**Computational Analysis of Adduct Formation between Benzaldehyde Derivatives and DNA**

Ekaterina Voytsekhovskaya
*Danae Quirk Dorr, Faculty Mentor, Chemistry (Science, Engineering and Technology)*
*Josh Marell, Faculty Mentor, Chemistry (Science, Engineering and Technology)*

Aldehydes have been previously found to be involved in the process of chromosomal aberrations and have the potential to form adducts as a result of DNA interactions. Structural examination of the formed adducts can contribute to the assessment of the level of genotoxicity of the reactive aldehydes as well as allow for the proposal of the reaction mechanism responsible for the formation of adducts. In this study, utilizing computational modeling and density-functional theory calculations aided the structure-property analysis of the adducts in order to yield information necessary to improve our understanding of the biological activity of the investigated benzaldehyde derivatives (cuminaldehyde, p-anisaldehyde, 3,4-dimethoxybenzaldehyde, and vanillin) commonly found in food. The aim of this research was to integrate computational techniques into an experimental study in order to explore the reactivity profiles of the aldehydes as well as determine the structural characteristics responsible for their reactivity toward DNA. Each aldehyde was allowed to independently react with DNA in the presence of L-arginine. The reaction mixtures and adducts were analyzed using HPLC and 1H NMR so that an extrapolative range of experimental data could be collected and used for further computational studying.