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Computational Analysis of O⁶-Methylated Guanine and Thioguanine Complexes

By Kristen Stinson and Michael Bowman

DNA methylation occurring on the O⁶ position of guanine has been linked to the formation of cancer. DNA complexes with O⁶-methylated guanine have been studied experimentally, yet questions remain concerning the carcinogenic properties of O⁶-methylguanine. Research conducted during the summer of 2023 explored the interaction between O⁶-methylguanine and its potential nucleobase pairs of cytosine and adenine in hopes of elucidating the mutagenic characteristics of O⁶-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 O⁶-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.