Lux et Fides: A Journal for Undergraduate Christian Scholars

Volume 2 Article 6

May 2024

# Computational Analysis of O6-Methylated Guanine and Thioguanine Complexes

Kirsten Stinson
*Taylor University*

Michael Bowman

# Computational Analysis of O6-Methylated Guanine and Thioguanine Complexes

By Kristen Stinson and Michael Bowman

DNA methylation occurring on the $O^6$ position of guanine has been linked to the formation of cancer. DNA complexes with $O^6$-methylated guanine have been studied experimentally, yet questions remain concerning the carcinogenic properties of $O^6$-methylguanine. Research conducted during the summer of 2023 explored the interaction between $O^6$-methylguanine and its potential nucleobase pairs of cytosine and adenine in hopes of elucidating the mutagenic characteristics of $O^6$-methylguanine. A variety of computational methods including Density Functional Theory, Symmetry Adapted Perturbation Theory, Noncovalent Interaction analysis, and Natural Bond Orbital analysis were employed to comprehensively probe this system.

Upon analysis of these results, it was observed that $O^6$-methylation causes a significant decrease in the interaction energy between the base pairs when compared to the canonical guanine-cytosine base pair. Methylated guanine also has a higher likelihood of mispairing with a only a modest preference for pairing with cytosine over thymine. Furthermore, when mis-paired with thymine, the complex loses a coplanar configuration, leading to instability within the DNA complex. This research may be leveraged to understand how cancer is formed and minimize the associated risks. Moreover, the wisdom of God is revealed to the world by studying the complex and robust mechanisms involved with DNA and the maintenance of life.