# SUPPLEMENTARY MATERIAL

Isoquinoline Alkaloids from *Asimina triloba*

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ABSTRACT

A new aporphine glycoside, (-)**-**anolobine-9-*O-β-*D-glucopyranoside was isolated from the twigs of pawpaw (*Asimina triloba*) along with 7 known alkaloids including five aporphine alkaloids (anolobine, nornuciferine, norushinsunine, liriodenine, and lysicamine), a proaporhine alkaloid (stepharine) and a tetrahydrobenzylisoquinoline alkaloid (coclaurine). Among these compounds, nornuciferine, lysicamine, stepharine, and coclaurine are reported for the first time from this plant. The structure of the new compound was elucidated by spectroscopic methods, including 1D, 2D NMR, and HRESI-​MS. The absolute configuration of compounds **1**, **2**, **7** and **8** was determined by CD experiment.

**Keywords:** Annonaceae, *Asimina triloba,* Anolobine-9-*O-β-*D-glucopyranoside, Aporphine, Alkaloids, NMR.

**Figure S1:** Key HMBC (→) and COSY (▬) correlations of 1



**Figure S2:** CD spectra of anolobine-9-*O-β-*D-glucopyranoside **1** and its aglycone (anolobine **2)**



**Figure S3:** CD spectrum of stepharine (**7**)



Figure S4: CD spectrum of coclaurine (**8**)



Table S1: 1H and 13C NMR data of anolobine-9-*O-β-*D-glucopyranoside (**1**) (DMSO-d6, 500 MHz/150 MHz)

|  |  |  |  |
| --- | --- | --- | --- |
| **No.** | **Mult.** | **δ 13C [ppm]** | **δ 1H [ppm]** |
| 1 | C | 141.7 | - |
| 2 | C | 146.5 | - |
| 3 | CH | 107.7 | 6.60 (s) |
| 3a | C | 127.6 |  |
| 4 | CH2 | 29.5 | 2.53 (m)2.79 (m) |
| 5 | CH2 | 43.3 | 2.77 (m)3.15 (m) |
| 6a | CH | 53.5 | 3.69 (overlapped)  |
| 7 | CH2 | 37.1 | 2.57 (t, J = 14.5, H-7α),2.83 (dd, J = 14.5, 4.8 Hz, H-7β) |
| 7a | C | 137.7 | - |
| 8 | CH | 116.3 | 6.97 (d, J = 2.3 Hz) |
| 9 | C | 157.1 | - |
| 10 | CH | 115.6 | 6.98 (dd, J = 9.4, 2.3 Hz) |
| 11 | CH | 128.1 | 7.90 (d, J = 9.4 Hz) |
| 11a | C | 125.0 | - |
| 11b | C | 115.0 | - |
| 11c | C | 128.5 | - |
| OCH2O | CH2 | 100.8 | 5.96, 6.09 (each brd. s) |
| 1' | CH | 100.9 | 4.90 (d, J = 7.5 Hz) |
| 2' | CH | 73.7 | 3.23 - 3.31 (overlapped) |
| 3' | CH | 77.1 | 3.23 - 3.31 (overlapped) |
| 4' | CH | 70.2 | 3.18 (t, J = 9.1 Hz) |
| 5' | CH | 77.6 | 3.35 (ddd, J = 9.1, 5.8, 2.1 Hz) |
| 6' | CH2 | 61.1 | 3.69 (overlapped)3.48 (dd, J =11.9, 5.8 Hz) |

# Original spectra for compound 1

1H NMR (500 MHz, DMSO-d6):

13C NMR (125 MHz, DMSO-d6):



DEPT 135:



HSQC:



H-H COSY:



HMBC:



IR (KBr):

