

Supporting Information

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A New Alkaloid from the Endophytic Fungus of *Crocus sativus* L., *Aspergillus fumigatus* Y0107

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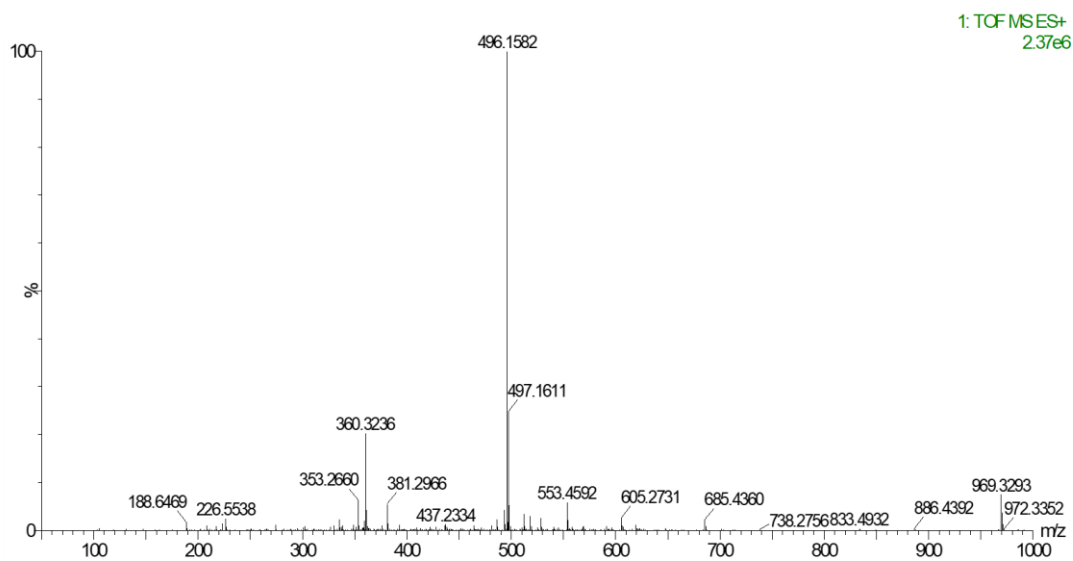


Figure S1: HR-ESI-MS spectrum of compound **1** (11-acetyl-pseurotin A₂)

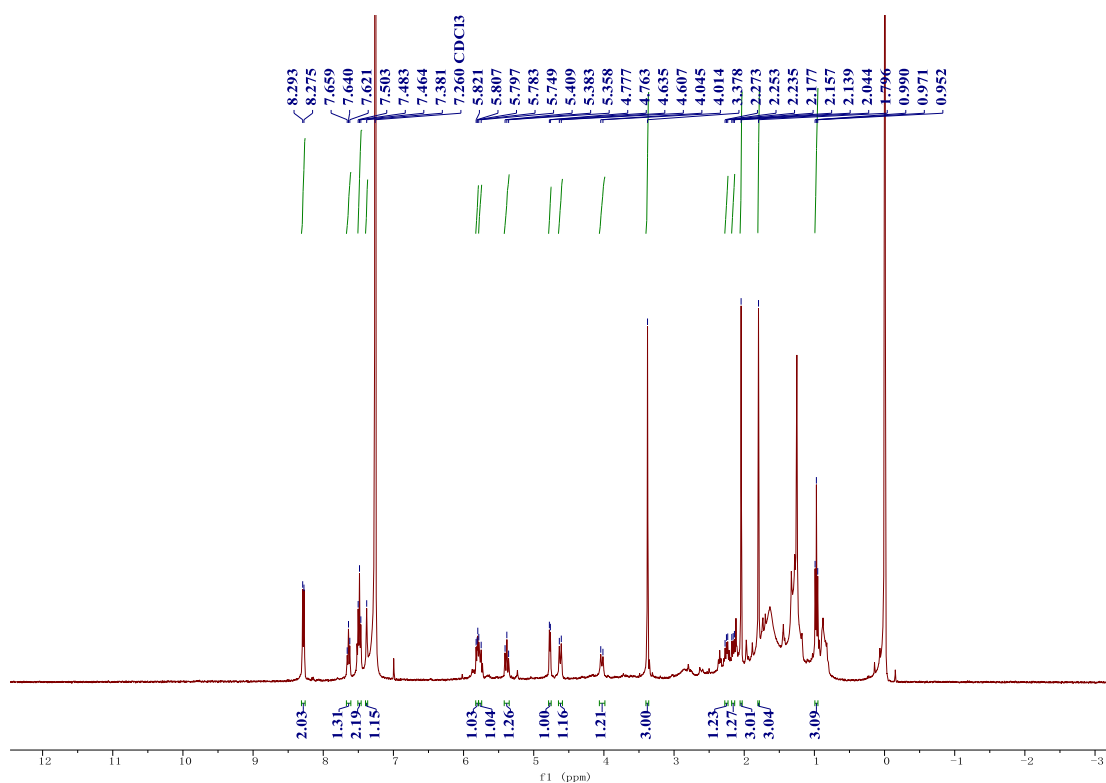
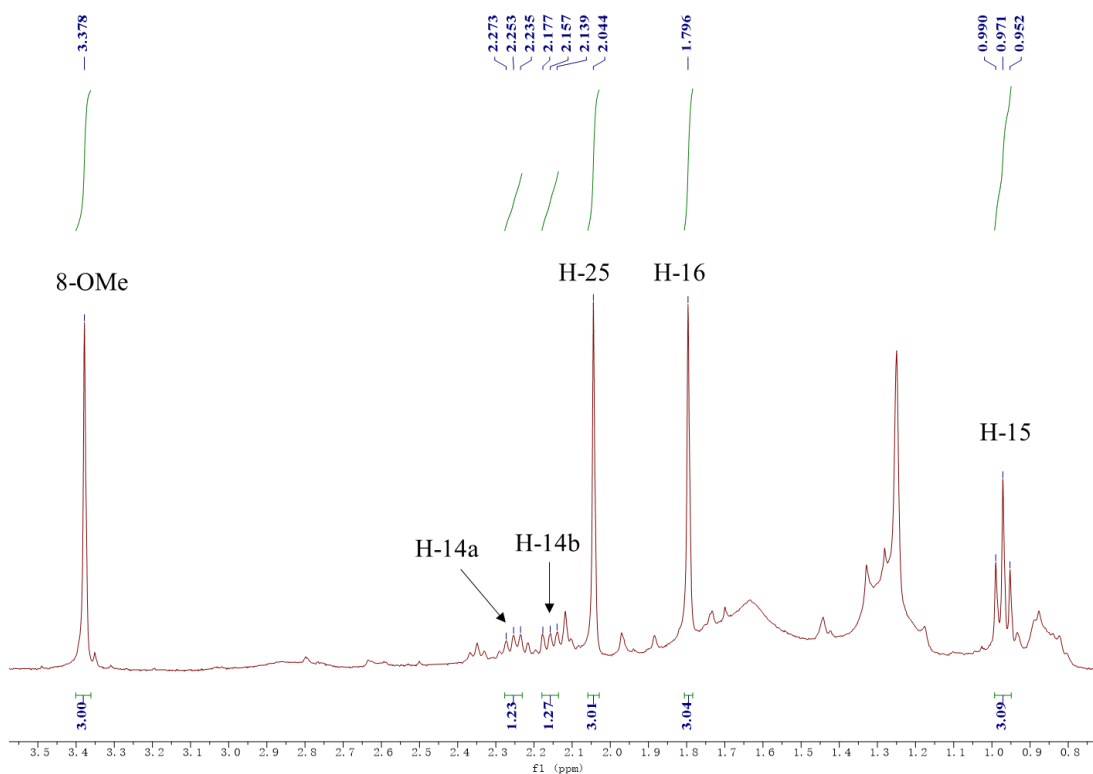
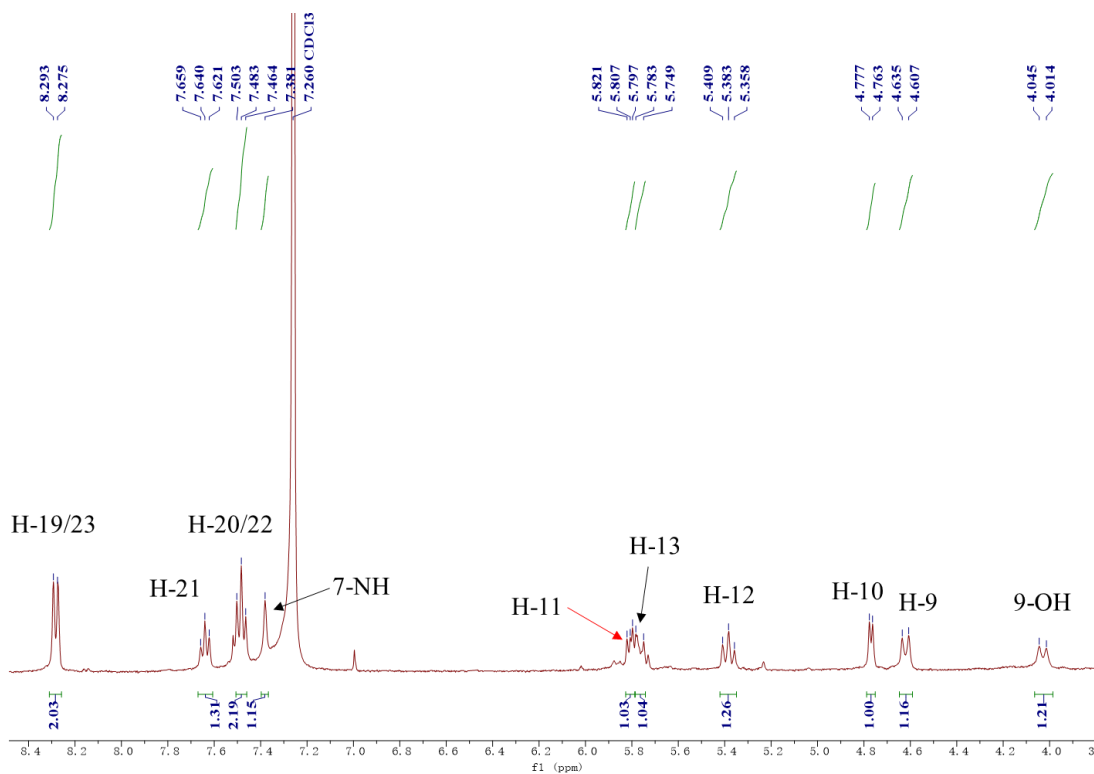


Figure S2: ¹H-NMR (400 MHz, CDCl₃) spectrum of compound **1** (11-acetyl-pseurotin A₂)



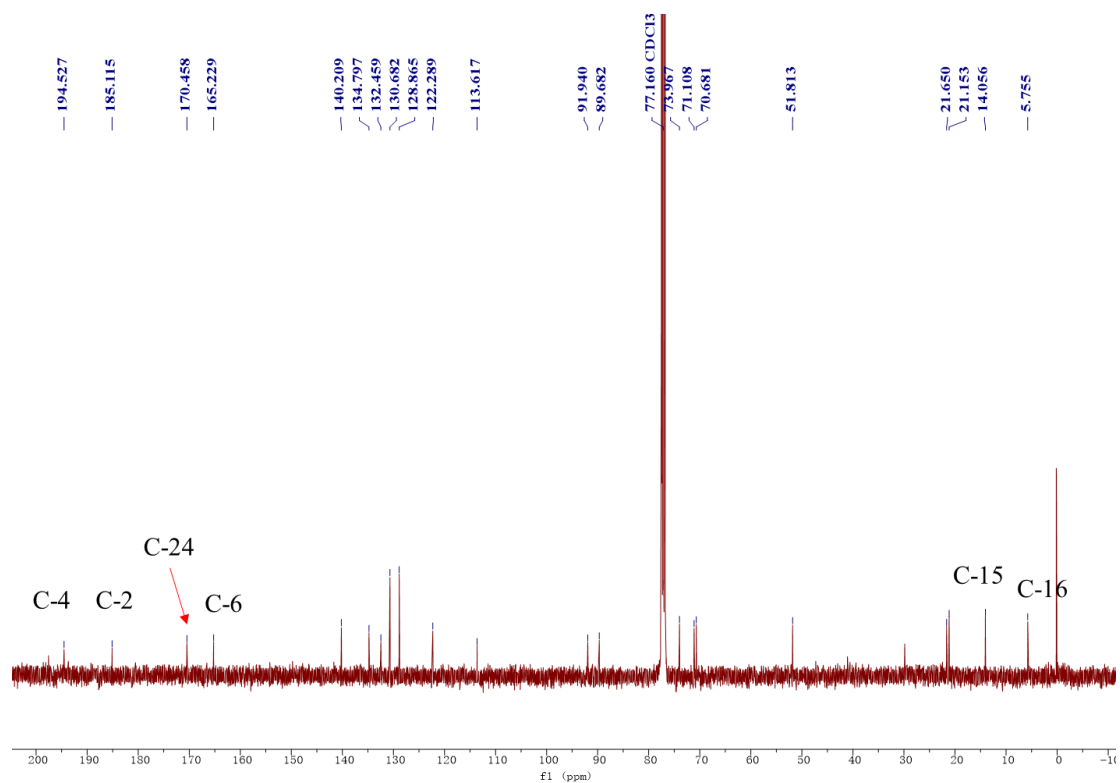


Figure S5: ^{13}C -NMR (100 MHz, CDCl_3) spectrum of compound **1** (11-acetyl-pseurotin A₂)

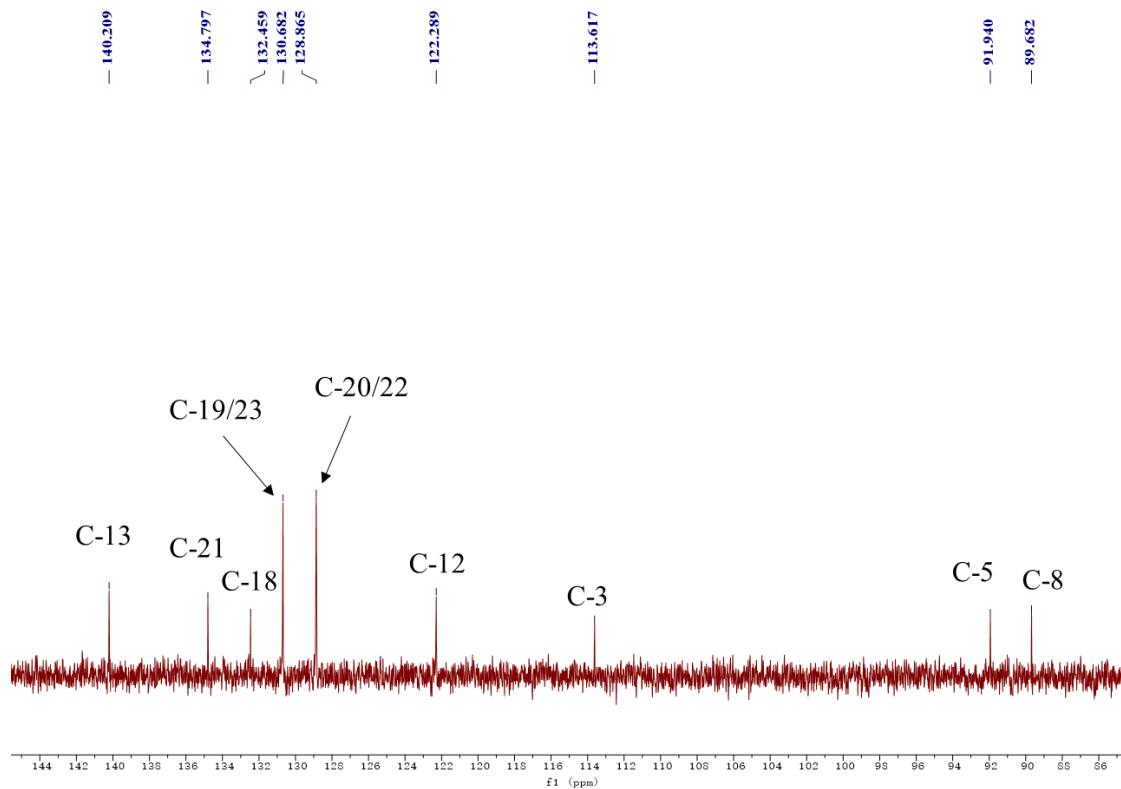


Figure S6: ^{13}C -NMR (100 MHz, CDCl_3) spectrum of compound **1** (11-acetyl-pseurotin A₂)

(From δ_C 85 ppm to δ_C 145 ppm)

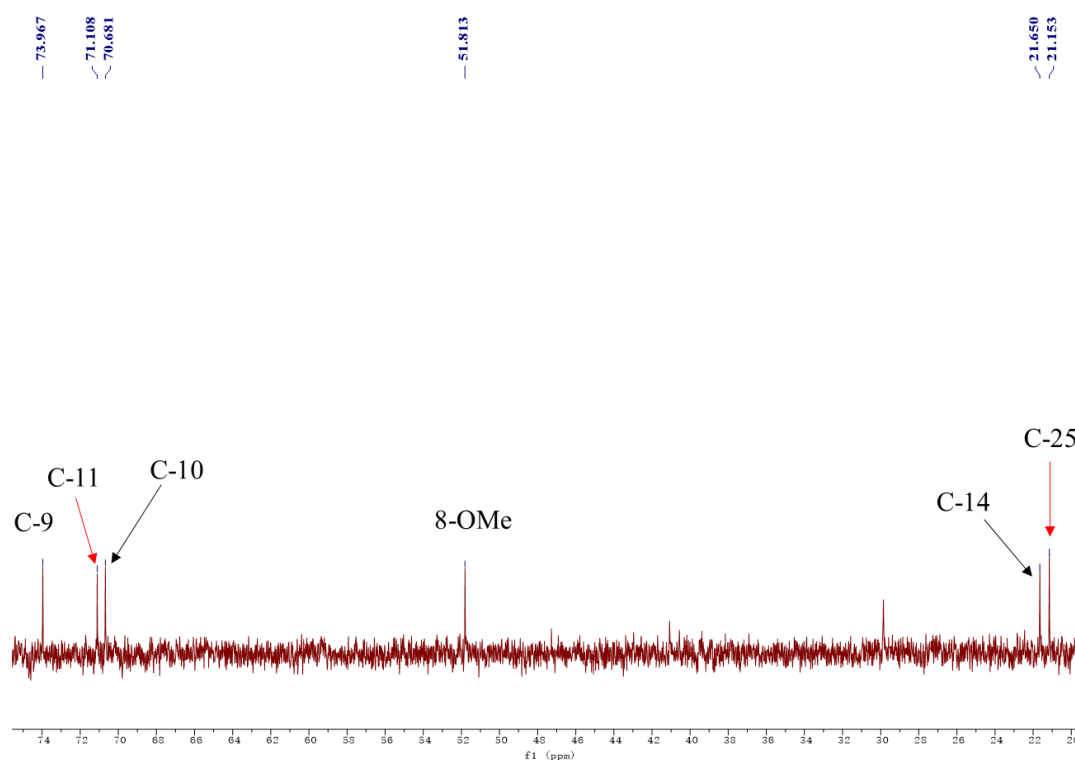


Figure S7: ^{13}C -NMR (100 MHz, CDCl_3) spectrum of compound **1** (11-acetyl-pseurotin A₂) (From δ_C 20 ppm to δ_C 75 ppm)

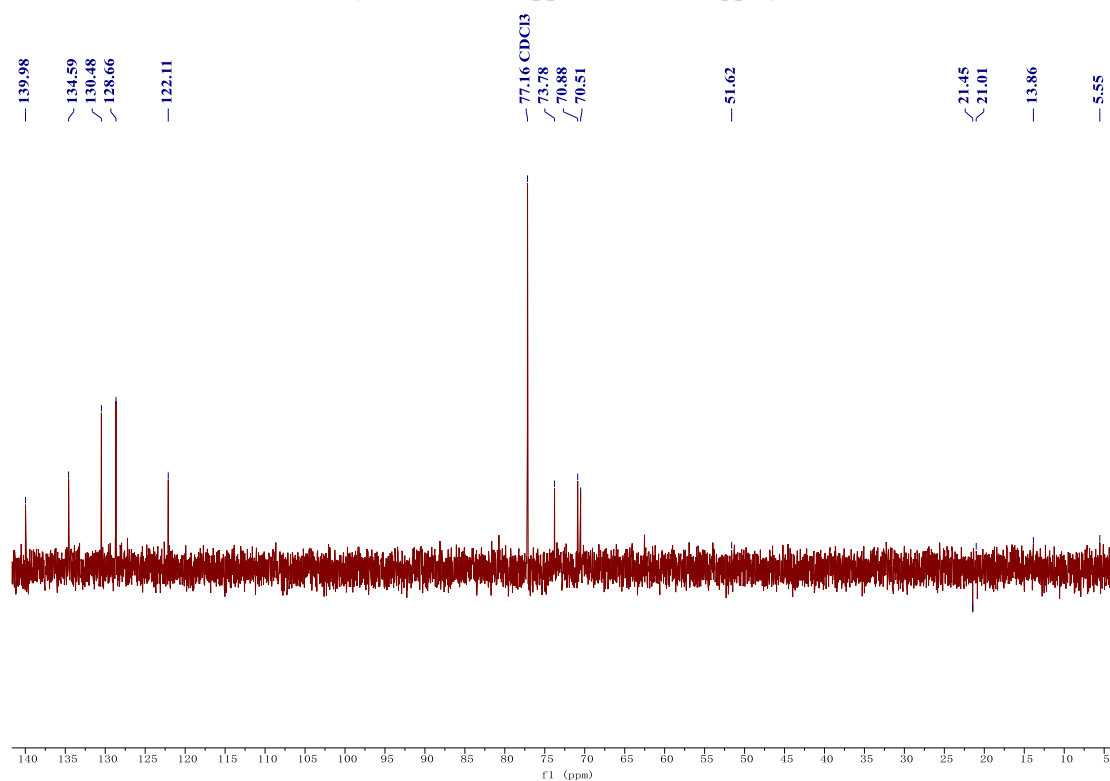


Figure S8: DEPT135 (100 MHz, CDCl_3) spectrum of compound **1** (11-acetyl-pseurotin A₂)

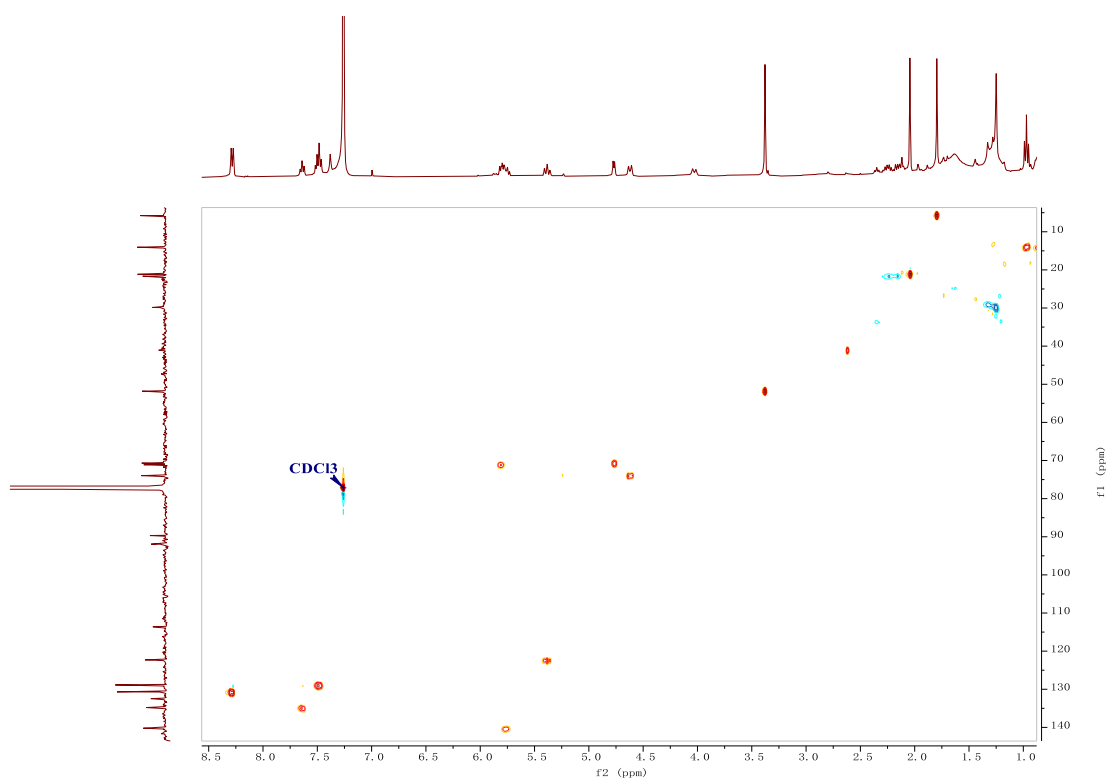


Figure S9: HSQC spectrum of compound **1** (11-acetyl-pseurotin A₂)

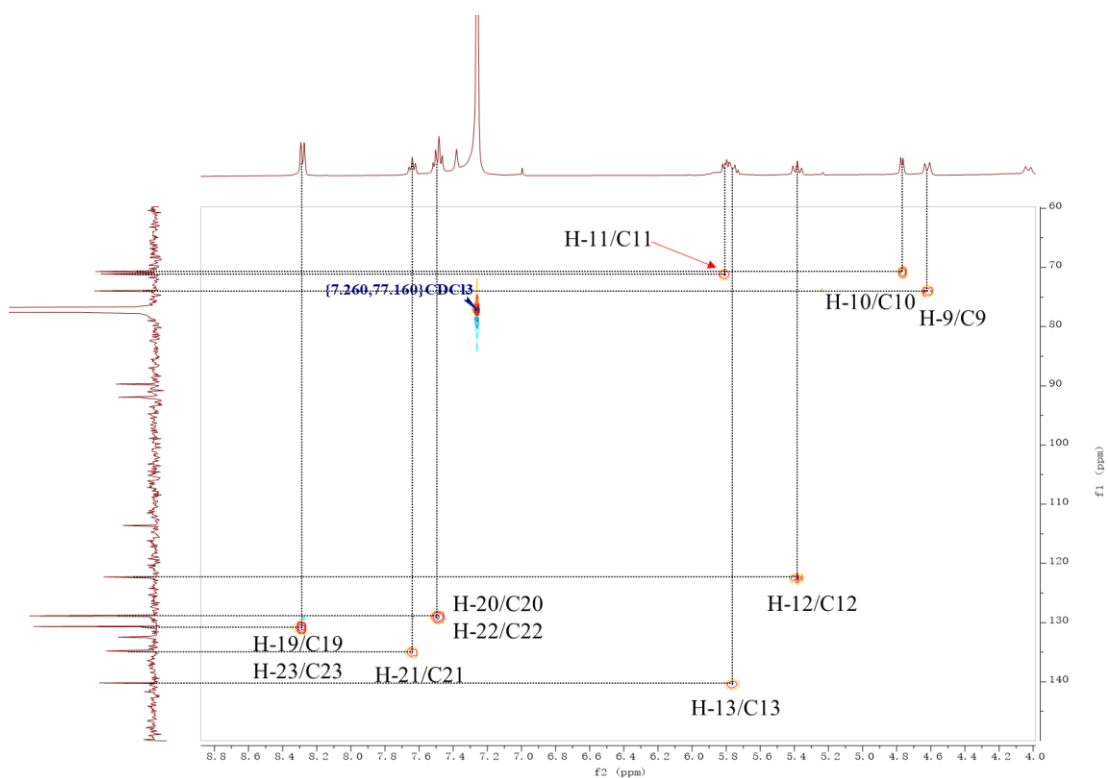


Figure S10: HSQC spectrum of compound **1** (11-acetyl-pseurotin A₂) (From δ_C 60 ppm to

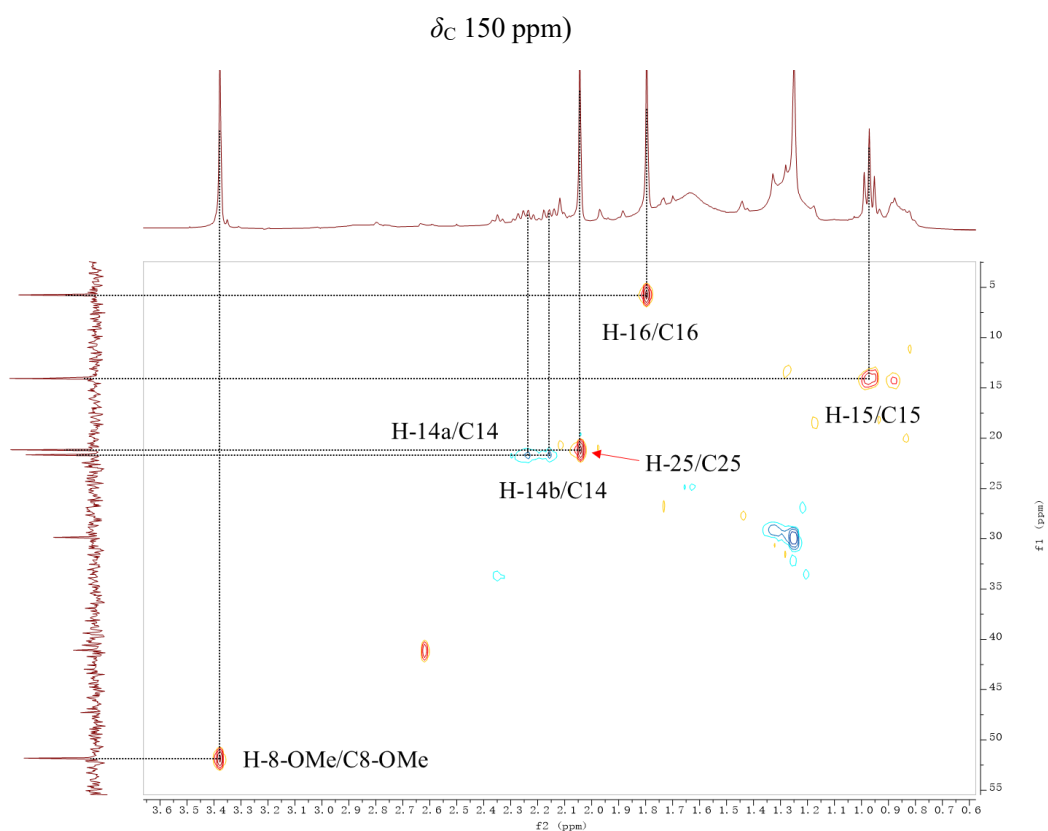


Figure S11: HSQC spectrum of compound **1** (11-acetyl-pseurotin A₂) (From δ_C 5 ppm to δ_C 55 ppm)

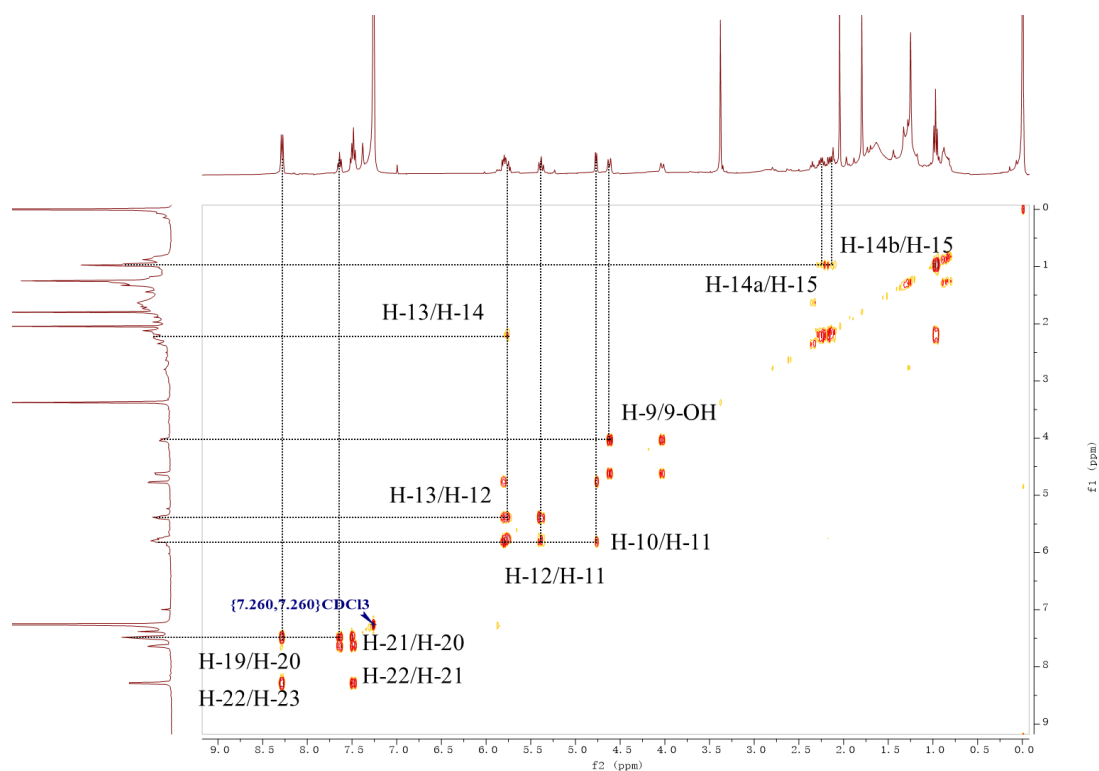


Figure S12: ^1H - ^1H COSY spectrum of compound **1** (11-acetyl-pseurotin A₂)

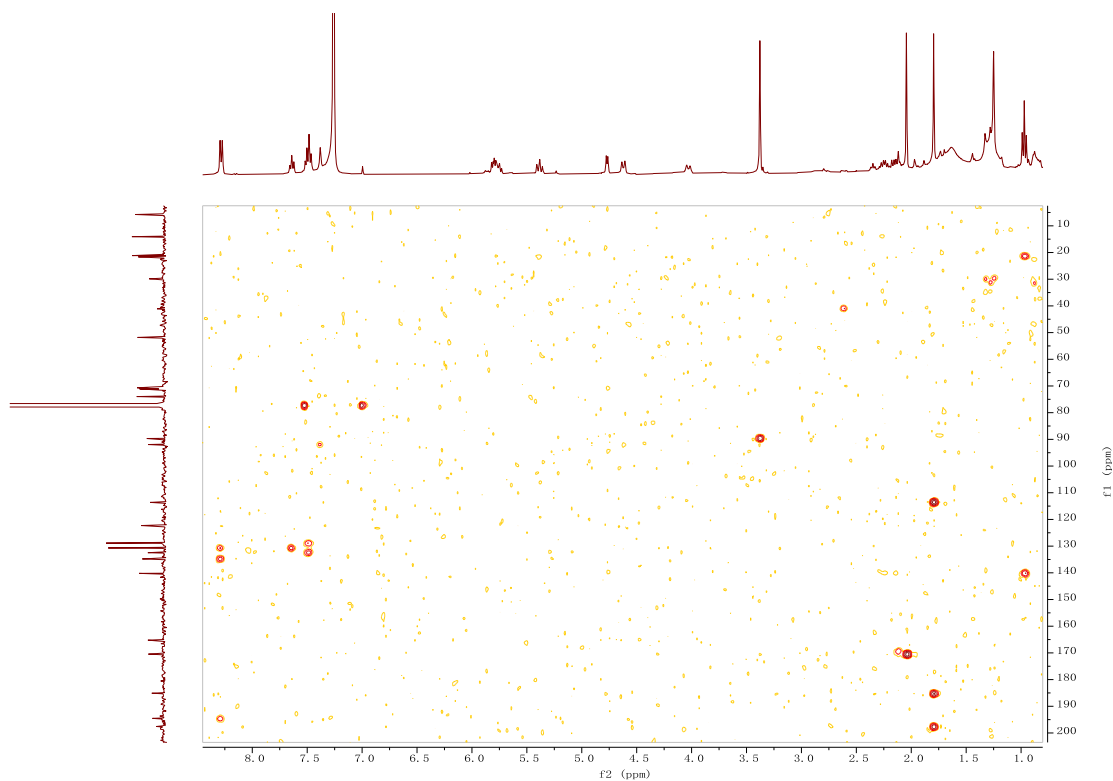


Figure S13: HMBC spectrum of compound **1** (11-acetyl-pseurotin A₂)

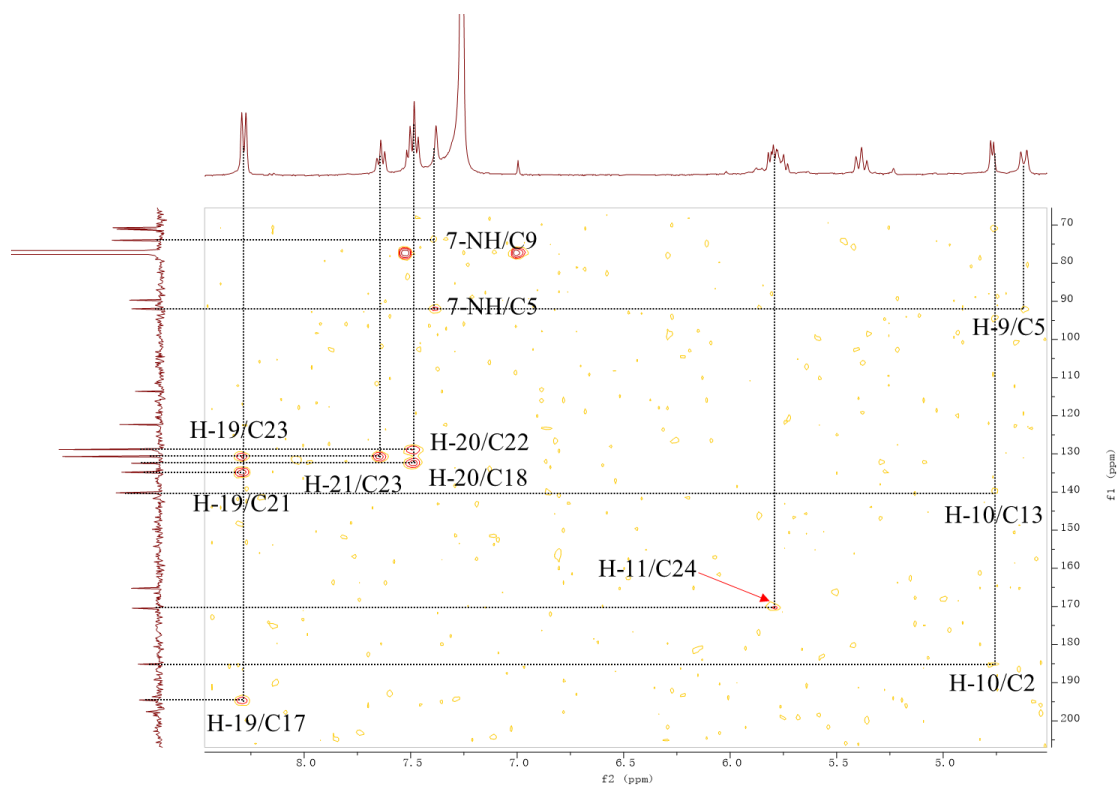


Figure S14: HMBC spectrum of compound **1** (11-acetyl-pseurotin A₂) (From δ_H 4.0 ppm to δ_H 9.0 ppm)

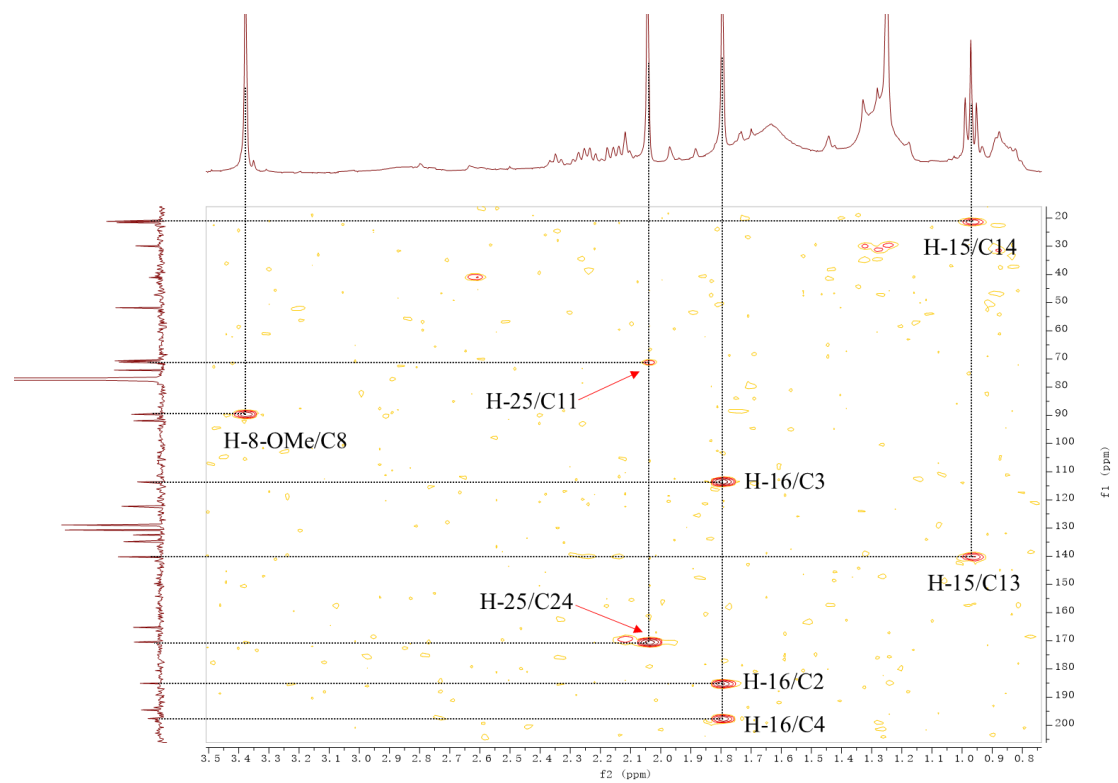


Figure S15: HMBC spectrum of compound **1** (11-acetyl-pseurotin A₂) (From δ_H 0.6 ppm to δ_H 3.6 ppm)

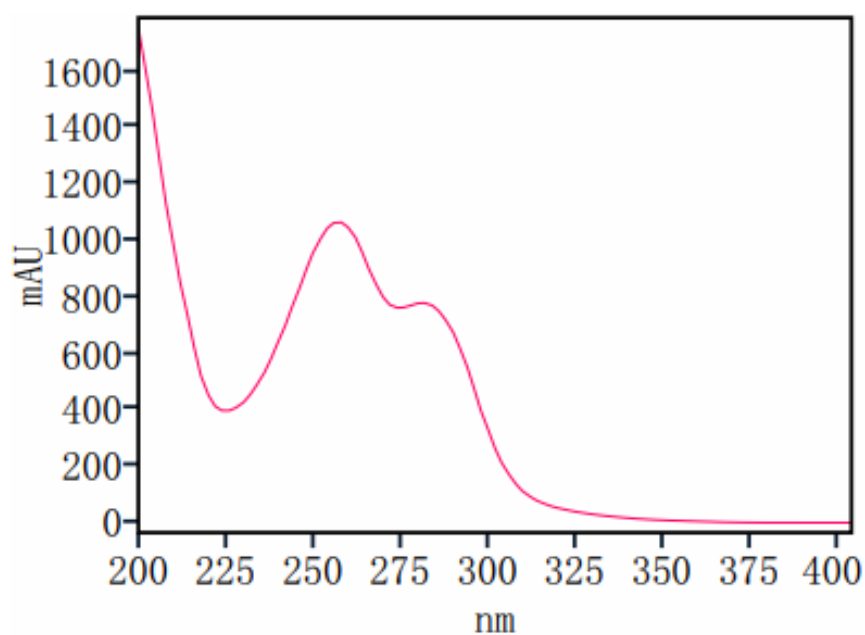


Figure S16: The UV spectrum of compound **1** (11-acetyl-pseurotin A₂)

Table S1. ¹H NMR data of compound **1**, pseurotin A₂ (2011), pseurotin A₂ (2016) and pseurotin A in CDCl₃

No	1	Pseurotin A₂ (2011)¹	Pseurotin A₂ (2016)¹	Pseurotin A²
2	-	-	-	-
3	-	-	-	-
4	-	-	-	-
5	-	-	-	-
6	-	-	-	-
7-NH	7.38 (s)	7.43 (s)	7.70 (s)	8.38 (s)
8	-	-	-	-
9	4.62 (d, 11.2)	4.45 (s)	4.42 (d, 11.8)	4.69 (br s)
10	4.77 (d, 5.6)	4.55 (br s)	4.74 (d, 2.5)	4.59 (d, 5.4)
11	5.80 (m)	4.70 (m)	4.94 (dd, 8.5, 2.8)	4.75 (dd, 10.8, 5.4)
12	5.38 (t, 10)	5.38 (t, 9.8)	5.28 (dd, 12.0, 7.7)	5.28 (dd, 11.2, 10.8)
13	5.75 (m)	5.70 (dt, 10.4, 7.6)	5.64 (m)	5.59 (dt, 11.2, 7.8)
14a	2.26 (m)	2.18-2.06 (m)	2.25-2.10 (m)	2.09 (m)
14b	2.15 (m)			2.15 (m)
15	0.97 (t, 7.6)	0.97 (t, 7.5)	1.03 (t, 7.5)	0.98 (t, 9.0)
16	1.80 (s)	1.71 (s)	1.67 (s)	1.68 (s)
17	-	-	-	-
18	-	-	-	-

19/23	8.28 (d, 7.2)	8.24 (d, 7.4)	8.34 (d, 7.6)	8.31 (d, 8.4)
20/22	7.48 (t, 8.0)	7.41 (t, 7.4)	7.48 (t, 7.8)	7.49 (t, 8.4)
21	7.64 (t, 7.6)	7.56 (t, 7.4)	7.62 (t, 7.3)	7.64 (t, 8.4)
24	-	-	-	-
25	2.04 (s)	-	-	-
8-OMe	3.38 (s)	3.25 (s)	3.30 (s)	3.44 (s)
9-OH	4.03 (d, 12.4)	-	-	-

References

- [1] G. R. Jachak, P. R. Tharra, P. Sevelde and J. Svenda (2021). Stereocontrolled synthesis of pseurotin A₂, *J. Org. Chem.* **86**, 11845-11861.
- [2] T. Yamada, M. Oshima, K. Yuasa, T. Kikuchi and R. Tanaka (2016). Assignment of the CD cotton effect to the chiral center in pseurotins, and the stereochemical revision of pseurotin A₂, *Mar. Drugs* **14**, 74.