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Design of new leads as novel therapeutics for tuberculosis - A computational approach

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Tuberculosis (TB) has been a global health threat currently affecting 9million new cases every year. In spite of chemotherapy and BCG vaccine, Mycobacterium tuberculosis (MTB) is causing one death in every 10 seconds. Major challenges and lacunae in the existing therapy are: prolonged therapy coupled with poor compliance of patients to drug administration and adaptation of the pathogen to evolve into multidrug resistant (MDR) and extensively drug resistant (XDR) TB strains.

In view of the latest technological information about the genome of the MTB and the mechanism of MTB manifestation, novel targets involved in various phases of life cycle of the bacteria may be considered for design of effective TB therapeutics. In the present work, proteins involved in (a) Transcription (b) Dormant stage and (c) Multidrug resistance of MTB, are explored for design of effective leads as antagonists for the mycobacterium pathogen. Computational techniques are applied to the targets, for 3D structural evaluation, identification of active site and novel leads are designed using virtual screening against the active site with molecular databases. Specific examples are presented and discussed. The study identifies new molecular entities for tuberculosis therapy.

Biography

Uma Vuruputuri is Professor at The Department of Chemistry, Nizam College, Osmania University since 1998. Her research interests include Molecular Modelling and Drug Designing with special reference to the Identification of NME's for the treatment of Cancer and Tuberculosis using Insilco Techniques. Prof. Uma's research group includes 10 Doctoral students, 8 Master's and M. Pharmacy students working towards their Thesis dissertation. She published several research papers in international peer reviewed Journals. Prof. Vuruputuri has reviewed several Research articles of international Journals, in the field of Chemical Biology, Bio Informatics and Molecular Modelling. Currently, Prof. Uma Vuruputuri is working on projects with special focus on Tuberculosis and Cancer, sponsored by DST and UGC, New Delhi, India. She is actively involved in academic administration of Nizam College and is a Governing Body member of Nizam College She is a resource person for designing the curriculum for UG and PG programs in the field of Pharmaco Informatics and Molecular modelling.

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