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MOLECULAR NETWORKING AS TOOL FOR DEREPLICATING COMPOUNDS WITH ANTI-INFLAMATORY POTENTIAL FROM BACCHARIS TRIMERA

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Baccharis trimera (Asteraceae), popular known as carqueja, is a medicinal plant widespread in Brazilian Cerrado with biological potential. This plant has been used in phytotherapy for stomach issues, but no usage of extract for skincare applications are known. Flavonoids, lactones and sesquiterpenes are chemical constituents previously known in the leaves of carqueja. In this view, this work aimed to investigate for anti-inflamatory potential of the leaves of this species and to dereplicate the active compounds for cosmetics application. Ethanolic solution of *B. trimera* (Sisgen A9D0265) was provided by Livealoe company and crude extract was obtained after removing the solvent in a rotatory evaporator. Fractionation was performed with hexane and ethyl acetate. THP-1 macrophage pro-inflammatory response assay was used to evaluate the ethanolic extract and fractions through the inhibition of pro-inflammatory cytokines (TNF-α, IL-1β, IL-6). The crude extract was dereplicated using hyphenated technique of Liquid Chromatography coupled to High Resolution Mass Spectrometry (LC-HRMS) and ionization in positive ion mode. The MS/MS data were analyzed using Bruker Smart Formula 3D, Compound Crawler, DataAnalysis 4.0 software, and Molecular Networking (GNPS). Biological investigation revealed that crude extract strongly inhibits IL-6 cytokine while polar fraction inhibit IL-6 with less intensity and apolar fraction inhibited TNF-α. GNPS data treatment exhibited 452 nodes, 534 edges and 38 clusters, where 28 compounds were annotated by platform. Analysis of data comparing ion fragments with literature led to eleven compounds, terpenes, sesquiterpenes, fatty acid, hydroxycinnamic acid derivative, and flavonoids. Among the secondary metabolites annotated, seven compounds are known for anti-inflammatory potential, dihydroxy-dimethoxy-isoflavone, apigenin-6,8-di-*C*-hexoside, isokaempferide, eupatorine, isoschaftoside, aristolone, and linolenic acid. These results bring insights of anti-inflammatory properties of carqueja leaf extract and revealed several related active compounds, as a source of material that could be further investigated for cosmetic application.

Keywords: *molecular networking, Baccharis trimera, anti-inflammatory potential*