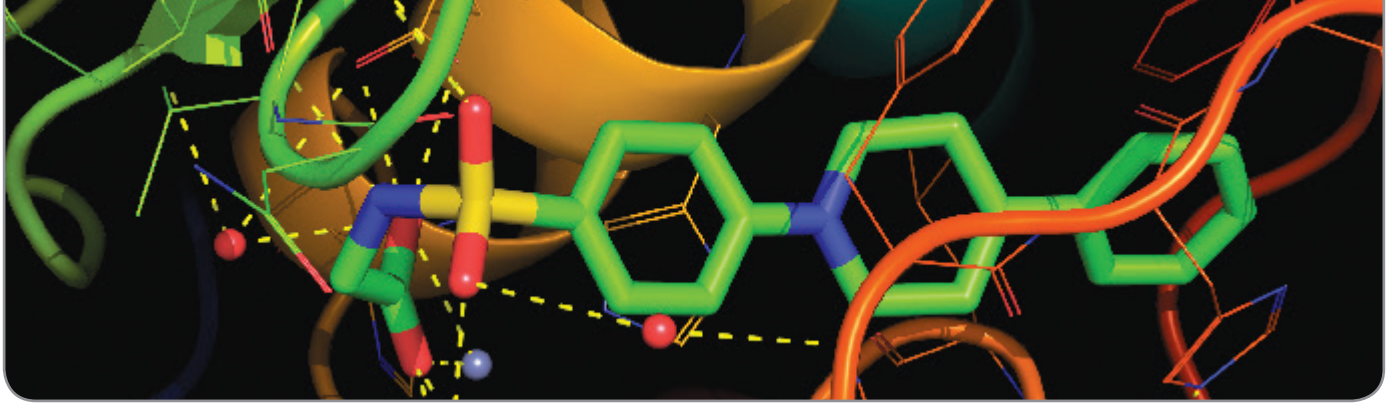
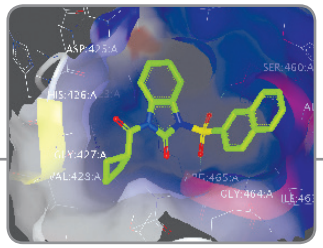


Improving drug discovery processes



The Genome Research Institute Discovery Platform, or GRIDP, provides Ohio academic researchers and educators with a user-friendly way to tap into the emerging field of computational drug discovery, encompassing bioinformatics, computational biology, and computational chemistry.

GRIDP gathers currently available computational biology and drug discovery software as well as other computational resources into one intuitive, Web-based interface. While pharmaceutical companies use similar tools that cost hundreds of thousands of dollars, this platform is the first of its kind for academia and harnesses the computational horsepower of the Ohio Supercomputer Center and expertise of the University of Cincinnati Genome Research Institute.

Effectively accessing and using the wealth of structural and chemical data currently available requires significant computing resources, talented programmers, and experienced high performance computing users familiar with the command line environment. GRIDP removes these technical hurdles by providing an intuitive graphical environment that delivers powerful resources, including software through the web. Students can focus on learning and researchers on discovery without being bogged down with technical details.

GRIDP, which was jointly developed by OSC and GRI scientists and programming experts, mirrors the discovery workflow and leads users through tasks such as protein model preparation and evaluation, binding site prediction, ligand preparation and docking/scoring, protein:ligand energy calculations, and chemical property analysis such as Lipinski's rules and distribution/absorption.

By modeling the interaction between target proteins and putative drug candidates, researchers can dramatically focus the set of compounds that need to be tested to a number that becomes reasonable—hundreds rather than tens of thousands. This allows academic researchers to play in an arena formerly reserved for big pharma.

"The most striking comment from biologists since we've launched GRIDP this summer is, 'I didn't know this was possible.' GRIDP opens a new realm of possibility, especially in drug discovery," said Matt Wortman, Ph.D., a researcher at the University of Cincinnati's Genome Research Institute and one of the lead investigators in GRIDP's development. "It gives researchers an entirely new research tool for discovering novel, biologically active chemicals."

OSC & UC PRESENT
GRIDP
OHIO'S DISCOVERY PLATFORM

OSC Partner:
University of Cincinnati's Genome Research Institute

Research Title:
Genome Research Institute Discovery Platform

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Principal Investigators:
Matthew D. Wortman, Ph.D., University of Cincinnati's Genome Research Institute

Co-Principal Investigators:
Steven Gordon, Ph.D., Ohio Supercomputer Center

For more information:
www.gridp.org