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Identification of cancer inhibitors from Hystrix brachyura bezoar extracts using LC-MS multivariate data analysis and in silico evaluation on Bcl-2, cyclin B/CDK1, VEGF and NM23-H1 [Identificación de inhibidores de cáncer a partir de extractos de bezoar de Hystrix branchyura usando análisis multivariado LC-MS y evaluación in silico en Bcl-2, cyclin B/CDK1, VEGF, y NM23-H1]

(2024) *Boletin Latinoamericano y del Caribe de Plantas Medicinales y Aromaticas*, 23 (1), pp. 41-60.

DOI: 10.37360/blacpma.24.23.1.4

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Abstract
Hystrix brachyura bezoar is calcified undigested material found in the gastrointestinal tract known for various medicinal benefits including as an anticancer agent. However, the H. brachyura population has been declining due to its demand and is under Malaysian law protection. Therefore, present study aimed to identify bezoar anticancer active compounds through metabolomics and in-silico approaches. Five replicates of bezoar powder were subjected to extraction using different solvent ratios of methanol-water (100, 75, 50, 25, 0% v/v). Cytotoxicity and metabolite profiling using liquid chromatography-mass spectrometry were conducted. Putative compounds identified were subjected to in-silico analysis with targeted anticancer proteins namely, Bcl-2, Cyclin B/CDK1 complex, VEGF and NM23-H1. The correlation of LC-MS and cytotoxicity profile pinpointed two compounds, mangiferin and propafenone. In-silico study showed both compounds exerted good binding scores to all proteins with hydrophobic interaction dominating the ligand-protein complex binding, suggesting the ligands act as hydrophobes in the interactions.

Author Keywords
Anticancer; Hystrix brachyura; LCMS; Metabolomics; Molecular docking

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Publisher: MS-Editions

ISSN: 07177917
Language of Original Document: English
Abbreviated Source Title: Bol.latinoam. y del Caribe de Plant.med.y aromat.
2-s2.0-85175322681
Document Type: Article
Publication Stage: Final
Source: Scopus