

Global AI Drug Discovery Software Supply, Demand and Key Producers, 2026-2032

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Abstracts

The global AI Drug Discovery Software market size is expected to reach \$ 2452 million by 2032, rising at a market growth of 15.4% CAGR during the forecast period (2026-2032).

AI drug discovery software is a software tool that accelerates the drug development process by utilizing artificial intelligence algorithms and technologies. This software integrates and analyzes a vast amount of bioinformatics data, chemical structure data, and clinical trial data to predict key properties such as compound bioactivity, pharmacokinetic characteristics, and toxicity. With the help of AI technology, drug researchers can more quickly and accurately screen potential candidate drugs, thereby reducing development costs, shortening development cycles, and improving success rates.

Upstream inputs include cloud computing infrastructure, GPUs and AI accelerators, chemical and biological databases, omics data, and experimental datasets generated by wet labs. Open-source AI frameworks and proprietary foundation models also form an important upstream layer. The midstream consists of AI drug discovery software vendors that develop platforms integrating algorithms, data management, molecular modeling, and workflow orchestration. Downstream customers are primarily pharmaceutical companies, biotechnology firms, and CROs, which use these tools either internally or through collaborative partnerships. Increasingly, AI software is embedded into broader R&D ecosystems rather than deployed as standalone tools. Gross margins in the AI Drug Discovery Software market are generally high due to its software-centric and IP-driven nature. Pure software or SaaS-based platforms typically achieve gross margins of 65-85%, supported by subscription licensing and relatively low marginal distribution costs. However, margins can be diluted when vendors adopt hybrid models that include customized projects, data curation, or experimental validation support, where gross margins often fall to the 50-65% range. Compute-

intensive workloads, particularly for large generative models, remain a key cost factor influencing margin sustainability.

This report studies the global AI Drug Discovery Software demand, key companies, and key regions.

This report is a detailed and comprehensive analysis of the world market for AI Drug Discovery Software, and provides market size (US\$ million) and Year-over-Year (YoY) growth, considering 2025 as the base year. This report explores demand trends and competition, as well as details the characteristics of AI Drug Discovery Software that contribute to its increasing demand across many markets.

Highlights and key features of the study

Global AI Drug Discovery Software total market, 2021-2032, (USD Million)

Global AI Drug Discovery Software total market by region & country, CAGR, 2021-2032, (USD Million)

U.S. VS China: AI Drug Discovery Software total market, key domestic companies, and share, (USD Million)

Global AI Drug Discovery Software revenue by player, revenue and market share 2021-2026, (USD Million)

Global AI Drug Discovery Software total market by Type, CAGR, 2021-2032, (USD Million)

Global AI Drug Discovery Software total market by Application, CAGR, 2021-2032, (USD Million)

This report profiles major players in the global AI Drug Discovery Software market based on the following parameters - company overview, revenue, gross margin, product portfolio, geographical presence, and key developments. Key companies covered as a part of this study include Merck KGaA, Atomwise Inc, BenevolentAI, BullFrog AI, Genesis Therapeutics, Pharma.AI, Recursion Pharmaceuticals, Verge Genomics, Schrödinger, Inc., XtalPi, etc.

This report also provides key insights about market drivers, restraints, opportunities, new product launches or approvals.

Stakeholders would have ease in decision-making through various strategy matrices used in analyzing the world AI Drug Discovery Software market

Detailed Segmentation:

Each section contains quantitative market data including market by value (US\$ Millions), by player, by regions, by Type, and by Application. Data is given for the years 2021-2032 by year with 2025 as the base year, 2026 as the estimate year, and 2027-2032 as the forecast year.

Global AI Drug Discovery Software Market, By Region:

United States

China

Europe

Japan

South Korea

ASEAN

India

Rest of World

Global AI Drug Discovery Software Market, Segmentation by Type:

Cloud Based

On Premise

Global AI Drug Discovery Software Market, Segmentation by Drug Discovery Stage:

Target Identification & Validation

Hit Discovery / Virtual Screening

Lead Optimization

ADMET & Toxicity Prediction

Candidate Selection & Preclinical Support

Global AI Drug Discovery Software Market, Segmentation by AI Task & Function:

Molecular Property Prediction

De Novo Molecule Generation

Protein?Ligand Interaction Modeling

Multi-Parameter Optimization

Knowledge Graph?Based Discovery

Global AI Drug Discovery Software Market, Segmentation by Application:

CRO and Universities

Pharmaceutical Company

Test Lab

Companies Profiled:

Merck KGaA

Atomwise Inc

BenevolentAI

BullFrog AI

Genesis Therapeutics

Pharma.AI

Recursion Pharmaceuticals

Verge Genomics

Schr?dinger, Inc.

XtalPi

Iktos

Key Questions Answered

1. How big is the global AI Drug Discovery Software market?
2. What is the demand of the global AI Drug Discovery Software market?
3. What is the year over year growth of the global AI Drug Discovery Software market?
4. What is the total value of the global AI Drug Discovery Software market?
5. Who are the Major Players in the global AI Drug Discovery Software market?
6. What are the growth factors driving the market demand?

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Figure 56. AI Drug Discovery Software Industrial Chain

Figure 57. Methodology

Figure 58. Research Process and Data Source

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