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Abstract

Computational aided virtual screening of natural epiesteriol as probable lead molecules towards prospective targets of multidrug resistant Acinetobacter baumannii

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Abstract:

Multidrug resistant Acinetobacter baumannii (MDRAb) declared as priority-I pathogen by WHO (2017) and screening of potential therapeutic agents has profound application. This study aimed to identify putative drug targets of MDRAb and validate the therapeutic potential of natural molecules by structure based drug screening and in vitro studies. Ten clinical isolates of Ab were subjected to antibiotic susceptibility testing against five carbapenems and two colistins. Based on the metabolic pathway and functional role analysis, Omp38, RecA, PyrE and PyrF were identified as potential drug targets by KEGG database search. The three dimensional structure of Omp38 was retrieved from PDB and others were computationally predicted and validated. 236 natural molecules were screened from various databases and subjected to virtual screening, molecular docking and molecular dynamic simulation. The therapeutic potential of computationally predicted molecules was validated by in vitro studies. The clinical isolates (n=10) showed extreme dug resistance to carbapenems and colistins ($p<0.05$). Computational screening suggested that 06 leads were qualified for drug likeliness, pharmacokinetic features and one molecule-natural epiesteriol (16b-Hydroxy-17a-estradiol) exhibited significant binding towards four drug targets in comparison with the binding of faropenem and polymyxin E towards their usual targets. MD simulations suggested that epiesteriol-receptor complexes demonstrated stability throughout the simulation. The growth curve and time kill assays revealed that MDRAb showed resistance to Faropenem and Polymyxin-E and the purified epiesteriol showed significant inhibitory properties (100 µg/mL) towards four drug targets in comparison with the controls ($p\leq0.5$).

Biography:

Dr. Sinosh Skariyachan, is working as Assistant Professor in the Department of Microbiology, St. Pius X College Rajapuram, Kasaragod, Kerala, India. He has pursued his post graduations in Microbiology (M. Sc) and Bioinformatics (M. Sc) and obtained his Ph. D in Biotechnology. He has sixteen years of experience in teaching and research. His key research domains are Computational Biology & Bioinformatics, Molecular Modeling and Computational Drug Designing, Chemoinformatics, Genomics and Proteomics and Medical Microbiology (Antimicrobial resistance). He is the member of 17 National and International scientific and professional societies. He has authored 52 International papers, 76 conferences proceedings, one text book and 7 invited book chapters. He has received several awards and travel grants for his research. He is the associate editor for computers in Biology and Medicine (Elsevier) serves as editorial board member and reviewer for more than 85 international journals published by reputed publishers. He has received grants from various funding agencies and honored as plenary speaker in various National and International conferences and symposiums.

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