Computational Explorations to Overcome the Anti-Microbial Resistance in Bacteria

Lakshmi P.T.V

Department of Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605014.
E-mail: lakshmiptv@yahoo.co.in; lakanna@bicpu.edu.in

Abstract

Multidrug-resistant (MDR) and in specific Methicillin-resistant Staphylococcus aureus (MRSA) which causes biofilm-associated infections like nosocomial and chronic disease, is a hot topic among microbiologist as it is related with high morbidity and mortality posing a global challenge to the scientific world today. Hence, there is an urgent need to identify novel compounds by applying the groundbreaking methods to pervade and clear biofilm-associated infections. Since, over the past decades, the computational strategies were found successful in screening and validating the effectiveness of potential natural molecules especially flavonoids from plants, which even at lower concentration have been suggested as effective drugs against pathogenic bacteria, studies in different directions have been attempted in our lab, mainly through computational strategies that includes molecular docking and simulation, and was further validated through in-vitro studies to evaluate the anti-bacterial and anti-quorum sensing ability of phyto-constituents. Thus, molecular docking and simulation studies to understand the molecular interaction of compound with regulatory proteins and Penicillin binding proteins of few gram positive bacteria gave some important observations to be disclosed for discussion during the presentation.