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# Computer aided design and optimization of kinase and phosphatase inhibitors

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Kinases and phosphatases are implicated in several disease states and a number of publications and patents have been published on the discovery of novel inhibitors for these classes of proteins. Newer targets are also coming into play with a need for small molecule inhibitors. More than 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 kinases and phosphatases. Lessons learned with these targets will be valuable in attempting to discover novel inhibitors to newly discovered kinases and phosphatases.

## Biography

Kal Ramnarayan is the Founder, President, Chief Scientific Officer of Sapient Discovery. Previously, he co-founded Structural Bioinformatics, Inc and Cengent Therapeutics. Prior to Structural Bioinformatics, Inc., he 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. He holds a PhD in molecular biophysics from the Indian Institute of Science, Bangalore and has multiple papers and patents and several other patents pending. He is also co-founder of Focus Synthesis, LLC., in San Diego.

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