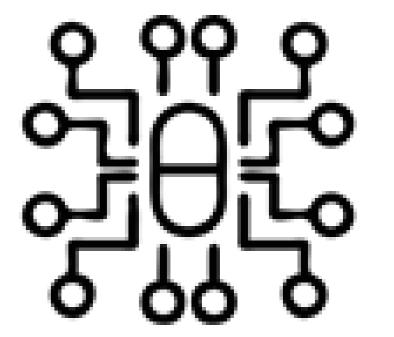
PREDICTION OF PROTEIN CANDIDATES FOR DRUG AND VACCINE DEVELOPMENT AGAINST PSEUDOMONAS AERUGINOSA INFECTIONS



SPECIAL INTEREST GROUP

DRUG-DESIGN

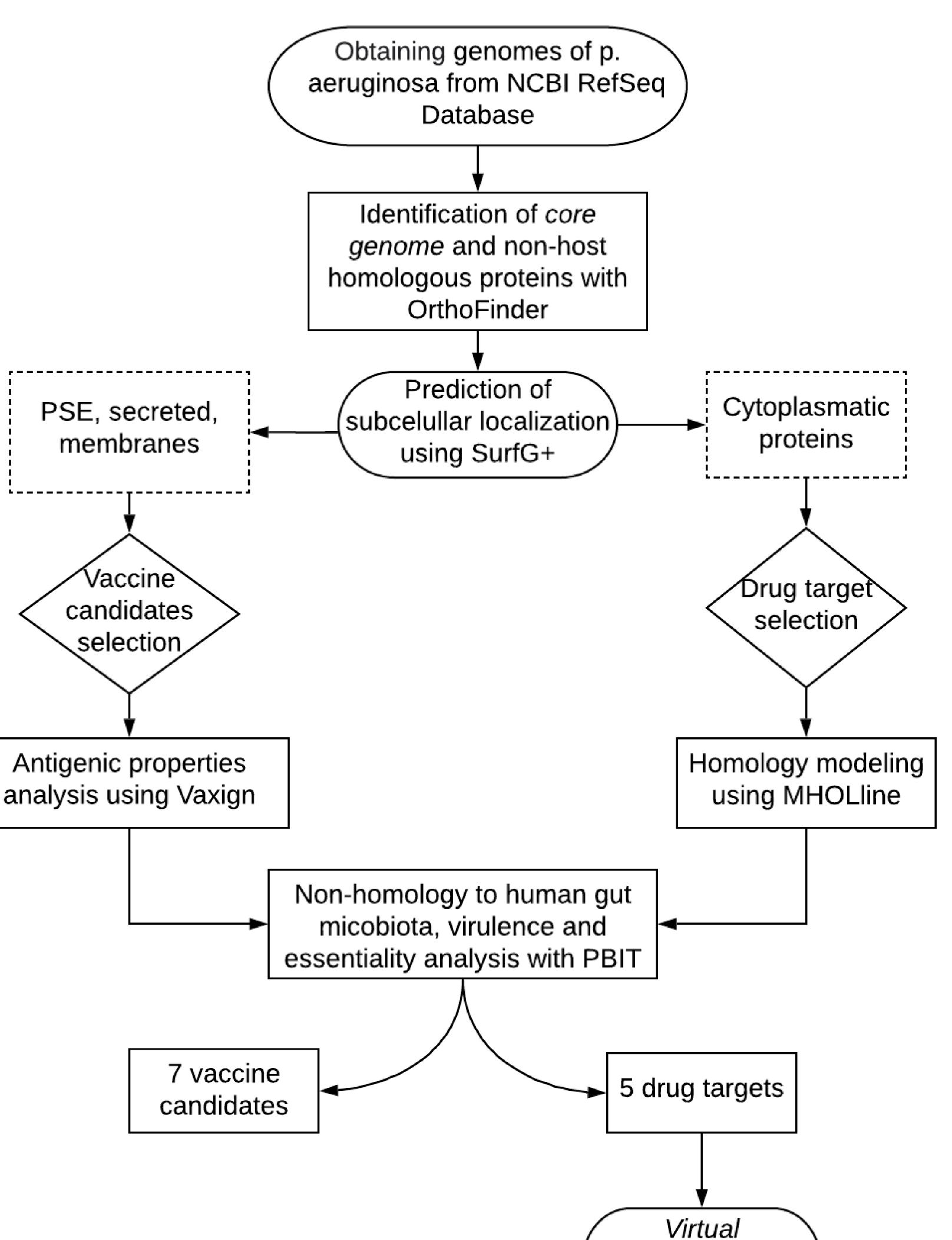
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Introduction

Pseudomonas aeruginosa is a Gram-negative and non-fermenting bacterium commonly present in soil and water. This opportunistic pathogen is one of the main agents of nosocomial infection in hospitals worldwide, causing high rates of morbidity and mortality in patients. The clinical importance of infection by *P. aeruginosa* is due to its high virulence and resistance to multiple antibiotics. Beyond the scarcity of effective pharmacological options, no vaccines ae available on the market.

Through the use of bioinformatics approaches, such as subtractive genomics and reverse vaccinology, this work aimed to identify proteins that could be used as targets in the development of new drugs and vaccines against *P. aeruginosa.*

Methods



>fasta sequence 2 GACCCcTCCCTtATCCTCTCCGCGTTCATC/ TCGCTACTCGTCAACGGCCAGGACCTCTCC TTCCCCACCGTAGCTCTCGCGGGGCCAGATGC ATCCTCTTCTCCCTTGGCGTCGCCTGGATTC CGCGCCAGCTCACAGATTCCTTTCTCGATGC GTGTTCGCCCTCCTATGCGTGCagCTCGCG/

Results

Adapted from: Getty Images, PDB

and bioinformatics.ibioba.gov.ar

PIBIC

UFBA

Prediction of subunit vaccine candidates resulted in 7 highly immunogenic antigens shared by all strains analyzed. In addition, the MHOLline workflow resulted in 29 very high and 42 high quality three-dimensional structures of P. aeruginosa cytoplasmic proteins shared by all strains. Among the modeled proteins, 5 were predicted to be virulent (1 also essential) and nonhomologous to the human gut microbiota. These proteins consist good target candidates to screen natural plant compounds that might be effective against the bacterial infection.

Acknowledgment



screening using

Figura 2: Structured workflow with the methodology of this work.



This study presents new directions for the development of therapies against *P. aeruginosa*. The 7 highly immunogenic proteins predicted could be tested as subunit vaccines in future works. The 5 virulent cytoplasmic proteins predicted in this study will be considered for the molecular docking using a library of 5.000 natural plant compounds.