

Supporting Information

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New Secondary Metabolites from an Endophytic Fungus in *Porodaedalea pini*

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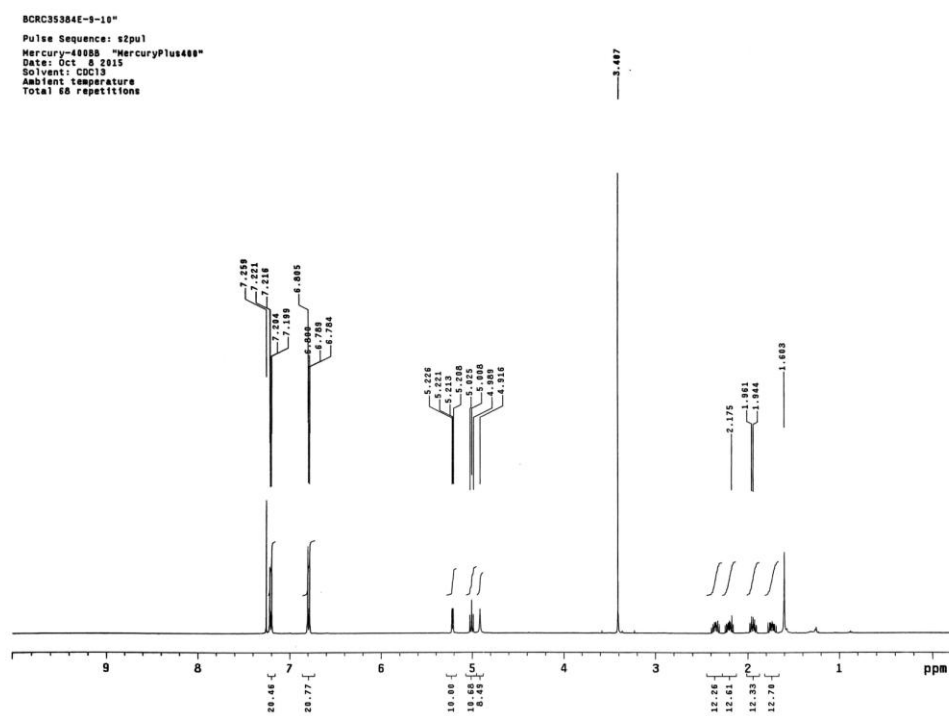
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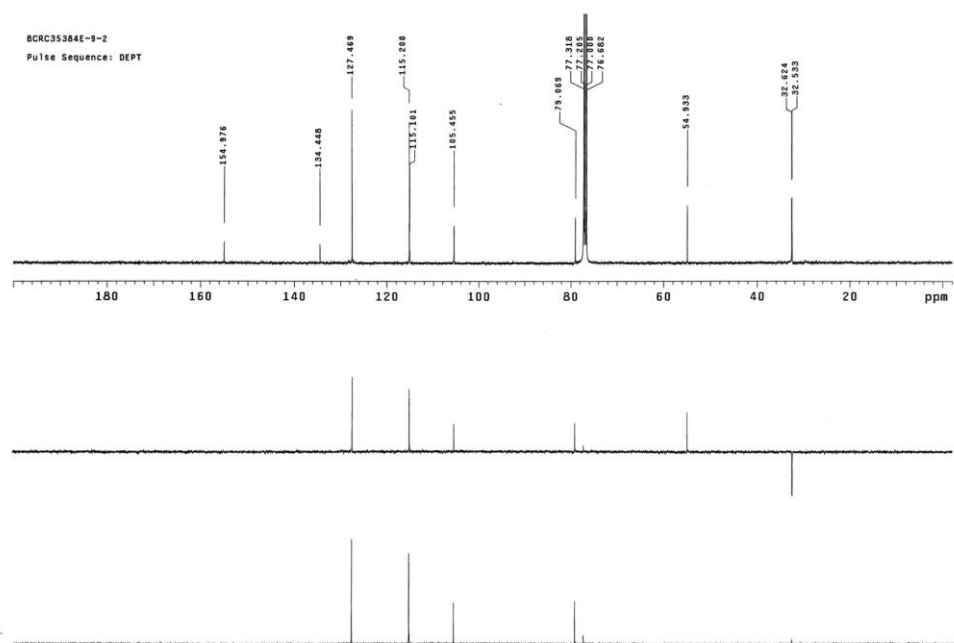
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S1: ¹H NMR spectrum of piniphenol A (**1**) in CDCl₃ at 400 MHz



S2: DEPT spectrum of piniphenol A (**1**) in CDCl₃ at 100 MHz

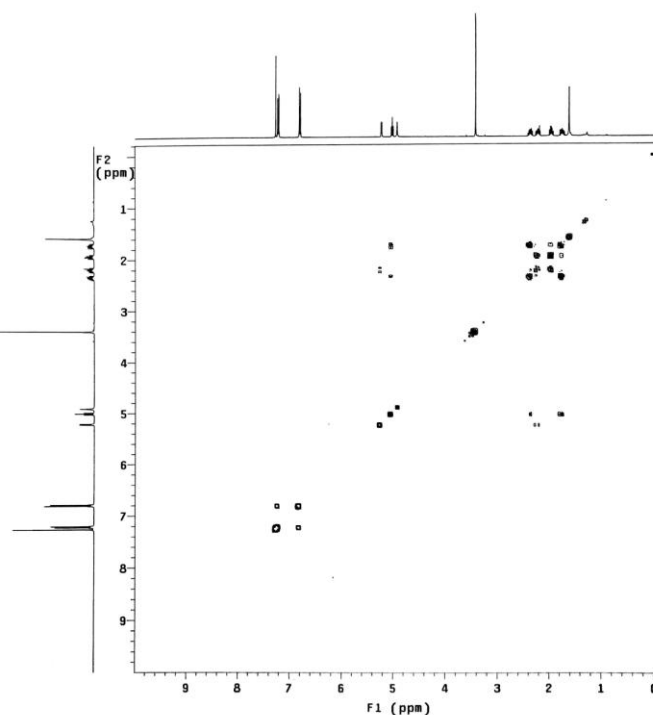
BCRC35384E-9-2

exp14 gCOSY

```

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date      Oct 8 2015      tsspl      n
solvent      CDCl3      hsglv1      992
sample      undefined
ACQUISITION      SPECIAL
sw      600.9      comp      not used
at      0.170      gain      30
np      2048      spin      0
fb      3480      F2 PROCESSING
ss      16      sb      -0.005
d1      1.008      sbx      not used
nt      48      fn      4096
2D ACQUISITION      F1 PROCESSING
sv1      600.9      sb1      -0.021
n1      168      sbx1      not used
TRANSMITTER      proc1      10
tp      400.485      fml      4096
ufq      61      vp      -01.5
tof      10.700      up1      -82.2
pw      GRADIENTS      wpl      4081.7
gzlv1      992      rfp1      941.2
gtl      0.001000      rfp      0
gstab      0.000500      rfl1      941.9
DECOUPLER      rfp1      0
dn      hs      PLOT      140.0
dm      nnn      wc      140.0
          vc      140.0
          vs      5.0
          th      694
          at      av      5

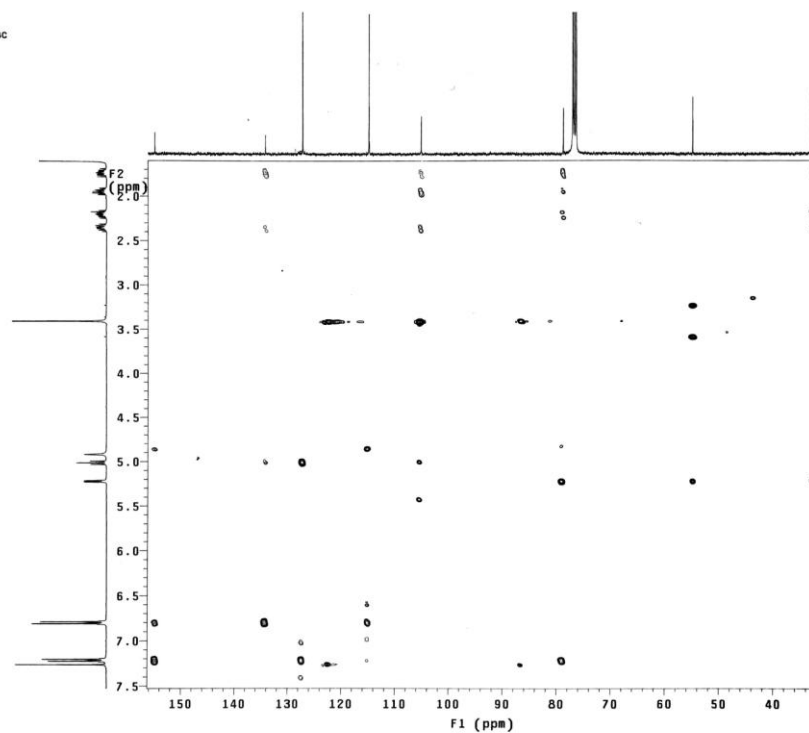
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S3: COSY spectrum of piniphenol A (1)

BCRC35384E-9-2

Pulse Sequence: gHMBC



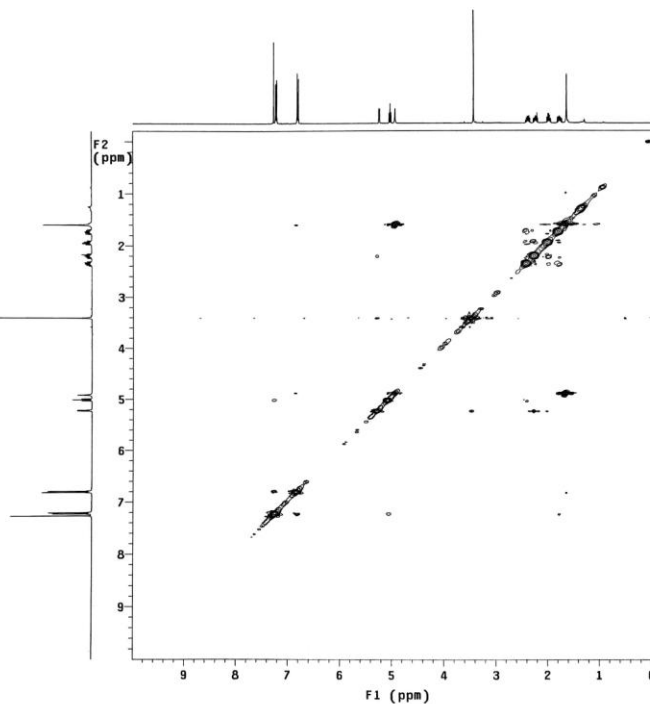
S4: HMBC spectrum of piniphenol A (1)

BCRC35384E-9-2
exp15 NOESY

```

SAMPLE          hs      FLAGS      n
date    OCT 8 2015  sspl      y
solvent  CDCl3      spul      y
sample   undefined  pfgf1q     y
ACQUISITION  hsglv      992
v1        600.5      temp    not used
at        0.179      gain    26
np        2048      spin    0
fs        not used  f2 PROCESSING 0
ss        32        gfs    not used
d1        1.289      f1      0.079
nt        48        f1      4096
2D ACQUISITION  f1 PROCESSING 0
v1        600.5      gfs1    0.023
n1        160      p1      not used
TRANSMITTER  H1      proc1    0
tn        400.489  f1      4096
t1f1      400.9      f1      4096
t1f2      400.9      f1      4096
pw        10.700  sp      400.1
NOESY      0.600  sp1      400.1
PRESATURATION  r1f1    400.0
satmode      nnnn    rfp      539.9
satpwr      0      r1f1    539.9
sat1v      0      rfp1    0
satf1q      0      PLOT    0
DECOUPLER  H1      sc      100.0
dn        nnn      wc2     140.0
dm        th      sc2     5.0
          al      th      894
          ph      3

```



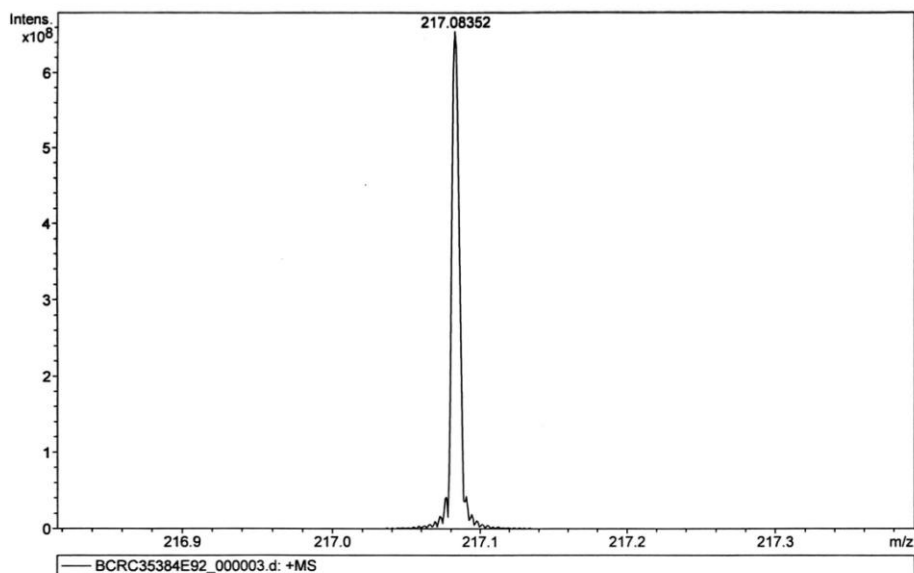
S5: NOESY spectrum of piniphenol A (1)

Mass Spectrum SmartFormula Report

Analysis Info

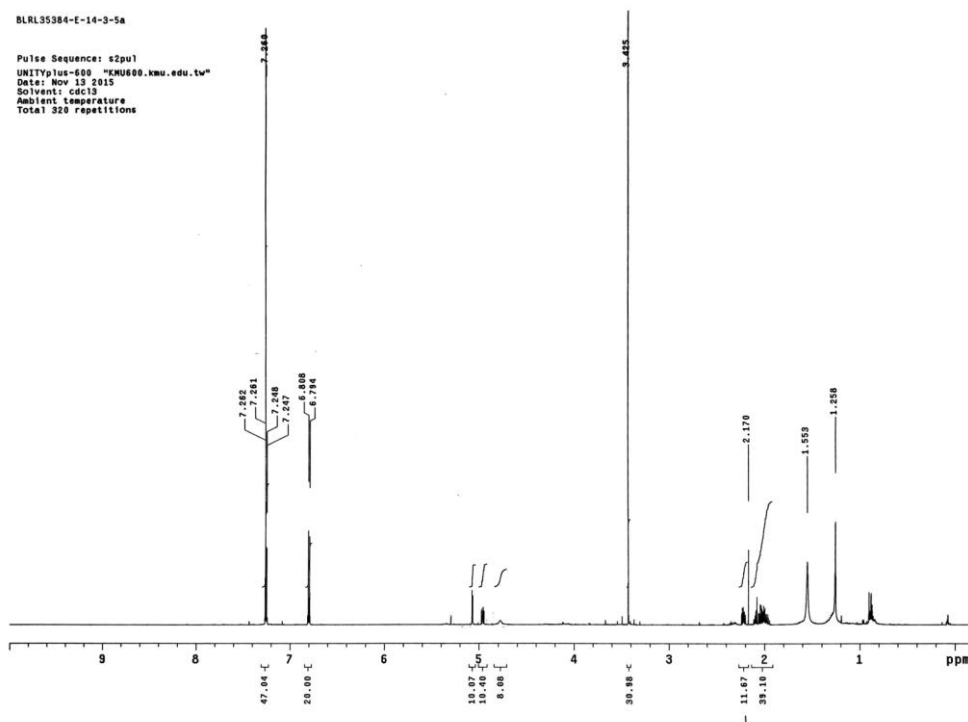
Analysis Name D:\Data\C3\BCRC35384E92_000003.d
Method broadband first signal
Sample Name BCRC35384-E-9-2
Comment ESI Positive

11/6/2015 2:56:45 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solarix

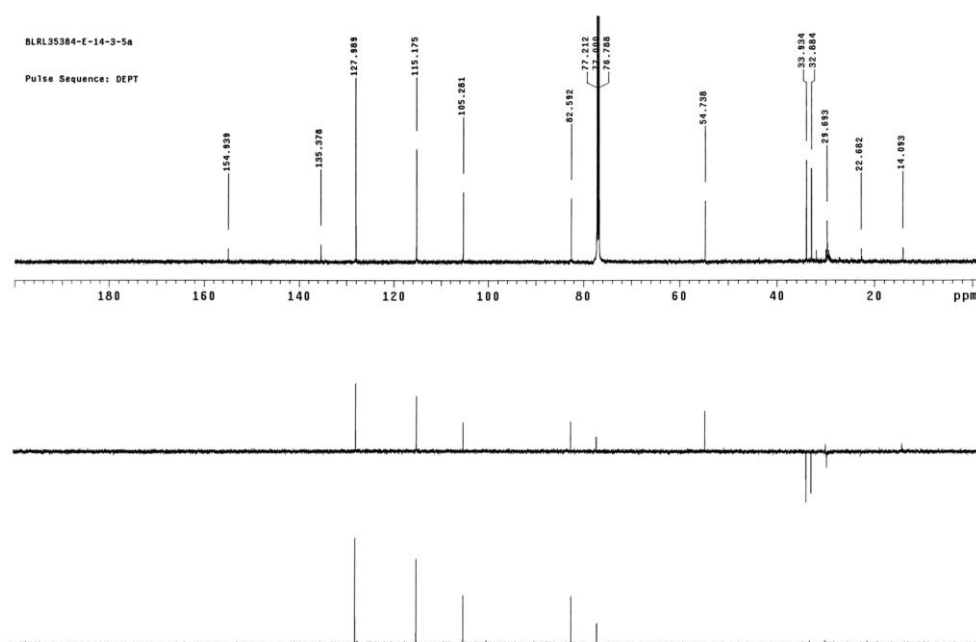


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
217.08352	1	C 11 H 14 Na O 3	100.00	217.08352	-0.01	-0.03	16.6	4.5	even	ok

S6: HRESIMS spectrum of piniphenol A (1)



S7: ^1H NMR spectrum of piniphenol B (2) in CDCl_3 at 600 MHz



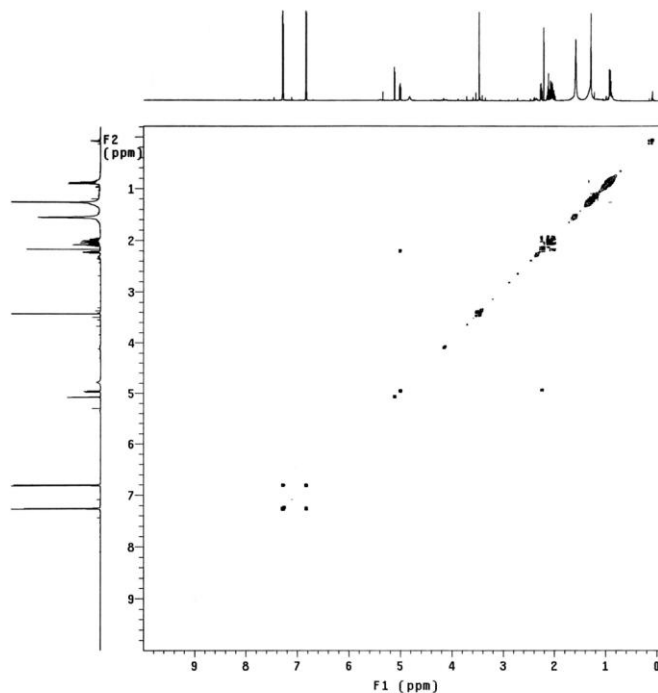
S8: DEPT spectrum of piniphenol B (2)

BLRL35384-E-14-3-5a
exp14 gCOSY

```

SAMPLE          FLAGS      nn
date   Nov 13 2015   he      Y
solvent cdc13      espu1    Y
sample  hsgv1      SPECIAL  5280
ACQUISITION
  sw      9542.0 temp      30.0
  at      0.150 gain      32
  np      2882 spin      0
  fd      4000 f2 PROCESSING 0
  ss      32 sb      -0.075
  d1      1.000 sbc      not used
  nt      40 f0      4096
2D ACQUISITION f1 PROCESSING
  sw1     9542.0 sb1      -0.013
  nt1     160 sbc1      not used
  d2      0 p1oc1      1p
  PRESATURATION fml      4096
  satmode      n DISPLAY -121.8
  wet          n sp      6088.5
  TRANSMITTER  H1 sp1      -121.1
  tn          597.315 vp1     6088.5
  tpf         597.3 rf1     1198.1
  tpm         58 rfp      0
  pw         12.000 rfp1    1202.1
  GRADIENTS    rf01      0
  g2iv1E      4405 PLOT    140.0
  g2E         0.001000 wc      5.0
  Edratio     1.000 sc      140.0
  g2mb        0.000500 wc2     5.0
  DECOUPLER    sc2      5.0
  dn          C13 vs      160
  dm          nm1 tn      8
  av

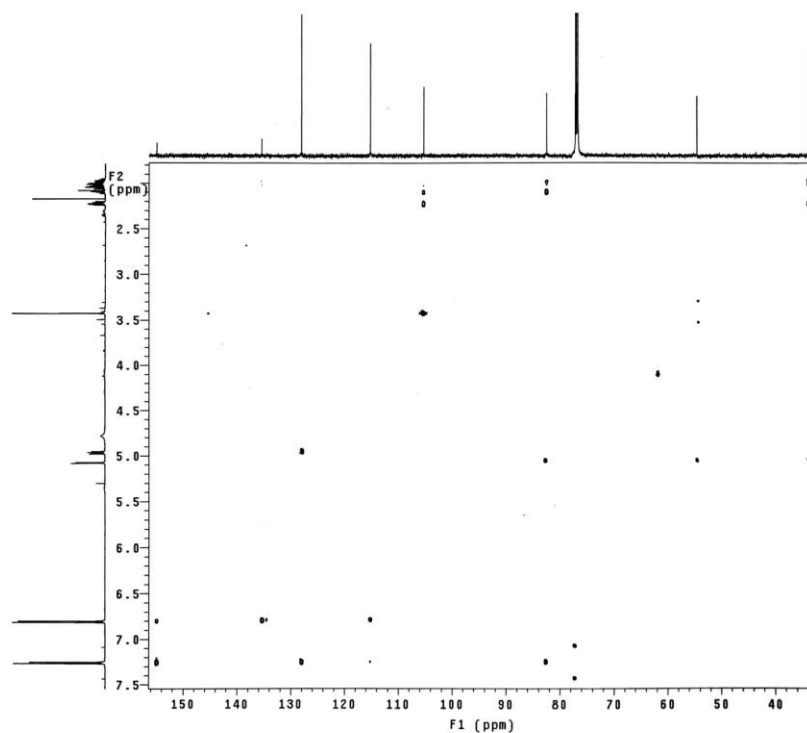
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S9: COSY spectrum of piniphenol B (2)

BLRL35384-E-14-3-5a

Pulse Sequence: gHMBCAD



S10: HMBC spectrum of piniphenol B (2)

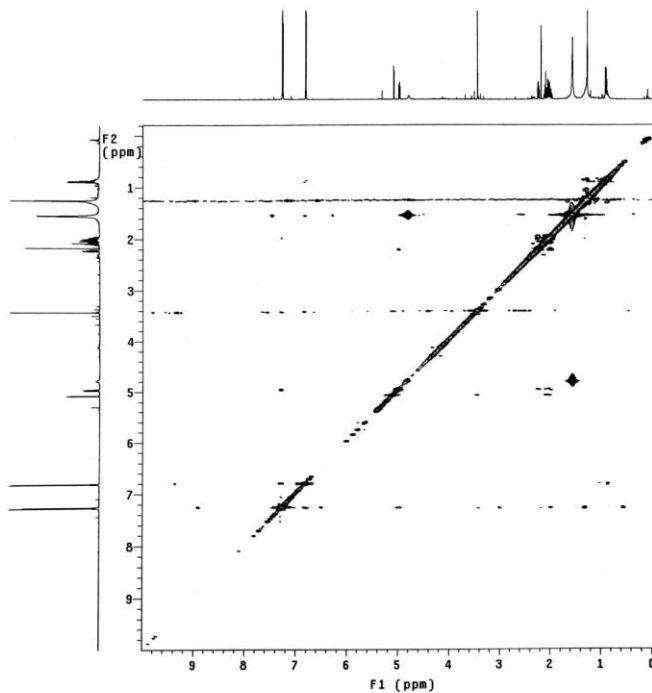
BRL35384-E-14-3-5a

exp5 NOESY

```

SAMPLE          date Nov 13 2015  hs  flags  nn
solvent          cdc13  sspul1  y
sample          PRDF1g  y
ACQUISITION      hsglv1  5280
sv              9542.0  temp  30.0
at              0.150  SPECIAL
np              2862  gain  48
fs              4000  spin  9
ss              16    f2 PROCESSING
d1              1.500  gf  0.969
nt              40    gfs  not used
2D ACQUISITION   f1  f3 PROCESSING
sv1             9542.0  gf1  0.014
n1              160    gf3  not used
TRANSMITTER      N1  procl  1p
tn              597.315  f1  4036
tof             597.3  DISPLAY
tpwr            58    sp  -123.3
pw             12.000  wp  6003.5
NOESY            0.600  sp1  -121.1
mixM            n  rf1  1199.6
PRESATURATION    n  rf2  0
satmode         n  rf3  1197.4
wet             n  rf4  0
DECOUPLER        C13  rf5  0
dm              nnn  PLOT
                  wc  140.0
                  sc  5.0
                  wc2 140.0
                  vc  5.0
                  th  400
                  al  ph  4

```



S11: NOESY spectrum of piniphenol B (2)

Data:BCRC35384-E-14-3-5c-3(1)

Comment:Method Set 1

Description:

Ionization Mode:ESI+

History:Average(MS[1] 0.56..0.58)

Acquired:1/21/2016 4:01:27 PM

Operator:AccuTOF

m/z Calibration File:20160121TFANa...

Created:1/22/2016 11:06:59 AM

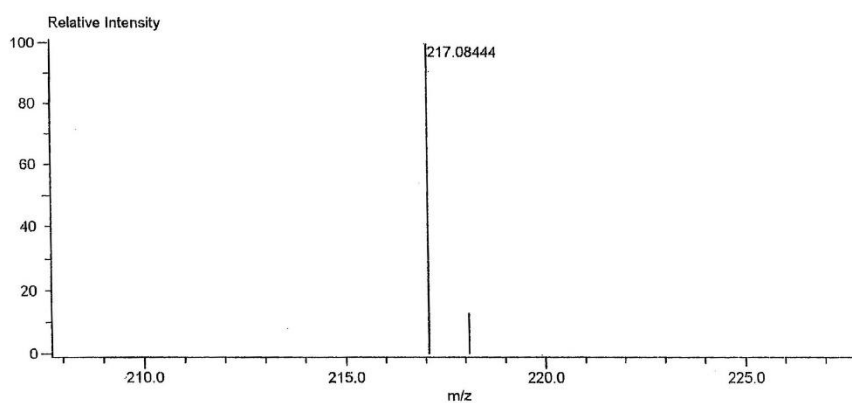
Created by:AccuTOF

Charge number:1

Tolerance:1.00[ppm], 1.00 .. 10.00[mDa]

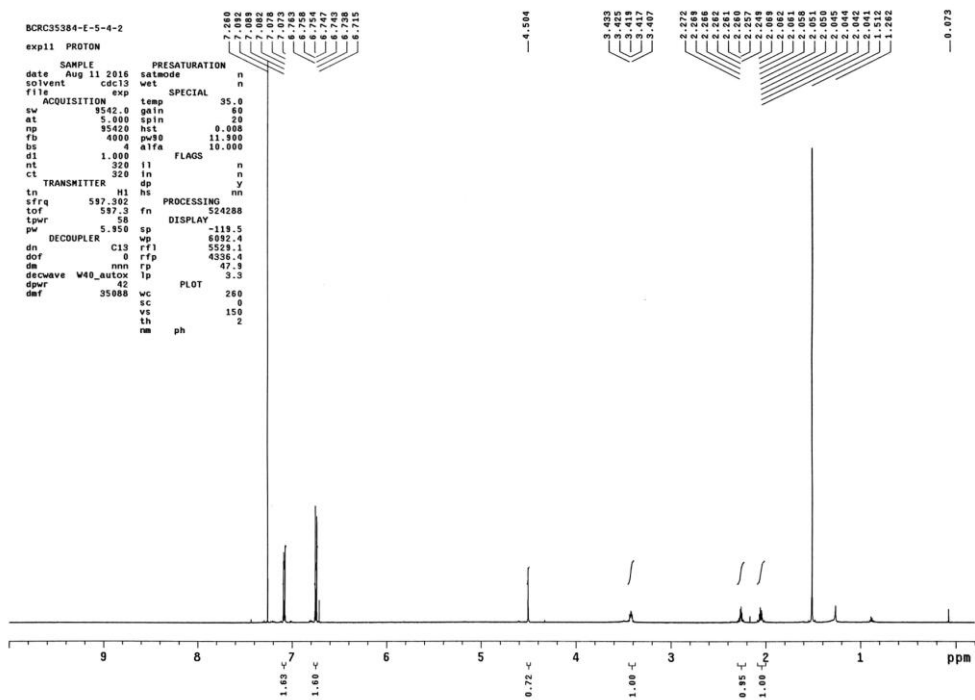
Unsaturation Number:-1.5 .. 20.0 (Frac...

Element:¹²C:0 .. 31, ¹H:0 .. 100, ¹⁴N:0 .. 3, ²³Na:0 .. 1, ¹⁶O:0 .. 10

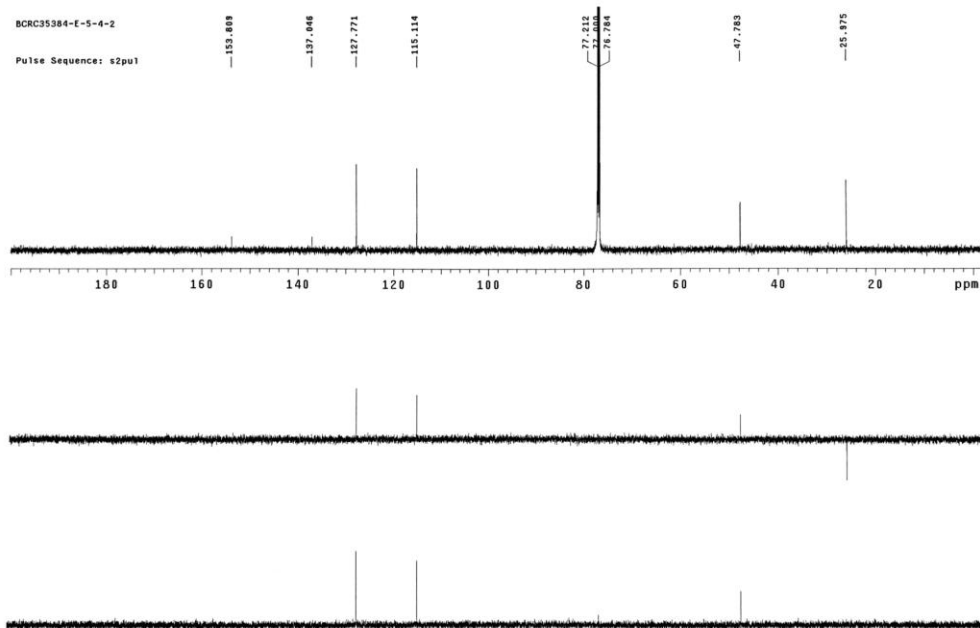


Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
217.08444	37276.38	217.08406	0.37	1.72	¹² C ₁₁ ¹ H ₁₄ ²³ Na ₁ ¹⁶ O ₃
		217.08513	-0.69	-3.17	¹² C ₁₁ ¹ H ₁₁ ¹⁴ N ₃ ¹⁶ O ₂

S12: HRESIMS spectrum of piniphenol B (2)



S13: ^1H NMR spectrum of piniphenol C (**3**) in CDCl_3 at 600 MHz



S14: DEPT spectrum of piniphenol C (**3**)

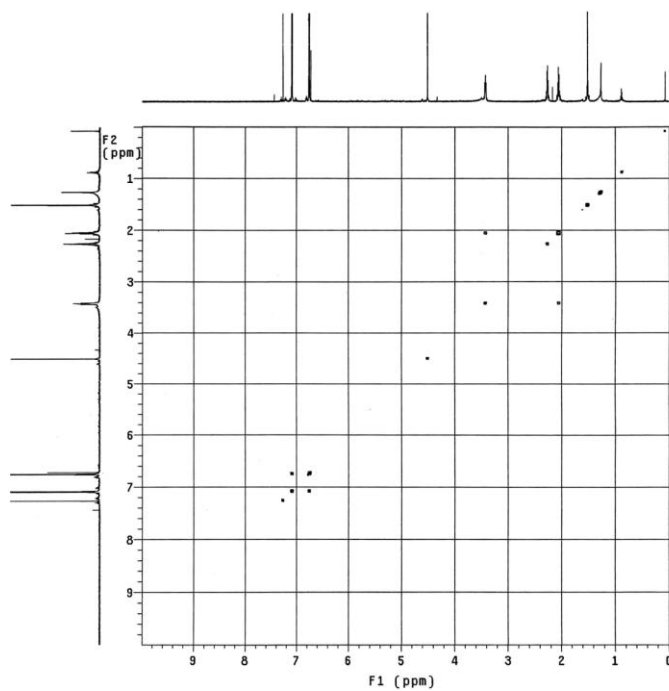
BCRC35384-E-5-4-2

exp14 gCOSY

```

SAMPLE          flags      nm
date Aug 11 2016  h5      Y
solvent cdc13  h5glv1  5280
sample          SPECIAL
sv 8542.0 temp 35.0
at 0.150 gain 80
np 2882 spin 0
fb 4000 f2 PROCESSING 0
ss 32 sb -0.075
d1 1.000 sbx not used
nt 48 fn 4096
2D ACQUISITION f1 PROCESSING
sv1 8542.0 sb1 -0.017
n1 160 sbol not used
d2 0 PROC1 lp
PRESATURATION fn1 4096
satmode n sp DISPLAY -1.8
wct n sp 5968.4
tn TRANSMITTER H1 sb1 -1.2
tfr 597.302 wp1 5968.4
tof 387.3 rfp1 1198.2
tpwr 58 rfp 0
pw 11.900 rfp1 1198.0
GRADIENTS 4485 PLOT
g2lvie 0.001000 wc 140.0
g1c 1.000 sc 5.0
g1stab 0.000500 wc2 140.0
DECOUPLER sc2 5.0
dn C13 va 450
dm nnn th 2
et cdc av 2

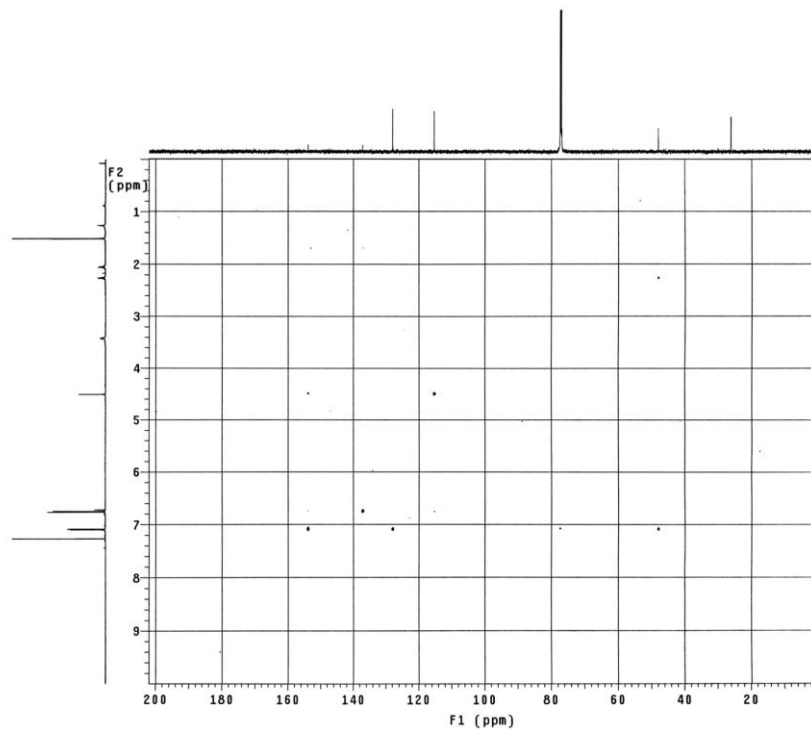
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S15: COSY spectrum of piniphenol C (3)

BCRC35384-E-5-4-2

Pulse Sequence: gHMBCAD



S16: HMBC spectrum of piniphenol C (3)

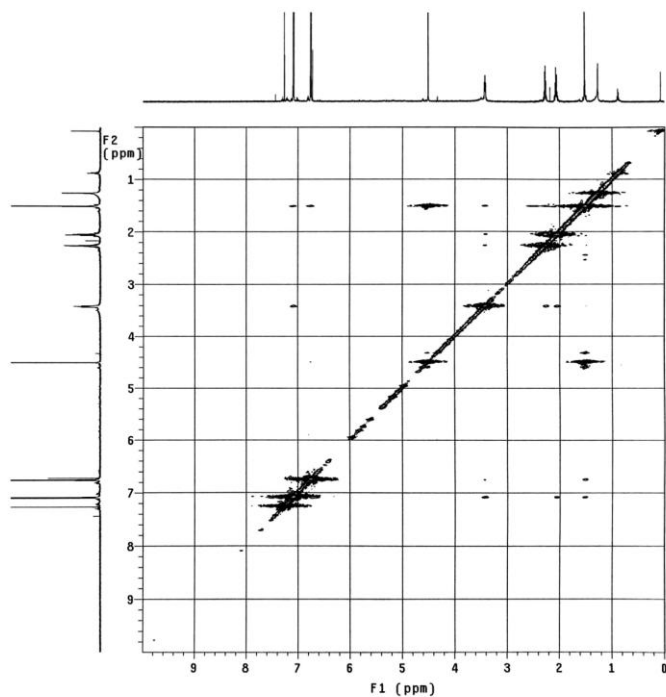
BCRC35384-E-5-4-2

exp15 NOESY

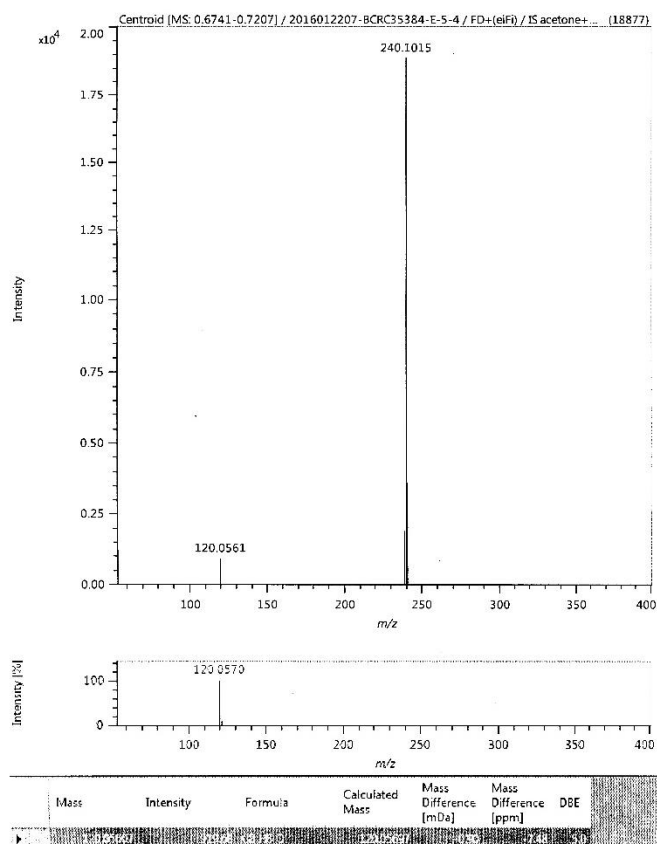
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solvent cdc13 sspul1 y
sample PFG1p hsglv1 y
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sv 0.150 temp 52
at 2862 gain 52
rs 4000 spin 0
ss 32 f2 PROCESSING 0
d1 1.500 gf not used
nt 48 gf 0.063
2D ACQUISITION 48 f1 not used
sv1 9542.0 f1 PROCESSING 4096
nt 160 gf1 0.016
TRANSMITTER H1 gf1 not used
tn 597.302 f1 proc1 lp
tofr 597.3 f1 DISPLAY -1.5
tpr 50 sp 5968.4
pw 11.900 wp1 -1.2
NOESY 0.600 wp1 5968.4
PRESATURATION n rf1 1198.9
satmode n rfp 0
wet n rf1 1194.0
DECOUPLER C13 n rf1 0
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dm nnn sc 5.0
wc2 140.0
vs 5.0
th 450
at cdc ph 2

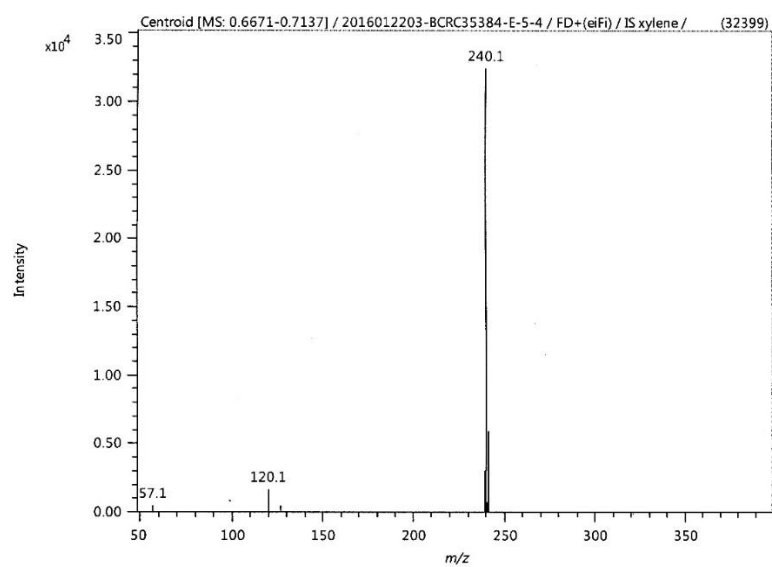
```



S17: NOESY spectrum of piniphenol C (3)



S18: HRFDMS spectrum of piniphenol C (3)



S19: FDMS spectrum of piniphenol C (3)