

Computational Insights in DNA Methylation: Catalytic and Mechanistic Elucidations for Forming 3-Methyl Cytosine

Mansour Almatarneh¹, Ghada Kayed¹, Mohammednoor Altarawneh², Yuming Zhao³, and Amita Verma⁴

¹University of Jordan

²United Arab Emirates University

³Memorial University of Newfoundland

⁴Sam Higginbottom University of Agriculture Technology and Sciences

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Abstract

abundantly occurring methylation process at CpG island, which has been well-known as an epigenetic modification linked to many human's diseases. Recently, another methylation approach has been discovered to show that DNA methyltransferases (DNMTs) promote the addition of methyl group at position 3 to yield 3mC. The existence of 3mC can cause severe damages to the DNA strand, such as blocking its replication, repair, and transcription, affecting its stability, and initiating a double-strand DNA break. To gain a deeper insight into the formation of 3mC, we have performed density functional theory (DFT) modeling studies at different levels of theory to clearly map out the mechanistic details for this new methylation approach. Our computed results are in harmony with pertinent experimental observations and shed light on a crucial off-target activity of DNMTs.

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