

Supporting Information

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9,11-Cycloneren-3,7-diol: a New Cyclonerane Sesquiterpene from the Marine-Sediment-Derived Fungus *Trichoerma harzianum* WH-22

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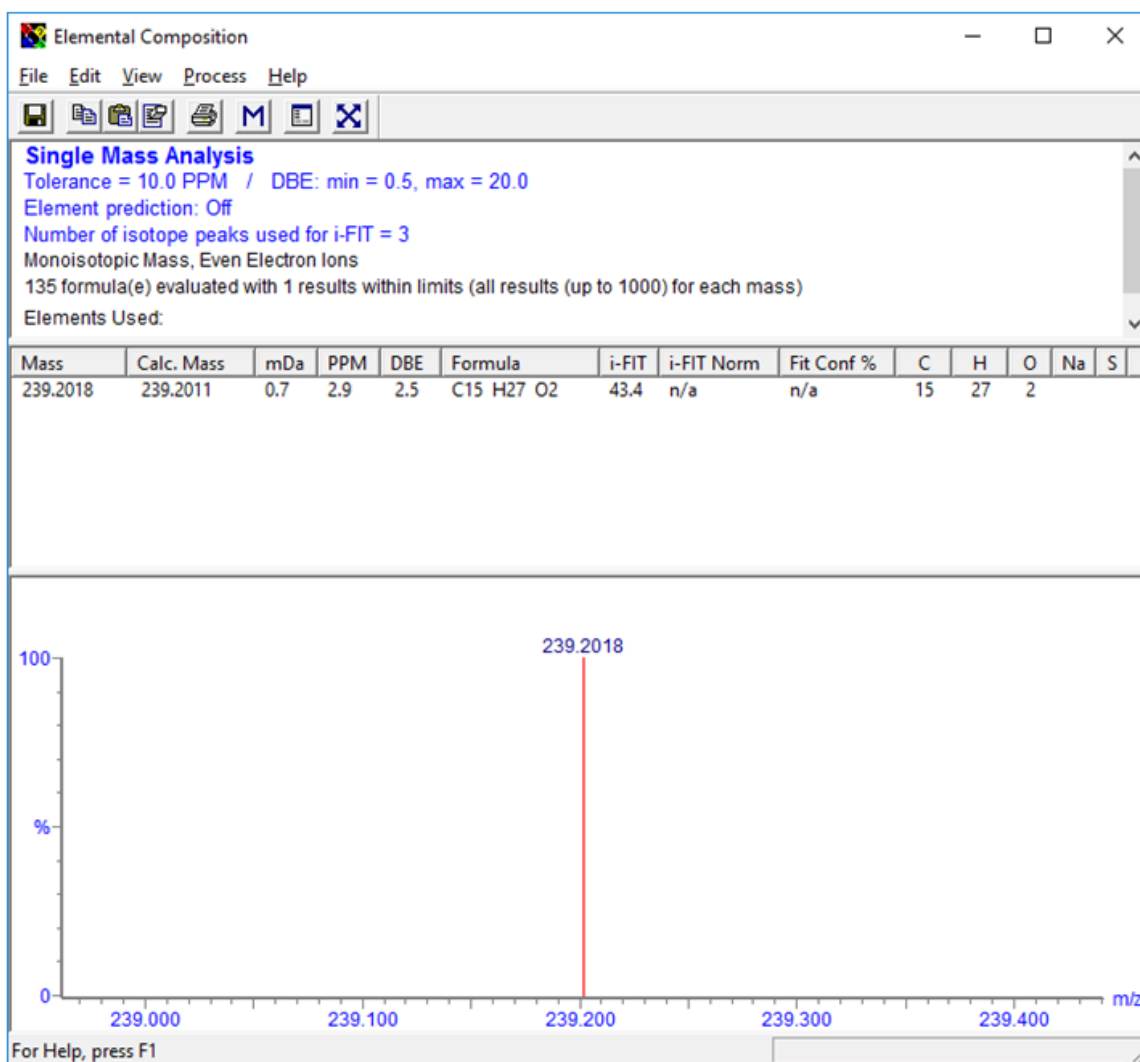


Figure S1: HR-ESI-MS spectrum of **1**

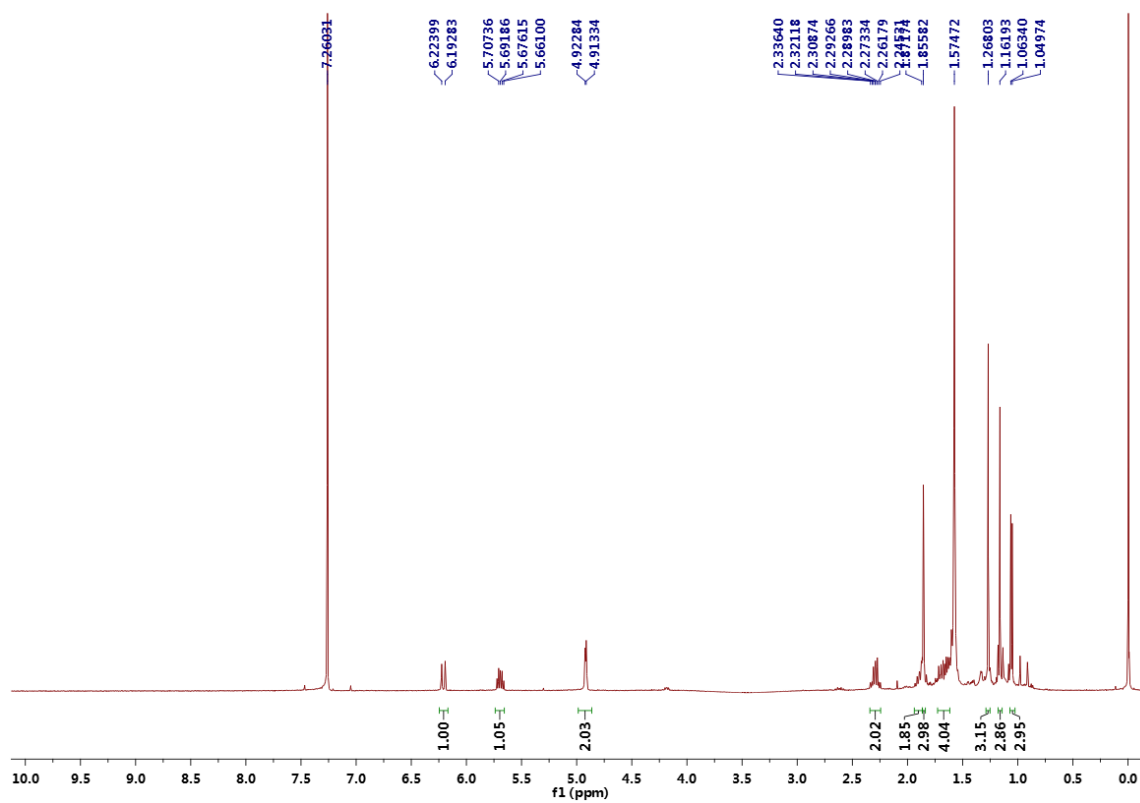


Figure S2: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of **1**

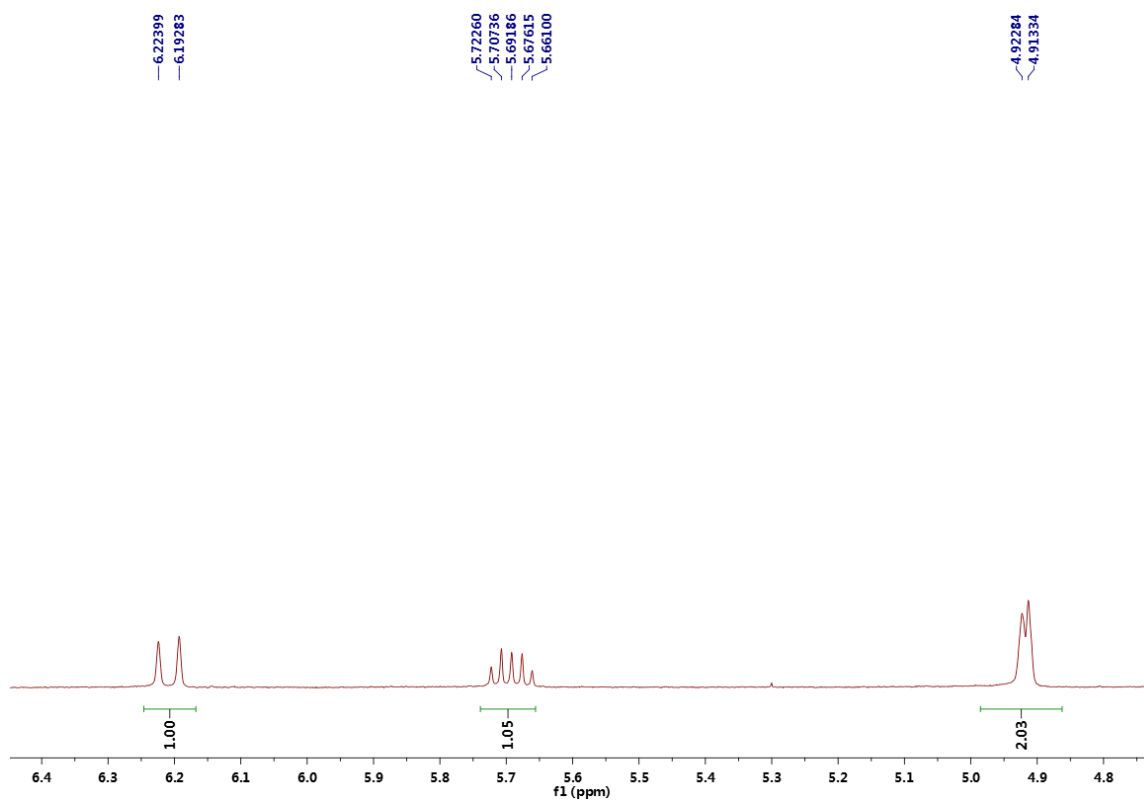


Figure S3: Enlarged $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of **1**

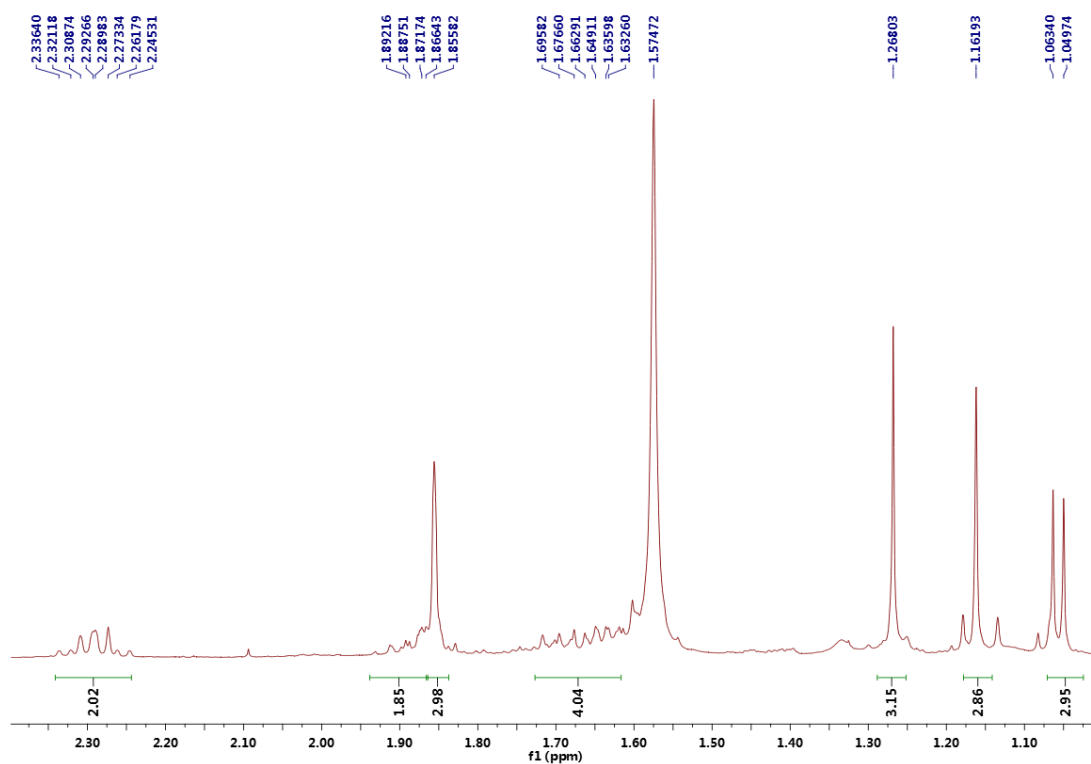


Figure S4: Enlarged $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of **1**

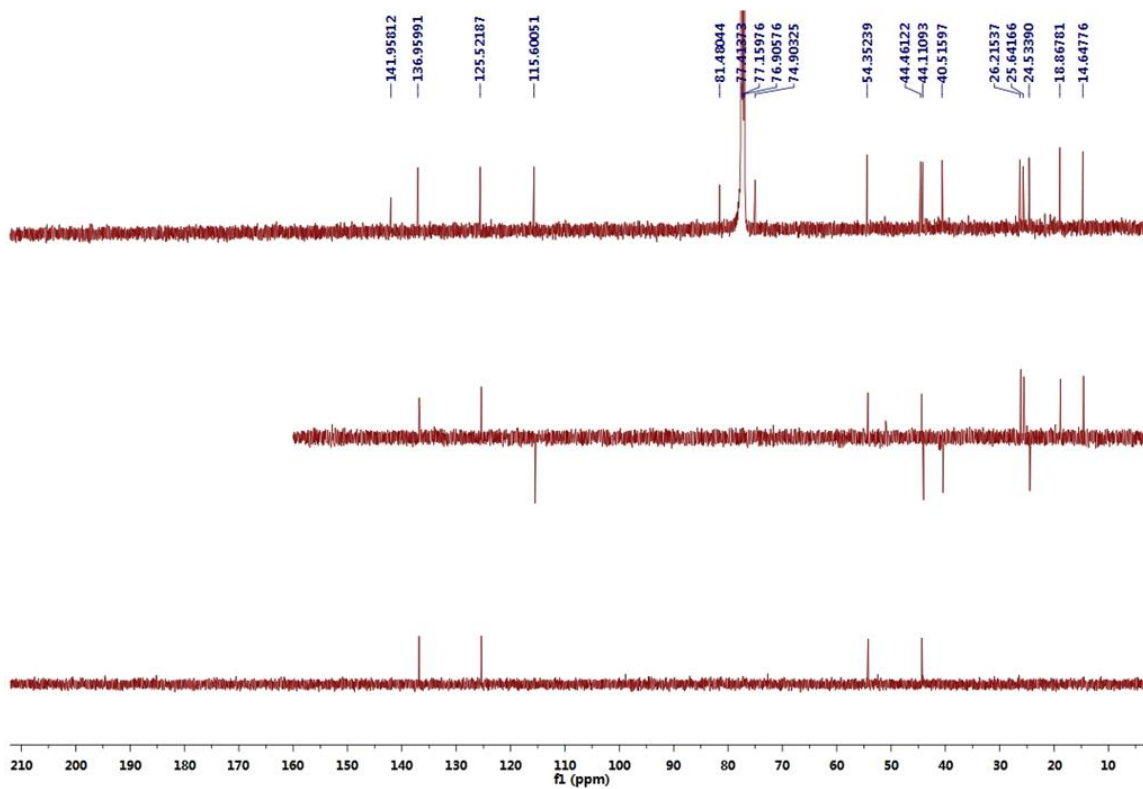


Figure S5: ^{13}C -NMR and DEPT (125 MHz, CDCl_3) spectra of **1**

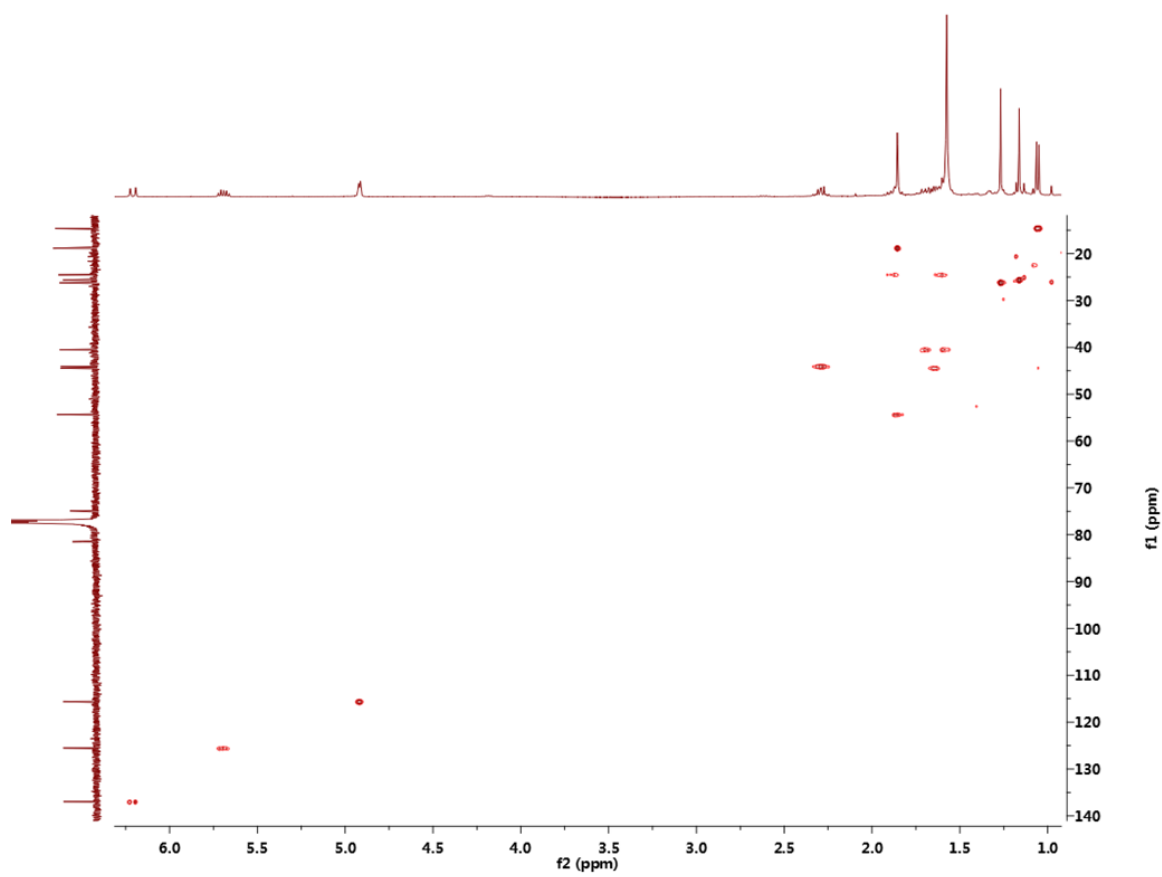


Figure S6: HSQC spectrum of **1**

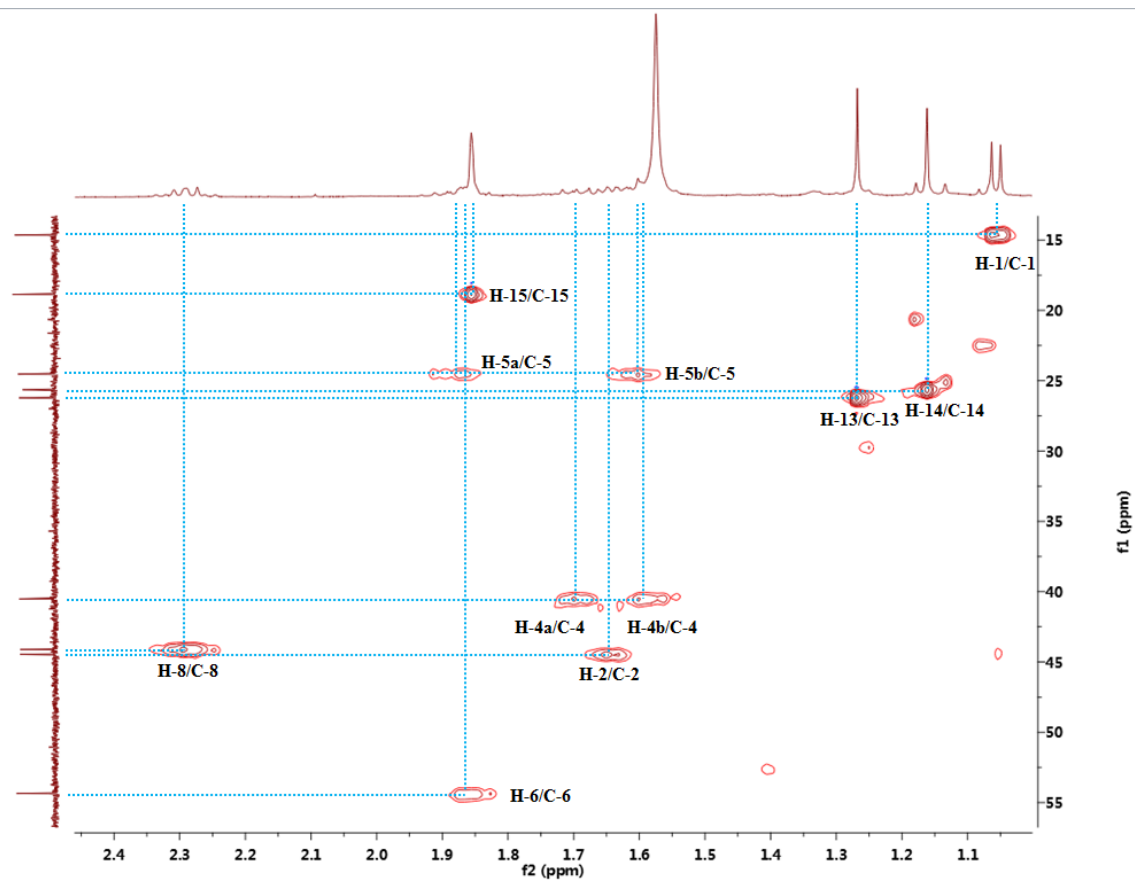


Figure S7: Enlarged HSQC spectrum of **1**

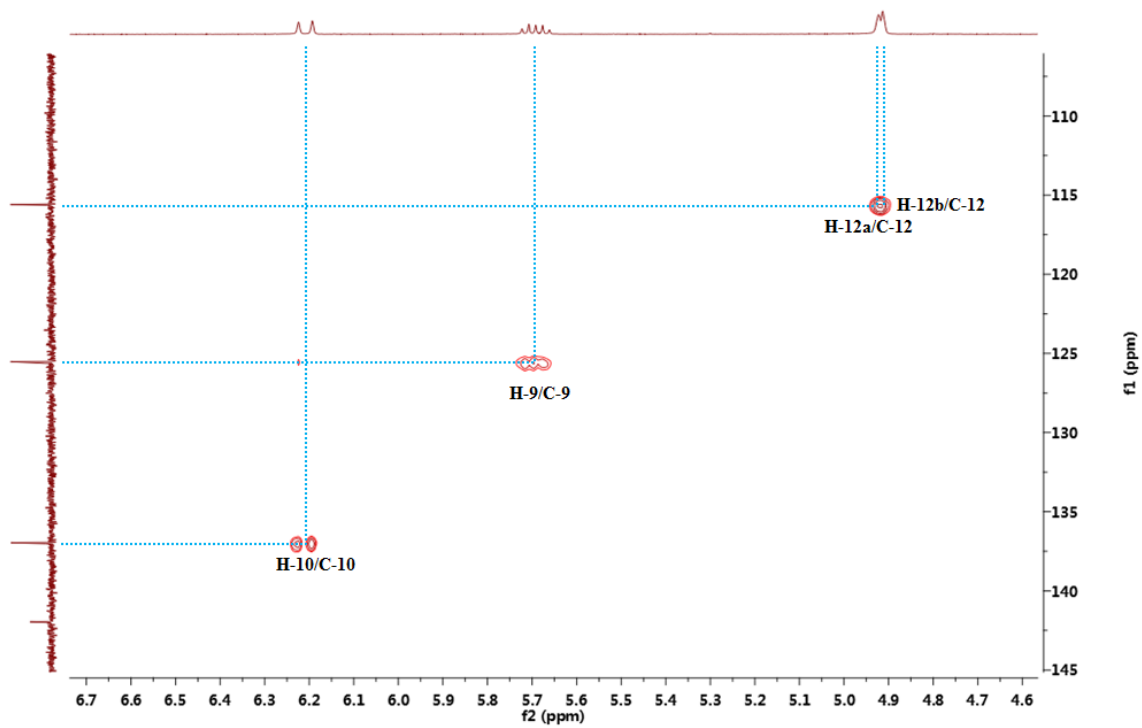


Figure S8: Enlarged HSQC spectrum of **1**

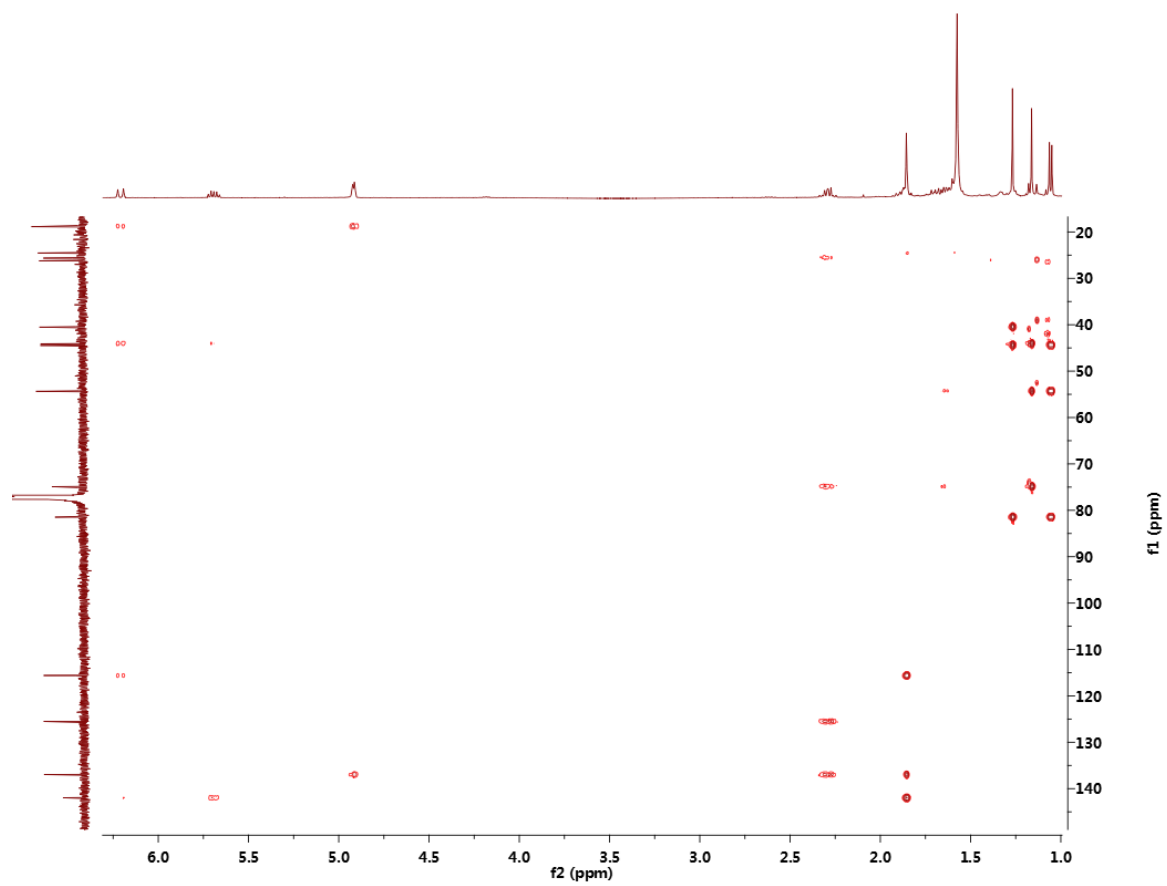


Figure S9: HMBC spectrum of **1**

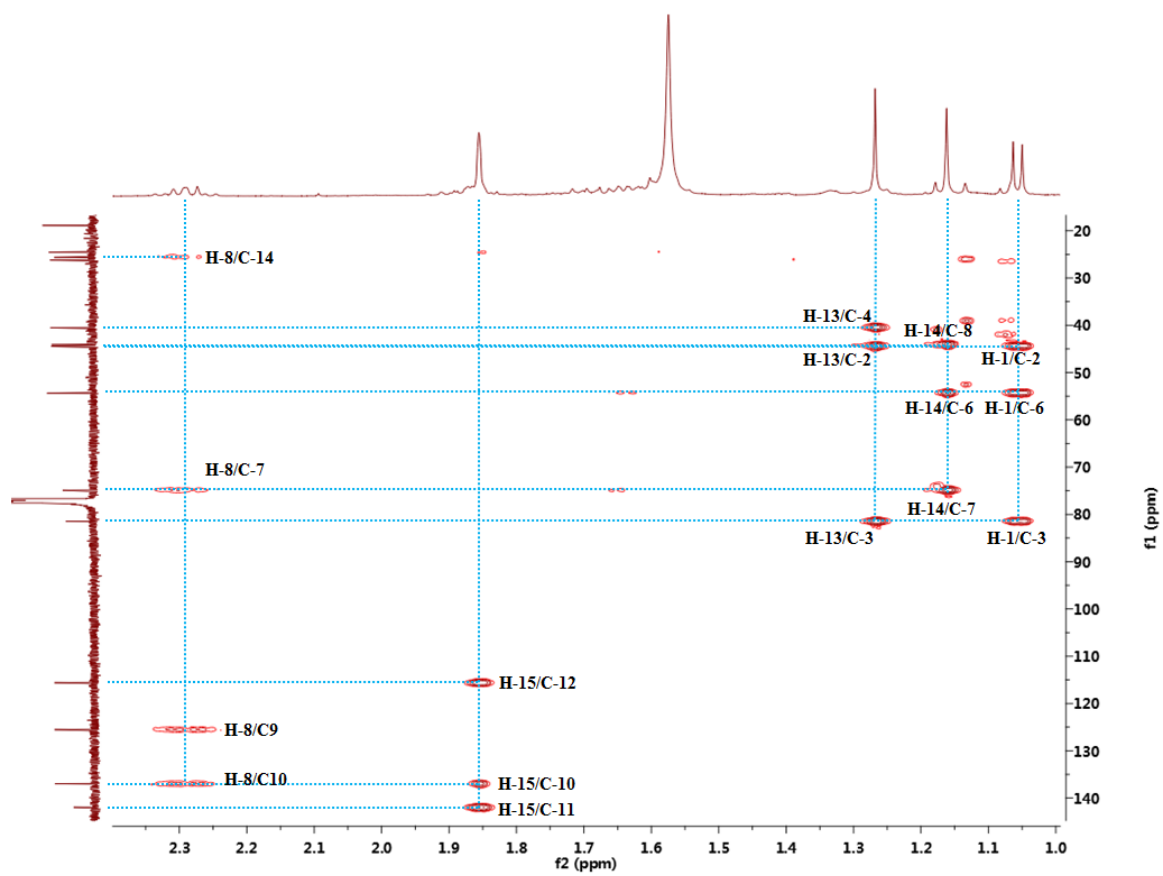


Figure S10: Enlarged HMBC spectrum of 1

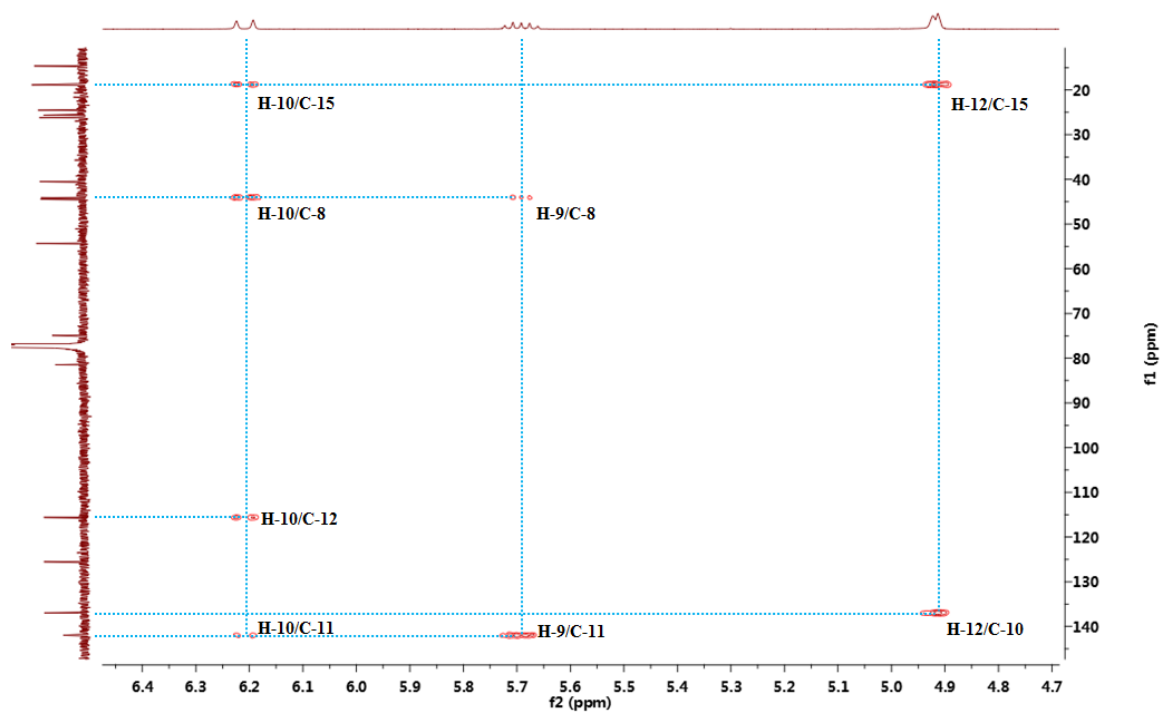


Figure S11: Enlarged HMBC spectrum of 1

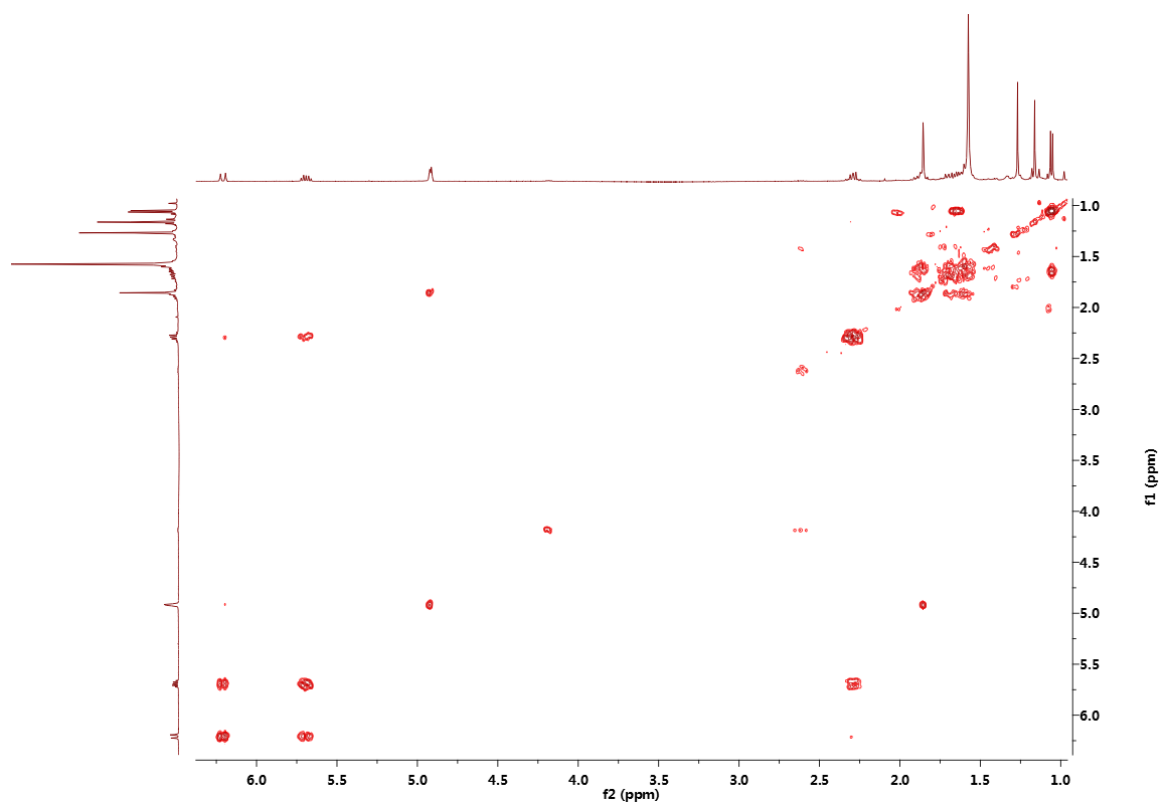


Figure S12: ^1H - ^1H COSY spectrum of **1**

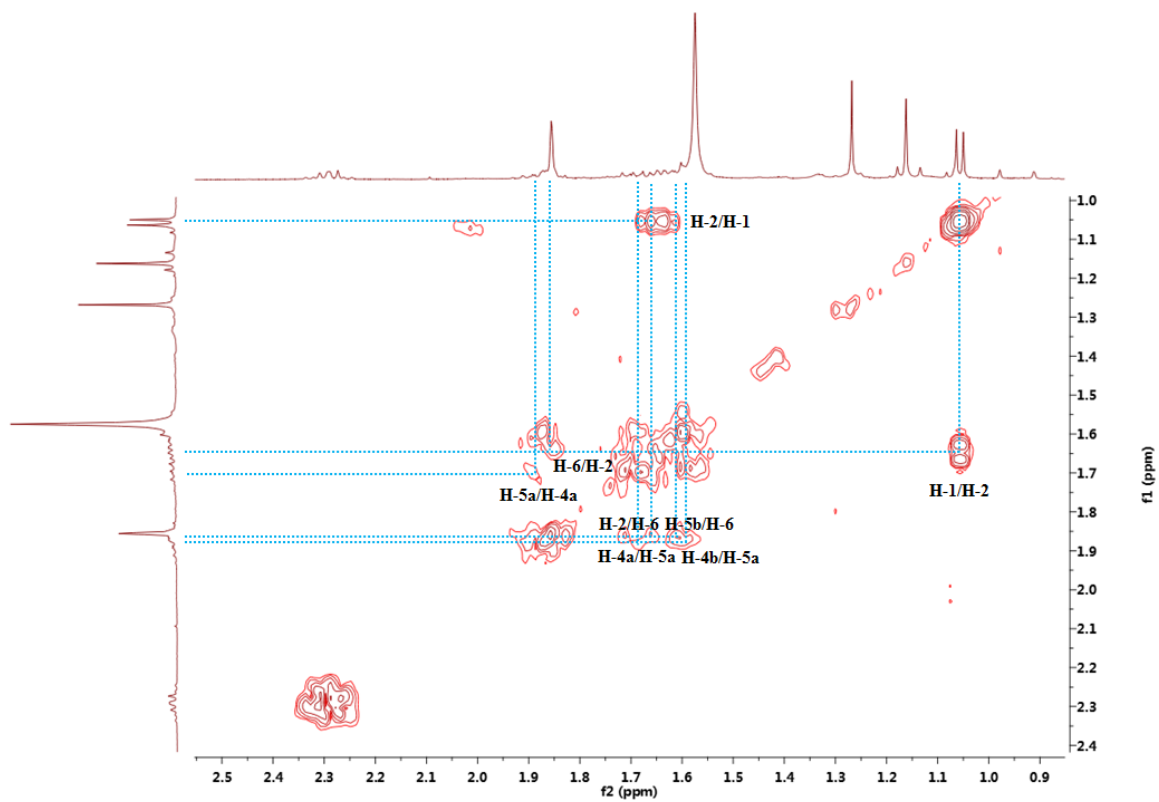


Figure S13: Enlarged ^1H - ^1H COSY spectrum of **1**

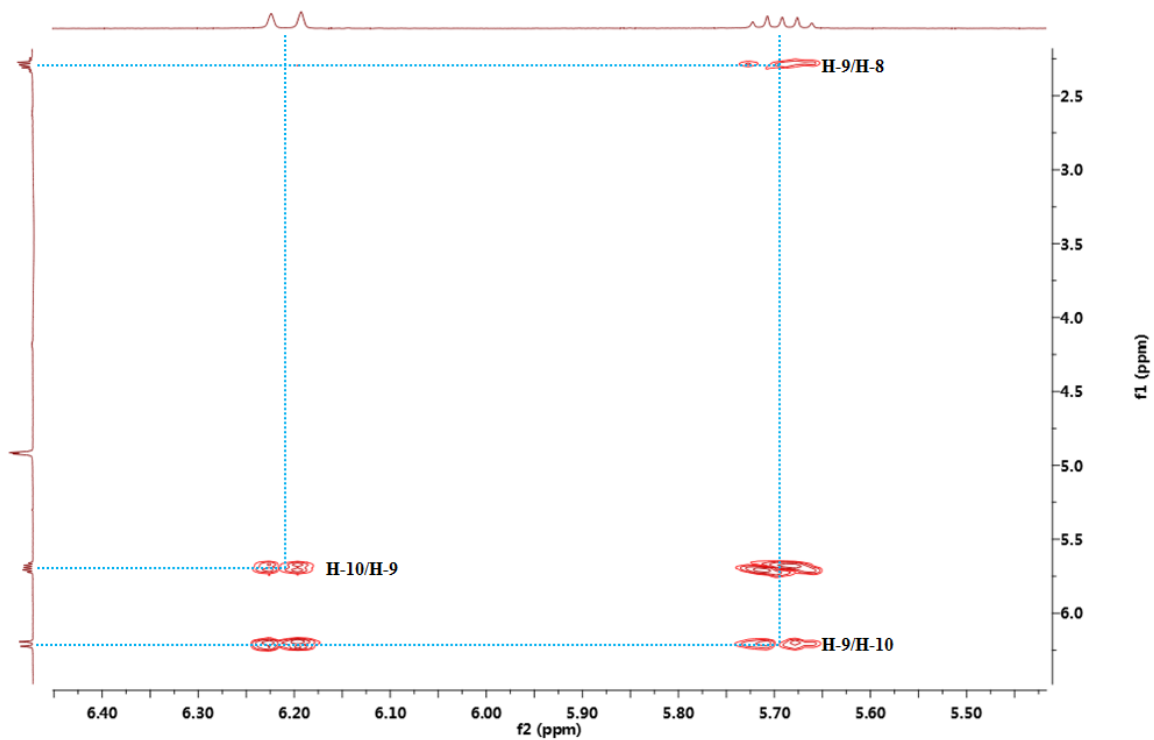


Figure S14: Enlarged ^1H - ^1H COSY spectrum of **1**

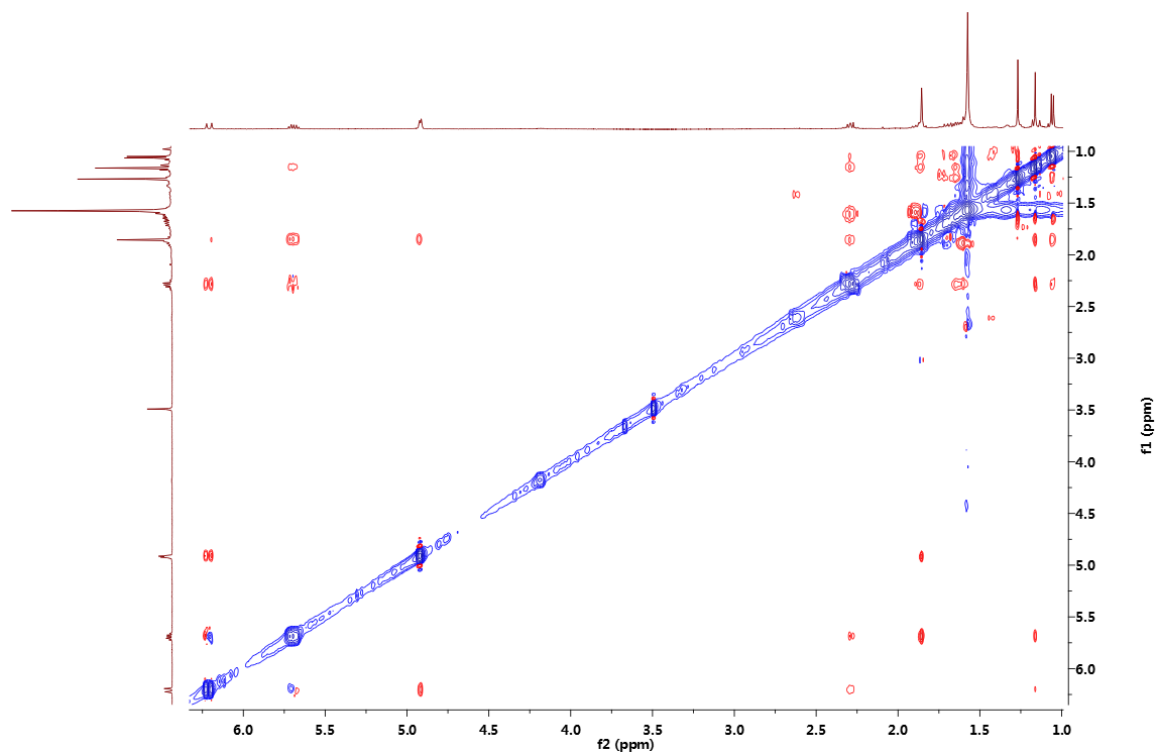


Figure S15: NOESY spectrum of **1**

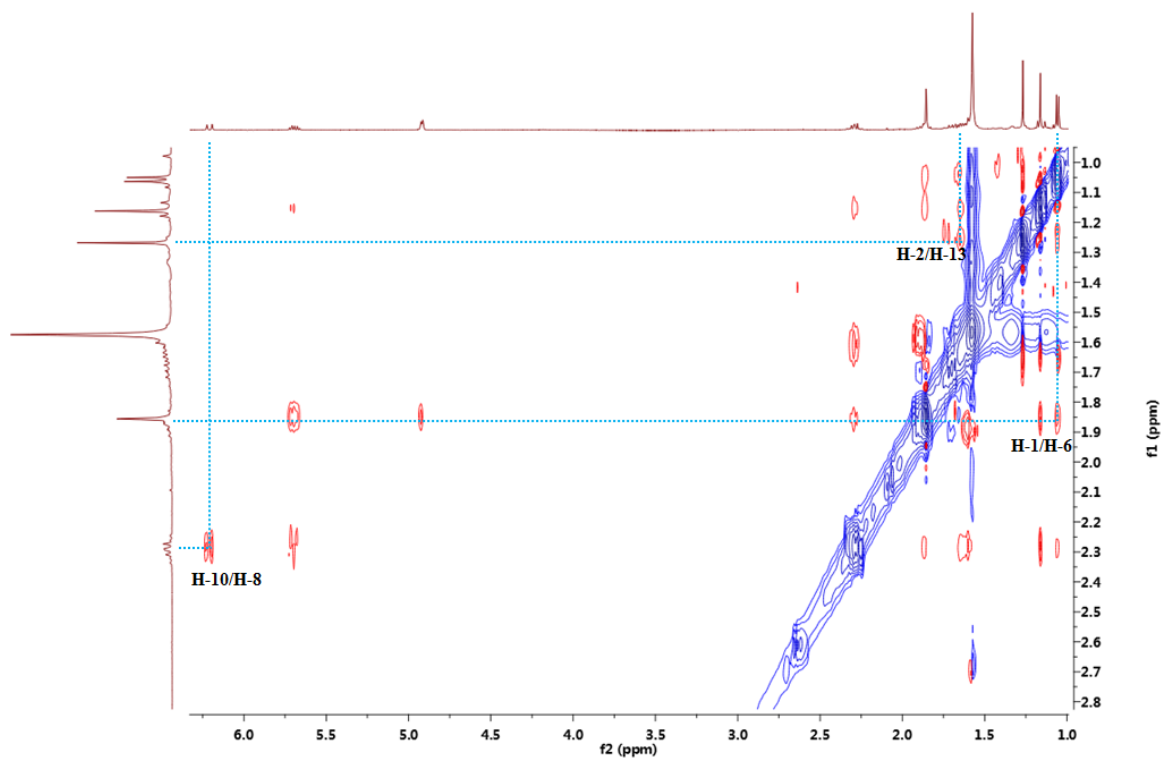


Figure S16: Enlarged NOESY spectrum of **1**

Structure Match

As Drawn (0)

Substructure (120)

Similarity (23K)

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Similarity

90-94 (2)

85-89 (14)

80-84 (40)

75-79 (195)

70-74 (992)

[View All](#)

Reaction Role

Product (7)

Reactant (1)

Reference Role

Filtering: Similarity: 2 Selected X Number of Components: 1 X [Clear All Filters](#)

16 Results Sort: Relevance View: Partial

1 94

125564-51-4

Absolute stereochemistry shown
Double bond geometry shown

$C_{15}H_{26}O_2$
(1R,2S,3R)-3-((3E)-5-Hydroxy-5-methyl-1-methylene-3-hexen-1-yl)-1,2-dimethylcyclopentane...

1 Reference 0 Reactions 0 Suppliers

2 92

125564-53-6

$C_{15}H_{26}O_3$
3,6-Heptadiene-1,2-diol, 6-(3-hydroxy-2,3-dimethylcyclopentyl)-2-methyl-

1 Reference 0 Reactions 1 Supplier

3 90

125564-52-5

Absolute stereochemistry shown
Double bond geometry shown

$C_{16}H_{28}O_2$
(1R,2S,3R)-3-((3E)-5-Methoxy-5-methyl-1-methylene-3-hexen-1-yl)-1,2-dimethylcyclopentane...

1 Reference 0 Reactions 0 Suppliers

4 89

28834-06-2

Absolute stereochemistry shown, Rotation (-)

$C_{15}H_{28}O_2$
Cyclonerodiol

64 Reference 32 Reactions 2 Suppliers

5 89

328902-04-1

Absolute stereochemistry shown

$C_{15}H_{28}O_2$
(1R,1S,2S,3R)-3-Hydroxy-α,2,3-trimethyl-α-(4-methyl-3-penten-1-yl)cyclopentanone...

2 Reference 0 Reactions 0 Suppliers

6 89

73465-86-8

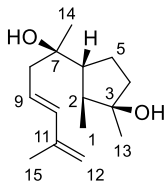
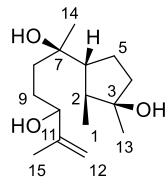
Relative stereochemistry shown

$C_{15}H_{28}O_2$
Cyclopentanemethanol, 3-hydroxy-α,2,3-trimethyl-α-(4-methyl-3-penten-1-yl)-, [1αR]...

2 Reference 1 Reactions 1 Supplier

Figure S17: Scifinder search results of 1

Table S1: NMR data of compound **1** and 11-cycloneren-3,7,10-triol

| No |  1 | |  11-cycloneren-3,7,10-triol | |
|-----|---|----------------------------|---|----------------------------|
| | δ_{H} (<i>J</i> in Hz) | δ_{C} , type | δ_{H} (<i>J</i> in Hz) | δ_{C} , type |
| 1 | 1.06, d (<i>J</i> = 6.8) | 14.6, CH ₃ | 1.02, d (<i>J</i> = 6.8) | 15.4, CH ₃ |
| 2 | 1.64, m | 44.5, CH | 1.64, m | 45.5, CH |
| 3 | | 81.5, C | | 82.1, C |
| 4a | 1.69, m | 40.5, CH ₂ | 1.63, m | 41.4, CH ₂ |
| 4b | 1.59, m | | 1.53, m | |
| 5a | 1.87, m | 24.5, CH ₂ | 1.81, m | 25.2, CH ₂ |
| 5b | 1.61, m | | 1.59, m | |
| 6 | 1.86, m | 54.4, CH | 1.81, m | 55.7, CH |
| 7 | | 74.9, C | | 75.4, C |
| 8a | 2.32, dd (<i>J</i> = 13.9, 7.6) | 44.1, CH ₂ | 1.52, m | 37.9, CH ₂ |
| 8b | 2.27, dd (<i>J</i> = 13.9, 7.9) | | 1.40, ddd (<i>J</i> = 12.1, 11.2, 4.0) | |
| 9a | 5.69, dt (15.6, 7.6) | 125.5, CH | 1.62, m | 30.2, CH ₂ |
| 9b | | | 1.56, m | |
| 10 | 6.21, br d (15.6) | 137.0, CH | 3.97, t (<i>J</i> = 6.4) | 77.4, CH |
| 11 | | 142.0, C | | 148.8, C |
| 12a | 4.92, br s | 115.6, CH ₂ | 4.91, br s | 111.6, CH ₂ |
| 12b | 4.91, br s | | 4.81, br s | |
| 13 | 1.27, s | 26.2, CH ₃ | 1.22, s | 26.1, CH ₃ |
| 14 | 1.16, s | 25.6, CH ₃ | 1.12, s | 24.8, CH ₃ |
| 15 | 1.86, s | 18.9, CH ₃ | 1.72, s | 17.4, CH ₃ |