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Genes to Leads: A rational structure guided lead discovery technology that works for both enzymes and protein-protein interaction targets

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Abstract

The entire life sciences industry is focused on only a few hundred protein targets for drug discovery. There are potentially many more novel targets, not only human proteins but also those present in infectious organisms likely to be relevant targets for important new drugs. The abundance of potential drug targets is a challenge for the pharmaceutical and biotech companies that have to focus their resources. At least 50% of all targets that go into HTS screens do not generate significant leads and hence other cost-effective technologies are required to generate novel lead molecules. We have developed a structure-based approach to develop lead molecules in 60 to 90 days, which has resulted in validated lead molecules for a diverse set of drug targets including targets that are involved in protein-protein interaction. Essential ingredients of the technology are: X-ray crystallography, protein modeling, virtual screening, docking and scoring. In this presentation we would like to discuss our technology with specific application examples in protein-protein interactions.

Biography

Dr. Kal Ramnarayan (Dr. Ram) is the Founder, President, Chief Scientific Officer of Sapient Discovery. Previously, Dr. Ramnarayan Co-founded Structural Bioinformatics, Inc and Cengent Therapeutics. Prior to Structural Bioinformatics, Inc., Dr. Ram was Head of Computational Chemistry at ImmunoPharmaceutics Inc., where he designed numerous drug leads, including highly specific endothelin-A receptor antagonists. This became Sitaxsentan, currently in Phase III clinical development by Encysive Pharmaceuticals. Dr. Ramnarayan holds a PhD in molecular biophysics from the Indian Institute of Science, Bangalore and has multiple papers and patents and several other patents pending. Dr. Ram is also Co-founder of Focus Synthesis, LLC, in San Diego.