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Computational chemistry and drug discovery platform at the University of Arizona's BIO5 Oro Valley and its application to the identification of potential small molecule therapeutics

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Recent advances in structural biology, x-ray crystallography, and high-performance computing and their synergistic application has led to a greater understanding about drugs and their interactions with biological targets. The BIO5 OV drug discovery and development center is equipped with a diversity of research industry-style resources and expertise in CADD and drug discovery technologies. Specifically, Computer-Aided Drug Discovery (CADD) has proved to be a valuable asset in the drug discovery and development process through virtual screening, structure-based design, and QSAR applications. The CADD group at BIO5 Oro Valley is an integral part of the chemical technology platform, which also includes structurally diverse chemotypes, in-house / commercial compound databases, the Arizona compound collection (BIO5-OV), and translational expertise. We are primed to assist in and enable the development of small molecule therapeutics for protein and biological targets.

The talk will describe the resources available at the BIO5 OV drug discovery and development center and the application of these resources to the identification and development of small molecule probes for the treatment of cancer and other diseases.

Biography

Vijay Gokhale completed his Ph.D. in 2001. His area of expertise and experience is in the field of computational and medicinal chemistry. His research focuses on the exploration of new and validated biological targets for the design and development of new chemical entities as drugs for the benefit of patients. In addition to his experience in computational and modeling techniques, he is also a medicinal chemist involved in the design and development of small molecules and was involved in moving potential drug molecules through various bioassays starting from ex-vivo systems to mouse xenograft models.

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