EightAdvisory

The AI Revolution in Drug Development

A new era empowering performance, innovation and care

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Summary

AI Across the Drug Development Lifecycle

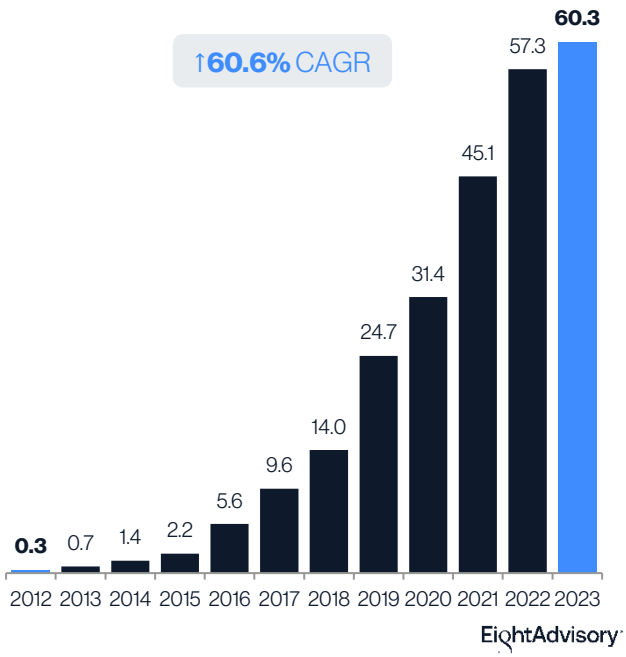
The rise of AI is reshaping pharmaceutical pipelines

From early discovery to post-market monitoring, artificial intelligence (AI) is becoming a transformative force across the drug development lifecycle. A 2024 World Health Organisation (WHO) report[1] suggests that in the future "every new drug" could involve some aspect of AI in its development. This optimism is backed by surging investment: global funding for top AI-focused pharma companies has grown **~27-fold** since 2015, reaching about **$60.3 billion** in 2023[2]. Such capital reflects high expectations that AI can help streamline the typical **10–15 year, ~$2 billion** drug R&D process.

Major pharmaceutical firms have been cautious but steadily increasing AI adoption. Currently, AI is largely used to *augment (not replace)* traditional R&D methods, with demonstrated benefits in all stages of development. Notable gains include *faster timelines, lower R&D costs, and improved success rates.* However, this is not without challenges to address such as: *data quality*, *algorithm transparency*, and *regulatory acceptance*[3].

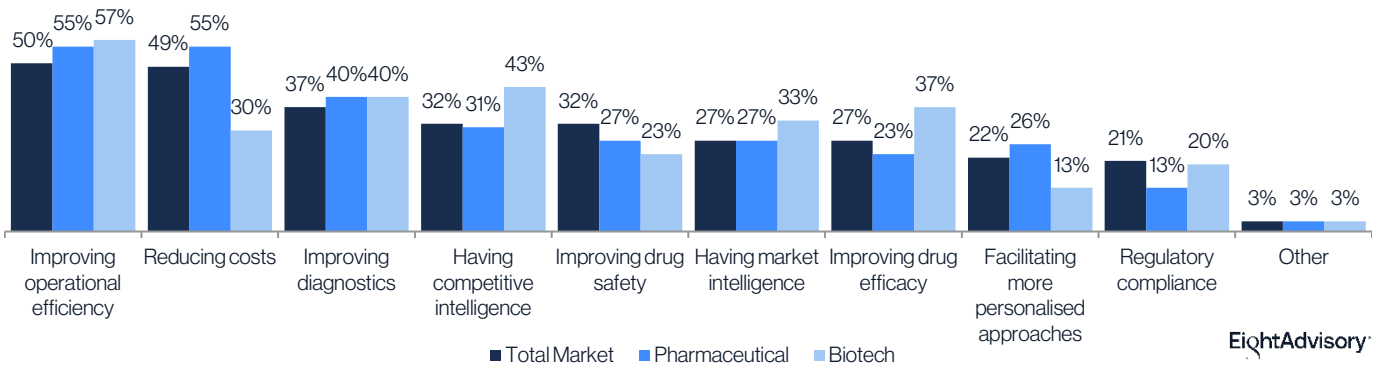
The following report summarises AI's impact at each stage of the drug development, with an emphasis on recent advances and the UK context.

Figure 1: Cumulative Investment in AI for Top 800 Pharma R&D Firms ($bn)



Source: Deep Pharma Intelligence (Artificial Intelligence for Drug Discovery Landscape Overview Q3 2023)

Figure 2: Main Benefits of Using AI in Pharmaceutical R&D according to industry survey respondents



Source: Norstella (State of the industry: AI advances in pharmaceutical R&D survey 2024)

[1] https://www.drugdiscoveryonline.com/doc/ai-and-pharmaceutical-development-who-calls-for-ethical-framework-good-governance-0001
[2] https://www.linkedin.com/pulse/global-state-ai-drug-discovery-defined-new-report/
[3] https://www.clinicalleader.com/doc/global-ai-in-clinical-trials-market-trends-current-partnerships-0001

AI in Drug Discovery and Preclinical Research

01. Target identification:

AI systems can mine genomics and proteomics data to identify novel drug targets such as disease-driving proteins. Furthermore, by analysing large datasets, AI can uncover hidden patterns that reveal secondary uses for existing drugs or unrecognised disease pathways[1].

02. Generative molecule design:

Once a target is selected, AI models can design potential drug molecules with desired properties. Generative adversarial networks and other deep learning models (sometimes termed '*ML-driven molecule design*') are now routinely used to propose novel chemical structures.

03. Virtual screening and prediction:

AI accelerates virtual screening by evaluating millions of chemical structures and predicting binding affinity using models trained on known actives. By forecasting bioactivity, solubility, permeability, and toxicity, it filters out weak or impractical candidates early, helping chemists avoid late-stage failures.

04. Preclinical testing:

During the preclinical phase, AI can enhance research and optimise experimental design. For example, deep learning applied to in vitro assay data or animal study results can detect subtle patterns such as changes in gene expression that may predict drug efficacy or side effects. Predictive toxicology models further reduce reliance on animal testing, while AI learning from prior results helps minimise experimental redundancy.

False starts and future potential

AI is transforming drug discovery by accelerating hit identification, designing novel chemical matter, and improving early-stage success rates. Globally, dozens of AI-designed or AI-discovered drug candidates have entered development pipelines. However, not all have succeeded. In 2023, several high-profile setbacks highlighted the complexity of biology. AI is not a panacea, and rigorous experimental validation remains essential.

Nonetheless, the trend is clear: AI has become an indispensable tool in early-stage drug research, with broad industry adoption expected to drive market growth from $1.7 billion in 2023 to a projected $12 billion by 2032[2].

Generative molecule design:

In 2020 **Exscientia** (an Oxford-based AI drug discovery firm) and **Sumitomo Dainippon Pharma** designed a new compound for obsessive-compulsive disorder entirely using AI, achieving in less than 12 months a stage of candidate nomination that normally takes 4–5 years. This AI-designed drug (DSP-1181) entered human trials in Japan in what was the first AI-created molecule to do so[2].

Target identification:

UK-based BenevolentAI used its AI to pinpoint baricitinib (an existing arthritis drug) as a treatment for COVID-19 in 2020, an insight that was later validated clinically. This kind of in silico target discovery accelerates the ideation of viable drugs.

Not all have succeeded:

Even though these experiences have advanced the use of AI in drug discovery and provided valuable learnings, **BenevolentAI**'s lead dermatitis drug (an AI-identified molecule) did not achieve its Phase II goals[1], and in Japan, **Sumitomo's AI-designed** psychiatric drug did not meet its Phase III[1] endpoint.

[1] https://www.drugdiscoveryonline.com/doc/ai-and-pharmaceutical-development-who-calls-for-ethical-framework-good-governance-0001
[2] https://cen.acs.org/pharmaceuticals/drug-development/Sumitomo-Dainippon-puts-drug-developed/98/i6

AI usage in Clinical Trials

In addition to growing use during the pre-clinical stages, AI is assisting clinical trials through:

01. Patient recruitment

Recruiting eligible patients remains one of the most significant bottlenecks in clinical research. AI can streamline this process by analysing electronic health records and real-world data to **match patients with trials more efficiently**. In oncology, where eligibility criteria are complex and suitable participants are limited, machine learning models can scan hospital records to identify candidates who meet inclusion requirements, significantly **reducing recruitment time**.

02. Intelligent trial design

AI supports more adaptive and efficient trial design than traditional fixed protocols. It can help identify *better endpoints*, *stratify patients by risk*, and even *adjust dosing in real time*.

Digital twins, or virtual patient simulations, allow researchers to explore multiple "what-if" scenarios before launching a trial, leading to more refined protocols. Jun Deng of Yale observed that each real patient can be modelled in numerous virtual forms, allowing researchers to expand sample size and test varying responses[1]. This is particularly useful in rare disease trials, where small patient populations make recruitment difficult. AI-powered simulations and Bayesian integration of historical data can enhance statistical power[2].

AI can also propose **adaptive trial rules**, such as discontinuing ineffective treatment arms early or dynamically adjusting inclusion criteria, which may **shorten trial timelines by 15% to 30%** without compromising scientific integrity[3].

03. Real-time monitoring

Throughout a trial, AI can continuously assess incoming data to **detect safety issues or efficacy trends** more quickly than traditional methods.

Machine learning models can uncover subtle signs of treatment response or highlight subgroups showing stronger outcomes, **enabling mid-trial adjustments**. Predictive models may forecast trial outcomes early, helping researchers make informed go or no-go decisions. In operational management, AI can flag underperforming sites, detect protocol deviations, and optimise logistics. Natural language processing also plays a role, automating tasks such as extracting patient data from medical records and matching trial criteria, which traditionally required substantial manual effort.

[1] https://www.healthcare-brew.com/stories/2024/12/12/how-digital-twins-could-change-clinical-trials
[2] https://pmc.ncbi.nlm.nih.gov/articles/PMC11263130
[3] https://www.clinicalleader.com/doc/global-ai-in-clinical-trials-market-trends-current-partnerships-0001

AI usage in Clinical Trials – Examples

As the integration of AI in clinical trials continues to revolutionise research methodologies, numerous real-world examples demonstrate its transformative impact:

Digital twins

Early adopters such as **AstraZeneca, Bayer, Sanofi, and Merck KGaA** have integrated digital twins into clinical trial design[1]. In one case, **Unlearn** used **AI-generated "virtual patients"** to replace part of the control arm, cutting its size by 33 percent. For a 1,000-patient trial, this could reduce enrolment time by 4 to 5 months[1]. Bayer also used digital twins to **optimise dosing in an anticoagulant study** where control groups were not feasible. U.S. federal support has followed, including a $6.0 million National Institutes of Health (NIH) and NSF programme launched in late 2024 to explore digital twin-based research[1].

Predictive power

IQVIA, a global provider of analytics to the life science industry, highlighted a case where an AI and machine learning platform **automated feasibility assessments for clinical sites**, **reducing the time required by 90%** and accelerating trial start-up[2]. In ongoing oncology trials, predictive models have improved patient stratification and **enabled earlier intervention, contributing to 15% - 25% lower cancer mortality** among trial participants[2]. While these outcomes may reflect controlled settings, they underscore AI's potential to identify optimal treatment paths during the trial itself.

Intelligent trial design

In a recent rare disease trial, AI replaced a traditional endpoint with frequent biomarker measurements, **reducing trial duration by nearly one-third**[2]. Major firms are following suit. AstraZeneca, in collaboration with **Immunai**, used AI-driven analytics to refine dose selection and biomarker strategy, achieving up to a 25% reduction in cancer trial durations[2].

Framing the Future

AI is making trials faster and more likely to succeed. Surveys suggest most trials will use AI within a decade. The business case is strong: **pharma–tech partnerships focused on AI rose ~30% from 2022 to 2024, while funding for top AI-in-pharma firms has grown ~ 27-fold since 2015**. The market for AI in clinical trials is projected to grow ~25% annually, reaching ~$8.5 billion by 2030. Regulators are cautiously supportive, requiring that AI decisions remain transparent and validated. As a result, adoption is accelerating but remains evidence-based[2].

[1] https://www.healthcare-brew.com/stories/2024/12/12/how-digital-twins-could-change-clinical-trials
[2] https://www.clinicalleader.com/doc/global-ai-in-clinical-trials-market-trends-current-partnerships-0001

UK Perspective and Recent Developments

UK leadership and initiatives

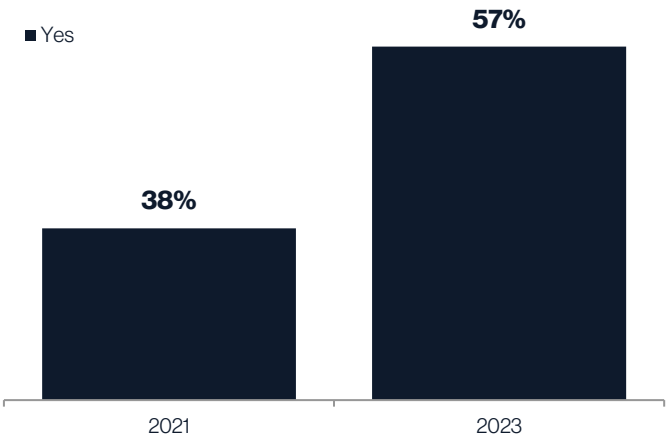
The UK's pharma sector is proactively adopting AI, with homegrown leaders like **Exscientia, BenevolentAI, and Healx**, along with major global firms such as GSK and AstraZeneca, investing heavily in AI research.

The MHRA's strategic roadmap for AI, published in April 2024, acknowledges AI's potential to expedite drug development and trial design while outlining a regulatory sandbox to promote safe innovation[1].

On the talent front, the UK is enhancing training in data science and AI for life sciences. A 2023 report from the Association of the British Pharmaceutical Industry (ABPI) revealed that 57% of UK pharma companies identified digital and AI skill gaps as a recruitment challenge, highlighting the urgent need for AI proficiency in drug R&D[2].

Various initiatives are addressing this, including new MSc programs in AI for drug discovery and industry-academia partnerships, such as **King's College London collaborating with GSK on AI-driven cancer drug discovery**[3].

Figure 3: Survey to UK pharma firms: *Are digital and AI skill gaps a recruitment challenge?*



Source: ABPI: Evolution of an innovation-based biopharmaceutical industry (2023)

Recent notable healthcare & AI partnerships:

Companies	Rationale
GSK & NVIDIA	GSK partnered with Nvidia to construct an AI lab to accelerate drug and vaccine discovery using genomic and biological data[4].
GSK & Cerebras	To enhance drug discovery process by using a deep learning model to integrate DNA sequences with large datasets[5].
AstraZeneca & ZS	Supporting clinical development through real-world evidence, aiming to enhance trial design, patient recruitment, and overall efficiency[6].
Merck KGaA & Unlearn.AI	Integration of Unlearn's Digital Twin trials capabilities, helping to reduce required participant numbers and maintain the integrity of randomised controlled trials[7].
Pfizer & IBM Watson	To aid immuno-oncology lead optimisation and identify clinical candidates faster than traditional methodology[8].

[1] https://www.raps.org/news-and-articles/news-articles/2024/5/euro-roundup-mhra-outlines-potential-impact-of-ai
[2] https://www.abpi.org.uk/media/news/2023/june/uk-life-sciences-in-search-for-ai-digital-and-data-talent
[3] https://www.mobihealthnews.com/news/emea/kings-college-london-and-gsk-collaborate-new-ai-led-cancer-research
[4] https://www.pharmaceutical-technology.com/news/nvidia-gsk-ai
[5] https://www.hpcwire.com/2022/01/28/cerebras-gsk-team-for-unprecedented-epigenomic-models
[6] https://www.zs.com/insights/astrazeneca-using-real-world-evidence-clinical-development
[7] https://www.businesswire.com/news/home/20220216005466/en
[8] https://www.clinicalleader.com/doc/global-ai-in-clinical-trials-market-trends-current-partnerships-0001

UK Perspective and Recent Developments

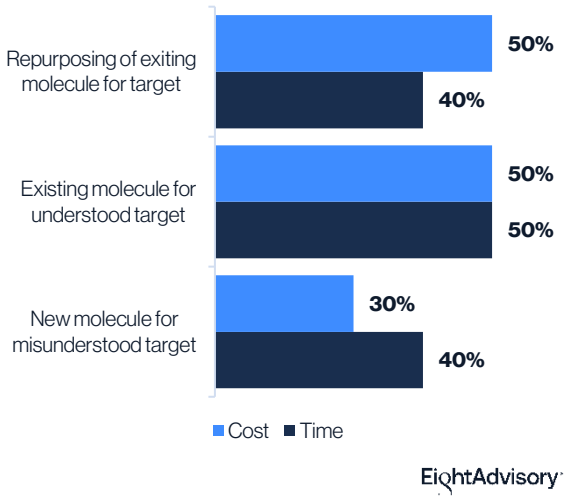
UK Government support

UK government initiatives are injecting substantial funding to drive AI in drug development. In October 2023, the UK government launched the **'AI Life Sciences Accelerator Mission'** with a **£100 million investment** specifically to leverage AI for new treatments targeting diseases like cancer and dementia[1]. More recently, in February 2025, the UK government announced £82.6 million in funding to support AI-driven cancer care, drug discovery, and water management research, including major projects like PharosAI, Bind Research, and MEMetic. It also committed £7.8 million to expand UK participation in the European High-Performance Computing partnership, reinforcing its plan to harness AI for healthcare innovation, economic growth, and scientific collaboration[2].

Impact on drug discovery and design

Recent data underscores how much AI is shortening the drug development process. It is estimated that AI workflows can introduce cost and time efficiencies, up to 30% and 40%[3], respectively, in bringing a new molecule to the preclinical candidate stage. While industry average success rates for Phase I success rates generally fall around 50%[4], AI-discovered compounds are showing early signs of better productivity. They show notably high Phase I success (80%-90%) and at least average Phase II success (~40%)[5]. If these trends hold as more AI-designed drugs advance, we could see a higher overall yield in drug pipelines – a major boost to productivity in an industry where ~90% of candidates fail to reach market. On the flip side, R&D timelines are contracting in areas where AI is applied. Several case studies report time savings of 1–2 years in discovery or trial phases due to AI.

Figure 4: Potential time and cost saving through AI usage in drug discovery, globally



Source: Coherent Solutions: Artificial Intelligence in Pharmaceuticals and Biotechnology: Current Trends and Innovations

Global Arms Race

Overall, the past few years have solidified AI's role from a novel experiment to a standard component of pharma strategy. The UK stands out as both a contributor and beneficiary of this trend – home to leading AI biotech firms, supportive policies, and major pharma activities. Yet, the global race is on; other regions (US, EU, China) are equally aggressive in deploying AI for drug discovery.

For UK pharma players, the key takeaway is that AI is no longer optional – it is becoming fundamental to remain competitive.

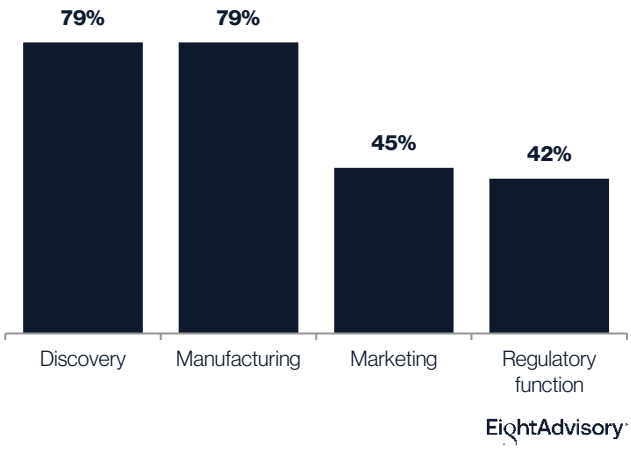
[1] https://www.pharmaceutical-technology.com/news/uk-ai-drug-development
[2] https://www.gov.uk/government/news/uk-backed-ai-companies-to-transform-british-cancer-care-and-spark-new-drug-breakthroughs
[3] https://www.coherentsolutions.com/insights/artificial-intelligence-in-pharmaceuticals-and-biotechnology-current-trends-and-innovations
[4] https://www.norstella.com/why-clinical-development-success-rates-falling
[5] https://pubmed.ncbi.nlm.nih.gov/38692505

Conclusion and Outlook

Future outlook

Success in this AI-driven paradigm necessitates addressing several critical challenges. Data quality and sharing pose significant hurdles; therefore, initiatives to curate large, diverse biomedical datasets while ensuring privacy protection will be essential. Companies must also build trust in AI by guaranteeing the transparency and validation of their models. This includes advancing efforts in explainable AI and implementing effective bias mitigation strategies to ensure that AI-driven decisions are both fair and generalisable[1]. Regulatory agencies are actively engaging with stakeholders to update guidelines and promote the responsible use of AI, as demonstrated by recent actions from the Food and Drug Administration (FDA and Medicines and Healthcare products Regulatory Agency (MHRA). These collaborative efforts are pivotal in determining how swiftly AI's potential can be translated into tangible benefits for patients through innovative therapeutics.

Figure 5: Estimated AI Integration by Drug Development Phase (2025)



Source: Arnold & Porter: The Convergence of Life Sciences and Artificial Intelligence: Seizing Opportunities While Managing Risk

In the next 5-10 years we can expect :

- Late-stage trials and potential approvals of AI-designed drugs.
- Digital twin-augmented trials to be standard, enabling faster, more accurate simulations and reducing the need for large trial groups.
- Greater regulatory clarity on the use of AI-derived evidence.
- Faster and more accurate diagnostics and decision-making due to multimodal AI entering workflows.
- Deeper integration of AI in real-world evidence and post-market surveillance.
- AI implementation in safety monitoring, allowing for real-time, proactive risk management.
- Personalised medicine approaches due to scalable datasets, helping improve efficacy and reduce adverse outcomes.

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Closing thoughts

AI is shifting drug development from an artisan craft to a more predictive, engineered process driven by big data and smart algorithms. The companies that master this AI integration, and do so with robust scientific and ethical rigor, will likely be the ones delivering the next generation of breakthroughs, faster and more affordably than ever before.

[1] https://www.drugdiscoveryonline.com/doc/ai-and-pharmaceutical-development-who-calls-for-ethical-framework-good-governance-0001

How We Can Support

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Value focused and integrated buy-side transaction services or integrated sell-side services tailored to your target.

Value Creation / Performance Improvement

Identification and implementation of actions to improve commercial, operational and financial value and performance.

Commercial Assessments

Alignment of strategic objectives, incorporating patient flow, R&D forecasts, regulatory requirements, commercial scenarios, market dynamics, and competitive landscape analysis, along with return-risk analysis.

Valuations & Financial Modelling

Valuations and modelling services to complete the deal process and provide ongoing support with managing investments.

Eight Advisory is an integrated transaction, transformation and restructuring advisory firm operating globally with over 950 professionals, including over 100 partners. We support clients in corporates, private equity funds and infrastructure investors, and navigate the complexities of a changing world: identifying, creating and realising value.

Contact our experts and see how we can help you!

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