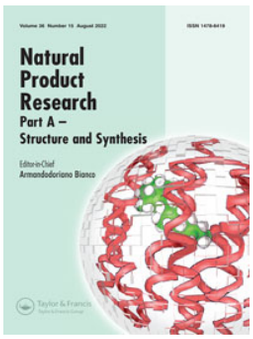

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SHORT COMMUNICATION

First report on the *Annona exsucca* DC. Essential oil and *in silico* identification of potential biological targets of its major compounds

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ABSTRACT

In the present study, the essential oil (EO) of *Annona exsucca* DC. or *Rollinia exsucca* was extracted by hydrodistillation, and the identification and quantification of volatile compounds were performed by GC-MS and GC-FID. *A. exsucca* leaves were collected from the Magalhães Barata, northeast of the State of Pará (Brazil) in March and September of 2019. Moreover, we used computational approaches to evaluate possible biological targets for the major compounds of the EO. In the sample obtained in March, 50 compounds were identified, with hydrocarbon sesquiterpenes being the predominant ones with the content of 80.52%. In the sample collected in September, 58 compounds were identified, and the chemical class of hydrocarbon monoterpenes and sesquiterpenes were the dominant ones with contents of 43.36 and 31.29%, respectively. Computational methods demonstrated that some major compounds have potential biological activity against some strains of pathogenic bacteria, as well as against molecular targets involved in cancer development.

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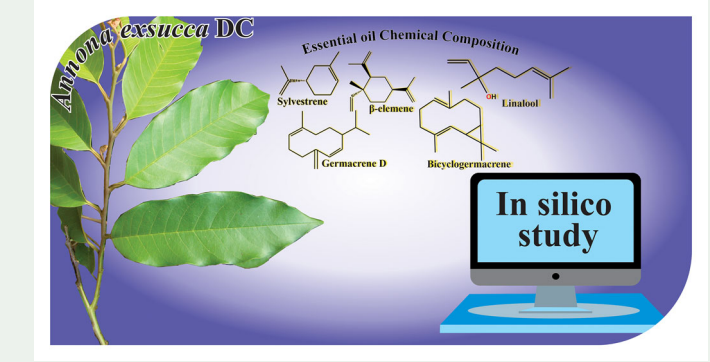

1. Introduction

Annonaceae is a dicotyledonous plant family comprising approximately 135 genera and more than 2500 species. Four subfamilies, Annonoideae, Anaxagoreoideae, Ambavioideae, and Malmeoideae are present in Brazil and are comprised of 386 species. It is estimated that approximately 75% of Annonaceae species are present in the Amazon region. *Annona* is one of the most common genus in the forests of Brazil (Anuragi et al. 2016). The relationship between the variation in the chemical composition of essential oils (EO) and their bioactivities have been investigated in several studies on plants (Do Nascimento et al. 2020).

Previous studies on this species have only reported its anatomical and physiological characteristics. Therefore, in the present study, we report the chemical composition of the EO of *A. exsucca*. or *R. exsucca* for the first time, and we also report the possible influence of climatological factors (at two different times of the year) on the chemical composition of *A. exsucca* EO. Finally, using a computational approach, we investigated potential biological activities of the major EO compounds of *A. exsucca*. The molecular modeling methods described in the present study have been extensively used to analyze compounds from natural and synthetic origin (Araújo et al. 2020; Mascarenhas et al. 2020; Santos et al. 2020).

2. Results and discussions

2.1. Chemical composition of essential oils

The chemical composition of the essential oils and the retention indices of their constituents are presented in Table S1. Hydrocarbon sesquiterpenes were predominant (80.52%) in the oils of specimens collected in March, whereas in the oils of specimen collected in September, hydrocarbon mono- (43.36%) and sesquiterpenes (31.29%) dominated.

The profile of EO can vary according to the age and organ of the plant. The principal constituents, (E)-caryophyllene, germacrene D, bicyclogermacrene, β-elemene, p-cymene, and linalool (Bicas et al. 2011; Naik and Sellappan 2020), have been reported in essential oils of other *Annona* species, indicating that this species has an essential oil composition typical for Annonaceae species. However, the hydrocarbon monoterpene sylvestrene, a

constituent found in a higher percentage in oil specimen collected in September, has not been described as a major constituent of any other *Annona* species to date.

To verify the possible influences of climatic variables on the chemical composition of the *A. exsucca* EOs, climatic parameters were obtained during the two collection periods (March and September) (Table S2). We can observe that the climatic conditions during sampling in March included higher relative humidity and along with lower average temperature and solar radiation than those during September sampling. This resulted in higher levels of (E)-caryophyllene , germacrene D , β-elemene, bicyclogermacrene, and α-humulene in March sample than those in September sample. The climatic factors may have favored a higher content of linalool and sylvestrene in September than that in March; in addition, significant levels of p-cymene, terpinolene, and 1,8-cineole that were absent in the March collection (Silva et al. 2018; dos Santos Ferreira et al. 2020; Silva et al. 2021).

2.2. Molecular targets of the essential oils compounds

Different computational methods have been applied to identify the molecular targets of bioactive compounds (Da Costa et al. 2019; Leão et al. 2020). We identified that (*E*)-caryophyllene showed a high similarity with 1 R-(+)-alpha-pinene, which has been shown to possess antibacterial activity against two pathogenic bacterial species, *Staphylococcus aureus* and *Vibrio parahaemolyticus*. Regarding bicyclogermacrene, our computational approach identified it as a possible inhibitor of *S. aureus*. Similarly, α-humulene and germacrene D showed structural matches with α-humulone and stigmasta-3,5-diene, respectively, and both compounds exhibited inhibitory activity against *Mycobacterium tuberculosis*.

Some compounds also exhibited a predicted inhibitory activity against cancer cell lines, such as CAKI-1 (β-elemene) and A549 (bicyclogermacrene), or molecular targets involved in carcinogenesis, such as arachidonate 15-lipoxygenase (linalool).

3. Conclusions

We observed qualitative and quantitative variations between the chemical compositions of *A. exsucca* EOs from leaves collected in March (rainy season) and September (dry season). We concluded that these differences in EO profiles were associated with different climatological conditions of both periods of sample obtention. Using a computational approach, we identified the molecular targets for the majority constituents of the investigated EO compounds, revealing their potential antimicrobial and anticancer activities.

Disclosure statement

No potential conflict of interest was reported by the authors.

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