

## CIDD Medicinal Chemistry and Synthesis Core Facility – Dr. Stanton McHardy (Director)



### **CENTER FOR INNOVATIVE DRUG DISCOVERY**

The Center for Innovative Drug Discovery (CIDD) is a joint venture between The University of Texas at San Antonio and The University of Texas Health Science Center to provide capabilities and core services in support of biomedical research related to drug discovery. CIDD is composed of two facilities: a High-Throughput Screening (HTS) Facility located at UTHSCSA and a Medicinal Chemistry and Synthesis Core Facility at UTSA. The ultimate intent of the CIDD is to provide a diverse array of core facilities and expertise to facilitate the translation of basic scientific discoveries into tangible pre-clinical candidate drugs that can be further

developed into clinical therapies for human disease.

**The Medicinal Chemistry Core Facility is a 2000 sq. ft. state-of-the-art technological center located on the west campus of UTSA that performs all necessary chemistry and synthesis services to support a large diversity of small molecule drug discovery efforts. The center will provide custom synthesis and medicinal chemistry research for small molecule drug discovery projects in any therapeutic area. The center will also provide collaboration, consultation and program strategy opportunities from investigators who have over 16+ years of pharmaceutical experience in taking small molecule compounds through all stages of the pre-clinical drug discovery process.**

### **SERVICES PROVIDED**

- Custom synthesis of non-commercial small molecules from milligram to multi-gram quantities.
- Design of “drug-like” molecules and analysis of physical chemical properties.
- Structure-based drug design.
- Full service medicinal chemistry suite, i.e. hit-to-lead activities, small library design and synthesis, de novo analog design and synthesis, structure-activity relationships (SAR).
- Analytical chemistry support, including drug stability, solubility and structural determinations.
- Synthetic route process development, improvement and scale up of biologically active compounds.
- Consultation, planning and strategy development for advancing small molecule drug discovery programs; including medicinal chemistry, ADME issues, pk/pd, toxicology, formulation, drug exposure and dosing options.

### **CAPABILITIES AND INSTRUMENTATION**

- 12 fully functional synthesis hoods with N<sub>2</sub>/high vacuum manifolds, stir plates, JKem controllers and block reactors, Buchi R-210 Rotovaps with V-700 vacuum pumps.
- Biotage Isolera One purification systems with UV detection and automatic fraction collections.
- Agilent DD2 400 MHz Nuclear Magnetic Resonance Spectrometer.
- Agilent 1290 HPLC with Agilent 6150 MS.
- Agilent SCF CO<sub>2</sub> 1260 Infinity HPLC w/ variable wavelength UV detection & auto sampler.
- Agilent 1260 Prep HPLC w/ variable wavelength UV detection, auto sampler & fraction collector.
- Anton Paar Monowave 300 microwave reactor with auto loader.
- Support for multiple FTE chemists at the BS/MS and PhD levels.

