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NIH COBRE-Natural Products Neuroscience Chemistry Services Under Chemistry and DM-PK CORE Facility

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CORE OVERVIEW

The Chemistry Facility is under Chemistry and DM-PK core is supported by the NIH COBRE Natural Products Neuroscience (NPN) program grant at the University of Mississippi. Our facility supports investigators with lead compound optimization, synthesis, The Chemistry Core has an advisory role for CORE-NPN investigators and Non-CORE NPN investigators that require expertise in the area of exploration of structure-activity relationships, metabolite activity relationships and pharmaceutical and chemical influences on solubility of test compounds and their formulations.

SYNTHESIS WORKFLOW

1. Synthetic Project Evaluation-Approval

2. Route Optimization and Scale-up

- Solution/Solid Phase Synthesis
- Single Reaction/Parallel Synthesis
- Intermediate/Target Purification
 - Flash Chromatography
 - Crystallization
 - Preparative HPLC
 - Mass Directed (LCMS Waters FractionLynx)
- Intermediate/Target Analysis-Purity Assessment
 - ¹H and ¹³C NMR (Teledyne-Isco EZ Combiflash)
 - HRMS (Q-TOF)
 - Elemental Analysis (CHN/SO)
 - LC-MS-PDA (purity assessment)
 - Enantiomeric -Diastereomeric Purity (where applicable)

3. Compound Delivery-Data Management

The Chemistry and DM-PK Research Facility is able to provide customized compounds to users for *in vitro* and *in vivo* assessments, based on natural products or synthetic compounds, and to provide early-stage DM-PK assessment of drug-like molecules.

Medicinal chemistry is one of the vital components of the iterative cycle of drug discovery: This component is embedded in hit-to-lead and lead optimization stages.

Ten years of collective experiences and services provided by this Chemistry Core in Phase I and II support the view that a majority of investigators are faced with two significant hurdles in advancing their research programs: compound acquisition and early-stage compound evaluation.

This Core has bridged the gap by providing investigators with consultation, training, and services in medicinal chemistry, helping alleviate the bottleneck associated with compound acquisition and evaluation.

SERVICES PROVIDED

Chemistry DM-PK Facility		Fee-for-Service Structure	
	Description of Service	Unit	Cost
	Consultation	No Charge	
1	Synthesis and purification	# of synthetic steps	Rate per step (for 100 mg) \$973
2	LC-MS (low resolution analysis) purity assessment	# of compounds:	Consumables cost/compound: \$15
3	CHN Analysis	# of compounds:	Consumables cost/compound: \$11
10	Physicochemical Characterization per compound	# of samples	Consumables cost per compound \$23

Rama S. Gadepalli



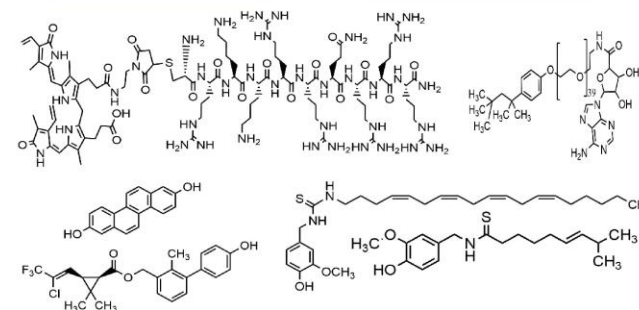
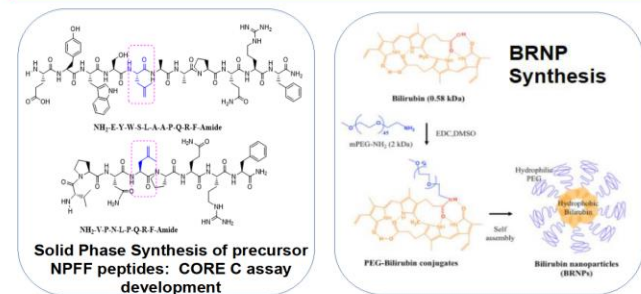
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EXAMPLES OF MOLECULES SYNTHESIZED



INSTRUMENTATION

NMR Facility

Combiflash



LCMS



FTIR



C,H,N Elemental Analyzer



Polarimetry

