

NDnano Undergraduate Research Fellowship (NURF) 2014 Project Summary

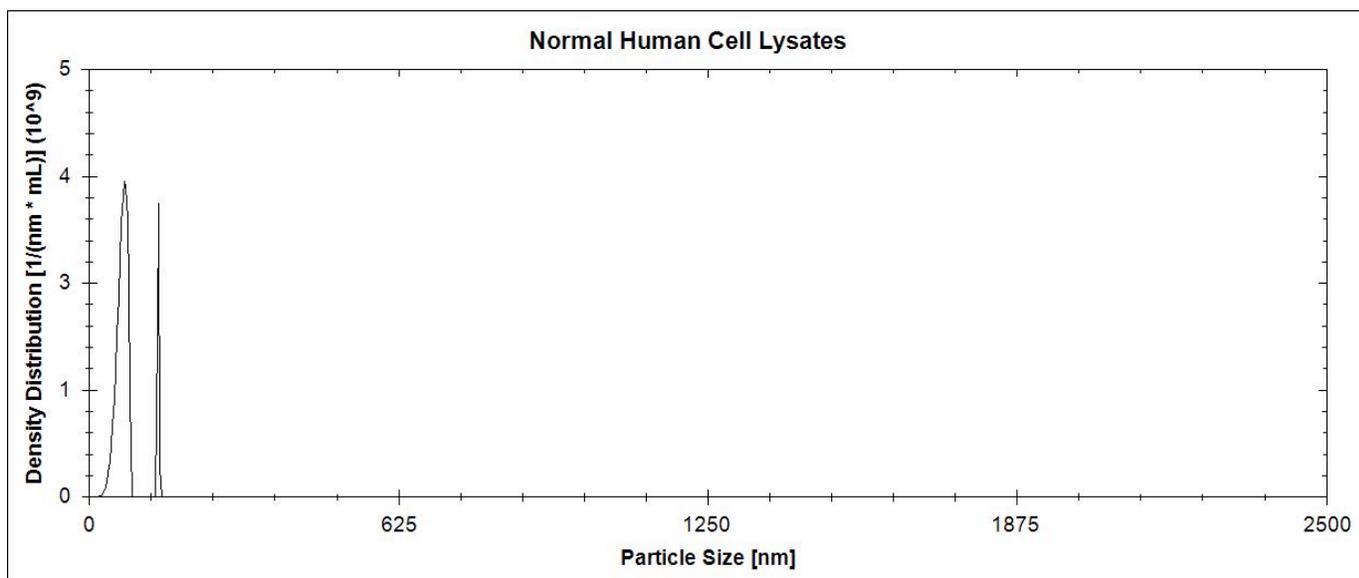
1. Student name: Roland Rebuyon Jr.
2. Faculty mentor name: Drs. Steven Ruggiero and Carol Tanner
3. Project title: Light Transmission Spectroscopy (LTS): A New Bio-molecular Tool
4. Briefly describe any new skills you acquired during your summer research:
 - Write code in FORTRAN computing language
 - Use Unix interface to complete tasks
 - Use the CRC's high-powered servers to run simulations
 - Run tests on valuable samples in laboratory setting
 - Use devices in biophysics laboratory for designing nanoparticle simulations
 - Gain proficiency in use of computer programs, including Excel and Mathematica
 - Gain understanding of relationship of nanoparticle size and light diffraction
 - Use light transmission spectroscopy to determine particle size and density
5. Briefly share a practical application/end use of your research: The LightSprite device, which uses LTS, has been used to determine the presence of pathogens in environmental settings and is a valuable tool in detecting invasive species in water supplies. Currently, the LightSprite is being used to determine the sizes and densities of lysates in human oral cancer cells with a higher degree of accuracy than dynamic light scattering analysis. This can greatly improve the practice of cancer diagnosis.

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

The current goal of the light transmission spectroscopy project is to use the LightSprite device as a medical research and diagnostics tool for the study of human cancer cells and their sub-cellular structures, including organelles and DNA/RNA molecules. By using light transmission spectroscopy through the LightSprite, a researcher will be able to trace the morphological changes of these structures through a detailed comparison of both healthy and cancerous human cells. Although many techniques, such as Raman spectroscopy and dynamic light scattering, have been used in order to study the properties of other cell systems, these techniques have not yet been used to study human cancer cells. Electron microscopy has determined that enlarged sub-cellular structures are a key indicator of the presence of cancerous growth within cells. Examples of structures that are enlarged in cancer cells are the nuclei, lysosomes, and mitochondria. The LightSprite device is now being used to create a mathematical model that defines the relationship between the sizes and the density distributions

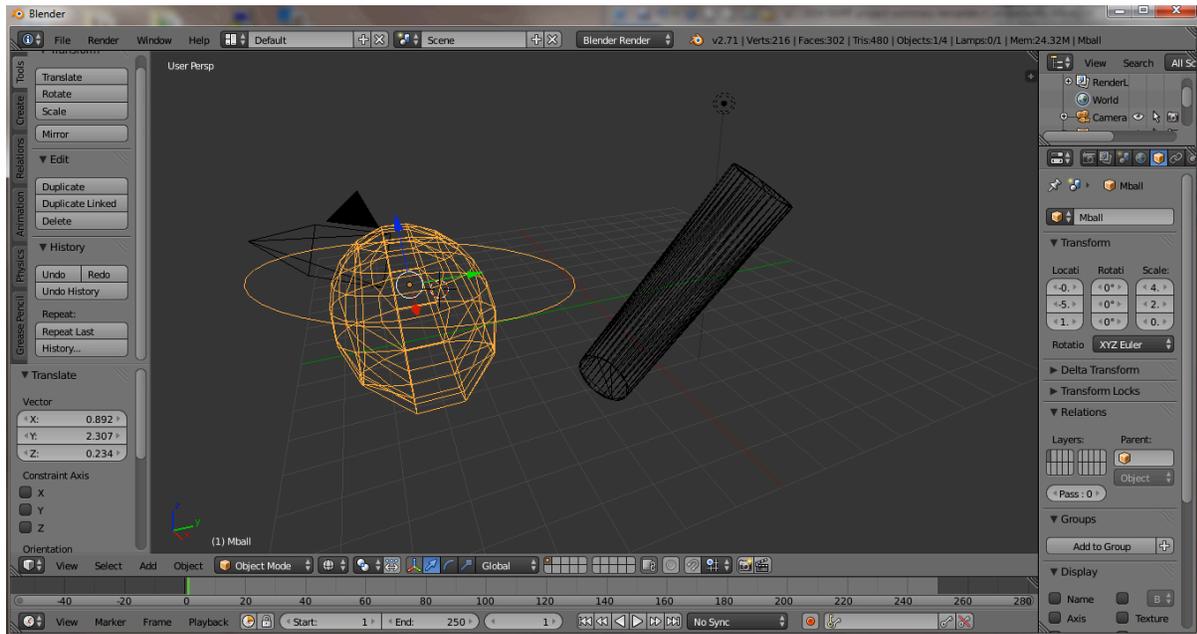
of suspended lysates of healthy and cancerous cells. Light transmission spectroscopy is well-suited for determining the optical properties of these lysates because it utilizes a spectral analysis of transmitted laser light over the UV and IR ranges and, therefore, can analyze nanoparticles with greater accuracy than other spectroscopy techniques.

My primary task this summer was to help Drs. Ruggiero and Tanner lay the groundwork for a library of particle size vs. density distribution graphs corresponding to different biological systems and chemical compounds, including the BSA protein, iron oxide, and silver nitrate. I also worked on verifying a specific set of data from human oral healthy and cancerous cells. Firstly, I had to familiarize myself with FTIKREG and MIEV0, which are two FORTRAN programs that, when compiled together, turn light extinction data from light transmission spectroscopy analyses of biomolecular systems into particle size vs. density distribution curves. These two programs are integrated into the LightSprite's software. Afterward, Alison Deatsch, my graduate student mentor, and I worked on replicating simulations from a thesis published by Frank Li, a PhD student whose work was supervised by Drs. Ruggiero and Tanner. These simulations involved using the LightSprite machine in order to glean both light extinction data and particle size/distribution graphs and modifying the FORTRAN programs. In order to tailor the FORTRAN programs to the specific nature of each of the molecules, we had to carefully fine-tune many of the programs' parameters. Then, we used 3D modeling software in order to create simulated targets and datasets in order to perform tests for molecules of different sizes and configurations. We eventually created simulations of both the BSA protein and cell lysates by replicating their shapes and dimensions through the modeling software and used the LightSprite to gather extinction data. Once we were pleased with our simulations, we turned our attention to the datasets from healthy and cancerous human oral cells in order to help verify experimental results that Drs. Ruggiero and Tanner will be using in their next publication. Using our modified FORTRAN programs and verifying our results with intensive LightSprite device testing, we were able to successfully replicate the results that will be used for the upcoming paper.



This is a graph taken from the LightSprite device depicting the particle size vs. density distribution curve from a dataset for normal (healthy) human cell lysates. The lysates show peaks of 72 and 141 nm, which represent particle sizes/diameters. Using the trapezoidal rule to find the

area under the peak at 72 nm, for example, we can conclude that the particles that are 72 nm in size have a density of 1.2×10^{11} particles/mL.



This is an image of the interface for the 3D modeling software, Blender, which we used to create simulations of different shapes, ranging from cylinders and ellipsoids to hearts and prisms, in order to verify the accuracy of the LightSprite's analyses. We used Blender in order to map out the shapes in the dimensions that we wanted, and then, we used publicly available software, such as DDSCAT and DDA Convert, in order to distribute dipoles within the shapes. This allowed for the simulation of light extinction data.

Publications (papers/posters/presentations): (still in the draft process)

Ruggiero, S. et al. Optical and Nanoparticle Analysis of Normal and Cancer Cells by Light Transmission Spectroscopy.