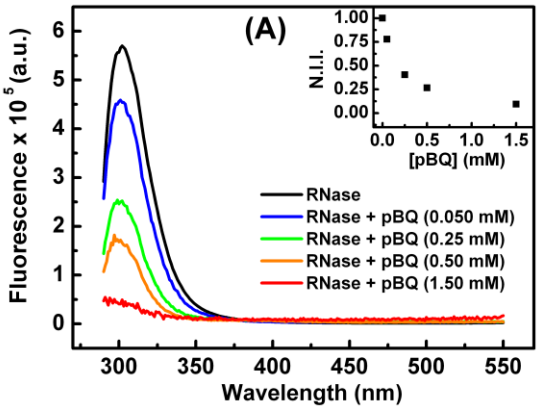
Computational and Experimental Research on Quinone Reactivity

Research Advisor: Dr. Titus V. Albu

The research in my group is focused on reactivity of quinones, and it can be either computational or experimental.

Experimental Project: *Fluorescence Studies of Protein Modifications Induced by Quinones*

This work is a collaborative project with Dr. Kim research group. It was found that quinones, as well as other polyaromatic hydrocarbon metabolites, are responsible for abnormal cell behavior. One of the possibilities for this behavior is the reaction of quinones with proteins leading to protein aggregation. Fluorescence techniques will be used to investigate these types of protein modifications. The current study will focus on reactivity of substituted benzoquinones and naphthoquinones, at various concentrations, solution pH values or temperatures.



Computational Project: *Studies of Quinones Reactivity toward N-Containing Compounds*

This project involves investigating reactions between a series of naphthoquinones and organic compounds containing amino groups. These reactions are relevant to the biological activity of quinones and are models for the reactions of quinones with proteins. The transition states (similar to the one aside) for these reactions will be determined using Gaussian software on Linux workstations. Solvent effects can be included in the computations. This study could lead to a better understanding of the quinone reactivity in biological systems because quantum mechanical studies typically provide complementary information that is difficult to be obtained experimentally.