WAYNE STATE
School of Medicine

Department of Biochemistry,
Microbiology and Immunology

Structural Biology and Drug Design Group (SBDDG)
Department of Biochemistry, Microbiology, and Immunology,
Wayne State University

SBDDG is a translational/drug discovery unit in the Department of Biochemistry, Microbiology, and Immunology at WSU. The SBDDG provides project-specific consulting for researchers with projects that have therapeutic potential. The SBDDG collection of pre-clinical drug discovery expertise includes high throughput protein expression, high throughput assay development, mechanism of action studies, X-ray crystallography, and modeling and drug design.

Therapeutic areas of unmet medical need include but are not limited to bacterial and viral infections, inflammatory disorders, oncology, maternal and fetal medicine, neurological disorders, cardiovascular disease, metabolic disorders, and obesity. The investigator and the SBDDG team strive to develop an executable drug discovery project plan. The SBDDG is open to WSU investigators and investigators throughout the Michigan research community.

In summary, the SBDDG brings together instrumentation and resources, intellectual expertise, and workshops and seminars related to structural biology and drug design.

The SBDDG operates on a joint project grant or fee for service model and includes the following capabilities:

Protein Purification

- Gene cloning into protein expression vectors
- Optimization of protein expression
- Protein purification

Structural Biology

- Crystallization of the drug target
- X-ray diffraction data collection at the Life Sciences Collaborative Access Team (LS-CAT) facility at Argonne National Laboratory (ls-cat.org/about.html). Current LS-CAT members are MSU, UM, WSU, Van Andel Research Institute, Northwester U., U. of Wisconsin, Vanderbilt U., and U. of Illinois
- Protein structure solution and refinement
- Structure analysis and preparation of publication-quality graphics for grants and publications

Molecular Modeling and Drug Design

- Schrodinger small-molecule drug discovery suite to accelerate lead discovery and lead optimization
- Some capabilities include:
  - Virtual compound screening
  - Target preparation
  - Ligand preparation

- ADME (absorption, distribution, metabolism, and excretion) properties prediction
- Molecular dynamics simulations
- Preparation of publication-quality graphics for grants and publications

Assay Development

- Protein stability assays
- Ligand binding assays
- Enzyme assay development
- Exploratory compound screening using 96-well plates

Mechanism of Action (MOA) Studies

- Kinetic studies of target enzyme inhibition
- Crystallographic studies of target-inhibitor complexes
- Target selectivity studies of lead compounds and drug candidates
- Drug resistance studies of anti-bacterial, anti-viral, and anti-neoplastic agents

For additional information please contact:

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