ND*nano* Undergraduate Research Fellowship (NURF)
2015 Project Summary

1. Student name: Roland Rebuyon, Jr.

2. Faculty mentor name: Dr. Steven Ruggiero and Dr. Carol Tanner

3. Project title: Light transmission spectroscopy: A new bio-molecular tool

4. Briefly describe any new skills you acquired during your summer research: During this summer project, I was able to build my proficiency in running complex computer simulations of light scattering properties of nanoparticles, including certain important bacterial pathogens. In addition, I learned to use simple engineering principles in order fine-tune the hardware of the LightSprite machine central to the project.

5. Briefly share a practical application/end use of your research: The simulations that I worked on this summer will be used to build a database that will describe the optical properties of a wide range of biological molecules, including both commensal and pathogenic bacteria, as well as metal and metalloid particles. Although this project will continue on into the foreseeable future, we have been able to use the LightSprite machine in order to compare our simulation results to other real-life samples, such as those of cancer cell lysates and E. coli.

Begin two-paragraph project summary here (~ one type-written page) to describe problem and project goal and your activities / results:

Working with Drs. Ruggiero and Tanner last summer, Alison Deatsch, my graduate student supervisor, and I worked on computer simulations of simple spheres, cylinders, and ellipsoids that formed the foundation of a database of simulations of biomolecules found in natural ecosystems, such as the Great Lakes, as well those found in the human body. At the end of the summer, we had successfully completed our task, and we were able to favorably compare the results of our tests to those of Frank Li, who had spearheaded the light transmission spectroscopy project in order to complete his PhD thesis, and the tests that Drs. Ruggiero and Tanner had previously completed with polystyrene samples. Upon returning to the lab last spring, I encountered problems running new tests with similar shapes because we had found that the success of our tests with simpler shapes may have been due to random chance, not just the accuracy of the software that we had used. The two programs that we used to replicate the light scattering properties of polystyrene and other biomolecules were FTIKREG and MIEV0. Using these programs, we gathered extinction values for each individual sample and mathematically inverted the data in order to graph peaks that corresponded to the particles' sizes and relative densities. However, these peaks became inaccurate when we attempted to invert extinction data of more complex shapes of different densities in solution. This summer, Alison and I attempted to rectify the problem by delving into the codes of these programs and replicating the code used by the LightSprite machine.

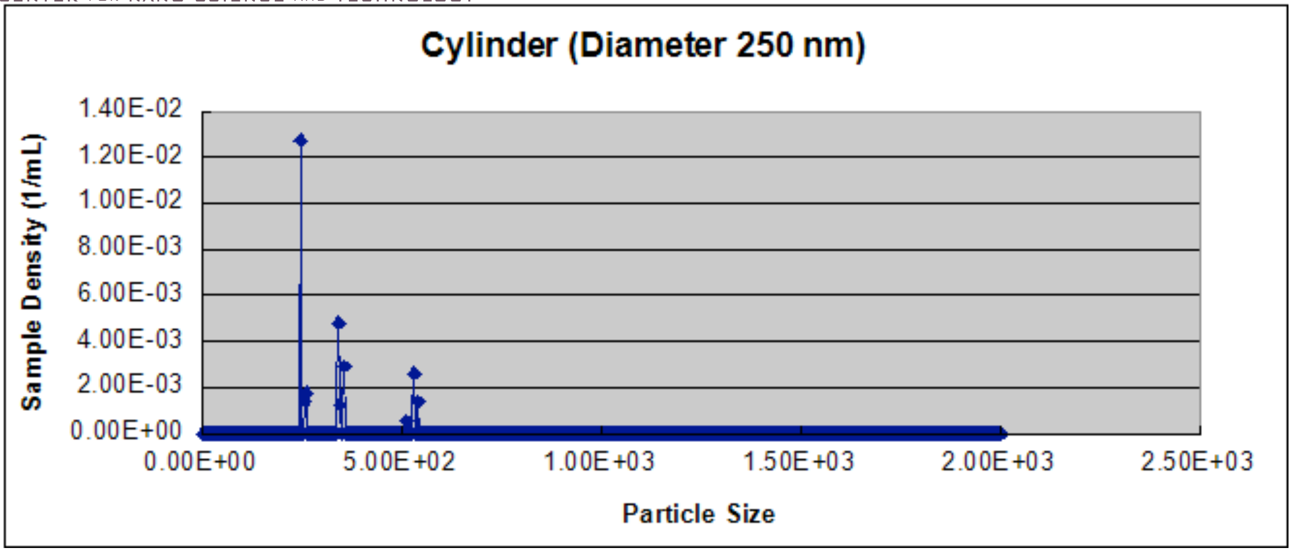

Figure 1: Example of an Inaccurate Cylinder Test

Even though the major peak in the graph represents a particle with a diameter of 244 nm (which is reasonably accurate), there is noise in the form of minor peaks that should not appear after a successful inversion of the extinction data.

After the publication of the most recent paper written by Drs. Ruggiero and Tanner, Alison and I were urged to continue our work on light transmission spectroscopy from last summer and obtained more accurate size vs. density tests. Over the course of 10 weeks, we altered the FTIKREG and MIEV0 code, and we used DDSCAT, a program that simulates the light extinction properties of many different shapes, in order to get more consistently accurate data. Using results of tests run by graduate student, Ariel Shogren, on E. coli and human cell lysates, we were able to successfully replicate peaks for polystyrene spheres and cylinders, which were of similar shapes and sample densities. This involved altering the values used by DDSCAT and MIEV0 in order to evaluate the refractive and dielectric indices of both the ambient medium and of the samples themselves. We repeated these simulation tests with the results of LightSprite tests using gold, silicon, and titanium and obtained favorable results. Meanwhile, Alison ran tests with E. coli and cancer cell lysates that we will use to supplement our database of the light scattering properties of different biomolecules.

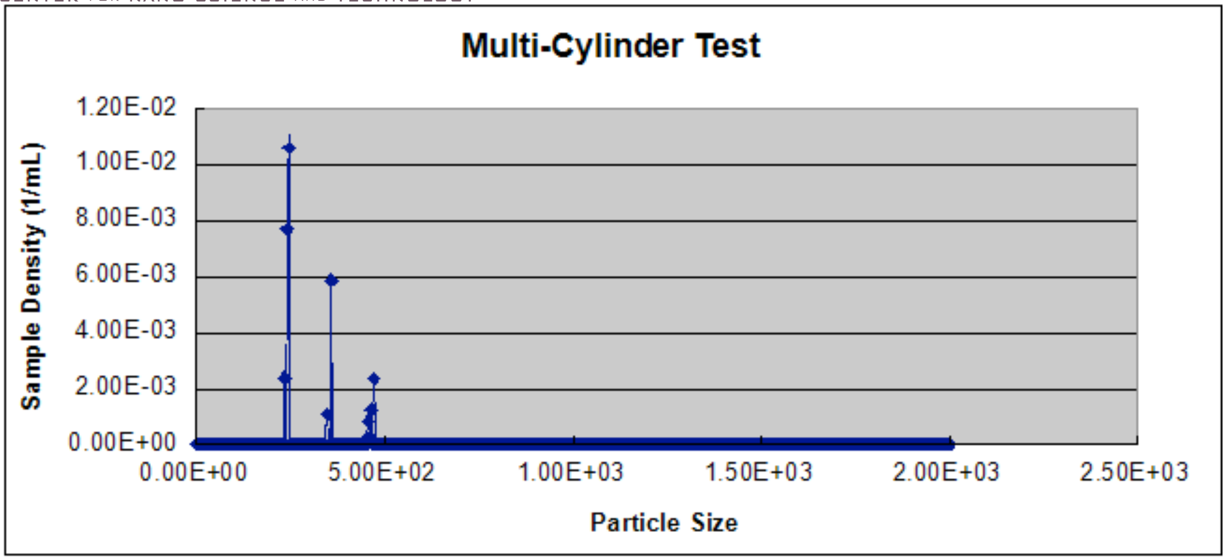

Figure 2: Example of a Successful Cylinder Test
We were able to obtain accurate peaks representing cylinders of diameters 245 nm, 360 nm, and 470 nm of different densities.

Although we are still trying to figure out how to consistently simulate accurate extinction data and inversion peaks for all of the particles tested in lab, we will be working diligently to further the project throughout the current school year.

Publications (papers/posters/presentations): N. Sun et. al, Nanoparticle analysis of cancer cells by light transmission spectroscopy. Analytical Biochemistry. Vol. 484. 58-65. 1 September 2015.