SUPPLEMENTARY MATERIAL

Two new benzolactones from the leaves of *Nicotiana tabacum* and their anti-tobacco mosaic virus activities

Qinpeng Shen \(^{a}\), Xingmeng Xu \(^{a,b}\), Fengmei Zhang \(^{a}\), Nengjun Xiang \(^{a}\), Pei He \(^{a}\), Xiaoxi Si \(^{a}\), Ruizhi Zhu \(^{a}\), Kunmiao Wang \(^{a}\), Zhihua Liu \(^{a}\), Chunbo Liu \(^{a*}\) and Mingming Miao \(^{a*}\)

\(^{a}\) Key Laboratory of Tobacco Chemistry of Yunnan Province, China Tobacco Yunnan Industrial Co., Ltd, Kunming 650231, P.R. China;

\(^{b}\) School of Pharmaceutical Science & Yunnan Key Laboratory of Pharmacology for Nature Products, Kunming Medical University, Kunming, Yunnan 650500, P.R. China

\(^{*}\)Corresponding author. Tel: +86 871 68315280. E-mail addresses: jszxtg_2015@163.com

**Abstract:** Two new benzolactones, 5-methyl-6-prenyl-isobenzofuran-1(3H)-one (1), 5-hydroxymethyl-6-prenyl-isobenzofuran-1(3H)-one (2), together with four known phenolic compounds (3-6), were isolated from the leaves of *Nicotiana tabacum*. Their structures were elucidated by spectroscopic methods, including extensive 1D- and 2D NMR techniques. Compounds 1-6 were evaluated for their anti-tobacco mosaic virus (anti-TMV) activities. The results showed that
compound 1-6 exhibited high anti-TMV activities with inhibition rates in the range of 16.9~26.2%, respectively.

**Keywords:** *Nicotiana tabacum*; benzolactones; anti-tobacco mosaic virus activities

*Figure S1*  
$^{13}$C NMR spectrum of 5-methyl-6-prenyl-isobenzofuran-1(3H)-one (1)
Figure S2  $^1$H NMR spectrum of 5-methyl-6-prenyl-isobenzofuran-1(3H)-one (1)
Figure S3 $^{13}$C NMR and DEPT spectra of 5-hydroxymethyl-6-prenyl-isobenzofuran-1(3H)-one (2)
Figure S4. $^{13}$C NMR and DEPT spectra of 5-hydroxymethyl-6-prenyl-isobenzofuran-1(3H)-one (2)

Figure S5. Key HMBC correlations of 1
Table S1. $^1$H NMR and $^{13}$C NMR Data (in C$_5$D$_5$N) of compounds 1 and 2

| No. | Compound 1 | | Compound 2 | |
|-----|------------| |------------|------------|
|     | $\delta$ (m) | $\delta$ (m, $J$, Hz) | $\delta$ (m) | $\delta$ (m, $J$, Hz) |
| 1   | 136.2 s    | | 133.7 s    | |
| 2   | 142.5 s    | | 146.1 s    | |
| 3   | 127.5 d    | 6.73 s                  | 125.9 d    | 6.77 s                  |
| 4   | 144.3 s    | | 145.0 s    | |
| 5   | 121.9 s    | | 122.7 s    | |
| 6   | 129.1 d    | 7.40 s                  | 130.7 d    | 7.44 s                  |
| 7   | 28.0 t     | 3.40 (d) 6.9            | 28.9 t     | 3.39 (d) 6.9            |
| 8   | 124.2 d    | 5.12 (t) 6.8            | 124.7 d    | 5.40 (t) 6.8            |
| 9   | 133.8 s    | | 133.1 s    | |
| 10  | 17.7 q     | 1.57 s                  | 16.1 q     | 1.51 s                  |
| 11  | 25.4 q     | 1.78 s                  | 26.1 q     | 1.67 s                  |
| 1’  | 16.9 q     | 2.29 s                  | 63.3 t     | 4.41 s                  |
| 2’  | 69.2 t     | 5.48 s                  | 69.0 t     | 5.50 s                  |
| 3’  | 168.1 s    | | 168.2 s    | |