

## Supporting Information

*Rec. Nat. Prod.* **10:2** (2016) 189-194

### Secondary Metabolites and Bioactivity of the Endophytic Fungus *Phomopsis theicola* from Taiwanese endemic plant

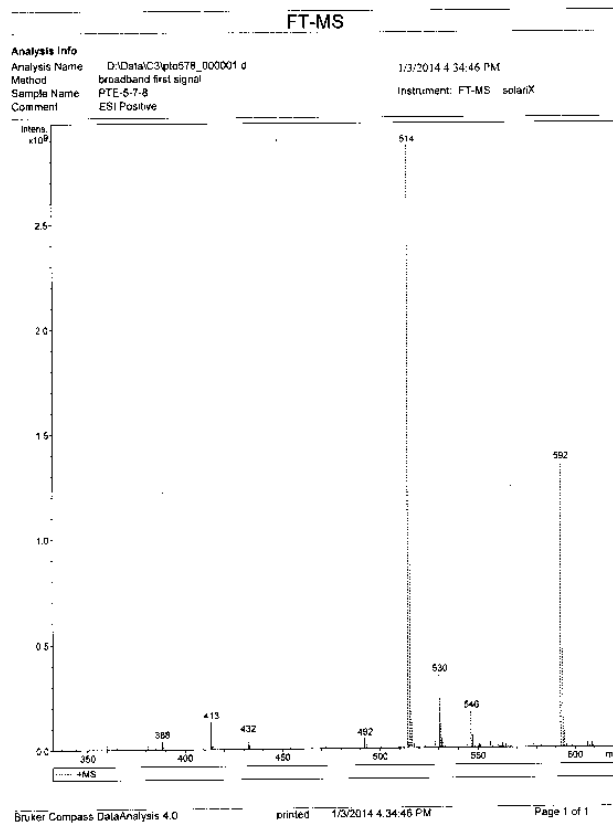
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**S1: ESI-MS Spectrum of Compound 1 (phomocytochalasin)**

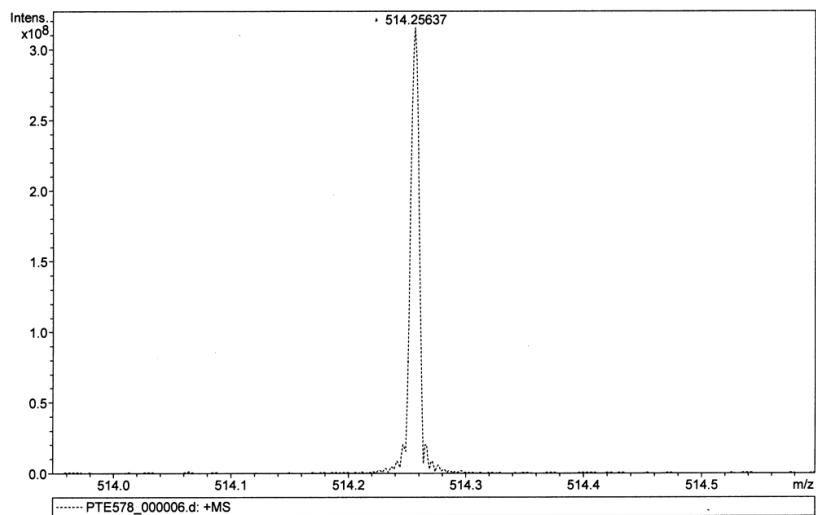
## Mass Spectrum SmartFormula Report

### Analysis Info

Analysis Name D:\Data\C3\PTE578\_000006.d  
Method broadband first signal  
Sample Name PTE5-7-8  
Comment ESI Positive

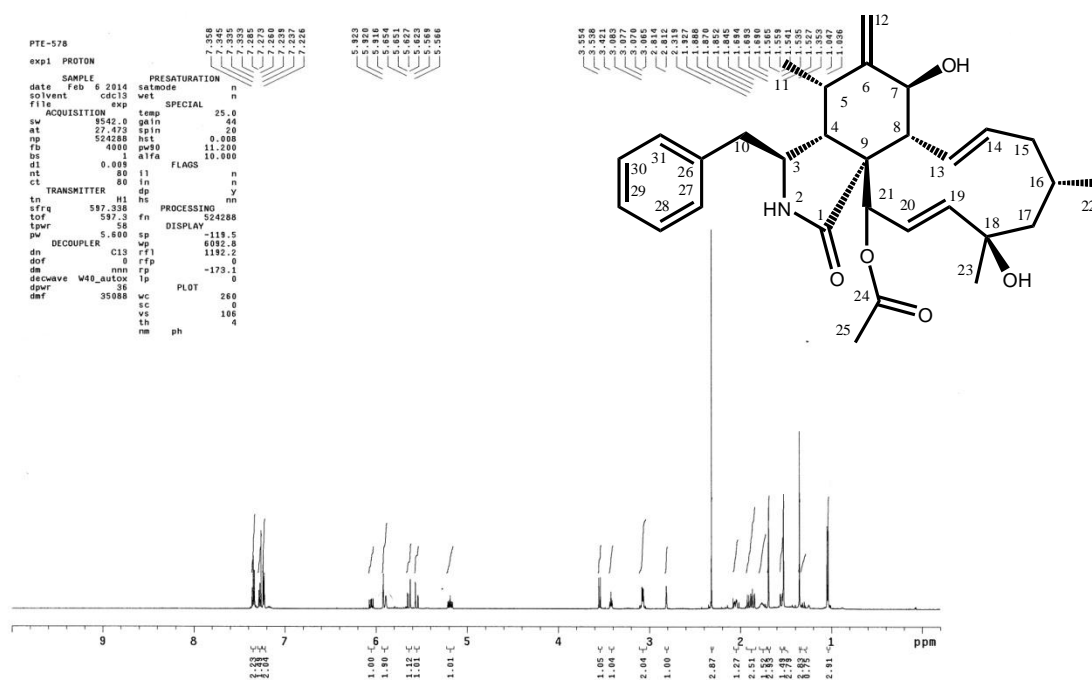
1/13/2014 3:00:29 PM

Instrument: FT-MS solarix



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
514.25637	1	C 30 H 37 N Na O 5	100.00	514.25639	0.03	0.05	6.6	12.5	even	ok

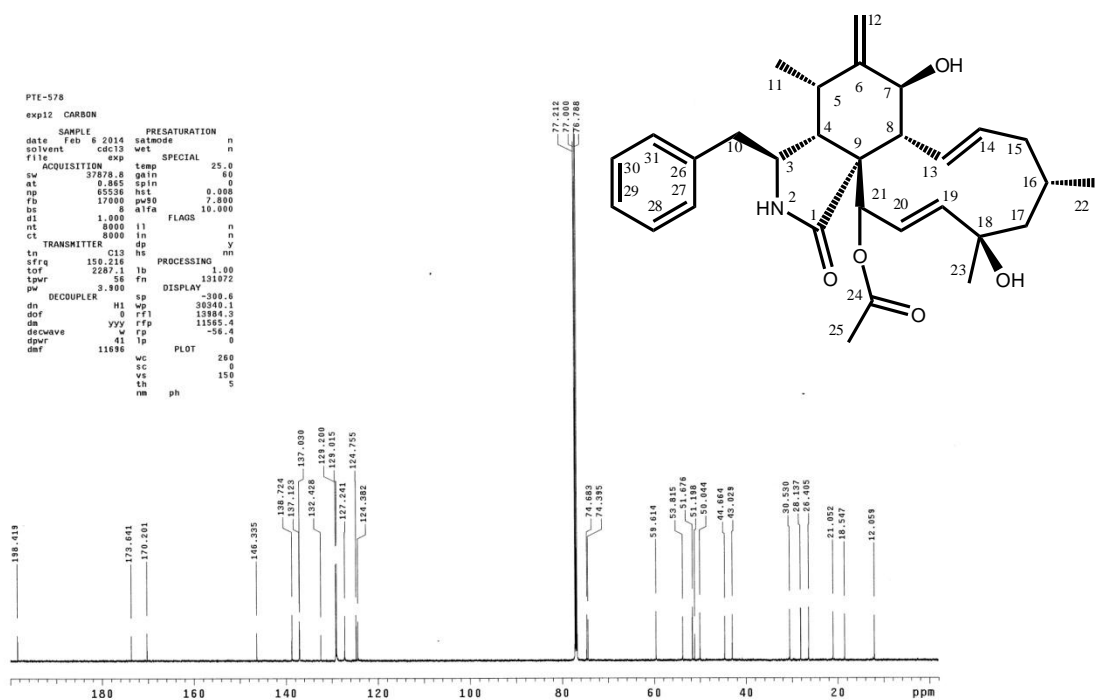
**S2: HRESI-MS Spectrum of Compound 1 (phomocytochalasin)**



### S3: <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>) Spectrum of Compound 1 (phomocytochalasin)

#### <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)

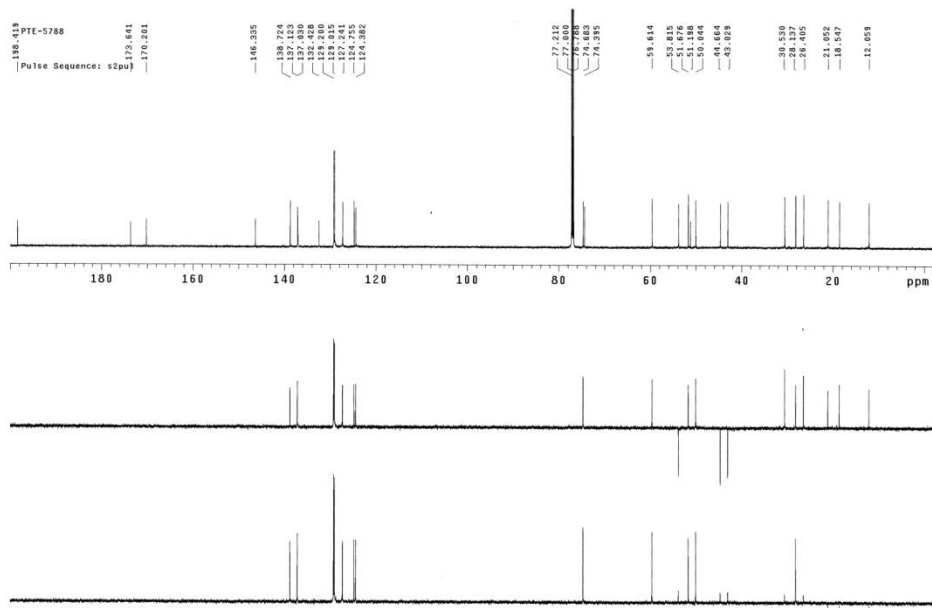
$\delta$  1.04 (3H, d,  $J = 6.6$  Hz, H-22), 1.35 (3H, s, H-23), 1.53 (3H, s, H-11), 1.55 (1H, dd,  $J = 14.4, 3.6$  Hz, H-17b), 1.69 (3H, s, H-12), 1.76 (1H, m, H-16), 1.86 (1H, dd,  $J = 14.4, 6.6$  Hz, H-17a), 1.90 (1H, br dd,  $J = 13.2, 1.8$  Hz, H-15b), 2.03 (1H, br dd,  $J = 13.2, 4.8$  Hz, H-15a), 2.32 (3H, s, H-25), 2.81 (1H, d,  $J = 1.5$  Hz, H-4), 3.06 (1H, dd,  $J = 13.8, 7.8$  Hz, H-10b), 3.07 (1H, dd,  $J = 13.8, 7.8$  Hz, H-10a), 3.42 (1H, tt,  $J = 7.8, 1.5$  Hz, H-3), 3.55 (1H, d,  $J = 9.6$  Hz, H-8), 5.19 (1H, ddd,  $J = 16.2, 10.8, 4.8$  Hz, H-14), 5.55 (1H, dd,  $J = 16.8, 2.4$  Hz, H-19), 5.64 (1H, dd,  $J = 16.8, 2.4$  Hz, H-20), 5.89 (1H, br s, NH-2, D<sub>2</sub>O exchangeable), 5.92 (1H, t,  $J = 2.4$  Hz, H-21), 6.05 (1H, ddd,  $J = 16.2, 9.6, 1.2$  Hz, H-13), 7.23 (2H, d,  $J = 7.2, 1.2$  Hz, H-27), 7.35 (2H, td,  $J = 7.2, 1.2$  Hz, H-28), 7.27 (1H, dd,  $J = 7.8, 1.2$  Hz, H-29), 7.35 (2H, td,  $J = 7.2, 1.2$  Hz, H-30), 7.23 (2H, d,  $J = 7.2, 1.2$  Hz, H-31)



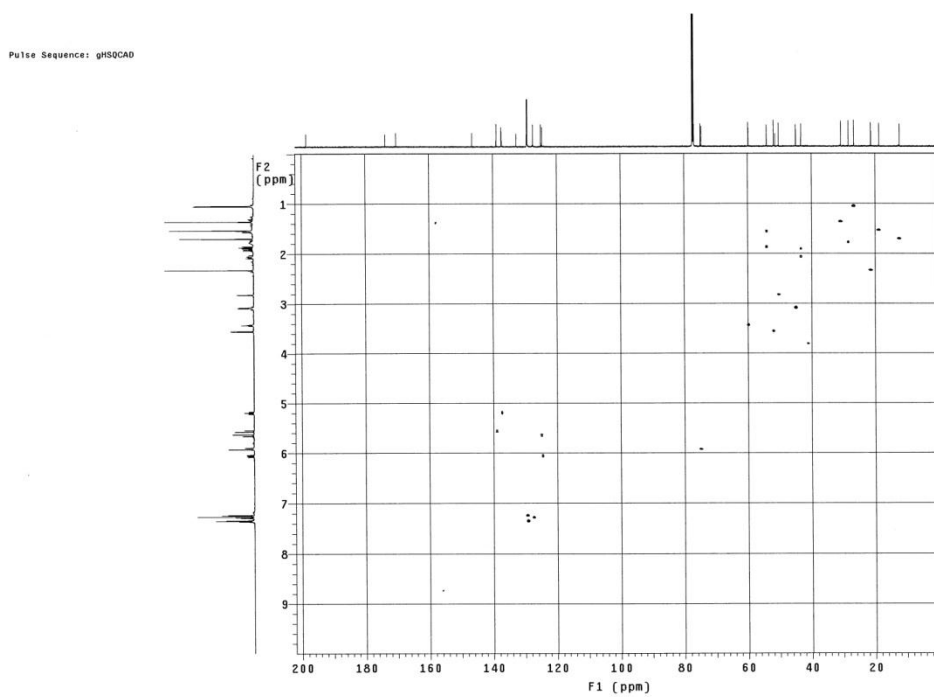
**S4:**  $^{13}\text{C}$ -NMR(150 MHz, $\text{CDCl}_3$ ) Spectrum of Compound **1** (phomocytchalasin)

$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )

$\delta$ 12.1 (C-12), 18.5 (C-11), 21.1 (C-25), 26.4 (C-22), 28.1 (C-16), 30.5 (C-23), 43.0 (C-15), 44.7 (C-10), 50.0 (C-4), 51.2 (C-9), 51.7 (C-8), 53.8 (C-17), 59.6 (C-3), 74.4 (C-18), 74.7 (C-21), 124.4 (C-13), 124.8 (C-20), 127.2 (C-29), 129.0 (C-28, 30), 129.2 (C-27, 31), 132.4 (C-6), 137.0 (C-26), 137.1 (C-14), 138.7 (C-19), 146.3 (C-5), 170.2 (C-24), 173.6 (C-1), 198.4 (C-7)



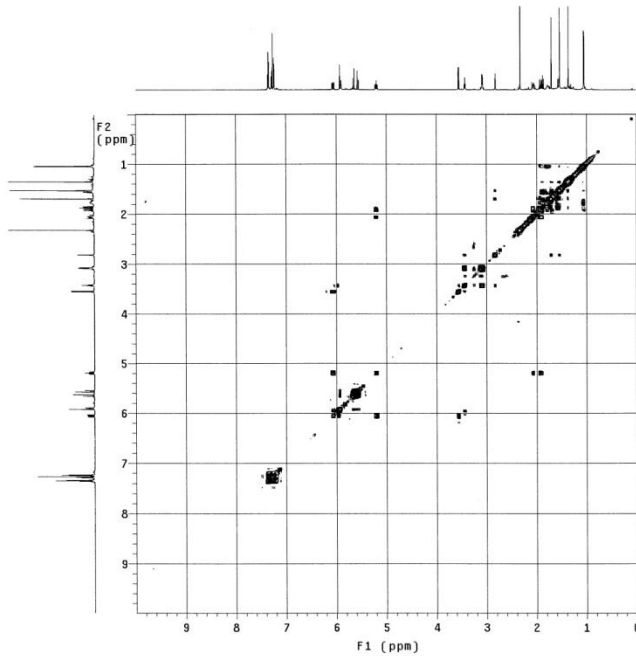
**S5: DEPT Spectrum of Compound 1 (phomocytochalasin)**



### S6: HSQC Spectrum of Compound 1 (phomocytochalasin)

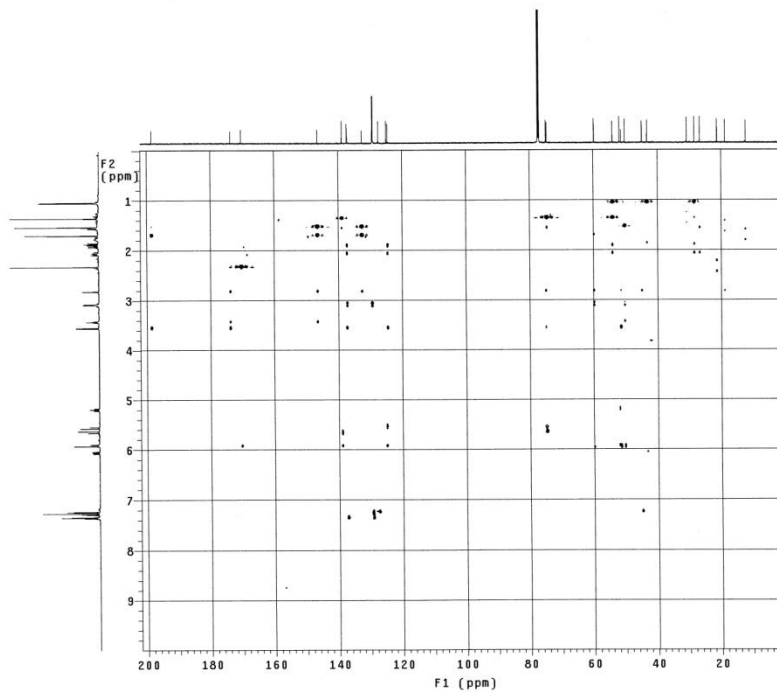
```

exp14 gCOSY
SAMPLE          hs   FLAGS      mn
date    Jan 17 2014  cdc13  spsu1   Y
solvent  cdc13      hsglvj   5328
sample
ACQUISITION    SPECIAL
sw         9542.0  temp       25.0
nt         0.150  gain       4.0
np         2862  spn        0
fs         4000   f2 PROCESSING 0
ss         32    sb       -0.075
d1         1.000  sb2     not used
nt         38    fn       4096
2D ACQUISITION  f1 PROCESSING 0
sw1        9542.0  sb1     -0.017
n1         160    sb2     not used
d2         0     proc1   1p
PRESATURATION  fn1     DISPLAY 4096
satmode       n       DISPLAY
wet           n       sp        -3.7
tn           n1      sp1       -3.7
rfra        597.258  wpl     5968.4
tor         597.4   rff     1191.8
tpwr        50     rfg       0
pw          11.200  rff1    1191.8
GRADIENTS     rfp1    0
gzlvie       4444   PLOT
gte          0.001000  wc      140.0
fdratio      1.000   sc       5.0
gstab        0.000500  wc2     140.0
DECOUPLER    cc2     5.0
dn           C13    vs       160
dm           nm    a1    cdc   av   2
  
```



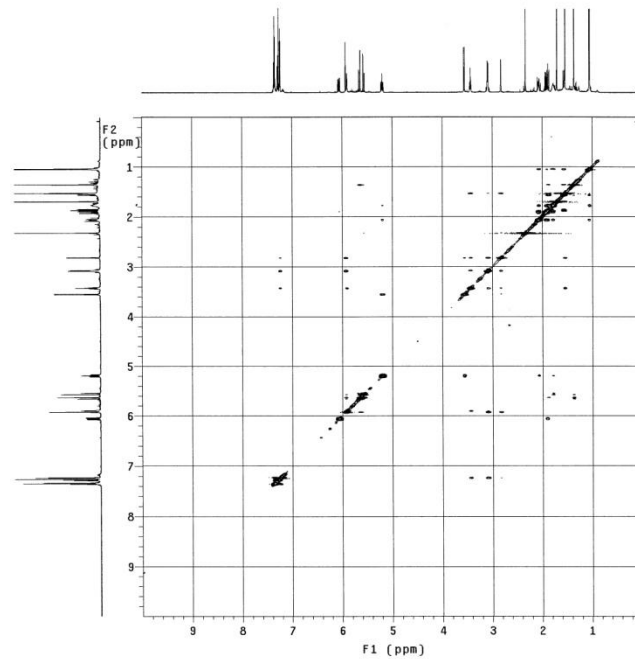
### S7: COSY Spectrum of Compound 1 (phomocytochalasin)

Pulse Sequence: gHMBCAD



### S8: HMBC Spectrum of Compound 1 (phomocytochalasin)

```
exp9 ROESY
SAMPLE
date Feb 6 2014 hs FLAGS nm
solvent cdc13 spsol y
sample POF1g y
ACQUISITION hsg1v1 SPECIAL 5328
sw 9542.0 SPECIAL
at 0.150 temp 25.0
np 2862 gain 28
fb 4900 spin 0
ss 15 F2 PROCESSING 0
d1 1.000 gf 0.059
nt 32 gfe not used
2D ACQUISITION fn 4096
sw1 9542.0 F1 PROCESSING
nl 160 gf1 0.018
tn TRANSMITTER h1 gf1 not used
sfrq 587.338 fn1 4096
tof 537.3 proc1 1p
tpwr 58 sp -4.2
pw 11.200 sp 5973.1
TQSY m1R sp1 -4.2
slpwR 46 rf1 1192.3
slpwK 47.350 rfp 0
trim 0.0020 rfp1 1192.3
PRESATURATION rfp1 0
satmode n PLOT
wet n wc 140.0
decopler n sc 0
dn C13 wc2 140.0
dm nmn cc2 5.0
vs 1096
th
nm ph 2
```



### S9: ROESY Spectrum of Compound 1 (phomocytochalasin)