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Short Note

Methyl 2,5-Dihydroxy-4-(3′-methyl-2′-butenyl)benzoate

Tjitjik Srie Tjahjandarie *, Ratih Dewi Saputri and Mulyadi Tanjung

Natural Products Chemistry Research Group, Organic Chemistry Division, Department of Chemistry, Faculty of Science and Technology, Universitas Airlangga, Surabaya 60115, Indonesia; duffputri@gmail.com(R.D.S.); mulyadi-t@fst.unair.ac.id (M.T.)

* Correspondence: tjitjiktjahjandarie@fst.unair.ac.id; Tel.: +62-31-593-6501; Fax: +62-31-593-6502

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Abstract: Methyl 2,5-dihydroxy-4-(3′-methyl-2′-butenyl)benzoate (**1**) was isolated from the root of *Erythrina subumbrans*. The chemical structure of **1** has been elucidated based on spectroscopy UV-Vis, HRESIMS, 1D and 2D NMR analysis.

Keywords: Methyl 2,5-dihydroxy-4-(3′-methyl-2′-butenyl)benzoate; Methyl benzoate derivative; *Erythrina subumbrans*

1. Introduction

The genus *Erythrina* (Euphorbiaceae) comprises more than 100 species that are widely distributed in tropical and subtropical regions. The evergreen plants of *Erythrina* occur in almost every part of Indonesia, from Sumatra to Irian and the plants is commonly known as 'dadap'. Many of these species are used indigenously as traditional medicines to treat various diseases, such as infection, cough, malaria, inflammation, and asthma. This genus has been shown to produce a number of phenolic compounds, particularly alkaloids [1], flavonoids [2,3], pterocarpans [4,5] and stilbenoids [6]. In continuation of our research into the phenolic compound in this medicinal plant, we report the isolation of methyl 2,5-dihydroxy-4-(3′-methyl-2′-butenyl)benzoate (**1**) from the methanol extract of the the root of *Erythrina subumbrans*. The chemical structure of compound **1** was established by UV, HRESIMS, 1D and 2D NMR, as well as by comparison with those related compounds previously reported. The antioxidant activity against DPPH radical scavenging of the isolated compound **1** is also briefly described.

2. Result and Discussion

Extraction of the dried milled of roots of *E. subumbrans* (1.5 kg) was carried out using methanol, and then methanol extract was partitioned with *n*-hexane and ethyl acetate. The ethyl acetate extract (18 g) was separated by vacuum liquid chromatography on silica gel and radial chromatography yielded methyl 2,5-dihydroxy-4-(3′-methyl-2′-butenyl) benzoate **1** (Figure 1).

Methyl 2,5-dihydroxy-4-(3′-methyl-2′-butenyl)benzoate (**1**) was isolated as white solid. The UV spectrum exhibited absorption maxima λ_{maks} 224 and 287 typical for a 4-methyl benzoate chromophore [7]. The HRESIMS spectrum showed a quasimolecular ion $[M-H]^-$ at m/z 235.0971 (calcd. 235.0970), which correspondend to the molecular formula of $C_{13}H_{15}O_4$. The ^{1}H-NMR (Table 1) spectrum of **1**, the presence of two singlet aromatic proton signals at δ_H 7.56 (1H, *s*, H-6) and 6.39 (1H, *s*, H-3) suggest that compound **1** is typical for a methyl benzoate with three substituents [8]. In the ^{13}C-NMR spectrum (Table 1), the results for **1** showed 13 carbon signals consistent for methyl isoprenylated benzoate structure, and two carbon signals at δ_C 52.0 and 170.4 were assigned to a methoxyl and carbonyl carbon from methyl benzoate structure. These spectroscopic data, therefore, suggested that **1** is a methyl benzoate containing an isoprenyl (3′-methyl-2′-butenyl) side chain.