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Appraising lead-likeness descriptors for selected drug targets

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Despite of the 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 useful for guiding the design and selection of compounds from libraries dictated by certain rule of thumbs. However, robust bio-technological 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 consider the specificity of biological target. In this pursuit, we have tried to appraise eight molecular properties for two major classes of biological targets 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.