Computational and Experimental Research on Chemical Reactivity

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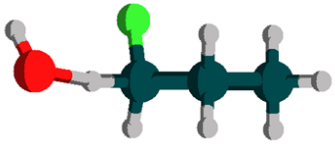
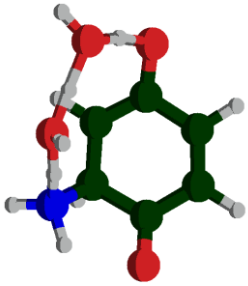
The research in my group in mainly computational in nature but an experimental project is also available. Besides the projects presented below, additional smaller computational projects are possible depending on student's interest and availability of resources.

Computational Project 1: *Computational Studies of Hydrogen Abstraction Reactions*



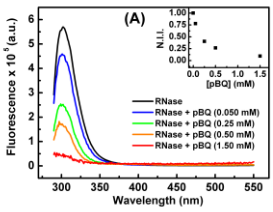
This project involves mainly the computation of reactivity parameters associated with different reaction pathways of hydrogen abstraction from hydrofluorocarbons and similar compounds. These reactions are relevant to the hydrofluorocarbons' residence time in atmosphere. The reactivity parameters (barrier height, transition state location, etc.) associated with various hydrogen-abstraction reactions from hydrofluorocarbons will be calculated using Gaussian software on Linux workstations. This study will extend the current knowledge of hydrofluorocarbons' reactivity and will lead to a better understanding of the environmental impact of these industrially important compounds.

Computational Project 2: *Studies of Quinones Reactivity toward N-Containing Compounds*



This project involves investigating reactions between a series of quinones 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. 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.

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.