New Withanolides from Two Varieties of *Jaborosa Caulescens*

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Abstract: The phytochemical study of two species of ***Jaborosa caulescens*** (***var. caulescens*** and ***var. bipinnatifida***) yielded the four new withanolides **1-4**. The structures of the new compounds were determined using a combination of spectroscopic techniques (including 1D and 2D NMR) and Molecular Modeling.

Introduction

The tribe ***Jaboroseae (Solanaceae***) is comprised by three genera: ***Jaborosa*** and ***Salpichroa,*** both Southamerican, and ***Nectouxia***, a monotipic genus endemic of Mexico.

Our research interest is focused on the phytochemical study of the ***Jaborosa*** genus. This genus is comprised by 23 species and 22 growth in Argentina [1-2].

Experimental

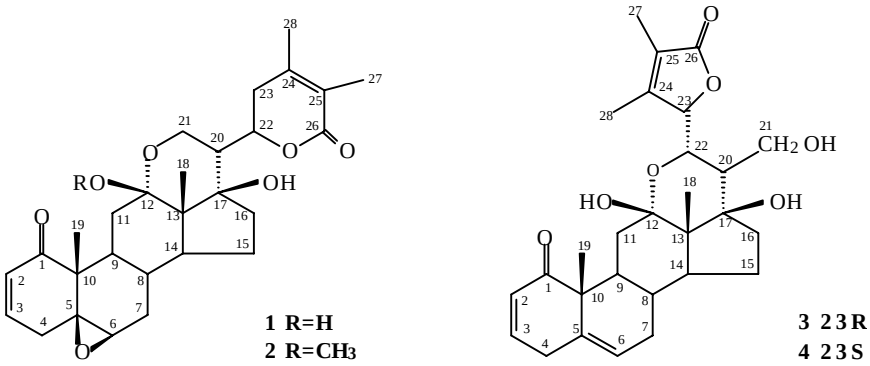
The aerial parts of ***Jaborosa caulescens var. caulescens*** and ***Jaborosa caulescens var. bipinnatifida*** were exhaustively extracted with ethanol. After evaporation of the solvent, the crude dried extract was partitioned with hexane-methanol-water (10:9:1). The methanol-water phase was then extracted with methylene chloride. The withanolides were isolated from this extract using different chromatografic techniques like CC, prep. TLC and prep. HPLC. The structures elucidation was performed by a combination of spectroscopic techniques (^{1}H-NMR, ^{13}C-NMR, DEPT, COSY, NOESY, HETCOR, IR, MS, CD) and Molecular Modeling.

Results and Discussion

J. caulescens var. caulescens yielded the withanolides **1** and **2**. These two compounds resemble the structures of Jaborosalactona R, S and T (isolated from ***J. sativa*** [3]), with respect to the presence of the hemiketal function between C-21 and C-12, but differ in the substitution pattern of ring A and B.

Compound **2**, once isolated from the plant extract, rapidily demethylate to give compound **1**. These evidences rule out the possibility that the methylation be an extraction artifact.

On the other side, compounds **3** and **4** were isolated from ***J. caulescens var. bipinnatifida***. Both compounds possessed a trechonolide type-structure. Their spectroscopic profiles were very similar and also showed the same molecular weight in the MS spectrum. A detailed analysis of the spectroscopic data led us to propose that both structures only differ in the stereochemistry at C-23. This was confirmed by Circular Dichroism experiments, in which the respective spectra of compound **3** and **4** showed opposite Cotton effect al 217 nm. The sign of the Cotton effect of compound **3** (-) was the same as trechonolide A, indicating the R stereochemistry.



References and Notes

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