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AI Drug Discovery Market Forecasts to 2032 – Global Analysis By Drug Type (Small Molecule Drug Discovery, Biologics Discovery, Peptide & Protein-Based Drugs, Regenerative & Cell Therapies, Gene Therapy Candidates, and Novel Therapeutic Modalities), Therapeutic Area, Technology, Application, End User, and By Geography.

https://marketpublishers.com/r/A178B047F43BEN.html
Date: December 2025
Pages: 200
Price: US$ 4,150.00 (Single User License)
ID: A178B047F43BEN

Abstracts

According to Stratistics MRC, the Global AI Drug Discovery Market is accounted for $4.8 billion in 2025 and is expected to reach $9.6 billion by 2032 growing at a CAGR of 10.4% during the forecast period. AI Drug Discovery involves deploying advanced algorithms to analyze biological data, predict molecular interactions, and accelerate identification of potential therapeutic candidates. Machine-learning platforms streamline target selection, lead optimization, and toxicity prediction, significantly reducing development time and costs. These systems enable rapid screening of vast compound libraries and simulate biochemical behavior before laboratory validation. As a result, pharmaceutical companies gain faster pathways to innovation, improved R&D productivity, and a higher probability of success in addressing complex and rare diseases.

According to Clinical Trials Arena's 2025 analysis, strategic partnerships between AI firms and pharmaceutical companies surged to 27 in 2024 from 4 in 2015, highlighting collaborative innovation in accelerating drug development and reducing preclinical failure rates.

Market Dynamics:

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Driver:

Rising demand for faster drug pipelines

Rising demand for faster drug pipelines is accelerating AI adoption as pharma companies strive to shorten discovery timelines and reduce R&D risks. Propelled by the need to identify lead compounds more efficiently, AI algorithms support high-throughput screening, molecular docking, and predictive modeling. Increasing pressure to commercialize therapeutics rapidly especially for complex diseases further boosts reliance on automation. As competitive intensity heightens, developers increasingly view AI-driven discovery engines as essential tools to enhance productivity and improve success rates across early-stage drug workflows.

Restraint:

High deployment costs for platforms

High deployment costs for platforms remain a significant barrier, especially for small and mid-sized biotech firms with limited capital. Advanced AI discovery engines require substantial investments in cloud computing, biological datasets, model training, and skilled personnel. Integration with legacy laboratory systems further increases expenditures, complicating scalability. Additionally, the need for ongoing algorithm refinement and data acquisition adds long-term operational costs. These financial constraints slow adoption and create disparities between large pharmaceutical companies and emerging research organizations.

Opportunity:

Advances in computational biology integration

Advances in computational biology integration create substantial growth opportunities by enabling deeper understanding of disease mechanisms. The fusion of omics data, molecular simulations, and AI-driven pathway analysis accelerates target identification and mechanism-of-action studies. As multi-modal datasets become more accessible, AI platforms gain the ability to predict therapeutic responses with higher accuracy. This synergy significantly enhances precision-drug development and broadens applicability across rare diseases, immunology, and personalized medicine. These advancements position AI as a transformative enabler of next-generation drug pipelines.

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Threat:

Data breaches affecting proprietary research

Data breaches affecting proprietary research pose a major threat, particularly as vast volumes of molecular data reside in cloud environments. Unauthorized access or model manipulation could compromise competitive strategies, delay regulatory submissions, or reveal confidential compound libraries. Increasing cyberattacks in the biotech sector amplify vulnerabilities, undermining trust in digitalized research workflows. Companies lacking robust security frameworks risk reputational damage and financial losses, emphasizing the necessity for stringent cybersecurity protocols across AI-driven discovery ecosystems.

Covid-19 Impact:

COVID-19 accelerated AI drug discovery adoption as pharma companies sought rapid solutions for antiviral and immunomodulatory candidates. AI tools supported virtual screening and repurposing efforts, significantly compressing early research timelines. The pandemic highlighted inefficiencies in traditional R&D approaches, prompting long-term investments in machine learning platforms. Additionally, global collaboration increased dataset availability, improving model accuracy. Post-pandemic, continued emphasis on rapid therapeutic response and preparedness sustains market momentum for AI-enabled discovery frameworks.

The small molecule drug discovery segment is expected to be the largest during the forecast period

The small molecule drug discovery segment is expected to account for the largest market share during the forecast period, resulting from its broad therapeutic applicability and well-established development pathways. AI platforms excel at optimizing molecular structures, predicting ADMET profiles, and accelerating lead optimization cycles. Pharmaceutical companies continue prioritizing small molecules due to their scalability, lower manufacturing complexity, and strong commercial success rates. These factors reinforce dominant adoption of AI technologies across small molecule pipelines compared to other drug classes.

The oncology segment is expected to have the highest CAGR during the forecast period

Over the forecast period, the oncology segment is predicted to witness the highest

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growth rate, propelled by rising demand for precision therapies and complex target identification. Cancer's heterogeneous biology requires extensive data modeling, making AI particularly valuable for biomarker discovery, pathway mapping, and personalized treatment design. Increasing investment in immuno-oncology and targeted inhibitors further boosts reliance on AI-driven insights. As cancer incidence climbs globally, developers accelerate adoption of advanced analytics, supporting this segment's exceptional growth trajectory.

Region with largest share:

During the forecast period, the Asia Pacific region is expected to hold the largest market share, attributed to expanding pharmaceutical R&D hubs across China, India, South Korea, and Japan. Strong government support for biotech innovation, increasing clinical trial activity, and growing AI research capabilities fuel demand. Regional cost advantages attract global companies to outsource discovery tasks. Additionally, rapidly developing health ecosystems and increasing investment in computational drug discovery strengthen Asia Pacific's leadership position.

Region with highest CAGR:

Over the forecast period, the North America region is anticipated to exhibit the highest CAGR associated with strong AI infrastructure, robust pharmaceutical innovation, and early adoption of advanced discovery tools. Leading biotech companies, AI start-ups, and research institutes accelerate integration of machine learning into drug pipelines. Favorable regulatory pathways for digital R&D tools further enhance uptake. High availability of curated datasets, venture funding, and interdisciplinary talent solidify North America as the fastest-expanding market for AI-driven drug discovery.

Key players in the market

Some of the key players in AI Drug Discovery Market include Pfizer, Roche, AstraZeneca, Moderna, Sanofi, Novartis, Johnson & Johnson, GSK, Eli Lilly, Bayer, Boehringer Ingelheim, Merck & Co., AbbVie, Schr?dinger, Exscientia, Atomwise and Insilico Medicine.

Key Developments:

In November 2025, AstraZeneca launched an AI collaboration with BenevolentAI, applying predictive algorithms to respiratory and cardiovascular drug pipelines, aiming

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to shorten discovery timelines and improve patient-specific treatment outcomes.

In October 2025, Pfizer advanced its AI-driven oncology pipeline, integrating machine learning for target identification and biomarker discovery, accelerating clinical trial readiness and enhancing precision medicine strategies across multiple cancer indications.

In September 2025, Roche expanded its AI-enabled drug discovery platform, focusing on immunology and rare diseases, leveraging deep learning to optimize molecular design and reduce early-stage attrition rates in therapeutic development.

Drug Types Covered:

- Small Molecule Drug Discovery
- Biologics Discovery
- Peptide & Protein-Based Drugs
- Regenerative & Cell Therapies
- Gene Therapy Candidates
- Novel Therapeutic Modalities

Therapeutic Areas Covered:

- Oncology
- Neurology
- Immunology
- Infectious Diseases
- Cardiology
- Rare & Orphan Diseases

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Technologies Covered:

- Machine Learning Platforms
- Deep Learning & Neural Networks
- Generative AI for Molecule Design
- Quantum AI Drug Modeling
- Structure-Based Drug Design Tools
- Omics Data Analysis Systems

Applications Covered:

- Target Identification
- Lead Generation & Optimization
- Compound Screening
- Preclinical Testing Automation
- Biomarker Identification
- Toxicity Prediction & Validation

End Users Covered:

- Pharmaceutical Companies & Biotechnology Companies
- Academic & Research Institutes
- Contract Research Organizations (CROs)

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- Hospitals & Clinical Labs
- Other End Users

Regions Covered:

- North America
  - US
  - Canada
  - Mexico
- Europe
  - Germany
  - UK
  - Italy
  - France
  - Spain
  - Rest of Europe
- Asia Pacific
  - Japan
  - China
  - India
  - Australia

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New Zealand

South Korea

Rest of Asia Pacific

South America

Argentina

Brazil

Chile

Rest of South America

Middle East & Africa

Saudi Arabia

UAE

Qatar

South Africa

Rest of Middle East & Africa

What our report offers:
- Market share assessments for the regional and country-level segments
- Strategic recommendations for the new entrants
- Covers Market data for the years 2024, 2025, 2026, 2028, and 2032
- Market Trends (Drivers, Constraints, Opportunities, Threats, Challenges, Investment Opportunities, and recommendations)
- Strategic recommendations in key business segments based on the market estimations
- Competitive landscaping mapping the key common trends

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- Company profiling with detailed strategies, financials, and recent developments
- Supply chain trends mapping the latest technological advancements

Free Customization Offerings:

All the customers of this report will be entitled to receive one of the following free customization options:

Company Profiling

Comprehensive profiling of additional market players (up to 3)

SWOT Analysis of key players (up to 3)

Regional Segmentation

Market estimations, Forecasts and CAGR of any prominent country as per the client's interest (Note: Depends on feasibility check)

Competitive Benchmarking

Benchmarking of key players based on product portfolio, geographical presence, and strategic alliances

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Contents

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11 KEY DEVELOPMENTS

12 COMPANY PROFILING

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List Of Tables

LIST OF TABLES

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Note: Tables for North America, Europe, APAC, South America, and Middle East & Africa Regions are also represented in the same manner as above.

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