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臭牡丹中一个新的过氧化物*

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摘要: 从四川眉山地区产的臭牡丹(*Clerodendrum bungei* Steud.)地上部分分离到一个新的过氧化物, 命名为 bungein A. 其结构通过各项波谱分析得到鉴定. 这是首次从马鞭草科赪桐属植物中分到的过氧化物。

关键词: 马鞭草科; 臭牡丹; 过氧化物; bungein A
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A New Peroxide Compound from *Clerodendrum bungei* *

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Abstract: A new peroxide compound, bungein A, was isolated from the aerial parts of *Clerodendrum bungei* Steud. collected at Meishan County, Sichuan, China. Its structure was elucidated by the spectroscopic methods. The peroxide compound was obtained from *Clerodendrum* genus for the first time.

Key words: *Clerodendrum bungei*; Verbenaceae; Peroxide compound; Bungein A

Clerodendrum bungei Steud., a shrub in the Verbenaceae family, distributed widely in most provinces of China. It has been used as folk medicine to treat headache, dizziness, furuncle (Wu *et al*, 1977) and hysteroptosis (Zhou *et al*, 1982) for a long time. Up to now, only a few papers (Zhou *et al*, 1982; He *et al*, 1997) concerned the chemical study of this plant. In order to find its biologically active components, this medicinal plant was reinvestigated carefully.

The study on *Clerodendrum bungei* led to the isolation and characterization of a new peroxide compound, bungein A.

Bungein A (**1**), no optical rotation, was obtained as colorless wax. Its molecular formula ($C_{16}H_{18}O_4$) was deduced from EIMS spectrum (m/z 274 $[M]^+$) and ^{13}C NMR spectrum. The IR absorption bands pointed to the presence of free hydroxyl groups (3147-3391 cm^{-1}) and aromatic rings (1599, 1512 and 819 cm^{-1}). The UV spectrum of **1** showed absorption maxims at 224, 278.5 and

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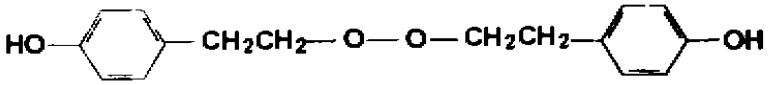
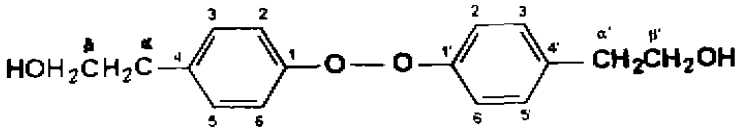
281.5 nm, which also suggested the existence of benzene moieties. Its ^{13}C NMR (Table 1) spectrum revealed only six carbon signals in **1**: two quaternary carbons (156.5 and 130.8 ppm), two methines (δ130.7 and 115.8 ppm), and two methylenes (δ64.2 and 39.3 ppm), exhibiting that **1** was a symmetric molecular. Its ^{1}H NMR (Table 1) spectrum displayed four groups of proton signals: δ7.03 (4H, dd, J = 8.4 and 2.9 Hz) and 6.73 (4H, dd, J = 8.4 and 2.9 Hz) due to aromatic protons, δ3.69 (4H, t, J = 7.2 Hz) owing to two equivalent methylenes bearing oxygen and 2.70 (4H, t, J = 7.2 Hz) assigned to two equivalent methylenes. Analysis of the coupling pattern of protons indicated the presence of some partial structures such as **A** and **B** (Fig. 1). From the above discussion, two possible structures **C** and **1** (Fig. 1) were suggested. In addition, **1** gave positive reaction with the reagent of Farbentwickler 3 merk; and after reacting with triphenyl phosphine, the above reaction was negative. It indicated 1 was a peroxide compound (Lou *et al*, 1997). This conclusion was also supported by the downfield carbon signals δ156.5 ppm (C-1 and C-1').

A　　B



C



1

Table 1　The ^{1}H and ^{13}C NMR spectral data of compound **1** in CD_3COCD_3

(400 MHz and 100.6 MHz, δ from TMS, J in Hz)

H/C	δ_H	δ_C
1, 1'		156.5 (s)
2, 6, 2', 6'	6.73 (4H, dd, J = 8.4, 2.9)	115.8 (d)
3, 5, 3', 5'	7.03 (4H, dd, J = 8.4, 2.9)	130.7 (d)
4, 4'		130.8 (s)
α, α'	2.70 (4H, t, J = 7.2)	39.34 (t)
β, β'	3.69 (4H, t, J = 7.2)	64.21 (t)

Moreover, further examination of the EIMS spectrum (m/z 274 $[M]^+$ (27), 256 $[M - H_2O]^+$ (4.5), 243 $[M - CH_2OH]^+$ (45), 225 $[256 - CH_2OH$ or $243 - H_2O]^+$ (23) and 138 (19)) of **1** excluded the structure **C**, since it can not explain the fragmentation pattern of EIMS of **1**. Accordingly, bungein A was identified as **1**. The structure of **1** containing a symmetric center and surface was consistent with no optical rotaion.

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