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Research Development Fund – FALL FY17

Application Title: Enabling Multinuclear, High-Resolution NMR for Applications in Chemical Sciences and Technology

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Key Participating Units: College of Science, College of Engineering, Health Science Center, Texas A&M Engineering Experiment Station

Anticipated Request Amount ($): 1,800,000

Executive summary of the intended application to utilize Research Development Funds. This proposal seeks to broaden the access to high-resolution NMR spectroscopy at TAMU, to further diverse research projects ranging from basic chemistry to polymers, materials science, energy, biomedical and environmental research. These and other applications in the chemical sciences and technology increasingly require the characterization of synthetic macromolecules and complex mixtures. Both cases result in NMR spectra subject to severe signal overlap. For example, many similar repeating units in polymers pose significant challenges for their structural characterization that can only be addressed by high-resolution instrumentation. Projects from these areas of chemical science and technology frequently also involve the detection of insensitive low-γ nuclei, or of nuclei that are otherwise not commonly available for NMR detection. Despite the University operating NMR instruments in several departments, equipment satisfying these requirements currently is not available on campus. With this project, the existing NMR capability at TAMU will be complemented and enhanced with a 700 MHz liquid state NMR spectrometer that includes broad-band detection capabilities. Solution NMR spectroscopy of most elements, both metals and non-metals encountered in the preparation and characterization of new materials, catalysts, ligands and other molecules will be enabled with broad-band detection. At the same time, a cryogenically cooled probe and the high magnetic field will provide the spectral resolution and sensitivity necessary for cutting-edge applications. Operationally, the instrument will be integrated with the NMR facility in the Chemistry Department and supported by existing personnel. This mode of operation provides for long term stability, does not require the staffing of a new facility and benefits from pre-existing infrastructure for maintenance and service. The facility staff is experienced in assisting all users across campus with highly diverse NMR applications. A current base of >400 individual registered users of the facility drawn from >40 research groups in various departments as well as from classes ensures broad access to the instrumentation. As a result of the new capabilities provided by the proposed instrumentation, the user base will further increase as described in the proposal. The augmented facility will provide leadership in the application of NMR spectroscopy to emerging areas of science and technology that are currently not well served, including polymeric materials for chemical and biomedical applications, environmental speciation, batteries, metal-organic frameworks, and others.