FENTON REACTION DAMAGING EFFECTS ON BIOLOGICAL MOLECULES: A THEORETICAL STUDY

Sharnek Walker and Glake Hill

Interdisciplinary Center for Nanotoxicity, Jackson State University, Jackson, MS 39217, USA

Abstract: The human body is introduced to metal ions through ingestion of contaminated foods and water, direct contact or injection. The toxic metal ions can be harmful to the human body and cause diseases like Alzheimer's disease and cancer. Metals, like iron, are present in the body, but in excess levels the effects of these metals could be detrimental to biological molecules and the functioning processes. For example, the metal ions can cause the production of reactive oxygen species (ROS), thus causing oxidative stress to biological molecules, like deoxyribonucleic acid (DNA). The Fenton reaction produces the hydroxyl radical, which is a ROS that is detrimental to the human body. Employing computational approaches provides a method for answering these unknowns that are less expensive and time consuming than traditional experimental approaches. In addition, computational data may help direct future experimental investigations. Traditional DFT methods were employed to investigate the interaction between the DNA bases and hydroxyl radicals produced from the Fenton reaction. Energy values are being compared to previous theoretical literature. Future studies will include solvent models to simulate biological systems in the body.

Key Words: Fenton Reaction, Reactive Oxygen Species (ROS), DNA, Hydroxyl Radical

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