SUPPLEMENTARY MATERIAL

Sesquiterpenes from the fruits of *Illicium simonsii* Maxim

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ABSTRACT

A new allo-cedrane sesquiterpene glycoside (1) and nine known compounds (2–10) were isolated from the ethanol extract of the fruit of *Illicium simonsii* Maxim. Their structures were elucidated by spectroscopic methods, including 1D-, 2D-NMR, and HRESIMS. The absolute configuration of compound 1 was confirmed by CD experiments. Among them, compounds 1, 4, 5, and 7 displayed moderate anti-inflammatory activities by use of an in vitro bioassay.

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S7. HRESIMS spectrum of compound 1

[Image of HRESIMS spectrum]

S8. Key HMBC and NOESY correlations of compound 1

[Diagram showing key HMBC and NOESY correlations]
S9. $^1$H and $^{13}$C NMR data of compound I in CD$_3$OD$^a$

| Position | $\delta_C$ | $\delta_H$ ($J$ in Hz) |
|----------|------------|----------------------|
| 1        | 46.1       | 1.78 (m)             |
| 2        | 75.4       | 4.26 (m)             |
| 3        | 35.0       | Ha 1.77 (m)          |
|          |            | Hb 1.71 (m)          |
| 4        | 46.4       | 3.06 (dd, 11.5, 7.5) |
| 5        | 51.8       |                      |
| 6        | 49.0$^b$   |                      |
| 7        | 29.1       | Ha 2.63 (m)          |
|          |            | Hb 1.28 (m)          |
| 8        | 30.6       | Ha 1.84 (m)          |
|          |            | Hb 1.43 (m)          |
| 9        | 45.5       |                      |
| 10       | 48.1       | Ha 2.34 (d, 19.5)    |
|          |            | Hb 2.05 (d, 19.5)    |
| 11       | 216.6      |                      |
| 12       | 15.3       | 0.97 (s, 3H)         |
| 13       | 175.4      |                      |
| 14       | 17.9       | 1.05 (s, 3H)         |
| 15       | 9.9        | 0.94 (d, 7.5, 3H)    |
| 1$'$     | 96.3       | 5.54 (d, 8.0)        |
| 2$'$     | 74.0       | 3.37 (m)             |
| 3$'$     | 78.4       | 3.41 (m)             |
| 4$'$     | 71.0       | 3.38 (m)             |
| 5$'$     | 78.9       | 3.38 (m)             |
| 6$'$     | 62.3       | Ha 3.84 (br d, 12.5) |
|          |            | Hb 3.69 (br d, 12.5) |

a. $^1$H NMR data ($\delta$) were measured at 500 MHz, and $^{13}$C NMR data ($\delta$) were measured at 125 MHz.
b. Signal overlapped by solvent peaks.