

## A Novel Dihydroflavone from the Roots of *Uvaria Macrophylla*

Si WANG, Pei Cheng ZHANG, Ruo Yun CHEN, Ying Hong WANG, Wen Yi HE,  
De Quan YU\*

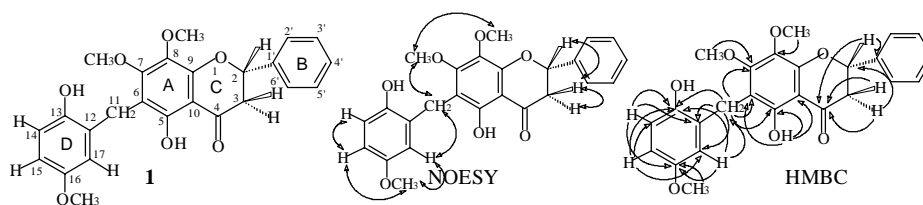
Institute of Materia Medica, Chinese Academy of Medical Sciences &  
Peking Union Medical College, Beijing 100050

**Abstract:** A new dihydroflavone (**1**), named macrophyllol A, was isolated from the roots of *Uvaria macrophylla*. Its structure was elucidated on the basis of spectroscopic evidence.

**Keywords:** *Uvaria macrophylla*, macrophyllol A.

*Uvaria macrophylla* (Annonaceae) is a tropical plant, widely distributed in Hainan, Guangdong and Guangxi provinces of southern China<sup>1</sup>. In the course of our ongoing screening for anticancer agents from Annonaceous plants, an ethanolic extract of the roots of the titled plant was found to possess strong cytotoxic activities against a number of human cancer cell lines. Purification of this extract yielded a new dihydroflavone, named macrophyllol A (**1**), together with nineteen known compounds including two dihydroflavones, three acetogenins, six polyoxygenated cyclohexens and eight alkaloids<sup>2-4</sup>. In this paper, we report the structure elucidation of the new compound by spectroscopic analysis.

**Figure 1** Structure and key HMBC and NOESY correlations for **1**



Macrophyllol A (**1**) was isolated as yellow powder, mp 124 -127°C,  $[\alpha]_D^{23}$  -67 (c 0.14, MeOH). Its molecular formula was determined as  $C_{25}H_{24}O_7$  by HREIMS,  $m/z$  436.1501  $[M]^+$  (calcd. 436.1522). The IR spectrum (KBr,  $cm^{-1}$ ) displayed absorption bands for hydroxyl (3467), carbonyl (1647) and aromatic moiety (1620 and 1500). Its UV spectrum exhibited characteristic absorptions for dihydroflavone  $[\lambda_{max}$  (log $\epsilon$ ): 285

\*E-mail: dqyu@imm.ac.cn

(4.56) and 204 (4.92) nm]. The  $^1\text{H}$  NMR spectrum of **1** showed the presence of a phenolic hydroxyl at  $\delta$  12.33 (s) ascribed to 5-OH, the signals at  $\delta$  7.38-7.68 (m, 5H) were assigned to the protons of ring B, the signals at  $\delta$  5.74 (dd, 1H,  $J = 13.5, 3.0$  Hz), 3.31 (dd, 1H,  $J = 17.6, 13.5$  Hz) and 2.96 (dd, 1H,  $J = 17.6, 3.0$  Hz) consisting of ABX system to H-2, H-3 $\alpha$  and H-3 $\beta$ , and the signals of another simplified ABX system at  $\delta$  6.48 (d, 1H,  $J = 2.7$  Hz), 6.61 (dd, 1H,  $J = 8.4, 2.7$  Hz) and 6.78(d, 1H,  $J = 8.4$ Hz) to the protons of ring D. The  $^{13}\text{C}$  and DEPT NMR spectra revealed 25 carbon signals including three primary, two secondary, nine tertiary and eleven quarternary carbons. Observation of the HMBC correlations of the protons at  $\delta$  3.91 (s, 2H) with the carbons at  $\delta$  160.9, 157.8, 149.8, 128.8, 115.7 and 114.3 suggested that a benzyl was linked to C-6 position, similarly the two methoxyl at  $\delta$  3.83(s, 3H) and 3.98(s, 3H) were determined to be located at C-7 and C-8 position respectively. In the NOESY spectrum, the aromatic proton at  $\delta$  6.48 (d, 1H,  $J = 2.7$ Hz) was correlated to the protons at  $\delta$  3.66 (s, 3H) and 3.91 (s, 2H) indicating that the methoxyl residue was substituted to C-16 position. The left hydroxyl should be attached to C-13 position according to its formula.

**Table 1.**  $^1\text{H}$  (500MHz) and  $^{13}\text{C}$  (125MHz) NMR data of **1** in  $\text{CD}_3\text{COCD}_3$

Position	$\delta_{\text{H}}$ J (Hz)	$\delta_{\text{C}}$	Position	$\delta_{\text{H}}$ J (Hz)	$\delta_{\text{C}}$
2	5.74 dd (13.5, 3.0)	80.1	14	6.78 d (8.4)	115.8
3	2.96 dd (17.6, 3.0)	44.0	15	6.61 dd (8.4, 2.7)	112.6
	3.31 dd (13.5, 17.6)		6		154.3
4		198.5	17	6.48 d (2.7)	115.7
5		157.8	1'		140.1
6		114.3	2'	7.68 m	128.5
7		160.9	3'	7.52 m	130.5
8		134.8	4'	7.41 m	130.5
9		155.2	5'	7.52 m	130.5
10		105.6	6'	7.68 m	128.5
11	3.91s	24.2	7-OCH <sub>3</sub>	3.98 s	61.7
12		128.8	8-OCH <sub>3</sub>	3.83 s	61.5
13		149.8	16-OCH <sub>3</sub>	3.66 s	55.8

## References

1. Editing Board of Flora of People's Republic of China, Chinese Academy of Sciences, *Flora of Reipublicae Popularis Sinicae* (in Chinese), Science Press, **1979**, 30 (2), 22.
2. H. L. Zhang, R. Y. Chen, *Chin. Chem. Lett.*, **2001**, 12 (9), 791.
3. H. N. Sohly, W. L. Lasswell, D. Hufford, *J. Nat. Prod.*, **1979**, 42, 264.
4. G. X. Zhou, L. E. Zhou, R. Y. Chen, D. Q. Yu, *J. Nat. Prod.*, **1999**, 62, 261.

Received 22 November, 2001