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Computational technique - A promising pathway for drug discovery: A case study

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Drug discovery is a complex process which involves an interdisciplinary approach to design effective feasible drugs (1). The development of new drugs with potential therapeutic applications is one of the most complex process in the pharmaceutical industry (2). Millions of dollars and man hours are dedicated to the discovery of new therapeutic agents. Rational drug discovery process combat and supersede the conventional process with the advent of proteomic, genomic and structural information (3).

The computational techniques and informatics assist in predicting the 3D structures, the active site, the binding modes of molecules and the ADME properties. The paramount of work is evident from recent publications in this area (4, 5 and the references therein). The present work showcases the application of structure based drug designing techniques, in the identification of new molecular entities with potential therapeutic value with reference to cancer and tuberculosis.

Novel proteins in Mycobacterium tuberculosis are targeted, their 3D structure evaluated, active site identified, virtual screening carried out using Glide software to identify novel leads to inhibit the target proteins. A similar procedure was also applied to the proteins which play an important role in apoptotic pathway. The identified lead molecules were synthesized and their biological activity tested which show promising results. These new molecular entities offer promising therapeutics for further stage of drug discovery.

Biography

Prof. Uma Vuruputuri is Professor at The Department of Chemistry, Nizam College, Osmania University since 1998, completed her Ph. D in Chemistry in the Year 1983.

Prof. Vuruputuri's research interests include Molecular Modeling 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.

Prof. Vuruputuri has reviewed several Research articles, of international Journals published in the field of Chemical Biology, Bio Informatics and Molecular Modeling.

At present, Prof. Uma Vuruputuri is working on projects sponsored by DST and UGC, New Delhi, India. She is actively involved in academic administration of Nizam College and The Chemistry Department, Osmania University.

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