

## A New Monoterpene Glycoside from *Swertia punicea*

Xin MING<sup>1</sup>, Ming Hua QIU<sup>1</sup>, Rui Lin NIE<sup>1</sup>, Guo Lin ZHANG<sup>2\*</sup>

<sup>1</sup> Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204

<sup>2</sup> Chengdu Institute of Biology, Chinese Academy of Sciences, Chengdu 610041

**Abstract:** A new monoterpene glycoside, 2,6-dimethyl-2*E*,6*E*-octadienoic acid 1,6'-lactone 8- $\beta$ -D-glucopyranoside, was isolated from *Swertia punicea*, accompanying with six known compounds 1-*O*-primeverosyl-3,7,8-trimethoxyxanthone, 1-*O*-primeverosyl-3,7,8-trimethoxyxanthone, 1,8-dihydroxy-3,7-dimethoxy xanthone and isovitexine. Their structures were elucidated based on spectral evidence.

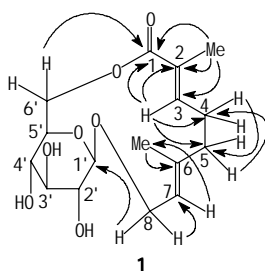
**Keywords:** *Swertia punicea*, monoterpene glycoside, xanthone, *epi*-eustomoside, isovitexine.

The plant *Swertia punicea* Hemsl. (Gentianaceae), distributed in Southwest China, is used in Chinese medicine for acute bilious hepatitis and cholecystitis<sup>1</sup>. Previous investigations of this plant have led the isolation of various compounds<sup>2</sup>. In this investigation, seven compounds were isolated from the whole plants of *S. punicea*, collected in E-Shan, Yunnan Province in July, 1997 and identified by P. Y. Bei in Kunming Institute of Botany, Chinese Academy of Sciences, where the specimen is deposited. On the basis of spectral data, they were determined to be new compound, 2,6-dimethyl-2*E*,6*E*-octadienoic acid 1,6'-lactone 8- $\beta$ -D-glucopyranoside (**1**), and known compounds 1-*O*-primeverosyl-3,7-dimethoxy-8-hydroxyxanthone<sup>3,4</sup>, 1-*O*-primeverosyl-3,7,8-trimethoxyxanthone<sup>3,5</sup>, *epi*-eustomoside<sup>6</sup>, 1-hydroxy-3,7,8-trimethoxyxanthone<sup>4</sup>, 1,8-dihydroxy-3,7-dimethoxyxanthone<sup>4</sup> as well as isovitexine<sup>7</sup>.

Compound **1**, mp. 100–101°C (MeOH),  $[\alpha]_D^{20} = 18.8$  (MeOH, c 1.0), white crystals, gives a base peak in FABMS (negative mode) at  $m/z$  655 ([2M-1]<sup>-</sup>). The EIMS showed the ion peaks at  $m/z$  327 ([M-1]<sup>+</sup>), 244, 166 ([M-C<sub>6</sub>H<sub>10</sub>O<sub>5</sub>]<sup>+</sup>), 121. UV  $\lambda_{\max}^{\text{MeOH}}$  nm: 268. IR  $\nu^{\text{KBr}}$  cm<sup>-1</sup>: 1709, 1647, 1448, 1418. Sixteen signals were observed in the <sup>13</sup>C NMR spectrum (DMSO-d<sub>6</sub>, **Table 1**). After hydrolysis **1** in 3 mol/L HCl (aq.) the sugar was identified as D-glucose by comparing with authentic sample in PTLC. The <sup>1</sup>H NMR signal at  $\delta$  4.09 (d, 1H,  $J=8$  Hz) and its corresponding <sup>13</sup>C NMR signal at  $\delta$  100.6 suggested the presence of  $\beta$ -D-glucopyranosyl. From <sup>1</sup>H NMR spectrum two methyl groups at  $\delta$  1.74 and 1.50 (each, 3H) and two olefinic protons at  $\delta$  6.60 (t, 1H,  $J=6.8$  Hz) and 5.27 (t, 1H,  $J=7.2$  Hz) were recognized. The IR absorption at  $\nu$  1709 cm<sup>-1</sup> and <sup>13</sup>C NMR signal at  $\delta$  166.8 suggested **1** is an ester. The <sup>13</sup>C NMR signals at  $\delta$  141.3, 139.3, 127.4 and 121.2 suggested two trisubstituted double bonds, whose configuration could be determined as *E* on the basis of <sup>13</sup>C NMR (in CD<sub>3</sub>OD) signals at  $\delta$  16.27 and 12.67 for 6-Me and 2-Me respectively, because the corresponding methyl groups in the *Z* analogue

resonate at  $\delta$  about 23<sup>8</sup> and 17 ppm<sup>9,10</sup>. According to HMQC and HMBC, the structure of **1** was thus elucidated as 2,6-dimethyl-2*E*,6*E*-octadienoic acid 1,6'-lactone 8- $\beta$ -D-glucopyranoside.

**Figure 1** Structure of **1**



**Table 1** <sup>1</sup>H- and <sup>13</sup>C NMR Data of **1** (for <sup>1</sup>H, 400 MHz; for <sup>13</sup>C, 100 MHz)

No	$\delta_c$ (DMSO-d <sub>6</sub> )	$\delta_c$ (CD <sub>3</sub> OD)	$\delta_H$ (DMSO-d <sub>6</sub> )	$\delta_H$ (CD <sub>3</sub> OD)
1	166.8	169.28		
2	127.4	129.06		
3	141.3	143.21	6.60 (t, 6.8)	6.75 (m)
4	25.6	27.11	2.28 (m)	2.39 (m)
5	37.4	39.94	2.15 (m)	2.23 (m)
6	139.3	140.07		
7	121.2	122.82	5.25 (t, 7.2)	5.39 (m)
8	64.3	65.54	4.10 (m)	4.15 (m), 4.25 (m)
2-Me	12.6	12.67	1.74 (s)	1.83 (s)
6-Me	15.3	16.27	1.50 (s)	1.63 (m)
1'	100.6	102.12	4.09 (d, 8.0)	4.12 (d, 8.0)
2'	73.2	75.37	2.94 (m)	3.47 (t, 7.0)
3'	73.8	77.96	3.30 (m)	3.35 (t, 7.0)
4'	70.9	72.47	2.96 (m)	3.18 (t, 7.0)
5'	76.5	75.02	3.12 (m)	3.15 (m)
6'	63.2	65.54	4.75 (d, 11.0)	4.56 (dd, 9.5, 1.5)
			3.96 (m)	4.15 (m)

### Acknowledgment

Di-Ao Science Foundation supported this work.

### References

1. Jiangsu New Medical College, "Dictionary of Chinese Medicine", Vol. 1, Shanghai Renming Publishing, Shanghai, **1977**, p.210.
2. P. Tan, Y. L. Lin, C.Y. Hou, *Yaoxue Xuebao*, **1993**, 28, 522.
3. K. Hostettmann, A. Jacot-Guillarmod, *Helv. Chim. Acta*, **1976**, 59, 165.
4. B. L. Hu, J. Y. Ding, H. F. Sun, S. F. Fan, *Zhiwu Xuebao*, **1991**, 33, 507.
5. M. Goetz, F. Manilho, A. Jacot-Guillarmod, *Helv. Chim. Acta*, **1978**, 61, 1549.
6. Y. H. Lo, R. L. Nie, *Yaoxue Xuebao*, **1992**, 27, 125.
7. D. Davoust, M. Massias, D. Molho, *Org. Mag. Res.*, **1980**, 13, 218.
8. B. Gering-Ward, P. Junior, *Planta Medica*, **1989**, 55, 75.
9. G. A. Gross, O. Sticher, C. Anklin, *Helv. Chim. Acta*, **1987**, 70, 91.
10. G.A. Gross, O. Sticher, *Helv. Chim. Acta*, **1986**, 69, 156.

Received 26 January 2000