The Role of AI in Drug Discovery in Africa

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The proliferation of artificial intelligence presents Africa's drug discovery landscape with a transformative opportunity to accelerate research and development (R&D) to address the continent's heavy disease burden. The integration of AI in drug discovery processes will help researchers by streamlining research pipelines and improving the design of clinical trials so that historically underserved populations can access cost-effective medication tailored to their needs. While challenges include AI skepticism, scarcity of data, and concerns about job losses, sustained advocacy and capacity-building can help to allay these concerns and facilitate widespread buy-in and adoption of AI tools across the continent. At a time of diminished funding for R&D globally, AI-assisted drug discovery – with its potential to alter fundamentally the pace and cost of R&D – should help Africa move toward a sustainable and innovative pharmaceutical paradigm led by Africans, out of Africa, for the global community.

Home to nearly one-fifth of the world's population, Africa bears a vastly disproportionate burden of infectious disease. This is best exemplified by malaria. The World Health Organization documented 263 million cases of malaria and 600,000 malaria deaths in 2023.[1] Africa accounted for about 95 percent of all malaria cases and mortalities, with African children under the age of five accounting for about 75 percent of all malaria deaths in the region. Other endemic diseases such as tuberculosis, HIV/AIDS, and neglected tropical diseases remain prevalent, and rising rates of noncommunicable diseases such as diabetes and hypertension create a double burden on fragile health systems. This means that Africa faces a unique set of health challenges that both mirror and diverge from those in other parts of the Global South.

The prevention and control of this disease burden in Africa are crucial if the world is to meet Sustainable Development Goal 3 (SDG 3, "to ensure healthy lives and promote well-being for all at all ages") and especially Target 3.3, which focuses on communicable diseases.[2] Meeting SDG 3 requires accelerated research and development (R&D) into lifesaving, innovative pharmaceutical interventions that

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are cost-effective and can be deployed across the continent at scale, together with urgent improvements to underfunded health infrastructure, fragmented data systems, and issues of access. However, due to a limited capacity to address these challenges locally, Africa has historically been compelled to rely on pharmaceutical interventions primarily from the Global North.

Reducing dependency on international aid and handouts is an increasingly prominent theme in the development discourse across Africa. While drug discovery research efforts have grown locally, they are still in a nascent stage, lacking a critical mass of skills and infrastructure. The challenge has been compounded by the continuous loss of talent from the continent (the "brain drain") and limited investment in R&D by African governments, along with a gradual decline in contributions from donor countries that has thrown many research projects and clinical trials out of gear. Unlike regions in Asia or Latin America that have made more sustained investments in biotechnology and digital health, Africa's health innovation ecosystem remains underdeveloped, leading to its underrepresentation in global pharmaceutical R&D.

We are at a critical juncture as well as unique moment of opportunity in Africa's history. With traditional channels of aid and support disrupted, Africa must rely on its own capabilities and build upon them to deliver cutting-edge, innovative medicines to the people who need it most.

Enter artificial intelligence. Even in its infancy, AI has had a transformative impact across virtually every sector of society. Consider its impact – and the recognition of it – in scientific research. In 2024, John Hopfield and Geoffrey Hinton were awarded the Nobel Prize in Physics for their work on artificial neural networks in machine learning (ML).[3] That same year, Demis Hassabis and John Jumper were awarded the Nobel Prize in Chemistry for their contributions in developing an AI tool, Google DeepMind's AlphaFold, that can predict the complex three-dimensional structures of proteins from the primary amino acid sequence. Apart from AlphaFold, David Baker also shared the Nobel Prize in Chemistry for his contributions to novel protein design.[4]

AI has the potential to accelerate health innovation and tailor drug discovery to Africa's disease burden. This is especially exciting in contexts like malaria or sickle cell disease, for which local prevalence is high and global pharmaceutical investment is limited. While its applications in drug discovery are incremental, AI is already catalyzing efforts to develop a malaria vaccine, combat drug-resistant bacteria, and mine local genomic and health data for new therapeutic insights.[5] These advances are possible because AI has the ability to identify patterns in data, process much larger datasets than humans, and automate complex tasks. While drug discovery is traditionally a time-consuming and expensive process, AI can potentially accelerate every step of the process, saving time and vast resources while providing novel insights.

Africa owes its limited capacity for drug discovery and development to several historical factors. One is the reliance on handouts and assistance mostly from the Global North. The continent is now enduring major disruptions to R&D in the wake of diminished donor funding. The problem is compounded by the historical general lack of investment in infectious disease R&D by African governments, the African private sector, as well as most innovative pharmaceutical companies due to low anticipated commercial returns.

Inequity in the global health landscape also puts Africa at a disadvantage, as the COVID-19 pandemic made clear. During the global rollout of vaccines, Africa received a minuscule allocation while countries in the Global North hoarded multiple doses for their citizens. By October 2022, nearly three years after the pandemic began, Africa had received only 540 million doses, or 6 percent of the 9 billion produced worldwide, with less than 10 percent of its population fully vaccinated by that time.[6]

This inequity also manifests itself in the paucity of clinical trials in Africa, which stood at 2.2 percent of all trials conducted worldwide between 2012 and 2023, despite the continent bearing 20 percent of the world's disease burden and greater genetic diversity than the rest of the world combined.[7] The absence of data on how drug dosages affect African genetics has led to serious consequences for the continent and its people. For example, the HIV/AIDS drug Efavirenz was launched as a first-line treatment in Zimbabwe in 2015 after being used successfully in the United States and Europe. But Zimbabwean HIV/AIDS patients experienced serious side effects that are associated in part with genetic mutations in the gene encoding for the enzyme responsible for the metabolism of Efavirenz. These mutations lead to a slow metabolizer phenotype, implying that Zimbabwean patients were effectively being overdosed, which accounts for the side effect profile in these patients. Dosing recommendations were based on the fact that such mutations are rare in Europeans and Americans (as low as 3 percent) but found in 20 percent of Africans.[8] Addressing such gaps will require including African data in drug discovery and development.[9] It is critical, therefore, for Africa to build its own drug discovery research capabilities to develop solutions for its most pressing disease challenges.

This is easier said than done. Financial constraints in low- and middle-income countries (LMICs) stand in the way of adequate infrastructure, including laboratories equipped with advanced technologies. Funding shortfalls result in a shortage of trained researchers and health care professionals. Drug discovery is also an inherently lengthy and costly process fraught with risk of failure. The journey of a drug from the laboratory to the shelf often takes a decade, if not more, with appropriate sustained investment. In Africa's case, the writing is on the wall. The challenges it faces are immense, but twenty-first-century tools like AI provide the continent with a unique opportunity to chart its own innovative pathways to drug discovery – *by Africans, out of Africa, for the global community*.

The Holistic Drug Discovery and Development (H3D) Center, Africa's first and leading world-class integrated drug discovery and development center, has been spearheading the continent's push for self-reliance in drug discovery.[10] I founded H3D at the University of Cape Town in 2010, and have directed it and the associated H3D Foundation since 2019. H3D works with a range of partners and collaborators to reduce barriers for African scientists, break new ground in the discipline of drug discovery, and expand the drug discovery ecosystem and community in Africa. H3D collaborated with the African Academy of Sciences, the Bill & Melinda Gates Foundation through its Grand Challenges initiative, and the Medicines for Malaria Venture to identify the best emerging African scientists and build a cohort of future leaders within Africa, thus strengthening the drug discovery discipline and mitigating the brain drain from the continent. This led to the initiation of the Grand Challenges Africa Drug Discovery Sentinel program in 2018, with H3D providing direct support to all the grantees.

In November 2023, the H3D Foundation, with $7.2 million in funding from the Gates Foundation and LifeArc, established the Grand Challenges African Drug Discovery Accelerator (GC ADDA), a network of drug discovery researchers working in Africa on unmet medical needs faced by the African patient.[11] By 2024, the network had already linked eight African countries and twenty-one research institutions. The GC ADDA seeks a future in which African patients have access to cost-effective, efficacious disease treatments tailored to their health needs. With four initial flagship projects, GC ADDA is working to create regional centers of excellence within the continent to grow and sustain self-reliant research in drug discovery.

The H3D Center's focus on innovation to develop platform technologies positions it as an early adopter of AI in drug discovery research. In 2021, H3D entered a partnership with the Ersilia Open Source Initiative (EOSI) with a mission to incorporate AI and ML tools into the H3D drug discovery pipeline.[12] This was an ideal partnership: H3D at that time had no in-house AI/ML expertise, and EOSI specialized in developing AI/ML tools for drug discovery in LMICs. In 2023, H3D received a major boost for AI-enabled drug discovery when I was awarded a Schmidt Sciences AI2050 Senior Fellowship through the H3D Foundation. The AI2050 work involves linking open-source AI to existing pharmacometrics (mathematical) modeling tools used in human dose prediction for clinical trials and boosting the development of ready-to-use AI models for malaria and tuberculosis drug discovery in Africa.[13]

Traditional methods of drug discovery are dependent upon an approach of examining large numbers of potential drug candidates and sorting through them to identify "lead" compounds. This is a cumbersome, expensive process, hamstrung by the limited availability of these compounds and the challenge of predicting how they will interact with the human body. Because AI algorithms can be applied across thematic domains and trained on a broad spectrum of data-

sets, they can be employed across different stages of the drug discovery pipeline to make the process much more time- and cost-effective. An example of this would be the chemistry-related or protein-related models that have been trained on network architectures inspired by large language models such as ChatGPT.

Training AI models on large datasets enables them to identify patterns in diseases and predict the potential composition of drugs that can treat them. Resources like AlphaFold, which can predict the 3D structure of proteins, can help accelerate this process. AI's ability to leverage statistical algorithms to anticipate how drug candidates will bind to specific targets and what properties they will have can also reduce the need for – and the costs associated with – physical testing of those compounds. Chemists can thus examine a much wider set of prospective compounds much more efficiently. AI-assisted approaches have also been known to rank promising drug candidates more accurately for further assessment compared with traditional methods.[14]

I had the privilege of being invited by the Wellcome Trust to join a Scientific Advisory Committee of about fifteen leaders in drug discovery across industries and geographies to offer input on and guide research led by the Boston Consulting Group for a new landscaping report on the impact of AI in drug discovery.[15] This report looked to understand at which points in drug discovery AI was being deployed, identify new areas to expand its use, and assess the extent of adoption of these tools across the drug discovery ecosystem. There was a strong focus on understanding where AI can be expanded across infectious disease drug development and how to increase adoption in LMIC settings.

A leading use case of AI for small molecule research is in the development of quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) prediction models to identify promising compounds prior to synthesis and increase the efficiency of the experimental pipeline. A prominent example of this approach is the end-to-end, fully automated implementation of an AI/ML tool for QSAR/QSPR modeling called ZairaChem. With no prior AI/ML capabilities, the H3D Center implemented ZairaChem, a first-of-its-kind deployment at scale of AI/ML tools in a research center operating in a low-resource setting.[16] With a light requirement for computational resources, the tool assisted H3D in developing a virtual screening cascade for malaria and tuberculosis drug discovery. Trained on the H3D Center's in-house compound library, the virtual screening cascade consists of a set of classification models that predict whether a given compound is likely to be "active" or "inactive" across various measured biological properties. Far from replacing lab-based scientists, expert insights from experimentalists are critical in developing relevant and accurate models. The AI models undergo retraining every six months to ensure they are updated with the most recent in-house data and remain aligned with ongoing research programs. Models can also be developed on request for specific drug discovery programs or for additional datasets of inter-

est. The periodic maintenance of AI models, including engaging with lab-based scientists during model development and regular upskilling of scientists in the use and interpretation of model outputs, is critical to maximizing the potential of AI in drug discovery research.[17] ZairaChem is now being applied to Gram-negative and Gram-positive pathogens responsible for antibiotic-resistant microbial diseases that are of global interest, given the threat of antimicrobial resistance.

More advanced applications include the use of generative AI techniques in the *de novo* design of small molecules. Considering the vastness of small-molecule chemical space, AI facilitates the exploration of this chemical space to generate safe and efficacious molecules. Generative AI methods produce vast libraries of virtual compounds that need to be logically filtered to a more manageable subset that balances chemical novelty with relevance to the project; the H3D Center has begun exploring these methods in programs across its different disease areas. Multimodal AI models link different data sources, such as images with assay data, to improve the accuracy of model predictions or answer new research questions. For example, image classification models can be trained on microscopy images to identify cell phenotypes associated with inhibiting specific proteins, an approach the H3D Center is exploring to understand potential malaria treatments. Thus, AI has enhanced researchers' ability to design drugs more efficiently and accurately and better understand disease biology.

Further AI applications include pharmacogenomics research, in which sophisticated AI tools are utilized to customize drug dosages and predict treatment outcomes based on genetic markers of specific diseases. This translates to a more personalized treatment of disease, which is vital for the African context. Despite being the most genetically diverse continent, Africa's severe paucity of clinical trials, as discussed earlier, has led to suboptimal treatment outcomes and raised questions about dose optimization for its population. AI-assisted data analysis of the clinical data landscape in Africa can improve clinical trial design and help increase the efficacy of clinical trials.[18] In these ways, AI can help to tailor drugs for the genetically diverse African population.[19]

At H3D, our initial contribution has been to apply a transfer-learning approach to mitigate the low-data paradigm and to identify relevant pharmacogenes for a given drug molecule. To do this, we integrated clinical and preclinical drug and gene data available in the public domain (that is, from prior experiments conducted globally). The Project Africa GRADIENT (Genomic Research Approach for Diversity and Optimizing Therapeutics) initiative explores the influence of the continent's genetic variability on existing therapies, especially for malaria and tuberculosis.[20] H3D's project within this initiative looked at the potential of AI/ML in pharmacogenomics to predict dosing adjustments for some drugs from a list of over thirty malaria and tuberculosis drugs prescribed in Africa. The predicted metabolism-related genes could then refine pharmacometrics models for human dose predictions to

optimize treatment for an individual's genetic makeup.[21] Genetic data collection conducted across the continent should greatly advance pharmacogenomics research in Africa enormously.

Despite the immense potential and noteworthy accomplishments of AI-assisted drug discovery research, there are significant challenges that stand in the way of its acceptance, adoption, and uptake. And within this context, there are the Africa-specific and major challenges of internet connectivity, low AI literacy, and limited digitalization. Further, the dominant discourse around AI is polarized, with sharp divides regarding the ethics of how AI models are trained, how they interact with intellectual property (IP) rights, and what tasks AI will "take over," possibly costing people their livelihoods.

The hype surrounding AI and the debates it spawns leave us with a paradigm in which many intended end users, including scientists, are skeptical of AI, if not hostile to it. End users are often not computationally trained, and their uptake of AI is hindered by a poor understanding of how to leverage insights from AI, as well as a lack of trust in predictions typically produced by "black box" models. It is reasonable to surmise that skepticism around AI is more pronounced and/or exacerbated in Africa due to the continent's history and limited access to the basic infrastructural ingredients that underpin AI.

An added challenge is that interaction with AI is fundamentally different from how society is accustomed to interacting with standard computer algorithms. Traditionally, computers have been used as "calculators" that follow a predefined formula to arrive at an output. However, AI output is intrinsically more probabilistic and leverages past learnings and context to make predictions. These are not – and will not always be – correct for every given input, but they still provide value at a larger scale over many molecules. Iterative testing can help bridge this lack of trust.

The biggest fear surrounding the proliferation of AI tools is that they will replace jobs. Though the experience in drug discovery so far has clearly shown that AI tools can neither substitute entirely for traditional research methodologies nor replace researchers' expertise, AI tools offer predictions and insights subject to the data they are provided with. Making sense of these insights in the context of the research requires human intervention. Skeptics have also suggested that scientists who do not embrace AI could lose their jobs. But we have already seen AI facilitate job creation, as in the context of digital health care. For Indian hiring companies, health informatics and medical AI are rapidly becoming two of the most promising career paths, evidenced by the number of informatics jobs created by hospitals, startups, government departments, and individuals who studied in technology fields.[22] The *complementary* design-make-test-analyze approach used for small molecule drugs – which takes advantage of AI's cost-effective, time-saving properties through the

rapid analysis of vast datasets or chemical spaces – alongside the skills and knowledge of human researchers is the way forward to optimizing drug discovery research.

Another major challenge concerns data. Researchers working with AI tools rely heavily on the availability of data to train their models and derive insights. While pharmaceutical datasets are vast, they are often severely access-limited. Datasets that are publicly available (such as clinical trial data) may be of poor quality, as they often are more biased due to being collected in a more-restricted context, and are smaller and heterogeneous, since they come from multiple sources. AI tools trained on such noisy data are susceptible to inaccurate predictions; this limits the applications of AI and the development of novel tools that could accelerate research. It could also lead to the development of drugs with limited efficacy in certain populations, as many African countries lack comprehensive biobanks, standardized health records, and data-sharing infrastructure. Existing datasets often reflect non-African populations, leading to models that may not generalize well in African contexts. There are also challenges around data governance, including ethical concerns, patient consent, and the risk of data exploitation. Addressing these issues requires investment in local data infrastructure, research capacity, and policies that promote equitable data ownership and sharing.

While the latest literature reports many new AI-driven drug discovery research tools, there is often little funding incentive to make these tools easily accessible, open-source, or regularly maintained through periodic retraining. As a result, the scientific literature on the development of AI tools for drug discovery grows rapidly with little emphasis on adoption of these tools postpublication.

EOSI is actively taking on this challenge with its Ersilia Model Hub. By disseminating AI models and published findings to researchers in the Global South, they enable the improvement of drug discovery efforts in low-resource regions. Most of the Hub's computational models are open-source and publicly available, contributed largely by data scientists and software engineers, and most users belong to drug discovery institutions across sub-Saharan Africa. Because they allow researchers to computationally simulate the interaction between a drug candidate and a specific disease pathogen, these models are cost-effective. H3D is EOSI's biggest partner in Africa.

As with all new technologies, the question of ethics is crucial. We must strike a balance between patient rights and the use of technology when we incorporate AI tools into drug discovery research. Sensitive data collected from patients for clinical trials must be treated with the utmost care and anonymity to ensure their privacy is not compromised. Informed consent is also essential to mitigate the continent's historical distrust of clinical trials. Regular audits of AI algorithms and their updates with the latest and most diverse datasets can address the challenge of bias in data that, as discussed, can reduce the efficacy of drugs produced for underserved populations. This is even more important in Africa. IP protection of drug discovery datasets is equally important. We need to find ways to incentivize

industry and African partners to share their datasets, if not publicly, then at least to train AI models for the benefit of the global community. It would be inequitable for Global North companies to retain their data confidentiality while African institutes are expected to relax their data confidentiality for the sake of AI progress.

These actions require collaboration between researchers, health care providers, data scientists, and software developers. Such practices help to build confidence in clinical trials and foster greater participation, allowing AI to enter the public health domain in an environment of positivity and trust. After all, new technologies are meant to enhance equity in public health rather than perpetuate existing inequalities and exacerbate social injustices. Hence, without addressing these structural gaps, AI risks reproducing existing inequities rather than resolving them. Alternatively, if developed in a locally relevant and inclusive way, AI could help reposition Africa from a passive recipient of health innovations to an active contributor to global biomedical research.

We are at a pivotal stage in the history of drug discovery and public health. The transition from traditional research methods to AI-assisted research will provide scientists and researchers with tools that catalyze processes and achieve better results. With the assistance of AI, the coming decades could see the Global South, especially Africa, make great progress to level the global playing field of pharmaceutical innovation and give the African people the cost-effective, efficacious treatments that they need. And while this essay has not placed much emphasis on generative chemistry and associated synthesis planning or on lab automation, all of which AI can facilitate, these can have critical importance in Africa, where the medicinal chemistry capacity is smaller than in the Global North. Furthermore, given the long history in Africa of exploring products from various natural sources, including African traditional medicines, for drug discovery, there is a tremendous opportunity to integrate AI into African natural products research. For example, AI can help to predict the activity of natural products like those derived from plants widely used in African traditional medicines, elucidate the composition of lab extracts, and help "simplify" natural product structures so they are more synthetically accessible.

Extensive training and consultations are the first steps toward growing literacy around AI tools and enabling the subsequent adoption of AI technologies. Ironically, it is this "human interaction" that minimizes the perceived barriers to the adoption of AI-based insights. In this regard, capacity-building activities such as workshops are crucial as they can aid the emerging networks of African scientists. This has already been demonstrated by workshops run jointly by the H3D Foundation and EOSI through my Schmidt Sciences AI2050 Senior Fellowship.

As AI becomes more prevalent in modern society, the importance of large-scale and high-quality data is becoming increasingly apparent. AI models need to be

trained on diverse and representative datasets to ensure biogeographical and/or ethnic representativeness. Truly democratized access to the benefits of AI will first require an increase in democratized access to data. These models must also be periodically reviewed and updated with newer data to ensure that their intervention follows the evolving realities of the infectious disease scenario in Africa.

Sensitive patient data such as medical histories and genetic information need to be protected to build wider trust in AI-assisted drug discovery processes, especially among governments, the media, and the larger public. Robust regulatory and ethical frameworks must consider how AI influences drug discovery processes to ensure that medicines developed with AI support continue to be held to the same rigorous standards as those that have been developed traditionally. "Federated learning" or "swarm learning," in which multiple institutions (such as hospitals) use their data to train an AI model jointly in a privacy-protected way, should be encouraged.

Historically, Africa has often been marginalized in global biomedical research, with its role largely limited to sites for occasional clinical trials, rather than as a hub for innovation. However, recent shifts – such as the growth of African genomics initiatives and the continent's increasing digital connectivity – signal a potential turning point. Looking ahead, the integration of AI into drug discovery offers a chance not only to leapfrog infrastructural limitations but also to redefine Africa's role in shaping global health solutions. If aligned with long-term investments in education, data sovereignty, and equitable research partnerships, the next five to ten years could see Africa moving from being underrepresented in the medical research pipeline to playing a leadership role in developing treatments for both local and global health challenges.

Around the world, AI has forced professionals to fundamentally rethink the way they approach their work. In science, AI has shown – and realized – great potential as a tool that augments the intellect and rigor of the scientist; a companion that catalyzes processes and allows humans to devote more time and thought to the problems they are trying to solve. Its relative cost-effectiveness democratizes scientific research and opens the door for researchers in the Global South, especially in Africa, to participate in the cutting-edge of drug discovery and achieve positive change for the people that need it the most.

The story of AI in African drug discovery is not only about present capabilities but also about reclaiming agency over future biomedical innovation. AI can be of interest in Africa for various applications, including better characterization of pathogen biology (in particular, to discover new essential/vulnerable proteins in poorly studied organisms), identification of drug repurposing opportunities, prediction of pathogen drug resistance, and elucidation of active natural products from medicinal plants.

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