Supporting Information

Rec. Nat. Prod. X:X (2023) XX-XX

Penicisepene, A New Sesquiterpenoid from the Fungus

Penicillium sp. LPFH-Q3

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Figure S1: ¹H NMR Spectrum of 1 in CDCl₃ (400 MHz)



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Figure S3: HSQC Spectrum of 1 in CDCl₃



Figure S4: HMBC Spectrum of 1 in CDCl₃







Figure S6: NOESY spectrum of compound 1 in CDCl₃.

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Figure S7: ¹H NMR Spectrum of 2 in DMSO-*d*₄ (400 MHz)



Figure S8: ¹³C NMR Spectrum of 2 in DMSO-*d*₄ (100 MHz)







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Figure S11: ¹H NMR Spectrum of 4 in CD₃OD (400 MHz)



Figure S12: ¹³C NMR Spectrum of 4 in CD₃OD (100 MHz)

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Figure S13: ¹H NMR Spectrum of 5 in DMSO-*d*₆ (400 MHz)



Figure S14: ¹³C NMR Spectrum of 5 in DMSO-*d*₆ (100 MHz)

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Figure S15: ¹H NMR Spectrum of 6 in DMSO-*d*₆ (400 MHz)



Figure S16: ¹³C NMR Spectrum of 6 in DMSO-*d*₆ (100 MHz)

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Figure S17: ¹H NMR Spectrum of 7 in CD₃OD (400 MHz)



Figure S18: ¹³C NMR Spectrum of 7 in CD₃OD (100 MHz)

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Figure S19: ¹H NMR Spectrum of 8 in CD₃OD (400 MHz)



Figure S20: HRESIMS Spectrum of 1

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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.	$\delta_{\rm C}$	$\delta_{\rm H}$
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, de	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 6.40, s	127.9, CH ₂
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