



IN SILICO EVIDENCE OF THE GASTROPROTECTIVE PROPERTIES OF *Aloysia polystachya*

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INTRODUCTION

Native to South America and widely distributed in Brazil, the plant species *Aloysia polystachya* (Griseb) Moldenke, commonly known as burrito, erva-serrana, or té-burro, is traditionally used to treat gastrointestinal problems. However, despite its widespread popular use and the bioactive potential of its compounds, research in silico is still scarce. Therefore, this study aimed to evaluate the gastroprotective potential of *A. polystachya* (Ap) through network pharmacology.

MATERIAL AND METHODS

The hydroalcoholic extract of *A. polystachya* (HEAp) was submitted to mass spectrometry (ESI-IT-MS) analysis to identify the phytoconstituents. The compounds that were in accordance with Lipinski's rule and that presented bioavailability more significant than 30 (>30) were selected for pharmacological target identification on the SwissPredict and SuperPred platforms. The common targets among the compounds were represented in a Venn diagram, and then crossed with the targets associated with gastric ulcer disease. Subsequently, a pharmacological interaction network was constructed on the Stitch platform. Finally, on the Cytoscape platform, the 10 most promising targets were ranked for subsequent enrichment analysis.

RESULTS

Four compounds were identified in the HEAp through mass spectrometry analyses: caffeic acid, *p*-coumaric acid, gallic acid, and epigallocatechin. In addition to these compounds, carvone, the major component of the plant's essential oil, was selected based on the literature. Among the five compounds, 27 common targets were identified, which were cross-referenced with 5010 targets related to gastric ulcer disease, resulting in 16 common targets between the compounds and the disease. These 16 targets generated a ranking with the top 10 that exhibited the highest binding scores. The proteins RELA, NFKB1, and BCL3 occupied the top positions.

CONCLUSIONS

Based on network pharmacology, the compounds of *Aloysia polystachya* exhibit potential gastroprotective properties. However, despite its ethnopharmacological use and promising in silico results, further studies are needed to corroborate the plant's use as an antiulcer agent.

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