

Research Development Fund

Application Title: Enhancing Access to NMR Spectroscopy

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Key Participating Units: College of Science, College of Engineering

Anticipated Request Amount (\$): 1,143,000

Executive summary of the intended application to utilize Research Development Funds. We are requesting funds to equip the NMR Facility with two broad-capability integrated autosampling NMRs. This will expand the use of NMR by researchers outside of the Chemistry Department by providing essentially immediate access to our most capable spectrometers by new and non-routine users. It will also avoid an oncoming crisis in the facility, and serve to enhance the retention and recruitment of researchers in both chemistry and related sciences. It will finally improve the quality of all NMR-dependent research through both the added capabilities of the NMRs and by removing substantial bottlenecks in the traditional application of NMR.

NMR spectroscopy is the most broadly used analytical technique in chemistry, and it is a critical supporting technique in many other areas. Since 2016, the NMR Facility in chemistry has seen use by 31 research groups in Chemistry, eight groups in BioMedical Engineering, four groups in Chemical Engineering, four groups in Petroleum Engineering, three in Mechanical Engineering, two in Materials Sciences, two in Biochemistry/Biophysics, two in Veterinary Medicine/Biomedical Sciences, one in the College of Medicine, and one in Pharmacy. The usage by out-of-chemistry groups was 1306 hours. The Facility averages over 400 users at any given time, including graduate students, postdocs, faculty, staff, and undergraduate research students. NMR is an essential component for over 50 current federal grants at Texas A&M. NMR is routinely used interactively versus laboratory experiments, and the interpretability of the complex results depends on the capability of the instrument. Because of this, the quality of research is intimately linked to the quality of the available NMR and the rapidity of its access.

The Chemistry NMR Facility faces a crisis due to the exit of the *Agilent* from the NMR business. Seven of the ten NMRs in the Facility were manufactured by Agilent. NMRs are normally long-lived, but they require unique parts, compatible software and operating systems, and specialized support services. Agilent promised some support for its latest machines through 2021, but not its older NMRs, where parts are already difficult to obtain. Some of our machines will be unrecoverable from their next major breakdown, and all will likely be lost from service within ten years.

The opportunity in this predicament is that two autosampling NMRs can take the place of four current spectrometers while increasing quality and providing a quantum broadening of access. NMR has traditionally been a hands-on technique, but this greatly inhibits new and occasional users who must either climb a considerable learning curve for access to the best spectrometers or deal with the limitations and cost of service work. Although most use NMR on a daily basis, graduate students and new postdocs in chemistry currently require months to gain access to the best spectrometers. Autosampling changes the equation by letting new, occasional, and short-term users have rapid access to the highest quality analyses with absolutely minimal impediment. Finally, the round-the-clock, no-human-time nature of autosampling affects all research by changing the approach to experimentation from serial to parallel.