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First protein drug target's appraisal of lead-likeness descriptors to unfold the intervening chemical space

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A plethora of literature has been published for unveiling the problems associated with lead and drug likeness. However, despite of these advances in combinatorial chemistry, high throughput methods and virtual screening, plethora of clinical studies disquiets due to lead and drug-likeness attrition. For mitigation, the knowledge of physicochemical properties is really useful for guiding the design and selection of compounds from libraries dictated by certain rule of thumbs. However, robust biotechnological and instrumental innovations have created exponential increase in novel compounds and databases which compelled rethinking of evaluation procedures. Known descriptive molecular property filters proposed by Lipinski, Verber and Hann are not efficient enough to encompass long array of compounds and do not take into account the specificity of biological target. In this pursuit, we have tried to appraise eight molecular properties for two major classes of biological targets viz. membrane proteins and ion channels binding ligands. It has been proposed that the target based knowledge of descriptors can guide the selection of molecules to pick compounds from high throughput screening. In this talk, efforts, challenges and success in filtering the compounds to answer the long pending questions on lead-likeness and drug-likeness will be addressed.

Biography

Mohd Athar is a Senior Research Fellow in Computational Chemistry Group at Central University of Gujarat. He holds the DST-INSPIRE Fellowship awarded by the Ministry of Science and Technology (DST) India. He has completed his Master's degree in Applied Chemistry at BBA Central University Lucknow and Bachelor's degree in Biotechnology from Hemwati Nandan Bahuguna Garhwal University. His major research is in the area of Medicinal Chemistry ranging from Drug Discovery, Combinatorial Chemistry, *In silico* Virtual Screening, Lead Optimization/Designing, Target Identification to its Validation.

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