Artificial Intelligence (AI) in Drug Discovery Market - Global Outlook & Forecast 2025-2030

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Report description:

The global AI in drug discovery market is expected to grow at a CAGR of 30.58% from 2024 to 2030.

MARKET TRENDS & DRIVERS

Integration of AI with Big Data and Omics Technologies

The integration of AI with big data and omics technologies is reshaping the global drug discovery market. By enabling a deeper understanding of biological systems, improving efficiency, and driving personalized medicine, this trend is creating unprecedented opportunities for innovation and growth. Overcoming existing challenges will further cement its role as a transformative force in the healthcare and pharmaceutical industries. The future of drug discovery is undeniably data-driven, with AI at its core.

Increasing Use of Generative AI Models

The increasing use of generative AI models in the global AI in drug discovery market marks a paradigm shift in how pharmaceutical research and development are conducted. By enabling faster, cheaper, and more precise drug development, these models are creating new opportunities across the healthcare ecosystem. As technology continues to evolve, generative AI is set to redefine the boundaries of what is possible in drug discovery, offering hope for faster cures, more personalized treatments, and a healthier future.

Emergence of AI-Driven Drug Repurposing

The emergence of AI-driven drug repurposing is a game-changer in the global drug discovery market, transforming traditional approaches and creating exciting new opportunities. By reducing costs, accelerating timelines, and addressing unmet medical

needs, AI-driven drug repurposing is shaping the future of pharmaceutical innovation. As AI technologies continue to evolve, their integration into drug repurposing will undoubtedly unlock even greater potential, benefiting both the industry and global healthcare systems.

Growing Partnerships between Pharmaceutical Companies and AI-focused Expertise

The growing partnerships between pharmaceutical companies and AI-focused expertise are transforming the global drug discovery landscape. By leveraging AI's capabilities to overcome traditional challenges, these collaborations are creating new opportunities for faster, more cost-effective, and innovative drug development. As the pharmaceutical industry continues to embrace AI, the synergies between these two domains will not only drive market growth but also pave the way for groundbreaking advancements in medicine, ultimately benefiting patients worldwide.

Advancements in Computing Power and Cloud Technologies

The convergence of computing power and cloud technologies has become a driving force in the global AI in drug discovery market. These advancements are empowering pharmaceutical companies and research institutions to revolutionize drug development processes, making them faster, more efficient, and more accessible. As technology continues to evolve, the synergy between AI, computing, and cloud platforms will play an increasingly central role in addressing unmet medical needs and advancing healthcare innovation worldwide.

Rising R&D Costs in Drug Discovery

The rising costs of R&D in drug discovery are pushing the pharmaceutical industry to embrace innovative solutions, and AI is emerging as a powerful enabler. By reducing expenses, improving success rates, and accelerating development timelines, AI is addressing critical pain points in the industry. As the global AI in drug discovery market continues to expand, it holds the potential to not only alleviate financial pressures but also revolutionize healthcare by delivering innovative treatments more efficiently and effectively.

Growing Volume of Biological and Clinical Data

The growing volume of biological and clinical data is a driving force in the global AI in drug discovery market. By enabling the analysis of vast and complex datasets, AI is revolutionizing target identification, drug screening, and personalized medicine. Although challenges remain, the synergy between AI and data promises to unlock new frontiers in drug discovery, improving global health outcomes and addressing unmet medical needs. As this trend continues, AI will remain at the forefront of innovation, reshaping the pharmaceutical landscape.

Increasing Prevalence of Chronic Diseases

The increasing prevalence of chronic diseases has created a pressing need for innovative and efficient drug discovery methods. AI has emerged as a transformative tool, enabling the rapid identification of potential drug candidates, optimizing clinical trials, and accelerating the development of personalized therapies. As chronic diseases continue to rise globally, the adoption of AI in drug discovery is poised to grow, driving advancements in healthcare and improving patient outcomes. With continued investments and collaborations, the global AI in drug discovery market is set to play a pivotal role in addressing one of the most significant healthcare challenges of our time.

SEGMENTATION INSIGHTS

INSIGHTS BY APPLICATION

The global AI in drug discovery market by application is segmented into drug repurposing, drug screening, drug design & optimization, and others. The drug repurposing segment held the largest market share. Drug repurposing refers to the identification of new therapeutic uses for existing drugs. AI significantly enhances this process by analyzing massive datasets, including genomics, clinical trials, and real-world evidence, to identify potential drug-disease pairings. Drug screening involves the evaluation of thousands of compounds to identify potential candidates for further development. AI-powered screening significantly accelerates this traditionally time-intensive process.
AI is revolutionizing drug design and optimization by generating novel molecular structures and refining existing compounds for improved efficacy, safety, and pharmacokinetics. Beyond the core applications, AI is being deployed in various other aspects of drug discovery, such as clinical trial optimization, biomarker discovery, and toxicity prediction. Furthermore, the global AI in drug discovery market is expected to witness sustained growth across all applications. Advances in AI technologies, increasing adoption of cloud computing, and deeper integration of AI into the pharmaceutical pipeline will drive innovation and efficiency. As more companies and research institutions embrace AI-driven approaches, the potential to bring safer, more effective therapies to market faster and at a lower cost is becoming a reality.

Segmentation by Application
- Drug Repurposing
- Drug Screening
- Drug Design & Optimization
- Others

INSIGHTS BY THERAPEUTIC AREA

The global AI in drug discovery market spans various therapeutic areas, leveraging AI to enhance research and development across diverse medical conditions. AI's ability to analyze vast datasets, identify potential drug candidates, and streamline development pipelines has significantly impacted therapeutic segments, addressing critical healthcare challenges. In 2024, the oncological disorders therapeutic area segment held the largest global AI in drug discovery market share. One of the primary applications of AI in oncological drug discovery is in identifying novel therapeutic targets. AI-powered algorithms analyze genomic and transcriptomic data to pinpoint genes and proteins involved in tumor progression. Furthermore, the integration of multi-omics data improved predictive analytics, and collaboration between stakeholders will further enhance therapeutic innovation, shaping the future of drug discovery worldwide.

Segmentation by Therapeutic Area
- Oncological Disorders
- CNS Disorders
- Infectious Diseases
- Immunological Disorders
- Cardiovascular Disorders
- Gastrointestinal Disorders
- Others

INSIGHTS BY DRUG TYPE

The small molecule drug type holds the most significant share of the global AI in drug discovery market, largely due to their established role in treating a broad range of diseases. These drugs are chemically synthesized, relatively inexpensive to manufacture, and have a proven track record in pharmaceutical applications. AI tools like generative models and machine

learning algorithms are extensively used to design and optimize small molecule drugs by predicting their interactions with biological targets, toxicity profiles, and pharmacokinetics. Biologics, including monoclonal antibodies, vaccines, and gene therapies, are gaining traction due to their specificity and efficacy in targeting complex diseases. AI technologies like neural networks are employed to analyze biological data, identify novel protein structures, and optimize biologics? development.

Segmentation by Drug Type
-Small Molecule
-Biologics

INSIGHTS BY TECHNOLOGY

The global AI in drug discovery market by technology is segmented into machine learning (ML), deep learning, natural language processing (NLP), and others. The machine learning (ML) segment holds the largest market share in 2024. ML is the most widely used technology in AI-driven drug discovery. It enables the analysis of large datasets, identifies hidden patterns, and accelerates the drug development process. Its ability to process vast amounts of structured and unstructured data makes it indispensable for drug discovery. Also, machine learning also plays a critical role in optimizing clinical trial design and execution. By analyzing patient data, ML algorithms can identify suitable patient cohorts for trials, predict patient responses, and reduce dropout rates. Deep learning uses artificial neural networks to analyze highly complex data, such as genomics, proteomics, and imaging. The deep learning segment is also projected to witness significant growth during the forecast period. Deep learning is particularly useful in structure-based drug design, biomarker discovery, and disease pathway analysis. Moreover, deep learning facilitates lead optimization by predicting the pharmacokinetics and toxicity profiles of drug candidates. Predictive models trained on historical data help refine chemical structures to enhance efficacy, safety, and bioavailability. This minimizes the chances of late-stage failures, a common challenge in traditional drug development.

Segmentation by Technology
-Machine Learning (ML)
-Deep Learning
-Natural Language Processing (NLP)
-Others

INSIGHTS BY END-USER

The global AI in drug discovery market by end-user is segmented into pharma & biotech companies, CROs & CDMOs, and others. The increasing adoption of AI across all end-user segments reflects the growing recognition of its transformative potential in drug discovery. Pharma & biotech companies will continue to lead the market, leveraging AI to address R&D inefficiencies and enhance drug pipelines. As AI technologies continue to advance, the role of pharma and biotech companies as end-users will be instrumental in shaping the future of medicine, addressing unmet medical needs, and improving global health outcomes. Meanwhile, CROs & CDMOs will see steady growth due to the rise in outsourcing trends, and academic institutions will remain pivotal in driving fundamental innovations. Government organizations will focus on fostering a regulatory and infrastructural environment conducive to AI adoption, ensuring the market's sustained expansion.

Segmentation by End-user
-Pharma & Biotech Companies
-Contract Research Organizations (CROs) & Contract Development and Manufacturing Organizations (CDMOs)
-Others

GEOGRAPHICAL ANALYSIS

The global AI in drug discovery market exhibits significant regional diversity, with each geography offering unique opportunities and challenges. North America leads the global AI in drug discovery market accounting for a global share of over 43% in 2024, driven by its advanced technological ecosystem, robust pharmaceutical and biotechnology sectors, and substantial investments in research and development. The region is home to key players, innovative startups, and extensive academic and research collaborations that position it at the forefront of AI adoption in drug discovery. Also, the U.S. is home to leading AI companies, research institutions, and pharmaceutical giants, fostering a strong ecosystem for AI integration in drug discovery. Companies such as IBM Watson, NVIDIA, and Google DeepMind are collaborating with pharmaceutical firms to accelerate AI-driven drug development.

Europe holds a significant share in the AI in drug discovery market, driven by its strong research networks, public-private partnerships, and supportive regulatory frameworks. European countries focus on secure data sharing and ethical AI deployment, supported by frameworks like GDPR. This ensures the responsible use of patient data in drug development. Also, strong Biotech Sector: Countries like Germany, France, and the UK are at the forefront of AI-driven drug discovery, with a thriving biotech industry and state-of-the-art research facilities.

Furthermore, the APAC region is witnessing exponential growth in the AI in drug discovery market, fueled by increasing healthcare investments, a growing pharmaceutical sector, and government support. Countries like China, Japan, and India have launched national AI strategies to boost innovation in drug discovery. For instance, China?s ?Next Generation Artificial Intelligence Development Plan? prioritizes AI integration across healthcare. Furthermore, the Middle East, Africa, and Latin America represent nascent but promising markets driven by government support and increasing investments in healthcare innovation. These regional dynamics collectively contribute to the global market's expansion, underscoring the transformative potential of AI in revolutionizing drug discovery.

Segmentation by Geography

- North America
  - The U.S.
  - Canada
- Europe
  - Germany
  - The U.K.
  - Switzerland
  - France
  - Italy
  - Spain
  - Netherlands
- APAC
  - China
  - Japan
  - India
  - South Korea
  - Australia
- Latin America
  - Brazil
  - Mexico
  - Argentina
  - Colombia
- Middle East & Africa

o Turkey
o South Africa
o Saudi Arabia
o UAE

VENDOR LANDSCAPE

The global AI in drug discovery market has witnessed significant growth in recent years as pharmaceutical companies increasingly adopt AI to accelerate and optimize drug discovery processes. AI-powered technologies, including machine learning (ML), deep learning, and natural language processing (NLP), are enabling researchers to navigate the complexity of biological systems, analyze vast biomedical datasets, and identify promising drug candidates faster and at reduced costs. The competitive landscape of the global AI in drug discovery market is marked by the presence of established pharmaceutical companies, AI technology providers, and emerging startups, all vying to gain a foothold in this rapidly evolving domain. Moreover, companies like IBM Watson Health, Google DeepMind, and NVIDIA, are significant players in the AI in drug discovery market offering advanced AI platforms tailored for drug discovery. For instance, IBM Watson leverages natural language processing and machine learning to mine scientific literature and identify drug targets. Google DeepMind, through its AlphaFold system, has revolutionized protein structure prediction, enabling faster and more precise identification of potential drug candidates.
Leading pharmaceutical firms such as Pfizer, Novartis, Roche, and AstraZeneca have incorporated AI technologies into their research pipelines. These companies are increasingly collaborating with AI startups to drive innovation. For example, AstraZeneca partnered with BenevolentAI to leverage machine learning algorithms for target identification and drug repurposing, showcasing the synergistic potential of AI in pharmaceutical R&D. Furthermore, startups and specialized AI companies, such as BenevolentAI, Insilico Medicine, Atomwise, Exscientia, and Recursion Pharmaceuticals, are at the forefront in the AI in drug discovery market. These companies have developed AI algorithms capable of analyzing complex biological data, predicting molecular interactions, and accelerating preclinical drug discovery stages.

Key Company Profiles

- Atomwise
- Amazon Web Services (AWS)
- BenevolentAI
- Google
- IBM
- Insilico Medicine
- Microsoft
- NVIDIA
- Recursion Pharmaceuticals

Other Prominent Vendors

- AbCellera
- Aitia
- BenchSci
- BioSymetrics
- BPGbio
- Centella
- Envisagenics
- EVAXION Biotech A/S

-Iktos
-Illumina
-insitro
-Merck KGaA
-Model Medicine
-NuMedii
-Owkin
-Predictive Oncology
-Relay Therapeutics
-Standigm
-Valo Health
-Verge Genomics
-XtalPi

KEY QUESTIONS ANSWERED:

1.How big is the global AI in drug discovery market?
2.What is the growth rate of the global AI in drug discovery market?
3.Which region dominates the global AI in drug discovery market share?
4.What are the significant trends in the AI in drug discovery industry?
5.Who are the key players in the global AI in drug discovery market?

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