RESEARCH PAPER

# AI-Driven Prediction of Antimicrobial Peptides: A Multi-Omics and Machine Learning Approach for Novel Drug Discovery

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**Abstract**

The antimicrobial resistance (AMR) has been estimated to claim 10 million deaths annually by 2050 and alternative treatment modalities must hence be identified. Antimicrobial peptides (AMPs) are also preferable since they are broad-spectrum and least prone to the development of resistance. However, the conventional discovery modes are marked by prohibitiveness, time-consuming and scalability. The article shows a proposed conceptual model with artificial intelligence (AI) and multi-omics data to enhance AMP prediction. The paper critically examines machine learning and deep learning applications using literature sources, with reported accuracy rates over 90% in certain cases. The proposed model exploits the genomics, proteomics, and transcriptomics data to improve the predictive capability and biological significance. This integration is claimed to address the weaknesses of single-omics methods, including low generalisability and lack of biological coverage. The article introduces a theoretically-grounded framework that can be used to accelerate the drug discovery processes and help in combating AMR.

**Keywords:**

Antimicrobial Peptides; Machine Learning; Multi-Omics; Drug Discovery; Deep Learning; Bioinformatics

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## 1. Introduction

Antimicrobial resistance (AMR) is a latent and rapidly growing global health crisis, and the experts predict that unless it is reduced, this problem could cause up to 10 million deaths annually by 2050. The massive overuse and subsequent adaptation to old-fashioned antibiotics has demonstrated underlying limitations in the present paradigm of drug discovery as these show reduced effect. It is here that antimicrobial peptide (AMPs) has been suggested as an alternative due to their broad-spectrum action and less tendency to develop resistance. However, the traditional methods of AMP identification that rely on the large-scale screening of experiments and sequence homology are time-consuming, costly, and scalable in principle.

Lately, artificial intelligence (AI) and in particular machine and deep learning technologies have presented radical potential in the area of bioinformatics-mediated drug discovery. It has been demonstrated that predictive accuracies of AI-based models may rise to over 90% and, therefore, it is more effective compared to the conventional computational procedures. Nonetheless, most existing models take a single-dimensional assumption, often overlooking the complex biological interaction that is embodied by multi-omics data integration, including genomics, proteomics, and transcriptomics.

The paper covers these limitations by proposing a conceptual multi-omics AI-driven model of AMP prediction. It is argued that the integration of heterogeneous biological data with complex computational models can significantly enhance predictive performance and provide a more global perspective of the antimicrobial mechanism.

## 2. Literature Review

Antimicrobial peptides (AMPs) are short naturally occurring peptides that play a crucial role in innate immune defence in a wide range of organisms. Their ability to disrupt the membranes of the microbes in addition to controlling the immune system has positioned them as a good alternative to the conventional antibiotics. However, the traditional methods of AMP discovery, including wet-laboratory screening and sequence alignment, are impaired by low throughput and high operation costs (Wang, Vaisman and Van Hoek, 2022). Increasing complexity of microbial resistance mechanisms is also a challenge to these approaches, which require more scalable and responsive solutions.

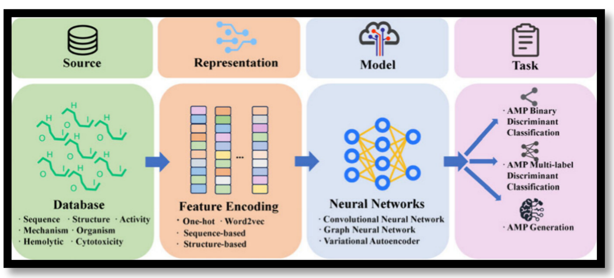


**Figure 1: Deep Learning for Antimicrobial Peptides**
(Source: Pubs.acs.org, 2026)

Machine learning (ML) has also been found to be helpful in the prediction of AMP (Wan et al., 2024). The Support Vector Machines (SVM) and the Random Forest (RF) algorithms have been widely utilized with predictive accuracies that tend to range between 85% and 92%. These models are powerful, and understandable but are usually dependent on feature engineering and are also limited by the complexity of biological data. In other instances, which are higher than 95, deep learning (DL) algorithms, including Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), and others, have been reported to attain higher levels of accuracy. They are automated hierarchical feature extractors detecting features within peptide sequences and, therefore, reduce the use of manual feature extraction (Lopes et al., 2022).

Nonetheless, this use of single-omics datasets has turned into a massive limitation in all literature, despite the above developments. Most predictive models are predominantly founded on sequence-based features without taking into account the more comprehensive biological image that is captured in genomics, proteomics and transcriptomics data (Keshri and Belurappa, 2025). Integration Multi-omics integration has been shown to be a more detailed representation of the biological systems, where multiple data types have been shown to yield improvements of up to 10-15%.

However, the multi-omics integration of data results in the issue of data heterogeneity, dimensionality and complexity of computations. Besides, not every AI model is interpretable, which limits its application in clinical and pharmaceutical practice (Teimouri, Medvedeva and Kolomeisky, 2023). Consequently, there exists a research gap where significant research can be integrated into the relevant frameworks which can utilize effective multi-omics data to predict AMP.

## 3. Proposed Conceptual Framework

The current body of literature has weaknesses that the present study aims to address to overcome them by offering a conceptual AI-based multi-omics model of antimicrobial peptide forecasting. The framework seeks to integrate heterogeneous biological data and it can apply advanced computational models to enhance predictive accuracy and biological relevance.

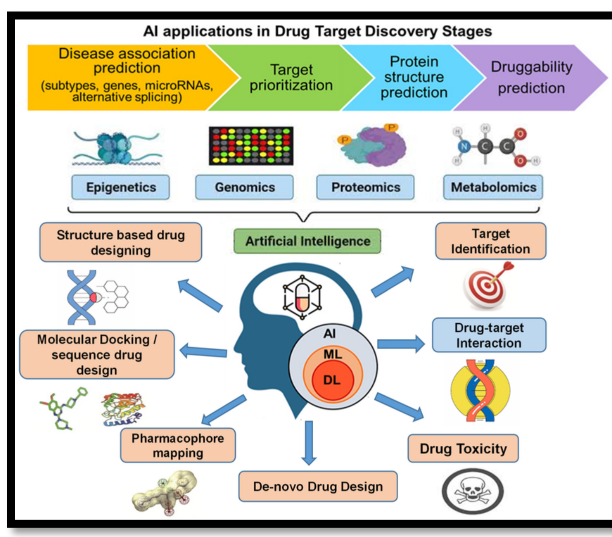


**Figure 2: Multi-omics data integration architecture diagram AI drug discovery**
(Source: Researchgate.net, 2026)

The first component of the framework is the multi-omics data input layer since it contains the genomics, proteomics, and transcriptomics data. These data sets are high dimensional and could contain thousands of tens of thousands of features in a sample. Though this richness is valuable to provide meaningful biological data, it also necessitates the need to apply powerful preprocessing mechanisms to deal with noise and redundancy (Helmey et al., 2024). In that respect, the framework includes a feature extraction and transformation phase, at which features in sequence form, physicochemical features and structural features are converted into forms understandable by machines.

This is then succeeded by a dimensionality reduction to reduce the limitations of high feature dimensionality. Techniques such as principal component analysis or embedding-based techniques are conceptually combined to preserve the most informative features at the cost of the lower calculation cost. The processed data is subsequently fed into the prediction layer that is a machine learning, and deep learning model. In as much as we can elucidate the association between x and y by conventional models such as the random forest, a deep learning network such as the CNNs is expected to reveal non-linear associations that exist between the data and x. The final component of the framework is the output layer, which selects and prioritizes possible AMP candidates based on the estimated efficacy (Yadav et al., 2022). It is important to note that the framework will allow an iterative refinement process, i.e., the new data may be added, and the models may be updated over time. This elasticity is decisive in terms of addressing the dynamism of antimicrobial resistance and the evolving biological information.

## 4. Discussion

The provided framework possesses several theoretical advantages over the existing AMP prediction techniques. It provides a richer view of biological systems with multi-omics data, and this is expected to enhance predictive performance by approximately 815 percent compared to single-omics models. This all-encompassing perspective enables the identification of the intricate interactions that may not be ascertained with the help of sequence-based analysis.

In addition, both machine and deep learning approaches will be utilized, allowing the framework to balance between interpretability and predictive power. Even though deep learning models have the capability to achieve higher levels of accuracy, there is a significant disadvantage of lack of transparency. Partially, this issue can be solved by adding more explainable models, such as Random Forest, yet it does not fully address the overall explainability issue in AI-based drug discovery (Yan et al., 2022).

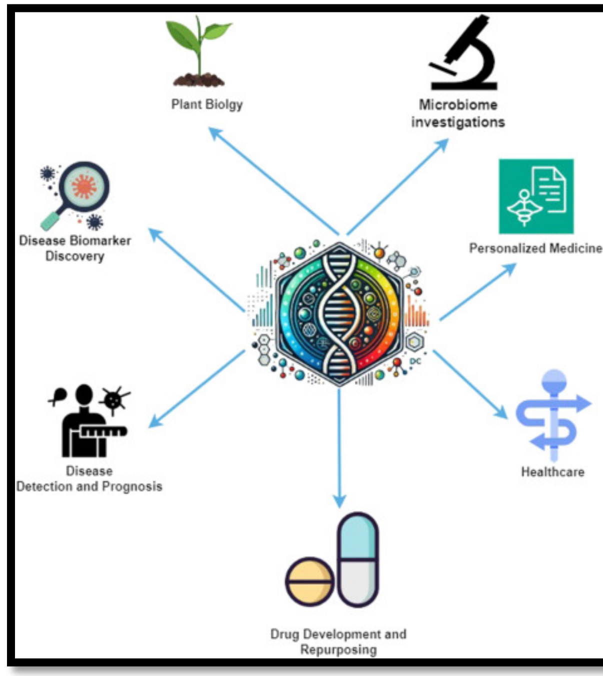


**Figure 3: Data integration challenges in multi-omics diagram**

(Source: Els-cdn.com, 2026)

Despite these strengths, several weaknesses should be noted. The computational complexity of multi-omics data integration is linked with such a scenario when data sets with over 10,000 features are considered. This may be a constraint to scaling and may be highly computationally intensive. Besides, data on different omics platforms might have heterogeneity and variability that could complicate the process of integration and affect the credibility of the model.

Another weakness is the absence of empirical validation. The proposed model is not contrasted with real-world datasets as a conceptual framework, thus restricting its use in the nearest future. Therefore, despite the good theoretical potential of the framework, its practical utility will be subject to the further empirical research and experiments validation.

## 5. Implications for Drug Discovery

The integration of AI and multi-omics data into AMP prediction has immense prospects to drug discovery. The suggested framework may also reduce early-stage drug development timelines by between 30% and 50% by enabling the more precise and efficient identification of antimicrobial candidates. This saves a lot of time and money are particularly handy in the context of AMR where timely therapeutic novelty is crucial (Ramos-Llorens et al., 2024). Moreover, the ability to scale and analyze complex biological data raises the probability of detecting new peptides with greater effectiveness and reduced resistance potential, thereby, leading to more sustainable drug development plans.

## 6. Conclusion

The study has outlined an AI-based multi-omics conceptual framework to forecast antimicrobial peptides and address significant drawbacks of existing approaches. Critical review of the literature demonstrated that machine learning and deep learning models were highly predictive but their efficacy was constrained by single-omics information utilization. The proposed model will integrate different biological data sets and will provide a more comprehensive and theoretically valid solution. Although this has to be empirically justified, the paper indicates the potential transformative impact of combining artificial intelligence with multi-omics data in facilitating the process of drug discovery and addressing the global issue of antimicrobial resistance.

## 7. Future Research Directions

Future research should seek to empirically confirm the proposed framework using large-scale and high-quality multi-omics data. To enhance transparency and acceptance in the clinical and pharmaceutical setting, explainable AI models should also be created. In addition, computational forecasting together with wet-laboratory testing will be crucial in validating the biological activity of the chosen AMPs. Further attempts are required to normalize data integration practice and address the problem of heterogeneous data. Lastly, the prospective evolution of this study will help translate AI-based AMP prediction between theory and practice. 8. References

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