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Methods

Aggregation-based *in silico* study for better understanding of related membrane interfering analogous of Amphotericin B

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Amphotericin B (AmB) is a choice antibiotic against fungal infections. Since AmB has many side effects, it is desired to come up with new molecules with similar activity and less toxicity. In this work, attempt has been made to design a series of molecules by chem/bioinformatics. The structure of AmB was divided into two fragments and the best modified molecules were chosen, according to binding energy obtained through *in silico* dock experiments. A similarity search was performed on the molecules, and the available similar compounds resulted to a set of structurally matched compounds with 70% and above for similarity value. Several molecules from the library were selected and evaluated for *in vitro* antifungal assay. The result of the evaluations was finding compounds, which their antifungal effect had not been reported before or proposed new mechanism of action possibly involve in binding to membrane components such as ergosterol.

Keywords: Amphotericin B; interaction energy; ergosterol; cholesterol; similarity search