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

Sardari Soroush, Saied Mostaan, Azerang Parisa

► To cite this version:

Sardari Soroush, Saied Mostaan, Azerang Parisa. Aggregation-based in silico study for better understanding of related membrane interfering analogous of Amphotericin B. Proceedings of the III International Conference on Environmental, Industrial and Applied Microbiology (BioMicroWorld2009), Dec 2010, Lisbon, Portugal. pp.668-671, 10.1000/ISBN978-981-4322-11-9 . pasteur-00746845

HAL Id: pasteur-00746845

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Submitted on 29 Oct 2012

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Microorganisms In Industry And Environment

From Scientific and Industrial Research to Consumer Products

Proceedings of the III International Conference on Environmental, Industrial and Applied Microbiology
(BioMicroWorld2009)

Lisbon, Portugal, 2 – 4 December 2009

S. Sardari, S. Mostaan, and P. Azerang (2010) Aggregation-based *in silico* study for better understanding of related membrane interfering analogous of Amphotericin B. Microorganisms In Industry And Environment: pp. 668-671.

Methods

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

S. Sardari

- Corresponding author: fax: (98-21) 6648 0780, phone: (98-21) 6695 3311.

Drug Design and Bioinformatics Unit, Medical Biotechnology Department, Biotechnology Research Center, Pasteur Institute of Iran, #69 Pasteur Ave., Tehran, Iran 13164, Iran

S. Mostaan

Drug Design and Bioinformatics Unit, Medical Biotechnology Department, Biotechnology Research Center, Pasteur Institute of Iran, #69 Pasteur Ave., Tehran, Iran 13164, Iran

P. Azerang

Drug Design and Bioinformatics Unit, Medical Biotechnology Department, Biotechnology Research Center, Pasteur Institute of Iran, #69 Pasteur Ave., Tehran, Iran 13164, Iran

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