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A New Macrocyclic Trichochecene from Soil Fungus

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Abstract: From fermentation broth of soil fungus 254-2 obtained from Yunnan province, a new macrocylic trichochecene was isolated. The structure was determined on the basis of spectroscopic evidences especially the 2-D NMR spectra.

Keywords: Soil fungus, macrocyclic trichochecene, spectral data.

The trichothecenes constitute an important class of mycotoxin which exhibit obviously biological activities[1]. In our previous paper, we have reported the isolation and structure elucidation of a series of metabolites from soil fungi[2]. In this paper, we wish to report the chemical studies on soil fungus 254-2, collected from Yunnan province. The fungus was fermented at 28°C for 5 days. Fermentation broth (6.5 L) was exhaustively extracted with EtOAc to give a crude extract. The EtOAc extract was chromatographed on a silica gel using gradient of MeOH in $CHCl_3$, resulted in the separation of a new macrocyclic trichochecene, compound 254-2-3.

254-2-3, was obtained as colorless crystals (from MeOH/$CHCl_3$ 1:1). Its molecular formula was $C_{29}H_{38}O_8$, which was deduced by a combination of the information from the ESI-MS spectrum (M^++1 at *m/z* 515) and NMR data. ^{1}H-NMR (300MHz, CD_3OD) and ^{13}C-NMR (75MHz, CD_3OD) made it clear that this compound was closely related to compounds roridin E which was isolated from soil fungus fermentations[3]. However, in the ^{13}C-NMR spectrum, the chemical shift of carbon C-6', C-13', are at δ_C 74.7 and 74.1 respectively, while in roridin E they are at δ_C 83.2 and 69.6. The signal of C-7' showed significant downfield shift of 7.0 ppm and the signal of C-5' showed highfield shift of 6.7 ppm. The above information indicated that compound 254-2-3 was different from roridin E at 6' and 13' positions. In HMQC spectrum, δ 3.70 (H-5') showed crosspeak with $_C$ 60.6 and in HMBC spectrum (**Figure 2**), H-13' (δ_H 4.89) showed C-H long-range correlation with carbon signal C-5' (δ_C 60.6). On the basis of HMQC and HMBC spectral data, the structure of 254-2-3 was established as shown in **Figure 1**. ^{1}H and ^{13}C-NMR data were assigned in **Table 1**.

Figure 1 Structure of 254-2-3

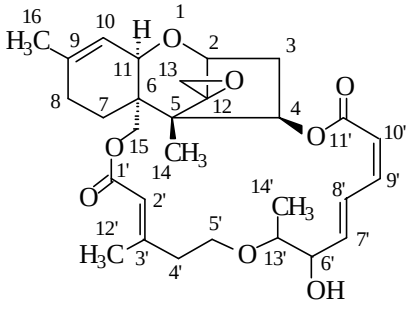

Figure 2 HMBC correlations of 254-2-3

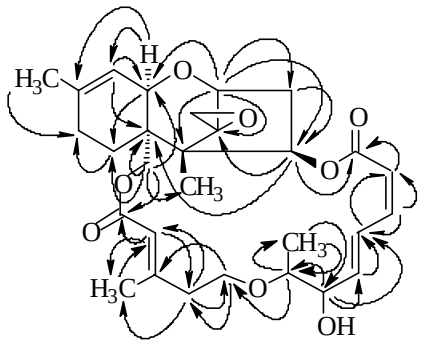

Table 1 NMR data of compound 254-2-3

No.	^{1}H-NMR	δ_C	No	^{1}H-NMR	δ_C
2	3.75(d, 1H, J=5.1Hz)	80.4	1'		167.6
3	1.98(m, 1H)	37.4	2'	5.75(s, 1H)	117.6
	2.54(dd, 1H, J=8.1,4.5Hz)				
4	5.87(m , 1H)	76.6	3'		159.5
5		50.2	4'	2.37(t, 2H, J=6.3Hz)	44.6
6		44.7	5'	3.70(t, 2H, J=6.3Hz)	60.6
7	2.02 (m, 2H)	22.2	6'	4.25(t, 1H, J=6.6Hz)	74.7
8	1.93 (m, 2H)	28.9	7'	6.07(dd, 1H, J=15.3, 6.6Hz)	143.2
9		141.9	8'	7.60(ddd, 1H,	129.6
10	5.41(d, 1H, J=5.1Hz)	119.6		J=11.4, 15.3, 3.6Hz)	
11	3.83(br d, 1H, J=5.1Hz)	68.3	9'	6.69(t, 1H, J=11.4Hz)	145.4
12		66.5	10'	5.67(dd, 1H, J=11.4,3.6Hz)	118.8
13	3.10(d, 1H, J=3.6Hz)	49.1	11'		167.2
	2.89(d, 1H, J=3.6Hz)				
14	0.79(s, 3H)	7.5	12'	2.18(s, 3H)	19.0
15	4.04(d, 1H, J=12.3Hz)	63.9	13'	4.89 (m, 1H)	74.1
	4.28(dd, 1H, J=12.3,5.1Hz)				
16	1.70(s, 3H)	23.2	14'	1.18 (d, 3H, J=6.3Hz)	16.2

Acknowledgment

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