The Future of AI in Drug Discovery: A Biology-First Asset Origination Model

Artificial Intelligence is here to stay. AI is now firmly embedded in drug discovery and, for senior scientific and business leaders, the strategic question is no longer whether AI will be used, but how it is applied in a way that creates durable scientific advantage and sustainable portfolio value. Over the past decade, AI has demonstrated clear utility in automating research tasks and accelerating medicinal chemistry. These advances have improved efficiency and reduced cost per programme, but they have not materially altered the fundamental economics of drug discovery. Failure rates remain stubbornly high, largely because the primary source of risk lies upstream in biology rather than downstream in chemistry.

The first phase of AI adoption in drug discovery focused on automation. AI systems have proven highly effective at standardising and accelerating activities such as image analysis, literature review, data curation, clinical trial logistics and manufacturing optimisation. These tools are now widely available and increasingly commoditised. They are valuable, but they no longer confer meaningful competitive advantage. Automation improves execution, but it does not change direction.

More recently, AI has delivered substantial gains in medicinal chemistry. Advances in molecular design, virtual screening, docking, and protein structure prediction have significantly accelerated the identification and optimisation of drug candidates. These tools allow organisations to move faster and explore chemical space more efficiently than ever before. However, faster molecule generation does not address the dominant cause of failure in drug discovery: insufficient understanding of disease biology and target relevance.

> "The greatest long-term impact of AI will … come not from further optimisation of chemistry, but from its application to the discovery and interpretation of human disease **biology**."
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> Dr Simon Haworth,
> CEO Intellomx

Without confidence in target selection, accelerated chemistry simply leads to faster attrition. Across therapeutic areas, the majority of programmes fail because the underlying biology is not sufficiently causal, context-appropriate, or translatable to patients.

This transition represents a shift from first-generation AI, focused on automation and optimisation, to second-generation AI, focused on biological discovery and causal understanding. Much of today's AI activity is concentrated on mining existing knowledge — the visible portion of scientific understanding represented by published literature and basic analyses of curated databases. While this has delivered incremental value, it addresses only a small fraction of the biological landscape. The majority of disease biology remains unexplored, undocumented, and inaccessible to either traditional methods or first-generation AI and LLMs.

The next generation of AI in drug discovery must therefore move beyond correlation and literature inference toward de novo modelling of disease systems. This requires approaches capable of extracting causal structure directly from human molecular data and of generating interpretable models that can be interrogated, validated, and acted upon. This is the domain in which Intellomx operates.

Intellomx applies proprietary, interpretable AI methods to large-scale human molecular datasets, most commonly transcriptomic data, to construct mathematical models of disease biology. These

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models are designed to reveal causal drivers of disease rather than downstream effects, enabling clear differentiation between targets that are biologically essential and those that are merely associated. Importantly, Intellomx advances this biology internally, validating targets experimentally and generating data packages that materially reduce biological uncertainty.

Intellomx engages with pharma and diagnostics partners using a twin-track business model covering in-house asset discovery and licensing, or a services and risk share model, typically in oncology, obesity/metabolic disease, autoimmune, neurodegeneration or infectious disease. Solid tumours in oncology, ALS in neurodegeneration and alternative approaches to GLP-1 in metabolic disease/obesity are currently in progress as our top priorities.

- In the **asset model**, programs are advanced internally to defined biological and translational milestones, creating assets that partners can access through structured options and downstream licensing arrangements. This approach aligns incentives, reflects the value of early biological risk reduction, and allows partners to secure early access to differentiated biology without committing full development capital before risk is sufficiently resolved;

- In the **services model**, Intellomx uses the in-house platform to analyse third-party data, alongside public and Intellomx datasets, for big pharma and diagnostic companies. Intellomx delivers novel targets based on biological understanding of each partner's area of focus. A material portion of our reward remains contingent on success, even in the services model.

A further advantage of Intellomx's approach lies in model interpretability and resource efficiency. Large, opaque AI models impose significant computational costs and present challenges for scientific and governance review. In contrast, Intellomx employs swarms of smaller, interpretable models that can be individually examined and collectively integrated. This architecture enables transparent decision-making, facilitates internal and external review, and supports use in regulated environments.

As biological understanding improves, second-generation AI also enables new approaches to translational risk management. Intellomx is developing increasingly sophisticated digital representations of human biology that allow prediction of off-target effects, assessment of target safety, and stratification of patient populations. In the near term, these capabilities inform trial design and companion diagnostic strategies. Over time, they may substantially reduce reliance on late-stage experimental failure.

Ultimately, successful drug discovery requires alignment of three factors: the right target, the right patient population, and the right drug. Our greatest contribution lies in strengthening the first two of these. By originating biologically de-risked assets and offering partners structured access through option and licensing models, Intellomx seeks to enable more confident decision-making, more efficient capital deployment, and improved outcomes across R&D portfolios.

AI will not eliminate failure from drug discovery, but it can ensure that resources are focused on the right biological questions. The strategic challenge for organisations in 2026 and beyond is to apply AI where it matters most: at the point where biological uncertainty is created or resolved.

Artificial Intelligence is indeed here to stay. But not perhaps as you know it.

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