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A New Phenylpropanoid from the Leaves of Flue-Cured Tobacco and Its Anti-Tobacco Mosaic Virus Activity

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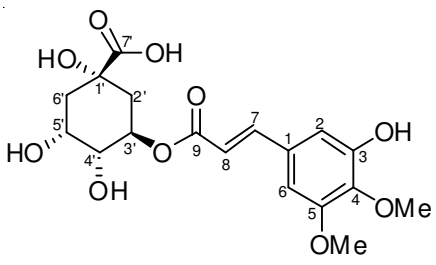
A new phenylpropanoid, nicotpanoid C (**1**), was isolated from the leaves of flue-cured tobacco (a variety of *Nicotiana tabacum* L). Its structure was elucidated by spectroscopic methods, including extensive 1D and 2D NMR techniques. Compound **1** was tested for its anti-tobacco mosaic virus (anti-TMV) activity and it shows modest anti-tobacco mosaic virus activity with inhibition rates of 22.4 %.

Keywords: Phenylpropanoid, Flue-cured tobacco, Anti-tobacco mosaic virus activity.

INTRODUCTION

Nicotiana tabacum L. is one of the most commercially valued agricultural crops in the world[1,2]. In addition to being used in cigarette industry, *N. tabacum* is also used as insecticide, anesthetic, diaphoretic, sedative and emetic agents in Chinese folklore medicine because of it containing many useful chemical compounds[1,3-5].

In previous work, a number of bioactive compounds, such as terpenoids[6-8], alkaloids[9,10], lignans[11,12], flavonoid[13], phenylpropanoids[14-16], and the homologous, were isolated from this plant. Motivated by search for bioactive metabolites from this plant, the investigation on the chemical constituents of the leaves of flue-cured tobacco (a variety of *Nicotiana tabacum* L) was carried out. As a result, a new phenylpropanoid, nicotpanoid C (**1**), was isolated from this plant. In addition, the anti-tobacco mosaic virus (anti-TMV) activity of **1** was evaluated. This article deals with the isolation, structural elucidation and biological activities of this new compound.



Structures of compound **1**

EXPERIMENTAL

Optical rotation was measured in Horiba SEPA-300 high sensitive polarimeter. IR spectra were obtained in KBr disc on a Bio-Rad Wininfmred spectrophotometer. ESI-MS were measured on a VG Auto Spec-3000 MS spectrometer. ^{1}H, ^{13}C and 2D NMR spectra were recorded on Bruker DRX-500 instrument with TMS as internal standard. Column chromatography was performed on silica gel (200-300 mesh), or on silica gel H (10-40 μm), Qingdao Marine Chemical Inc., China). Preparative HPLC was used an agilent 1100 HPLC equipped with ZORBAX-C_{18} (21.2 × 250 mm, 7.0 μm) column and DAD detector.

The leaves of flue-cured tobacco were collected in Yuxi Prefecture, Yunnan Province, People's Republic of China, in September 2011. The identification of the plant material was verified by Prof. Chen Y. J (Yunnan University of Nationalities).

Extraction and isolation: The air-dried and powdered leaves of oriental tobacco (2.8 kg) were extracted four times with 90 % methanol (4 × 2.5 L) at room temperature and filtered to yield a filtrate. The crude extract (151 g) was applied to silica gel (200-300 mesh) column chromatography, eluting with a $CHCl_3$-$(CH_3)_2CO$ system (20:1, 9:1, 8:2, 7:3, 6:4, 5:5), to give six fractions A - F. The further purification of fraction D (7:3, 18.3 g) by silica gel column chromatography, eluted with $CHCl_3$-MeOH (9:1, 8:2, 7:3, 6:4, 5:5), yielded mixtures D1 - D5. Fraction D2 (8:2, 1.82 g) was subjected to preparative HPLC (28 % MeOH-H_2O, flow rate 12 mL/min) to yield compound **1** (12.6 mg).

TABLE-1
^{1}H NMR AND ^{13}C NMR DATA OF COMPOUND **1** (C_5D_5N, δ, ppm, /Hz)

No.	δ_C (mult.)	δ_H (mult, *J*, Hz)	No.	δ_C (mult.)	δ_H (mult, *J*, Hz)
1	132.4 s		2'	38.3 t	2.75-2.84, overlap
2	106.8 d	6.52, d, *J* = 1.8			2.94-2.98, overlap
3	148.6 s		3'	71.6 d	6.20 m
4	139.5 s		4'	73.5 d	4.38 m
5	152.2 s		5'	70.8 d	4.82 m
6	104.9 d	6.65, d, *J* = 1.8	6'	39.0 t	2.75-2.84, overlap
7	145.2 d	7.76, d, *J* = 15.5	7'	176.8 s	10.8 brs
8	116.8 d	6.82, d, *J* = 15.5	4-OMe	55.8 q	3.79 s
9	167.8 s		5-OMe	61.2 q	3.81, s
1'	76.6 s		Ar-OH		11.85 brs

Nicotpanoid C (1): Obtained as a pale yellow gum; $[\alpha]_D^{25}$ -46.8 (*c* 0.20, MeOH); UV (MeOH), λ_{max} (log ε) 326 (3.92), 300 (3.68), 242 (4.08), 210 (4.36) nm; IR (KBr, ν_{max}, cm^{-1}) 3382, 2955, 2873, 1718, 1705, 1618, 1536, 1469, 1421, 1375, 1250, 1185, 1055, 958, 864; ^{1}H NMR and ^{13}C NMR data (C_5D_5N, 500 MHz and 125 MHz, respectively), see Table-1; ESIMS (positive ion mode), *m/z* 421 $[M+Na]^+$; HRESIMS (positive ion mode), *m/z* 421.1118 $[M+Na]^+$ (calcd. 421.1111 for $C_{18}H_{22}NaO_{10}$).

RESULTS AND DISCUSSION

Compound **1** was obtained as pale yellow gum. Its molecular formula was determined as $C_{18}H_{22}O_{10}$ by HRESIMS, *m/z* 421.1118 $[M+Na]^+$ (calcd. 421.1111), corresponding to eight degrees of unsaturation. Its ^{1}H and ^{13}C NMR spectral data (Table-1) showed signals to 22 hydrogens and 18 carbons, respectively, corresponding to one aromatic ring (δ_C 132.4 s, 106.8 d, 148.6 s, 139.5 s, 152.2 s, 104.9 d) with two aromatic protons (δ_H 6.52 (d) *J* = 1.8 and 6.65 (d) *J* = 1.8), one acryl group (δ_C 145.2, 116.8, 167.8; δ_H 7.76 (d) *J* = 15.5, 6.82 (d) *J* = 15.5), one 3-*O*-quinic acid group (δ_C 76.6 s, 38.3 t, 71.6 d, 73.5 d, 70.8 d, 39.0 t, 176.8 s; δ_H 2.75-2.84 overlap, 2.94-2.98 overlap, 6.20 m, 4.38 m, 4.82 m, 2.75-2.84 overlap, 10.8 brs), two methoxy groups (δ_C 55.8 q, 61.2 q; δ_H 3.79 s, 3.81 s) and one phenolic hydroxy group (δ_H 11.85). Strong absorption bands accounting for hydroxy (3382 cm^{-1}), carbonyl (1718, 1705 cm^{-1}) and aromatic group (1618, 1536, 1469, 1421 cm^{-1}) could be observed in its IR spectrum. The UV spectrum of **1** showed absorption maxima at 326, 300, 242 and 210 nm also confirmed the existence of the aromatic function. The HMBC correlations (Fig. 1) of H-8 (δ_H 6.82) with C-1 (δ_C 132.4), of H-7 (δ_H 7.76) with C-1 (δ_C 132.4), C-2 (δ_C 106.8) and C-6 (δ_C 104.9), of H-2 (δ_H 6.52) with C-7 (δ_C 145.2) and of H-6 (δ_H 6.65) with C-7 (δ_C 145.2) suggested the acryl (-CH=CH-COO-) unit was attached to C-1. The long-range correlations of two methoxy proton signals (δ_H 3.79 and 3.81) with C-4 (δ_C 139.5) and C-5 (δ_C 152.2) clearly indicated that two methoxy groups located at C-4 and C-5. The HMBC correlations of phenolic hydroxy proton signal (δ_H 11.85) with C-2 (δ_C 106.8), C-3 (δ_C 148.6) and C-4 (δ_C 139.5) indicated that the hydroxy group should be located at C-2. The HMBC correlation of H-3' (δ_H 6.20) with C-9 (δ_C 167.8) indicated that the 3-*O*-quinic acid group should be located at C-9. Thus, the structure of **1** was established and it was named as nicotpanoid C.

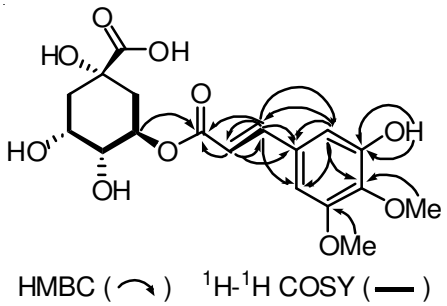


Fig. 1. The key HMBC and ^{1}H-^{1}H COSY correlations of **1**

Since certain of the phenylpropanoids exhibit potential Anti-TMV activity, compounds **1** was tested for it anti-tobacco mosaic virus activity. The anti-TMV activities were tested using the half-leaf method[17]. Ningnanmycin (2 % water solution), a commercial product for plant disease in China, was used as a positive control. The results showed that compound **1** exhibited inhibition rates of 22.4 %.

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