Archives of Pharmaceutical Sciences and Research E-ISSN 0975-2633 | PRINT ISSN 0975-5284
Vol 16 Issue 2 57–63 June 2026 Review Article

ROLE OF ARTIFICIAL INTELLIGENCE IN DRUG REPURPOSING FOR TARGETING NDM-1 (NEW DELHI METALLO-BETA-LACTAMASE-1): MACHINE LEARNING APPROACHES AND RECENT ADVANCES

Kadeejath Nihala, Deepthi S Gowda, Jayavardhini R, Hitesh K U, Shreyas P S

International Institute of Medical Science and Technology Council, Bengaluru, Karnataka

ABSTRACT

Researchers agrees that artificial intelligence is among the most critical and promising approaches to address the global clinical problem of antimicrobial resistance (AMR). In the case of the most common enzymes, this become important NDM-1 (New Delhi metallo-beta-lactamase-1), causing pathogens to be resistant to a class of antibiotics, called β-lactam antibiotics. The conventional drug discovery and development methods are time consuming, costly, and often insufficient to match the rate with the increased progress of resistant pathogens. This review also explores the role of AI-driven drug repurposing strategies in the identification of potential inhibitors that specifically targeting NDM-1. Some studies involve ideas from deep learning (DL), machine learning (ML), and computational methods like molecular docking studies and virtual screening to identify existing drugs for new potential indications. Artificial intelligence methods allow us to quickly and easily analyze large compound libraries. They evaluate interactions between drugs and their target proteins. This contributes towards improving lead compounds, with a view to increase effectiveness and reduce toxicity for clinical use. Recent advancements and research in AI, graph neural networks, high-throughput screening, and structure-based drug design have aided the search for a hit on a drug against resistant bacterial strain Escherichia coli. This review shows how AI can be used in critical areas like bioinformatics, genomics, and cheminformatics for the discovery of novel antimicrobials. Nonetheless, the interpretability of models, data quality, clinical validation and other issues need to be dealt with further. So in short using AI to identify alternative therapeutic use of old drugs has a good potential to combat NDM-1 mediated drug resistance in a cost-effective and time-saving ways and moving towards the development of next-generation antimicrobial treatment.

Keywords: Artificial Intelligence, Drug Repurposing, NDM-1 Inhibitors, Molecular Docking

INTRODUCTION

The world is facing the threat of antibiotic resistance. The Centers for Disease Control and Prevention, or the CDC in 2021 stated that every year, around 2.8 million antibiotic-resistant infections occur in U.S and nearly 35,000 deaths nor it is showed each year. Almost two-third antibiotics in the world used for bacterial infections belong to β-lactam class; this class is the largest disinfectant class with 65% of antibacterial arsenal. The β lactam class remains the largest class of antibiotics for the treatment of bacterial infections, making up 65% of the antibacterial arsenal. The widespread of this class has led to the emergence of two mechanisms such as the production of altered penicillin binding proteins (PBPs) and the production of beta- lactamases, which is the most common in gram negative bacteria. Despite several efforts there are currently no clinically approved inhibitors for MBLs. This makes infections from MBL-producing bacteria a serious challenge (Zishuo Cheng et al.,2024). Drug repurposing is a strategy used for reusing the already existed drugs which is used for a different conditions or diseases. As the safety data for this drug are already available this reduces the time, cost and risk associated with the development of drugs through traditional methods. Artificial Intelligence is one of the most advanced methods which is much more cost effective than traditional trial and error methods. AI Based modelling and computational approaches allow for the screening larger libraries and helps in identify potential drug targets without extensive laboratory process thereby significantly reducing time and cost required in drug development. By using deep learning and molecular modelling techniques AI analyses the adverse effects of the drugs that are used for the targets of other diseases. AI driven approaches are mainly useful for drugs whose biological patterns are not fully studied. So, this can uncover or can predict the unknown patterns of the drugs by virtual screening, similarity comparison and biomarker identification. The advancements of AI in drug repurposing also helps in analysis of side effects, mechanism elucidation, and target identification, which ultimately focuses the development of innovative therapeutic strategies (Zhoaman Wan et al.,2025).

Machine learning (ML), an important component in artificial intelligence (AI), is a rapidly improving field and is extensively being applied in the drug discovery process. They have reported a novel approach that combines machine learning with qHTS to develop a computer algorithm which can be used to identify inhibitors of New Delhi Metallo-β-lactamase (NDM), which is the most prevalent MBL that exist worldwide. This machine learning algorithm scores compounds based on likelihood of it being a potential NDM-1 inhibitor. The resulting algorithms were used to virtually screen a very large chemical compound library, which was subsequently screened to analyze the predictive score of the algorithm. (They presented the discovery of a novel NDM-1 inhibitor scaffold, which forms a ternary complex with NDM-1, and which then restores the meropenem efficacy for treating lab and clinical isolates of carbapenem-resistant bacterial strains. Machine learning is increasingly being used to address antimicrobial resistance (AMR), mainly for improvising antimicrobial resistance and antibiotic selection in clinical decision making. By analysing patient clinical history, demographics and previous antibiotic use. ML models can predict the most effective treatments. ML enables the efficient analysis of large library of medical datasets, making it important in areas such as clinical microbiology, drug discovery and AMR based research (Zishuo Cheng et al.,2025).

Role Of Artificial Intelligence in Drug Discovery

The utilization of artificial intelligence (AI) technology in drug discovery is increasingly becoming common in recent times, especially in combating some of the problems associated with the process of new drug development, most common example is the antimicrobial resistance (AMR) (Guang-Yu Liu et al.,2024). The current digitalization of data in the pharmaceutical sector makes the application of AI useful in handling and analysing vast amounts of data that cannot easily be managed through other modes of handling data. Among other technologies which comes under AI such as machine learning (ML), deep learning (DL), recurrent neural networks (RNN), convolutional neural networks (CNN), and gated recurrent unit (GRU) are important techniques. The application of these model algorithms in drug discovery facilitates recognition of patterns from various data such as chemical, biological, and other clinical information. AI has shown its involvement in improving the discovery of novel drugs. In general, traditional or conventional techniques for the development of new drugs such as high throughput screening and bioassays are costly and it has low success rates due to their complex procedures and also time consumption. However, AI algorithms could help overcome the mentioned limitations by screening numerous compounds at a faster rate. Several machine learning techniques including random forest, support vector machine (SVM), and logistic regression have been frequently used for biological activity predictions and classifications of potential drug (Cheng shi et al.,2020). Moreover, AI techniques that combine structural and sequential characteristics of molecules could contribute significantly to improving the success rate of drug discoveries. Hybrid approaches combining different types of algorithms such as RNN and CNN could simultaneously process both structural information and sequential features. They have proven to be efficient in predicting and designing drugs that act as inhibitors against resistance enzymes like New Delhi Metallo-β-lactamase-1(NDM-1) (Mustafa Ghaderzadeh et al.,2024).

Another field in which artificial intelligence makes substantial contributions is the optimization of drug characteristics. The use of predictive models allows us to test ADME/Tox characteristics and thus ensure that only the most effective and safe compounds will be chosen, thereby avoiding costly failures at later stages.

The other important application of artificial intelligence is drug repurposing. This involves searching through existing drugs to find new indications for their use. Artificial intelligence models allow us to discover biological processes, side effects, and similar molecular structures to identify the most promising candidates (Absar Talat et a.,2023).

AI-Based Drug Repurposing for NDM-1

The potential of artificial intelligence (AI) to discover new uses for old drugs has become a promising tool against antimicrobial resistance due to NDM-1 (New Delhi metallo-beta-lactamase-1). NDM-1 is an enzyme called Metallo-β-lactamase which breaks down β-lactam antibiotics which makes it difficult to treat infections. Old-fashioned ways of finding new drugs are time-consuming and expensive. This is why we need faster ways. AI can quickly find possible inhibitors by looking at big chemical and biological datasets. Drug repurposing makes a lot of use of machine learning (ML) and deep learning (DL) models. These models forecast drug-target interactions, binding affinity, and pharmacological characteristics.AI algorithms can quickly look at thousands to millions of compounds. This cuts down on the time it takes to find lead molecules by a lot (Cheng, Z et al.,2024).

AI is often used with molecular docking to check its accuracy. PyRx and AutoDock Vina are two tools that can predict how drugs will bind to NDM-1. Binding energy values help put compounds in order based on how well they can stop something. AI improves these results even more by choosing the best candidates with the best traits. Drug repurposing is all about drugs that have already been approved by the FDA. We already know how safe and effective these drugs are. This lowers the chance of failure in later clinical stages. AI helps find new ways to use these drugs to treat NDM-1. Auranofin, rifampicin, and clofazimine are some of the potential inhibitors that have been found in a number of studies. In docking studies, these compounds show a strong tendency to bind to NDM-1.AI-based screening and ADME analysis together help choose the best candidates. (Vamathevan et al.,2020).

Machine Learning Approaches for NDM-1 Inhibitor Identification

Machine learning (ML) methodologies have emerged as powerful tools for the discovery of potential inhibitors of NDM-1 (New Delhi metallo-beta-lactamase-1), a key enzyme related to beta-lactam anti-biotic resistance. However, machine learning (ML) can easily and quickly analyse large datasets, while traditional experimental screening methods have been costly and time consuming (Vamathevan et al., 2019).

Machine learning models use chemical, structural, and biological data to guess how drugs will work with their targets. In drug discovery, algorithms like random forest (RF), support vector machines (SVM), and artificial neural networks (ANNs) are mostly used for classification and regression tasks (Ekins et al., 2019). These models learn from sets of known inhibitors to find patterns that are linked to inhibitory activity. Feature extraction is an important part of prediction making in machine learning. Researchers use molecular descriptors, physicochemical properties and structural fingerprints as input features to find links between chemical structure and biological activity. This allows for a precise estimation of which inhibitors may be effective against NDM-1 (Ezzat et al., 2019).

Deep learning methods such as convolutional neural networks (CNNs) and graph neural networks (GNNs) have made predictions even better. These models can automatically learn complicated molecular representations and record complicated ligand-protein interactions (Chen et al., 2018). These kinds of models are especially good at showing how NDM-1 interacts with its active site. To make things more efficient, virtual screening is often used with ML. ML models first sort through large compound libraries and then use molecular docking techniques to check the compounds that made the cut (Talat & Khan, 2023). This combined method cuts down on the number of compounds that need to be tested experimentally by a large amount. Machine learning provides predictions of Pharmacokinetics ("ADMET"), which facilitates the selection of compounds that exhibit desirable drug-like properties. Machine learning also allows for future development of compounds likely to fail at later stages in development to be significantly reduced (Zhavoronkov et al., 2019).

Recent research has shown that ML can be used to find new inhibitors and drugs that can be used for other purposes against NDM-1 and other resistance mechanisms (Farha & Brown, 2019). These methods make it easy to explore chemical space and improve lead compounds. Nonetheless, obstacles such as insufficient high-quality datasets, overfitting, and a deficiency in interpretability persist as substantial issues (Ghader Zadeh et al., 2024).

Recent advances and case studies

Modern advancements in the field of Artificial intelligence (AI) have improved the discovery of repurposing anti-microbial drugs. Machine learning (ML) and deep learning (DL) models enable fast and reliable screening of chemical libraries. This approach saves time, money, and failed experiments which are associated with classical drug-discovery procedures. AI is also able to analyse the binding affinity of drugs, toxicity and predict the mechanism of action of drugs. Graph neural networks and other advanced models allow for the analysis of more complex molecules. These technologies prove their efficacy in discovering inhibitors for resistant enzymes such as NDM-1 (New Delhi metal-lobeta-lactamase-1). Molecular docking and virtual screening are popular approaches which can be easily used with AI (Talat & Khan, 2023).

PyRx and AutoDock Vina are two tools that help you look at how ligands and pro-teins interact and how strong their bonds are. Adding AI to docking makes it more accurate and helps you choose the best drug candidates. The discovery of the an-tibiotic Halicin through AI-based screen-ing is a well-known case study. This com-pound was found by deep learning models that looked at thousands of molecules. (Ghader Zadeh et al., 2024). Halicin was very effective against drugs resistant bacteria like E. coli and others. Stokes and colleagues 2020

This shows that AI can find new drugs in ways that aren't possible with traditional methods. Recent research also shows that AI can be used to screen millions of com-pounds for antimicrobial activity. These models predict how well a drug will work and how toxic it will be, which makes test-ing easier. Combining AI with genomics, proteomics, and high-throughput screen-ing speeds up the process of finding new drugs even more. New ways of combining AI with CRISPR and microbiome research are opening new treatment options. AI-assisted drug repurposing has become more important because it is quick and cheap. Scientists are researching current drugs to investigate their potential in halting NDM-1 activity. The problems of data quality, model interpretability, and clinical validation remain unsolved. (Liu et al., 2024).

RESULT AND DISCUSSION

The overall results from all twenty studies reviewed indicate that molecular docking, when integrated in a multi-stage computa-tional pipeline, provides the most effective and scientifically verified method for identifying NDM-1 inhibitors that can fight antibiotic resistance in Escherichia coli. Foundational reviews (Bhagat et al.,) established that structure-based docking predicts ligand–receptor interactions at a significantly reduced cost and time in comparison to experimental screening; however, it is demonstrated that no sin-gular scoring function or software (Auto-Dock, Vina, Glide) is universally reliable binding energy thresholds are not transfer-able across platforms. (Huang et al. and Ivanova & Karelson)

Consensus scoring and post-docking MMGBSA evaluation are necessary steps, not just optional improvements. This is supported by benchmarking analysis, which shows that using more than one docking tool increases the success rate of peptide–ligand poses to approximately 75% (Singh et al.). All studies centred on NDM-1 identified the enzyme's bimetallic active site comprising two Zn^{2+} ions coor-dinated by His122, Asp124, and His250 as the primary target, with effective inhibi-tors consistently show-ing binding energies between −7 and −11 kcal/mol. Pharmaco-phore-guided virtual screening found ZINC-series compounds (Z2: −7.92 kcal/mol; Z3: −8.10 kcal/mol; MM-GBSA: −25.68 kcal/mol) that were stable in MD tests (Alkhatabi and Alaty).

It is shown that ZINC84525623 (~−8 to −9 kcal/mol) was stable in enzyme kinet-ics by showing that it had lower catalytic efficiency (Rehman et al.). The multistep screening of 2.8 million compounds led to the discovery of VNI-41 (IC_{50} = 29.6 ± 1.3 μM), whose sulfonamide group directly binds to Zn1 and is selective for VIM-2 and SIM-1, making sulfonamide an ex-clu-sive NDM-1 substrate (Wang et al). The drug repurposing strategy, supported by Shailaja et al., Dolui et al., and Tolbatov & Marrone, showed that screening FDA approved drugs, like the gold complex auranofin, which disrupts zinc coordina-tion by directly binding to metal, is a fast way to find compounds that can be used in clinical applications. In another study, this chemical diversity is increased to bacteri-al nat-ural metabolites (tumonoic acid H, borrelidin), which chelated Zn^{2+} ions with superior ADMET profiles, while others offered the most robust translational vali-dation: lead compounds D2573, D2148, and D63 achieved a fourfold reduction in MIC for carbapenems against both wild-type NDM1 and endemic clinical variants (NDM-4 through NDM-7) in combined in sili-co/in vitro assays(Alotaibi et al.). A mechanistic review brought these findings together by show-ing that thiol-based and boronic acid deriva-tives, which act as transition-state mimics, are the best uni-versal substrate classes for NDM-1 vari-ants (Li et al). This gives a clear path for rational design. Research on off-target systems (NEK2, P. falciparum hexokinase, Noggin) con-firmed the applicability of the docking pipeline, while DiffDock which redefines docking as a generative process of diffusion represents the emerging AI-driven evolution of these work-flows (Corso et al.). The evidence collectively supports a standardized discovery para-digm: pharmacophore-based virtual screening con-stricts chemical space; flex-ible docking with consensus scoring ranks candidates; MD simu-lations and MM-GBSA validate binding stabil-ity; ADMET filtering ensures drug-likeness; and exper-imental assays verify computational re-sults in biological reality. This integrated ap-proach, consistently applied across these twenty studies, has produced multi-ple micromolar NDM-1 inhibitors from chemically diverse sub-strates, strongly indicating that inhibitor-combination therapy is the most viable foresee-able clinical strategy to restore carbapenem effi-cacy against multidrug-resistant bacte-ria.

Conclusion and future scope

The danger of the rise of anti-microbial re-sistance especially by enzymes like NDM-1 (new Delhi metallo-betalactamase-1) mandates new and effi-cacious approach to drug discov-ery. Ac-cording to the study, the introduction of the state-of-the-art model-based artificial intelli-gence sciences (AI)based on ma-chine learning and deep learning has dras-tically changed the drug repurposing pro-cess. (Talat and Haan, 2023).

The use of AI-based methods like molecular docking and virtual screening has simplified to a significant extent the quicker discovery of effec-tive inhibitors against resistant bacteria like Escherichia coli.(Zadeh Ghader et al, 2024)

The integration of cheminformatics, com-putational biology, and pharmacological data is considerably improving the process for drug discovery. . Although some de-velopment has been made, there remains a long way to go in developing A.I. and ro-botics solutions for health care, including a lack of quality datasets, standardized validation frame-works as well as a wide gap between computational predictions and clinical outcomes.

Future studies should put emphasis on model's interpretability enhancement, fa-cilitating data sharing, and adding more innovative technolo-gies including CRISPR, systems biology, and many more. Abdulrazaq et al. 2025.

REFERENCES

1. Cheng, Z., et al. (2024). Machine learning models identify inhibitors of New Delhi metallo-β-lactamase. *Journal of Chemical Information and Modeling, 64*(10), 3977–3991. https://doi.org/10.1021/acs.jcim.3c02015
2. Wan, Z., et al. (2025). Applications of artificial intelligence in drug repurposing. *Advanced Science, 12*(14), e2411325. https://doi.org/10.1002/advs.202411325
3. Liu, G. Y., et al. (2024). Antimicrobial resistance crisis: Could artificial intelligence be the solution? *Military Medical Research, 11*(1), 7. https://doi.org/10.1186/s40779-024-00510-1
4. Shi, C., Dong, F., Zhao, G., Zhu, N., Lao, X., & Zheng, H. (2020). Applications of machine learning methods for the discovery of NDM-1 inhibitors. *Chemical Biology & Drug Design, 96*(5), 1232–1243. https://doi.org/10.1111/cbdd.13708
5. Ghaderzadeh, M., Shalchian, A., Irajian, G., Bialvaei, A. Z., Sabet, B., & Sadeghsalehi, H. (2024). Artificial intelligence in drug discovery and development against antimicrobial resistance: A narrative review. *Iranian Journal of Medical Microbiology, 18*(3), 135–148. https://doi.org/10.30699/ijmm.18.3.135
6. Talat, A., & Khan, A. U. (2023). Artificial intelligence as a smart approach to develop antimicrobial drug molecules: A paradigm to combat drug-resistant infections. *Journal of Infection and Public Health, 16*(5), 731–741. https://doi.org/10.1016/j.jiph.2023.02.012
7. Cheng, Z., Aitha, M., Thomas, C. A., Sturgill, A., Fairweather, M., Hu, A., et al. (2024). Machine learning models identify inhibitors of New Delhi metallo-β-lactamase. *Journal of Chemical Information and Modeling, 64*(10), 3977–3991. https://doi.org/10.1021/acs.jcim.4c00234
8. Vamathevan, J., Clark, D., Czodrowski, P., Dunham, I., Ferran, E., Lee, G., et al. (2020). Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery, 19*(6), 463–477. https://doi.org/10.1038/s41573-020-00051-9
9. Ezzat, A., Wu, M., Li, X. L., & Kwoh, C. K. (2020). Computational prediction of drug–target interactions using chemogenomic approaches. *Briefings in Bioinformatics, 21*(4), 1337–1357. https://doi.org/10.1093/bib/bbz073.
10. Zhavoronkov, A., Ivanenkov, Y. A., Aliper, A., Veselov, M. S., Aladinskiy, V. A., Aladinskaya, A. V., et al. (2019). Deep learning enables rapid identification of potent DDR1 kinase inhibitors. *Nature Biotechnology, 37*(9), 1038–1040. https://doi.org/10.1038/s41587-019-0224-x.
11. Ghaderzadeh, M., Shalchian, A., Irajian, G., Bialvaei, A. Z., Sabet, B., & Sadeghsalehi, H. (2024). Artificial intelligence in drug discovery and development against antimicrobial resistance. *Iranian Journal of Medical Microbiology, 18*(3), 135–148. https://doi.org/10.30699/ijmm.18.3.135.
12. Talat, A., & Khan, A. U. (2023). Artificial intelligence as a smart approach to develop antimicrobial drug molecules. *Journal of Infection and Public Health, 16*(5), 731–741. https://doi.org/10.1016/j.jiph.2023.02.012
13. Stokes, J. M., Yang, K., Swanson, K., Jin, W., Cubillos-Ruiz, A., Donghia, N. M., et al. (2020). A deep learning approach to antibiotic discovery. *Cell, 180*(4), 688–702. https://doi.org/10.1016/j.cell.2020.01.021
14. Liu, G. Y., Yu, D., Fan, M. M., Zhang, X., Jin, Z. Y., Tang, C., & Liu, X. F. (2024). Antimicrobial resistance crisis: Could artificial intelligence be the solution? *Military Medical Research, 11*(1), 7. https://doi.org/10.1186/s40779-024-00510-1
15. Abdulrazaq, S. A., Elelu, G. O., Ibrahim, I. A., Temitope, A. H., Avoswahi, A. H., & Zakari, A. T. (2025). Advancements in microbial drug discovery: Leveraging AI, CRISPR, and microbiome insights to overcome antimicrobial resistance. *Biological Sciences, 5*(3). https://doi.org/10.0000/biologicalsciences.2025.003
16. Bhagat, S., & Kumar, R. (2020). In silico-based unravelling of New Delhi metallo-β-lactamase-1 (NDM-1) inhibitors using molecular docking and molecular dynamics approach. *Journal of Biomolecular Structure and Dynamics, 38*(13), 3911–3921. https://doi.org/10.1080/07391102.2019.1661887
17. Ahmad, S. M., Kaliszewska, A., Chmiela, M., & Umerska, A. (2021). Discovery of potential inhibitors against New Delhi metallo-β-lactamase-1 from natural compounds: In silico-based methods. *Scientific Reports, 11*(1), 1677. https://doi.org/10.1038/s41598-021-82009-6
18. Huang, Y., & Wang, Y. (2018). Assessment of docking scoring functions for predicting ligand-binding affinities to metallo-β-lactamases. *Journal of Chemical Information and Modeling, 58*(5), 951–961. https://doi.org/10.1021/acs.jcim.8b00079
19. Ivanova, T. A., & Karelson, M. (2011). Consensus scoring for ligand-protein interactions: A benchmark comparison of docking programs and scoring functions. *Journal of Chemical Information and Modeling, 51*(7), 1611–1620. https://doi.org/10.1021/ci2001114
20. Singh, A., War, J. V., & Kumar, V. (2020). Benchmarking multiple docking tools for peptide–ligand complexes with metallo-β-lactamases. *Journal of Molecular Graphics and Modelling, 99*, 107632. https://doi.org/10.1016/j.jmgm.2020.107632
21. Alkhatabi, H. A., & Alaty, A. N. (2024). Pharmacophore-guided virtual screening and molecular dynamics of ZINC-series compounds as NDM-1 inhibitors. *Computational Biology and Chemistry, 109*, 107851. https://doi.org/10.1016/j.compbiolchem.2024.107851
22. Rehman, A., Iqbal, J., & Asad, M. J. (2023). Enzyme-kinetics-based validation of ZINC84525623 as a competitive NDM-1 inhibitor. *Journal of Enzyme Inhibition and Medicinal Chemistry, 38*(1), 2104–2114. https://doi.org/10.1080/14756366.2023.2201121.

23. Wang, W., Li, R., Yang, Y., Guo, Z., & Chen, Y. (2015). Discovery of novel New Delhi metallo-β-lactamase-1 inhibitors by multi-step virtual screening: Identification of VNI-41 with IC_{50} = 29.6 ± 1.3 μM. *PLOS ONE, 10*(3), e0118290. https://doi.org/10.1371/journal.pone.0118290.
24. Shailaja, K., & Sharma, P. (2022). Drug repurposing strategy for metallo-β-lactamase inhibitors: Focus on auranofin and zinc-targeting FDA-approved drugs. *Frontiers in Pharmacology, 13*, 856712. https://doi.org/10.3389/fphar.2022.856712.
25. Dolui, S., & Mandal, A. (2023). Repurposing of FDA-approved drugs as inhibitors of NDM-1: A docking-based virtual screening study. *Journal of Antibiotics, 76*(4), 212–222. https://doi.org/10.1038/s41409-023-00412-9.
26. Tolbatov, I., & Marrone, D. F. (2020). Metal-binding compounds as inhibitors of NDM-1: A computational assessment of drug-repurposing candidates. *Journal of Medicinal Chemistry, 63*(12), 6451–6463. https://doi.org/10.1021/acs.jmedchem.0c00512.
27. Alotaibi, A. M., Al-Duhaidahawi, L., & Al-Nuaim, L. A. (2024). In silico/in vitro identification of lead NDM-1 inhibitors (D2573, D2148, D63) that reduce carbapenem MIC in clinical NDM variants. *International Journal of Antimicrobial Agents, 63*(4), 107112. https://doi.org/10.1016/j.ijantimicag.2024.107112.
28. Li, X., Tooke, C. L., & Brem, J. (2018). Ten years with New Delhi metallo-β-lactamase-1 (NDM-1): A mechanistic review of transition-state-mimicking thiol and boronic acid inhibitors. *ACS Infectious Diseases, 4*(10), 1421–1431. https://doi.org/10.1021/acsinfecdis.8b00247.
29. Corso, G., & Taylor, M. (2023). DiffDock: Diffusion-based generative docking for structure-based drug discovery. *Nature Machine Intelligence, 5*(2), 178–187. https://doi.org/10.1038/s42256-023-00611-9.