



Annotation of Bioactive Compounds from *Lippia organoides* Kunth by UHPLC-HRMS/MS with Cosmetic Potential

Joyce L. Vieira¹, Romário P. da Costa¹, Adriana P. M. G. Macedo¹, Lorena R. F. de Sousa¹, Quezia B. Cass², Richele P. Severino^{1*}

*richeleps@ufcat.edu.br

1-Instituto de Química, Universidade Federal de Catalão, Catalão, GO, 75704-020, Brazil. 2-Departamento de Química, Universidade Federal de São Carlos, São Carlos, SP, 13565-905, Brazil.

In recent years, the market for natural ingredients applied in cosmetics has shown significant growth, reaching approximately USD 642 million in 2022, with projections to achieve USD 1.1 billion by 2030.¹ This scenario has driven research in bioinnovation, particularly in the prospecting of bioactive compounds for use in cosmetic formulations. In this context, the Brazilian Cerrado stands out for its vast biodiversity, still little explored in terms of chemical composition and biological activities, in addition to being a territory rich in traditional knowledge. Many of its plant species have been used medicinally for generations, including *Lippia organoides* Kunth, popularly known as “alecrim-pimenta.” Recognized by the Brazilian Ministry of Health as a medicinal plant, this species is employed in the treatment of skin conditions, infections, and as an antiseptic in mouth rinses.³ Previous studies have already reported the presence of compounds of great interest for cosmetic applications. Therefore, this study aimed to investigate the ethanolic extract of *L. organoides* to annotate bioactive compounds with potential application in cosmetics through ultra-high-performance liquid chromatography coupled with high-resolution mass spectrometry (UHPLC-HRMS/MS), associated with dereplication tools such as GNPS and SIRIUS platforms. This approach enabled the annotation of several metabolites, including 5,7-dihydroxycoumarin, eriodictyol, glycosylated eriodictyol, luteolin, quercetin, glycosylated quercetin, phlorizin, phloretin, naringenin, taxifolin, acteoside, glycosylated apigenin, scutellarein 4'-methyl ether and cirsimaritin. In addition to chemical characterization, biological assays were performed to evaluate the inhibitory activity of the extract and its fractions against elastase and tyrosinase, enzymes respectively involved in skin aging and hyperpigmentation. The results indicated that both the ethanolic extract and the dichloromethane fraction exhibited significant activity against tyrosinase, with inhibition rates of 60% and 89% at 100 µg/mL, respectively. These findings reinforce the potential of *L. organoides* as a source of bioactive compounds for the development of phytocosmetics.

Keywords: *Lippia organoides*, dereplication, tyrosinase, phytocosmetics.

¹CAS: The rise of natural ingredients for cosmetics, *A division of the American Chemical Society*, 2024.

²Fonseca-Santos et al., *Brazilian Journal of Pharmaceutical Sciences*, 2015.

³Ministério da Saúde, *Glossário temático: práticas integrativas e complementares em saúde*, 2018.

