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Antibacterial Activity and Virtual Screening by Molecular Docking of Lycorine from *Pancratium Foetidum* Pom (Moroccan Endemic Amaryllidaceae)

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ABSTRACT

Lycorine is an alkaloid isolated from bulbs of *Pancratium foetidum* Pom Amaryllidaceae of the genus Lycoris. It has very strong pharmacodynamics properties and biological effects, among others, antimalarial, antiviral, antitumor, and anti-inflammatory. Lycorine has been identified and characterized by thin layer chromatography, IR and NMR (¹H and ¹³C NMR, COZY, HMBC, HSQC and NOESY).

The antibacterial activity of lycorine has been evaluated. Lycorine has a moderate antibacterial activity on the majority of strains studied, nevertheless it is more effective than Streptomycin and Ampicillin against bacteria: *P. aeruginosa*, *En. cloacae*. To confirm these results, it is necessary to use qualitative techniques and methods, etc...

We performed a virtual docking ligand-lycorine protein screening study to predict and characterize their mode of interaction with the LpxC receptor. Docking results have shown that lycorine can interact with target amino residues studied by hydrogen and metal-ion bonds. In addition, the ADME-Tox profile study has shown that lycorine is all in agreement, either with Lipinski's critics or with the toxicity standards.

Keywords: Lycorine, *Pancratium foetidum*, Antibacterial power, LpxC receiver, ADME-Tox profile, Lipinski.

1.Introduction

Medicinal plants have been used for a long time to relieve and cure human diseases. In fact, their therapeutics properties are due to the presence of hundreds or even thousands of bioactive natural compounds called: secondary metabolites. Natural substances isolated from plants have multiple interests in the field of biotechnology [1], the food industry [2], cosmetics and pharmaceuticals [3]. Alkaloids are part of secondary metabolites of plants, which are subsequently accumulated in different organs and sometimes in specialized cells of the plant. Currently, the development of microbial resistance to antibiotics, leads researchers

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