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Bioinformatics and Biomedical Computing

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The rapid advancement of high-throughput sequencing technologies and the explosive growth of biological data have revolutionized the field of bioinformatics and biomedical computing [1-4]. The generation of vast amounts of genomic, transcriptomic, proteomic, and metabolomic data has created unprecedented opportunities for understanding the complexities of biological systems and their implications for human health [5-6]. Moreover, the emergence of spatial omics technologies, such as spatial transcriptomics and spatial proteomics, has added a new dimension to our understanding of the spatial organization and heterogeneity of biological systems. These cutting-edge technologies enable the mapping of molecular information at a high spatial resolution, providing valuable insights into the tissue microenvironment and the interplay between cells in various physiological and pathological conditions [7-10].

Bioinformatics effectively processes various biomedical data, playing a crucial role in addressing the numerous challenges faced by global health, particularly in the prevention, diagnosis, and treatment of diseases. For instance, by integrating multi-omics data and machine learning algorithms, bioinformatics enables the identification of key genes, biomarkers, and risk factors associated with diseases, facilitating early warning and precise stratification of diseases [11-13]. Moreover, employing computational methods to simulate the mechanisms of drugtarget interactions can significantly accelerate the drug discovery process and reduce the cost of drug development [14]. Furthermore, the cross-integration of bioinformatics with cutting-edge technologies such as artificial intelligence and big data analysis is driving the transition of personalized medicine from concept to clinical application. By integrating multi-dimensional data from patients' genomes, physiology, and pathology, and combining advanced computational modelling and analysis tools, bioinformatics is empowering physicians to develop personalized and precise diagnostic and treatment plans, significantly enhancing the effectiveness of disease prevention and treatment [15-17]. Despite the remarkable progress made in bioinformatics and biomedical computing, there remain numerous challenges and opportunities for further advancement. The integration and analysis of multi-omics data, the development of more efficient and accurate computational methods, and the translation of bioinformatics findings into clinical practice are among the key areas of focus. Additionally, the ethical, legal, and social implications of bioinformatics research, particularly in the context of personal genomic data privacy and security, require careful consideration and governance.

This special issue of Fundamental Research focuses on bioinformatics and biomedical computing, presenting a collection of one review article and six original research articles. Wu et al. [18] provide a review of deep learning methods for drug virtual screening and discuss the existing challenges and future directions in this field. Wang et al. [19] develop a user-friendly web pipeline ASTool to detect the associations between individual single nucleotide polymorphisms (SNPs) and phenotypes for exploring the genetic mechanism. Hong et al. [20] present an Increment of Diversity for Trajectory Inference (IDTI) method to infer the cell state trajectory of time-series scRNA-seq data. Yu et al. [21] introduce a comprehensive study of the generation of barcodes and design a tool to select optimal DNA barcode sets and demultiplexing. Wei et al. [22] present a deep association model to analyze the transcriptome and methylation data of childhood asthma. Peng et al. [23] construct a biological knowledge-driven deep learning model to capture and characterize the complex, non-linear associations among SNPs for scoring the risk of common diseases. Liu et al. [24] combine a range of classic machine-learning methods to probe the dynamical $\alpha - \beta$ transition process induced by ILs of 1-alkyl-3-methylimidazolium chloride and its molecular mechanism in neurodegenerative diseases. These articles provide valuable insights into the field of bioinformatics and biomedical computing, driving progress in this field and pointing out future research directions. Finally, we sincerely express our heartfelt gratitude to all the authors who made remarkable contributions to this special issue. Additionally, we extend our appreciation to the esteemed members of the editorial board and the editorial office for their invaluable support and assistance.

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