

## A New Perylenequinone from *Hypomyces* sp.

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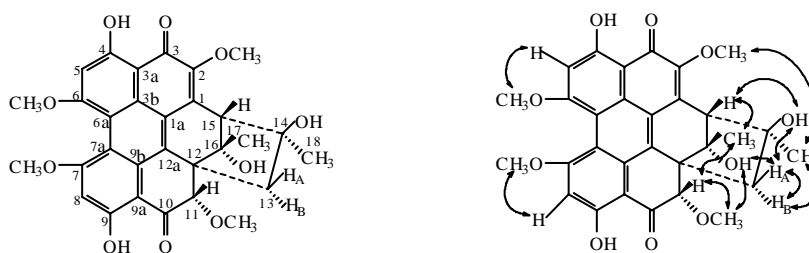
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**Abstract:** A new perylenequinone, named hypomycin A, was isolated from the mycelia of *Hypomyces* sp.. Its structure was elucidated on the basis of spectroscopic methods.

**Keywords:** *Hypomyces* sp., perylenequinone, hypomycin A.

Some metabolites of fungi and plants containing perylenequinones have been used as folk medicine for the treatment of many diseases<sup>1,2</sup>. A filamentous fungus, Ascomycetes Hypocreaceae *Hypomyces* (Fr.) Tul. sp., was found from the northwestern mountains of Yunnan Province, and cultured successfully in the laboratory. A new perylenequinone, named hypomycin A (**1**), was isolated from its mycelia. In this paper the structure elucidation of **1** was described.

**Figure 1** The structure of compound **1** **Figure 2** The key correlations of **1** in the NOESY



Compound **1**, red crystals, mp 166~169°C (EtOH);  $[\alpha]_D^{25} +350.6$  (c, 0.15, CHCl<sub>3</sub>). The FAB-MS spectrum showed a  $[M+1]^+$  ion peak at  $m/z$  549. Its molecular formula, C<sub>30</sub>H<sub>28</sub>O<sub>10</sub>, was established by FAB-MS, <sup>1</sup>H and <sup>13</sup>C NMR (**Table 1**) spectroscopy. The IR absorptions at 3422, 1624 and 1583 cm<sup>-1</sup> indicated the presence of hydroxy and hydrogen-bonded extended quinone carbonyl groups. The UV-vis spectrum  $\lambda_{max}^{MeOH}$  nm (lg  $\epsilon$ ) 212 (4.45), 286 (4.52), 395 (4.23), 416 (4.31), 495 (3.89) and 527 (3.92), was similar to those of elsinochromes<sup>3</sup> and other perylene-quinones<sup>4</sup>, but hypsochromic obviously. Furthermore, compound **1** showed a remarkable upfield shift of one phenyl hydroxy ( $\delta$  12.71), a downfield shift of one quinone carbonyl group ( $\delta$  197.2), and only

the  $\delta$  values of 18 carbons were more than 99 (common perylenequinones<sup>5</sup> at least 20 carbons). So compound **1** was a perylenequinone whose one carbonyl group lacked a conjugated double bond.

In the HMBC experiment, the correlations of H-11 with C-10, C-12, C-12a, C-13 and C-16, H<sub>A</sub> and H<sub>B</sub>-13 with C-12 and C-12a, H-15 with C-1, C-1a, C-2, C-12 and C-16, and H-17 with C-12, C-15 and C-16, indicated C-16 and C-13 connected with C-12, C-15 with C-1, and C-16 with C-15. In addition, the correlations of H-18 with C-13, C-14 and C-15, and H-15 with C-13 and C-14, showed that C-14 connected with C-15 and C-13. Together with other correlations, the basic structure of **1** was established. All proton and carbon data were assigned on the basis of the HMQC and HMBC spectra.

The relative stereochemistry of **1** was deduced by the NOESY (**Figure 2**) experiment. If H<sub>A</sub>-13 were in  $\beta$ -configuration, the correlations of H<sub>A</sub>-13 with 16-OH, H-11 with H-17, and H<sub>B</sub>-13 with H-18 revealed that H-11 and 17-CH<sub>3</sub> were in  $\beta$ -configuration, and 18-CH<sub>3</sub> was in  $\alpha$ -configuration. Thus, the structure of **1** was determined.

**Table 1** The <sup>1</sup>H and <sup>13</sup>C NMR data of compound **1** (500MHz,  $\delta$  ppm, CDCl<sub>3</sub>, TMS)

	<sup>1</sup> H	<sup>13</sup> C		<sup>1</sup> H	<sup>13</sup> C		<sup>1</sup> H	<sup>13</sup> C
1		135.9s	8	6.76(s)	100.3d		16	85.8s
1a		121.8s	9		165.4s		17	20.8q
2		149.6s	9a		102.4s		18	0.88(s)
3		181.2s	9b		127.3s	2-OCH <sub>3</sub>	4.13(s)	60.9q
3a		106.7s	10		197.2s	6-OCH <sub>3</sub>	4.10(s)	56.3q
3b		124.6s	11	4.56(s)	81.1d	7-OCH <sub>3</sub>	4.08(s)	56.2q
4		169.9s	12		55.4s	11-OCH <sub>3</sub>	3.92(s)	60.6q
5	6.77(s)	99.5d	12a		139.6s	14-OH	4.83(s)	
6		164.5s	13	H <sub>A</sub> 2.94(d, 13.5)	46.3t	16-OH	5.60(s)	
6a		112.1s		H <sub>B</sub> 1.84(d, 13.5)		4-OH	15.19(s)	
7		164.1s	14		80.5s	9-OH	12.71(s)	
7a		115.4s	15	3.85(s)	58.2d			

## References

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