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Artificial Intelligence in Drug Discovery Market by Process (Target, Lead), Use Case (Design & Optimisation: Vaccine, Antibody; Disease understanding, PK/PD), Therapy (Cancer, CNS, CVS), Tool (ML:DL (CNN, GAN)), End User & Region - Global Forecast to 2029

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Abstracts

The global artificial intelligence (AI) in drug discovery market is projected to reach 6.89 billion by 2029 from 1.86 billion in 2024, at a CAGR of 29.9% from 2024 to 2029. Increasing cross-industry collaborations and partnerships drive the growth of the artificial intelligence (AI) in drug discovery market by combining expertise, resources, and technology from various aspects of the drug discovery supply chain. For instance, in March 2024, Cognizant collaborated with NVIDIA to use generative AI through the BioNeMo platform, with the goal of transforming drug discovery and accelerating the development of life-saving therapies. Similarly, in August 2024, Exscientia Recursion and Exscientia plc announced a agreement, combining their technologies to enhance drug discovery. The integrated Recursion OS will enhance drug discovery through patient-centric target discovery, AI-driven design, quantum mechanics modeling, automated chemical synthesis, and other features. The combined company plans to complete 10 clinical trials within 18 months. Exscientia shareholders will receive Recursion stock, with Recursion shareholders owning 74% of the combined company. The deal is worth USD 850M in cash and is expected to close by early 2025.

“Oncology held the largest market share in the artificial intelligence (AI) in drug discovery market, by therapeutic area in 2023.”

Based on therapeutic areas, the artificial intelligence (AI) in drug discovery market is

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segmented into oncology, infectious diseases, neurology, metabolic diseases, cardiovascular diseases, immunology, mental health, and others (respiratory diseases, nephrology, dermatological diseases, genetic disorders, inflammatory diseases, and gastrointestinal). The oncology segment held the largest market share in the artificial intelligence (AI) in drug discovery market due to high prevalence of cancer and the complex nature of tumor biology, which necessitates innovative approaches for drug development. There were approximately 20 million new cancer cases and 9.7 million cancer-related deaths worldwide in 2022. Similarly, in 2024, 2.0 million new cancer cases and 611,720 cancer deaths are projected to occur in the US. The growing availability of biomedical data from cancer research, patient records, genomic studies, multi-omics datasets (genomics, proteomics, transcriptomics), and clinical trials provides an opportunity to leverage AI for pattern recognition and predicting drug interactions. The high demand for personalized medicine and targeted therapies in oncology, large commercial returns, emerging focus on immuno-oncology (especially checkpoint inhibitors and T-cell therapies), and exhaustive data availability drive investment in AI-driven solutions, elevating it to the forefront of the drug discovery landscape.

“Understanding disease use case to witness the fastest growth during the forecast period.”

Based on the use case, artificial intelligence (AI) in drug discovery market is segmented into understanding the disease, drug repurposing, de novo drug design, drug optimization, and safety & toxicity. The understanding disease is poised to be the fastest-growing use case over the forecast period. AI’s capacity to assess complex biological data and identify disease mechanisms is critical in early-stage drug development. AI helps researchers better understand disease pathways, genetic factors, and biomarkers, all of which are necessary for developing targeted therapies. Understanding diseases is required to identify potential drug targets, which enhances the efficiency of subsequent stages such as drug design and testing. The growth use of AI for phenotypic screening, image analysis, detecting anomalies in genetic perturbations on cellular or tissue morphology, biomarker identification, (-omics) data mining is expected to fuel the market growth.

“North America to dominate the market over the forecast period.”

Based on the region, the artificial intelligence (AI) in drug discovery market is segmented into five major regional segments: North America, Europe, Asia Pacific, Latin America, and Middle East & Africa. The North American region dominated the

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artificial intelligence (AI) in drug discovery market in 2023. Several factors contribute to this dominance, including significant investment in healthcare technology, strong cross-sector collaborations, the presence of large pharmaceutical and biotechnology companies, and a favorable regulatory environment. The total investments in AI in Drug Development companies are USD 60.2 billion as of March 2023. A large wave of proof-of-concept studies and substantial advances in democratizing AI technology are also propelling the growth of the market. For example, in January 2023, AbSci created and validated de novo antibodies in silico with generative AI. Furthermore, in February 2023, the FDA granted an Orphan Drug Designation to a drug discovered and designed with AI. Insilico Medicine and began a global Phase I trial for the drug.

In-depth interviews have been conducted with chief executive officers (CEOs), Directors, and other executives from various key organizations operating in the authentication and brand protection marketplace.

Breakdown of supply-side primary interviews by company type, designation, and region:

By Company Type: Tier 1 (31%), Tier 2 (28%), and Tier 3 (41%)

By Designation – Demand Side: Purchase Managers (45%), Heads of Artificial Intelligence, Machine Learning, Drug Discovery, and Computational Molecular Design (30%), and Research Scientists (25%)

By Designation – Supply Side: C-level Excecutives & Director level (35%), Managers (40%), and Others (25%)

By Region: North America (45%), Europe (30%), Asia Pacific (20%), and Rest of the world (5%)

List of Companies Profiled in the Report

NVIDIA Corporation (US)

Exscientia (UK)

Google (US)

BenevolentAI (UK)

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Recursion (US)

Insilico Medicine (US)

Schr?dinger, Inc. (US)

Microsoft (US)

Atomwise Inc. (US)

Illumina, Inc. (US)

Numedii, Inc. (US)

Xtalpi Inc. (US)

Iktos (France)

Tempus (US)

DEEP GENOMICS (Canada)

Verge Genomics (US)

BenchSci (Canada)

Insitro (US)

Valo Health (US)

BPGBio, Inc. (US)

Merck KGaA (Germany)

IQVIA (US)

Tencent Holdings Limited (China)

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Predictive Oncology, Inc. (US)

CytoReason (Israel)

Owkin, Inc. (US)

Cloud Pharmaceuticals (US)

Evaxion Biotech (Denmark)

Standigm (South Korea)

BIOAGE (US)

Envisagenics (US)

Abcellera (US)

Centella (India)

The study includes an in-depth competitive analysis of these key players in the artificial intelligence (AI) in drug discovery market, with their company profiles, recent developments, and key market strategies.

Research Coverage

This research report categorizes the artificial intelligence (AI) in drug discovery market by process (target identification & selection, target validation, hit identification & prioritization, hit-to-lead identification/lead generation, lead optimization, and candidate selection & validation), by use case (understanding disease, drug repurposing, de novo drug design [small molecule design, vaccines design, antibody & other biologics design], drug optimization [small molecule optimization, vaccines optimization, antibody & other biologics optimization], and safety and toxicity), by therapeutic area (oncology, infectious diseases, neurology, metabolic diseases, cardiovascular diseases, immunology, mental health, others), by player type (end-to-end solution providers, niche/point solutions providers, AI technology providers, business process service providers), by tools (machine learning, natural language processing, context-aware process and computing, computer vision, image analysis (including optical character

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recognition)), by deployment (on-premise, cloud-based, SaaS-based), by end user (pharmaceutical & biotechnology companies, contract research organizations (CROs), and research centers, academic institutes, & government organizations) and by region (North America, Europe, Asia Pacific, Latin America, and Middle East & Africa). The scope of the report covers detailed information regarding the major factors, such as drivers, restraints, challenges, and opportunities, influencing the growth of the artificial intelligence (AI) in drug discovery market. A detailed analysis of the key industry players has been done to provide insights into their business overview, solutions, and services, key strategies such as product launches and enhancements, investments, partnerships, collaborations, agreements, joint ventures, funding, acquisitions, expansions, conferences, FDA clearances, sales contracts, alliances, and other recent developments associated with the artificial intelligence (AI) in drug discovery market. Competitive analysis of upcoming startups in the artificial intelligence (AI) in drug discovery market ecosystem is covered in this report.

Reasons to buy this report

The report will help the market leaders/new entrants in this market with information on the closest approximations of the revenue numbers for the artificial intelligence (AI) in drug discovery market and the subsegments. This report will help stakeholders understand the competitive landscape and gain more insights to position their businesses better and to plan suitable go-to-market strategies. The report also helps stakeholders understand the pulse of the market and provides them with information on key market drivers, restraints, challenges, and opportunities.

The report provides insights on the following pointers:

- Analysis of key drivers (growing cross-industry collaborations and partnerships, growing need to reduce time and cost of drug discovery and development, patent expiry of several drugs, AI application in oncology areas, integration of multi-omics data, initiatives for research on rare diseases and orphan drugs), restraints (shortage of AI workforce and ambiguous regulatory guidelines for medical software, interpretability of AI), opportunities (growing biotechnology industry, increasing focus on emerging markets, focus on developing human-aware AI systems, increasing use of AI in single cell analysis, rapid expansion of biomarker, disease types, and subtypes identification, growing demand for precision and personalized medicine), and challenges (limited availability of data sets, lack of required tools and usability, computational limitations of advanced AI models, challenges regarding the accessibility of high-quality data)

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influencing the growth of the artificial intelligence (AI) in drug discovery market

Product Development/Innovation: Detailed insights on upcoming technologies, research & development activities, and new product & service launches in the artificial intelligence (AI) in drug discovery market

Market Development: Comprehensive information about lucrative markets – the report analyses the artificial intelligence (AI) in drug discovery market across varied regions.

Market Diversification: Exhaustive information about new products & services, untapped geographies, recent developments, and investments in the artificial intelligence (AI) in drug discovery market

Competitive Assessment: In-depth assessment of market shares, growth strategies and service offerings of leading players such as NVIDIA Corporation (US), Exscientia (UK), Google (US), BenevolentAI (UK), Recursion (US), Insilico Medicine (US), Schr?dinger, Inc. (US), Microsoft (US), Atomwise Inc. (US), Illumina, Inc. (US), Numedii, Inc. (US), Xtalpi Inc. (US), Iktos (France), Valo Health (US), and Merck KGaA (Germany), among others in artificial intelligence (AI) in drug discovery market.

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