A New Oligostilbene from the Roots of Vitis Amurensis

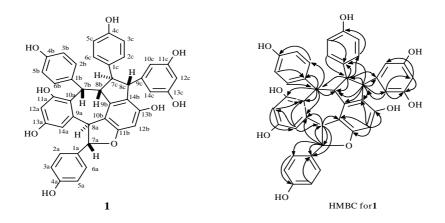
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Abstract: A new resveratrol trimer, amurensin G (1), was isolated from the roots of *Vitis amurensis* Rupr. Its structure and relative configuration were established on the basis of spectral evidence, especially on HMBC spectrum and NOE difference experiments.

Keywords: Vitis amurensis, Vitaceae, oligostilbene, amurensin G, resveratrol.

Our continuous research on chemical constituents of the roots of *Vitis amurensis* resulted in the isolation of another new oligostilbene amurensin G (1), besides oligostilbenes we reported before¹. In this paper, we report the structure determination of 1, including 2D-NMR studies.



Amurensin G (1) was isolated as colorless amorphous powder, $[\alpha]_{D}^{19}=+20.1$ (c 0.072, MeOH). Its molecular formula $C_{42}H_{32}O_9$ was determined on the basis of FAB-MS (m/z 681 [MH]⁺) and ¹H, ¹³C-NMR data, which indicated that it should be a resveratrol trimer. The ¹H-NMR spectrum of 1 displayed the following features: In lower field, there were three sets of signals for 4-hydroxybenzene moieties, one set of signals for a 3,5-dihydroxybenzene moiety, two *meta*-coupled doublets due to two aromatic protons and a singlet of an aromatic proton. In higher field, there were signals

for six aliphatic protons. The ¹H-NMR and ¹³C-NMR data of **1** were similar to those of ampelopsin C², but in the HMBC spectrum of **1**, the long range couplings between H-8c and C-10(14)c, H-10(14)c and C-8c suggested that the 3,5-dihydroxybenzene group should be attached to C-8c position; meanwhile, the long range couplings between H-7c and C-2(6)c, H-2(6)c and C-7c indicated that the 4-hydroxybenzene group should be attached to C-7c position, thus the planar structure of amurensin G was determined as **1**, a stereo-isomer of suffruticosol A and B³. Its ¹H and ¹³C-NMR data were assigned as **Table 1**.

To clarify the relative stereochemistry of **1**, NOE difference experiments have been carried out. Irradiation of H-8a signal enhanced H-2(6)a and H-2(6)b signals, suggesting the *trans* orientation for H-8a and H-7a, as well as for H-8a and H-7b. The significant NOEs between H-7b and H-8b, H-8b and H-8c indicated the *cis* orientation of H-7b, H-8b and H-8c, the H-7c situated in *trans* position to them was demonstrated by the NOEs between H-7c and H-2(6)b, H-7c and H-10(14)c, H-8b and H-2(6)c, therefore the relative stereochemistry of amurensin G was determined as shown in structure **1**, which was different from suffruitcosol A or B.

No.	$^{1}\mathrm{H}$	¹³ C	No.	^{1}H	¹³ C
1a		130.7	8b	3.59 dd (11.8, 3.4).	52.4
2(6)a	7.23 d (8.6)	130.1	9b		144.0
3(5)a	6.77 d (8.6)	116.1	10b		116.0
4a		158.6	11b		159.4
7a	5.80 d (11.8)	90.6	12b	6.13 s	96.5
8a	4.43 d (11.8)	48.9	13b		154.7
9a		141.6	14b		121.1
10a		124.7	1c		132.6
11a		155.9++	2(6)c	6.96 d (8.6)	129.9
12a	6.33 d (2.0)	101.7	3(5)c	6.69 d (8.6)	115.8
13a		156.8^{+}	4c		156.7 ⁺
14a	6.13 d (2.0)	105.8	7c	3.73 dd (11.8, 9.7)	61.7
1b		133.3	8c	4.20 d (9.7)	57.4
2(6)b	7.14 d (8.6)	130.5	9c		146.8
3(5)b	6.65 d (8.6)	115.4	10(14)c	6.17 d (2.2)	107.4
4b		155.8++	11(13)c		159.2
7b	5.23 d (3.4)	37.5	12c	6.16 t (2.2)	101.7

Table 1. ¹H and ¹³C-NMR data for 1 in CD₃COCD₃ (500MHz, δ in ppm, J in Hz)[§]

[§] All assignments were confirmed by 2D ¹H-¹H COSY, ¹H-¹³C COSY, HMBC spectra.

⁺, ⁺⁺: Maybe interchangeable

References

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Received 9 May 1999