IV SIMPÓSIO INTERNACIONAL EM INVESTIGAÇÕES QUÍMICO-FARMACÊUTICAS

UNIVALI

Área: FAR

NETWORK PHARMACOLOGY IN THE INVESTIGATION OF THE GASTROPROTECTIVE POTENTIAL OF *Plectranthus barbatus*

Khetlyn Freschi[1]*, Cristian A. Dalla Vecchia[1], Ana L. T. Borba[1], Amanda M. Steffler[1], Daniela Miorando[1], Juliana C. Maccagnan[1], Lincon B. Somensi[1], Iuri R. Giacomelli[1], Maria I. Roman[1], Walter A. Roman Junior[1].

[1]*Community University of Chapecó Region, Brazil.* *khetlyn_@outlook.com*.*

INTRODUCTION

Plectranthus barbatus Andrews (Lamiaceae) is native to Africa and India and is known in Brazil as a false-boldo. Its leaves are widely used in popular medicine for the treatment of gastrointestinal and liver disorders. However, despite its traditional use, in silico studies evaluating the hypothesis that your phytoconstituents are active in gastric ulcers have not yet been carried out. In this context, this research aims to evaluate the gastroprotective potential of the hydroalcoholic extract of *P. barbatus* (HEPb) through Network Pharmacology.

MATERIAL AND METHODS

The compounds present in the hydroalcoholic extract of *P. barbatus* (HEPb) were identified using mass spectrometry (ESI-MS), and their targets were predicted through the SwissPredict and SuperPred databases. The common targets among all identified compounds were represented in a Venn diagram, which was subsequently cross-referenced with targets associated with gastric ulcers predicted in the DisGiNet and GeneCards databases. The Stitch platform was then used to construct pharmacological networks, which were analyzed in Cytoscape to rank the principal targets. These targets were then subjected to enrichment analysis in the SRPlot database.

RESULTS

Four compounds were identified through chemical analysis: caffeic acid, coumaric acid, barbatusol, and epigallocatechin. Additionally, forskolin was selected based on literature reviews, as it is the predominant compound in the plant under study. The five chosen compounds shared 27 common targets among themselves, and when cross-described with the 5,010 targets associated with gastric ulcers, 19 shared targets were identified. The rank of the targets with the highest interaction pointed to RELA, NFκB1, and NFBIA.

CONCLUSIONS

The compounds of Plectranthus barbatus demonstrated a strong association with key targets in the inflammatory pathway, indicating that the modulation of these proteins may partly explain a gastroprotective effect. However, further studies are needed to better understand the pharmacological mechanism.

ACKNOWLEDGMENTS

Community University of Chapecó Region, Coordination of Improvement of Personal Higher Education (CAPES) – Brazil.