

This article was downloaded by:

On: 22 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Journal of Asian Natural Products Research

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713454007>

A new phenanthraquinone from the stems of *Bauhinia variegata* L.

Y. -Y. Zhao; C. -B. Cui; B. Cai; B. Han; Q. -S. Sun

To cite this Article Zhao, Y. -Y. , Cui, C. -B. , Cai, B. , Han, B. and Sun, Q. -S.(2005) 'A new phenanthraquinone from the stems of *Bauhinia variegata* L.', Journal of Asian Natural Products Research, 7: 6, 835 — 838

To link to this Article: DOI: 10.1080/10286020410001721140

URL: <http://dx.doi.org/10.1080/10286020410001721140>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

A new phenanthraquinone from the stems of *Bauhinia variegata* L.

Y.-Y. ZHAO†‡, C.-B. CUI¶*, B. CAI†, B. HAN† and Q.-S. SUN‡*

†The School of Traditional Chinese Materia Medica, Shenyang Pharmaceutical University, Shenyang 110016, China

‡Marine Drug and Food Institute, Ocean University of China, Qingdao 266003, China

¶Beijing Institute of Pharmacology and Toxicology (AMMS), Beijing 100850, China

(Received 13 January 2004; revised 14 April 2004; in final form 21 April 2004)

A new phenanthraquinone, named bauhinione (**1**), has been isolated from *Bauhinia variegata* L., and its structure has been elucidated as 2,7-dimethoxy-3-methyl-9,10-dihydrophenanthrene-1,4-dione on the basis of spectroscopic analysis.

Keywords: Bauhinione; Phenanthraquinone; Leguminosae; *Bauhinia variegata*

1. Introduction

The genus *Bauhinia* (Leguminosae) consists of about 40 species distributed in the south and southwest region of China. Many species are used in Yunnan folk medicine for the treatment of rheumatism. Few components of *Bauhinia variegata* L. have been studied [1]. During our screening for new antitumor constituents from natural sources, the extract of the stems of *Bauhinia variegata* L. showed antitumor activity on human myeloid leukemia K562 cells and a new compound named bauhinione (**1**) was then obtained. This is the first time a quinone has been obtained from this genus. The structural elucidation of compound **1** is described in this paper.

2. Results and discussion

Bauhinione (**1**) was isolated as orange colored needles, mp 130–131°C. It has a molecular formula of C₁₇H₁₆O₄, on the basis of a quasi-molecular ion peak [M + NH₃]⁺ at *m/z* 301.1310 in the positive ion HR-ESIMS spectrum. In the ¹H NMR spectrum of **1**, the ABX-type signals at δ 6.71 (1H, dd, *J* = 8.4, 2.9 Hz), 6.69 (1H, d, *J* = 2.9 Hz) and

*Corresponding authors. E-mail: cuicb@sohu.com; sunqishi@sina.com

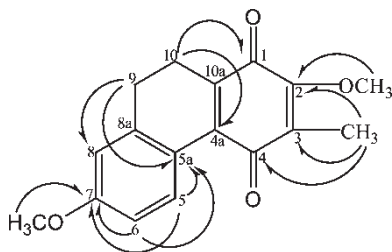


Figure 1. Key HMBC correlations of **1**.

7.13 (1H, d, $J = 8.4$ Hz) show the presence of a 1,3,4-trisubstituted benzene ring. In addition, the ^1H NMR spectrum exhibits a methyl singlet at δ 1.98 (3H, s), two methoxys at δ 3.79 (3H, s) and 3.98 (3H, s) as well as two methylene signals at δ 3.01 (2H, m) and 2.78 (2H, m). The ^{13}C NMR and DEPT spectra showed 17 carbon signals: one methyl, two methoxys, two methylenes, six aromatic carbons, four olefinic quaternary carbons and two carbonyl carbons, suggesting a trisubstituted benzene ring and a quinone moiety in the molecule. This was supported by IR absorption bands at 1663 and 1644 ($\text{C}=\text{O}$) cm^{-1} and the characteristic UV absorptions at λ_{max} 201, 276 and 342 nm.

In the ^1H - ^1H COSY spectrum of **1**, the signal of H-9 correlates with H-10, indicating a $-\text{CH}_2-\text{CH}_2-$ unit. In the HMBC spectrum (figure 1), H-9 shows long-range correlations with C-5a and C-8, and H-10 is correlated with C-4a and C-1. These facts reveal connections between C-9 and C-8a, and between C-9 and C-10a. Furthermore, the HMBC spectrum shows correlations of the methyl protons with C-2, C-3 and C-4, as well as two methoxy signals with C-2 and C-7, respectively. Thus, the methyl group was assigned to C-3 and the two methoxy groups to C-2 and C-7. Considering the ten degrees of unsaturation of the molecule and chemical shifts of C-4a and C-5a, the connection between C-4a and C-5a was established. Therefore, the structure of **1** is formulated as 2,7-dimethoxy-3-methyl-9,10-dihydrophenathrene-1,4-dione (figure 2).

3. Experimental

3.1 General experimental procedures

Melting points were measured on XT micromelting point apparatus and are uncorrected. UV spectra were determined on a Shimadzu UV-2501PC UV-VIS spectrophotometer and IR spectra were taken on a Bio-Rad FTS3000. Both 1D and 2D NMR spectra were taken on

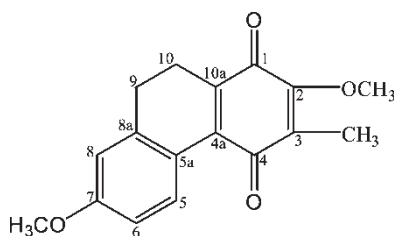


Figure 2. Compound **1**.

a Jeol Eclips-600 instrument with TMS as internal reference. ESI-MS was measured on an Esquire LC mass spectrometer.

3.2 Plant material

The plant material was collected in the Mengla area of Yunnan province, China, in September 1999, and identified as *Bauhinia variegata* L. by Professor Q.-S. Sun of Shenyang Pharmaceutical University, China. A voucher specimen has been deposited at the Herbarium of the Shenyang Pharmaceutical University, China.

3.3 Extraction and isolation

Dried, powdered *B. variegata* L. stems (8.4 kg) were extracted with 95% EtOH (3 ×) to give a crude extract (1.8 kg). The whole extract was then suspended in water and extracted successively with CHCl₃, EtOAc and n-BuOH. The CHCl₃ extract (45 g) was subjected to vacuum liquid chromatography over silica gel and eluted with light petroleum–acetone (from 100:1 to 1:1) and CHCl₃–MeOH (from 10:1 to 1:1) to give Fractions 1–9. Fraction 2 (1.4 g) was chromatographed on a silica-gel column and eluted with n-hexane–EtOAc (from 100:2 to 100:5) to obtain fractions A–D; the orange fraction C was further subjected to ODS column chromatography and eluted with MeOH–H₂O (4: 6) to yield **1** (5 mg).

Bauhinione (**1**): C₁₇H₁₆O₄, orange needles, mp 130–131°C. UV (MeOH) λ_{max} (nm) (log ε): 202 (4.25), 227 (3.75), 278 (3.87), 340 (3.00); IR (KBr) ν_{max} (cm⁻¹): 2950, 2937, 2922, 1663, 1644, 1613, 1496, 1429, 997, 980, 866, 812. ¹H and ¹³C NMR data see table 1. ESIMS *m/z* 323 [M + K]⁺, 301 [M + NH₃]⁺. HRESIMS *m/z* [M + NH₃]⁺ 301.1310 (calcd for C₁₇H₁₆O₄ + NH₃, 301.1314).

Table 1. ¹H (600 MHz) and ¹³C (150 MHz) NMR spectral data of **1** in CDCl₃.

Positions	δ _H (J in Hz)	¹ H– ¹ H COSY	δ _C (ppm)	HMBC	
				² J _{CH} (Hz)	³ J _{CH} (Hz)
1	–	–	183.94 s	–	10
2	–	–	155.59 s	–	2–OCH ₃ , 3–CH ₃
3	–	–	126.47 s	3–CH ₃	–
4	–	–	183.07 s	–	3–CH ₃
4a	–	–	152.80 s	–	10
5a	–	–	149.65 s	5	6, 8, 9
5	7.13 d (8.4)	6	121.75 d	–	–
6	6.71 dd (8.4, 2.9)	5, 8	112.22 d	–	8
7	–	–	156.95 s	8	5, 7–OCH ₃
8	6.69 d (2.9)	6	114.23 d	–	6, 9
8a	–	–	134.21 s	9	5, 10
9	3.01 (2H) m	10	29.93 t	10	8
10	2.78 (2H) m	9	26.05 t	9	–
10a	–	–	122.96 s	10	9
3–CH ₃	1.98 s	–	8.67 q	–	–
2–OCH ₃	3.98 s	–	61.08 q	–	–
7–OCH ₃	3.79 s	–	55.61 q	–	–

Acknowledgements

This work was financially supported by the Fund from the National Natural Science Foundation of China (no. 39825126), the Fund for the 973-Project from the Ministry of Science and Technology of China (no. 1988051113), and the Fund from the Chung Kong Scholars Program administered by the Ministry of Education of China.

References

- [1] A.K. Gupta, T.J. Vidyapati, J.S. Chauhan. *Planta Med.*, **38**, 174 (1980).