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A New Flavan from *Sinacalia tangutica*

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Abstract: A new flavan named 4α, 5-dimethoxy-8-formyl-7-hydroxy-6-methylflavan (**1**) was isolated from *Sinacalia tangutica.* Its structure was determined using spectroscopic methods and X-ray diffraction experiments.

Keywords: *Sinacalia tangutica*, Compositae, flavan, X-ray.

Sinacalia tangutica has been used for expectorant, anti-cough and cathartic purposes and curing distention of chest and hypochondrium[1]. There have been no prior chemical studies on this plant. Herein we report the structured elucidation of a new flavan **1** and five known compounds **2-6** from the stems of *S. tangutica*.

Compound **1**, colourless needles, mp 110-111℃. The IR spectrum of **1** indicated the presence of a carbonyl group (1648 cm^{-1}) and aromatic ring (1464, 900-363 cm^{-1}). The molecular formula, $C_{19}H_{20}O_5$, was determined by HRESIMS (*m/z* 351.1198 $[M+Na]^+$, calcd. 351.1203). In the ^{1}H-NMR spectrum, the presence of two one-proton doublet of doublets at δ 5.29 (H-2) and δ 4.50 (H-4) and the methylene protons multiplets of ABMX at δ 2.42 (H-3eq) and δ 1.90 (H-3ax) suggested that compound **1** was 4-substituted flavan[2,3]. The ^{13}C-NMR spectrum [signals at δ 33.6 (C-3), δ 73.9 (C-2), δ 67.8 (C-4)] also justified a flavan skeleton for **1** (**Table 1**). The appearance of H-4 (t, J=2.6Hz) as a triplet implied a *trans* configuration[3]. In addition, the ^{1}H-NMR spectrum showed the presence of two methoxyl groups, a hydroxyl group, an aromatic methyl, an aldehydic group and a typical five proton multiplet (at δ 7.44) which confirmed the unsubstituted B-ring and fully substituted A-ring. The EIMS of **1** displayed a

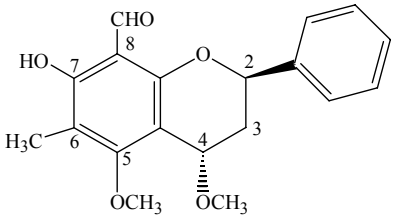

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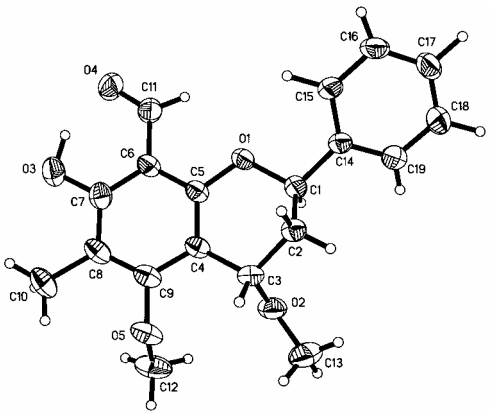
Figure 1 ORTEP diagram of the crystal structure of **1**



molecular ion at *m/z* 328 $[M]^+$, the fragmentation ions at *m/z* 224 $[A]^+$ and *m/z* 104 $[B]^+$ which also confirmed the unsubstituted B-ring. The localization of the methoxyl (δ 3.52) at C-4 position was deduced from the long-range coupling of C-4 (δ 67.8) with methoxyl protons (δ 3.52). The positions of the substituents in A-ring were determinted by HMBC experiments. The structure of **1** and its relative stereochemistry were unequivocally established by X-ray diffraction analysis (**Figure 1**). Therefore, the structure of **1** was determined as 4α, 5-dimethoxy-8-formyl-7-hydroxy-6-methylflavan.

Table 1 ^{1}H - and ^{13}C-NMR data of compound **1** ($CDCl_3$, 400MHz, δ_{ppm})

C	δ_C	H	δ_H
2	73.9 (CH)	2	5.29 dd (12.4,1.7)
3	33.6 (CH_2)	3	2.42 dt (14.7,2.2)
4	67.8 (CH)		1.90ddd(14.7,12.4,2.8)
5	165.8(C)	4	4.50 t (2.6)
6	111.1(C)		
7	163.8(C)		
8	107.1(C)		
9	157.0(C)		
10	107.3(C)	7-OH	12.51 s
1′	140.3(C)		
2′,6′	126.2(CH)	2′,6′	7.44 m
3′,5′	128.7(CH)	3′,5′	7.44 m
4′	128.3(CH)	4′	7.44 m
CH_3	7.96 (CH_3)	CH_3	2.13 s
OCH_3	61.4 (CH_3)	OCH_3	3.91 s
	55.9 (CH_3)		3.52 s
CHO	193.0(CH)	CHO	10.22s

The structure of known compounds **2-6** were determined to be desmosflavone **2**[4], lawinal **3**[5,6], isounonal **4**[7], 5,7-dihydroxy-8-formyl-6-methylflavone(Unonal) **5**[7], 5,7-dihydroxy-6,8-dimethylflavanone **6** [5,8] by comparison of MS, ^{1}H-NMR, ^{13}C-NMR and DEPT data with reported values in the literature.

Acknowledgments

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