

Supporting Information

Rec. Nat. Prod. X:X (202X) XX-XX

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

Aspergillus terreus LPFH-1

Jingmin Wu ¹, Linlin Qiu¹, Yanli Zhou ¹, Shen Yao ¹

and Dabu Zhu ^{1, 2*}

¹ The First People's Hospital of Linping District, Hangzhou 311100, China

² Collaborative Innovation Center of Yangtze River Delta Region Green Pharmaceuticals,
Zhejiang University of Technology, Hangzhou 310014, China

Table of Contents	Page
Figure S1: ¹ H NMR Spectrum of 1 in CD ₃ OD (400 MHz)	2
Figure S2: ¹³ C NMR Spectrum of 1 in CD ₃ OD (100 MHz)	2
Figure S3: HSQC Spectrum of 1 in CD ₃ OD	3
Figure S4: HMBC Spectrum of 1 in CD ₃ OD	3
Figure S5: ¹ H- ¹ H COSY Spectrum of 1 in CD ₃ OD	4
Figure S6: NOESY Spectrum of 1 in CD ₃ OD	4
Figure S7: ¹ H NMR Spectrum of 2 in CD ₃ OD (400 MHz)	5
Figure S8: ¹³ C NMR Spectrum of 2 in CD ₃ OD (100 MHz)	5
Figure S9: HSQC Spectrum of 2 in CD ₃ OD	6
Figure S10: HMBC Spectrum of 2 in CD ₃ OD	6
Figure S11: ¹ H- ¹ H COSY Spectrum of 2 in CD ₃ OD	7
Figure S12: ¹ H NMR Spectrum of 3 in CD ₃ OD (400 MHz)	7
Figure S13: ¹³ C NMR Spectrum of 3 in CD ₃ OD (100 MHz)	8
Figure S14: HSQC Spectrum of 3 in CD ₃ OD	8
Figure S15: HMBC Spectrum of 3 in CD ₃ OD	9
Figure S16: ¹ H NMR Spectrum of 4 in CD ₃ OD (400 MHz)	9
Figure S17: ¹³ C NMR Spectrum of 4 in CD ₃ OD (100 MHz)	10
Figure S18: ¹ H NMR Spectrum of 5 in CD ₃ OD (400 MHz)	10
Figure S19: ¹³ C NMR Spectrum of 5 in CD ₃ OD (100 MHz)	11
Figure S20: ¹ H NMR Spectrum of 6 in CDCl ₃ (400 MHz)	11
Figure S21: ¹³ C NMR Spectrum of 6 in CDCl ₃ (100 MHz)	12
Figure S22: ¹ H NMR Spectrum of 7 in CDCl ₃ (400 MHz)	12
Figure S23: ¹³ C NMR Spectrum of 7 in CDCl ₃ (100 MHz)	13
Figure S24: ¹ H NMR Spectrum of 8 in DMSO- <i>d</i> ₆ (400 MHz)	13
Figure S25: ¹³ C NMR Spectrum of 8 in DMSO- <i>d</i> ₆ (100 MHz)	14
Figure S26: HRESIMS Spectrum of 1	14

Figure S27: ESIMS Spectrum of 2	15
Figure S28: ESIMS Spectrum of 3	15
Figure S29: Scifinder similarity report for compound 1	16
Table S1. ^1H and ^{13}C NMR Data of 1 and the analog aspterric A in Methanol- d_4 .	17

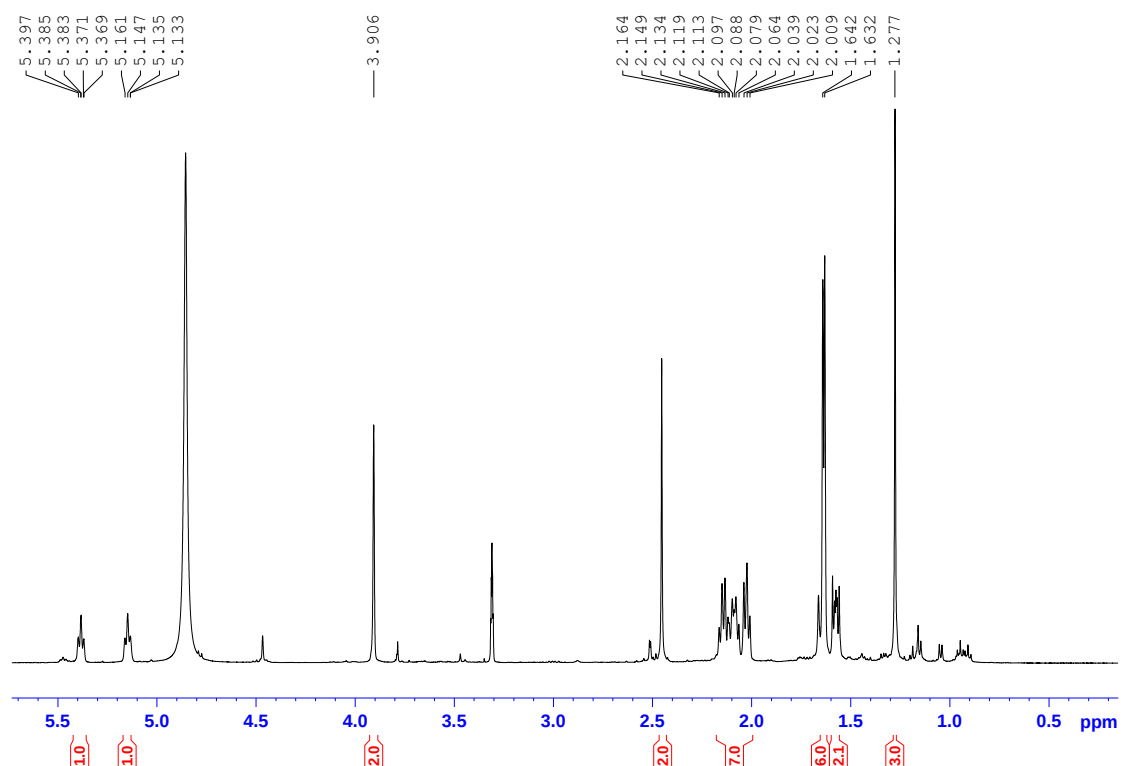


Figure S1: ¹H NMR Spectrum of **1** in CD₃OD (400 MHz)

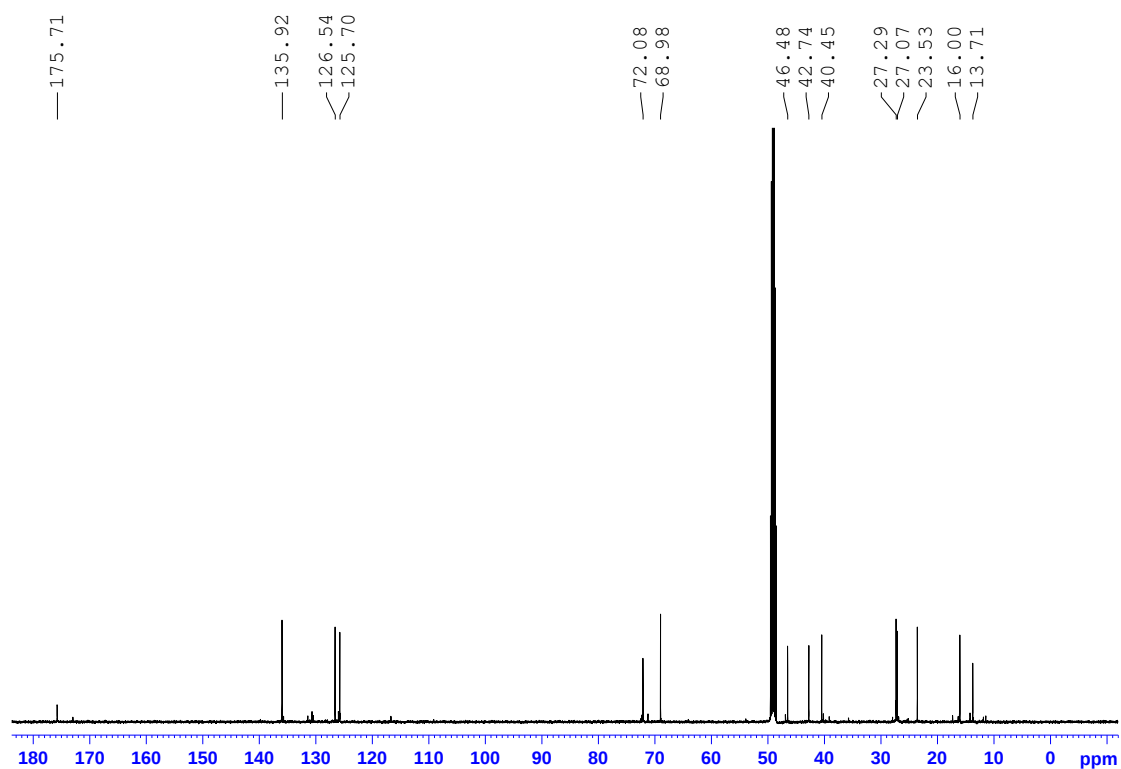


Figure S2: ¹³C NMR Spectrum of **1** in CD₃OD (100 MHz)

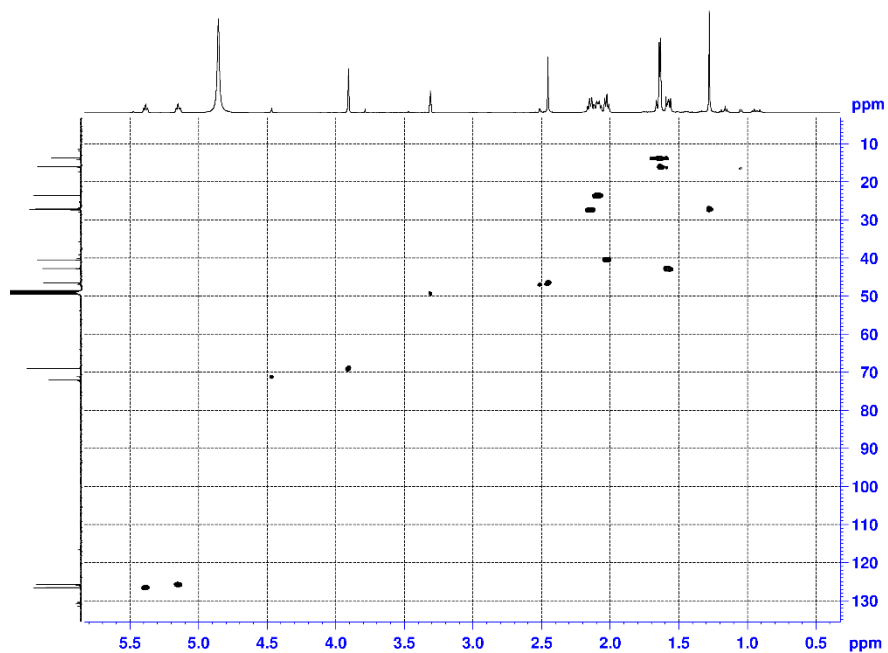


Figure S3: HSQC Spectrum of **1** in CD₃OD

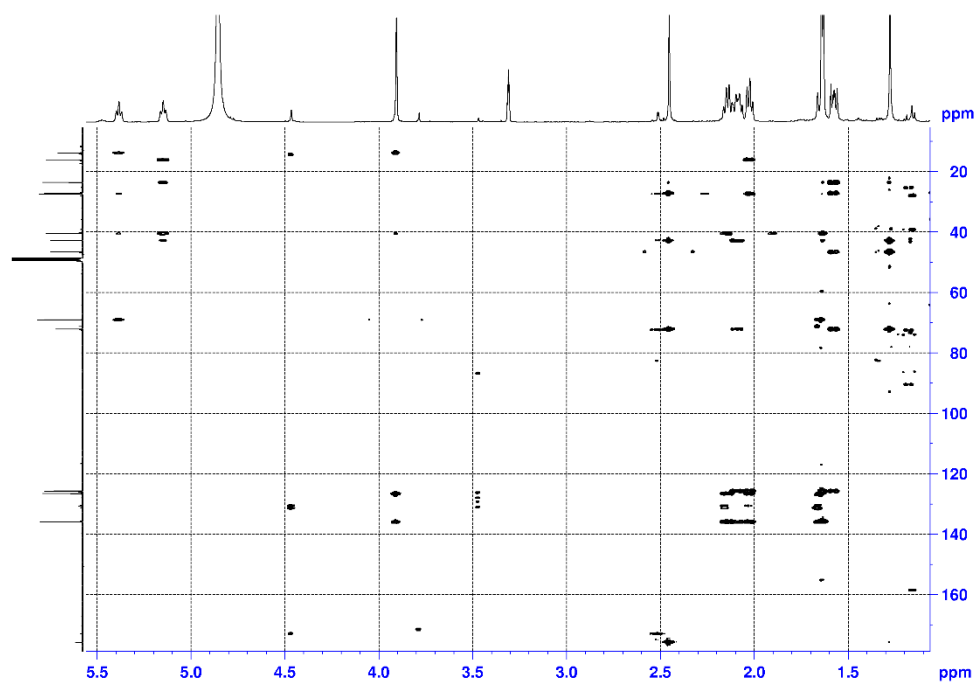


Figure S4: HMBC Spectrum of **1** in CD₃OD

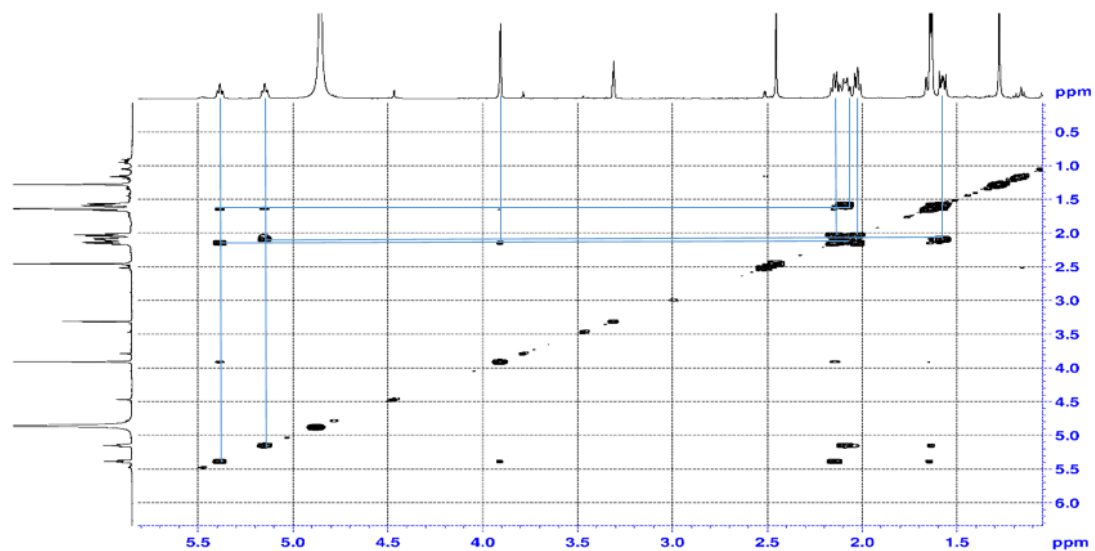


Figure S5: ^1H - ^1H COSY Spectrum of compound **1** in CD_3OD

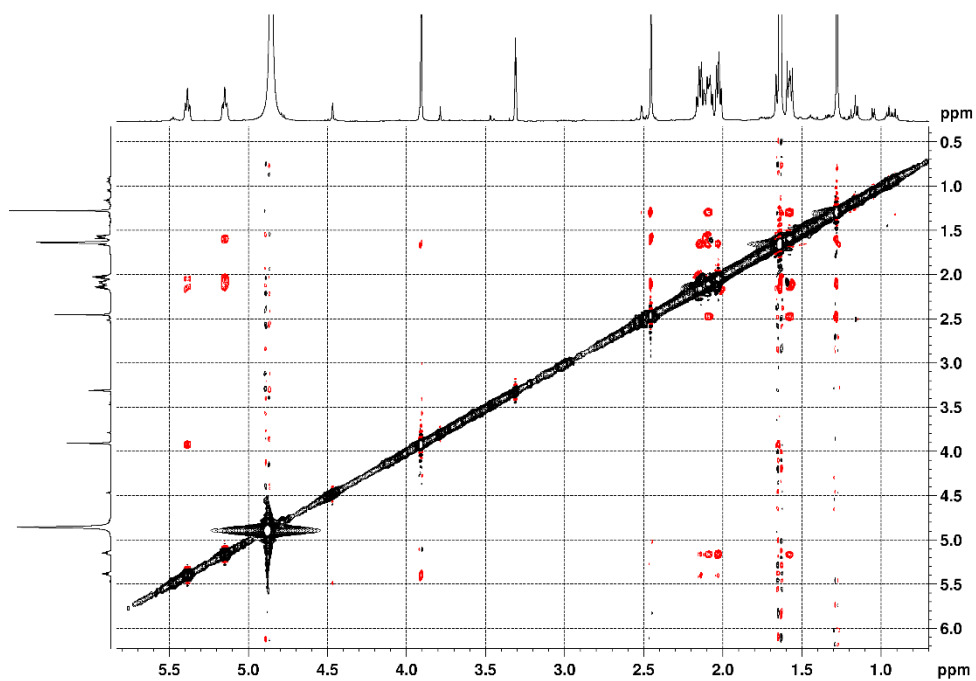


Figure S6: NOESY spectrum of compound **1** in CD_3OD

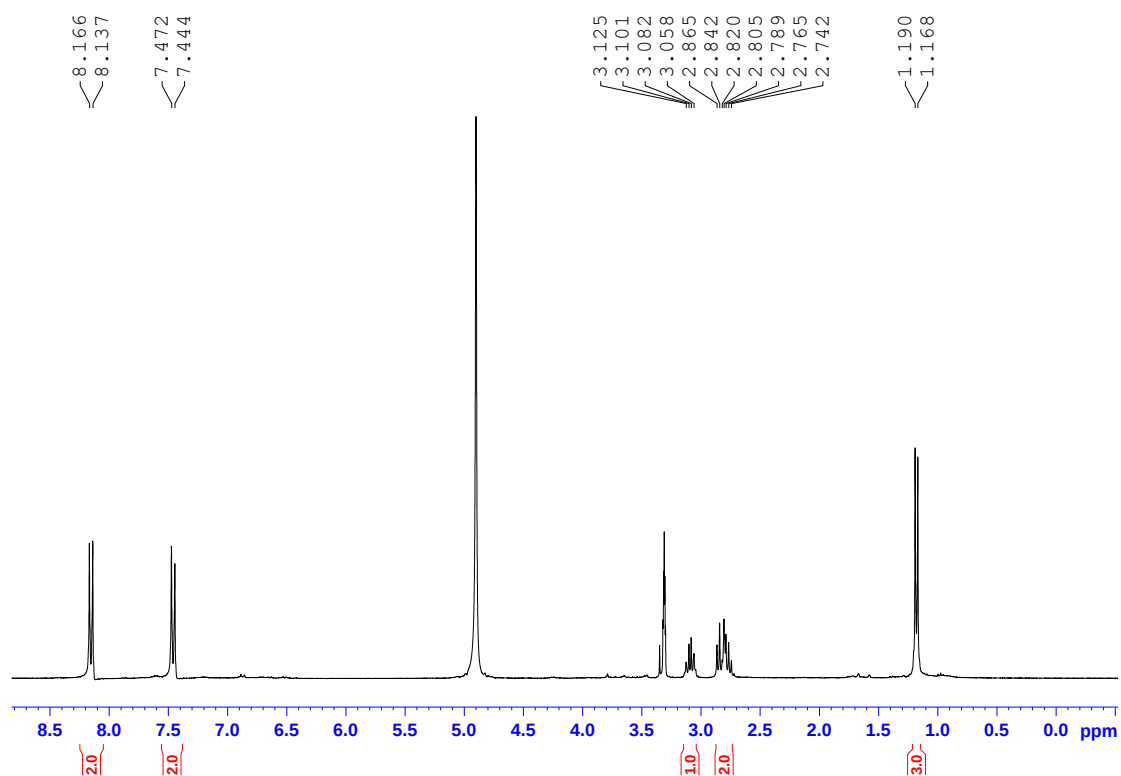


Figure S7: ¹H NMR Spectrum of **2** in CD₃OD (400 MHz)

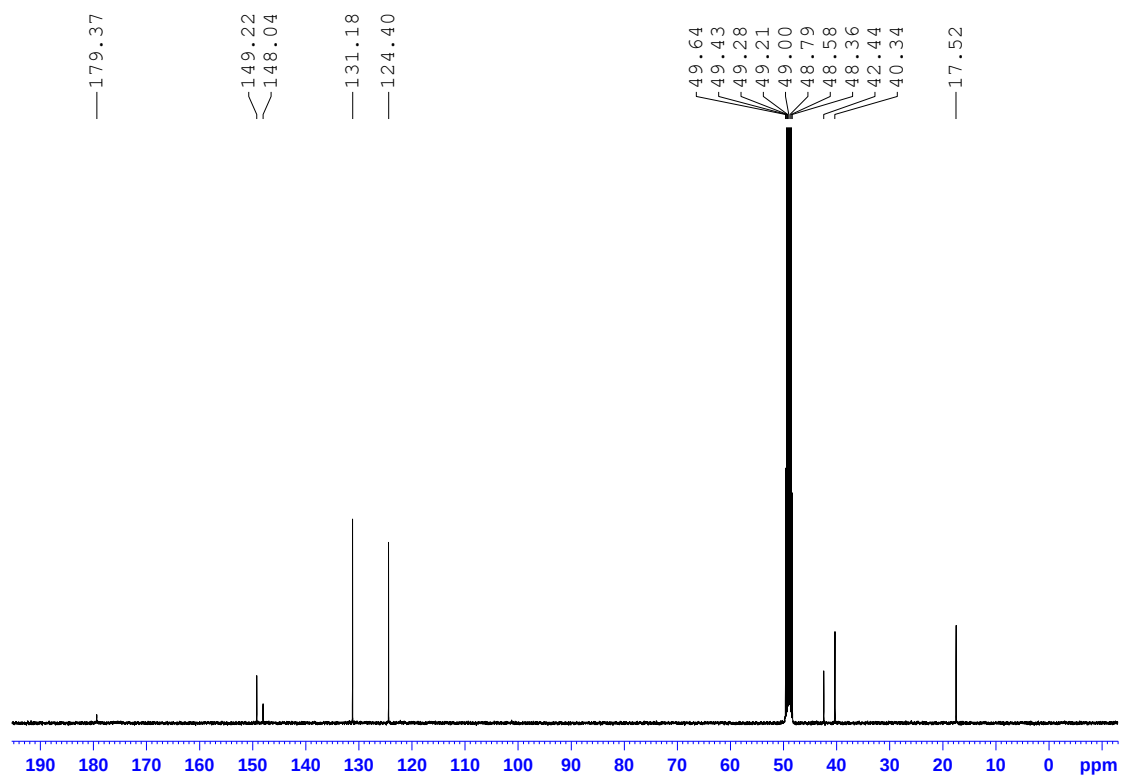


Figure S8: ¹³C NMR Spectrum of **2** in CD₃OD (100 MHz)

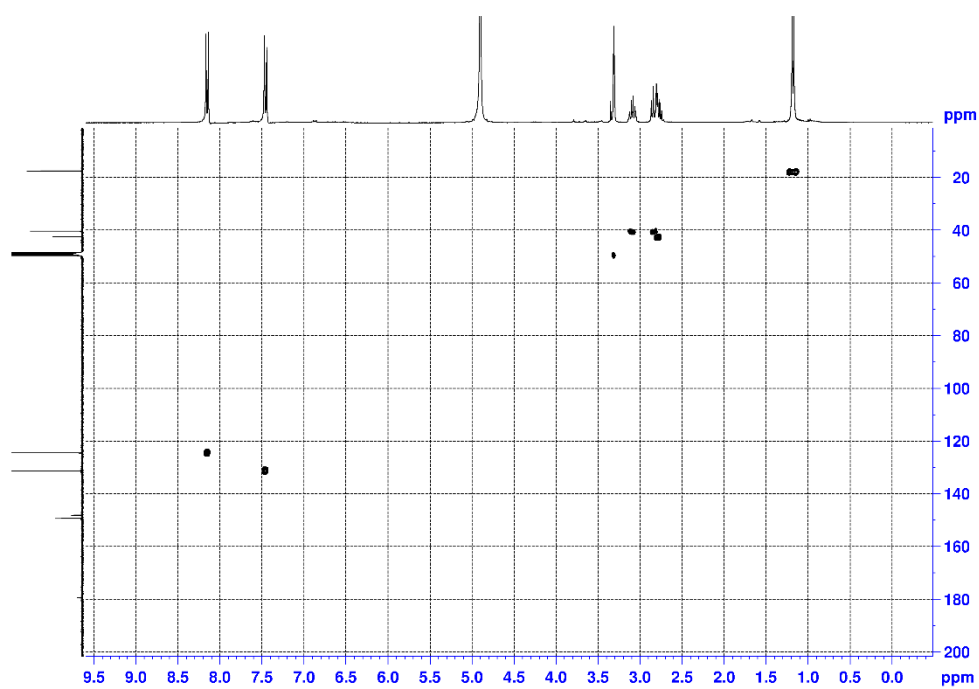


Figure S9: HSQC Spectrum of **2** in CD₃OD

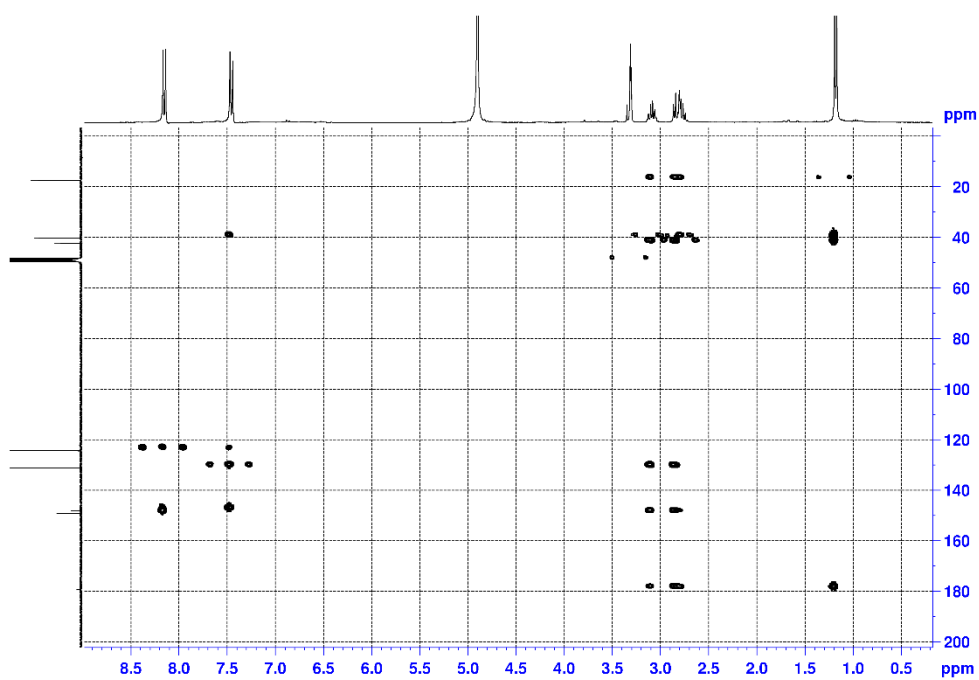


Figure S10: HMBC Spectrum of **2** in CD₃OD

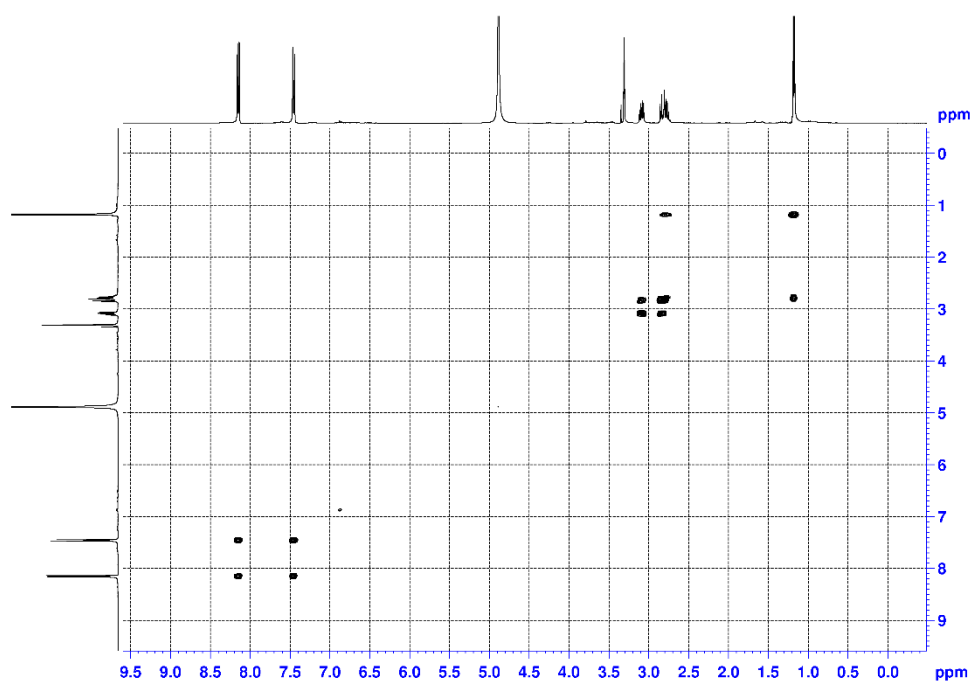


Figure S11: ^1H - ^1H COSY Spectrum of **2** in CD_3OD

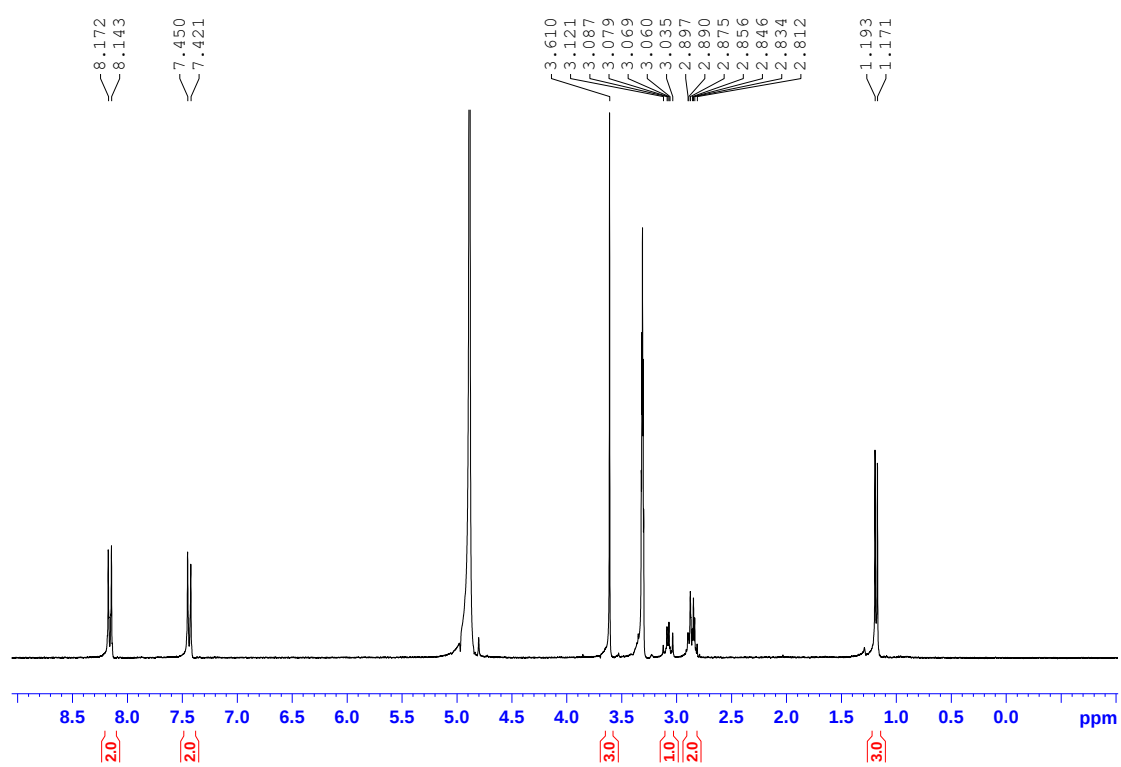


Figure S12: ^1H NMR Spectrum of **3** in CD_3OD (400 MHz)

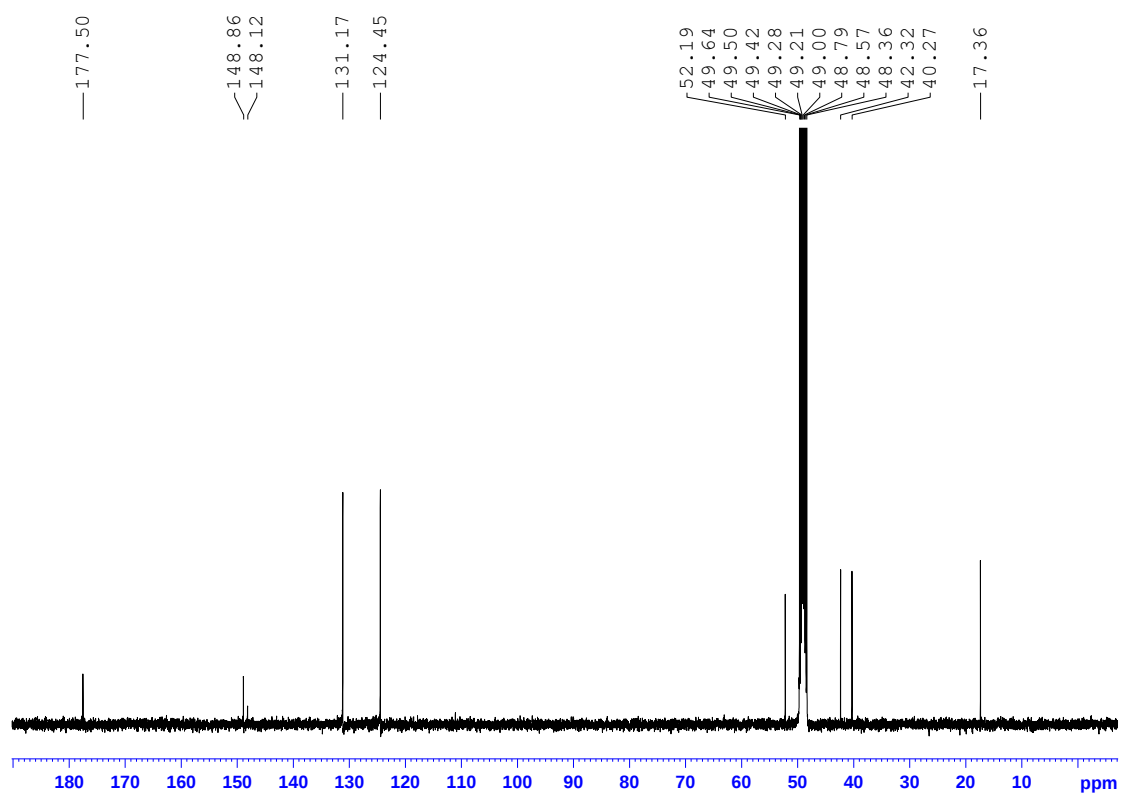


Figure S13: ^{13}C NMR Spectrum of **3** in CD_3OD (100 MHz)

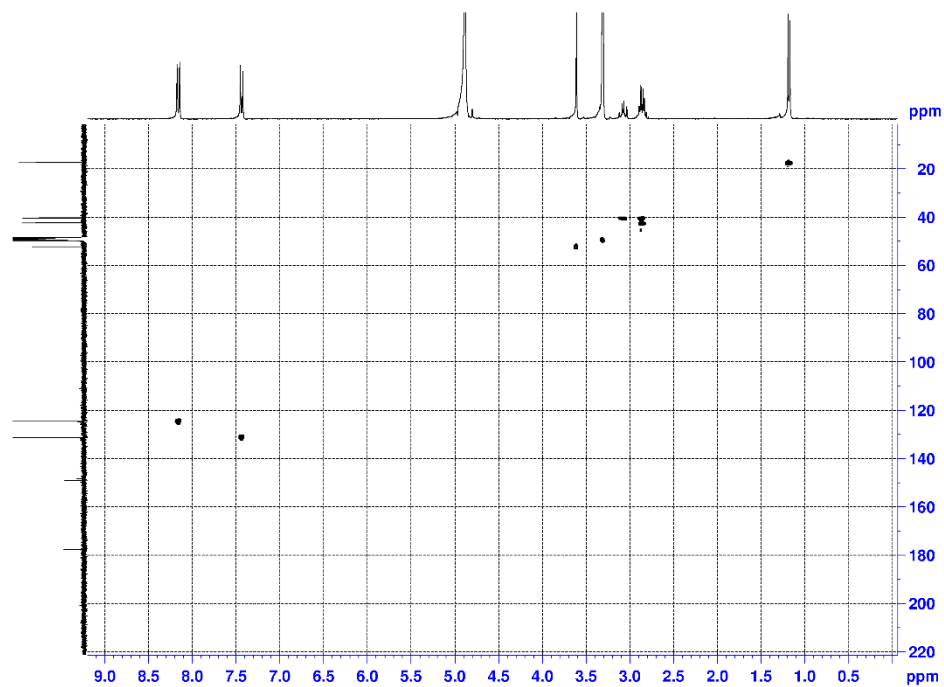


Figure S14: HSQC Spectrum of **3** in CD_3OD

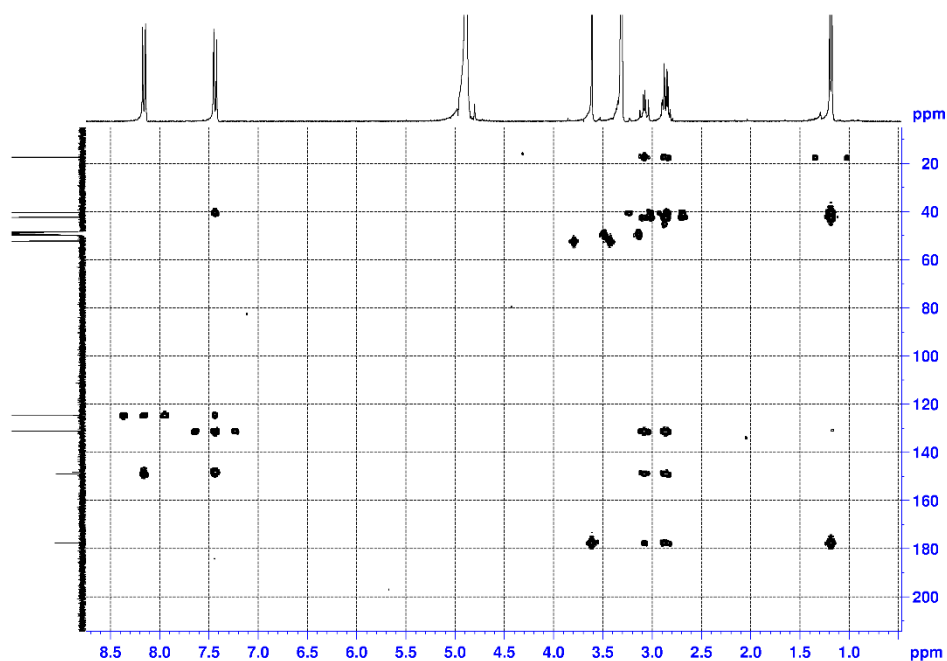


Figure S15: HMBC Spectrum of **3** in CD₃OD

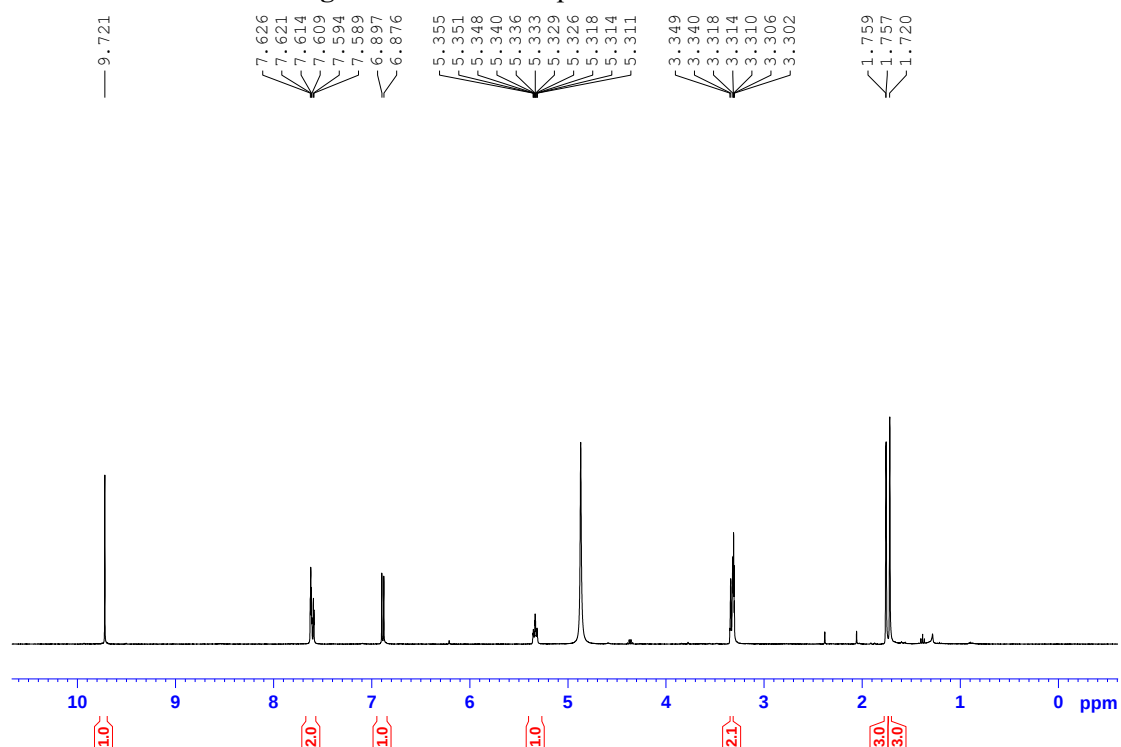


Figure S16: ¹H NMR Spectrum of **4** in CD₃OD (400 MHz)

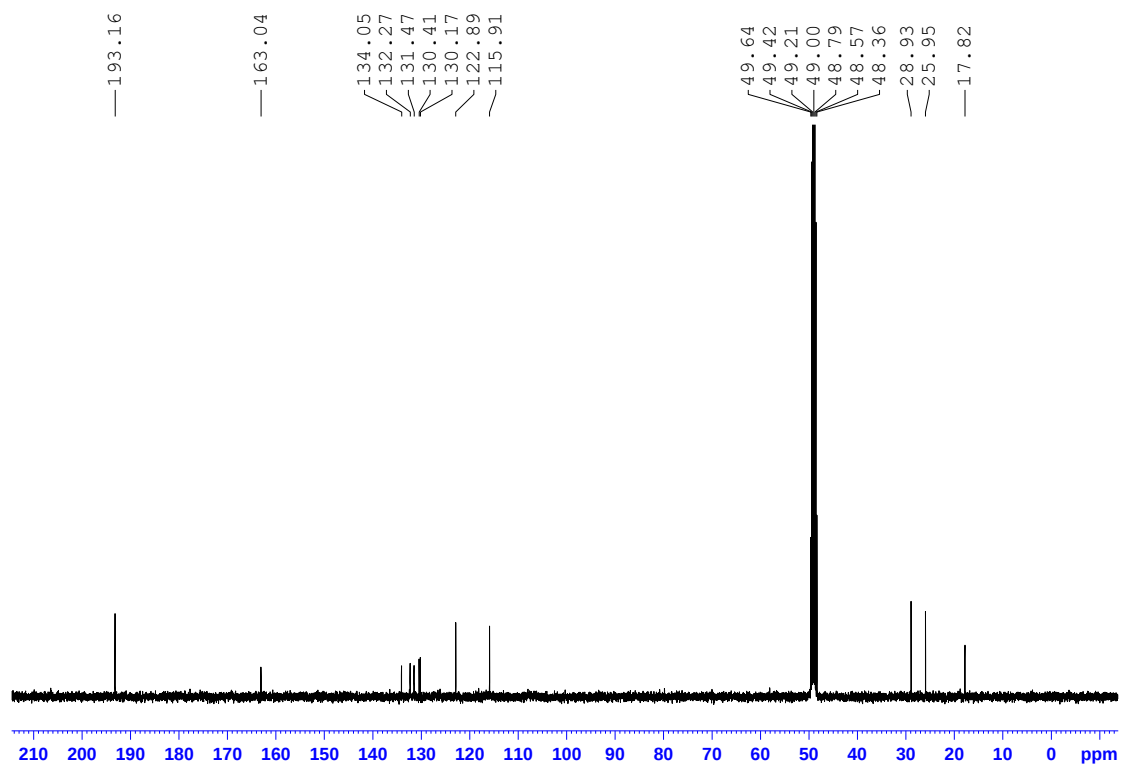


Figure S17: ^{13}C NMR Spectrum of **4** in CD_3OD (100 MHz)

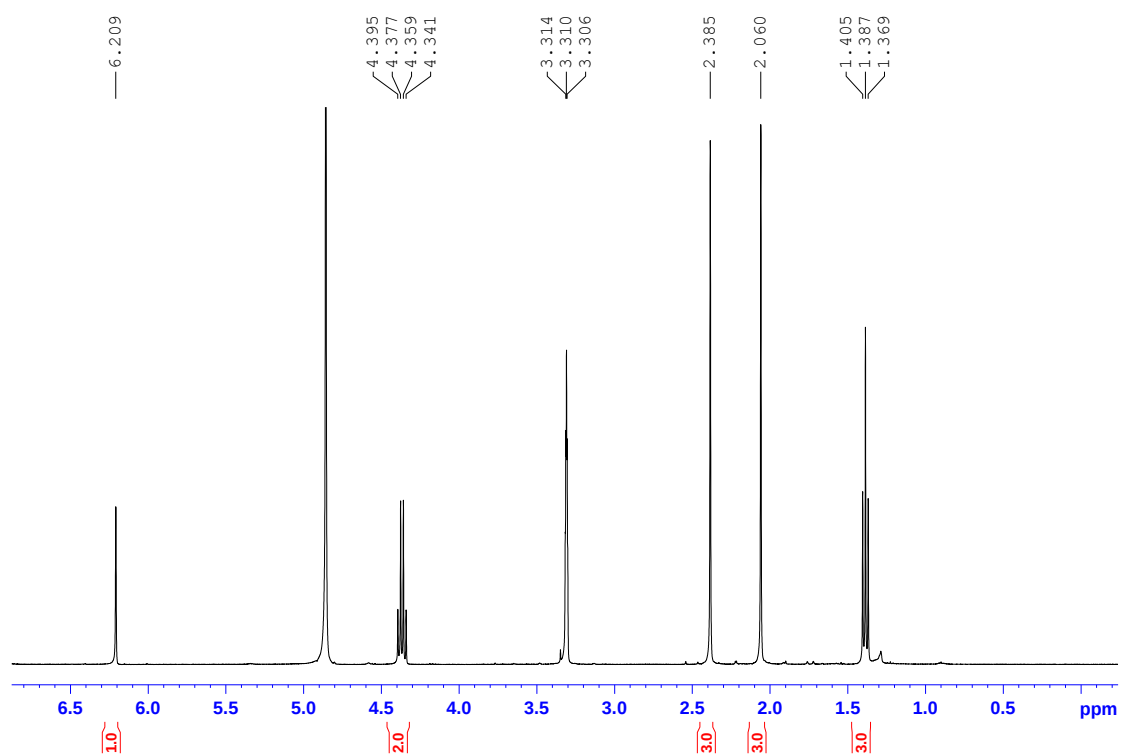


Figure S18: ^1H NMR Spectrum of **5** in CD_3OD (400 MHz)

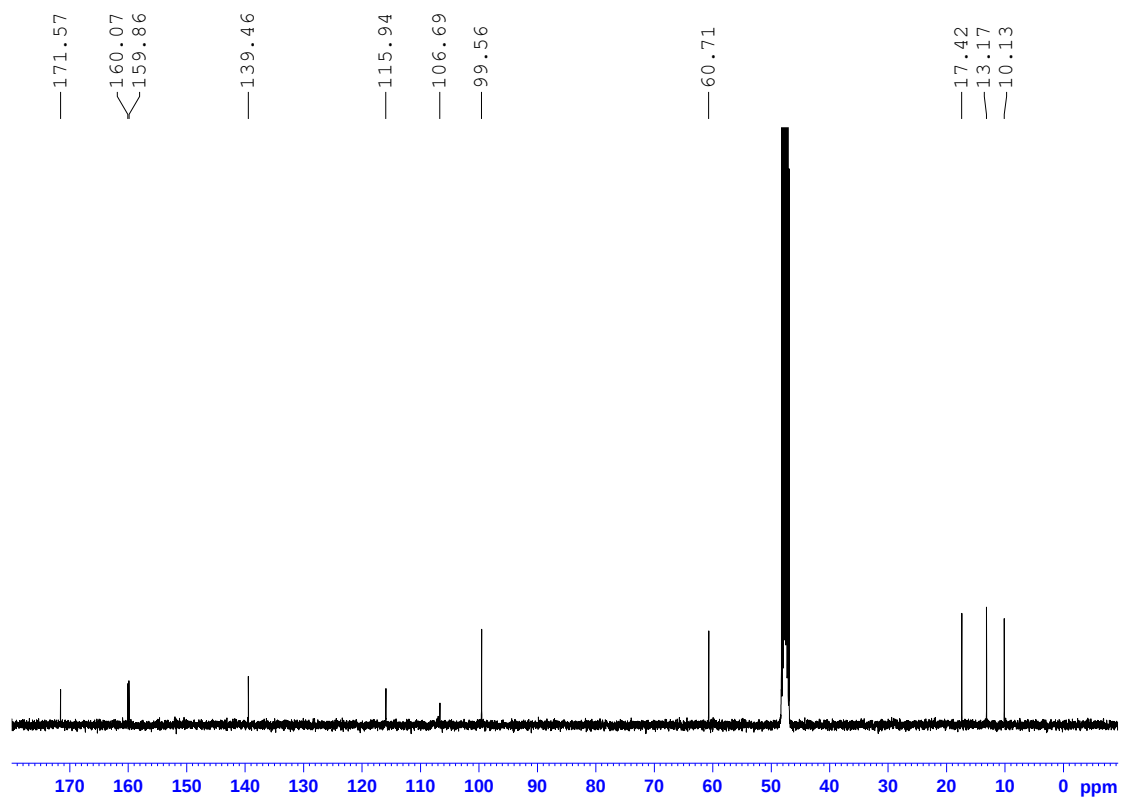


Figure S19: ^{13}C NMR Spectrum of **5** in CD_3OD (100 MHz)

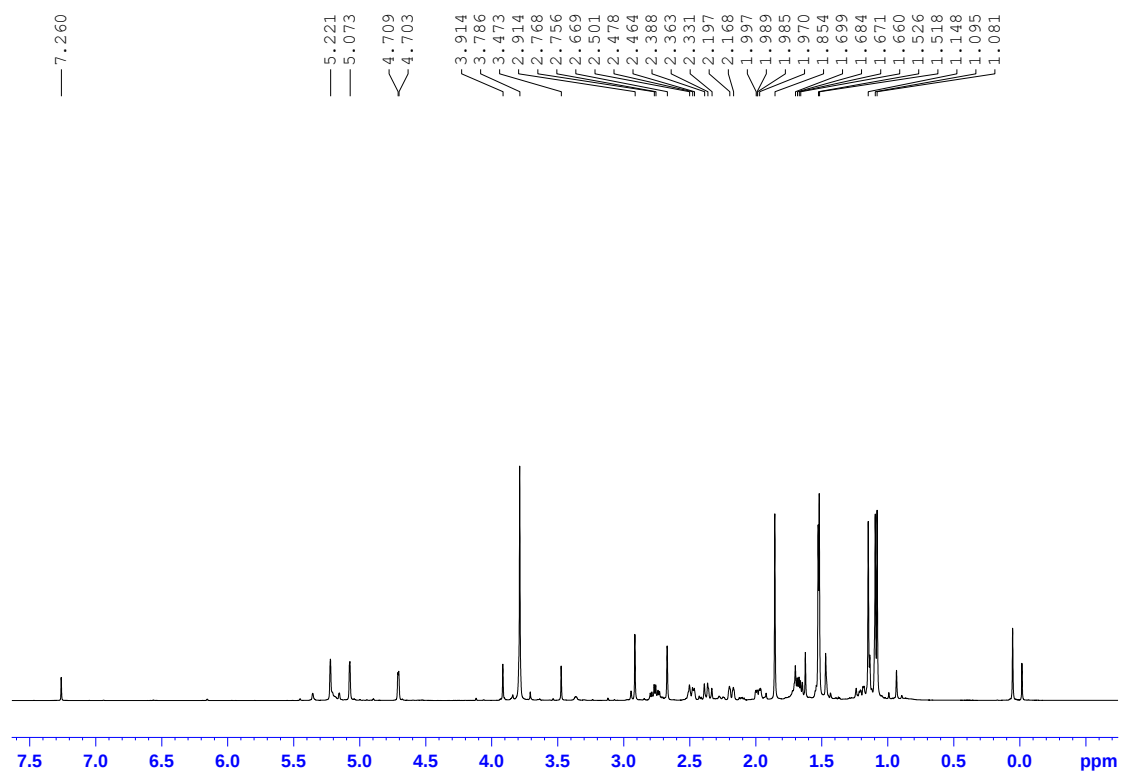
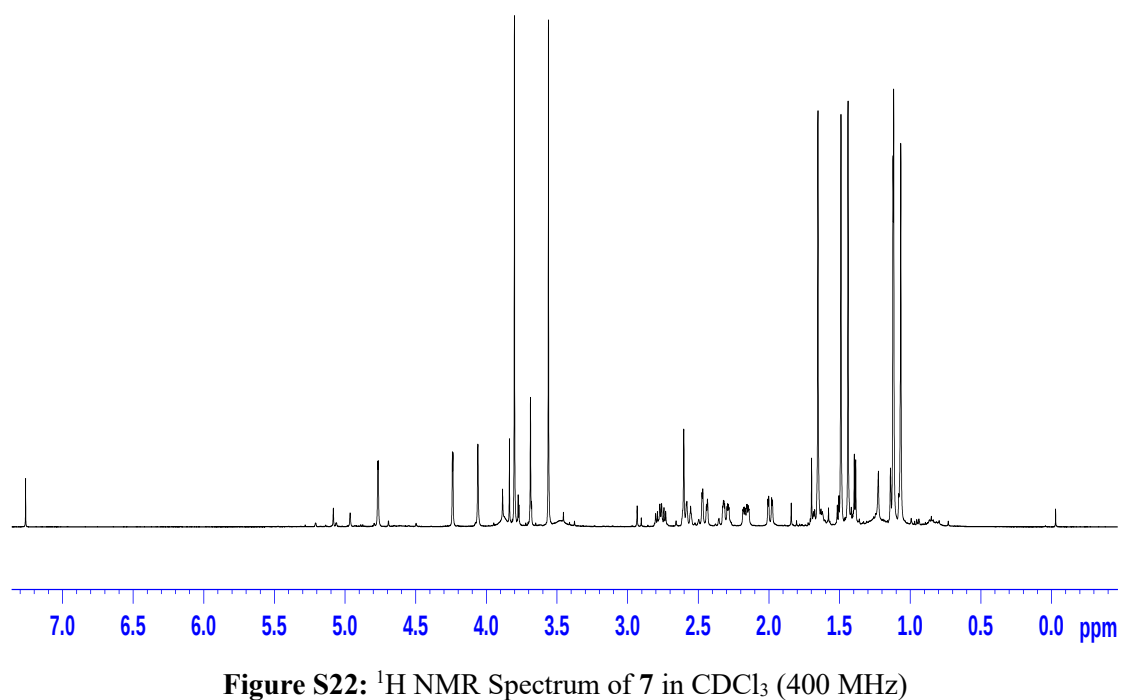
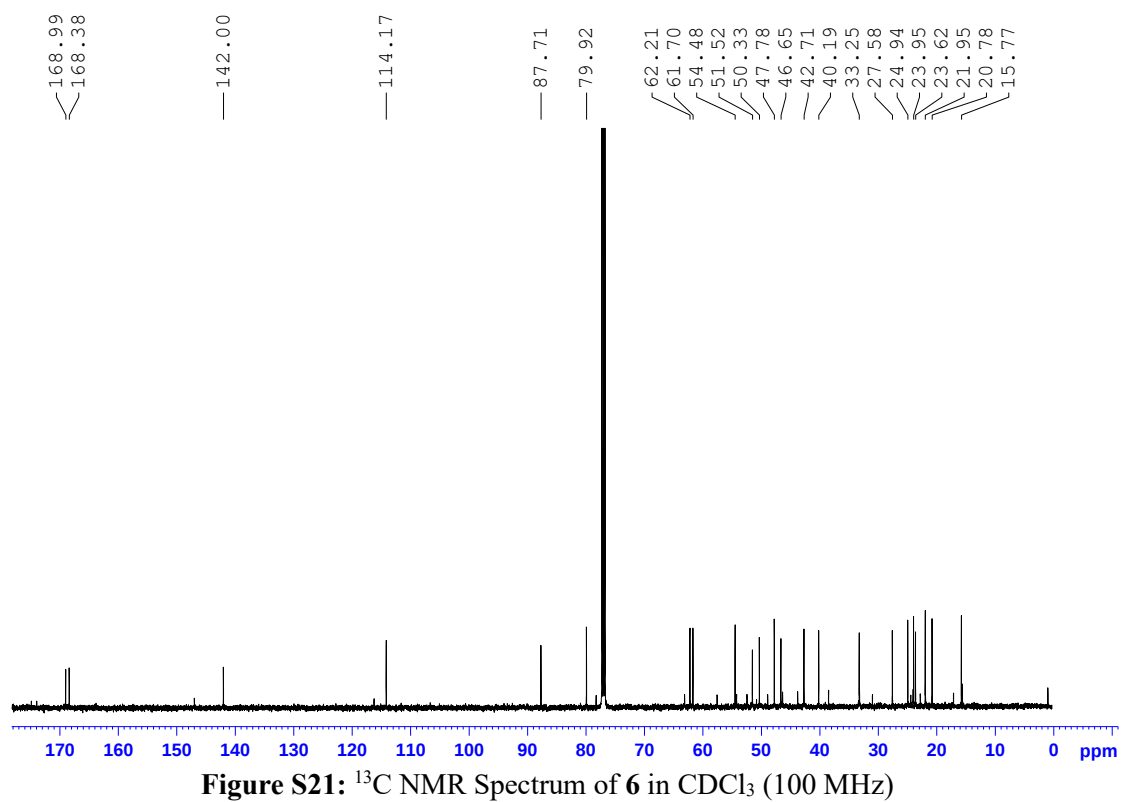


Figure S20: ^1H NMR Spectrum of **6** in CDCl_3 (400 MHz)



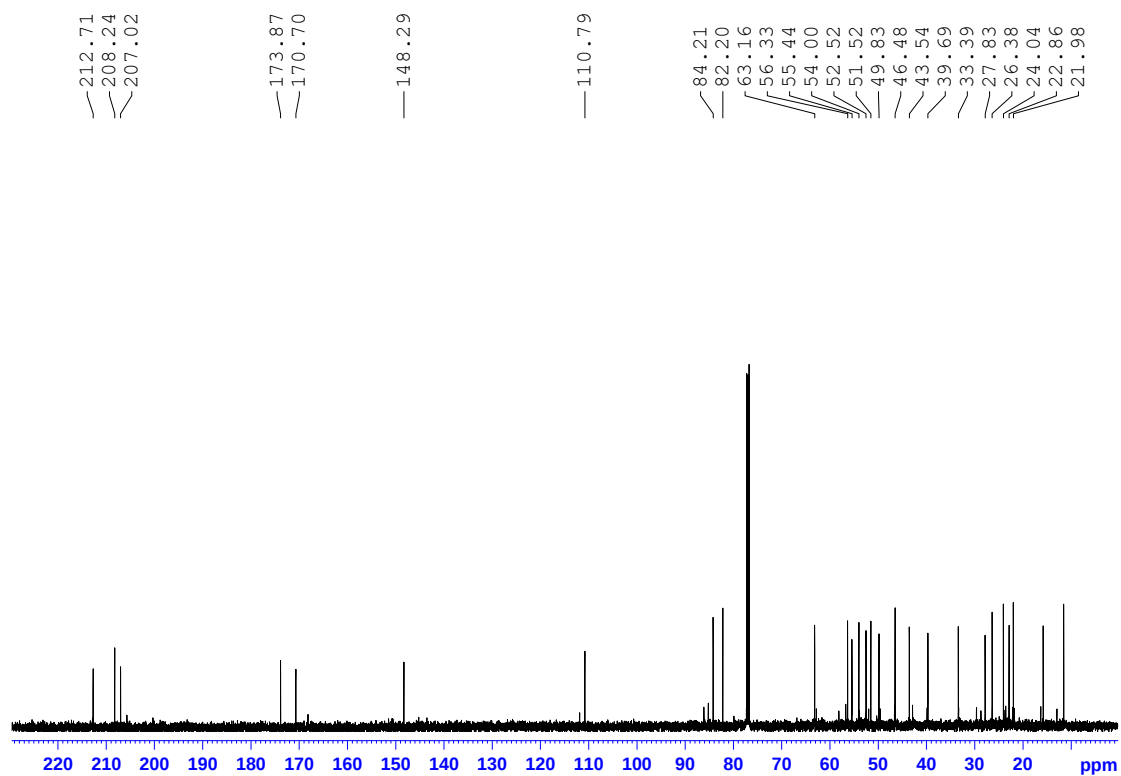


Figure S23: ^{13}C NMR Spectrum of **7** in CDCl_3 (100 MHz)

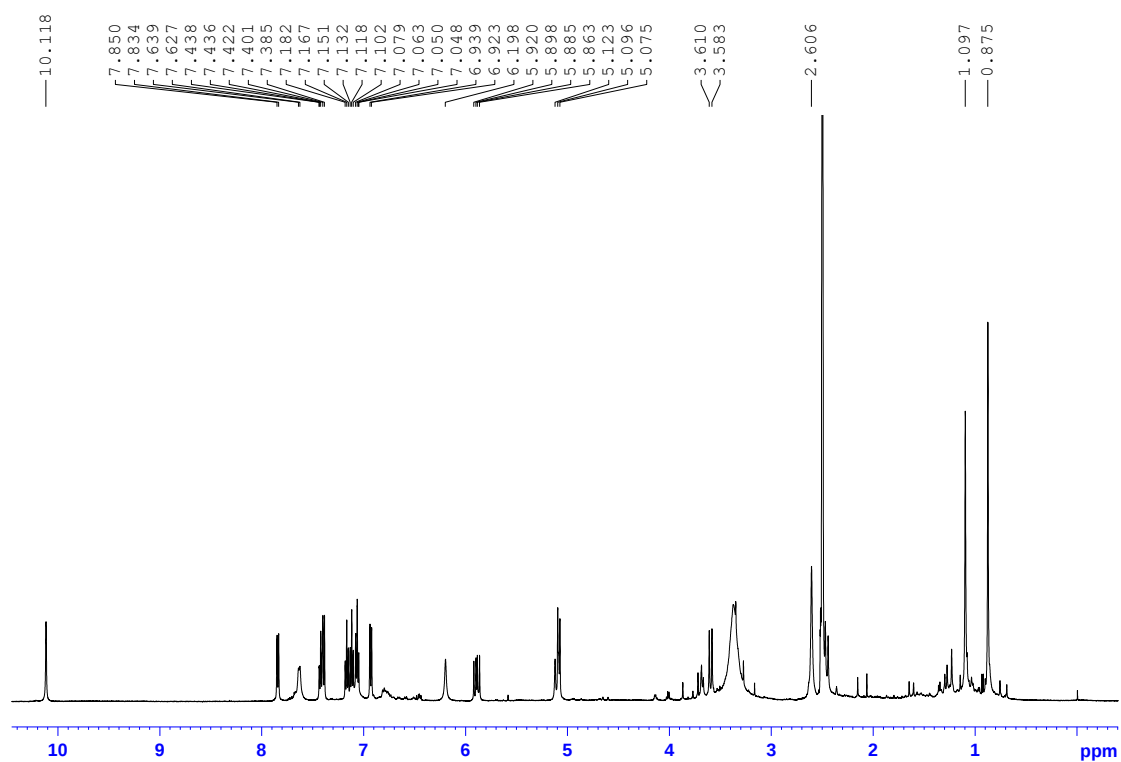


Figure S24: ^1H NMR Spectrum of **8** in CD_3OD (400 MHz)

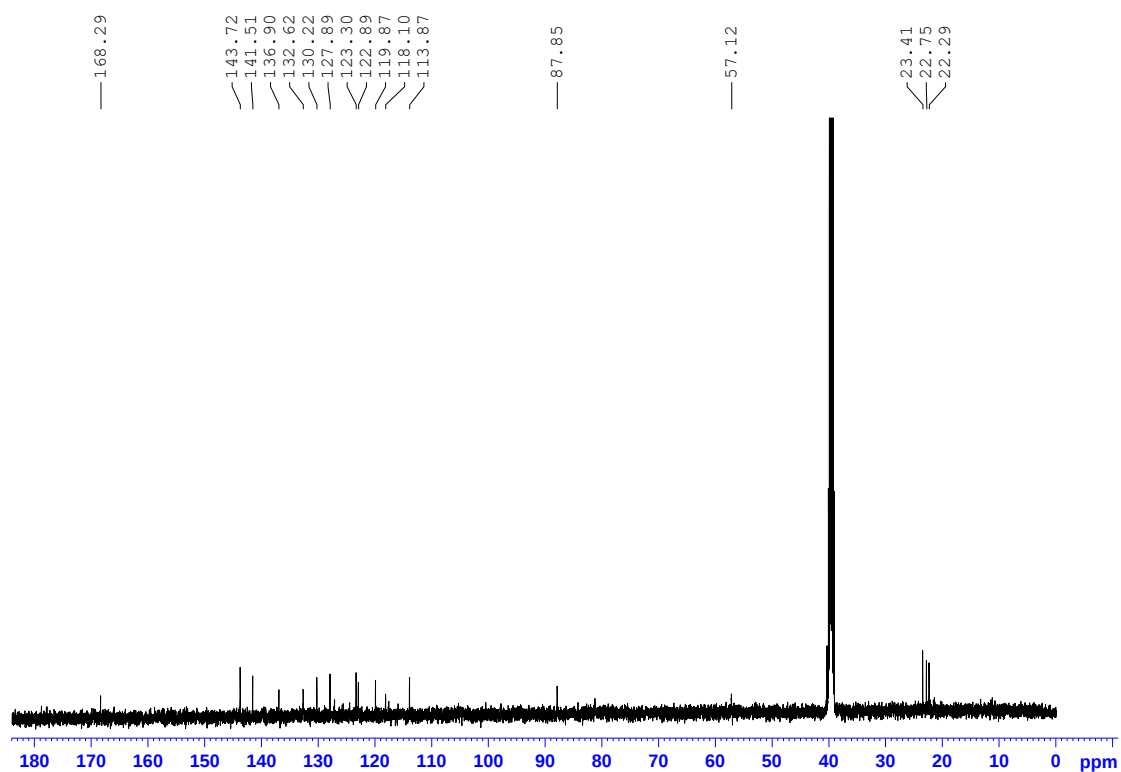


Figure S25: ^{13}C NMR Spectrum of **8** in CD_3OD (100 MHz)

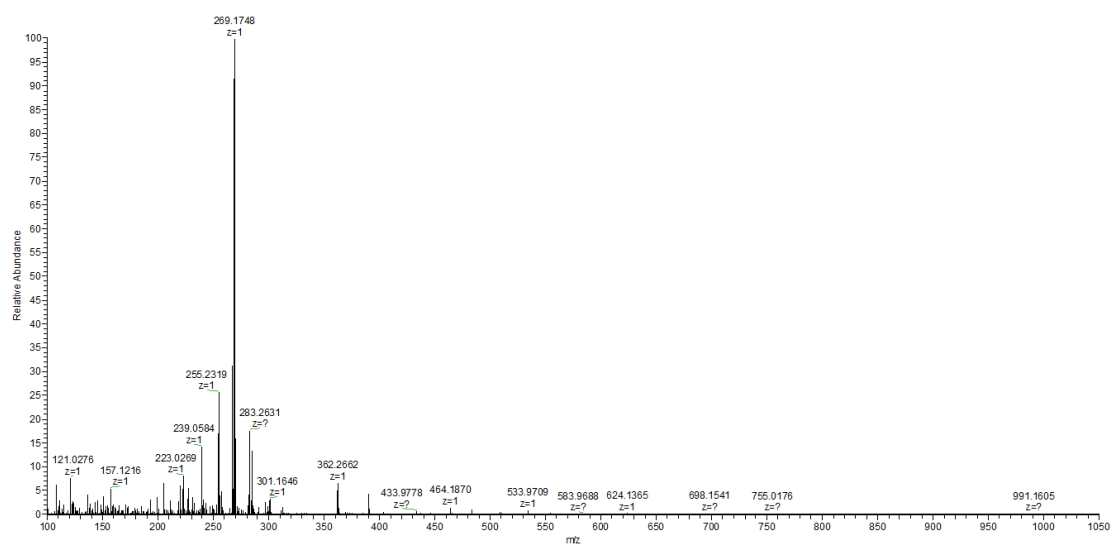


Figure S26: HRESIMS Spectrum of **1**

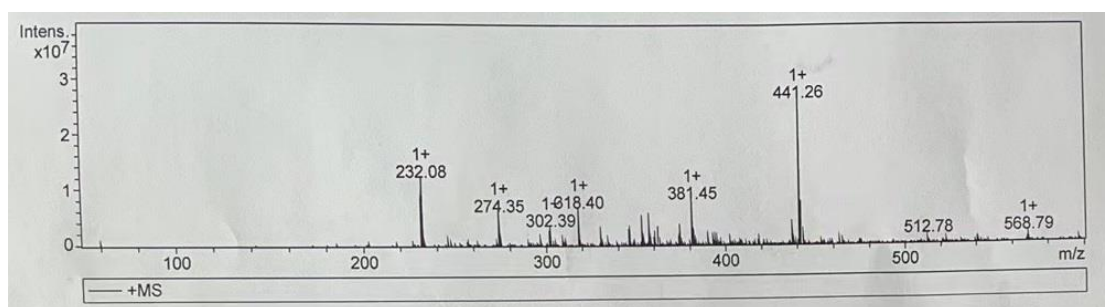
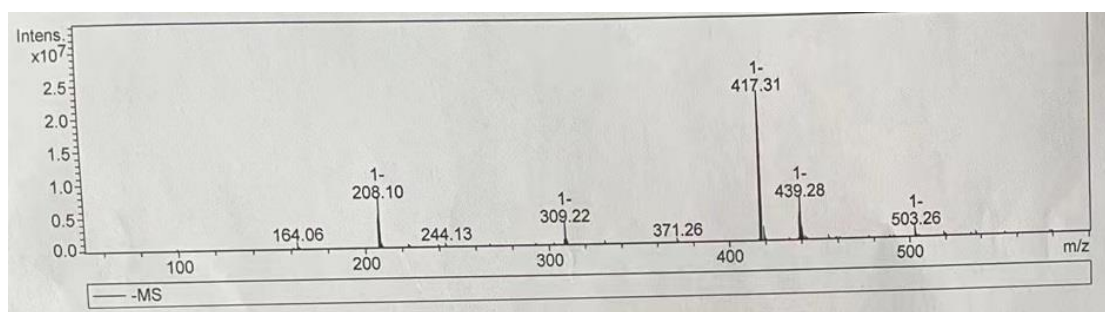


Figure S27: ESIMS Spectrum of 2

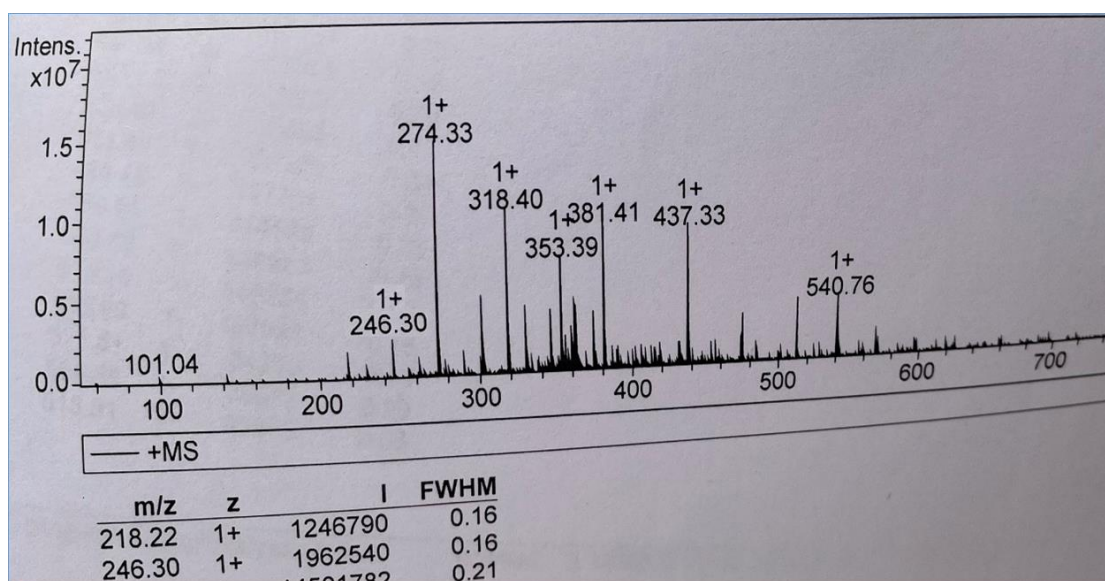


Figure S28: ESIMS Spectrum of 3

REFERENCES

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

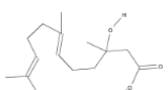
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:



Click image to change structure or view detail.
Import CXF
Search
Advanced Search

Search Type:

☐ Exact Structure
☐ Substructure
☒ Similarity

☐ Show precision analysis

ChemDraw

Launch a SciFinder/SciFinder[®] substance or reaction search directly from the latest version of ChemDraw. [Learn More](#)

Chemical Structure similarity

SUBSTANCES

Select All Deselect All

0 of 8 Similarity Candidates Selected

≥ 99 (most similar)

95-98

90-94

85-89

80-84

75-79

70-74

65-69

0-64 (least similar)

0

1

8

115

1226

7499

16873

23275

69140

Get Substances

Chemical Structure similarity > substances (9) > 107058-67-3 > get references (3)

SUBSTANCES

Get References
Get Reactions
Get Commercial Sources
Tools

Create Keep Me Posted Alert
Send to SciPlanner
Display Options

Analyze Refine

Analyze by:

Substance Role

Preparation

Biological Study

Reactant or Reagent

Uses

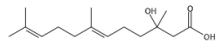
Show More

Sort by: Similarity Score

0 of 9 Substances Selected

Score: 98

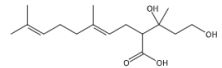
1. 107058-67-3



$C_{15}H_{26}O_3$
6,10-Dodecadienoic acid, 3-hydroxy-3,7,11-trimethyl-
Key Physical Properties

Score: 94

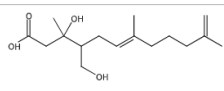
2. 101726-17-4



$C_{16}H_{28}O_4$
4,8-Dodecadienoic acid, 2-(1,3-dihydroxy-1-methylpropyl)-5,9-dimethyl- (6CI)
Key Physical Properties

Score: 94

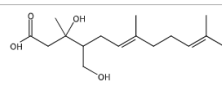
3. 107525-30-4



$C_{16}H_{28}O_4$
6,11-Dodecadienoic acid, 3-hydroxy-4-(hydroxymethyl)-3,7,11-trimethyl- (6CI)
Key Physical Properties

Score: 94

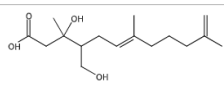
4. 860439-79-8



$C_{16}H_{28}O_4$
Mevalonic acid, 4-geranyl- (6CI)
Key Physical Properties

Score: 91

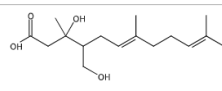
5. 53042-57-2



$C_{15}H_{26}O_3$
6,10-Dodecadienoic acid, 3-hydroxy-3,7,11-trimethyl-
Key Physical Properties

Score: 91

6. 53042-58-3



$C_{15}H_{26}O_3$
6,10-Dodecadienoic acid, 3-hydroxy-3,7,11-trimethyl-
Key Physical Properties

Figure S29: Scifinder similarity report for compound 1

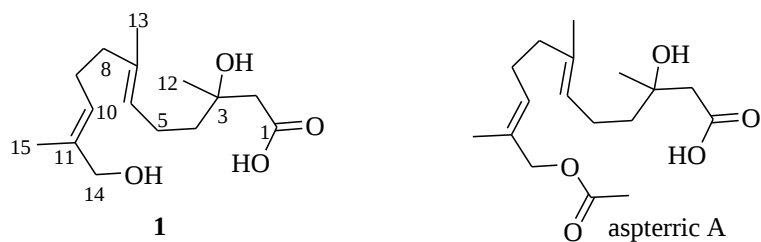


Table S1: ^1H and ^{13}C NMR Data of **1** and the analog Aspterric A in Methanol- d_4 .^a

No.	1		aspterric A	
	δ_{H}	δ_{C}	δ_{H}	δ_{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

^a ^1H NMR recorded at 400 MHz, ^{13}C NMR recorded at 100 MHz.