Opinion

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Building Structures of Viruses and Beyond

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ABSTRACT

Carrying out structural examination of viruses and cells at atomic resolution presents formidable challenges due to the substantial computational resources required to handle intricate complexes comprising millions and billions of atoms. Despite these difficulties, I firmly believe that this endeavor is of paramount importance for elucidating fundamental biological mechanisms at the organismic level. Consequently, the utilization of computers is indispensable to attain this objective, including the construction of structures from individual proteins and the examination of their molecular dynamics, in this case, those of viruses, cell organelles, or cells. To achieve this goal, the development of more powerful computers, including quantum computers, which can exponentially improve the outcome, will be fundamental. Recently, structures of complete viruses have been built, demonstrating the validity of this approach.

Keywords: Structure; Virus; Computational Biology; Chimera; Molecular Dynamics

Abbreviations: VMD: Visual Molecular Dynamics; NAMD: Nanoscale Molecular Dynamics

Main Text

The challenges that were associated with conducting structural analysis of proteins before the year 2000 were considerable, primarily due to the limitations imposed by outdated computing technology. However, the advent of new computer systems and the internet has since facilitated the determination of protein structures at atomic resolution. Furthermore, the development of cutting-edge techniques, such as cryoEM structural determination, has recently achieved resolutions comparable to those obtained through X-ray crystallography, thereby significantly advancing the field of protein structural determination. By the years 2000s, the Protein Data Bank and Electron Microscopy Data Bank have been established, providing the necessary structures and maps to construct larger structures, such as complete viruses. Using low resolution maps, individual proteins can be matched in the right position in the map, making it possible to construct larger structures, such as viral heads with all their components, the tails, and other parts of the virus. The final result is an accurate structure of a complete organism, in this case, a virus such as bacteriophage T4, and other viruses, including bacteriophages, coronaviruses, Nipah viruses, HIV, and so on [1]. The size of viruses is within the limits of current computational powers, although a high-performance computer is necessary. However, for larger structures like cell organelles, bacteria, and finally cells, more computational power is necessary, which is not currently available.

The application of atomic resolution viral structures permits the investigation of protein-protein interactions in both static and dynamic settings, thereby furnishing a wealth of information at the amino acid and atomic levels. This knowledge bolsters human capability to address intricate problems in the medical field and other sectors that profit from molecular insights into proteins, microorganisms, and microscopic cells. In the years to come, a revolution in structural analysis will likely bring about numerous breakthroughs in a wide range of human activities. By leveraging this knowledge, we will be able to develop more effective drugs, design antibodies in silico to combat diseases, engineer viruses to target unwanted bacteria for various purposes such as phage therapy, food preservation, and agricultural applications, among other fields. The primary software applications that I rely upon for conducting structural analyses are UCSF Chimera and VMD/NAMD [2-4]. These tools are currently considered to be the most effective options available, and have consistently proven their value in achieving the desired outcomes of the analyses. As evidenced in Figure 1, this software has enabled the visualization of bacterial infection structures at the atomic level of resolution. Please visit https://www.drvictorpadillasanchez.com/ and https://

studio.youtube.com/channel/UCJjVolkp5os9qtXd3A_-VCw/videos/upload?filter=%5B%5D&sort=%7B%22columnType%22%3A%22date%22%2C%22sortOrder%22%3A%22DESCENDING%22%7D for further information.

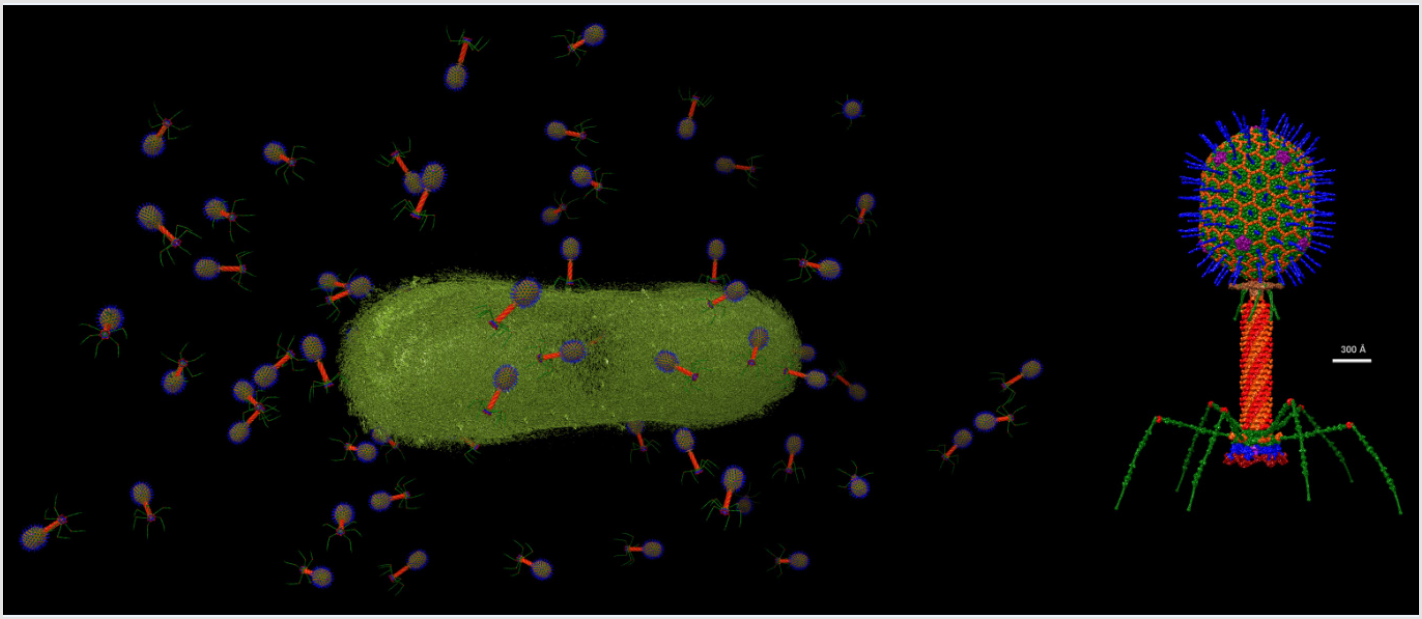

Figure 1: The structure of bacteriophage T4 during its infection of an *Escherichia coli* cell, as well as the structure of T4 at atomic resolution, have been studied and analyzed. The length of the Escherichia coli cell is approximately 2.8 μm, while the bar denotes 300 Angstroms.

Conclusion

Considering the present state of structural determinations, we are poised to take the next step, which involves a significant leap from protein structure determination to constructing structures of microorganisms and even cells at the atomic resolution. These structures will afford unprecedented insights into a wide range of fields of study, thereby facilitating the development of innovative solutions to long-standing biological problems. In light of these developments, it is crucial that extensive research be conducted in this area to enhance our understanding of biology and to identify novel strategies for addressing the complex challenges that lie ahead.

Conflict of Interest

The author declares no conflict of interests.

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