

# ChemCore

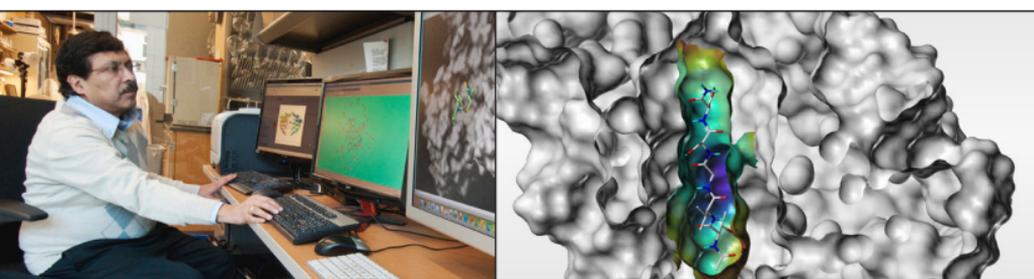
Medicinal and Synthetic Chemistry Core

[www.cmidd.northwestern.edu/chemcore](http://www.cmidd.northwestern.edu/chemcore)  
[drugdiscovery@northwestern.edu](mailto:drugdiscovery@northwestern.edu)

## *In Silico* Services

- Cost- and time-efficient hit ID and lead discovery process
- Leverage chemical and biological information about ligands and/or targets to identify and optimize new drugs
- Design in silico filters to eliminate compounds with undesirable properties (poor activity and/or poor ADMET) and select the most promising candidates
- Virtual high throughput screening of drug-like libraries for novel therapeutic targets
- ADMET property evaluation of drug-like candidates
- Construction of protein homology models and 3-D analysis, structure-focused & ligand-based pharmacophore design
- Dynamic QSAR modeling to predict relationship of chemical structure and pharmacological activity

Contact our Cheminformatics Specialist, Dr. Rama Mishra at [r-mishra@northwestern.edu](mailto:r-mishra@northwestern.edu)



## Compound Purification Services

- Mass-directed analytical-to-preparative (A2Prep) HPLC purification system (full-service only)
- Reverse phase analytical and preparative HPLC systems equipped with UV and ELS detection
- Compound drying capabilities: GeneVac HT-4X Plus centrifugal evaporator and a VirTis shelf lyophilizer
- High pressure microreactor/hydrogenation system

Contact our Purification Lab Manager, Dr. Arsen Gaisin at [arsen.gaisin@northwestern.edu](mailto:arsen.gaisin@northwestern.edu)



## Medicinal and Synthetic Chemistry Services

- Provides comprehensive medicinal chemistry support in drug discovery and research
- Hit-to-lead and lead optimization medicinal chemistry to enhance the drug-like properties of a compound
- Design and synthesis of novel analogs with improved potency, ADME and IP properties
- Novel scaffold design and synthesis
- Preparation of biotinylated and fluorescently-tagged molecules for chemical biology applications

Contact our Director of Chemistry, Dr. Gary Schiltz at [gary-schiltz@northwestern.edu](mailto:gary-schiltz@northwestern.edu)



## Metabolic Stability Services

Optimizing a compound's drug-like properties to enable evaluation *in vivo* is crucial in therapeutic development, and the costly assessment of a compound's pharmacokinetics is a critical step in the process. To facilitate this compound development, ChemCore offers *in vitro* services to measure metabolic stability and improve characterization and optimization of compounds through microsomal, S9, and plasma assays.

### Microsomal Stability Assay

- Most common metabolizing fraction in drug discovery
- Liver microsomes represent the major portion of metabolizing enzymes and can be used to estimate the intrinsic *in vitro* clearance of a compound

### S9 Fractions Stability Assay

- Contains a wide variety of both phase I & phase II enzymes
- Species-specific S9 fractions can be used to enable an understanding of interspecies differences in drug metabolism

### Plasma Stability Assay

- Instability in plasma can result in misleading *in vitro* data which can be difficult to interpret
- Plasma stability is very useful for screening of prodrugs and antedrugs, where rapid conversion in plasma is desirable

*Interested in our metabolic stability services?*

Contact us at [drugdiscovery@northwestern.edu](mailto:drugdiscovery@northwestern.edu)

