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RPPR Final Report
as of 28-Feb-2018

Agency Code:

Proposal Number: 68935CHREP

Agreement Number: W911NF-16-1-0412

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Final Report for Period Beginning 25-Jul-2016 and Ending 25-Jul-2017

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STEM Degrees:

STEM Participants:

Major Goals: This grant was used to purchase a new, state-of-the-art 400MHz Bruker Avance III Nuclear Magnetic Resonance (NMR) Spectrometer to support both research and teaching applications. The NMR was installed successfully in May 2017. The NMR has become vital to new and existing research programs at the university. These projects include isolating and analyzing natural products that could treat human diseases, developing smart polymers that have interesting biomedical and material science applications, developing materials that have novel sensor capabilities, and synthesizing new molecules that could treat neurological disorders, such as traumatic brain injuries. The NMR is also becoming incorporated into the academic courses for students studying analytical chemistry. Most students do not get hands-on training with an NMR within their classroom or laboratory courses. The NMR will provide unique opportunities to our students as they train to become the next generation of scientists, doctors, and engineers.

Accomplishments: Introduction

The grant Using NMR to Expand Chemistry Research and Educational Experiences at North Carolina Central University, an Historically Black University (GRANT12037919) was used for the purchase of a new 400MHz Bruker Avance III HD nuclear magnetic resonance spectrometer (NMR)1 within the Department of Chemistry and Biochemistry of North Carolina Central University (NCCU; Durham, NC) to support and expand research and educational opportunities. The NMR was successfully installed in May 2017. This new NMR replaced an aging 300MHz Varian NMR within the NCCU chemistry department. The new NMR is more powerful, smaller, and easier to use and maintain. This report will describe the expanded research capabilities and the additional educational opportunities afforded by this NMR.

The new NMR has allowed the initiation of two new research projects within the chemistry department. The first project is within Prof. Omar Christian's group. This research isolates and determines the molecular structure of

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medicinally promising compounds from native plants. These compounds are then assayed to anti-inflammatory activity to treat medical conditions such as hypertension and arteriosclerosis, which disproportionately affect minority populations.² This research will be extended to include isolating and characterizing natural product active metabolites responsible for the antibacterial, anti-inflammatory, antioxidant and mosquitocidal activities observed in various local, native plants. This research project would have been incredibly more difficult without the power and speed of the new NMR.

The second newly initiated project within Prof. Nathan Wymer's research group attaches the immunosuppressant cyclosporine A (CyA) onto a carrier protein in order to shuttle the CyA across the blood brain barrier. Research studies have shown that CyA can protect the mitochondria within neural cells for patients suffering from various degenerative neurological disorders, including traumatic brain injuries,³ Alzheimer's disease,⁴ multiple sclerosis,⁵ and amyotrophic lateral sclerosis (ALS).⁶ The CyA must be chemically linked to the carrier protein. This project is currently using the NMR to support these synthetic efforts to prepare various chemical linkers.

The new NMR has been used to support the day-to-day needs of the synthetic chemistry needs of the department's research, as described within the original application. These projects include designing and synthesizing stimuli-responsive polymers and "smart" materials within Prof. Darlene Taylor's group.⁷ Taylor's group is also engineering novel hole transport materials that can be used in a variety of fields, such as efficient solar cells.⁸ Prof. Fei Yan's group is synthesizing and investigating nanotechnology technologies that can measure reactive oxygen species within cells to determine their impact on human health.⁹

Each of these research groups contains significant number of undergraduate and graduate students performing advanced chemical and biochemical research. The new NMR purchased with this grant will help the department sustain this high number of research opportunities for NCCU students.

Works Cited

- 1 <<https://http://www.bruker.com/products/mr/nmr/avance-iii-hd/overview.html>>
- 2 Christian, O. E. et al. Redetermination and absolute configuration of (+)-7-epiclusianone. *Acta crystallographica. Section E, Structure reports online* 68, o3222-3223, doi:10.1107/S1600536812043784 (2012).
- 3 Li, P. A., Kristian, T., He, Q. P. & Siesjo, B. K. Cyclosporin A enhances survival, ameliorates brain damage, and prevents secondary mitochondrial dysfunction after a 30-minute period of transient cerebral ischemia. *Experimental neurology* 165, 153-163, doi:10.1006/exnr.2000.7459 (2000).
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- 5 Forte, M. et al. Cyclophilin D inactivation protects axons in experimental autoimmune encephalomyelitis, an animal model of multiple sclerosis. *Proceedings of the National Academy of Sciences of the United States of America* 104, 7558-7563, doi:10.1073/pnas.0702228104 (2007).
- 6 Kirkinezos, I. G., Hernandez, D., Bradley, W. G. & Moraes, C. T. An ALS mouse model with a permeable blood-brain barrier benefits from systemic cyclosporine A treatment. *J. Neurochem.* 88, 821-826, doi:10.1046/j.1471-4159.2003.02181.x (2004).
- 7 Koepnick, B. D., Lipscomb, J. S. & Taylor, D. K. Effect of Substitution on the Optical Properties and HOMO-LUMO Gap of Oligomeric Paraphenylenes. *Journal of Physical Chemistry A* 114, 13228-13233 (2010).
- 8 Le, K., Chand, L. B., Griffin, C., Williams, A. L. & Taylor, D. K. Paraphenylene Dimers with Diphenylamine Donor Groups: Synthesis and Photophysics. *Tetrahedron Letters* 54, 3097-3100 (2013).
- 9 Yan, F., Zhang, Y., Kim, K. S., Yuan, H. & Vo-Dinh, T. Intracellular photodynamic therapy using methyleneblue-containing protein nanocages. *Photochemistry and Photobiology* 86, 662-666 (2010).

Training Opportunities: Education

The NMR will also be incorporated in the analytical chemistry courses within the NCCU Department of Chemistry and Biochemistry. The ease of use and automated sample changer allow for students to prepare their own samples, get experience in using the NMR instrument and software, and interpreting real world NMR spectra.

Results Dissemination: Nothing to Report

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

RPPR Final Report
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PARTICIPANTS:

Participant Type: PD/PI

Participant: Nathan Wymer

Person Months Worked: 12.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co PD/PI

Participant: Darlene Taylor

Person Months Worked: 12.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: PD/PI

Participant: Fei Yan

Person Months Worked: 12.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

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15. SUBJECT TERMS Nuclear Magnetic Resonance Spectrometer (NMR)					
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Department of Defense - Research and Education Program for Historically Black Colleges and Universities and Minority-Serving Institutions (HBCU/MI) Equipment/Instrumentation (W911NF-15-R-0025)

Final Technical Report on *Using NMR to Expand Chemistry Research and Educational Experiences at North Carolina Central University, an Historically Black University* (GRANT12037919)

Introduction

The grant *Using NMR to Expand Chemistry Research and Educational Experiences at North Carolina Central University, an Historically Black University* (GRANT12037919) was used for the purchase of a new 400MHz Bruker Avance III HD nuclear magnetic resonance spectrometer (NMR)¹ within the Department of Chemistry and Biochemistry of North Carolina Central University (NCCU; Durham, NC) to support and expand research and educational opportunities. The NMR was successfully installed in May 2017. This new NMR replaced an aging 300MHz Varian NMR within the NCCU chemistry department. The new NMR is more powerful, smaller, and easier to use and maintain. This report will describe the expanded research capabilities and the additional educational opportunities afforded by this NMR.



Figure 1: The Bruker Avance III NMR installed in May 2017 within the NCCU Department of Chemistry and Biochemistry

Research

The new NMR has allowed the initiation of two new research projects within the chemistry department. The first project is within Prof. Omar Christian's group. This research isolates and determines the molecular structure of medicinally promising compounds from native plants. These compounds are then assayed to anti-inflammatory activity to treat medical conditions such as hypertension and arteriosclerosis, which disproportionately affect minority populations.² This research will be extended to include isolating and characterizing natural product active metabolites responsible for the antibacterial, anti-inflammatory, antioxidant and mosquitocidal activities observed in various local, native plants. This research project would have been incredibly more difficult without the power and speed of the new NMR.

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Education

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- 9 Yan, F., Zhang, Y., Kim, K. S., Yuan, H. & Vo-Dinh, T. Intracellular photodynamic therapy using methyleneblue-containing protein nanocages. *Photochemistry and Photobiology* **86**, 662-666 (2010).