

Supporting Information

Rec. Nat. Prod. 17:4 (2023) 671-677

Penicisepene, A New Sesquiterpenoid from the Fungus

Penicillium sp. LPFH-Q3

Linlin Qiu*, Jingmin Wu, and Yanli Zhou

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

Table of Contents	Page
Figure S1: ¹ H NMR Spectrum of 1 in CDCl ₃ (400 MHz)	2
Figure S2: ¹³ C NMR Spectrum of 1 in CDCl ₃ (100 MHz)	2
Figure S3: HSQC Spectrum of 1 in CDCl ₃	3
Figure S4: HMBC Spectrum of 1 in CDCl ₃	3
Figure S5: ¹ H- ¹ H COSY Spectrum of compound 1 in CDCl ₃	4
Figure S6: NOESY spectrum of compound 1 in CDCl ₃	4
Figure S7: ¹ H NMR Spectrum of 2 in DMSO- <i>d</i> ₄ (400 MHz)	5
Figure S8: ¹³ C NMR Spectrum of 2 in DMSO- <i>d</i> ₄ (100 MHz)	5
Figure S9: ¹ H NMR Spectrum of 3 in CD ₃ OD (400 MHz)	6
Figure S10: ¹³ C NMR Spectrum of 3 in CD ₃ OD (100 MHz)	6
Figure S11: ¹ H NMR Spectrum of 4 in CD ₃ OD (400 MHz)	7
Figure S12: ¹³ C NMR Spectrum of 4 in CD ₃ OD (100 MHz)	7
Figure S13: ¹ H NMR Spectrum of 5 in DMSO- <i>d</i> ₆ (400 MHz)	8
Figure S14: ¹³ C NMR Spectrum of 5 in DMSO- <i>d</i> ₆ (100 MHz)	8
Figure S15: ¹ H NMR Spectrum of 6 in DMSO- <i>d</i> ₆ (400 MHz)	9
Figure S16: ¹³ C NMR Spectrum of 6 in DMSO- <i>d</i> ₆ (100 MHz)	9
Figure S17: ¹ H NMR Spectrum of 7 in CD ₃ OD (400 MHz)	10
Figure S18: ¹³ C NMR Spectrum of 7 in CD ₃ OD (100 MHz)	10
Figure S19: ¹ H NMR Spectrum of 8 in CD ₃ OD (400 MHz)	11
Figure S20: HRESIMS Spectrum of 1	12
Figure S21: Scifinder similarity report for compound 1	12
Table S1: Comparisons of NMR data of penicisepene (1) and acremeremophilane B	

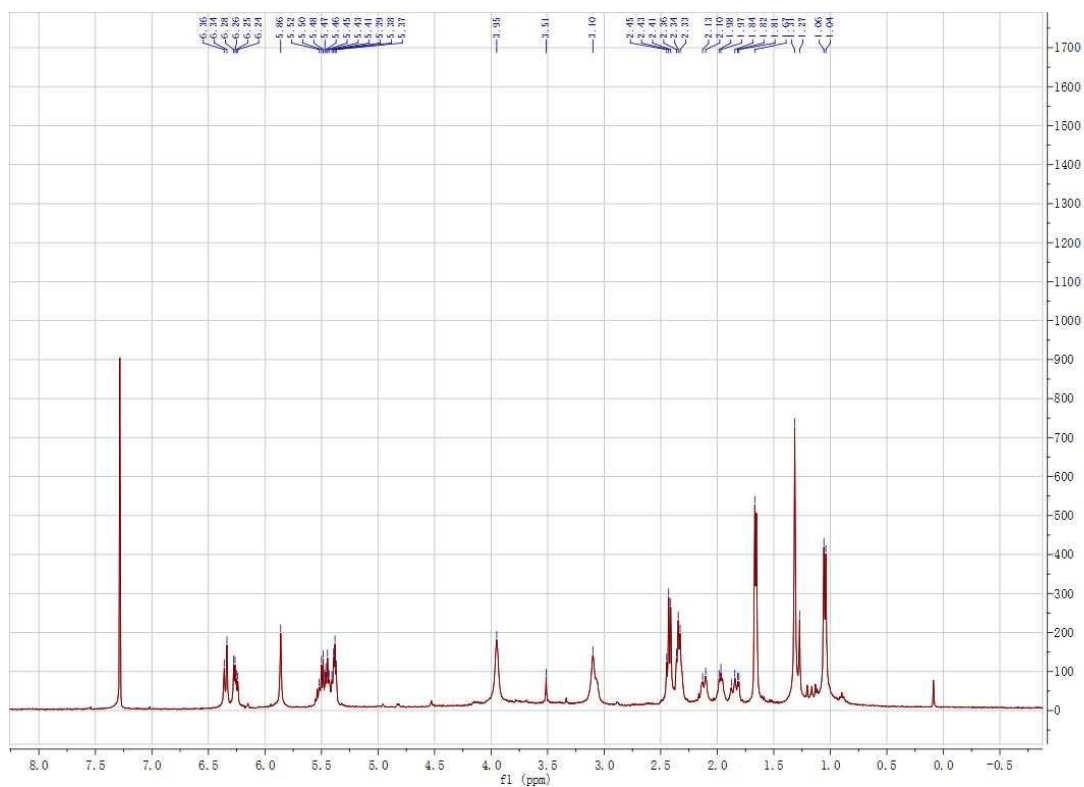


Figure S1: ^1H NMR Spectrum of **1** in CDCl_3 (400 MHz)

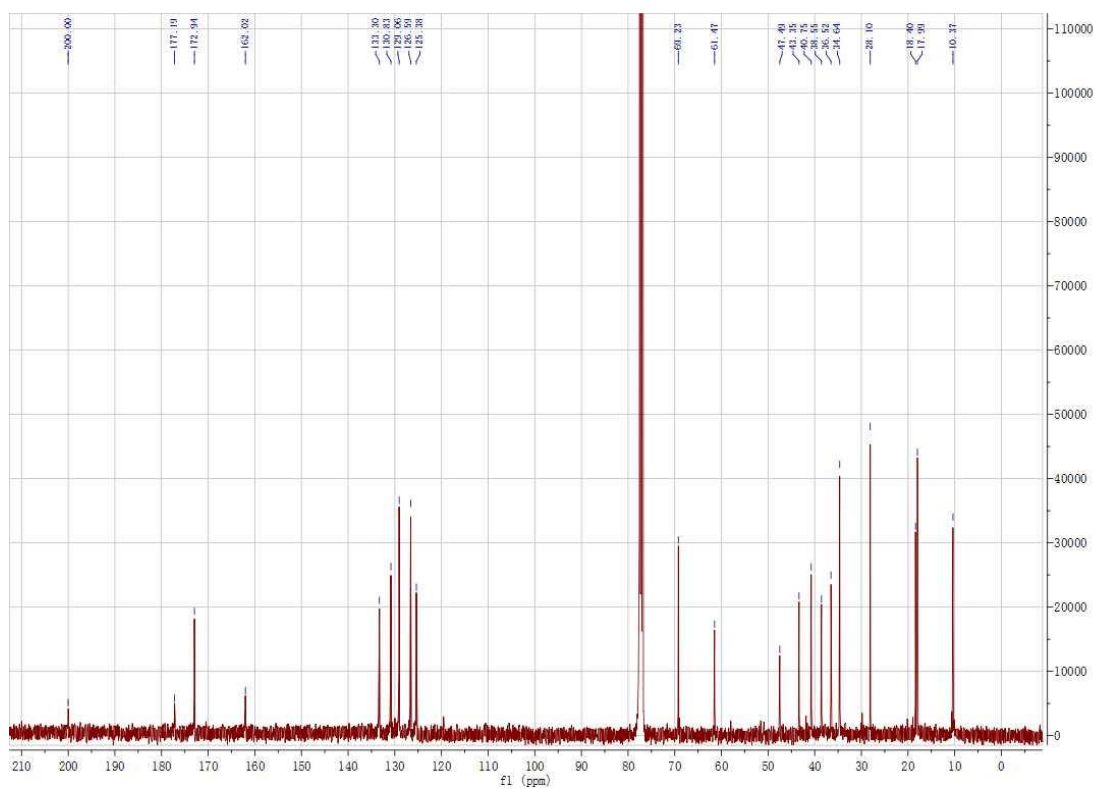


Figure S2: ^{13}C NMR Spectrum of **1** in CDCl_3 (100 MHz)

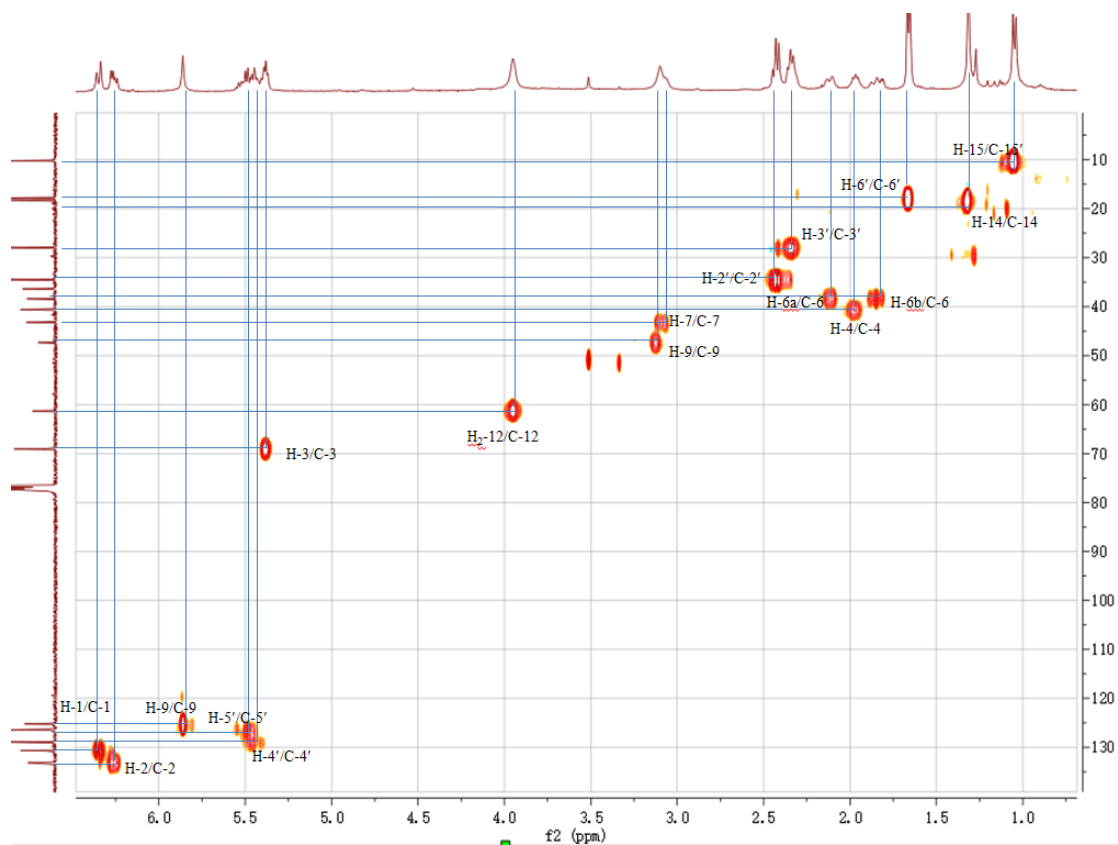


Figure S3: HSQC Spectrum of **1** in CDCl_3

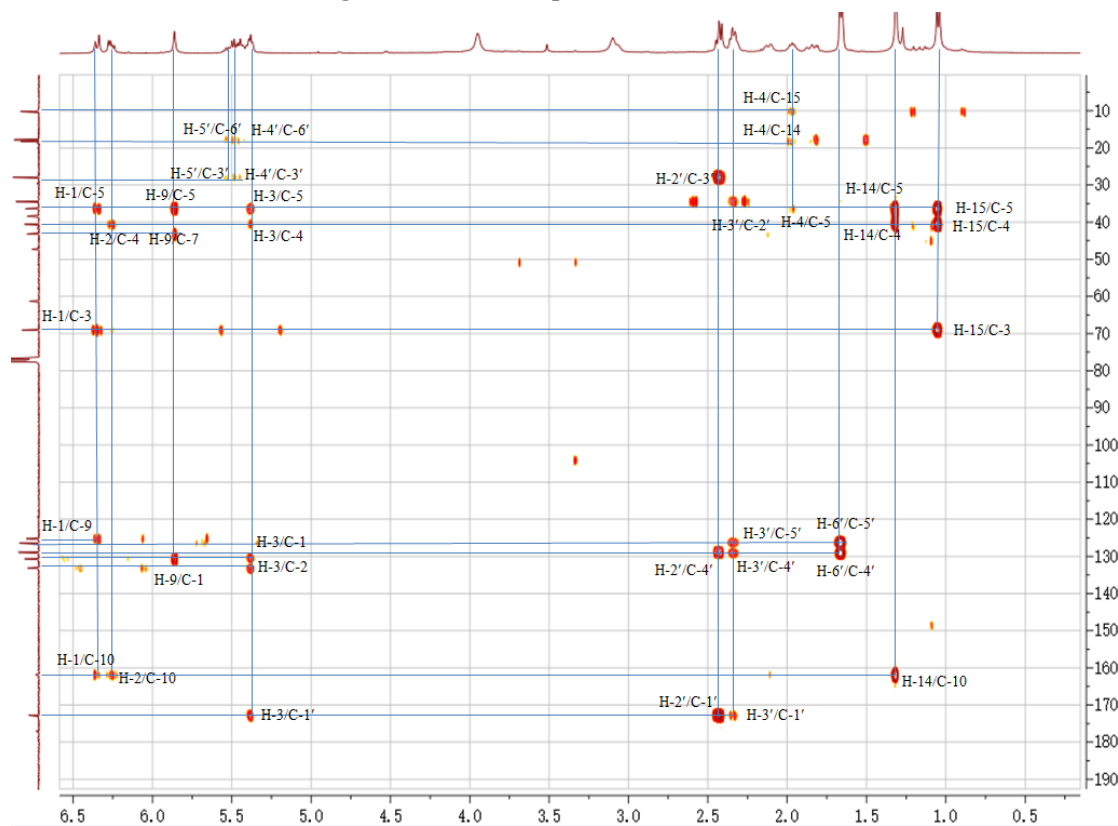


Figure S4: HMBC Spectrum of **1** in CDCl_3

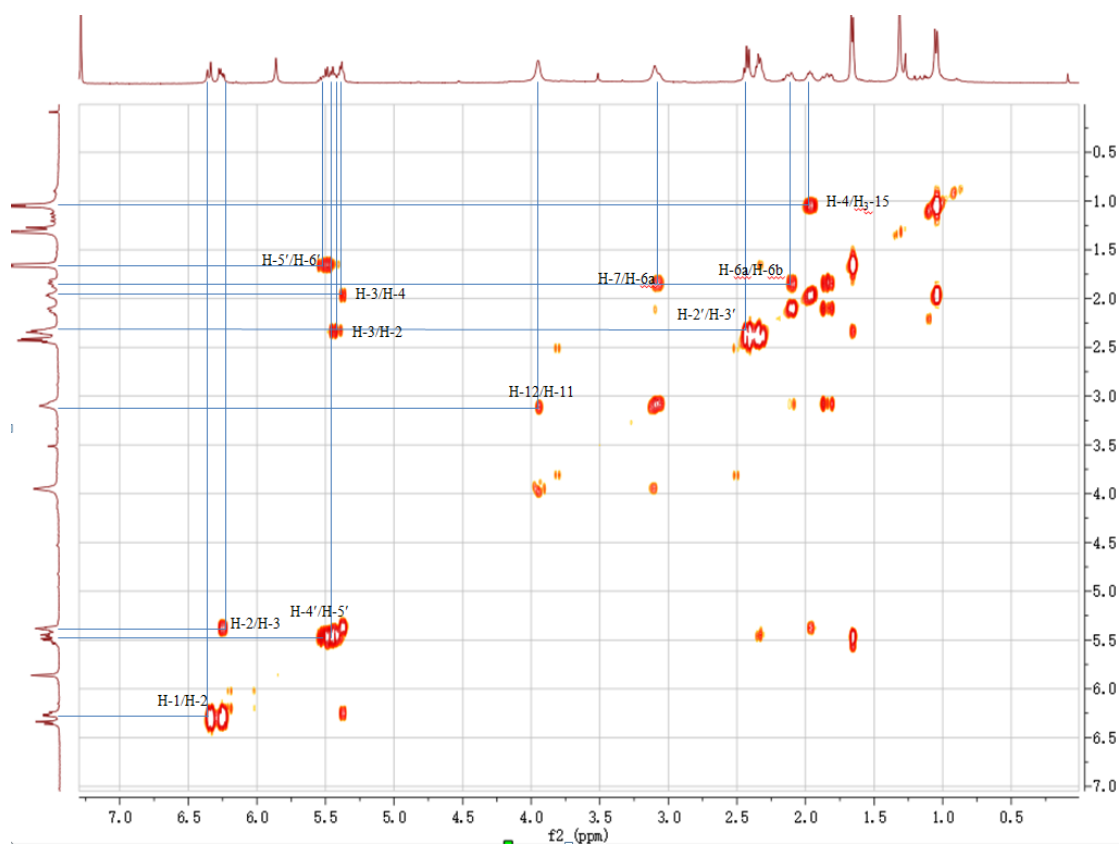


Figure S5: ^1H - ^1H COSY Spectrum of compound **1** in CDCl_3

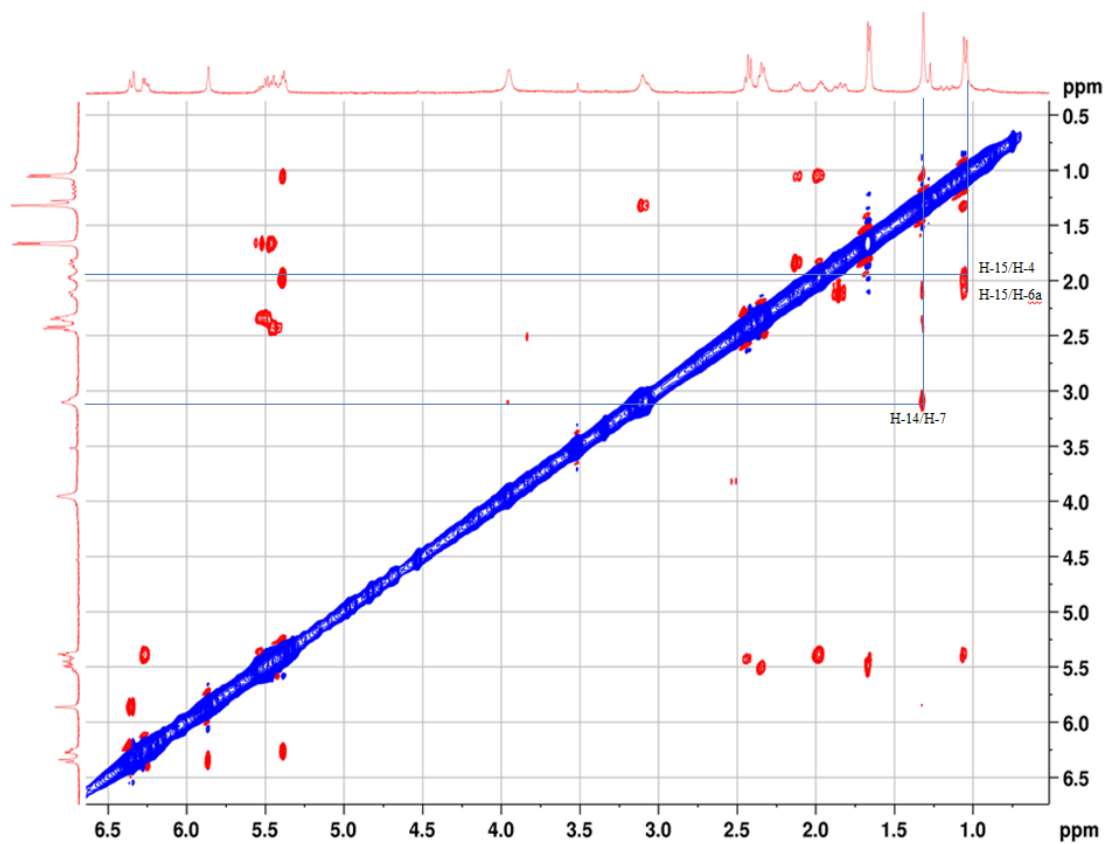


Figure S6: NOESY spectrum of compound **1** in CDCl_3 .

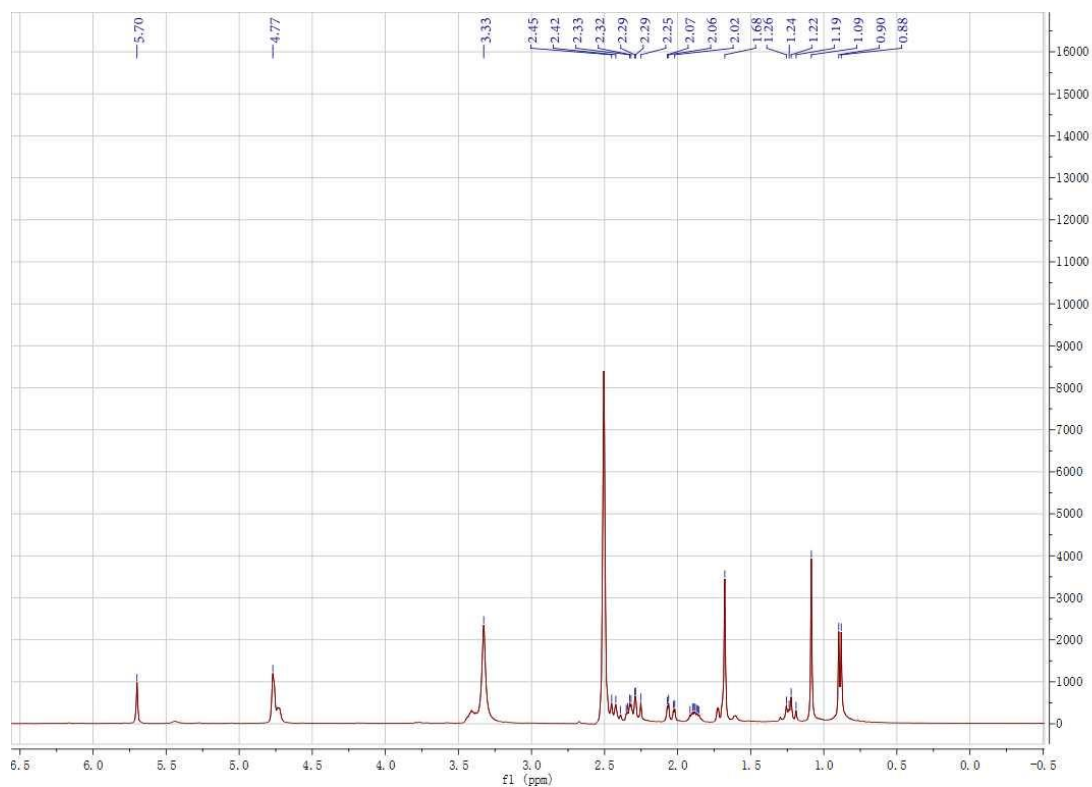


Figure S7: ^1H NMR Spectrum of **2** in $\text{DMSO-}d_4$ (400 MHz)

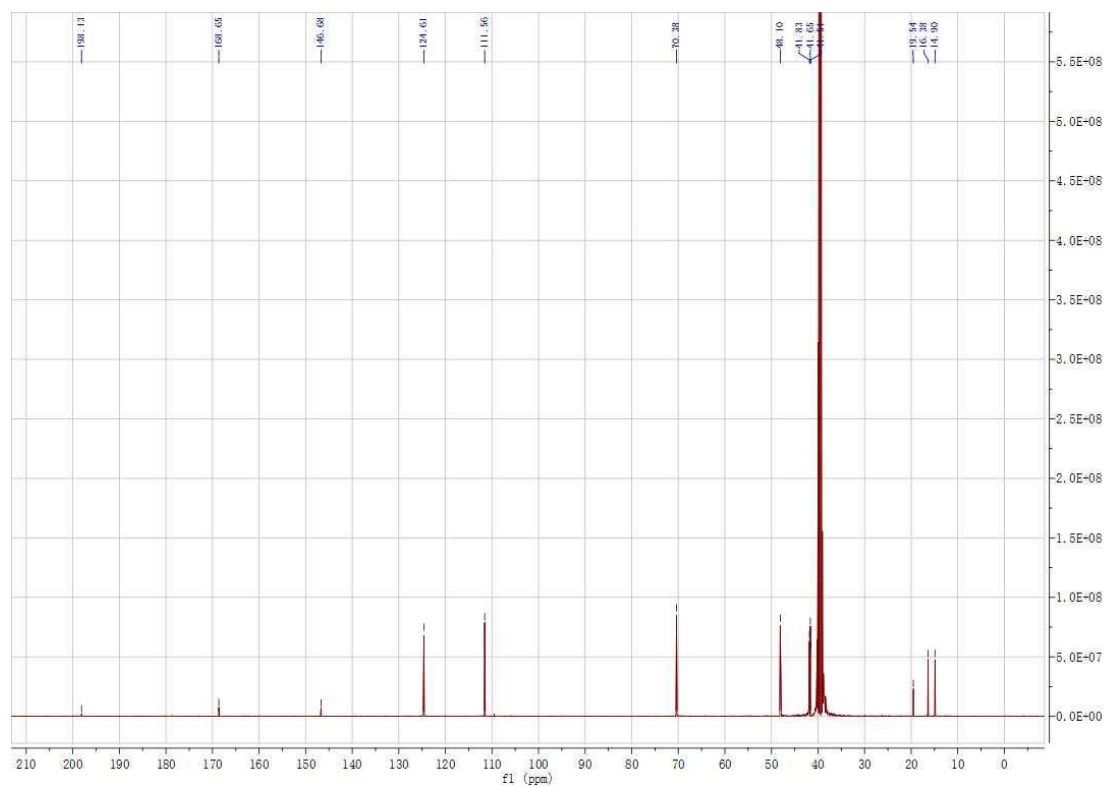


Figure S8: ^{13}C NMR Spectrum of **2** in $\text{DMSO-}d_4$ (100 MHz)

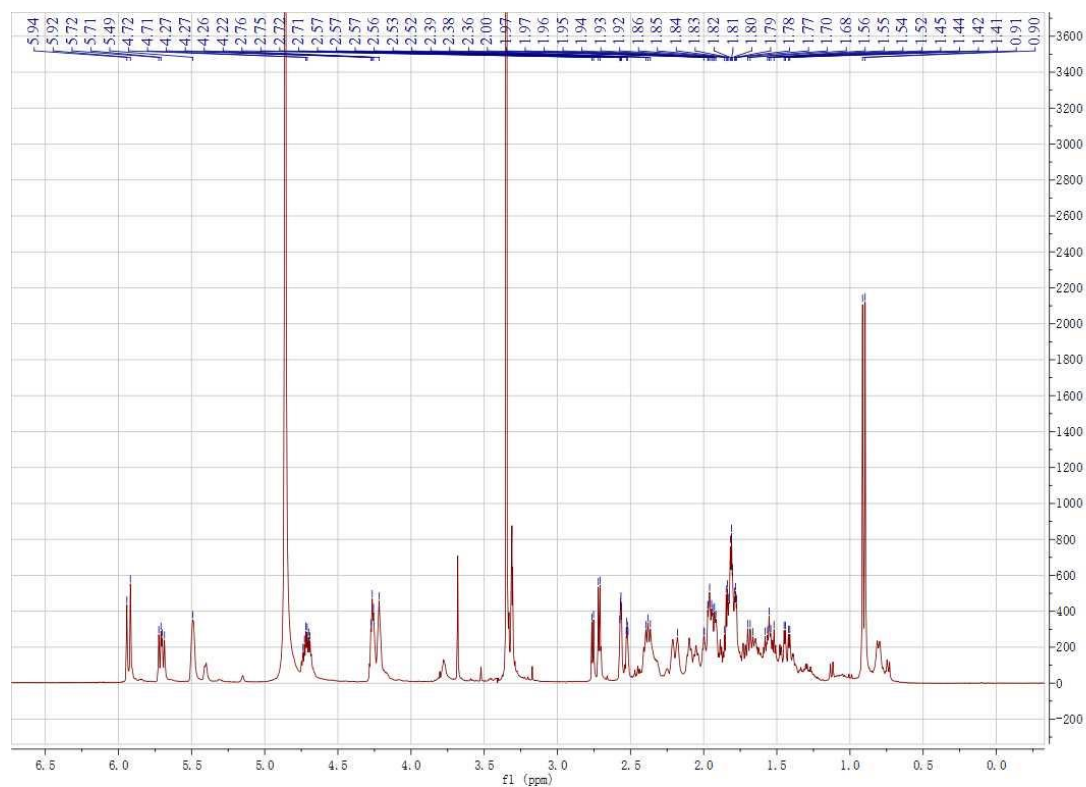


Figure S9: ^1H NMR Spectrum of **3** in CD_3OD (400 MHz)

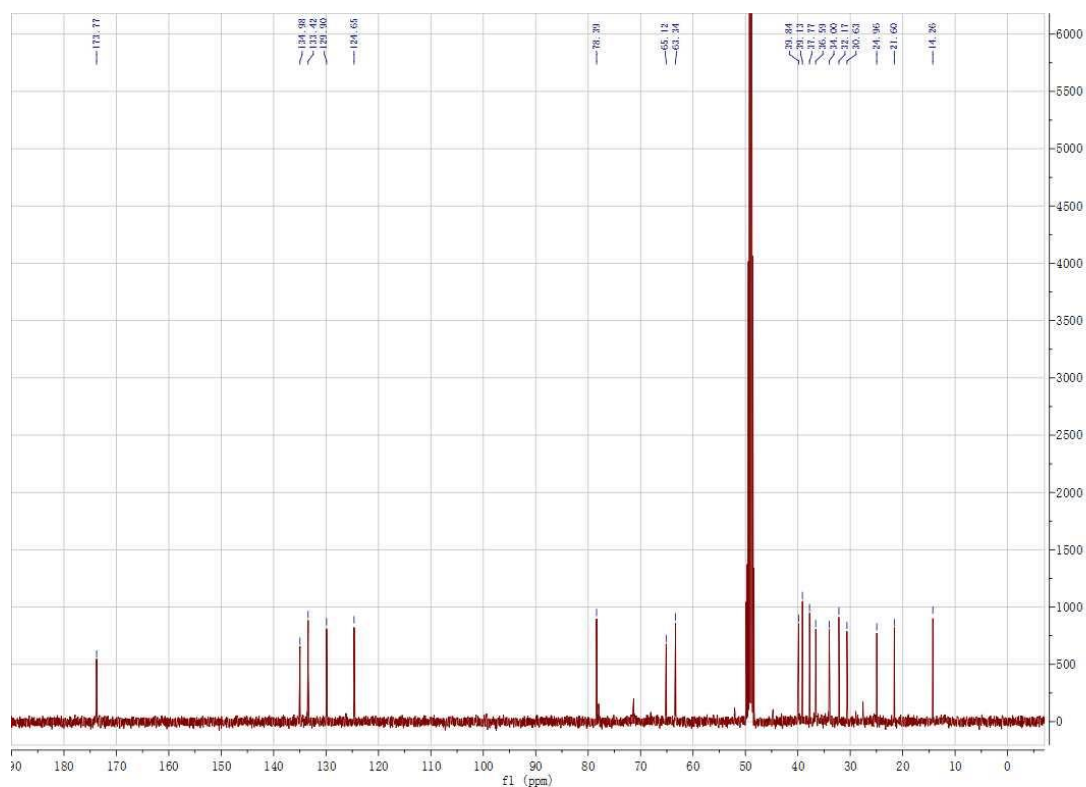


Figure S10: ^{13}C NMR Spectrum of **3** in CD_3OD (100 MHz)

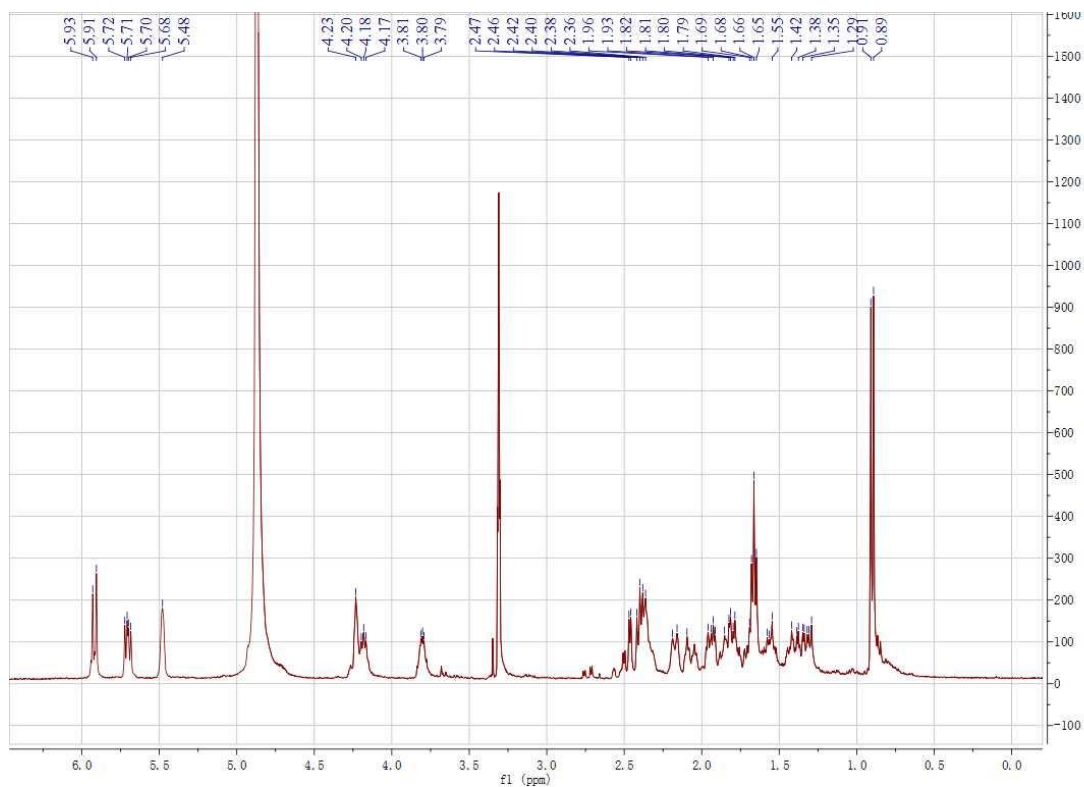


Figure S11: ^1H NMR Spectrum of **4** in CD_3OD (400 MHz)

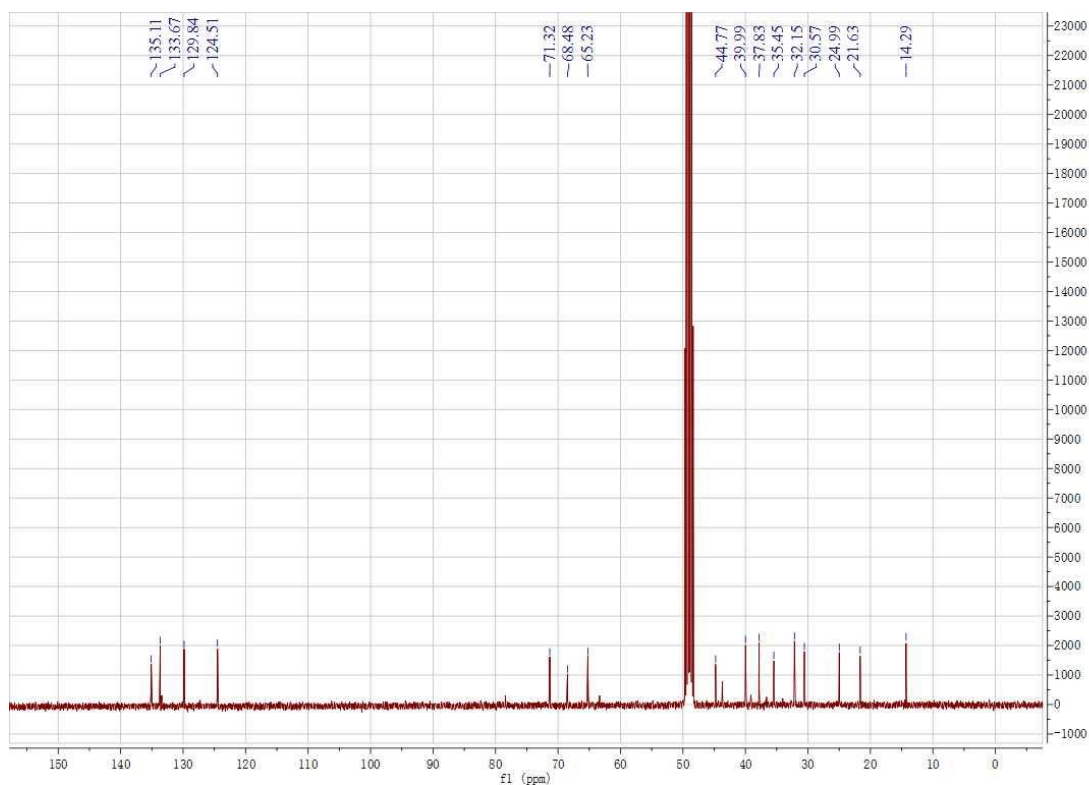


Figure S12: ^{13}C NMR Spectrum of **4** in CD_3OD (100 MHz)

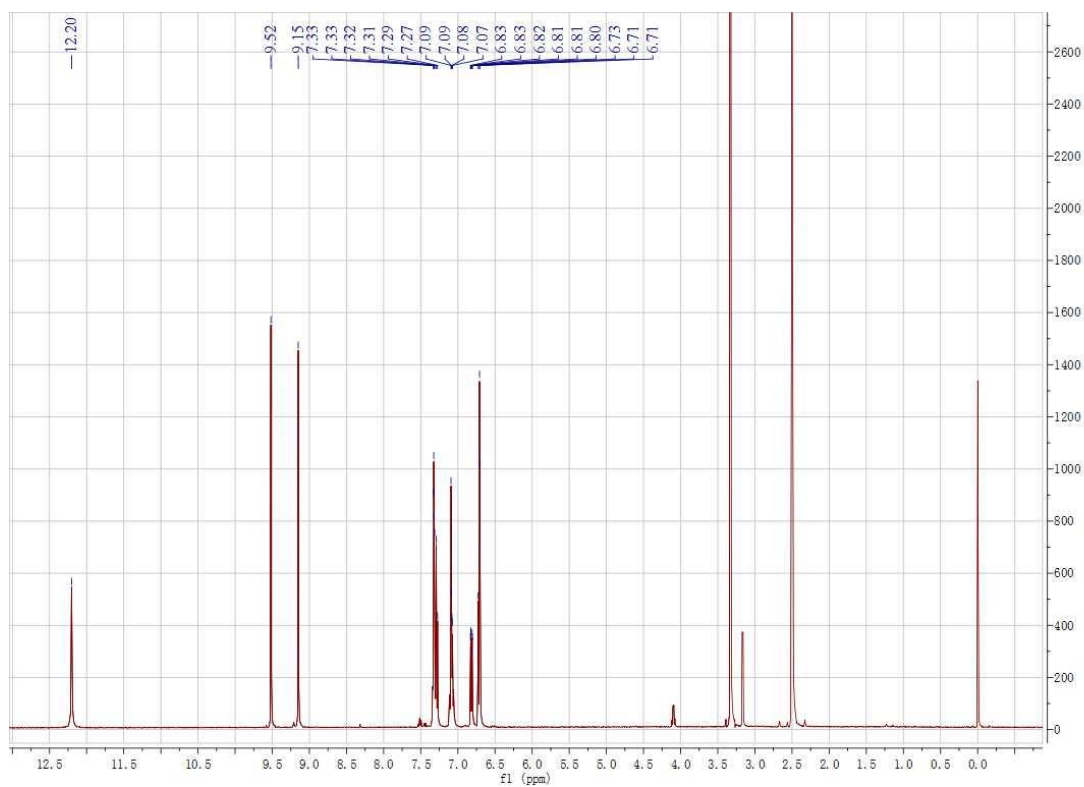


Figure S13: ^1H NMR Spectrum of **5** in $\text{DMSO-}d_6$ (400 MHz)

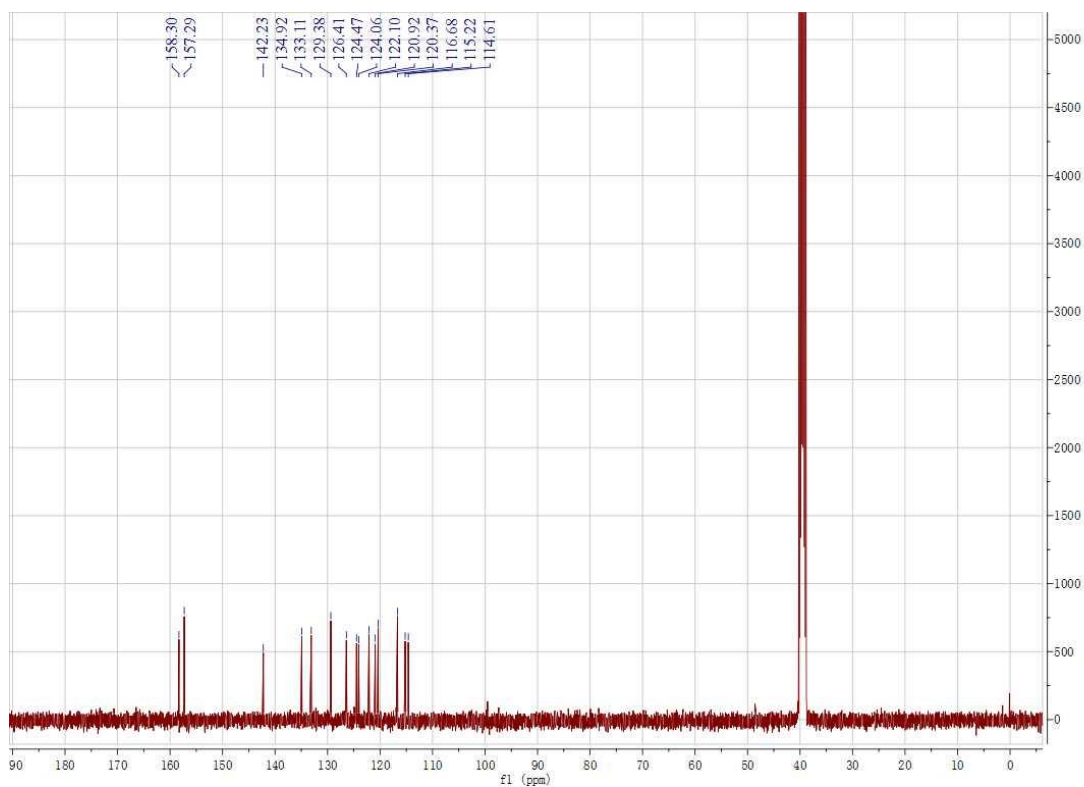


Figure S14: ^{13}C NMR Spectrum of **5** in $\text{DMSO-}d_6$ (100 MHz)

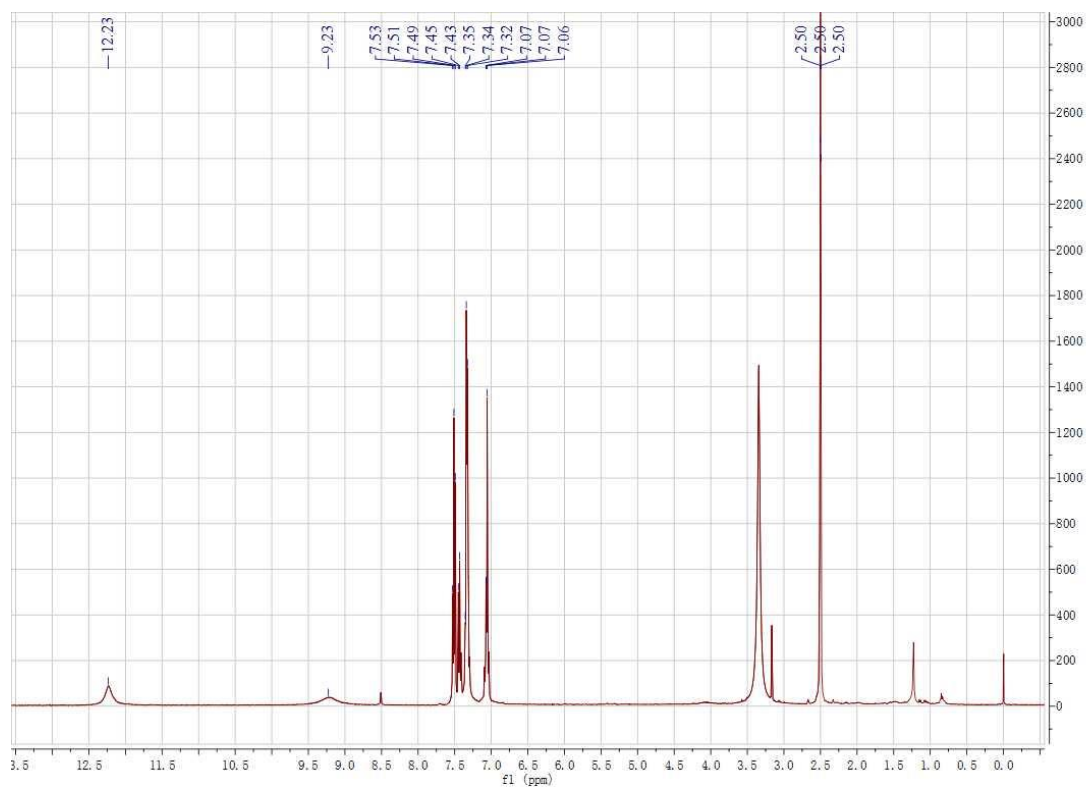


Figure S15: ^1H NMR Spectrum of **6** in $\text{DMSO-}d_6$ (400 MHz)

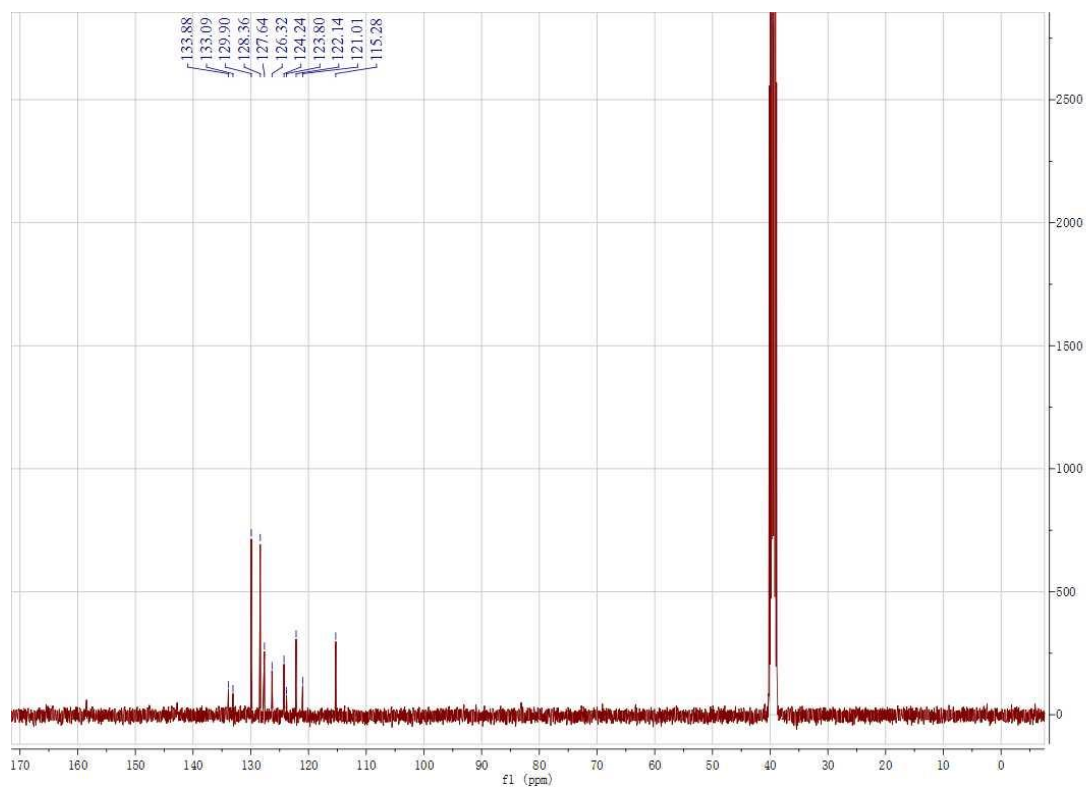


Figure S16: ^{13}C NMR Spectrum of **6** in $\text{DMSO-}d_6$ (100 MHz)

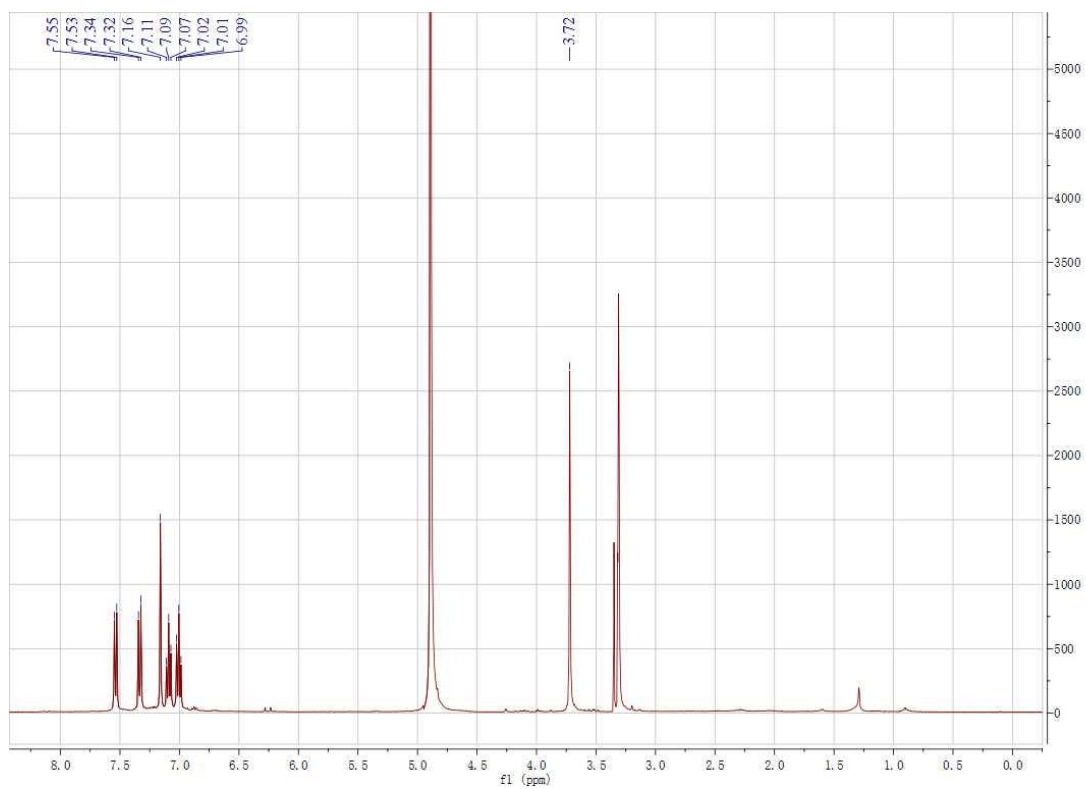


Figure S17: ^1H NMR Spectrum of **7** in CD_3OD (400 MHz)

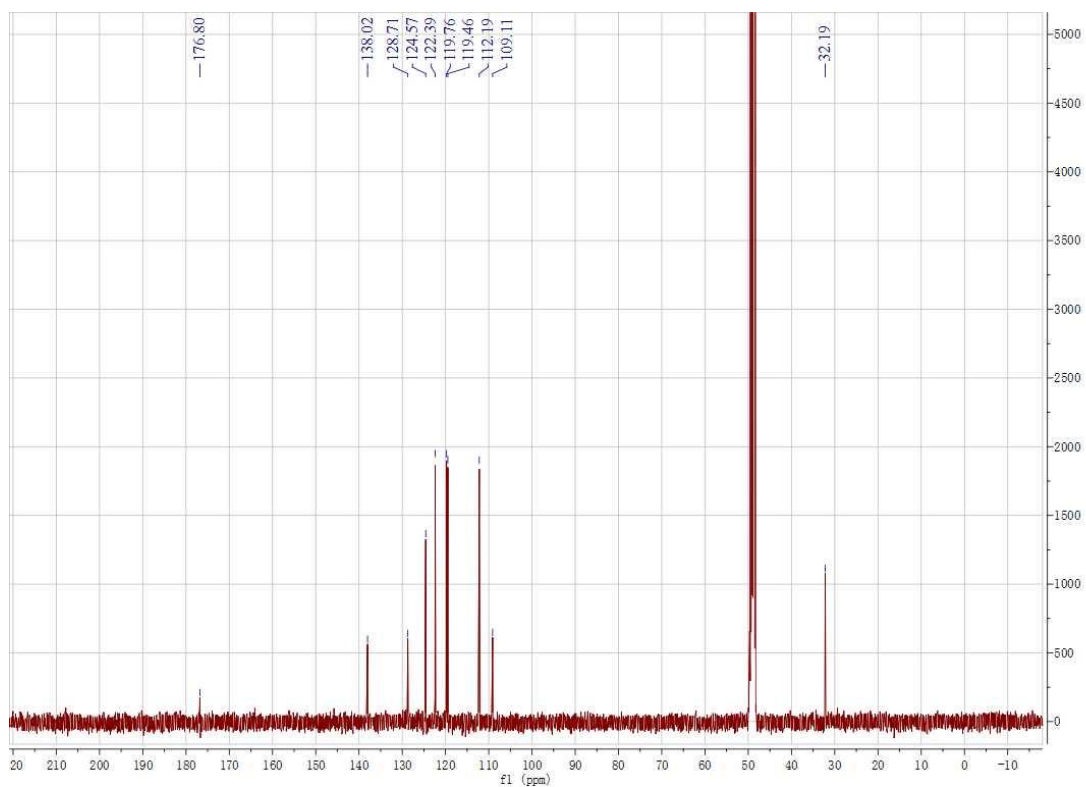


Figure S18: ^{13}C NMR Spectrum of **7** in CD_3OD (100 MHz)

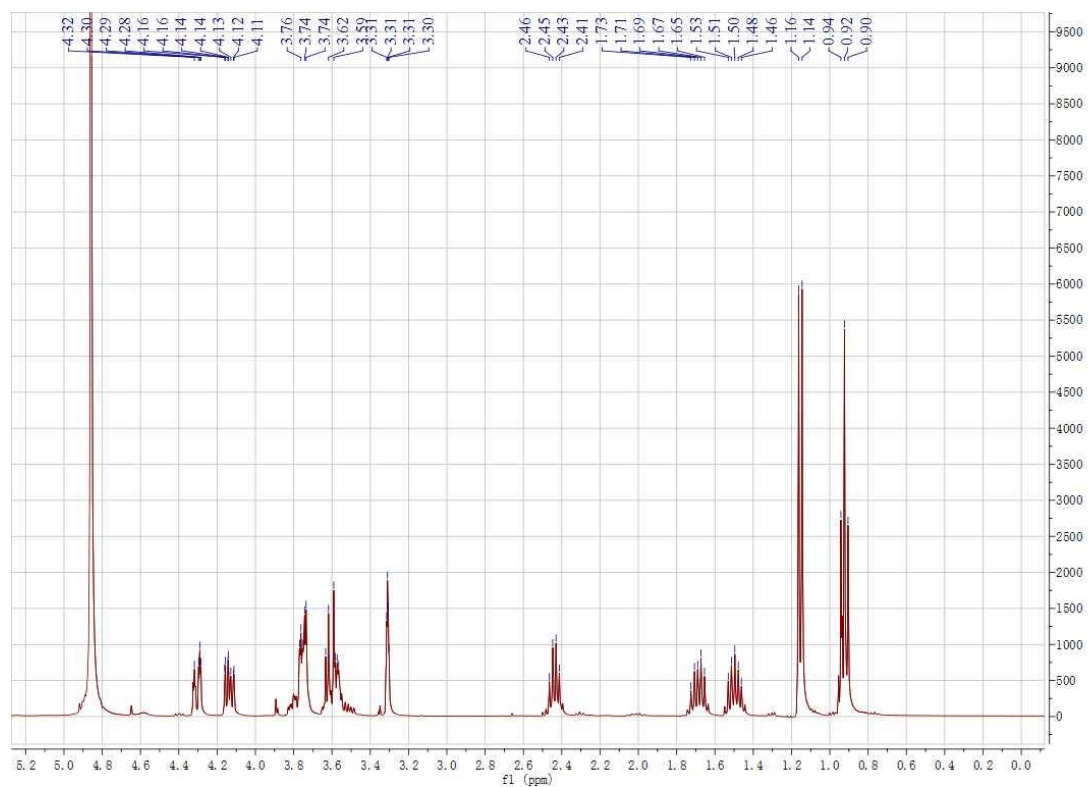


Figure S19: ^1H NMR Spectrum of **8** in CD_3OD (400 MHz)

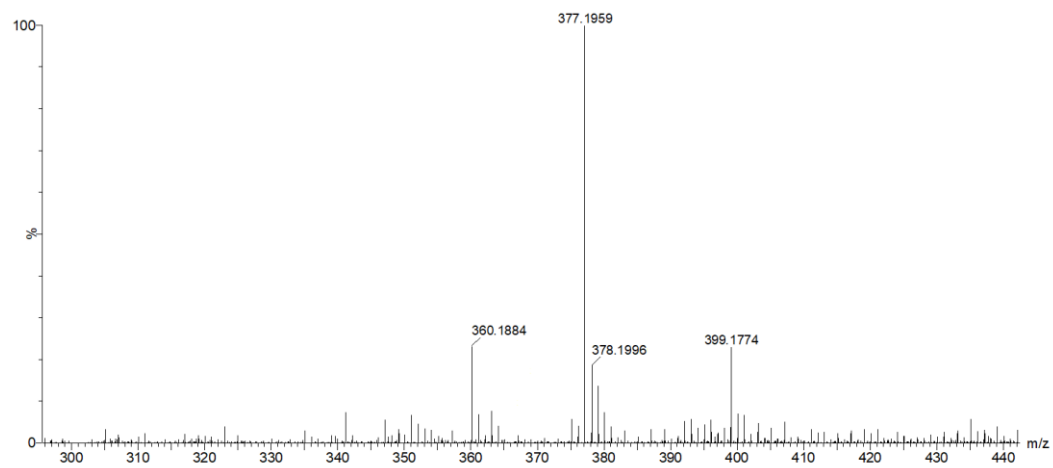


Figure S20: HRESIMS Spectrum of **1**

Chemical Structure similarity

SUBSTANCES

Select All Deselect All

0 of 7 Similarity Candidates Selected

Similarity Score	Substances
> 99 (most similar)	0
95-98	0
90-94	1
85-89	13
80-84	73
75-79	858
70-74	1459
65-69	19180
0-64 (least similar)	48360

Get Substances

Analyze Refine

Sort by: Similarity Score

0 of 14 Substances Selected

Analyze by: Substance Role

Biological Study 11

Occurrence 8

Preparation 5

Properties 5

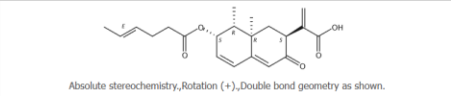
Uses 5

Reactant or Reagent 3

Show More

Score: 93

1. **1883548-70-6**

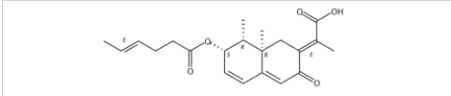


Absolute stereochemistry, Rotation (+), Double bond geometry as shown.

C₂₁H₂₆O₅
2-Naphthaleneacetic acid, 1,2,3,7,8,8a-hexahydro-8,8a-dimethyl-α-methylene-3-oxo-7-[[[(4E)-1-oxo-4-hexen-1-yl]oxy]-, (2S,7S,8R,8aR)-
Key Physical Properties

Score: 89

2. **1883548-71-7**

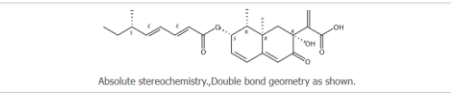


Absolute stereochemistry, Rotation (+), Double bond geometry as shown.

C₂₁H₂₆O₅
4-Hydroxonic acid, (1R,2S,7E,8aR)-7-(1-carboxylethylidene)-1,2,6,7,8,8a-hexahydro-1,8a-dimethyl-6-oxo-2-naphthalenyl ester, (4E)-
Key Physical Properties

Score: 88

3. **1893385-99-3**

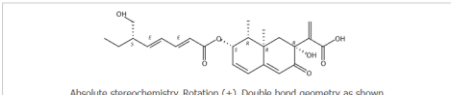


Absolute stereochemistry, Double bond geometry as shown.

C₂₄H₃₀O₆
2-Naphthaleneacetic acid, 1,2,3,7,8,8a-hexahydro-2-hydroxy-8,8a-dimethyl-α-methylene-7-[[[(2E,4E,6S)-6-methyl-1-oxo-2,4-octadien-1-yl]oxy]-3-oxo-, (2R,7S,8R,8aR)-
Key Physical Properties

Score: 88

4. **1893386-01-0**



Absolute stereochemistry, Rotation (+), Double bond geometry as shown.

C₂₄H₃₀O₇
2-Naphthaleneacetic acid, 1,2,3,7,8,8a-hexahydro-2-hydroxy-7-[[[(2E,4E,6S)-6-(hydroxymethyl)-1-oxo-2,4-octadien-1-yl]oxy]-8,8a-dimethyl-α-methylene-3-oxo-, (2R,7S,8R,8aR)-
Key Physical Properties

Figure S21: Scifinder similarity report for compound 1

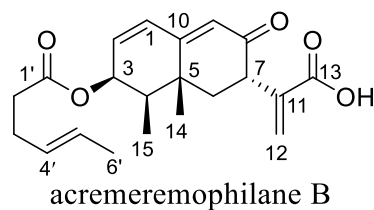
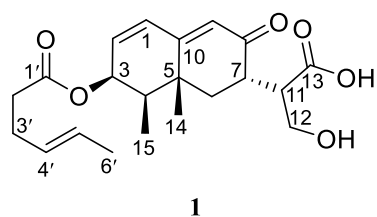


Table S1: Comparisons of NMR data of penicisepene (**1**) and acremeremophilane B

No.	δ_C	δ_H	No.	δ_C	δ_H
1	130.8, CH	6.35, d (9.7)		6.31, d (10.0)	130.9, CH
2	133.3, CH	6.26, dd (9.7, 5.2)		6.20, dd (5.2, 10.0)	132.2, CH
3	69.2, CH	5.38, dd (5.2, 4.6)		5.35, dd (4.8, 5.2)	69.1, CH
4	40.7, CH	1.97, m		1.97, dq (4.8, 7.2)	40.6, CH
5	36.5, C				36.2, C
6	38.5, CH ₂	2.11, dd (12.7, 4.0)		2.02, dd (5.2, 12.8)	40.6, CH ₂
		1.84, dd (12.7, 12.7)		2.13, dd (12.8, 13.4)	
7	43.3, CH	3.07, m		3.57, dd (5.2, 13.4)	46.8, CH
8	200.0, C				197.8, C
9	125.4, C	5.86, s		5.81, s	125.4, CH
10	162.0, C				160.5, C
11	47.5, CH	3.11, m			139.8, C
12	61.5, CH ₂	3.95, br s		5.68, s	127.9, CH ₂
				6.40, s	
13	177.2, C				168.5, C
14	18.4, CH ₃	1.32, s		1.30, s	18.4, CH ₃
15	10.4, CH ₃	1.05, d (7.0)		1.00, d (7.2)	10.1, CH ₃
1'	172.9, C			2.41, t (6.8)	172.7, C
2'	34.6, CH ₂	2.43, m		2.31, dt (5.6, 6.8)	34.4, CH ₂
3'	28.1, CH ₂	2.35, m		5.42, dt (5.6, 16.0)	27.8, CH ₂
4'	129.1, CH	5.43, m		5.51, dq (5.6, 16.0)	128.8, CH
5'	126.6, CH	5.50, m		1.63, d (5.6)	126.3, CH
6'	18.0, CH ₃	1.66, d (5.9)			17.7, CH ₃