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Special Issue Reprint

Computational Approaches in Discovery & Design of Antimicrobial Peptides

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Antimicrobial resistance remains a major concern in medicine, especially during the COVID-19 pandemic, where microbial infections were frequent complications. To combat drug-resistant pathogens, there has been a renewed interest in the use of antimicrobial peptides (AMPs). This reprint focuses on the in-silico approaches used for the rational discovery and design of AMPs. Such computational methodologies range from classical homology-based and machine-learning prediction algorithms to complex similarity networks and evolutionary algorithms that use models of sequence evolution. Furthermore, the reprint explores the improvement of high-throughput screening techniques in the discovery of AMPs from biological samples, which has also led to the evolution of computational approaches that aid in this biodiscovery process. The reprint contains original research and review papers, which serve as valuable references for researchers dedicated to peptide drug development.

