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A New Sesquiterpene Polyol Ester from *Celastrus Angulatus*

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Abstract: A new sesquiterpene polyol ester, angulatin D, has been isolated from the root bark of *Celastrus angulatus.* The chemical structure is elucidated on the basis of spectral analysis.

Keywords: *Celastrus angulatus*, root bark, sesquiterpene, β –dihydroagarofuran, angulatin D.

The genus *Celastrus* has been shown a rich source of sesquiterpene. The sesquiterpenes polyol esters with a β–dihydroagarofuran skeleton possess various biological activities. In our previous papers[1,2], we have reported some angulatin constituents from *Celastrus angulatus.* In the present paper, we describe the isolation and the structural elucidation of a new sesquiterpene polyol ester, angulatin D (**1**), from the root bark of *Celastrus Angulatus* by column chromatography on silica gel followed by recrystallization.

Angulatin D is an amorphous yellow powder, the molecular formula was determined as $C_{30}H_{38}O_{15}$ by EIMS. Elemental analysis gave C% 56.44 and H% 6.00 (requires: C% 56.43 and H% 5.96). The IR spectrum indicated the presence of hydroxyl group (3550 cm^{-1}) and ester group (1745 cm^{-1}). EIMS exhibited fragment ions attributable to the presence of $CH_3C{\equiv}O^+$ (*m/z* 43), $C_4H_3OC{\equiv}O^+$ (*m/z* 95), M - CH_3 $C{\equiv}O^+$ (*m/z* 595) and M^+ (*m/z* 638). The signals of ^{1}H-NMR (400MHz, $CDCl_3$) spectrum are assigned as: δ_H 5.24 (d, 1H, H-1, J=2.4), 5.53 (m, 2H, H-2 and H-8), 2.11 (m, 2H, H-3), 6.51 (s, 1H, H-6), 2.63 (d, 1H, H-7, J=2.0), 5.43 (s, 1H, H-9), 4.53 and 5.07 (d, 2H, H-15, J=13.2), 8.00 (m, 1H, H-1′), 6.72 (m, 1H, H-3′), 7.44 (m, 1H, H-4′). The methyl protons of H-12, H-13 and H-14 appeared as three singlets at δ_H 1.48, 1.56 and 1.61, respectively. The acetate protons appeared as five singlets at δ_H 1.65, 2.10, 2.11, 2.19 and 2.28, respectively. The signals of ^{13}C-NMR (100MHz, $CDCl_3$) are assigned as: δc 67.8 (C-1), 70.5 (C-2), 41.9 (C-3), 69.8 (C-4), 91.5 (C-5), 75.2 (C-6), 53.3 (C-7), 76.5 (C-8), 72.9 (C-9), 54.2 (C-10), 83.2 (C-11), 24.5, 25.4, 29.4 (C-12, C-13, C-14), 65.6 (C-15), 21.5, 21.2, 21.2, 21.1, 20.5 (acetates, CH_3), 170.5, 169.9, 169.7, 169.6, 169.5 (acetates, C=O), 149.0 (C-1′), 117.8 (C-2′), 109.7(C-3′), 144.1(C-4′), 161.0 (furoylate, C=O). Based on the above results and related literatures[1-4], Angulatin D can be regarded as a β–dihydro-

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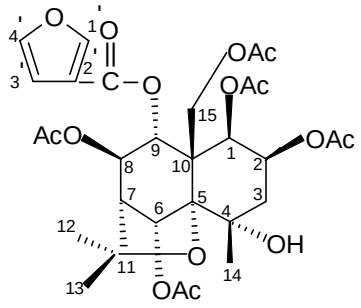
Figure 1 The Structure of Compound **1**



agarofuran derivative with seven substituted groups on the β–dihydroagarofuran skeleton. The seven substituents at 1, 2, 4, 6, 8, 9, 15-carbons are a hydroxyl, a furancarboxy and five acetoxyl groups. A free hydroxyl group is usually at C-4 position[3]. Among the five acetoxyl groups, the proton signal at δ_H 1.65 ppm, which is less than 1.90 ppm, is indicated that an acetoxyl group and the furancarboxy group are located at C-1 and C-9 positions[4]. The fragment ion ($C_{11}H_{12}O_3^{+\cdot}$, *m/z*192) indicated that the furancarboxy group is located at C-9 position[4]. Therefore, the five acetoxyl groups are located at C-1, C-2, C-6, C-8 and C-15 positions, respectively.

Generally, the substituted groups at C-1 and C-2 positions are in *cis*-form and β-configuration, the hydroxyl group at C-4 position and the substituted group at C-6 position are in α-configuration[4]. The substituted group at C-9 is confirmed as a α-configuration by the signal of C-15 (δ 65.5 ppm) on the ^{13}C-NMR spectrum[3]. The protons of H-8 and H-9 appeared as a single peak illuminated that H-8 and H-9 are situated on equatorial bond[4], the acetoxyl group at C-8 position is confirmed as a β-configuration. Therefore, the substituted groups at C-8 and C-9 are in *trans*-form. From the above analysis, we can conclude that the structure of angulatin D is 1β, 2β, 6α, 8β, 15-pentaacetoxy-4α-hydroxy-9α-(β-furancarboxy)-β-dihydroagarofuran (**1**).

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