

Review of: "Expansion of the Experimental Antifungal Activities Through in Silico Docking Study of Compounds From Albizia Lebbeck"

Raúl Díaz-Molina¹

¹ Autonomous University of Baja California

Potential competing interests: No potential competing interests to declare.

The abstract is confusing. The authors must be very clear about the objective of the work, the methodology used, and the results obtained. What the authors describe in the abstract and introduction is confusing with the objective and methodology of this work.

The authors must be very clear in this work with the following questions: Were the mentioned natural products isolated in this work? Were the effects of natural products on bacteria evaluated in this work?

The methodology of this work does not accurately describe the procedures used for the extraction of the mentioned natural products (2.2. Plant Material, Extraction and Isolation, and Experimental Characterization).

In section 2.1 General Experimental Procedures, the authors do not describe the methodologies used for the identification of the mentioned natural products (the technical characteristics of the spectroscopic and spectrometric machines).

Only the methodology used should be described in section 2.5 Experimental Antimicrobial Assay (this should be improved). In this section, it is mentioned that only natural products 2 and 7 were evaluated with this test, however, this is an aspect related to the results of the work (docking results).

In the first paragraph of the Results and Discussion section, the authors mention that "*only lebbeckisoetin A (2) and chiakine (7) were experimentally assayed for their antimicrobial activities against five microbial strains (one fungal: Candida albicans and four bacterial: Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Enterococcus faecalis) (Table S1)*"; however, the authors do not present the results obtained in the study carried out on these bacteria.

The authors present results of the minimum inhibitory concentration, however, the method used is not described in the Materials and Methods section.

Why was the antimicrobial effect of quericitrin (1) not evaluated? (This product presented the most negative docking score (Table 1)).

The last section of the manuscript is 2.7 Molecular Docking Simulation Studies, it seems to me that there is an error in the numbering.

It seems to me that it is a mistake to indicate in the conclusions section the objective of the work (the objective should be indicated in the abstract and at the end of the introduction).

The study's conclusions are not clear.