

Research Development Fund - Fall 2023

Application Title: New 500 MHz NMR Spectrometer with Increased Sensitivity Probe for ALL Nuclei.

Lead contact for RDF Application:

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Key Participating Units: College of Arts and Sciences

RDF Amount Requested (\$): \$994,779.13

Executive Summary

This application seeks to secure a state-of-the-art Bruker 500 MHz NMR spectrometer to enhance the core research infrastructure at Texas A&M University for sample limited compounds to address questions of molecular structure and kinetic interest in solution-state chemistry. This proposal outlines the following specific objectives for research enhancement:

1. Replacement of an obsolete Varian with a new Bruker NMR, which would provide significantly higher sensitivity, increased capability, and improved quality (e.g. resolution).
2. Facilitation of sample limited studies involving all observable nuclei by offering the dramatically increased sensitivity from a modern cryoprobe.
3. Increased competitiveness for extramural research funding by improving research productivity and scope.

The NMR facility within the Department of Chemistry has successfully maintained high-field spectrometers for decades, owing in large part to the expertise of our staff scientists. Their skills have significantly extended the lifespan of the facility's instruments, which has resulted in lower user costs and prolific research output from investments made up to 30 years ago. However, with Varian/Agilent ceasing their NMR operations, it has become impossible to fully support or upgrade this aging equipment. Bruker BioSpin currently holds the most prominent position in the NMR instrumentation industry. The proposed Bruker NMR system here offers not only the opportunity to access improved features and advancements over our existing capabilities, but also ensures Texas A&M University remains open to future developments in NMR spectroscopy for years to come. This upgrade and functionality is crucial, as just within the chemistry department over \$10 million in grant proposals rely on this technique and these instruments. A significant breakdown of this instrumentation disrupts research across multiple groups and may jeopardize external funding.

Given the pressing need for replacing these outdated spectrometers, it is prudent to upgrade our NMR facility's capabilities to meet today's research standards. Currently, the chemistry department only has a single system capable of looking at sample limited compounds, but it is limited to experiments on ^1H and ^{13}C . A system that can offer such increased sensitivity for all observable nuclei has the ability to look at lower concentration samples, nuclei that have inherently low natural abundance, accomplish more time-limited (including mechanistic) studies, and showcase the utility of NMR in advancing our understanding of chemistry and its applications. As a whole, NMR is underutilized across Texas A&M University due to infrastructure limitations, and so has significant untapped potential for answering questions of chemical interest. The addition of an instrument with these capabilities would not only expedite research but also facilitate our securing external grants across various departments. Across Texas A&M University, any research project involving compatible chemical analyses, such as degradation studies, kinetic investigations, or mechanistic studies, could benefit greatly from the proposed system.