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How AI Is Accelerating Drug Repurposing & Therapeutic Innovation in India

01 September 2025 | Views | By Dhaval Vasavada, Associate Director - Information, Data and Technology (IDT), Healthark

With India facing increasing disease burdens and deficiencies in healthcare infrastructure, AI is becoming a driving force for quicker, more intelligent therapeutic advancements. Indian startups and institutions are making significant contributions through drug repurposing, enhancing diagnostics, genomics, and clinical research.



India's healthcare system is at a pivotal moment. The numbers tell a stark story - non-communicable diseases now cause 66 per cent of all deaths while a staggering 2.4 million hospital bed shortfall intensifies the pressure on limited infrastructure. Add to that a highly cost-sensitive market where over 50 per cent of healthcare expenses are paid out-of-pocket, and the urgency for faster, more efficient treatment pathways becomes clear.

One promising solution gaining momentum is drug repurposing - the game changing strategy of finding new therapeutic uses for existing drugs. This is accelerated by the growing adoption of artificial intelligence (AI) tools that can cut early-stage development costs by up to 50 per cent.

AI plays a crucial role in unlocking the full potential of drug repurposing by analysing vast and complex datasets such as clinical records, biomedical literature, molecular pathways, and real-world evidence to uncover hidden drug-disease relationships. Unlike traditional methods, AI enables faster hypothesis generation, predictive modeling, and risk profiling at scale. In India, where time and cost constraints are particularly acute, this ability to accelerate discovery and reduce trial-and-error makes AI not just a helpful tool, but a transformative enabler across drug development and other therapeutic areas like oncology, rare diseases, and infectious conditions.

AI in Drug Repurposing: Use Cases from India

AI-powered drug repurposing is rewriting the rulebook, cutting development time and costs by 50-60 per cent compared to building drugs from scratch. Across India, pioneering platforms are harnessing machine learning, natural language processing, and molecular modeling to breathe new life into existing compounds

Game changing AI workflows in action

Advanced platforms are leveraging deep learning, cheminformatics, and molecular modeling to accelerate both novel drug discovery and drug repurposing. These systems integrate capabilities like target identification, virtual screening, and compound property prediction (e.g., ADMET, toxicity, reaction outcomes) to efficiently prioritise candidates for lab validation. Sravathi AI, a Bengaluru-based pharma-tech startup is using this approach for integrating AI workflow to identify and validate repurposed drug candidates, thereby supporting drug repositioning efforts

Breathing new life into safe compounds

AI is also enabling the rescue and repositioning of approved drugs and late-stage clinical assets by identifying new indications with strong safety profiles. Using a combination of generative AI, deep learning, and chemical data processing, these platforms aim to accelerate development in hard-to-treat domains like rare diseases, oncology, and inflammation. This approach is exemplified by Peptris Technologies, which raised \$1 million in 2023 to expand its pipeline. A landmark case is PEPR124 (RT001): India's first AI-discovered drug candidate, repurposed for Duchenne muscular dystrophy (DMD). Licensed to Revio Therapeutics in March 2025, the asset retains commercialisation rights in BRICS countries with Peptris, while Revio will drive global development outside BRICS.

Next-Gen Generative Platforms

Modular, multi-agent platforms are also emerging to streamline the design of small molecules, clinical trial simulation, and protein engineering. Tools within these systems handle retrosynthetic planning, multi-omics analysis, and digital twin modeling, enabling end-to-end AI-guided drug development.

A prominent example is Boltzmann Labs, which began using its in-house suite (BoltChem, ReBolt, BoltBio, BoltPro, ClinBolt) on internal discovery programmes in 2023, backed by \$113,000 in total funding including a \$200,000 ML Elevate grant.

AI Applications Beyond Drug Repurposing in India

AI's impact extends far beyond drug repurposing, revolutionising diagnostics, genomics, and hospital operations across India. The country's recent launch of its first 10,000 whole genome sequence dataset signals a major leap toward population-scale precision medicine.

AI-powered imaging tools are transforming medical diagnostics by enabling rapid interpretation of chest X-rays, brain scans, and CTs, especially in under-resourced regions. These solutions aid in early detection of diseases such as tuberculosis, stroke, and lung cancer, making timely care more accessible across both urban and rural healthcare systems. Qure.ai, one of the leaders in this space, whose suite including qXR, qER, and qCT, has been using this technology widely to bridge diagnostic gaps in India and beyond.

Generative AI is also reshaping medical research by streamlining systematic literature reviews (SLRs), clinical evidence reports (CERs), and targeted literature reviews (TLRs). These platforms can reduce review time by nearly 50 per cent, with 90 per cent+ accuracy in title and abstract screening and over 80 per cent accuracy in data extraction, dramatically accelerating insights generation. Such capabilities are showcased by MadeAi, developed by CapeStart, which also received the 2025 Artificial Intelligence Excellence Award and is in use by leading pharmaceutical companies worldwide.

Building India's AI Healthcare Empire

India is laying foundational infrastructure to support the growth of AI across health and biotech, driven by digital public goods, academic partnerships, and strategic funding. Some recent examples attest to the significance of these elements in shaping up India's AI healthcare ecosystem.

- In September 2024, the National Health Authority and Indian Institute of Technology (IIT) Kanpur signed a Memorandum of Understanding (MoU) to build federated learning, consent, and benchmarking platforms under Ayushman Bharat Digital Mission (ABDM). This initiative aims to enhance AI model validation while protecting patient data privacy.
- The 2025 Union Budget allocated Rs 500 crore for establishing AI Centres of Excellence, including AIIMS, IITs, and others, bolstering healthcare-focused AI research.
- Initiatives like Atal Innovation Mission, IIT Hub Gujarat, and Bengaluru's new Global Innovation Hub are nurturing deep-tech startups, providing lab facilities, investor access, and mentoring for scaling AI-driven health solutions.

Shaping AI-driven Drug Discovery

As India grapples with rising disease burdens and healthcare infrastructure gaps, AI is emerging as a catalyst for faster, smarter therapeutic innovation. From repurposing drugs to advancing diagnostics, genomics, and clinical research, Indian startups and institutions are delivering real-world impact.

What amplifies this momentum is growing ecosystem readiness, unified health data under ABDM, dedicated AI Centers of Excellence, and a surge in industry-academic collaboration. If India continues to connect these strengths, it could accelerate not just its own healthcare transformation, but help shape the global future of AI-driven drug discovery.

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