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AI in Drug Discovery Market Forecasts to 2032 – Global Analysis By Type (Preclinical and Clinical Testing, Molecule Screening, Target Identification and De Novo Drug Design), Drug Type, Offering, Technology, Application, End User and By Geography

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Abstracts

According to Stratistics MRC, the Global AI in Drug Discovery Market is accounted for $2.6 billion in 2025 and is expected to reach $17.8 billion by 2032 growing at a CAGR of 31.7% during the forecast period. Artificial Intelligence (AI) in drug discovery refers to the application of machine learning and data-driven algorithms to accelerate and optimize the process of developing new drugs. AI can analyze vast datasets—from molecular structures to clinical trial results—to identify promising drug candidates, predict drug-target interactions, and even design novel compounds. It reduces the time, cost, and failure rate associated with traditional drug development methods. By simulating biological systems and learning from existing data, AI helps researchers uncover patterns and make decisions with greater precision.

According to the estimates by WHO, in 2022, 20 million new cancer cases and 9.7 million deaths were reported globally.

Market Dynamics:

Driver:

Rising R&D Costs and Time Pressure

Rising R&D costs and time pressure are accelerating the adoption of AI in drug discovery, acting as catalysts for innovation. These challenges push pharmaceutical

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companies to embrace AI-driven solutions that streamline target identification, optimize clinical trials, and reduce costly failures. As a result, AI enhances R&D productivity, shortens development timelines, and improves success rates. This urgency fosters investment in intelligent technologies, transforming traditional workflows and enabling faster, more cost-effective drug development to meet growing healthcare demands.

Restraint:

Lack of Standardized, High-Quality Data

The lack of standardized, high-quality data severely hampers AI's effectiveness in drug discovery. Inconsistent formats, incomplete annotations, and biased datasets compromise model accuracy and reproducibility. These data issues lead to flawed predictions, increased development costs, and delayed timelines. Without harmonized data, AI struggles to identify viable drug candidates or predict outcomes reliably, limiting its transformative potential and widening the gap between research innovation and real-world pharmaceutical application.

Opportunity:

Explosion of Biomedical Data

The explosion of biomedical data is fueling a transformative leap in AI-driven drug discovery. With vast datasets from genomics, proteomics, and clinical records, AI models can now uncover hidden patterns, predict drug-target interactions, and accelerate lead identification. This data abundance enhances precision, reduces trial-and-error, and supports personalized medicine. As a result, pharmaceutical R&D becomes faster, more efficient, and cost-effective. The synergy between big data and AI is reshaping drug development into a smarter, data-powered frontier.

Threat:

High Implementation Costs

High implementation costs significantly hinder the adoption of AI in drug discovery, especially among small and mid-sized pharmaceutical firms. These expenses include advanced infrastructure, skilled personnel, and ongoing system maintenance. Such financial barriers delay integration, limit innovation, and widen the gap between large

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corporations and emerging players. As a result, the full potential of AI remains underutilized, slowing progress in developing faster, cost-effective, and personalized therapeutic solutions.

Covid-19 Impact

The COVID-19 pandemic significantly accelerated the adoption of AI in drug discovery, as pharmaceutical companies urgently sought faster, cost-effective solutions. AI tools were pivotal in identifying therapeutic targets, repurposing drugs, and optimizing vaccine development. This surge in demand led to increased investments, collaborations, and integration of AI platforms across R&D pipelines. The pandemic ultimately highlighted AI's transformative potential, establishing it as a critical asset in future pharmaceutical innovation and crisis response.

The oncology segment is expected to be the largest during the forecast period

The oncology segment is expected to account for the largest market share during the forecast period due to the urgent demand for precise, personalized cancer treatments. AI accelerates biomarker discovery, predicts therapeutic responses, and enhances clinical trial design, especially in complex cancers like lung and breast cancer. With oncology accounting for the largest share of AI drug discovery investments, it fosters innovation in targeted therapies and immuno-oncology. This synergy improves success rates, reduces development time, and positions AI as a transformative force in cancer research and treatment.

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

Over the forecast period, the deep learning segment is predicted to witness the highest growth rate as it enables rapid analysis of complex biomedical data. Its ability to model intricate biological interactions accelerates target identification, optimizes compound screening, and enhances de novo drug design. Deep learning reduces development time and costs by improving prediction accuracy and minimizing trial failures. As pharmaceutical companies increasingly adopt these models, they unlock scalable, data-driven innovation—transforming drug discovery into a faster, more precise, and cost-effective process.

Region with largest share:

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During the forecast period, the Asia Pacific region is expected to hold the largest market share due to robust R&D ecosystems, government support, and a surge in biotech startups. Countries like China, India, and Japan are leveraging AI to accelerate clinical trials, reduce costs, and enhance precision medicine. With vast genomic datasets and digital infrastructure, the region fosters innovation in oncology, immunology, and rare diseases. This momentum positions Asia Pacific as a global leader, transforming drug development into a faster, smarter, and more accessible process.

Region with highest CAGR:

Over the forecast period, the North America region is anticipated to exhibit the highest CAGR, owing to robust pharmaceutical infrastructure and leading tech innovators, the region leads global adoption. AI enables rapid compound screening, predictive modeling, and personalized medicine development. Strategic collaborations between biotech firms and AI startups are fueling innovation, while regulatory support fosters growth. This synergy is driving a projected market surge, positioning North America as a powerhouse in AI-driven pharmaceutical breakthroughs

Key players in the market

Some of the key players profiled in the AI in Drug Discovery Market include Atomwise, Inc., BenevolentAI, Insilico Medicine, Exscientia Ltd., Recursion Pharmaceuticals, BioXcel Therapeutics, Deep Genomics, Cloud Pharmaceuticals, Numerate, Inc., Cyclica Inc., Iktos, Evaxion Biotech, BERG LLC, Verge Genomics, Healx, PathAI, NVIDIA Corporation, IBM Watson Health, Google DeepMind and Schrodinger, Inc.

Key Developments:

In August 2022, Atomwise and Sanofi have launched a strategic, exclusive collaboration to harness Atomwise’s AtomNet® AI platform for structure-based drug discovery targeting up to five molecular targets.

In March 2020, Atomwise and Bridge Biotherapeutics struck potential $1 billion research collaboration, aiming to develop up to 13 AI-driven small-molecule programs targeting inflammation-related proteins, especially Pellino E3 ubiquitin ligases.

Types Covered:

Preclinical and Clinical Testing

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- Molecule Screening
- Target Identification
- De Novo Drug Design

Drug Types Covered:

- Small Molecules
- Large Molecules

Offerings Covered:

- Software
- Services

Technologies Covered:

- Machine Learning
- Deep Learning
- Natural Language Processing (NLP)
- Other Technologies

Applications Covered:

- Oncology
- Neurology

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- Infectious Diseases
- Cardiovascular Diseases
- Metabolic Diseases
- Immunology
- Other Applications

End Users Covered:

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

Regions Covered:

- North America
  - US
  - Canada
  - Mexico
- Europe
  - Germany
  - UK

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- Italy
- France
- Spain
- Rest of Europe

Asia Pacific

- Japan
- China
- India
- Australia
- New Zealand
- South Korea
- Rest of Asia Pacific

South America

- Argentina
- Brazil
- Chile
- Rest of South America

Middle East & Africa

- Saudi Arabia

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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 2022, 2023, 2024, 2026, and 2030
- 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
- 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

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

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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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