

Supporting Information

Rec. Nat. Prod. 18:1 (2024) 171-175

A New Phenolic Bisabolane Sesquiterpenoid from the Fungus *Aspergillus* sp. Hvtc-2021zx1

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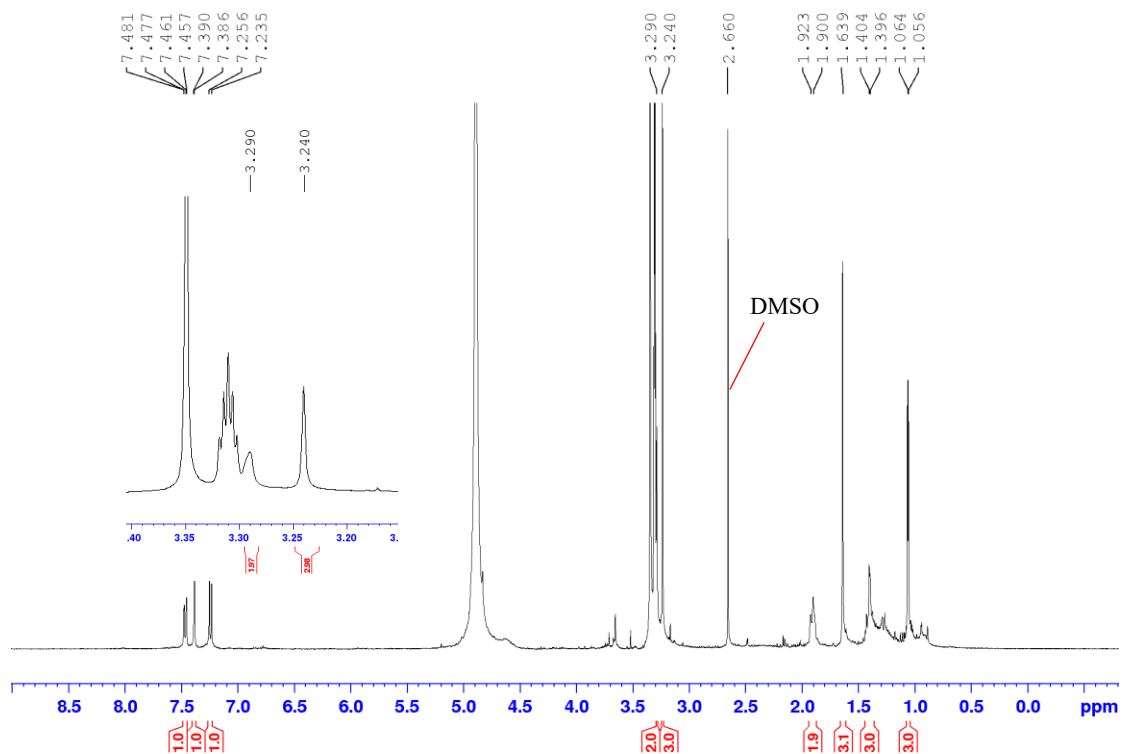


Figure S1: ^1H NMR Spectrum of **1** in CD_3OD (400 MHz)

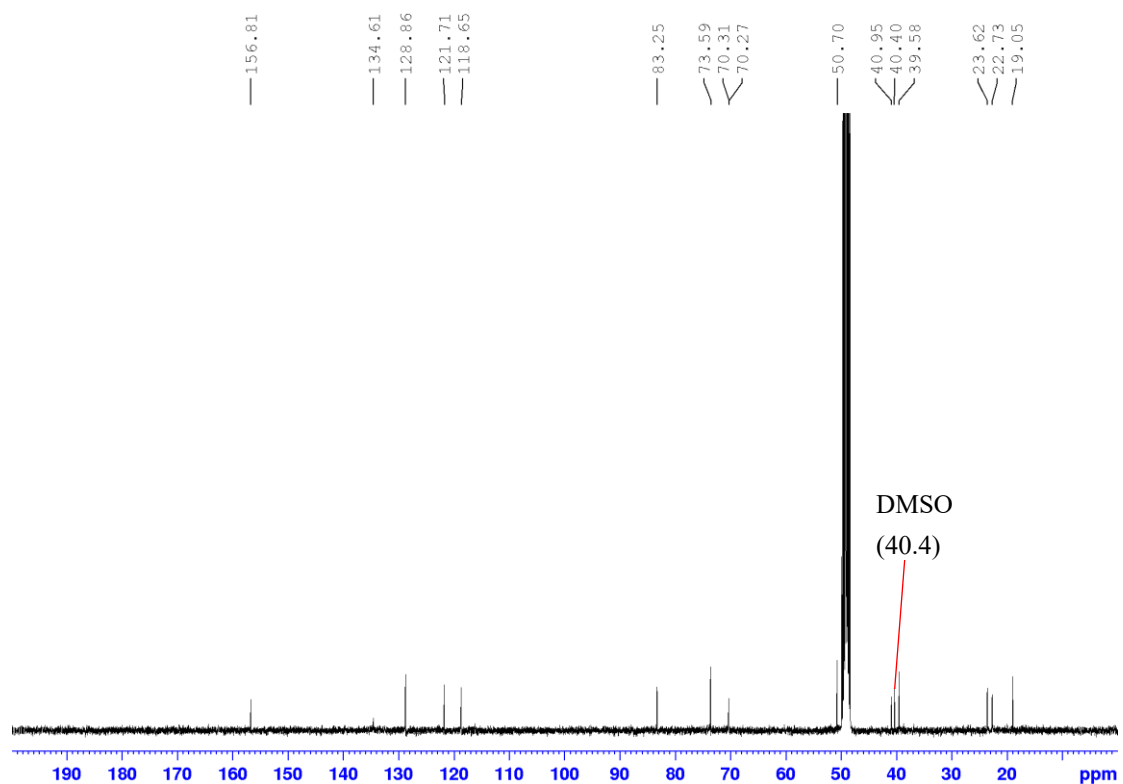


Figure S2: ^{13}C NMR Spectrum of **1** in CD_3OD (100 MHz)

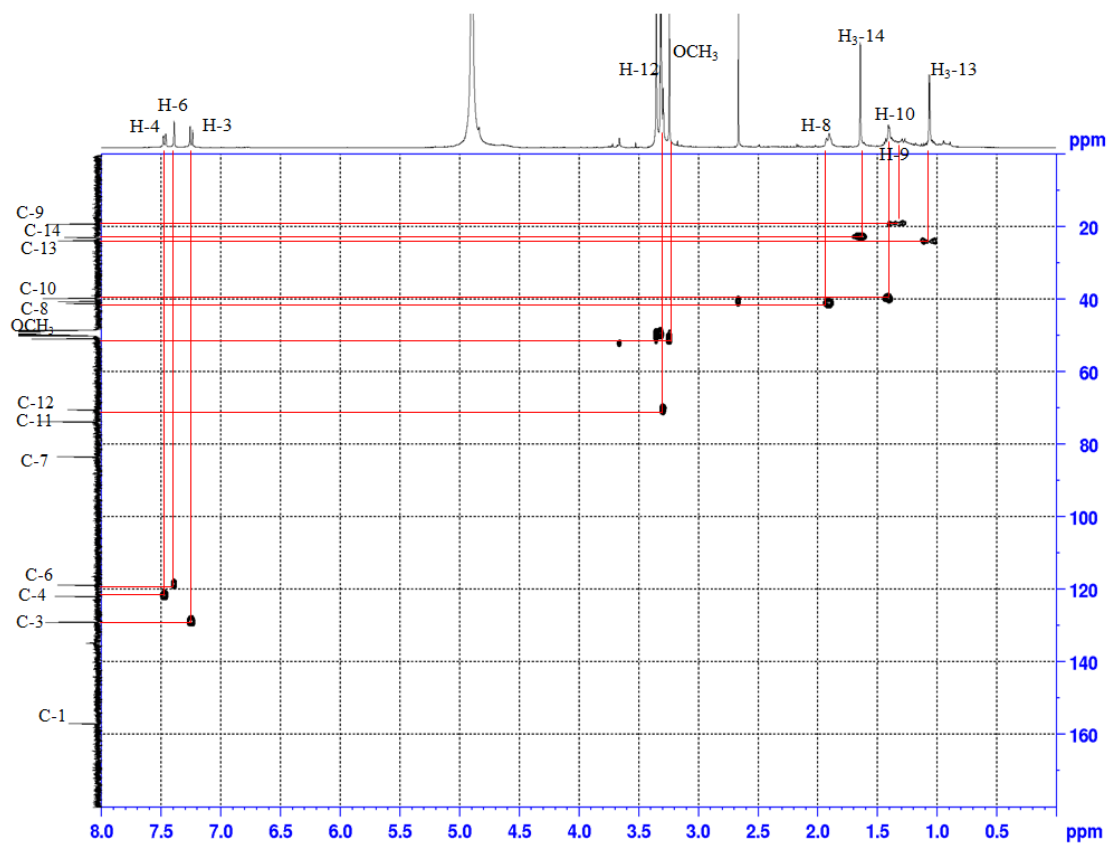


Figure S3: HSQC Spectrum of **1** in CD₃OD

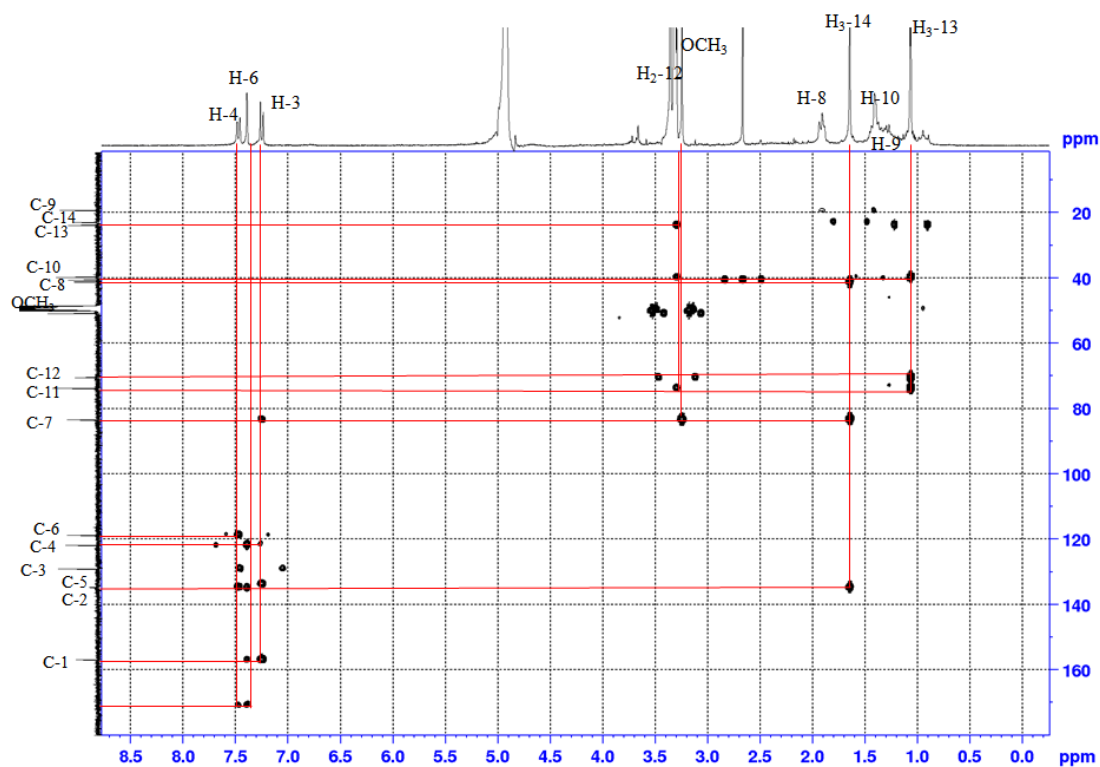


Figure S4: HMBC Spectrum of **1** in CD₃OD

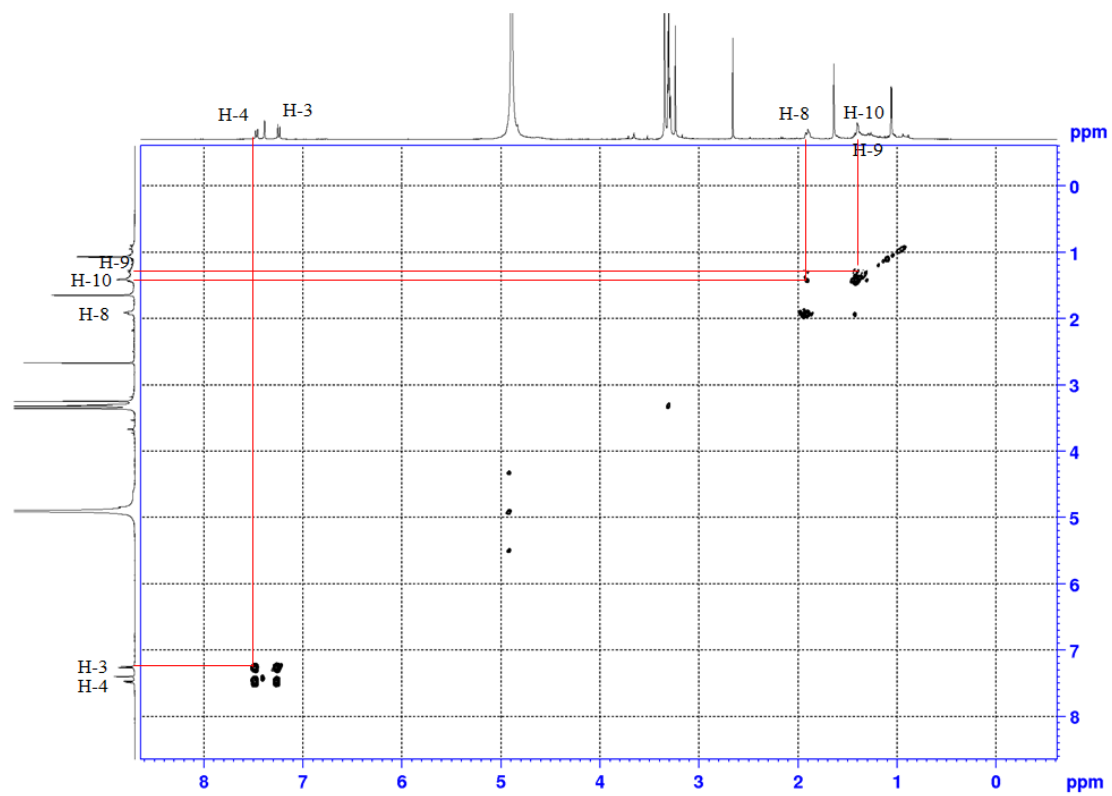


Figure S5: ^1H - ^1H COSY Spectrum of compound **1** in CD_3OD

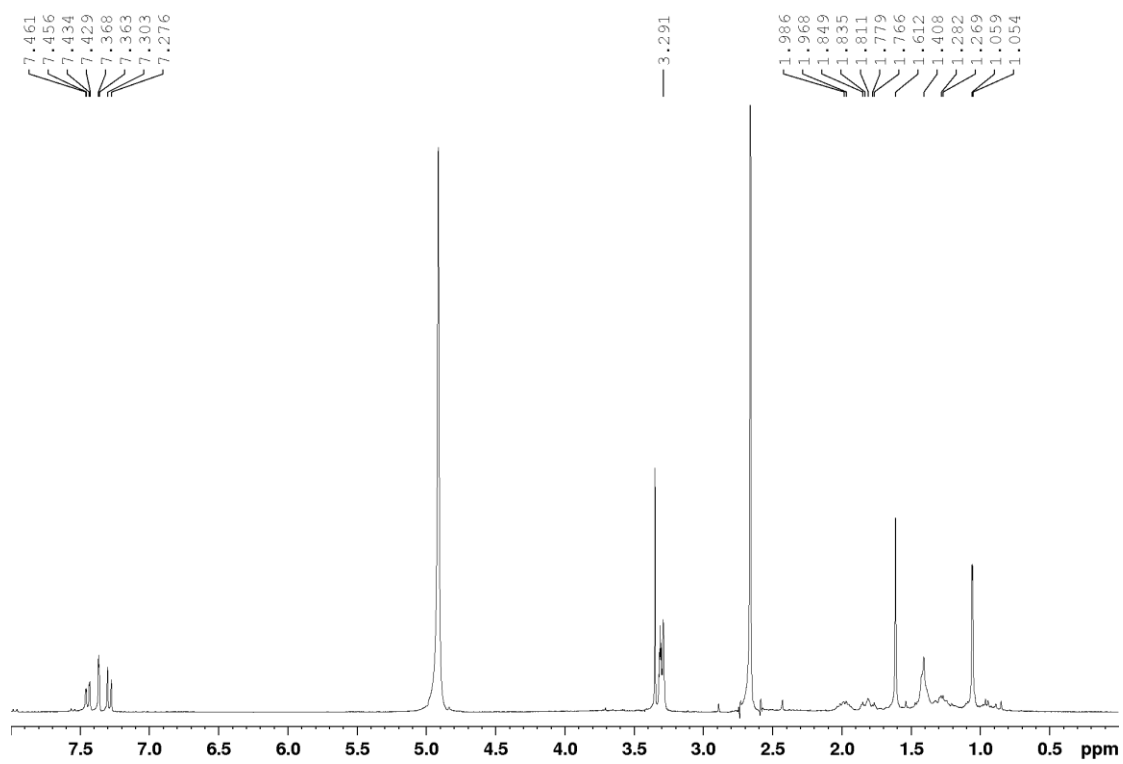


Figure S6: ^1H NMR Spectrum of **2** in CD_3OD (400 MHz)

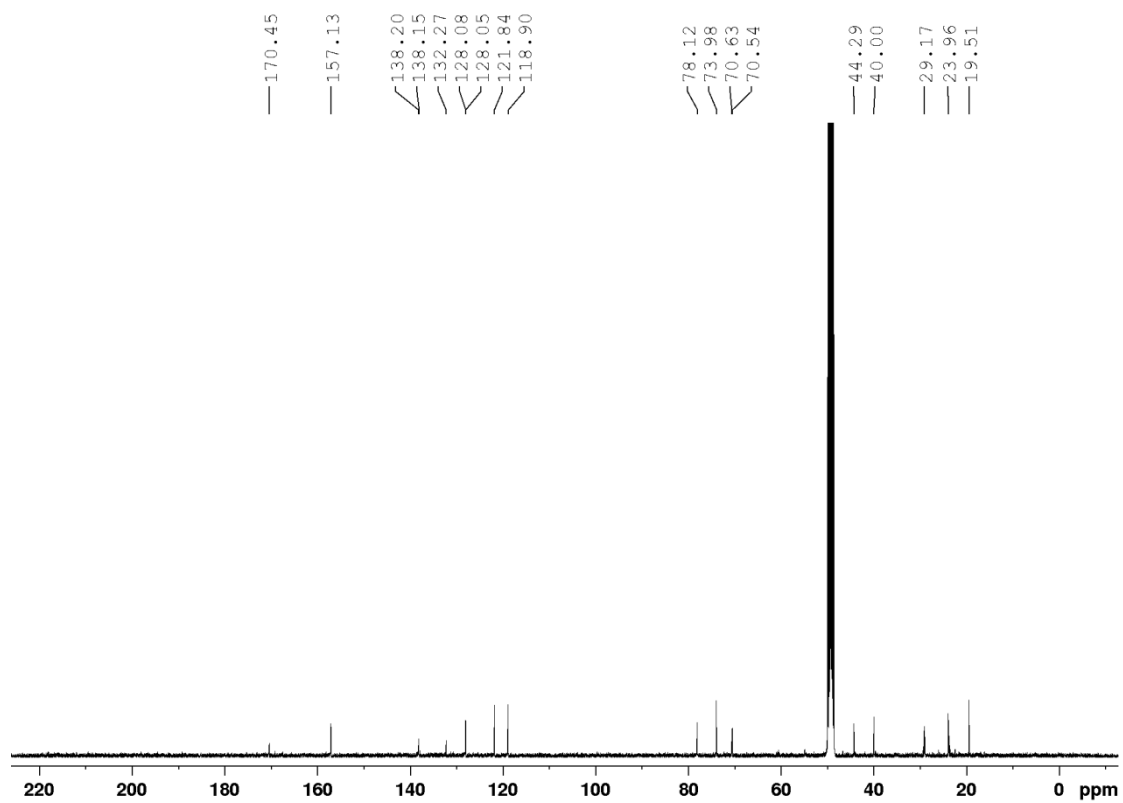


Figure S7: ^{13}C NMR Spectrum of **2** in CD_3OD (100 MHz)

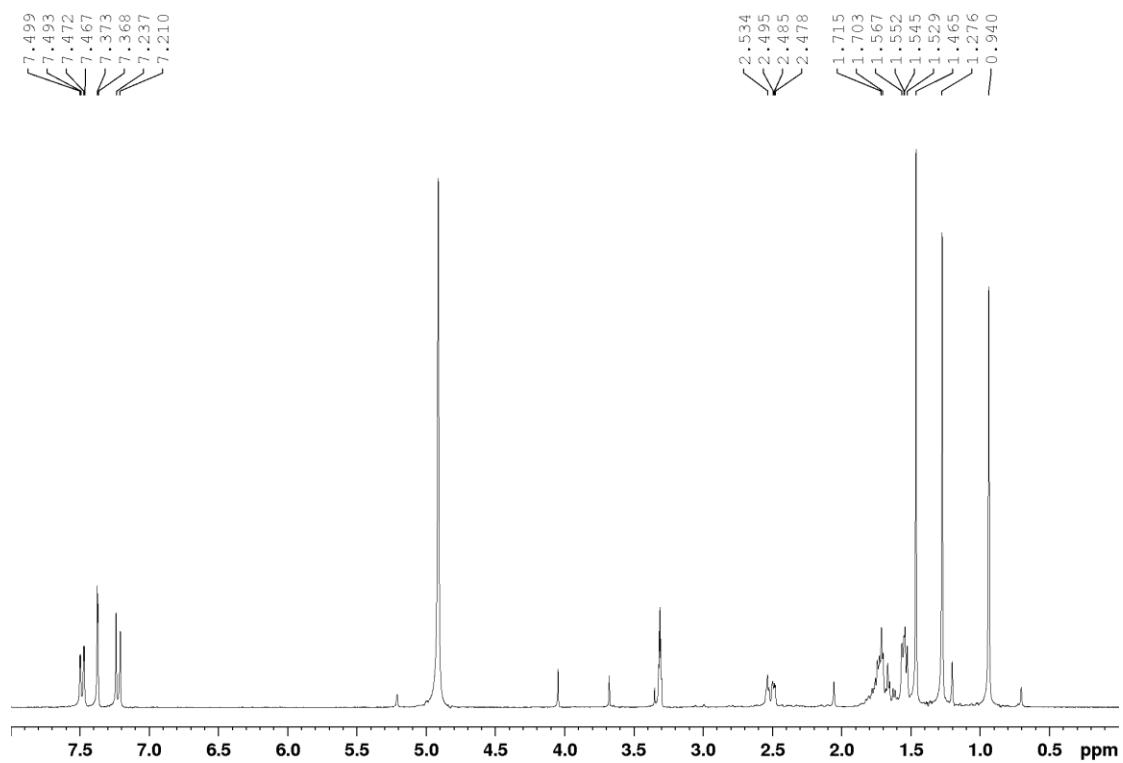


Figure S8: ^1H NMR Spectrum of **3** in CD_3OD (400 MHz)

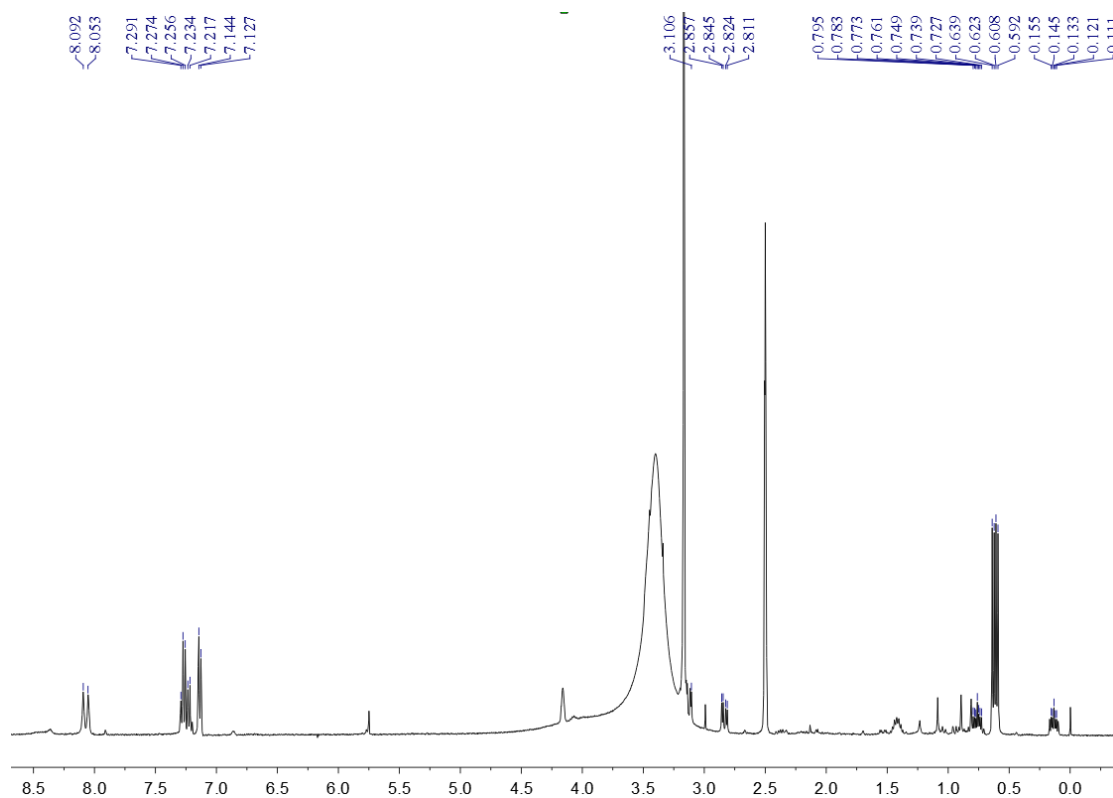


Figure S9: ^1H NMR Spectrum of **4** in CD_3OD (400 MHz)

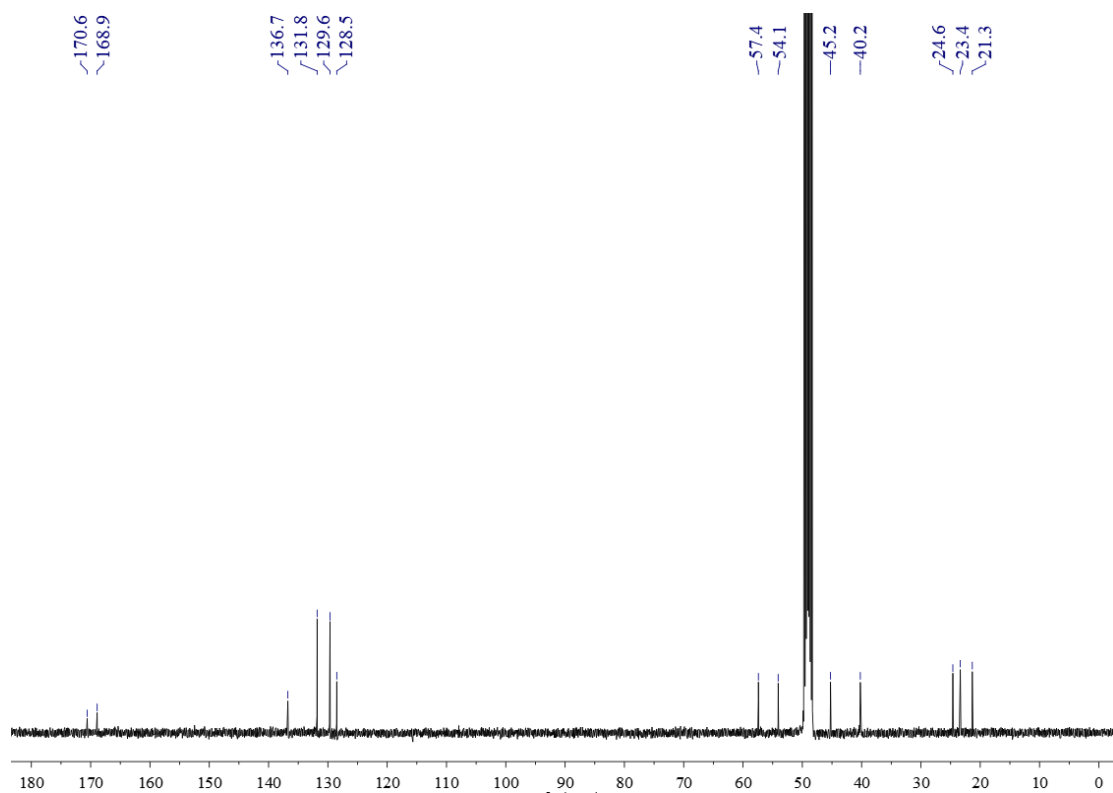


Figure S10: ^{13}C NMR Spectrum of **4** in CD_3OD (100 MHz)

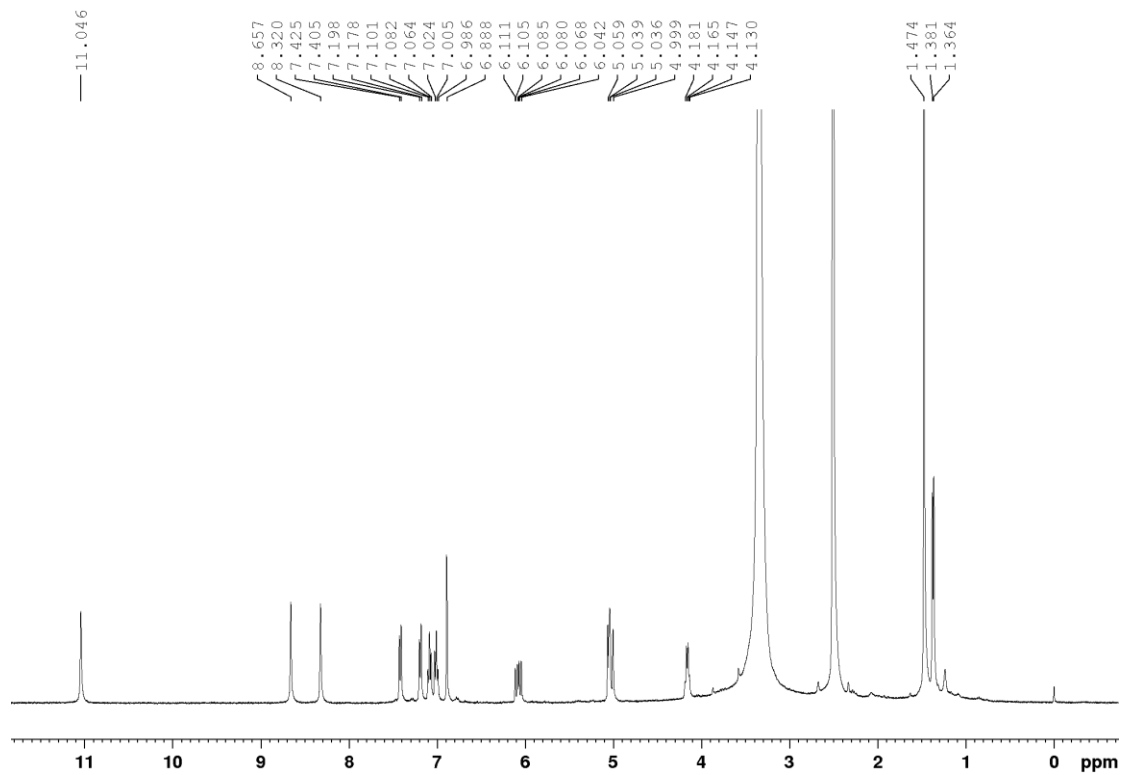


Figure S11: ^1H NMR Spectrum of **5** in $\text{DMSO-}d_6$ (400 MHz)

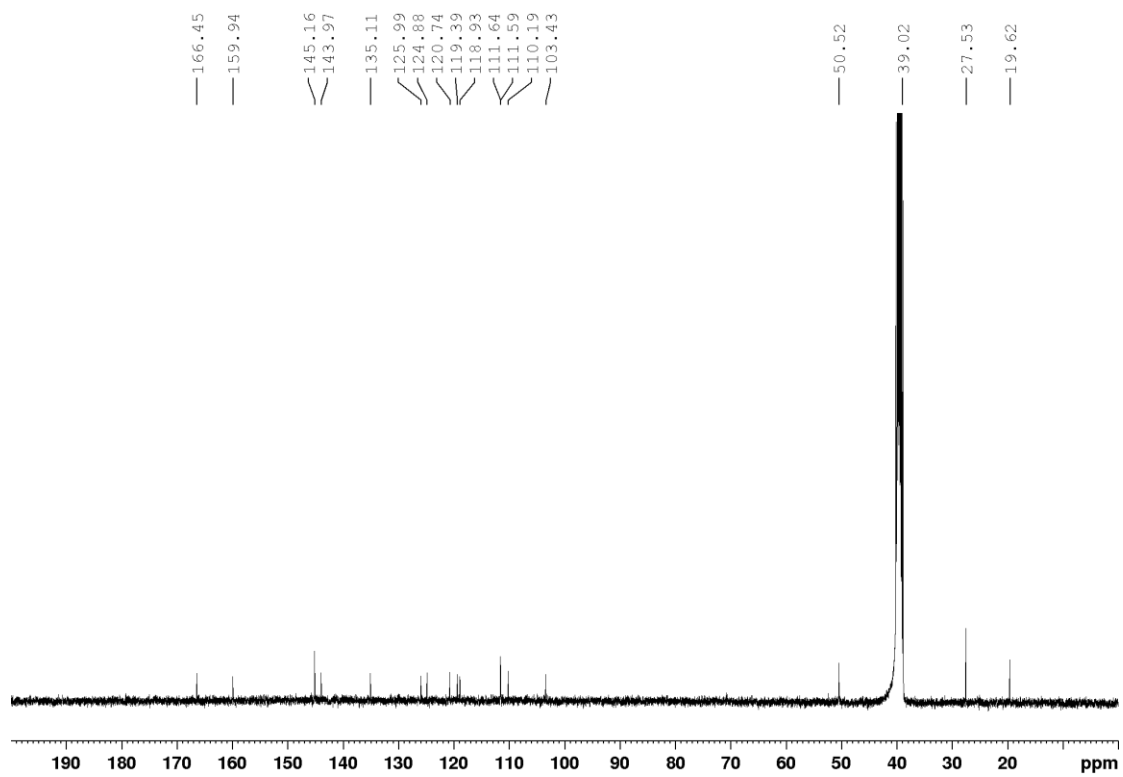


Figure S12: ^{13}C NMR Spectrum of **5** in $\text{DMSO-}d_6$ (100 MHz)

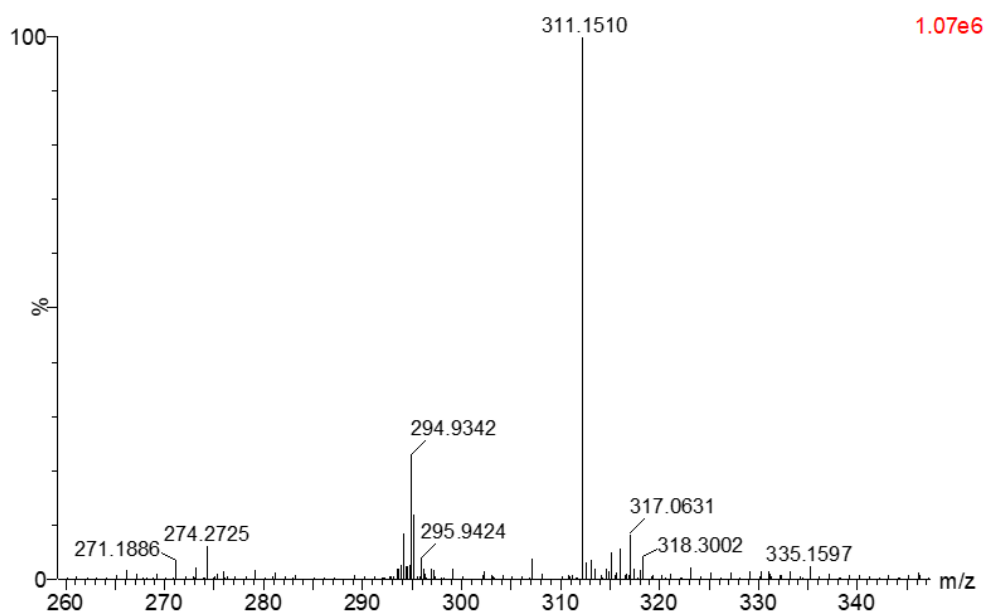


Figure S13: HRESIMS Data of compound 1

As Drawn (0) | Substructure (0) | Similarity (393K)

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Search Within Results
Similarity
 95-98 (3)
 90-94 (14)
 85-89 (56)
 80-84 (505)
 75-79 (3,553)
[View All](#)

17 Results | Sort: Relevance | View: Partial

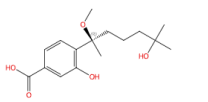
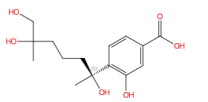
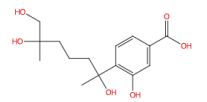
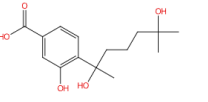
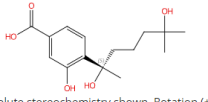
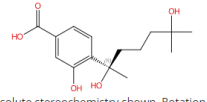
<p>1 98</p> <p>2479401-59-5</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₁₆H₂₄O₅ 3-Hydroxy-4-[(1R)-5-hydroxy-1-methoxy-1,5-dimethylhexyl]benzoic acid</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>2 95</p> <p>1919065-41-0</p>  <p>Available stereochemistry shown, Rotation (+)</p> <p>C₁₅H₂₂O₆ 3-Hydroxy-4-[(1S)-1,5,6-trihydroxy-1,5-dimethylhexyl]benzoic acid</p> <p>3 References 0 Reactions 0 Suppliers</p>	<p>3 95</p> <p>1246066-82-9</p>  <p>C₁₅H₂₂O₆ Benzoic acid, 3-hydroxy-4-(1,5,6-trihydroxy-1,5-dimethylhexyl)-</p> <p>2 References 0 Reactions 2 Suppliers</p>
<p>4 94</p> <p>1649441-60-0</p>  <p>C₁₅H₂₂O₅ 4-(1,5-Dihydroxy-1,5-dimethylhexyl)-3-hydroxybenzoic acid</p>	<p>5 94</p> <p>1675975-90-2</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>C₁₅H₂₂O₅ 4-[(1S)-1,5-Dihydroxy-1,5-dimethylhexyl]-3-hydroxybenzoic acid</p>	<p>6 94</p> <p>1908414-19-6</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₁₅H₂₂O₅ 4-[(1R)-1,5-Dihydroxy-1,5-dimethylhexyl]-3-hydroxybenzoic acid</p>

Figure S14: Similarity report for compound 1