

# DANIEL CHABEDA

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## EDUCATION

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### Yale University

Pursuing a B.S. in Chemistry

Member of the Yale American Chemical Society Chapter

*August 2018 - Present*

### North Carolina School of Science and Math Online

Concentration: Computational Science

*August 2016 - May 2018*

### Community School of Davidson

High School Diploma

*August 2014 - May 2018*

## RESEARCH EXPERIENCE

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### North Carolina School of Science and Math Online

*Comparative Study of the Chemical, Biological, and Pharmacological Properties of Calcineurin*

*Inhibitors*

March 2018 - May 2018

*Advisor: Robert Gotwals*

- Utilized MO calculations, ADME(T) parameters, and Cresset's molecular field technology to compare the structural chemistry of three immunosuppressant drugs: Tacrolimus, Cyclosporine A, and Sirolimus.
- Conducted protein-ligand docking calculations using the Schrodinger Bioluminate Suite and Molegro Virtual Docker to determine the binding affinity of each drug to its target.

### North Carolina School of Science and Math Online

*Investigation of Solvatochromism in  $\pi$ -Conjugated Chromophores Using Computational*

*UV-Vis Spectroscopy*

November 2017 - January 2018

*Advisor: Robert Gotwals*

- Examined solvatochromic shifts of 1,3-butadiene, 2-furoic acid, and naphthalene UV-Vis spectra in various solvents using TD-DFT UV-Vis/Excited State calculations coupled with the Polarizable Continuum Matrix model.

### Summer Ventures in Science and Mathematics

*Providing K-12 Students Access to Digital Fabrication Technologies Through the Implementation of Community-Based Makerspaces*

June 2017 - July 2017

*Advisor: Daniel Zuberbier*

- Conducted educational technology research on the cognitive benefits of digital fabrication experience and employed the design-thinking process to design a community-centered model to make 3D-printers and other digital fabrication tools widely available.

## TECHNICAL STRENGTHS

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### Software & Tools

Gaussian, Molegro Virtual Docker, Schrodinger Materials Science Suite, StarDrop  
LaTeX, Excel, Mathematica, Gnuplot

## ACADEMIC ACHIEVEMENTS

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National AP Scholar with Distinction

Member of the National Honors Society

Awarded first place in the Project for Innovation, Energy, and Sustainability's Green Idea Factory Competition.