Available online at www.sciencedirect.com
SCIENCE DIRECT
Biochemical Systematics and Ecology 33 (2005) 551–554
biochemical systematics and ecology
www.elsevier.com/locate/biochemsyseco

Benzoxazinoid glucosides from *Baphicacanthus cusia*

Haihui Xie[a], Huanhuan Wei[a], Masayuki Yashikawa[b], Nianhe Xia[a], Xiaoyi Wei[a,*]

[a]*South China Botanical Garden, Chinese Academy of Sciences, Guangzhou 510650, China*
[b]*Kyoto Pharmaceutical University, Misasagi, Yamashina-ku, Kyoto 607-8412, Japan*

Received 26 March 2004; accepted 20 August 2004

Keywords: *Baphicacanthus cusia*; *Strobilanthes cusia*; Strobilanthinae; Acanthaceae; Benzoxazinoids

1. Subject and source

Baphicacanthus cusia (Nees) Bremek. (Acanthaceae, subfamily Ruellioideae, tribe Ruellieae and subtribe Strobilanthinae), sometimes assigned to the genus *Strobilanthes* as *Strobilanthes cusia* (Nees) O. Kuntze, is a herbaceous plant native to northeast India, Myanmar, Thailand, and southern part of China (Hu et al., 2002). Its roots were collected from Dinghushan, Guangdong, China in June 2001. An authenticated voucher specimen (HC160580) was deposited at the herbarium of South China Botanical Garden, Chinese Academy of Science, Guangzhou, China.

* Corresponding author. Tel.: +86 20 37252638; fax: +86 20 37252615.
E-mail address: wxy@scbg.ac.cn (X. Wei).

doi:10.1016/j.bse.2004.08.008

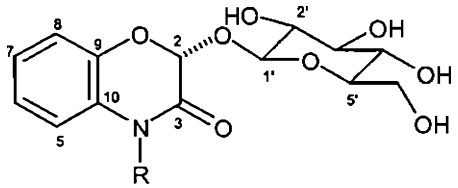
2. Previous work

Indigoid indole alkaloids, quinazolinone alkaloids, triterpenes, and sitosterols had been reported (Honda and Tabata, 1979; Chen et al., 1987; Li et al., 1993; Yang et al., 1995).

3. Present study

Powdered dry roots of *B. cusia* (4.7 kg) were extracted with MeOH. The resulting MeOH solution was concentrated under vacuum. The residue (350 g) was suspended in H_2O and partitioned successively with petroleum ether, EtOAc, and *n*-BuOH. The *n*-BuOH extract (52.1 g) was subjected to silica gel column chromatography (CC) eluted with $CHCl_3$–MeOH–H_2O mixtures (10:3:1, 7:3:1, and 6:4:1) of increasing polarities, to obtain seven fractions (I–VII). Fraction IV (5.4 g), obtained on elution with $CHCl_3$–MeOH–H_2O (7:3:1), was rechromatographed on an ODS column eluted with MeOH–H_2O mixtures (3:7, 1:1, and 7:3) to obtain four subfractions (IV-1–IV-4). Part (0.77 g) of subfraction IV-2 (total 2.8 g) was separated by HPLC (column: Develosil C30-UG-5; mobile phase: 10% aqueous CH_3CN) to afford **1** (102.8 mg) and **2** (72.7 mg).

The isolated compounds were identified as (2*R*)-2-*O*-β-D-glucopyranosyl-2*H*-1,4-benzoxazin-3(4*H*)-one (**1**) (Kanchanapoom et al., 2001; Tietze et al., 1991) and (2*R*)-2-*O*-β-D-glucopyranosyl-4-hydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one (**2**) (Hartenstein and Sicker, 1994; Kanchanapoom et al., 2001) by interpretation of their spectral (FABMS, HRFABMS, 1D NMR, and 2D NMR) data as well as by comparison of their data with those published.



1 R = H
2 R = OH

(2*R*)-2-*O*-β-D-Glucopyranosyl-2*H*-1,4-benzoxazin-3(4*H*)-one (**1**): white amorphous powder, $[\alpha]_D^{25}$ +89.0 (*c* 0.5, MeOH); FABMS (positive ion mode): *m*/*z* 328 $[M + H]^+$, 166 $[M + H - Glc]^+$; HRFABMS: *m*/*z* 328.0860 $[M + H]^+$ (calcd for $C_{14}H_{18}NO_8$, 328.1032); ^1H (500 MHz) and ^{13}C (125 MHz) NMR: see Table 1.

(2*R*)-2-*O*-β-D-Glucopyranosyl-4-hydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one (**2**): white amorphous powder, $[\alpha]_D^{25}$ +80.1 (*c* 1.0, MeOH); FABMS (positive ion mode): *m*/*z* 344 $[M + H]^+$, 182 $[M + H - Glc]^+$; HRFABMS: *m*/*z* 344.0827 $[M + H]^+$ (calcd for $C_{14}H_{18}NO_9$, 344.0982); ^1H (500 MHz) and ^{13}C (125 MHz) NMR: see Table 1.