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ASIA EDITION

APAC takes centre-stage in AI-driven drug discovery

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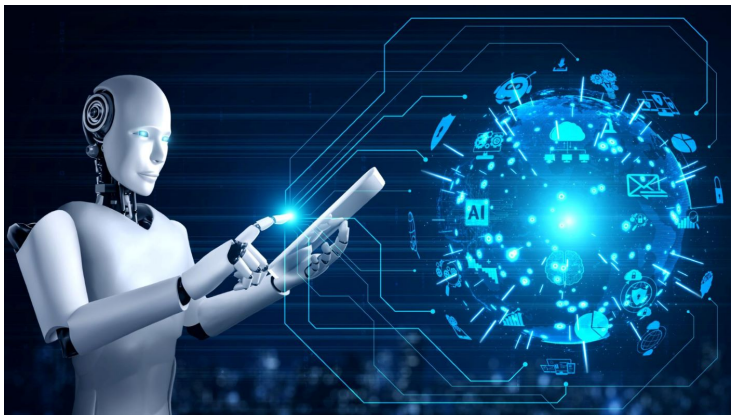
The Asia-Pacific (APAC) region is rapidly emerging as a leader in AI-driven drug discovery, fueled by robust research ecosystems and strong industry collaboration. Substantial investments, cutting-edge technologies, and strategic partnerships are optimising drug development efficiency. As Artificial Intelligence (AI) has become more embedded into many facets of everyday life, it has become an indispensable part of the drug discovery landscape. 2024 was the year of reckoning when AI in drug discovery received the highest validation—three researchers who leveraged the neural network AI programme AlphaFold to predict protein structures won the Nobel Prize in Chemistry. The industry is pushing ahead, using tech to make the business of drug development faster, safer, and more economical. Morgan Stanley estimates that AI's use in drug development could lead to 50 more successful treatments over a decade, potentially creating a $50 billion market. Let's explore the region's efforts in accelerating drug development through AI.



Drug discovery is a lengthy and costly process, typically requiring billions of dollars and nearly a decade to bring a drug to market. AI holds the promise of reducing both the costs and the timelines involved in this process. A study published by the Boston Consulting Group (BCG) found that at least 75 drug candidates developed by companies using AI in their discovery process were in clinical trials over the past decade. Impressively, 80-90 per cent of the candidates that entered phase I clinical testing were successful, a success rate considerably higher than the industry average of 50-60 per cent.

AI research in drug discovery primarily focuses on small molecules, with oncology as the leading area due to the growing global cancer burden. Immunology follows, with 21 per cent of companies using AI for immunological treatments. Fewer programmes target neurology and inflammation, according to Deep Pharma Intelligence.

Big pharma and AI

Big pharma has stepped up its efforts in the race to develop AI-based drugs, with nearly 100 partnerships identified between AI vendors and major pharmaceutical companies since 2015 as per a report from GlobalData. Among the leaders in this space are Pfizer, Takeda, and AstraZeneca, each with eight deals. Other pharmaceutical companies recently forging AI-related deals include Novartis, Bristol Myers Squibb (BMS), Roche, Janssen, Merck KGaA, Boehringer Ingelheim, Bayer, GSK, and Sanofi.

Noteworthy recent deals include an AI partnership between Eli Lilly and Novartis with Alphabet's digital biotech company Isomorphic Labs in January 2024. These companies will leverage Isomorphic's AI platform to develop small-molecule drugs for undisclosed targets. In November 2023, Roche also announced a multi-year research collaboration with chipmaker NVIDIA, marking one of (at least) eight AI deals Roche has signed since 2019.

Asia scenario

While the US and Europe remain leaders in AI drug discovery, the APAC region is rapidly catching up with the commoditisation of AI tools and resources.

"Countries in the APAC region, including China, Taiwan, Singapore, South Korea, and Japan, are emerging as key players in AI-driven drug discovery, due to substantial investments in research, strong academic institutions, and efforts to attract top talent. The region is making significant strides in areas such as drug repurposing (identifying new uses for existing drugs), drug asset management (licensing undervalued assets, redeveloping them with AI, and advancing them through the pipeline), and the development of novel AI algorithms like GenAI and Causal AI. Additionally, many governments in the region are providing significant funding and policy support to foster the growth of AI in healthcare, further fueling innovation and progress in the drug discovery space," said Dr Yu-Feng Wei, CEO, Vizuro LLC.

Sanjay Vyas, President and Managing Director, Parexel India observed that AI-driven drug discovery has become the mainstay in the APAC region. "Around 11 per cent of the total number of AI-driven drug development companies are in Asia. Leading the group in Asia is China and South Korea as per the Deep Pharma Intelligence report. Around 700 companies across Asia are using AI to decrease the failure rate of new chemical entities (NCE) during early development into final drug approval and commercialisation. AI has shown success in certain stages of NCE development and has been in use in late-stage clinical trials – site selection, patient identification, monitoring and retention," added Vyas.

According to a report by Deep Pharma Intelligence, an analysis of 92 companies in Asia developing AI-based drugs revealed key insights into the current landscape of drug development. Of the 152 reported drug candidates, 92 are at the discovery stage. Additionally, 10 drugs are in Phase II, and 16 are in Phase I. The majority of the drug candidates, 66 out of 152, are focused on various types of cancer, with the most common benign solid tumours, breast cancer, and prostate cancer. Another 17 candidates have undisclosed therapeutic areas, and 11 are aimed at treating neurodegenerative disorders, including amyotrophic lateral sclerosis and Parkinson's disease.

The report also highlights the leading countries in Asia developing AI-driven drugs. South Korea leads with 72 of the 152 drug candidates, of which four have reached Phase I of clinical trials. China follows with 53 drug candidates, including nine in Phase I, six in Phase II, and one in Phase III. Japan ranks third, with 12 drug candidates, all still in the discovery stage. Hong Kong and Singapore contribute smaller numbers, with 10 and 5 drug candidates under development, respectively.

"The APAC region, particularly China, India and Japan, is at the forefront of AI-driven drug discovery, with rapid advancements in machine learning, deep learning, and natural language processing shaping the future of pharmaceutical research. In China alone, over 100 AI pharmaceutical companies have emerged, supported by substantial investments exceeding $1.26 billion in 2021. This surge in innovation is facilitated by a supportive regulatory environment that encourages faster clinical trials and the integration of real-world data to assess treatment effectiveness. The growing investment in AI technologies, combined with strong academic and industry collaborations, is creating an ecosystem where innovation can thrive. With a supportive regulatory environment and a focus on real-world evidence, the region is poised to significantly impact global drug development, driving faster, more efficient solutions for unmet medical needs," said Vera Zheng, Senior Vice President, Asia Pacific Strategy and Head of Greater China, Parexel International.

Let's take a closer look at the efforts of these countries in advancing AI-based drug discovery.

Singapore

Singapore is bullish on becoming a biomedical powerhouse and the government has been actively pursuing the advancement of frontier technologies such as AI to support its biomedical science and healthcare ecosystems. As part of its

Research, Innovation and Enterprise (RIE) 2025 plan, the government has invested over SGD 25 billion in science and technology research.

One of the initiatives is the launch of the Ignition AI accelerator. Through collaboration with Digital Industry Singapore (DISG), Ignition AI Accelerator aims to attract top international AI startups to Singapore, fostering a robust ecosystem for frontier technologies. In October 2024, the Ignition AI Accelerator announced a strategic partnership with Pfizer to transform its drug discovery and development processes through the integration of AI.

The Experimental Drug Development Centre (EDDC), Singapore's national platform for drug discovery and development, has inked several deals with AI-driven companies such as Partex and XtalPi. In the partnership with Partex, the focus is on leveraging AI-powered technologies such as target identification, molecule generation, and structure-activity relationship (SAR) optimisation to accelerate the development of novel therapeutics. Partex will bring its knowledge graph and small molecule screening library, while EDDC will contribute its extensive drug discovery expertise to drive clinical development. On the other hand, the XtalPi-EDDC collaboration, which expands on an earlier partnership, aims to integrate automated synthesis solutions and large language models (LLMs) to enhance pharmaceutical research, particularly in targeted therapies. By combining AI, automation, and scientific expertise, both partnerships aim to streamline drug development, reduce time and costs, and expedite the conversion of scientific discoveries into viable drug candidates.

Apart from this, several startups have also mushroomed, of which, BluMaiden Biosciences has secured funding to advance small molecule drug discovery using AI-guided computational genetics and chemistry. Similarly, Engine Biosciences, focused on precision oncology, raised $27 million in a Series A extension, bringing its total to $86 million. Engine’s platform decodes biological networks to identify genetic interactions, enabling the development of targeted therapeutics for cancers such as ovarian, colorectal, liver, lung, and prostate.

Australia

Australia is making significant strides in AI-driven drug discovery, with various platforms and collaborations accelerating the process. Researchers at Monash University have developed an AI tool called PSICHIC (PhySIcoCHemICal) to expedite drug discovery by using sequencing data to understand protein-molecule interactions, reducing reliance on costly traditional methods. Meanwhile, Commonwealth Scientific and Industrial Research Organisation (CSIRO) is working on new AI tools to fast-track drug discovery for emerging infectious diseases.

Algorae Pharmaceuticals has also made progress with its Algorae Operating System (AlgoraeOS) platform, finalising an initial catalogue of 24 drug targets. Developed in collaboration with University of New South Wales AI experts, these targets will undergo preclinical studies in an Australian pharmaceutical lab.

Several strategic partnerships further bolster Australia’s AI-driven drug discovery landscape. The University of Sydney has signed an MoU with Pharos Therapeutics (the Australian arm of South Korea’s Pharos iBio) to use AI in identifying compounds for cancer and rare disease treatments. The partnership grants access to Chemiverse, Pharos’s proprietary AI platform, and provides the university with a top-tier research infrastructure.

Additionally, Queensland Institute of Medical Research (QIMR) Berghofer Medical Research Institute has partnered with Syntekabio of South Korea to apply AI and high-performance computing in the development of new cancer and chronic inflammation treatments. Clinical-stage company PYC Therapeutics has also unveiled a collaboration with Google Cloud and other specialised partners to leverage AI for developing innovative medicinal drugs.

South Korea

South Korea is taking significant strides in AI-driven drug discovery, launching the South Korea AI Roadmap, a five-year initiative to integrate AI into healthcare. The roadmap, extending through 2028, aims to strengthen AI R&D in healthcare and drug development while advancing medical data systems for safe applications. In November 2024, a consortium of South Korean research institutes was formed to leverage AI and national supercomputers in discovering novel drugs for lung cancer treatment.

Leading the charge in AI drug discovery are companies such as Syntekabio, Standigm, Pharos iBio, and Oncocross. Syntekabio uses its DeepMatcher platform, combining AI with genomic big data, to discover new drug candidates. The company is also conducting research on cancer drug screening, immune typing, pharmacogenomics, and multi-omics-based side-effect prediction, along with developing neoantigen prediction technologies for use with vaccines and cell therapies.

Pharos iBio has developed Chemiverse, an AI-based platform that supports the entire drug discovery process, from target identification to clinical development. Their first AI-driven drug is currently in clinical trials. Daewoong Pharmaceutical, another major player, has unveiled an AI-powered drug development system supported by an 800 million-compound

database.

Standigm has built a workflow AI-driven drug discovery platform. With a global presence, it uses AI for novel target identification and compound design, generating First-in-Class compounds in as little as seven months. Its Standigm ASK and Standigm BEST platforms are fully automated, streamlining the entire drug discovery process.

Oncocross specialises in AI-driven drug discovery for in vitro and in vivo analysis. Oncocross has entered into a joint research agreement with JW Pharmaceutical to develop new drugs using its AI platform. The company recently completed a Phase 1 global clinical trial for OC514, a drug targeting sarcopenia and other rare muscle diseases.

China

China has placed a significant emphasis on AI in the pharmaceutical industry under its 'Made in China 2025' plan, to become a global leader in advanced manufacturing, including AI technologies. The country leads the global AI landscape, housing over 60 per cent of big data experts across various sectors. Since 2018, over 100 AI startups have emerged in China's healthcare space, responding to growing demand.

A notable success story from this region is Insilico Medicine, a Hong Kong-based startup pioneering AI-based drug discovery. Their lead drug, INS018-055, is the first AI-discovered drug, designed by generative AI, to enter Phase 2 clinical trials for idiopathic pulmonary fibrosis (IPF). Founded in 2014, when AI in drug discovery was still nascent, Insilico has made major strides, with its partnerships—including those with Janssen Pharmaceuticals—showcasing the increasing reliance on AI in the field. Insilico's approach involves using its AI target-discovery engine, PandaOmics, to process vast amounts of data, including omics, compounds, and clinical information, to discover new drug targets. This data is then used to design small molecule inhibitors through their Chemi platform. Additionally, the company's Pharma.ai suite, which includes tools like PandaOmics, Chemistry42, and inClinico, has helped accelerate the drug discovery process by predicting the success of clinical trial transitions.

Another key player, XtalPi Holdings, is transforming the biopharmaceutical industry by combining AI and robotics to improve drug development. The company integrates AI-driven dry lab algorithms with large-scale wet lab robotics, collaborating with major pharmaceutical firms like Eli Lilly and Janssen to enhance their drug discovery efforts.

In addition, global tech giants such as NVIDIA and Huawei are pushing the envelope in AI-driven drug discovery. NVIDIA BioNeMo, a generative AI platform, is accelerating drug development by providing customisable foundation models for pharmaceutical research. Huawei Cloud's Pangu Drug Molecule Model, co-developed with the Shanghai Institute of Materia Medica, has notably reduced the lead compound development cycle from years to just one month, showcasing significant improvements in drug design efficiency.

Japan

Japan has identified AI as a key technology in its drive to become a global leader in drug discovery. The Ministry of Economy, Trade, and Industry has launched initiatives to promote AI-based drug discovery. All the major pharmaceutical companies such as Takeda, Astellas, Chugai, Ono, and Daiichi Sankyo integrate AI into their research and development processes.

Astellas Pharma has made significant strides with its 'Human-in-the-Loop' drug discovery platform, which combines human input, AI, and robotics to accelerate the drug discovery process. This platform has successfully reduced the time from hit compound identification to drug candidate selection by approximately 70 per cent. The process revolves around a DMTA cycle: Design, Make, Test, and Analyse, enabling continuous improvements based on AI-driven insights.

Chugai Pharmaceutical leverages AI for target exploration and molecule design, especially in therapeutic areas where the company is already a leader. In collaboration with Preferred Networks and other partners, Chugai is developing internal AI technologies using machine learning and deep learning to analyse massive datasets and create innovative drugs.

On the technological front, Mitsui and NVIDIA have teamed up to develop the Tokyo-1 supercomputer, the world's first generative AI supercomputer dedicated to pharmaceutical drug discovery. Set to launch later this year, the supercomputer will be available to Japan's pharmaceutical companies and startups, aiming to accelerate AI adoption in drug development. Major players such as Astellas, Daiichi Sankyo, and Ono Pharmaceutical are already planning to use Tokyo-1 in their AI-driven drug discovery projects.

Additionally, Fujitsu and the RIKEN Center for Computational Science have developed an AI-powered technology to predict structural changes of proteins from electron microscope images, generating 3D density maps using generative AI. This breakthrough promises to enhance understanding of protein behaviour and accelerate the development of novel therapeutics.

India

India too is catching up in utilising the technology for drug discovery. Key Indian startups, including Peptris Technologies, Sravathi AI Technology, Molecule AI, and Aurigene Pharmaceutical Services, are developing their platforms to augment drug development.

Peptris Technologies, for instance, is leveraging AI to enhance the pre-clinical phase of drug discovery by integrating AI-driven chemical prediction algorithms and advanced machine learning models. By reducing both the cost and timeline of the pre-clinical phase, Peptris is aiming to make drug discovery more accessible and less financially prohibitive, which could lead to faster innovation in addressing unmet medical needs. Peptris Technologie claims their AI platform could reduce this phase from five years to just 1.5 years, and reduce the cost from $700 million to $400,000.

Sravathi AI Technology has developed a proprietary AI platform that can accurately predict chemical reactions, drug molecule properties, and formulation designs. Another startup Molecule AI has developed Molecule GEN, a built-in intelligence and heuristics that allow users of all skill levels and backgrounds, namely biologists, chemists, and AI researchers alike, to effectively translate their research ideas in no time and expedite the discovery of new therapeutic candidates. As a SaaS (software as a service) platform, Molecule GEN does away with the complex setup and maintenance processes and offers a frictionless way to use many built-in, tailor-made workflows for rational and AI-based de novo drug design.

Aurigene Pharmaceutical Services, an arm of Dr. Reddy's Laboratories, has developed the Aurigene.AI platform, which combines predictive AI models, physics-based simulations, and computer-aided drug design (CADD) to assist in every step of the drug discovery process.

Leading AI drug discovery companies in Asia

S.No	Company	Details
1	BluMaiden Biosciences, Singapore	Leverages its MAIDENTM platform combining comp chemistry to advance small molecule drug discovery
2	Engine Biosciences, Singapore	Leveraging machine learning and high-throughput bi develop precision oncology medicines
3	Algorae Pharmaceuticals, Australia	Undertaking AI enhanced drug discovery and develo improve the wellbeing of people with serious disease
4	Syntekabio, South Korea	Developed disease-agnostic synthetic drug candidat
5	Standigm, South Korea	Built a workflow AI-driven drug discovery platform
6	Pharos iBio, South Korea	Developed Chemiverse, an AI-based platform that su discovery process
7	Oncocross, South Korea	Innovating the drug development process through its
8	Insilico Medicine, Hong Kong	Pioneer in AI based drug discovery. Only AI based co 2 trial
9	XtalPi Holdings, China	Deveoped AI based drug disocvery platform
10	Peptris Technologies, India	Developing AI/ML based computational platform to a of finding novel drugs ·
11	Sravathi AI, India	Focused on creating, discovering, and developing inn pharma and chemical products
12	Molecule AI, India	Developed Molecule GEN as a SaaS (software as a s AI-based de novo drug design.

Immense potential

AI in drug discovery is not without its challenges. There is still a lack of regulatory clarity, and agencies are working to establish the best ways to govern and support the technology, not to mention concerns around data privacy. Moreover, sceptics are questioning the technology's potential in developing blockbuster drugs—pharma's Achilles' heel.

S&P analysts do not expect AI to produce more blockbuster drugs, but rather to shorten development timelines. According to a report from S&P Global, clinical development timelines with the use of this technology range from three to five years, compared to the typical seven to nine years without AI.

Nonetheless, AI has become a crucial tool in drug discovery, and Asia is leading the charge in this transformation. As AI technologies continue to evolve, they have immense potential for breakthroughs in cancer, neurological disorders, and beyond.

Setbacks in AI-driven drug development

Despite the rapid progress of AI in drug discovery, not all has been smooth sailing. Several AI-developed drug candidates have encountered significant setbacks in 2023.

The UK-based biotech Exscientia announced in October 2023 the termination of its early clinical trial for the AI-driven cancer drug candidate EXS-21546. According to both clinical and preclinical data, the drug was unlikely to achieve an adequate therapeutic index. Consequently, the Phase 1/2 trial was halted, and further research on the target was discontinued.

Similarly, BenevolentAI, a London-based company, reported disappointing results for its AI-designed drug, BEN-2293, in April 2023 in a Phase 2a clinical trial for atopic dermatitis. The double-blind, placebo-controlled study showed the drug failed to outperform the placebo.

Japanese firms Sumitomo Pharma and Otsuka Pharmaceutical faced a setback when their AI-developed schizophrenia drug failed to outperform a placebo in two Phase 3 trials in July 2023.

Drug design on Supercomputers

Researchers in China are exploring the potential of next-generation computing technologies, including quantum computing, to revolutionise drug design, reduce development timelines, and lower costs.

A team of Chinese scientists has developed a model pipeline that integrates quantum computing with classical systems to address two critical challenges in drug discovery: computing reaction barriers and molecular dynamics simulations. Their approach, published in Scientific Reports, combines quantum-classical hybrid computing platforms and the ddCOSMO solvation model for solvation energy calculations. This hybrid method aims to accelerate the identification of promising drug candidates.

In December 2024, China established its first quantum computing and data medicine research institute to further explore the use of quantum computing in drug discovery. Another Chinese University Bengbu Medical University, in collaboration with Origin Quantum, is investigating quantum computing's role in accelerating small molecule drug development, leveraging China’s third-generation superconducting quantum computer, Wukong.

Meanwhile, Insilico Medicine, in partnership with the Acceleration Consortium at the University of Toronto, has combined quantum computing with generative AI and classical computing methods to create molecules targeting the cancer-linked KRAS protein, previously deemed undruggable. This breakthrough demonstrates the powerful synergy between AI and quantum computing in advancing drug discovery, opening new possibilities for previously uncharted therapeutic targets.

Elsewhere, in Japan, D-Wave Quantum and Japan Tobacco's pharmaceutical division have partnered on a proof-of-concept project using quantum computing and AI to enhance small molecule drug development. The collaboration aims to accelerate the discovery of ‘first-in-class’ compounds, utilising D-Wave’s quantum annealing technology to optimise AI training for drug design.

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