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SECONDARY METABOLITES FROM THE STEMS OF *Synsepalum dulcificum*

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Synsepalum dulcificum Daniell (Sapotaceae) is an evergreen shrub native to tropical West Africa; its fruit and red berries have the property of remarkably altering the sour taste to a sweet taste [1]. This explains why the berry has been called "miracle fruit or mysterious fruit". In the course of screening for chemically novel agents from plants, *S. dulcificum* was chosen for further phytochemical investigation [2–5]. In this study, the MeOH extract of its stems was subjected to chromatographic separation to afford six pure compounds, including propane-1,2,3-triol (**1**), 2,5-dimethoxyphenol (**2**), 3,4,5-trimethoxybenzoic acid (**3**), nicotinic acid (**4**) [6], *β*-sitosterol (**5**), and stigmasterol (**6**) [7]. Among them, **2** was isolated from natural sources for the first time though they had been synthesized previously [8], and **1–4** were obtained for the first time from this plant [2–5]. In this paper, we report the isolation and structure elucidation of **2**.

2,5-Dimethoxyphenol (**2**) was obtained as a brown powder. Its molecular formula was deduced as $C_8H_{10}O_3$ by HR-ESI-MS *m/z* 177.0521 ($[M + Na]^+$; calcd 177.0528). The UV spectroscopic absorptions at 225, 265, and 305 and the IR spectrum show absorptions for the hydroxyl group (3400 cm^{-1}) and an aromatic moiety (1590 and 1510 cm^{-1}). The ^1H NMR spectrum clearly indicated the presence of two methoxy groups at δ 3.88 (3H, s) and 3.91 (3H, s), one hydroxy group at δ 7.32 (1H, s), and three ABX methine protons at δ 6.90 (1H, d, J = 8.3, H-3), 7.55 (1H, d, J = 1.8, H-6), and 7.58 (1H, dd, J = 8.3, 1.8, H-4). The carbons of the 2,5-dimethoxyphenol were assigned, from ^{13}C NMR and DEPT experiments, to two methyls at δ 56.4 (5-OCH_3) and 56.7 (2-OCH_3), three methines at δ 108.2 (C-6), 113.7 (C-4), and 124.1 (C-3), and three quaternary carbons at δ 145.4 (C-2), 148.7 (C-1), and 155.1 (C-5). The structure of **2** was also confirmed by 2D NMR experiments. A COSY correlation was observed between the H-3 and H-4. The HSQC experiment showed that the carbon signals at δ 108.2 for C-6, 113.7 for C-4, and 124.1 for C-3 were correlated to the proton signals at δ 7.55 for H-6, 7.58 for H-4, and 6.90 for H-3, respectively. In the HMBC spectra, the significant correlations between δ_H 6.90 (H-3) and δ_C 148.7 (C-1)/155.1 (C-5)/56.7 (2-OCH_3), δ_H 7.58 (H-4) and δ_C 145.4 (C-2)/108.2 (C-6)/56.4 (5-O*C*H_3), as well as δ_H 7.55 (C-6) and δ_C 145.4 (C-2)/113.7 (C-4)/56.4 (5-OCH_3) suggested that each substituent OH, OCH_3, and OCH_3 was connected to C-1, C-2, and C-5 of the benzenoid moiety, respectively. The observation of the NOESY correlation from H-3 to H-4 and 2-OCH_3 and from H-6 to 5-OCH_3 suggested that the two methoxy groups were in C-2 and C-5 of this phenol structure. Thus, the structure of **2** was determined to be 2,5-dimethoxyphenol.

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