

James & Esther King Biomedical Research Program

McLaughlin, Mark

Chemistry
University of South Florida

2009 Program
Shared Instrument Grant
(1-year project)

Project Title: Acquisition of a High-Throughput 500 MHz NMR for the Characterization of Potential Anti-Cancer and Anti-Stroke Therapeutics (USF-HT-NMR)

Project Summary: Drug design and synthesis is very much analogous to architecture and construction, respectively. An architect designs a building to fit a 3D space to serve its function as a home or a place of business and the resulting construction techniques will hopefully produce a robust building that will survive Florida's weather for at least 100 years. Drug design involves the design of molecules to fit a defined three-dimensional space, which is usually a protein-binding site. The synthesis of molecules to fit the protein-binding site is complicated by numerous additional constraints. The designed drug must fit the protein-binding site with at least competitive binding as compared with the natural molecule fitting that binding site. Instead of needing to survive Florida storms, the drug molecules must be stable for storage and for some period of time in the body of the patient. These and other reasons require that several structurally related molecules be prepared and tested to determine which molecules will best fit the protein-binding site. Nuclear Magnetic Resonance (NMR), which is analogous to MRI, is the best method of structurally characterizing molecules, and the high-throughput NMR instrument obtained through this grant will expedite the structural analysis of drug candidates. This instrument will therefore speed our progress in finding drug candidates to treat tobacco-related diseases such as cancer and stroke.