Project Summary: Acquisition of a 400 MHz NMR Spectrometer for Use in Research, Teaching and Research Training at Earlham College

The Departments of Chemistry and Biology at Earlham College are requesting a high-field NMR spectrometer to support research, teaching, and research training programs. Because student/faculty research is an integral part of the education of science majors at Earlham, this instrument will have immediate and substantial benefits for majors in chemistry and biology. Earlham has a long history of providing opportunities for undergraduate research. Earlham has maintained and strengthened its ability to offer significant projects through recent facility renovations, substantial acquisition of new instrumentation, and the development of endowment programs for the support of academic year and summer research programs. At this time, the lack of high-field NMR remains the single important barrier to our ability to conduct a full range of significant student research projects, particularly in organic synthesis, biochemistry, and molecular biology. Two chemistry faculty members and one biologist will be most involved with the projects and the management of the new spectrometer.

Dr. Mark Stocksdale and his students will investigate the synthetic applications of ring expansions and contractions of a series of cyclic β–hydroxy tertiary amines under Mitsunobu and modified Mitsunobu conditions. A second project will synthesize and investigate analogues of phytosiderophores, natural compounds that may facilitate active transfer of molecules into the roots of grasses. Given the complexities of the molecules, the possibility of product mixtures, and the interest in investigating intermediates, high-field NMR is essential. Product determination and characterization will rely on ^{1}H and ^{13}C 1D and 2D NMR methods. Reaction studies will require the capacity for variable temperature NMR experiments.

Dr. Michael Deibel, a bioanalytical chemist whose research interests concern the effects of oxidative damage on proteins, will utilize ^{19}F and ^{13}C NMR to examine the consequences of such damage on the structure and function of transferrin. His students will compare effects at two different metal binding sites, and will also investigate the role of damage at key sites in the protein secondary structure. The sensitivity and resolution of the 400 MHz NMR is critically important to this work. His work will also take advantage of the water suppression capabilities of the gradient probe.

Dr. Nathan Trueblood and his students will study the effects of an NAD^{+} precursor on high-energy phosphate metabolism (ATP, PCr) and glycolysis in hearts from diabetic rats. ^{31}P-NMR spectra (using the wide-bore ^{31}P probe) will be generated from isolated, perfused (beating) rat hearts, and ^{1}H- and ^{13}C-NMR spectra will be generated from tissue homogenates. The requested spectrometer will provide needed water-suppression methods and ^{13}C decoupling capability. The goal of this basic research project is to evaluate the effectiveness of metabolic interventions on cardiovascular function and susceptibility to injury (heart attack).

In addition to these primary research uses, the instrument will find substantial use in undergraduate organic chemistry, as well as in particular experiments within courses such as inorganic chemistry, molecular biology, physical chemistry, anatomy and physiology, modern physics, and hydrology. The proposal includes plans and funding to support training for the PIs and to support operation and maintenance of the instrument.