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Review

THE USE OF AI IN FINDING NEW ANTIMICROBIALS

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Abstract: *The pressing need for new antimicrobial drugs has been highlighted by the growing problem of antimicrobial resistance (AMR). The quick creation of efficient medicines is hampered by the time-consuming and expensive nature of traditional drug discovery techniques. Artificial intelligence (AI) has recently surfaced as a potentially useful technology to speed up the discovery of novel antimicrobials. From anticipating chemical interactions to improving drug candidates, artificial intelligence (AI) technologies including machine learning, deep learning, and natural language processing have been used at different phases of antimicrobial development. AI can find previously undiscovered chemicals and forecast their effectiveness against resistant infections by examining enormous datasets of chemical structures, biological activity, and genomic data. This study examines the use of AI in antimicrobial drug discovery, emphasizing how it can expedite the drug development process, increase target identification precision, and encourage the creation of new compounds with improved potency and selectivity. We also go over the drawbacks and difficulties of incorporating AI into antimicrobial research, such as the requirement for interdisciplinary cooperation, data quality, and model interpretability. Finally, AI-driven strategies present a promising opportunity to tackle the worldwide AMR epidemic and quicken the creation of critically required antibiotic treatments. As an alternative to traditional antibiotics, antimicrobial peptides (AMPs) show promise as agents against antimicrobial resistance. AMP discovery was transformed by artificial intelligence (AI) using both generation and discrimination techniques. The vast field of drug discovery is always looking for new and creative ways to find and create peptide-based medicines. The development of novel peptide medications has undergone a radical change since the introduction of artificial intelligence (AI). A variety of computer tools and algorithms provided by AI allow researchers to expedite the development of therapeutic peptides.*

Keywords: artificial intelligence, antimicrobial peptides, antibiotics, machine learning

INTRODUCTION

In recent years, the rise of antimicrobial resistance (AMR) has emerged as a global health crisis, threatening our ability to treat infections effectively. As traditional antimicrobial discovery faces increasing challenges, artificial intelligence (AI) is stepping in as a transformative tool in the search for new antimicrobial agents. Since its recent technological advancement, AI has been quickly used into medication research, significantly increasing the effectiveness of finding new antibiotics (Liu et al., 2024b).

This narrative review explores how AI is being utilized in the discovery of new antimicrobials, the possible benefits it offers, as well as future prospects, with particular attention to antimicrobial peptides.

Antibiotics have emerged as the mainstay of contemporary medicine since the discovery of penicillin. However, because antibiotic-resistance determinants are spreading throughout the world, it is unknown if these

necessary medications will remain effective (Stokes et al., 2020).

Antibacterial peptides (ABPs) are a family of peptides found in nature that play a crucial role in the innate immune systems of organisms. These ABPs offer several advantages over widely used antibiotics. As a result, they have recently received a lot of attention as potential replacements for currently available antibiotics. But it is expensive and time-consuming to identify ABPs from natural sources, AI-based approaches could facilitate screening and optimization of AMP candidates (Sharma et al., 2024).

In reaction to environmental challenges, pathogens undergo various changes in their genomes, resulting in AMR. As a consequence of AMR, these pathogens become unresponsive to antibiotics (Sharma et al., 2024).

AI has significantly sped the development of novel antibiotics in recent years (Cesaro et al., 2023; Stokes et al., 2020; Wong et al., 2023). New AI-based antibiotic candidates can now be discovered in hours due to computational screening, compared to conventional discovery workflows that take years. Millions of individuals still pass away from infections every year despite these scientific and technological advancements (Murray et al., 2022; Naghavi et al., 2024). More than 4 million people died in 2019 alone as a result of pan-drug-resistant bacteria that have emerged because of the overuse and abuse of antibiotics. However, antibiotic-resistant genes are not the only reason why antimicrobial treatments fail to successfully cure people and eradicate infections. Antibiotic failure is caused by a variety of circumstances, including intricate systems underpinning serious clinical situations like sepsis (Cesaro et al., 2023). This complex problem is becoming a major worldwide concern.

Since its recent technological advancement, AI has been quickly used into medication research, significantly increasing the effectiveness of finding new antibiotics (Liu et al., 2024b).

1.Artificial Intelligence in Drug Development

AI is anticipated to streamline and expedite pharmaceutical development in the future. By using robotics and models of genetic targets, medications, organs, diseases and their course, pharmacokinetics, safety, and efficacy, AI can transform the labour-intensive process of drug development into one that requires capital and data (Naik et al., 2022). The drug discovery and development process can be accelerated and made more economical and efficient with the application of AI. AI was previously used to find possible Ebola virus medications, but like with any pharmacological study, finding a lead compound does not ensure the creation of a safe and effective treatment (Stephenson, 2021).

AI has the ability to close gaps in rural communities and resource-poor nations, increasing access to healthcare services. AI could be used to conduct screening and evaluation in settings with limited resources if insufficient medical expertise is available, a common challenge in many resource-poor settings (Stephenson, 2021).

Using algorithms that can produce and assess a huge number of peptide sequences according to desired characteristics, like target affinity, selectivity, and bioavailability, is known as AI-driven peptide design. Compared to conventional techniques, these algorithms are more thorough and effective at exploring vast chemical regions (Nissan et al., 2024).

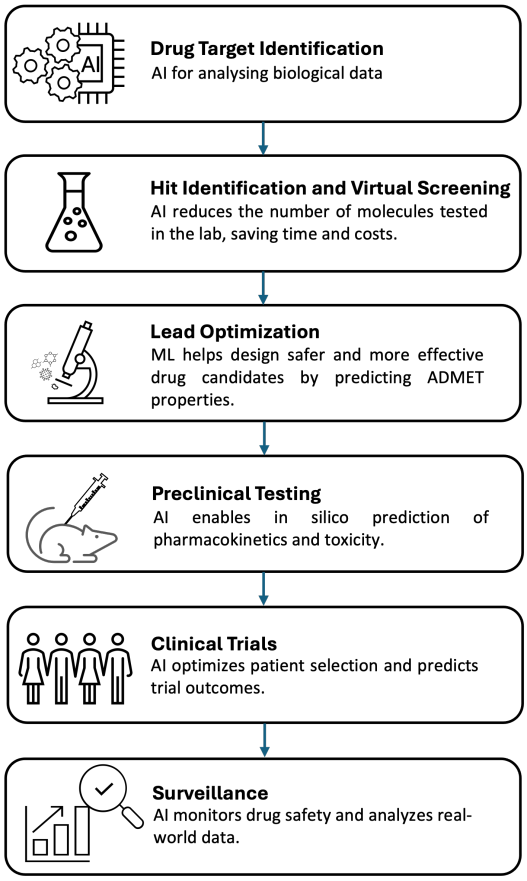

Figure 1. Schematic representation of AI in drug development.

2. Machine learning (ML)

With its many uses in computer vision, language processing, gaming, and computational biology, machine learning (ML), a subfield of artificial intelligence, has advanced significantly. Some machine learning models make use of deep learning (DL), a technique that uses deep networks (DNNs) to predict outcomes and extract hidden features from complicated datasets, such as biomolecular structures and photographs (Liu et al., 2024b; Stokes et al., 2020; Wan et al., 2024a).

In addition to producing medicines, machine-learning (ML) models have been used to forecast antimicrobial resistance, haemolysis, and antimicrobial activity (Wan et al., 2022).

ML can be used to predict macromolecular structures and therapeutic features, including antibiotic activity and absorption, distribution, metabolism, excretion, and toxicity (ADMET) (Wan et al., 2024b).

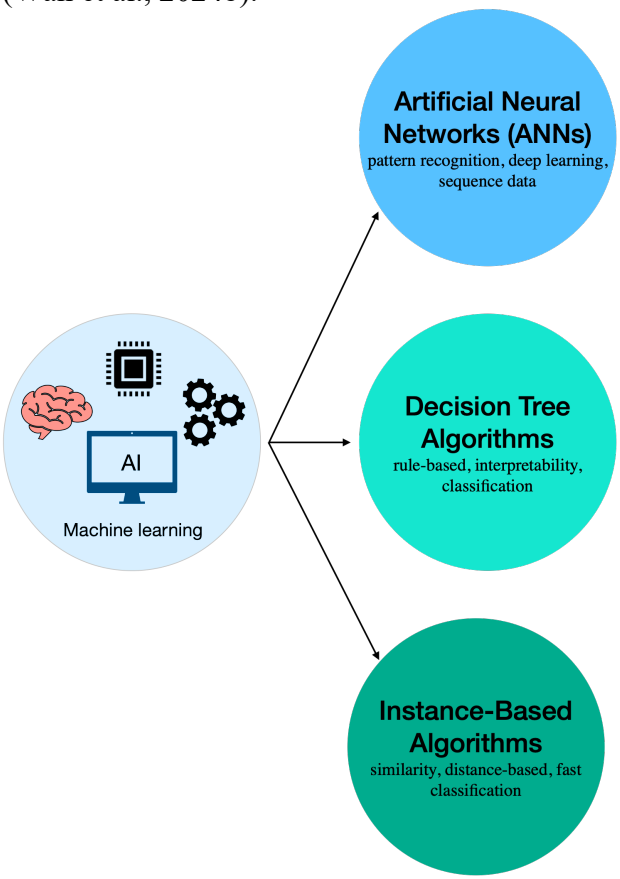

Figure 2. Schematic representation of ML.

The use of AI in the development of novel peptide drugs has bright future prospects and has the potential to completely transform the peptide drug discovery process. To fully realize the potential of AI-driven techniques and guarantee their successful incorporation into the drug development pipeline, a number of obstacles must be overcome. Expanding and improving AI models through the use of more extensive and varied datasets is one of the fundamental prerequisites (Bilal et al., 2025).

For example, machine learning has identified genetic traits associated with antibiotic sensitivity in *Escherichia coli* across various sequence types (STs) (Bilal et al., 2025). These genetic markers help elucidate how STs evolve and spread within populations that are likely to facilitate dissemination (Shaik et al., 2022). Similarly, it was used to predict *Streptococcus pneumoniae* susceptibility to β-lactam antibiotics by correlating penicillin-binding protein (PBP) sequences with minimum inhibitory concentrations (MIC) values (Zhang et al., 2019).

Intricate patterns in a variety of data can be found using AI/ML methods, which can shed light on the processes behind the emergence of drug resistance (Liu et al., 2024a). An AI-based tool called PathogenWatch makes it possible to analyze and visualize microbial genome sequences in real-time in both geographical and phylogenetic settings, which enhances the tracking and monitoring of pathogen outbreaks (Vashisht et al., 2023). Real-time monitoring enabled by AI/ML helps to promptly modify containment and treatment plans (Vashisht et al., 2023).

Using a dataset of 312 antibiotics and 936 non-antibiotic medications, researchers trained eight distinct algorithms—including extreme gradient boosting, random forest, deeper neural networks, and gradient boosting classifier—to predict novel antimicrobial compounds. With five-fold cross-validation, the top four classifiers obtained over 80% accuracy in both test and blind data (Jana et al., 2024).

Table 1. A list of antimicrobial agents and peptides discovered or designed using artificial intelligence (AI) and machine learning (ML)

Antimicrobial Agent	Methods Used	Properties	References
SPR206	Structure-activity relationship (SAR) models	Reduced nephrotoxicity, high efficacy	(Hazrat et al., 2025; Zhang et al., 2020)
QPX9003	AI-guided structure optimization	Improved safety profile, effective at lower doses	(Castanheira et al., 2019)
MRX−8	Predictive modeling	Lower toxicity, enhanced pharmacokinetics	(Duncan et al., 2022)
Murepavadin	Iterative peptidomimetic design	High specificity, effective in biofilms	(Sader et al., 2018)
IB−367	AI peptide design	Safe but limited efficacy in clinical settings	(Mosca et al., 2000)
SCH−79797	ML based dual mechanism profiling	Broad-spectrum efficacy	(Martin et al., 2020; Mosca et al., 2000)
Bactenecin	Machine-learning classifer	Broad-spectrum efficacy	(Wu et al., 1999)
DP7	AI-driven sequence optimization	Low cytotoxicity, strong biofilm activity	(Wu et al., 2014)
Lead AMPs	PanCleave random forest modeling	Low toxicity, high specificity	(Maasch et al., 2023)

3. Deep Learning

Deep learning models have shown promise in predicting molecular properties and biological activities of compounds. Deep-learning approaches applied to antibiotic discovery include graph neural networks (GNN) and message-passing neural networks (MPNN) for molecular activity prediction, convolutional neural networks (CNNs) and transformers for compound or antimicrobial peptide classification, and generative architectures such as autoencoders and variational autoencoders (VAEs), generative adversarial networks (GANs), diffusion models, and reinforcement-learning frameworks for the de novo design and optimization of antibacterial molecules. By training on datasets that include chemical structures and their associated biological responses, these models can suggest novel compounds that may not have been previously considered. HydrAMP is a deep-learning model that learns the main structural features of peptides together with their antimicrobial properties, allowing it to generate new peptide sequences or improved analogues of known peptides. By combining this design process with computational screening and molecular dynamics simulations, HydrAMP can prioritize promising candidates for experimental testing and improve the chances of identifying active antimicrobial peptides. This approach was used to obtain Hydraganan-1, an analogue of pexiganan and showed strong activity against *E. coli* (Szymczak et al., 2023). DeepAMP is a peptide language-based deep generative framework designed to discover potent, broad-spectrum antimicrobial peptides. It was successfully used to generate 18 candidates with strong activity against both Gram-positive and Gram-negative bacteria, reduced potential for resistance development, and three of them demonstrated efficacy in an in vivo wound infection model (Li et al., 2024). AMP-Diffusion is a generative AI platform that combines latent diffusion modeling with protein language embeddings to design novel antimicrobial peptides. By using this model the authors obtained a high experimental success rate of the AMPS tested against both susceptible and multidrug-resistant bacteria, with low toxicity and promising in vivo efficacy for two peptides, comparable to clinically used antibiotics (Torres et al., 2025).

4. Challenges and Future Directions

While the use of AI in antimicrobial discovery is promising, several challenges remain. Data quality, accessibility, and the need for interdisciplinary collaboration are all crucial for advancing this field. Additionally, regulatory and ethical considerations must be addressed as AI-driven solutions become more prevalent in drug development. The use of AI in the development of novel peptide drugs has bright future prospects and has the potential to completely transform the peptide drug discovery process. To fully realize the potential of AI-driven techniques and guarantee their successful incorporation into the drug development pipeline, a number of obstacles must be overcome. Expanding and improving AI models through the use of more extensive and varied datasets is one of the fundamental prerequisites (Nissan et al., 2024).

CONCLUSIONS

AI is revolutionizing and overall, increasingly contributing to the discovery of new antimicrobials, offering efficient, accurate, and innovative approaches to combat antimicrobial resistance. As researchers continue to leverage AI technologies, the hope for effective solutions to tackle resistant infections becomes increasingly attainable. Embracing this interdisciplinary approach may hold the key to safeguarding public health against the ever-evolving threat of resistant pathogens. However, all AI-generated predictions still require an experimental validation process.

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DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES

During the preparation of this work, the authors used ChatGPT-4 to assist with grammar checking. After utilizing this tool, the authors reviewed and edited the content as necessary and take full responsibility for the final content of the publication.

REFERENCES

Bilal, H., Khan, M.N., Khan, S., Shafiq, M., Fang, W., Khan, R.U., Rahman, M.U., Li, X., Lv, Q.-L., Xu, B., 2025. The role of artificial intelligence and machine learning in predicting and combating antimicrobial resistance. Computational and Structural Biotechnology Journal 27, 423-439.

Castanheira, M., Lindley, J., Huynh, H., Mendes, R.E., Lomovskaya, O., 2019. 690. Activity of a novel polymyxin analog, QPX9003, tested against resistant Gram-negative pathogens, including carbapenem-resistant Acinetobacter, Enterobacterales, and Pseudomonas, Open Forum Infectious Diseases, p. S313.

Cesaro, A., Bagheri, M., Torres, M., Wan, F., de la Fuente-Nunez, C., 2023. Deep learning tools to accelerate antibiotic discovery. Expert Opinion on Drug Discovery 18, 1245-1257.

Duncan, L.R., Wang, W., Sader, H.S.J.A.A., Chemotherapy, 2022. In vitro potency and spectrum of the novel polymyxin MRX-8 tested against clinical isolates of gram-negative bacteria. 66, e00139-00122.

Hazrat, B., Muhammad Nadeem, K., Sabir, K., Muhammad, S., Wenjie, F., Rahat Ullah, K., Mujeeb Ur, R., Xiaohui, L., Qiao-Li, L., Bin, X., 2025. The role of artificial intelligence and machine learning in predicting and combating antimicrobial resistance. Computational and Structural Biotechnology Journal 27, 423-439.

Jana, T., Sarkar, D., Ganguli, D., Mukherjee, S.K., Mandal, R.S., Das, S.J.I.J.o.M.R., 2024. ABDpred: Prediction of active antimicrobial compounds using supervised machine learning techniques. 159, 78-90.

Li, T., Ren, X., Luo, X., Wang, Z., Li, Z., Luo, X., Shen, J., Li, Y., Yuan, D., Nussinov, R., Zeng, X., Shi, J., Cheng, F., 2024. A Foundation Model Identifies Broad-Spectrum Antimicrobial Peptides against Drug-Resistant Bacterial Infection. Nature Communications 15, 7538.

Liu, G.Y., Yu, D., Fan, M.M., Zhang, X., Jin, Z.Y., Tang, C., Liu, X.F., 2024a. Antimicrobial resistance crisis: could artificial intelligence be the solution? Military Medical Research 11.

Liu, G.Y., Yu, D., Fan, M.M., Zhang, X., Jin, Z.Y., Tang, C., Liu, X.F., 2024b. Antimicrobial resistance crisis: could artificial intelligence be the solution? Military Medical Research 11, 7.

Maasch, J.R., Torres, M.D., Melo, M.C., de la Fuente-Nunez, C.J.C.H., Microbe, 2023. Molecular de-extinction of ancient antimicrobial peptides enabled by machine learning. 31, 1260-1274. e1266.

Martin, J.K., Sheehan, J.P., Bratton, B.P., Moore, G.M., Mateus, A., Li, S.H.-J., Kim, H., Rabinowitz, J.D., Typas, A., Savitski, M.M.J.C., 2020. A dual-mechanism antibiotic kills gram-negative bacteria and avoids drug resistance. 181, 1518-1532. e1514.

Mosca, D.A., Hurst, M.A., So, W., Viajar, B.S., Fujii, C.A., Falla, T.J.J.A.a., chemotherapy, 2000. IB-367, a protegrin peptide with in vitro and in vivo activities against the microflora associated with oral mucositis. 44, 1803-1808.

Murray, C.J.L., Ikuta, K.S., Sharara, F., Swetschinski, L., Robles Aguilar, G., Gray, A., Han, C., Bisignano, C., Rao, P., Wool, E., Johnson, S.C., Browne, A.J., Chipeta, M.G., Fell, F., Hackett, S., Haines-Woodhouse, G., Kashef Hamadani, B.H., Kumaran, E.A.P., McManigal, B., Achalapong, S., Agarwal, R., Akech, S., Albertson, S., Amuasi, J., Andrews, J., Aravkin, A., Ashley, E., Babin, F.-X., Bailey, F., Baker, S., Basnyat, B., Bekker, A., Bender, R., Berkley, J.A., Bethou, A., Bielicki, J., Boonkasidecha, S., Bukosia, J., Carvalheiro, C., Castañeda-Orjuela, C., Chansamouth, V., Chaurasia, S., Chiurchiù, S., Chowdhury, F., Clotaire Donatien, R., Cook, A.J., Cooper, B., Cressey, T.R., Criollo-Mora, E., Cunningham, M., Darboe, S., Day, N.P.J., De Luca, M., Dokova, K., Dramowski, A., Dunachie, S.J., Duong Bich, T., Eckmanns, T., Eibach, D., Emami, A., Feasey, N., Fisher-Pearson, N., Forrest, K., Garcia, C., Garrett, D., Gastmeier, P., Giref, A.Z., Greer, R.C., Gupta, V., Haller, S., Haselbeck, A., Hay, S.I., Holm, M., Hopkins, S., Hsia, Y., Iregbu, K.C., Jacobs, J., Jarovsky, D., Javanmardi, F., Jenney, A.W.J., Khorana, M., Khusuwan, S., Kissoon, N., Kobeissi, E., Kostyanev, T., Krapp, F., Krumkamp, R., Kumar, A., Kyu, H.H., Lim, C., Lim, K., Limmathurotsakul, D., Loftus, M.J., Lunn, M., Ma, J., Manoharan, A., Marks, F., May, J., Mayxay, M., Mturi, N., Munera-Huertas, T., Musicha, P., Musila, L.A., Mussi-Pinhata, M.M., Naidu, R.N., Nakamura, T., Nanavati, R., Nangia, S., Newton, P., Ngoun, C., Novotney, A., Nwakanma, D., Obiero, C.W., Ochoa, T.J., Olivas-Martinez, A., Olliaro, P., Ooko, E., Ortiz-Brizuela, E., Ounchanum, P., Pak, G.D., Paredes, J.L., Peleg, A.Y., Perrone, C., Phe, T., Phommasone, K., Plakkal, N., Ponce-de-Leon, A., Raad, M., Ramdin, T., Rattanavong, S., Riddell, A., Roberts, T., Robotham, J.V., Roca, A., Rosenthal, V.D., Rudd, K.E., Russell, N., Sader, H.S., Saengchan, W., Schnall, J., Scott, J.A.G., Seekaew, S., Sharland, M., Shivamallappa, M., Sifuentes-Osornio, J., Simpson, A.J., Steenkeste, N., Stewardson, A.J., Stoeva, T., Tasak, N., Thaiprakong, A., Thwaites, G., Tigoi, C., Turner, C., Turner, P., van Doorn, H.R., Velaphi, S., Vongpradith, A., Vongsouvath, M., Vu, H., Walsh, T., Walson, J.L., Waner, S., Wangrangsimakul, T., Wannapinij, P., Wozniak, T., Young Sharma, T.E.M.W., Yu, K.C., Zheng, P., Sartorius, B., Lopez, A.D., Stergachis, A., Moore, C., Dolecek, C., Naghavi, M., 2022. Global burden of bacterial antimicrobial resistance in 2019: a systematic analysis. The Lancet 399, 629-655.

Naghavi, M., Vollset, S.E., Ikuta, K.S., Swetschinski, L.R., Gray, A.P., Wool, E.E., Robles Aguilar, G., Mestrovic, T., Smith, G., Han, C., Hsu, R.L., Chalek, J., Araki, D.T., Chung, E., Raggi, C., Gershberg Hayoon, A., Davis Weaver, N., Lindstedt, P.A., Smith, A.E., Altay, U., Bhattacharjee, N.V., Giannakis, K., Fell, F., McManigal, B., Ekapirat, N., Mendes, J.A., Runghien, T., Srimokla, O., Abdelkader, A., Abd-Elsalam, S., Aboagye, R.G., Abolhassani, H., Abualruz, H., Abubakar, U., Abukhadijah, H.J., Aburuz, S., Abu-Zaid, A., Achalapong, S., Addo, I.Y., Adekanmbi, V., Adeyeoluwa, T.E., Adnani, Q.E.S., Adzigbli, L.A., Afzal, M.S., Afzal, S., Agodi, A., Ahlstrom, A.J., Ahmad, A., Ahmad, S., Ahmad, T., Ahmadi, A., Ahmed, A., Ahmed, H., Ahmed, I., Ahmed, M., Ahmed, S., Ahmed, S.A., Akkaif, M.A., Al Awaidy, S., Al Thaher, Y., Alalalmeh, S.O., AlBataineh, M.T., Aldhaleei, W.A., Al-Gheethi, A.A.S., Alhaji, N.B., Ali, A., Ali, L., Ali, S.S., Ali, W., Allel, K., Al-Marwani, S., Alrawashdeh, A., Altaf, A., Al-Tammemi, A.B., Al-Tawfiq, J.A., Alzoubi, K.H., Al-Zyoud, W.A., Amos, B., Amuasi, J.H., Ancuceanu, R., Andrews, J.R., Anil, A., Anuoluwa, I.A., Anvari, S., Anyasodor, A.E., Apostol, G.L.C., Arabloo, J., Arafat, M., Aravkin, A.Y., Areda, D., Aremu, A., Artamonov, A.A., Ashley, E.A., Asika, M.O., Athari, S.S., Atout, M.M.d.W., Awoke, T., Azadnajafabad, S., Azam, J.M., Aziz, S., Azzam, A.Y., Babaei, M., Babin, F.-X., Badar, M., Baig, A.A., Bajcetic, M., Baker, S., Bardhan, M., Barqawi, H.J., Basharat, Z., Basiru, A., Bastard, M., Basu, S., Bayleyegn, N.S., Belete, M.A., Bello, O.O., Beloukas, A., Berkley, J.A., Bhagavathula, A.S., Bhaskar, S., Bhuyan, S.S., Bielicki, J.A., Briko, N.I., Brown, C.S., Browne, A.J., Buonsenso, D., Bustanji, Y., Carvalheiro, C.G., Castañeda-Orjuela, C.A., Cenderadewi, M., Chadwick, J., Chakraborty, S., Chandika, R.M., Chandy, S., Chansamouth, V., Chattu, V.K., Chaudhary, A.A., Ching, P.R., Chopra, H., Chowdhury, F.R., Chu, D.-T., Chutiyami, M., Cruz-Martins, N., da Silva, A.G., Dadras, O., Dai, X., Darcho, S.D., Das, S., De la Hoz, F.P., Dekker, D.M., Dhama, K., Diaz, D., Dickson, B.F.R., Djorie, S.G., Dodangeh, M., Dohare, S., Dokova, K.G., Doshi, O.P., Dowou, R.K., Dsouza, H.L., Dunachie, S.J., Dziedzic, A.M., Eckmanns, T., Ed-Dra, A., Eftekharimehrabad, A., Ekundayo, T.C., El Sayed, I., Elhadi, M., El-Huneidi, W., Elias, C., Ellis, S.J., Elsheikh, R., Elsohaby, I., Eltaha, C., Eshrati, B., Eslami, M., Eyre, D.W., Fadaka, A.O., Fagbamigbe, A.F., Fahim, A., Fakhri-Demeshghieh, A., Fasina, F.O., Fasina, M.M.,

Fatehizadeh, A., Feasey, N.A., Feizkhah, A., Fekadu, G., Fischer, F., Fitriana, I., Forrest, K.M., Fortuna Rodrigues, C., Fuller, J.E., Gadanya, M.A., Gajdács, M., Gandhi, A.P., Garcia-Gallo, E.E., Garrett, D.O., Gautam, R.K., Gebregergis, M.W., Gebrehiwot, M., Gebremeskel, T.G., Geffers, C., Georgalis, L., Ghazy, R.M., Golechha, M., Golinelli, D., Gordon, M., Gulati, S., Gupta, R.D., Gupta, S., Gupta, V.K., Habteyohannes, A.D., Haller, S., Harapan, H., Harrison, M.L., Hasaballah, A.I., Hasan, I., Hasan, R.S., Hasani, H., Haselbeck, A.H., Hasnain, M.S., Hassan, I.I., Hassan, S., Hassan Zadeh Tabatabaei, M.S., Hayat, K., He, J., Hegazi, O.E., Heidari, M., Hezam, K., Holla, R., Holm, M., Hopkins, H., Hossain, M.M., Hosseinzadeh, M., Hostiuc, S., Hussein, N.R., Huy, L.D., Ibáñez-Prada, E.D., Ikiroma, A., Ilic, I.M., Islam, S.M.S., Ismail, F., Ismail, N.E., Iwu, C.D., Iwu-Jaja, C.J., Jafarzadeh, A., Jaiteh, F., Jalilzadeh Yengejeh, R., Jamora, R.D.G., Javidnia, J., Jawaid, T., Jenney, A.W.J., Jeon, H.J., Jokar, M., Jomehzadeh, N., Joo, T., Joseph, N., Kamal, Z., Kanmodi, K.K., Kantar, R.S., Kapisi, J.A., Karaye, I.M., Khader, Y.S., Khajuria, H., Khalid, N., Khamesipour, F., Khan, A., Khan, M.J., Khan, M.T., Khanal, V., Khidri, F.F., Khubchandani, J., Khusuwan, S., Kim, M.S., Kisa, A., Korshunov, V.A., Krapp, F., Krumkamp, R., Kuddus, M., Kulimbet, M., Kumar, D., Kumaran, E.A.P., Kuttikkattu, A., Kyu, H.H., Landires, I., Lawal, B.K., Le, T.T.T., Lederer, I.M., Lee, M., Lee, S.W., Lepape, A., Lerango, T.L., Ligade, V.S., Lim, C., Lim, S.S., Limenh, L.W., Liu, C., Liu, X., Liu, X., Loftus, M.J., M Amin, H.I., Maass, K.L., Maharaj, S.B., Mahmoud, M.A., Maikanti-Charalampous, P., Makram, O.M., Malhotra, K., Malik, A.A., Mandilara, G.D., Marks, F., Martinez-Guerra, B.A., Martorell, M., Masoumi-Asl, H., Mathioudakis, A.G., May, J., McHugh, T.A., Meiring, J., Meles, H.N., Melese, A., Melese, E.B., Minervini, G., Mohamed, N.S., Mohammed, S., Mohan, S., Mokdad, A.H., Monasta, L., Moodi Ghalibaf, A., Moore, C.E., Moradi, Y., Mossialos, E., Mougin, V., Mukoro, G.D., Mulita, F., Muller-Pebody, B., Murillo-Zamora, E., Musa, S., Musicha, P., Musila, L.A., Muthupandian, S., Nagarajan, A.J., Naghavi, P., Nainu, F., Nair, T.S., Najmuldeen, H.H.R., Natto, Z.S., Nauman, J., Nayak, B.P., Nchanji, G.T., Ndishimye, P., Negoi, I., Negoi, R.I., Nejadghaderi, S.A., Nguyen, Q.P., Noman, E.A., Nwakanma, D.C., O'Brien, S., Ochoa, T.J., Odetokun, I.A., Ogundijo, O.A., Ojo-Akosile, T.R., Okeke, S.R., Okonji, O.C., Olagunju, A.T., Olivas-Martinez, A., Olorukooba, A.A., Olwoch, P., Onyedibe, K.I., Ortiz-Brizuela, E., Osuolale, O., Ounchanum, P., Oyeyemi, O.T., P A, M.P., Paredes, J.L., Parikh, R.R., Patel, J., Patil, S., Pawar, S., Peleg, A.Y., Peprah, P., Perdigão, J., Perrone, C., Petcu, I.-R., Phommasone, K., Piracha, Z.Z., Poddighe, D., Pollard, A.J., Poluru, R., Ponce-De-Leon, A., Puvvula, J., Qamar, F.N., Qasim, N.H., Rafai, C.D., Raghav, P., Rahbarnia, L., Rahim, F., Rahimi-Movaghar, V., Rahman, M., Rahman, M.A., Ramadan, H., Ramasamy, S.K., Ramesh, P.S., Ramteke, P.W., Rana, R.K., Rani, U., Rashidi, M.-M., Rathish, D., Rattanavong, S., Rawaf, S., Redwan, E.M.M., Reyes, L.F., Roberts, T., Robotham, J.V., Rosenthal, V.D., Ross, A.G., Roy, N., Rudd, K.E., Sabet, C.J., Saddik, B.A., Saeb, M.R., Saeed, U., Saeedi Moghaddam, S., Saengchan, W., Safaei, M., Saghazadeh, A., Saheb Sharif-Askari, N., Sahebkar, A., Sahoo, S.S., Sahu, M., Saki, M., Salam, N., Saleem, Z., Saleh, M.A., Samodra, Y.L., Samy, A.M., Saravanan, A., Satpathy, M., Schumacher, A.E., Sedighi, M., Seekaew, S., Shafie, M., Shah, P.A., Shahid, S., Shahwan, M.J., Shakoor, S., Shalev, N., Shamim, M.A., Shamshirgaran, M.A., Shamsi, A., Sharifan, A., Shastry, R.P., Shetty, M., Shittu, A., Shrestha, S., Siddig, E.E., Sideroglou, T., Sifuentes-Osornio, J., Silva, L.M.L.R., Simões, E.A.F., Simpson, A.J.H., Singh, A., Singh, S., Sinto, R., Soliman, S.S.M., Soraneh, S., Stoesser, N., Stoeva, T.Z., Swain, C.K., Szarpak, L., T Y, S.S., Tabatabai, S., Tabche, C., Taha, Z.M.-A., Tan, K.-K., Tasak, N., Tat, N.Y., Thaiprakong, A., Thangaraju, P., Tigoi, C.C., Tiwari, K., Tovani-Palone, M.R., Tran, T.H., Tumurkhuu, M., Turner, P., Udoakang, A.J., Udoh, A., Ullah, N., Ullah, S., Vaithinathan, A.G., Valenti, M., Vos, T., Vu, H.T.L., Waheed, Y., Walker, A.S., Walson, J.L., Wangrangsimakul, T., Weerakoon, K.G., Wertheim, H.F.L., Williams, P.C.M., Wolde, A.A., Wozniak, T.M., Wu, F., Wu, Z., Yadav, M.K.K., Yaghoubi, S., Yahaya, Z.S., Yarahmadi, A., Yezli, S., Yismaw, Y.E., Yon, D.K., Yuan, C.-W., Yusuf, H., Zakham, F., Zamagni, G., Zhang, H., Zhang, Z.-J., Zielińska, M., Zumla, A., Zyoud, S.e.H.H., Zyoud, S.H., Hay, S.I., Stergachis, A., Sartorius, B., Cooper, B.S., Dolecek, C., Murray, C.J.L., 2024. Global burden of bacterial antimicrobial resistance 1990–2021: a systematic analysis with forecasts to 2050. The Lancet 404, 1199-1226.

Naik, N., Hameed, B.M.Z., Shetty, D.K., Swain, D., Shah, M., Paul, R., Aggarwal, K., Ibrahim, S., Patil, V., Smriti, K., Shetty, S., Rai, B.P., Chlosta, P., Somani, B.K., 2022. Legal and Ethical Consideration in Artificial Intelligence in Healthcare: Who Takes Responsibility? 9.

Nissan, N., Allen, M.C., Sabatino, D., Biggar, K.K., 2024. Future Perspective: Harnessing the Power of Artificial Intelligence in the Generation of New Peptide Drugs. 14, 1303.

Sader, H.S., Dale, G.E., Rhomberg, P.R., Flamm, R.K.J.A.A., Chemotherapy, 2018. Antimicrobial activity of murepavadin tested against clinical isolates of Pseudomonas aeruginosa from the United States, Europe, and China. 62, 10.1128/aac. 00311-00318.

Shaik, S., Singh, A., Suresh, A., Ahmed, N., 2022. Genome Informatics and Machine Learning-Based Identification of Antimicrobial Resistance-Encoding Features and Virulence Attributes in Escherichia coli Genomes Representing Globally Prevalent Lineages, Including High-Risk Clonal Complexes. 13, e03796-03721.

Sharma, R., Shrivastava, S., Singh, S.K., Kumar, A., Singh, A.K., Saxena, S., 2024. Artificial Intelligence-Based Model for Predicting the Minimum Inhibitory Concentration of Antibacterial Peptides Against ESKAPEE Pathogens. Ieee Journal of Biomedical and Health Informatics 28, 1949-1958.

Stephenson, J., 2021. WHO Offers Guidance on Use of Artificial Intelligence in Medicine. JAMA Health Forum 2, e212467-e212467.

Stokes, J.M., Yang, K., Swanson, K., Jin, W., Cubillos-Ruiz, A., Donghia, N.M., MacNair, C.R., French, S., Carfrae, L.A., Bloom-Ackermann, Z., Tran, V.M., Chiappino-Pepe, A., Badran, A.H., Andrews, I.W., Chory, E.J., Church, G.M., Brown, E.D., Jaakkola, T.S., Barzilay, R., Collins, J.J., 2020. A Deep Learning Approach to Antibiotic Discovery. Cell 180, 688-702.e613.

Szymczak, P., Możejko, M., Grzegorzek, T., Jurczak, R., Bauer, M., Neubauer, D., Sikora, K., Michalski, M., Sroka, J., Setny, P., Kamysz, W., Szczurek, E., 2023. Discovering highly potent antimicrobial peptides with deep generative model HydrAMP. Nature Communications 14, 1453.

Torres, M.D.T., Chen, L.T., Wan, F., Chatterjee, P., de la Fuente-Nunez, C., 2025. Generative latent diffusion language modeling yields anti-infective synthetic peptides. Cell Biomaterials 1.

Vashisht, V., Vashisht, A., Mondal, A.K., Farmaha, J., Alptekin, A., Singh, H., Ahluwalia, P., Srinivas, A., Kolhe, R.J.B., 2023. Genomics for emerging pathogen identification and monitoring: Prospects and obstacles. 3, 1145-1177.

Wan, F., Kontogiorgos-Heintz, D., de la Fuente-Nunez, C., 2022. Deep generative models for peptide design. Digital Discovery 1, 195-208.

Wan, F., Torres, M.D.T., Peng, J., de la Fuente-Nunez, C., 2024a. Deep-learning-enabled antibiotic discovery through molecular de-extinction. Nature Biomedical Engineering 8, 854-871.

Wan, F., Wong, F., Collins, J.J., de la Fuente-Nunez, C., 2024b. Machine learning for antimicrobial peptide identification and design. Nature Reviews Bioengineering 2, 392-407.

Wong, F., de la Fuente-Nunez, C., Collins, J.J., 2023. Leveraging artificial intelligence in the fight against infectious diseases. 381, 164-170.

Wu, M., Hancock, R.E.J.A.a., chemotherapy, 1999. Improved derivatives of bactenecin, a cyclic dodecameric antimicrobial cationic peptide. 43, 1274-1276.

Wu, X., Wang, Z., Li, X., Fan, Y., He, G., Wan, Y., Yu, C., Tang, J., Li, M., Zhang, X.J.A.a., chemotherapy, 2014. In vitro and in vivo activities of antimicrobial peptides developed using an amino acid-based activity prediction method. 58, 5342-5349.

Zhang, C., Ju, Y., Tang, N., Li, Y., Zhang, G., Song, Y., Fang, H., Yang, L., Feng, J., 2019. Systematic analysis of supervised machine learning as an effective approach to predicate β-lactam resistance phenotype in Streptococcus pneumoniae. Briefings in Bioinformatics 21, 1347-1355.

Zhang, Y., Zhao, C., Wang, Q., Wang, X., Chen, H., Li, H., Zhang, F., Wang, H.J.J.o.A.C., 2020. Evaluation of the in vitro activity of new polymyxin B analogue SPR206 against clinical MDR, colistin-resistant and tigecycline-resistant Gram-negative bacilli. 75, 2609-2615.

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