Structure Based Drug Design Lab

Our goal is to assist medical researchers with novel drug discovery and development. Pursuant to this goal we specialize in three primary tasks: lead discovery, lead optimization, and x-ray crystallography.

Lead optimization is perfomed on compounds that have been discovered through computational and/or assay-based lead discovery. Two primary tools exist for lead optimization: RACHEL and CHARLIE, both SYBYL modules.

X-ray crystallography primarily consists of three stages: crystallization trials, data collection, and structure determination & refinement. A successful x-ray crystallography run results in three-dimensional coordinates of a novel target protein that can be used for lead discovery and/or three-dimensional coordinates of lead compounds bound to validated targets to serve as a basis for lead optimization.