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POLYPHENOLIC PROFILES AND ANTIFUNGAL POTENTIAL OF Eugenia SPECIES AGAINST Candida auris: in vitro AND in silico INSIGHTS

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The genus *Eugenia* is the largest neotropical representative of the *Myrtaceae* family. It is widely distributed in Brazil and recognized for its diversity of secondary metabolites with potential pharmacological applications. This study investigated the diversity of polyphenolic metabolites in leaf extracts of *E. uniflora, E. dysenterica, E. pyriformis,* and *E. stipitata,* correlating these profiles with their antifungal potential, and assessed whether molecular modelling could support the *in vitro* findings. Leaves were collected, identified, registered (A74AD6E), stabilized, and subjected to turbolysis (5% w/v) with 50% (v/v) ethanol. Phytochemical profiles were then obtained by LC-ESI(-)MS. Antifungal activity against *Candida auris* CDCP (11903) was evaluated using broth microdilution, while molecular modelling targeted lanosterol 14α-demethylase (PDB 3LD6) with Autodock Vina. Distinct phytochemical profiles were observed among the species. *E. uniflora* was rich in glycosylated flavonoids of myricetin (myricitrin, myricetin-O-glucoside, myricetin-O-pentoside), quercetin derivatives (quercitrin, quercetin-O-deoxyoside), and hydrolysable tannins. *E. dysenterica* contained abundant procyanidins (dimeric and trimeric), catechin, and rutin. *E. pyriformis* presented epigallocatechin, procyanidin B, and quercetin, whereas *E. stipitata* showed catechin, quercetin-O-glucuronide, and ellagic acid derivatives. In antifungal assays, *E. uniflora* displayed the strongest activity (MIC: 62.5 µg/mL), followed by *E. pyriformis* and *E. stipitata* (both 250 µg/mL), while *E. dysenterica* showed the weakest effect. These results suggest that glycosylated myricetin and quercetin derivatives contribute to the stronger activity of *E. uniflora*, whereas species rich in procyanidins and ellagic acid derivatives displayed intermediate to lower activity. The *in silico* analyses supported these findings: quercetin-3-O-gallate (-11.5 kcal/mol), dismantin (-10.0), myricitrin (-9.7), myricetin-3-O-glucoside (-9.6), and epigallocatechin gallate (-9.5) showed strong binding affinities at the enzyme's active site. Therefore, the phytochemical, biological, and modelling data highlight the central role of polyphenolic compounds in the antifungal activity of *Eugenia* species, reinforcing their potential as sources of innovative antifungal molecules.

Keywords: *flavonoids, pitanga, uvaia, cagaita, araçá-boi.*