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Research on potent TLR2 inhibitors based on Machine Learning approaches for the treatment of Mycoplasma Pneumoniae Disease

Muhammad Ishfaq

Huanggang Normal University, China

Statement of the Problem: Mycoplasma pneumoniae (MP) is one of the most common pathogens that causes acute respiratory tract infections. Children experiencing MP infection often suffer severe complications, lung injury, and even death. Previous studies have demonstrated that Toll-like receptor 2 (TLR2) is a potential therapeutic target for treating the MP-induced inflammatory response. However, the screening of natural compounds has received more attention for the treatment of bacterial infections to reduce the likelihood of bacterial resistance. Methodology & Theoretical Orientation: Herein, we screened compounds by combining molecular docking and machine learning approaches to find potential lead compounds for treating MP infection. Currently, AI and machine learning explicitly improve the use of data obtained from several sources to predict drug bioactivities for various diseases, accelerating the drug discovery process through the development of faster, more economical, and more efficient solutions. Findings: First, all compounds were docked with the TLR2 receptor protein to screen for potential candidates. To predict drug bioactivity, a machine learning model (random forest (RF)) was trained for TLR2 inhibitors to obtain the predictive model. The model achieved significant squared correlation coefficient (R^2) values for the training set (0.85) and validation set (0.84) of compounds. The developed machine learning model was then used to predict the pIC50 values of the top 50 candidates from the Traditional Chinese compounds and Discovery Diversity sets of compounds. Conclusion & Significance: As a result, these compounds can inhibit the inflammatory response induced by MP. However, prior to bringing these compounds to market, it is necessary to verify these results with additional biological testing, including preclinical and clinical studies. Moreover, the present study provides a theoretical basis for the use of natural compounds as potential candidates to treat pneumonia caused by MP.

Biography

ISHFAQ completed his PhD degree in Veterinary Pharmacology and Toxicology from Northeast Agricultural University, China, in year 2021. His research areas of interest are In-silico pharmacology, Machine learning, Molecular Pharmacology and Toxicology, Drugs and Toxins, Cell signaling pathways, Drug targets, Inflammation, and Infectious Disease models. Dr. ISHFAQ has published several research articles in various prestigious international journals with good impact factor. He is working as a volunteer reviewer in different prestigious journals. He is currently working on machine learning-based drug discovery and design and focusing on developing cutting edge technology on AI integrating biomedical big data searching for drugs targeting various diseases