

IN SILICO BIOACTIVITY OF SECONDARY METABOLITES FROM *LICANIA TOMENTOSA* (BENTH.) FRITSCH FRUITS (CHRYSOBALANACEAE)

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RESUMO

Licania tomentosa (Benth.) Fritsch (Chrysobalanaceae), is a specie that presents an arboreal habit, its fruits are considered to have potential application as food, but whose benefits of its adoption have not been clearly evaluated. In this sense, it is thought that by observing the probable biological activities of the fruits of *L. tomentosa*, it is associated with the maintenance of health, may are possible to create mechanisms to attract interest in their consumption and to developing of technologies that use the specie or compounds of its secondary metabolism, in order to employ this resource that is little used in present. For that, we sought to observe the compounds already isolated in *L. tomentosa*, in afterwards, betulinic acid, oleanolic acid, eutin, catechin, palmitoleic acid, kaempferol and gallic acid were selected, whose molecular configurations were obtained in the PubChem database for computer analysis. The PASS algorithm (Prediction of Activity Spectra for Substances) was used for the computational screening of possible biological effects. After the prediction of the bioactivity spectrum, several potential biological activities were observed, among them probable hepatoprotective, antineoplastic, chemopreventive, antineoplastic, anticarcinogenic, antimutagenic, vasoprotective, cardioprotective, free radical inhibitory, lipid peroxidase action and possible action antioxidant. The evaluated compounds belong to the classes of triterpenes, flavonoids and phenolic acids, groups of substances whose several bioactive properties have already been reported, such as antioxidant, chemoprotective and anti-inflammatory activity. Hereupon, it could be observed that some of the bioactive effects already reported in compounds of the species were observed in in silico analysis, which contributes to validation of the computational analyzes. As a result, it is presumed that the fruits of *L. tomentosa* potentially present several biological activities that can contribute to the maintenance of the health of its consumers and will make it attractive to develop new technologies based on it or compounds derived from its metabolism.

PALAVRAS-CHAVE: Applied botany, chemistry of natural products, computational chemistry, food science, phytochemistry.

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