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Two New Cassane-Type Diterpenes from *Calliandra californica* with Antituberculosis and Cytotoxic Activities

Abstract

From the root of *Calliandra californica* two new cassane-type diterpenes were isolated and characterized, escobarine A (**1**) and B (**2**), which showed promising activities against two *Mycobacterium tuberculosis* strains. The microplate alamar blue assay was used to determine the minimum inhibitory concentrations (MIC) of **1** and **2** against *M. tuberculosis* H37Rv and the resistant CIBIN/UMF15:099 strains. The MIC of **1** against the resistant *M. tuberculosis* strain showed a value 8 times lower than that of ri-

fampin. The structures of the bioactive constituents were established by extensive NMR data analyses (including 1D and 2D NMR). The relative configuration of **2** was confirmed by X-ray analysis and the absolute configurations of **1** and **2** were determined by the circular dichroism method. Additionally, **1** and **2** displayed remarkable cytotoxic activity when evaluated against five human tumor cell lines.

Calliandra californica Benth (Fabaceae) is a perennial endemic shrub distributed over desert washes, gravelly flats, and hillsides from the Sierra of San Pedro Martir to the Cape region of Baja California Sur, México [1]. This species is locally known as "Tabardillo", "Zapotillo", and "Pelo de angel" and the decoction of flowers, roots, or branches, together or separate, is used in folk medicine to treat kidney ache, cystitis, urethritis, prostate inflammation, fever, tooth-ache, and cramps [2]. Previous reports on *C. californica* have shown that the crude ethanol extract of the aerial parts was active against *Staphylococcus aureus*, *Bacillus subtilis*, and *Candida albicans*, and also showed prostaglandin synthetase inhibitory activity [3]. Additionally, it has been noted that the antimicrobial activity of *C. californica* is caused by the presence of flavones [4].

From the known information, we hypothesized that *C. californica* may contain other potential antimicrobial compounds. Thus, as

part of our research on medicinal plants from the Peninsula of Baja California Sur, we investigated the antimicrobial ethyl acetate extract obtained from the roots of *C. californica*. The fractionation of this extract resulted in the isolation and characterization of two new cassane-type diterpenoids (Fig. 1), which were named escobarine A (**1**) and escobarine B (**2**). Escobarine A showed promising antituberculosis activity against the *M. tuberculosis* and *M. tuberculosis* CIBIN/UMF15:099 strains, the latter of which is resistant to the first-line antituberculosis drugs. Additionally, these compounds were evaluated against five human tumor cell lines and showed promising cytotoxic activities. This paper deals with the structural elucidation of these compounds and the determination of their potential as antituberculosis and cytotoxic natural products.

Escobarine A (**1**) was obtained as a white amorphous solid, which had the molecular formula C₂₀H₂₆O₄ as can be deduced

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Bibliography

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