

## **Molecular Dynamics Studies of Retinoid Ligands in the Fatty Acid Binding Protein FABP5 as a Potential Cancer Therapy**

Nathanael Hunter, Chrystal D. Bruce  
John Carroll University

Department of Chemistry, John Carroll University, University Heights, OH 44118

Treatment of cancer cells with retinoic acid, a fatty acid, can either lead to proliferation or inhibition of cancer cells depending on the relative ratio of two proteins in the cancer cell: FABP5 and CRABP-II. Inhibiting the action of FABP5, or fatty-acid binding protein by binding with retinoic acid may lead to the observed reduction in cell proliferation. The goal of this project was to examine the binding of retinoic acid and its isomer, 9-cis-retinoic acid in the binding pocket of FABP5 in a molecular dynamics simulation. Results of the molecular dynamics production run, performed using AMBER12 software, as well as free energy approximations, calculated using molecular mechanics/generalized born surface area and normal mode harmonic entropy approximations, will be presented. These will be compared to preliminary docking results found using AutoDock Vina docking software.