**Pharma Insights #5** By: Dr. June Choon

# TRANSFORMING DRUG DEVELOPMENT: WHERE THE PHARMACEUTICAL BIG GUNS ARE WITH AI

The pharmaceutical industry has witnessed a rapid acceleration in the integration of artificial intelligence (AI) technologies over the past decade. This growing interest promises profound impacts, not only benefiting healthcare providers and patients dealing with challenging conditions but also significantly influencing the biotech sector.

Al is now being utilised to enhance efficiency, accuracy, and outcomes in pharmaceutical R&D, addressing critical challenges that have long hindered drug discovery and development. According to Morgan Stanley Research, even slight improvements in early-stage drug development success rates, powered by Al, could result in approximately 50 additional innovative treatments over the next ten years—a significant boost for patients and healthcare systems worldwide. This surge in drug approvals could also represent a market opportunity of over \$50 billion, making Al one of the most valuable technological advancements for the industry.

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### Healthcare industry prioritises Al investment

Al has emerged as a top priority for healthcare professionals and companies, surpassing many other technologies in perceived value and transformative potential. A 2022 report by GlobalData found that 50% of healthcare professionals and executives identify Al as the foremost area for investment. This outpaces other prominent technologies such as big data (38%), digital media (37%), cloud computing (31%), and real-world evidence (27%).

Al's potential in healthcare and pharmaceuticals is profound because it allows for more precise data analysis and decision-making. This helps reduce the risks and uncertainties associated with drug development, a process that typically takes over a decade and costs billions of dollars. The pharmaceutical industry alone is projected to invest over \$3 billion in Al by 2025, reflecting its commitment to leveraging Al to streamline research and development (R&D) and bring effective treatments to market faster.

## Al-powered drug discovery and disease modeling

One of the most promising applications of AI in pharmaceuticals is drug target discovery and disease modeling. Traditional drug discovery often involves labor-intensive processes to identify biological targets associated with diseases. AI, however, enables researchers to analyse vast amounts of data to uncover these targets more efficiently and accurately.

Al companies like CytoReason and BenevolentAl are pioneering efforts to develop advanced disease models that can predict how diseases progress and respond to treatments. AstraZeneca's collaboration with BenevolentAl is a notable example. Together, they identified and validated a new target for idiopathic pulmonary fibrosis (IPF), a chronic lung disease. BenevolentAl's Al-driven platform discovered the serum response factor (SRF) as a potential target, and AstraZeneca conducted rigorous testing, including genome editing using clustered regularly interspaced short palindromic repeats (CRISPR) screening approach, to confirm its effectiveness in disease models. This partnership has led to five Al-generated targets entering AstraZeneca's research portfolio, showcasing how Al can revolutionise target discovery for challenging conditions.

In another collaboration, AstraZeneca and Illumina have partnered to accelerate drug target discovery by combining AI-powered genome analysis with cutting-edge deoxyribonucleic acid (DNA) sequencing technologies. By utilising tools such as Illumina's PrimateAI and SpliceAI, and AstraZeneca's JARVIS, this partnership seeks to enhance drug discovery efficiency and accuracy. The collaboration highlights the potential for AI-driven insights to transform how we identify and validate drug targets based on human omics data. Slavé Petrovski, head of AstraZeneca's Centre for Genomics Research, Discovery Sciences, R&D, remarked:

"Continuous innovation in the AI tools and frameworks that are applied to the growing human genomics, transcriptomics, and proteomics medical research resources will enable us to answer some of the toughest questions and contribute to our aims of uncovering novel drug targets with a higher probability of success while also characterising patient subgroups that are most likely to benefit from the treatments we discover."

#### Advancing drug design and lead optimisation

In addition to target discovery, AI plays a crucial role in drug design and lead optimisation steps that involve identifying the most promising compounds for development. Traditional approaches to drug design often involve screening libraries of potential compounds, a process that is costly and time-consuming. AI accelerates this process by predicting which compounds are likely to succeed based on their molecular structures and biological effects.

Sanofi's collaboration with Atomwise, an Al-driven drug discovery company, is a prime example. Sanofi is leveraging Atomwise's AtomNet<sup>®</sup> platform, which uses deep learning to screen a library of over three trillion synthesisable compounds. This collaboration allows Sanofi to identify and optimise potential drug candidates for challenging targets. Sanofi's upfront investment of \$20 million reflects the high stakes involved, with potential payments exceeding \$1 billion if key milestones are achieved.

Eli Lilly has also ventured into Al-powered drug design by partnering with XtalPi, an Al and robotics company. Together, they aim to design and test new compounds using Al-driven de novo synthesis, speeding up the discovery process. XtalPi's platform enables rapid identification and testing of chemical compounds, allowing Eli Lilly to advance the most promising candidates through clinical trials. This partnership demonstrates how Al can reduce the time and cost associated with traditional drug development processes.

#### Improving clinical trials with AI

Clinical trials are one of the biggest bottlenecks in drug development, accounting for the largest share of time and costs in the R&D process. Many drug candidates with promising preclinical data fail in clinical trials due to issues with patient selection, trial protocols, or unforeseen side effects. Al is transforming this phase by enabling more efficient trial design, patient selection, and real-time monitoring.

Pharmaceutical giant GlaxoSmithKline (GSK) has embraced AI to optimise its clinical trial processes. In collaboration with PathAI, GSK is running a Phase 2b clinical trial for nonalcoholic steatohepatitis (NASH), a severe liver disease. The trial measures improvements in liver histology with GSK4532990 compared with placebo in participants with NASH and advanced fibrosis. PathAI's role is to generate, digitise, and analyse liver biopsy slides for



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central pathologist evaluation in addition to Al-powered histologic evaluation using PathAl's Al-based Measurement of NASH Histology (AIM-NASH) tool. In addition, GSK has also partnered with Tempus, an Al-driven tech vendor, to enhance trial design and patient enrolment, particularly for oncology trials. Tempus' ΔI platform, which includes a large library of de-identified patient data, helps GSK improve trial outcomes and streamline the enrolment process.

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AstraZeneca is also employing AI to enhance trial recruitment, especially in oncology. In partnership with Oncoshot, AstraZeneca uses AI-powered analytics to match eligible patients with relevant cancer trials. This approach not only speeds up the recruitment process but also ensures that trials are better aligned with patient needs, improving outcomes and supporting local healthcare systems.

#### Al for drug formulation and development

Beyond discovery and trials, AI is increasingly applied in optimising drug formulations. In April 2023, Merck partnered with XtalPi to explore how computational workflows can streamline formulation processes. Together, they used AI to predict how additives would affect the crystal structure of metformin, a diabetes medication, and confirmed these predictions through lab experiments. This collaboration highlights a "digital-first" approach to formulation, where AI predictions are tested in wet lab settings to improve efficiency and precision in drug development.

## A shift towards AI partnerships and outsourcing

As AI becomes more integral to pharmaceutical R&D, companies are shifting towards strategic partnerships, R&D outsourcing, and mergers to access specialised expertise in AI. Developing AI-based drug discovery capabilities requires costly infrastructure and skilled data scientists, which are in limited supply. By forming alliances with AI-driven companies, pharmaceutical companies can integrate these technologies more swiftly and focus on their core expertise.

Partnerships like those between AstraZeneca and BenevolentAl, or Sanofi and Atomwise, reflect this trend, where big pharma collaborates with tech firms to enhance drug discovery and development. This approach not only accelerates innovation but also allows companies to adapt to the fast-evolving Al landscape, which is transforming how medicines are discovered, developed, and delivered.

In a nutshell, AI is ushering in a new era in pharmaceutical R&D, promising faster and more efficient drug development, enhanced precision in clinical trials, and optimised formulations. As Malaysia and other countries look to improve healthcare outcomes, the integration of AI offers a compelling pathway to advance medical science and improve patient access to innovative treatments. By embracing AI-driven partnerships, the pharmaceutical industry is set to deliver transformative solutions to some of the most pressing health challenges of our time.

## **About the Author**



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Dr. Choon is an academic and health economics researcher. She serves on various advisory boards for multinational pharmaceutical companies and the Ministry of Health. Her passion lies in improving patient access to life-saving innovative medicines in Malaysia.