# 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 before ${ }^{1}$. In this paper, we report the structure determination of $\mathbf{1}$, including 2D-NMR studies.


1


HMBC for 1

Amurensin $G$ (1) was isolated as colorless amorphous powder, $[\alpha]^{19}=+20.1$ (c $0.072, \mathrm{MeOH})$. Its molecular formula $\mathrm{C}_{42} \mathrm{H}_{32} \mathrm{O}_{9}$ was determined on the basis of FAB-MS ( $\mathrm{m} / \mathrm{z} 681[\mathrm{MH}]^{+}$) and ${ }^{1} \mathrm{H},{ }^{13} \mathrm{C}-\mathrm{NMR}$ data, which indicated that it should be a resveratrol trimer. The ${ }^{1} \mathrm{H}$-NMR spectrum of $\mathbf{1}$ 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 ${ }^{1} \mathrm{H}$-NMR and ${ }^{13} \mathrm{C}$-NMR data of $\mathbf{1}$ were similar to those of ampelopsin $\mathrm{C}^{2}$, but in the HMBC spectrum of $\mathbf{1}$, the long range couplings between $\mathrm{H}-8 \mathrm{c}$ and $\mathrm{C}-10(14) \mathrm{c}, \mathrm{H}-10(14) \mathrm{c}$ and $\mathrm{C}-8 \mathrm{c}$ suggested that the 3,5 -dihydroxybenzene group should be attached to $\mathrm{C}-8 \mathrm{c}$ position; meanwhile, the long range couplings between $\mathrm{H}-7 \mathrm{c}$ and $\mathrm{C}-2(6) \mathrm{c}, \mathrm{H}-2(6) \mathrm{c}$ and $\mathrm{C}-7 \mathrm{c}$ indicated that the 4-hydroxybenzene group should be attached to $\mathrm{C}-7 \mathrm{c}$ position, thus the planar structure of amurensin G was determined as $\mathbf{1}$, a stereo-isomer of suffruticosol A and B ${ }^{3}$. Its ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}-\mathrm{NMR}$ 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 $\mathrm{H}-8 \mathrm{a}$ and $\mathrm{H}-7 \mathrm{a}$, as well as for $\mathrm{H}-8 \mathrm{a}$ and $\mathrm{H}-7 \mathrm{~b}$. The significant NOEs between $\mathrm{H}-7 \mathrm{~b}$ and $\mathrm{H}-8 \mathrm{~b}, \mathrm{H}-8 \mathrm{~b}$ and $\mathrm{H}-8 \mathrm{c}$ indicated the cis orientation of $\mathrm{H}-7 \mathrm{~b}, \mathrm{H}-8 \mathrm{~b}$ and $\mathrm{H}-8 \mathrm{c}$, the $\mathrm{H}-7 \mathrm{c}$ situated in trans position to them was demonstrated by the NOEs between $\mathrm{H}-7 \mathrm{c}$ and $\mathrm{H}-2(6) \mathrm{b}, \mathrm{H}-7 \mathrm{c}$ and $\mathrm{H}-10(14) \mathrm{c}, \mathrm{H}-8 \mathrm{~b}$ and $\mathrm{H}-2(6) \mathrm{c}$, therefore the relative stereochemistry of amurensin $G$ was determined as shown in structure 1, which was different from suffruticosol A or B.

Table $1 .{ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$-NMR data for $\mathbf{1}$ in $\mathrm{CD}_{3} \mathrm{COCD}_{3}(500 \mathrm{MHz} \text {, } \delta \text { in ppm, } \mathrm{J} \text { in } \mathrm{Hz})^{8}$

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

${ }^{8}$ All assignments were confirmed by $2 \mathrm{D}{ }^{1} \mathrm{H}-{ }^{1} \mathrm{H}$ COSY, ${ }^{1} \mathrm{H}-{ }^{13} \mathrm{C}$ COSY, HMBC spectra.
${ }^{+},{ }^{++}$: Maybe interchangeable

## References

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