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## Phenylpropanoids produced by *Streptomyces* sp.3C, a commensal microbe of *Maytenus hookeri*

LU Chun-hua, SHEN Yue-mao

(The State Key Laboratory of Phytochemistry and Plant Resources in West China,  
Kunming Institute of Botany, Chinese Academy of Science, Kunming 650204, China)

**Abstract:** Two phenylpropanoids (1 and 2) were isolated from the fermentation extracts of commensal microbe of *Maytenus hookeri* (*Streptomyces* sp. 3C). Their structures were elucidated on the basis of NMR and EIMS techniques and compound 2 was a new one. Their acetylated products, 1a, 1b and 2a, were obtained by acetylation with Ac<sub>2</sub>O-pyridine. The antibacterial activities of all the five compounds were performed by paper-disc assay method, and potential activities were observed.

**Key words:** medicinal chemistry; structural identification; NMR; *Streptomyces* sp. 3C; *Maytenus hookeri*; phenylpropanoids

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## 云南美登木共生放线菌菌株 3C 产生的苯丙素类化合物

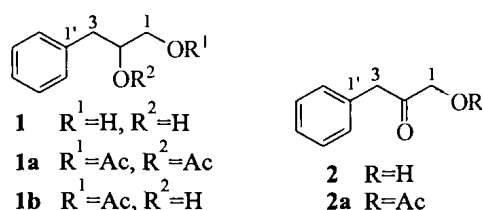
鲁春华, 沈月毛

(中国科学院昆明植物研究所 西部植物化学和植物资源重点实验室, 云南 昆明 650204)

**摘 要:** 从云南美登木共生放线菌菌株 3C 的发酵提取物中分离得到两个苯丙素类化合物 1 和 2。通过谱学特征鉴定了化合物的结构, 其中, 化合物 2 为新化合物。通过乙酰化反应得到了相应的乙酰化产物, 并通过纸片扩散法测定了所有化合物的抗菌活性。

**关键词:** 药物化学; 结构鉴定; 核磁共振波谱; 放线菌菌株 3C; 云南美登木; 苯丙素类化合物

The strain 3C, isolated from the fresh stem barks of *Maytenus hookeri*, was identified as *Streptomyces* sp. on the genus level. Investigation on the secondary metabolites led to the isolation of two phenylpropanoids (1 and 2) including a new one (2) by column chromatography. Their structures were elucidated based on the NMR data. Their acetylated products (1a, 1b and 2a) were obtained through acetylation with Ac<sub>2</sub>O-pyridine.



Compound 1: The NMR data including <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, DEPT, HMQC and HMBC (Table 1) revealed that it was a phenylpropanoid type compound. The <sup>13</sup>C-NMR and DEPT spectra

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**Biographies:** LU Chun-hua (1975 - ), female (Han nationality), was born in Shandong Province; SHEN Yue-mao (1965 - ), male (Han nationality), was born in Anhui, Professor, and was major in natural products chemistry, E-mail: yshen@mail.kib.ac.cn.

of **1** showed nine carbon signals for two methylene, six methine, and one quaternary carbon atoms. The  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR resonances of **1** were assigned by HMQC and HMBC experiments. The protons at  $\delta$ : 7.16(m, 2H), 7.20(m, 2H) and 7.26(m, 1H)<sup>[1]</sup> indicated a single substitute aryl ring was exist in the structure. The proton at  $\delta$  3.60 and  $\delta$  3.44(H-1) showed long-range correlation with C-3 and C-2, and protons at  $\delta$  2.70 and  $\delta$  2.66(H-3) with C-2, which indicated the exist of the fragment of propanediol, and the  $^1\text{H}$ - $^{13}\text{C}$  long-range correlation of the proton at  $\delta$  2.70 and  $\delta$  2.66(H-3) with the carbons at  $\delta$  137.8(C-1') and  $\delta$  129.8(C-2') indi-

cated the linkage between C-3 and C-1'. Therefore, compound **1** was determined to be 3-phenyl-1, 2-propanediol, which was consistent with the molecular ion peak at  $m/z$  152 in EI-MS. The absolute configuration was determined in (*R*)-form by comparing the optical rotation  $[\alpha]_{\text{D}}^{20} + 81^\circ$  ( $c$  2.5, MeOH) with literature data<sup>[1]</sup>.

The  $^{13}\text{C}$ -NMR and DEPT spectra of **2** showed nine carbon signals for two methylene, five methine, and two quaternary carbon atoms including one carbonyl. According to the NMR data, and further compared with those of compound **1**. Compound **2** was identified to be 1-hydroxyl-3-phenyl acetone (Table 1).

Table 1 The NMR data for **1** and **2**

Position	Compound 1			Compound 2	
	$^{13}\text{C}$	$^1\text{H}$	HMBC	$^{13}\text{C}$	$^1\text{H}$
1'	137.8(s)	/	/	132.6(s)	/
2'	129.8(d)	7.16(m, 2H)	C-1', C-3'	129.2(d)	7.20(d, $J = 7.6$ Hz, 2H)
3'	128.5(d)	7.20(m, 2H)	C-1', C-2', C-4'	128.9(d)	7.34(t, $J = 7.2$ Hz, 2H)
4'	126.5(d)	7.26(m, 1H)	C-2', C-3'	127.4(d)	7.26(d, $J = 6.8$ Hz, 1H)
5'	128.5(d)	/	/	128.9(d)	/
6'	129.8(d)	/	/	129.2(d)	/
1	65.9(t)	3.60(m), 3.44(m)	C-3, C-2	67.7(t)	4.27(s)
2	73.0(d)	3.86(m, 1H)	/	207.3(s)	/
3	39.7(t)	2.70(m), 2.66(m)	C-1', C-2', C-2	45.7(t)	3.70(s)

Note: The NMR data for compounds **1** and **2** were recorded on Bruker AM-400 in  $\text{CDCl}_3$  at room temperature

The antimicrobial activities were tested by paper disc diffusion methods<sup>[2]</sup>. The activities were illustrated by the diameters of inhibitory zones against tested pathogenic strains at a given amount

of tested compound. The results were summarized in Table 2. Streptomycin was used as positive control in the antibacterial assays.

Table 2 Antimicrobial activity against some pathogens of compounds **1**, **2** and their acetylated products

Compound	Tested microorganism		
	<i>Staphylococcus aureus</i>	<i>Mycobacterium tuberculosis</i>	<i>Streptococcus pneumoniae</i>
<b>1</b>	— (200)	— (200)	— (200)
<b>1a</b>	8 (200)	— (200)	— (200)
<b>1b</b>	10 (40), 15(80)	10 (20), 15(40)	10 (20), 15(40)
<b>2</b>	8 (100)	— (200)	8 (100)
<b>2a</b>	— (160)	7 (40), 9(80)	7 (40), 9(80)
streptomycin	13 (5), 16(10)	13 (5), 16(10)	/

Note: The diameter of paper disc is 5 mm; "—" means no inhibitory activity; The diameter of inhibitory zone in mm with certain amount of compounds ( $\mu\text{g}$ , in parentheses) per disc

新化合物。

实验用植物药材麻叶千里光由长春华康制药有限公司提供,经长春中医药研究院严仲凯研究员鉴定为 *S. cannabifolius* Less. 的全草。

麻叶千里光苷 D 为黄色液体, Molish 反应呈阳性, 反相 HPLC [Cosmosil 5 C<sub>18</sub>-AR-II, 10 mm × 250 mm, Nacalai Tesque, 15% (φ) MeOH-H<sub>2</sub>O-1% (φ) THF, UV λ 254 nm, 3.0 mL·min<sup>-1</sup>], 测得 *t<sub>R</sub>* ≈ 29 min。薄层酸水解色谱只检测出葡萄糖, 由 <sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>, 400 MHz) 谱中的糖端基质子信号 δ 4.24 (1H, d, *J* = 8.0 Hz) 判断为 β-D-吡喃型葡萄糖。正离子源 ESI-MS 谱给出 *m/z* 403 [M+H]<sup>+</sup> 等准分子离子峰, 结合其核磁共振波谱, 确定化合物 1 的结构如图 1 所示。<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>, 100 MHz) δ: 208.9 (C-2), 197.6 (C-3), 118.4 (C-1'), 101.2 (C-1''), 99.6 (C-1), 76.7 (C-3'), 73.4 (C-5'), 73.4 (C-2'), 70.6 (C-4'), 70.4 (C-2'), 70.0 (C-4''), 61.0 (C-6'), 46.9 (C-5'), 46.0 (C-3'), 35.5 (C-6'), 31.6 (C-9'), 30.3 (C-7'), 28.7 (C-8'), 26.2 (C-4)。

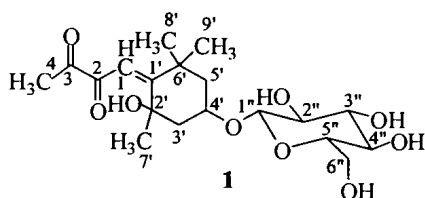


Figure 1 The structure of compound 1

麻叶千里光苷 E 为淡黄色油状物, Molish 反应呈阳性, 反相 HPLC [Cosmosil 5 C<sub>18</sub>-AR-II, 10 mm × 250 mm, Nacalai Tesque, 25% (φ) MeOH-H<sub>2</sub>O, UV λ 254 nm, 3.0 mL·min<sup>-1</sup>], 测得 *t<sub>R</sub>* ≈ 32 min。薄层酸水解色谱只检测出葡萄糖, 由 <sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>, 400 MHz) 谱中的糖端基质子 δ 4.29 (1H, d, *J* = 7.6 Hz), 确定为 β-D-吡喃型葡萄糖。正离子源 ESI-MS 谱给出 *m/z* 387 [M+H]<sup>+</sup> 等准分子离子峰, 结合其核磁共振波谱, 确定化合物 2 的结构如图 2 所示。<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>, 100 MHz) δ: 199.9 (C-1), 159.3 (C-3), 139.5 (C-8), 126.9 (C-2), 125.4 (C-7), 101.1 (C-1'), 76.8 (C-3'), 76.7 (C-5'), 75.0 (C-9), 73.7 (C-2'), 69.7 (C-4'), 68.5 (C-6), 60.8 (C-6'), 45.7 (C-5), 36.3 (C-4), 30.0 (C-12), 25.5 (C-13), 20.7 (C-10), 13.4 (C-11)。

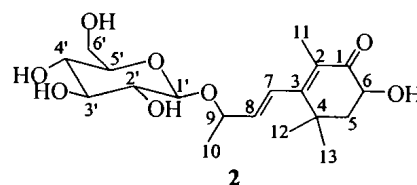


Figure 2 The structure of compound 2

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Compound 1 is a simple phenylpropanoid compound, and it was reported as a derivative of phenylalanine<sup>[1]</sup>. It was firstly reported that compound 1 was produced by fermentation of microorganism with high yield (22%). Compound 2 is a new compound and is the oxidized form of 1. Compound 2 and the acetylated derivatives showed potential antibacterial activity.

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