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A New Biflavonoid from *Stellera chamaejasme* L.

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Abstract: A new biflavonoid, stelleranol, was isolated from the roots of *Stellera chamaejasme* L.. Its structure was determined by the analysis of MS and NMR data, especially 2D NMR spectra.

Keywords: *Stellera chamaejasme* L., flavonoids, biflavonoids**.**

Stellera chamaejasme L. (Thymelaeaceae) is widespread in the north of China. *S. chamaejasme* L. has been known to contain biflavonoids and up to now a few biflavonoids have been isolated from this plant [1-4]. During investigation of chemical constituents of the roots of this plant, a new biflavonoid, stelleranol has been isolated.

Stelleranol was isolated as brown powder, mp 264~266°C (MeOH/H_2O). $[\alpha]_D$=-103 (c0.26, MeOH). Positive $FeCl_3$ reaction showed the existence of phenolic hydroxy groups. Its molecular formula was deduced to be $C_{30}H_{22}O_{11}$ through the information of ESI-MS ($[M-H]^-$=557) and NMR data. In ^{1}H NMR (acetone-d_6) signals at δ 7.22 (d, 2H, J=8.6Hz), 6.83 (d, 2H, J=8.6Hz), 6.71 (d, 2H, J=8.6Hz) and 6.62 (d, 2H, J=8.6Hz) suggested two 4-oxyphenyl groups. Signals at δ 6.16 (d, 1H, J=2.2Hz), 6.14 (d, 1H, J=2.2Hz) indicated the presence of a 1, 2, 4, 6-tetra substituted aromatic ring. Signals at δ 2.66 (d, 1H, J=17.0Hz), 2.49 (dd, 1H, J=17.0, 3.7Hz) corresponded to a $-CH_2-$ group. ^{1}H NMR also showed 4 –CH- signals at δ 6.09, 5.70, 4.96 and 4.18. Besides those functional groups described above, ^{13}C NMR (acetone-d_6) indicated 2 carbonyls (δ 191.8, 187.8) and 2 oxygen attached quaternary carbons (δ 86.4, 81.0) too.

The foregoing spectra studies and further HMBC experiment on stelleranol suggested its similarity to genkwanol B and genkwanol C isolated from the roots of *Dapnhe genkwa* [5, 6]. *J* values between H-2 and H-3 in genkwanol B and genkwanol C were 8.4, 6.2 respectively. But that of stelleranol was so little that H-2 and H-3 showed singlet signals [H-2 at 4.96 (s, 1H), H-3 at 4.18 (s, 1H)]. These suggested that configuration at C-2/C-3 of genkwanol B and genkwanol C was *trans* , while it was *cis* in stelleranol. The chemical shifts of H-2 and H-3 are similar to those of (-)-epicatechin [7], through which configurations at C-2 and C-3 were both deduced to be α. The assignments of ^{1}H NMR and ^{13}C NMR data were finished by HMQC and HMBC

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analysis as shown in **Table 1**.

Figure 1 Structures and main HMBC correlations of stelleranol

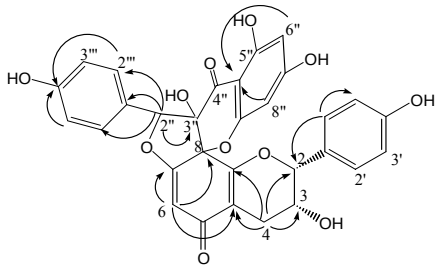

Table 1 ^{1}H NMR and ^{13}C NMR data of stelleranol

	^{1}H NMR	^{13}C NMR		^{1}H NMR	^{13}C NMR
2	4.96 (s, 1H)	81.2	2"	6.09 (s, 1H)	91.2
3	4.18 (brs, 1H)	65.4	3"		81.0
4	2.66（d, 1H, *J*=17.0Hz）， 2.49（dd, 1H, *J*=17.0, 3.7Hz）	27.6	4"		191.8
4a		110.0	4"a		100.9
5		87.8	5"		162.0
6	5.70 (s, 1H)	101.8	6"	6.14（d, 1H, *J*=2.2Hz）	97.9
7		169.5	7"		168.9
8		86.4	8"	6.16（d, 1H, *J*=2.2Hz）	97.4
8a		159.2	8"a		165.0
1'		129.4	1'''		123.7
2'	6.71（d, 1H, *J*=8.6Hz）	128.3	2'''	7.22（d, 1H, *J*=8.6Hz）	130.7
3'	6.62（d, 1H, *J*=8.6Hz）	115.4	3'''	6.83（d, 1H, *J*=8.6Hz）	115.6
4'		157.5	4'''		159.0
5’	6.62（d, 1H, *J*=8.6Hz）	115.4	5’’’	6.83（d, 1H, *J*=8.6Hz）	115.6
6’	6.71（d, 1H, *J*=8.6Hz）	128.3	6’’’	7.22（d, 1H, *J*=8.6Hz）	130.7

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