Supporting Information

Idesolide: A New Spiro Compound from *Idesia polycarpa*

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Supporting Information Available

Experimental Section

1. The ESIMS spectrum of idesolide
2. The EIMS spectrum of idesolide
3. The HRFABMS spectrum of idesolide
4. The IR spectrum of idesolide
5. The ^1H NMR spectrum of idesolide
6. The ^{13}C NMR spectrum of idesolide
7. The HMQC spectrum of idesolide
8. The HMBC spectrum of idesolide
9. The ^1H - ^1H COSY spectrum of idesolide

Experimental Section

The ^1H and ^{13}C NMR measurements were carried out in a Bruker AMX 400 spectrometer operating at 400 and 100 MHz, respectively. Solvent were used as an internal standard. HMQC, HMBC, and ^1H - ^1H COSY NMR experiments were performed on the same spectrometer. EIMS spectrum was obtained on a VG Trio II spectrometer. FAB-MS were recorded on VG 70-VSEQ mass spectrometer with direct inlet system using PEG600/glycerol as a matrix. High resolution mass spectral analysis was obtained on a JEOL JMS AX 505 WA spectrometer. FT-IR spectra were recorded on a Perkin Elmer 1710 spectrophotometer. Optical rotation was measured with a Jasco DIP-1000 digital polarimeter.

The fruits of *I. polycarpa* were collected in Beagwoon Mountain, Gwangyang city, Jeollanam-do, Korea, in September 2003 and authenticated by Dr. Jong Hee Park, professor of Pusan National University. A voucher specimen (CS76) has been deposited at the Herbarium of the Medicinal Plant Garden, College of Pharmacy, Seoul National University, Koyang, Korea. The fresh fruits (9kg) were ground and extracted with MeOH ($3 \times 10\text{L}$) at room temperature. The MeOH extract was concentrated in vacuo to give a crude extract (1.2kg) and then partitioned successively with *n*-hexane, CHCl_3 , ethylacetate and *n*-BuOH. The CHCl_3 fraction (32g) which showed the most potent anti-inflammatory activity was subjected to ODS gel column chromatography with a gradient elution of H_2O –MeOH to give nine fractions (CI to CIX). CII was applied on silica gel column using a mixture of CHCl_3 –MeOH as an eluting solvent to give two subfractions (CII-1 to CII-2). Idesolide (130mg) was isolated from CII-1 by semi-preparative HPLC (Microsorb C_{18} 80-299, $10 \times 250\text{mm}$, $\text{H}_2\text{O}:\text{MeOH} = 80:20$, 20ml/min , $t_r=25.8\text{min}$).

1. The ESIMS spectrum of idesolide

2. The EIMS spectrum of idesolide

3. The HRFABMS spectrum of idesolide

[Theoretical Ion Distribution]

Molecular Formula : C16 H20 O8 Na

(m/z 363.1056, MW 363.3198, U.S. 6.5)
Base Peak : 363.1056, Averaged MW : 363.3203(a), 363.3210(w)

m/z	INT.
363.1056	100.0000 *****
364.1090	18.4005 *****
365.1111	3.1977 **
366.1138	0.3808
367.1162	0.0400
368.1186	0.0035
369.1210	0.0003

[Theoretical Ion Distribution]

Molecular Formula : C16 H21 O8

(m/z 341.1236, MW 341.3379, U.S. 6.5)
Base Peak : 341.1236, Averaged MW : 341.3385(a), 341.3392(w)

m/z	INT.
341.1236	100.0000 *****
342.1271	18.4155 *****
343.1292	3.2004 **
344.1319	0.3813
345.1342	0.0400
346.1367	0.0035
347.1391	0.0003

4. The IR spectrum of idesolide

Sample Name: CII

Resolution: 4 cm-1

Apodization: Cosine

Accumulation: 11

Date/Time: 104-12-23 9:41 오전

5. The ^1H NMR spectrum of idesolide

6. The ^{13}C NMR spectrum of idesolide

7. The HMQC spectrum of idesolide

8. The HMBC spectrum of idesolide