A pattern recognition study of anthocyanins found in beans from Brazil, and the correlation between their physicochemical properties and the incidence of neoplasms associated with their low consumption

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RESUMO

Este estudo descreve uma análise de reconhecimento de padrões de antocianinas (flavonoides polifenólicos) presentes em feijões brasileiros para classificar suas propriedades físico-químicas e examinar correlações com a incidência de câncer. Seis grupos de antocianinas foram identificados, dos quais se destacam por suas peculiaridades os compostos do grupo G1, que apresentam baixas massas moleculares e alta lipofilicidade, predominam nos feijões e cumprem a regra de Lipinski, sugerindo boa biodisponibilidade, e os compostos do grupo G3, antocianinas de alta concentração conjugadas com carboidratos. Dados nutricionais e de saúde pública sugerem uma relação inversa entre o consumo de feijão e cânceres do sistema nervoso, sugerindo que uma menor ingestão de feijões na adolescência esteja correlacionada a maiores taxas de câncer, enquanto maior consumo em idosos correlaciona-se com redução na incidência. Os resultados sugerem que antocianinas presentes nos feijões podem contribuir para a prevenção do câncer dada sua capacidade antioxidante que está associada ao combate a diversas comorbidades, o que pode ser útil em estudos sobre a importância de alimentos ricos em polifenóis na nutrição em saúde pública.

Palavras-chave: polyphenols, anthocyanins, cancer, food, nutrition.

Introduction

Polyphenols are compounds derived from the secondary metabolism of plants, characterized by a common structure consisting of a benzene ring bonded to multiple hydroxyl groups. Their biosynthesis is induced by biotic and abiotic stresses, such as herbivores, pathogens, temperature and pH effects, salt stress, carbon dioxide, ozone, heavy metal stress, and ultraviolet radiation[1]. Polyphenols can be classified into several groups, including anthocyanins, which belong to the flavonoid class. These compounds are obtained from various plant sources, such as fruits and grains. The pharmacological applications of polyphenols, often associated with their antioxidant properties[2], are diverse, with notable efficacy in combating various types of cancer.

Methods

This study conducted a statistical classification analysis of anthocyanins from the Phenol-Explorer database[3] using a pattern recognition analysis (PCA) to identify relationships between their available properties in the database and those calculated from empirical ADMET models, comparing them with their occurrence in beans. Subsequently, a comparison was established between bean consumption across different population segments and the incidence of various cancer types. Some of the analyzed properties (some related to Lipinski's rule) included: druglikeness, polar surface area, irritant potential, molecular flexibility, SVD globularity, aromatic rings, small rings, and molecular complexity.

Results and Discussion

The pattern recognition analysis enabled the identification of six distinct groups (Figure 1). The groups exhibited the following characteristics: G1 comprised compounds with low molecular weight, high lipophilicity, low SVD globularity, few H-acceptors and H-donors, low total surface area, low polar surface area, and a small number of non-hydrogen atoms. In contrast, G5 compounds displayed opposite traits to those of G1. G2 compounds were notable for their high lipophilicity and numerous aromatic rings.

Compound **76** (which did not belong to any of the identified groups) exhibited high irritancy, low lipophilicity, and poor druglikeness. The compounds in G1 satisfied Lipinski's rule. Additionally, all G2 compounds were found to be conjugated with carbohydrates and stilbenes. Following an assessment of the occurrence and concentration of each anthocyanin in beans, as reported in the Phenol-Explorer database, it was observed that all G1 compounds were present in beans, along with a significant portion of G3 compounds and only one compound from G2 (**95**). Two G4 compounds (**71** and **74**) were also detected in beans. G3 contained the compounds found in beans at the highest concentrations, namely **28**, **12**, and **9**, all of which conjugated with carbohydrates.

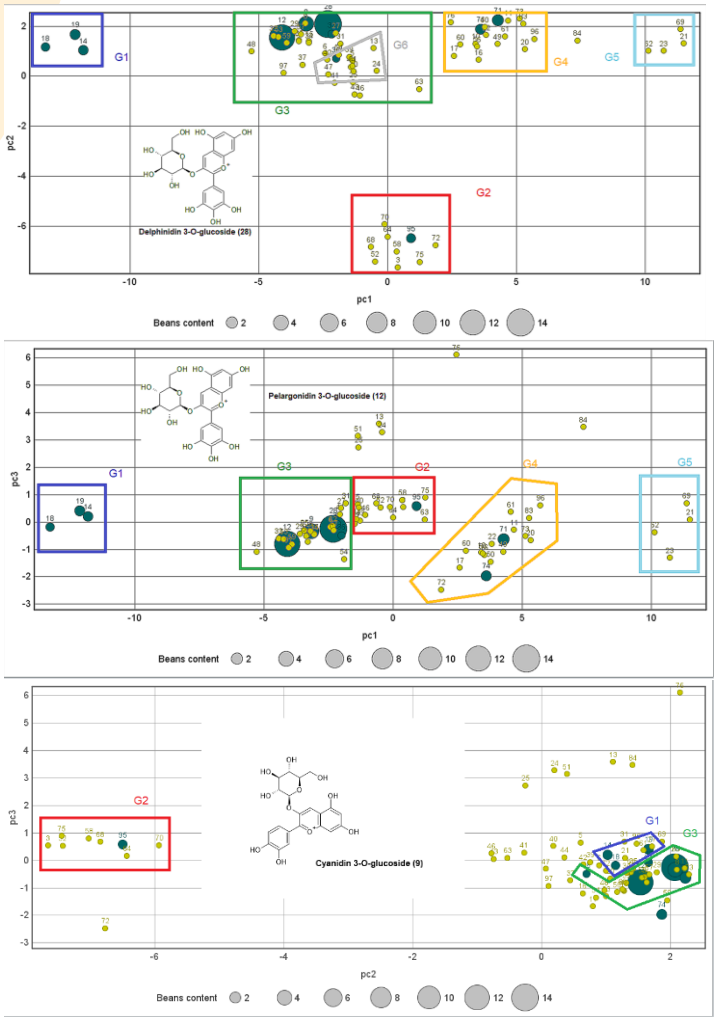
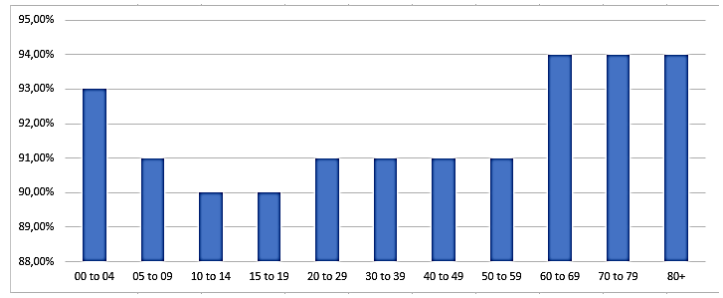


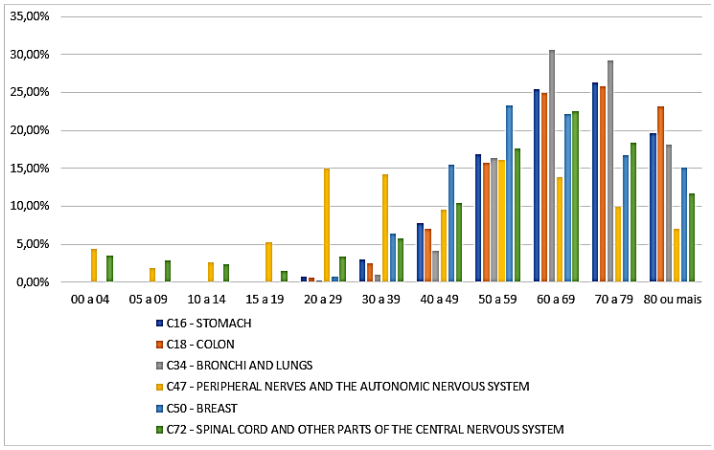
Figure 1. Principal component analysis (PCA) of bean anthocyanins, showing their correlation with concentration levels, sourced from the Phenol Explorer database. Anthocyanin most abundant in beans are highlighted. Source: author content.

The survey of the incidence of different cases of cancer among the different age groups in Brazil (Figure 2) suggests that adult and elderly population is the most affected. Data on the consumption of beans, an important source of anthocyanins, indicate a significant percentage decrease in adolescence and an increase in old age (Figure 2 (a)).

An inverse variation is also observed in the reported cases of cancer in the peripheral nerves and autonomic nervous system in these two age groups (Figure 2 (b)), suggesting a possible correlation between the consumption of these antioxidant compounds and the depletion of associated diseases.



(A)



(B)

Figure 2. (A) Beans consumption per age group (2015-2020). (B) Cancer incidence per age group (2012-2022). Source: IBGE/INCA.

Conclusions

This study provided a deeper understanding of the relationships between polyphenols present in the Brazilian diet, their pharmacological effects—particularly their potential antineoplastic properties—and the consumption of foods where they are typically found. Such insights enable further discussions on national and regional nutritional considerations.

Ackowledgments

FAPEMIG, CNPq, CEFET-MG, DECAQ-CEFET-MG.

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