

Supplementary Materials: An Unusual Conformational Isomer of Verrucosidin Backbone from a Hydrothermal Vent Fungus, *Penicillium* sp. Y-50-10

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Table S1. Gibbs Free Energy (Hartree/Particle) of compound **1**.

Table S2. Total Energy (Hartree/Particle) of different transition states.

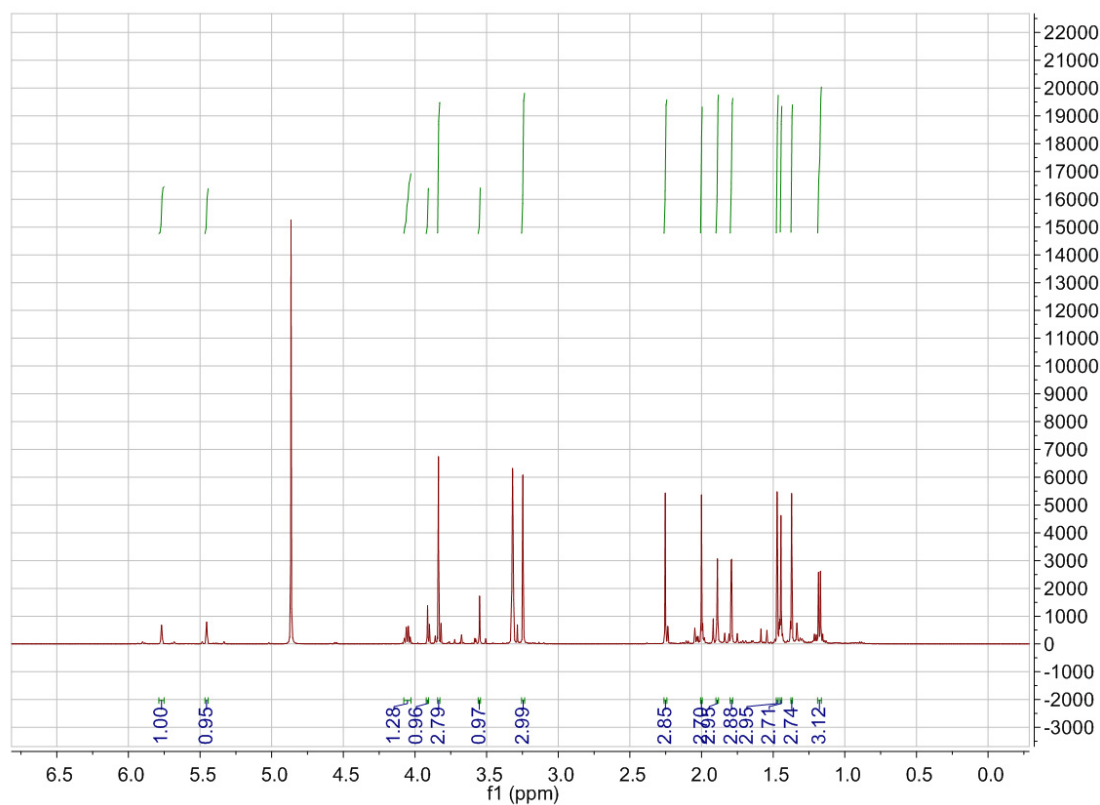


Figure S1. ¹H NMR in CD₃OD for compound 1.

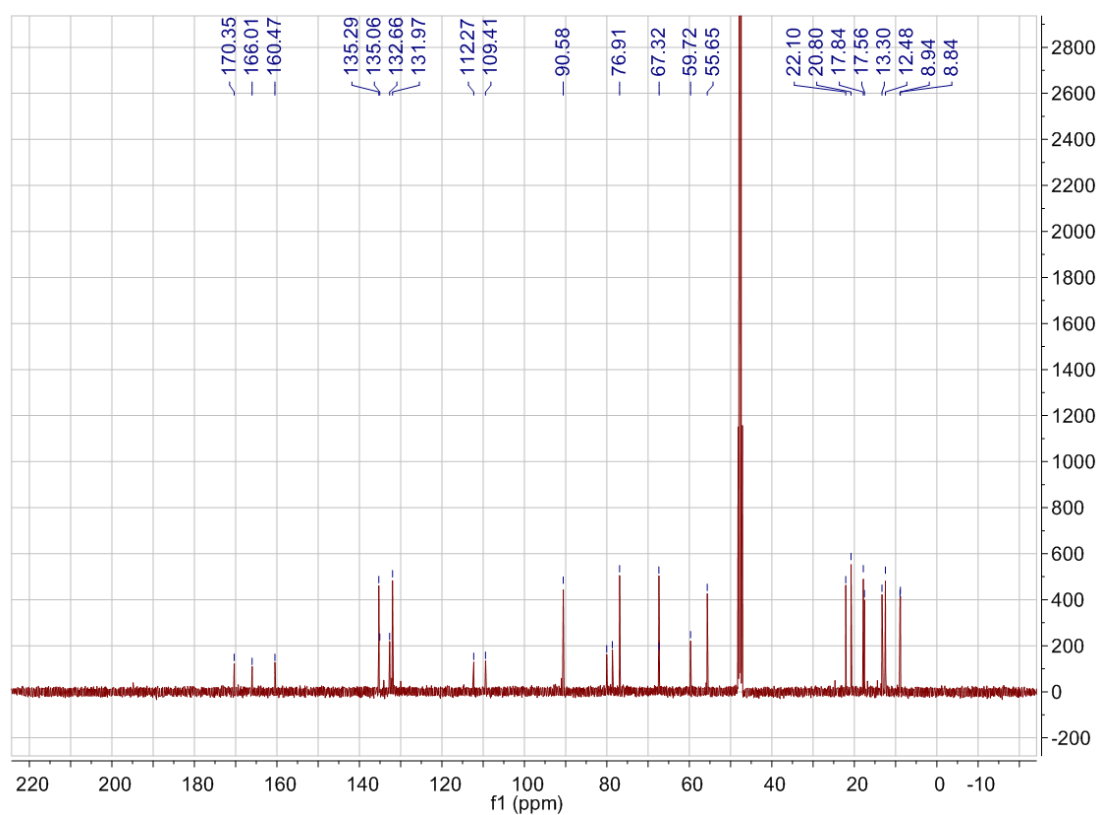


Figure S2. ¹³C NMR in CD₃OD for compound 1.

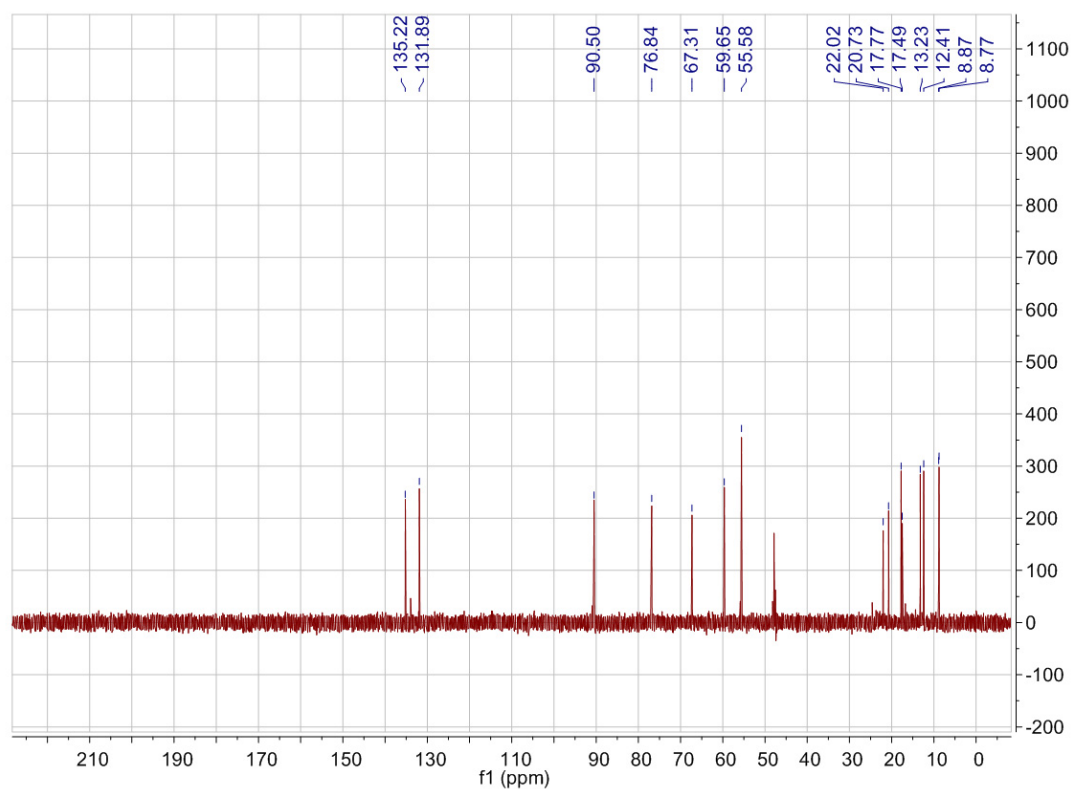


Figure S3. DEPT in CD₃OD for compound 1.

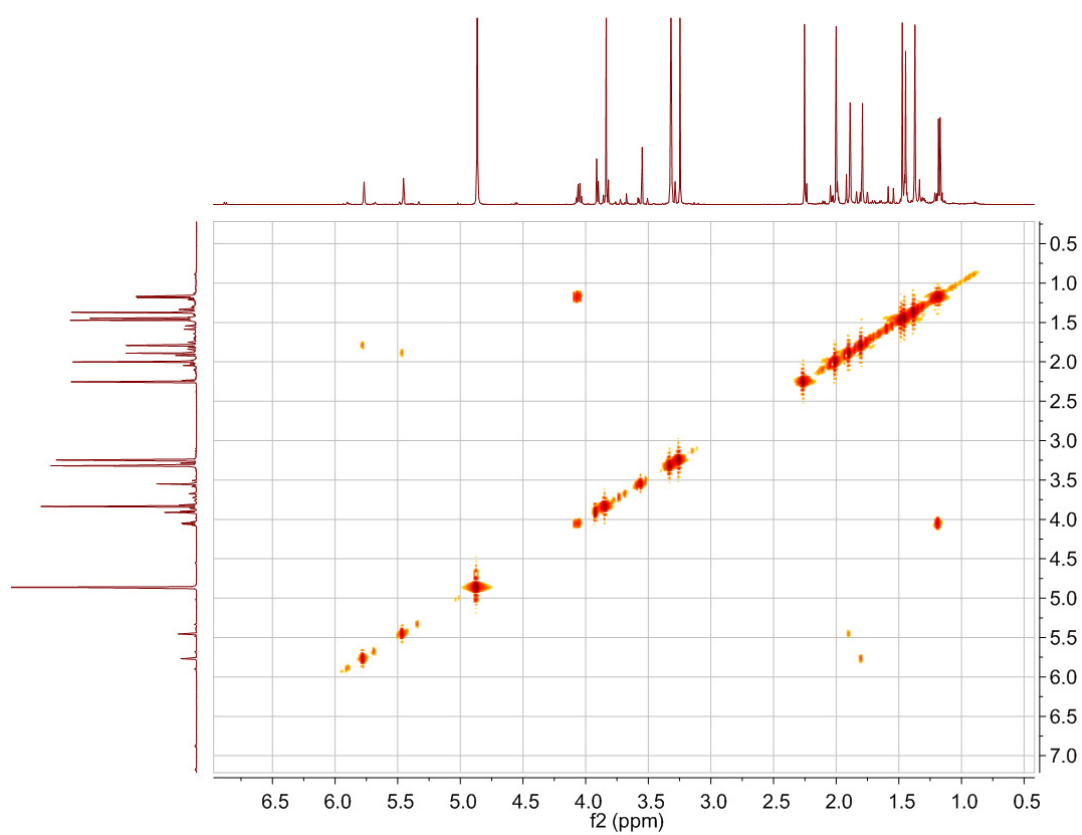


Figure S4. COSY in CD₃OD for compound 1.

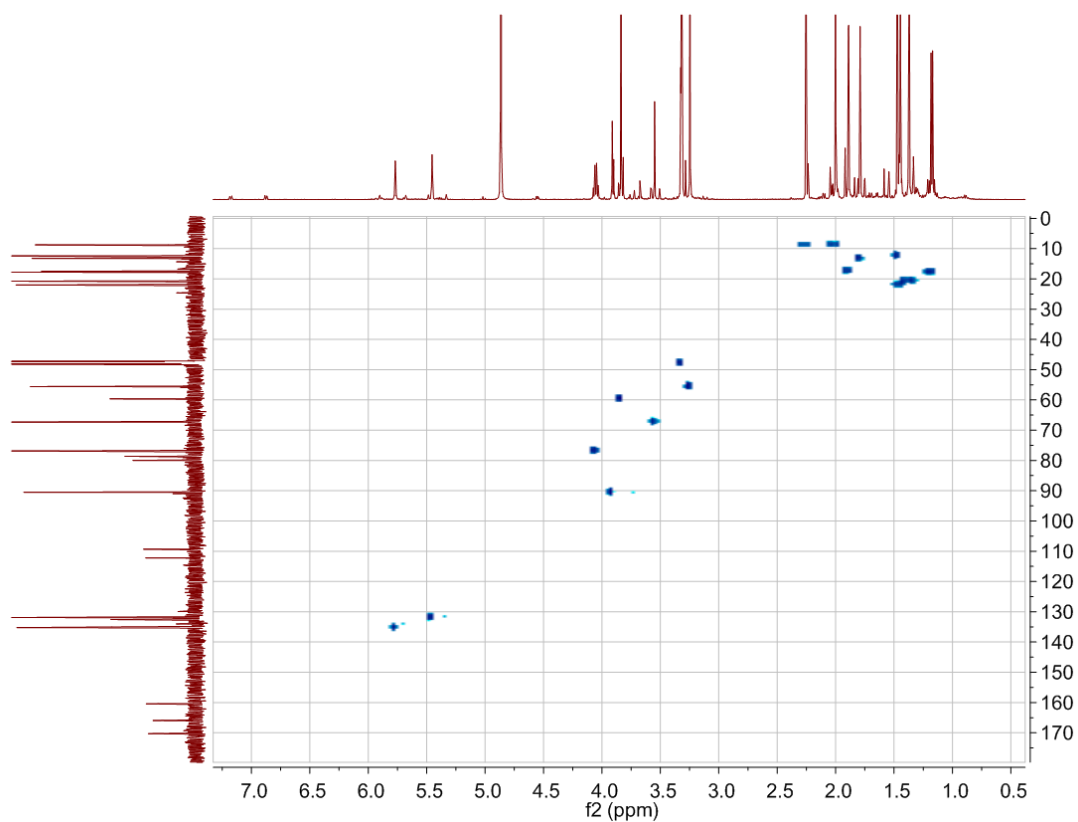


Figure S5. HMQC in CD₃OD for compound 1.

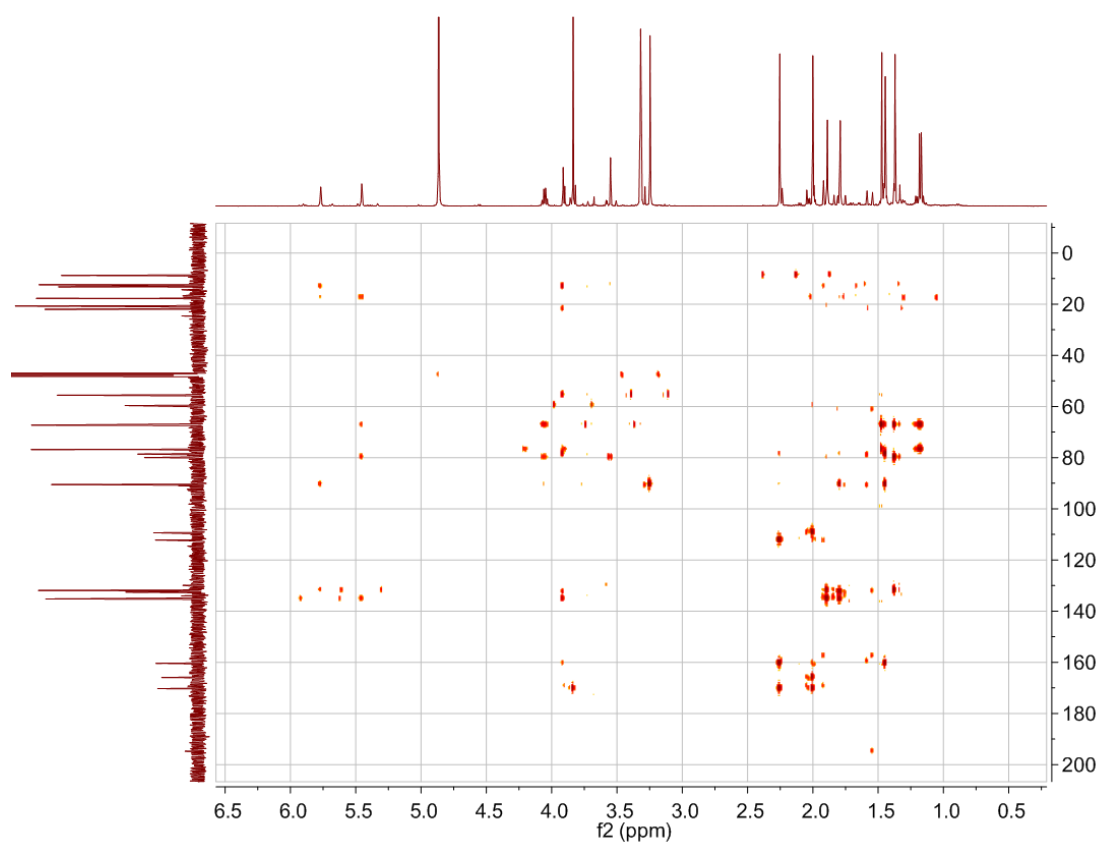


Figure S6. HMBC in CD₃OD for compound 1.

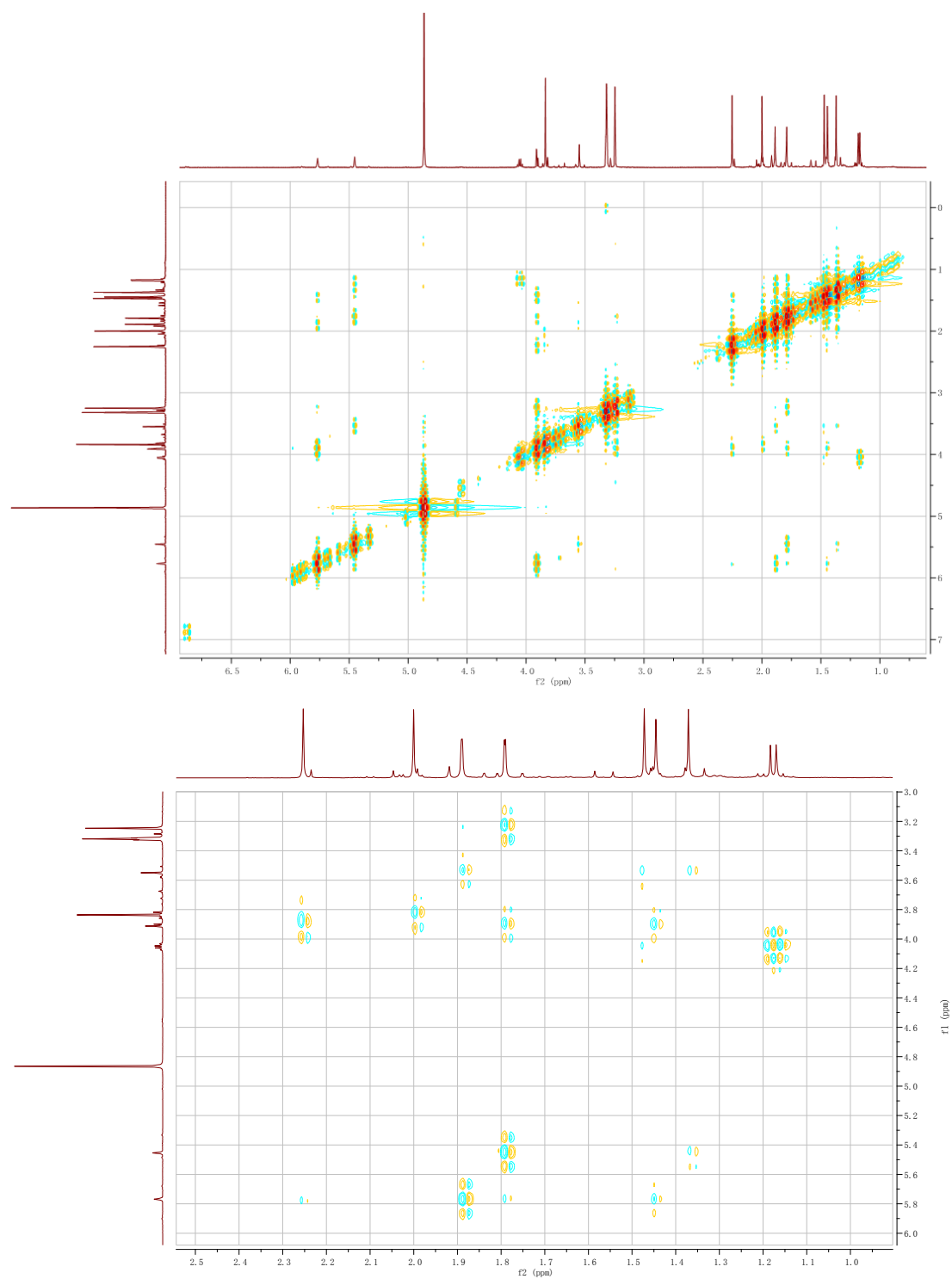


Figure S7. NOESY in CD₃OD for compound 1.

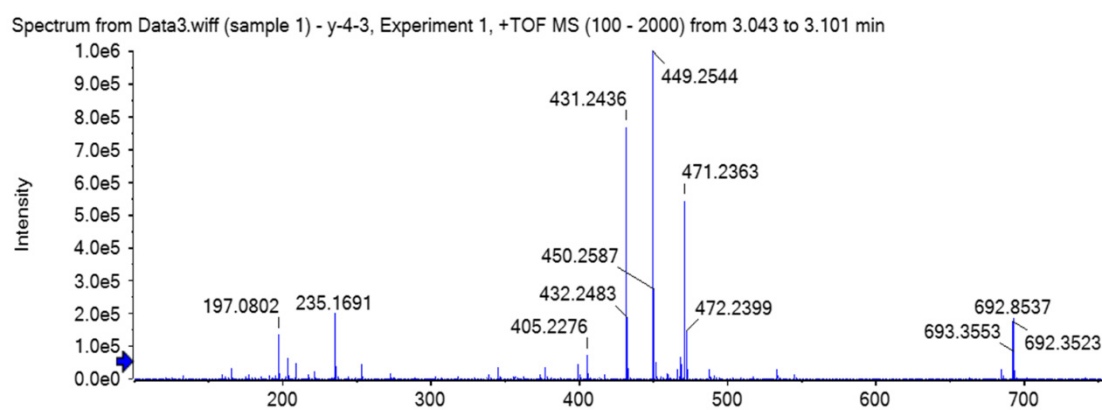


Figure S8. HRESIMS for compound 1.

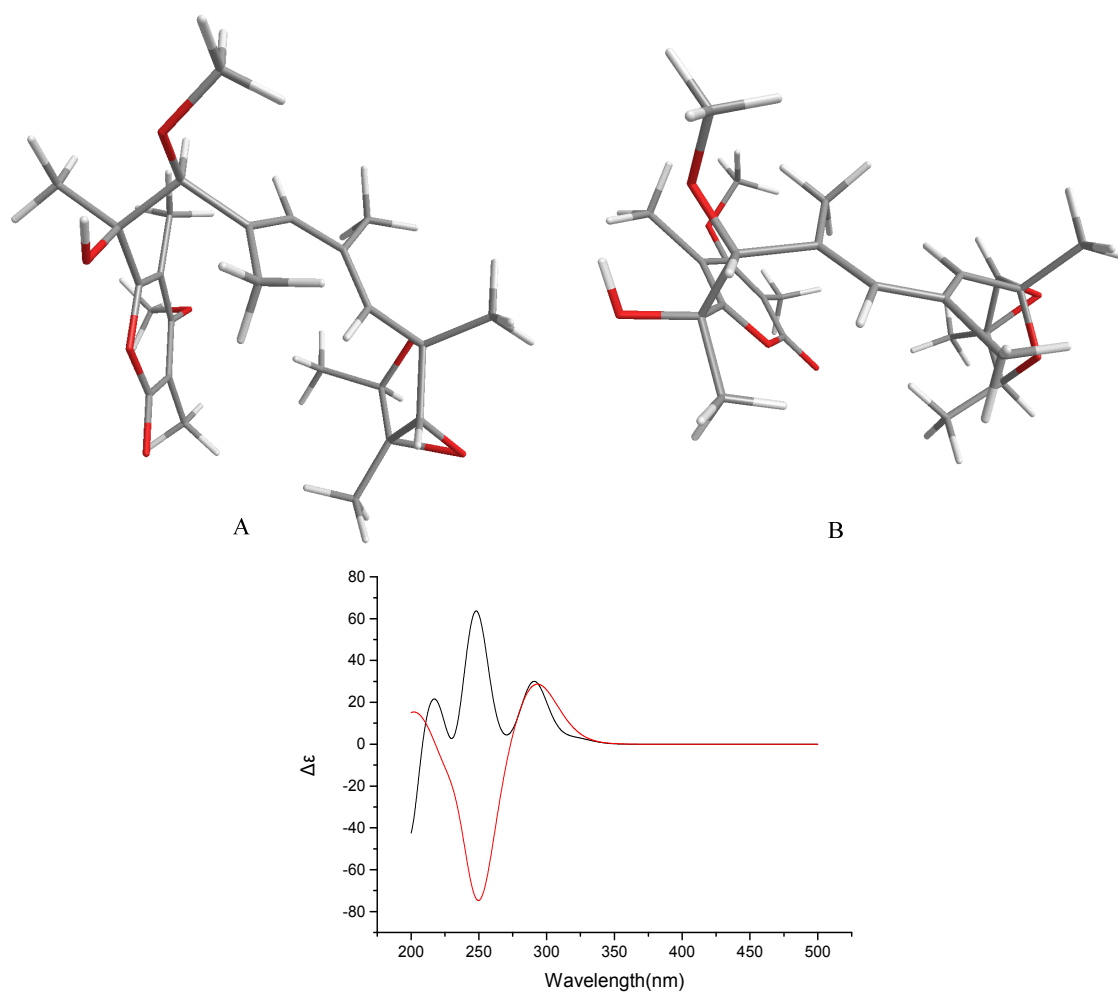


Figure S9. B3LYP/6-31+G(d,p) calculated ECD data for conformations of A (red) and B (black) of compound 1.

TIC

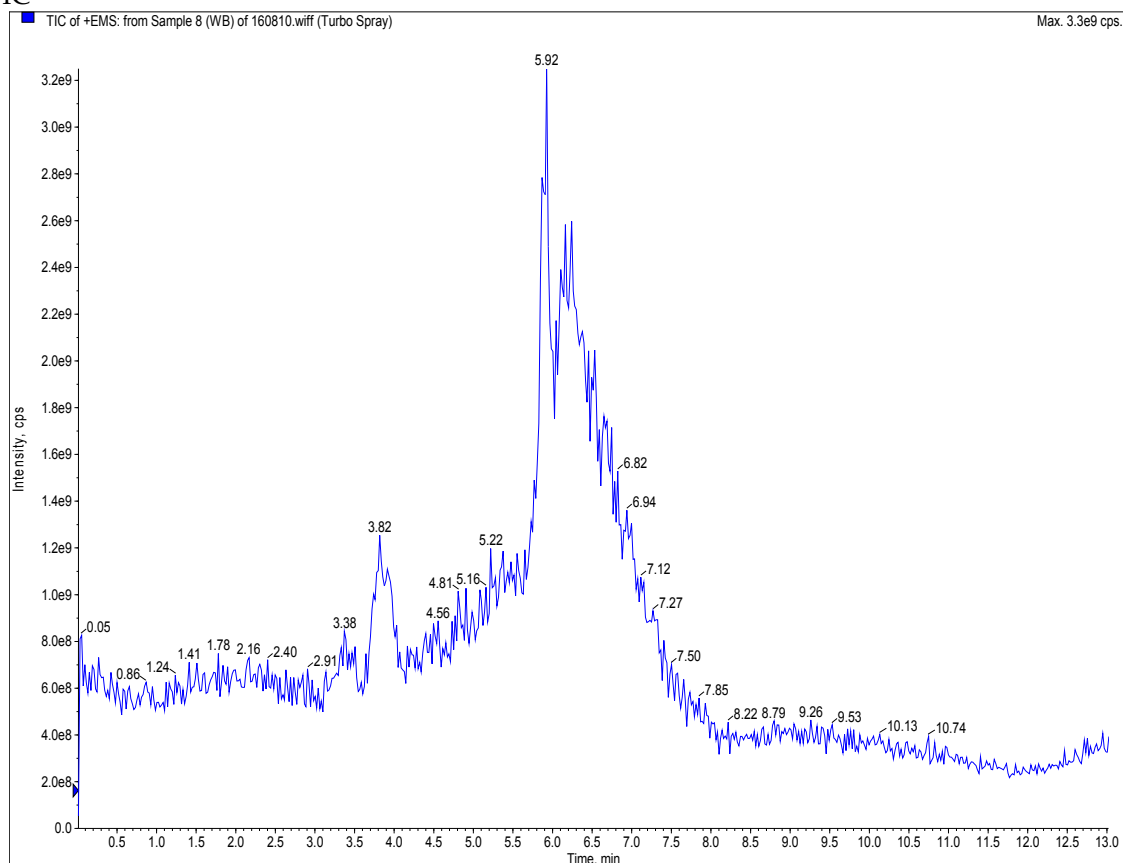
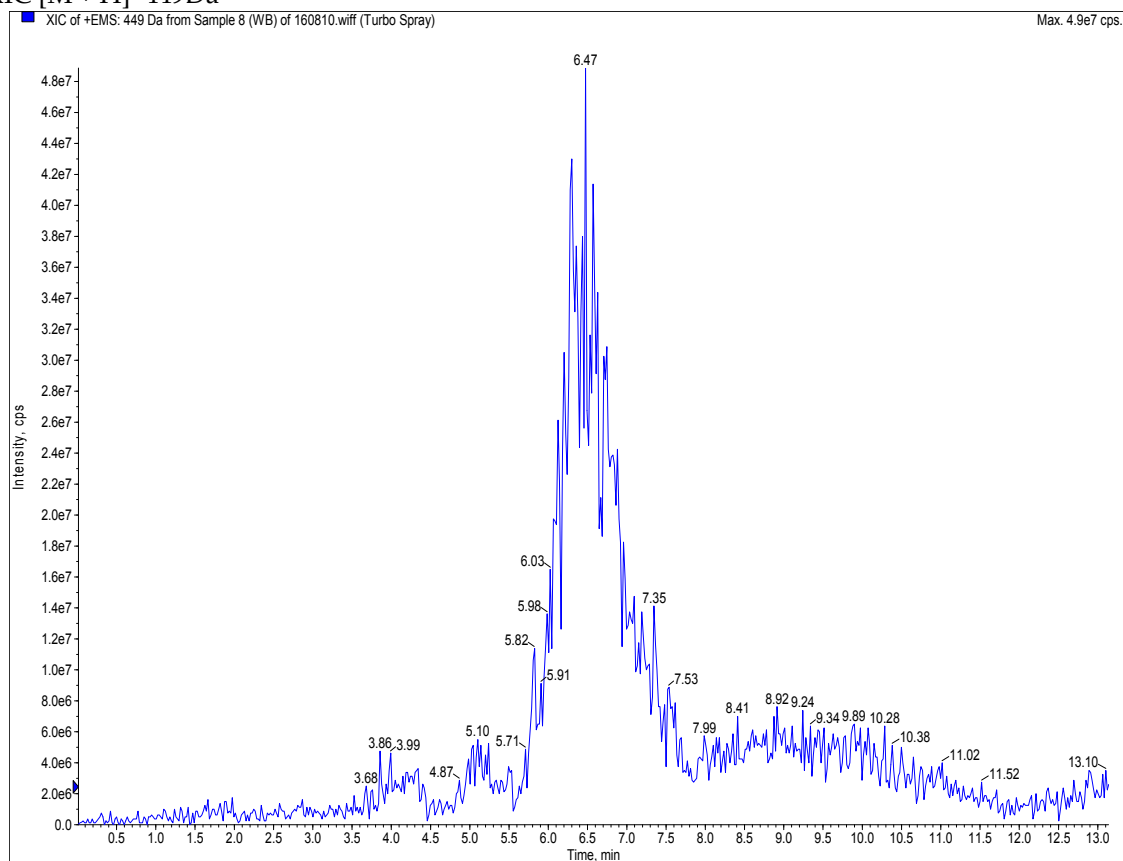
XIC [M + H]⁺ 449Da

Figure S10. Cont.

6.47 min

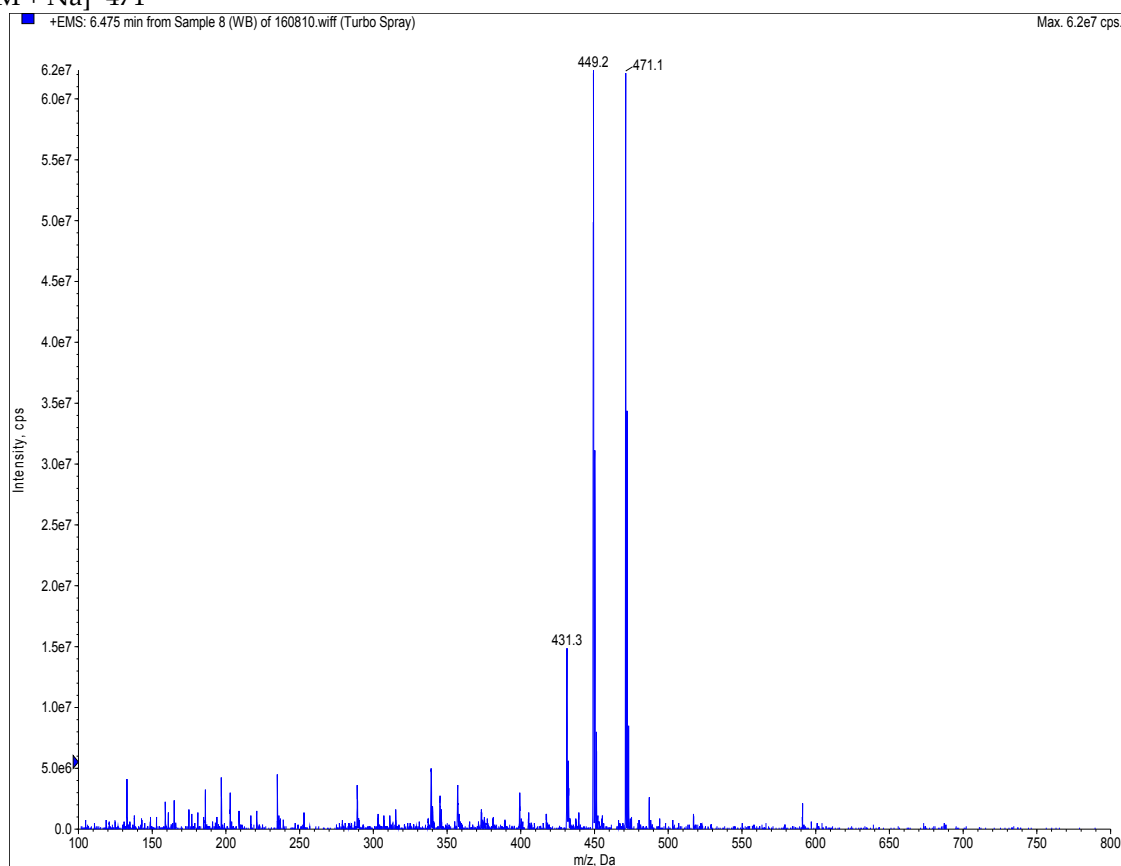
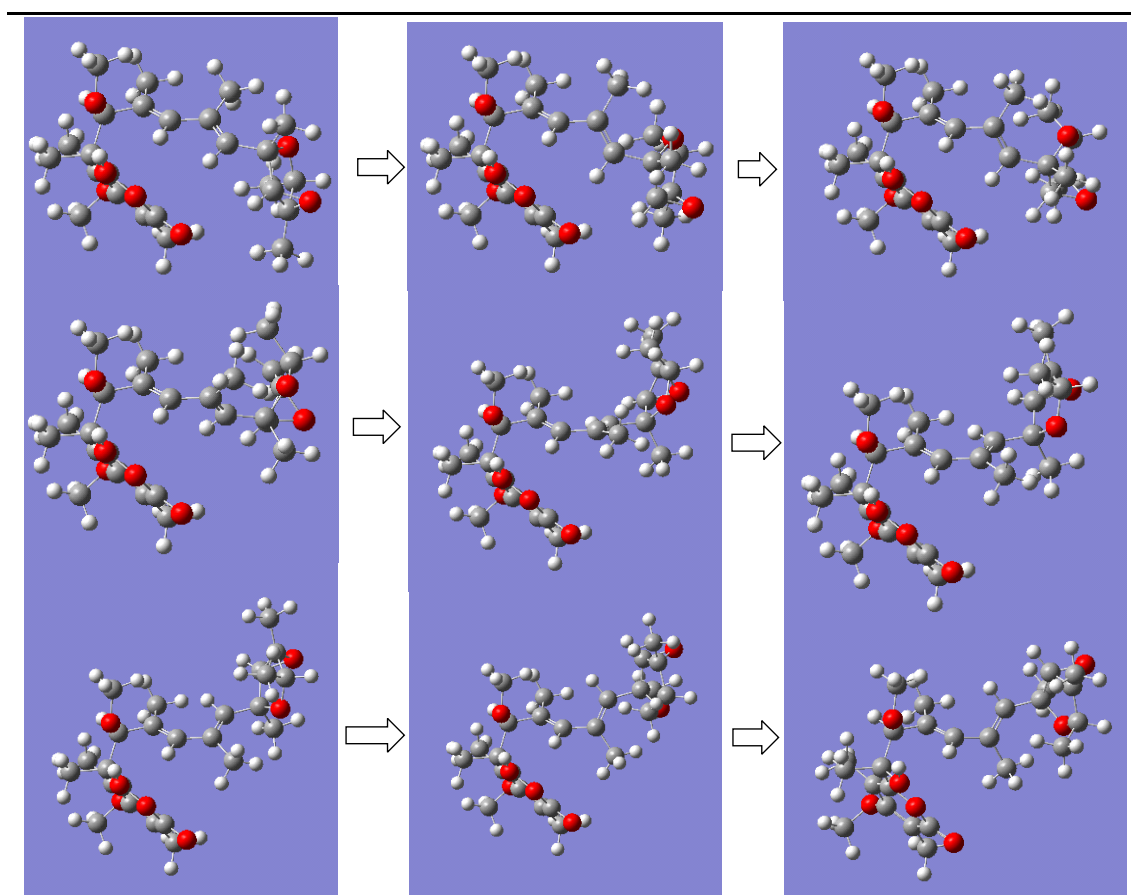
 $[M + H]^+$ 449 $[M + Na]^+$ 471Figure S10. MS data (TIC and XIC $[M + H]^+$ 449 Da) for acetonitrile dissolved *Penicillium* sp. Y-50-10 extract.

Table S1. Gibbs Free Energy (Hartree/Particle) of compound 1.

Zero-Point Correction	0.577812 (Hartree/Particle)
Thermal correction to Energy	0.608788
Thermal correction to Enthalpy	0.609732
Thermal correction to Gibbs Free Energy	0.516601
Sum of electronic and zero-point Energies	−1499.793597
Sum of electronic and thermal Energies	−1499.762620
Sum of electronic and thermal Enthalpies	−1499.761676
Sum of electronic and thermal Free Energies	−1499.854807

Table S2. Total Energy (Hartree/Particle) of different transition states.**Scan of Total Energy**

# X-Axis: Scan Coordinate	# Y-Axis: Total Energy (Hartree)
-166.1186100000	-1500.3629599400
-146.1186100000	-1500.3615611600
-126.1186100000	-1500.3576511800
-106.1186100000	-1500.3554275500
-86.1186100000	-1500.3536596900
-66.1186100000	-1500.3554050000
-46.1186100000	-1500.3551308200
-26.1186100000	-1500.3517034100
-6.1186100000	-1500.3391024800
13.8813900000	-1500.3436973200
33.8813900000	-1500.3553624000
53.8813900000	-1500.3573404300
73.8813900000	-1500.3545908000