Metabolic Profile of Spent Coffee Grounds Extracts: Pharmacological Potential

Naira Linhares Sabino[1], Rafael Vieira[2], Cristiano Soleo de Funari[3], Kelly Johana Dussán[1]

[1.] UNESP, Universidade Estadual Paulista - Instituto de Química, Av. Prof. Francisco Degni, 55 - Jardim Quitandinha, Araraquara - SP, 14800-900, Brasil;
[2.] IFRO, Instituto Federal de Educação, Ciência e Tecnologia de Rondônia, R. Rio Amazonas, 151 - Jardim dos Migrantes, Ji-Paraná, RO, 76900-730, Brasil;
[3.] UNESP, Universidade Estadual Paulista - Faculdade de Ciências Agrárias, Av. Universitária 3780, Botucatu, SP, 18610-034, Brasil;

Introduction: The increasing generation and disposal of solid and liquid wastes are significant global issues affecting the environment. Effective waste management is critical for sustainable development and achieving the Sustainable Development Goals (SDGs), including proper waste treatment and resource conservation. Brazil\'s coffee production in the 2022/23 harvest was 65.49 million bags, with 650 kg of coffee grounds generated per ton of green coffee processed. Spent coffee grounds (SCG) contain approximately 26% extractable compounds, including phenolic compounds, fatty acids, hydrocarbons and triterpenes, which have potential applications in the pharmaceutical, cosmetic and food industries. This study investigates the metabolic profile of the non-polar extract of SCG, known to contain compounds with various beneficial properties, and analyzes target compounds with antioxidant, anti-inflammatory, and immunomodulatory properties through molecular docking for potential binding to interleukin-6 (IL-6), a protein involved in inflammatory responses.

Materials and Methods: A solid-liquid ratio of 1:10 was used for the extraction process with an apolar solvent combination, specifically ethyl acetate (5:1:4 v/v). The extraction was performed at 30°C with stirring at 1400 rpm for 30 minutes. The extracts were analyzed by gas chromatography (5% phenyl-methyl column) and mass spectrometry, with mass spectra compared to NIST data and retention index values compared to literature. Errors of less than 20% in retention index values were accepted. The CAS SciFinder tool was used to validate compound annotations. Molecular docking analysis was performed on selected target compounds to evaluate their activity against skin inflammatory episodes.

Results and Discussion: The ethyl acetate extract had a mass extraction yield of 9.80±1.94%, higher than the literature reported yield of 4.47±0.81% for SCG extracts with hydroethanol/n-heptane using the same extraction method. The combination of ethyl acetate and hydroethanol yielded a high total number of peaks in both polar and apolar phases, indicating a wider range of annotated compounds. The major extracted compounds with prominent percentage peak areas included cycloeucalenol (2.14), ?-sitosterol (1.91), caffeine (1.85), trilinolein (1.83), stigmasterol (1.27), and campesterol (0.96). Among these compounds, cycloeucalenol, ?-sitosterol and campesterol were analyzed by molecular docking with IL-6 protein (PDB code 8D82) due to their anti-inflammatory properties. Campesterol showed the best binding affinity (-5.7 kcal.mol-1), followed by cycloeucalenol (-5.4 kcal.mol-1) and ?-sitosterol (-5.2 kcal.mol-1), outperforming the co-crystallized standard ligand 2-acetamido-2-deoxy-beta-D-glucopyranose (-3.7 kcal.mol-1). These results indicate that the analyzed phytosterols, especially campesterol, are promising for interrupting inflammatory processes and potentially alleviating skin inflammatory symptoms such as atopic dermatitis.

Conclusions: This study highlights the potential of SCG as a source of high value-added products. The extracts showed significant yields of biologically active compounds with potential pharmaceutical applications. Phytosterols such as campesterol, cycloeucalenol and ?-sitosterol

showed promising interactions with IL-6 protein, suggesting their potential as anti-inflammatory agents for the treatment of skin diseases such as atopic dermatitis.

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