

Supporting Information

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Three New Polyketides from the Insect-Associated Fungus *Letendraea* sp. 5XNZ4-2

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Table of Contents	Page
1. MTPA esters of Compound 1	3
2. Cytotoxic assay	3
3. Antibacterial assay	4
Table S1: Optimized Cartesian Coordinates for the lowest energy conformers reoptimized at b3lyp/6-31+g(d,p) level in MeOH for 4 <i>R</i> , 7 <i>S</i> , 10 <i>R</i> - 3 (C1, C2) and 4 <i>R</i> , 7 <i>S</i> , 10 <i>S</i> - 3 (C3, C4)	5
Figure S1: ¹ H NMR (500 MHz, CD ₃ OD) spectrum of letendronol D (1)	8
Figure S2: ¹³ C NMR (125 MHz, CD ₃ OD) spectrum of letendronol D (1)	9
Figure S3: DEPT (CD ₃ OD) spectrum of letendronol D (1)	10
Figure S4: HMQC (CD ₃ OD) spectrum of letendronol D (1)	11
Figure S5: HMQC (CD ₃ OD) spectrum of letendronol D (1) (From δ _C 25 ppm to δ _C 70 ppm)	12
Figure S6: ¹ H- ¹ H COSY (CD ₃ OD) spectrum of letendronol D (1)	12
Figure S7: HMBC (CD ₃ OD) spectrum of letendronol D (1)	13
Figure S8: HMBC (CD ₃ OD) spectrum of letendronol D (1) (From δ _C 60 ppm to δ _C 145 ppm)	14
Figure S9: NOESY (CD ₃ OD) spectrum of letendronol D (1)	14
Figure S10: HRESIMS spectrum of letendronol D (1)	15
Figure S11: IR spectrum of letendronol D (1)	15
Figure S12: CD spectrum of letendronol D (1)	15
Figure S13: ¹ H NMR (600 MHz, CD ₃ OD) spectrum of phomopsiketone H (2)	16
Figure S14: ¹³ C NMR (150 MHz, CD ₃ OD) spectrum of phomopsiketone H (2)	17
Figure S15: DEPT (CD ₃ OD) spectrum of phomopsiketone H (2)	18
Figure S16: HMQC (CD ₃ OD) spectrum of phomopsiketone H (2)	19
Figure S17: HMQC (CD ₃ OD) spectrum of phomopsiketone H (2) (From δ _C 10 ppm to δ _C 45 ppm)	19
Figure S18: HMQC (CD ₃ OD) spectrum of phomopsiketone H (2) (From δ _C 45 ppm to δ _C 85 ppm)	20
Figure S19: ¹ H- ¹ H COSY (CD ₃ OD) spectrum of phomopsiketone H (2)	20
Figure S20: HMBC (CD ₃ OD) spectrum of phomopsiketone H (2)	21
Figure S21: HMBC (CD ₃ OD) spectrum of phomopsiketone H (2) (From δ _H 1.7 ppm to δ _H 4.7 ppm)	21

Figure S22: NOESY (CD ₃ OD) spectrum of phomopsiketone H (2)	22
Figure S23: HRESIMS spectrum of phomopsiketone H (2)	22
Figure S24: IR spectrum of phomopsiketone H (2)	23
Figure S25: CD spectrum of phomopsiketone H (2)	23
Figure S26: ¹ H NMR (600 MHz, DMSO) spectrum of phomopsiketone I (3)	24
Figure S27: ¹³ C NMR (150 MHz, DMSO) spectrum of phomopsiketone I (3)	25
Figure S28: HSQC (DMSO) spectrum of phomopsiketone I (3)	26
Figure S29: HSQC (DMSO) spectrum of phomopsiketone I (3) (From δ _C 5 ppm to δ _C 45 ppm)	26
Figure S30: ¹ H- ¹ H COSY (DMSO) spectrum of phomopsiketone I (3)	27
Figure S31: HMBC (DMSO) spectrum of phomopsiketone I (3)	28
Figure S33: NOESY (DMSO) spectrum of phomopsiketone I (3)	29
Figure S34: HRESIMS spectrum of phomopsiketone I (3)	29
Figure S35: IR spectrum of phomopsiketone I (3)	30
Figure S36: CD spectrum of phomopsiketone I (3)	30
Figure S37: ¹ H NMR (600 MHz, CDCl ₃) spectrum of 1a	31
Figure S38: ¹ H NMR (600 MHz, CDCl ₃) spectrum of 1b	32
Figure S39: HRESIMS spectrum of 1a	33
Figure S40: HRESIMS spectrum of 1b	33
Figure S41: HPLC chromatogram of compound 2 (15%CH ₃ CN+H ₂ O, 1 mL/min, 230 nm)	33
Figure S42: HPLC chromatogram of compound 3 (15%CH ₃ CN+H ₂ O, 1 mL/min, 230 nm)	34
Figure S43: SciFinder Search Results of 1	35
Figure S44: SciFinder Search Results of 2	36
Figure S45: SciFinder Search Results of 3	37

1. MTPA Esters of Compound 1

4, 7, 10-tri-S-MTPA Ester of 1 (1a): White amorphous solid. ¹H NMR (600 MHz, in CDCl₃) δ_H 7.24–7.52 (15H, m, MTPA-Ar), 5.52 (1H, brs, H-7), 5.48 (1H, brs, H-4), 5.26 (1H, ddd, *J* = 9.2, 3.6, 2.0 Hz, H-10), 4.95 (1H, m, H-9), 4.59 (1H, dd, *J* = 13.6, 3.6 Hz, H-2a), 4.54 (1H, ddd, *J* = 13.6, 6.0, 2.0 Hz, H-2b), 3.51 (3H, brs, MTPA-OMe), 3.46 (3H, brs, MTPA-OMe), 3.45 (3H, brs, MTPA-OMe), 1.93 (1H, m, H-6a), 1.87 (1H, m, H-5a), 1.83 (1H, m, H-6b), 1.77 (1H, m, H-5b), 1.70 (1H, m, H-11a), 1.40 (1H, m, H-12a), 1.35 (1H, m, H-11b), 1.30 (1H, m, H-12b), 0.87 (3H, t, *J* = 7.2 Hz, H-13).

4, 7, 10-tri-R-MTPA Ester of 1 (1b): White amorphous solid. ¹H NMR (600 MHz, in CDCl₃) δ_H 7.25–7.52 (15H, m, MTPA-Ar), 5.58 (2H, brs, H-7, H-4), 5.21 (1H, m, H-10), 4.87 (1H, m, H-9), 4.57 (1H, dd, *J* = 13.7, 3.3 Hz, H-2a), 4.46 (1H, ddd, *J* = 13.7, 6.1, 2.0 Hz, H-2b), 3.53 (3H, brs, MTPA-OMe), 3.50 (3H, brs, MTPA-OMe), 3.47 (3H, brs, MTPA-OMe), 2.13 (1H, m, H-6a), 2.11 (1H, m, H-5a), 1.96 (1H, m, H-6b), 1.94 (1H, m, H-5b), 1.54 (1H, m, H-11a), 1.20 (1H, m, H-11b), 1.15 (1H, m, H-12a), 1.10 (1H, m, H-12b), 0.78 (3H, t, *J* = 7.3 Hz, H-13).

2. Cytotoxic Assay

Cytotoxicity of **1** were measured by the MTT assay [1] against the prostate cancer PC3 cell line (more sensitive than other cancer cells). Tumor cell lines were seeded in 96-well plates (4000 per well in 100 μL). After 24 h of incubation cells were treated with gradient concentrations (100 μM, 50 μM, 25 μM, 12.5 μM, 6.25 μM, 3.125 μM) for another 72h. Afterwards, MTT solution (5.0 mg/mL in RPMI-1640 media, Sigma, St. Louis, MO, USA) was added (20 μL/well) and then plates were incubated for another 4 h at 37°C. The compounds were dissolved in DMSO and cell growth inhibition assay was performed as reported previously. Doxorubicin (ADR) was used as a positive control. compound **1** didn't exhibit cytotoxicity against PC₃ cells (the cell growth inhibition rate was 13% at 10 μg/mL).

3. Antibacterial Assay

The antibacterial activities of **1** was evaluated with *S. aureus*, *S. epidermidis*, *E. coli*, *M. albicans* and *P. aeruginosa* using Kirby–Bauer Diffusion method [2] and gentamicin, vancomycin, ampicillin, amphotericin B and gentamicin served as the positive drugs, respectively.

The stock solution of compound **1** was prepared in methanol with a series of concentration (25, 5.0, 1 and 0.2 mg/mL). Positive control drugs gentamicin, vancomycin and ampicillin were dissolved in purified water with the concentration of 500 ug/mL, amphotericin B was dissolved in DMSO with the concentration of 100 ug/mL.

S. aureus, *S. epidermidis*, *E. coli*, *M. albicans* and *P. aeruginosa* were activated in nutrient broth at 37°C for 6~8 h with 200 rpm and the culture broth was poured on the surface of MEB Agar (20 g MEB and 20 g agar in 1 L water) plates inside the cabinet.

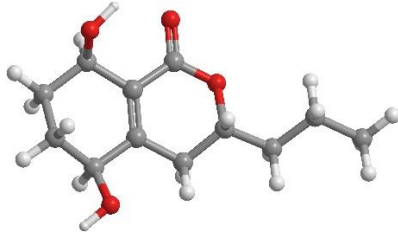
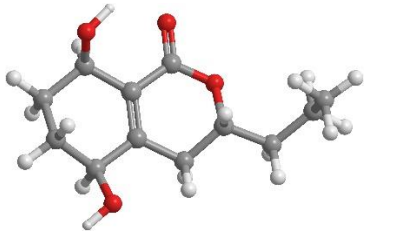
(Make sure to have a uniform distribution of cells on the plates). Label the location of negative control (methanol), the positive drug and different contents of tested compounds (100 µg, 20 µg, 4 µg and 0.8 µg for **1**) on the agar side of the plate and outside the lid. Arrange the discs as to mimic their positions outside the lid and add 4 µL of corresponding concentrations of tested compounds and methanol to the discs. The contents of the positive drugs gentamicin, ampicillin and amphotericin B were 3 ug, 1.5 ug and 0.35 ug, respectively. Transfer the discs from the lid to the agar plate using a sterile forcep. Finally, place the plates in an incubator agar side up at 37°C for 12 h to observe the inhibition zone.

Unfortunately, compound **1** didn't show any inhibition zone to the tested microbials at all the concentrations (100 µg, 20 µg, 4 µg and 0.8 µg/disc).

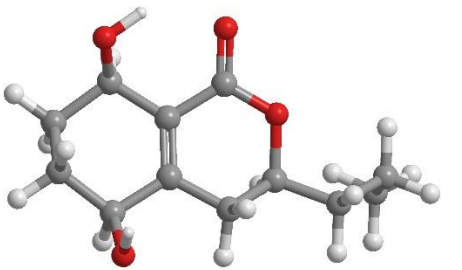
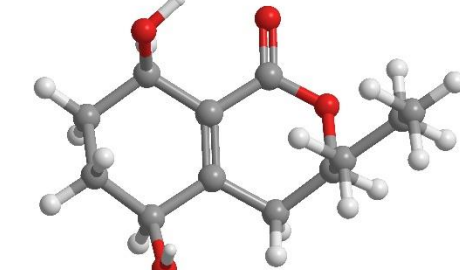
References

- [1] T. Mosmann (1983). Rapid colorimetric assay for cellular growth and survival: Application to proliferation and cytotoxicity assays, *J. Immunol. Meth.* **65**, 55-63.
- [2] A. W. Bauer, W. M. Kirby, J. C. Sherris and M. Turck (1966). Antibiotic susceptibility testing by a standardized single disk method, *Amer. J. Clin. Pathol.* **45**, 493:496.

Table S1. Optimized Cartesian Coordinates for the lowest energy conformers reoptimized at b3lyp/6-31+g(d,p) level in MeOH for 4*R*, 7*S*, 10*R*-**3** (C1, C2) and 4*R*, 7*S*, 10*S*-**3** (C3, C4).

 <p>C1 74.03%</p>				 <p>C2 25.97%</p>			
-768.9420838 Hartree				-768.9410956 Hartree			
C	3.53081900	-0.26677200	-0.35131800	C	3.45371900	-0.36517600	-0.14520000
C	3.24826200	1.08303000	0.31337200	C	3.15369000	0.99560700	0.48894200
C	1.98719400	1.70648100	-0.28798400	C	1.98523300	1.66236200	-0.23936500
C	0.82628600	0.73221600	-0.29078500	C	0.79299300	0.73322800	-0.34957400
C	1.02656400	-0.60306900	-0.23056400	C	0.93765800	-0.60863000	-0.27362700
C	2.39108700	-1.26347100	-0.14107800	C	2.26242900	-1.31925300	-0.05800200
C	-0.56904400	1.27701700	-0.44895400	C	-0.56131000	1.32910600	-0.63132800
C	-1.59976400	0.33357300	0.15021400	C	-1.67506500	0.42226200	-0.13258800
O	-1.37450200	-1.03834300	-0.31878700	O	-1.45859000	-0.95502800	-0.58859600
C	-0.12259400	-1.53542800	-0.32355700	C	-0.23140900	-1.49847800	-0.47420000
O	0.02390900	-2.74939200	-0.43321100	O	-0.12025100	-2.71753000	-0.56889200
C	-3.04020600	0.69222400	-0.19105600	C	-3.06261700	0.83774800	-0.60742700
C	-4.09508500	-0.16599100	0.52009600	C	-4.22917300	-0.00866200	-0.06969700
C	-5.52680000	0.25511900	0.16951300	C	-4.43668900	0.08308300	1.44778300
O	2.56701700	-1.89165400	1.14841500	O	2.28617200	-1.96221000	1.23593100
O	1.57440600	2.88329500	0.42209600	O	1.55294900	2.86330900	0.41615400
H	3.66868700	-0.12044300	-1.43000900	H	3.70960600	-0.22560500	-1.20308800
H	4.45531600	-0.70946000	0.03100300	H	4.31605500	-0.84142500	0.33068300
H	4.09451800	1.76481300	0.17375100	H	4.03421000	1.64541900	0.43783200
H	3.09758600	0.95895200	1.39206500	H	2.88847000	0.88041400	1.54638900
H	2.18353100	1.97679700	-1.34000600	H	2.29565400	1.91166600	-1.26871100
H	2.44732400	-2.04288600	-0.90960800	H	2.36581400	-2.09553500	-0.82500600
H	-0.64861000	2.24939100	0.04223900	H	-0.65726700	1.50595400	-1.71334500
H	-0.76887400	1.44414500	-1.51816400	H	-0.65023000	2.30283500	-0.14429100
H	-1.47004000	0.30272000	1.24022200	H	-1.63836800	0.38392300	0.96289700
H	-3.18361600	1.74624500	0.08055200	H	-3.20371400	1.88480300	-0.30853100
H	-3.17018900	0.62635600	-1.27948800	H	-3.06778100	0.81913600	-1.70457500
H	-3.94709200	-1.21934000	0.25596100	H	-5.14276200	0.32663500	-0.57559100
H	-3.94635900	-0.09202600	1.60583000	H	-4.08383000	-1.05532800	-0.36149900

H	-6.26091100	-0.36943400	0.68950700	H	-5.32189300	-0.48539200	1.75243500
H	-5.71404300	1.29779400	0.45234200	H	-3.58416500	-0.31950000	2.00585100
H	-5.71331300	0.16347400	-0.90706700	H	-4.58213300	1.12277900	1.76487600
H	1.93307200	-2.62214300	1.20315000	H	1.62058400	-2.66595000	1.21924100
H	2.27606300	3.54422200	0.34223000	H	2.28276500	3.49766800	0.39334600

 <p style="text-align: center;">C3 98.61%</p>				 <p style="text-align: center;">C4 1.39%</p>			
-768.9441117 Hartree				-768.9400902 Hartree			
C	-3.16369500	-0.31106000	1.11524600	C	-3.16369500	-0.31106000	1.11524600
C	-3.24922600	0.96726500	0.27490800	C	-3.24922600	0.96726500	0.27490800
C	-1.90360200	1.69443500	0.27668700	C	-1.90360200	1.69443500	0.27668700
C	-0.74488000	0.75307400	-0.00353500	C	-0.74488000	0.75307400	-0.00353500
C	-0.86605400	-0.58760000	0.11429600	C	-0.86605400	-0.58760000	0.11429600
C	-2.13524400	-1.29446300	0.55713100	C	-2.13524400	-1.29446300	0.55713100
C	0.57607800	1.34950900	-0.41469300	C	0.57607800	1.34950900	-0.41469300
C	1.72376200	0.42845800	-0.02424600	C	1.72376200	0.42845800	-0.02424600
O	1.46090000	-0.92854000	-0.52090000	O	1.46090000	-0.92854000	-0.52090000
C	0.24257900	-1.46268500	-0.32909200	C	0.24257900	-1.46268500	-0.32909200
O	0.07398500	-2.65401800	-0.58476700	O	0.07398500	-2.65401800	-0.58476700
C	3.07592600	0.85369700	-0.58361800	C	3.07592600	0.85369700	-0.58361800
C	4.27118900	-0.01743900	-0.16016100	C	4.27118900	-0.01743900	-0.16016100
C	4.58787600	0.02040300	1.34069800	C	4.58787600	0.02040300	1.34069800
O	-2.73568800	-2.00742800	-0.54343000	O	-2.73568800	-2.00742800	-0.54343000
O	-1.88842700	2.81640000	-0.61596100	O	-1.88842700	2.81640000	-0.61596100
H	-2.88329200	-0.05707900	2.14500600	H	-2.88329200	-0.05707900	2.14500600
H	-4.13440000	-0.81383800	1.16245300	H	-4.13440000	-0.81383800	1.16245300
H	-3.51791000	0.71461300	-0.75907300	H	-3.51791000	0.71461300	-0.75907300
H	-4.02265500	1.63885200	0.65975600	H	-4.02265500	1.63885200	0.65975600
H	-1.72976400	2.13833500	1.26698200	H	-1.72976400	2.13833500	1.26698200
H	-1.87208500	-2.02306500	1.33593000	H	-1.87208500	-2.02306500	1.33593000
H	0.58345800	1.53868500	-1.49711500	H	0.58345800	1.53868500	-1.49711500
H	0.71401500	2.32215100	0.06842300	H	0.71401500	2.32215100	0.06842300
H	1.76400600	0.34961700	1.06870400	H	1.76400600	0.34961700	1.06870400
H	3.00272100	0.87334700	-1.67823900	H	3.00272100	0.87334700	-1.67823900
H	3.24581900	1.88886300	-0.25960500	H	3.24581900	1.88886300	-0.25960500
H	4.09663400	-1.05253800	-0.47643000	H	4.09663400	-1.05253800	-0.47643000

H	5.14869600	0.32993200	-0.71890600	H	5.14869600	0.32993200	-0.71890600
H	5.48800300	-0.56332400	1.56098600	H	5.48800300	-0.56332400	1.56098600
H	4.76424400	1.04759400	1.68204400	H	4.76424400	1.04759400	1.68204400
H	3.77458500	-0.39653100	1.94477300	H	3.77458500	-0.39653100	1.94477300
H	-2.05546400	-2.62148800	-0.86628700	H	-2.05546400	-2.62148800	-0.86628700
H	-2.14103200	2.51299800	-1.50066100	H	-2.14103200	2.51299800	-1.50066100

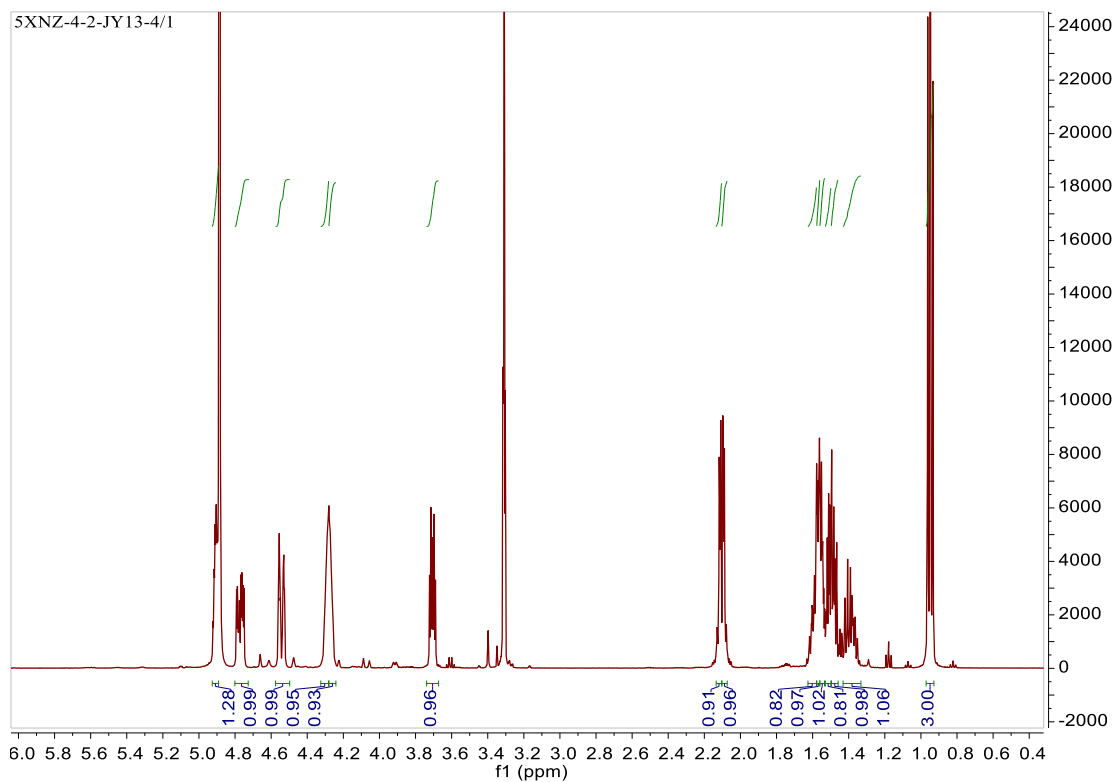


Figure S1: ^1H NMR (500 MHz, CD_3OD) spectrum of letendronol D (**1**)

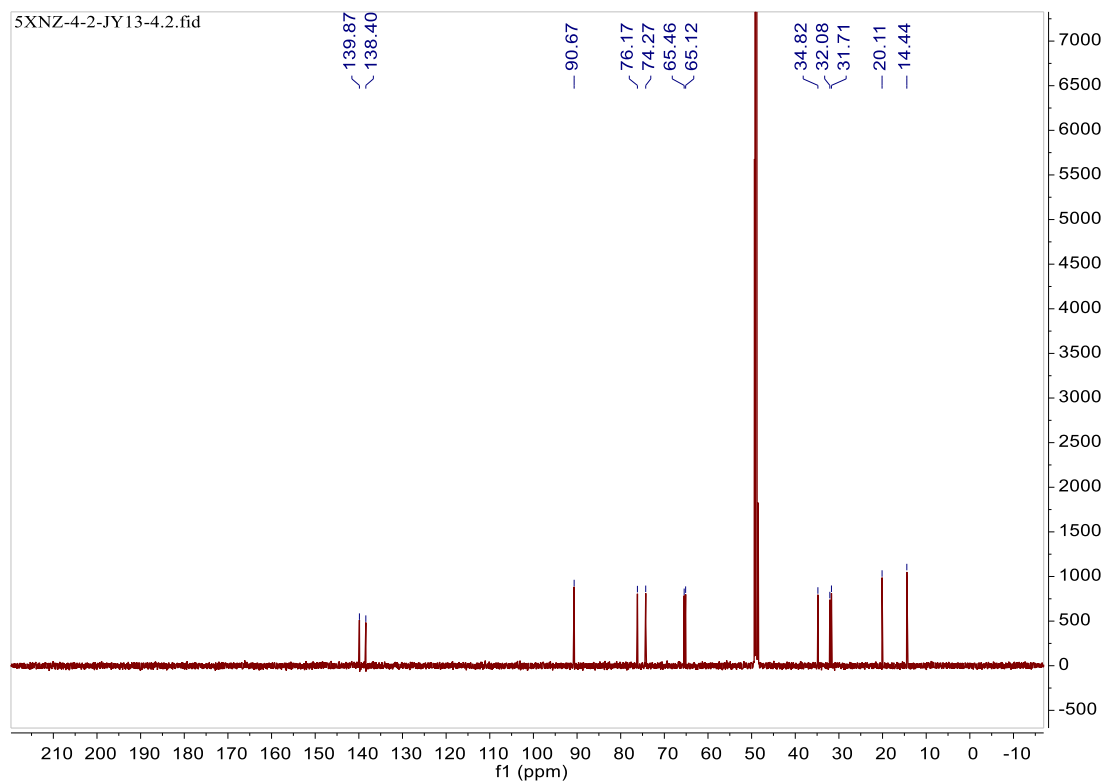


Figure S2: ^{13}C NMR (125 MHz, CD_3OD) spectrum of letendronol D (**1**)

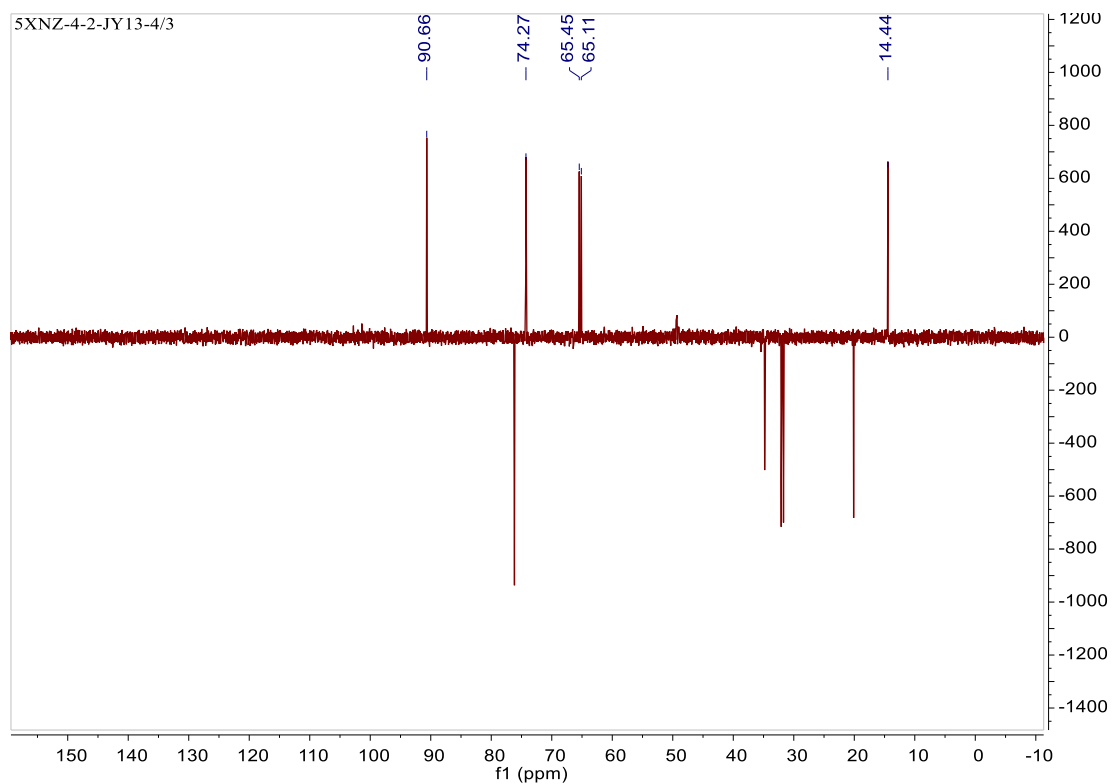


Figure S3: DEPT (CD₃OD) spectrum of letendronol D (**1**)

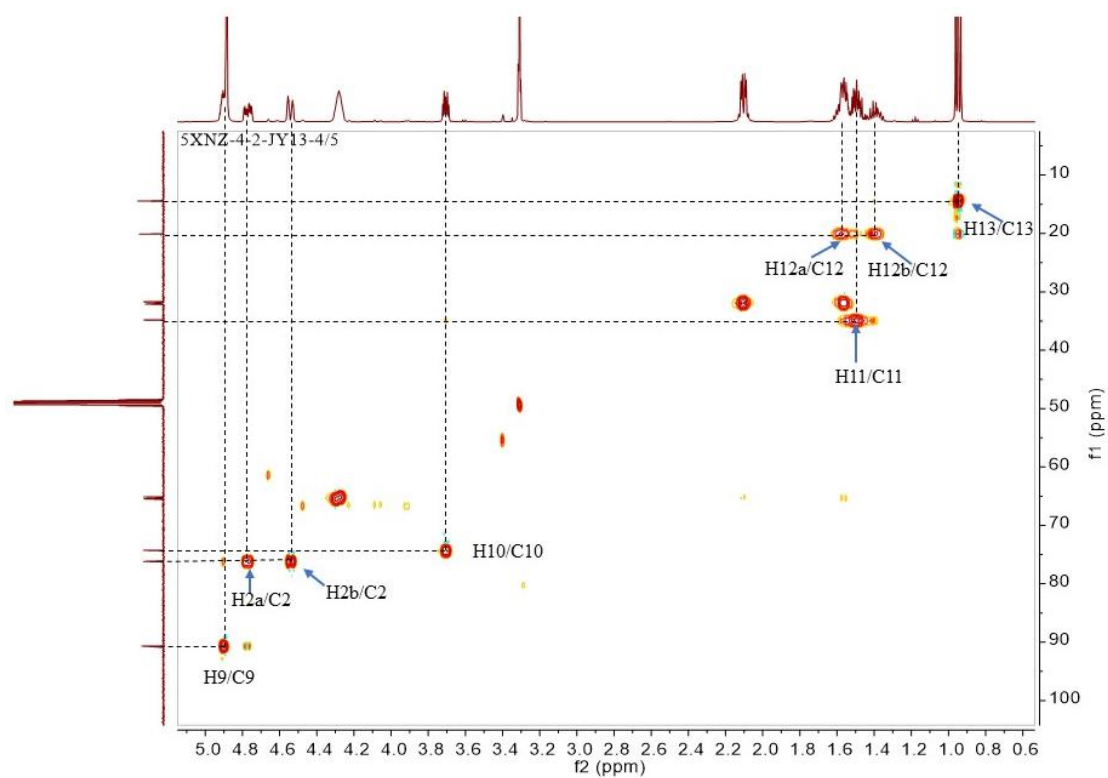


Figure S4: HMQC (CD₃OD) spectrum of letendronol D (**1**)

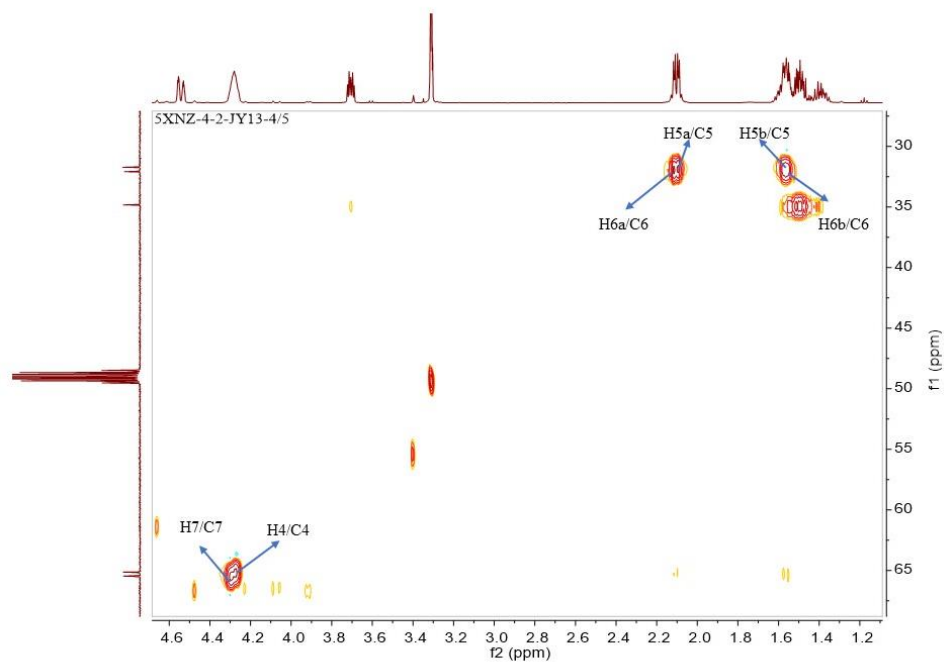


Figure S5: HMQC (CD₃OD) spectrum of letendronol D (**1**) (From δ_C 25 ppm to δ_C 70 ppm)

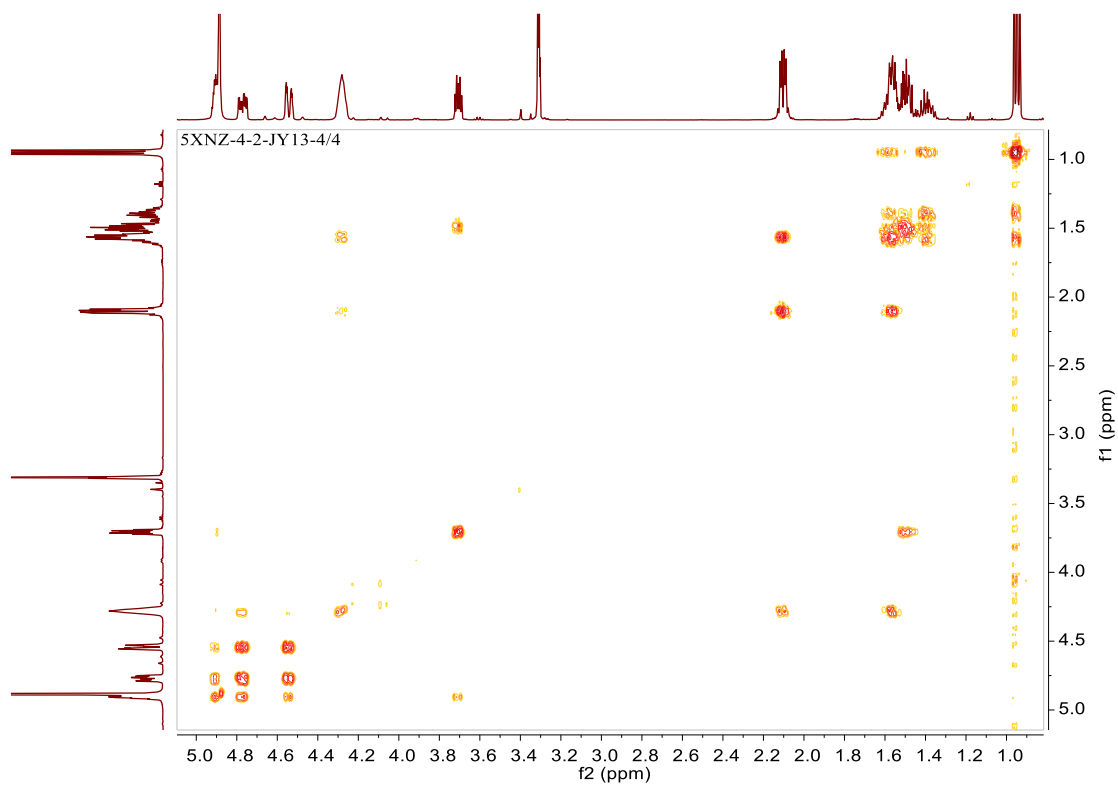


Figure S6: ^1H - ^1H COSY (CD_3OD) spectrum of letendronol D (**1**)

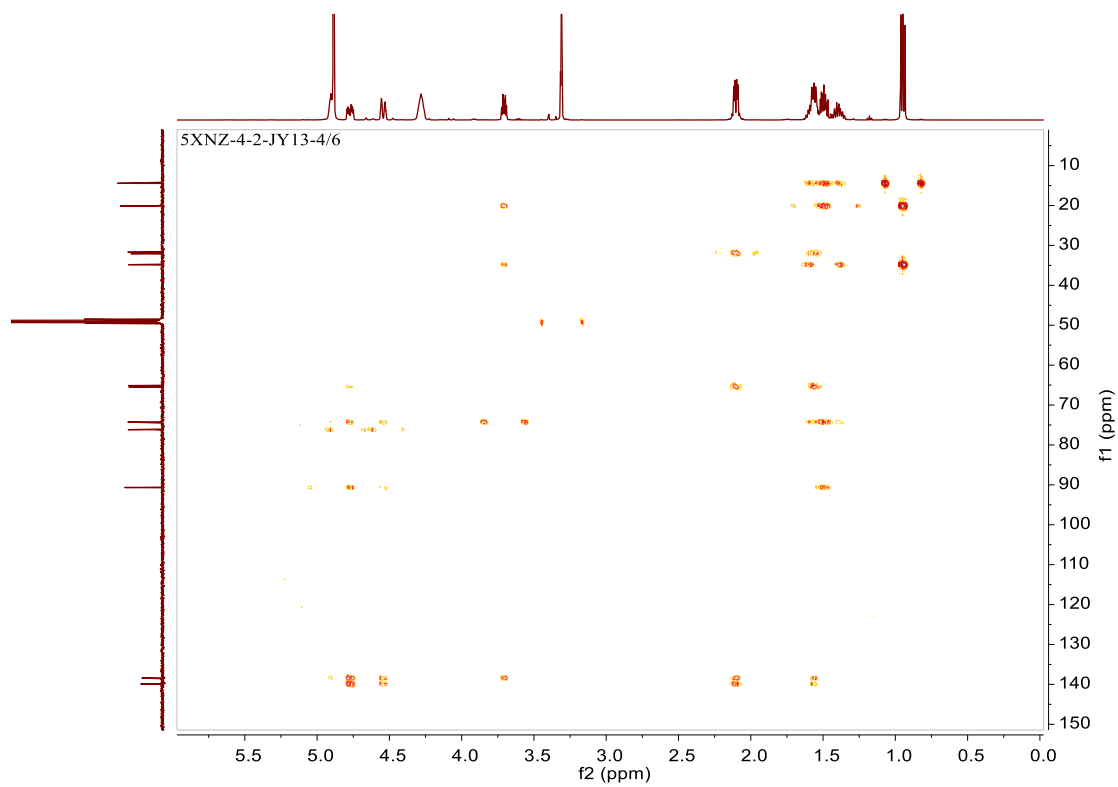


Figure S7: HMBC (CD_3OD) spectrum of letendronol D (**1**)

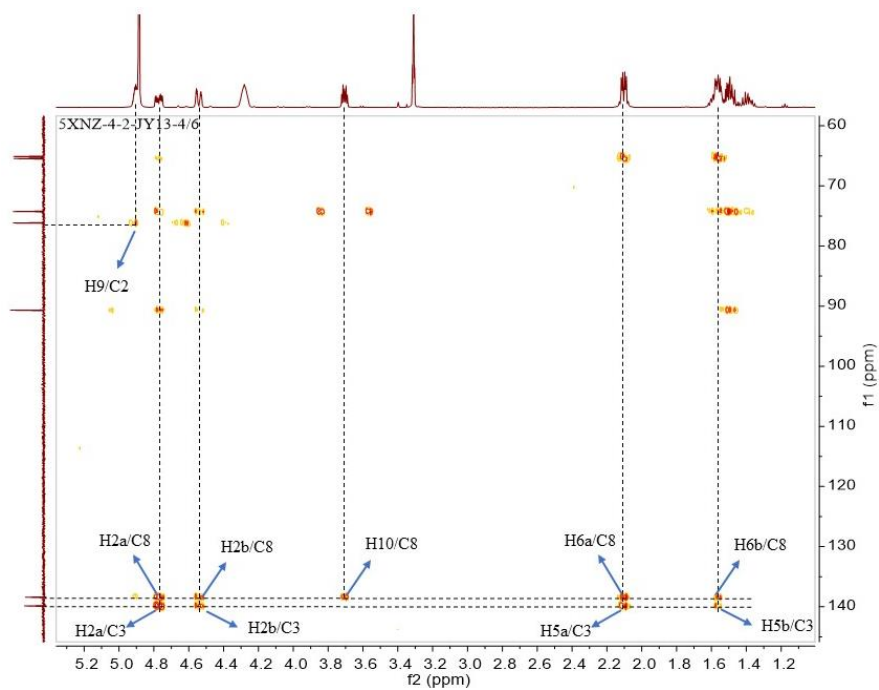


Figure S8: HMBC (CD₃OD) spectrum of letendronol D (**1**) (From $\delta_{\text{C}}60$ ppm to $\delta_{\text{C}}145$ ppm)

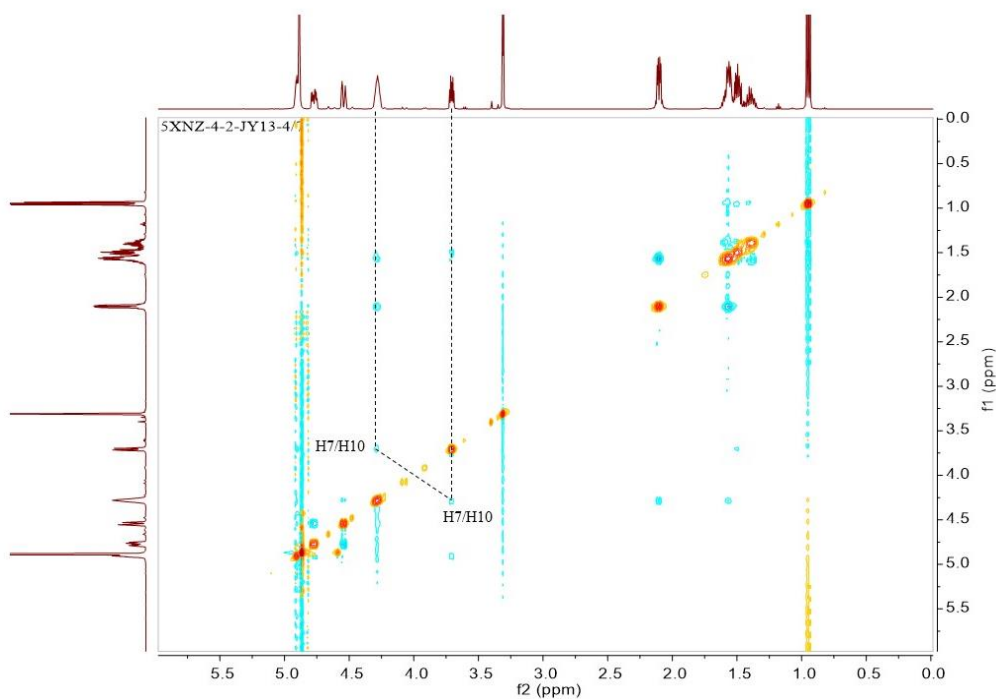


Figure S9: NOESY (CD₃OD) spectrum of letendronol D (**1**)

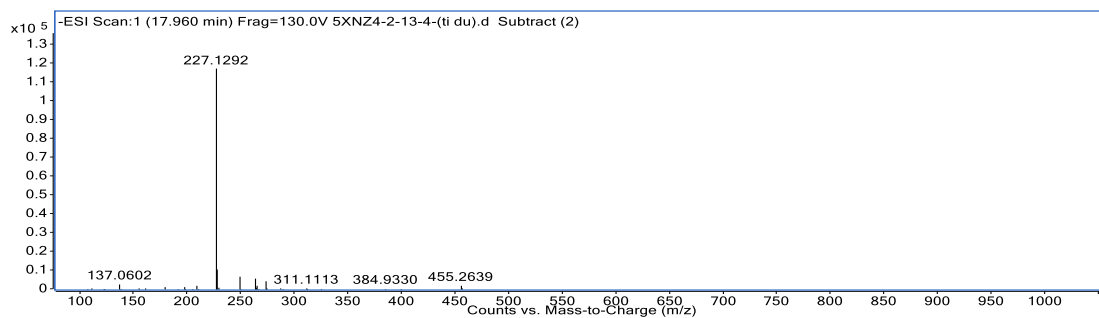


Figure S10: HRESIMS spectrum of letendronol D (1)

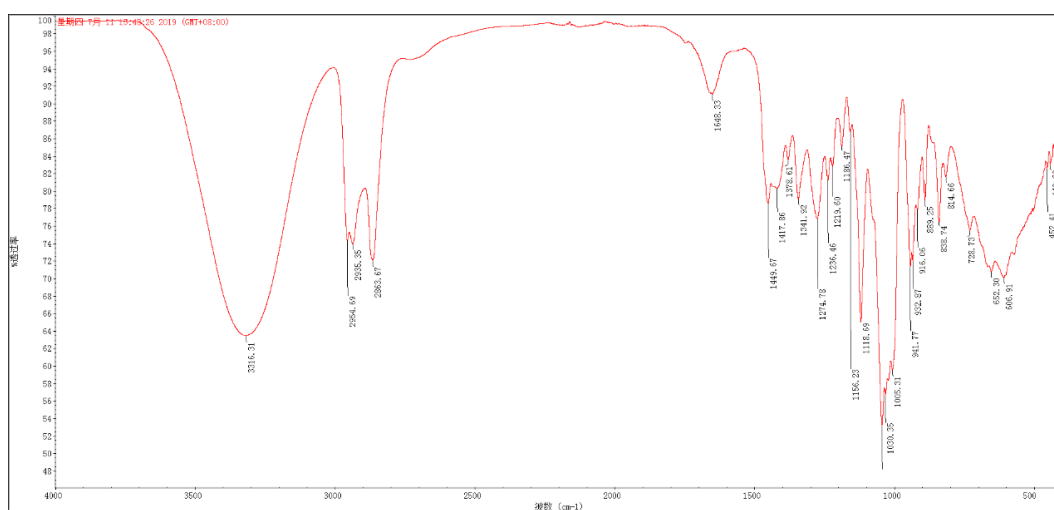


Figure S11: IR spectrum of letendronol D (1)

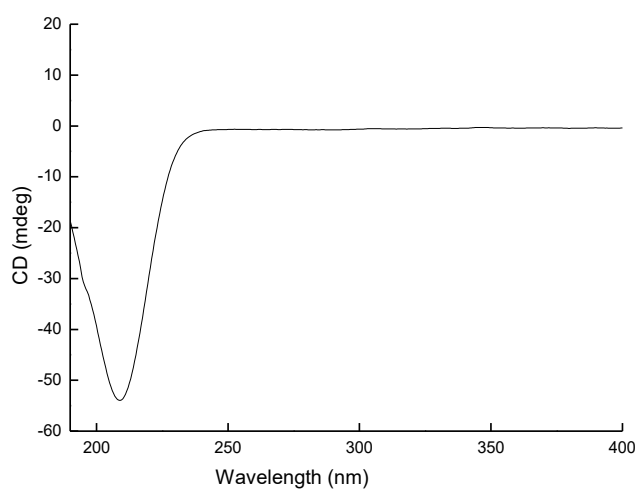


Figure S12: CD spectrum of letendronol D (1)

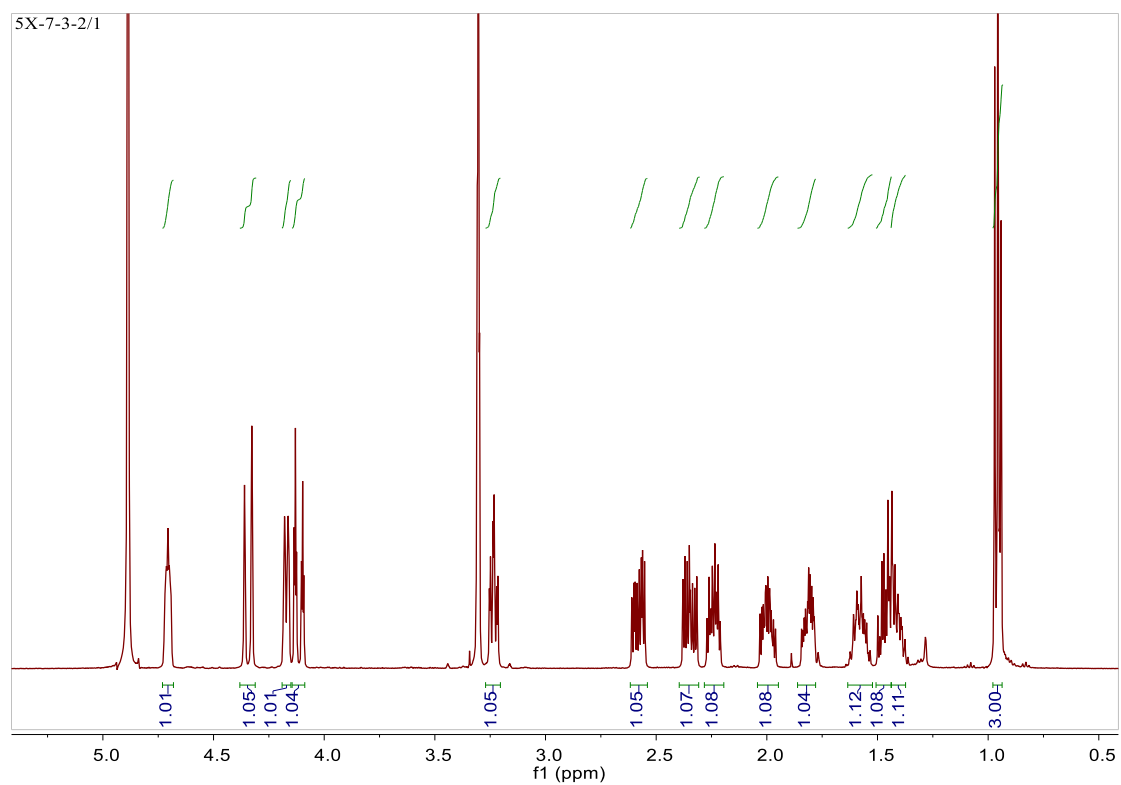


Figure S13: ^1H NMR (600 MHz, CD_3OD) spectrum of phomopsiketone H (**2**)

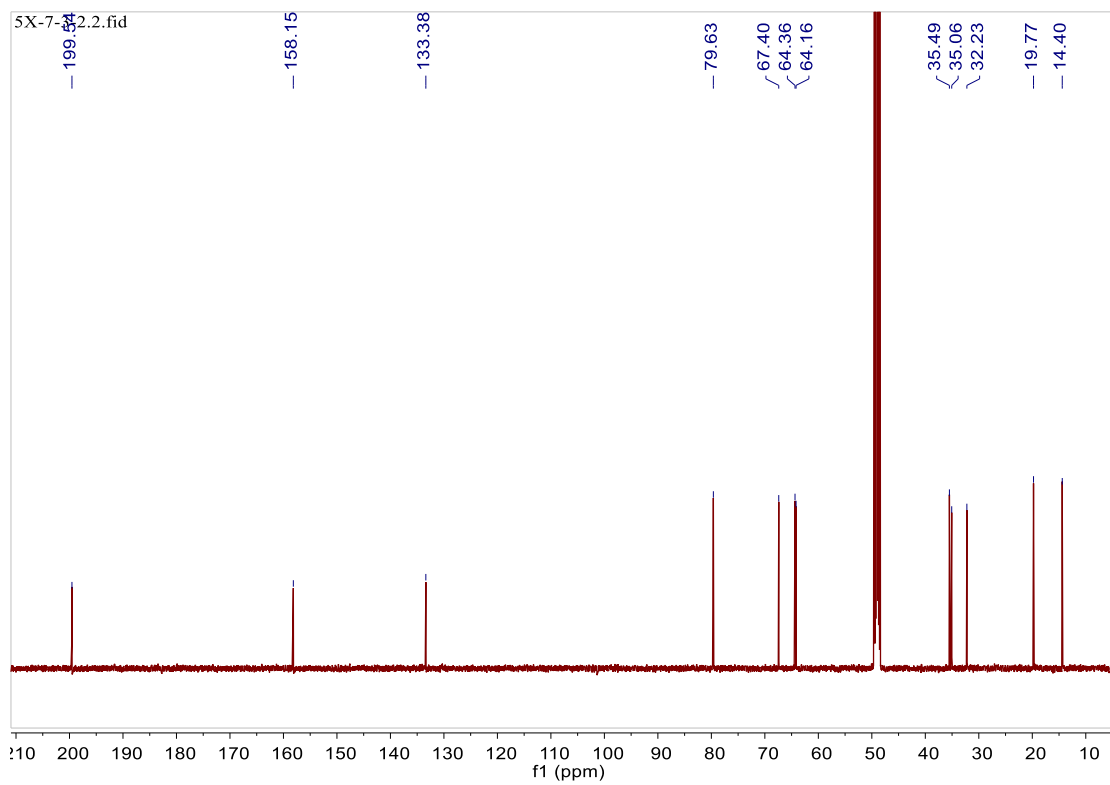


Figure S14: ^{13}C NMR (150 MHz, CD_3OD) spectrum of phomopsiketone H (**2**)

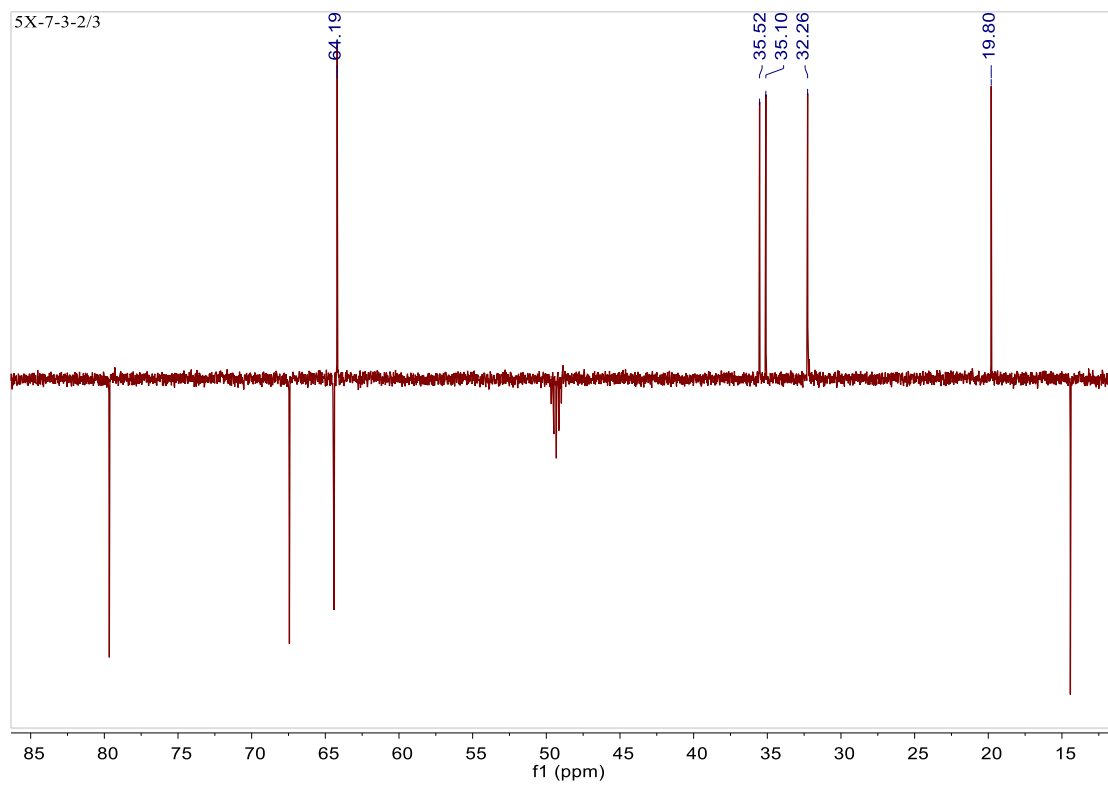


Figure S15: DEPT (CD₃OD) spectrum of phomopsiketone H (2)

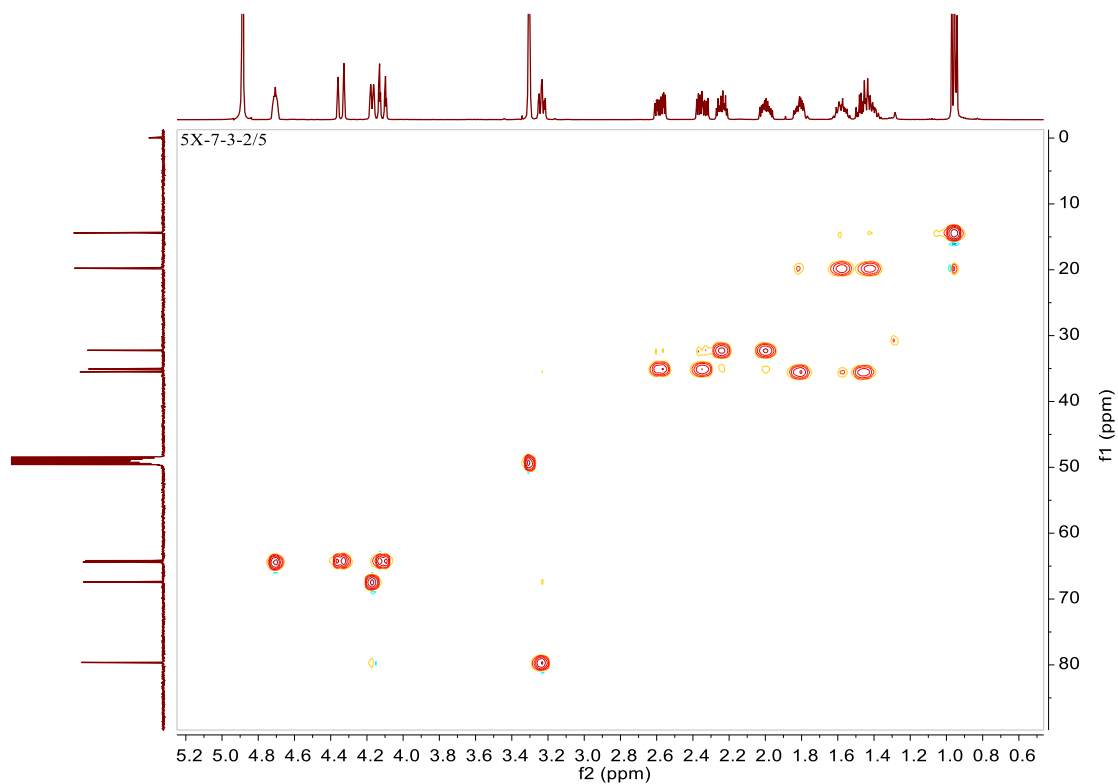


Figure S16: HMQC (CD₃OD) spectrum of phomopsiketone H (**2**)

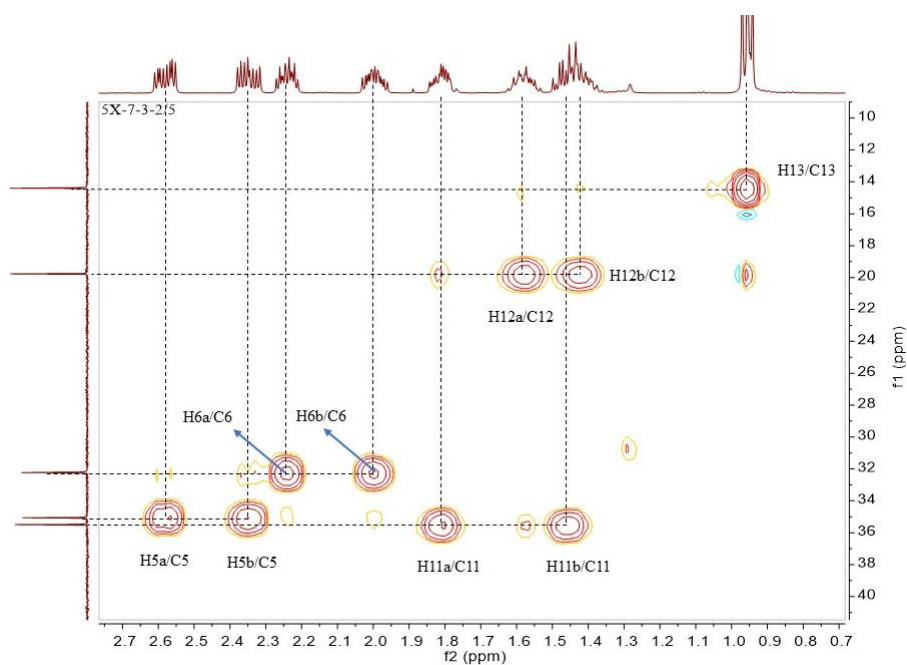


Figure S17: HMQC (CD_3OD) spectrum of phomopsiketone H (**2**) (From δ_{C} 10 ppm to δ_{C} 45 ppm)

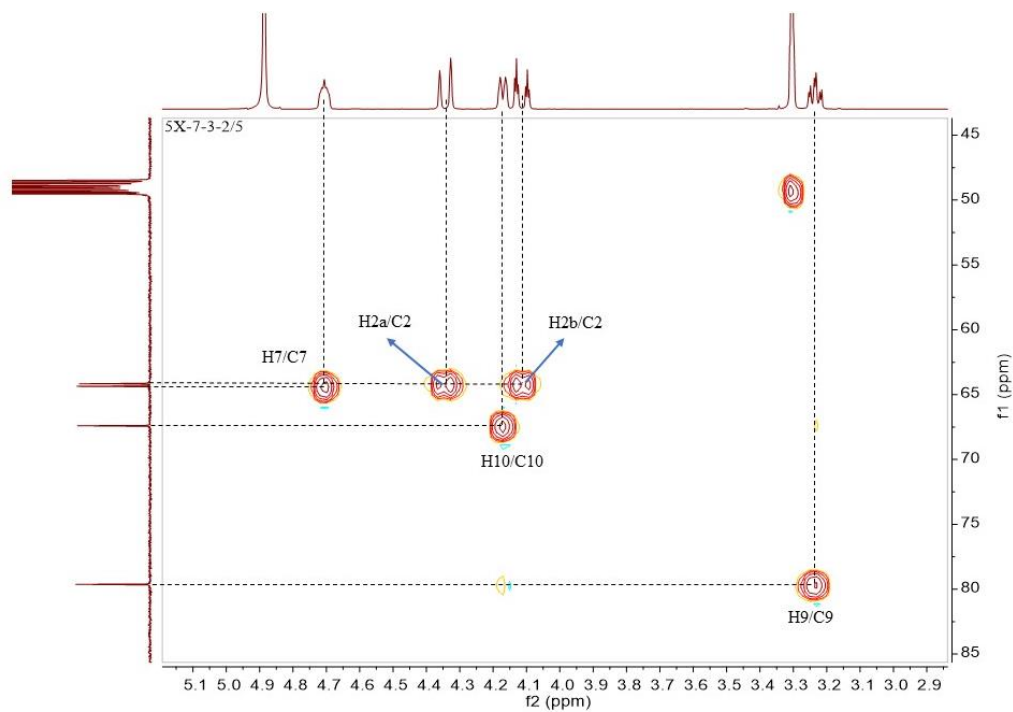


Figure S18: HMQC (CD_3OD) spectrum of phomopsiketone H (**2**) (From δ_{C} 45 ppm to δ_{C} 85 ppm)

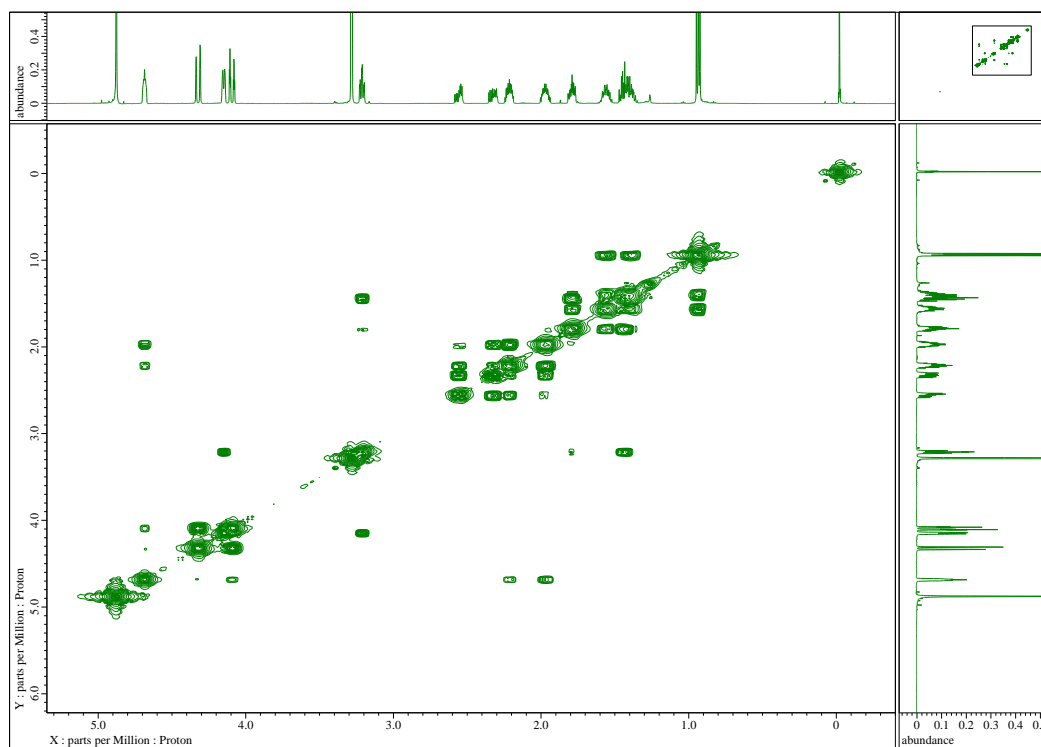


Figure S19: ^1H - ^1H COSY (CD_3OD) spectrum of phomopsiketone H (**2**)

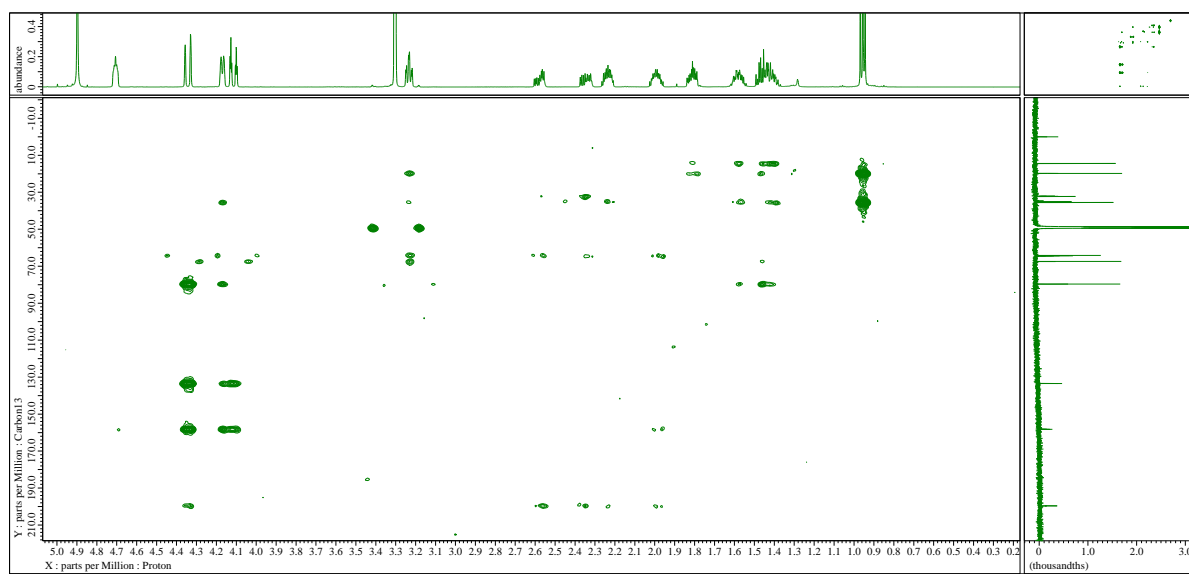


Figure S20: HMBC (CD_3OD) spectrum of phomopsiketone H (**2**)

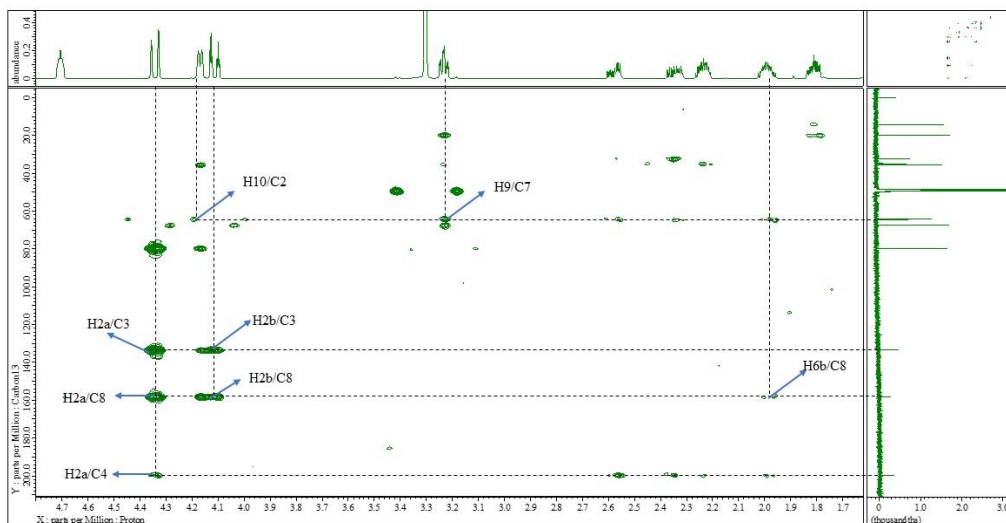


Figure S21: HMBC (CD_3OD) spectrum of phomopsiketone H (**2**) (From δ_{H} 1.7 ppm to δ_{H} 4.7 ppm)

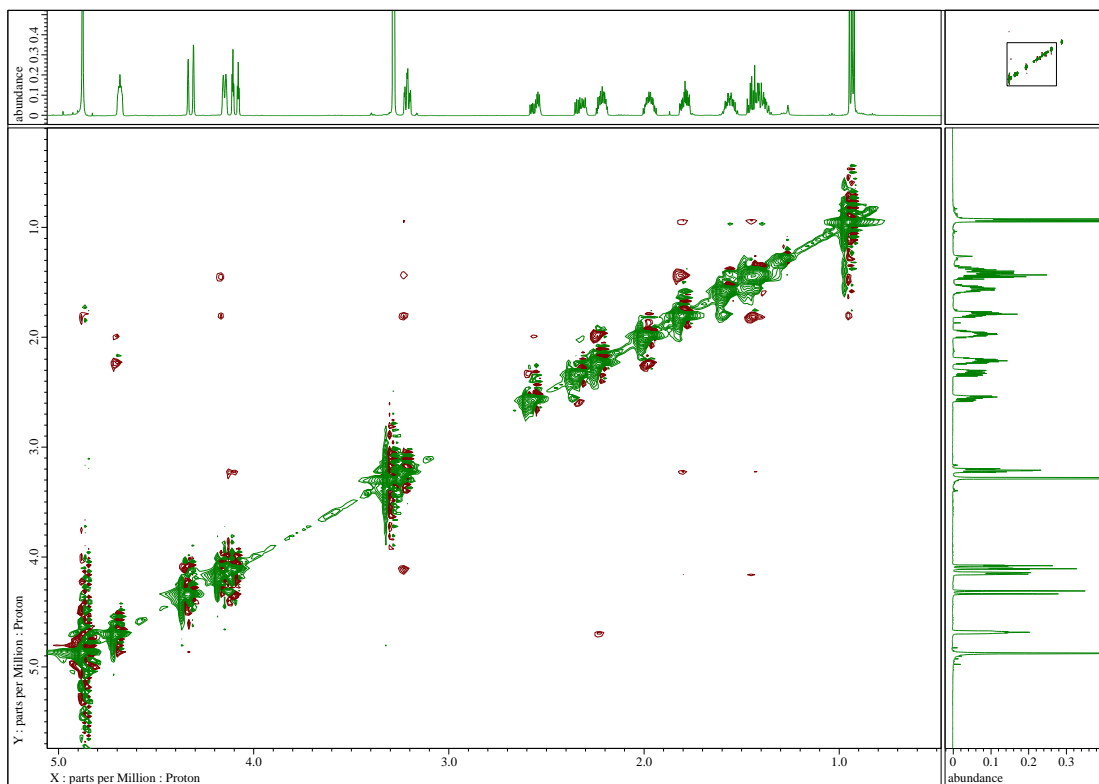


Figure S22: NOESY (CD₃OD) spectrum of phomopsiketone H (2)

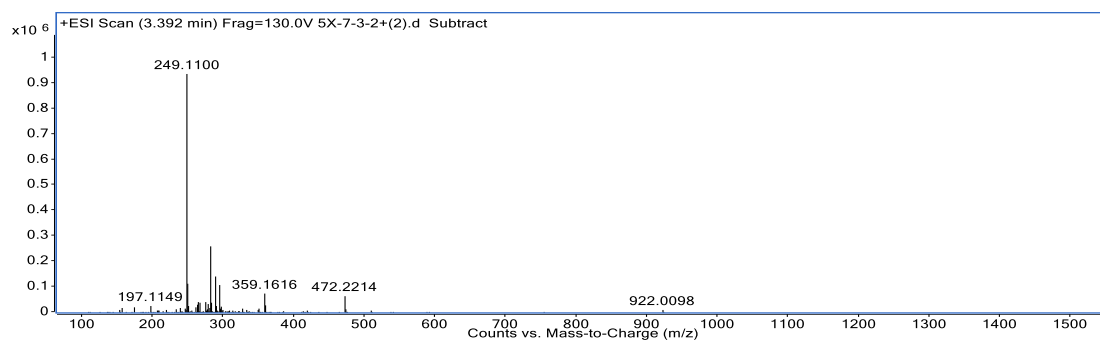


Figure S23: HRESIMS spectrum of phomopsiketone H (2)

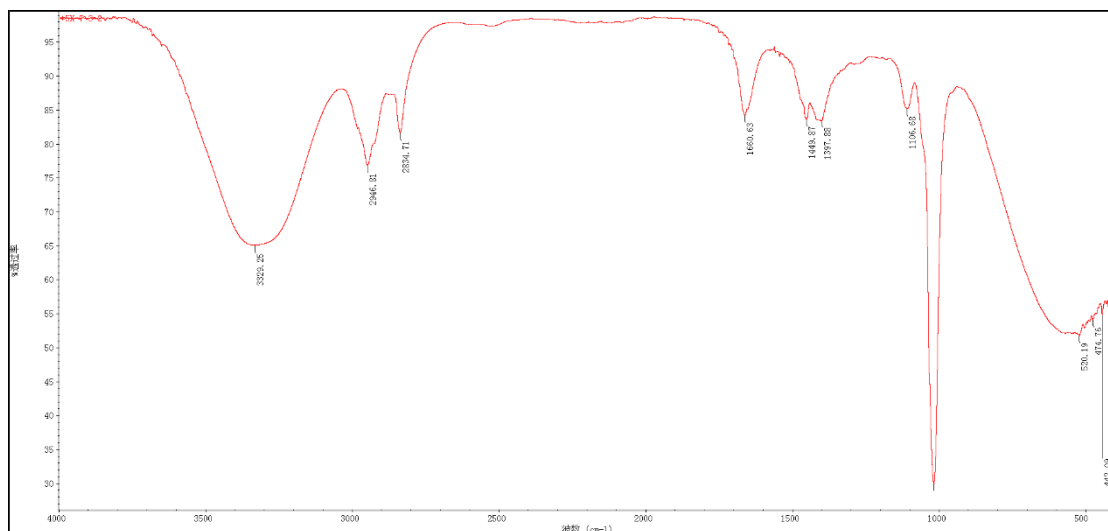


Figure S24: IR spectrum of phomopsiketone H (2)

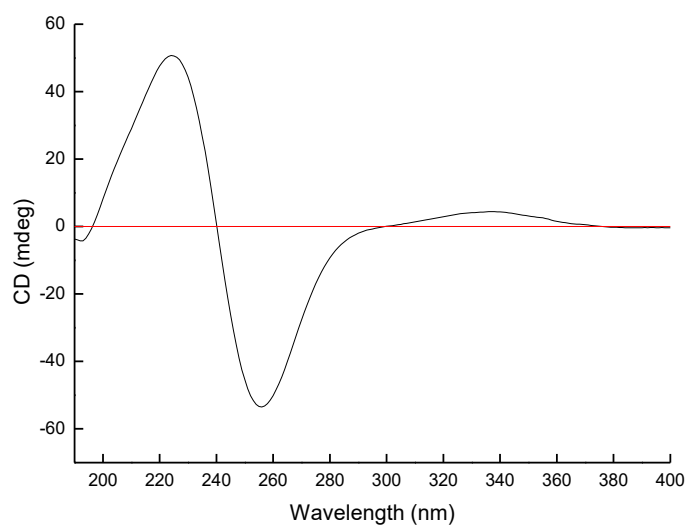


Figure S25: CD spectrum of phomopsiketone H (2)

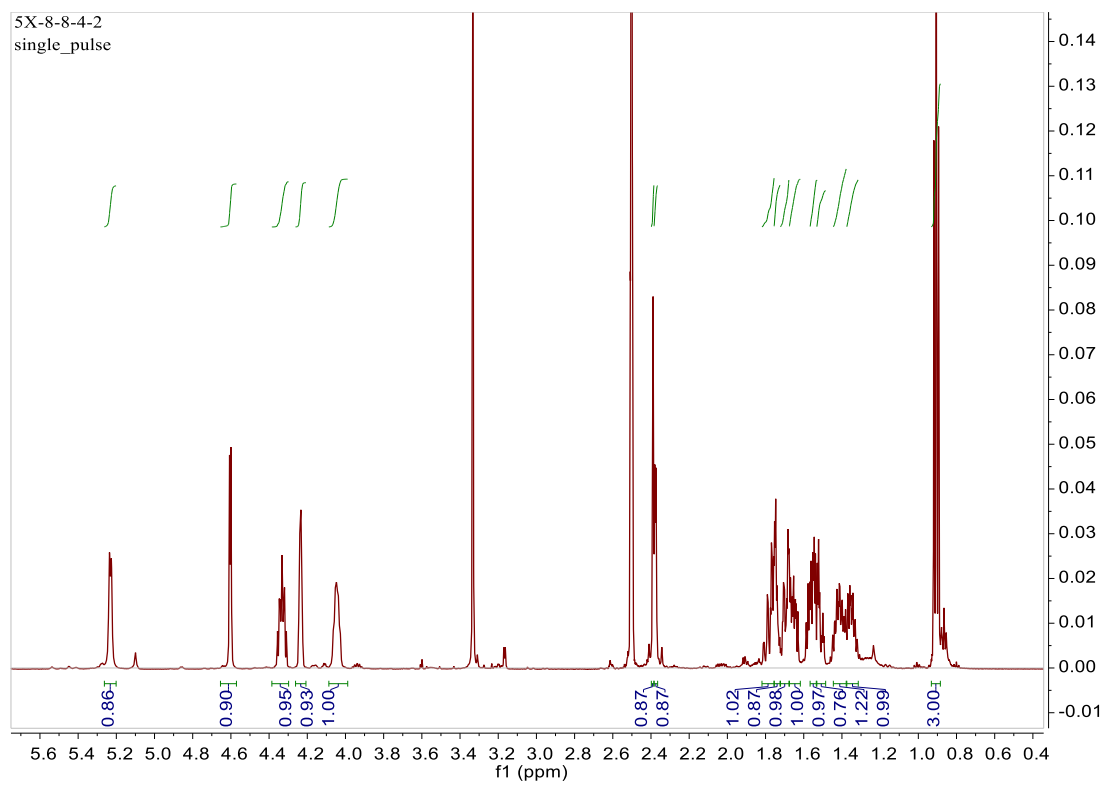


Figure S26: ^1H NMR (600 MHz, DMSO) spectrum of phomopsiketone I (**3**)

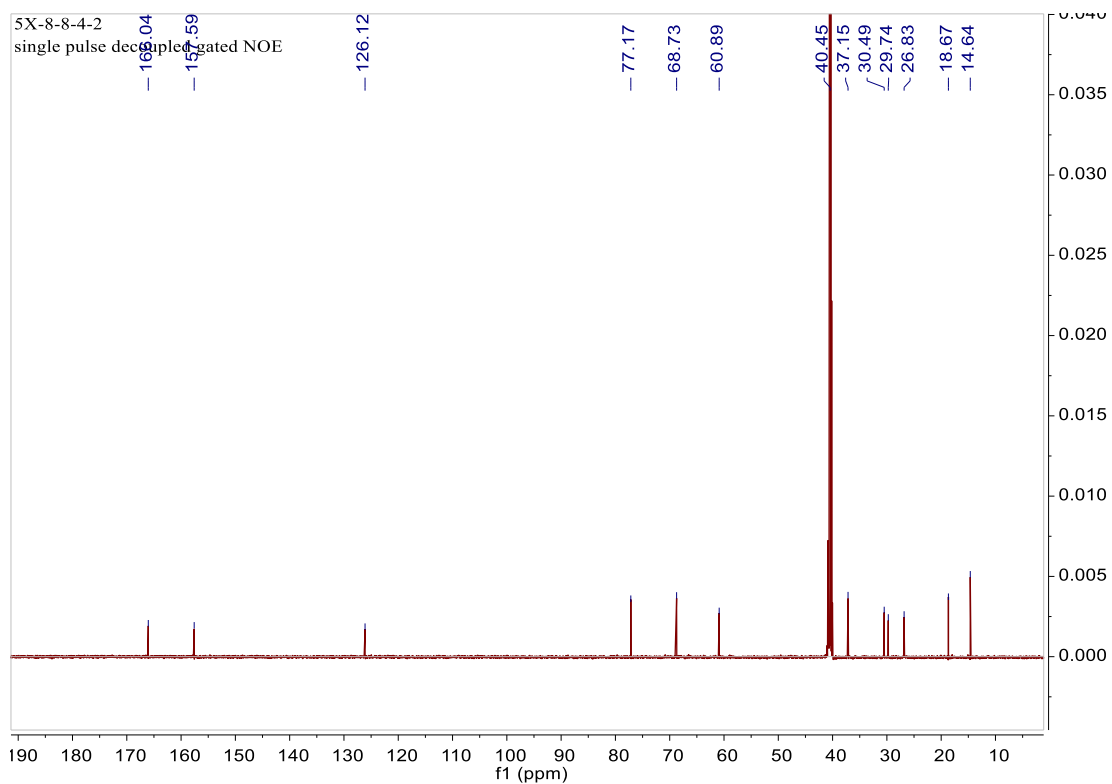


Figure S27: ^{13}C NMR (150 MHz, DMSO) spectrum of phomopsiketone I (**3**)

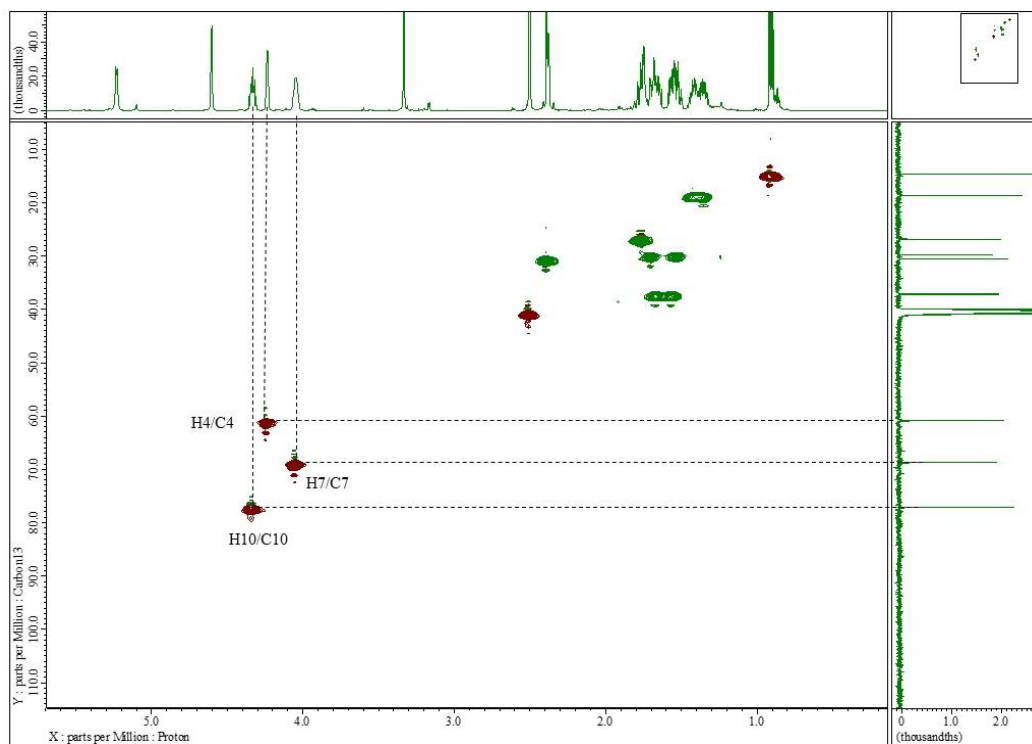


Figure S28: HSQC (DMSO) spectrum of phomopsiketone I (**3**)

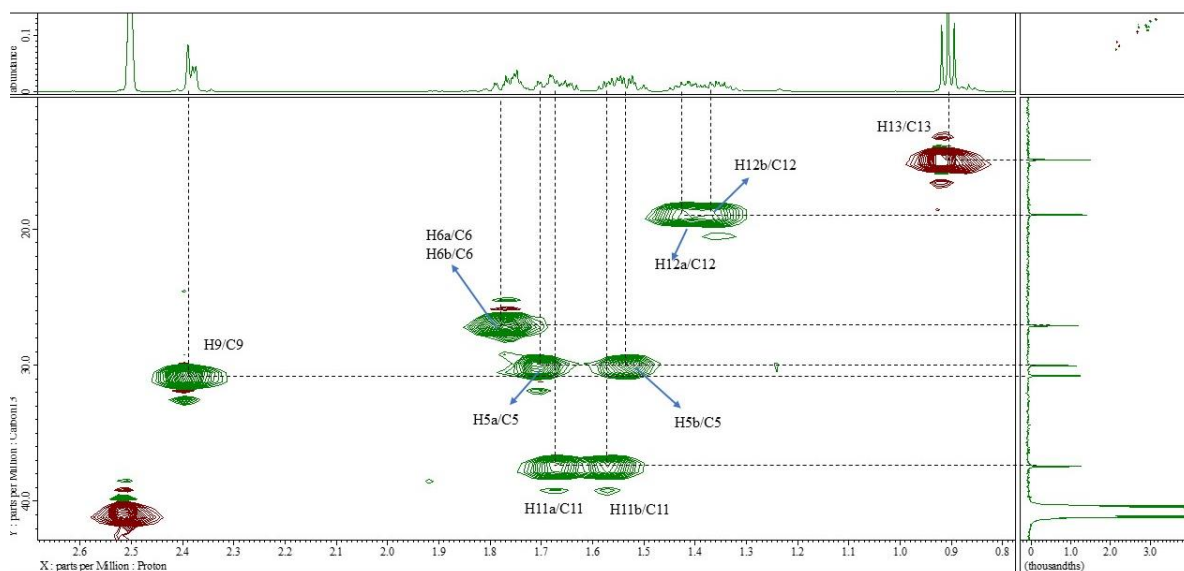


Figure S29: HSQC (DMSO) spectrum of phomopsiketone I (**3**) (From δ_C 5 ppm to δ_C 45 ppm)

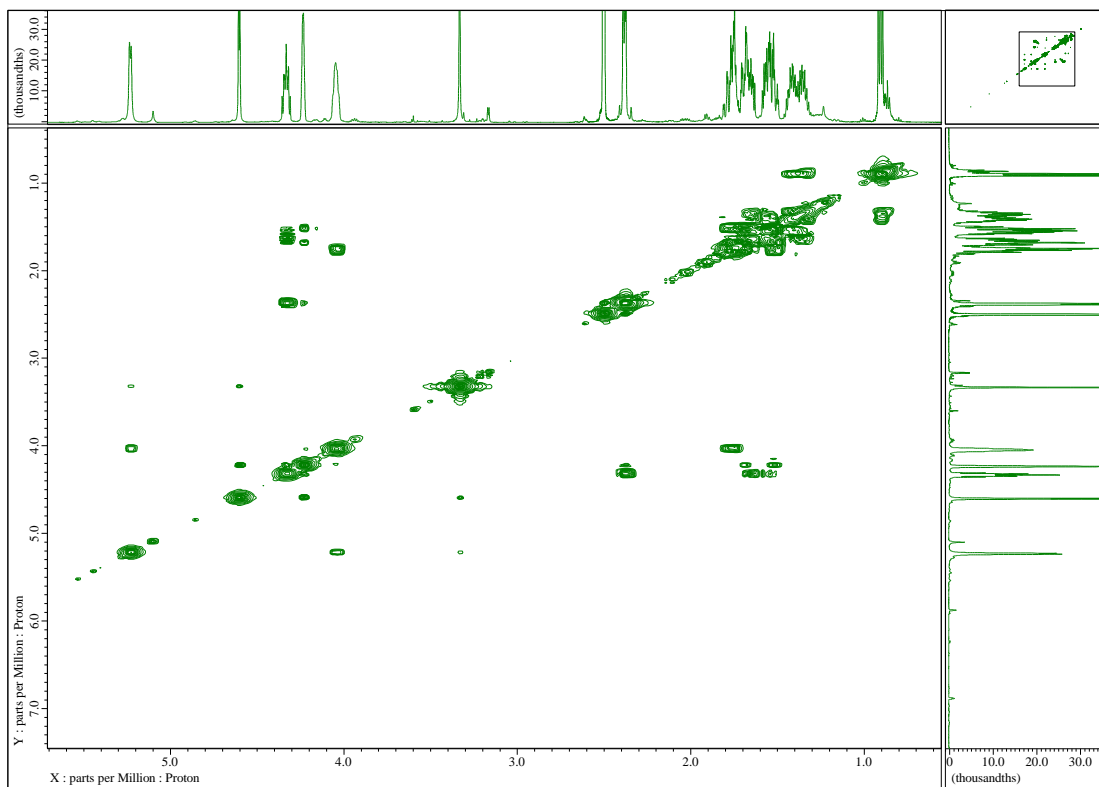


Figure S30: ^1H - ^1H COSY (DMSO) spectrum of phomopsiketone I (**3**)

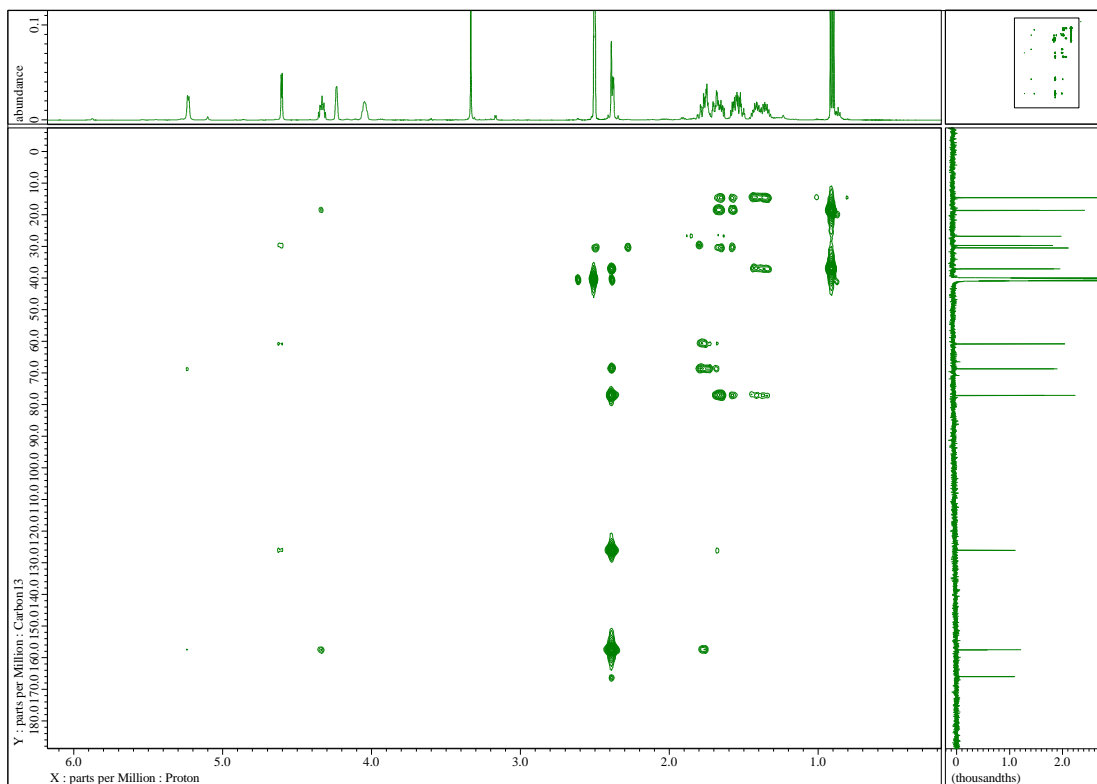


Figure S31: HMBC (DMSO) spectrum of phomopsiketone I (**3**)

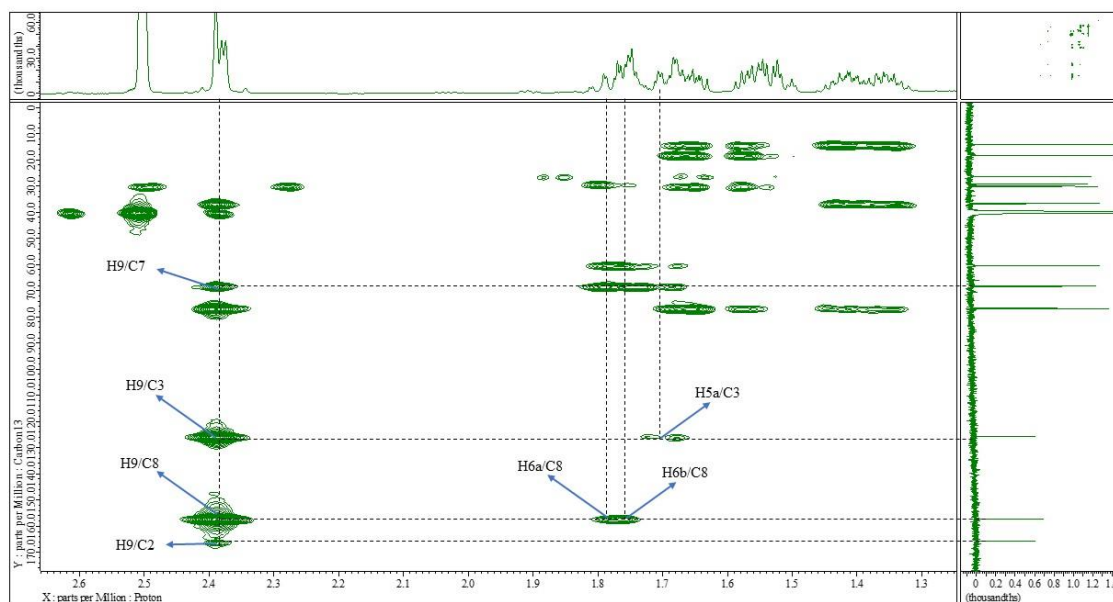


Figure S32: HMBC (DMSO) spectrum of phomopsiketone I (**3**) (From δ_H 1.3 ppm to δ_H 2.5 ppm)

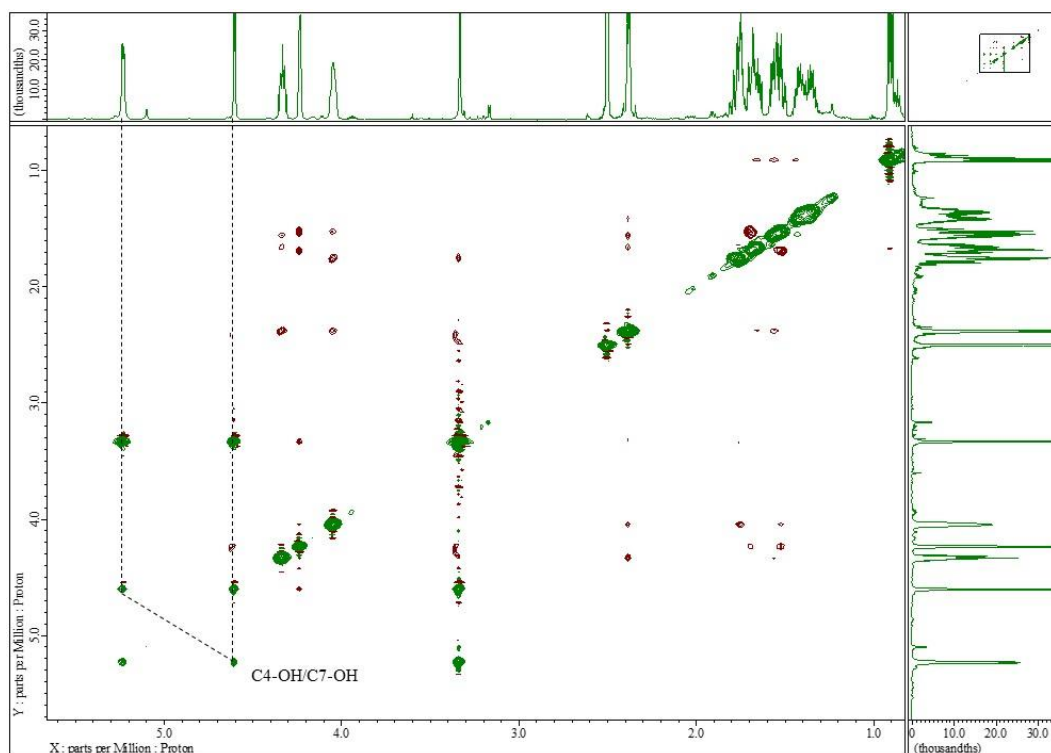


Figure S33: NOESY (DMSO) spectrum of phomopsiketone I (3)

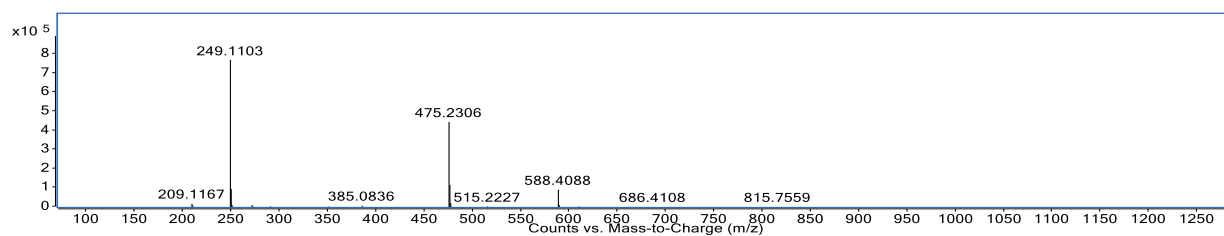


Figure S34: HRESIMS spectrum of phomopsiketone I (3)

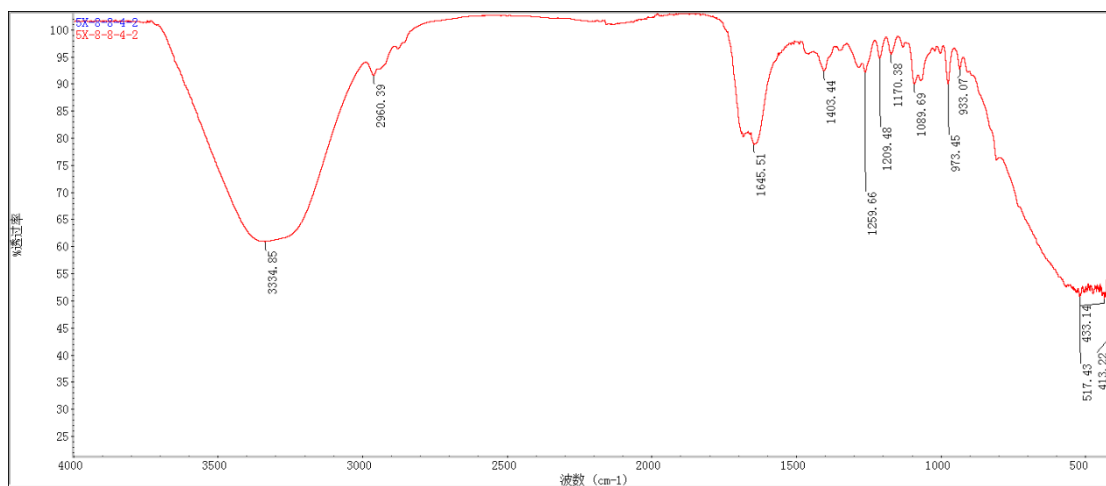


Figure S35: IR spectrum of phomopsiketone I (3)

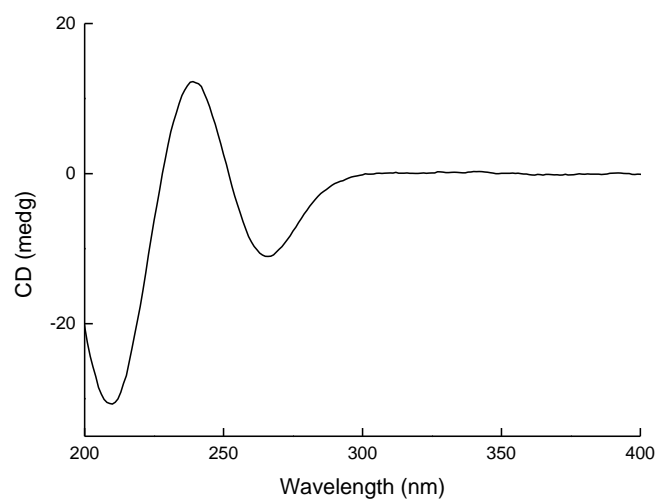


Figure S36: CD spectrum of phomopsiketone I (3)

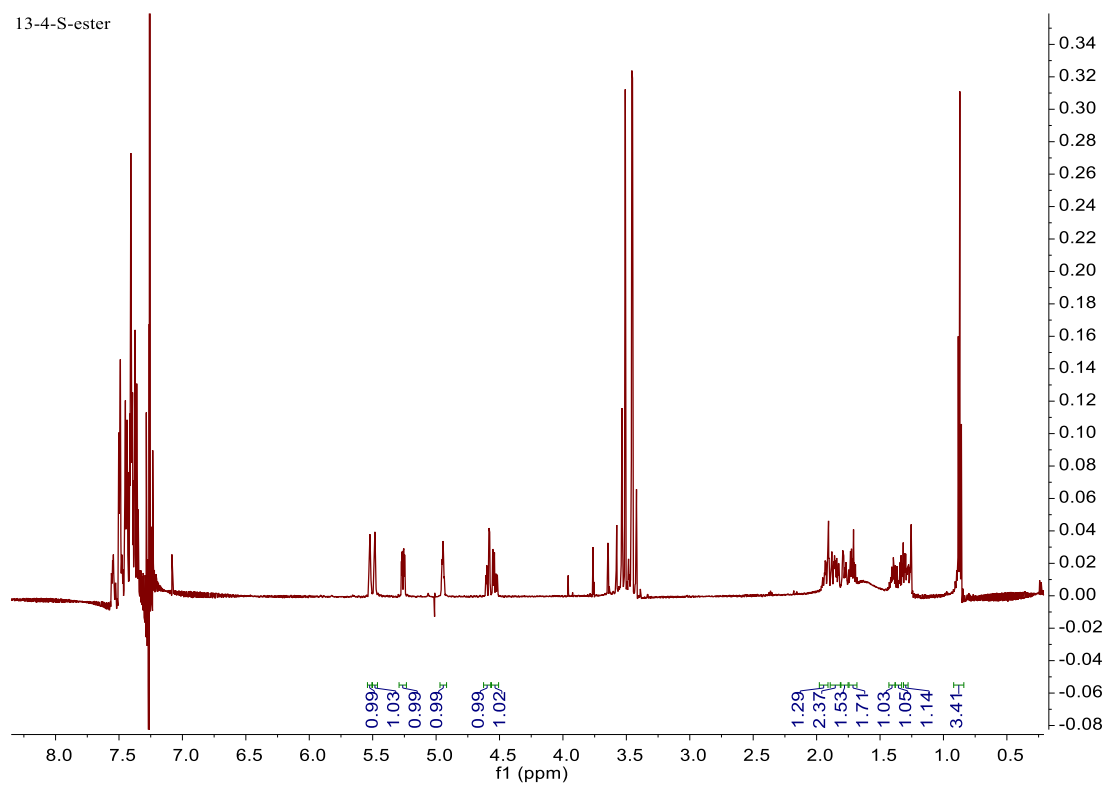


Figure S37: ^1H NMR (600 MHz, CDCl_3) spectrum of **1a**

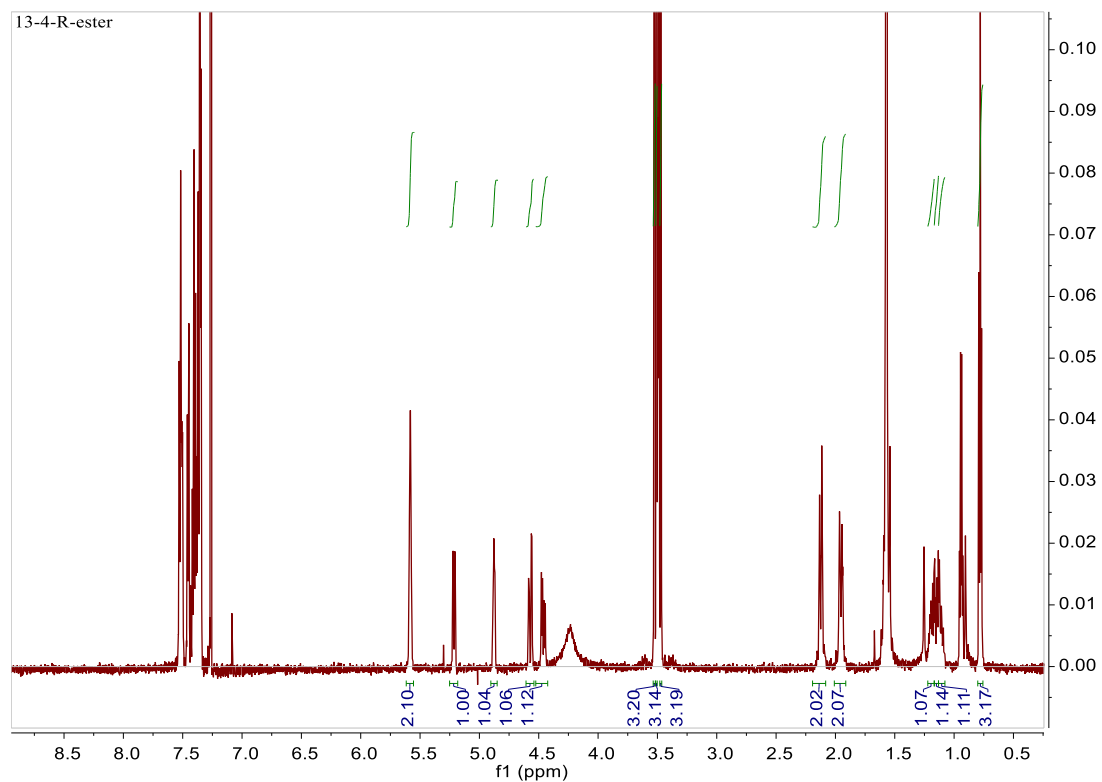


Figure S38: ^1H NMR (600 MHz, CDCl_3) spectrum of **1b**

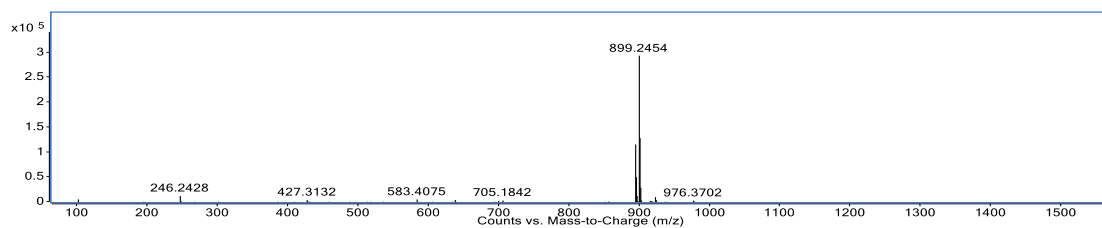


Figure S39: HRESIMS spectrum of 1a

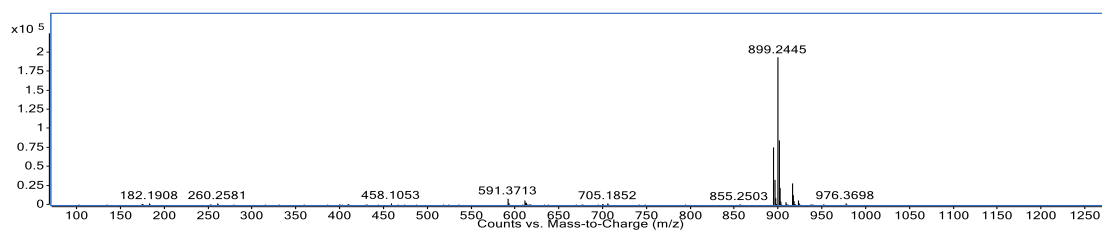


Figure S40: HRESIMS spectrum of 1b

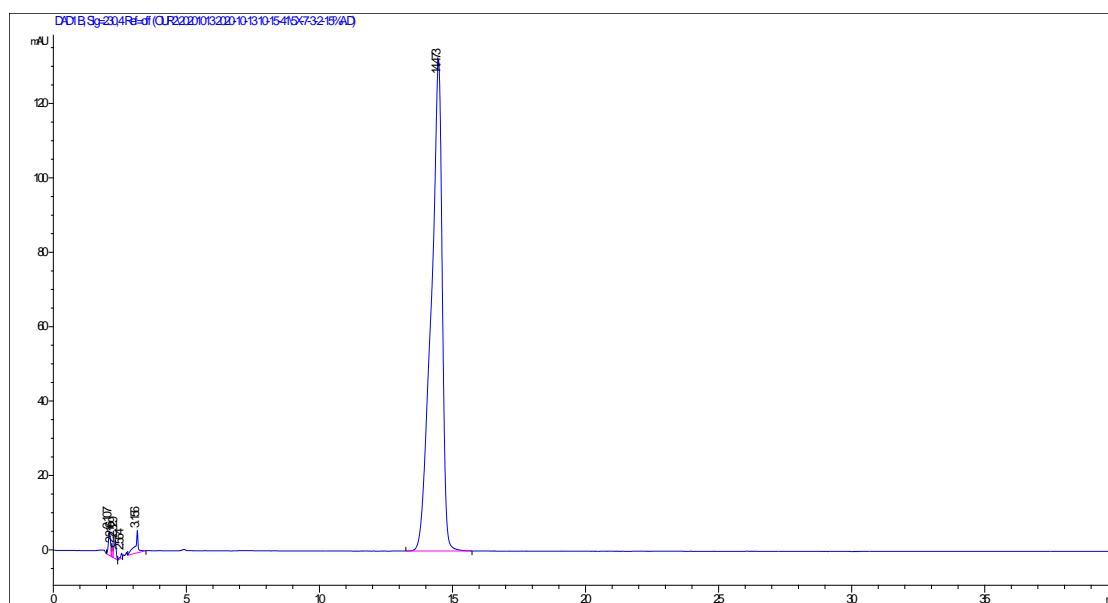


Figure S41: HPLC chromatogram of compound 2 (15% CH₃CN+H₂O, 1 mL/min, 230 nm)

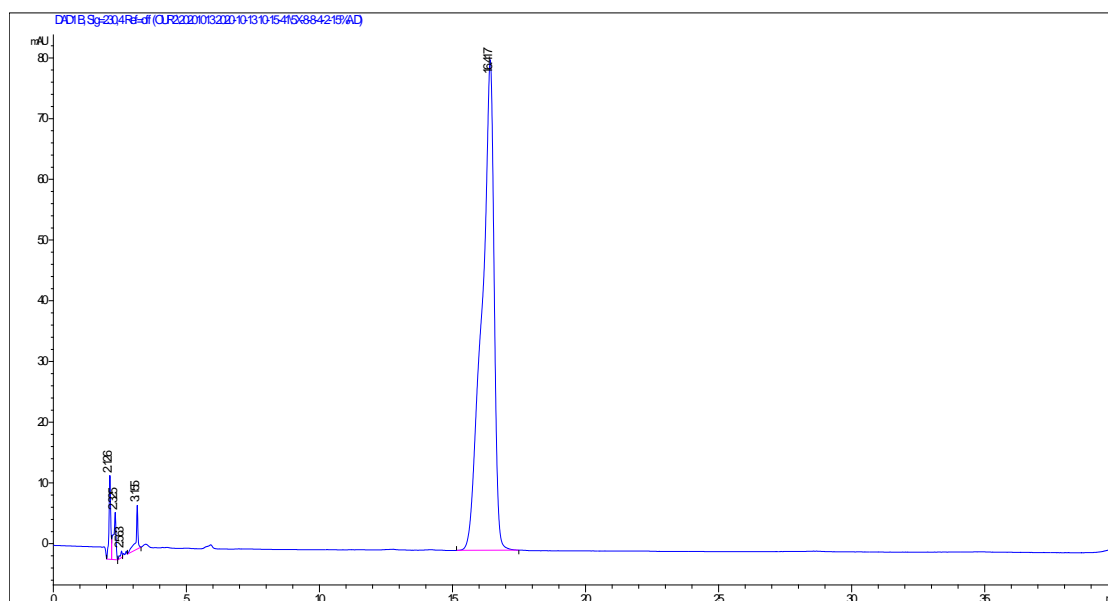
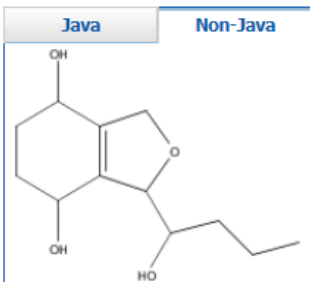


Figure S42: HPLC chromatogram of compound **3** (15% CH₃CN+H₂O, 1 mL/min, 230 nm)

Structure Editor:

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Search Type:

Exact Structure

Substructure

Similarity

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 ChemDraw

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0 of 7 Similarity Candidates Selected	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	3
<input type="checkbox"/> 85-89	1
<input type="checkbox"/> 80-84	1
<input type="checkbox"/> 75-79	26
<input type="checkbox"/> 70-74	43
<input type="checkbox"/> 65-69	211
<input type="checkbox"/> 0-64 (least similar)	1575

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Analyze by:

Substance Role

Biological Study 1

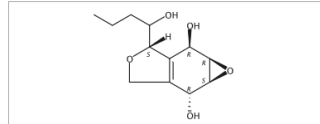
Occurrence 1

Properties 1

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Score: 90

1. [877418-45-6](#)



Currently available stereo shown. Absolute stereochemistry unknown. Rotation (-).

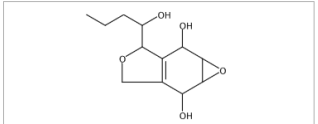
C₁₂ H₁₈ O₅
Oxireneol [Isobenzofuran-2,6-diol, 1a,2,3,5,6,6a-hexahydro-5-(1-hydroxybutyl)-, (1aR,2,5R,6,5,6a,5)-ref(-)]

[Key Physical Properties](#)

Spectra

Score: 90

2. [1235343-92-6](#)

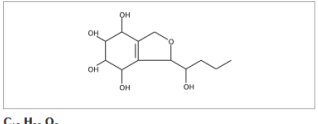


C₁₂ H₁₈ O₅
Oxireneol [Isobenzofuran-2,6-diol, 1a,2,3,5,6,6a-hexahydro-3-(1-hydroxybutyl)-]

[Key Physical Properties](#)

Score: 90

3. [1236255-29-0](#)



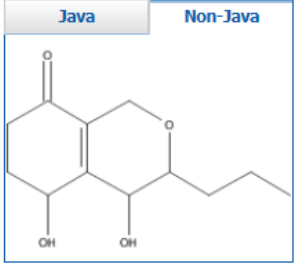
C₁₂ H₂₀ O₆
4,5,6,7-Isobenzofurantetrol, 1,3,4,5,6,7-hexahydro-1-(1-hydroxybutyl)-

[Key Physical Properties](#)

Figure S43: SciFinder Search Results of 1

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF

Search Type:

- Exact Structure
- Substructure
- Similarity

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	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	1
<input type="checkbox"/> 90-94	4
<input type="checkbox"/> 85-89	3
<input type="checkbox"/> 80-84	6
<input type="checkbox"/> 75-79	56
<input type="checkbox"/> 70-74	209
<input type="checkbox"/> 65-69	1194
<input type="checkbox"/> 0-64 (least similar)	6207

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SUBSTANCES

Analyze Refine

Analyze by: Substance Role

Preparation 4

Biological Study 3

Properties 2

Uses 2

Occurrence 1

Process 1

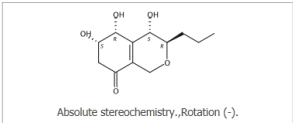
Show More

Sort by: Similarity Score

0 of 5 Substances Selected

Score: 95

1. 2095879-67-5



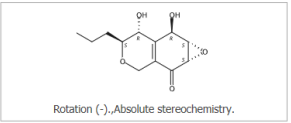
Absolute stereochemistry, Rotation (-).

C₁₂H₁₈O₅
8#7-2-Benzopyran-8-one, 1,3,4,5,6,7-hexahydro-4,5,6-trihydroxy-3-propyl-, (3*R*,4*S*,5*R*,6*S*)

Key Physical Properties

Score: 91

2. 193481-66-2



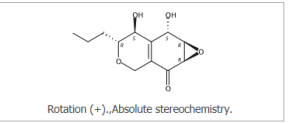
Rotation (-), Absolute stereochemistry.

C₁₂H₁₆O₅
2#9-Oxirenol[*g*][2]benzopyran-2-one, 1*a*,3,5,6,7,7*a*-hexahydro-6,7-dihydroxy-5-propyl-, (1*a*,5*S*,6*R*,7*R*,7*a*,5*S*)

Key Physical Properties

Score: 91

3. 384835-66-9



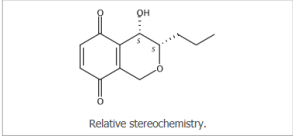
Rotation (+), Absolute stereochemistry.

C₁₂H₁₆O₅
2#9-Oxirenol[*g*][2]benzopyran-2-one, 1*a*,3,5,6,7,7*a*-hexahydro-6,7-dihydroxy-5-propyl-, (1*a*,5*R*,6*S*,7*S*,7*a*,5*R*)

Key Physical Properties

Score: 90

4. 95330-50-0



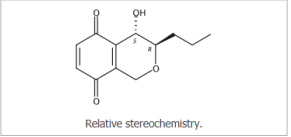
Relative stereochemistry.

C₁₂H₁₄O₄
1#5-Benzopyran-8-one, 3,4-dihydro-4-hydroxy-3-propyl-, (3*R*,4*S*)

Key Physical Properties

Score: 90

5. 95330-53-3



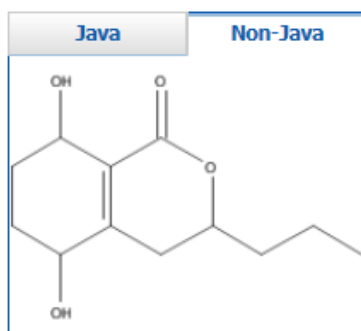
Relative stereochemistry.

C₁₂H₁₄O₄
1#5-Benzopyran-8-one, 3,4-dihydro-4-hydroxy-3-propyl-, (3*S*,4*R*)

Key Physical Properties

Figure S44: SciFinder Search Results of 2

Structure Editor:



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Import CXF

Search Type:

- Exact Structure
 Substructure
 Similarity

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Select All Deselect All

0 of 7 Similarity Candidates Selected

Similarity Range	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	2
<input type="checkbox"/> 85-89	9
<input type="checkbox"/> 80-84	30
<input type="checkbox"/> 75-79	171
<input type="checkbox"/> 70-74	522
<input type="checkbox"/> 65-69	1861
<input type="checkbox"/> 0-64 (least similar)	8092

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Sort by: Similarity Score

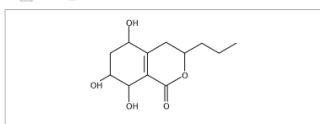
0 of 2 Substances Selected

Analyze by: Substance Role

Biological Study 1
Occurrence 1
Preparation 1
Properties 1
Uses 1

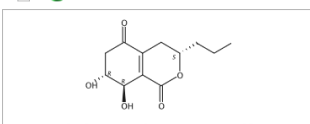
Show More

Score: 92
1. 1236262-66-0



$C_{12}H_{16}O_5$
1*H*-2-Benzopyran-1-one, 3,4,5,6,7,8-hexahydro-5,7,8-trihydroxy-3-propyl-
Key Physical Properties

Score: 90
2. 189828-33-9



Absolute stereochemistry, Rotation (-).
 $C_{12}H_{16}O_5$
1*H*-2-Benzopyran-1,5(3*H*)-dione, 4,6,7,8-tetrahydro-7,8-dihydroxy-3-propyl-, (3*S*,7*R*,8*R*)-
Key Physical Properties
Experimental Properties

Figure S45: SciFinder Search Results of 3