

Award No. DE-SC0005129

Recipient: The Research Foundation of State University of New York

Project Title: Molecular Structure Laboratory: Fourier Transform Nuclear Magnetic Resonance (FTNMR) Spectrometer and Ancillary Instrumentation at SUNY Geneseo

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Executive Summary: An Agilent 400-MR nuclear magnetic resonance (NMR) spectrometer and ancillary equipment and supplies were purchased. The instrument is part of Geneseo's Molecular Structure Laboratory. Five faculty members received training from the manufacturer on the use of the instrument. The instrument is being used to further the research efforts of participating faculty members in the areas of organic, inorganic and analytical chemistry. In addition, the instrument is a major tool for structure elucidation that is used for instructional purposes in the introductory and advanced organic chemistry and the inorganic techniques laboratories. On average, the instrument benefits approximately 70 students/semester in research and advanced laboratories and ~200 students/semester in the introductory organic chemistry laboratory. The instrument has had a direct impact on neighboring schools, which have used the instrument in teaching (Houghton College) and research (The University of Rochester).

Attainment of Goals: The original goals included the establishment of Geneseo's Molecular Structure Laboratory with the purchased NMR spectrometer as the centerpiece instrument, training of faculty and students, incorporation of the instrument in teaching laboratories and in the research efforts of faculty and providing the opportunity of neighboring schools to use the instrument. All of these goals have met. The instrument is used routinely in Organic Chemistry Laboratory (Chem 216), Synthesis and Techniques in Organic Chemistry (Chem 313), Laboratory Techniques in Inorganic Chemistry (Chem 331), Directed Study Research (Chem 399), and Honors Research (Chem 393). The instrument is an integral part of the research efforts of six faculty members in SUNY-Geneseo's chemistry department. It has been used on several occasions as an instructional tool by faculty at Houghton College and has been used in a collaborative research effort with the University of Rochester.

Activity summary: During reporting period 7/10-9/10, the NMR users group was formed, vendor site visits were made for instrument demonstrations, and quotes from vendors were obtained. Negotiations with the vendor chosen (Agilent) continued through 3/11 and the instrument, robotic sample changer and the air-handling systems were sited in 5/11. The instrument was fully commissioned in 6/11. Two of the NMR users group members received manager training at the vendor site and they developed the protocols for use in the research and teaching laboratories. In addition, deuterated solvents and the associated storage cabinets

were purchased for sample preparation for use with the instrument. Training of students and routine use of the instrument commenced during 9/11. During the first quarter of 2012, one of the the NMR spectrometer probes malfunctioned. However, it was under warranty and was replaced. Fortunately, the secondary probe allowed for continued use of the instrument during this time. During the second quarter of 2012, the data analysis software was upgraded. A suite of structure predication software was purchased during the third quarter of 2012. The new software enhanced our ability to train students in structure elucidation techniques. During spring 2013, the NMR spectrometer was introduced into our first year laboratory course for chemistry majors. The air-drying unit for the spectrometer failed and was replaced during the third quarter of 2013. An upgraded workstation was purchased during the second quarter of 2014. The instrument vendor (Agilent) closed its NMR business during the third quarter of 2014. This precluded training at the vendor site. In place of training, permission to use funds to present findings obtained using instrumentation in the molecular structure laboratory at national meetings was obtained. During the fourth quarter of 2014, the battery module on the backup power supply failed wand was replaced. Deuterated solvent supplies were replenished. During the remainder of the grant period, routine use of the NMR spectrometer continued.

Technology transfer activities:

Publications citing the grant

Hilimire TA, Bennett RP, Stewart RA, Garcia-Miranda P, Blume A, Becker J, Sherer N, Helms ED, Butcher SE, Smith HC, Miller BL.; "N-Methylation as a Strategy for Enhancing the Affinity and Selectivity of RNA-binding Peptides: Application to the HIV-1 Frameshift-Stimulating RNA"; ACS Chemical Biology, 2015, Article ASAP; DOI: 10.1021/acscchembio.5b00682; Publication Date (Web): October 23, 2015.

Conference papers citing the grant

Helms, E. D., "Using an Elimination Reaction of Tropic Acid as a Simple Example of an E1cb Reaction." 23rd Biennial Conference on Chemical Education, Grand Valley State University, Grand Rapids, MI, August 6th, 2014

Geiger, D. K.; Geiger, H. C. "Crystallographic characterization of three furan-substituted benzimidazoles and calculation of C-H/ π and π/π interaction energies." 249th ACS National Meeting, March 22-26, 2015, Denver, CO.

Geiger, H. C.; Geiger, D. K. "Synthesis and Spectroscopic Characterization of Chiral Biphenyl-Cholesterol Gels." 26th International CHIRALITY Conference, July 27-30, 2014, Prague, Czech Republic.

Parsons, D. E.; Geiger, D. K. "Structural characterization of novel acetato-bridged (benzene-1,2-diamine- κ N)lead(II) complexes." 247th ACS National Meeting & Exposition, March 16-21, 2014, Dallas, TX.

DeStefano, M. R.; Nellist, M. R.; Geiger, D. K. "Synthesis and structural characterization of new benzimidazole derivatives," 245th National ACS Meeting, April 7-11, 2013, New Orleans, LA.

