

Global AI Drug Discovery Software Market 2026 by Company, Regions, Type and Application, Forecast to 2032

<https://marketpublishers.com/r/G0D925CBAEA7EN.html>

Date: January 2026

Pages: 114

Price: US\$ 3,480.00 (Single User License)

ID: G0D925CBAEA7EN

Abstracts

According to our (Global Info Research) latest study, the global AI Drug Discovery Software market size was valued at US\$ 887 million in 2025 and is forecast to a readjusted size of US\$ 2452 million by 2032 with a CAGR of 15.4% during review period.

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 is a detailed and comprehensive analysis for global AI Drug Discovery Software market. Both quantitative and qualitative analyses are presented by company, by region & country, by Type and by Application. As the market is constantly changing, this report explores the competition, supply and demand trends, as well as key factors that contribute to its changing demands across many markets. Company profiles and product examples of selected competitors, along with market share estimates of some of the selected leaders for the year 2025, are provided.

Key Features:

Global AI Drug Discovery Software market size and forecasts, in consumption value (\$ Million), 2021-2032

Global AI Drug Discovery Software market size and forecasts by region and country, in consumption value (\$ Million), 2021-2032

Global AI Drug Discovery Software market size and forecasts, by Type and by Application, in consumption value (\$ Million), 2021-2032

Global AI Drug Discovery Software market shares of main players, in revenue (\$ Million), 2021-2026

The Primary Objectives in This Report Are:

To determine the size of the total market opportunity of global and key countries

To assess the growth potential for AI Drug Discovery Software

To forecast future growth in each product and end-use market

To assess competitive factors affecting the marketplace

This report profiles key 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.

Market segmentation

AI Drug Discovery Software market is split by Type and by Application. For the period 2021-2032, the growth among segments provides accurate calculations and forecasts for Consumption Value by Type and by Application. This analysis can help you expand your business by targeting qualified niche markets.

Market segment by Type

Cloud Based

On Premise

Market segment by Drug Discovery Stage

Target Identification & Validation

Hit Discovery / Virtual Screening

Lead Optimization

ADMET & Toxicity Prediction

Candidate Selection & Preclinical Support

Market segment by AI Task & Function

Molecular Property Prediction

De Novo Molecule Generation

Protein-Ligand Interaction Modeling

Multi-Parameter Optimization

Knowledge Graph-Based Discovery

Market segment by Application

CRO and Universities

Pharmaceutical Company

Test Lab

Market segment by players, this report covers

Merck KGaA

Atomwise Inc

BenevolentAI

BullFrog AI

Genesis Therapeutics

Pharma.AI

Recursion Pharmaceuticals

Verge Genomics

Schrödinger, Inc.

XtalPi

Iktos

Market segment by regions, regional analysis covers

North America (United States, Canada and Mexico)

Europe (Germany, France, UK, Russia, Italy and Rest of Europe)

Asia-Pacific (China, Japan, South Korea, India, Southeast Asia and Rest of Asia-Pacific)

South America (Brazil, Rest of South America)

Middle East & Africa (Turkey, Saudi Arabia, UAE, Rest of Middle East & Africa)

The content of the study subjects, includes a total of 13 chapters:

Chapter 1, to describe AI Drug Discovery Software product scope, market overview, market estimation caveats and base year.

Chapter 2, to profile the top players of AI Drug Discovery Software, with revenue, gross margin, and global market share of AI Drug Discovery Software from 2021 to 2026.

Chapter 3, the AI Drug Discovery Software competitive situation, revenue, and global market share of top players are analyzed emphatically by landscape contrast.

Chapter 4 and 5, to segment the market size by Type and by Application, with consumption value and growth rate by Type, by Application, from 2021 to 2032.

Chapter 6, 7, 8, 9, and 10, to break the market size data at the country level, with revenue and market share for key countries in the world, from 2021 to 2026. and AI Drug Discovery Software market forecast, by regions, by Type and by Application, with

consumption value, from 2027 to 2032.

Chapter 11, market dynamics, drivers, restraints, trends, Porters Five Forces analysis.

Chapter 12, the key raw materials and key suppliers, and industry chain of AI Drug Discovery Software.

Chapter 13, to describe AI Drug Discovery Software research findings and conclusion.

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