

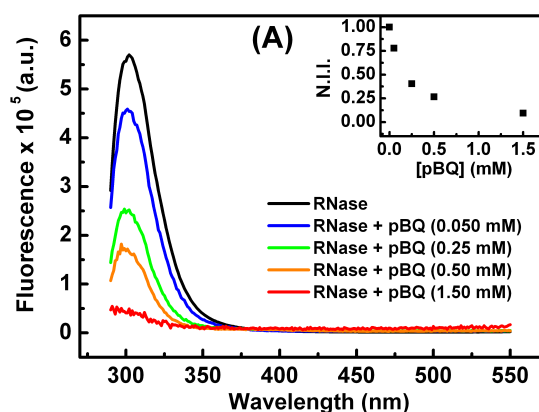
## Computational and Experimental Research on Quinone Reactivity

Research Advisor: Dr. Titus V. Albu

A research area in my group focuses on investigating both computationally and experimentally the reactivity of quinones.

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

It was found that quinones modify proteins like RNase or Lysozyme through adduct formation, oligomerization and polymerization. In this project, fluorescence techniques and UV-Vis spectroscopy will be used to investigate these types of protein modifications. The current study will focus on reactivity of substituted benzoquinones and naphthoquinones toward proteins in the presence of metal ions. This work is a collaborative project with Dr. Kim research group.



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

This project involves investigating reactions between quinones or naphthoquinones and organic compounds containing amino groups. These reactions are relevant to the biological activity of the quinones and are models for the reactions of quinones with proteins. The study will focus in understanding the dependence of pH on the reactivity. The transition states (similar to the one aside) for these reactions will be determined using Gaussian software on Linux workstations. 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.

