

AI in Drug Discovery Market is growing at a CAGR of 29.8% during 2025–2035

AI in Drug Discovery Market is gaining momentum amid growing investments in healthcare AI by biotech firms and governments worldwide.

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/EINPresswire.com/ -- [AI in Drug Discovery Market](#) was valued at \$1.88 billion in 2024 and is projected to grow at a CAGR of 29.8% during the forecast period (2025-2035). The pharmaceutical industry is changing with a paradigm shift, as artificial intelligence (AI) is revolutionizing the discovery, testing, and marketing of drugs. The implementation of AI technologies is making it possible for researchers to speed up drug discovery processes, reduce costs, and improve the success rate of new drug candidates. Machine learning, natural language processing (NLP), deep learning, and other AI models are assisting researchers in predicting molecular behavior, discovering drug targets, and designing drugs.

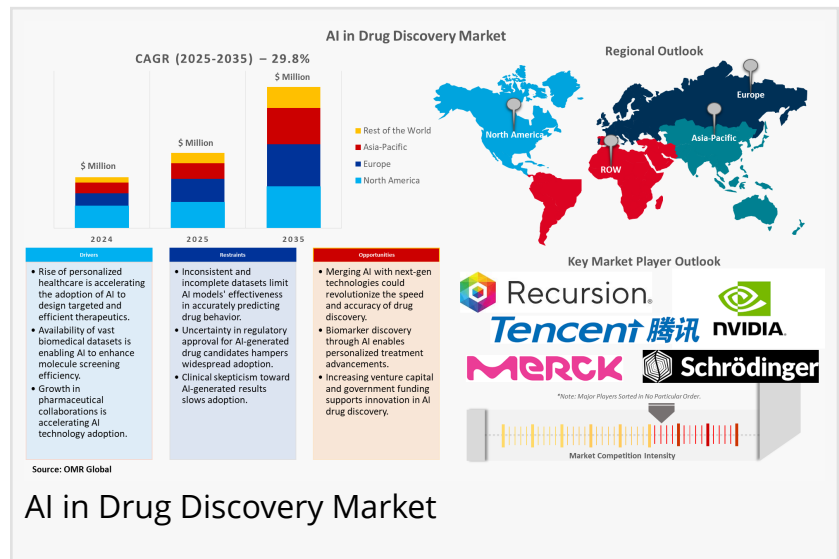
Several pharma companies are collaborating with technology companies to co-design AI-based drug discovery software. For instance, in 2024, Bayer AG announced its collaboration with Google DeepMind to improve AI-assisted target discovery and molecule optimization. Likewise, Insilico Medicine and Recursion Pharmaceuticals are creating headlines with AI-discovered drug candidates already advancing in clinical trials.

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Market Trends

Increasing Drug Discovery with AI-Based Tools and Emphasis on Innovative Drugs

The increasing prevalence of chronic diseases, pharmaceutical firms to accelerate their research



on new drugs to address disease indications. For accelerating drug development, various industrial players moved towards AI-based platforms and tools for drug discovery and development, which is expected to be the major growth driver of AI in the drug discovery market. For instance, in July 2024, researchers at the Broad Institute of MIT and Harvard reported the creation of new AI-based models that have the potential to screen the biological effects of therapeutic drug candidates even before they reach the body. The effective results of therapeutic drugs in clinical trials using AI-based models and constant developments on AI models to accelerate drug discovery are expected to be the key driver for AI in drug discovery market.

Growing Partnerships and Investment in the Emerging Market

From overcoming several challenges, various industrial participants engaged in this sector are persistently making substantial investments and signing agreements to supply developed AI-powered platforms for drug research. For instance, in January 2025, Novo Nordisk widened its collaboration with Valo Health for the quicker development of novel therapies for cardiometabolic diseases using AI and vast human datasets. Additionally, in May 2024, Accenture invested through Accenture Ventures in Turbine (a global predictive simulation leader) to advance its use of AI-driven cell simulation for biopharma R&D guiding and accelerate significant drug development workstreams.

In addition, the growing number of new entrants in this sector reflects the rising research in AI-based programming, software, and tools to speed up drug discovery. For instance, in March 2024, AION Labs introduced CombinAble.AI to solve the issues regarding antibody designs to raise the research and development of useful therapeutic drugs. Company will develop a platform that integrates AI with computational methods for biomolecule simulations, aiming on developing new biotherapeutics. Influenced by the increasing investments and partnerships among industry players, there are various opportunities to make investments in this space to foster innovations, that is expected to propel AI in the drug discovery market growth throughout the forecast period.

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Regional Outlook

Increasing research by several companies in the Asia-Pacific region

The Asia-Pacific region is likely to expand due to increased government funding for research and precision medicine initiatives in nations such as South Korea, China, and India, as well as increased utilization of AI-based technologies for drug discovery research and development by major pharmaceutical companies in the region. For instance, in April 2025, Elucidata, an Indian company, empowering biotech labs to deploy AI models using localized datasets, accelerating

regional drug discovery pipelines. They were working on specific deployment challenges that are slowing time-to-market for life-saving drugs, and addressing them while bringing new therapies to patients sooner. The position of the region in the AI drug discovery market is further strengthened by its commitment to promoting innovation through partnerships between industry, academia, and technology providers. For instance, in June 2024, China's National Medical Products Administration (NMPA) invites public comments until July 24, 2024, to expedite the fast-track clearance process for foreign innovative medicines with unmet clinical needs.

North America Holds a Major Market Share

North America is the largest share due to several AI in drug discovery firms and providers such as NuMedii, Inc., Recursion Pharmaceuticals Inc., NVIDIA Corp., Schrödinger, Inc., and XtalPi Inc. within the region. The growth in the market is due to more medication research, design, and repurposing. The top US IT companies have partnered with prestigious institutes. AI is also being utilized to study diseases and make pertinent conclusions that can assist in disease management. For instance, in March 2024, NVIDIA Healthcare launched generative AI Microservices to accelerate drug discovery, MedTech, and Digital Health. Furthermore, NVIDIA accelerated software development kits and tools such as Parabricks, MONAI, Riva, NeMo, and Metropolis can now be used as NVIDIA CUDA-X microservices to speed up healthcare workflows in drug discovery, medical imaging, and genomics analysis.

Market Segmentation and Growth Areas

Oncology is anticipated to have the Largest Segment

The oncology segment is projected to have the major market share. The key drivers behind the growth are making existing AI systems that are designed to sort through huge data sets and extract knowledge. AI can be used to offer patients customized treatments. Besides supplying patient histories and genetic codes, scans can create a pattern for cancer detection at its early stages and patient-specific medication administration. For instance, in April 2024, the National Institutes of Health (NIH) created an artificial intelligence tool that can predict, with data from individual cells within tumors, whether a person's cancer will be responsive to a particular drug. In this recent study, researchers tested whether they could use a machine learning strategy known as transfer learning to train an AI model to forecast drug responses based on widely available bulk RNA sequencing data, and then further fine-tune that model on single-cell RNA sequencing data.

Drug Optimization and Repurposing Segment to Hold a Significant Market Share

The drug optimization and repurposing segment is projected to grab a significant share of the market. Drug effectiveness, as well as side effects, can be studied with the help of new AI systems such as Deep Learning (DL) and drug modeling. The advancement of AI technology has helped in studying, comparing, and repurposing drugs into more effective forms, minimizing

side effects, and maximizing overall effectiveness. For instance, in January 2024, Accenture introduced a strategic investment, via Accenture Ventures, in QuantHealth, a clinical trial design firm powered by AI that runs clinical trials in the cloud, enabling pharma and biotech firms to develop treatments for patients more quickly and at lower cost. By running trials at scale, QuantHealth's platform can reduce risks, accelerate, and streamline drug development.

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Market Limitations and Challenges

- **Expensive Deployment:** It is costly to develop and sustain AI drug discovery platforms as they demand huge investments in data infrastructure, talented individuals, and validation processes.
- **Skilled Workforce Shortage:** There is a lack of professionals with cross-disciplinary skills in AI, drug development, and bioinformatics.

Market Players Outlook

The key players operating in the AI in drug discovery market are Merck KGaA, NVIDIA Corp., Recursion Pharmaceuticals Inc., Schrödinger, Inc., and Tencent Holdings Ltd., among others. The market players are shifting their focus towards business growth and product development by adopting strategies such as collaborations, mergers, and acquisitions to remain competitive in the market. For instance, in January 2025, Advanced Micro Devices (AMD) invested \$20 million in AI-driven drug discovery firm Absci Corp. AMD will also join forces with Absci to assist its research initiatives.

Recent Developments

- In Jan 2025, Adnexus Biotechnologies Inc. launched Trapiacolast, a groundbreaking antimalarial drug developed using its AI-powered Sutra platform. This innovative medication targets dual mechanisms in the Plasmodium parasite, focusing on the apicoplast and vesicular trafficking pathways, with the help of AI-discovered ADX1 and ADX2.
- In Jan 2025, Collaborations Pharmaceuticals, Inc. (CPI) collaborated with Bausch + Lomb for the use of CPI's AI and machine learning capabilities in the discovery of novel treatments for eye diseases. The financial terms of the collaboration have not been disclosed.
- In January 2025, Predictive Oncology is acquired by Renovaro to utilize their complementary AI and machine learning platforms to improve patient outcomes in various cancer indications.
- In October 2024, Iambic Therapeutics, a biotech company, announced a breakthrough artificial intelligence model that could potentially reduce the time and expense involved with developing new drugs.
- In September 2024, Insilico Medicine collaborated with Inimmune to utilize its proprietary AI platform, Chemistry42, in accelerating the discovery and development of future

immunotherapeutics.

- In August 2024, Exscientia plc and Recursion entered into a definitive agreement, merging their technologies for accelerating small-molecule drug discovery. The combined Recursion OS will advance drug discovery using patient-directed target discovery, AI-based design, quantum mechanics-based modeling, automated chemical synthesis, and much more. Together, the companies aim to finish 10 clinical trials over 18 months. Exscientia shareholders are entitled to share Recursion stock, with 74% stake going to Recursion shareholders in the combined firm. The deal, worth USD 850 million in cash, aims for USD 100 million in annual synergies and is expected to close by early 2025.
- In July 2024, Exscientia plc declared that it would be extending its partnership with Amazon Web Services (AWS) to leverage the cloud provider's machine learning and artificial intelligence capabilities to power its end-to-end drug discovery and automation platform.
- In May 2024, Google introduced AlphaFold 3, an innovative AI model from Google DeepMind and Isomorphic Labs. The firm asserts that the model accurately predicts the structure of DNA, RNA, proteins, and ligands and how they interact, with the potential to revolutionize the understanding of the biological world and drug discovery.
- In May 2024, Sanofi Open AI, Formation Bio announced a collaboration that would create AI-driven software meant to speed drug development and drive the efficiency of getting new medications to patients more quickly. Working together, the companies aimed to build tailored, purpose-built solutions that would drive different stages in the drug development process, enhancing processes and delivering better outcomes across pharmaceutical innovation.
- In May 2024, Lantern Pharma and Oregon Therapeutics initiated a strategic AI collaboration to maximize the development of first-in-class drug candidate XCE853, a highly effective inhibitor of cancer metabolism.
- In April 2024, Xaira Therapeutics, a drug discovery and development firm with AI capabilities, raised more than \$1 million in a co-funding round with ARCH Venture Partners and Foresite Labs. Xaira Therapeutics applies machine learning, data generation models, and therapeutic product development to address historically difficult drug targets.
- In April 2024, Odyssey Therapeutics, Inc., a biopharmaceutical firm leading the charge in next-generation precision medicines, disclosed that it signed a strategic research partnership with Janssen Pharmaceutica NV, a company of Johnson & Johnson, to co-discover and optimize small-molecule drugs against certain therapeutic targets. The two firms will share their strengths in AI, ML, computational chemistry, and drug discovery to de-risk challenging-to-drug targets.
- In February 2024, QIAGEN launched an AI-generated biomedical knowledge base to speed data-driven drug discovery. QIAGEN Biomedical KB-AI has more than 640 million biomedical relationships, such as gene, disease, and drug causal relationships, to support data-driven drug discovery.

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Some of the Key Companies in the AI in Drug Discovery Market Include-

- AiCure, LLC
- Atomwise Inc.
- BenevolentAI Group
- BioXcel Therapeutics Inc.
- BPGbio Inc.
- Cloud Pharmaceuticals
- Cyclica Inc.
- Deep Genomics Inc.
- Envisagenics
- Euretos Services BV
- Exscientia Plc.
- Healx Ltd.
- Iktos
- Insilico Medicine
- Lantern Pharma Inc.
- Merck KGaA
- NVIDIA Corp.
- NuMedii Inc.
- Pepticom Ltd.
- PHARNEXT SCA
- Predictive Oncology Inc.
- Recursion Pharmaceuticals Inc.
- Schrödinger, Inc.
- Tencent Holdings Ltd.
- Turbine Ltd.
- Valo Health Inc.
- XtalPi Inc.

AI in Drug Discovery Market Segmentation Analysis

Global AI in Drug Discovery Market by Component

- Software
- Services

Global AI in Drug Discovery Market by Therapeutic Area

- Oncology
- Infectious Diseases
- Neurology
- Metabolic Diseases
- Cardiovascular Diseases
- Immunology
- Other (Inflammatory Diseases)

Global AI in Drug Discovery Market by Application

- Drug Optimization and Repurposing
- Preclinical Testing
- Drug Screening
- Global AI in Drug Discovery Market by End-Users
- Pharmaceutical & Biotechnology Companies
- Contract Research Organizations (CROs)
- Research Centers and Academic & Government Institutes

Regional Analysis

- North America
 - o United States
 - o Canada
- Europe
 - o UK
 - o Germany
 - o Italy
 - o Spain
 - o France
 - o Rest of Europe
- Asia-Pacific
 - o China
 - o India
 - o Japan
 - o South Korea
 - o ASEAN Economies (Singapore, Thailand, Vietnam, Indonesia, and Other)
 - o Australia and New Zealand
 - o Rest of Asia-Pacific
- Rest of the World
 - o Latin America
 - o Middle East and Africa

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