Newby Research Group

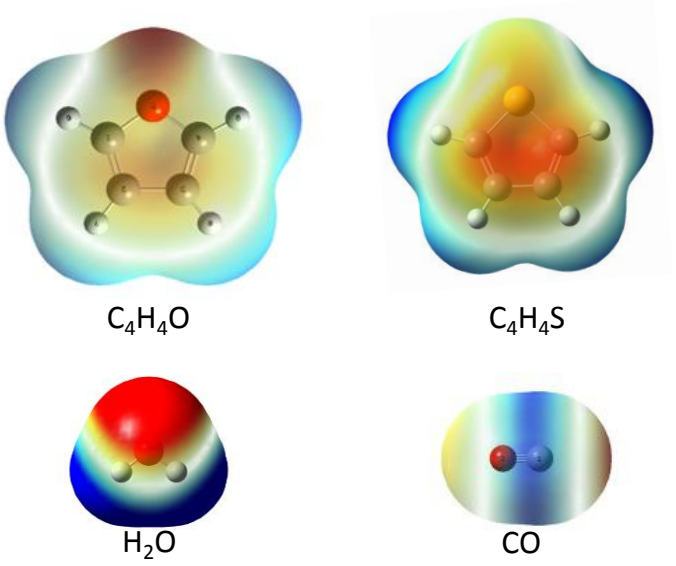
NRG 2021
(L-R: Rachael Vasilchenko, Emily Weaver, Annabelle Carney, Kenny Mogauro, Xavier Solivan, and Dr. Newby)

The Newby Group spent the summer of 2021 working to better understand solvation, intermolecular forces (IMFs), how IMFs influence geometry, and techniques for studying molecular geometry. The bulk of our studies made use of computational chemistry software. The program uses quantum mechanics to find the energy of molecular structures. To use this program, the group made use of supercomputers at San Diego Supercomputing Center as part of an XSEDE grant.

Annabelle, Emily, and Kenny spent the summer working to identify the minimum energy structures of complexes of water with lactones. Lactones are cyclic esters that are often found in flavorings and fragrances or can also be used in the synthesis of illicit drugs.

Computed minimum energy structures of γ-hydroxybutyrate with water.

Xavier and Rachael worked to find the minimum energy complexes of the heterocycles furan and thiophene. These heterocycles are important in chemical synthesis and petroleum. We are interested if the complex geometry preferences are affected by the polarity of the interacting molecule. Previous studies focused on the heterocycles with water (highly polar) where Xavier and Rachael explored the interactions with carbon monoxide (mildly polar).



Computed electron density maps of the furan, thiophene, water and carbon monoxide.

Additionally, the group helped Dr. Newby start putting together the custom spectrometers that will be used to experimentally study these complexes. The lab being built in the basement of Peckham Hall will use cryogenic chambers, supersonic expansions, mass spectrometry, and laser spectroscopy to better understand how weakly bound molecules come together.

Building a spectroscopy lab in Peckham!

Did we mention Chemistry won the Inaugural Summer Research Games? The AMAZING trophy is proudly on display on the third floor of Peckham Hall.

Look at this great group of awesome scientists!