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Designing of inhibitors for cancer phenotype: An experimental and computational approach

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Cancer is a major public health problem worldwide and is the second leading cause of death in the United States. The discovery and ontogenesis of small molecule inhibitors of cancer have been remodeled with technological innovation. The application of computational techniques has been quickly ratified by the scientists in the field of targeted drug designing. The pharmacokinetic parameters (ADME) are important for the designing as well as targeted delivery to the site of infection/disease. The highly expressed proteins phenotypes in cancer are targeted through signaling pathways, leading to gene expression. In the present study computer-aided drug designing techniques are used to design drugs and potential binding affinities to understand the pharmacokinetic aspects of the lead i.e., ADME. Successful case studies will be discussed to understand the target specificity and site specificity. Bioinformatic tools are used for refining the 3D structure of the target protein, validation of the active site, virtual screening carried out to identify the leads (inhibitors), and synthesis of leads, *in vitro* and *in vivo* studies.

Biography

Navaneetha Nambigari, Assistant Professor, Department of Chemistry, University College of Science, Saifabad, Osmania University, Hyderabad. She has done PhD in Bio-Inorganic Chemistry and Post Doctoral work in Computational Chemistry. Her core research areas are Spectroscopic Investigations of Metal Complexes and Their Applications (Bioinorganic chemistry) and *in silico* Drug designing techniques, based on targeted approaches. Drug designing with special reference for identifying New leads against cancer and rheumatoid arthritis. She has several awards to her credit "Best Presentation Award" at Drug Design 2017, JNU Convention Centre, New Delhi, India, and April 2017 and at recent advances in applied nano materials, Osmania University, Hyderabad (2016). "Young Faculty Award" by Venus International Foundation, Chennai. (2015) and "Young Chemist Award", by Royal Society of Chemistry, London, UK at 42nd IUPAC Conference, "Chemistry Solutions", Glasgow, UK (2009). She has 13 years of teaching and 16 years of research experience with 5 Graduate students and 6 PhD scholars working for their thesis dissertation.

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