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Artificial Intelligence in Drug Discovery: A Theoretical Framework of Target Identification, Molecular Design and the Translation Gap for Diseases of the Global South

Paul Idowu Bamigbola[1], NWOGBOJI Emmanuel Usulor[2], Igwe Emmanuel Sunday[3], OGAH SUNDAY OGBO[4]

[1,2,3,4] Veristzon Global Research Lab

ABSTRACT

Artificial intelligence (AI) has compressed stages of drug discovery that once required years. It predicts protein structures, screens virtual libraries, generates candidate molecules and forecasts their properties, and the first AI-discovered molecules have entered clinical trials. This paper asks whether that acceleration will reach the diseases that burden the Global South, drawing on the pharmaceutical-sciences literature on AI-driven discovery, the economics of pharmaceutical innovation and neglected diseases, and recent research on machine learning for target identification, de novo molecular design and property prediction. It distinguishes three stages, target identification, molecular design and translation to the clinic, and argues that AI has transformed the first two while leaving the third constrained by the factors that constrained it before: the cost of trials, the absence of commercial incentive for low-margin diseases, and weak research and regulatory infrastructure where those diseases occur. On this basis the paper advances the view that AI's effect on the global distribution of new medicines depends on three variables: who owns the models, whose disease targets and chemical spaces the models are trained upon, and whether reductions in the cost of discovery are carried through into the development of unprofitable indications. It then considers the conditions under which African pharmaceutical research institutions might participate in AI-driven discovery for malaria, neglected tropical diseases and antimicrobial resistance, rather than remaining downstream consumers of its products. The paper derives a set of propositions about when AI-driven discovery reaches neglected diseases, and argues that participation on terms that build local capacity, rather than consumption of tools designed elsewhere, is what would allow African institutions to shape the chemical spaces and disease targets on which the models are trained.

Keywords: drug discovery; artificial intelligence; machine learning; molecular design; target identification

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1. INTRODUCTION

Drug discovery has long been slow, expensive and uncertain. Identifying a biological target, finding a molecule that modulates it, optimising that molecule into a candidate with acceptable properties, and demonstrating its safety and efficacy in humans has typically taken more than a decade, and most candidates fail along the way. Artificial intelligence promises to change the early part of this process: machine-learning models predict protein structures, identify candidate targets from multi-omic data, screen virtual libraries of billions of compounds, generate novel molecules with specified properties, and predict their absorption, distribution, metabolism, excretion and toxicity. Reviews document the spread of AI across the discovery pipeline, from target identification to clinical-trial design (Inoue et al., 2026).

The first AI-discovered molecules have now entered clinical trials, and early analysis of their performance offers an initial test of AI's promise. Jayatunga et al. (2024), analysing the clinical pipelines of AI-native biotechnology companies, found that AI-discovered molecules showed higher Phase I success rates than historical industry averages while their Phase II success rates remained broadly in line with historical levels. This pattern suggests that AI improves the early, molecule-level properties that determine safety and tolerability more than it improves the biological validity of the targets that determine efficacy.

This paper poses a question that the enthusiasm surrounding AI-driven discovery has largely passed over: whom will the acceleration benefit? The diseases that impose the heaviest burden on the Global South include malaria, neglected tropical diseases, tuberculosis and drug-resistant bacterial infections, most of which have long been underserved by pharmaceutical innovation because those who suffer from them cannot pay prices that would reward investment. Machine-learning approaches to neglected tropical diseases have been explored precisely because these diseases are common in countries lacking the resources for conventional drug development (Breslin & Pham, 2023). Whether AI narrows or widens the gap between the diseases of the rich and those of the poor is not a technical question alone; it depends on who owns the models, on the data those models are trained upon, and on whether reductions in the cost of discovery translate into investment in development.

The analysis is theoretical, integrating recent research on AI in drug discovery (Inoue et al., 2026; Jayatunga et al., 2024; Liu et al., 2024; Nussinov et al., 2023; Pathak, 2026; Thomas et al., 2024), on data-limited and privacy-preserving machine learning (Pallikkavaliyaveetil & Chandrasekaran, 2026; Smajić et al., 2023), on the incentives of pharmaceutical innovation (Kinch, 2023; Sachs et al., 2023), on AI for malaria, neglected diseases and antimicrobial resistance (Breslin & Pham, 2023; Cesaro et al., 2023; Gholami & Asadollahi-Baboli, 2025; Wan et al., 2024), and on African disease burden, clinical research and regulation (Adebisi et al., 2025; Assefa et al., 2024; Kwizera et al., 2025; Ncube et al., 2024; Sagandira, 2025; Salami & Agogo, 2026; Sibomana, 2024).

2. LITERATURE REVIEW

2.1 Three Stages of Drug Discovery

The discovery and development of a medicine may be divided into three stages, target identification, molecular design and translation to the clinic, and AI relates to each in a distinct manner.

The first stage is the identification of a biological target, typically a protein whose modulation is expected to alter the course of a disease. Target identification draws on genetic, genomic, proteomic and clinical data to link molecular mechanisms to disease, and AI has strengthened it by integrating heterogeneous data at scale, identifying associations that would escape conventional analysis, and prioritising targets by their predicted relevance and tractability (Inoue et al., 2026). Protein structure prediction has been particularly influential, making it possible to assess the druggability of targets whose structures had never been determined experimentally and to design molecules against them (Nussinov et al., 2023). Yet this is also the stage at which AI's limitations bear most heavily on clinical success. The Phase II failures that dominate drug development reflect, in large part, targets that appeared promising but did not alter disease in patients; AI can identify associations in data, but whether modulating a target will produce clinical benefit depends on biology that data may not reveal, and the finding that AI-discovered molecules have

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not yet improved Phase II success rates (Jayatunga et al., 2024) is consistent with this interpretation.

The second stage is the discovery and optimisation of molecules that act on the target with sufficient potency, selectivity and drug-like properties, and it is here that AI has made its most visible contribution. Virtual screening uses machine-learning models to predict which compounds within vast libraries will bind a target; deep generative models design new molecules with specified properties (Liu et al., 2024); property-prediction models estimate absorption, toxicity and other characteristics before synthesis; and structure-based approaches using predicted protein structures extend these methods to targets lacking experimental structures, though benchmarking studies reveal both their capabilities and their limits for medicinal chemistry (Pathak, 2026), and frameworks for scoring and benchmarking generative models have been developed so that their outputs may be compared and evaluated (Thomas et al., 2024). The acceleration at this stage is real but data-dependent: generative and predictive models perform best where large, high-quality datasets of measured activities and properties exist for related targets and chemical series, and less reliably where data are sparse, as for many targets relevant to neglected diseases. Strategies for data-limited drug discovery, transfer learning, few-shot learning and data augmentation, mitigate this difficulty without eliminating it (Pallikkavaliyaveetil & Chandrasekaran, 2026).

The third stage is translation: demonstrating in humans that a candidate is safe and effective, and securing regulatory approval and access. Translation encompasses preclinical development, the phases of clinical trials, regulatory review, manufacturing and distribution, and it is by far the most expensive and time-consuming part of bringing a medicine to patients. AI is applied here as well, in trial design, patient selection and the analysis of trial data (Inoue et al., 2026); but the fundamental costs of translation, recruiting patients, conducting trials over months or years, manufacturing to quality standards and navigating regulation, are not substantially reduced by computation. Translation is constrained by institutions, infrastructure and incentives far more than by the methods of discovery.

2.2 The Translation Gap

The central claim of the framework is that AI has transformed the first two stages of drug discovery while leaving the third largely unchanged, producing what this paper terms a translation gap. The pipeline of candidate molecules can now be filled faster and more cheaply, but the capacity to carry candidates through clinical development has not grown correspondingly. For diseases that already attract investment, the gap may be closed by the ordinary operation of pharmaceutical markets, since companies holding promising AI-discovered candidates for profitable indications will fund their development; for diseases that do not attract investment, the gap may widen, as candidates generated by cheaper discovery accumulate without the resources to test them.

The economics of pharmaceutical innovation explain this asymmetry. Pharmaceutical firms invest in development where expected revenues justify the cost and risk, and the incentives of innovation, from patent protection to pricing and reimbursement policy, are structured around this logic, so that proposals for reform must address the whole system of incentives rather than any single lever (Sachs et al., 2023). Kinch (2023) describes a pharmaceutical innovator's dilemma in which the structure of the industry shapes which innovations are pursued. Under these conditions, reducing the cost of discovery does not of itself alter which diseases receive investment: discovery constitutes a small fraction of total development cost, and the revenue prospects that govern investment are unchanged.

The translation gap is compounded by the infrastructure of clinical research, since the diseases of the Global South must ultimately be studied in the populations that suffer them. Clinical-trial capacity in sub-Saharan Africa remains limited by shortages of trained investigators, research infrastructure, funding and regulatory capacity (Kwizera et al., 2025); regulatory systems across the continent are fragmented, though harmonisation initiatives and the establishment of the African Medicines Agency offer prospects of change (Ncube et al., 2024; Ngum et al., 2023); and recommendations for the Agency's strategic priorities identify fragmented regulation, inadequate regulation of clinical trials and limited capacity for drug development as core challenges (Salami & Agogo, 2026). Until these constraints are addressed, faster discovery will continue to produce candidates that cannot be developed where they are needed.

2.3 AI and the Distribution of New Medicines

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The framework holds that AI's effect on the global distribution of new medicines depends on three variables. The first is the ownership of models and data. The most capable AI drug-discovery systems are developed by technology companies, pharmaceutical firms and well-funded biotechnology start-ups, overwhelmingly in North America, Europe and East Asia, and their models, training data and computing infrastructure are proprietary; where these systems are applied to neglected diseases, it is usually through philanthropic partnerships or open-science initiatives rather than ordinary commercial activity. Privacy-preserving and federated approaches allow models to be trained across data held by different organisations without sharing the data itself (Smajić et al., 2023), which could enable collaboration that includes institutions in the Global South, but such approaches do not of themselves alter who controls the resulting models.

The second variable is the composition of the training data. AI models learn from the data on which they are trained, and the chemical, biological and clinical data available for training reflect past research priorities: targets and chemical series associated with profitable diseases are richly represented, those associated with neglected diseases are not, and models trained on such data will be most capable for the targets and chemical spaces already well studied and least capable for those that are not (Breslin & Pham, 2023; Pallikkavaliyaveetil & Chandrasekaran, 2026). The same consideration applies to human genetic and clinical data. African populations possess the greatest human genetic diversity, with implications for drug response and precision medicine, yet they remain underrepresented in genomic research (Sibomana, 2024), so that models trained on data from other populations may predict drug responses in African patients poorly.

The third variable is the allocation of cost savings. Where AI reduces the cost of discovery, the savings may be captured as profit, reinvested in profitable indications, or directed to unprofitable ones; market incentives favour the first two (Kinch, 2023; Sachs et al., 2023), and the third occurs only where public, philanthropic or policy mechanisms direct it. AI will therefore not of itself redirect pharmaceutical innovation toward the diseases of the Global South; it will do so only where mechanisms exist to channel the savings it generates into the development of medicines for those diseases.

Taken together, these variables indicate that the default effect of AI on the distribution of new medicines is to widen existing disparities, since models owned in the Global North, trained on data reflecting past priorities and deployed under market incentives, will accelerate discovery for diseases that already receive attention. Altering this outcome requires deliberate action on all three variables: broader participation in model development, investment in data for neglected targets and populations, and mechanisms to fund translation for unprofitable indications.

2.4 Malaria, Neglected Tropical Diseases and Antimicrobial Resistance

Three disease areas illustrate both the potential and the limits of AI-driven discovery for the Global South. Malaria remains among Africa's heaviest disease burdens, and the emergence of resistance threatens the artemisinin-based combination therapies on which treatment depends. Artemisinin partial resistance has emerged in East Africa and the Horn of Africa (Assefa et al., 2024), and a new focus of probable partial resistance has been identified in southern Africa (Martinez-Vega et al., 2026), so that the need for new antimalarials with novel mechanisms is urgent. Machine learning has been applied to antimalarial discovery, for instance in ensemble models predicting the activity of inhibitors against parasite kinases (Gholami & Asadollahi-Baboli, 2025). Because malaria benefits from substantial public and philanthropic investment and from established product-development partnerships, AI-discovered antimalarial candidates have a pathway to development that many neglected diseases lack.

Neglected tropical diseases present the translation gap in its starkest form, affecting large numbers of people, chiefly in low-income settings, while attracting little commercial investment. Breslin and Pham (2023), reviewing machine-learning approaches to drug discovery for these diseases, note that the increasing availability of data from high-throughput screening makes such approaches feasible, and that the diseases are common in countries lacking the resources for research and development. AI can lower the cost of finding candidates for these diseases, but without funded pathways for development, candidates will remain candidates.

Antimicrobial resistance presents the problem in a different form. Drug-resistant bacterial infections

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impose a heavy and growing mortality burden in Africa, including East Africa (Adebisi et al., 2025). Deep learning has produced notable advances in antibiotic discovery, with tools to accelerate the process reviewed by Cesaro et al. (2023) and deep learning used to mine the proteomes of extinct organisms for antibiotic peptides through molecular de-extinction (Wan et al., 2024); but the economics of antibiotics are poor even in wealthy markets, since new antibiotics must be held in reserve to slow resistance, which limits sales. Here the translation gap is global rather than specific to the Global South, though its consequences fall most heavily where resistance is highest and alternatives fewest.

2.5 Validating AI-Discovered Candidates

A further constraint on the translation of AI-driven discovery concerns validation, the experimental work required to establish that computationally generated candidates actually possess the properties predicted for them, and it bears on the Global South because validation requires laboratory infrastructure that is unevenly distributed.

The predictions on which AI-driven discovery rests have recognised limitations. Predicted protein structures have transformed structure-based design, but they are models rather than measurements: their reliability varies across protein families, conformational states and binding sites, and benchmarking against experimental structures reveals cases in which predicted structures mislead medicinal chemistry (Pathak, 2026), with allosteric sites and conformational dynamics, important for many drug targets, posing particular difficulty (Nussinov et al., 2023). Generative models can propose molecules that score well on computational objectives yet prove difficult to synthesise, unstable, or inactive in practice, which is precisely why frameworks for evaluating and benchmarking generative models exist (Thomas et al., 2024), and property predictions are least reliable for molecules far from the chemical space represented in the training data (Pallikkavaliyaveetil & Chandrasekaran, 2026).

Every AI-discovered candidate must therefore be synthesised and tested, for activity against the target, for activity in cells and organisms, for selectivity, for toxicity and for pharmacokinetic properties, and these steps require medicinal-chemistry laboratories, biological assays, animal facilities and analytical instrumentation. For neglected diseases they further require access to relevant pathogens, parasite strains and disease models; the discovery of antibiotics by deep learning, for example, has relied upon experimental confirmation of predicted antimicrobial activity in laboratory and animal studies (Wan et al., 2024).

It follows that the democratisation of computational discovery does not democratise validation. Access to predicted structures, open chemical libraries and pretrained models allows researchers anywhere to generate candidates, but converting candidates into credible leads requires experimental capacity that remains concentrated in well-resourced institutions. For African institutions this points to a strategic priority: investment in validation capacity, medicinal chemistry, screening against locally relevant pathogens and strains, and preclinical pharmacology, may yield more than investment in computation, since it addresses the step that computation cannot replace and that determines whether AI-generated candidates become credible leads. It also points to a role for partnerships in which computational discovery performed anywhere is coupled to validation performed where the relevant pathogens, strains and patient populations are found.

3. CONCEPTUAL FRAMEWORK

The argument may be summarised in a set of propositions, framed as conditional claims for research and as principles for policy on pharmaceutical innovation and AI.

The first concerns the location of AI's effect: AI accelerates target identification and molecular design substantially more than it accelerates translation to the clinic, so that the resulting translation gap prevents faster discovery from producing proportionally faster delivery of new medicines (Inoue et al., 2026; Jayatunga et al., 2024). Within this, AI improves the molecule-level properties that determine early clinical success more than it improves the biological validity of targets that determine efficacy, so that the principal source of clinical attrition, failure to demonstrate efficacy, will persist (Jayatunga et al., 2024; Nussinov et al., 2023).

A second group of propositions concerns the direction of benefit. AI models perform best for targets and chemical spaces richly represented in the training data, and because these reflect past research priorities, AI will be least capable for the neglected targets and underrepresented populations of the

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Global South unless data for them are deliberately generated (Breslin & Pham, 2023; Pallikkavaliyaveetil & Chandrasekaran, 2026; Sibomana, 2024). Reductions in the cost of discovery will not of themselves redirect pharmaceutical investment toward unprofitable indications, which requires public, philanthropic or policy mechanisms to fund their translation (Kinch, 2023; Sachs et al., 2023). Where established product-development pathways exist, as for malaria, AI-discovered candidates have a realistic route to patients; where they do not, as for many neglected tropical diseases, AI will increase the stock of candidates without increasing the supply of medicines (Breslin & Pham, 2023; Gholami & Asadollahi-Baboli, 2025).

A final group concerns African participation. Clinical-trial and regulatory capacity in sub-Saharan Africa is a binding constraint on translating AI-discovered medicines for African diseases, so that investment in that capacity, together with the effective operation of the African Medicines Agency, will determine how much of AI's acceleration reaches African patients (Kwizera et al., 2025; Ncube et al., 2024; Salami & Agogo, 2026). African research institutions can participate in AI-driven discovery as contributors rather than consumers to the extent that they generate high-quality data on local diseases and populations, build computational and medicinal-chemistry expertise, and secure governance arrangements affording them a share in the models and medicines that result (Sagandira, 2025; Sibomana, 2024; Smajić et al., 2023).

4. ANALYSIS AND DISCUSSION

4.1 African Pharmaceutical Research Institutions

African pharmaceutical research institutions face a choice in the age of AI-driven discovery: they may remain downstream consumers of medicines discovered and developed elsewhere, or they may become participants in discovery and development for the diseases that burden their populations. Four conditions determine whether participation is possible.

The first is data. AI-driven discovery depends on data, and the data most valuable for African diseases are generated in Africa, clinical isolates of resistant pathogens, parasite samples carrying resistance mutations, genomic and pharmacogenomic data from African populations, and clinical-outcome data from African patients. The genetic diversity of African populations has direct implications for drug response and precision medicine (Sibomana, 2024), and institutions that generate, curate and govern such data well will be indispensable partners in AI-driven discovery for African diseases, a source of leverage that can secure a share in the benefits of discovery. The second condition is expertise. Participation requires scientists who combine computational skills with medicinal chemistry, pharmacology and disease biology, a dual competence scarce globally and especially so in Africa; building it requires investment in training, in research careers that retain trained scientists, and in collaborations that transfer capability rather than merely extract data.

The third condition is translational infrastructure. Even where African institutions contribute to discovery, the resulting medicines must be developed, tested, manufactured and regulated. Clinical-trial capacity remains a significant constraint (Kwizera et al., 2025); local manufacturing of active pharmaceutical ingredients could strengthen health security and economic development (Sagandira, 2025); and the establishment of the African Medicines Agency, together with the harmonisation of regulatory systems across the continent, could reduce the fragmentation that impedes development and access (Ncube et al., 2024; Ngum et al., 2023; Salami & Agogo, 2026). The fourth condition is governance. Collaborations between African institutions and the owners of AI models must be structured so that African partners share in the intellectual property, the models and the medicines that result, not merely in the authorship of papers. Privacy-preserving and federated approaches can allow African data to contribute to model training without leaving local control (Smajić et al., 2023), but the terms of collaboration, including access to the resulting models and medicines, are a matter of negotiation and depend on the leverage African institutions can bring to bear.

For Nigeria, the framework indicates specific priorities. Nigeria carries a heavy malaria burden and faces substantial challenges from antimicrobial resistance and neglected tropical diseases, and its pharmaceutical research institutions, universities and manufacturers could position themselves as partners in AI-driven discovery by building high-quality data resources on these diseases, investing in computational pharmaceutical sciences,

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strengthening clinical-trial capacity, and engaging with continental regulatory harmonisation. The aim should not be to replicate the AI infrastructure of global technology firms, which would be neither feasible nor necessary, but to become an indispensable contributor of the data, expertise and translational capacity that AI-driven discovery for African diseases requires.

4.2 Implications

For pharmaceutical scientists, the framework implies that the value of AI-driven discovery should be judged by its contribution to medicines that reach patients, not by the speed or novelty of candidate generation, and that attention should accordingly concentrate on the stages where AI's contribution is weakest: the biological validation of targets, which determines efficacy, and translation, which determines access (Jayatunga et al., 2024). For funders and policymakers, it implies that AI will not of itself correct the neglect of the diseases of the Global South: public and philanthropic funding for the translation of AI-discovered candidates for neglected indications, together with incentive mechanisms that reward development for unprofitable diseases, is required if reductions in the cost of discovery are to benefit those diseases (Kinch, 2023; Sachs et al., 2023), while investment in data generation for neglected targets and underrepresented populations is a high-leverage intervention, since it improves the capability of all models trained on the data (Breslin & Pham, 2023; Pallikkavaliyaveetil & Chandrasekaran, 2026).

For African governments and regional bodies, the framework underscores the strategic importance of clinical-trial capacity, regulatory harmonisation and local manufacturing (Kwizera et al., 2025; Sagandira, 2025; Salami & Agogo, 2026), which are the translational capacities that determine whether AI-discovered medicines for African diseases reach African patients, and which policy can influence within a reasonable time frame. For African research institutions, it recommends a strategy of indispensable contribution: generating and governing high-quality data on local diseases and populations, building computational and medicinal-chemistry expertise, and negotiating collaborations that share benefits (Sibomana, 2024; Smajić et al., 2023).

Several questions remain open for research. Will the early pattern of AI-discovered molecules' clinical performance persist as more candidates advance? How far does the underrepresentation of neglected targets in the training data limit AI's usefulness for those diseases, and how far can targeted data generation overcome it? Which mechanisms most effectively direct AI-enabled reductions in cost toward unprofitable indications? And how can collaborations between African institutions and the owners of AI models be structured for equitable benefit? Answering these questions requires research that follows AI-discovered candidates through development, not only through discovery.

5. CONCLUSION AND RECOMMENDATION

Artificial intelligence has transformed the early stages of drug discovery. Targets can be identified, structures predicted and molecules designed faster and more cheaply than before, and the first AI-discovered molecules are proceeding through clinical trials. This paper has argued that this transformation does not of itself change the distribution of new medicines across the world's diseases, because AI has accelerated target identification and molecular design while translation remains constrained by cost, incentives and infrastructure, and the resulting translation gap is widest for the diseases of the Global South.

Whether AI narrows or widens the gap between the diseases of the rich and those of the poor depends on three variables, who owns the models, what data they are trained upon, and where the cost savings are directed, and by default all three favour diseases that already receive attention. Altering this outcome requires deliberate action: data must be generated for neglected targets and underrepresented populations, translation for unprofitable indications must be funded, and the clinical, regulatory and manufacturing capacity of the regions where these diseases occur must be strengthened.

For African pharmaceutical institutions, the age of AI-driven discovery offers an opportunity to move from the periphery of pharmaceutical innovation toward its centre for the diseases that matter most to African populations, an opportunity to be realised not by competing with the computational resources of global firms, but by becoming an indispensable contributor of the data, expertise and translational capacity without which AI-discovered candidates cannot become medicines for African patients.

6. CONTRIBUTION TO EXISTING KNOWLEDGE

The paper contributes an analysis of artificial intelligence across the three stages of drug

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discovery, target identification, molecular design and translation, and argues that AI has transformed the first two while leaving the third, the translation gap, constrained by the economic and infrastructural factors that constrained it before.

It gives researchers, funders and African pharmaceutical institutions a basis for judging where AI will and will not alter the global distribution of new medicines, and for directing effort toward the diseases of the Global South rather than assuming that technical acceleration alone will reach them.

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