

Sequence-based computational protein analysis MDR pumps for use in epidemiology and drug design

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Motivation and Aim: Antibiotic resistance is a pressing problem in modern healthcare. Attempts to predict the effect of a drug on specific strains usually do not lead to positive results. We chose to model MDR pump genes known for their variability. Multidrug-resistant (MDR) pumps are essential for protecting bacteria from antibiotics. These pumps offer a basis for the non-specific defense of bacteria and are categorized into six families of MDR pumps [1].

Methods and Algorithms: To solve our problem of predicting the right antibiotic for treatment, we use methods from molecular microbiology, sequence alignment, molecular docking and molecular biology, which allows us to obtain reliable results.

Results: Using molecular microbiology, we validate data obtained through sequence analysis. Using molecular biology methods, strains will be created to create pathogen resistance systems in the laboratory. Using molecular docking, we study how the mutation process can affect the antibacterial substances we are developing.

Conclusion: We have developed a pipeline for analyzing pump sequences. This allows us to predict resistance to the antibiotics we are developing based on the primary structure of a set of certain bacterial pump genes.

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References

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