

Global AI Drug Discovery Software Market Growth (Status and Outlook) 2026-2032

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Abstracts

The global AI Drug Discovery Software market size is predicted to grow from US\$ 843 million in 2025 to US\$ 2450 million in 2032; it is expected to grow at a CAGR of 16.3% from 2026 to 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.

LPI (LP Information)' newest research report, the 'AI Drug Discovery Software Industry Forecast' looks at past sales and reviews total world AI Drug Discovery Software sales in 2025, providing a comprehensive analysis by region and market sector of projected AI Drug Discovery Software sales for 2026 through 2032. With AI Drug Discovery Software sales broken down by region, market sector and sub-sector, this report provides a detailed analysis in US\$ millions of the world AI Drug Discovery Software industry.

This Insight Report provides a comprehensive analysis of the global AI Drug Discovery Software landscape and highlights key trends related to product segmentation, company formation, revenue, and market share, latest development, and M&A activity. This report also analyses the strategies of leading global companies with a focus on AI Drug Discovery Software portfolios and capabilities, market entry strategies, market positions, and geographic footprints, to better understand these firms' unique position in an accelerating global AI Drug Discovery Software market.

This Insight Report evaluates the key market trends, drivers, and affecting factors shaping the global outlook for AI Drug Discovery Software and breaks down the forecast by Type, by Application, geography, and market size to highlight emerging pockets of opportunity. With a transparent methodology based on hundreds of bottom-up qualitative and quantitative market inputs, this study forecast offers a highly nuanced view of the current state and future trajectory in the global AI Drug Discovery Software.

This report presents a comprehensive overview, market shares, and growth opportunities of AI Drug Discovery Software market by product type, application, key players and key regions and countries.

Segmentation by Type:

Cloud Based

On Premise

Segmentation by Drug Discovery Stage:

Target Identification & Validation

Hit Discovery / Virtual Screening

Lead Optimization

ADMET & Toxicity Prediction

Candidate Selection & Preclinical Support

Segmentation by AI Task & Function:

Molecular Property Prediction

De Novo Molecule Generation

Protein-Ligand Interaction Modeling

Multi-Parameter Optimization

Knowledge Graph-Based Discovery

Segmentation by Application:

CRO and Universities

Pharmaceutical Company

Test Lab

This report also splits the market by region:

Americas

United States

Canada

Mexico

Brazil

APAC

China

Japan

Korea

Southeast Asia

India

Australia

Europe

Germany

France

UK

Italy

Russia

Middle East & Africa

Egypt

South Africa

Israel

Turkey

GCC Countries

The below companies that are profiled have been selected based on inputs gathered from primary experts and analyzing the company's coverage, product portfolio, its market penetration.

Merck KGaA

Atomwise Inc

BenevolentAI

BullFrog AI

Genesis Therapeutics

Pharma.AI

Recursion Pharmaceuticals

Verge Genomics

Schrödinger, Inc.

XtalPi

Iktos

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