

## Supporting Information

*Rec. Nat. Prod.* 17:3 (2023) 516-521

# A New Sesquiterpenoid and Two Nitro-containing Phenylpropionic Acid Derivatives from the Fungus

## *Aspergillus terreus* LPFH-1

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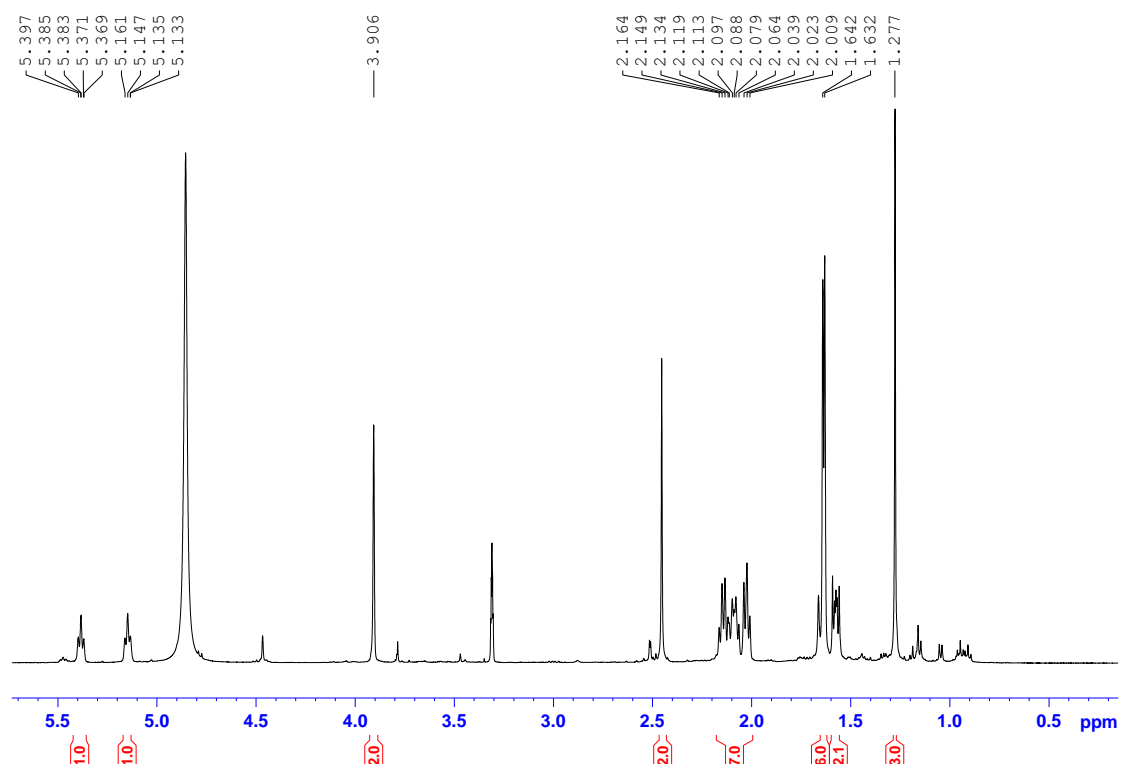


Figure S1:  $^1\text{H}$  NMR Spectrum of **1** in  $\text{CD}_3\text{OD}$  (400 MHz)

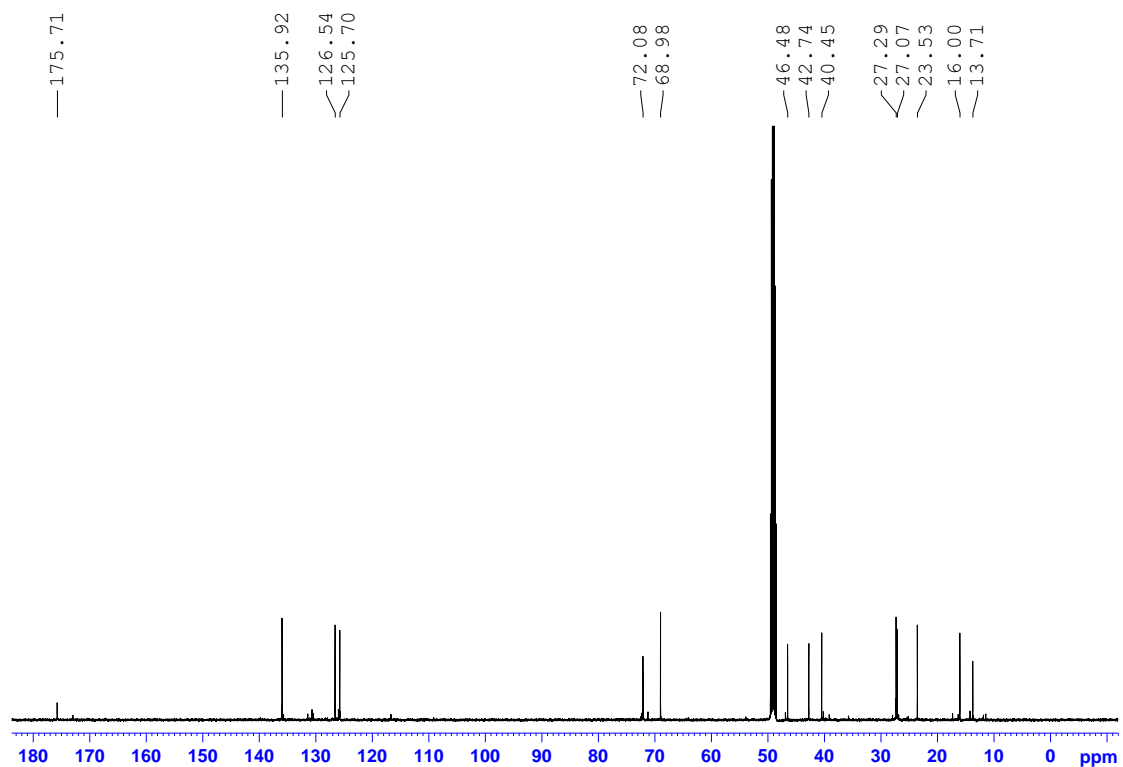
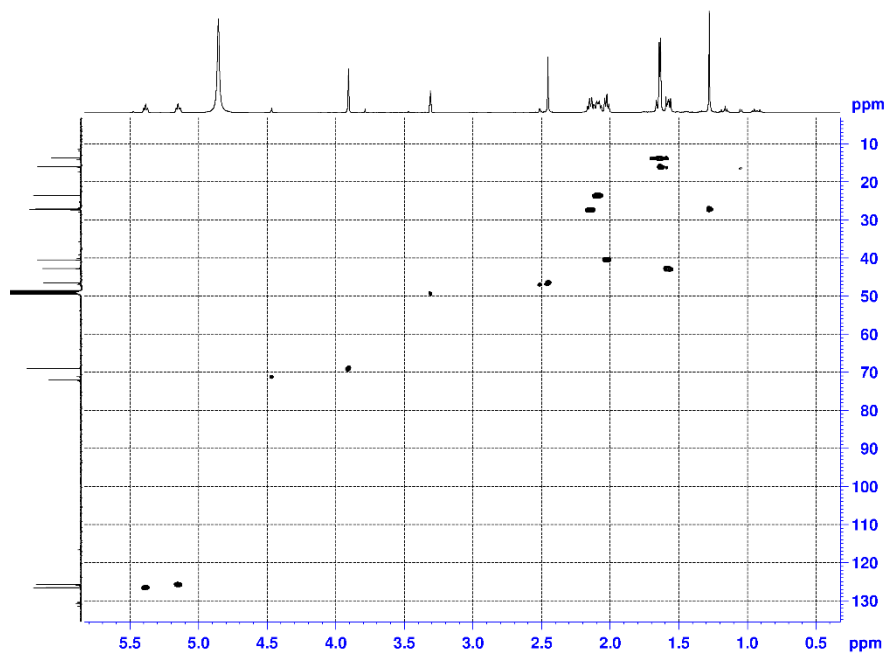
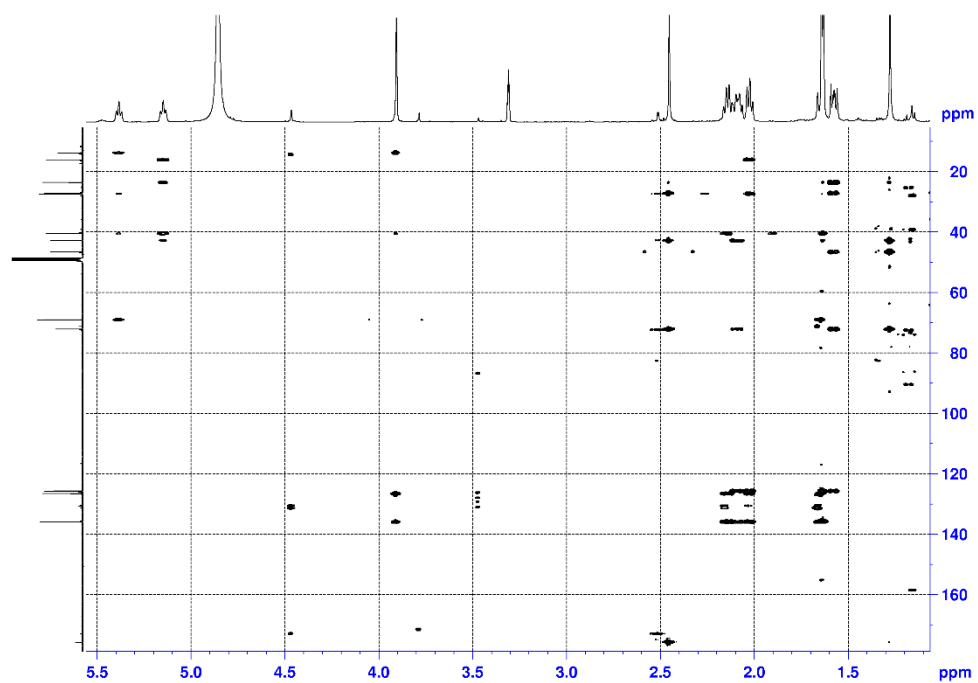


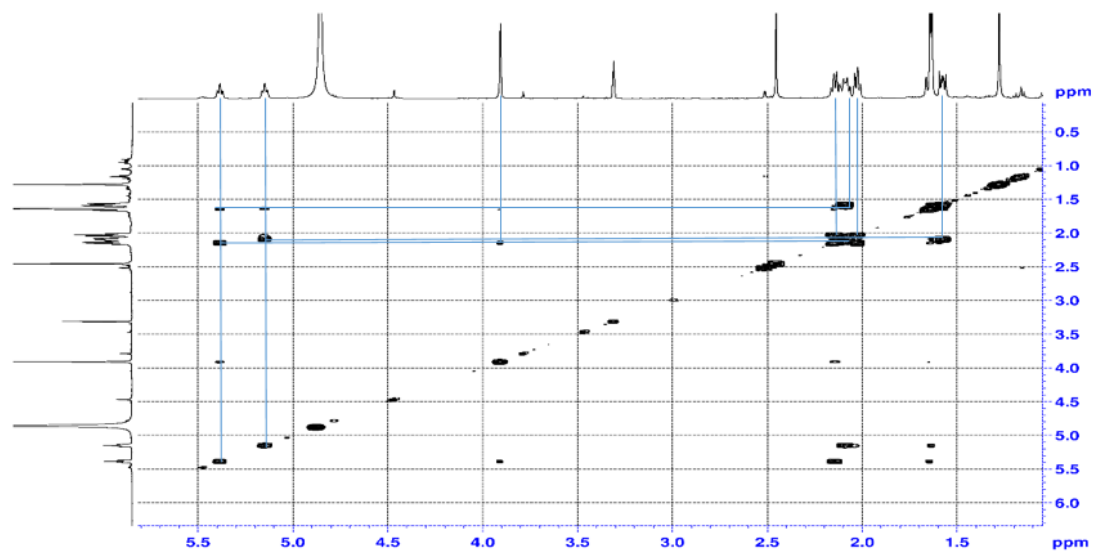
Figure S2:  $^{13}\text{C}$  NMR Spectrum of **1** in  $\text{CD}_3\text{OD}$  (100 MHz)



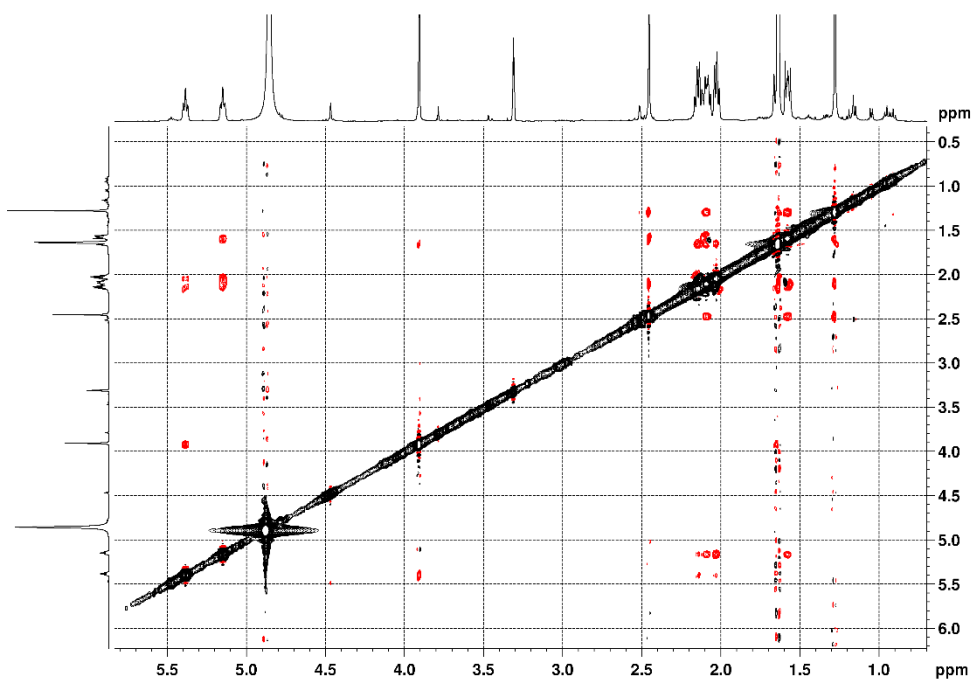
**Figure S3:** HSQC Spectrum of **1** in CD<sub>3</sub>OD



**Figure S4:** HMBC Spectrum of **1** in CD<sub>3</sub>OD



**Figure S5:**  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of compound **1** in  $\text{CD}_3\text{OD}$



**Figure S6:** NOESY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

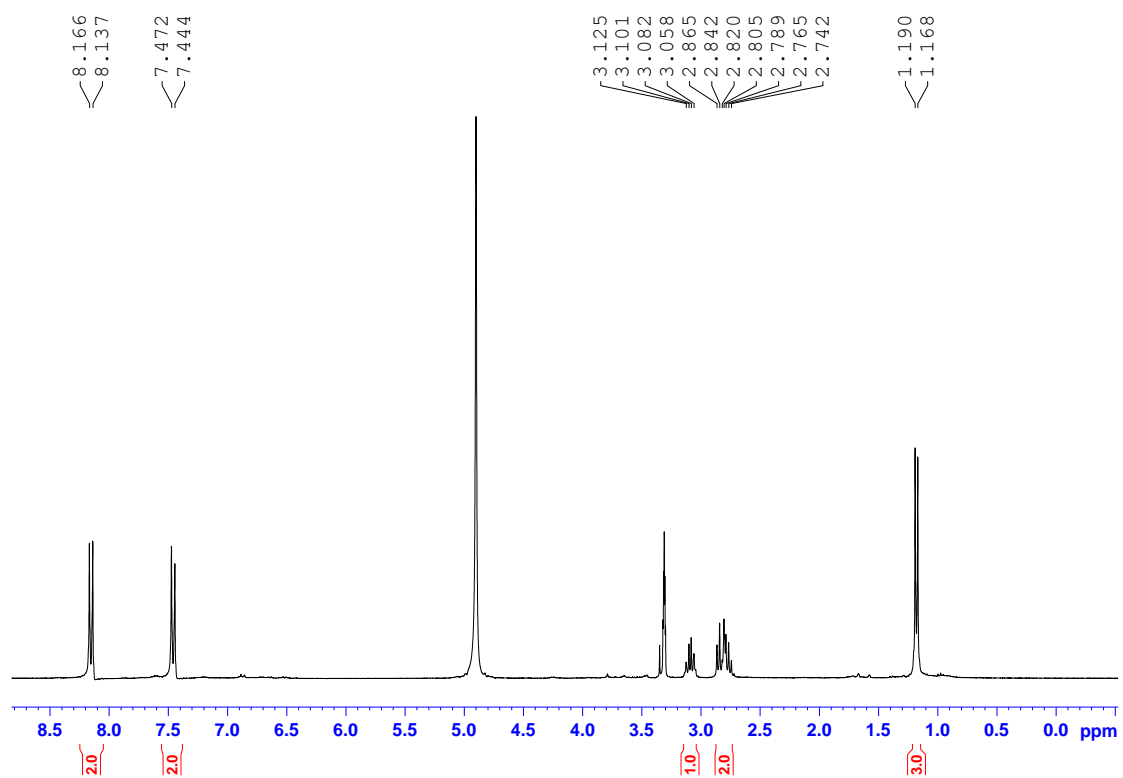


Figure S7:  $^1\text{H}$  NMR Spectrum of **2** in  $\text{CD}_3\text{OD}$  (400 MHz)

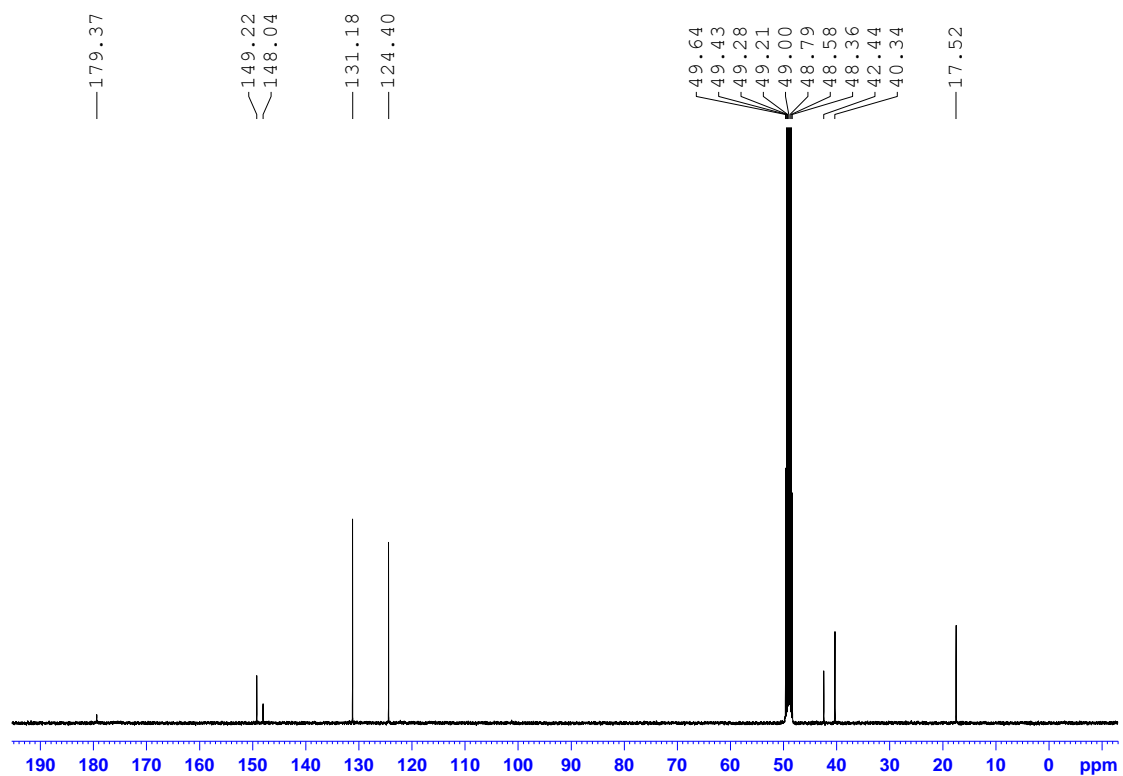
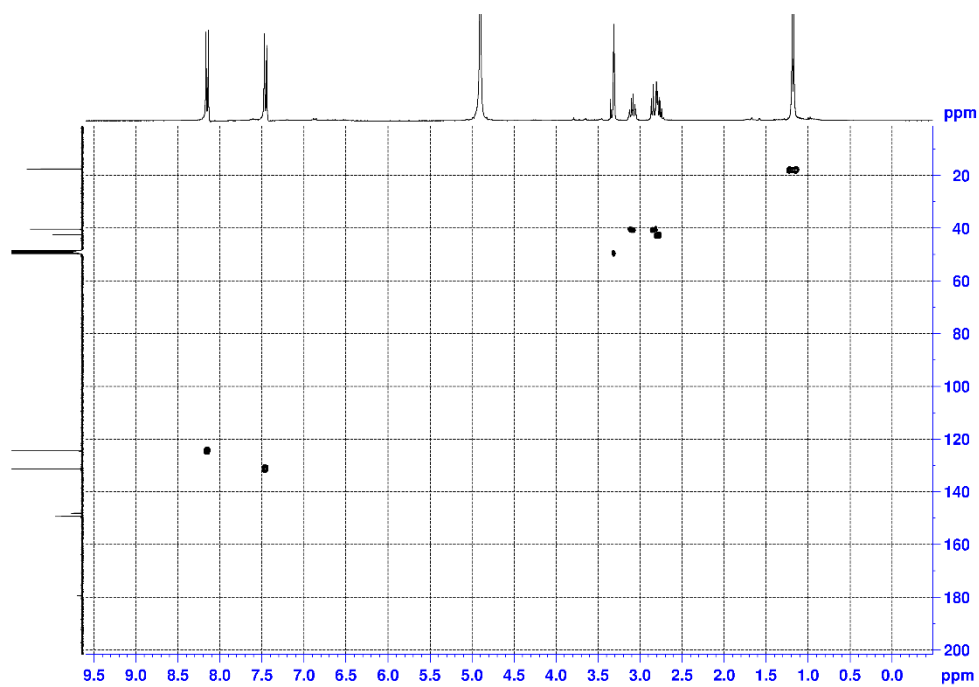
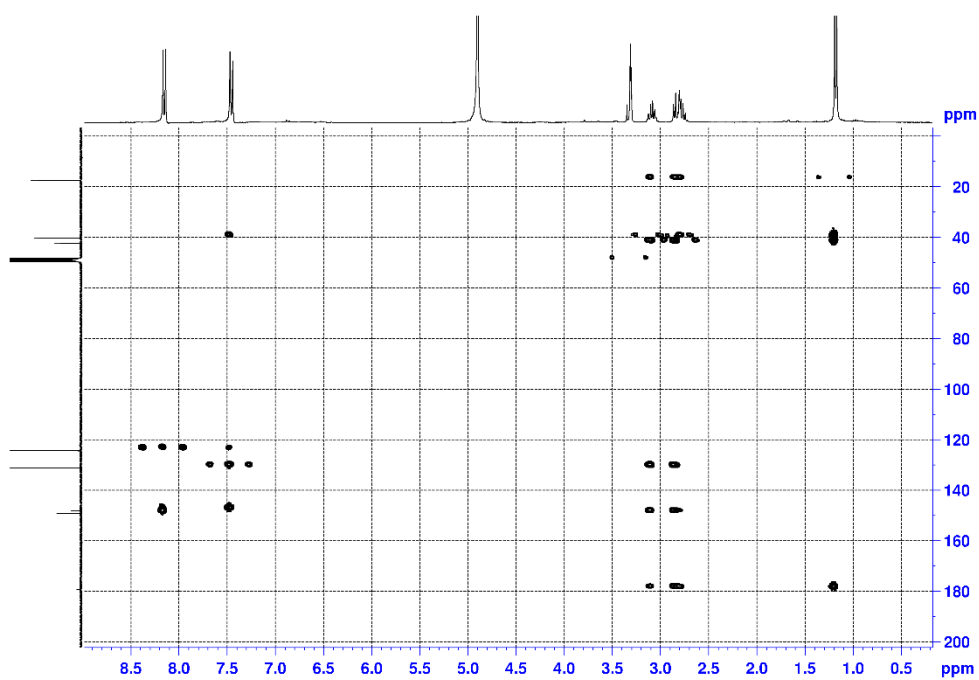


Figure S8:  $^{13}\text{C}$  NMR Spectrum of **2** in  $\text{CD}_3\text{OD}$  (100 MHz)



**Figure S9:** HSQC Spectrum of **2** in CD<sub>3</sub>OD



**Figure S10:** HMBC Spectrum of **2** in CD<sub>3</sub>OD

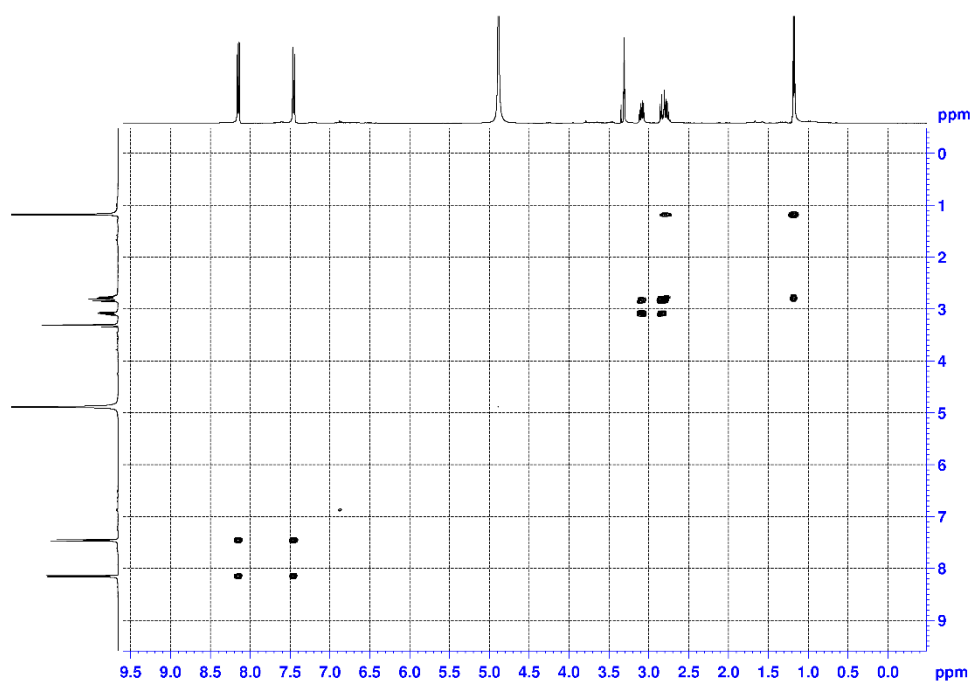


Figure S11:  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of **2** in  $\text{CD}_3\text{OD}$

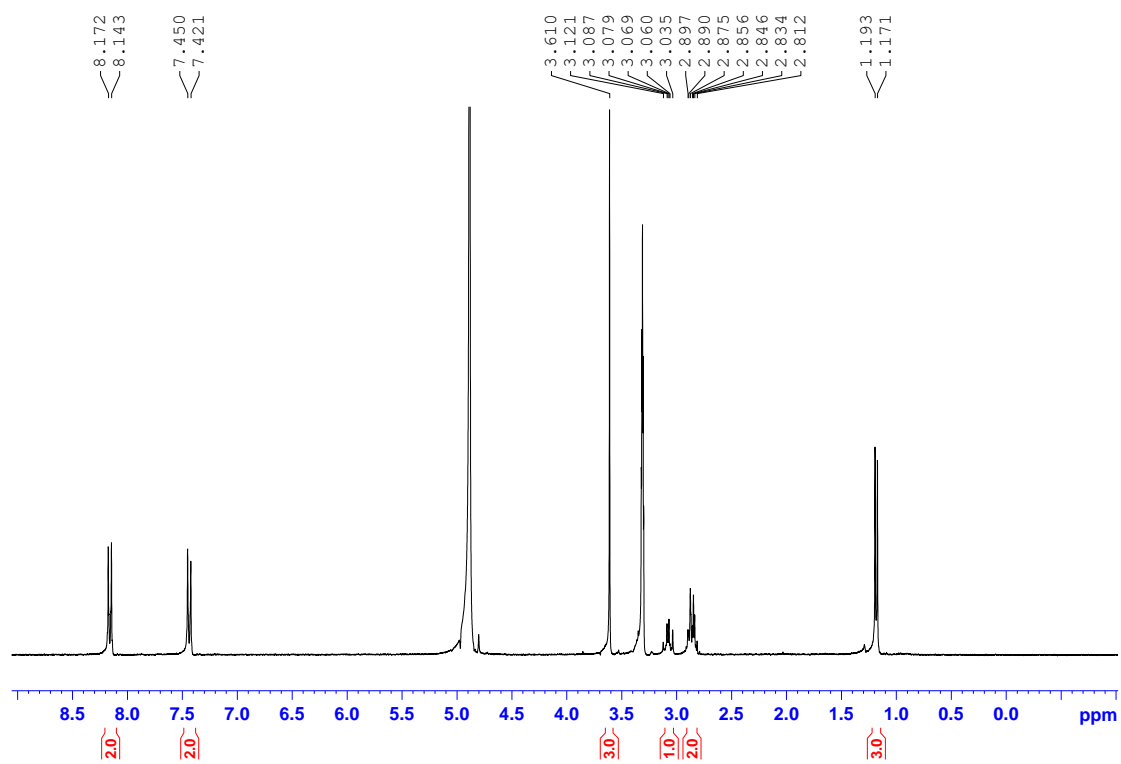


Figure S12:  $^1\text{H}$  NMR Spectrum of **3** in  $\text{CD}_3\text{OD}$  (400 MHz)



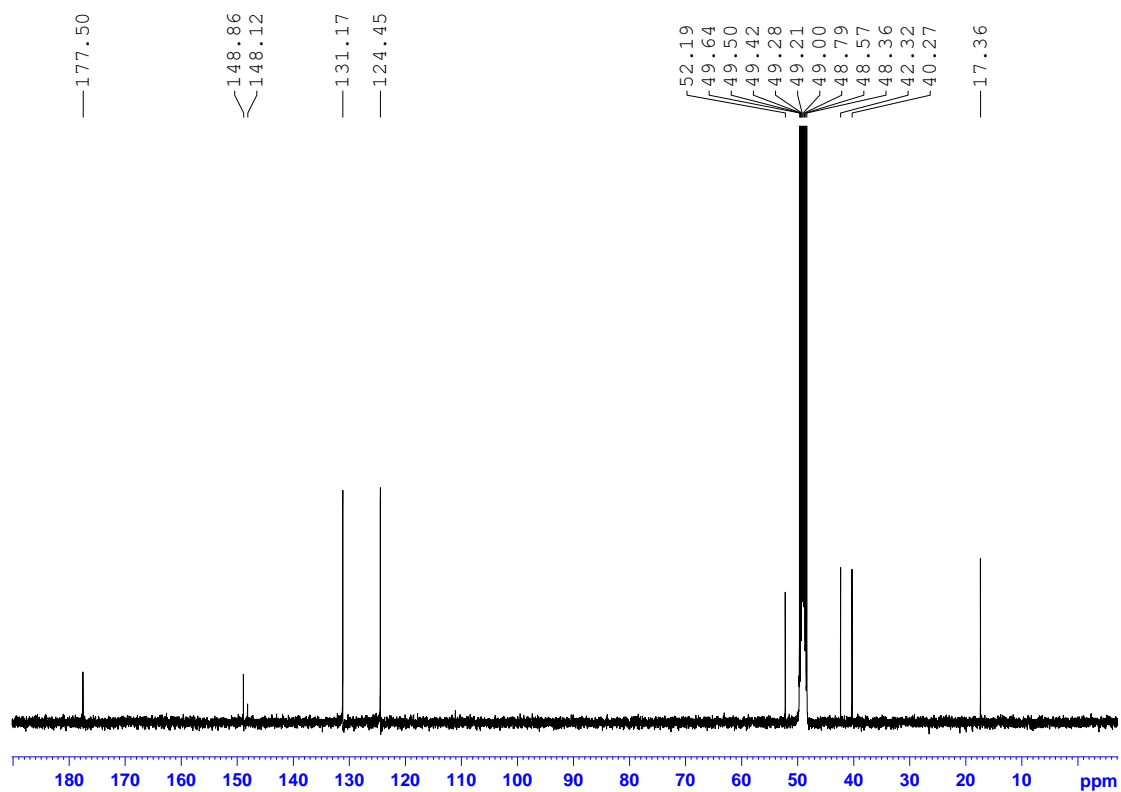


Figure S13:  $^{13}\text{C}$  NMR Spectrum of **3** in  $\text{CD}_3\text{OD}$  (100 MHz)

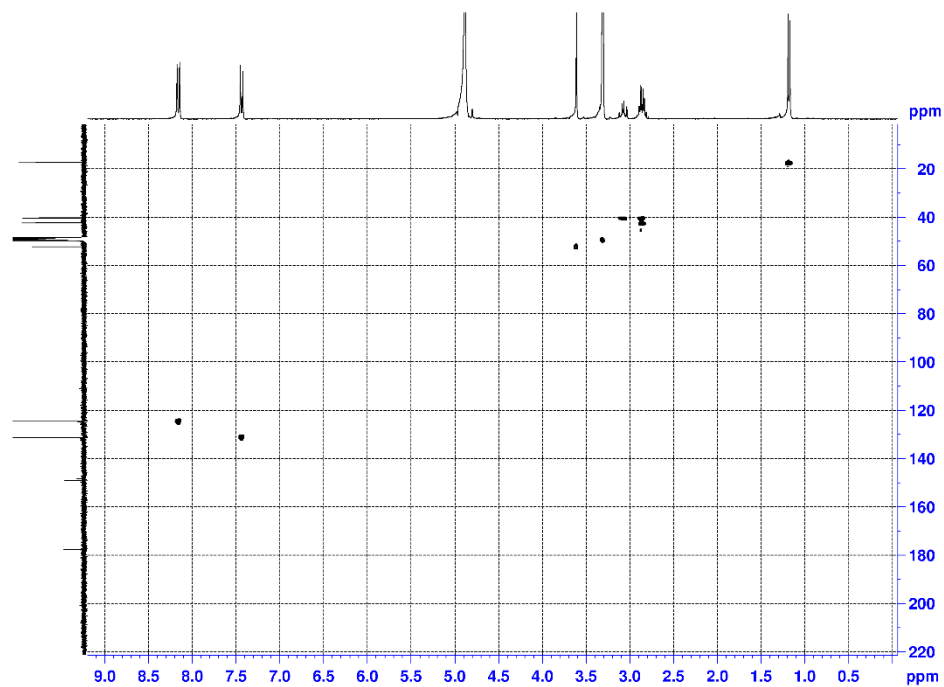


Figure S14: HSQC Spectrum of **3** in  $\text{CD}_3\text{OD}$

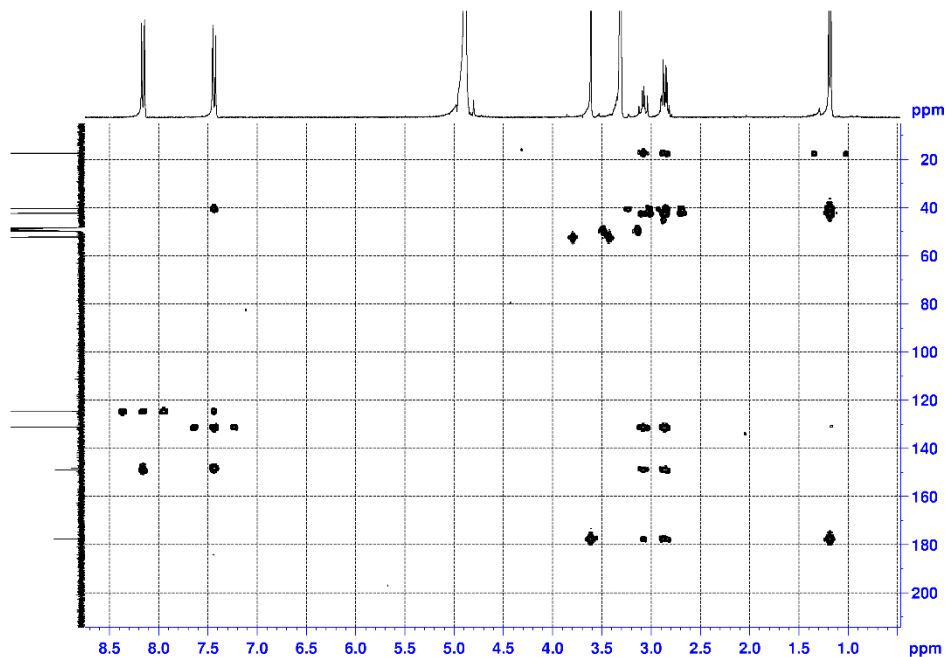


Figure S15: HMBC Spectrum of 3 in CD<sub>3</sub>OD

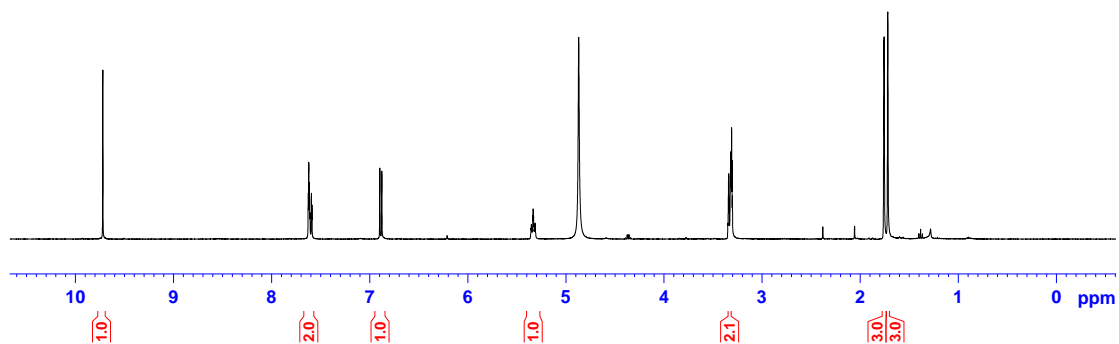
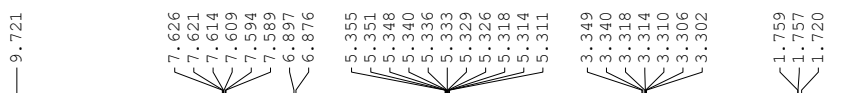


Figure S16: <sup>1</sup>H NMR Spectrum of 4 in CD<sub>3</sub>OD (400 MHz)

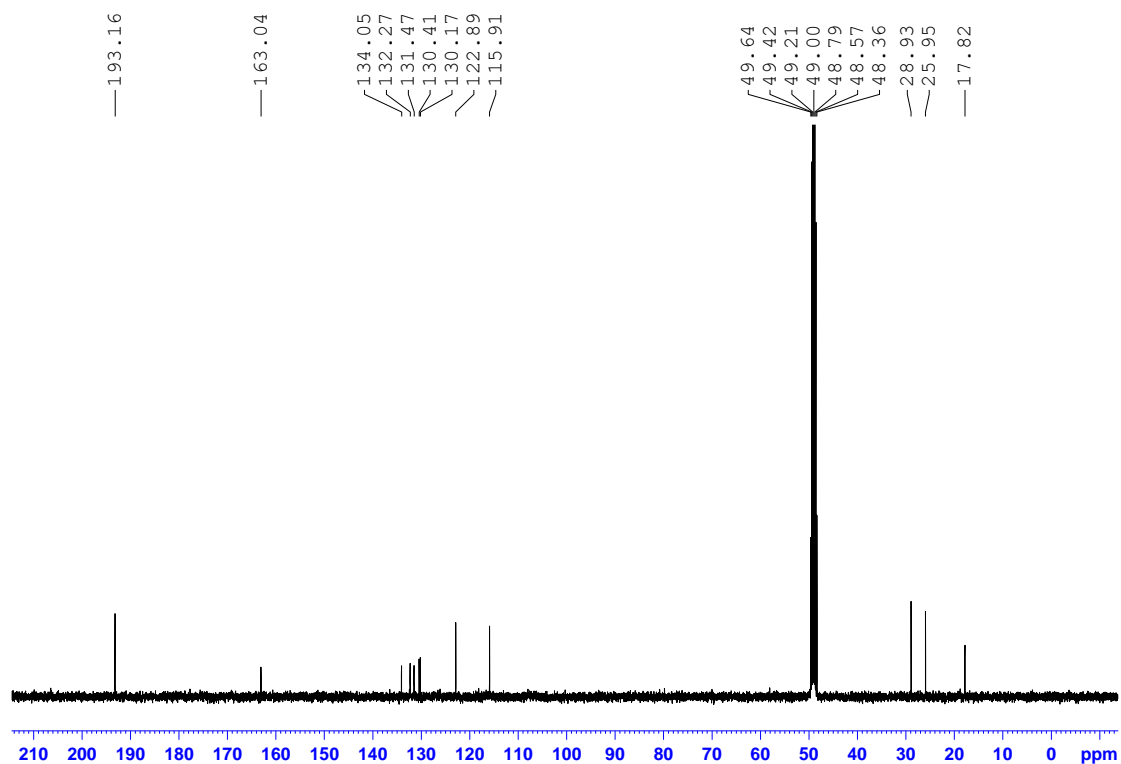


Figure S17:  $^{13}\text{C}$  NMR Spectrum of **4** in  $\text{CD}_3\text{OD}$  (100 MHz)

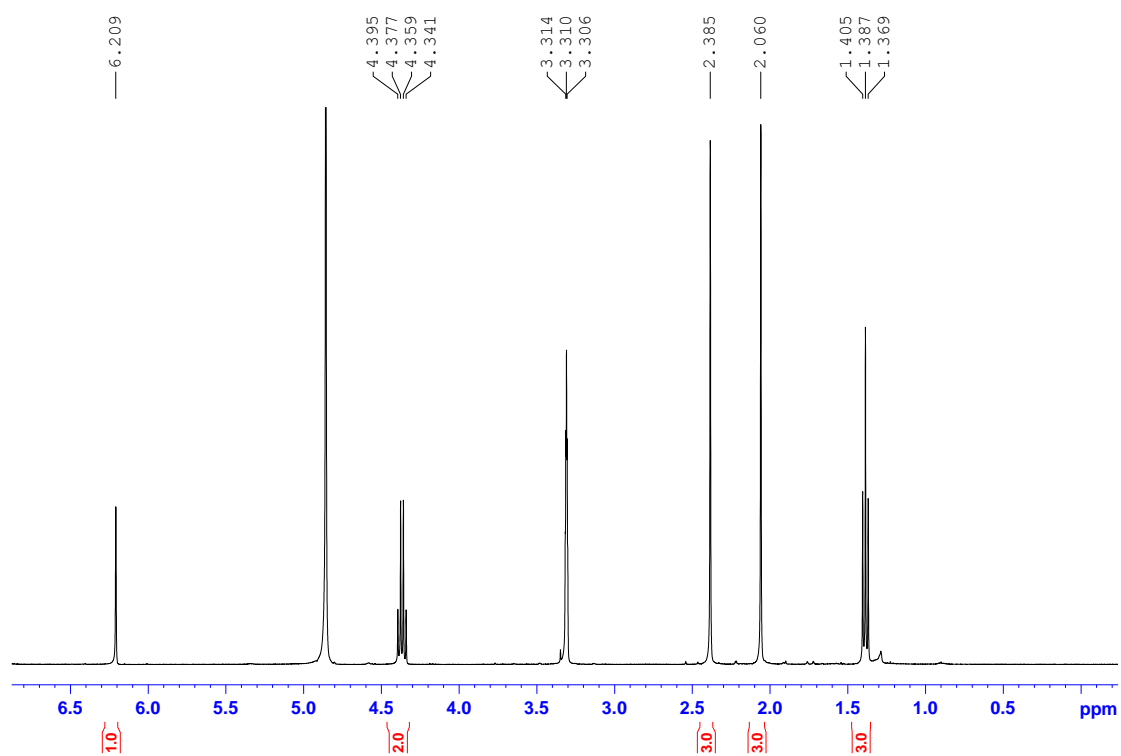


Figure S18:  $^1\text{H}$  NMR Spectrum of **5** in  $\text{CD}_3\text{OD}$  (400 MHz)

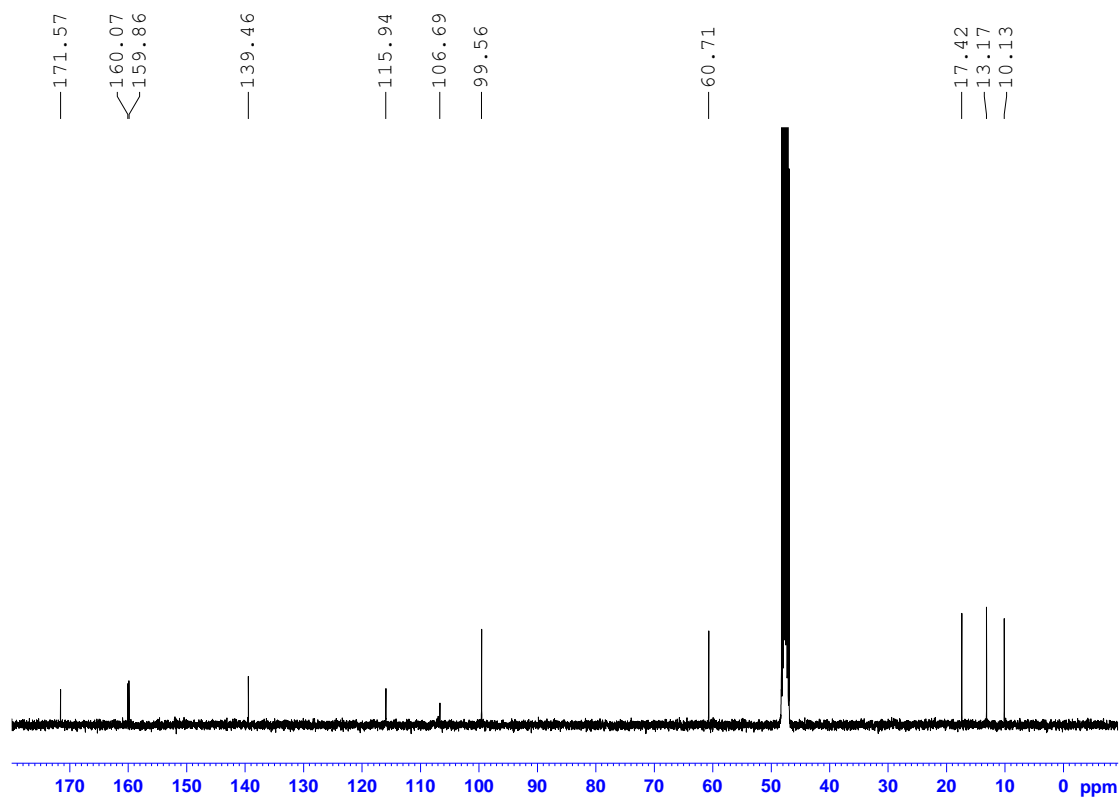


Figure S19:  $^{13}\text{C}$  NMR Spectrum of **5** in  $\text{CD}_3\text{OD}$  (100 MHz)

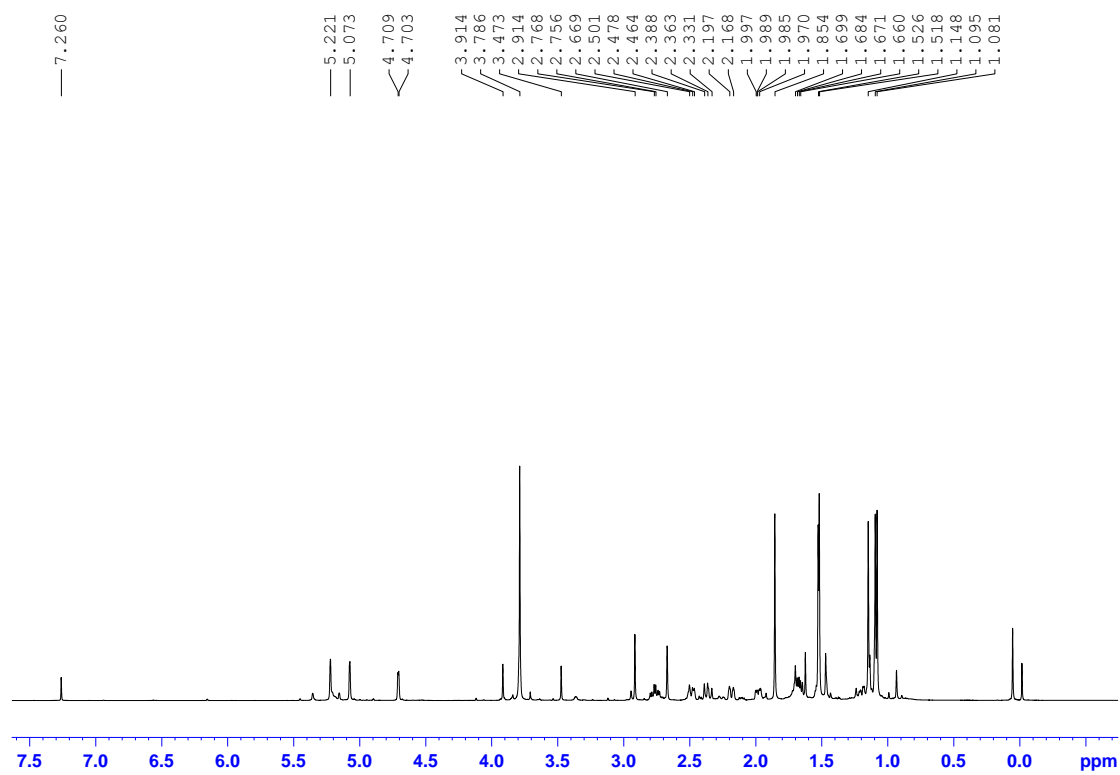
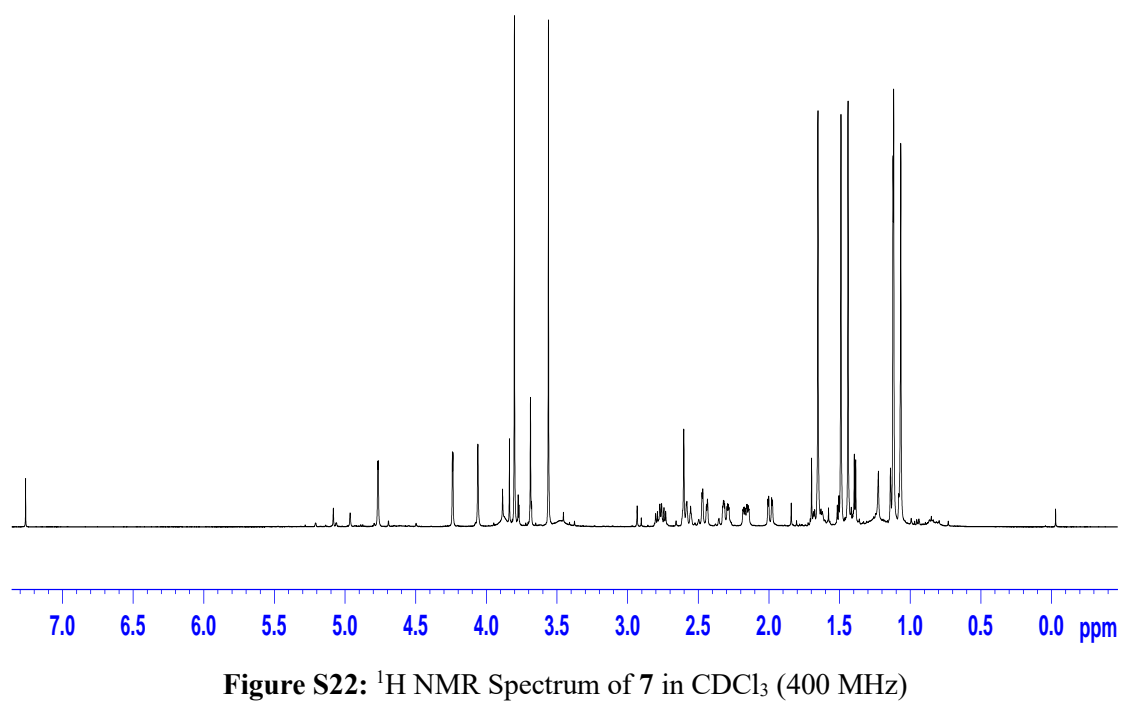
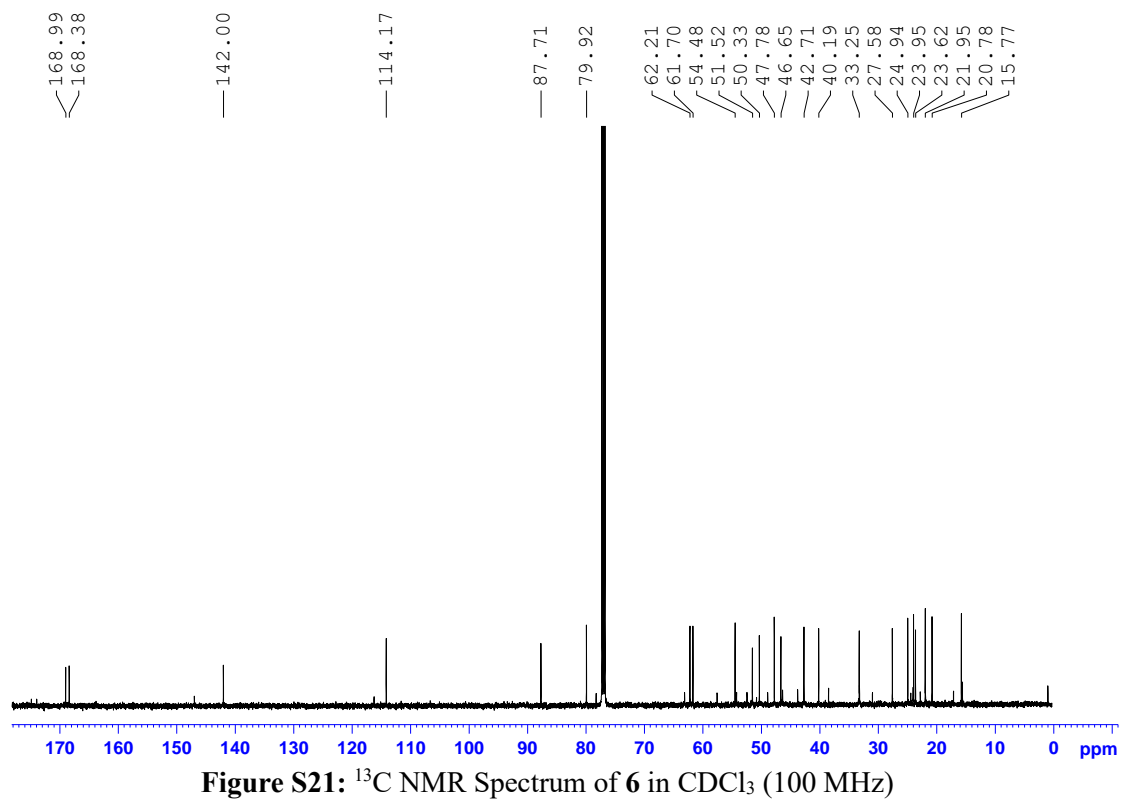


Figure S20:  $^1\text{H}$  NMR Spectrum of **6** in  $\text{CDCl}_3$  (400 MHz)



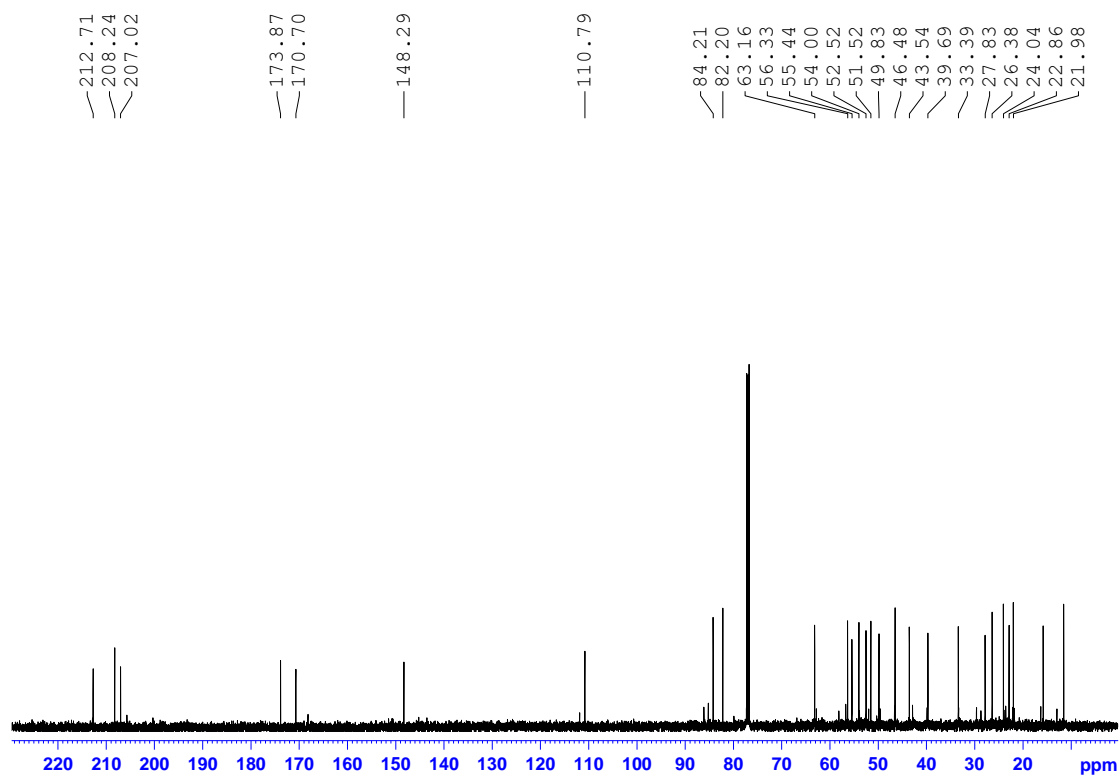


Figure S23:  $^{13}\text{C}$  NMR Spectrum of **7** in  $\text{CDCl}_3$  (100 MHz)

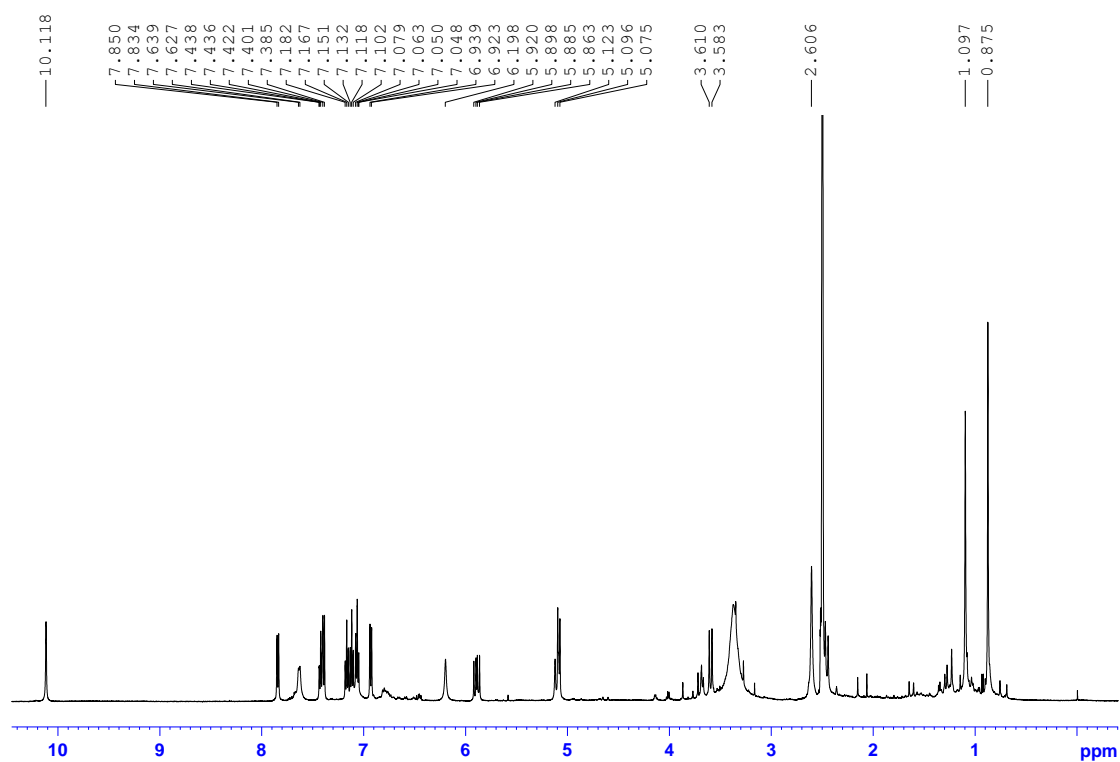


Figure S24:  $^1\text{H}$  NMR Spectrum of **8** in  $\text{CD}_3\text{OD}$  (400 MHz)

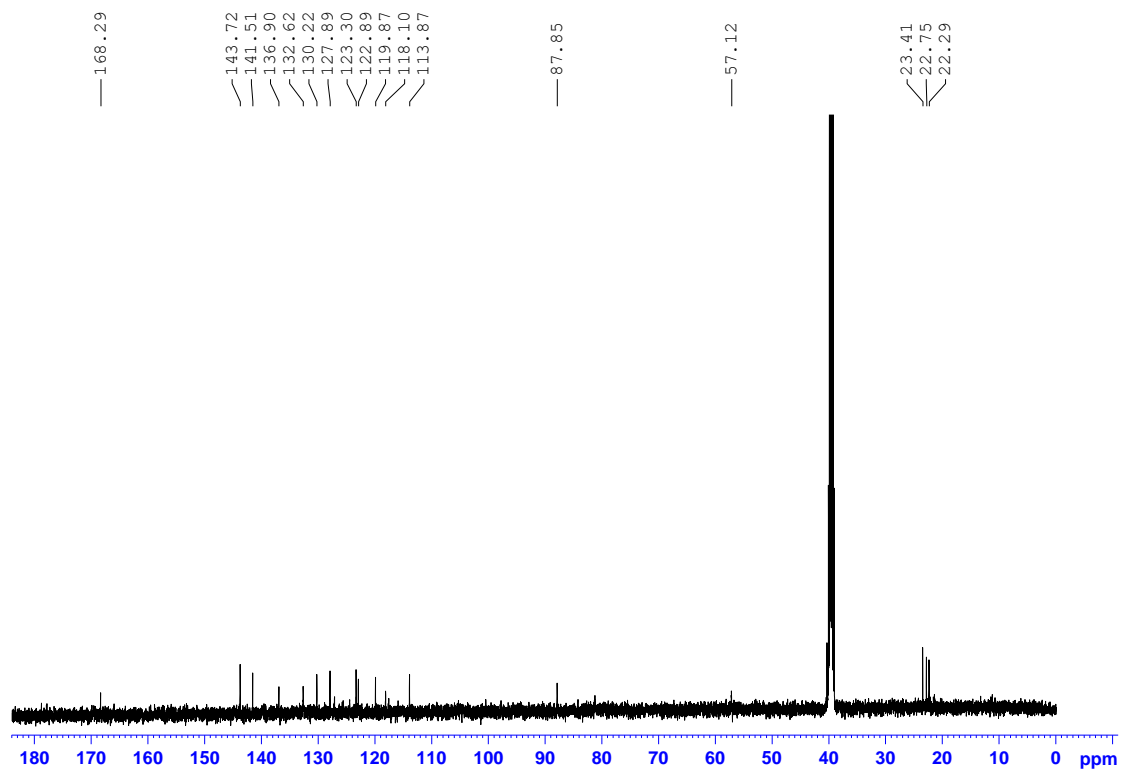


Figure S25:  $^{13}\text{C}$  NMR Spectrum of **8** in  $\text{CD}_3\text{OD}$  (100 MHz)

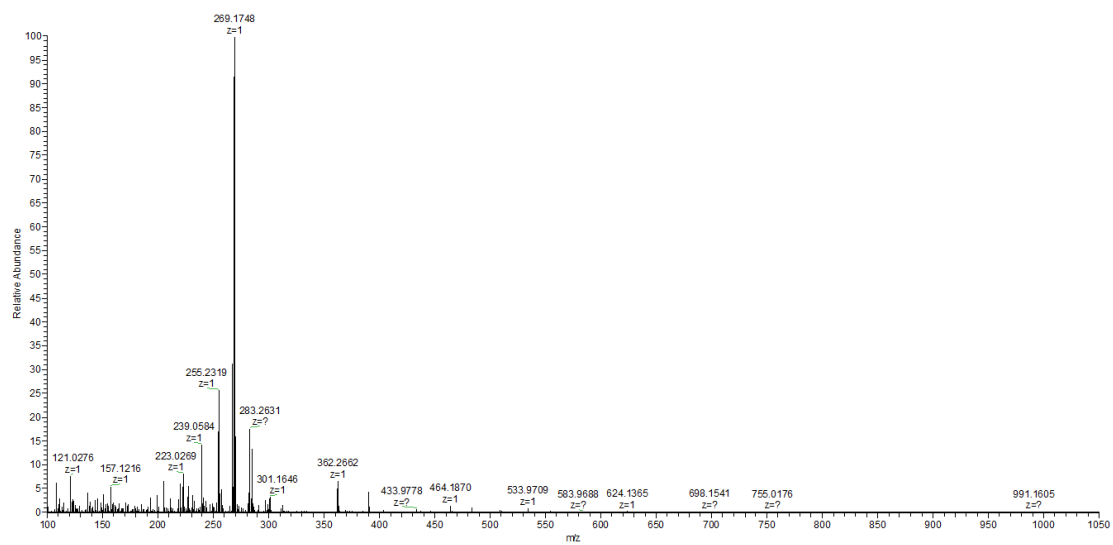
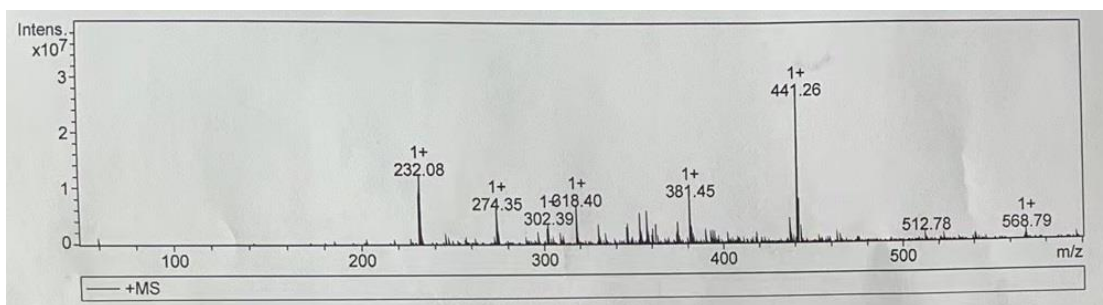
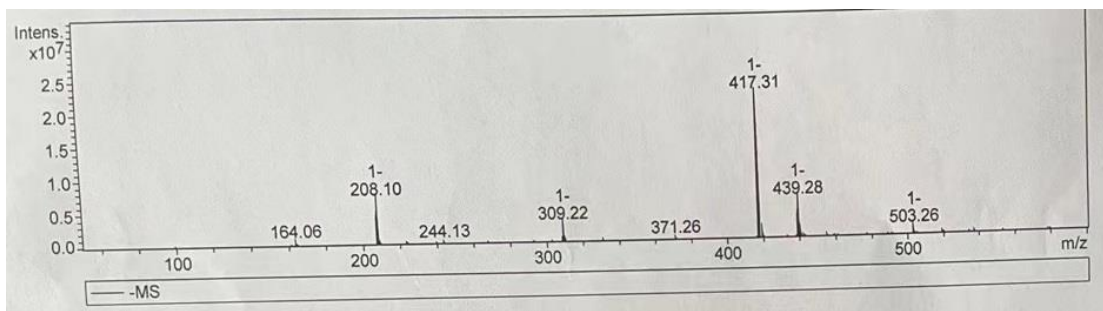
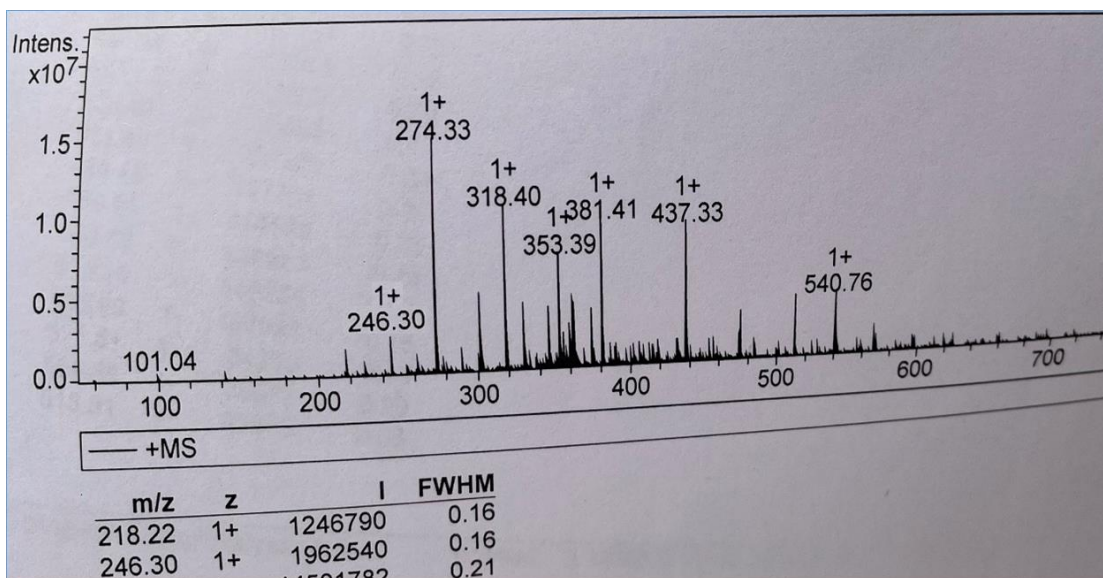


Figure S26: HRESIMS Spectrum of **1**



**Figure S27: ESIMS Spectrum of 2**



**Figure S28: ESIMS Spectrum of 3**



REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

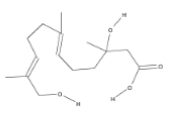
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- Molecular Formula
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| 85-89                | 115        |
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| 75-79                | 7499       |
| 70-74                | 16873      |
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Biological Study 2

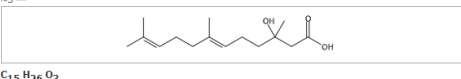
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Uses 1

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Score: 98

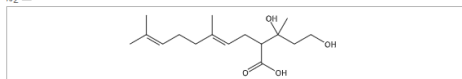
1. 107058-67-3



**C<sub>15</sub>H<sub>26</sub>O<sub>2</sub>**  
6,10-Dodecadienoic acid, 3-hydroxy-3,7,11-trimethyl-  
• Key Physical Properties

Score: 94

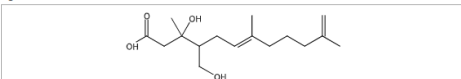
2. 101726-17-4



**C<sub>16</sub>H<sub>28</sub>O<sub>4</sub>**  
4,8-Dodecadienoic acid, 2-(1,3-dihydroxy-1-methylpropyl)-5,9-dimethyl- (6CI)  
• Key Physical Properties

Score: 94

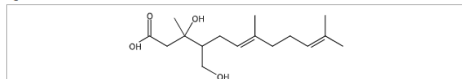
3. 107525-30-4



**C<sub>16</sub>H<sub>28</sub>O<sub>4</sub>**  
6,11-Dodecadienoic acid, 3-hydroxy-4-(hydroxymethyl)-3,7,11-trimethyl- (6CI)  
• Key Physical Properties

Score: 94

4. 860439-79-8



**C<sub>16</sub>H<sub>28</sub>O<sub>4</sub>**  
Mevalonic acid, 4-geranyl- (6CI)  
• Key Physical Properties

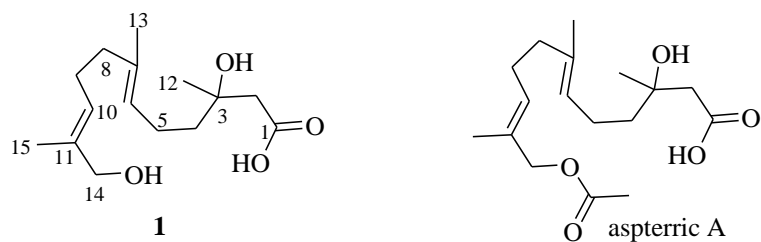
Score: 91

5. 53042-57-2

Score: 91

6. 53042-58-3

Figure S29: Scifinder similarity report for compound 1



**Table S1:**  $^1\text{H}$  and  $^{13}\text{C}$  NMR Data of **1** and the analog Aspterric A in Methanol- $d_4$ .<sup>a</sup>

| No. | <b>1</b>            |                     | aspterric A         |                     |       |
|-----|---------------------|---------------------|---------------------|---------------------|-------|
|     | $\delta_{\text{H}}$ | $\delta_{\text{C}}$ | $\delta_{\text{H}}$ | $\delta_{\text{C}}$ |       |
| 1   |                     | 175.7               | 1                   | 175.9               |       |
| 2   | 2.45, s             | 46.5                | 2                   | 2.45, s             | 46.5  |
| 3   |                     | 72.1                | 3                   |                     | 72.1  |
| 4   | 1.58, m             | 42.7                | 4                   | 1.57, m             | 42.7  |
| 5   | 2.09, m             | 23.5                | 5                   | 2.09, m             | 23.5  |
| 6   | 5.15, t (7.0)       | 125.7               | 6                   | 5.14, t (7.1)       | 125.9 |
| 7   |                     | 135.9               | 7                   |                     | 135.6 |
| 8   | 2.02, t (7.0)       | 40.4                | 8                   | 2.03, m             | 40.1  |
| 9   | 2.14, q (7.0)       | 27.3                | 9                   | 2.16, m             | 27.1  |
| 10  | 5.38, t (7.0)       | 126.5               | 10                  | 5.46, t (7.0)       | 130.3 |
| 11  |                     | 135.9               | 11                  |                     | 131.4 |
| 12  | 1.28, s             | 27.1                | 12                  | 1.28, s             | 27.2  |
| 13  | 1.63, s             | 16.0                | 13                  | 1.63, s             | 16.0  |
| 14  | 3.91, s             | 69.0                | 14                  | 4.44, s             | 71.3  |
| 15  | 1.64, s             | 13.7                | 15                  | 1.65, s             | 14.0  |
|     |                     |                     |                     | 2.04, s             | 20.8  |
|     |                     |                     |                     |                     | 172.9 |

<sup>a</sup>  $^1\text{H}$  NMR recorded at 400 MHz,  $^{13}\text{C}$  NMR recorded at 100 MHz.