The DISRUPT Framework

AI in Drug Discovery

GLOBAL X
by Mirae Asset

The DISRUPT Framework: Understanding the Future of Innovation

In the rapidly evolving world of artificial intelligence (AI), staying ahead of the curve is more crucial than ever. For investors, it's not just about spotting the next trend—it's about identifying where AI is making a true impact and how that translates into real opportunities. The challenge lies in cutting through the noise to find which developments are transformative and which may be overhyped. That is why Global X developed The DISRUPT Framework, a systematic tool to evaluate and track the progress of AI and other groundbreaking technologies.

Expected Outcome

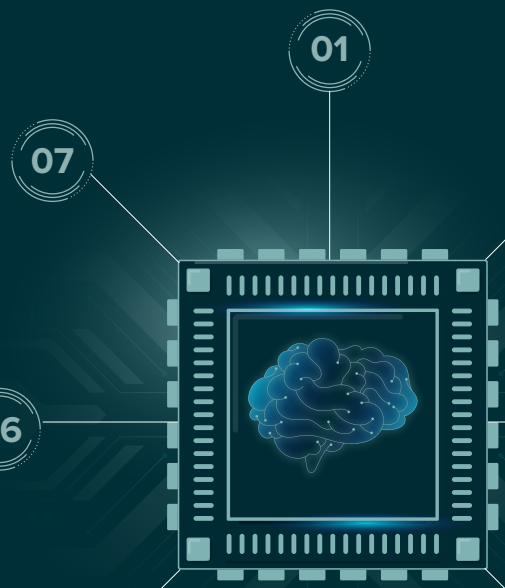
The DISRUPT Framework evaluates seven criteria: disruption, innovation, scalability, resilience, uptake, potential, and transformation. Each element combines to paint a picture on a specific innovation, its lifecycle stage, and investment potential. A five-level rating system is then used to assess the maturity of these technologies, from early-stage development (Nascent) to full-scale implementation (Fully Realised).

	Component	Objective	Guidelines
D	**D**isruption	Identify and analyse technologies causing major disruptions in various industries.	• Identify Technologies • Assess Impact • Market Dynamics
I	**I**nnovation	Track cutting-edge innovations driving change and breakthroughs.	• Research and Development • Technological Breakthroughs • Patents and Publications • Industry Awards
S	**S**calability	Assess the scalability and growth potential of disruptive technologies.	• Market Size • Growth Rates • Barriers to Entry • Adoption Catalysts
R	**R**esilience	Evaluate how technologies contribute to business resilience and adaptability.	• Risk Management • Sustainability • Business Continuity • Adaptability
U	**U**ptake	Monitor the market uptake and adoption rates of disruptive technologies.	• Adoption Curves • User Engagement • Market Penetration • Competitor Analysis
P	**P**otential	Assess the future potential and impact of disruptive technologies.	• Long-term Forecasts • Strategic Partnerships • Investment Opportunities • Regulatory Environment
T	**T**ransformation	Analyse how disruptive technologies are transforming industries and societies.	• Industry Changes • Economic Impact • Societal Impact

Rating	Description
Nascent	Early stages of development with limited real-world application.
Developing	Progressing, but significant advancements needed before becoming mainstream.
Established	Proven and widely used, though room for further growth and improvements remains.
Advanced	Highly developed, with few obstacles, close to full-scale implementation and monetisation.
Fully Realised	Fully adopted and delivering maximum impact across industries.

AI in Drug Discovery is in the "Developing" Stage of The DISRUPT Framework

AI in drug discovery is in the "Developing" stage, showing potential and progress in disruption, resilience, and innovation. While it has achieved many breakthroughs, especially in speeding up the discovery process and improving clinical trials, it is still developing in terms of scalability, uptake, and realising its full potential. The next signal for moving forward will be broader adoption across late-stage trials and greater scalability across therapeutic areas.



01 DISRUPTION

Rating: Developing

Fact: Exscientia's AI-designed drug for OCD entered human trials in just 12 months, five times faster than traditional methods.[1]

02 INNOVATION

Rating: Developing

Fact: While AI has shown a 90% accuracy in predicting protein structures, the broader application in personalised therapies is still evolving.[2]

03 SCALABILITY

Rating: Nascent

Fact: AI-driven platforms are beginning to screen billions of compounds simultaneously, but large-scale, cross-disease applications are still in development.[3]

04 RESILIENCE

Rating: Developing

Fact: AI models can adapt to regulatory changes quickly, but widespread adoption across late-stage trials and regulatory agencies is not yet fully realised.[4]

05 UPTAKE

Rating: Nascent

Fact: Over 15 AI-designed drugs have entered clinical trials as of 2023, signalling a growing acceptance of AI's potential in pharmaceutical R&D.[5]

06 POTENTIAL

Rating: Developing

Fact: AI has reduced drug identification time for rare diseases by up to 70%, but broader application in rare and complex diseases remains in early stages.[6]

07 TRANSFORMATION

Rating: Developing

Fact: AI-driven repurposing of drugs for conditions like Alzheimer's and Parkinson's is in its infancy, highlighting a major area of future potential.[7]

[1] BBC. (2024, Jan 31). Artificial intelligence-created medicine to be used on humans for first time.
[2] Nature. (2021, Jul 22). DeepMind's AI predicts structures for a vast trove of proteins.
[3] Nature. (2022, January). A virtual drug-screening approach to conquer huge chemical libraries.
[4] MDPI. (2024, March). Advances in AI for Protein Structure Prediction: Implications for Cancer Drug Discovery and Development.
[5] CAS. (2022). AI drug discovery: assessing the first AI-designed drug candidates for humans.
[6] MDPI. (2023). The Impact of Artificial Intelligence in the Odyssey of Rare Diseases.
[7] ScienceDaily. (2021, March 4). Artificial intelligence reveals current drugs that may help combat Alzheimer's disease.

Disruption: How is AI Revolutionising Drug Discovery by Improving Efficacy?

In 2019, the AI-driven drug discovery company Exscientia, in collaboration with Sumitomo Dainippon Pharma, used AI to design a drug candidate for obsessive-compulsive disorder in just 12 months - five times faster than traditional methods. This marked the first AI-discovered drug to enter human clinical trials.[1]

AI's integration into drug discovery has fundamentally reshaped how new drugs are developed. Since its early impact in the 2010s, AI use has rapidly expanded across the entire pipeline, from compound identification to clinical trial predictions.

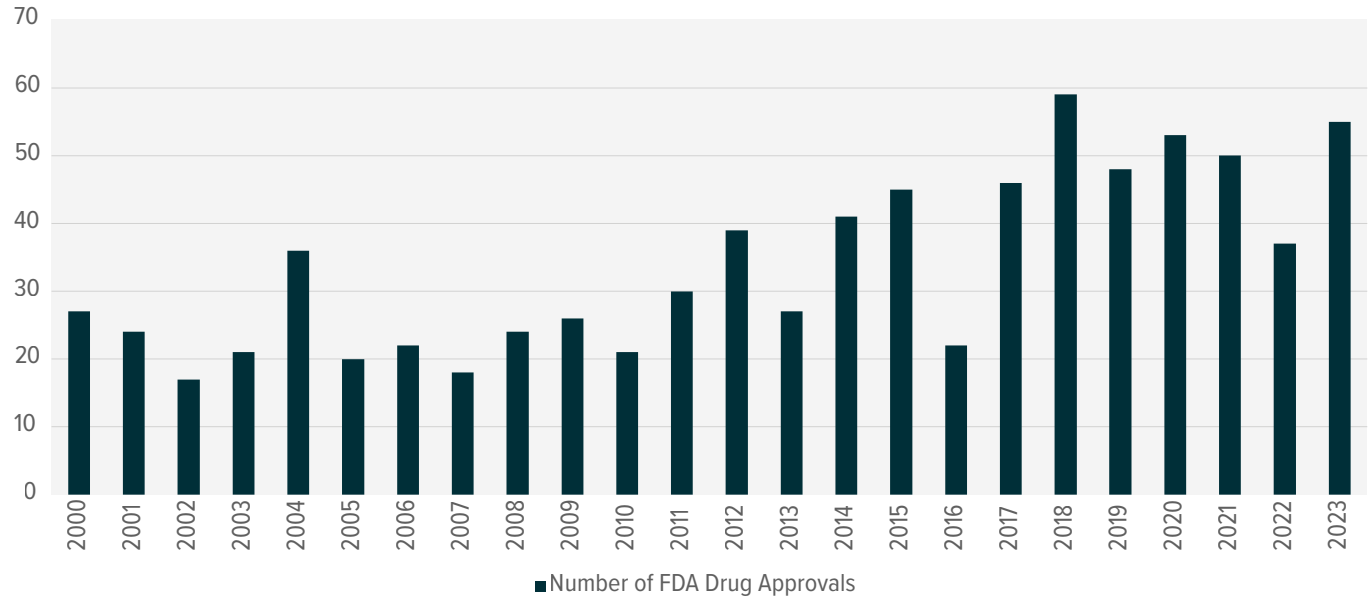
AI's impact is clear in the numbers. In 2000, only 27 new drugs were approved by the US Food and Drug Administration (FDA); by 2023, that figure nearly doubled to 55,[2] largely thanks to AI's efficiency. For instance, Insilico Medicine screened over 6,000[3] molecules quickly, whereas traditional methods might screen only a few hundred. This speed accelerates drug candidates into clinical trials.

Clinical trial success rates have improved significantly over the years. The overall probability of drug approval has risen from around 8% in 2000 to 13.8% in 2023, as documented in various studies, including those from MIT. AI's role in drug development has been increasingly recognised for enhancing trial design and patient selection. For example, success rates from Phase 1 to Phase 2 have shown improvement, driven by the application of AI in predicting drug interactions and optimising clinical trial protocols. While exact figures vary, AI continues to demonstrate a positive impact on trial efficiency and outcomes.[4]

AI has also reshaped the pharmaceutical landscape, shortening timelines, improving trial accuracy, and cutting costs. Pfizer, Novartis, and AI-native firms like BenevolentAI now use the technology to identify novel compounds, optimise trials, and repurpose drugs. Recursion Pharmaceuticals, for example, used NVIDIA's AI to predict drug-protein interactions for 36 billion compounds in a week[5] - a process that would traditionally take 100,000 years.

NUMBER OF FDA DRUG APPROVALS HAVE ALMOST DOUBLED SINCE 2000

Source: FDA's Center for Drug Evaluation and Research (CDER)



DID YOU KNOW

AI has the potential to reduce drug development costs by up to 40%.[5] A study by the Tufts Center for the Study of Drug Development found that AI can reduce the cost of bringing a new drug to market by automating early-stage research and speeding up clinical trials, potentially saving billions of dollars in R&D costs.

Innovation: Breakthroughs in Drug Discovery

In 2019, Atomwise used its AI platform to identify promising compounds to treat Ebola in less than a day by virtually screening millions of molecules, bypassing years of lab work.[6]

AI has not only accelerated drug discovery timelines but also driven major innovations in molecular design. Companies like Atomwise use AI to predict how drug molecules interact with biological targets, drastically reducing the time needed to identify viable compounds. What once took years of trial and error can now be achieved in weeks, optimising structures for efficacy and safety.

AI has also revolutionised protein structure prediction, a crucial step in drug development. Techniques like X-ray crystallography used to take years, but AI models like AlphaFold can now predict 3D protein structures with near-perfect accuracy in a fraction of the time,[7] opening new possibilities for diseases like Alzheimer's.

Clinical trial optimisation has benefited as well, with AI predicting which patients are most likely to respond to treatments using historical data and genetics. Exscientia is improving trial efficiency by using AI to select the right populations and better predict side effects.[8]

Additionally, AI is driving advancements in personalised medicine, with companies like BenevolentAI developing cancer therapies that target specific genetic mutations, offering more effective treatments tailored to individual genetic profiles.[9]

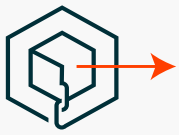
AI CAN BE USED TO ACCELERATE DRUG DISCOVERY PROCESS

Source: Nature.com

Deep Search

Knowledge extraction using AI for text and image understanding.

Teams of scientists used Deep Search to extract knowledge from the COVID-19 Open Research Dataset.



Generative Toolkit for Scientific Discovery

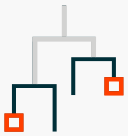
Accelerated hypothesis-generation for molecular research.

Researchers from IBM and the University of Oxford used generative modeling for de novo design of antimicrobial therapeutics in only 48 days.

Simulation Toolkit for Scientific Discovery

AI-enhanced molecular simulation for virtual experiments.

IBM Research demonstrated advanced simulation techniques offer a 30-40x speedup in the discovery of antimalarial drugs.



RXN for Chemistry

An AI lab partner for chemical synthesis.

IBM Researchers used RXN to shortlist candidates and narrow chemical recipes to use for the creation of new photoresists.

DID YOU KNOW

AI models like AlphaFold have achieved a success rate of over 90% in predicting protein structures, compared to traditional methods like X-ray crystallography, which often took years to complete. This innovation has unlocked new possibilities in drug development, particularly for diseases with previously unknown protein structures, like Alzheimer's and Parkinson's.[10]

Scalability: Extending AI's Reach in Drug Discovery

In 2021, Pfizer expanded its AI platform to target multiple therapeutic areas at once, from cancer to autoimmune diseases, cutting years off development times.[11]

AI's scalability is a major strength, enabling its application across various diseases, from cancer to rare genetic disorders, without requiring new frameworks. Companies like Recursion Pharmaceuticals use AI to screen billions of compounds in different therapeutic areas, dramatically reducing the time required for traditional methods. This flexibility allows firms to quickly shift focus to new opportunities.[12]

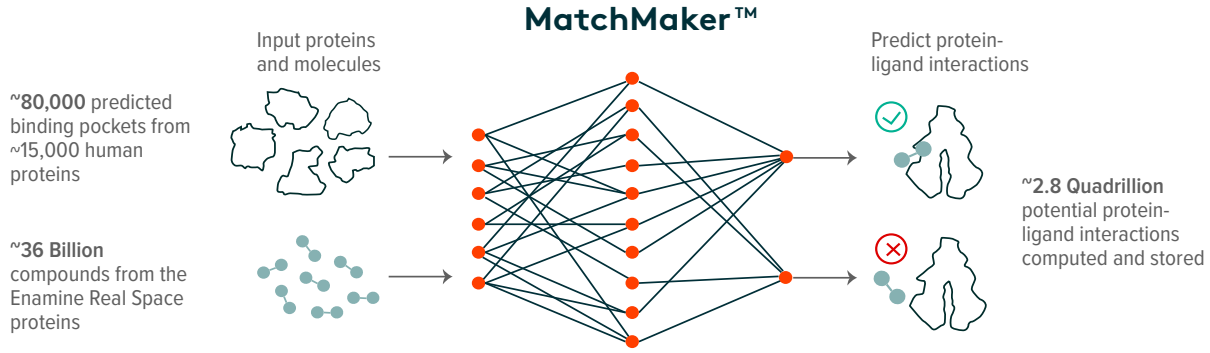
AI also handles vast datasets in parallel, including genomic data and clinical trial information. Schrödinger's platform, for example, models billions of molecules at once, accelerating compound discovery in oncology, virology, and immunology.

Cost-efficiency is another advantage. AI reduces the resources needed for drug development, with scalable systems managing larger datasets and multiple disease targets without a proportional increase in cost or time. A 2021 Tufts study showed AI can cut drug development costs by 20-40%, underscoring its financial benefits.[13]

By scaling AI, pharmaceutical companies can explore more drug candidates and therapeutic areas simultaneously, boosting efficiency and increasing the likelihood of success.

AI MAKES INTERACTION PREDICTIONS AT LIGHTNING SPEED

Source: Recursion investor relations.



Computation at Scale
Recursion partnered with NVIDIA to integrate and optimise MatchMaker (acquired via CYCUCA) for massive scale GPU-based computation on BioHive-1 and the DGXCloud.

Computation at Speed
This tool was deployed to predict protein-ligand interaction for ~36 Billion compounds from the Enamine Real Space, less than 90 days post-acquisition of cyclica and less than 30 days post-partnership with NVIDIA.

Computation as a Data-Layer
Recursion will use the predicted interactions as a data-layer in its multi-omic dataset for honing mechanistic predictions from its wet-labs and for accelerating SAR cycles through better predictions for its internal pipeline and within its partnerships.

DID YOU KNOW

AI's scalability enables the screening of billions of compounds in parallel, cutting early-stage drug discovery times by 50% and allowing firms to rapidly shift focus across diseases.[14]

Resilience: Ensuring Stability and Flexibility in Pharmaceutical Innovation

In 2020, Moderna leveraged AI to adapt its mRNA vaccine development in real-time as new variants of COVID-19 emerged. By processing real-time data, Moderna tweaked vaccine formulations without delaying clinical trials, illustrating how AI ensures resilience in drug development by allowing rapid adjustments during crises.[15]

AI's integration into drug discovery has made the entire process more resilient, allowing pharmaceutical companies to adapt swiftly to disruptions, whether they are global health crises, regulatory shifts, or setbacks during clinical trials. One of the core advantages of AI is its ability to continuously process data and adjust models without pausing development efforts, ensuring that the drug discovery pipeline remains intact even in uncertain conditions.

During the COVID-19 pandemic, AI systems were quickly adapted to identify antiviral candidates for SARS-CoV-2. AI platforms processed vast amounts of viral data and suggested existing drugs for repurposing, significantly speeding up the initial phases of research. This rapid response highlights AI's ability to pivot swiftly in response to emerging threats or unforeseen challenges.[16]

AI also enhances resilience by identifying early signs of trial failure. Traditionally, trial failures could result in months or even years of delays. However, AI systems can quickly rerun simulations or screen additional compounds, ensuring setbacks do not derail an entire development process. Furthermore, AI models can adapt to new regulatory standards in real-time, ensuring compliance without delaying drug development timelines.[17]

By maintaining this flexibility and allowing seamless transitions between targets, clinical trial phases, or regulatory standards, AI ensures that pharmaceutical companies are less vulnerable to unforeseen setbacks, creating a more robust and agile drug discovery ecosystem.

DID YOU KNOW

AI-driven drug discovery platforms are capable of rerunning simulations in hours when drug candidates fail, preventing months of delays typically caused by trial setbacks. This capability ensures that development timelines stay on track, even in the face of unexpected failures.[18]

Uptake: Accelerating the Adoption of AI in Drug Discovery

In 2021, the pharmaceutical startup Verge Genomics raised US$98 million to advance its AI-powered drug discovery platform. The success of such projects has significantly accelerated AI adoption in the drug development industry, attracting interest from investors and major pharmaceutical companies.[19]

The adoption of AI in drug discovery has been accelerating as pharmaceutical companies, biotech firms, and research institutions increasingly recognise its transformative potential. A key reason for this growth is AI's ability to significantly reduce the time and costs associated with traditional drug development, attracting large industry players and startups alike.

Data availability is a major success driver. Advances in genomics, molecular databases, and patient data are feeding AI models. Companies are using AI to manage these massive datasets, which would be impossible to handle manually, accelerating everything from target identification to clinical trials and improving R&D pipelines.

Collaborations between tech companies and pharmaceutical firms have also sped up AI adoption. Partnerships with companies like Google DeepMind and IBM Watson are helping pharmaceutical giants develop AI models that predict drug efficacy and identify new compounds,[20] expanding AI's role in the industry.[21]

Regulatory support has further boosted adoption. Agencies like the US FDA and the European Medicines Agency (EMA) are increasingly open to AI in clinical trials, offering clearer guidelines for its use. This support is critical for AI-driven drug discovery to gain broader acceptance.

While challenges like data privacy, intellectual property, and evolving regulatory frameworks remain, as more success stories emerge and AI proves itself in trials, its adoption in drug discovery is set to keep growing.

AI-DRIVEN BIOTECH FUNDING ROUNDS IN DRUG DISCOVERY AND DESIGN

Source: Verge Genomics. (2021). Verge Genomics Secures $98 Million in Series B Financing to Advance AI-Powered Platform for Neurodegenerative Diseases., Recursion Pharmaceuticals. (2020). Recursion Raises $239 Million to Advance AI-Powered Drug Discovery., Exscientia. (2020). Exscientia Raises $60 Million to Expand AI-Driven Drug Design and International Growth.

Name	Date	Size (USD)	Background
Verge Genomics	Dec-21	$98 million	Raised to advance its AI-powered platform for neurodegenerative diseases.
Recursion Pharmaceuticals	Sep-20	$239 million	Raised to enhance AI-powered drug discovery using cellular imaging.
Exscientia	May-20	$60 million	Raised to expand AI-driven drug design and international growth.

DID YOU KNOW

The FDA approved its first AI-designed drug to enter clinical trials in 2020, a significant milestone that has encouraged regulatory agencies worldwide to embrace AI in drug development. This regulatory support is paving the way for more widespread adoption of AI in pharmaceutical R&D.[22]

Potential: Unlocking New Horizons with AI in Drug Discovery

In 2020, AI-powered drug discovery identified a treatment for Duchenne Muscular Dystrophy in just a few months. This marked a monumental leap in a historically underfunded area, highlighting AI's transformative potential in rare diseases.[23]

AI's potential in drug discovery extends far beyond its current applications, offering a unique chance to revolutionise the pharmaceutical industry.

One significant area where AI's potential is clear is in discovering treatments for rare diseases. Historically, these conditions have been under-researched due to high costs and limited financial incentives. AI can reduce the time and resources needed to explore drug candidates for such conditions, making treatments for diseases like cystic fibrosis or muscular dystrophy more feasible.[24] With its ability to process vast datasets and predict outcomes more efficiently, rare diseases are becoming a more viable focus for R&D.

AI also holds great promise in personalised medicine. By analysing genomic data, AI can help create treatments tailored to individual patients, ensuring more effective therapies. This could lead to a future where patients receive therapies designed specifically for their genetic makeup, reducing side effects and improving efficacy. AI's role in drug repurposing is another promising area. By analysing existing drugs to find new uses, AI reduces the time it takes to bring treatments to market, saving both time and costs by bypassing much of the early-stage development process. AI has already shown success in repurposing drugs, and its ability to continue exploring these opportunities holds great potential.

Generative AI is also set to push drug discovery forward. By creating novel drug molecules from scratch and optimising them for specific targets, AI could greatly expand the pool of drug candidates, leading to treatments that are faster, more precise, and more effective.

AI's potential in drug discovery is not just about speeding things up—it's about enabling entirely new ways of developing treatments, from personalisation to drug repurposing. As AI evolves, the possibilities it can unlock in drug discovery are virtually limitless.

DID YOU KNOW

AI models can analyse vast genetic and molecular datasets, enabling the discovery of treatments for rare diseases that would otherwise be too costly or time-consuming to explore. In fact, AI has reduced the time needed to identify drug candidates for rare diseases by up to 70%, creating new hope for previously neglected conditions.[25]

Transformation: Redefining Drug Discovery with AI

In 2021, AI identified a potential new treatment for a rare genetic disorder, Niemann-Pick disease, by analysing existing drug data. This breakthrough happened in just months, illustrating the immense potential of AI to unlock new treatments for diseases that had been historically under-researched.[26]

AI is driving a fundamental transformation in drug discovery by enabling entirely new approaches that were previously unimaginable. Beyond just speeding up the process, AI is changing how pharmaceutical companies think about research and development from the ground up.[27]

One significant transformation is the shift from hypothesis-driven experiments to data-driven discoveries.[28] In the past, drug discovery was largely reliant on researchers' hypotheses and traditional experimentation. Now, AI enables companies to explore drug candidates without prior assumptions, uncovering hidden patterns and connections in vast datasets. This opens up new possibilities for uncovering treatments that would have otherwise been overlooked.

AI is also transforming how drugs are tested and developed in virtual environments. Using advanced simulations, researchers can now model how potential drugs will interact with biological systems, reducing the need for early-stage in-vitro testing. These simulations can test thousands of variables in parallel, providing insights into drug efficacy, safety, and potential side effects before human trials even begin.[29]

Moreover, AI-driven collaboration tools are transforming the pharmaceutical industry's approach to R&D. Cross-border, interdisciplinary collaboration is becoming more efficient as AI platforms allow researchers across the globe to work on the same projects in real-time, sharing data and insights instantly. This is fostering a more integrated and global approach to drug development, with researchers no longer constrained by geographic or organisational silos.

In addition to improving efficiency, AI is fostering a shift towards a more sustainable drug discovery model. By reducing the resources required for trial and error, AI not only cuts costs but also reduces the environmental impact of extensive laboratory testing. This shift aligns the pharmaceutical industry with broader global sustainability goals, marking a key transformation in how new medicines are developed.

Beyond identifying new treatments, AI's role in drug repurposing is another major transformation. By analysing existing drugs and finding new uses for them, AI reduces the need for early-stage development, significantly cutting down time and costs.

DID YOU KNOW

AI's drug repurposing capabilities have already identified existing drugs that could be effective for diseases like Alzheimer's and Parkinson's, reducing the need for new drug development. This approach has the potential to bring treatments to market much faster and at a lower cost.[30]

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About The Author

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Billy joined Global X in 2024 and is responsible for investment research and ETF analysis in the technology sector. Billy has over a decade of experience in financial services, focusing on equities and technology, previously working as Equity Analyst at Optiver in Sydney, and was the Director of Equity Research for China Internet at Haitong International in Hong Kong. Billy has been a top ranked equity analyst for regional software and internet by Asiamoney. Billy holds a Bachelor of Commerce from the University of Melbourne and is a qualified CPA Australia.

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