A New Isoprenylated flavonol from the Leaves of *Broussonetia kazinoki*

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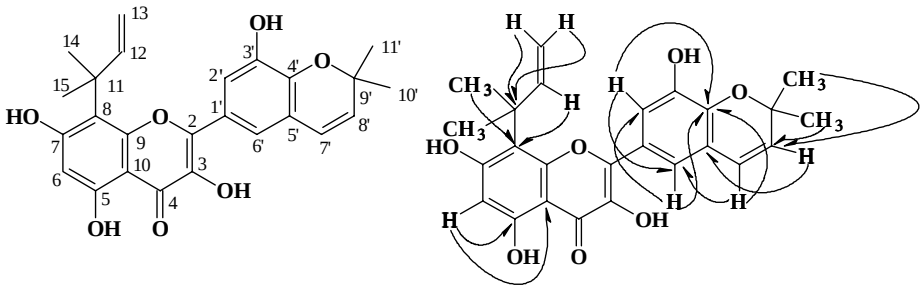
Abstract: A new isoprenylated flavonol, named broussonol A (**1**) was isolated from the leaves of *Broussonetia kazinoki* Sieb. The structure of broussonol A was characterized by chemical and spectral methods.

Keywords: *Broussonetia kazinoki*, moraceae, isoprenyl flavonol, broussonol A.

Broussonetia kazinoki Sieb (Moraceae) is distributed throughout China and Japan. Previous investigations of this plant revealed the presence of isoprenylated flavans, isoprenylated flavonoids, isoprenylated 1,3-diphenylpropanes[1] and alkaloids[2,3]. Natural prenylated flavonoids have shown potent inhibition against human hepatoma PLC/PRF/5 and epidermoid carcinoma KB cells in *vitro*[4]. In order to search for its biologically active compounds, chemical study on this plant was carried out and led to the isolation of a new isoprenylated flavonol, named broussonol A (**1**).

Figure 1 Strccture and key HMBC for **1**



Broussonol A (**1**) was obtained as yellow powder, mp 162-164°C, exhibiting a positive ferric chloride test and magnesium hydrochloric acid test. The IR spectrum of **1** showed the presence of hydroxyl groups [3430 (br) and 3269 (sh) cm^{-1}], aromatic rings [1589 and 1549 cm^{-1}], and a conjugated carbonyl group [1651 cm^{-1}]. The HREIMS of

1indicated a molecular ion peak at *m/z* 436.1546 , which corresponded to a molecular formula $C_{25}H_{24}O_7$. The ^{1}H NMR spectrum of **1** (**Table 1**) indicated the presence of a 1,1-dimethylallyl group at δ 1.68 (6H, s, 2 CH_3), 4,88 (1H, d, *J*=10.0 Hz), 4.93 (1H, d, *J*=17.5 Hz), and 6.35 (1H, dd, *J*=10.0, 17.5 Hz) and a 2,2-dimethylpyran ring at δ 1.46 (6H, s, 2 CH_3), 5.82 (1H, d, *J*=9.6 Hz), and 6.47 (1H, d, *J*=9.6 Hz), as well as three aromatic proton signals at δ 6.33 (1H, s, H-6), 7.71 (1H, d, *J*=2.1Hz, H-2′), and 7.51 (1H, d, *J*=2.1Hz, H-6′) and four phenolic hydroxyl proton signals at δ 12.52 (1H, s, 5-OH), 9.37 (1H, s, 7-OH) and 7.80 (2H, s, 3, 3′-OH). EIMS of **1** showed a molecular ion peak at *m/z* 436 $[M]^+$ and significant fragments at *m/z* 421$[M\text{-}CH_3]^+$, 393, 353. The ^{13}C NMR data (**Table 1**) showed 25 carbons, the number of carbons suggesting a flavonoid nucleus and two prenyl groups. The chemical shift value of the carbonyl carbon (δ 176.5) was similar to those of flavonols[5]. The chemical shift values of C-2 to C-10 were similar to those of the corresponding data for 8-isoprenyl-5,7-dihydroxylflavonol[5]. The carbon signals of 8-prenyl group appeared at δ 30.4 (CH_3), 30.4 (CH_3), 41.8 (C), 150.9 (CH) and 109.6 (CH_2), indicating that 8-prenyl group was 1,1-dimethyallyl. The substitution patterns of a hydroxyl group and 2,2-dimethyl chromene group in ring B were determined at C-3′, C-4′ and C-5′ positions by HMQC and HMBC (**Figure 1**). All these results indicated that the structure of broussonol A is represented by formula **1**.

Table 1 ^{1}H and ^{13}NMR spectral data for **1** (acetone-d_6, multiplicity, *J*, Hz)

Position	^{1}H	^{13}C	Position	^{1}H	^{13}C
2		147.4	15	1.68s	30.4
3	7.80 (OH)	136.6	1′		124.2
4		176.7	2′	7.71d(2.1)	116.9
5	12.52 (OH)	160.1	3′	7.80s(OH)	146.0
6	6.33s	100.3	4′		142.7
7	9.37 (OH)	163.4	5′		122.0
8		111.8	6′	7.51d (2.1)	118.9
9		156.2	7′	6.47d (9.6)	122.6
10		105.1	8′	5.82d (9.6)	132.2
11		41.8	9′		78.0
12	6.35dd (10.0, 17.5)	150.9	10′	1.46s	28.1
13	4.88d (10.0) 4.93d (17.5)	109.6	11′	1.46s	28.1
14	1.68s	30.4			

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