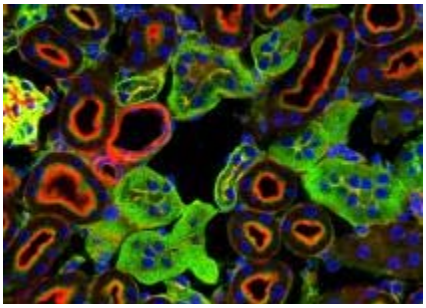
Center for Molecular Design and Preformulations (CMDP)

This center offers research and development support for interdisciplinary areas related to new drug discovery. The facility is led by **Dr. Lakshmi P. Kotra** and Dr. Ping I. Lee.



Service Department(s): Research Communications

Overview

Core competencies include the ability to integrate and conduct research in computer modelling, synthetic medicinal chemistry, bioassays and animal models to develop new therapeutic solutions. With expertise in specialty areas such as prodrug design and protein-drug conjugates, our resources span state-of-the-art computer modelling, synthetic medicinal chemistry and preformulations infrastructure. All projects are conceived with the unique therapeutic angle and experimental proof of concept is streamlined accordingly.

Available Equipment

- REMEDI Visualization and Computer Modelling Suite (MaRS/TMDT 7-1000)
  - Hardware: 400 core Linux server and 44 processor Onyx; 4 workstations with high-end graphics capabilities; movie-screen size (1.6x3.4 m2) HD stereo visualization system; 100 TB storage
  - Software tools for drug discovery, image processing, stats and visualization: Sybyl, Gaussian, Spartan, GOLD, Amber, Amira, Comsol, IDL, Matlab
- Medicinal Chemistry Suite (MaRS/TMDT 5-401 and UHN-Shanghai)
  - State-of-the-art infrastructure: mg to 100 g scale synthesis; ability to deploy up to 25 chemists
  - Focused library generation; integration with computer modelling and preformulations
  - Sirius T3, Thermal activity monitor, DSC, PXRD, nanomill, microfluidizer, particle size analyzer, viscometer, lyophilizer etc.; cost-effective solutions (work carried out by UHN-Shanghai)
- Preformulations Suite (MBRC 5R-423)
  - LogP/LogD/pKa/solubility (Sirius T3); Confocal Raman Microscope, and Differential Scanning Calorimeter; Powder X-Ray Diffractor; Hot stage microscope; Nanomill, microfluidizer, particle size analyzer, viscometer, lyophilizer etc.

Core Scientific Expertise

- In silico database screening and docking

    - Virtual screening, docking to a receptor site, identifying novel core structures/molecules, designing focused libraries. Docking and in silico screening to test small molecule target binding, to create a short list of compounds
- Homology modelling
    - Homology modelling to predict the 3D structures for proteins using the primary sequence of a protein, or using homologous proteins, with energy refinements and structure validations
- Lead characterization
    - Identification of most promising biologically potent compounds through physicochemical characterization, and elucidation of metabolism and toxicology parameters
    - Structural biology: Referrals provided for structural biologists capable of determining 3D structures in collaboration with Toronto Proteomics Initiative
- Three dimensional visualization
    - A powerful, unparalleled 3D Reality Center provides a venue for discussing complex structurebased projects in large group settings
- Synthetic chemistry and medicinal chemistry
    - State-of-the-art synthetic chemistry infrastructure and the ability to enhance efficiency while reducing costs through our own Shanghai (China) chemistry operations
    - Sophisticated analytical equipment for compound characterization
    - Capability to build focused libraries and difficult-to-accomplish reactions
    - Gram-scale reactions

Quick Links

- **Wepage**

Contacts

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