ABSTRACT

A new homosesquiterpenoid, cinnamastemol (1) was isolated from the roots of Cinnamomum macrostemon (Lauraceae). The structure of the new homosesquiterpenoid was elucidated by chemical and physical evidence.

Keywords
Cinnamomum macrostemon, Lauraceae, Homosesquiterpenoid.

Introduction

Cinnamomum macrostemon Hayata is a medium-sized evergreen tree, and it is endemic in Taiwan, distributed at medium altitudes throughout the island. In the course of screening for biologically and chemically novel agents from Formosan Lauraceous plants, C. macrostemon Hayata was chosen for further phytochemical investigation. Previously, we isolated 12 compounds, including three coumarins, two benzenoids, two steroids, two lignan and three dibenzocycloheptenes from the roots of this plant. In the course of screening for biologically and chemically novel agents from Formosan plants in the family Lauraceae [1-79], C. macrostemon was chosen for further phytochemical investigation. In this paper, we report the isolation and structural elucidation of this new homosesquiterpenoid.

Cinnamastemol (1) was obtained as a colorless oil. Its molecular formula was established as C_{16}H_{28}O by HRESIMS (m/z 259.2035 [M + Na]^+; calc. 259.2038). The IR spectrum revealed the presence of hydroxyl group absorption at 3300 cm\(^{-1}\). The \(^1\)H NMR spectrum of 1 showed four methyl groups at \(\delta\) 0.77 (3H, d, J = 7.2), 0.92 (3H, d, J = 7.2), 1.11 (3H, s) and 1.67 (3H, br s), five methine protons at \(\delta\) 1.03, 1.23, 1.75, 2.16 and 5.50, five methylene protons at \(\delta\) 1.14/1.64, 1.28/1.99, 1.28/2.02, 1.29 and 1.44/1.81, indicating that 1 was probably a sesquiterpene possessing a hydroxyl group in the structure. The \(^13\)C NMR spectrum and a DEPT experiments indicated that compound 1 had a total of 16 carbons, with the skeleton consisting of 16 carbons, consistent with a homosesquiterpenoid. The carbons of the homosesquiterpenoid were assigned, from \(^13\)C NMR and DEPT experiments, as four methyls at \(\delta\) 15.1, 20.8, 21.5 and 23.8; five methylenes at \(\delta\) 21.9, 22.6, 29.7, 30.9 and 42.2; five methines at \(\delta\) 26.0, 39.8, 46.7, 50.0 and 122.3 and two quaternary carbons at \(\delta\) 72.4 and 135.0. The structure of 1 was also confirmed by 2D NMR experiments. Examination of the \(^1\)H-\(^1\)H COSY and \(^1\)H-\(^13\)C COSY spectra provided one continuous fragment as shown.
by bold lines in Figure 1. The HETCOR experiment showed that
the carbon signals at δ 22.6 for C-1, 30.9 for C-2, 122.3 for C-4,
39.8 for C-4a, 46.7 for C-5, 21.9 for C-6, 29.7 for C-7, 42.2 for
C-8, 50.0 for C-9a and 26.0 for C-11 were correlated to the proton
signals at δ 1.28/2.02 for H-1, 1.28/1.99 for H-2, 5.50 for H-4, 1.75
for H-4a, 1.03 for H-5, 1.14/1.64 for H-6, 1.29 for H-7, 1.44/1.81
for H-8, 1.23 for H-9a and 2.16 for H-11, respectively. The relative
stereochemistry of 1 was determined through 2D NOESY analysis
(Figure 2). Thus, the structure of this compound was determined to be
a new homosesquiterpenoid, which was further confirmed by HMBC
experiments (Table 1). The structure of 1 was determined to be a new
homosesquiterpenoid and has been named cinnamastemol (1).

![Chemical structure (a) and COSY (b) correlations of 1.](image1)

**Figure 1:** Chemical structure (a) and COSY (b) correlations of 1.

**Experimental**

**General**

UV spectra were obtained in MeCN, IR spectra were measured on
a Hitachi 260-30 spectrophotometer. 1H NMR (500 MHz, CDCl3)
and NOESY spectra were obtained on a Varian (Unity Plus) NMR
spectrometer. Low-resolution ESI-MS spectra were obtained on an
API 3000 (Applied Biosystems) and high-resolution ESI-MS
spectra on a Bruker Daltonics APEX II 30e spectrometer. Silica
gel 60 (Merck, 70–230 mesh, 230–400 mesh) was used for column
chromatography. Precoated silica gel plates (Merck, Kieselgel 60 F-254), 0.20 mm and 0.50 mm, were used for analytical TLC and
preparative TLC, respectively, and visualized with 50% H2SO4.

**Plant Material**

The roots of *Cinnamomum macrostemon* Hayata were collected
from Pinglin Hsiang, Taipei County, Taiwan, and November 2009.
Dr. Fu-Yuan Lu (Department of Forestry and Natural Resources
College of Agriculture, National Chiayi University) identified
plant material. A voucher specimen (*Cinnamo. 9*) was deposited
in the School of Medical and Health Sciences, Fooyin University,
Kaohsiung, Taiwan.

**Extraction and Isolation**

The air-dried roots of *C. macrostemon* (2.3kg) were extracted with
MeOH (10 L×5) at room temperature and a MeOH extract (90.3g)
was obtained upon concentration under reduced pressure. The
residue was placed on a silica gel column and eluted with CHCl3,
gradually enriched with MeOH to afford 4 fractions. Part of fraction
4 (15.2g) was subjected to silica gel CC, eluting with CH2Cl2–MeOH
(10:1) and enriched gradually with MeOH, to obtain 5
fractions (4-1-4-5). Fraction 4-1 (2.8g) was further separated
by silica gel CC using the same solvent system and purified by
preparative TLC (CH2Cl2–MeOH, 90:1) to cinnamastemol (1)
(4mg).

**Cinnamastemol (1):** Colorless oil. UV λmax (MeCN, log ε) 193
(3.11), 208 (2.56) nm. IR (neat) νmax 3300 (br, OH), 1550, 1015 cm–1;
ESI-MS m/z 259 [M+Na]+; HR-ESI-MS m/z 259.2035 [M+Na]+
(called for C15H28ONa, 259.2038); 1H NMR: see Table 1; 13C NMR:
see Table 1.

**Acknowledgment**

This investigation was supported by a grant from the National
Taiwan University awarded to S. L. Liu and the Yuan’s General
Hospital (YGH-22-006) awarded to C. T. Chang.

**References**

of the stem bark of *Neolitsea acuminatissima*. J Nat Prod.
shift of rhamnosides from the stem of *Cinnamomum


© 2022 Chang CT, et al. This article is distributed under the terms of the Creative Commons Attribution 4.0 International License