**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*

**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*
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

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