



ACID TRITERPENES AND A BETA-CARBOLINE ALKALOID FROM LEAVES OF *SIMIRA SAMPAIOANA* (STANDL.) STEYERM (RUBIACEAE)

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Abstract: *Simira sampaioana* (Standl.) Steyerm is a plant species, popularly known as Maiate or Arariba, belonging to the Rubiaceae family and occurring in the states of São Paulo, Rio de Janeiro, Minas Gerais and Goiás [1]. Its bark is used in reforestation and, so far, there is only one report of chemical studies on this species [2]. *S. sampaioana* was collected in Itatiaia National Park, Rio de Janeiro state and its leaves were dried, crushed and subjected to extraction with methanol. Methanol extract was subsequently submitted to a partition with dichloromethane, ethyl acetate and acetone. The ethyl acetate fraction were refractionated by adsorption chromatography on a silica gel column and led to isolation of two compounds and two more were identified in a mixture. ¹H and ¹³C NMR data (1D or 2D) allowed their structural identification as the triterpenes pomolic acid, which possesses a skeleton of the ursan-type, sumaresinolic acid, with a oleanane-type skeleton and a mixture of two position isomers known as hederagenin (oleanane-type) and 23-hydroxy-ursolic acid (ursane-type). Pomolic acid, 23-hydroxyursolic acid, hederagenin and sumaresinolic acid possess significant biological activities reported in the literature such as anti-cancer and anti-depressant of the central nervous system [3,4]. These triterpenes have been previously isolated from species of Rubiaceae, but have never been reported in *Simira* genus. An alkaloid extract obtained from the leaves of *S. sampaioana* was analyzed by ESI-MS and showed the presence of harmane, a β-carboline alkaloid which is the chemotaxonomic marker for the genus *Simira*, demonstrating the efficacy of an instrumental technique in a study of dereplication of plant extracts. The results are of great interest to chemotaxonomic studies and add data to the chemical knowledge of the species and studied genus.

References:

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