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A New Sesquiterpene from Transformation of Curdione by Cell Suspension Culture of *Platycodon Grandiflorum*

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Abstract: A new sesquiterpene was isolated from transformation of curdione by cell suspension culture of *Platycodon grandiflorum*. The structure of the new compound was elucidated on the basis of spectral methods including 2D NMR.

Keywords: *Platycodon grandiflorum*, biotransformation, curdione, sesquiterpene.

Curcuma aromatica (Family *Zingiberaceae*) is an important medicinal plant and its rhizome has been used as a traditional Chinese medicine possessing activities of anticancer, antioxidation and bile secretion promotion. Curdione, compound **1**, with a germacrane skeleton is one of its major active constituents. Recently, curdione was reported to exhibit hepatoprotective activity [1, 2]. In an endeavor to find new chemical entities, we examined the plant cell suspension cultures of *Platycodon grandiflorum* for its capability to transform curdione. Incubation of curdione with *P. grandiflorum* for 6 days yielded a new compound, 1α, 10β-epoxy-11-hydroxyl-curdione (compound **2**) (**Figure 1**).

Compound **2** afforded as colorless oil, $[\alpha]_D^{22}$ +79.2 (*c* 0.3, MeOH). Its HR-FABMS provided a *quasi*-molecular ion $[M+H]^+$ at *m/z* 269.1748 (calcd. 269.1746), suggesting the molecular formula of $C_{15}H_{24}O_4$. Compared to that of compound **1**, the ^{1}H-NMR spectrum of compound **2** showed disappearance of the olefin proton and appearance of a new proton (δ 2.71, dd, 1H, *J* = 10.0, 2.0 Hz), in higher field. The ^{13}C-NMR spectrum of compound **2** also showed disappearance of olefin carbons and presence of two oxygen-bearing carbons (δ 62.8 and 58.4). In HMBC, the proton signals at δ 1.31 (Me-15) correlated with the carbon signals of C-1 (δ 62.8) and C-10 (δ 58.4). These data indicated that compound **2** was the C-1, 10 epoxide of compound **1**. In addition, when compared the ^{1}H-NMR spectrum with that of compound **1**, the methyl signals at δ 0.89 (d, 3H, *J* = 7.0 Hz, C-12) and δ 0.94 (d, 3H, *J* = 7.0 Hz, C-13) shifted to δ 1.15 (s, Me-12) and δ 1.27 (s, Me-13), respectively.

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Figure 1 The structures of compounds **1** and **2**

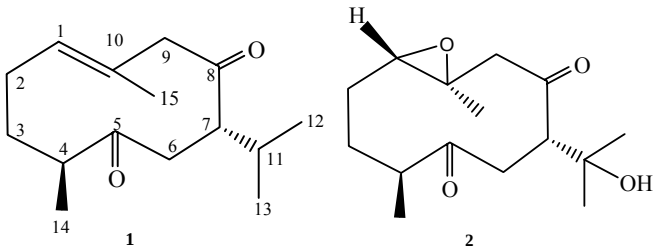

Table 1 ^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) data of **2** ($CDCl_3$, δ ppm, *J* Hz)

No.	δ_H	δ_C	No.	δ_H	δ_C
1	2.71 (dd, 10.0, 2.0)	62.8	9	2.27 (d, 10.0) 2.86 (d, 10.0)	56.2
2	1.29 (m) 2.08 (m)	26.0	10	-	58.4
3	1.71 (m) 2.16 (m)	30.6	11	-	72.0
4	2.57 (m)	46.9	12	1.15 (s)	26.9
5	-	214.2	13	1.27 (s)	28.4
6	2.73 (dd, 15.0, 7.0) 2.82 (dd, 15.0, 2.5)	40.4	14	1.12 (d, 7.0)	17.6
7	3.27 (dd, 7.0, 2.5)	55.5	15	1.31 (s)	16.8
8	-	214.5			

In the ^{13}C-NMR spectrum of compound **2**, the carbon signal (δ 30.0, C-11) of compound **1** shifted downfield to δ 72.0. In HMBC spectrum, the carbon signal of C-11 (δ 72.0) correlated with the proton signals of δ 1.15 (CH_3-12), δ 1.27 (CH_3-13), δ 2.73 (H_a-6), δ 2.82 (H_b-6) and δ 3.27 (H-7), which suggested that compound **2** possessed 11-hydroxyl group. In NOE spectrum, the proton signal at δ 2.27 (d, 1H, *J* = 10.0 Hz, H_b-9) with the signal at δ 3.27 (dd, 1H, *J* = 7.0, 2.5 Hz, βH-7) and the signal at δ 2.71 (dd, 1H, *J* = 10.0, 2.0 Hz, H-1) have the NOE enhancements. No enhancement between δ 2.71 (H-1) and δ 1.31 (CH_3-15) was observed, but NOE enhancement between δ 1.31 (CH_3-15) and δ 2.57 (H-4) was observed. On the basis of the above analysis, compound **2** was identified as 1α, 10β-epoxy-11-hydroxycurdione. All the ^{1}H- and ^{13}C-NMR spectral data were unambiguously assigned by 2D-NMR spectra (**Table 1**).

Acknowledgments

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