A New Flavanone from the Bark of *Morus macoura* Miq.

Sheng Guo SUN, Ruo Yun CHEN*, De Quan YU

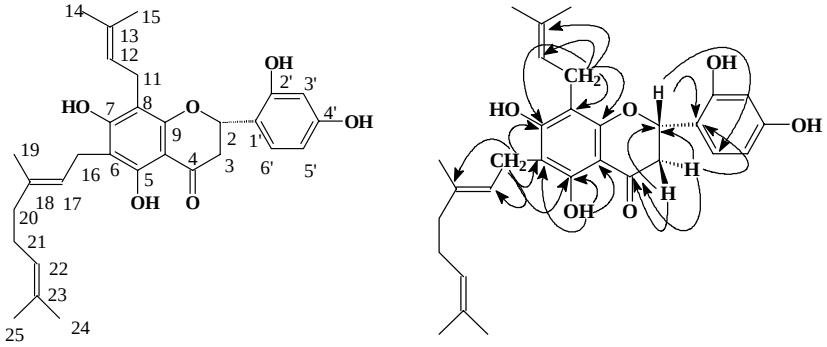
Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing 100050

Abstract: A new flavanone named macrouroine **C** (**1**) was isolated from the bark of *Morus macroura* Miq.. The structure of **1** was elucidated mainly on the basis of spectroscopic evidence.

Keywords: *Morus macroura* Miq., flavanone, macrourone **C**.

"Sang Bai Pi", the bark of mulberry, has been used as herbal medicine to treat diabetes, arthritis, rheumatism for thousands of years. Phytochemical studies on some *Morus* species revealed that they contained phenolic compounds[1]. Macrourone **C** (**1**) was isolated from *Morus macroura* Miq. In this paper, the structure of **1** was elucidated on the basis of spectoscopic evidence.

Figure 1 Structure and Key HMBC for **1**



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Macrourone **C** (**1**), a yellow powder, exhibited dark blue fluorescence under UV light at 254 nm, mp 128 °C (dec.). The HREI-MS of **1** give M^+ at *m/z* 492.2517 corresponding to the molecular formula $C_{30}H_{36}O_6$ (for $C_{30}H_{36}O_6$, calcd. 492.2512). The IR spectrum of **1** showed the presence of hydroxyls (3384 cm^{-1}, br), aromatic groups (1603, 1450cm^{-1}) and a carbonyl group (1630 cm^{-1}). The UV spectrum of **1** [λ_{max}^{EtOH} (logε) 204 (4.00), 295 (3.45) nm] suggested the flavanone skeleton. In the ^{1}H-NMR spectrum of **1**, there was one proton singlet at δ 12.36 being typical of C-5 hydroxyl correlated to C-(5, 6, 10) in the HMBC analysis. Besides, there was only one set of ABX

system signals in the downfield region: δ 6.45 (1H, d, *J* = 2.0 Hz, 3′-H), 6.42 (1H, dd, *J* = 2.0, 8.5 Hz, 5′-H) and 7.09 (1H, d, *J* = 8.5 Hz, 6′-H). So B ring must be a 2,4-dihydroxybenzene and the protons of A ring must all be substituted. Furthermore, there was another ABX system signals at δ 2.86 (1H, dd, *J* = 2.5, 17.0 Hz, 3-βH), 3.12 (1H, dd, *J* = 13.0, 17.0 Hz, 3-αH) and 5.53 (1H, dd, *J* = 2.5, 13.0 Hz, 2-H) in the ^{1}H-NMR. The ^{13}C–NMR datum of **1** was corresponding with its ^{1}H-NMR, showing a carbonyl group signal at δ 196.7, C-2 and C-3 signals at δ 77.5 and 41.9 respectively. The ^{1}H and ^{13}C -NMR spectra of **1** also indicated the presence of a 3-methyl-2-butenyl (prenyl) moiety which was similar to that of enchrenone $\mathbf{a}_7$[2] and a 3,7-dimethyl-2, 6-octanedienyl (geranyl) group similar to that of kuwanon **E**[3]. In the HMBC spectrum of **1**, the CH long-range correlation between H-11/C- (7, 8, 9, 12, 13) and H-16/C- (5, 6, 7, 17, 18) suggested that the prenyl was linked to C-8 and the geranyl linked on C-6. The absolute configuration at C-2 was determined as S by CD analysis, which showed a positive Cotton effect at 315 ($\Delta\varepsilon$ 0.58), a negative Cotton effect at 293 ($\Delta\varepsilon$ -9.77) (peak) and a positive Cotton effect at 258 ($\Delta\varepsilon$ 0.41) nm[4]. Based on the above evidence, the structure of **1** was established and named as macrourone **C**.

Table 1 ^{1}H-NMR and ^{13}C-NMR Chemical Shift for Macrourone **C** (**1**)

NO.	H[a]	C[b]	NO.	H[a]	C[b]
2	5.53 dd (13.0, 2.5)	77.5	17	5.14 t (7.0)	121.8
3	α 3.12 dd (17.0, 13.0)	41.9	18		139.3
	β 2.86 (17.0, 2.5)		19	1.82 s	16.2
4		196.7	20	2.60 m	39.7
5	OH 12.36 s	159.4	21	2.60 m	26.3
6		107.3	22	5.04 t (7.5)	123.9
7		162.4	23		132.0
8		107.2	24	1.69 s	25.8
9		157.0	25	1.60 s	17.8
10		102.7	1´		116.9
11	3.28 d (7.0)	21.8	2´		155.4
12	5.24 t (7.0)	121.3	3´	6.45 d (2.0)	104.3
13		138.8	4´		157.1
14	1.71 s	25.7	5´	6.42 dd (8.5, 2.0)	107.8
15	1.69 s	17.7	6´	7.09 d (8.5)	128.0
16	3.38 d (7.0)	21.2			

[a]Recorded at 500 MHz in $CDCl_3$, [b]Recorded at 125 MHz in $CDCl_3$. Coupling constants (*J*) are in parentheses.

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