Supporting Information

***Rec. Nat. Prod*. 17:1 (2022) 106-112**

First 6, 7-*Seco*-Clerodane Furan Diterpenoid from *Croton morifolius*

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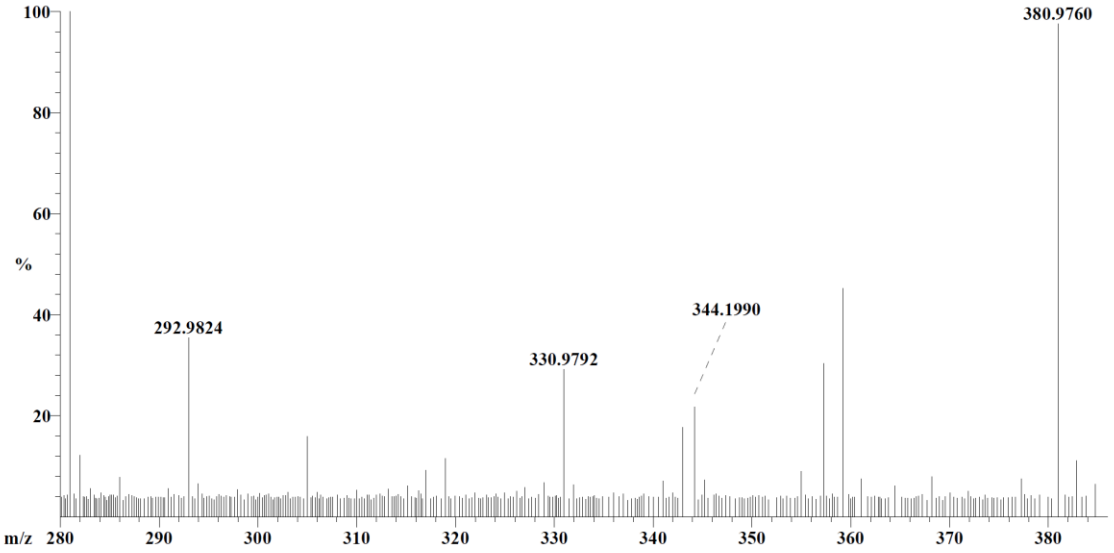
File: EBT COMPUESTO3-211221Date Run: 12-21-2021 (Time Run: 12:04:18)
Sample: EBT-COMP-3
Instrument: JEOL GCmate
Inlet: My Inlet **Ionization mode: EI+**

Scan: 94 **R.T.: 1.26**
Base: m/z 281; 2.1%FS TIC: 383056 **#Ions: 330**



Selected Isotopes : $H_{0-28}C_{0-21}O_{0-4}$ **Error Limit : 50 ppm** **Unsaturation Limits : 0 to 50**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*	*Unsaturation*
344.1990	21.8%	$C_{21}H_{28}O_4$	344.1988	0.7	8.0

Figure S1: EIHRMS spectrum of Morifolin A.

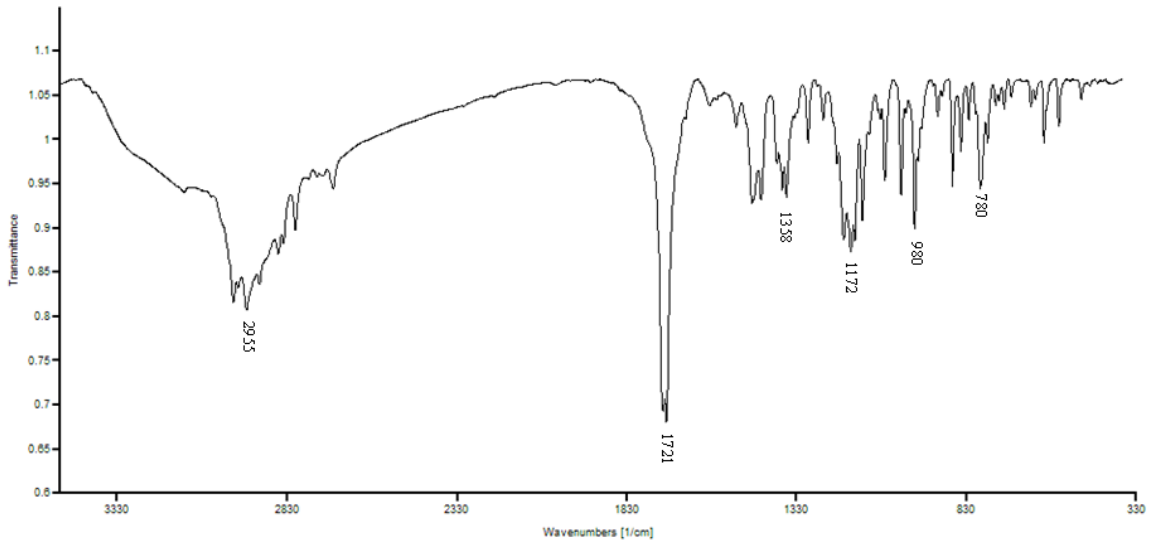


Figure S2: IR spectrum of Morifolin A.

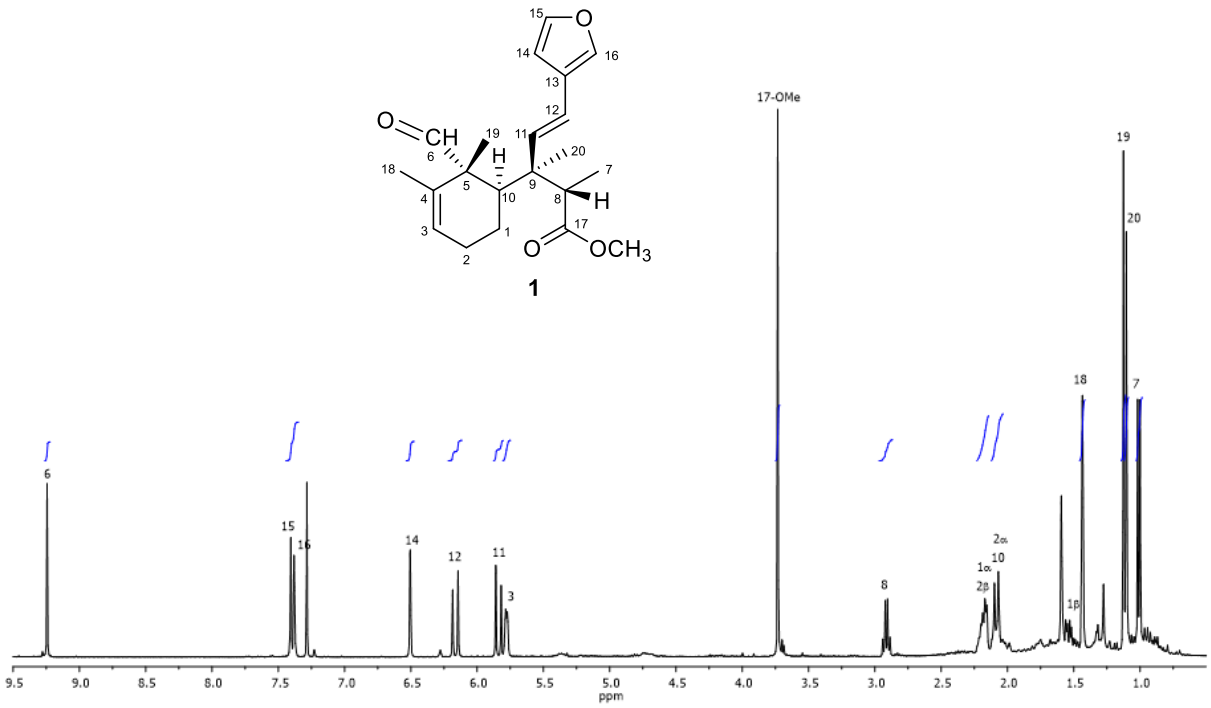


Figure S3: ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of Morifolin A.

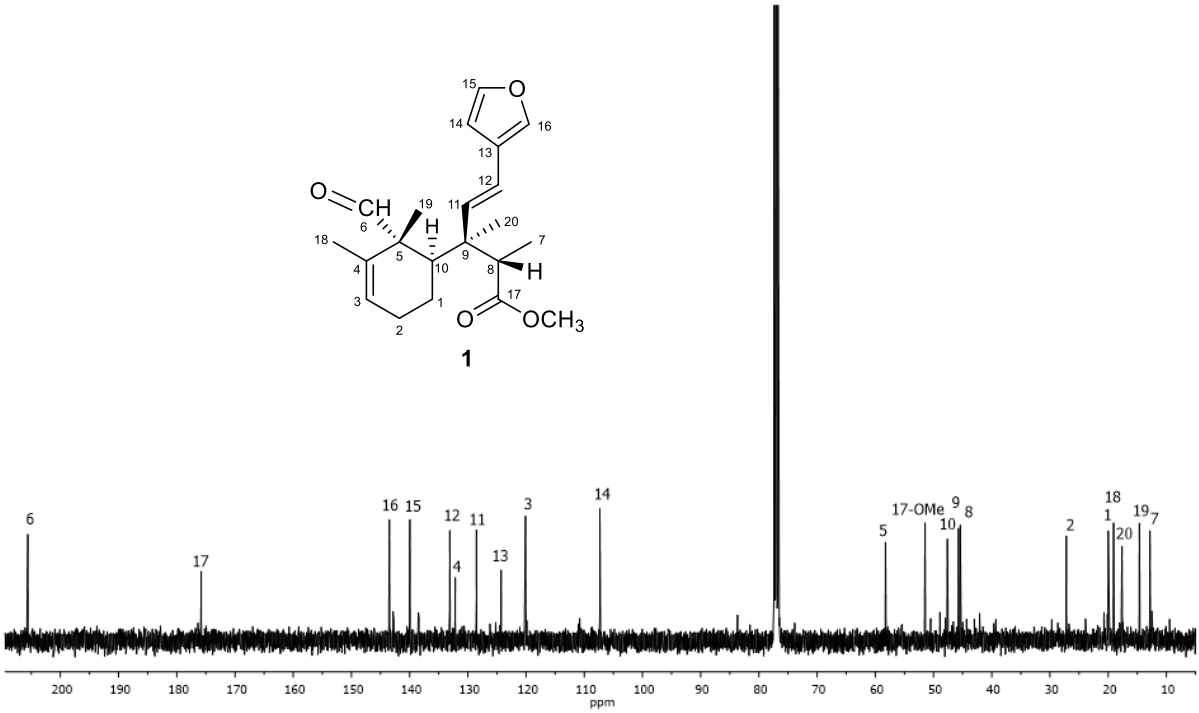


Figure S4: ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of Morifolin A.

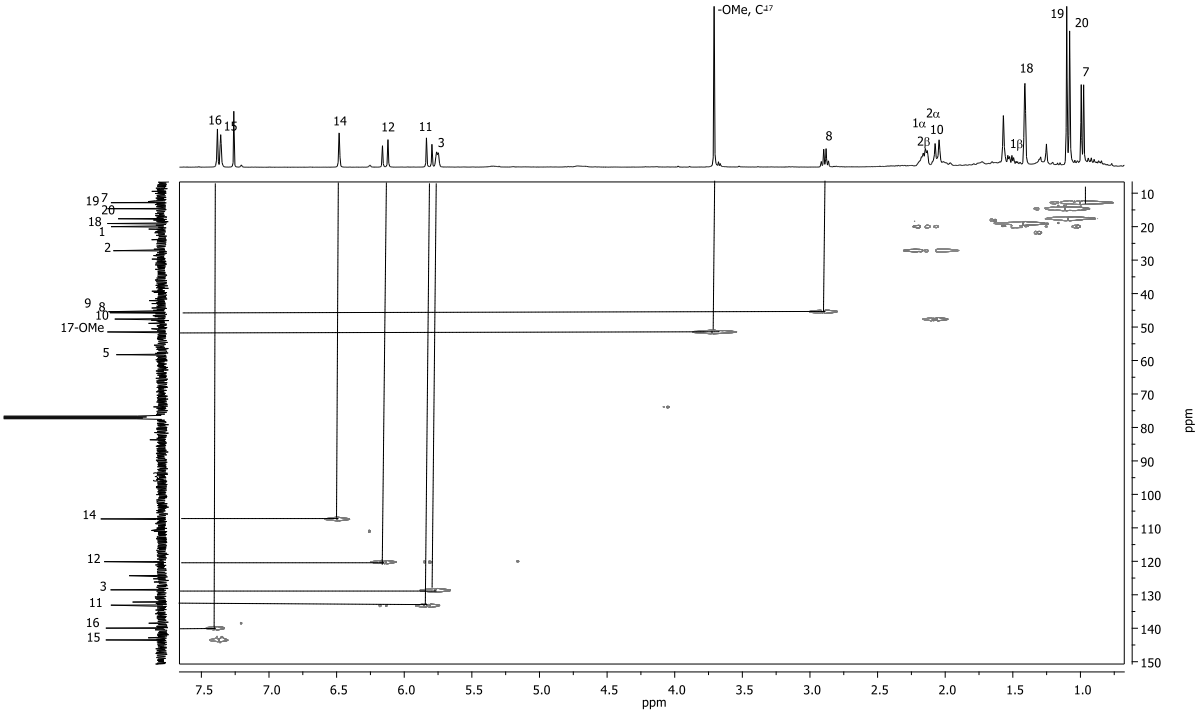


Figure S5: HSQC spectrum of Morifolin A

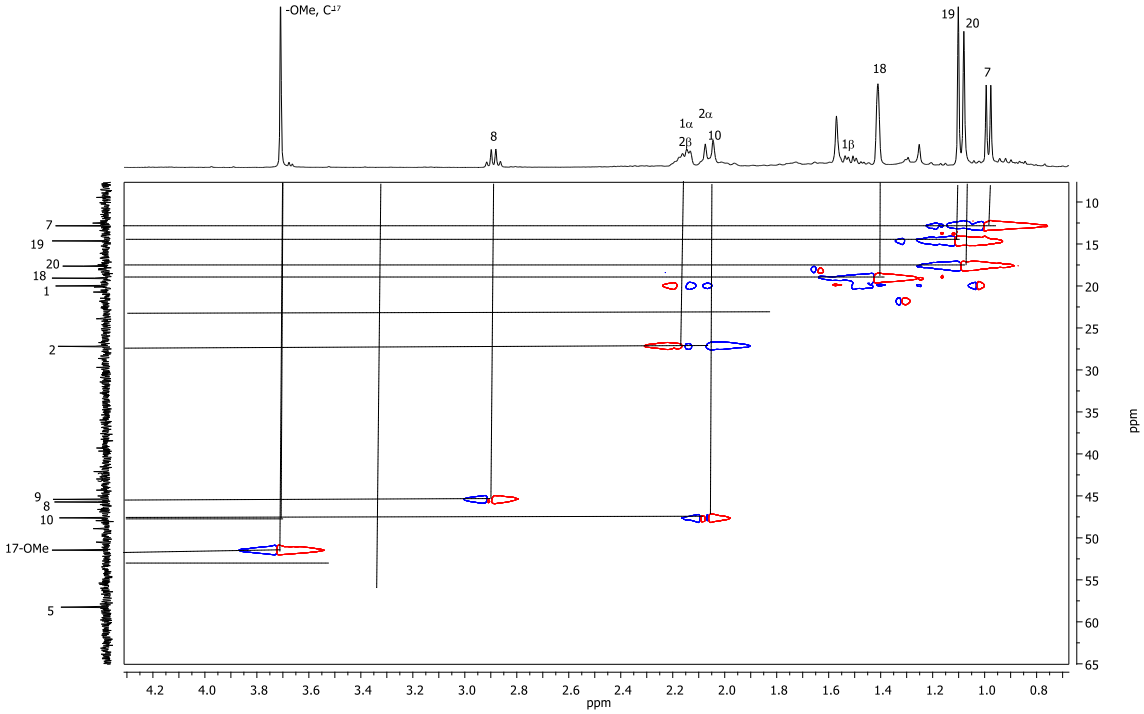


Figure S6: HSQC spectrum of Morifolin A (δC= 10 – 65 ppm)

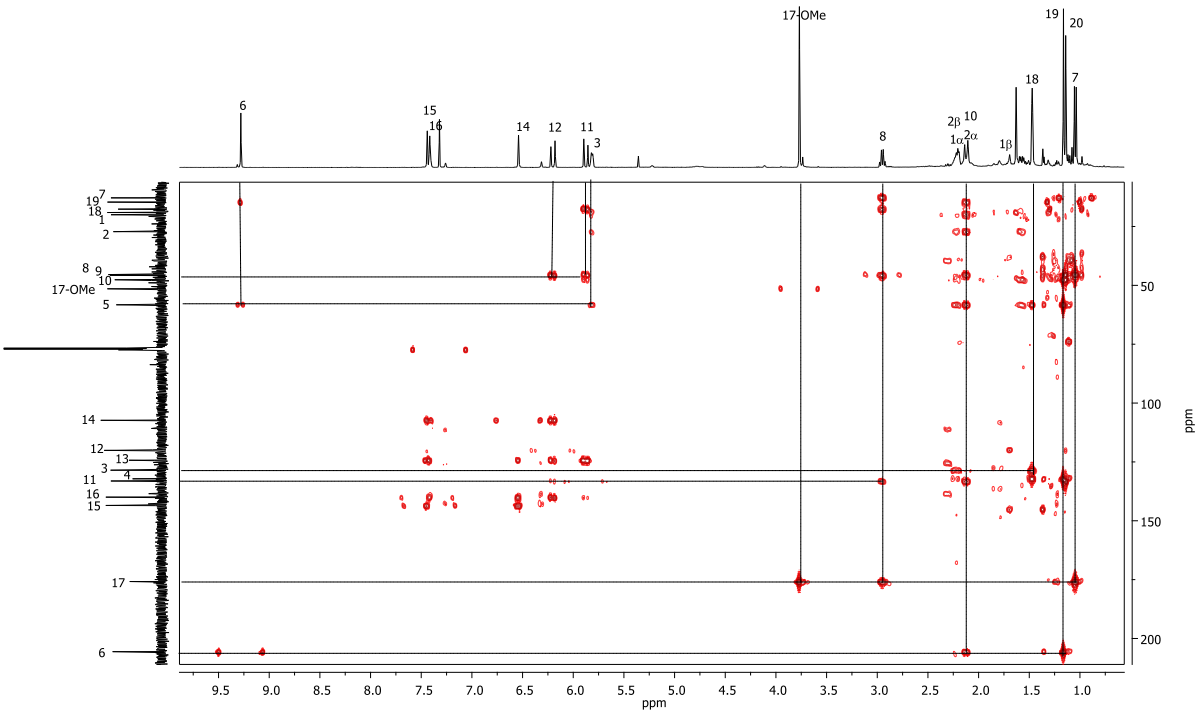


Figure S7: HMBC spectrum of Morifolin A

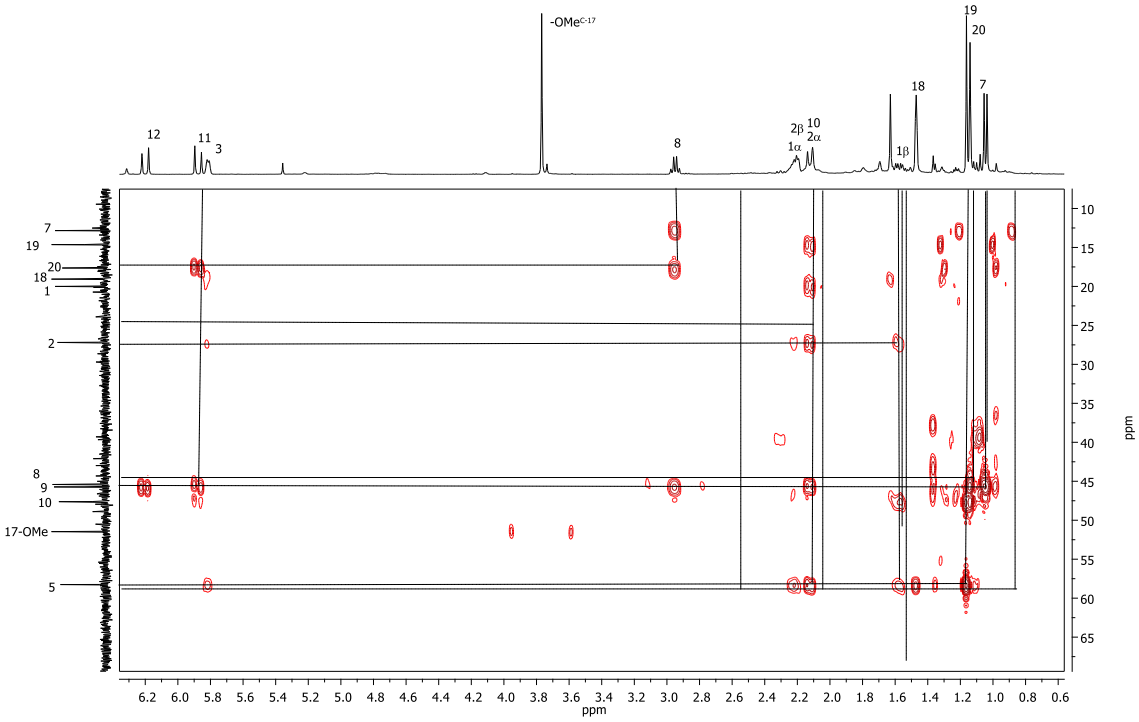


Figure S8: HMBC spectrum of Morifolin A (δC = 10 – 65 ppm)

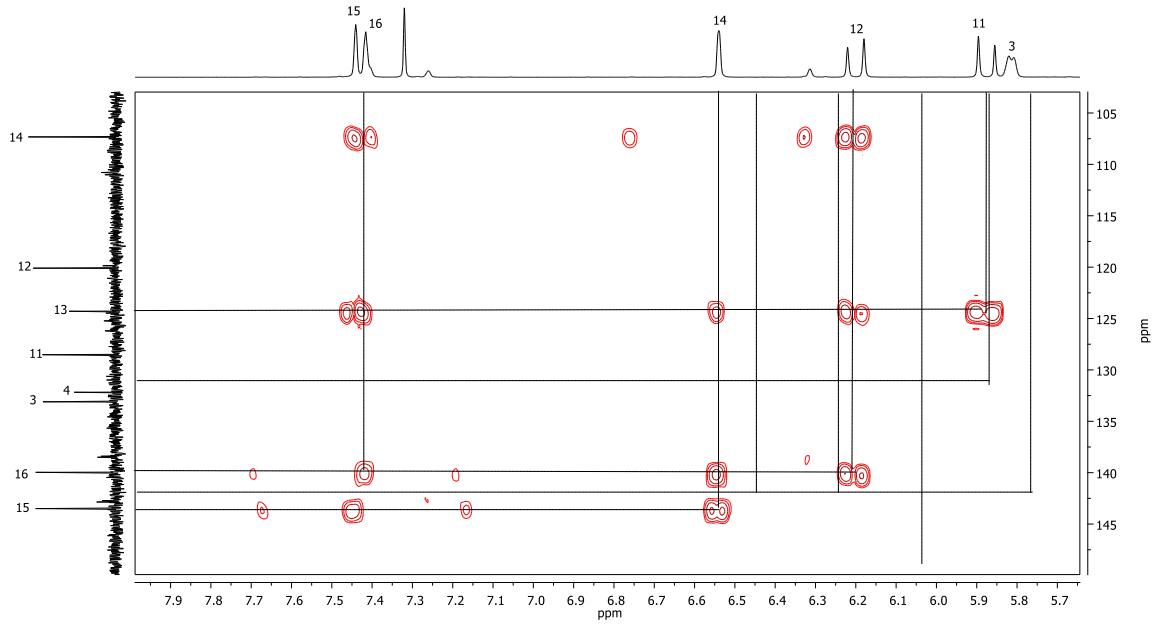


Figure S9: HMBC spectrum of Morifolin A (δC = 105 – 145 ppm)

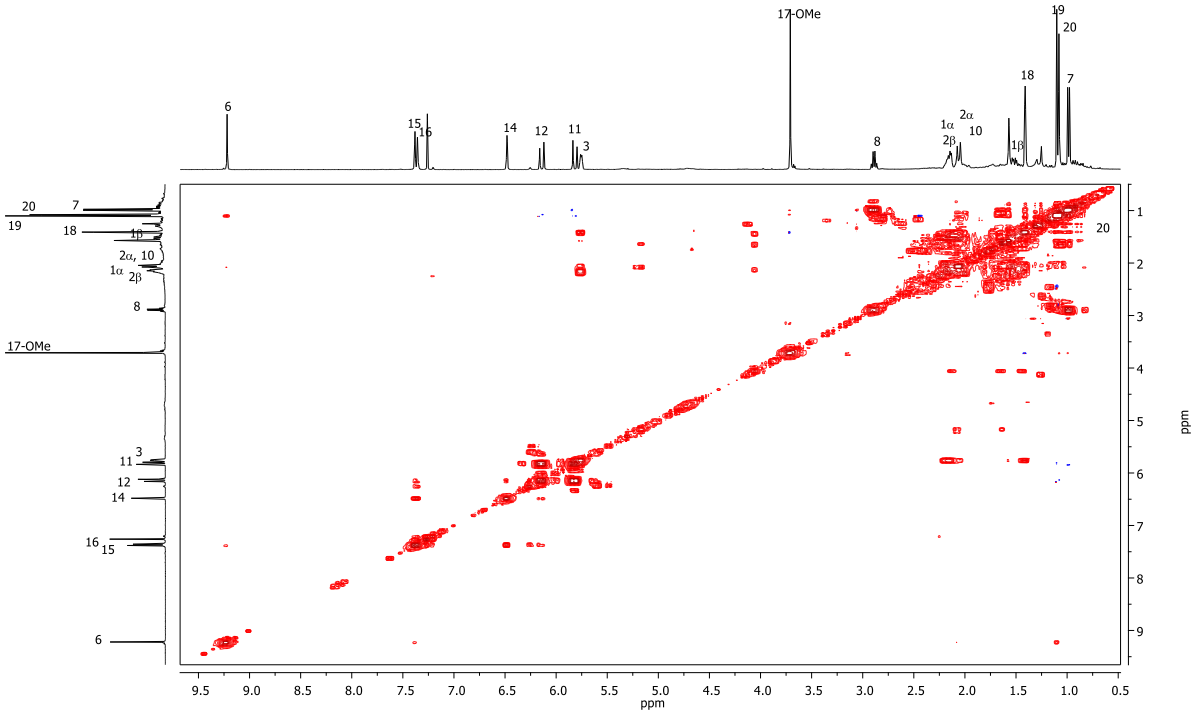


Figure S10: ^{1}H-^{1}H COSY spectrum of Morifolin A

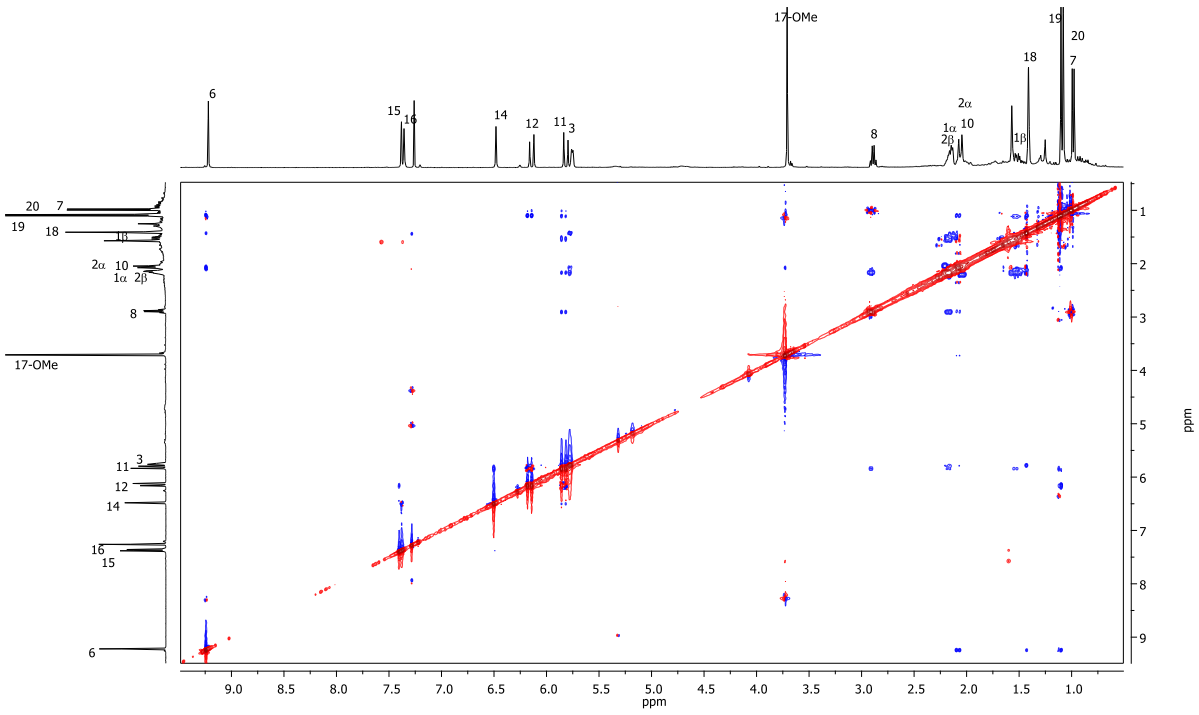
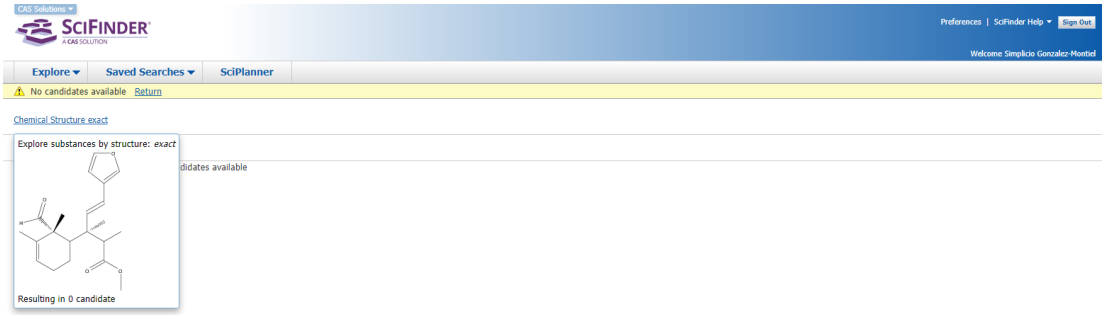
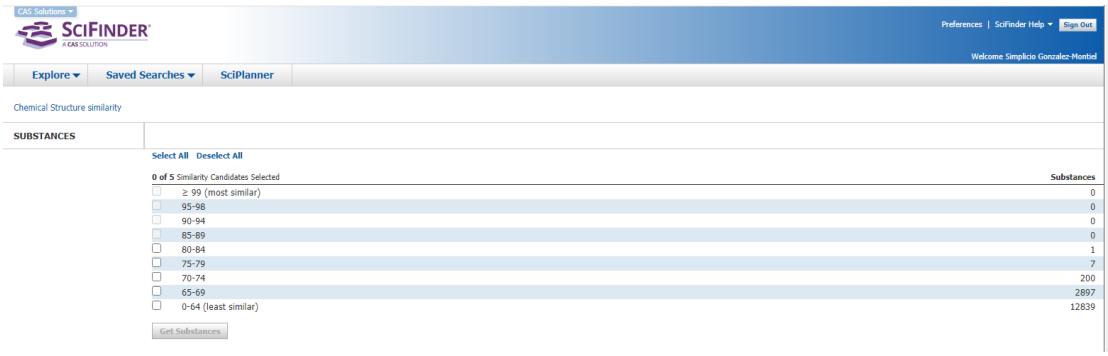


Figure S11: NOESY spectrum of Morifolin A

1) Exact search" resulted in zero hit.



2) Similarity search" led to a structure with 80 - 84% similarity to Morifolin A.



3) Only one structure with ≥ 80 - 84% similarity to Morifolin A.

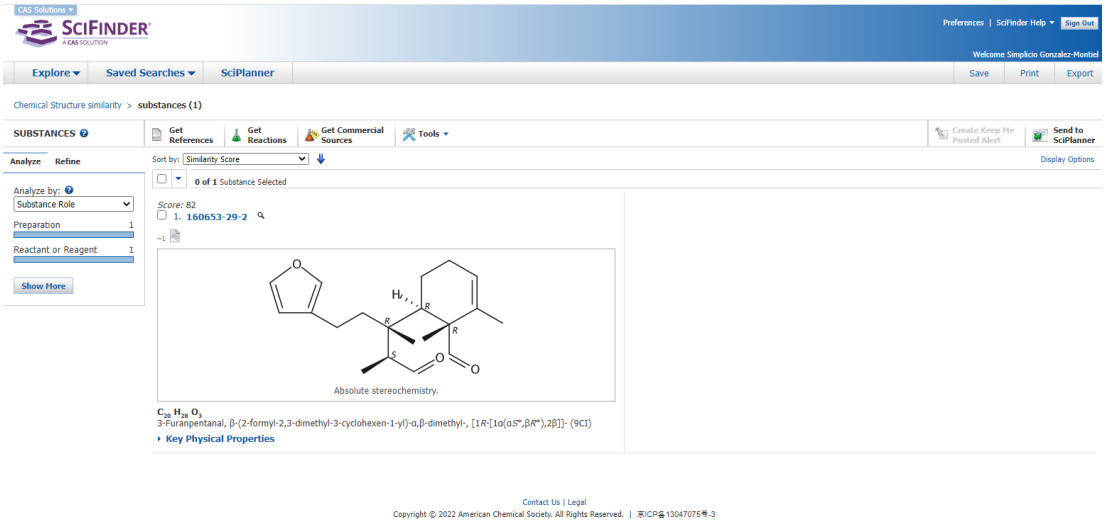


Figure S12: Scifinder search report for Morifolin A

Table S1. Details of crystal data and structure refinement parameters for Morifolin A.

Compound	**Morifolin A**
Empirical formula	$C_{21}H_{28}O_4$
Formula weight	344.43
Temperature (K)	100(2)
Crystal size (mm^3)	0.34 × 0.25 × 0.21
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a(Å)	9.09710(10)
d(Å)	10.14580(10)
c(Å)	19.9631(2)
α(°)	90
β(°)	90
γ(°)	90
Volume ($Å^3$)	1842.54(3)
Z	4
ρ_{calc} (g/cm^3)	1.242
μ (mm^{-1})	0.678
F(000)	744.0
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection (°)	8.858 to 143.538
Index ranges	$-11 \leq h \leq 10$ $-12 \leq k \leq 12$ $-24 \leq l \leq 24$
Reflections collected	29211
Independent reflections	3595 [R_{int} = 0.0332, R_{sigma} = 0.0131]
Data/restraints/parameters	3595/0/231
Goodness-of-fit on F2	1.083
Final R indexes [I>=2σ (I)]	R_1 = 0.0275, wR_2 = 0.0733
Final R indexes [all data]	R_1 = 0.0276, wR_2 = 0.0734
Largest diff. peak/hole (e $Å^{-3}$)	0.18/-0.16
Flack, Parsons and Hooft parameters	0.01(18), 0.01(3) and 0.03(2)
Inverted Flack, Parsons and Hooft parameters	1.00(18), 0.98(3) and 0.97(2)

Table S2: Check cif of morifolin A

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3

```
Bond precision:   C-C = 0.0020 A          Wavelength=1.54178

Cell:              a=9.0971(1)      b=10.1458(1)      c=19.9631(2)
                   alpha=90         beta=90           gamma=90
Temperature:       100 K

                 Calculated                Reported
Volume           1842.54(3)                1842.54(3)
Space group      P 21 21 21                P 21 21 21
Hall group       P 2ac 2ab                 P 2ac 2ab
Moiety formula   C21 H28 O4                C21 H28 O4
Sum formula      C21 H28 O4                C21 H28 O4
Mr               344.43                    344.43
Dx,g cm-3        1.242                     1.242
Z                4                         4
Mu (mm-1)        0.678                     0.678
F000             744.0                     744.0
F000'            746.23
h,k,lmax         11,12,24                  11,12,24
Nref             3615[ 2080]               3595
Tmin,Tmax        0.817,0.866               0.703,0.753
Tmin'            0.795

Correction method= # Reported T Limits: Tmin=0.703 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.73/0.99        Theta(max)= 71.769

R(reflections)= 0.0275( 3586)                wR2(reflections)=
                                             0.0734( 3595)
S = 1.083                  Npar= 231
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

```
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..............    0.00010 Ang.
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O4             106.0 Degree
PLAT791_ALERT_4_G Model has Chirality at C2          (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C3          (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C9          (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C13         (Sohnke SpGr)         S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         6 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        13 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock 3 - ellipsoid plot