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Identification of promising antibacterial chemical compounds using pharmacoinformatics approaches

Bacterial resistance to antibiotics is of great concern in the development of new infectious therapeutics especially as there are two million deaths due to bacterial infection annually worldwide. There is therefore a paramount requirement to develop innovative and novel antibacterial agents with new mechanisms of action and activity against resistant bacterial strains. For this purpose, a set of benzothiazole and N-phenylpyrrolamides derivatives reported in the literature as DNA Gyrase B (GyrB) inhibitors were collected and docked inside the receptor cavity of GyrB (PDB ID: 5L3J). The binding energy and binding interactions were analysed and the best ten docked complexes used to identify novel antibacterial chemical agents through a de novo design approach in the online server eLEA3D. Initially 300 new chemical analogues were generated. The best six analogues were identified using screening with a set of criteria followed by pharmacoinformatics analysis. The binding mode and molecular interactions of the best six analogues were explored and we found that all molecules formed a number of critical interactions with catalytic amino residues of the GyrB with high binding energy. The RMSD, RMSF and radius of gyration parameters obtained from the 100ns molecular dynamics simulation study clearly explained that all six analogues were efficient enough to form stable complexes with GyrB. Finally, the binding affinities of the proposed analogues acting on GyrB were checked using binding energy calculations by the MM-GBSA method. High negative binding energy of all molecules explained the strong affinity towards the GyrB. Therefore, the proposed de novo designed molecules can be considered as promising antibacterial chemical agents that should subjected to experimental validation, in vitro.

Presenter Biography

The presenter, Dr. Mohammed Ataul Islam is a prior recipient of the Young Scientist award from the Indian Chemical Society in the field of molecular modelling and drug design. Currently he is working as a Post-Doctoral researcher at the Department of Chemical Pathology, University of Pretoria, South Africa. Dr. Islam is a bioinformatician, focussing on the pharmacoinformatics approaches on small and macro- molecules to design new chemical entities for the treatment of the different diseases including hormone responsive bacterial infection, breast cancer, AIDS, genetic diseases and diabetes. Thus far, he has published 29 research articles delivered more than twenty five conference presentations.

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