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# Generative AI Molecule Discovery & Repurposing Market Forecasts to 2034 – Global Analysis By Product (AI-Driven Drug Design Platforms, Molecule Generation Software, Drug Repurposing Engines, Virtual Screening Platforms, Other Products), By Component, By Technology, By Application, By End User and By Geography

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## Abstracts

According to Stratistics MRC, the Global Generative AI Molecule Discovery & Repurposing Market is accounted for $4.6 billion in 2026 and is expected to reach $49.5 billion by 2034 growing at a CAGR of 30% during the forecast period. Generative AI Molecule Discovery & Repurposing involves the use of artificial intelligence models to design new chemical compounds or identify new therapeutic uses for existing drugs. These AI systems analyze large biological and chemical datasets to generate potential drug candidates with optimized properties. They can simulate molecular interactions, predict efficacy, and accelerate early-stage drug discovery. By reducing research timelines and development costs, generative AI helps pharmaceutical companies identify promising treatments more efficiently while expanding opportunities for repurposing approved drugs for new diseases.

**Market Dynamics:**

**Driver:**

Accelerating drug discovery with AI

AI algorithms enable rapid identification of novel molecules and predictive modeling of

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therapeutic outcomes. This significantly reduces the time and cost associated with traditional drug development. Pharmaceutical and biotech firms are increasingly adopting AI platforms to enhance R&D efficiency. Partnerships between AI developers and research institutions are further strengthening adoption. This technological momentum continues to propel global market growth.

**Restraint:**

High computational infrastructure costs

Generative AI platforms require advanced hardware, cloud computing resources, and specialized expertise. Smaller firms and startups often struggle to afford these investments. Ongoing maintenance and data management add to operational expenses. Limited access to affordable infrastructure slows adoption in emerging regions. These financial barriers continue to restrict broader market penetration.

**Opportunity:**

Repurposing existing drugs for new indications

Generative AI can analyze molecular structures and predict alternative applications for approved drugs. This approach reduces development timelines and regulatory hurdles compared to novel drug creation. Pharmaceutical firms are leveraging AI-driven repurposing to expand product pipelines. Collaborations with healthcare providers and research institutions are enhancing credibility. This opportunity is expected to drive innovation and cost efficiency in the sector.

**Threat:**

Regulatory uncertainty for AI-designed drugs

Approval processes for AI-designed molecules remain unclear in many jurisdictions. Lack of standardized frameworks creates challenges for commercialization. Regulatory delays discourage investment in AI-driven drug discovery. Concerns about transparency and explainability of AI models further complicate compliance. This uncertainty continues to challenge the scalability of generative AI in pharmaceuticals.

**Covid-19 Impact:**

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The Covid-19 pandemic accelerated interest in AI-driven drug discovery. Urgent demand for treatments and vaccines highlighted the need for faster R&D processes. Generative AI platforms were leveraged to identify potential molecules and repurpose existing drugs. Increased funding for biotech and AI startups boosted innovation. Remote collaboration tools supported global research efforts during lockdowns. Overall, Covid-19 reinforced the relevance of AI in building resilient drug discovery pipelines.

The software platforms segment is expected to be the largest during the forecast period

The software platforms segment is expected to account for the largest market share during the forecast period as AI-driven tools form the backbone of molecule discovery. Pharmaceutical and biotech firms rely on advanced platforms for predictive modeling and molecular design. Continuous innovation in algorithms enhances accuracy and efficiency. Cloud-based solutions are expanding accessibility across regions. Rising demand for integrated platforms further strengthens this segment's dominance.

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

Over the forecast period, the biotechnology companies segment is predicted to witness the highest growth rate due to their agility in adopting AI-driven solutions. Biotech firms are increasingly leveraging generative AI to accelerate drug pipelines and repurpose molecules. Rising venture capital investments are fueling adoption among startups. Collaborations with AI developers and pharmaceutical firms are driving innovation. Growing demand for precision medicine is further boosting this segment.

**Region with largest share:**

During the forecast period, the North America region is expected to hold the largest market share owing to advanced healthcare infrastructure and strong R&D investments. The U.S. leads in AI adoption for drug discovery, with established pharmaceutical and biotech firms driving innovation. Regulatory frameworks and funding initiatives further support commercialization. Strong venture capital presence accelerates startup growth. Academic collaborations enhance credibility and adoption.

**Region with highest CAGR:**

Over the forecast period, the Asia Pacific region is anticipated to exhibit the highest CAGR driven by rapid advancements in healthcare and biotechnology. Countries such

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as China, India, and Japan are witnessing increased adoption of AI-driven drug discovery platforms. Government-backed initiatives and funding programs are boosting innovation. Local startups are entering the market with cost-effective solutions, expanding accessibility. Expansion of digital infrastructure and cloud computing is further supporting growth.

**Key players in the market**

Some of the key players in Generative AI Molecule Discovery & Repurposing Market include Insilico Medicine, Exscientia plc, BenevolentAI, Recursion Pharmaceuticals, Inc., Schr?dinger, Inc., Atomwise, Inc., XtalPi Inc., Generate Biomedicines, Deep Genomics Inc., Relay Therapeutics, Inc., IBM Corporation, Alphabet Inc., Microsoft Corporation, NVIDIA Corporation and Absci Corporation.

**Key Developments:**

In January 2026, Insilico launched the Science MMAI Gym, a new domain-specific training environment designed to transform general-purpose Large Language Models (LLMs) into high-performance engines for pharmaceutical-grade drug discovery tasks.

In February 2024, Exscientia signed a collaboration worth up to $674 million with the German Merck to discover novel small-molecule candidates across oncology, neurology, and immunology. The deal included a $20 million upfront payment for three initial research programs.

Products Covered:

AI-Driven Drug Design Platforms

Molecule Generation Software

Drug Repurposing Engines

Virtual Screening Platforms

Other Products

Components Covered:

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- Software Platforms
- AI Algorithms & Models
- Data Libraries
- Cloud Infrastructure
- Computational Chemistry Tools
- Other Components

Technologies Covered:

- Deep Learning
- Transformer Models
- Graph Neural Networks
- Reinforcement Learning
- Other Technologies

Applications Covered:

- Oncology Drug Discovery
- Rare Disease Drug Development
- Infectious Disease Research
- CNS Drug Discovery
- Immunology & Inflammation
- Other Applications

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End Users Covered:

- Pharmaceutical Companies
- Biotechnology Companies
- CROs
- Academic Research Institutes
- Other End Users

Regions Covered:

- North America
  - United States
  - Canada
  - Mexico
- Europe
  - United Kingdom
  - Germany
  - France
  - Italy
  - Spain
  - Netherlands

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- Belgium
- Sweden
- Switzerland
- Poland
- Rest of Europe

Asia Pacific

- China
- Japan
- India
- South Korea
- Australia
- Indonesia
- Thailand
- Malaysia
- Singapore
- Vietnam
- Rest of Asia Pacific

South America

- Brazil
- Argentina

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- Colombia
- Chile
- Peru
- Rest of South America

Rest of the World (RoW)

- Middle East
  - Saudi Arabia
  - United Arab Emirates
  - Qatar
  - Israel
  - Rest of Middle East
- Africa
  - South Africa
  - Egypt
  - Morocco
  - Rest of 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 2023, 2024, 2025, 2026, 2027, 2028, 2030, 2032 and 2034

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- 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

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

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