

## Research Development Fund – Fall 2021

**Application Title:**            **New 500 MHz NMR Spectrometer with Increased VT-Capabilities**

Lead contact for RDF Application:

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Key Participating Units:    College of Science

**RDF Amount Requested (\$): \$703,080.60**

### EXECUTIVE SUMMARY

The objective of this application is to acquire a state-of-the-art Bruker 500 MHz NMR spectrometer to improve Texas A&M's core research infrastructure for solution state structural and kinetic analyses. Specific research enhancement goals of this proposal include: (1) replacement of an aging 30-year-old Varian system with a new Bruker NMR that provides for higher sensitivity and spectra with superior resolution; (2) upgrade our variable temperature (VT) capabilities to the standard in the NMR spectroscopy field and (3) increase competitiveness for extramural research funding *via* increased and higher quality research output.

The Department of Chemistry's NMR facility has maintained several high field spectrometers for decades which is in part due to the high caliber staff scientists employed. This has led to dramatic increases in the lifetime of all the spectrometers located within our facility leading to lower user costs and extensive research output from the initial investments within our facility over 30 years ago. However, with Varian/Agilent closing their doors aging equipment can no longer be supported or easily upgraded. Purchasing temporary fixes to this problem would likely only lead to increased overall cost and as such would be a poor investment of resources. Bruker Biospin is currently the leading company for NMR instrumentation and is widely used across academia and industry. The new Bruker system described in this proposal provides not only a venue to obtain improved features and advancements over our current analytical capabilities, but would allow TAMU to keep pace with future advancements in NMR spectroscopy for years to come. It is imperative that we upgrade our system expediently because over 10 million dollars of grant proposals rely on these instruments within the chemistry department alone. A major breakdown of this instrument would halt research progress across multiple research groups and jeopardize external funding.

Since this outdated spectrometer is in need of replacement, it is prudent to upgrade our NMR facility's capabilities to at least the standard in the field. Currently, our variable temperature (VT) abilities are lacking entirely. VT experiments are an indispensable tool in the study of reaction mechanisms and highlight the utility of NMR. Gaining insight into the mechanistic underpinnings of any reaction advances our basic understanding of chemistry and its applications. Across TAMU this is a sorely underutilized resource due to the lack of infrastructure. Adding an instrument with these capabilities would speed up the time to complete more sophisticated experiments and thus would improve the chances to obtain external grants across multiple departments. Any research project requiring chemical analysis such as degradation, kinetic or mechanistic studies would benefit immensely from this proposed instrument.