



THREE GLUCOSYL ALKALOIDS FROM *SIMIRA GRAZIELAE* P. RUBIACEAE

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Abstract: Rubiaceae family, Angiospermae, has 660 genus and 11.150 species [1]. The species of *Simira* genus are popularly known as "arariba" [2]. *S. grazielae* P., known as "red arariba", is found in the Northeast of Bahia and Southeast of Espírito Santo state, Brazil [3]. The objective of this work was to realize the phytochemical study of wood of *Simira grazielae*, contribute to the knowledge of Rubiaceae chemical composition, and the chemotaxonomic profile of this genus. The used material of this study, was collected at forest reserve of Vale do Rio Doce Company, in Linhares city, Espírito Santo State, Brazil, and was identified by the taxonomist Domingos A. Folli. A voucher specimen (CVRD 357) was deposited at the company's herbarium (CVRD). The dried and powdered wood of *S. grazielae* P. (4.5 kg) was extracted with MeOH by maceration at room temperature, affording 271.63 g of crude methanolic extract. 235.13 g of the residue was solubilized with MeOH/H₂O (7:3) and subjected to successive liquid/liquid extraction with solvents: *n*-C₆H₁₄ (SMH, 5.34 g), CH₂Cl₂ (SMD, 11.44 g), AcOEt (SMAC, 12.44 g) and BuOH (SMB, 42.25 g). SGD (9.0 g) was chromatographed on a silica gel column (230-400 mesh) (50 cm x 6 cm), using hexane, CH₂Cl₂, AcOEt, MeOH and H₂O, pure or in gradient of increasing polarity, as eluents. The group of fractions 3-6, obtained from the elution with AcOEt/MeOH (9:1) and AcOEt/MeOH (8:1), was filtered on a Sephadex LH-20 column (40 cm x 3 cm) using MeOH 100% as eluent, and furnished the compounds **1** (6.0 mg) and **2** (4.0 mg). Fraction SGB (3.26 g) was washed with distilled water. The water-soluble fraction was lyophilized, re-suspended in water and purified by chromatography RP-2 column (40 cm x 3 cm; eluted with mixture of water/methanol) and the compound **3** (20.0 mg) was obtained. The structures of compounds were defined by of ¹H NMR (500 MHz), ¹³C NMR (125 MHz), HSQC, HMBC, COSY and ESI-MS the analysis besides comparison with literature data. The compounds were identified as alkaloids: lyalosidic acid (**1**) [4], lyaloside (**2**) [5] and ophiorine B (**3**) [6]. To the best of our knowledge this is the first report for the compounds **1** and **2** in *Simira grazielae*.

References:

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