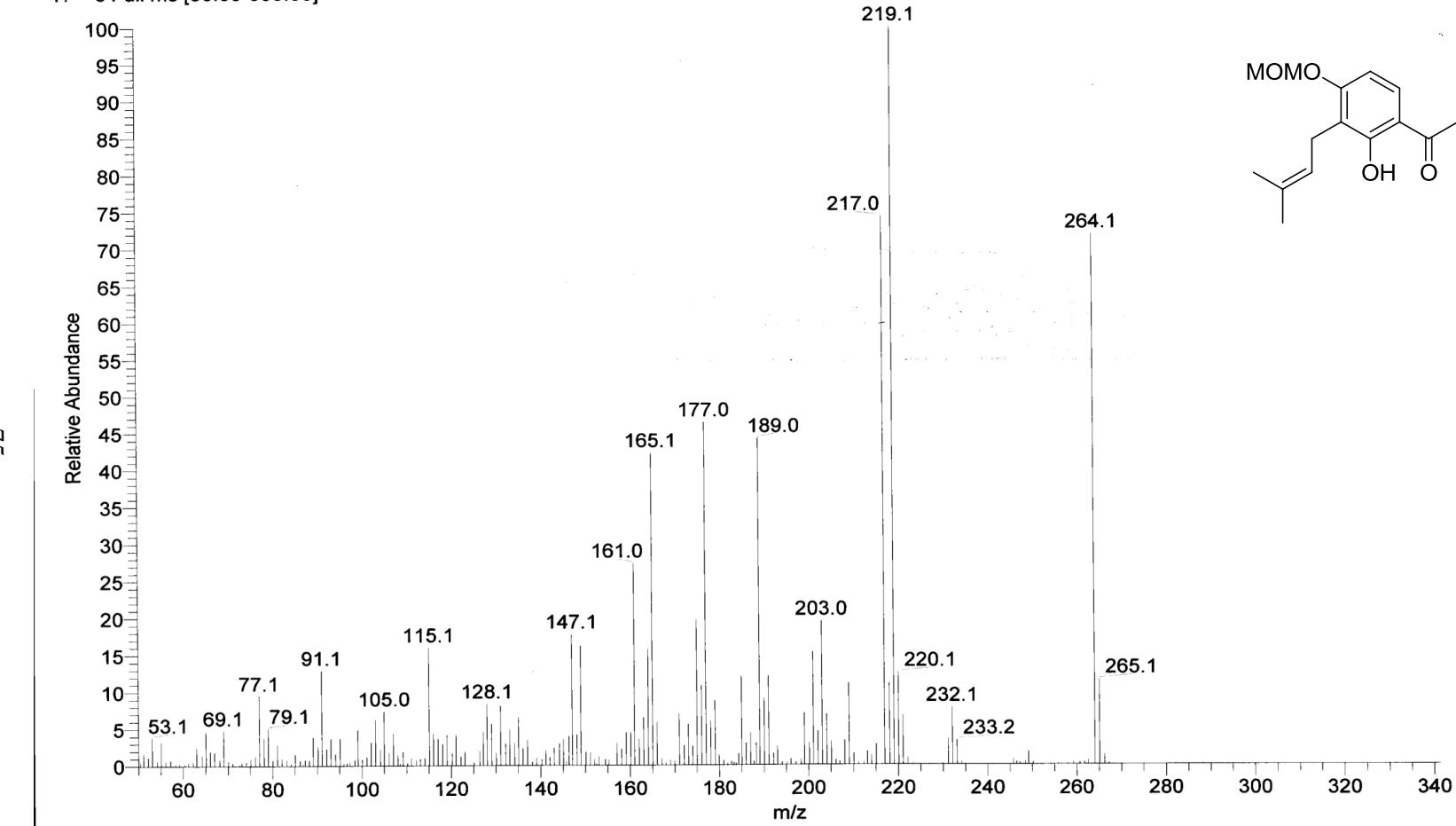


Fig. 24. 1-(2-Hydroxy-4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)ethanone (**13**) 的 EI-MS 圖譜

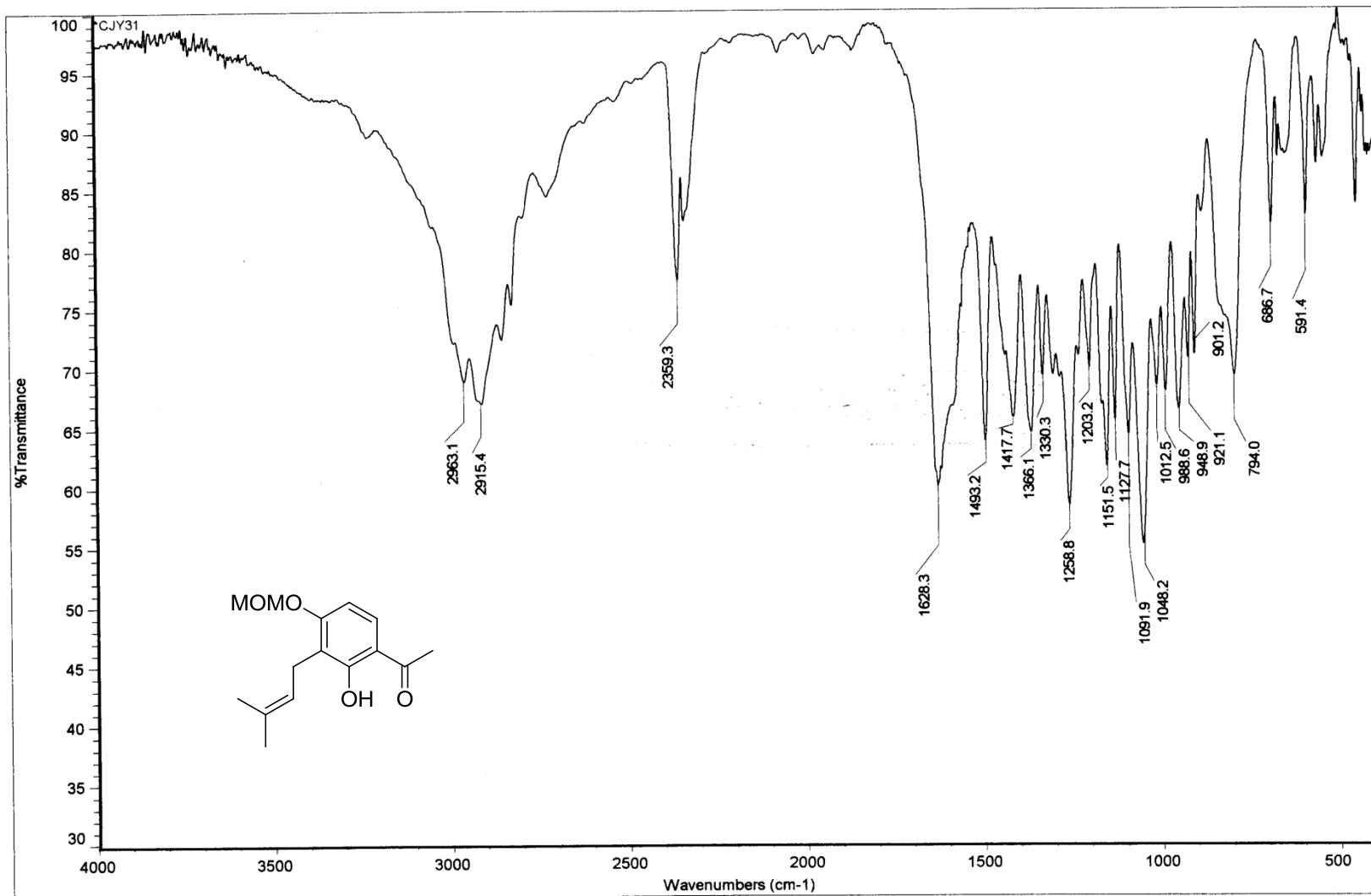


Fig. 25. 1-(2-Hydroxy-4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)ethanone (**13**) 的FTIR圖譜

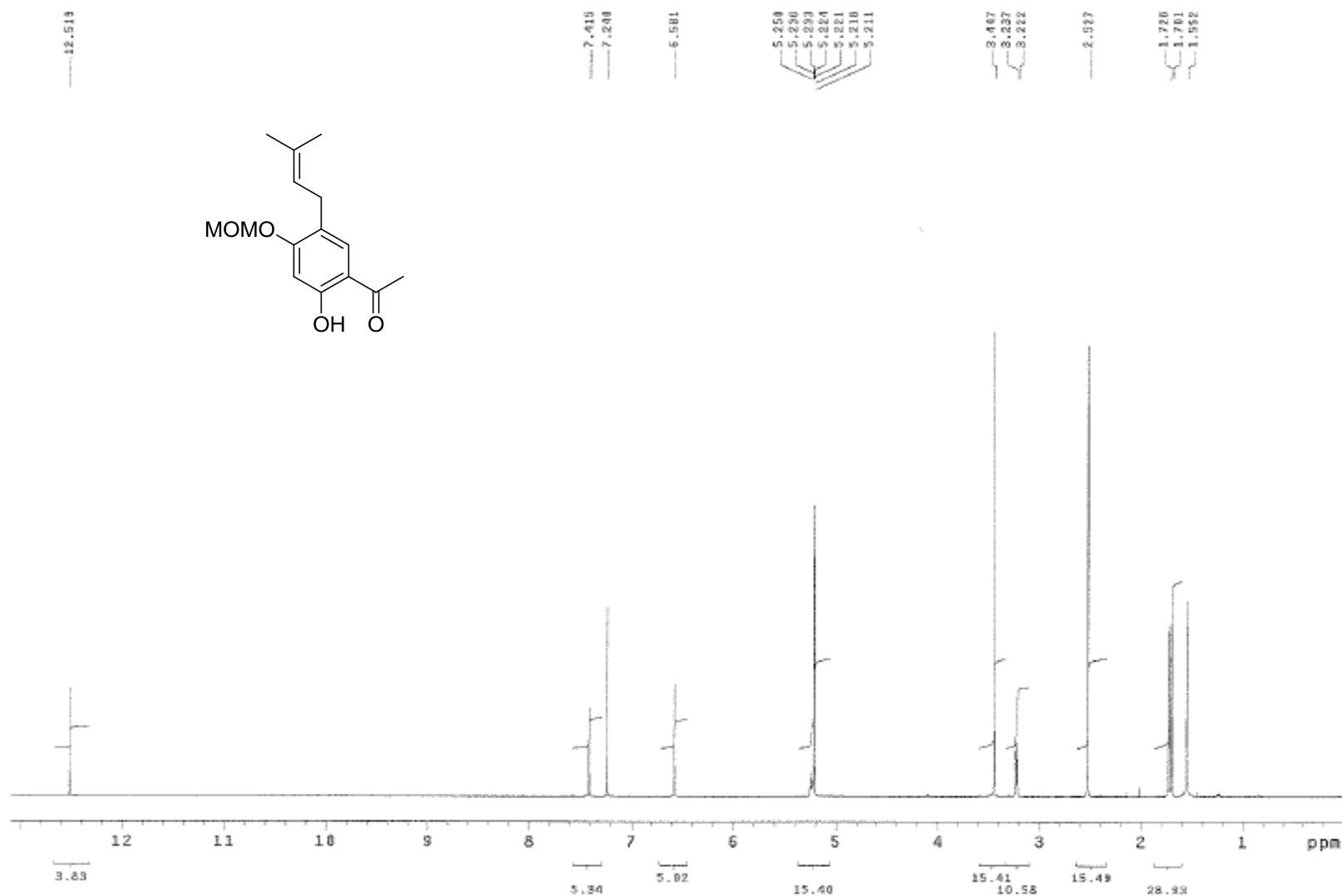


Fig. 26. 1-(2-Hydroxy-4-(methoxymethoxy)-5-(3-methylbut-2-enyl)-phenyl)ethanone (**14**) 的 $^1\text{H-NMR}$ 圖譜

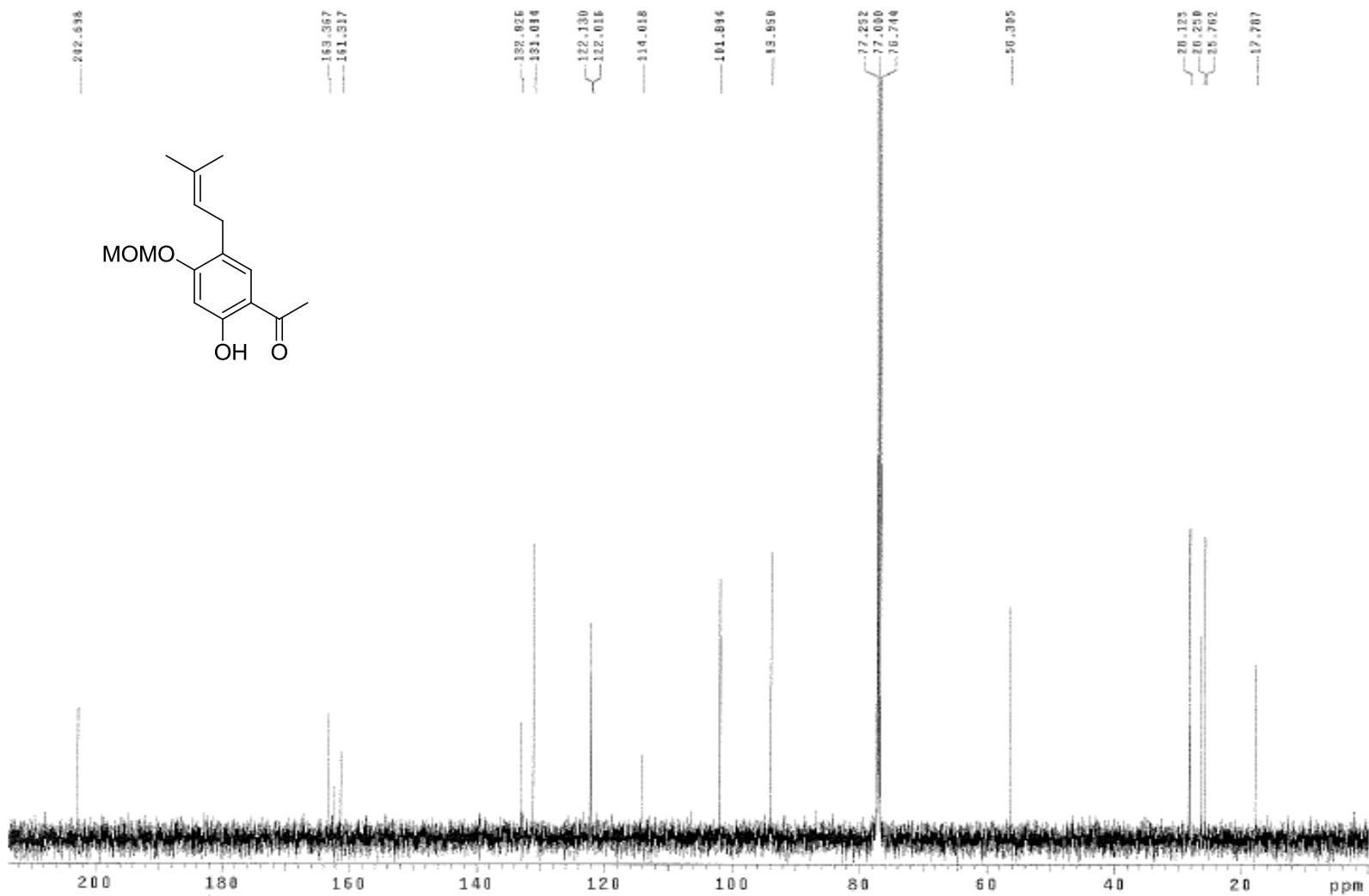


Fig. 27. 1-(2-Hydroxy-4-(methoxymethoxy)-5-(3-methylbut-2-enyl)-phenyl)ethanone (14) 的 ^{13}C -NMR 圖譜

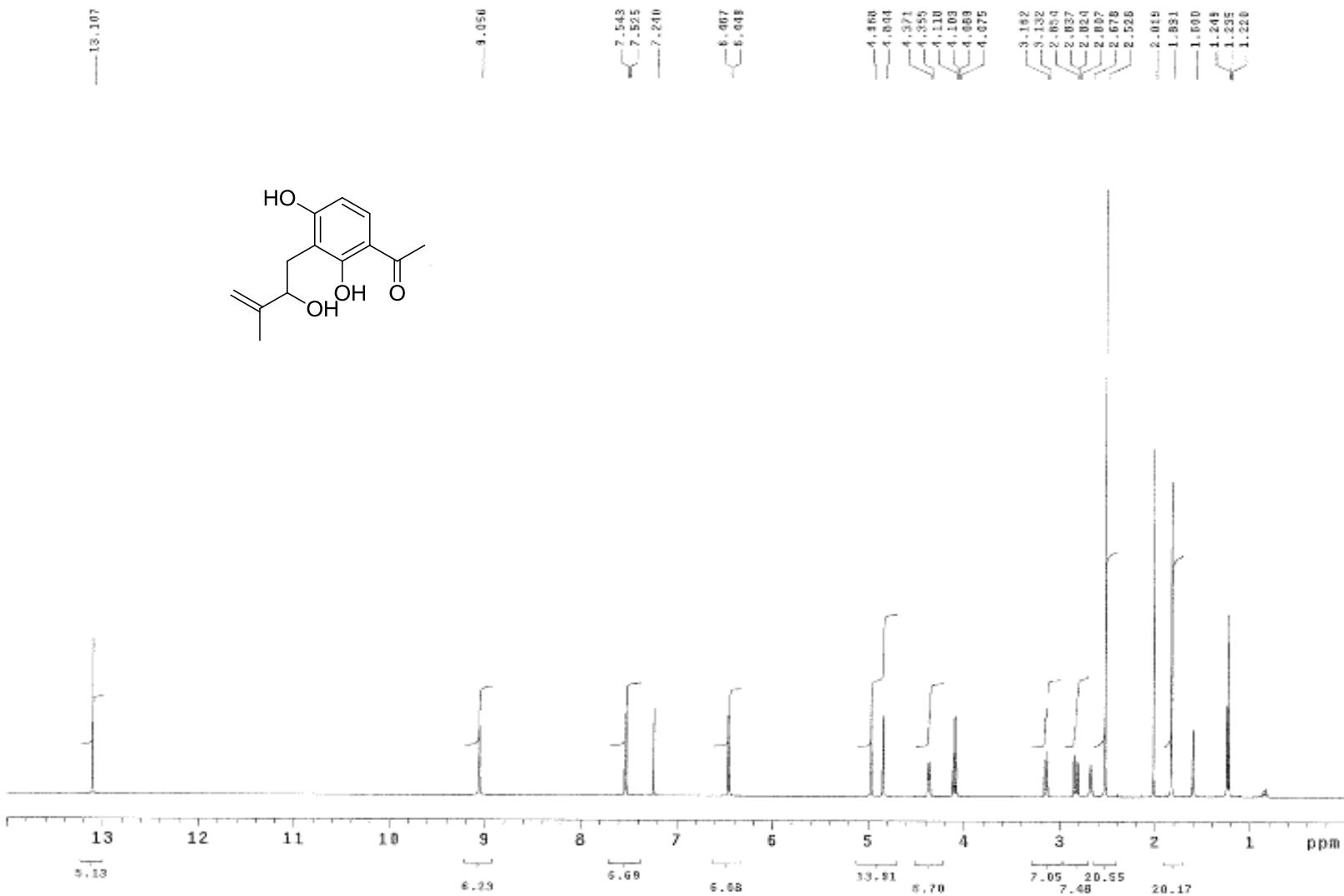


Fig. 28. 1-(2,4-Dihydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-phenyl)ethanone (**15**) 的¹H-NMR 圖譜

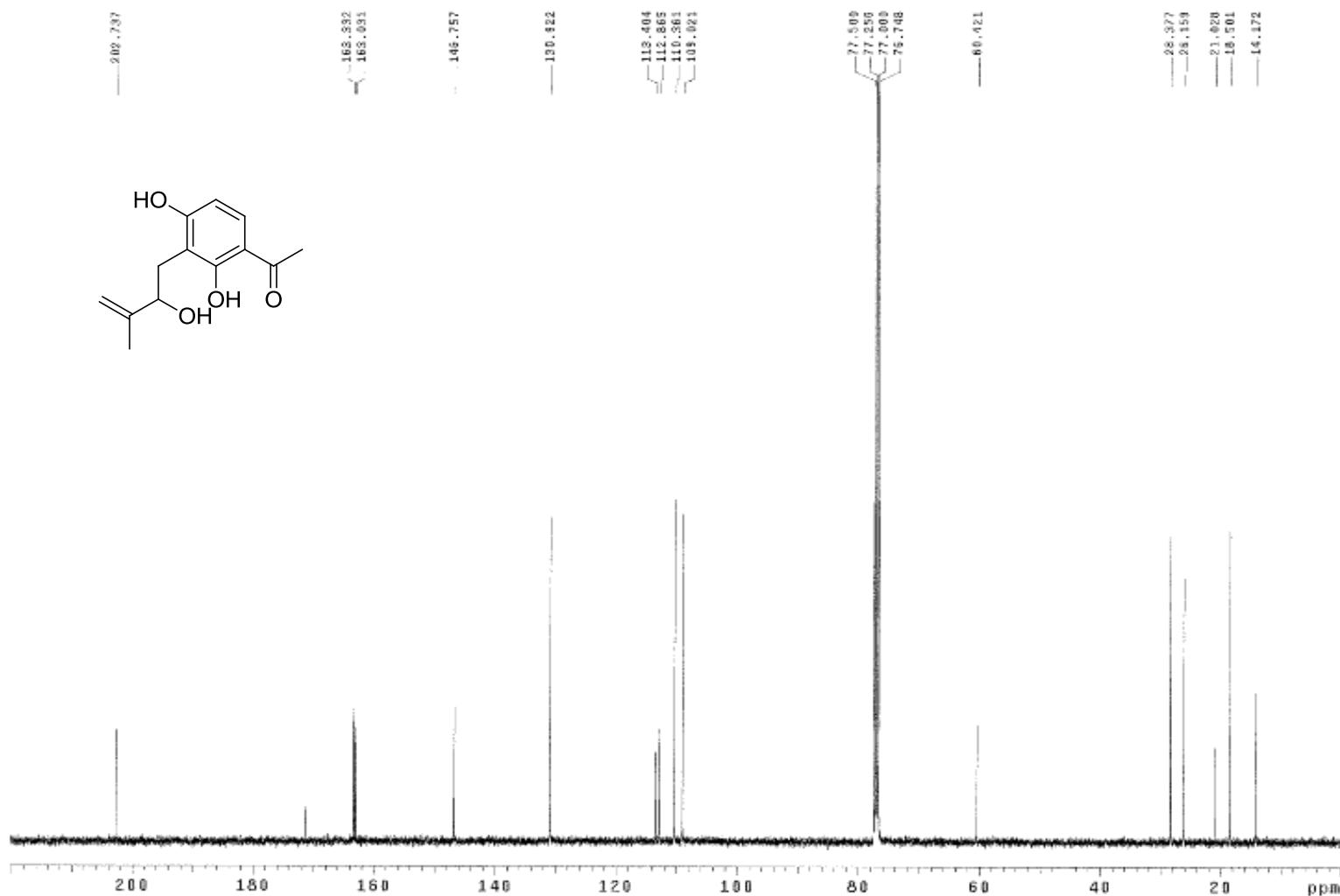


Fig. 29. 1-(2,4-Dihydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-phenyl)ethanone (15) 的 ^{13}C -NMR 圖譜

C:\Xcalibur\data\MJD\CJY-21

DIP-EI-70ev

CJY-21 #113 RT: 2.33 AV: 1 NL: 8.68E5

T: + c Full ms [50.00-650.00]

12/23/2011 1:45:44 PM

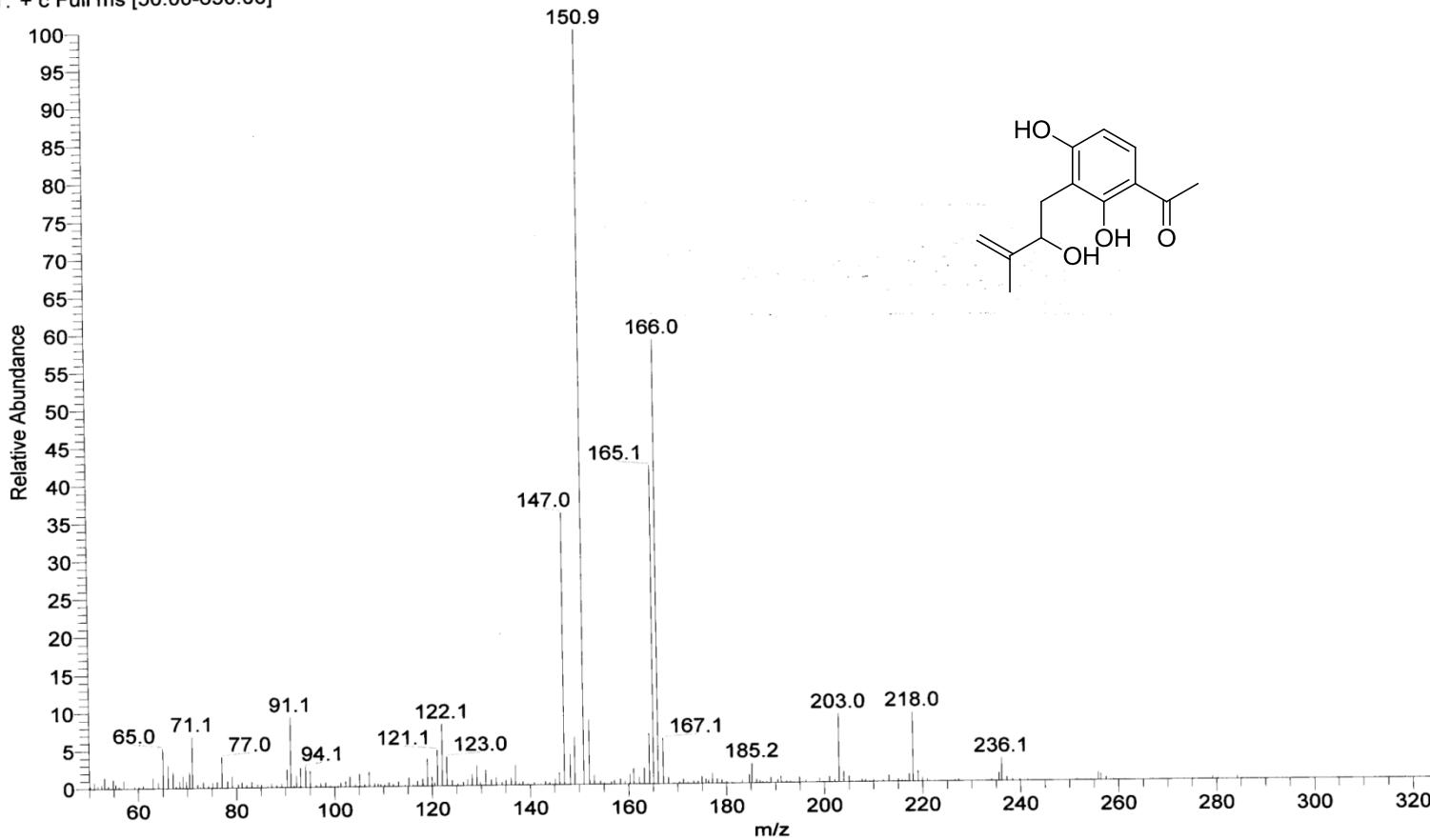


Fig. 30. 1-(2,4-Dihydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-phenyl)ethanone (**15**) 的EI-MS圖譜

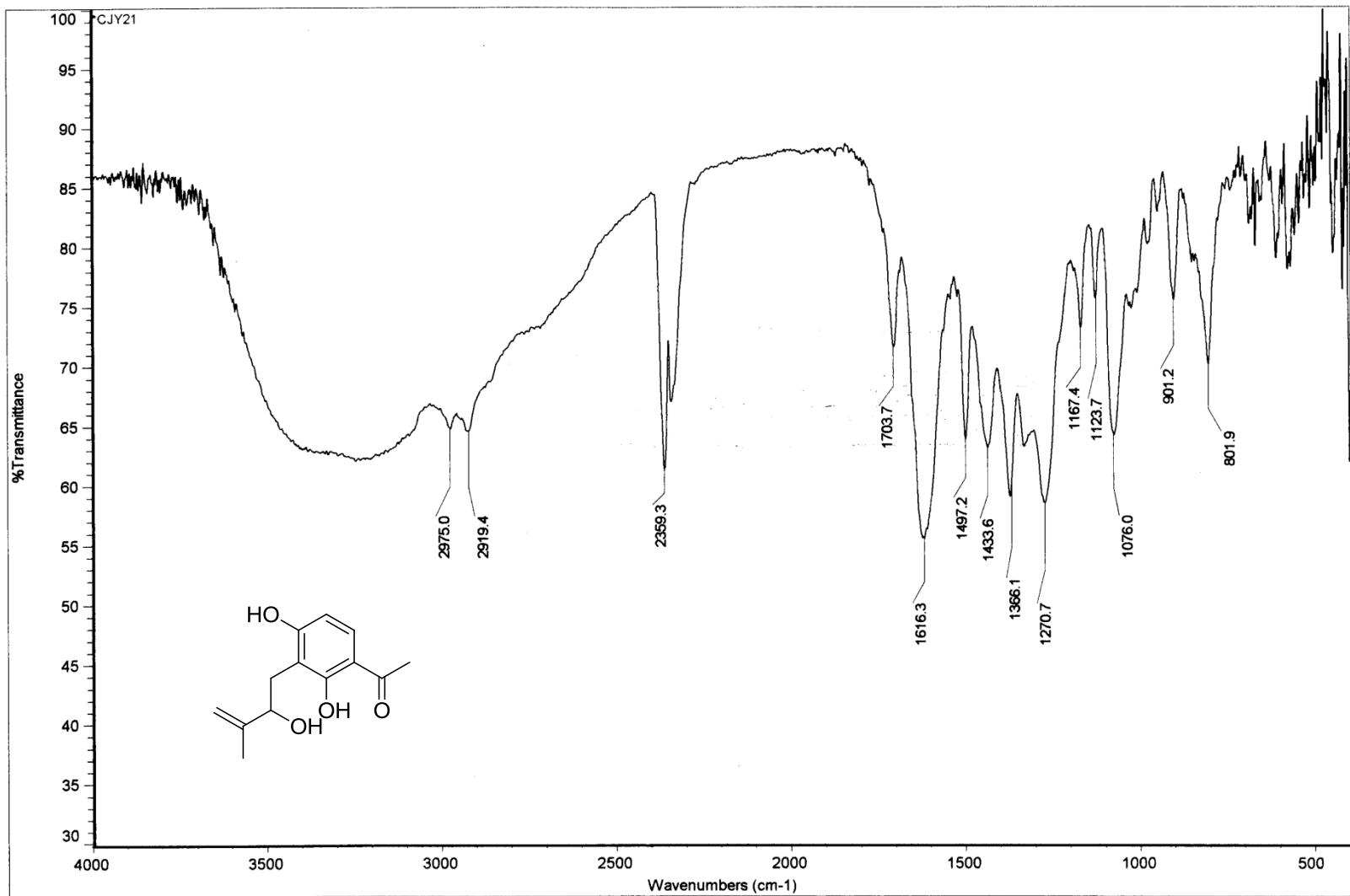


Fig. 31. 1-(2,4-Dihydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-phenyl)ethanone (**15**) 的FTIR圖譜

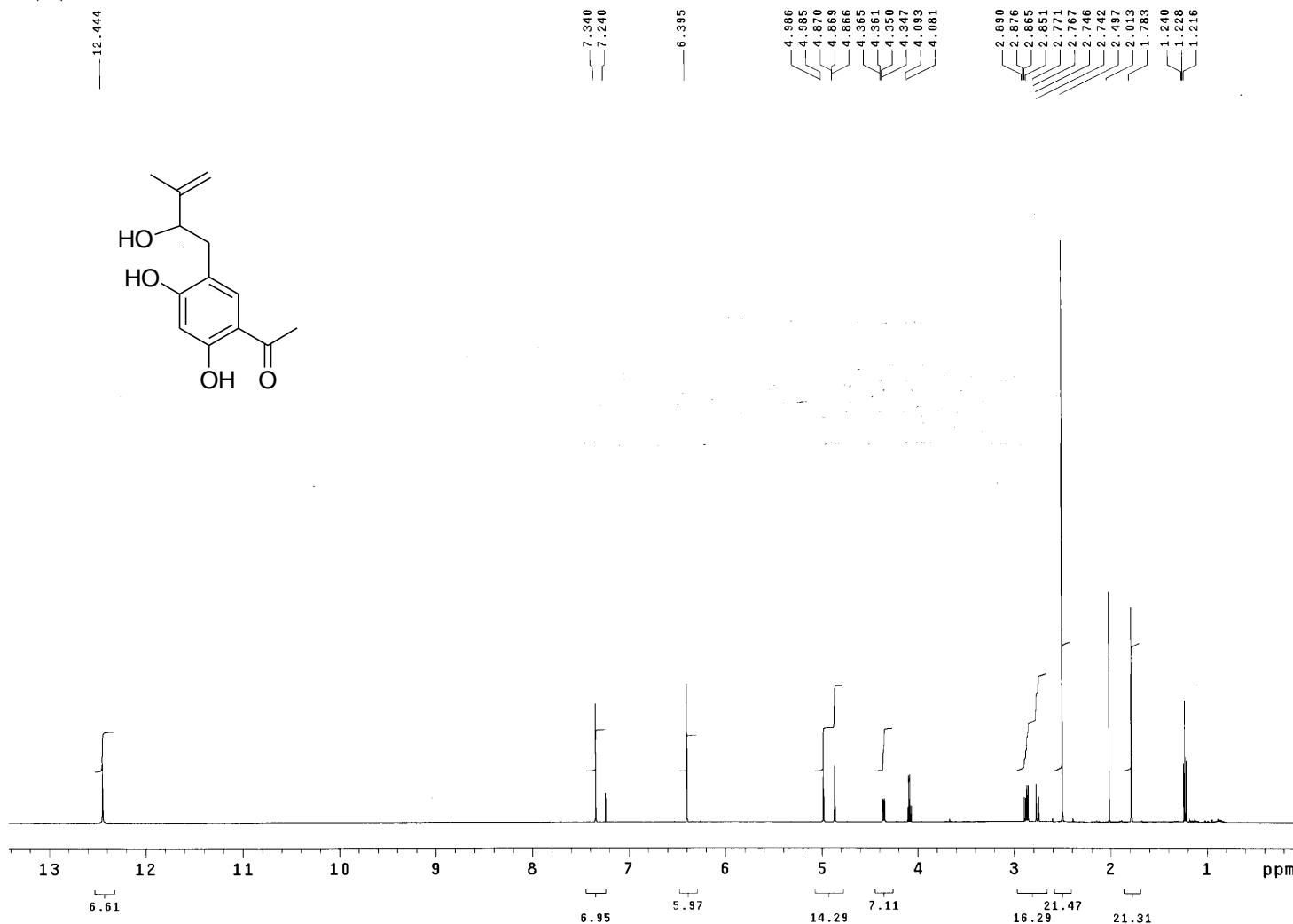


Fig. 32. 1-(2,4-Dihydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-phenyl)ethanone (**16**)的¹H-NMR圖譜

CJY06a_CDC13_600
11/03/09

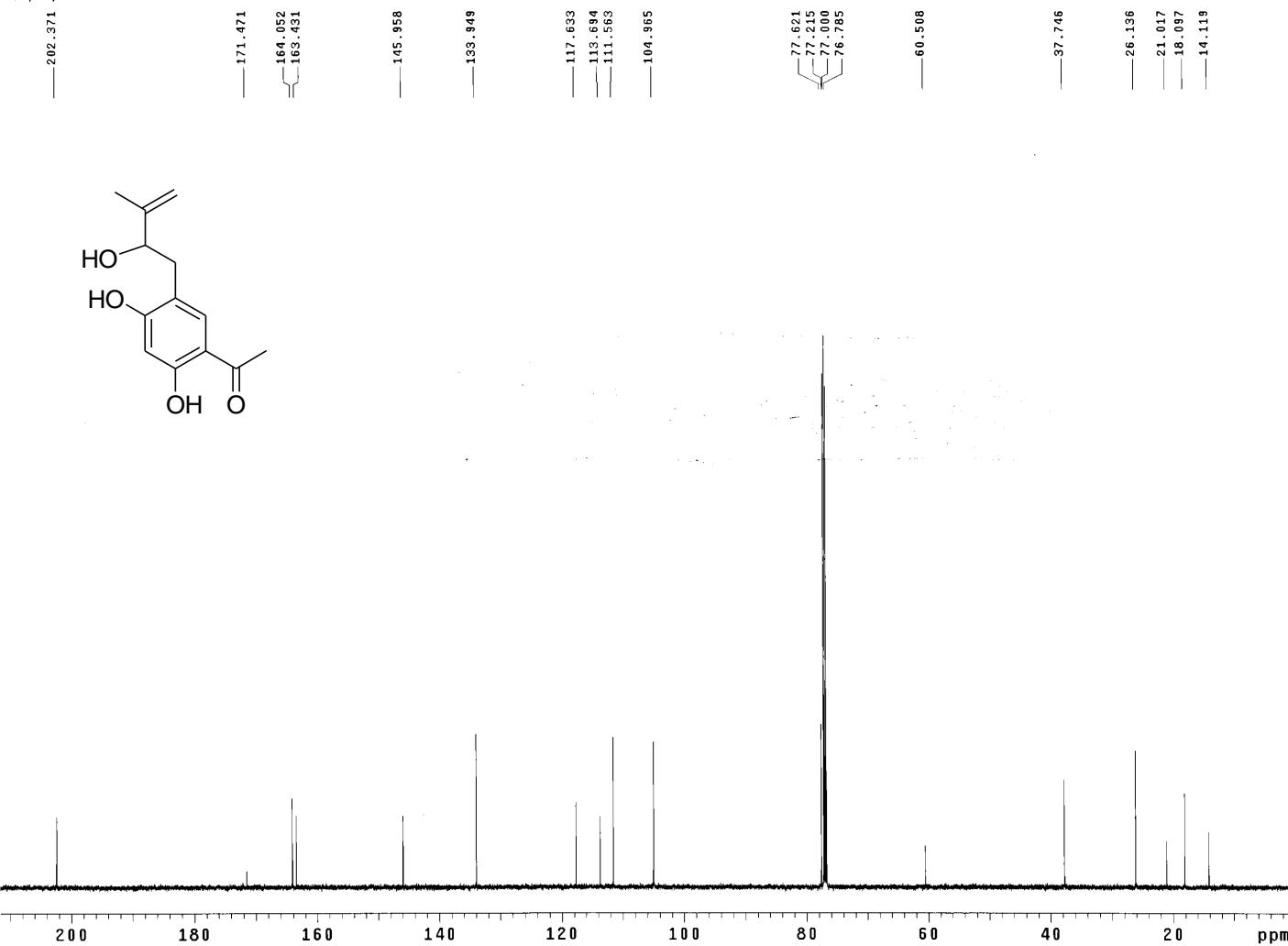


Fig. 33. 1-(2,4-Dihydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-phenyl)ethanone (16)的¹³C-NMR圖譜

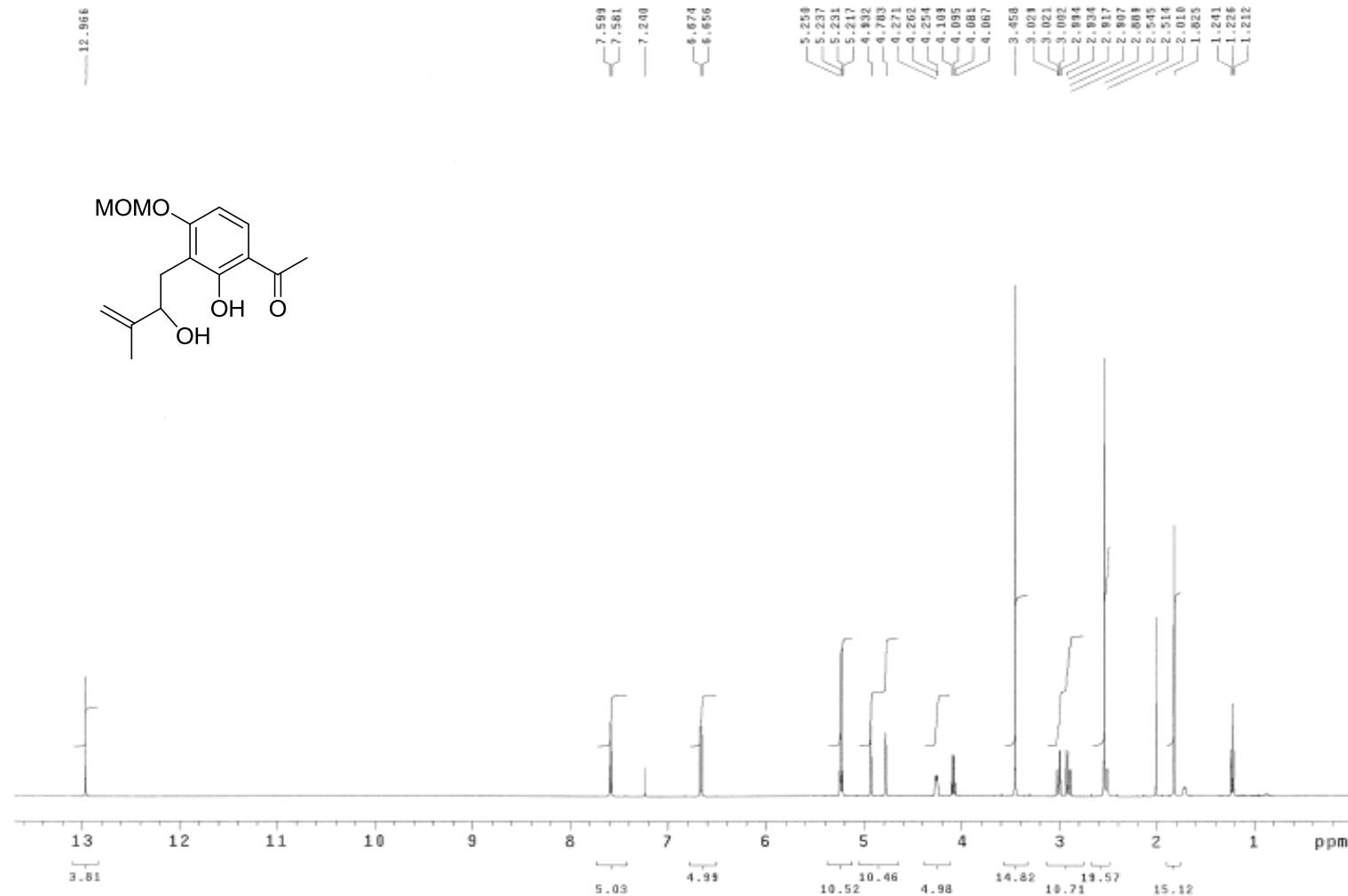


Fig. 34. 1-(2-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxy-methoxy)phenyl)ethanone (**17**) 的¹H-NMR 圖譜

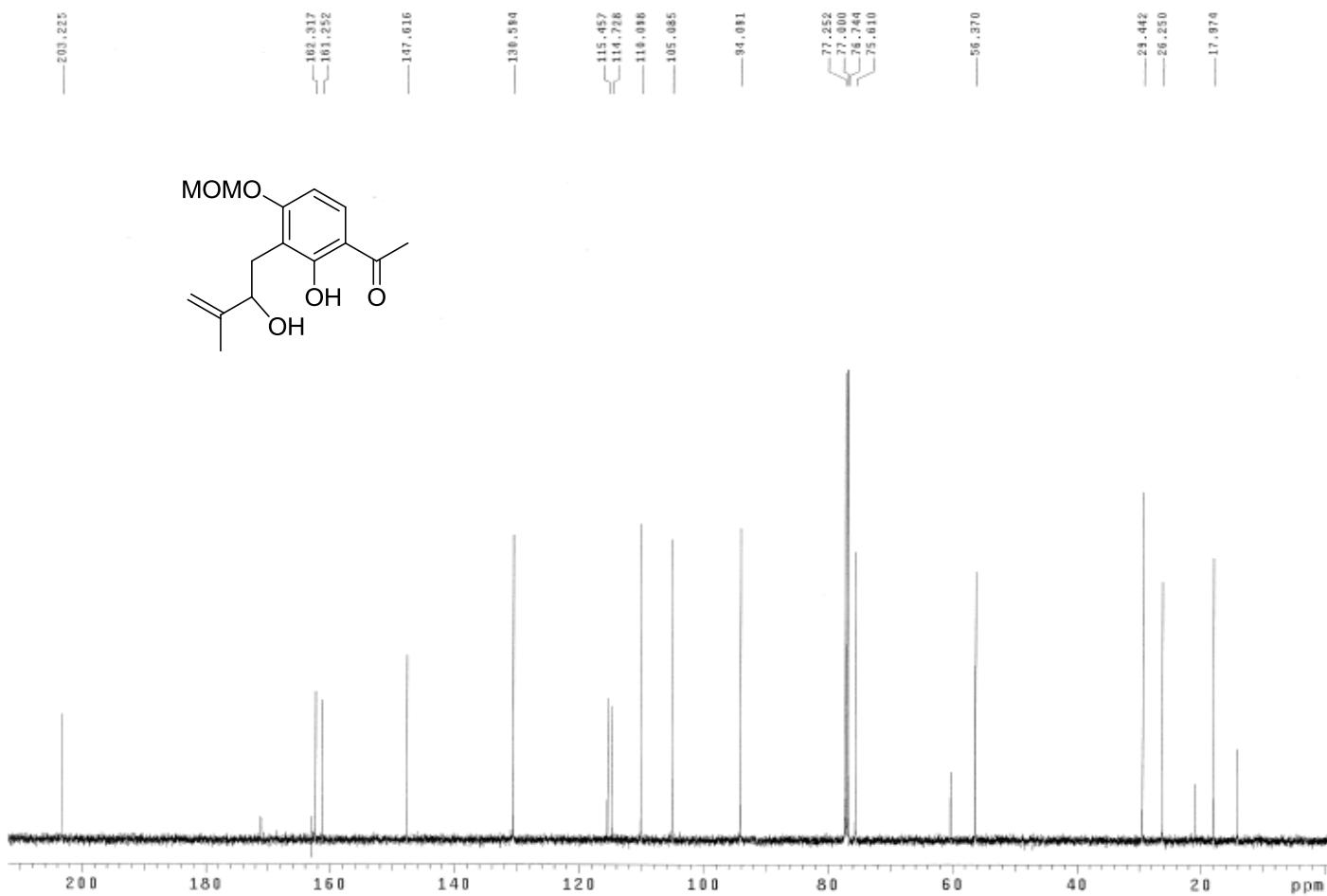


Fig. 35. 1-(2-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxy-methoxy)phenyl)ethanone (**17**) 的 ^{13}C -NMR 圖譜

C:\Xcalibur\data\MJD\CJY-26b
DIP-EI-70ev

12/23/2011 2:11:13 PM

CJY-26b #21 RT: 0.45 AV: 1 NL: 2.06E5
T: + c Full ms [50.00-650.00]

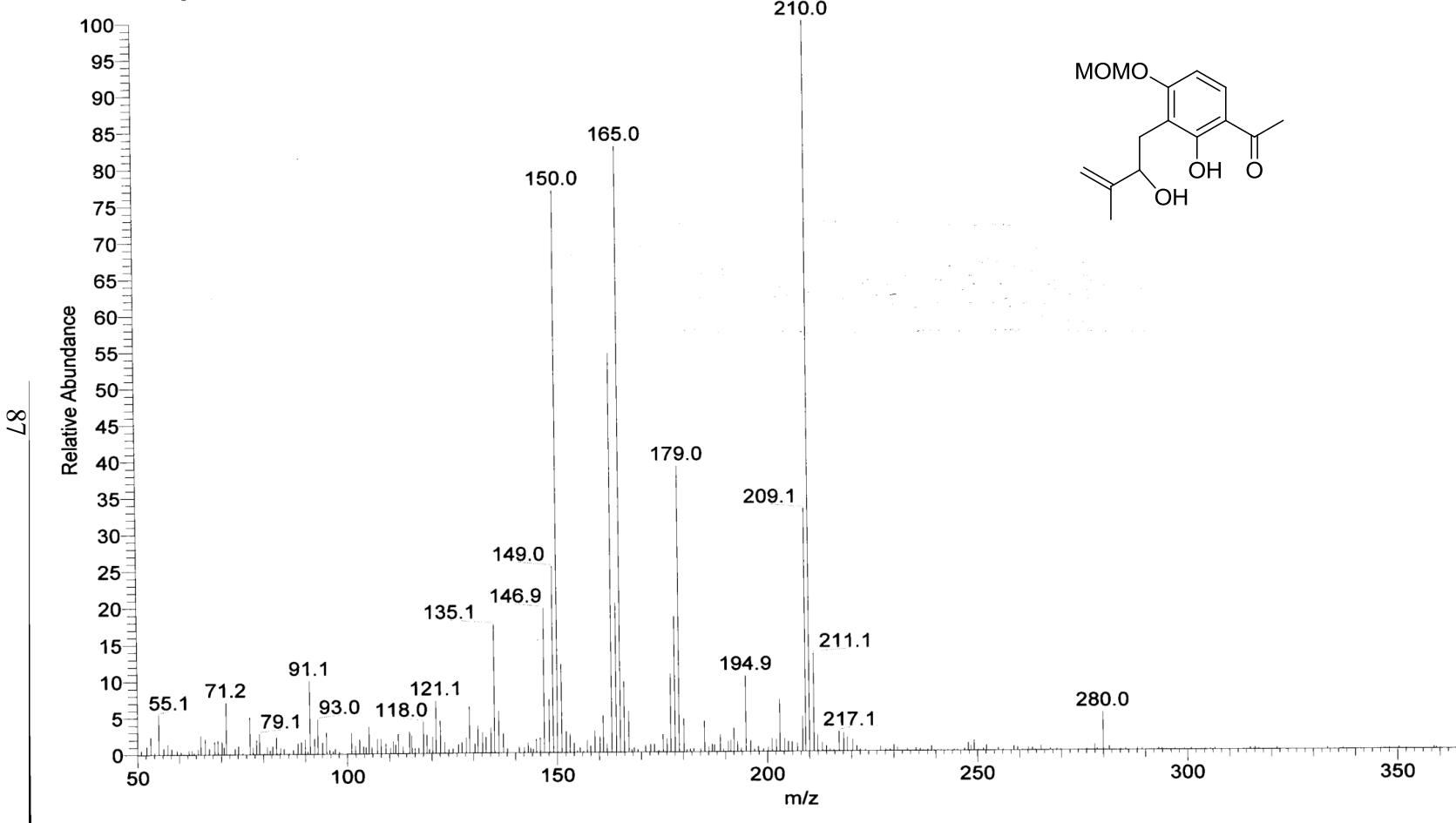


Fig. 36. 1-(2-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxy-methoxy)phenyl)ethanone (17) 的 EI-MS 圖譜

CJY 266

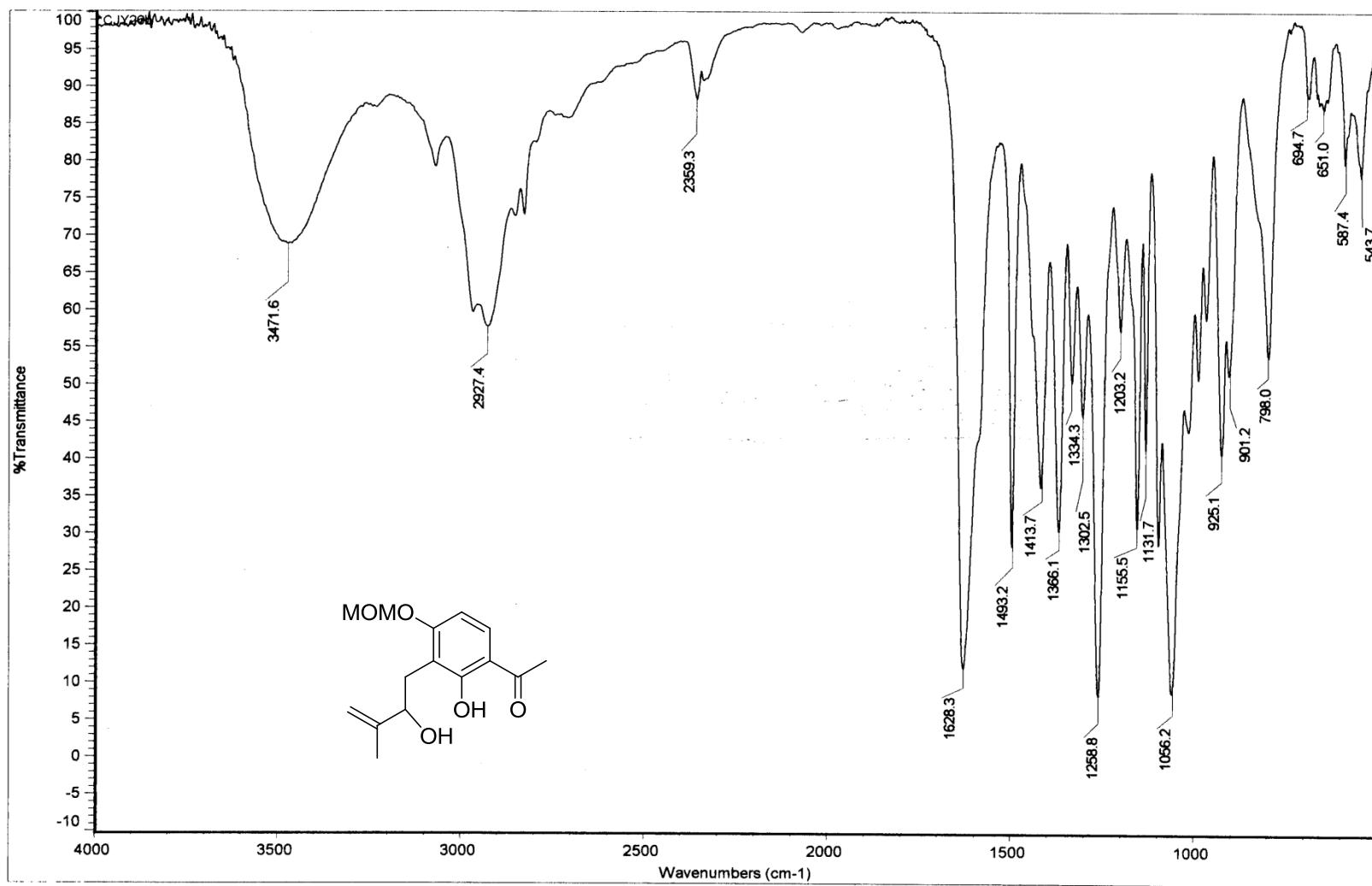


Fig. 37. 1-(2-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)ethanone (**17**) 的FTIR圖譜

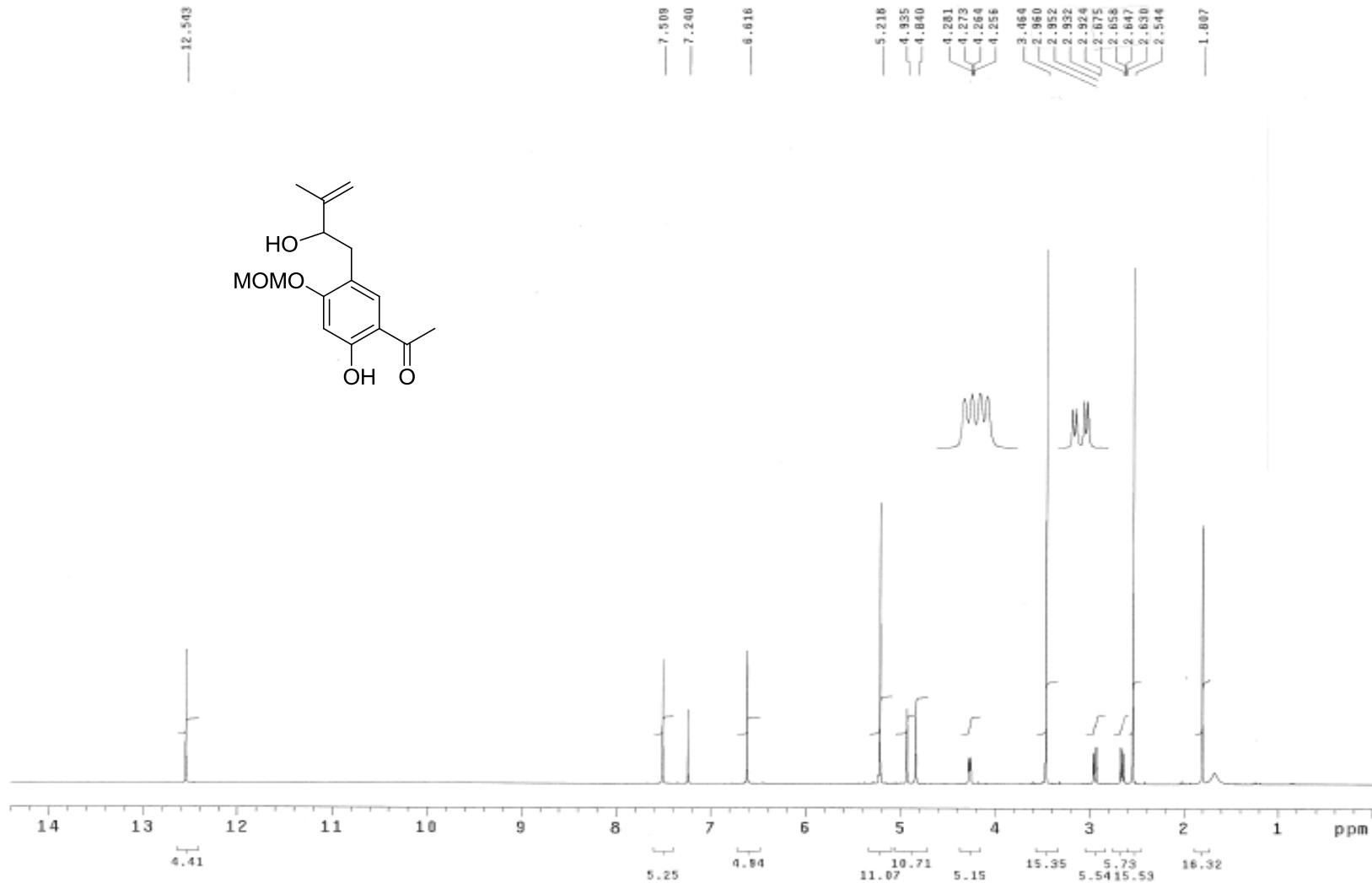


Fig. 38. 1-(2-Hydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)-phenyl)ethanone (**18**) 的¹H-NMR 圖譜

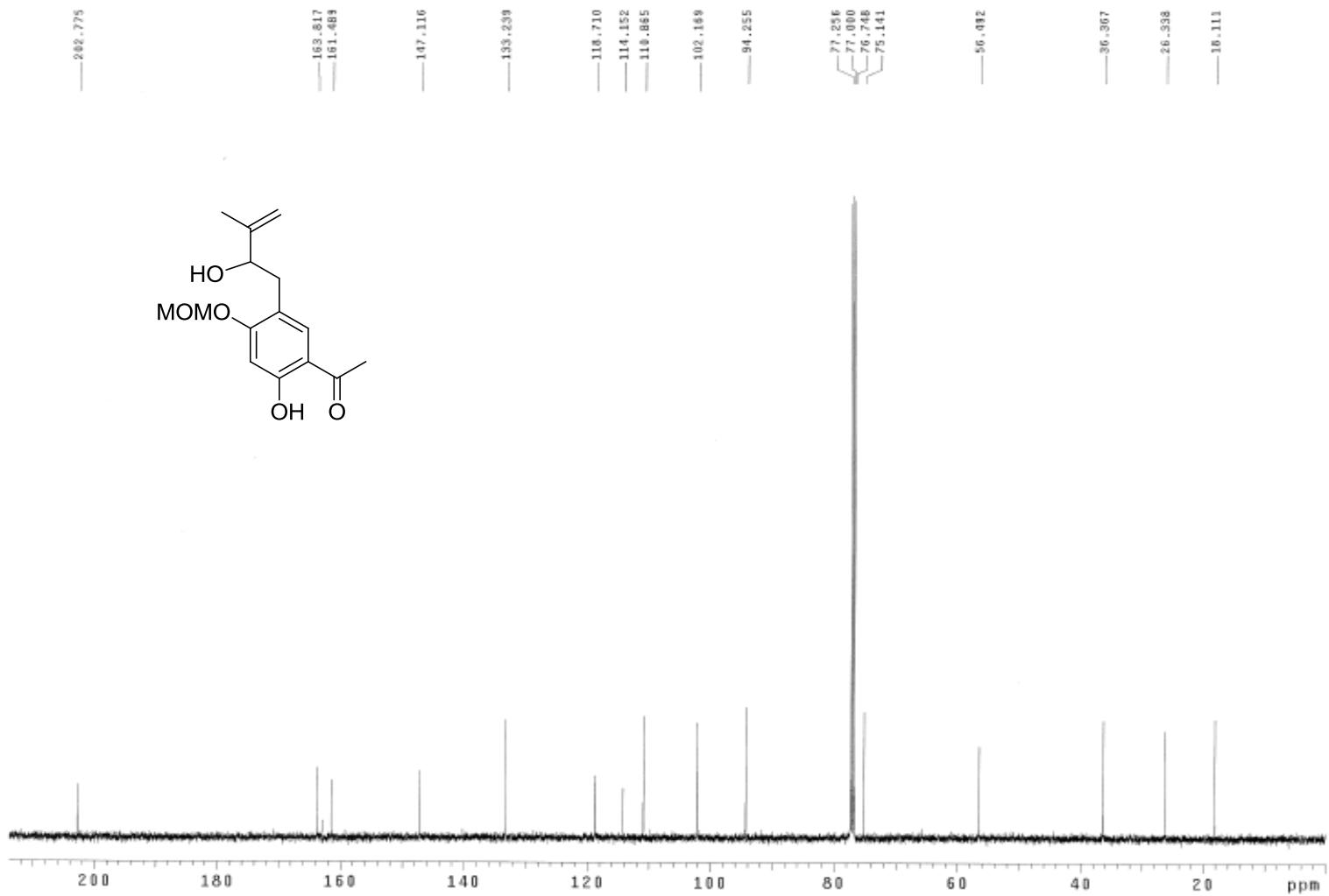
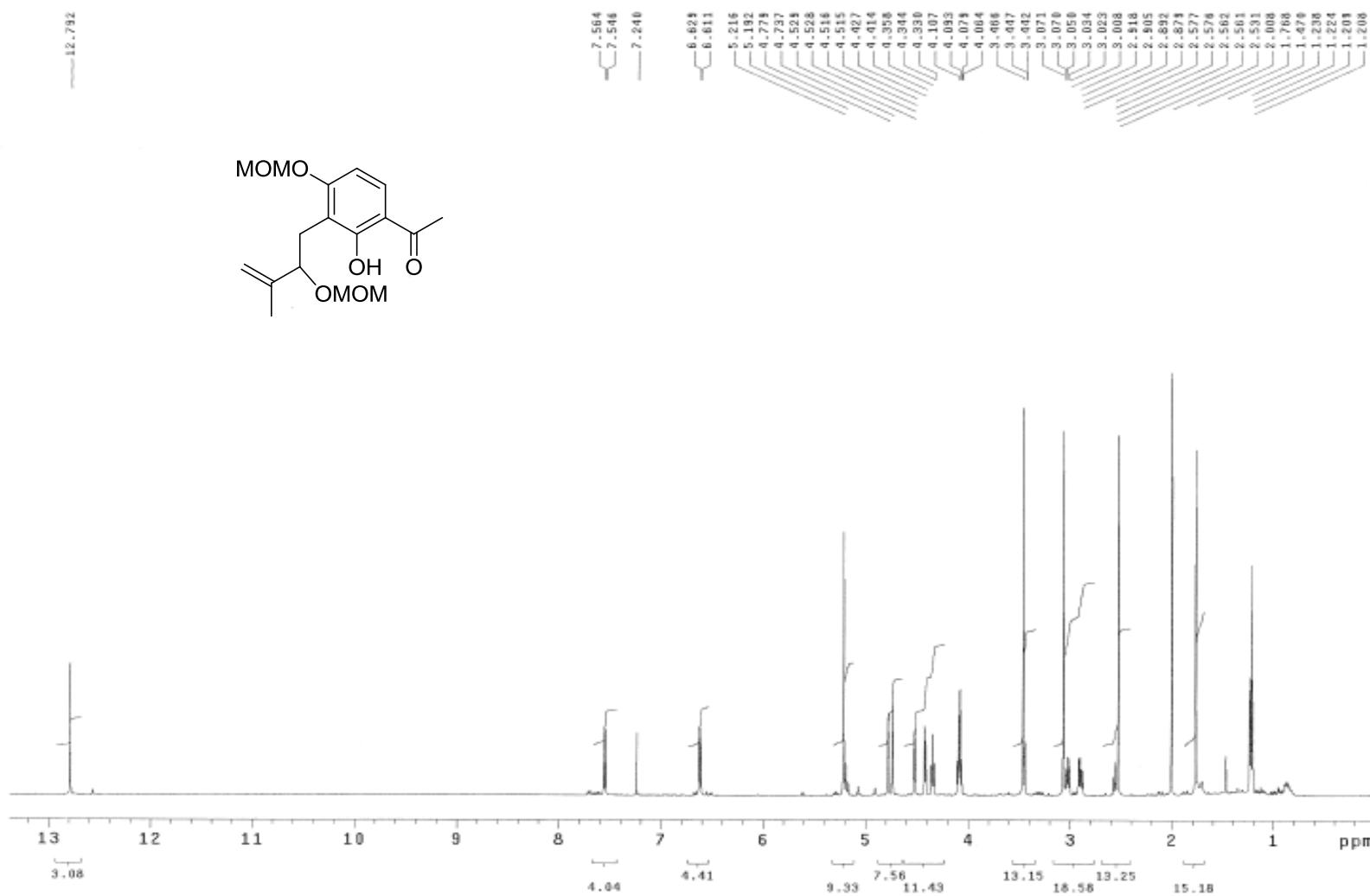


Fig. 39. 1-(2-Hydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)-phenyl)ethanone (**18**) 的 ^{13}C -NMR 圖譜



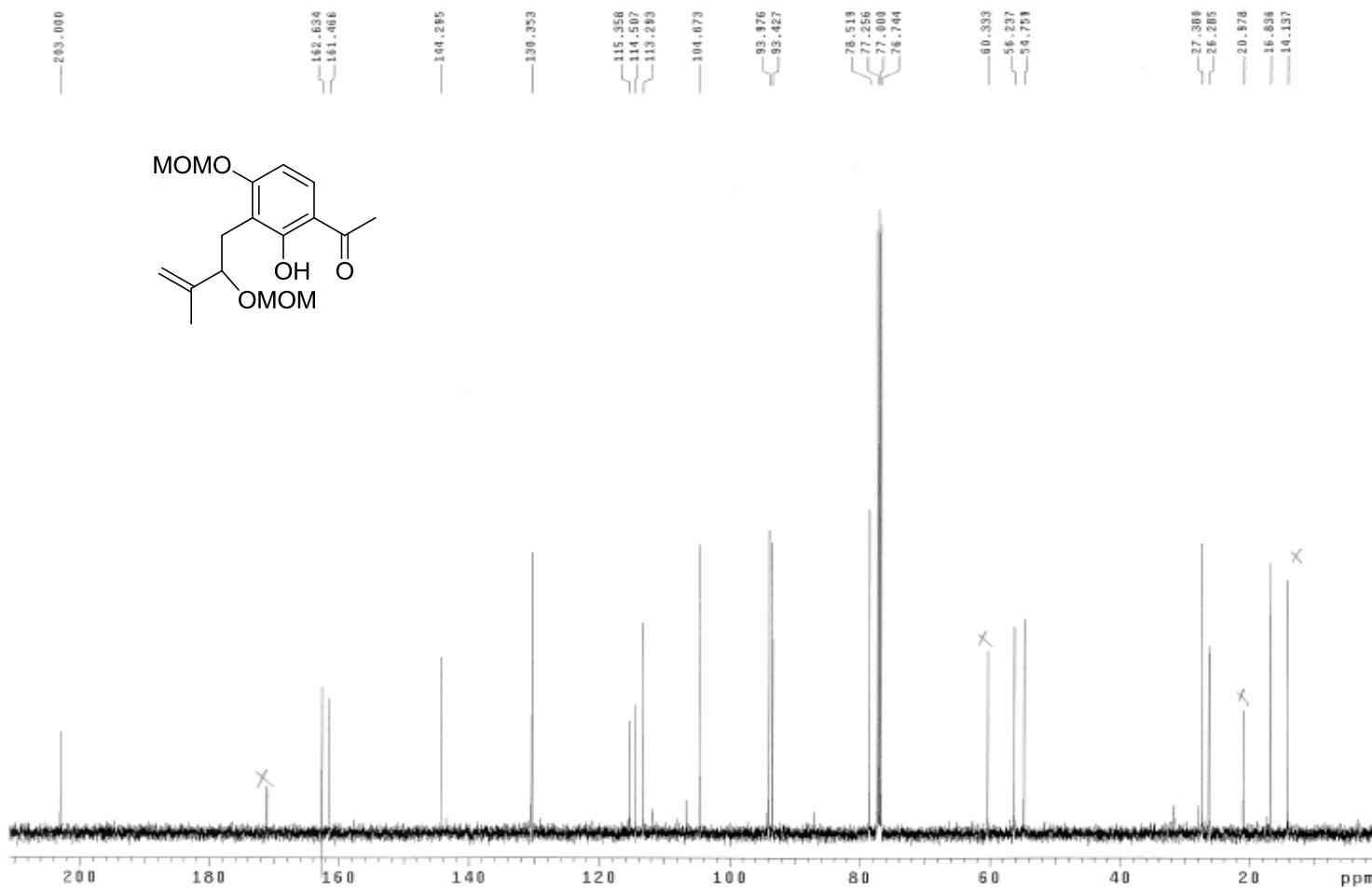


Fig. 41. 1-(2-Hydroxy-4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)ethanone (**19**) 的 ^{13}C -NMR 圖譜

C:\Xcalibur\data\MJD\CJY-26a

12/23/2011 2:15:51 PM

DIP-EI-70ev

CJY-26a #17-18 RT: 0.37-0.39 AV: 2 NL: 5.12E5

T: + c Full ms [50.00-650.00]

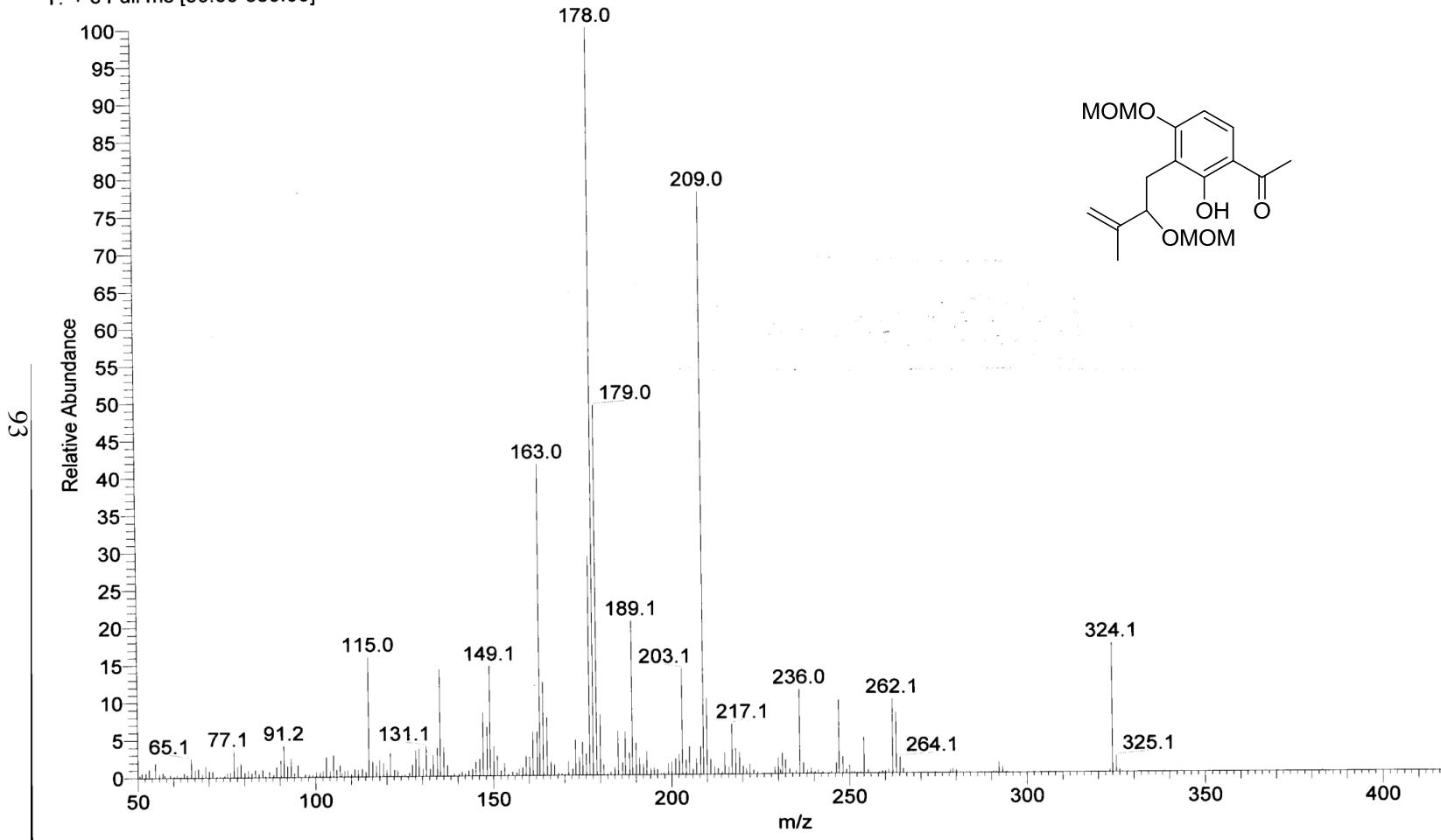


Fig. 42. 1-(2-Hydroxy-4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)ethanone (**19**) 的 EI-MS 圖譜

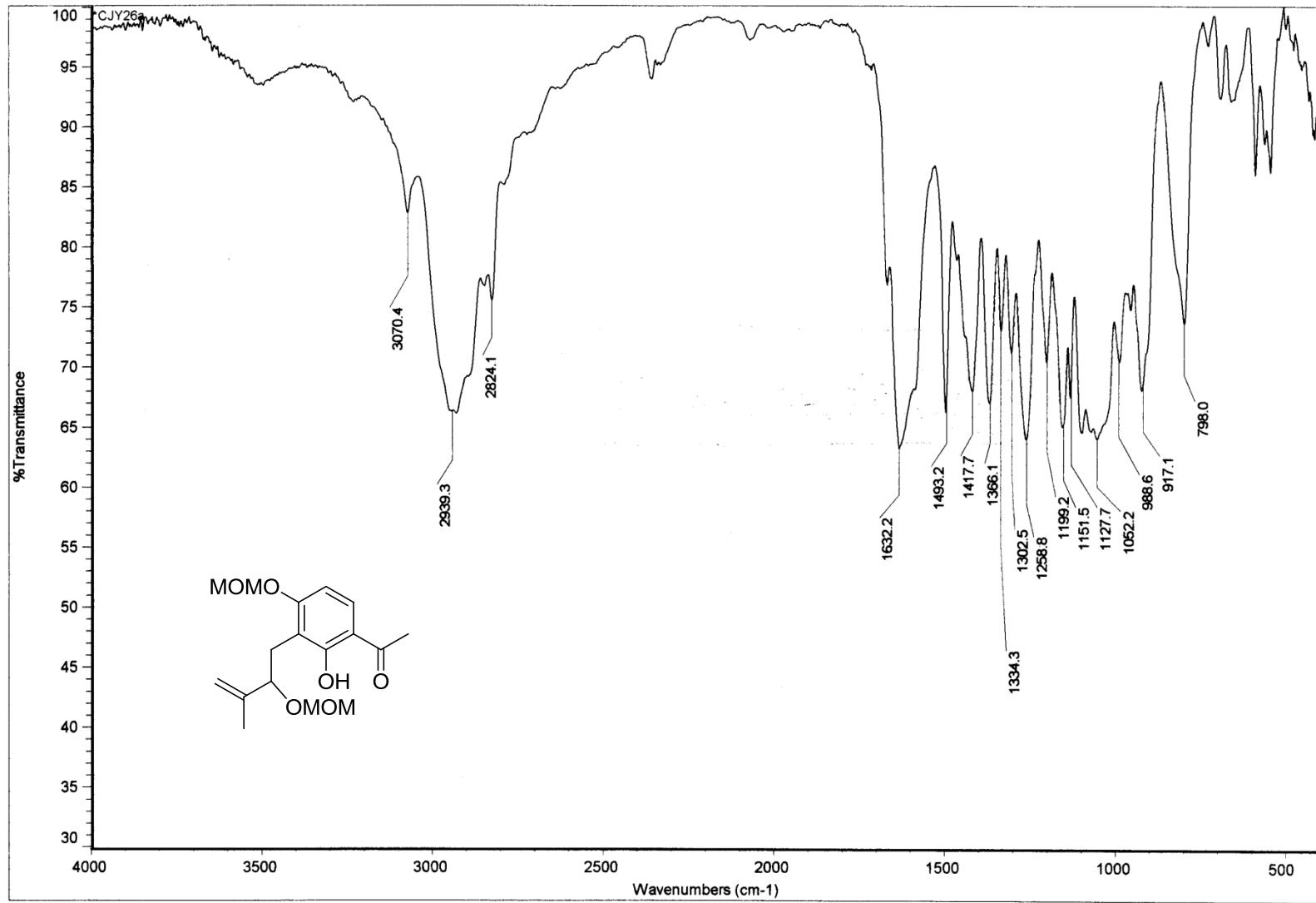


Fig. 43. 1-(2-Hydroxy-4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)ethanone (19) 的FTIR圖譜

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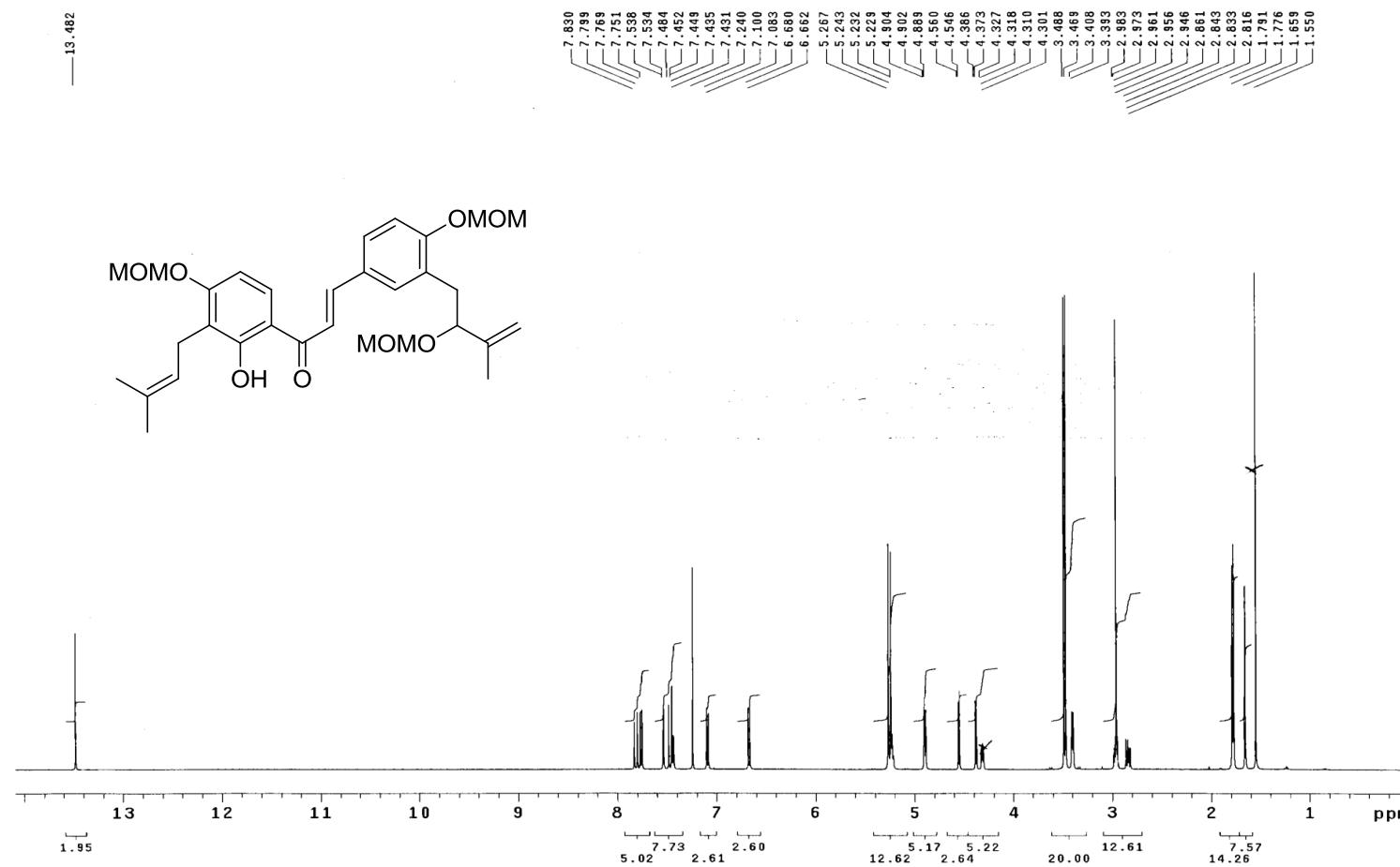


Fig. 44. (E)-1-(2-Hydroxy-4-(methoxymethoxy)-3-(3-methylbut-2-enyl)- phenyl)-3-(4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methyl- but-3-enyl)phenyl)prop-2-en-1-one (**20**) 的¹H-NMR 圖譜

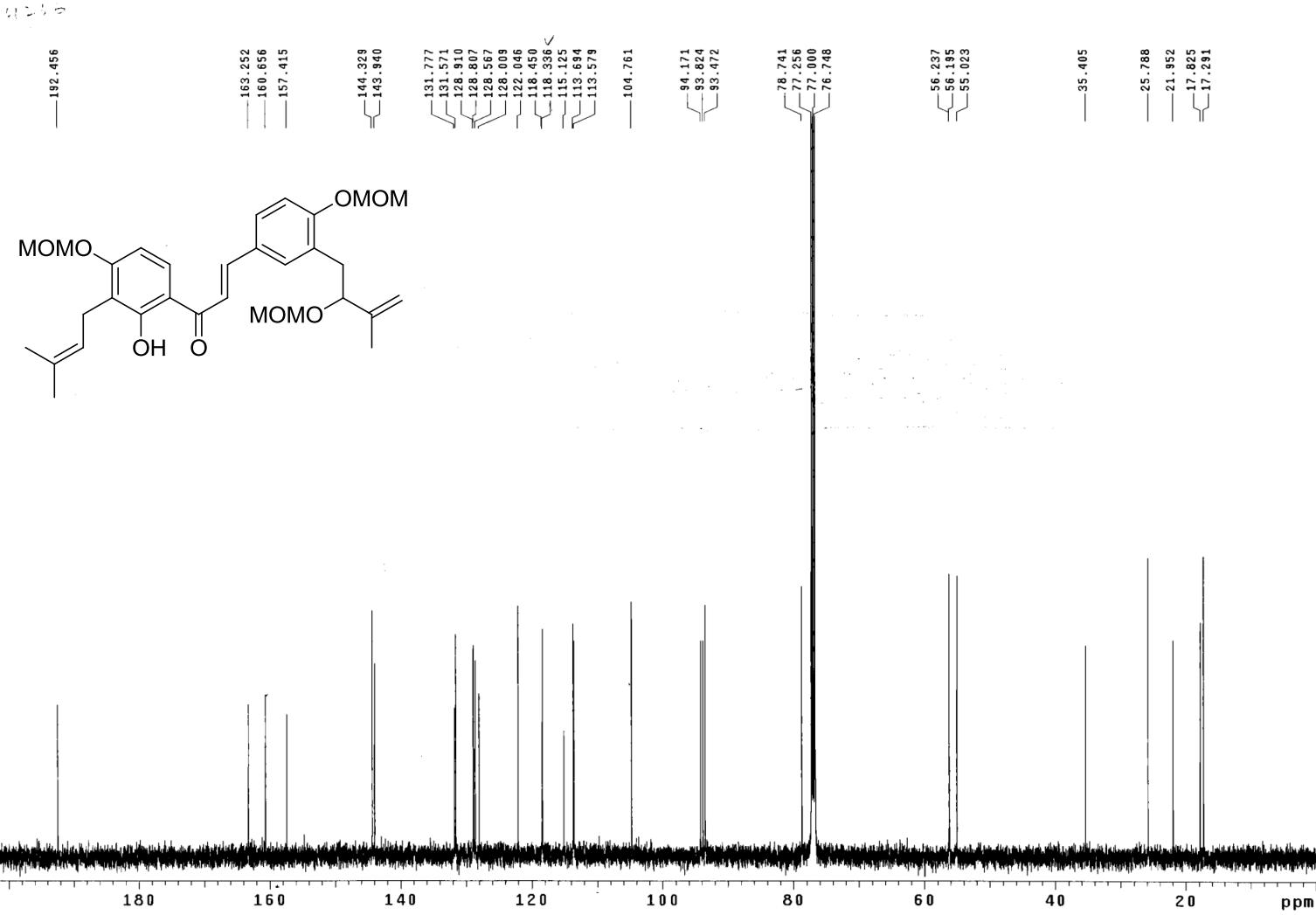


Fig. 45. (E)-1-(2-Hydroxy-4-(methoxymethoxy)-3-(3-methylbut-2-enyl)- phenyl)-3-(4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methyl- but-3-enyl)phenyl)prop-2-en-1-one (**20**) 的 ^{13}C -NMR 圖譜

CSH-236 #212 RT: 4.35 AV: 1 NL: 9.37E5
T: + c Full ms [50.00-650.00]

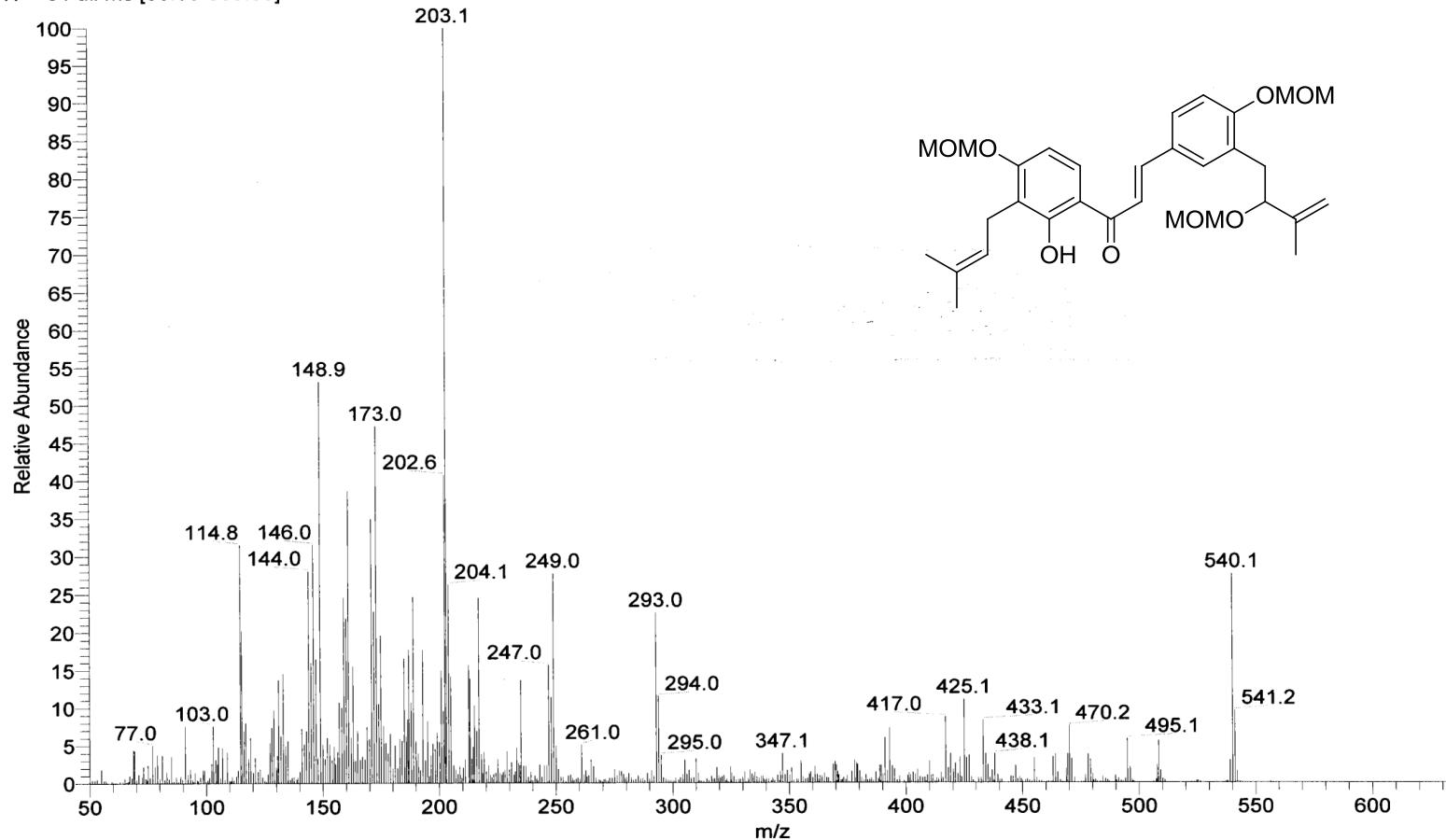


Fig. 46. (E)-1-(2-Hydroxy-4-(methoxymethoxy)-3-(3-methylbut-2-enyl)- phenyl)-3-(4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)prop-2-en-1-one (**20**) 的 EI-MS 圖譜

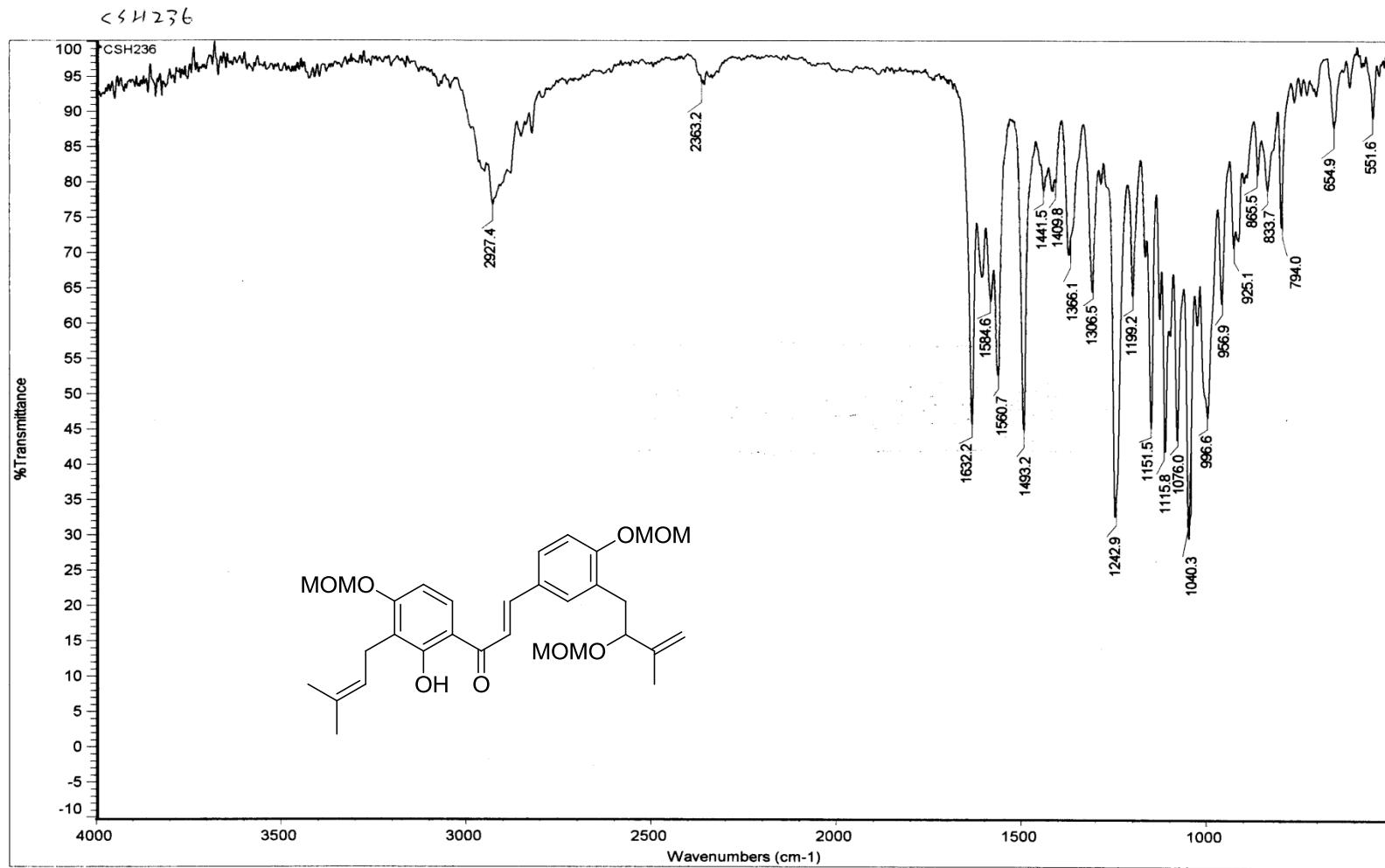


Fig. 47. (E)-1-(2-Hydroxy-4-(methoxymethoxy)-3-(3-methylbut-2-enyl)-phenyl)-3-(4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)prop-2-en-1-one (**20**) 的 FTIR 圖譜

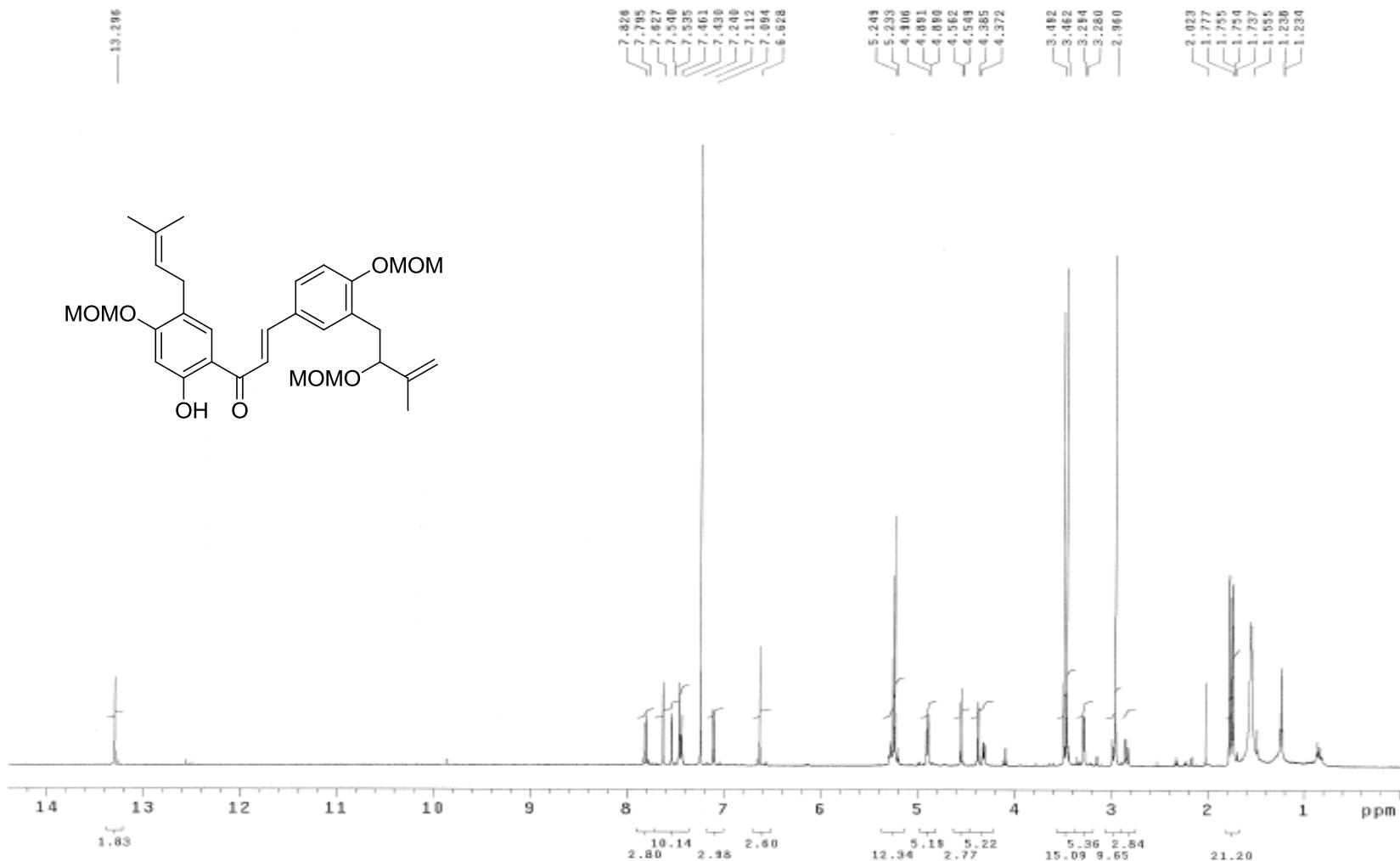


Fig. 48. (E)-1-(2-Hydroxy-4-(methoxymethoxy)-5-(3-methylbut-2-enyl)- phenyl)-3-(4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methyl- but-3-enyl)phenyl)prop-2-en-1-one (**21**) 的¹H-NMR圖譜

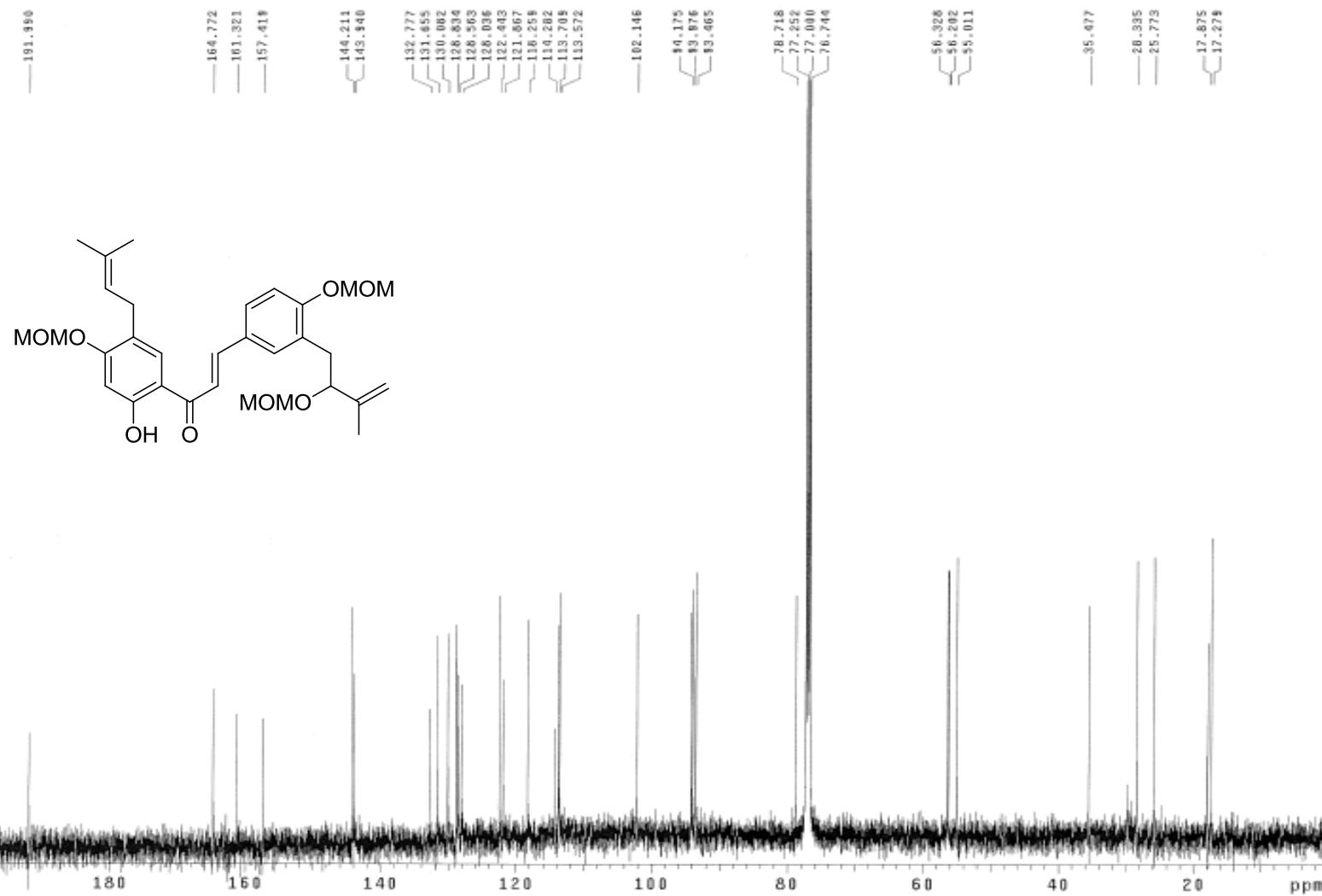


Fig. 49. (E)-1-(2-Hydroxy-4-(methoxymethoxy)-5-(3-methylbut-2-enyl)- phenyl)-3-(4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)prop-2-en-1-one (**21**) 的¹³C-NMR圖譜

C:\Xcalibur\data\MJD\CSH-235

DIP-EI-70ev

CSH-235 #199 RT: 4.08 AV: 1 NL: 4.63E4

T: + c Full ms [50.00-650.00]

12/23/2011 3:07:57 PM

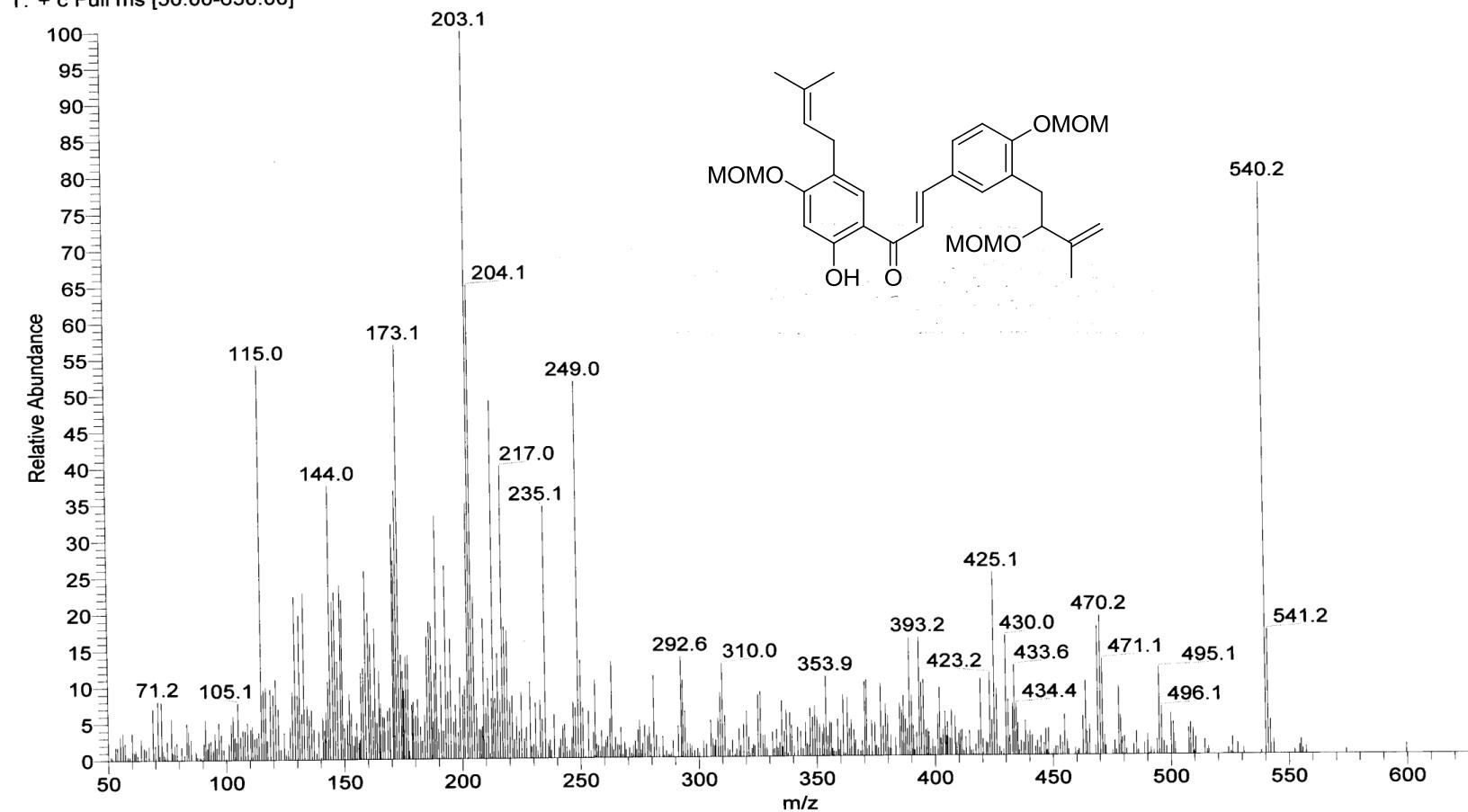


Fig. 50. (E)-1-(2-Hydroxy-4-(methoxymethoxy)-5-(3-methylbut-2-enyl)-phenyl)-3-(4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)prop-2-en-1-one (**21**) 的EI-MS圖譜

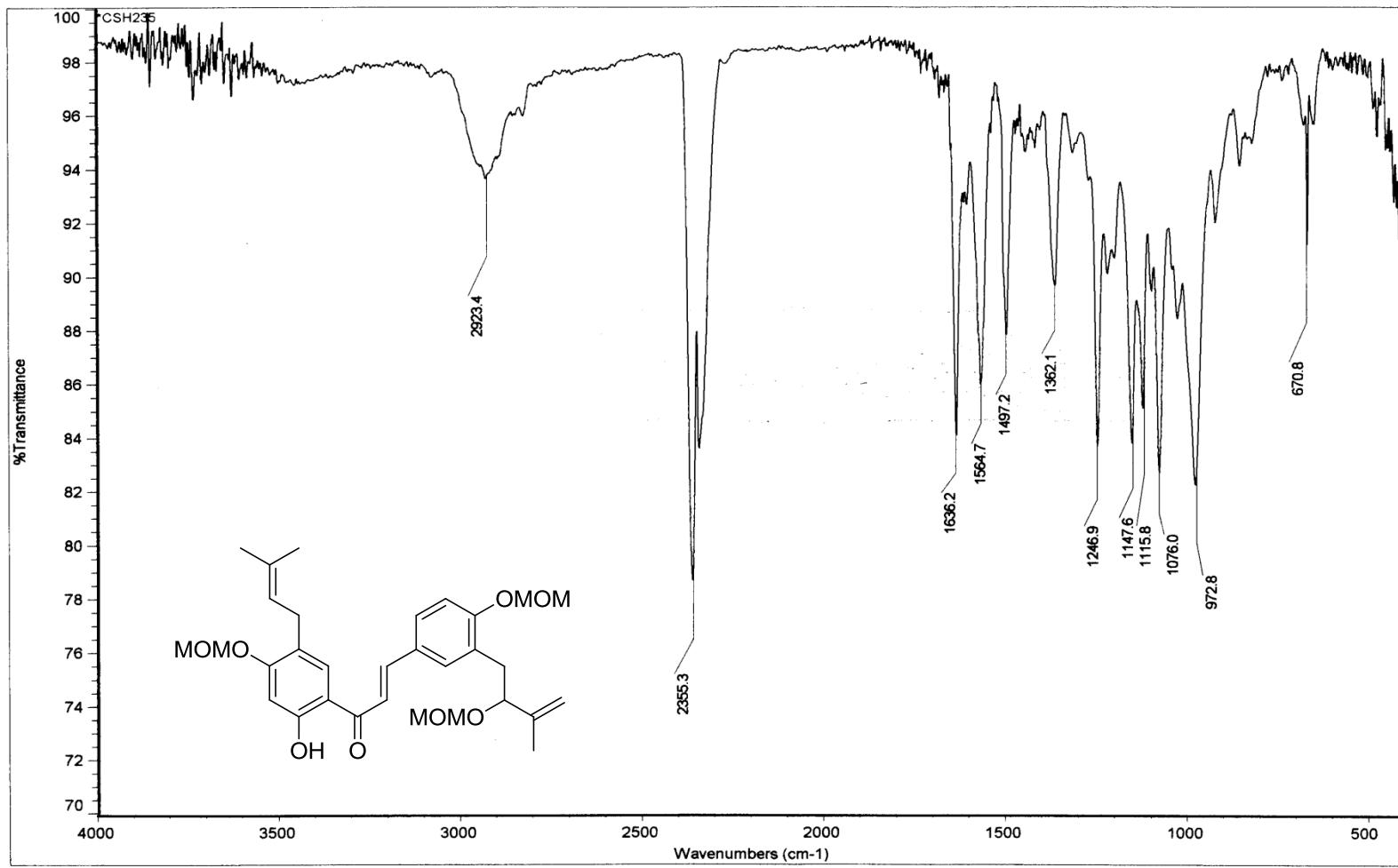


Fig. 51. (E)-1-(2-Hydroxy-4-(methoxymethoxy)-5-(3-methylbut-2-enyl)-phenyl)-3-(4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methyl- but-3-enyl)phenyl)prop-2-en-1-one (**21**) 的FTIR圖譜

546

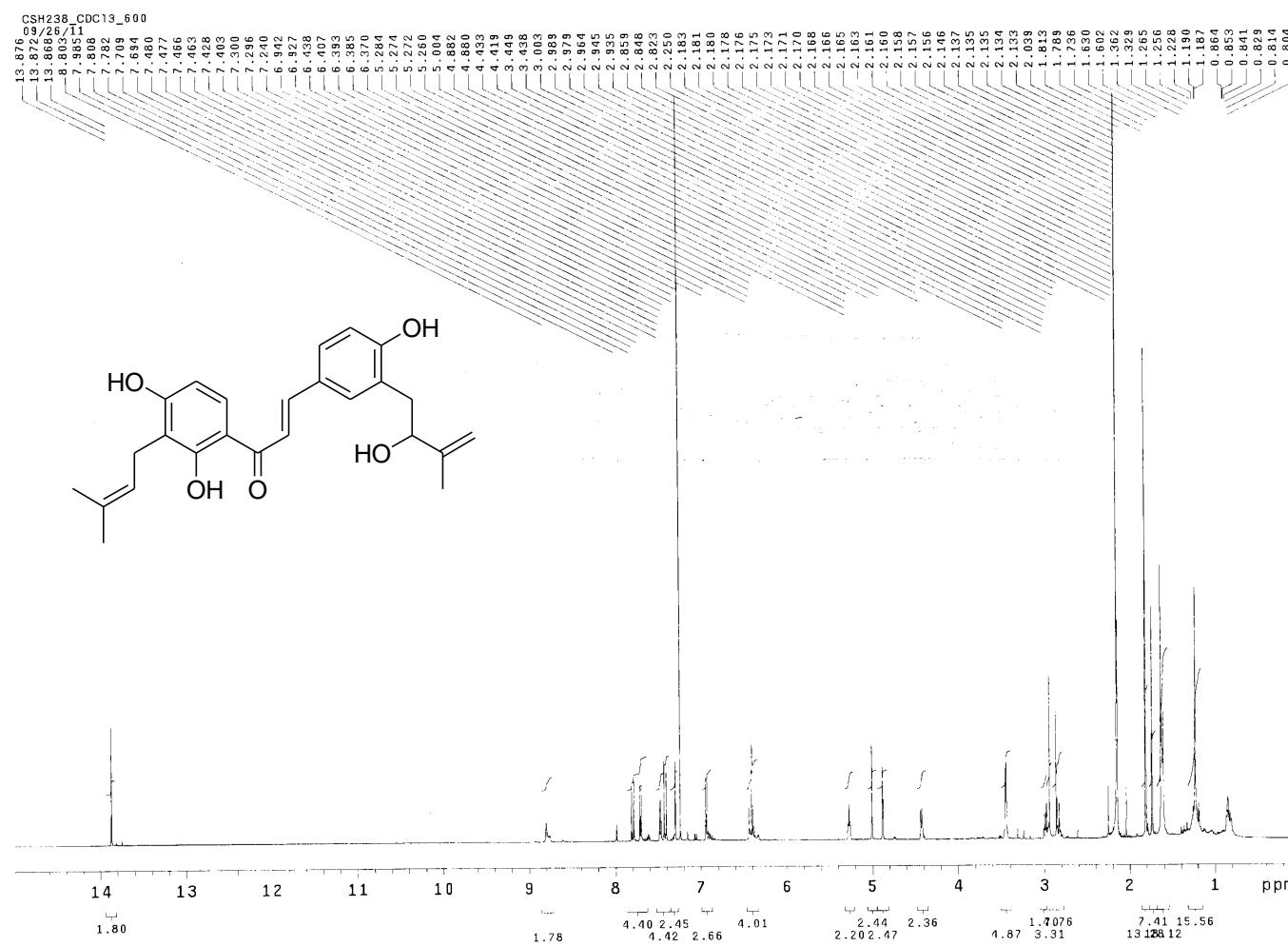


Fig. 52. Paratocarpin D (**1**) 的¹H-NMR圖譜

104

541

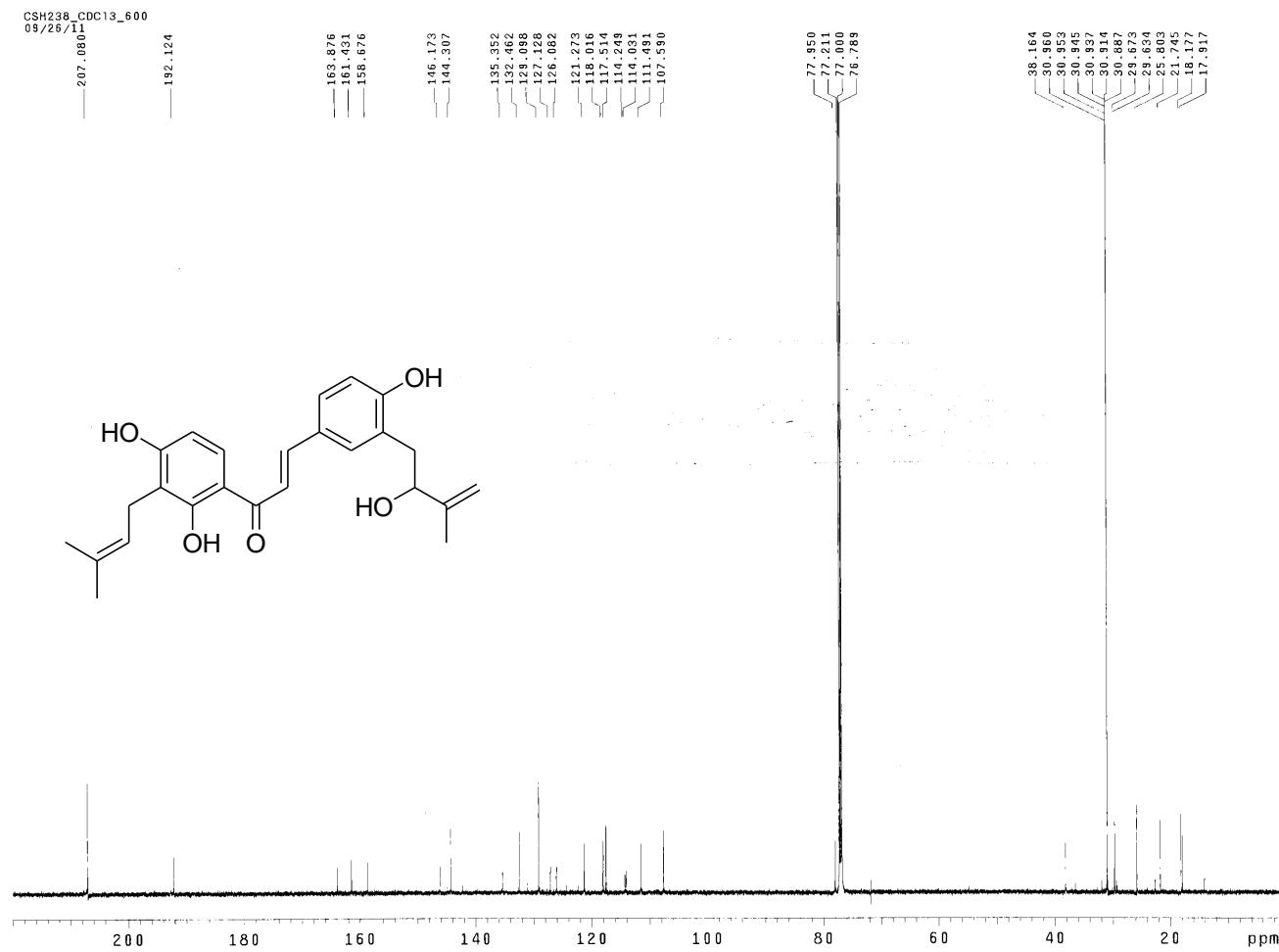


Fig. 53. Paratocarpin D (**1**) 的¹³C-NMR圖譜

CSH238_CDCl₃_600
09/26/11

ErrorLog:
auto_20110920_01 loc:9 (day)
CARBON_01 Acquisition error: 16 16

exp6 gCOSY

SAMPLE	FLAGS
date Sep 26 2011	hs nm
solvent cdc13	sspul y
sample CSH238_01	hsgv1v1 5040
ACQUISITION SPECIAL	
sw 9815.4	temp 25.0
at 0.150	gain 30
np 2884	spin not used
fb 4000	F2 PROCESSING
ss 32	sb -0.075
di 1.000	sbs not used
nt 4	fn 4096
2D ACQUISITION F1 PROCESSING	
sw1 9615.4	sb1 -0.013
ni1 128	sbs1 not used
d2 0	proc1 ip
PRESATURATION fn1 4096	
satmode n	DISPLAY
wet	n sp 11.1
TRANSMITTER wp	8986.3
tn H1	Sp1 11.1
sfrq 599.871	wp1 8986.3
tof 1199.7	rfl 608.6
tpwr 61	rfp 0
pw 12.300	rfl1 608.6
GRADIENTS 4201 PLOT	
g2l1v1 0.001000	wc 150.0
gTE 0.001000	sc 0
EDratio 1.000	wc2 150.0
gstab 0.000500	sc2 0
DECOPULER C13 vs 709	
dn nn	th ai cdc av

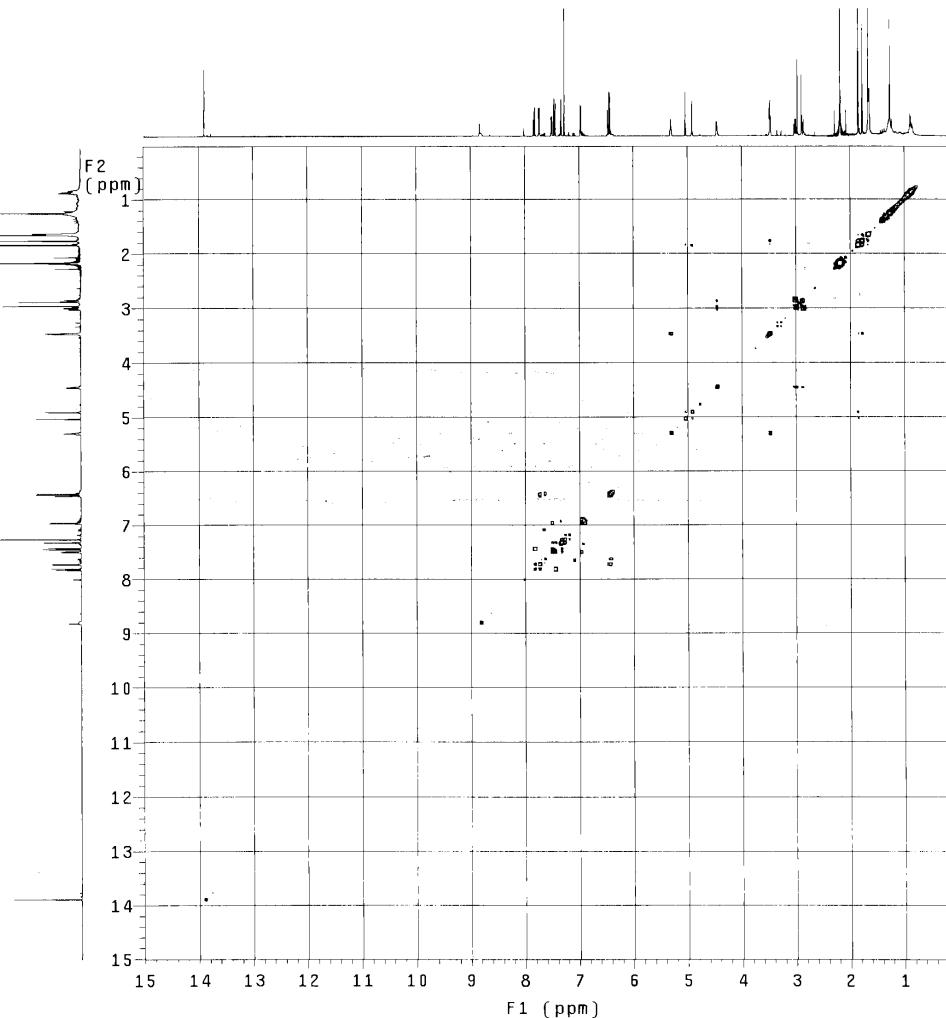
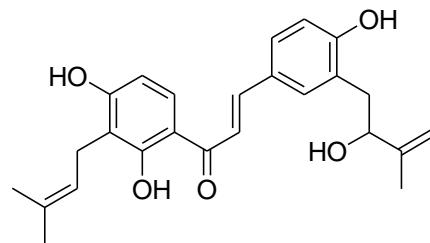


Fig. 54. Paratocarpin D (1)的COSY圖譜

4C1

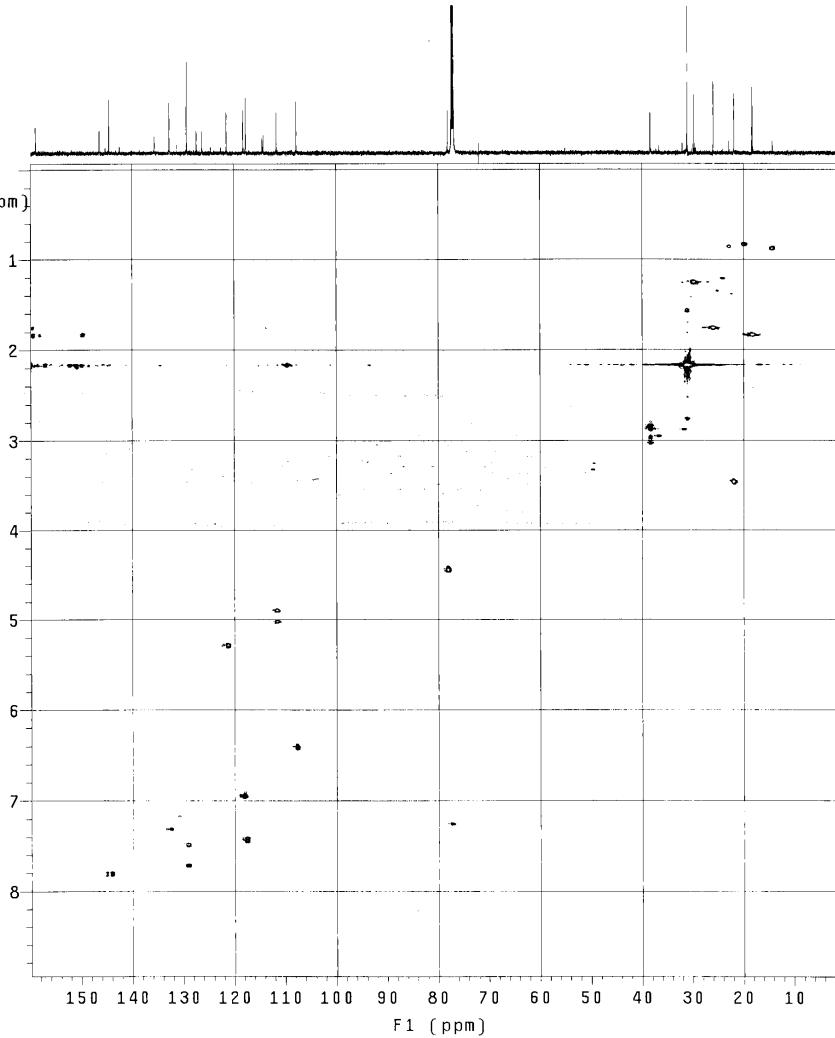
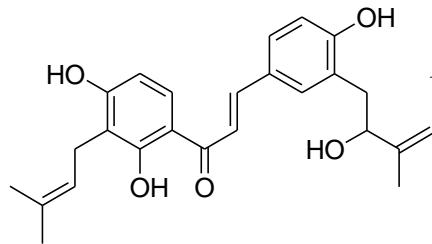
CSH238_CDC13_600
09/26/11ErrorLog:
auto_20110920_01 loc:9 (day)
CARBON_01 Acquisition error: 16 16

exp? gHMQC

```

SAMPLE          FLAGS      ACQUISITION ARRAYS
date   Sep 26 2011 hs       nn      array
solvent    cdc13  sspul     y      arraydim
sample   CSH238_01 PFGrig    y
ACQUISITION          phase
sw      9815.4 SPECIAL    1
at      0.150 temp       25.0
np      2884 gain        30
fb      4000 spin        not used
ss      .32 GRADIENTS
d1      1.000 gzlVIE    4201
nt      8 gxE        0.002000
2D ACQUISITION   EDratio   3.976
sw1     25641.0 gstab     0.000500
n1      128 F2 PROCESSING
phase    arrayed   gf      0.069
PRESATURATION  gfs      not used
satmode   n fn      4096
wet      n Fi PROCESSING
TRANSMITTER   gfi     0.009
tn      H1 gfs1     not used
sfrq    599.871 proc1    1p
tof     1199.7 fn1      2048
tpwr     61 DISPLAY
pw      12.300 sp      -40.5
DECOUPLER    wp      5408.7
dn      C13 spi      19.6
dof     -2981.5 wp1     24063.5
dm      mnv r11      608.1
decwave   W40.COLD rfp
dmf     35088 rfp1     1507.8
dpwr     43 rfp1     0
pwxv1l    59 PLOT
pwx     13.800 wc      150.0
      HMQC sc      0
jixh    146.0 wc2     150.0
nullfig   y sc2      0
mult     2 vs      709
      th      1
      ai cdc ph

```



106

Fig. 55. Paratocarpin D (1)的HMQC圖譜

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CSH238_CDC13_600
09/26/11ErrorLog:
auto_20110920_01 loc:9 (day)
CARBON_01 Acquisition error: 16 16

exp8 gHMBCAD

```

SAMPLE          Sep 26 2011   hs      nn      array
date           Sep 26 2011   hs      nn      array
solvent        cdc13    ssppul   y      arraydim
sample         CSH238_01   PGFflg   y
ACQUISITION    hsgv1v1   5040    i      phase
sw             9615.4   SPECIAL   1      1
at             0.150    temp     25.0   2
np             2884     gain     30
fb             4000     spin    not used
ss             32       GRADIENTS
d1             1.000   gzlvl1  420
nt             8        gtl1    0.001000
2D ACQUISITION gzlvl13 1260
sw1            36199.1  gt3     0.001000
n1             200     gstab    0.000500
phase          arrayed   F2 PROCESSING
PRESATURATION st       -0.075
satmode        n        sbs     not used
wetmode        n        fns    4096
TRANSMITTER    H1      gfp1    0.005
sfrq           599.871  gfs1    not used
tof             1199.7   proc1   1p
tpwr           61       fnl    4096
pw             12.300   DISPLAY
DECOUPLER      sp      -45.2
dn             C13     wp     8881.6
dof            1542.6   sp1    71.4
dm             nnn     wp1    30012.7
decwave        W40_COLD rfp1   608.6
dmf            35088   rfp1   0
dpwr           43      rf11   2261.7
pxwlvl1       59      rf11   0
pxw           13.800   PLOT
HMBC           wc      150.0
j1xh           146.0   sc      0
jnxh           8.0     wc2    150.0
ADIABATICCIC sc      0
pxw180ad      COLD_ad300 vs     709
pxw1v1180     57     th     1
pxw180         400.0   ai     cdc  av

```

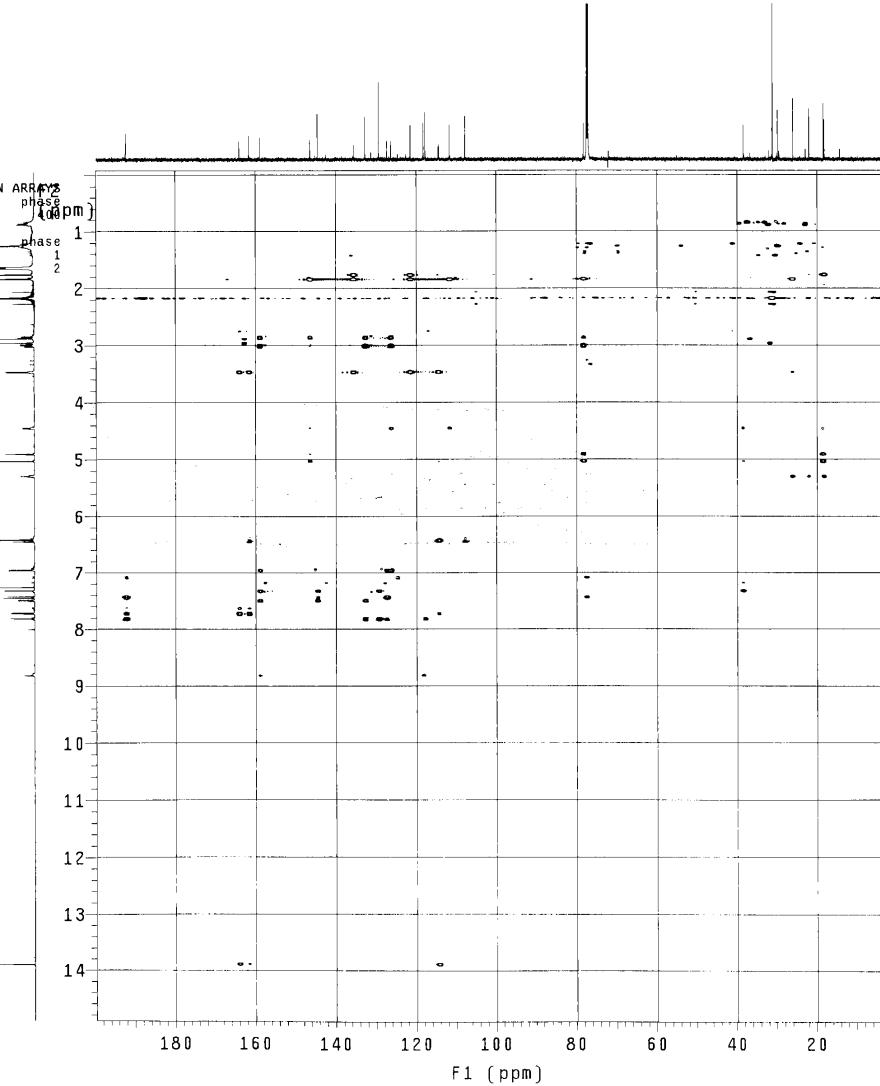
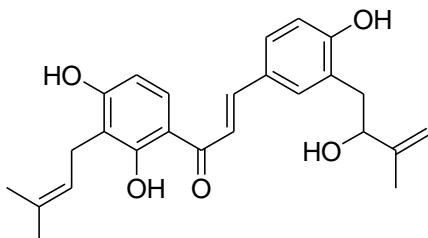


Fig. 56. Paratocarpin D (1)的HMBC圖譜

C:\Xcalibur\data\MJD\CSH-238
DIP-EI-70ev

12/23/2011 11:39:43 AM

CSH-238 #191 RT: 3.92 AV: 1 NL: 8.24E5
T: + c Full ms [50.00-650.00]

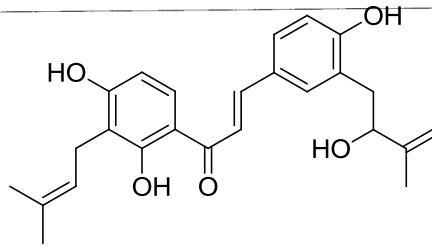
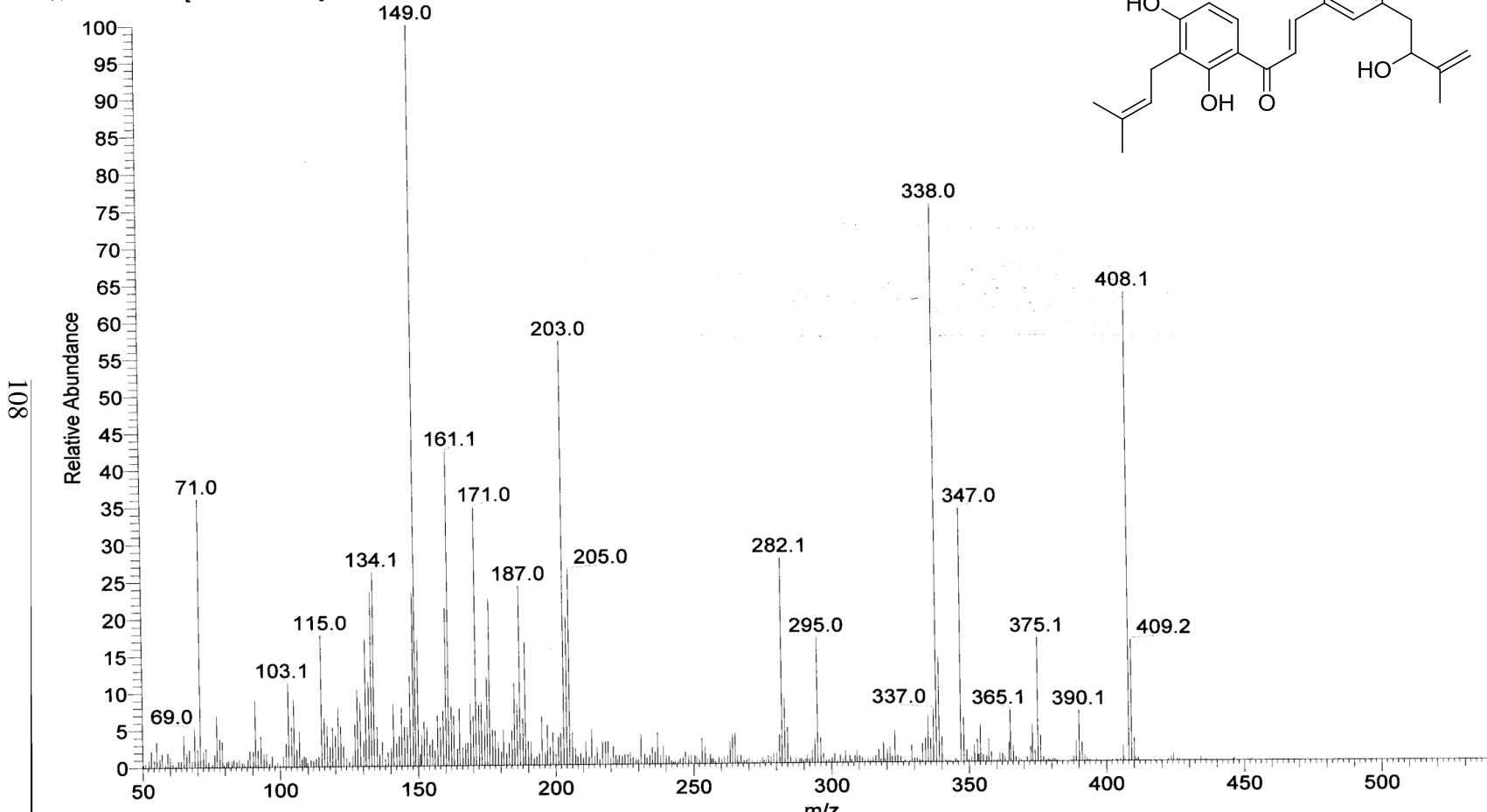


Fig. 57. Paratocarpin D (1)的EI-MS圖譜

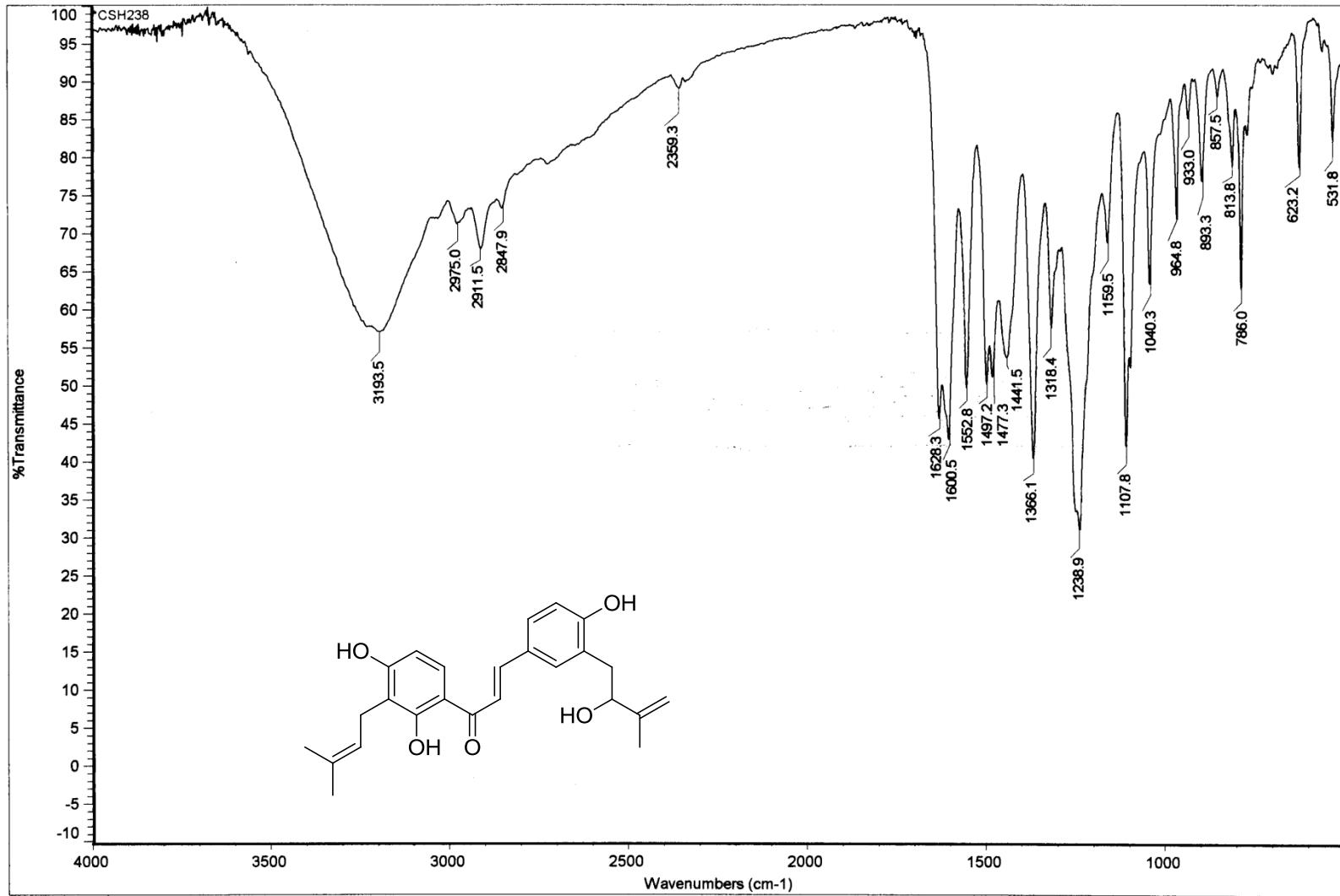


Fig. 58. Paratocarpin D (1)的FTIR圖譜

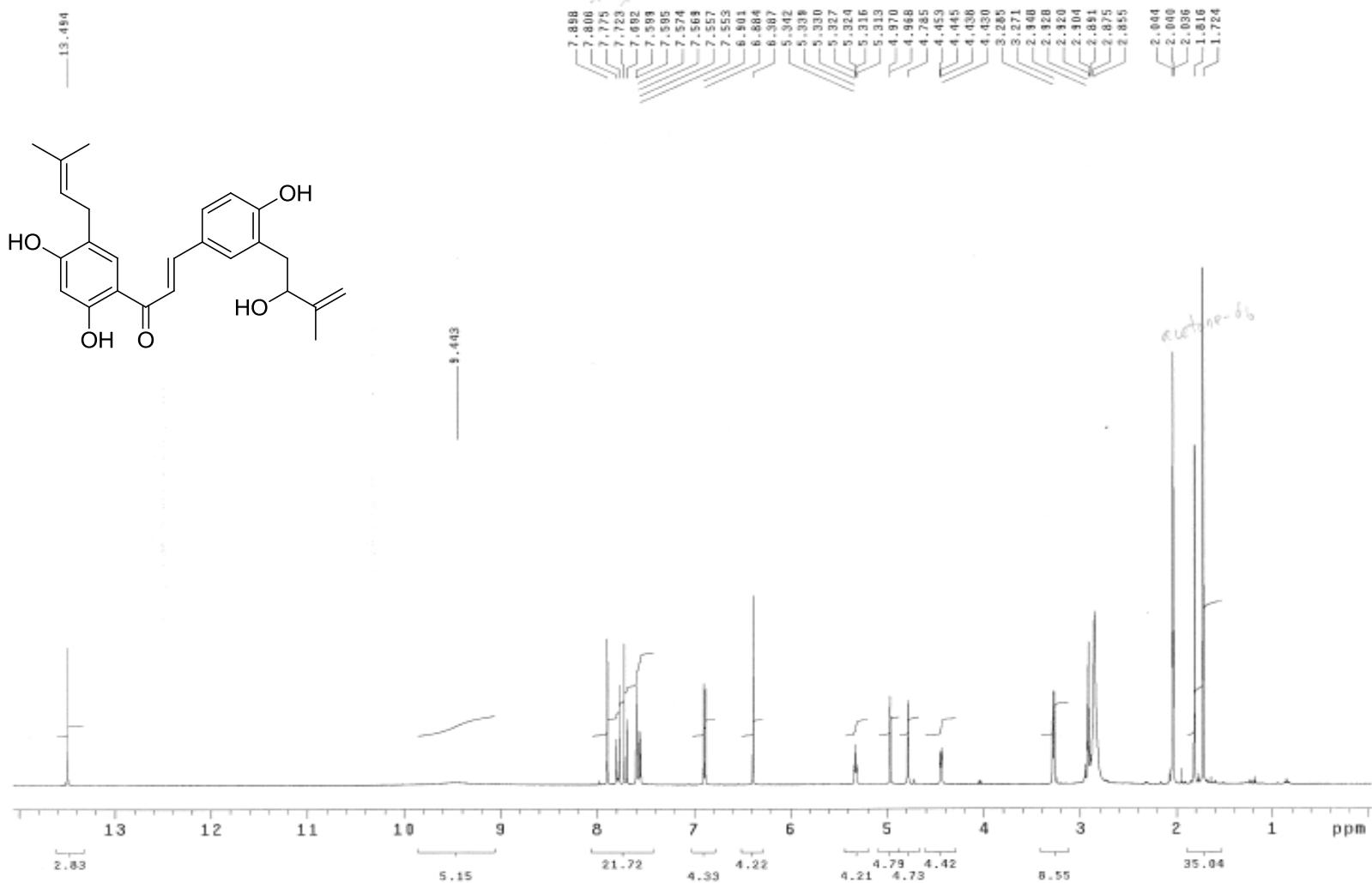


Fig. 59. Bartericin D (**4**) 的¹H-NMR 圖譜

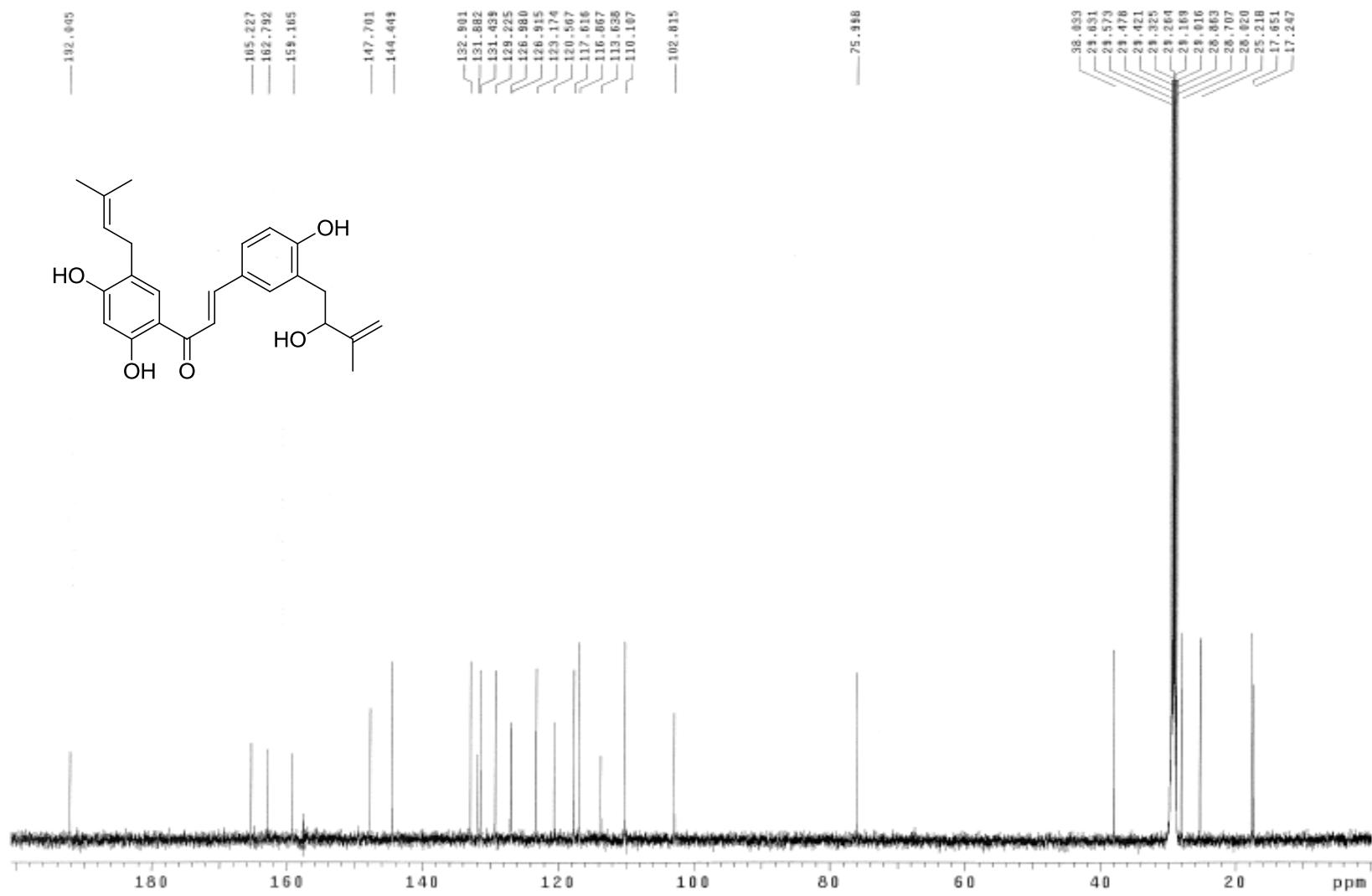


Fig. 60. Bartericin D (4)的 ^{13}C -NMR圖譜

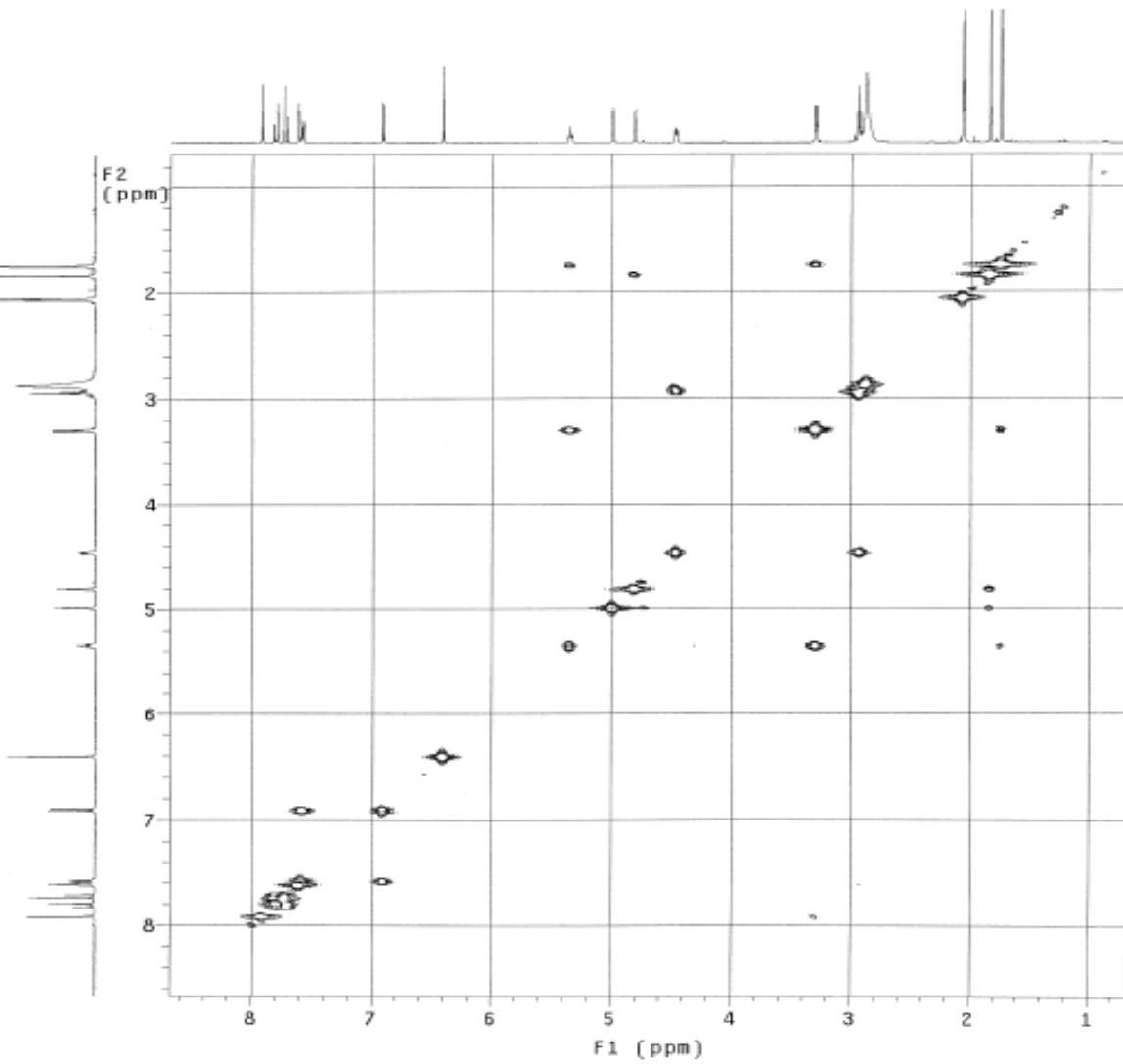
CSH237

exp3 Gcosy

```

SAMPLE          FLAGS
date   Jun 19 2010 hs      nn
solvent acetone sspul    n
sample      hsgv11  4651
ACQUISITION      SPECIAL
sw       8000.0 temp     25.0
dt       0.128 gain     48
np      2048 spin    not used
fb      not used F2 PROCESSING
ss        16 sb      0.064
di      1.301 sbs    not used
nt         4 f1      2048
2D ACQUISITION      F1 PROCESSING
sw1      8000.0 sb1    0.032
n1       128 sb1    not used
PRESATURATION      proc1    1p
satnode    mnm f1i    2048
satdly     0 DISPLAY
satfrq    499.8 sp      302.9
satpwr    -13 wp      3992.2
TRANSMITTER      spl      335.1
tn       H1 wpl    4000.0
sfrq    499.854 rfp    500.8
tof      593.7 rfp    0
tpwr      59 rfp1   500.8
pw       8.600 rfp1   0
tpwr_cf   0.049 PLOT
GRADIENTS      wc      150.0
g2v11    4651 sc      0
gti      0.001000 wc2    150.0
gstab    0.000500 sc2    0
DECOUPLER      vs      872
dm       C13 th      5
dn       mnm ai      cdc av

```

Fig. 61. Bartericin D (**4**)的COSY圖譜

CSH237

expd Ghmqc

```

SAMPLE          FLAGS      ACQUISITION ARRAYS
date   Jun 19 2010 hs        n    array    phase
solvent acetone sspul      y    arraydim  256
sample
ACQUISITION    hsgv11   4651  1    phase
sw     800.0   SPECIAL   1
at     0.128   temp      25.0  2
np     2048    gain      4B
fb     not used spin      not used
ss     32      GRADIENTS
d1     1.000   gztv11   0.0651
nt     16      gztv12   0.061800
2D ACQUISITION  gztv13   2333
sw1    21367.5 gt3       0.081800
m1     128     gztab    0.080500
phase  arrayed F2 PROCESSING
TRANSMITTER   gf       0.059
tn     H1      gfs      not used
sfrq   499.884 fn       4086
tof    399.7   F1 PROCESSING
tpwr   59      gfi      0.006
pw     9.600   gfsi     not used
DECOUPLER    proc1    1p
dn     C13     fn1     2048
dof    -2515.4 DISPLAY
ds     sp       475.2
dm     CCP      wp      3808.6
dmf    32258   spl     1623.0
dpwr   35      wpl     17340.2
pw1v1l 51      rfi     500.8
pxc    14.500   rfp     0
HMOC   140.0   rfp1    1256.6
j1xh   140.0   rfp1l   0
null1g y       PLOT
ai     cdc     ph

```

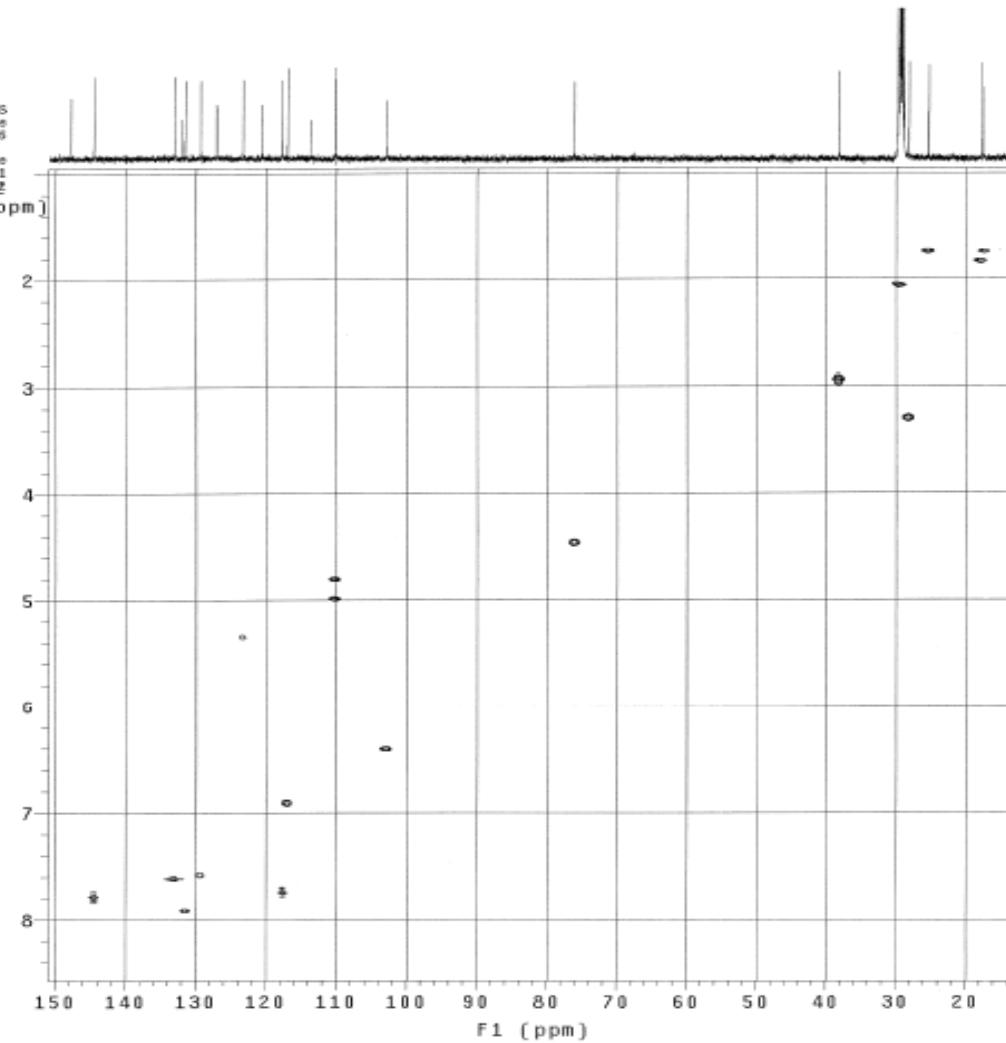
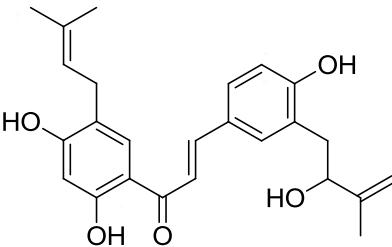


Fig. 62. Bartericin D (4)的HMQC圖譜

CSH297

exp5 Ghmhc

```

SAMPLE          FLAGS
date   Jun 19 2010 hs      n
solvent acetone sspp1    n
sample          PFOF1g   y
ACQUISITION    heavy1  4651
sw     8000.0  SPECIAL
at     0.12s  temp     25.0
res    2048   gain     14
f1b    not used spin     not used
ss     32     GRADIENTS
dl     1.000  g2lv11  4651
nt     16     g2lv13  2333
sw1    30185.9 gts9    0.001000
ni     256    gstab   0.000500
phase   0     F2 PROCESSING
prfsATURATION sb2    0.064
satnme  nnn    sb5    not used
satdly  0      tn     2048
satfrq  499.8  f1 PROCESSING
satpwz  -13    sb1    0.007
TRANSMITTER sb81   not used
tn     H1     proc1  1p
strq   499.884 fml    2048
t0f    393.7   DISPLAY
tpwr   3.600  sp     452.3
pm     59     sp     6640.6
DECOUPLER   cpl    1149.3
din    C13    wpl   23626.0
dof    1255.4 rfp    500.8
dm    nnn    rfp    0
dnf    32258  rfp1   1885.0
dpwpr  35     rfp1   0
pxwlvl  51     PLOT
pxw   14.500 wc    150.0
j1xh   HMBC   sc    0
jnxh   140.0  wc2   150.0
jnxh   8.0    sc2   0
                vs    32702
                th    2
                ai    cdc  av

```

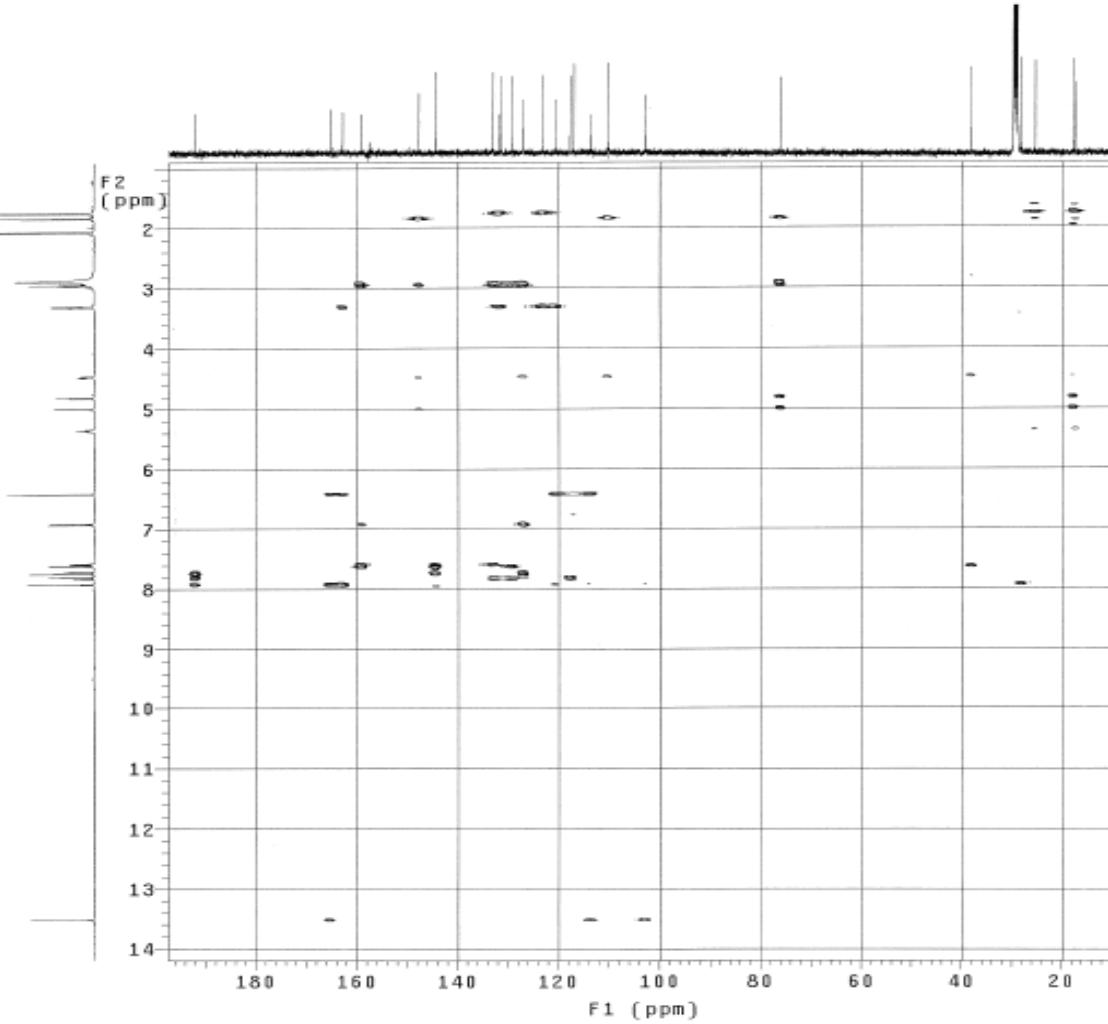
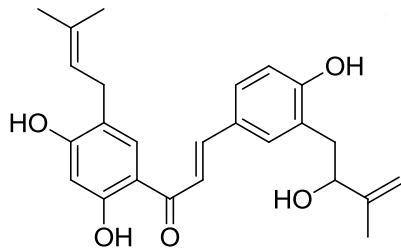


Fig. 63. Bartericin D (4)的HMBC圖譜

C:\Xcalibur\data\MJD\CSH-237

DIP-EI-70ev

CSH-237 #199 RT: 4.08 AV: 1 NL: 1.37E6

T: + c Full ms [50.00-650.00]

12/23/2011 10:53:15 AM

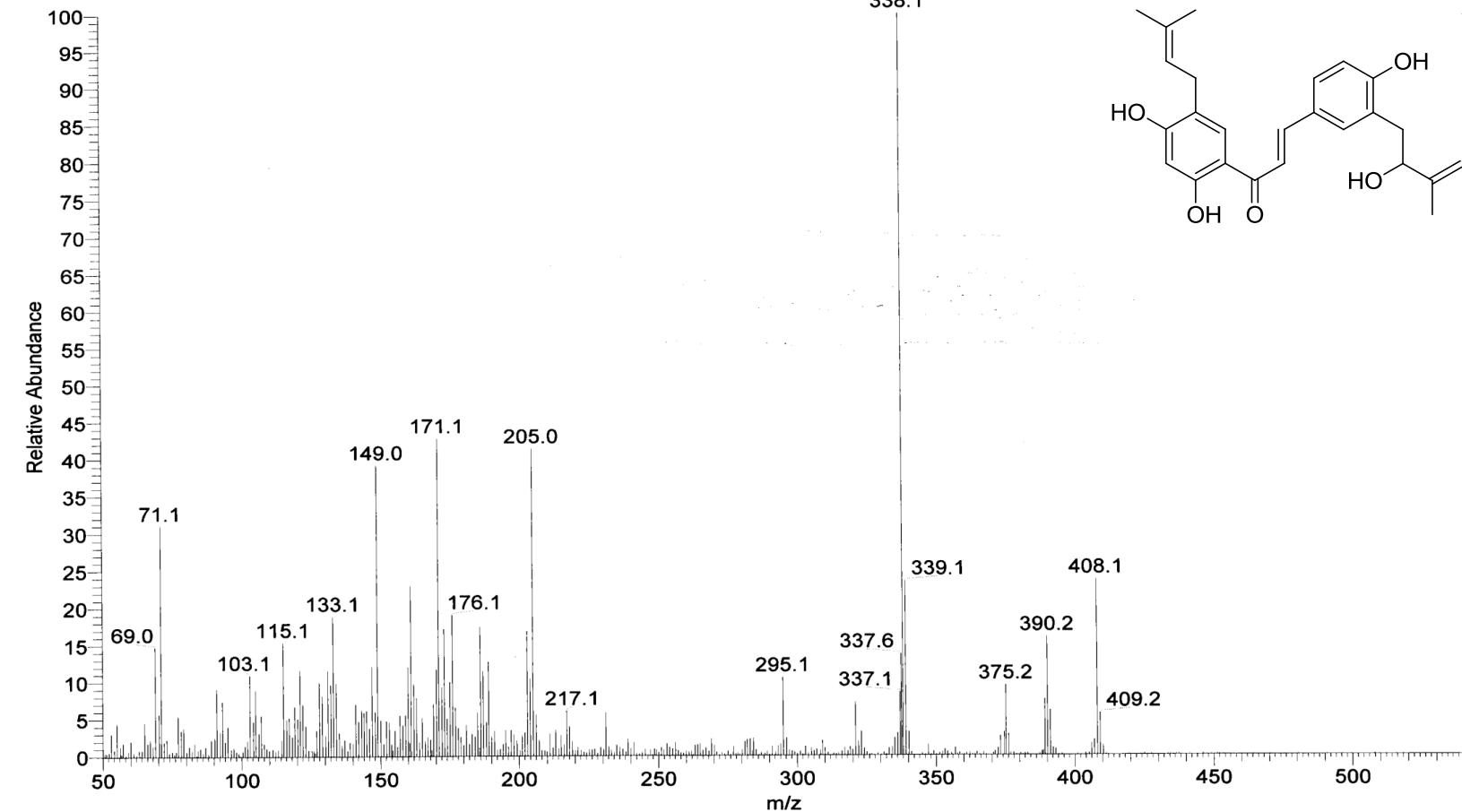


Fig. 64. Bartericin D (4)的EI-MS圖譜

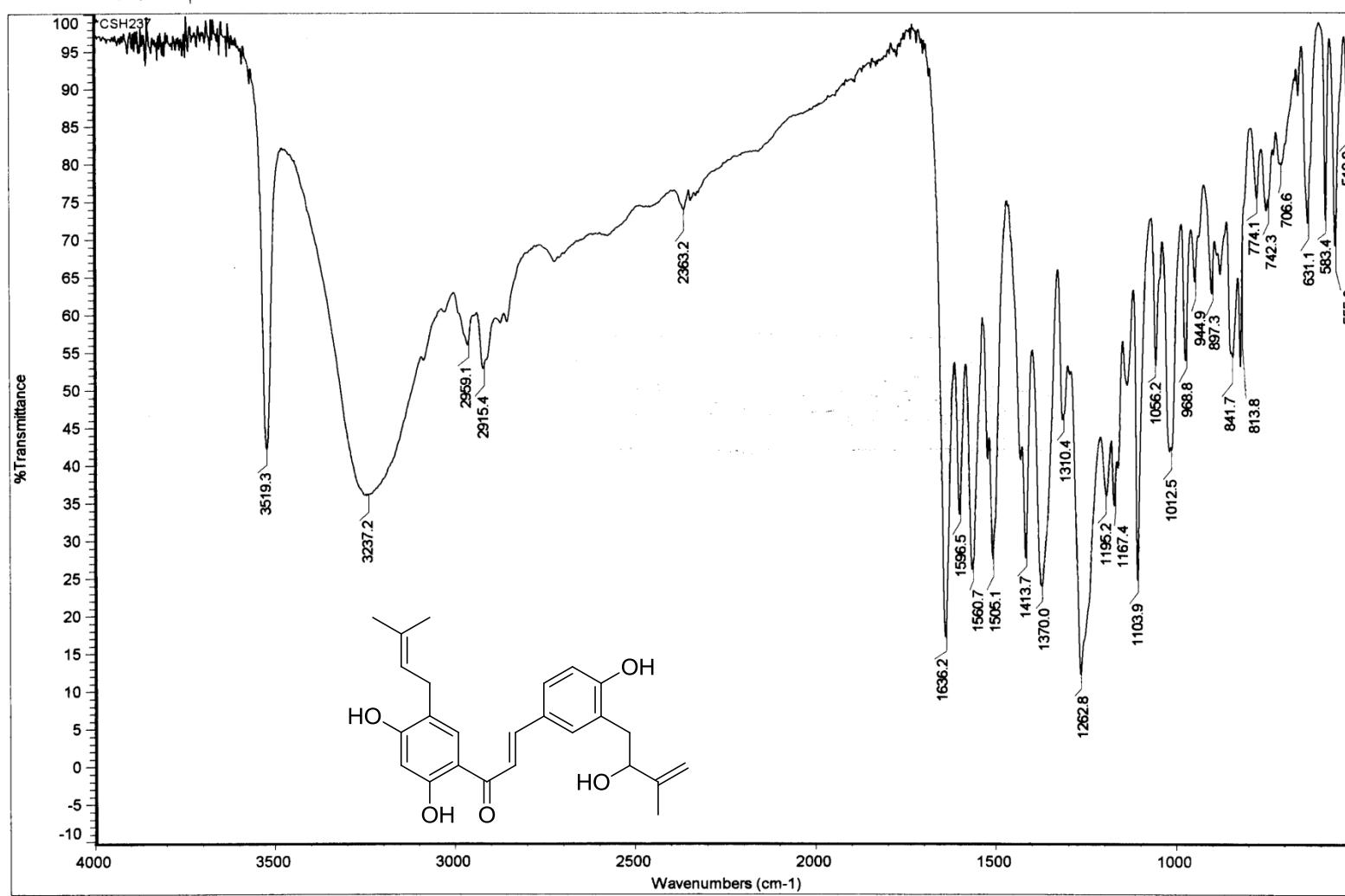


Fig. 65. Bartericin D (4)的FTIR圖譜

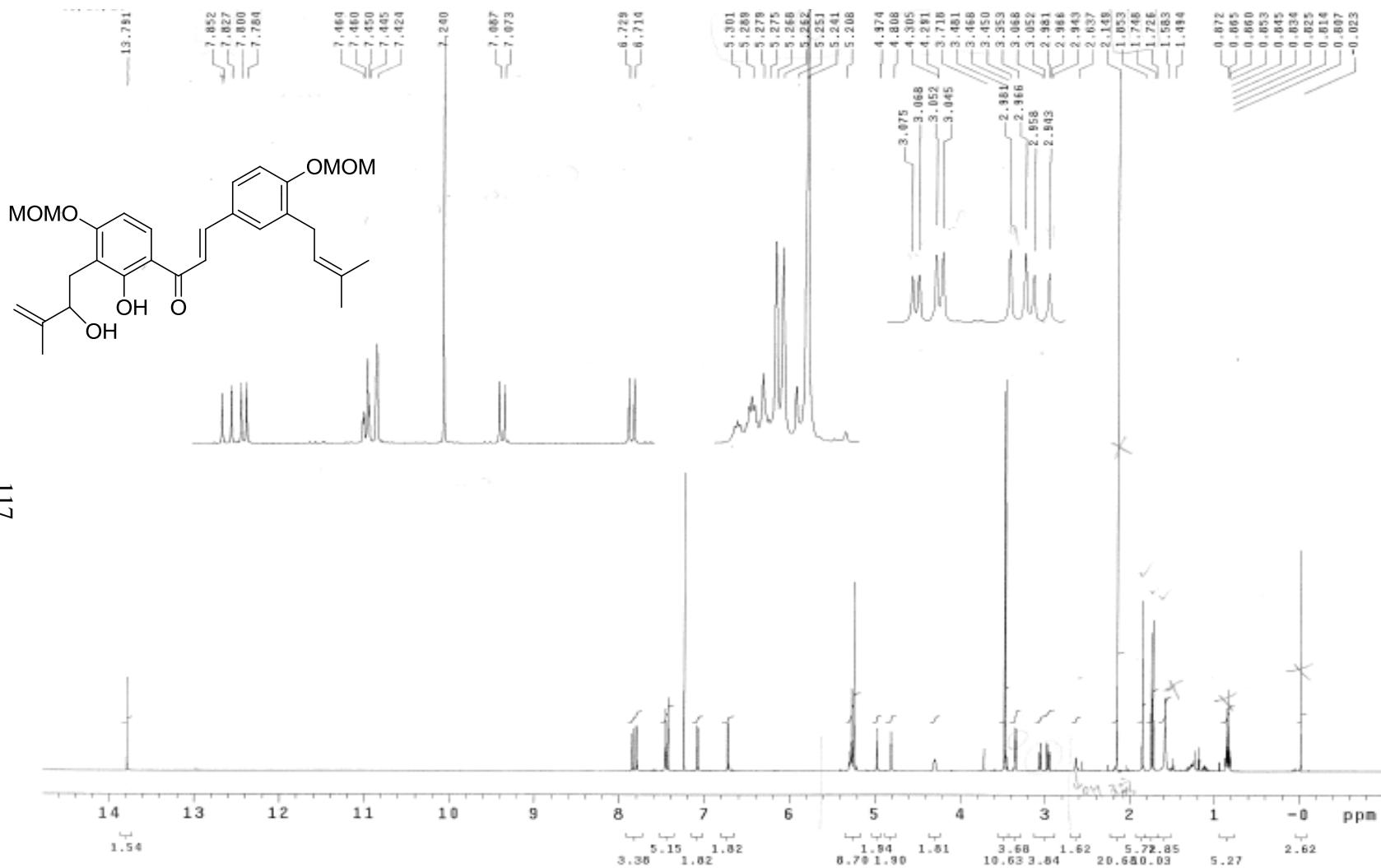


Fig. 66. (E)-1-(2-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)-3-(4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)prop-2-en-1-one (**22**) 的¹H-NMR 圖譜

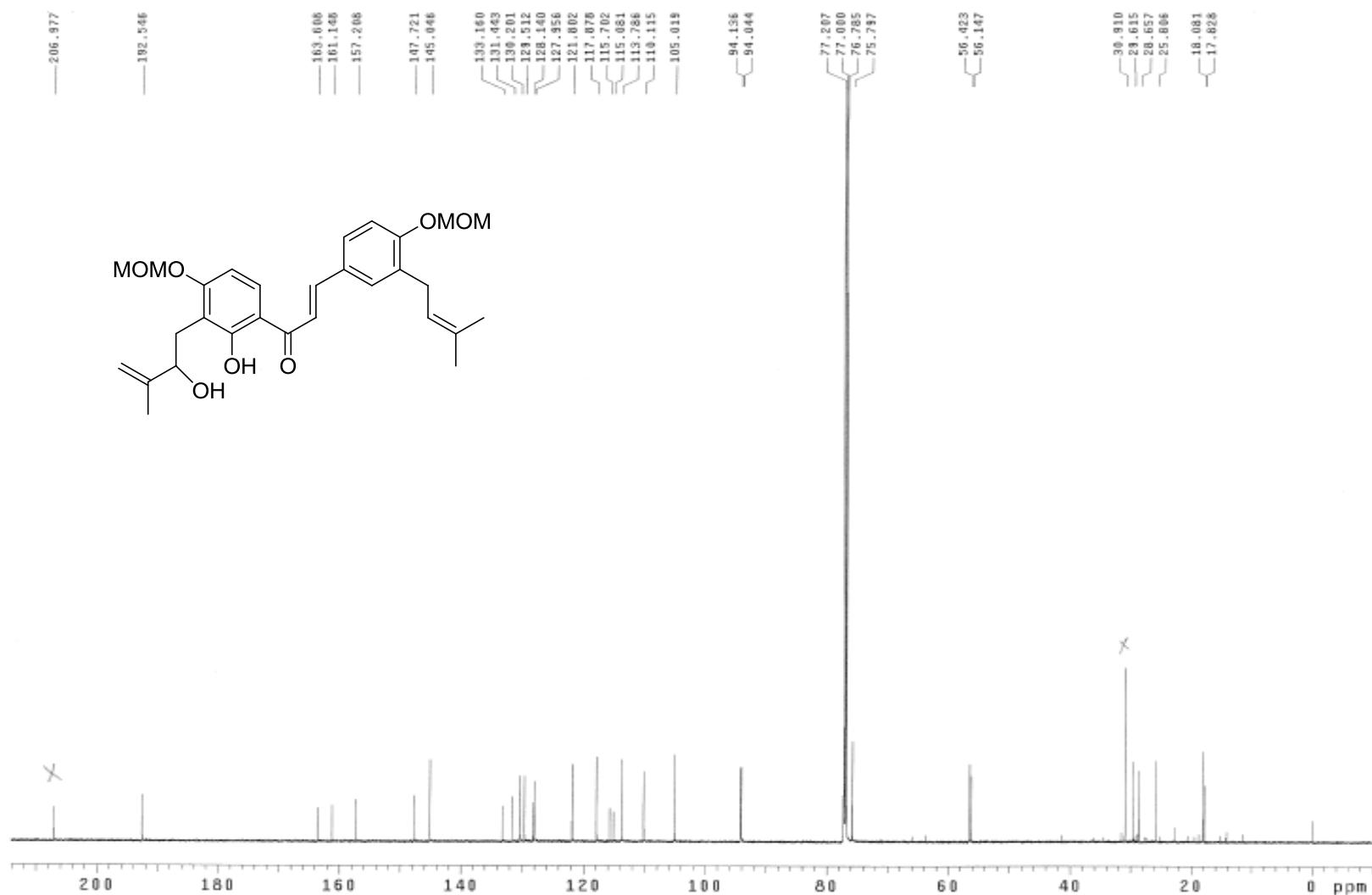


Fig. 67. (E)-1-(2-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)-3-(4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)prop-2-en-1-one (22) 的 ^{13}C -NMR 圖譜

C:\Xcalibur\data\MJD\CSH-220

DIP-EI-70ev

CSH-220 #180 RT: 3.69 AV: 1 NL: 7.03E5

T: + c Full ms [50.00-650.00]

12/23/2011 11:24:02 AM

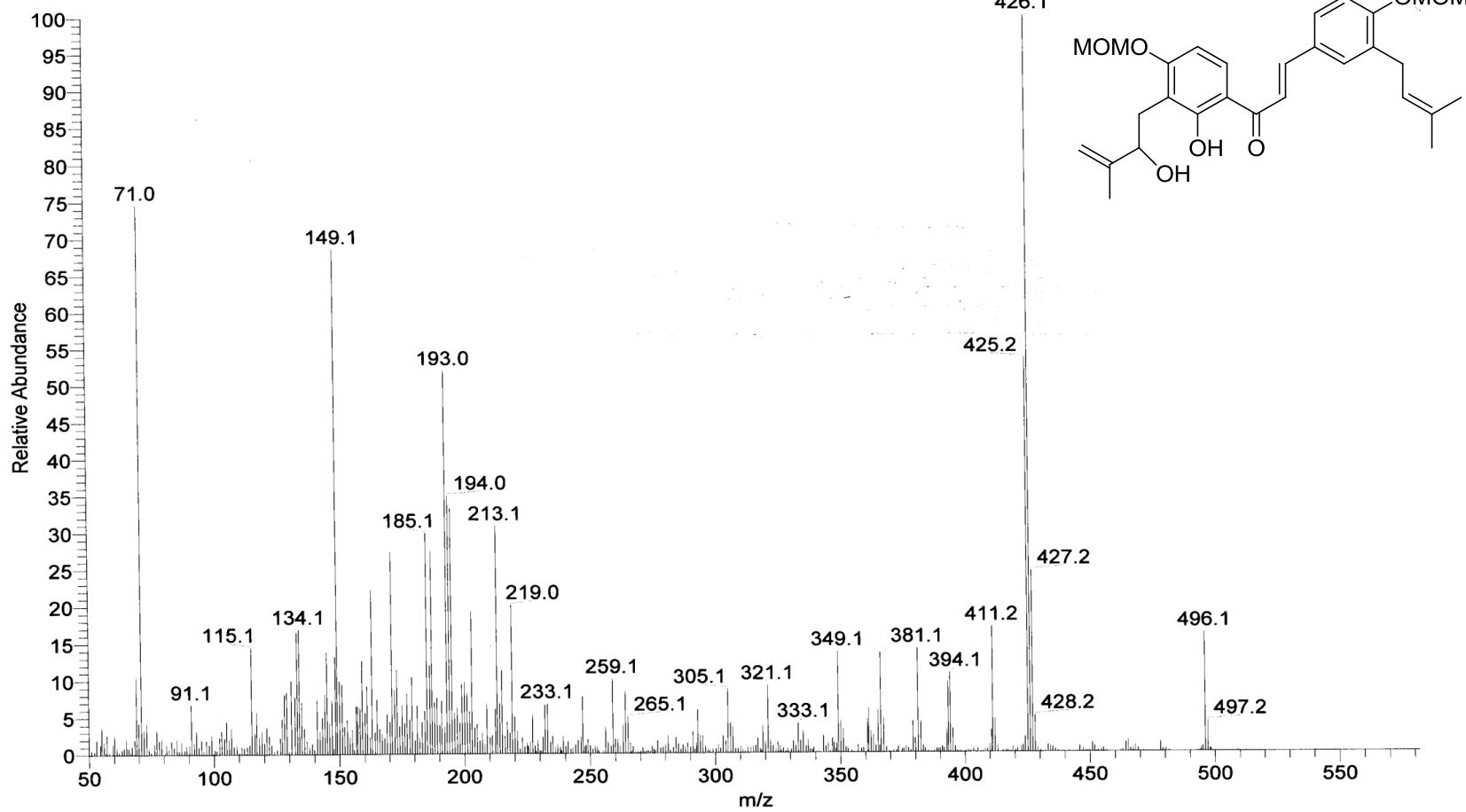


Fig. 68. (E)-1-(2-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)-3-(4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)prop-2-en-1-one (22) 的 EI-MS 圖譜

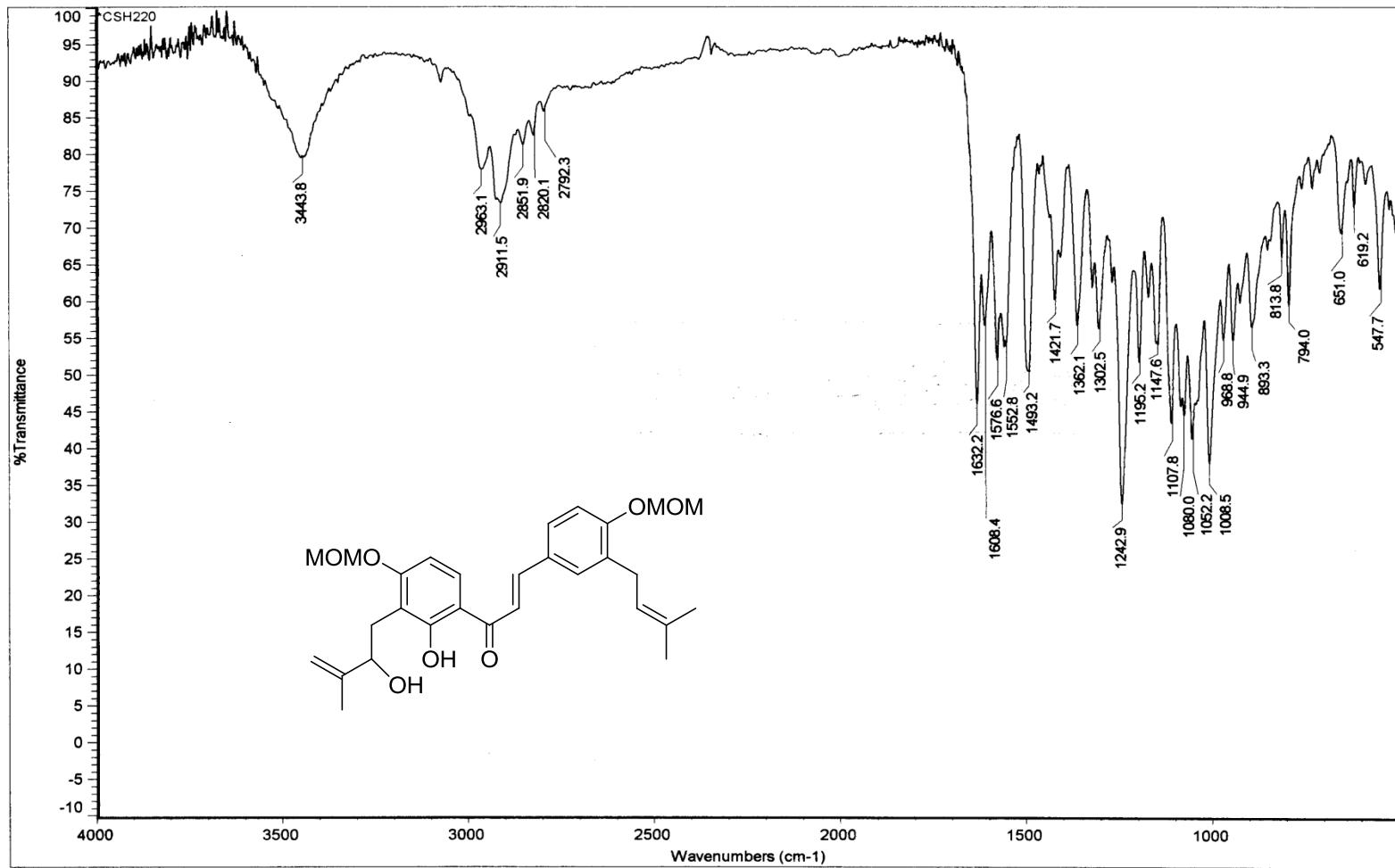


Fig. 69. (E)-1-(2-Hydroxy-3-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)-3-(4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)prop-2-en-1-one (22) 的FTIR圖譜

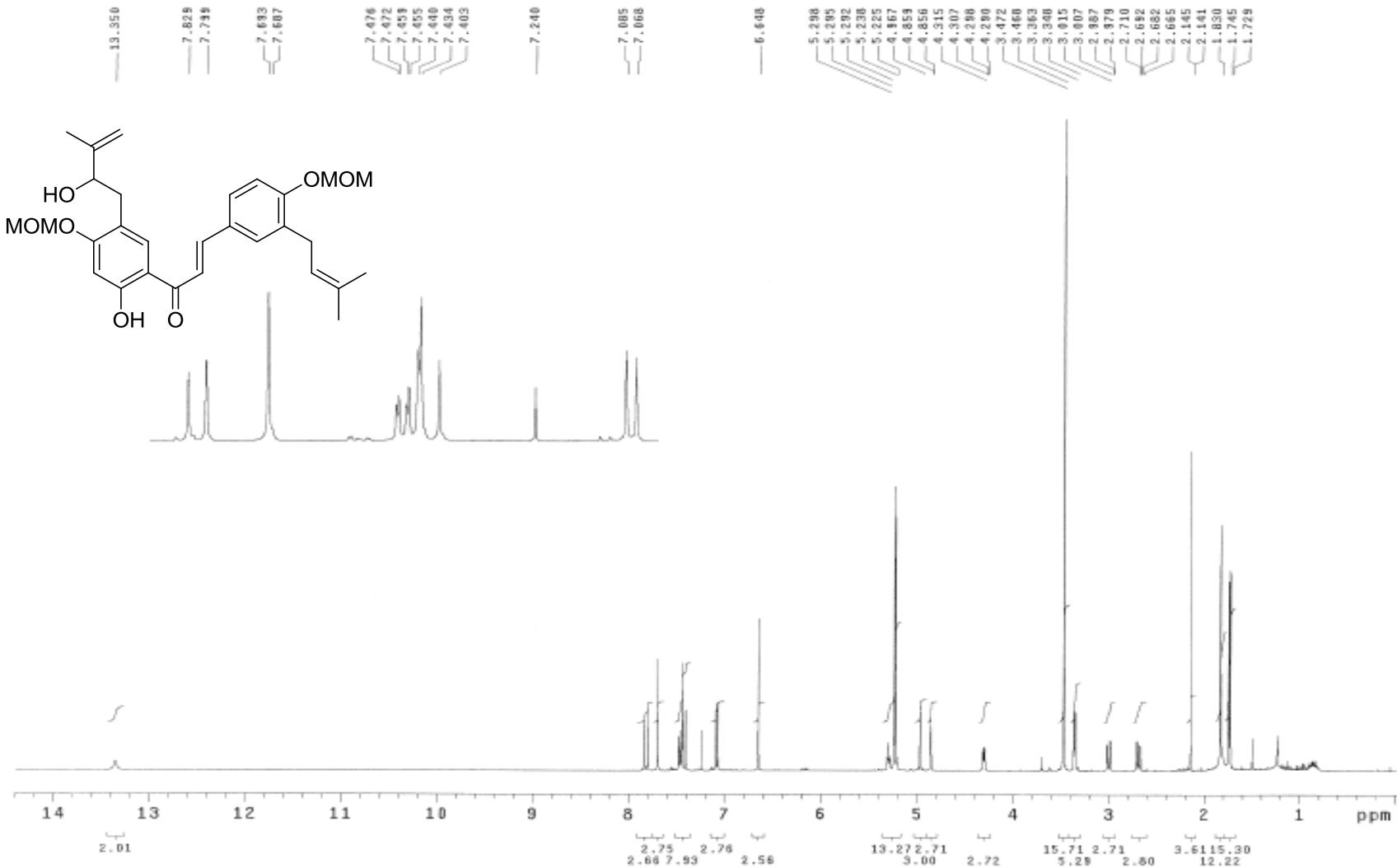


Fig. 70. (E)-1-(2-Hydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)-3-(4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)prop-2-en-1-one (**23**) 的¹H-NMR圖譜

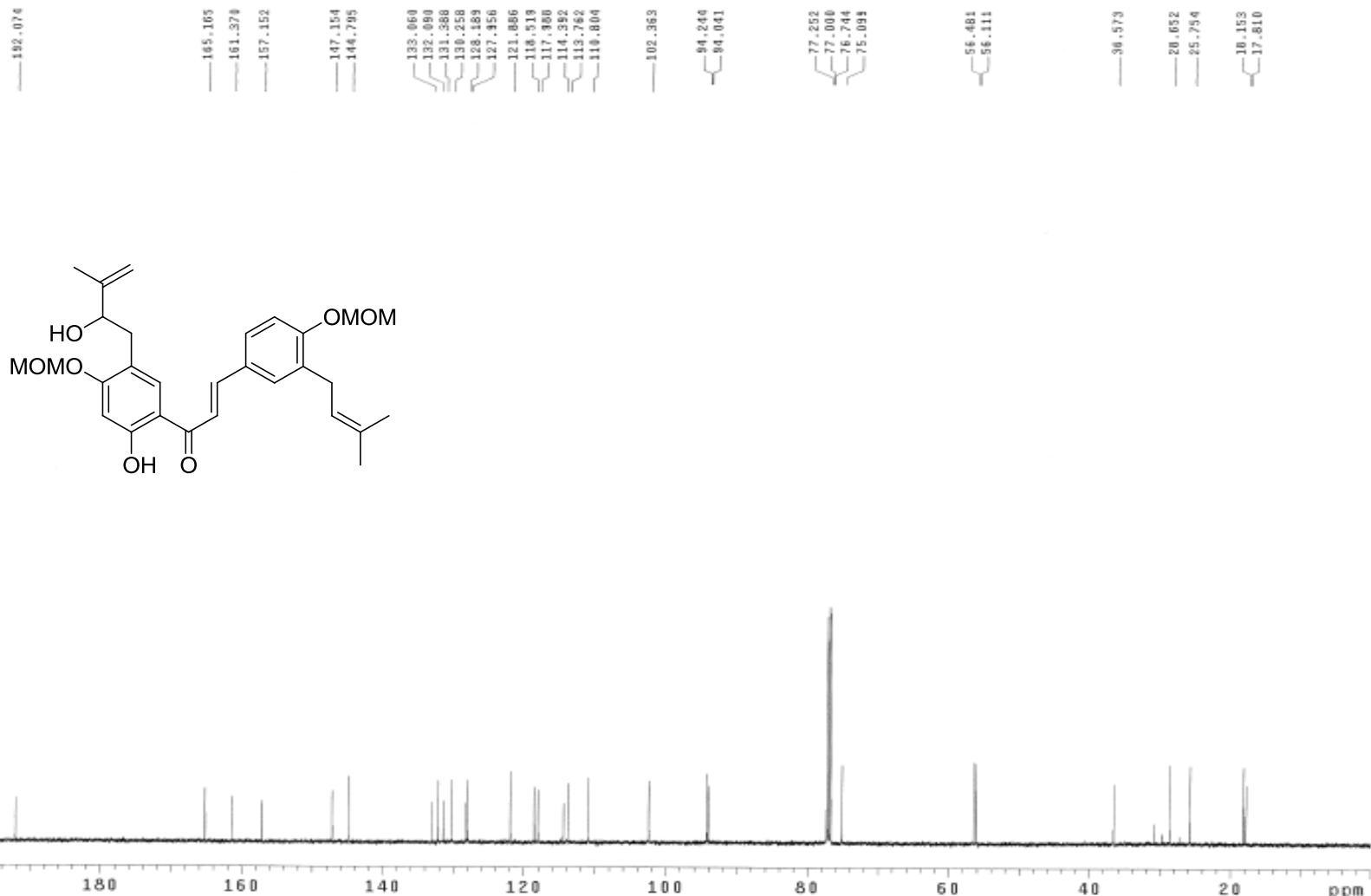


Fig. 71. (E)-1-(2-Hydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)-3-(4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)prop-2-en-1-one (23) 的 ^{13}C -NMR圖譜

C:\Xcalibur\data\MJD\CSH-218
DIP-EI-70ev

12/23/2011 1:55:27 PM

CSH-218 #211 RT: 4.33 AV: 1 NL: 1.36E5
T: + c Full ms [50.00-650.00]

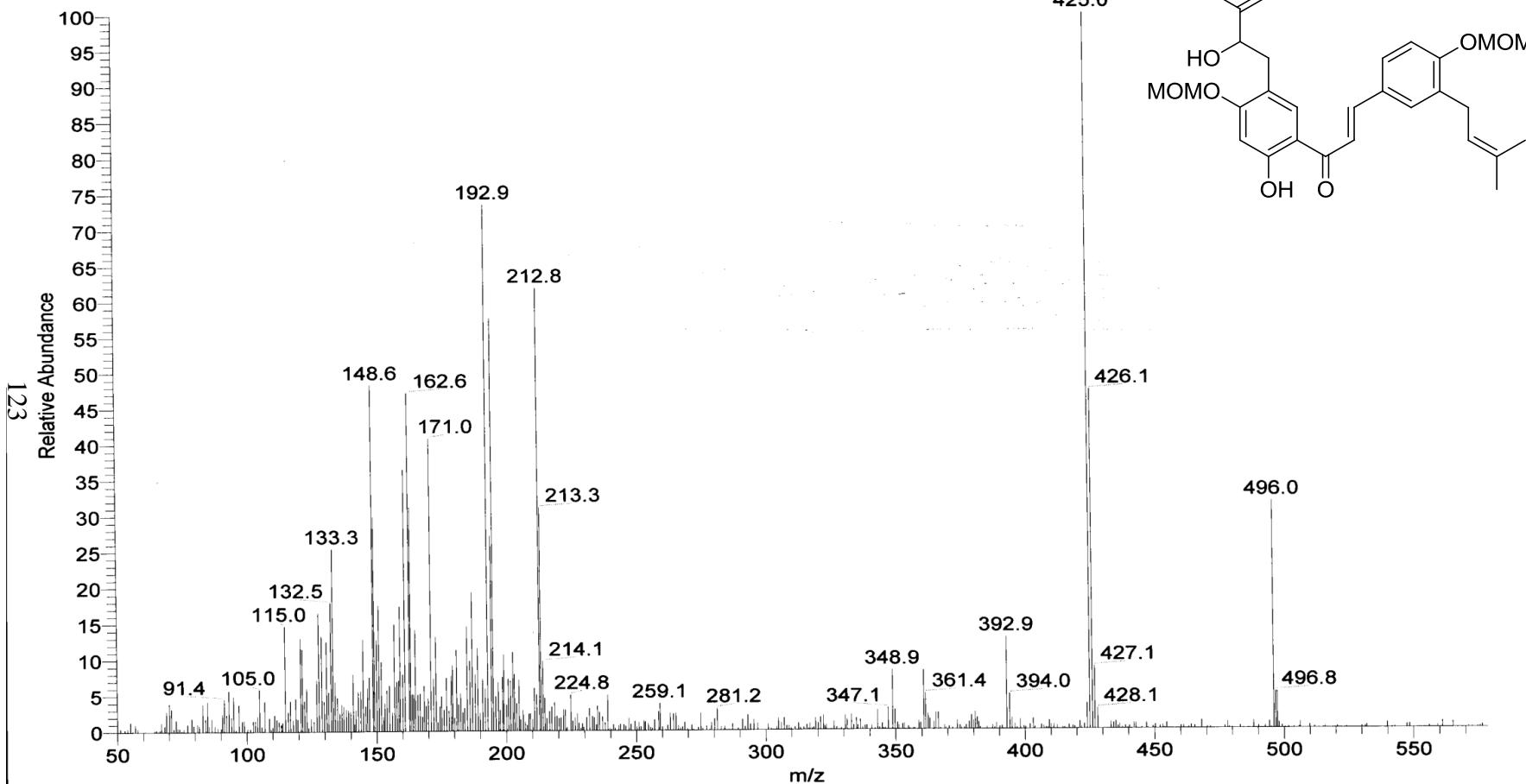


Fig. 72. (E)-1-(2-Hydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)-3-(4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)prop-2-en-1-one (23) 的 EI-MS 圖譜

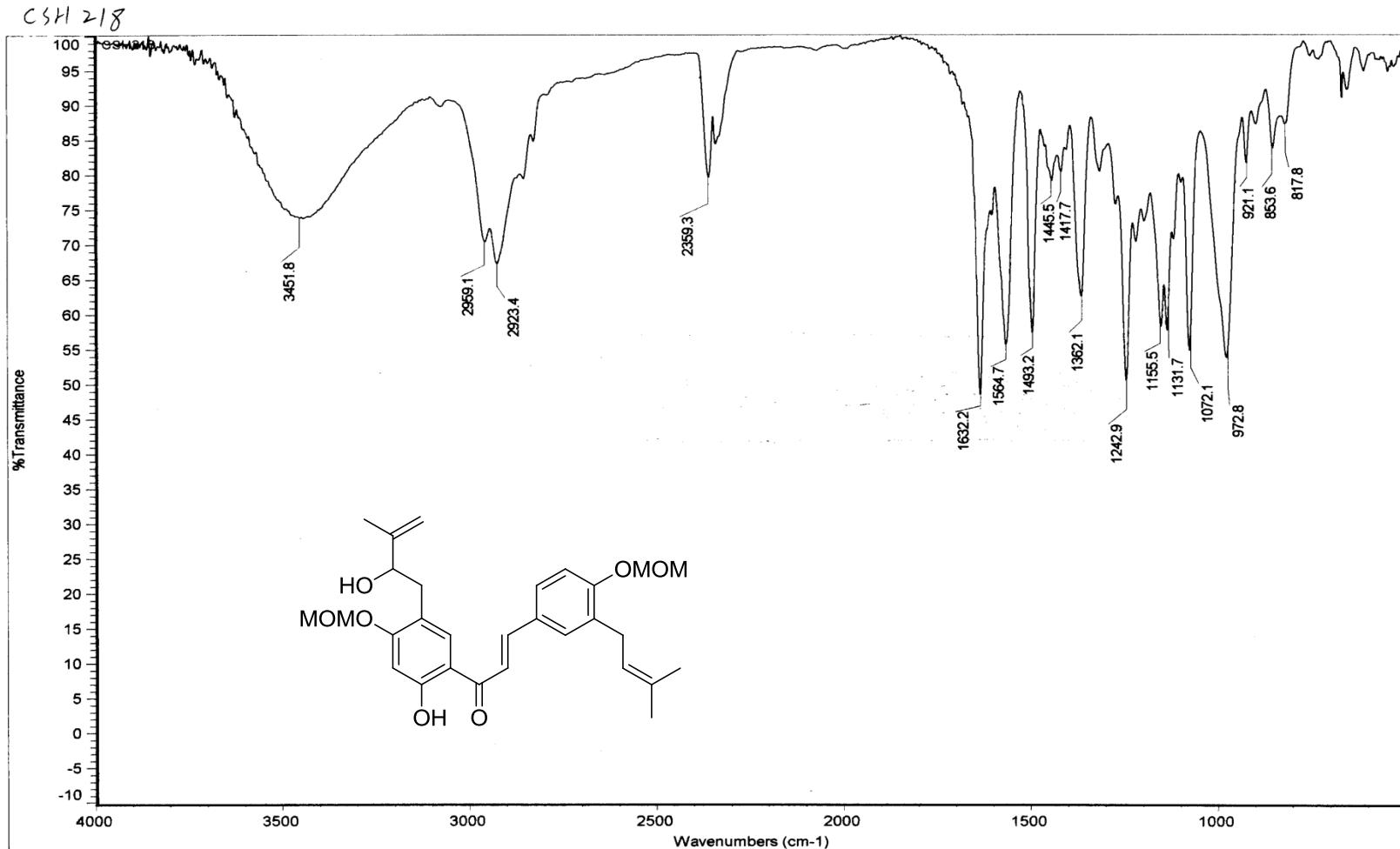


Fig. 73. (E)-1-(2-Hydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-4-(methoxymethoxy)phenyl)-3-(4-(methoxymethoxy)-3-(3-methylbut-2-enyl)phenyl)prop-2-en-1-one (**23**) 的 FTIR 圖譜

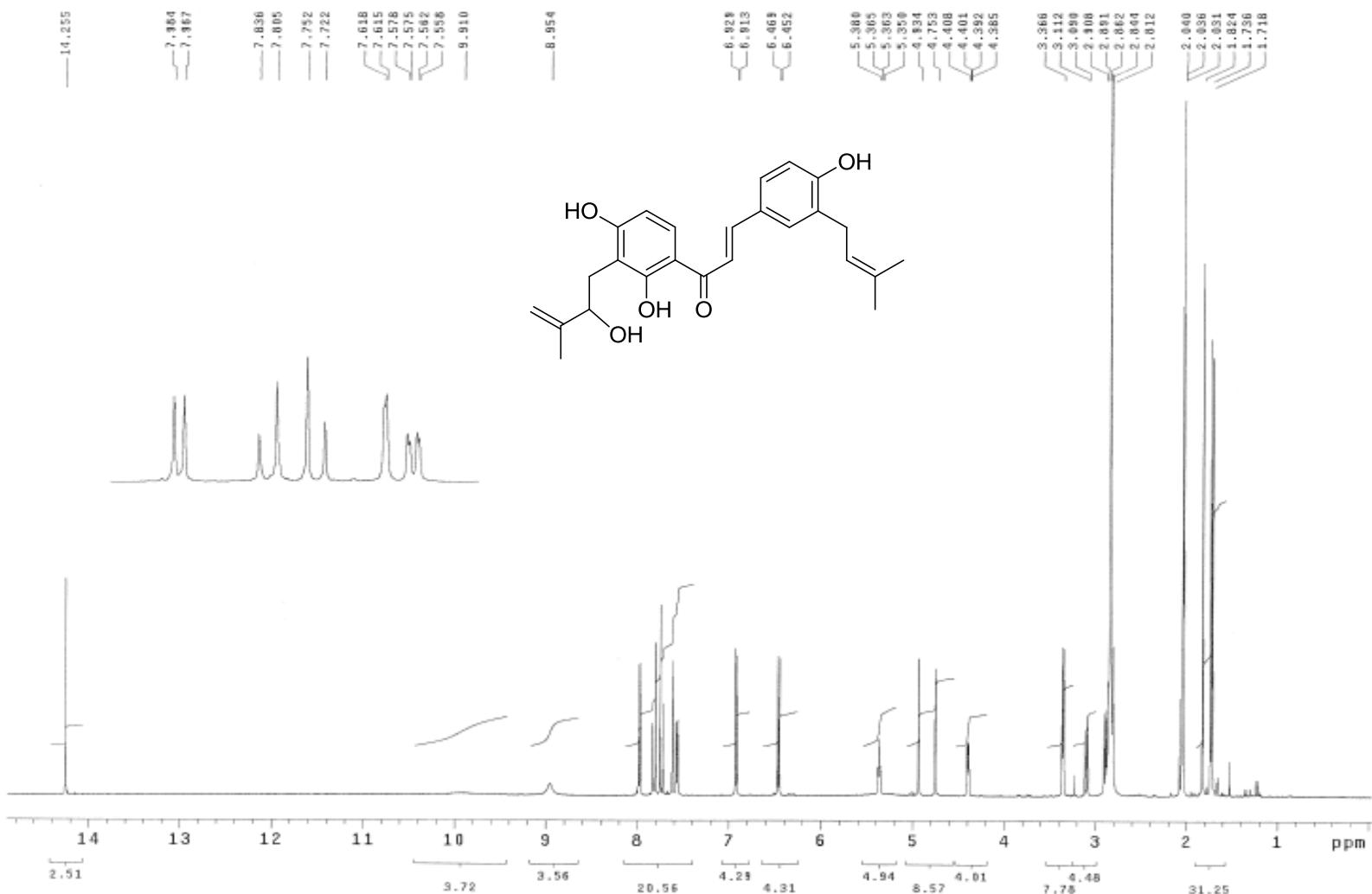


Fig. 74. Paratocarpin E (2)的¹H-NMR圖譜

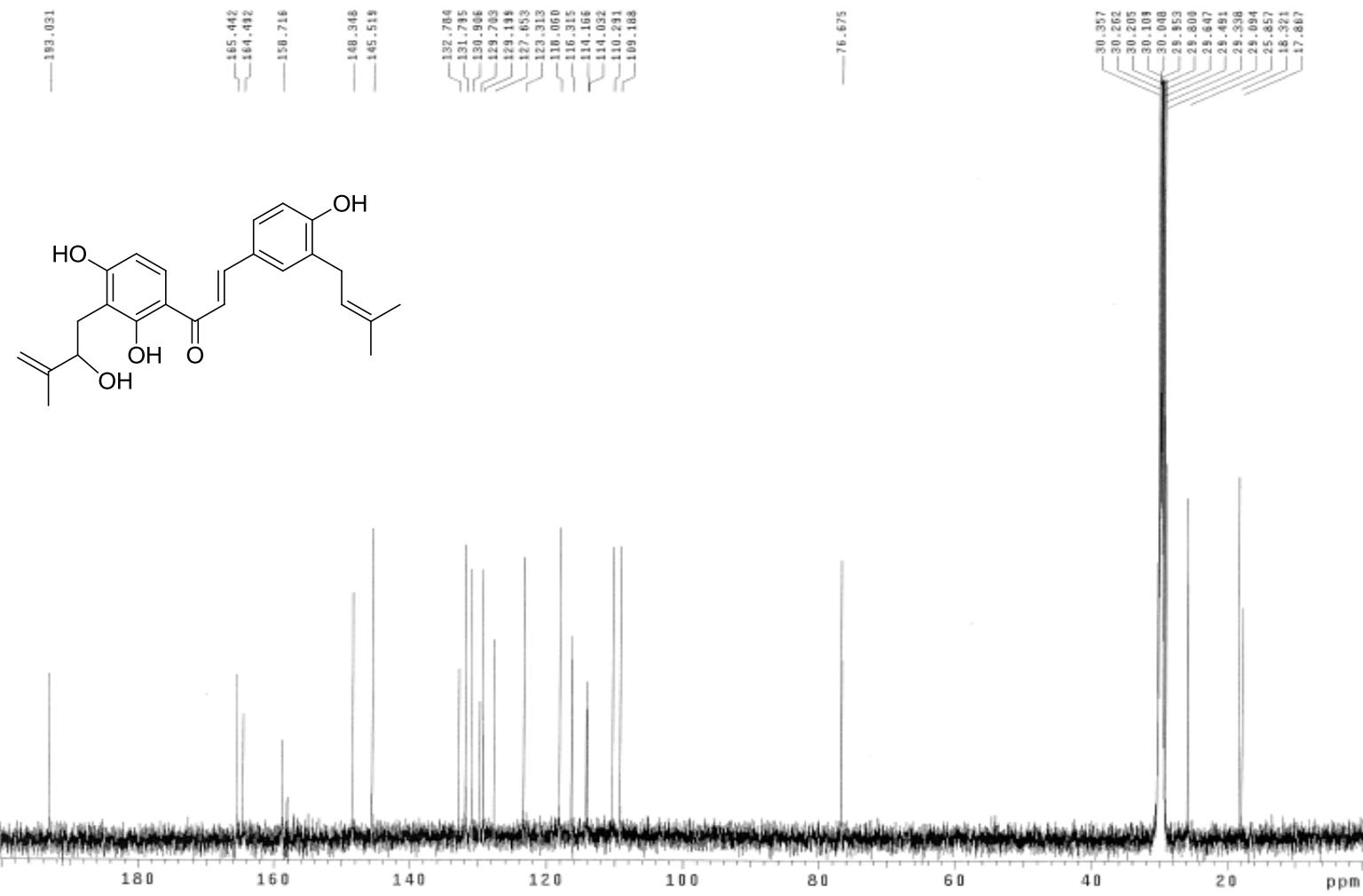


Fig. 75. Paratocarpin E (2)的¹³C-NMR圖譜

CSH228

exp3 Gcosy

```

SAMPLE      hs      FLAGS
date  Mar 25 2010 hs      nm
solvent acetone spul    n
sample   hsgv1    4651
          ACQUISITION SPECIAL
sw       8000.0  temp  25.0
at        0.128  gain   48
np       2048   spin  not used
fb        not used  F2 PROCESSING
ss        16     sb   0.054
d1       1.301  sbs  not used
nt        5     fn   2048
          2D ACQUISITION f1 PROCESSING
sw1      8000.0  sb1  0.032
n1        128   sb1  not used
          PRESATURATION proc1  1p
satnode  mnn   fn1  2048
satdry   0     DISPLAY 451.4
satfrq   459.8  sp   451.4
satpwrf -13    wp   3742.2
          TRANSMITTER sp1  459.2
tn        H1    wpl  3742.2
sfreq    459.884 r11  500.8
t1f      339.7  rfp   0
tpwr     5%    r111  500.8
pw       9.600  rfp1  0
tpwrcf  0.949 PLOT
          GRADIENTS wc   155.0
g2l1v11  4651  sc   10.0
gt1     0.001000 wc2  155.0
gstab   0.000500 sc2   0
          DECOUPLER vs   872
dn        C13 th   4
dm      mnn ai   cdc av

```

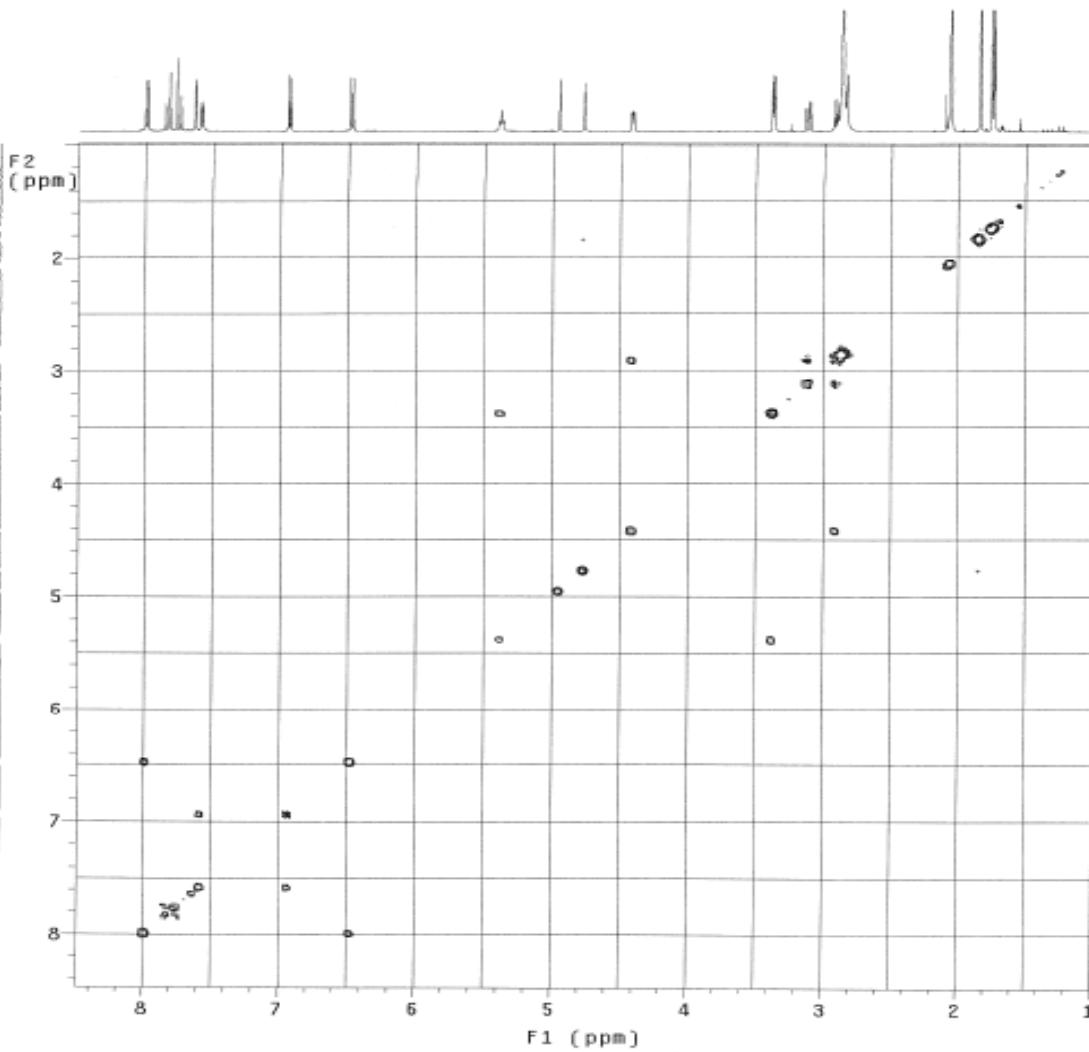
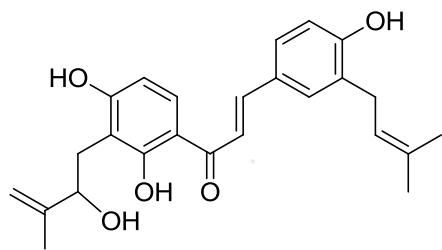


Fig. 76. Paratocarpin E (2)的COSY圖譜

CSH22B

expd4 Ghmc

```

SAMPLE          FLAGS
date Mar 25 2010 hs
solvent acetone ssPUL
sample          PGf1g1
ACQUISITION    hsgv1 4651 s
sw      8000.0 SPECIAL
at      0.128 temp 25.0
np      2048 gain 48
fb      not used spin not used
ss      32 GRADIENTS
sl      1.000 g2v1v1 4651
nt      16 g1 0.001000
2D ACQUISITION sw1 21367.5 g1v13 2333
sw1 21367.5 g1s 0.001000
m1      128 gstab 0.000500
phase     arrayed F2 PROCESSING
TRANSMITTER   gf 0.053
tn      H1 gfs not used
sfra   499.884 f1 4996
t0f    999.7 F1 PROCESSING
tpwr   51 g1 0.006
pw      9.600 g1s1 not used
DECOUPLER    C13
dn      -2515.4 DISPLAY
dm      rny sp 518.7
dma    ccp w1 3753.9
dmr   32258 sp1 1458.6
dpwr   35 w1 17528.0
pwx1v1 51 w1 508.8
pwx  14.500 rfp 0
HMOC   140.0 rfp1 1256.8
j1xh   140.0 rfp1 0
nullflg Y PLOT
          wc 150.0
          sc 0
          wc2 150.0
          sc2 0
          vs 328
          th 6
          ai cdc ph

```

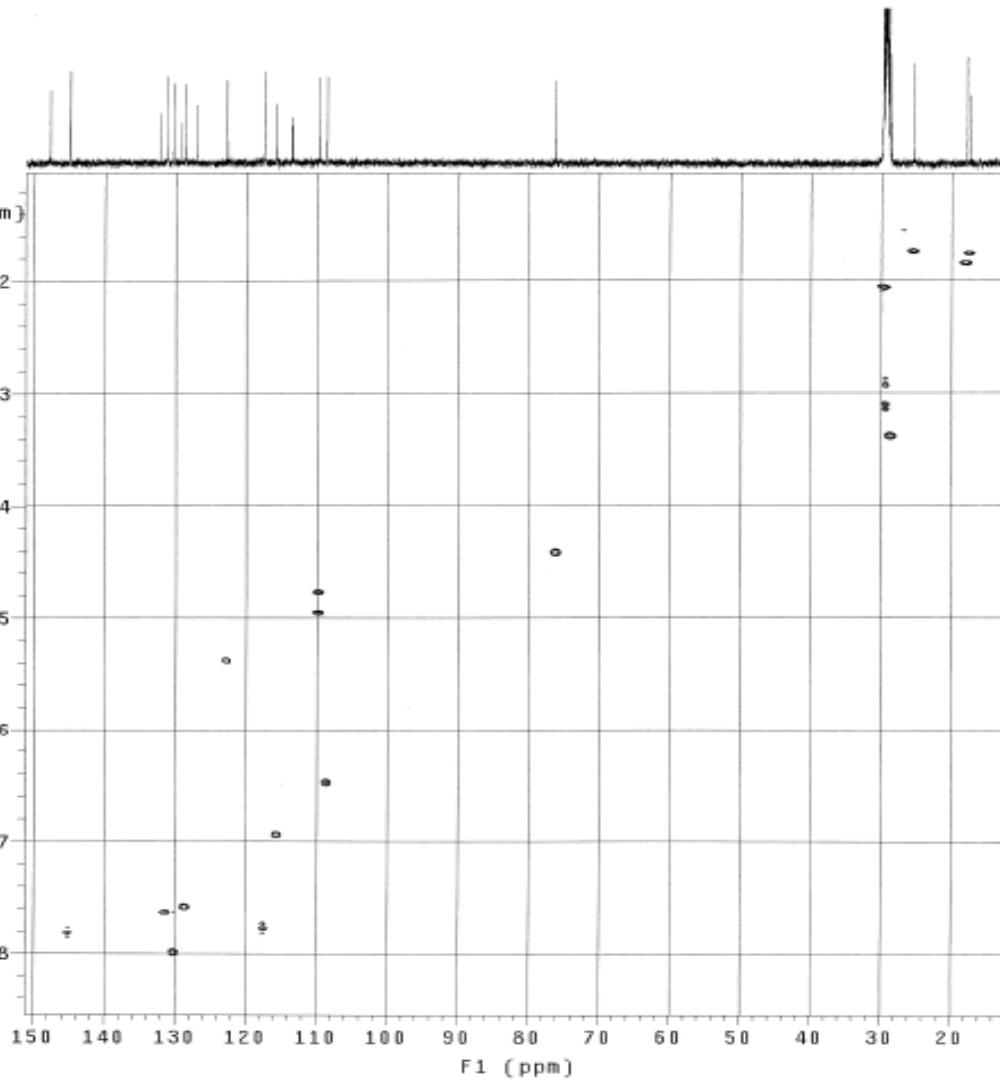
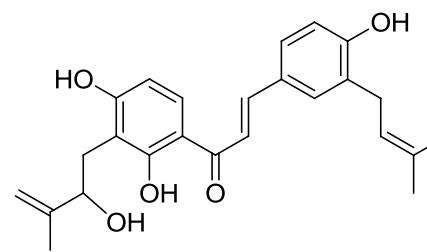


Fig. 77. Paratocarpin E (2)的HMQC圖譜

CSH22B

exp5 Ghabc

```

SAMPLE          FLAGS
date Mar 25 2010 hs      n
solvent acetone ssppul   n
sample PFGrf9  gsn      y
ACQUISITION hsgv1v1 4651
sw    8000.0 SPECIAL
et    0.128 temp    25.0
np    2668  gain    48
fb    not used spin    not used
ss    32    GRADIENTS
di    1.000 gztv1v1 4651
dt    32    gti     0.001000
nt    32    gtl     0.001000
2D ACQUISITION gztv1v3 2333
sw1   30165.4 gts     0.001000
ml    256   gtab    0.000500
phase 0      F2 PROCESSING
PRESATURATION s1     0.064
satnode mn1   sbs     not used
satdly 0      fn     2048
satfrq 499.8 F1 PROCESSING
satpwr -13   sb1   sbs1  not used
TRANSMITTER H1    proc1  lp
tn    499.884 fni    2048
sfreq 499.884
t1of  99.7    DISPLAY
tpwr  59    sp     402.5
pw    8.000 wp    6906.2
DECOUPLER C13  wpl    23596.6
dm    1255.4 rrf1   500.0
dn    1255.4 rfp    0
dmf   32258 rrf11  1885.0
dpwr  35    rfp1   0
pwxtv1 51    PLOT
pxw   14.500 wc     150.0
j1xh  140.0  wc2   150.0
jnxh  8.0    sc2    0
vs    32702 th     12
ai    cdc  av

```

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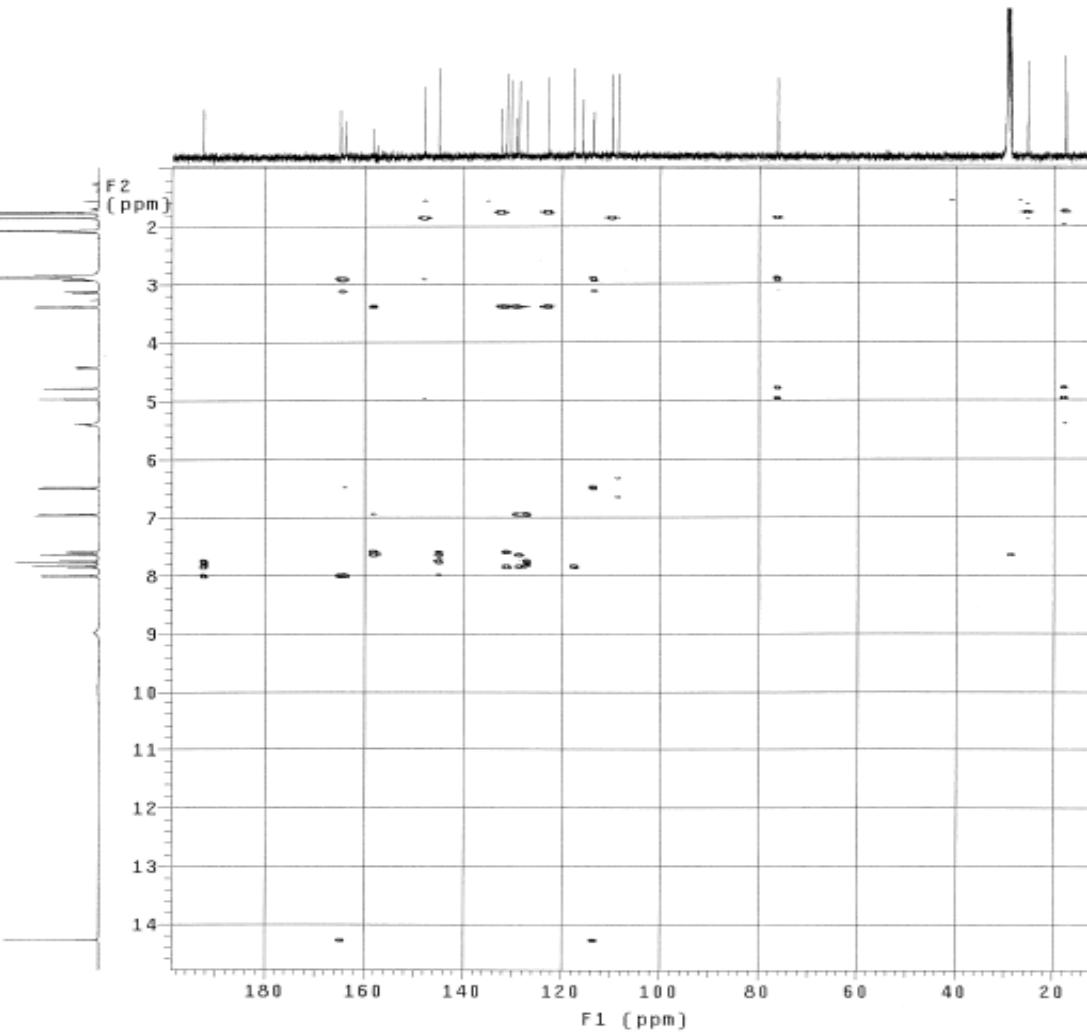
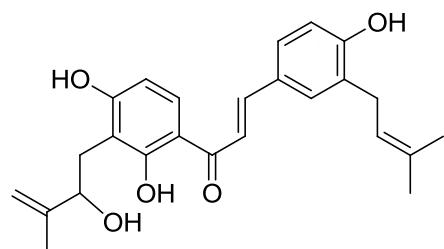


Fig. 78. Paratocarpin E (2)的HMBC圖譜

C:\Xcalibur\..\MJD\CSH-228_111223132648
DIP-EI-70ev

12/23/2011 1:26:48 PM

CSH-228_111223132648 #185 RT: 3.80 AV: 1 NL: 2.23E6
T: + c Full ms [50.00-650.00]

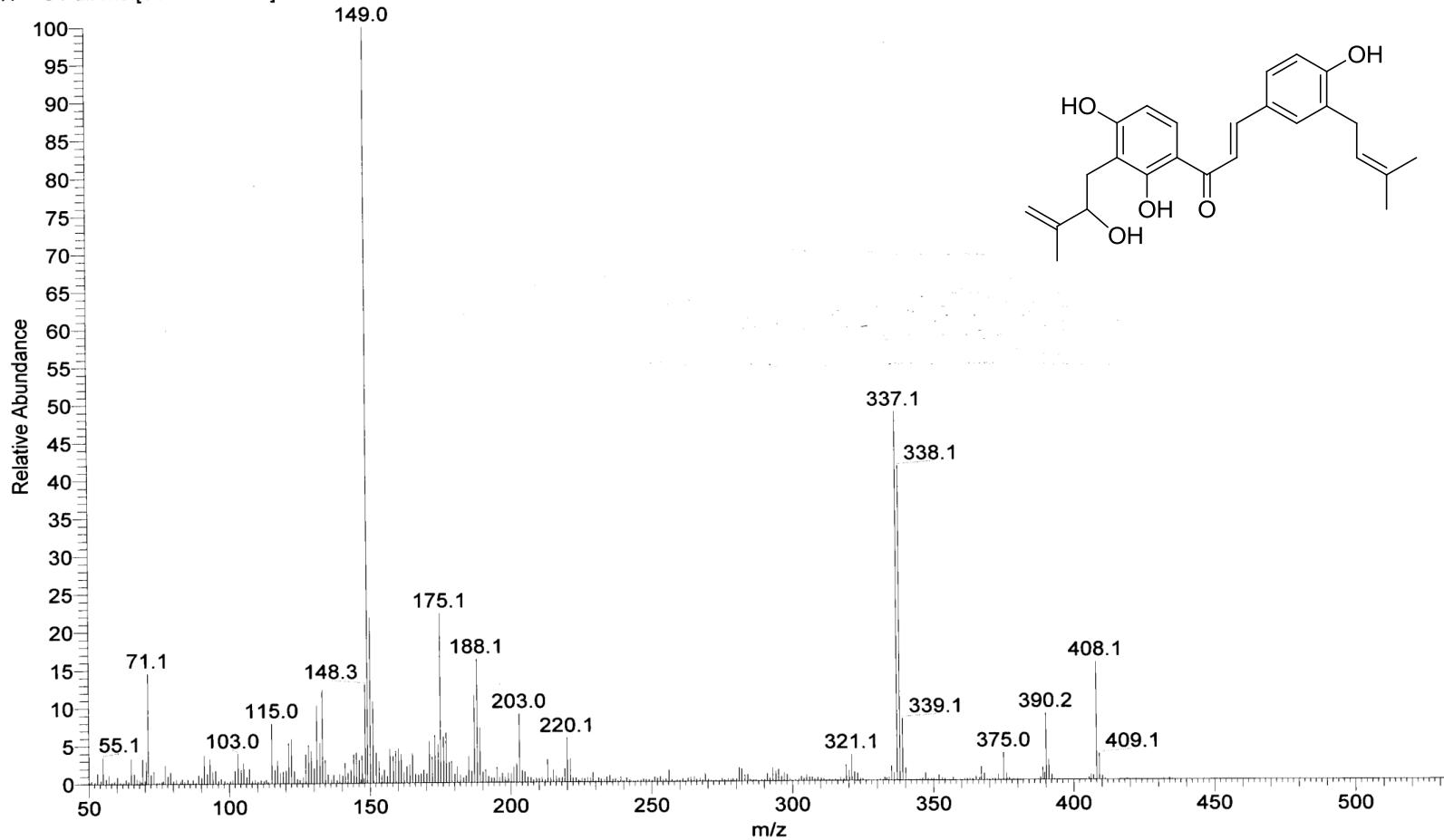


Fig. 79. Paratocarpin E (2)的EI-MS圖譜

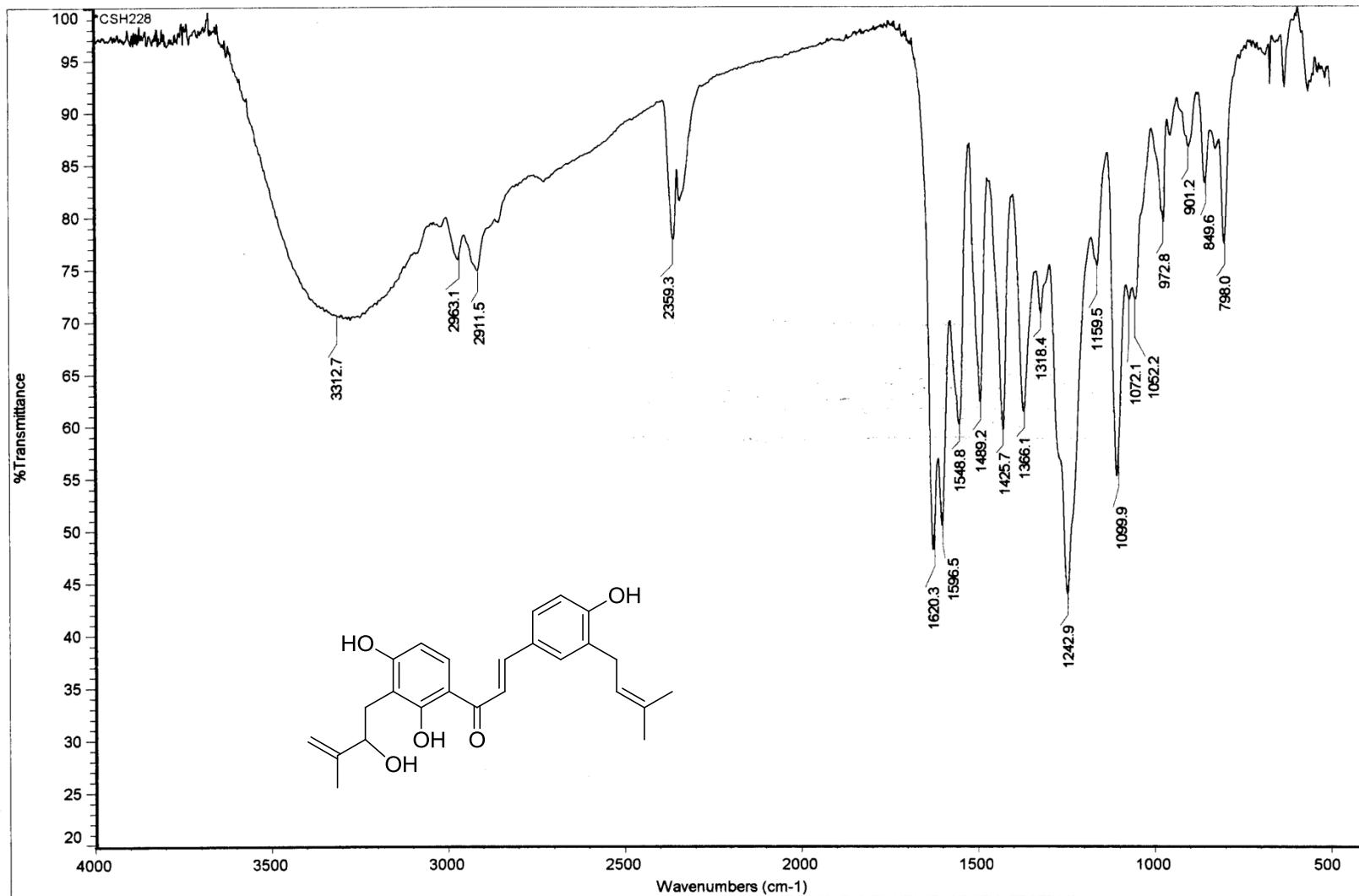


Fig. 80. Paratocarpin E (2)的 FTIR 圖譜

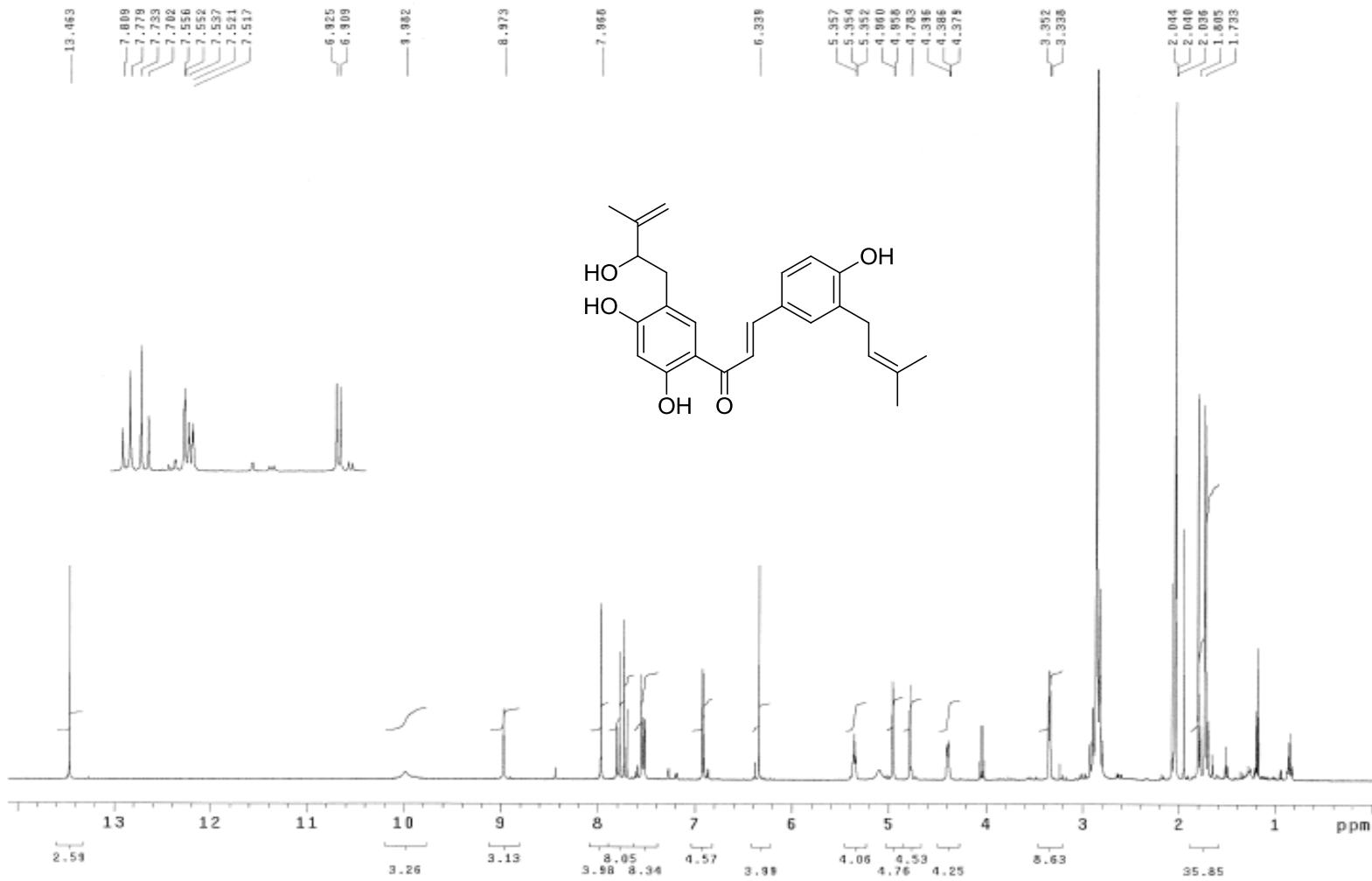


Fig. 81. Bartericin A (3)的¹H-NMR圖譜

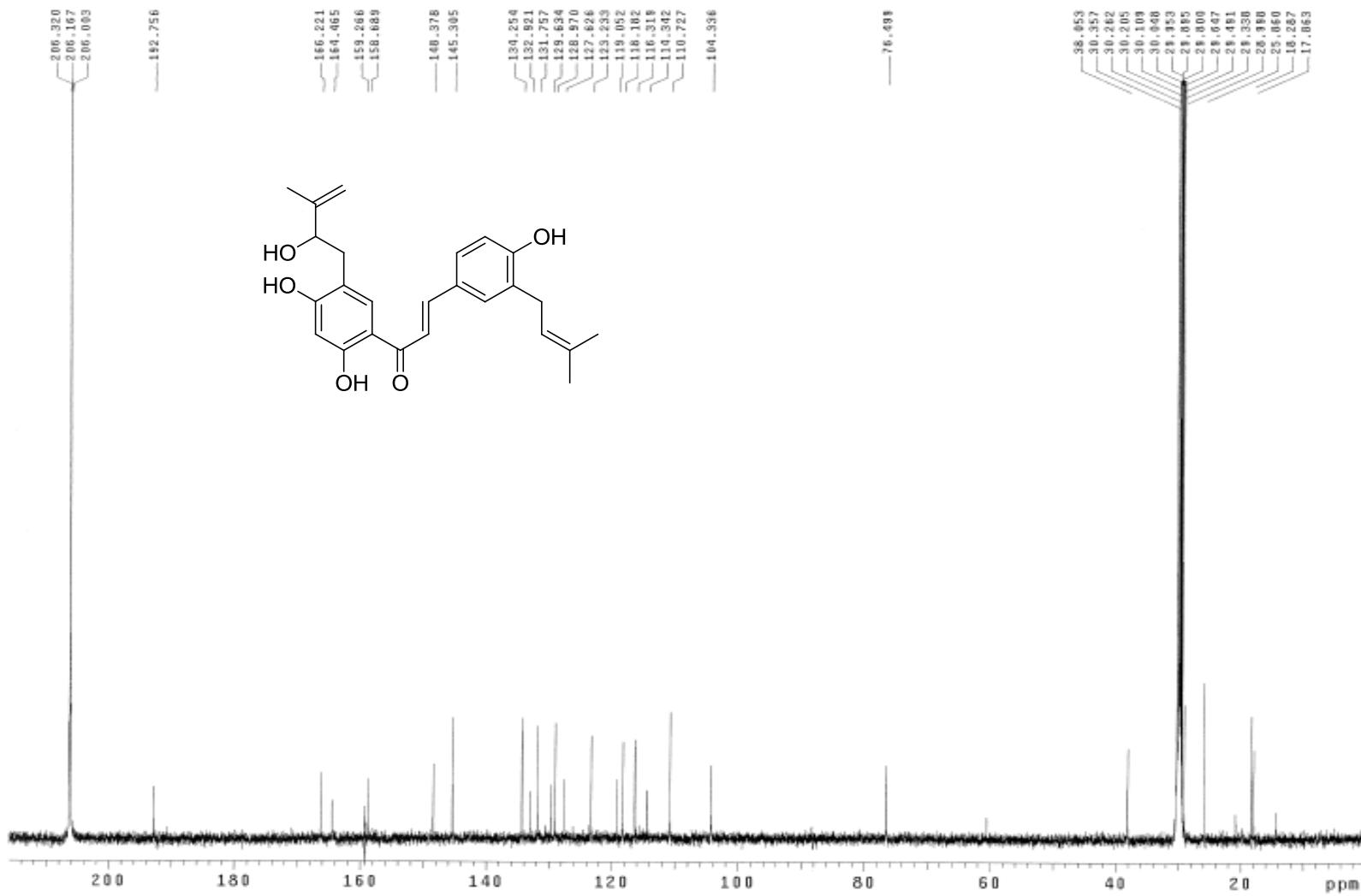


Fig. 82. Bartericin A (3) 的 ^{13}C -NMR 圖譜

CSH230
exp11 Gcosy

SAMPLE	Mar 25 2010	hs	nn
solvent	acetone	sspul	n
sample		hsgv11	4651
ACQUISITION		SPECIAL	
sw	8000.0	temp	25.0
at	0.128	gain	48
np	2048	spin	not used
fb	not used	F2 PROCESSING	
ss	16	sb	0.064
di	1.301	sbs	not used
nt	4	fn	2048
2D ACQUISITION		F1 PROCESSING	
sw1	8000.0	sbl	0.032
tn	128	sbs1	not used
PRESATURATION		proc1	1p
satnode	nnn	fni	2048
satdry	0	DISPLAY	
satfri	499.8	sp	-0.8
satpowr	-13	wp	4773.4
TRANSMITTER		spl	-0.8
tn	H1	wpl	4773.4
sf1	499.884	rfl	500.8
tof	999.7	rfp	0
tpwr	53	rfl1	500.8
pw	9.600	rfp1	0
tpwr_cf	0.949	PLOT	
GRADIENTS		wc	150.0
g2v11	4651	sc	0
gt1	0.001000	wc2	150.0
gstab	0.000500	sc2	0
DECOUPLER		vs	872
din	C13	th	0
dm	nnn	ai	cde

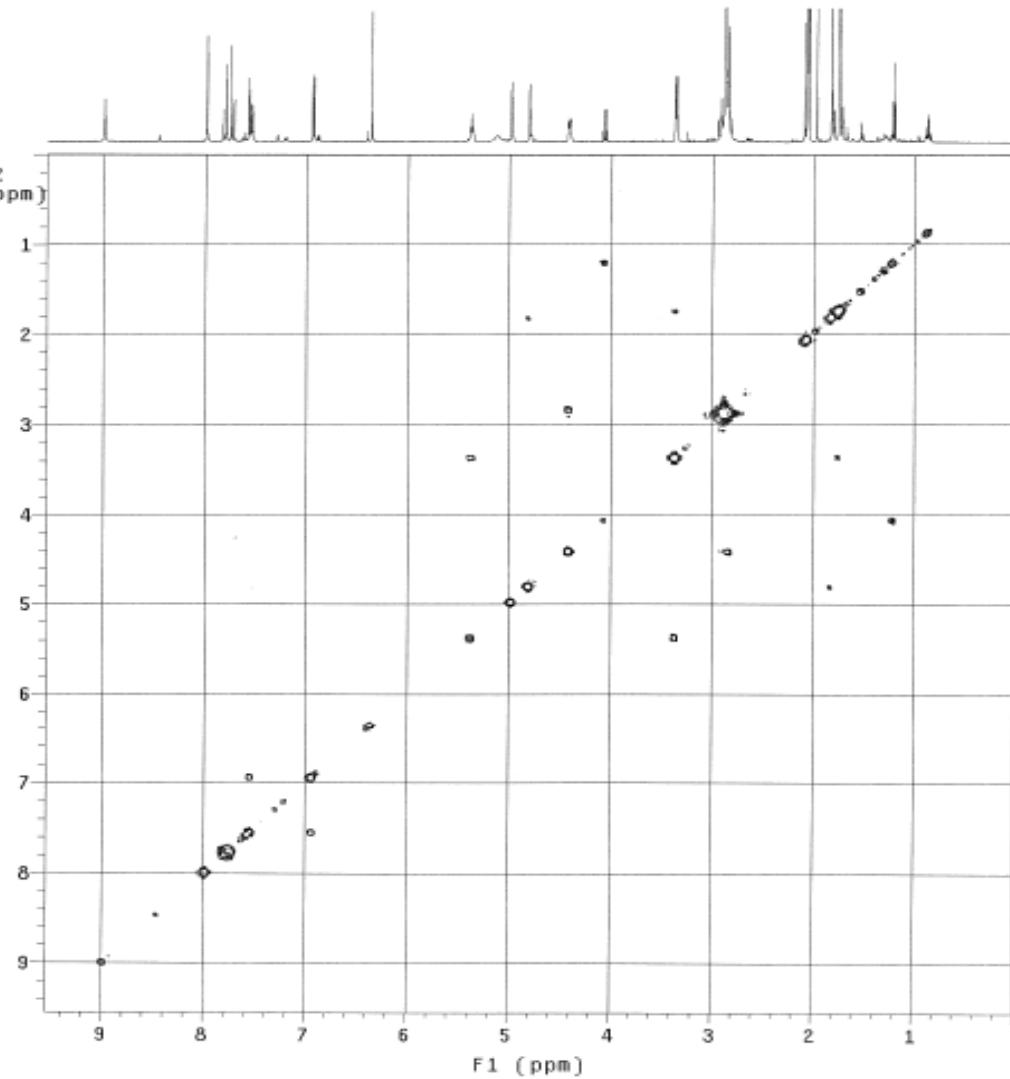
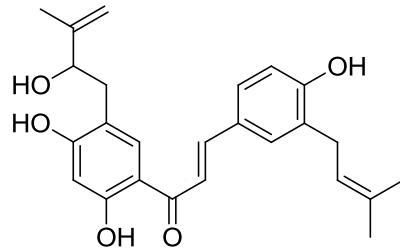


Fig. 83. Bartericin A (3)的COSY圖譜

CSH230

exp12 Chem3D

```

SAMPLE          FLAGS
date   Mar 25 2010 hs
solvent acetone sspe1
sample hsgv1g    y
ACQUISITION      arraydim
sw     8000.0   SPECIAL 4651 1
at     0.128   temp    25.0 2
np     2048    gain    48
fb     not used spin   not used
ss     32      GRADIENTS
di     1.000   gzl1v11 4651
nt     0.01000
2D ACQUISITION      F2
sw1   21367.5  gzl1v13 2333
ni     128     gt3    0.001000
phase  arrayed
F2 PROCESSING
TRANSMITTER        gfs    0.059
tn     H1      gfs    not used
sfrq  499.884  fn     4036
t0f   999.7    F1 PROCESSING
tpwr  59      gfl    0.006
pw     9.600   gfs1   not used
proc1
DECOUPLER          C13    fml    2048
dn     -2515.4  DISPLAY
dm     nny     sp     -36.0
dmcn  CCP     sp1    4523.4
dmrf  3225.0  CCP     sp1    -4.6
dmrf  35       CCP     sp1    20094.7
dpwcr 35      rfp1   500.8
pwxlv1 14.500  rfp1   1256.6
pwx   14.500  rfp1   0
HMOC   140.0   rfp1   0
nullflg Y      PLOT
al     cdc     wc    150.0
sc     0       sc2   150.0
sc2   0       vs    328
th     6
ph

```

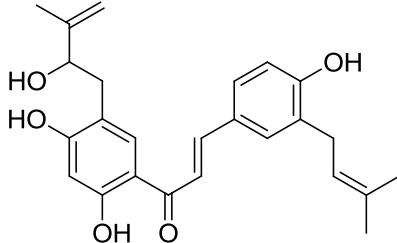
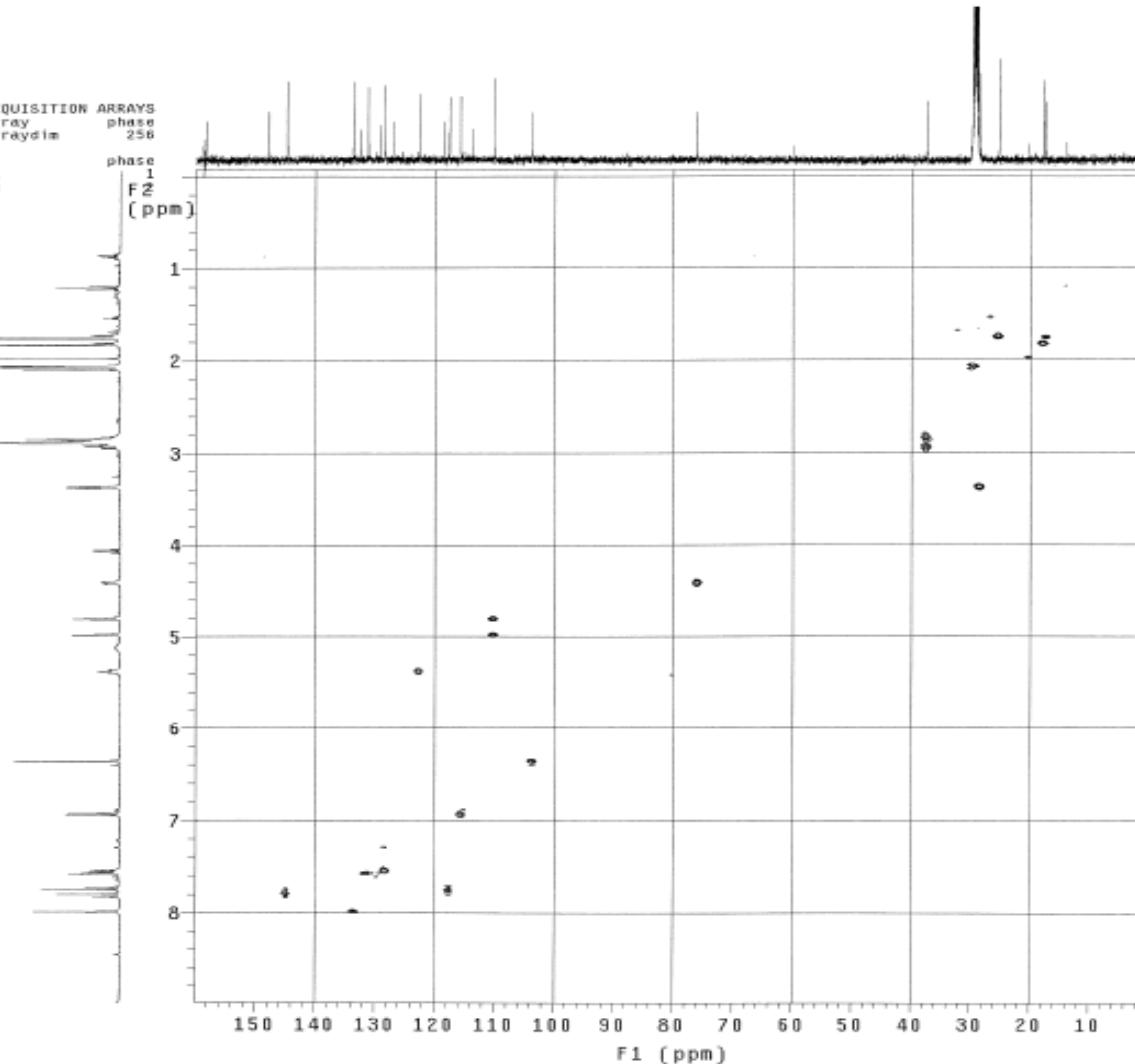


Fig. 84. Bartericin A (3)的HMQC圖譜

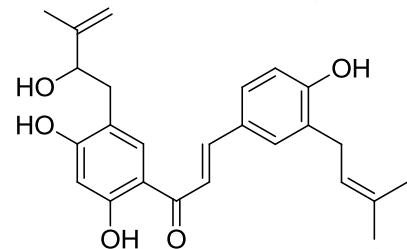
CSM230

exp13 Ghmhc

```

SAMPLE          FLAGS
date  Mar 25 2010 hs      n
solvent acetone ssppul   y
sample          PFG1q
ACQUISITION    insq1v1  4651
sw   8000.0   SPECIAL
at   0.128   temp    25.0
np   2048    gain    48
fb   not used
ss   32      spin    not used
di   1.000
nt   32      GRADIENTS
        gztv11  4651
        gztv13  0.001060
        gt3     0.001060
        gstab   0.000560
        F2 PROCESSING
        sb      0.064
        sbs     not used
        fn      2048
        F1 PROCESSING
        sbl     0.008
        sbtl    not used
        proc1   1p
        fml    2048
        DISPLAY
        H1      -0.8
        sp      7203.1
        sp1     -28.1
        Wp      26886.0
        Wp1    500.5
        rfp     0
        rfp1   1885.0
        rfp1i  0
        PLOT
        HMBC
        14.500 wc      150.0
        j1xh   140.0 sc      0
        jmxh   8.0    sc2    150.0
                           0
                           s     32782
                           th    12
                           al    cdc av

```



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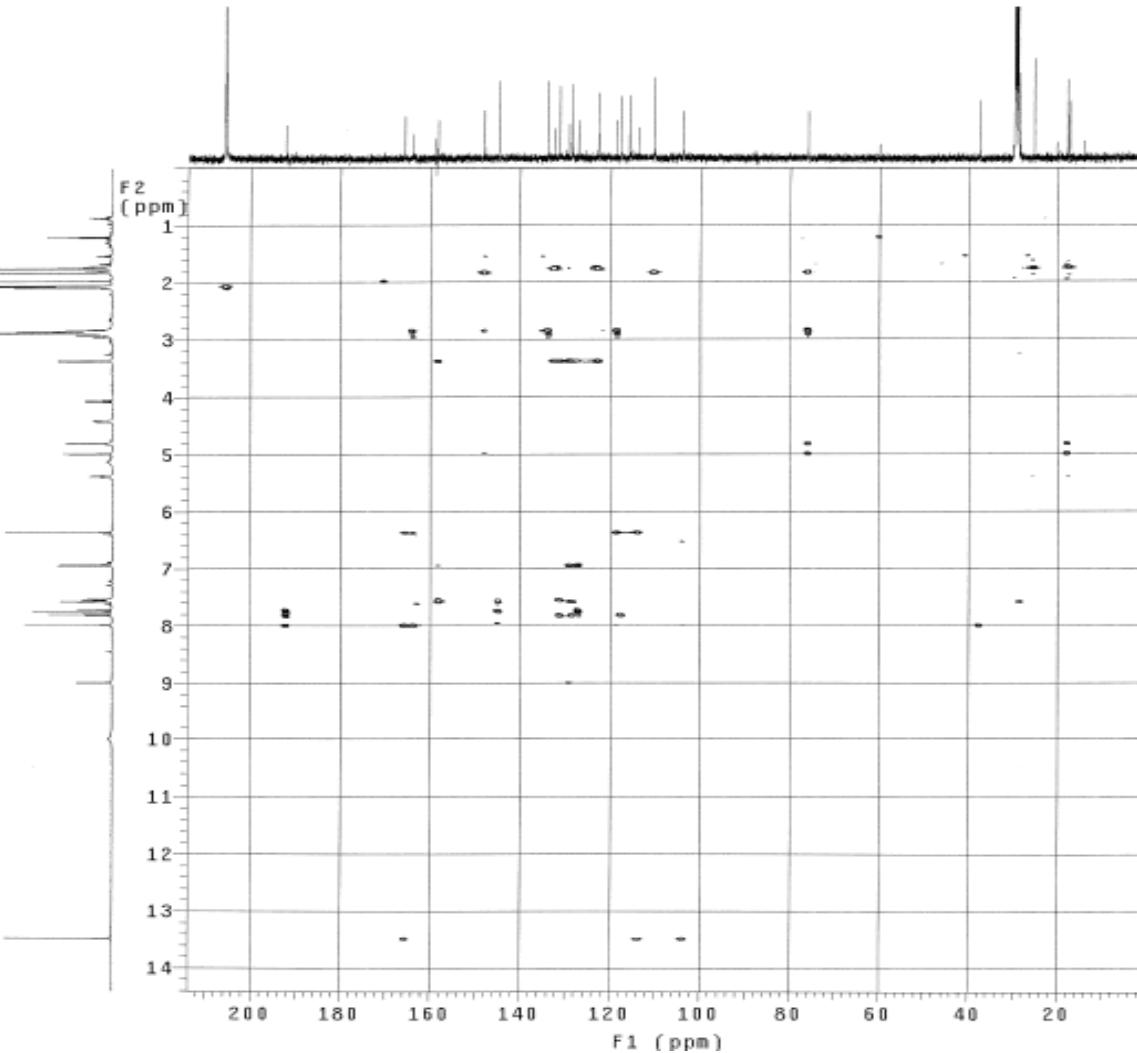


Fig. 85. Bartericin A (3)的HMBC圖譜

C:\Xcalibur...\MJD\CSH-230_111223121045

12/23/2011 12:10:45 PM

DIP-EI-70ev

CSH-230_111223121045 #212 RT: 4.35 AV: 1 NL: 1.39E6

T: + c Full ms [50.00-650.00]

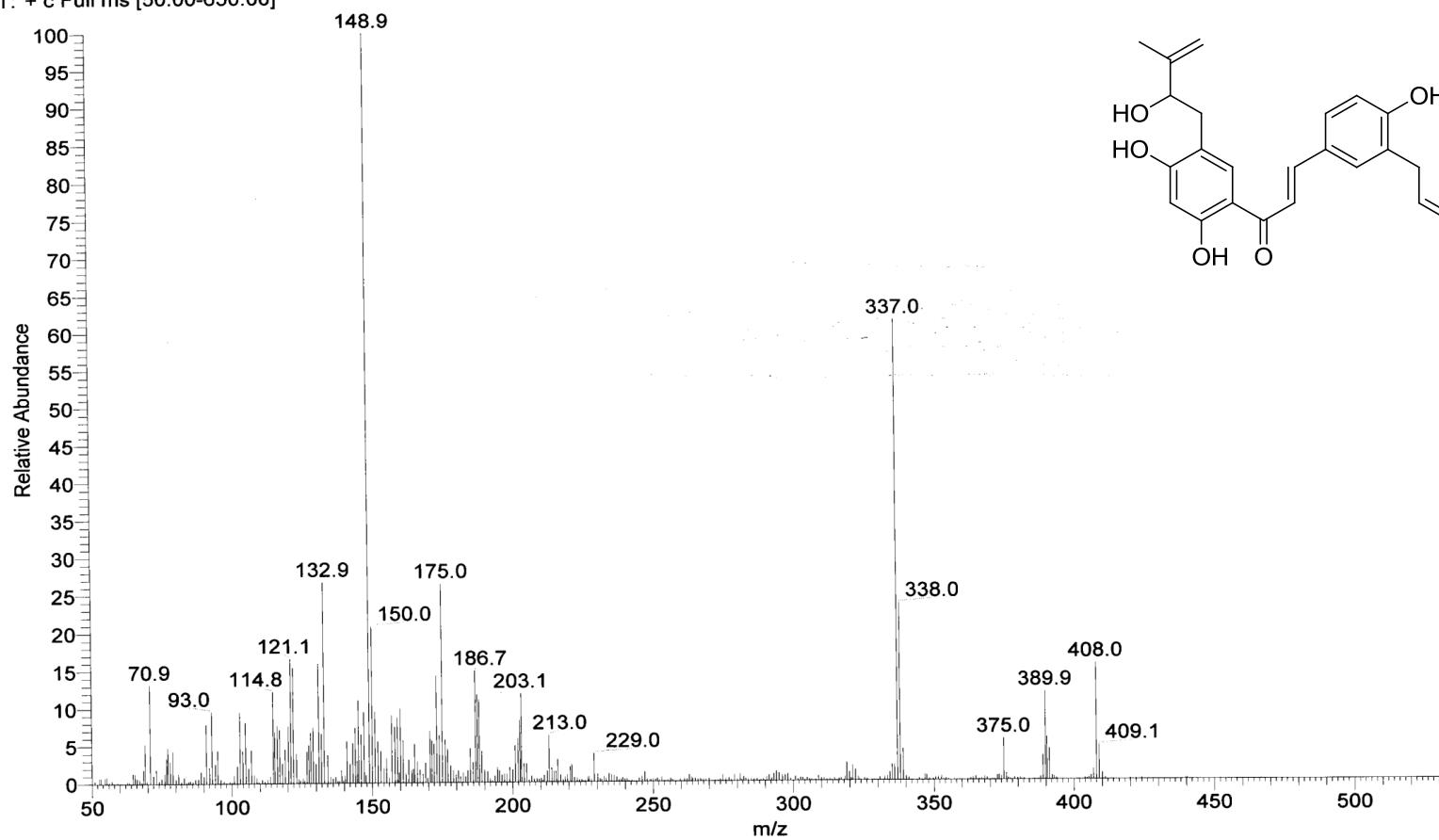


Fig. 86. Bartericin A (3)的EI-MS圖譜

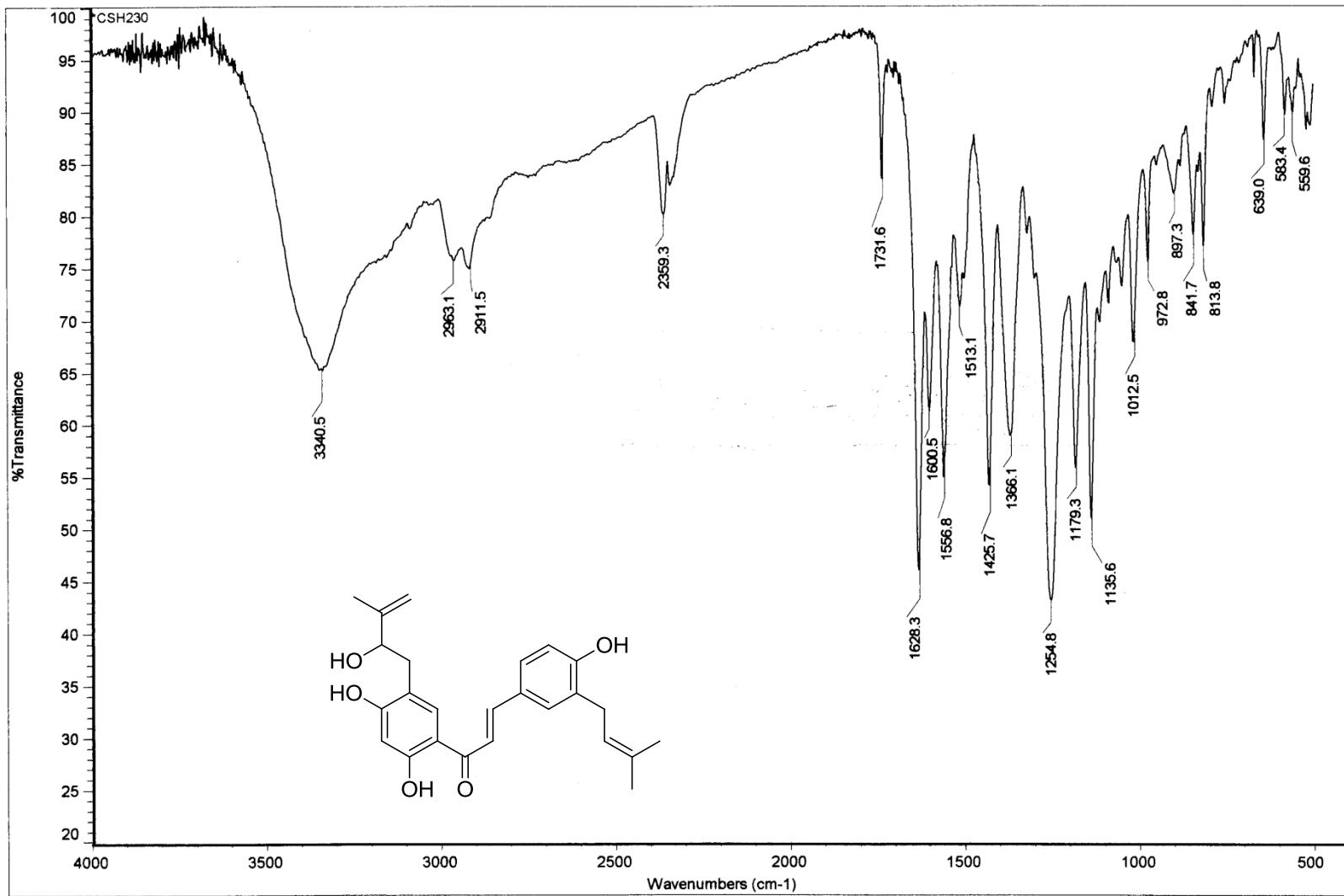


Fig. 87. Bartericin A (3)的FTIR圖譜

CSH233d_CDC13_500
12/21/11

12.58

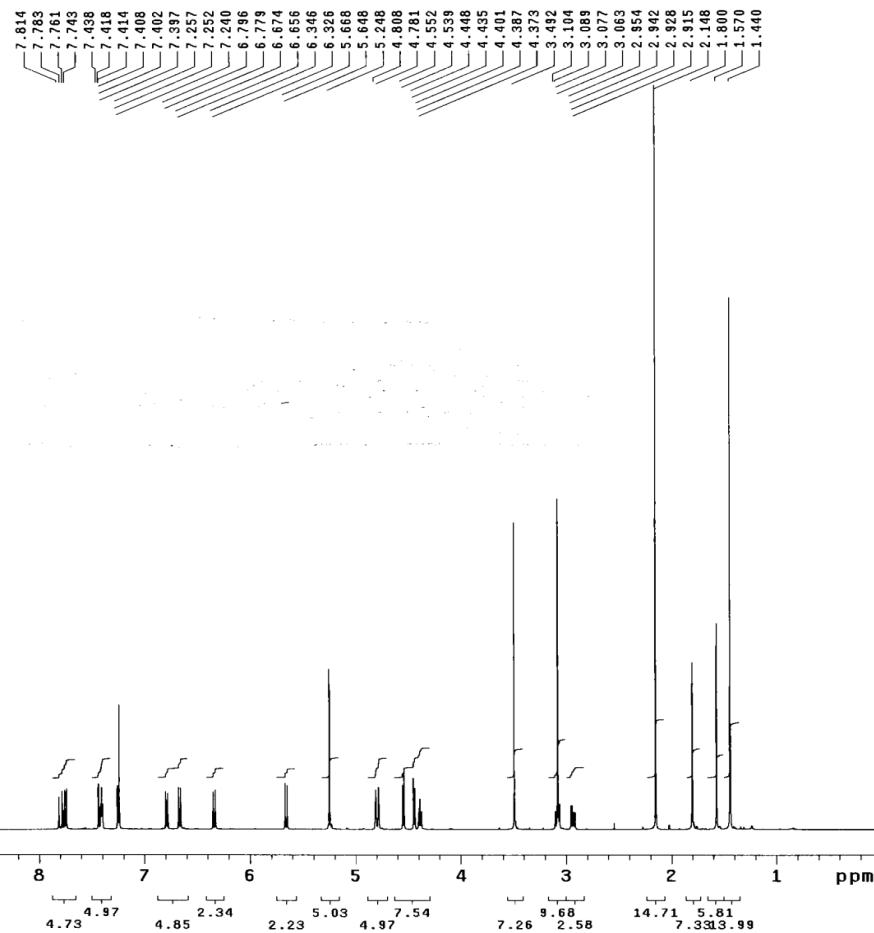
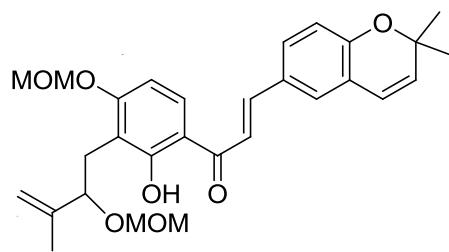


Fig. 88. (E)-3-(2,2-Dimethyl-2H-chromen-6-yl)-1-(2-hydroxy-4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)- prop-2-en-1-one (24) 的 ^1H -NMR 圖譜

CSH233d_CDC13_500
12/21/11

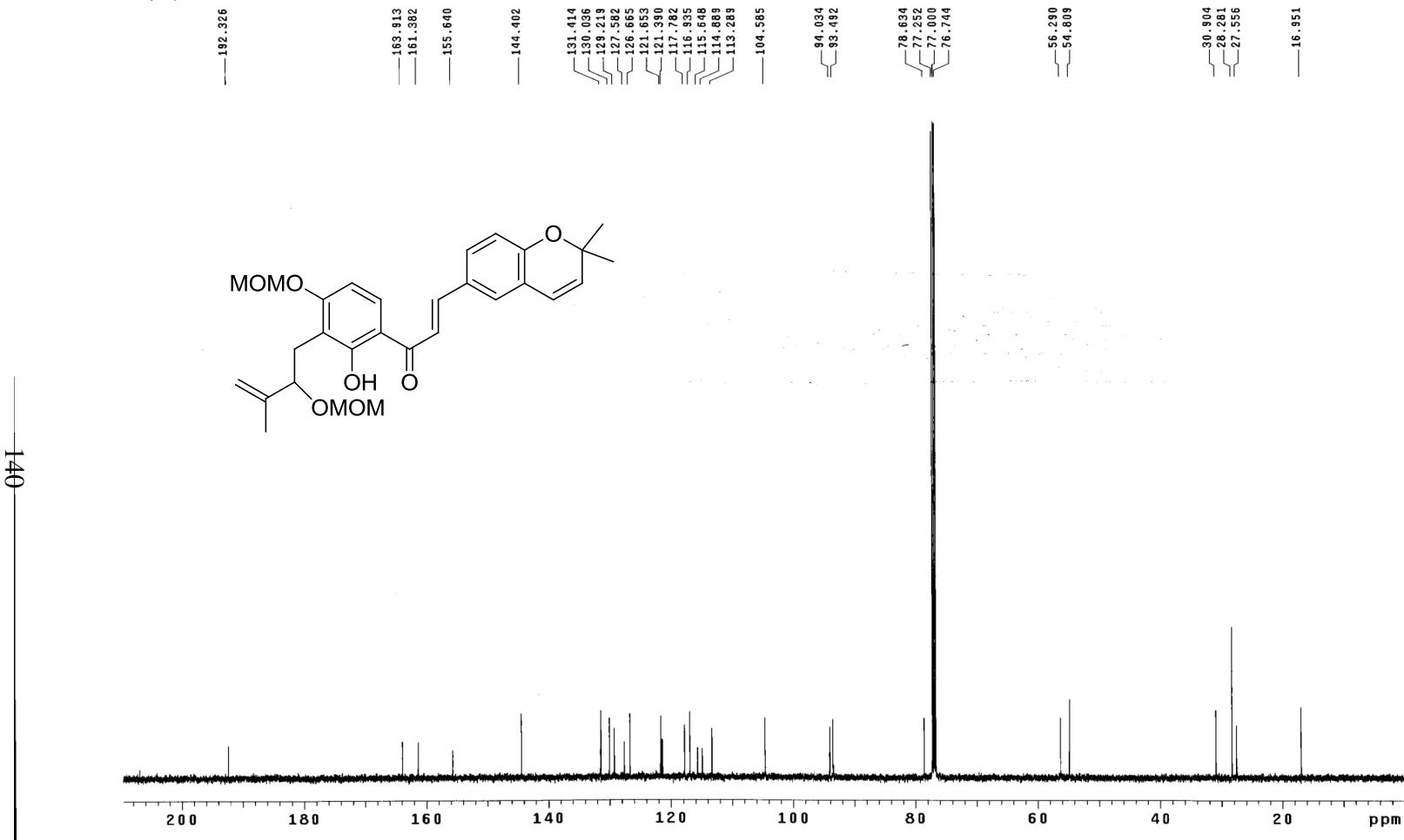


Fig. 89. (E)-3-(2,2-Dimethyl-2H-chromen-6-yl)-1-(2-hydroxy-4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)- prop-2-en-1-one (**24**) 的 ^{13}C -NMR 圖譜

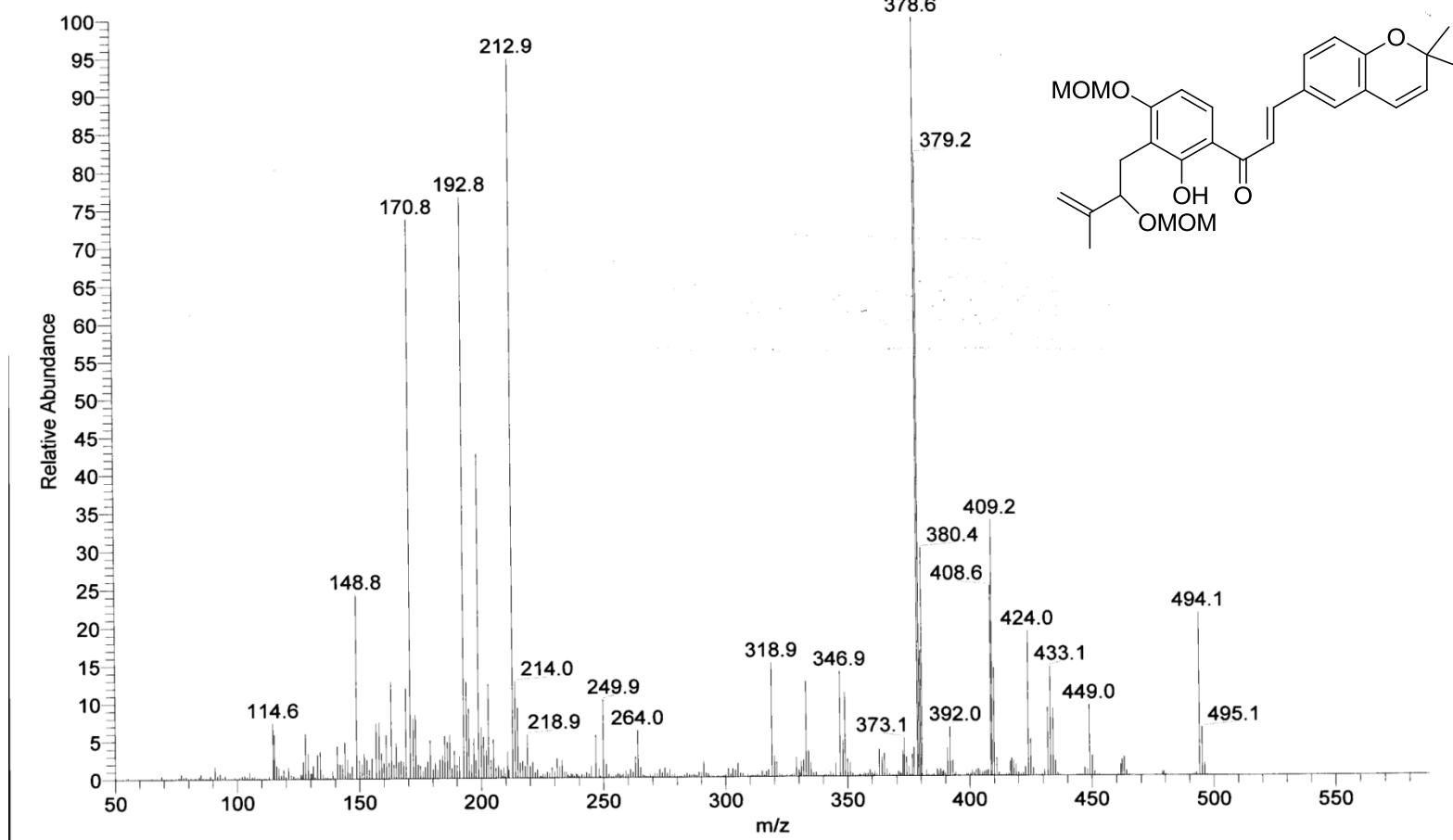


Fig. 90. (E)-3-(2,2-Dimethyl-2H-chromen-6-yl)-1-(2-hydroxy-4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)- prop-2-en-1-one (**24**) 的 EI-MS 圖譜

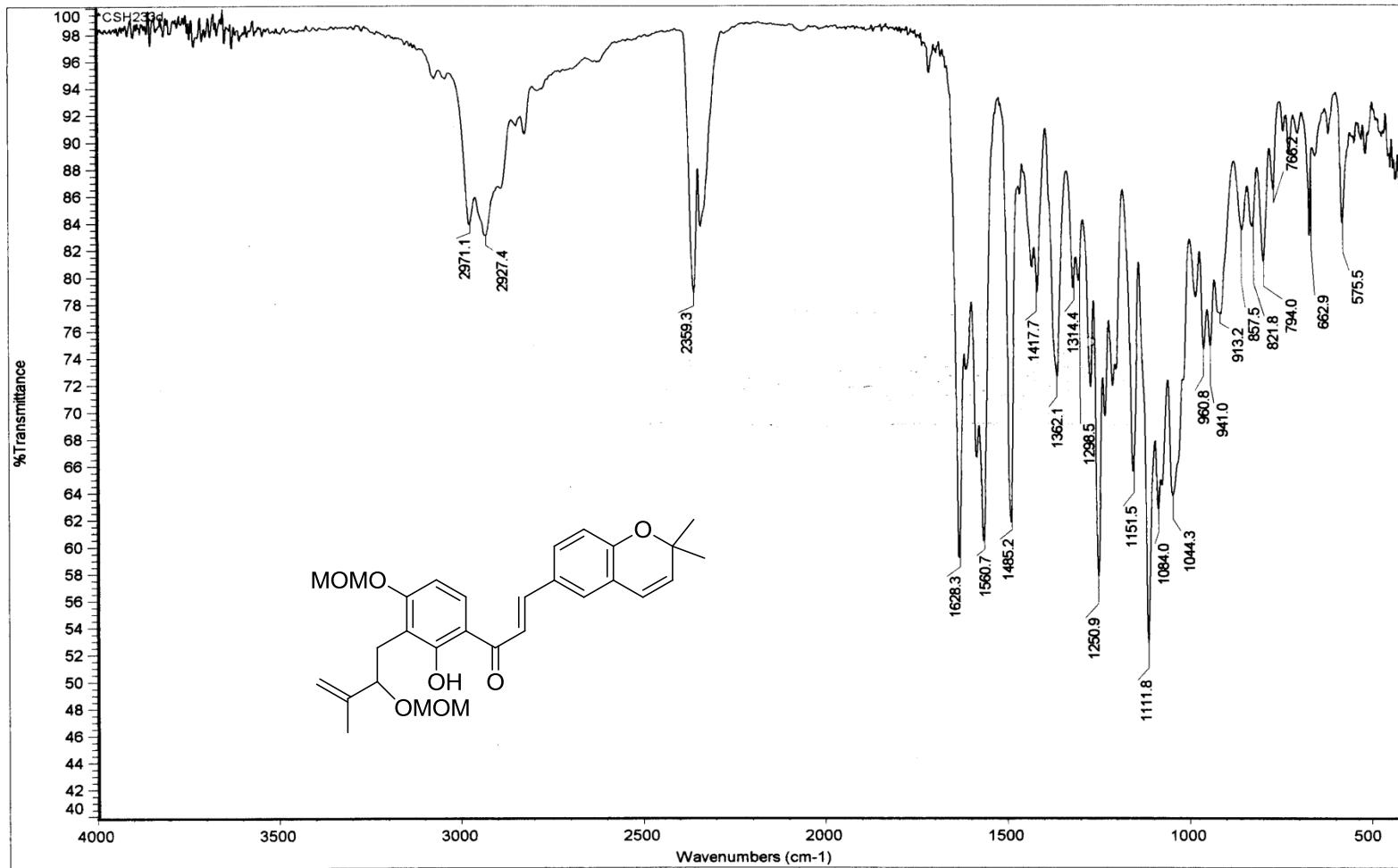


Fig. 91. (E)-3-(2,2-Dimethyl-2H-chromen-6-yl)-1-(2-hydroxy-4-(methoxymethoxy)-3-(2-(methoxymethoxy)-3-methylbut-3-enyl)phenyl)- prop-2-en-1-one (**24**) 的FTIR圖譜

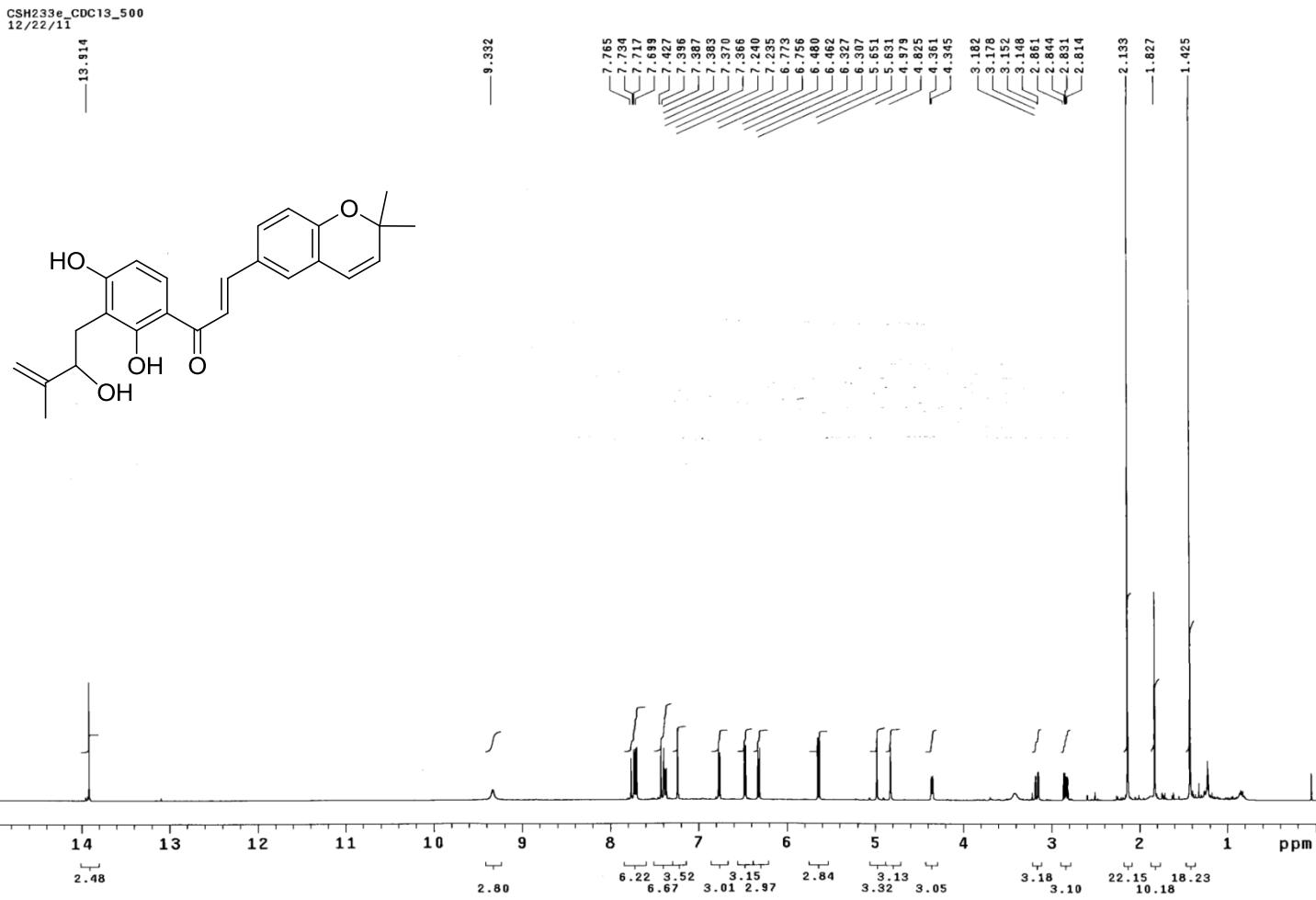


Fig. 92. Angusticornin A (5)的¹H-NMR圖譜

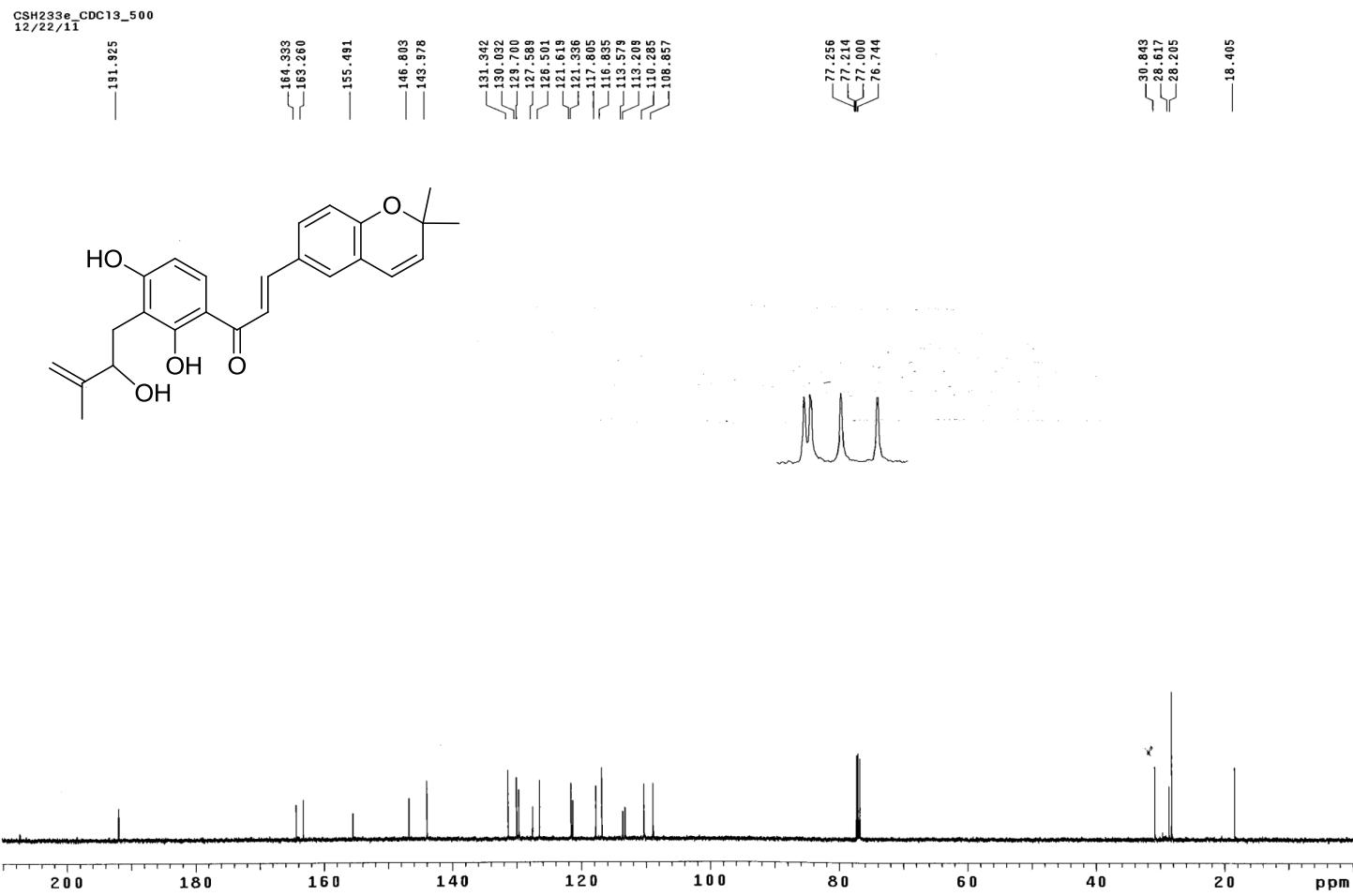


Fig. 93. Angusticornin A (**5**)的 ^{13}C -NMR圖譜

CSH239e_CDC13_500
12/22/11

exp60 Gcosy

```

SAMPLE          FLAGS
date Dec 23 2011 hs      nn
solvent   cdc13 sspul   n
sample    hsglv1 4672

ACQUISITION      SPECIAL
sw     8000.0 temp   25.0
at      0.128 gain    32
np      2048 spin   not used
fb      not used F2 PROCESSING
ss      16 sb     0.064
d1     1.301 sbs    not used
nt      4 f1     2048

2D ACQUISITION   F1 PROCESSING
sw1    8000.0 sb1    0.032
ni      128 shs1   not used
PRESATURATION    proc1   1p
satmode   nnn fn1    2048
satdly    0      DISPLAY
satfrq   499.8 sp     -8.7
satpwr   -13    wp     7476.6
TRANSMITTER      spi    22.6
tn      H1      w1i    7466.8
sfrq    499.881 rfp1   500.9
t0f     999.7 rfp1   500.9
tpwr     59    rfp1   500.9
pw      9.500 rfp1   0
tpwr_cf  0.790 PLOT
GRADIENTS       wc    150.0
gzlv11  4672  sc    0
gt1     0.001000 wc2   150.0
gstab   0.000500 sc2   0
DECOUPLER        vs    872
dn      C13 th    2
dm      nnn ai    cdc av

```

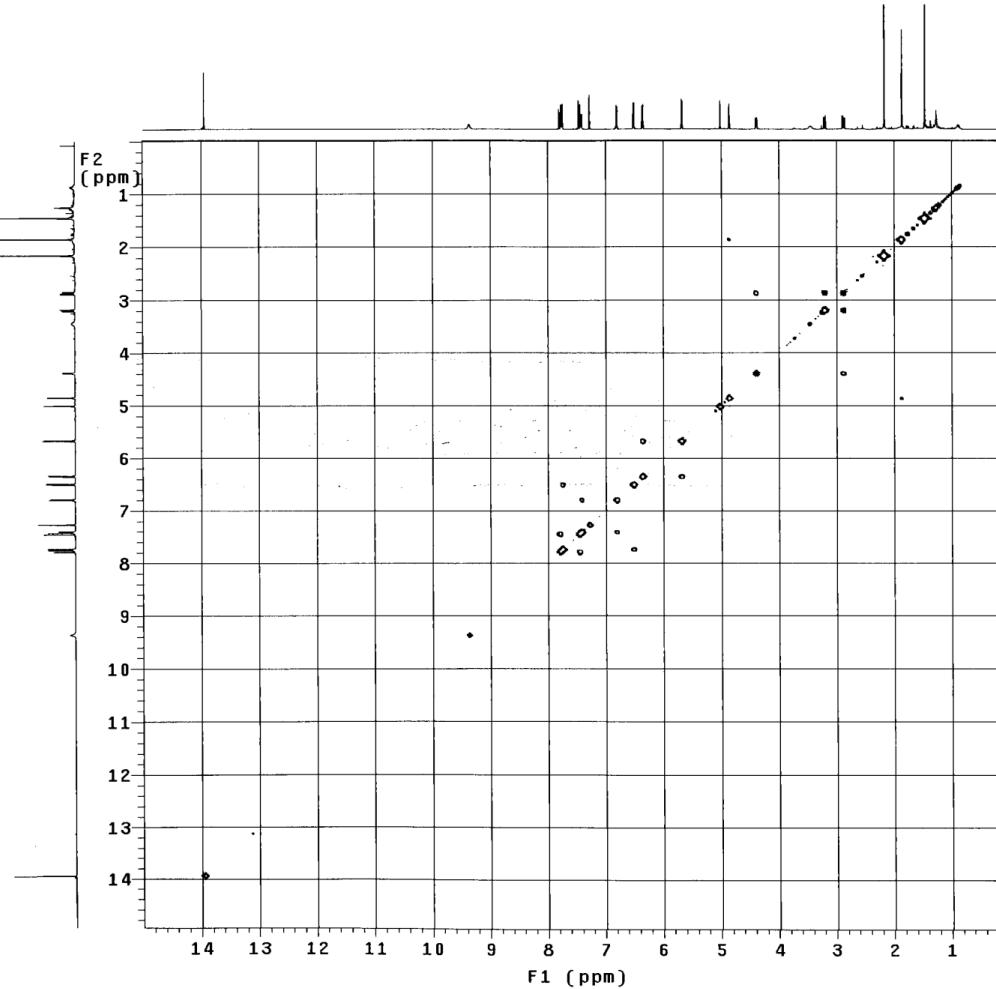
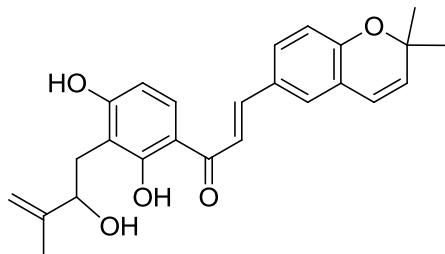


Fig. 94. Angusticornin A (5)的COSY圖譜

CSH233e_CDC13_500
12/22/11

exp61 Ghmqc

```

SAMPLE          FLAGS          ACQUISITION ARRAYS
date  Dec 23 2011 hs      n      array      phase
solvent   cdc13  sepul   y      arraydim  256
sample    P56flg          y
ACQUISITION   hsgv11      4672  1
sw      8000.0  SPECIAL
at      0.128  temp     25.0  2
np      2048   gain     32
fb      not used  spin    not used
ss      32      GRADIENTS
dt      1.000  gzlv11  4672
nt      16      gzlv13  2344
2D ACQUISITION 2D
sw1    21367.5  gt1     0.001000
ni      128    gstab   0.000500
phase   arrayed  F2 PROCESSING
TRANSMITTER   H1      gf      0.059
tn      1       gfs     not used
sfrq   499.881  f1      4096
t0f    939.7   f1 PROCESSING
tpwr   59      gfs1   not used
pw      9.500   proc1  1p
DECOUPLER    C13    fn1    2048
dn      -2515.4  DISPLAY
dof    1
dm      nny    sp      -8.7
dmn    ccp    sp      4480.5
dmf    3225.8  sp1     37.9
dpwr   35      wpl    20032.1
pwxlv1 50      rfp    500.9
pwx   16.100   rfp1   0
HMOC   140.0   rfp1  1256.7
j1xh
nullflg  y      PLOT
          wc      150.0
          sc      0
          wc2     150.0
          sc2     0
          vs      328
          th      1
ai      cdc ph

```

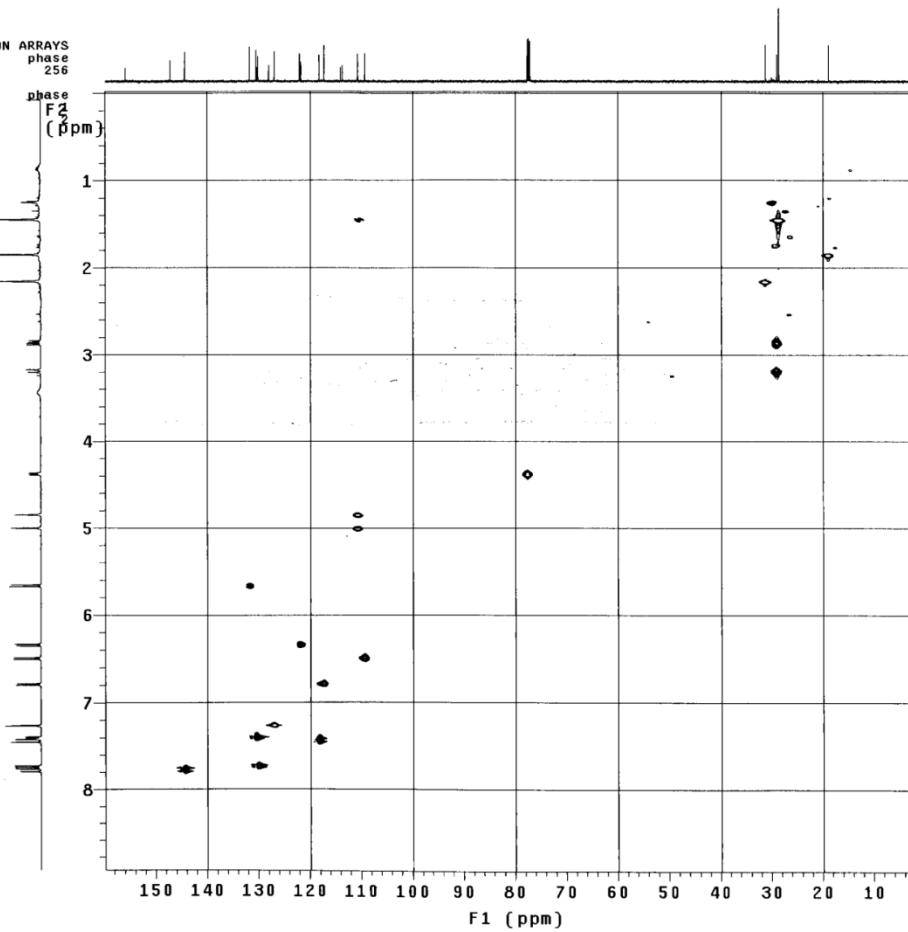
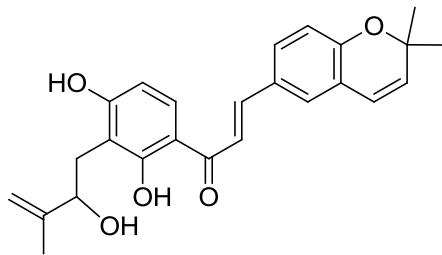


Fig. 95. Angusticornin A (5)的HMQC圖譜

CSH233e_CDC13_500
12/22/11

exp62 Ghmbc

SAMPLE FLAGS
date Dec 23 2011 hs n
solvent cdc13 sspul n
sample PFGr1g y
ACQUISITION hsgv1 4672
sw 8000.0 SPECIAL
et 0.128 temp 25.0
rf 2048 gain 32
tp not used spin not used
ss 32 GRADIENTS
d1 1.000 gzl1 4672
nt 32 gtl1 0.001000
2D ACQUISITION gzl1v13 2344
sw1 30165.9 gt3 0.000000
ri 256 gstab 0.000500
phase 0 F2 PROCESSING
PRESATURATION sb 0.064
satmode nnn sbs not used
satddy 0 fn 2048
satfrq 499.8 F1 PROCESSING
satpwr -13 sb1 0.008
TRANSMITTER sb51 not used
tn H1 ploc1
sfreq 499.881 fn1 2048
tof 999.7 DISPLAY
tpwr 59 sp -39.9
pw 9.500 wp 7476.6
DECOUPLER C13 sp1 -58.6
dn C13 w1 25747.9
dof 1255.4 rf1 500.9
dm nnn rfp 0
dmf 32258 rf11 1885.1
dpwr 35 rfp1 0
pwxy1 50 PLOT
pwx 16.100 w 150.0
HMBC 140.0 sc 0
j1xh 8.0 wc2 150.0
jnkh 8.0 sc2 0
vs 32702
th 8
ai cdc av

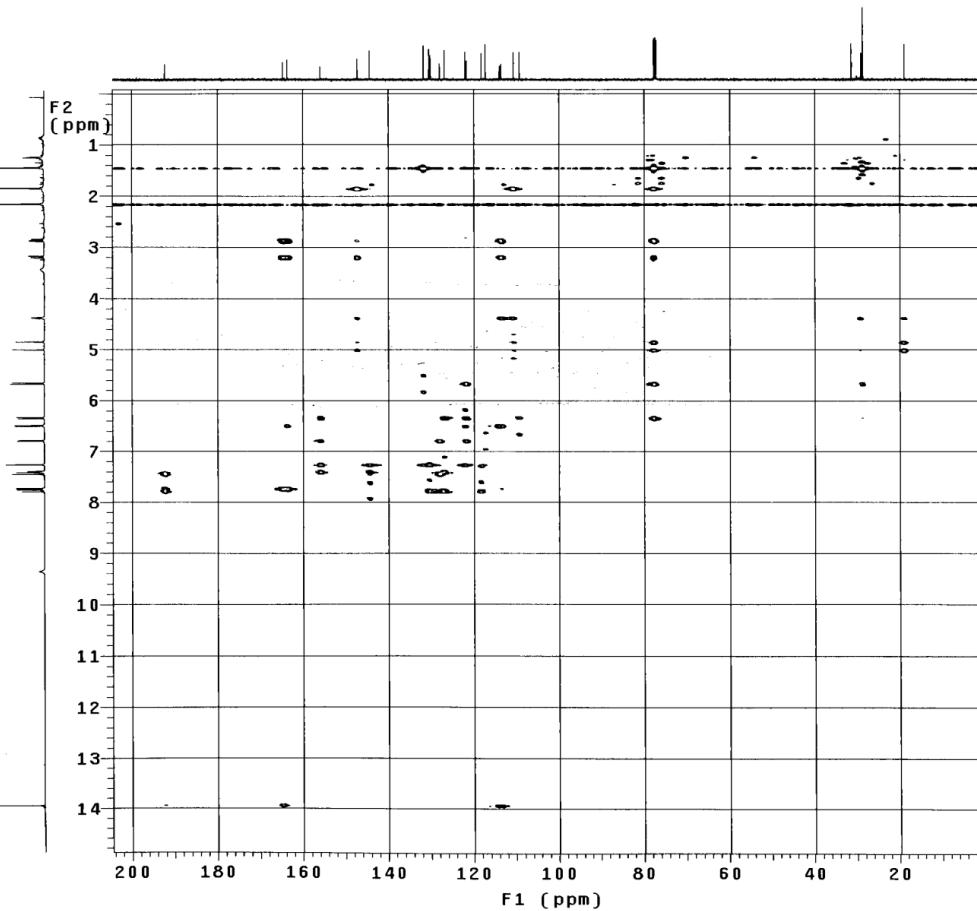


Fig. 96. Angusticornin A (5)的HMBC圖譜

C:\Xcalibur\data\MJD\CSH-233e
DIP-EI-70ev

12/23/2011 2:33:01 PM

CSH-233e #166-168 RT: 3.41-3.45 AV: 3 NL: 1.08E6
T: + c Full ms [50.00-650.00]

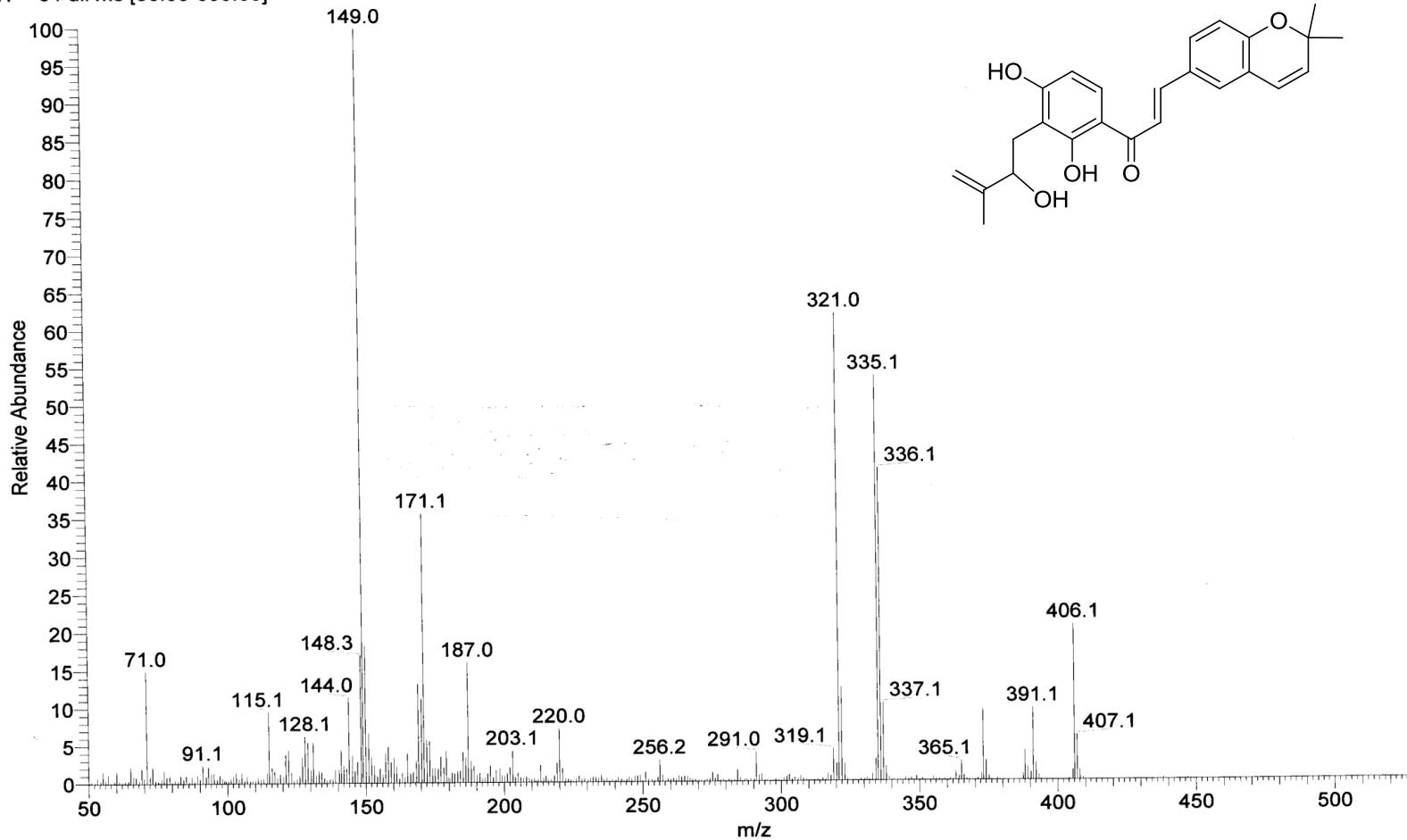


Fig. 97. Angusticornin A (5)的EI-MS圖譜

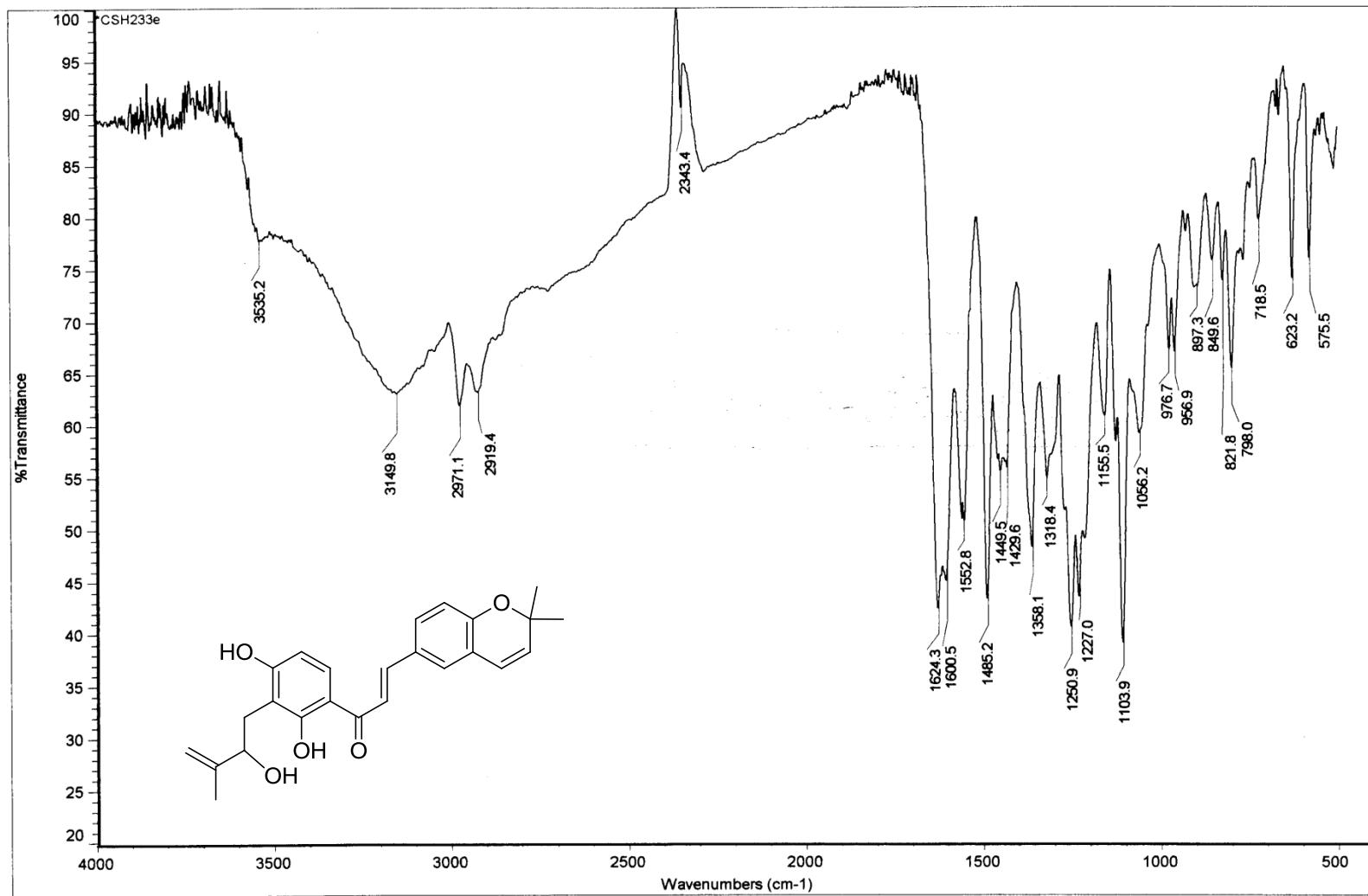


Fig. 98. Angusticomin A (5)的FTIR圖譜