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Research Article

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Evaluating Hypericin as A Therapeutic Agent Against Neisseria Gonorrhoeae

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Abstract

This study employed molecular docking simulations to investigate potential interactions between natural molecules and the Fe(3+) ions import ATP-binding protein fbpC in Neisseria gonorrhoeae FA 1090. Among the screened molecules, Hypericin exhibited a remarkable binding energy of approximately -13.2 kcal/mol, indicating a robust and favorable binding affinity with the target protein. This promising outcome suggests that Hypericin could serve as a potential candidate for further exploration as a therapeutic agent against Neisseria gonorrhoeae infections. However, it is imperative to emphasize that these in silico findings necessitate experimental validation through in vitro and in vivo studies to ascertain the actual efficacy and safety of Hypericin as a treatment option.

Keywords: Hypericin, Neisseria Gonorrhoeae, Docking Analysis, Autodock Vina.

1. Introduction

Neisseria gonorrhoeae, also known as Neisser's gonococcus, is the causative agent responsible for gonorrhea (or blenorrhagia) [1,2]. This Gram-negative bacterium belongs to the Neisseriaceae family and is morphologically similar to Neisseria meningitidis, the causative agent of meningococcal meningitis. Both are gram-negative cocci that often occur in pairs [1-6]. Neisseria gonorrhoeae is transmitted mainly through sexual contact and can cause a variety of symptoms involving the genital system and, in some cases, other areas such as the throat or anus [1-6]. Increasing resistance to antibiotics has made the management of gonorrhea a challenge, underscoring the importance of safe sexual practices and timely identification and appropriate treatment of infections [1-4].

This Gram-negative diplococcus primarily infects the genital and reproductive tract mucosa but can also affect the throat and rectum [1,2].

Neisseria gonorrhoeae is transmitted through unprotected sexual contact and can lead to a range of symptoms, including genital discharge, pain during urination, and in some cases, complications such as pelvic inflammatory disease [1-6].

The emergence of antibiotic-resistant strains of Neisseria gonorrhoeae has posed challenges for treatment, emphasizing the importance of early detection and appropriate antibiotic therapy. Regular testing, safe sexual practices, and awareness are crucial for preventing and managing infections caused by Neisseria gonorrhoeae [5,6].

2. Material and Methods

-Fe(3+) ions import ATP-binding protein fbpC (PDB Code: 3fvq) Grid box Coordinates of binding Center X (-18,1105), Y(-13,5136), Z(39,4644)

3. Results and Discussion

This short theoretical computational study based on Molecular Docking [7,9-10] aims to investigate natural molecules against Neisseria gonorrhoea [1-6].

Neisseria gonorrhoeae is a bacterium responsible for the sexually transmitted infection (STI) known as gonorrhea. This bacterium infects the mucous membranes of the reproductive tract, including the cervix, uterus, and fallopian tubes in women, and the urethra in both men and women. It can also infect the throat, rectum, and eyes [1-6].

Gonorrhea is primarily transmitted through sexual contact, including vaginal, anal, and oral sex.Transmission from an infected mother to her child can also occur during childbirth [1-6].

Particular attention docking calculation was performed against Fe(3+) ions import ATP-binding protein fbpC by Neisseria gonorrhoeae [8].

Performing a docking calculation allows to understand the potential binding modes and strength of interaction between the Fe(3+) ions and the fbpC protein [8].

This information can be crucial in understanding the role of this protein in iron import processes in Neisseria gonorrhoeae. Docking analysis was conducted by Mcule Server by Autodock Vina [9,10].

The observation that Hypericin demonstrated an excellent binding energy of about -13.2 kcal/mol against the Fe(3+) ions import ATP-binding protein fbpC in Neisseria gonorrhoeae FA 1090 is noteworthy. A lower binding energy typically indicates a stronger and more stable interaction between the molecule and the target protein.

This calculation suggests its potential utility as a candidate for further exploration in combating Neisseria gonorrhoeae infections.

However, it's important to note that in silico docking studies provide predictions, and experimental validation is crucial to confirm the actual biological activity and effectiveness of Hypericin against Neisseria gonorrhoeae.

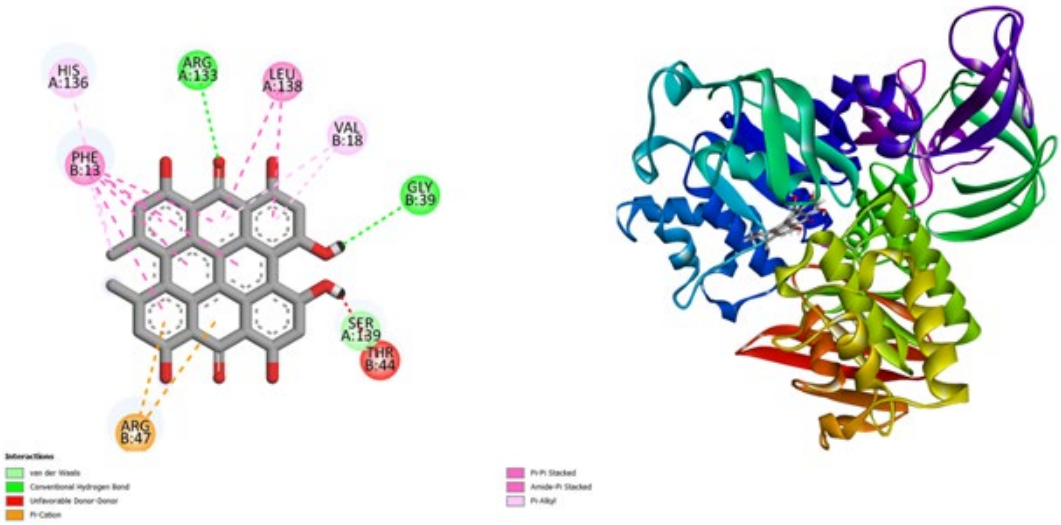

Figure 1: displays the docking outcomes of Fe(3+) ions import ATP-binding protein fbpC in conjunction with Hypericin -13.2 kcal/mol within the Ligand Binding Site, as analyzed by Autodock Vina through the Mcule Database. On the left side, 2D diagrams illustrate the residue interactions between the protein and Hypericin. Meanwhile, the right side exhibits the Ligand Binding Site of the protein, highlighting the specific location of Hypericin.

4. Conclusion

In conclusion, the molecular docking study revealed that Hypericin exhibits a notable and favorable binding affinity with the Fe(3+) ions import ATP-binding protein fbpC in Neisseria gonorrhoeae FA 1090, as evidenced by a robust binding energy of approximately -13.2 kcal/mol. This finding suggests the potential of Hypericin as a candidate for further investigation as a therapeutic agent against Neisseria gonorrhoeae infections. However, it is crucial to acknowledge that these computational results serve as a preliminary step, and experimental validation through in vitro and in vivo studies is essential to confirm the actual antimicrobial efficacy and safety of Hypericin.

Conflicts of Interest:

The authors declare no conflicts of interest.

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