

## A New Phenolic Compound from *Thamnoia vermicularis*

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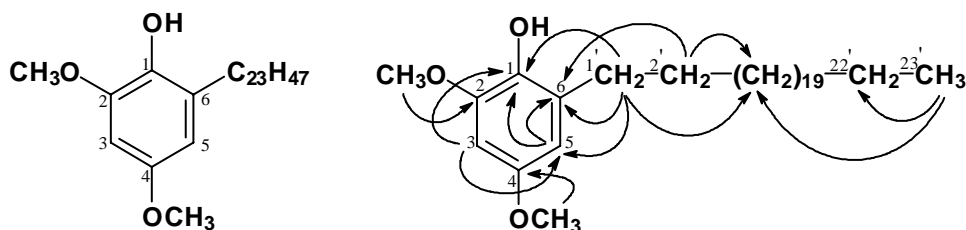
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**Abstract:** A new phenolic compound, thamnolin (**1**), was isolated from the extract of *Thamnoia vermicularis*. Its structure was determined as 6-tricosyl-2,4-dimethoxy-phenol by spectral methods.

**Keywords:** *Thamnoia vermicularis*, phenolic compound, thamnolin.

*Thamnoia vermicularis* (Sw.) Ach., an alga-fungus symbiont with a commercial name “Xuecha”, has long been used for medicinal purposes in common people of Yunnan province to cure sore throats, hypertension, cough caused by lung-heat, tidal fever due to *yin* deficiency, summer-heat and neurasthenia<sup>1</sup>. It was reported previously that several phenolic compounds, thamnolic acid<sup>2</sup>, vermicularin<sup>3</sup> and baemycesi acid<sup>3</sup>, had been isolated from this plant and some of those had been identified to be the main bio-active constituents of the plant<sup>1,3</sup>. In continuation of our research on phenolic compounds in the *Thamnoia* species, a new compound, thamnolin (**1**), as well as several known compounds, are obtained from the EtOAc extract of *T. vermicularis*. In this paper, we wish to report the structural elucidation of **1**.

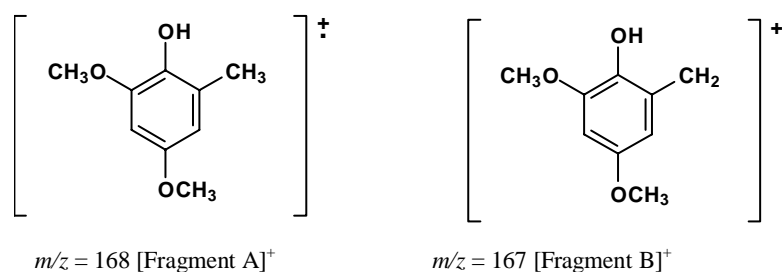
**Figure 1** Key HMBC correlations of compound **1**



Thamnolin (**1**), amorphous substance, IR (KBr)  $\nu_{\max}$  3379 (br), 2918, 2850, 1616, 1503, 1466, 1430, 1388, 1302, 1221, 1200, 1151, 1114, 1077, 1052, 926, 823, 811, 787, 722  $\text{cm}^{-1}$ ; EIMS  $m/z$  (rel. int %) 476 ( $\text{M}^+$ , 3), 462 (5), 448 [ $\text{M}^+ - \text{CH}_2 = \text{CH}_2$ ] (58), 434 (19), 420 [ $\text{M}^+ - 2 \times \text{CH}_2 = \text{CH}_2$ ] (52), 406 (2), 392 [ $\text{M}^+ - 3 \times \text{CH}_2 = \text{CH}_2$ ] (100), 378 (4), 194 [ $\text{M}^+ - \text{C}_{20}\text{H}_{42}$ ] (2), 180 [ $\text{M}^+ - \text{C}_{21}\text{H}_{44}$ ] (5), 168 [Fragment A]<sup>+</sup> (98), 167 [Fragment B]<sup>+</sup> (52) (**Figure 2**)<sup>4</sup>, 153 (14), 139 (38), 137 (13), 125 (5), 109 (3), 95 (6), 83 (4), 77 (6), 69 (8),

57 (12). It had a molecular formula of  $C_{31}H_{56}O_3$  established by HREIMS (obsd 476.4237, calcd 476.4230). From its spectral data of IR,  $^1H$  and  $^{13}C$  NMR, it was clearly observed that compound **1** possessed a basic skeleton of phenol with the substitutes of two methoxy groups and one alkyl. Also observed from the spectra of EIMS and DEPT were that the alkyl was tricosyl, a linear alkyl group, because it consisted of twenty-two methylenes and one methyl. The positions of all substitutes were determined by the experiment of HMBC, and the key correlations of HMBC were shown in **Figure 1**. Thus, compound **1** was elucidated as 6-tricosyl-2,4-dimethoxy-phenol. The assignments of  $^1H$  and  $^{13}C$  NMR data for compound **1** vide **Table 1**.

**Figure 2** Characteristic mass spectral fragments of compound **1**



**Table 1**  $^1H$  NMR and  $^{13}C$  NMR Data for Compound **1** in  $CDCl_3$

| proton | $^1H$ NMR (400 MHz)<br>$\delta$ ppm (mult, <i>J</i> in Hz) | carbon | $^{13}C$ NMR (100 MHz)<br>$\delta$ ppm (multiplicity) |
|--------|--|--------|---|
| 3      | 6.33 (1H, d, 2.80)   | 1      | 137.66 (s)  |
| 5      | 6.26 (1H, d, 2.80)   | 2      | 146.76 (s)  |
| 1'     | 2.58 (2H, t, 7.76)   | 3      | 96.77 (d)   |
| 2'     | 1.57 (2H, m)   | 4      | 152.79 (s)  |
| 3'     | 1.30 (2H, m)   | 5      | 106.01 (d)  |
| 4'-22' | 1.23 (38H, overlap)  | 6      | 128.80 (s)  |
| 23'    | 0.86 (3H, t, 6.8)  | 1'     | 31.91 (t)   |
| OMe-2  | 3.82 (3H, s)   | 2'     | 30.03 (t)   |
| OMe-4  | 3.73 (3H, s)   | 3'-20' | 29.67 (t)   |
|        |  | 21'    | 29.33 (t)   |
|        |  | 22'    | 22.65 (t)   |
|        |  | 23'    | 14.03 (q)   |
|        |  | OMe-2  | 55.97 (q)   |
|        |  | OMe-4  | 55.75 (q)   |

## References

1. Z. W. Xie, C. S. Fan, Z. Y. Zhu *et al*, *The collection of Chinese Traditional and Herbal Drugs*, The People's Health Publishing House, Beijing, **1996**, Section B, 527-528.
2. C. A. Wachtmeister, *Acta Chem. Scand.*, **1955**, 9, 1395.
3. H. D. Sun, X. Y. Shen and Z. W. Lin, *Acta Botanica Yunnanica*, **1985**, 7, 109-113.
4. A. G. González, J. B. Barrera, E. M. R. Pérez and C. E. H. Padrón, *Planta Med.*, **1992**, 58, 214-218.

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