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

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Potential competing interests: No potential competing interests to declare.

This work deals with the computational study of certain compounds isolated from the fruit of Albizia lebbeck: quercitrin (1), lebbeckisoetin A (2), quercetin-3-O-β-D-glucopyranoside (3), acid (E)-p-coumaric (4), eugenol (5), eugenol, 1-acetate (6), chiakine (7), bis[(2S), 2,3-dihydroxypropyl] hexancosan-1',26'dioate (8), oleanolic acid (9), betulin (10), hopan-29-ol (11), hopan-30-ol (12), 22hydroxyhopan-3-ol (13), and lupeol (14). The two compounds lebbeckisoetin A (2) and chiakine (7) were evaluated for their antimicrobial activities on five strains (fungal: Candida albicans and bacteria: Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Enterococcus faecalis). The results revealed powerful antifungal activities. Then, the authors carried out a theoretical study on the virtual screening of antimicrobial activity using the crystal structures of sterol 14-alpha demethylase (CYP51) from Candida albicans in complex with the tetrazole antifungal drug candidate VT1161 (VT1) (PDB Id: 5TZ1) and the crystal structure of sterol 14-alpha demethylase (CYP51) from the pathogenic yeast Candida albicans in complex with the antifungal drug posaconazole (PDB Id: 5FSA). The results show that compounds (1 to 10) reveal an interesting binding strength with the 5TZ1 and 5FSA proteins, with a docking score ranging from -7.892 to -5.256, supporting the experimental results. Compounds (1-9) are primarily active due to the formation of π-π interactions, H-bonds, and hydrophobic interactions, as well as π-cation and salt bridge interactions, with both 5TZ1 and 5FSA. The results are numerous and interesting; the article corresponds perfectly to the objectives of the journal. I recommend its publication after a few corrections.

1. Review English errors and punctuation throughout the text;
2. Can the methods cited in this work be used to study other diseases or other viruses...? If yes, the authors must cite bibliographical references on work already carried out.
3. Justify the choice of the in-silico study with a link to the respective mechanisms of action of the studied activities in this work
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5. In the conclusion, the authors should describe a strategy to draw concrete conclusions from this paper;
6. Authors must cite work published in this journal and other journals on in-silico investigations:

    a. https://doi.org/10.1016/j.arabjc.2023.105262
    b. J. Infect. Dis., 192 (8) (2005), pp. 1422-2149, 10.1086/466536
    c. J. Biomol. Struct. Dyn. (2022), pp. 1-11, 10.1080/07391102.2022.2152871

d. 10.1080/07391102.2019.1707122

e. https://doi.org/10.1007/s42250-023-00744-x