

A New Cyclohexene Oxide from *Uvaria tonkinensis* var. *subglabra*

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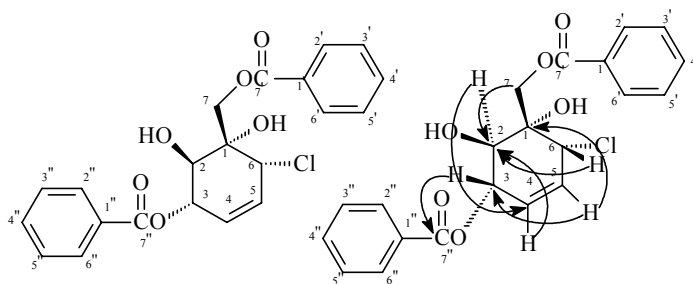
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Abstract: A new compound, subglain B, was isolated from the stems of *Uvaria tonkinensis* var. *subglabra* and its structure was identified as 1S, 2R, 3S, 6R-1-benzoyloxymethylene-1,2-dihydroxy-3-benzoyloxy-6-chlorocyclohex-4-ene (**1**), by spectral evidences.

Keywords: *Uvaria tonkinensis* var. *subglabra*, subglain B, cyclohexene.

In order to discover new antitumour agents from the plant sources, one species of *Uvaria* genus, *Uvaria tonkinensis* var. *subglabra*, growing in Hainan Island of China, was subjected to phytochemical studies. A new compound, named as subglain B, was isolated from 95% ethanol extract fraction and identified by means of various spectral techniques, by silica gel and Sephdax LH-20.

Figure 1 The key HMBC for compound **1**



Compound **1** was isolated as white solid, mp 187-189°C, $[\alpha]_D^{20}$ -133 (c 0.75, CHCl₃). The exact molecular weight was determined by HR-TOF-MS to be m/z 403.0943 ($[M^+ + H]$, calcd. 403.0942), corresponding to molecular formula C₂₁H₁₉O₆Cl. The IR spectrum showed absorptions at 3340 cm⁻¹ (OH), 1700 cm⁻¹ (O-C=O), 1290 cm⁻¹ (ether), 720 cm⁻¹ (monosubstituted benzene). The EI mass spectrum showed prominent peaks at m/z 367 (M-Cl)⁺, 249, 215, 163, 122, 105 (base peak). Its ¹H NMR and ¹³C NMR spectrum displayed characteristics of cyclohexene oxide compounds^{1,2}. The ¹H NMR spectrum exhibited a ten protons multiplet at δ 7.53~8.06 belonging to

the phenyl protons of two benzoyloxy groups, two *cis* olefinic protons at δ 5.82 and δ 5.99 ($J=9.5$ Hz), two hydroxyl protons at δ 5.61 and δ 5.83 and five protons on the substituted carbons at δ 4.1~6.0 ppm (**Table 1**). The ^1H - ^1H COSY spectrum showed that the protons at δ 4.16 and δ 5.68 were correlated ($J=7$ Hz), the protons at δ 4.80 and δ 5.99 were correlated ($J=4$ Hz). Analysis of the HMQC spectrum, the relationship between all the H and C were determined (**Table 1**). Analysis of the HMBC spectrum (**Figure 1**), the doublet at δ 4.80 (H-6) coupled with C-2 at δ 68.5; the doublet at δ 5.68 (H-3) coupled with C at δ 165.6, indicated that one benzoyl group was located at C-3. The relative stereochemical structure of **1** was determined by the coupling constant of the H-2 and H-3 ($J_{2,3}=7$ Hz), showed that H-2 and H-3 had to be *trans*-diaxial^{2,3}. And the coupling constant of H-5 and H-6 ($J_{5,6}=4$ Hz), which indicated that the chloro group was in axial conformation¹. The NOESY spectrum showed H-6 (δ 4.80) and H $_{\beta}$ -7 (δ 4.52) were interacted, which indicated H-6 and H-7 were on the same side of the molecule. Its CD spectrum showed strongly positive cotton effect ($\epsilon +50$) at λ 228 nm, which suggested the benzoyloxy groups located at C-7 and C-3 in clockwise manner⁴. Thus, the absolute stereochemical configuration of compound **1** can be 1S, 2R, 3S, 6R. This a new natural product is named subglain B (see **Figure 1**).

Table 1: ^1H (500 MHz) and ^{13}C (125 MHz) NMR data of compound **1** (CDCl_3)

Position	δ_{H}	δ_{C}
1		74.7
2	4.16 (t, 1H, $J=7$ Hz)	68.5
3	5.68 (d, 1H, $J=7$ Hz)	73.8
4	5.82 (m)	127.8
5	5.99 (dd, 1H, $J=4, 12$ Hz)	127.8
6	4.80 (d, 1H, $J=4$ Hz)	57.5
7	4.60, 4.52 (each d, 1H, $J=11.5$ Hz)	67.7
1', 1''		128.5
2', 6', 2'', 6''	8.06 (each d, 4H, $J=7.5$ Hz)	129.6
3', 5', 3'', 5''	7.53 (each m, 4H)	128.5
4', 4''	7.66 (each m, 2H)	133.2
7', 7''	5.61 (s), 5.83 (d, $J=7$ Hz)	165.5
1-OH, 2-OH		

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