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Addressing blood-brain barrier in CNS drug discovery using fragment based approach

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Central nervous system (CNS) related disorders affect over one billion people worldwide. The treatment cost in USA alone is expected to be over $600 billion per year with an economic impact exceeding over a trillion dollar. The two major challenges that impact the treatment of CNS diseases are: (i) effective delivery of drugs and (ii) discovery and development of drug molecules that can cross the blood-brain barrier. Given the fact, that CNS drugs require a more restricted profile of molecular properties (MW: <450 Da; LogP: ≤4.0 and polar surface area (PSA): ≤ 80 $Å^2$) than the Lipinski 'Rule of Five', hits identified using conventional compound library (MW: 500 Da; LogP: 5.5 and polar surface area: 140 $Å^2$) limits the possibility of evolving and optimizing them into promising lead candidates suitable for advancing into *in vivo* proof of concept and development studies. An efficient and alternate approach to overcome and address this limitation is to initiate the lead optimization starting with hits identified using fragment based approach and combine with rational structure-based drug design methods. We have used this approach to discover novel, potent and CNS permeable inhibitors of the molecular chaperone, heat shock protein-90, which have demonstrated selective portioning into the CNS, target engagement and pharmacodynamics effects *in vivo*.

Biography

G. Sridhar Prasad is the co-founder and VP of Research of CalAsia Pharmaceuticals. He has been the core member of multiple drug discovery teams, including the marketed drug, NESINA (Alogliptin, DPPIV Inhibitor) and clinical candidate MK-4965, for the treatment of HIV-1 AIDS. He obtained his Ph.D. from Indian Institute of Science, Bangalore, India and post-doctoral training at University of Minnesota Medical School and the Scripps Research Institute, La Jolla, California, where he grew to the ranks of Assistant Professor. He has co-authored over 45 peer reviewed research articles, holds six US and international patents. He serves on the editorial board of *Current Protein and Peptide Science*.

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