

Review of: "Expansion of the antifungal activities through in silico docking study of compounds from Albizia lebbeck fruits"

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Potential competing interests: No potential competing interests to declare.

The present work represents the development of new computational and experimental techniques that are efficient, fast, and accurate and has become a priority for researchers in all domains around the world. The present manuscript deals with the computational investigation of some naturally isolated compounds, including quercitrin (1), lebbeckisoetin A (2), quercetin-3-O-β-D-glucopyranoside (3), (E)-p-coumaric acid (4), eugenol (5), eugenol 1-acetate (6), chiakine (7), hexancosan-1',26'-dioate of bis[(2S), 2,3-dihydroxypropyl] (8), oleanolic acid (9), betulin (10), hopan-29-ol (11), hopan-30-ol (12), 22-hydroxyhopan-3-ol (13), and lupeol (14). These compounds were all isolated from the fruit of Albizia lebbeck. Only lebbeckisoetin A (2) and chiakine (7) were evaluated for their experimental antimicrobial activities on five microbial strains (fungal: Candida albicans, and bacteria: Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Enterococcus faecalis), which both revealed potent antifungal activities. This theoretical study was undertaken in the framework of better understanding the experimental results at the atomic level and to expand the antimicrobial assays of the other non-tested compounds.

Authors have done great work; however, I have some observations as follows:

- 1. Please double-check for spelling and English grammar errors in the manuscript.
- 2. The style of references must be in a similar way; please check it.
- 3. Figures must be in good quality.
- 4. Tables must be revised.
- 5. The authors wrote the introduction section in an impressive way, but it is too long. So, it must be reduced to some extent considering the readers' time.

In view of the above points, I feel the work has great knowledge that may be useful in future research. I therefore recommend the manuscript be accepted after these comments are revised (accepted after minor revision).

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