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Editorial: Editing DNA and RNA through Computations

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Gene editing is a process in which the DNA of an organism is deliberately altered, modified, or corrected at specific locations within its genome.[1] The goal of gene editing is to make precise changes to the genetic material of organisms to achieve the desired characteristics, correct genetic mutations, or study gene functions. Gene editing has a wide range of potential applications across various fields, including medicine, agriculture, and biotechnology, alongside basic research.

One of the most revolutionary advancements in gene editing technology is CRISPR-Cas9 (Clustered Regularly Interspaced Short Palindromic Repeats and CRISPR-associated protein 9). CRISPR-Cas9 allows scientists to target specific DNA sequences within a given genome and make changes by either adding, deleting, or replacing genetic material. While CRISPR-Cas9 is the most well-known and widely used gene editing system, several other systems can process DNA and RNA, opening Pandora's box for the development of new gene editing technologies.[2]

Nucleic acid manipulation goes beyond gene editing to include a variety of techniques and applications to manipulate and engineer DNA and RNA molecules. Macromolecular machines acting on genes are at the center of life's fundamental processes. DNA replication and repair, chromatin packaging, transcription, translation, and RNA splicing involve multiple protein/nucleic acid complexes that have profound biological implications. In this multifaceted scenario, RNA has emerged as the main player in driving biochemical and therapeutic transformations. Recent advancements in nucleic acid manipulation have led to the development of RNA-based vaccines, such as the mRNA vaccines for COVID-19.

These fast scientific advancements open new opportunities and challenges for computational chemistry. By using computational methods, scientists are now able to predict the structure, dynamics, and function of large macromolecules involved in processing and editing nucleic acids. Computational studies of CRISPR-Cas9 and other genome editors,[3] RNA splicing systems, replication and transcription machineries, nucleosomes, and chromatin factors, as well as the ribosome, are paving the way for harnessing computations toward new discoveries.[4]

To foster the discussion on how computational chemistry can give a critical contribution to the gene editing revolution, the *Journal of Chemical Information and Modeling* (JCIM) is announcing the publication of a Virtual Special Issue on the topic of **Editing DNA and RNA through Computations**. This special issue welcomes the most exciting computational studies in the field of protein/nucleic acids. We call for the most innovative applications in the simulation proteins and nucleic acids and for methodological advances in terms of force fields and computational methods. We welcome computational studies of gene editing systems including but not limited to CRISPR, as well as RNA splicing, DNA replication and repair, gene transcription and regulation, chromatin packaging, and other macromolecular machines acting on genes.

Our Virtual Special Issue will offer a computational journey through the field of nucleic acid processing and editing, welcoming studies based on multiscale approaches, ranging from quantum-classical (QM/MM) simulations to characterize enzymatic reactions, to all-atom and coarse-grained simulations, including also enhanced sampling methods to study long-time scale conformational changes. We welcome studies harnessing novel machine-learning techniques and methodological development, including but not limited to force-field development. Advanced computational methods and innovative applications will be featured to showcase the power of computational methods in describing what is unseen through experimental techniques.

We welcome all types of manuscripts that fit the scope of JCIM, such as articles, perspectives, viewpoints, reviews, letters, and application notes. Please find more information on the manuscript type at JCIM's official site.

We are requesting interested authors to submit their manuscripts by August first, 2024. We look forward to your contributions. Submissions will be peer-reviewed and, if accepted, will be published in a regular issue of the *Journal of Chemical Information and Modeling*. Once the Virtual Special Issue is complete, all articles will be publicized in a virtual collection, providing additional exposure to their work. We look forward to your contribution.

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Notes

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