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(I) Computer Simulations of Modified Nucleic Acids: From Biomolecular Structure to Chemical Reactivity

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Nucleic acids are the most basic molecules of life, being tasked with storing and transmitting genetic information in all living organisms. Both DNA and RNA are composed of fundamental building blocks that each include a nucleobase (A, G, C, T/U), sugar ([deoxy]ribose), and phosphate moiety. To enhance nucleic acid programmability and stability, and aid the formation of functional 3D shapes, nucleotides are commonly modified in nature. Indeed, DNA nucleobases are methylated to control gene expression, while the identification of over 130 distinct modifications in RNA has led to the emerging field of epitranscriptomics. Furthermore, the ease of synthesis of nucleic acids functionalized at any nucleobase, sugar, or phosphate site, as well as the ability of modifications to impact pairing, chemical stability, conformation, and interactions with proteins, has led to the development of a wealth of unique modifications with far-reaching applications. For example, modified nucleic acids have been designed for medicinal uses such as drugs, vaccines, bioprobes, antimicrobials and tissue engineering, as well as for nanomaterials to build nanowires, nanomachines and nanorobots. Unfortunately, the lack of known structure–function relationships for a range of modified nucleic acids raises questions such as why does nature introduce modifications and how can modifications be used to their full potential in valued applications. This talk will provide a survey of some of the recent topics of interest in my lab that use computer modeling to gain a fundamental understanding of the diverse chemistry of modified nucleic acids. The information gained from computer simulations fills knowledge gaps by providing a greater understanding of the role of nucleic acid modifications in nature and improving the design of original modified nucleotides for novel applications.

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Keyword-2

Biomolecular Simulations

Keyword-3

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